Full wwPDB EM Validation Report ⓘ

Sep 10, 2024 – 04:23 PM JST

PDB ID	:	8IAR
EMDB ID	:	EMD-35316
Title	:	Respiratory complex CIII2, focus-refined of type I, Wild type mouse under thermoneutral 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:

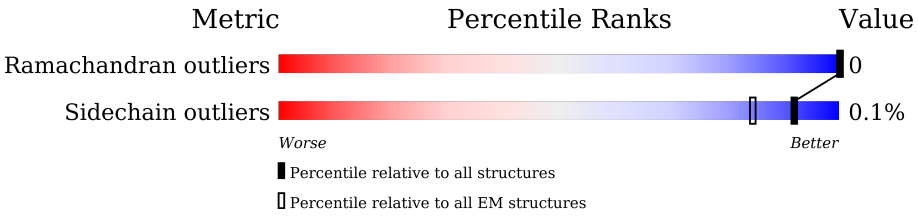
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	84% 16%
1	Aa	480	85% 14%
2	AB	453	5% 92% 8%
2	Ab	453	91% 9%
3	AC	381	7% 97%
3	Ac	381	5% 98%
4	AD	325	8% 74% 26%
4	Ad	325	6% 74% 26%
5	AE	274	42% 68% 31%

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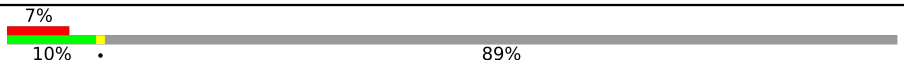
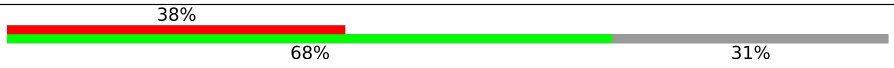
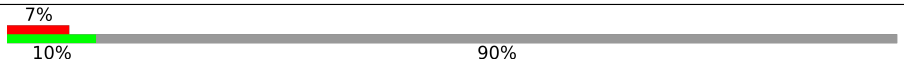
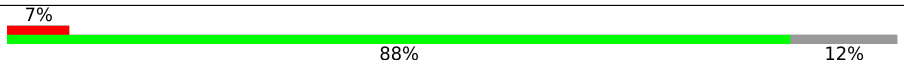
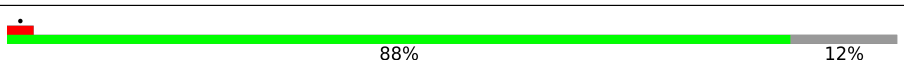
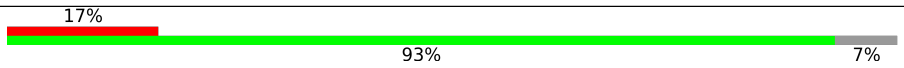
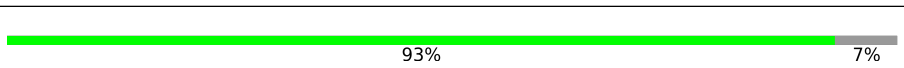
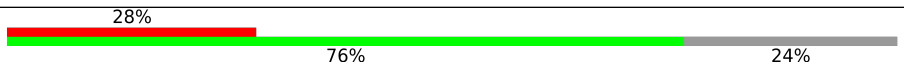
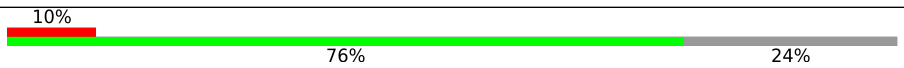
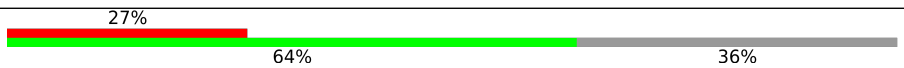
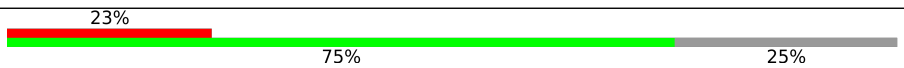
Mol	Chain	Length	Quality of chain
5	AI	274	
5	Ae	274	
5	Ai	274	
6	AF	111	
6	Af	111	
7	AG	82	
7	Ag	82	
8	AH	89	
8	Ah	89	
9	AJ	64	
9	Aj	64	
10	AK	56	
10	Ak	56	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32253 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	403	Total	C	N	O	S	0	0
			3153	1970	560	607	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	412	Total	C	N	O	S	0	0
			3094	1945	542	598	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	240	Total	C	N	O	S	0	0
			1912	1221	328	349	14		
4	Ad	240	Total	C	N	O	S	0	0
			1912	1221	328	349	14		

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

Mol	Chain	Residues	Atoms	AltConf	Trace
5	AE	188	Total C N O S 1451 916 254 274 7	0	0
5	AI	30	Total C N O 217 138 42 37	0	0
5	Ae	188	Total C N O S 1451 916 254 274 7	0	0
5	Ai	28	Total C N O 207 133 40 34	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	68	Total C N O S 562 343 103 111 5	0	0
8	Ah	68	Total C N O S 562 343 103 111 5	0	0

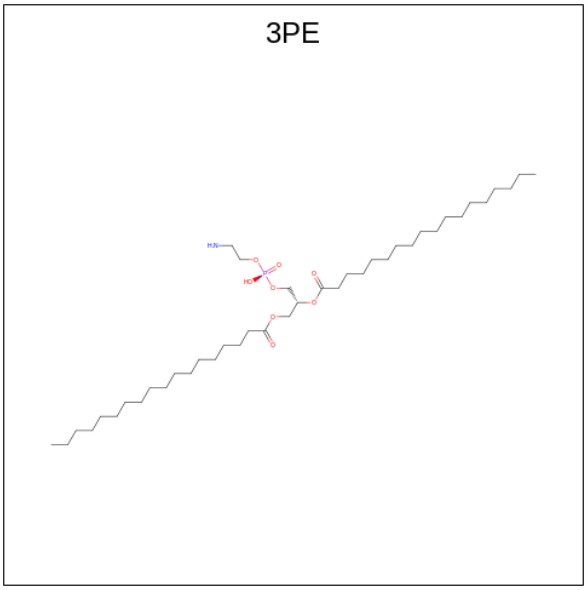
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

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 391 257 66 68	0	0

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

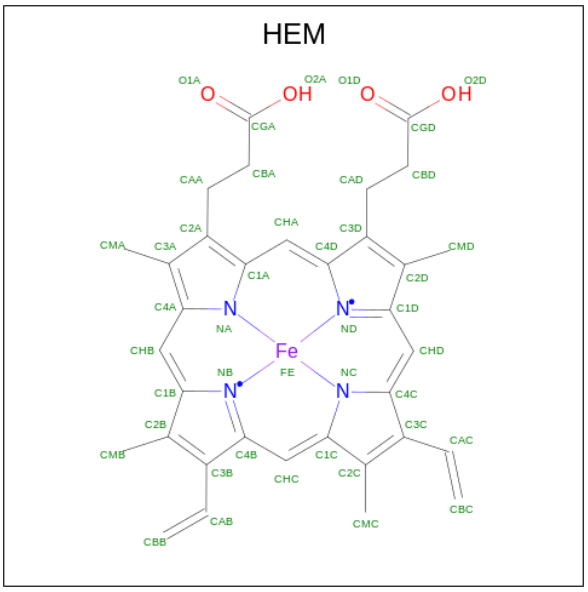
Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	49	Total	C	N	O	S	0	0
			401	266	71	63	1		
10	Ak	49	Total	C	N	O	S	0	0
			401	266	71	63	1		

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



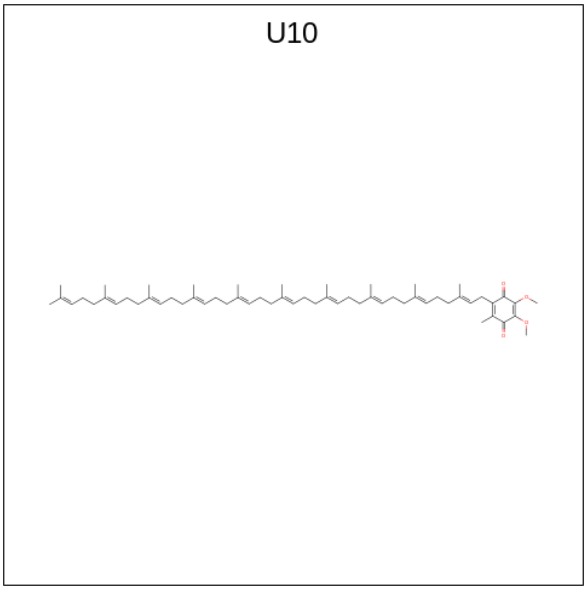
Mol	Chain	Residues	Atoms					AltConf
11	AC	1	Total	C	N	O	P	0
			23	13	1	8	1	
11	AC	1	Total	C	N	O	P	0
			35	25	1	8	1	
11	AG	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	Aa	1	Total	C	N	O	P	0
			23	13	1	8	1	
11	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
11	Ag	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



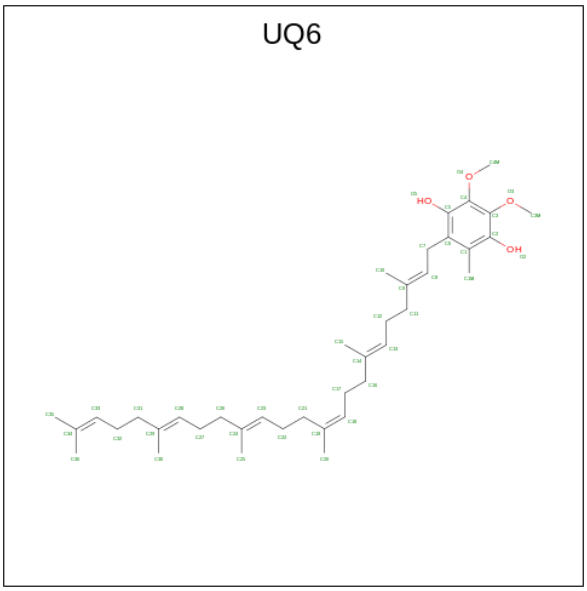
Mol	Chain	Residues	Atoms					AltConf
12	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



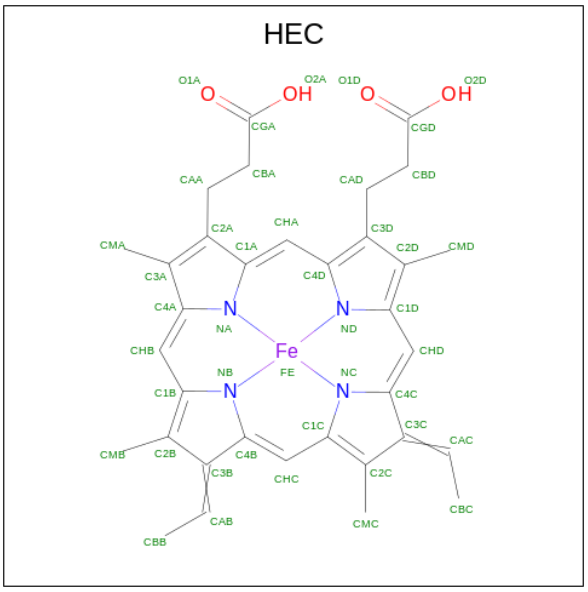
Mol	Chain	Residues	Atoms	AltConf
13	AC	1	Total C O 23 19 4	0
13	Ac	1	Total C O 23 19 4	0

- 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).



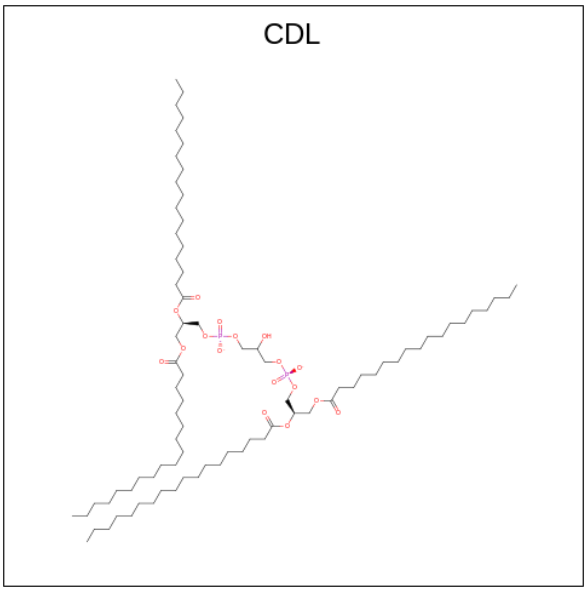
Mol	Chain	Residues	Atoms	AltConf
14	AC	1	Total C O 28 24 4	0
14	Ac	1	Total C O 28 24 4	0

- Molecule 15 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
15	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 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
16	AG	1	Total	C	O	P	0
			42	23	17	2	

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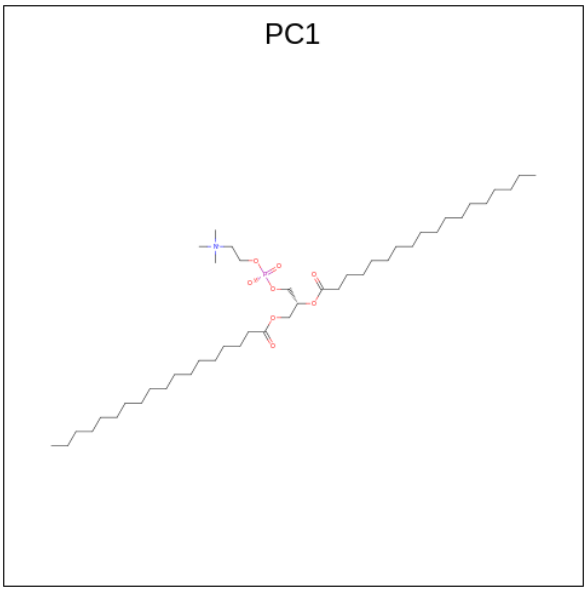
Mol	Chain	Residues	Atoms				AltConf
16	AG	1	Total	C	O	P	0
			56	37	17	2	
16	Aa	1	Total	C	O	P	0
			46	27	17	2	
16	Ag	1	Total	C	O	P	0
			42	23	17	2	
16	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



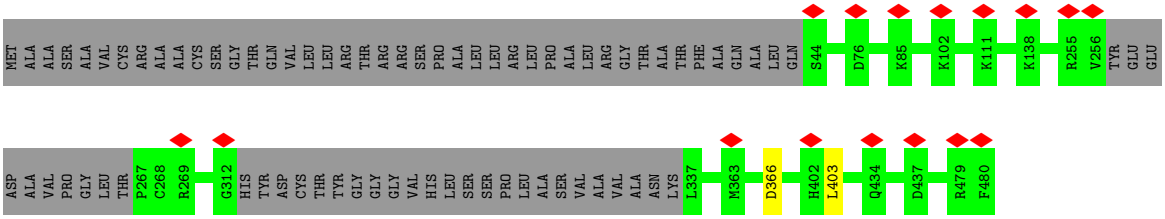
Mol	Chain	Residues	Atoms					AltConf
17	Ae	1	Total	C	N	O	P	0
			35	25	1	8	1	

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.

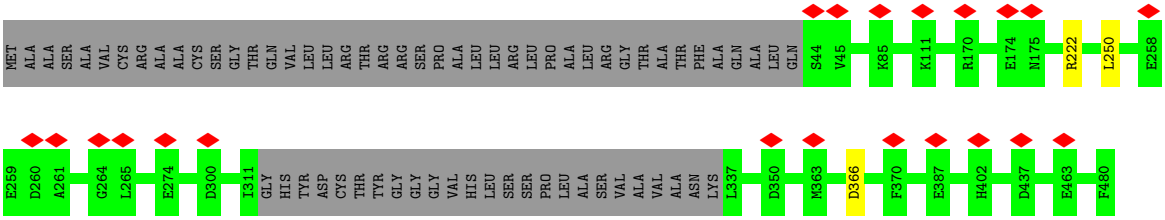
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AA:



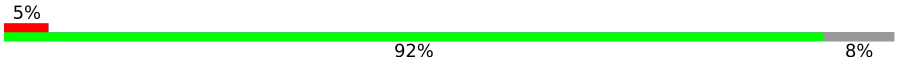
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

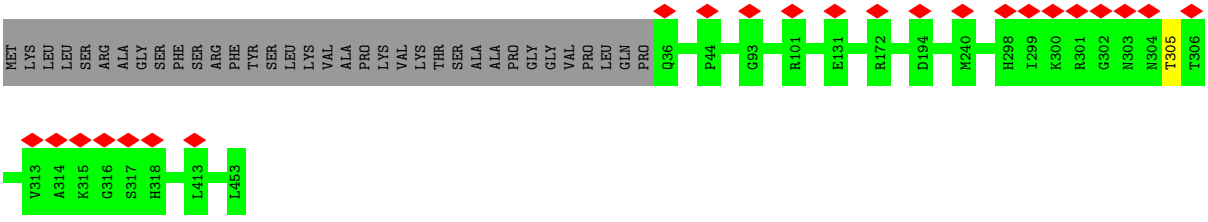
Chain Aa:



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

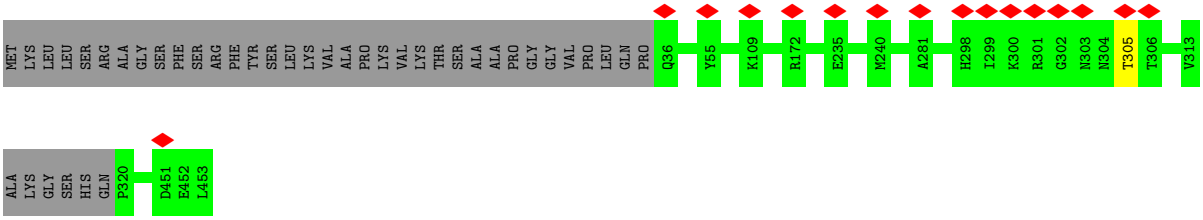
Chain AB:



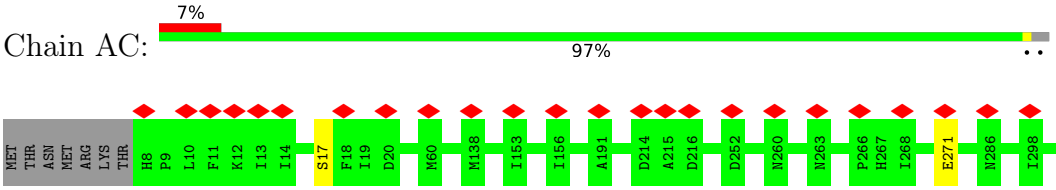


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

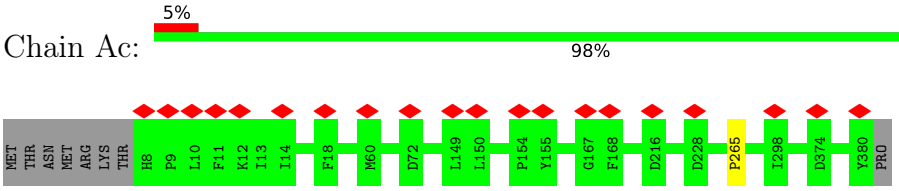
Chain Ab:



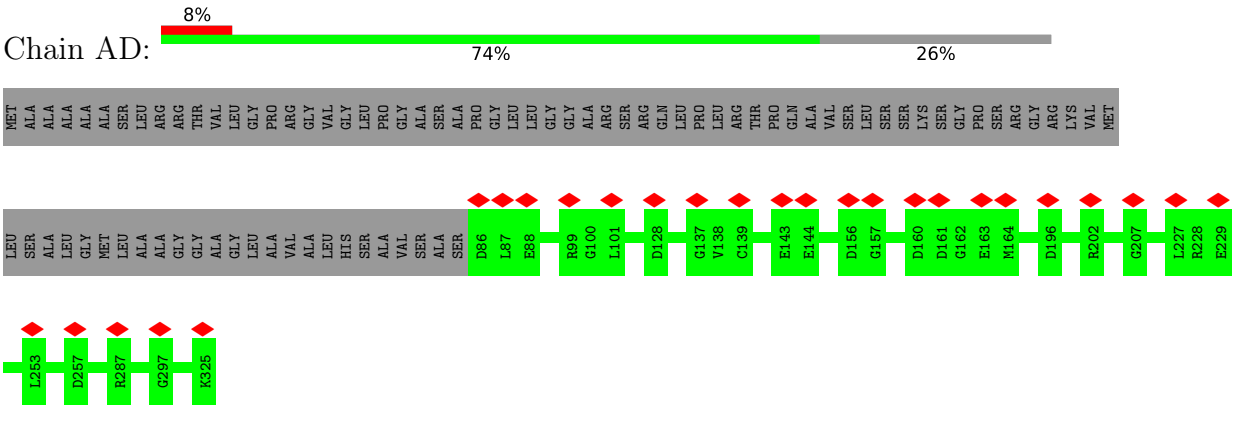
• Molecule 3: Cytochrome b



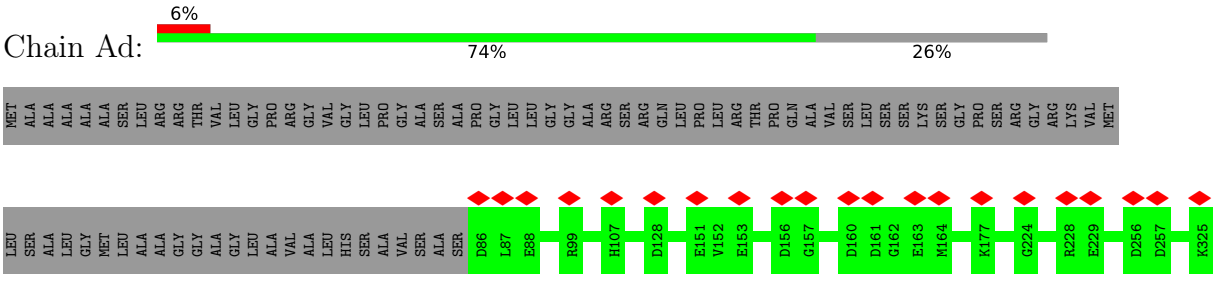
• Molecule 3: Cytochrome b



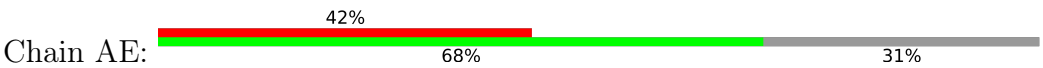
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

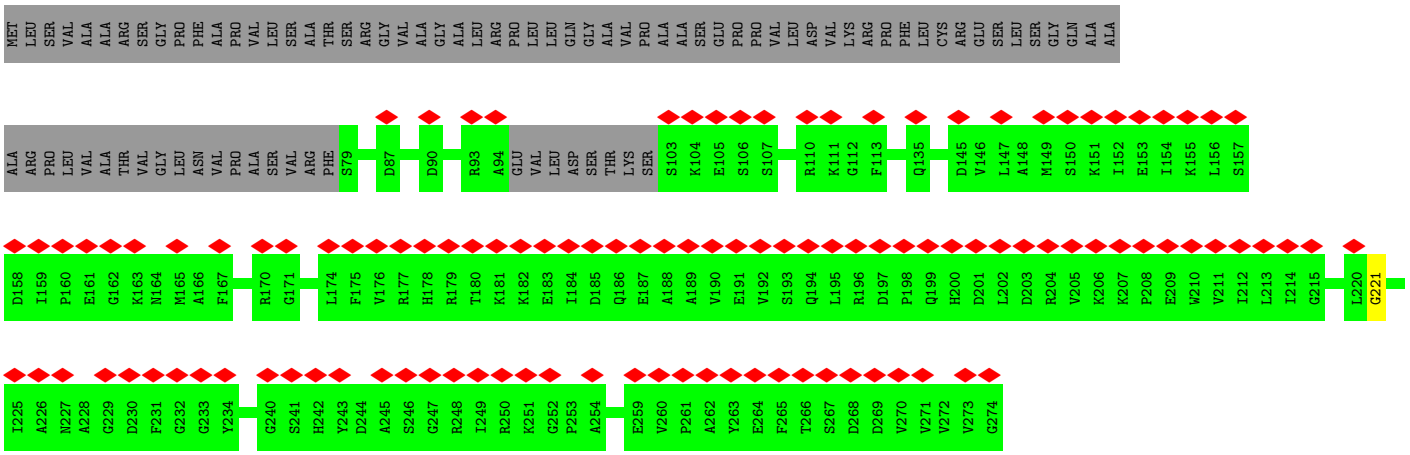


• Molecule 4: Cytochrome c1, heme protein, mitochondrial



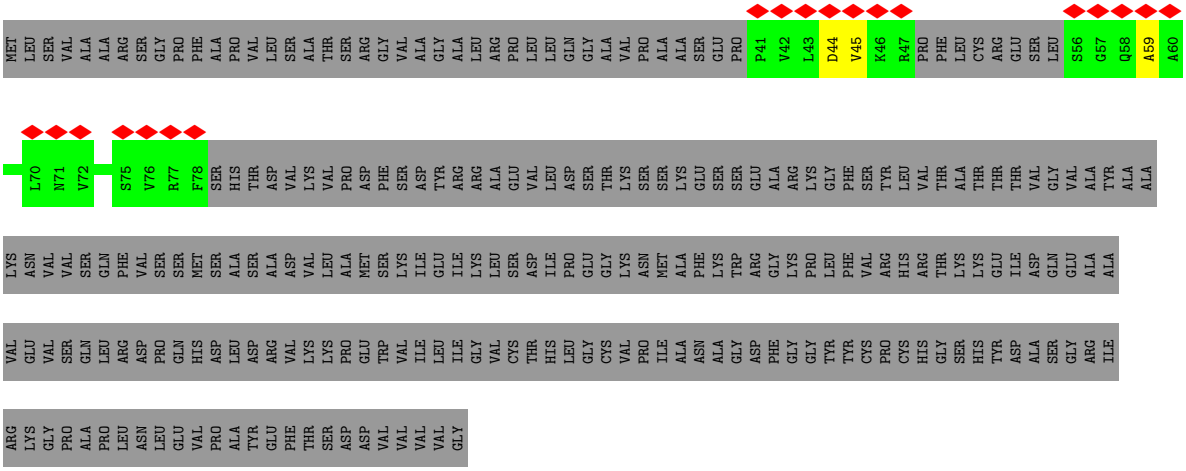
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial





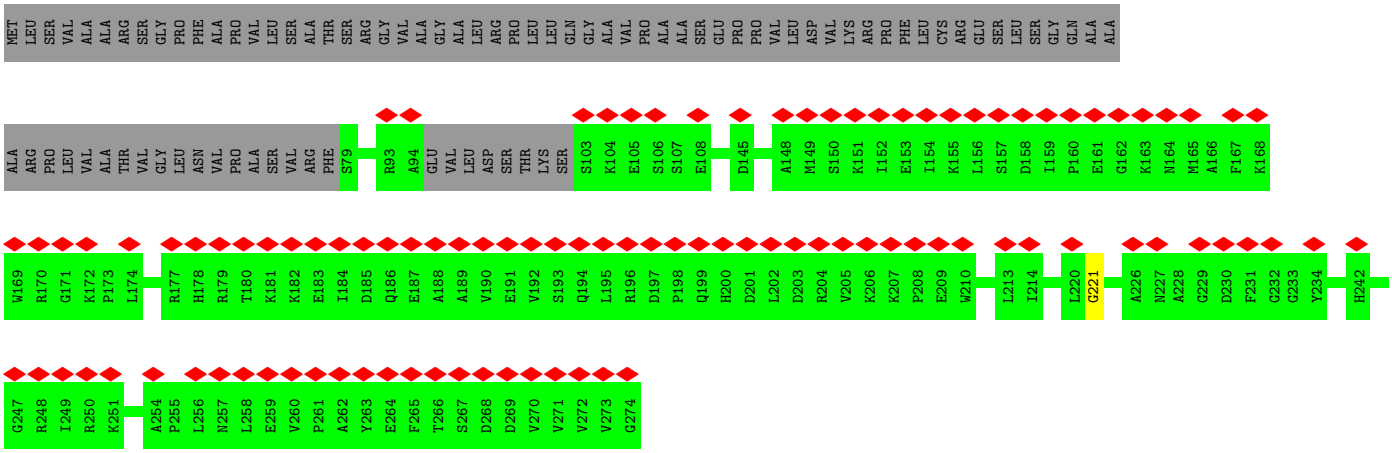
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AI:



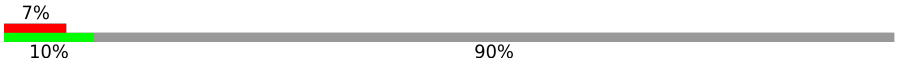
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

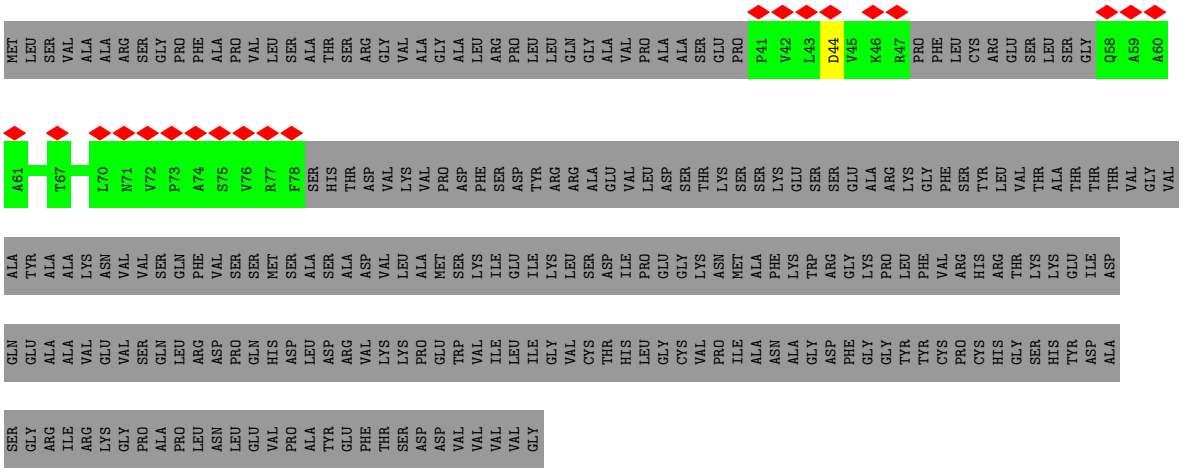
Chain Ae:



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

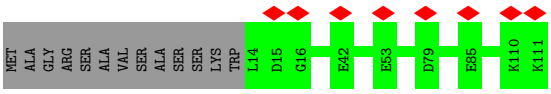
Chain Ai:





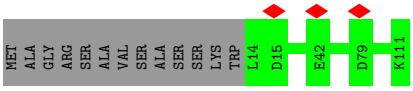
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain AF:



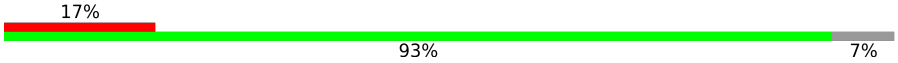
• Molecule 6: Cytochrome b-c1 complex subunit 7

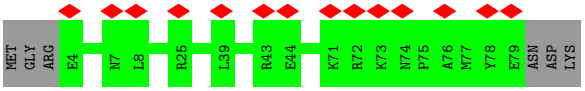
Chain Af:



• Molecule 7: Cytochrome b-c1 complex subunit 8

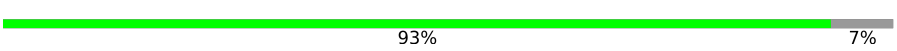
Chain AG:

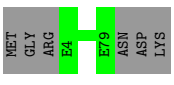




• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain Ag:

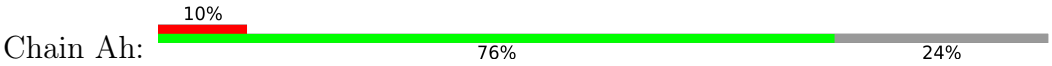


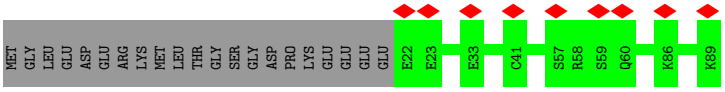


• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

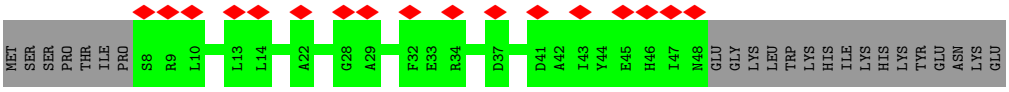
Chain AH:

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

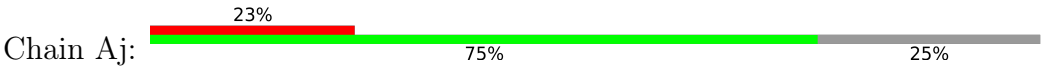


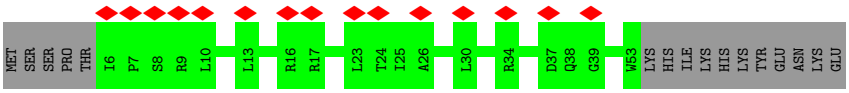


• Molecule 9: Cytochrome b-c1 complex subunit 9

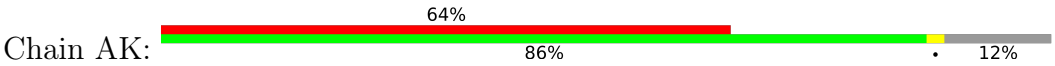


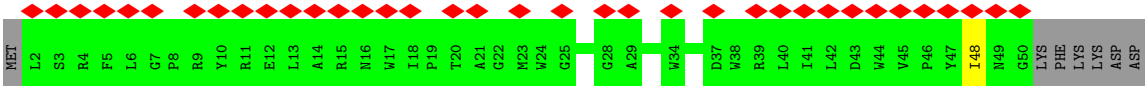
• Molecule 9: Cytochrome b-c1 complex subunit 9



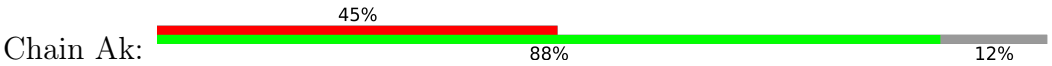


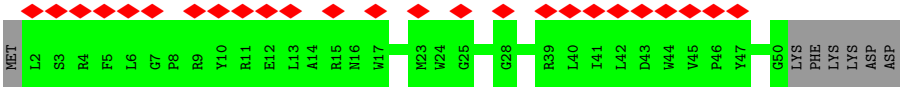
• Molecule 10: Cytochrome b-c1 complex subunit 10





• Molecule 10: Cytochrome b-c1 complex subunit 10





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85845	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 ($e^-/Å^2$)	46.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.363	Depositor
Minimum map value	-1.370	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.5	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: PC1, CDL, U10, HEM, HEC, UQ6, 3PE

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	0.34	0/3213	0.60	1/4355 (0.0%)
1	Aa	0.38	1/3288 (0.0%)	0.60	2/4462 (0.0%)
2	AB	0.32	0/3187	0.57	1/4308 (0.0%)
2	Ab	0.34	0/3142	0.56	1/4246 (0.0%)
3	AC	0.37	1/3089 (0.0%)	0.55	1/4221 (0.0%)
3	Ac	0.38	1/3089 (0.0%)	0.56	0/4221
4	AD	0.33	0/1971	0.53	0/2677
4	Ad	0.37	0/1971	0.50	0/2677
5	AE	0.45	0/1483	0.62	1/2007 (0.0%)
5	AI	0.87	2/219 (0.9%)	0.98	3/296 (1.0%)
5	Ae	0.45	0/1483	0.62	1/2007 (0.0%)
5	Ai	0.65	1/209 (0.5%)	0.72	1/283 (0.4%)
6	AF	0.32	0/884	0.50	0/1184
6	Af	0.33	0/884	0.50	0/1184
7	AG	0.37	0/662	0.55	0/895
7	Ag	0.38	0/662	0.56	0/895
8	AH	0.33	0/569	0.59	0/763
8	Ah	0.33	0/569	0.59	0/763
9	AJ	0.35	0/339	0.48	0/457
9	Aj	0.37	0/401	0.47	0/542
10	AK	0.33	0/416	0.64	1/571 (0.2%)
10	Ak	0.34	0/416	0.52	0/571
All	All	0.37	6/32146 (0.0%)	0.57	13/43585 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	250	LEU	C-N	10.79	1.58	1.34
5	AI	45	VAL	C-N	8.53	1.53	1.34
3	Ac	265	PRO	N-CD	8.12	1.59	1.47
5	Ai	44	ASP	C-N	7.84	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AI	44	ASP	C-N	7.84	1.52	1.34
3	AC	271	GLU	C-N	7.81	1.52	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	366	ASP	CB-CG-OD1	9.44	126.79	118.30
1	Aa	366	ASP	CB-CG-OD1	9.42	126.78	118.30
1	Aa	250	LEU	O-C-N	-6.55	112.22	122.70
5	AI	59	ALA	N-CA-CB	-6.21	101.40	110.10
3	AC	17	SER	N-CA-CB	-5.62	102.06	110.50
5	AE	221	GLY	N-CA-C	5.51	126.88	113.10
5	Ae	221	GLY	N-CA-C	5.49	126.83	113.10
10	AK	48	ILE	CB-CA-C	-5.34	100.93	111.60
5	AI	44	ASP	O-C-N	5.33	131.23	122.70
5	Ai	44	ASP	O-C-N	5.32	131.22	122.70
5	AI	45	VAL	C-N-CA	-5.23	108.62	121.70
2	AB	305	THR	N-CA-CB	-5.21	100.41	110.30
2	Ab	305	THR	N-CA-CB	-5.19	100.43	110.30

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	397/480 (83%)	388 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	408/480 (85%)	395 (97%)	13 (3%)	0	100	100
2	AB	416/453 (92%)	406 (98%)	10 (2%)	0	100	100
2	Ab	408/453 (90%)	396 (97%)	12 (3%)	0	100	100
3	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
3	Ac	371/381 (97%)	368 (99%)	3 (1%)	0	100	100
4	AD	238/325 (73%)	230 (97%)	8 (3%)	0	100	100
4	Ad	238/325 (73%)	225 (94%)	13 (6%)	0	100	100
5	AE	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
5	AI	26/274 (10%)	23 (88%)	3 (12%)	0	100	100
5	Ae	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
5	Ai	24/274 (9%)	23 (96%)	1 (4%)	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%)	74 (100%)	0	0	100	100
8	AH	66/89 (74%)	66 (100%)	0	0	100	100
8	Ah	66/89 (74%)	66 (100%)	0	0	100	100
9	AJ	39/64 (61%)	39 (100%)	0	0	100	100
9	Aj	46/64 (72%)	46 (100%)	0	0	100	100
10	AK	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
10	Ak	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
All	All	3916/5178 (76%)	3811 (97%)	105 (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	341/398 (86%)	340 (100%)	1 (0%)	91 95
1	Aa	349/398 (88%)	348 (100%)	1 (0%)	91 95
2	AB	328/356 (92%)	328 (100%)	0	100 100
2	Ab	324/356 (91%)	324 (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	205/260 (79%)	205 (100%)	0	100 100
4	Ad	205/260 (79%)	205 (100%)	0	100 100
5	AE	158/224 (70%)	158 (100%)	0	100 100
5	AI	23/224 (10%)	23 (100%)	0	100 100
5	Ae	158/224 (70%)	158 (100%)	0	100 100
5	Ai	22/224 (10%)	22 (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	65/83 (78%)	65 (100%)	0	100 100
8	Ah	65/83 (78%)	65 (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	39/46 (85%)	39 (100%)	0	100 100
10	Ak	39/46 (85%)	39 (100%)	0	100 100
All	All	3361/4304 (78%)	3359 (100%)	2 (0%)	92 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	403	LEU
1	Aa	222	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	87	ASN

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Mol	Chain	Res	Type
1	AA	160	GLN
1	AA	173	GLN
1	AA	181	ASN
1	AA	207	ASN
1	AA	402	HIS
2	AB	167	GLN
2	AB	298	HIS
2	AB	304	ASN
2	AB	415	GLN
3	AC	312	GLN
3	AC	341	GLN
4	AD	115	GLN
5	AE	242	HIS
5	AI	71	ASN
10	AK	16	ASN
1	Aa	87	ASN
1	Aa	173	GLN
1	Aa	181	ASN
1	Aa	207	ASN
2	Ab	167	GLN
2	Ab	298	HIS
2	Ab	304	ASN
2	Ab	415	GLN
3	Ac	201	HIS
3	Ac	312	GLN
3	Ac	341	GLN
4	Ad	115	GLN
4	Ad	190	ASN
5	Ae	242	HIS
7	Ag	65	GLN
10	Ak	16	ASN

5.3.3 RNA (i)

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)

22 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	$\#\|Z\| > 2$
17	PC1	Ae	301	-	34,34,53	1.17	2 (5%)	40,42,61	1.18	4 (10%)
13	U10	AC	405	-	23,23,63	1.24	3 (13%)	28,31,79	2.10	7 (25%)
11	3PE	Aa	501	-	22,22,50	1.37	2 (9%)	25,27,55	1.20	2 (8%)
16	CDL	AG	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.33	6 (12%)
12	HEM	AC	403	3	41,50,50	1.27	3 (7%)	45,82,82	1.72	9 (20%)
11	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.21	3 (8%)
16	CDL	Ag	102	-	55,55,99	0.39	0	61,67,111	0.33	0
11	3PE	AC	404	-	34,34,50	1.10	2 (5%)	37,39,55	1.14	3 (8%)
15	HEC	AD	401	4	32,50,50	2.16	3 (9%)	24,82,82	1.62	5 (20%)
12	HEM	Ac	401	3	41,50,50	1.22	4 (9%)	45,82,82	1.68	8 (17%)
14	UQ6	Ac	405	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
12	HEM	Ac	402	3	41,50,50	1.25	3 (7%)	45,82,82	1.71	8 (17%)
12	HEM	AC	402	3	41,50,50	1.23	4 (9%)	45,82,82	1.70	8 (17%)
13	U10	Ac	404	-	23,23,63	1.24	3 (13%)	28,31,79	2.08	7 (25%)
16	CDL	Aa	502	-	45,45,99	1.34	4 (8%)	51,57,111	1.36	6 (11%)
11	3PE	AG	103	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
11	3PE	AC	401	-	22,22,50	0.47	0	25,27,55	0.73	1 (4%)
14	UQ6	AC	406	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
16	CDL	Ag	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.35	6 (12%)
16	CDL	AG	102	-	55,55,99	1.20	4 (7%)	61,67,111	1.25	6 (9%)
11	3PE	Ag	103	-	50,50,50	0.31	0	53,55,55	0.29	0
15	HEC	Ad	401	4	32,50,50	2.17	3 (9%)	24,82,82	1.64	5 (20%)

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
17	PC1	Ae	301	-	-	7/38/38/57	-
13	U10	AC	405	-	-	6/15/39/87	0/1/1/1
11	3PE	Aa	501	-	-	7/26/26/54	-
16	CDL	AG	101	-	-	8/52/52/110	-
12	HEM	AC	403	3	-	6/12/54/54	-
11	3PE	Ac	403	-	-	3/38/38/54	-
16	CDL	Ag	102	-	-	13/66/66/110	-
11	3PE	AC	404	-	-	1/38/38/54	-
15	HEC	AD	401	4	-	0/10/54/54	-
12	HEM	Ac	401	3	-	7/12/54/54	-
14	UQ6	Ac	405	-	-	13/21/21/39	0/1/1/1
12	HEM	Ac	402	3	-	6/12/54/54	-
12	HEM	AC	402	3	-	7/12/54/54	-
13	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
16	CDL	Aa	502	-	-	13/56/56/110	-
11	3PE	AG	103	-	-	9/54/54/54	-
11	3PE	AC	401	-	-	7/26/26/54	-
14	UQ6	AC	406	-	-	13/21/21/39	0/1/1/1
16	CDL	Ag	101	-	-	7/52/52/110	-
16	CDL	AG	102	-	-	15/66/66/110	-
11	3PE	Ag	103	-	-	10/54/54/54	-
15	HEC	Ad	401	4	-	0/10/54/54	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Ad	401	HEC	C3C-C2C	-6.46	1.34	1.40
15	AD	401	HEC	C3C-C2C	-6.40	1.34	1.40
15	Ad	401	HEC	C2B-C3B	-6.15	1.34	1.40
15	AD	401	HEC	C2B-C3B	-6.07	1.34	1.40
15	Ad	401	HEC	C3D-C2D	5.48	1.53	1.37
15	AD	401	HEC	C3D-C2D	5.41	1.53	1.37
17	Ae	301	PC1	O31-C31	4.33	1.46	1.33
16	Aa	502	CDL	OA8-CA7	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Aa	502	CDL	OB8-CB7	4.24	1.45	1.33
16	AG	101	CDL	OA8-CA7	4.24	1.45	1.33
11	AC	404	3PE	O31-C31	4.23	1.45	1.33
11	Aa	501	3PE	O31-C31	4.22	1.45	1.33
11	Ac	403	3PE	O31-C31	4.22	1.45	1.33
11	AG	103	3PE	O31-C31	4.21	1.45	1.33
16	Ag	101	CDL	OB8-CB7	4.20	1.45	1.33
16	Ag	101	CDL	OA8-CA7	4.16	1.45	1.33
16	AG	101	CDL	OB8-CB7	4.16	1.45	1.33
16	AG	102	CDL	OB8-CB7	4.16	1.45	1.33
16	AG	102	CDL	OA8-CA7	4.15	1.45	1.33
11	Aa	501	3PE	O21-C21	4.14	1.46	1.34
11	AG	103	3PE	O21-C21	4.14	1.46	1.34
16	Aa	502	CDL	OB6-CB5	4.11	1.45	1.34
17	Ae	301	PC1	O21-C21	4.10	1.45	1.34
16	AG	101	CDL	OA6-CA5	4.10	1.45	1.34
16	Ag	101	CDL	OA6-CA5	4.05	1.45	1.34
16	AG	101	CDL	OB6-CB5	4.04	1.45	1.34
16	Ag	101	CDL	OB6-CB5	4.03	1.45	1.34
16	AG	102	CDL	OA6-CA5	4.01	1.45	1.34
16	Aa	502	CDL	OA6-CA5	4.01	1.45	1.34
11	AC	404	3PE	O21-C21	3.94	1.45	1.34
11	Ac	403	3PE	O21-C21	3.93	1.45	1.34
16	AG	102	CDL	OB6-CB5	3.92	1.45	1.34
12	AC	403	HEM	C4D-ND	-3.81	1.33	1.40
12	Ac	402	HEM	C4D-ND	-3.73	1.33	1.40
12	AC	402	HEM	C4D-ND	-3.67	1.34	1.40
12	Ac	401	HEM	C4D-ND	-3.59	1.34	1.40
12	AC	403	HEM	C1B-NB	-3.26	1.34	1.40
12	Ac	402	HEM	C1B-NB	-3.21	1.34	1.40
12	AC	402	HEM	C1B-NB	-3.06	1.35	1.40
12	Ac	401	HEM	C1B-NB	-3.06	1.35	1.40
14	Ac	405	UQ6	O2-C2	-2.96	1.30	1.37
14	AC	406	UQ6	O2-C2	-2.95	1.30	1.37
13	AC	405	U10	C6-C5	-2.93	1.38	1.46
13	Ac	404	U10	C6-C5	-2.92	1.38	1.46
13	Ac	404	U10	C4-C3	2.90	1.48	1.36
13	AC	405	U10	C4-C3	2.89	1.48	1.36
12	AC	403	HEM	C1D-ND	-2.72	1.33	1.38
12	Ac	402	HEM	C1D-ND	-2.69	1.33	1.38
12	AC	402	HEM	C1D-ND	-2.55	1.33	1.38
13	Ac	404	U10	C3-C2	-2.50	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AC	405	U10	C3-C2	-2.47	1.41	1.48
12	Ac	401	HEM	C1D-ND	-2.45	1.33	1.38
12	AC	402	HEM	CHB-C1B	2.06	1.40	1.35
12	Ac	401	HEM	CHB-C1B	2.06	1.40	1.35

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	AC	405	U10	C6-C1-C2	7.80	125.35	119.18
13	Ac	404	U10	C6-C1-C2	7.71	125.28	119.18
12	AC	402	HEM	CHC-C4B-NB	4.74	129.58	124.43
12	Ac	401	HEM	CHC-C4B-NB	4.66	129.49	124.43
12	AC	403	HEM	C4D-ND-C1D	4.47	109.69	105.07
11	AG	103	3PE	O21-C21-C22	4.44	121.07	111.50
12	Ac	402	HEM	C4D-ND-C1D	4.38	109.59	105.07
12	AC	403	HEM	CHC-C4B-NB	4.20	128.99	124.43
12	Ac	402	HEM	CHC-C4B-NB	4.19	128.99	124.43
16	Aa	502	CDL	OA6-CA5-C11	4.17	120.49	111.50
13	AC	405	U10	C1-C6-C5	-4.14	115.69	119.58
13	Ac	404	U10	C1-C6-C5	-4.09	115.73	119.58
11	Ac	403	3PE	O21-C21-C22	4.07	120.27	111.50
17	Ae	301	PC1	O21-C21-C22	4.03	120.19	111.50
12	Ac	402	HEM	CHB-C1B-NB	3.99	129.31	124.38
16	AG	102	CDL	OA6-CA5-C11	3.97	120.06	111.50
16	AG	102	CDL	OB6-CB5-C51	3.97	120.06	111.50
12	AC	403	HEM	CHB-C1B-NB	3.95	129.26	124.38
12	Ac	401	HEM	CHB-C1B-NB	3.94	129.24	124.38
16	AG	101	CDL	OB6-CB5-C51	3.92	119.94	111.50
12	AC	402	HEM	CHB-C1B-NB	3.87	129.16	124.38
15	Ad	401	HEC	CMC-C2C-C1C	-3.79	122.64	128.46
15	AD	401	HEC	CMC-C2C-C1C	-3.78	122.66	128.46
16	Ag	101	CDL	OB6-CB5-C51	3.75	119.59	111.50
11	AC	404	3PE	O21-C21-C22	3.70	119.48	111.50
16	Ag	101	CDL	OA6-CA5-C11	3.36	120.17	110.80
16	Aa	502	CDL	OB6-CB5-C51	3.34	120.11	110.80
16	Ag	101	CDL	OB8-CB7-C71	3.33	120.12	111.38
12	AC	402	HEM	C4D-ND-C1D	3.29	108.48	105.07
16	Aa	502	CDL	OB8-CB7-C71	3.29	120.00	111.38
13	Ac	404	U10	C4-C3-C2	-3.28	114.23	120.68
11	Aa	501	3PE	O21-C21-C22	3.27	119.92	110.80
13	AC	405	U10	C4-C3-C2	-3.25	114.30	120.68
12	AC	403	HEM	C1B-NB-C4B	3.23	108.41	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	AC	403	HEM	CHD-C1D-ND	3.22	127.92	124.43
12	Ac	401	HEM	C4D-ND-C1D	3.21	108.39	105.07
12	Ac	402	HEM	C1B-NB-C4B	3.20	108.38	105.07
12	Ac	402	HEM	CHD-C1D-ND	3.17	127.88	124.43
16	AG	101	CDL	OA6-CA5-C11	3.12	119.49	110.80
16	AG	101	CDL	OB8-CB7-C71	3.11	119.53	111.38
12	Ac	401	HEM	C1B-NB-C4B	3.09	108.27	105.07
12	AC	402	HEM	C1B-NB-C4B	3.07	108.24	105.07
16	AG	102	CDL	CA4-OA6-CA5	-2.87	110.72	117.79
12	AC	402	HEM	CHD-C1D-ND	2.87	127.55	124.43
12	Ac	401	HEM	CHD-C1D-ND	2.82	127.49	124.43
16	AG	102	CDL	CB4-OB6-CB5	-2.79	110.93	117.79
15	Ad	401	HEC	CMB-C2B-C1B	-2.77	124.20	128.46
16	Aa	502	CDL	CB4-OB6-CB5	-2.73	111.07	117.79
11	Ac	403	3PE	C2-O21-C21	-2.72	111.08	117.79
15	AD	401	HEC	CMB-C2B-C1B	-2.70	124.31	128.46
16	Ag	101	CDL	CA4-OA6-CA5	-2.69	111.16	117.79
11	Ac	403	3PE	O31-C31-C32	2.68	120.31	111.91
17	Ae	301	PC1	O31-C31-C32	2.66	120.25	111.91
13	AC	405	U10	C7-C6-C5	2.64	121.66	118.48
11	AC	404	3PE	O31-C31-C32	2.63	120.17	111.91
16	AG	101	CDL	OA8-CA7-C31	2.62	120.11	111.91
16	Aa	502	CDL	CA4-OA6-CA5	-2.61	111.36	117.79
16	AG	101	CDL	CB4-OB6-CB5	-2.60	111.38	117.79
13	Ac	404	U10	C7-C6-C5	2.59	121.60	118.48
17	Ae	301	PC1	C2-O21-C21	-2.59	111.42	117.79
12	AC	402	HEM	CHA-C4D-ND	2.58	127.57	124.38
13	Ac	404	U10	O4-C4-C5	-2.55	107.94	116.56
13	AC	405	U10	O4-C4-C5	-2.55	107.95	116.56
11	Aa	501	3PE	O31-C31-C32	2.53	119.85	111.91
16	Ag	101	CDL	OA8-CA7-C31	2.49	119.71	111.91
12	Ac	401	HEM	CHA-C4D-ND	2.46	127.42	124.38
16	AG	102	CDL	OB8-CB7-C71	2.46	119.61	111.91
16	AG	102	CDL	OA8-CA7-C31	2.45	119.59	111.91
12	Ac	402	HEM	CHB-C1B-C2B	-2.44	119.98	126.72
12	AC	403	HEM	CHB-C1B-C2B	-2.43	120.00	126.72
11	AG	103	3PE	O31-C31-C32	2.43	119.52	111.91
16	Aa	502	CDL	OA8-CA7-C31	2.42	119.51	111.91
17	Ae	301	PC1	C11-C12-N	-2.41	107.73	115.78
15	Ad	401	HEC	CBD-CAD-C3D	-2.41	108.51	112.62
12	Ac	401	HEM	C4B-C3B-C2B	-2.37	105.23	107.11
11	AC	404	3PE	C2-O21-C21	-2.37	111.96	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	AC	402	HEM	C4B-C3B-C2B	-2.37	105.24	107.11
15	AD	401	HEC	CBD-CAD-C3D	-2.36	108.59	112.62
15	Ad	401	HEC	C1D-C2D-C3D	-2.36	105.35	107.00
12	AC	403	HEM	CHA-C4D-ND	2.31	127.24	124.38
15	AD	401	HEC	C1D-C2D-C3D	-2.31	105.39	107.00
16	AG	101	CDL	CA4-OA6-CA5	-2.29	112.16	117.79
16	Ag	101	CDL	CB4-OB6-CB5	-2.27	112.20	117.79
12	Ac	401	HEM	CHB-C1B-C2B	-2.25	120.50	126.72
12	Ac	402	HEM	CHA-C4D-ND	2.25	127.16	124.38
12	AC	402	HEM	CHB-C1B-C2B	-2.24	120.53	126.72
11	AC	401	3PE	C2-O21-C21	2.23	123.29	117.79
11	AG	103	3PE	C2-O21-C21	-2.22	112.31	117.79
12	AC	403	HEM	CAD-C3D-C4D	2.07	128.28	124.66
15	AD	401	HEC	CAA-CBA-CGA	-2.07	107.96	113.76
12	Ac	402	HEM	CAD-C3D-C4D	2.04	128.22	124.66
13	Ac	404	U10	C3M-O3-C3	2.04	123.69	116.47
15	Ad	401	HEC	CAA-CBA-CGA	-2.04	108.05	113.76
13	AC	405	U10	C3M-O3-C3	2.03	123.66	116.47
13	AC	405	U10	O4-C4-C3	2.02	131.26	123.64
13	Ac	404	U10	O4-C4-C3	2.00	131.20	123.64
12	AC	403	HEM	CMC-C2C-C3C	2.00	128.42	124.68

There are no chirality outliers.

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AC	401	3PE	C11-O13-P-O12
11	AC	401	3PE	O13-C11-C12-N
11	AG	103	3PE	C1-O11-P-O12
11	AG	103	3PE	C1-O11-P-O13
11	AG	103	3PE	C1-O11-P-O14
11	AG	103	3PE	C11-O13-P-O14
11	Aa	501	3PE	C11-O13-P-O12
11	Ag	103	3PE	C1-O11-P-O12
11	Ag	103	3PE	C1-O11-P-O14
11	Ag	103	3PE	C11-O13-P-O11
11	Ag	103	3PE	O13-C11-C12-N
12	AC	402	HEM	C2B-C3B-CAB-CBB
12	AC	403	HEM	C2B-C3B-CAB-CBB
12	AC	403	HEM	C4B-C3B-CAB-CBB
12	Ac	401	HEM	C2B-C3B-CAB-CBB
12	Ac	402	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	Ac	402	HEM	C4B-C3B-CAB-CBB
13	AC	405	U10	C7-C8-C9-C10
13	AC	405	U10	C7-C8-C9-C11
13	Ac	404	U10	C7-C8-C9-C10
13	Ac	404	U10	C7-C8-C9-C11
14	AC	406	UQ6	C1-C6-C7-C8
14	AC	406	UQ6	C7-C8-C9-C10
14	AC	406	UQ6	C7-C8-C9-C11
14	AC	406	UQ6	C12-C13-C14-C15
14	AC	406	UQ6	C12-C13-C14-C16
14	AC	406	UQ6	C13-C14-C16-C17
14	AC	406	UQ6	C15-C14-C16-C17
14	AC	406	UQ6	C17-C18-C19-C20
14	Ac	405	UQ6	C1-C6-C7-C8
14	Ac	405	UQ6	C7-C8-C9-C10
14	Ac	405	UQ6	C7-C8-C9-C11
14	Ac	405	UQ6	C12-C13-C14-C15
14	Ac	405	UQ6	C12-C13-C14-C16
14	Ac	405	UQ6	C13-C14-C16-C17
14	Ac	405	UQ6	C15-C14-C16-C17
14	Ac	405	UQ6	C17-C18-C19-C20
16	AG	101	CDL	CA2-OA2-PA1-OA4
16	AG	101	CDL	CB2-OB2-PB2-OB3
16	AG	102	CDL	C1-CB2-OB2-PB2
16	AG	102	CDL	CB2-OB2-PB2-OB4
16	AG	102	CDL	CB3-OB5-PB2-OB2
16	AG	102	CDL	CB3-OB5-PB2-OB3
16	AG	102	CDL	CB3-OB5-PB2-OB4
16	Aa	502	CDL	CA2-OA2-PA1-OA5
16	Aa	502	CDL	CA3-OA5-PA1-OA3
16	Aa	502	CDL	CB2-OB2-PB2-OB3
16	Aa	502	CDL	CB2-OB2-PB2-OB4
16	Ag	101	CDL	CB2-OB2-PB2-OB3
16	Ag	101	CDL	CB2-OB2-PB2-OB4
16	Ag	101	CDL	CB2-OB2-PB2-OB5
16	Ag	101	CDL	CB3-OB5-PB2-OB2
16	Ag	101	CDL	CB3-OB5-PB2-OB3
16	Ag	101	CDL	CB3-OB5-PB2-OB4
16	Ag	102	CDL	CB2-OB2-PB2-OB5
16	Ag	102	CDL	CB3-OB5-PB2-OB4
17	Ae	301	PC1	C1-O11-P-O12
17	Ae	301	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
13	AC	405	U10	C12-C13-C14-C15
13	AC	405	U10	C12-C13-C14-C16
13	Ac	404	U10	C12-C13-C14-C15
13	Ac	404	U10	C12-C13-C14-C16
14	AC	406	UQ6	C17-C18-C19-C21
14	Ac	405	UQ6	C17-C18-C19-C21
17	Ae	301	PC1	O32-C31-O31-C3
11	Aa	501	3PE	C22-C21-O21-C2
17	Ae	301	PC1	C32-C31-O31-C3
14	AC	406	UQ6	C9-C11-C12-C13
14	AC	406	UQ6	C14-C16-C17-C18
14	Ac	405	UQ6	C9-C11-C12-C13
14	Ac	405	UQ6	C14-C16-C17-C18
11	Aa	501	3PE	O22-C21-O21-C2
12	AC	402	HEM	C2A-CAA-CBA-CGA
12	Ac	401	HEM	C2A-CAA-CBA-CGA
11	Ag	103	3PE	C32-C33-C34-C35
11	AC	401	3PE	C11-O13-P-O11
11	AG	103	3PE	C11-O13-P-O11
11	Ag	103	3PE	C1-O11-P-O13
16	AG	101	CDL	CB2-OB2-PB2-OB5
16	AG	102	CDL	CB2-OB2-PB2-OB5
16	Aa	502	CDL	CB2-OB2-PB2-OB5
16	Aa	502	CDL	CB3-OB5-PB2-OB2
16	Ag	102	CDL	CB3-OB5-PB2-OB2
11	AG	103	3PE	C32-C33-C34-C35
11	Ag	103	3PE	C3C-C3D-C3E-C3F
16	AG	101	CDL	C31-CA7-OA8-CA6
16	Aa	502	CDL	C51-CB5-OB6-CB4
11	Ag	103	3PE	C37-C38-C39-C3A
16	Ag	102	CDL	C74-C75-C76-C77
16	Aa	502	CDL	OB7-CB5-OB6-CB4
11	AG	103	3PE	C37-C38-C39-C3A
16	AG	101	CDL	OA9-CA7-OA8-CA6
16	AG	102	CDL	C31-CA7-OA8-CA6
16	AG	102	CDL	C74-C75-C76-C77
12	AC	402	HEM	C4B-C3B-CAB-CBB
12	Ac	401	HEM	C4B-C3B-CAB-CBB
16	AG	102	CDL	C51-CB5-OB6-CB4
11	Aa	501	3PE	C11-O13-P-O11
16	AG	101	CDL	CA2-OA2-PA1-OA5
16	Ag	102	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
16	AG	102	CDL	OA9-CA7-OA8-CA6
17	Ae	301	PC1	C2-C1-O11-P
16	Ag	102	CDL	OB5-CB3-CB4-CB6
16	Aa	502	CDL	C71-CB7-OB8-CB6
17	Ae	301	PC1	C1-O11-P-O13
16	Ag	102	CDL	OB5-CB3-CB4-OB6
16	AG	102	CDL	OB7-CB5-OB6-CB4
16	AG	102	CDL	C1-CA2-OA2-PA1
11	Aa	501	3PE	C3-C2-O21-C21
16	Aa	502	CDL	OB9-CB7-OB8-CB6
16	AG	102	CDL	CB4-CB3-OB5-PB2
16	Ag	102	CDL	CB4-CB3-OB5-PB2
11	AC	401	3PE	C11-O13-P-O14
11	AG	103	3PE	C11-O13-P-O12
11	Aa	501	3PE	C11-O13-P-O14
11	Ag	103	3PE	C11-O13-P-O12
16	AG	101	CDL	CA2-OA2-PA1-OA3
16	AG	101	CDL	CB2-OB2-PB2-OB4
16	Aa	502	CDL	CA2-OA2-PA1-OA4
16	Aa	502	CDL	CB3-OB5-PB2-OB3
16	Aa	502	CDL	CB3-OB5-PB2-OB4
16	Ag	102	CDL	CB2-OB2-PB2-OB4
17	Ae	301	PC1	C1-O11-P-O14
16	Ag	102	CDL	C1-CA2-OA2-PA1
16	AG	102	CDL	C71-CB7-OB8-CB6
16	AG	102	CDL	OB9-CB7-OB8-CB6
11	Ag	103	3PE	C35-C36-C37-C38
11	AG	103	3PE	C35-C36-C37-C38
16	Ag	101	CDL	C1-CA2-OA2-PA1
13	AC	405	U10	C12-C11-C9-C10
13	Ac	404	U10	C12-C11-C9-C10
12	AC	403	HEM	CAD-CBD-CGD-O1D
12	Ac	402	HEM	CAD-CBD-CGD-O1D
12	AC	402	HEM	CAD-CBD-CGD-O1D
12	AC	402	HEM	CAD-CBD-CGD-O2D
12	Ac	401	HEM	CAD-CBD-CGD-O2D
12	AC	402	HEM	CAA-CBA-CGA-O2A
12	Ac	401	HEM	CAA-CBA-CGA-O2A
12	Ac	401	HEM	CAD-CBD-CGD-O1D
12	AC	403	HEM	CAD-CBD-CGD-O2D
12	Ac	402	HEM	CAD-CBD-CGD-O2D
12	AC	402	HEM	CAA-CBA-CGA-O1A

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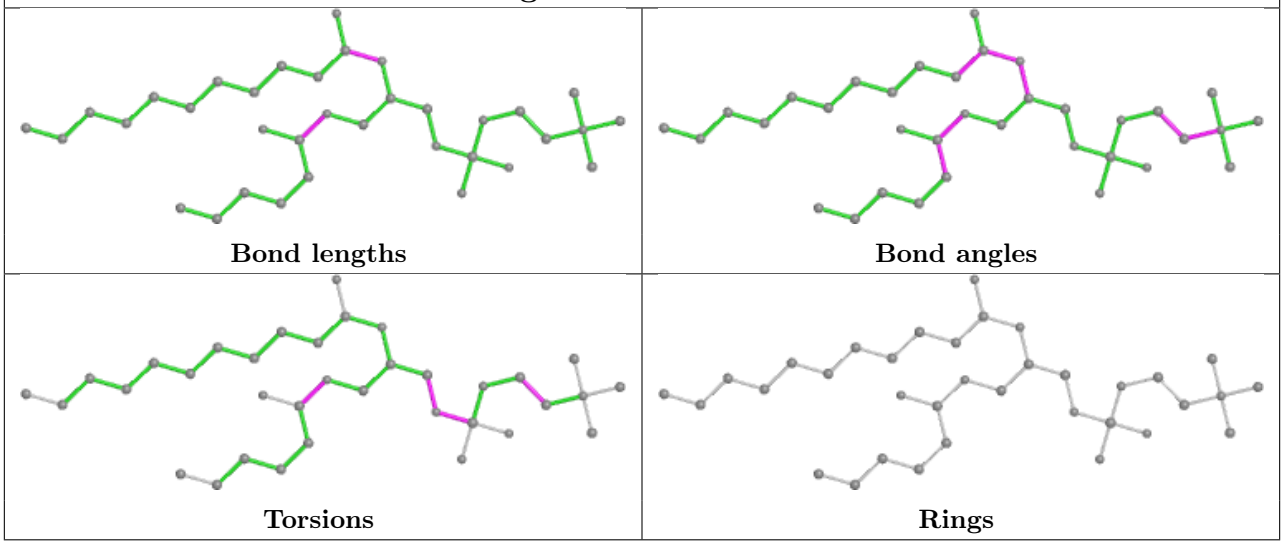
Mol	Chain	Res	Type	Atoms
12	Ac	401	HEM	CAA-CBA-CGA-O1A
13	AC	405	U10	C12-C11-C9-C8
13	Ac	404	U10	C12-C11-C9-C8
14	AC	406	UQ6	C5-C6-C7-C8
14	Ac	405	UQ6	C5-C6-C7-C8
16	Ag	102	CDL	C72-C73-C74-C75
12	AC	403	HEM	CAA-CBA-CGA-O2A
12	Ac	402	HEM	CAA-CBA-CGA-O2A
16	Ag	102	CDL	C52-C51-CB5-OB6
12	Ac	402	HEM	CAA-CBA-CGA-O1A
12	AC	403	HEM	CAA-CBA-CGA-O1A
11	Ac	403	3PE	C23-C24-C25-C26
11	AC	401	3PE	O31-C31-C32-C33
14	AC	406	UQ6	C6-C7-C8-C9
14	Ac	405	UQ6	C6-C7-C8-C9
11	AC	404	3PE	C11-O13-P-O14
11	Aa	501	3PE	C1-O11-P-O14
11	Ac	403	3PE	C11-O13-P-O14
16	Ag	102	CDL	CB2-C1-CA2-OA2
11	Ac	403	3PE	C22-C23-C24-C25
11	AC	401	3PE	O21-C21-C22-C23
11	AC	401	3PE	O32-C31-C32-C33

There are no ring outliers.

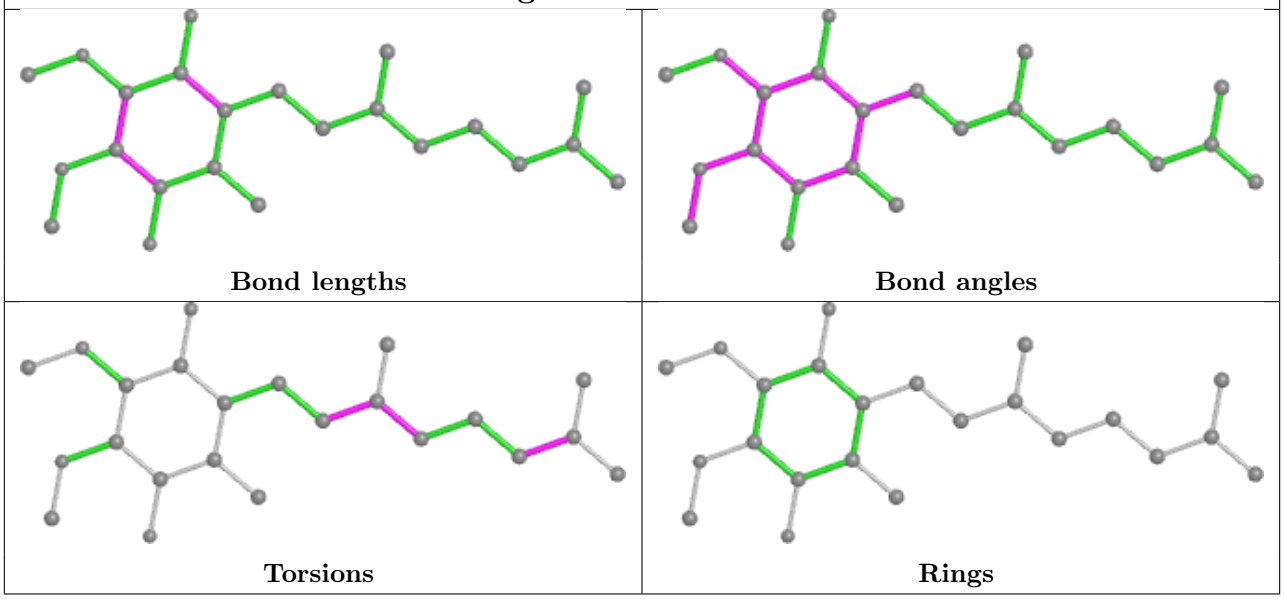
No monomer is involved in short contacts.

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.

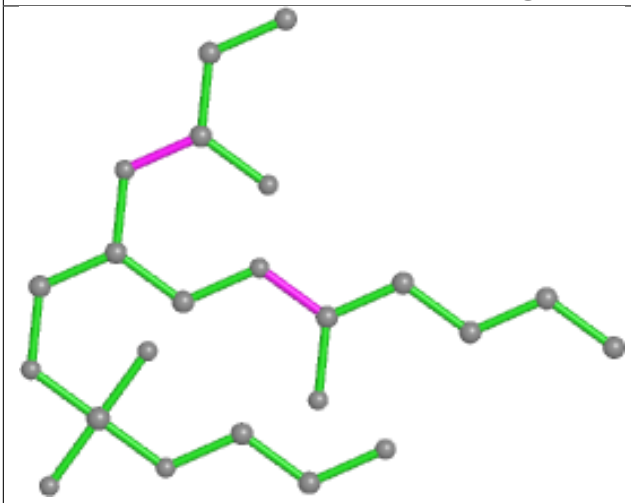
Ligand PC1 Ae 301



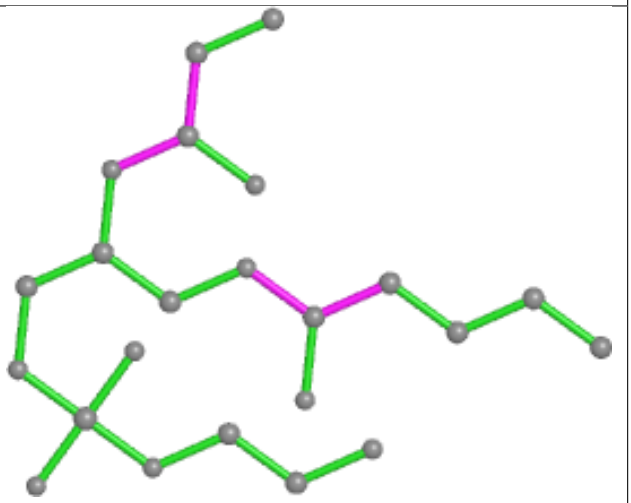
Ligand U10 AC 405



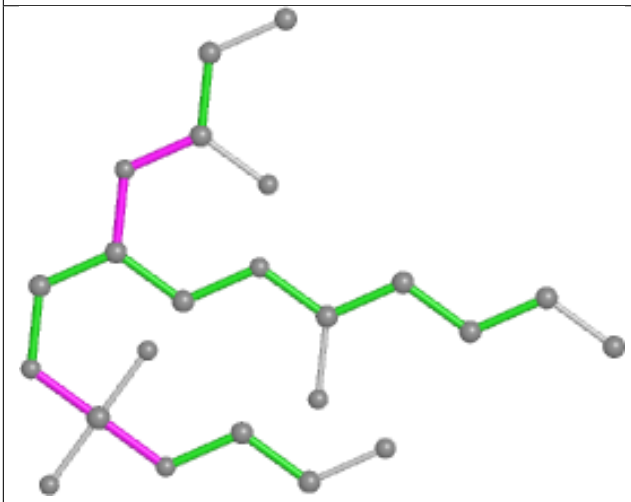
Ligand 3PE Aa 501



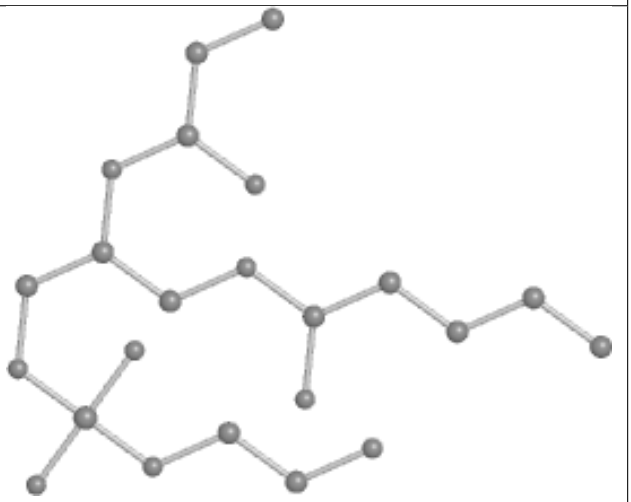
Bond lengths



Bond angles

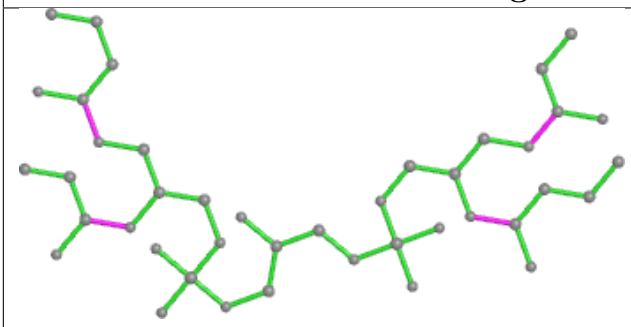


Torsions

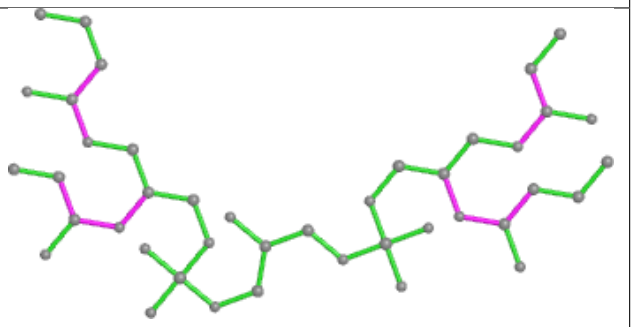


Rings

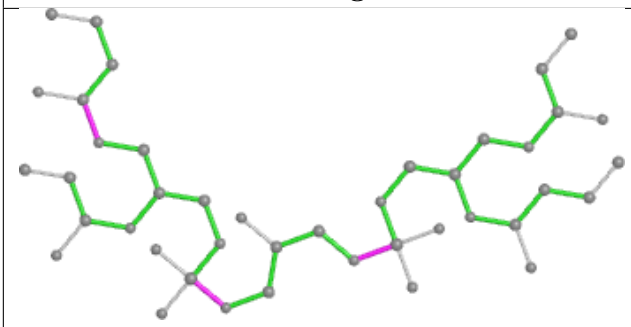
Ligand CDL AG 101



Bond lengths



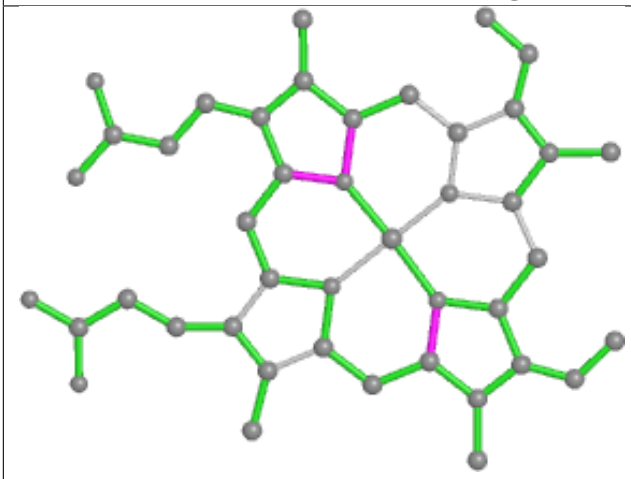
Bond angles



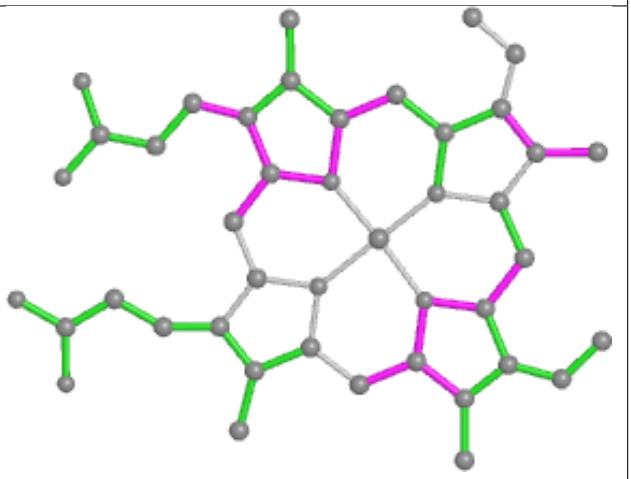
Torsions

Rings

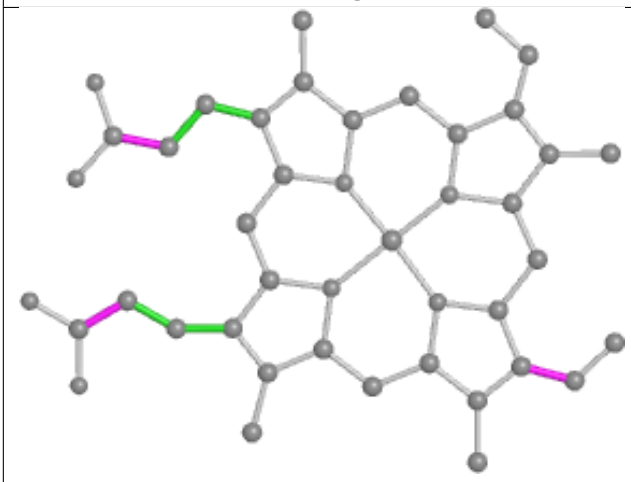
Ligand HEM AC 403



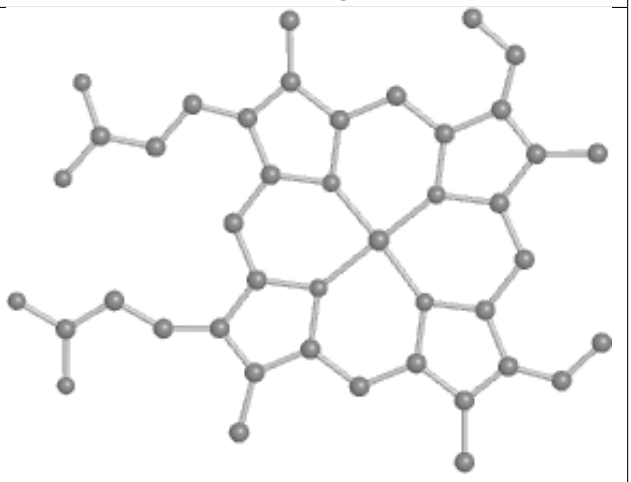
Bond lengths



Bond angles

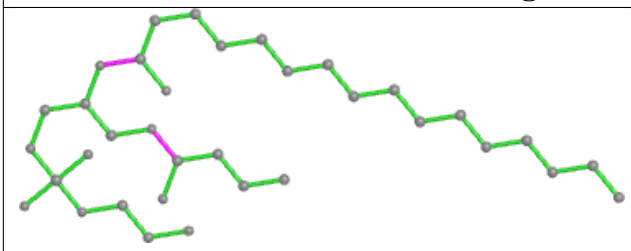


Torsions

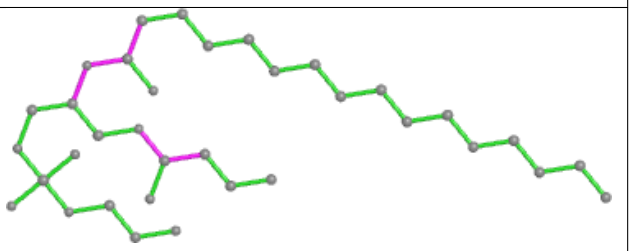


Rings

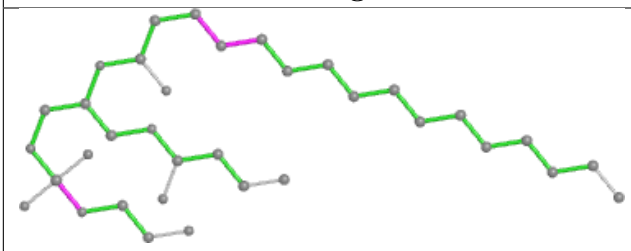
Ligand 3PE Ac 403



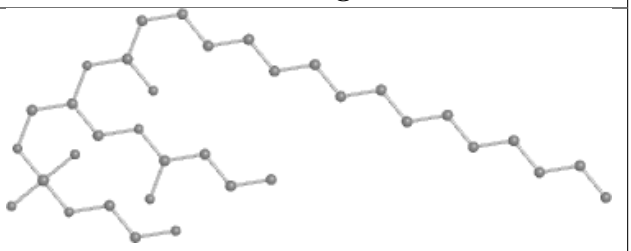
Bond lengths



Bond angles

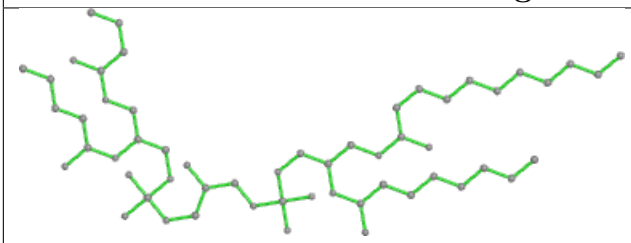


Torsions

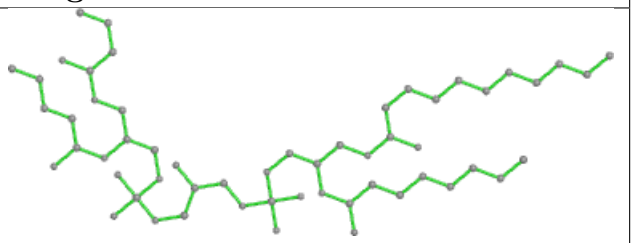


Rings

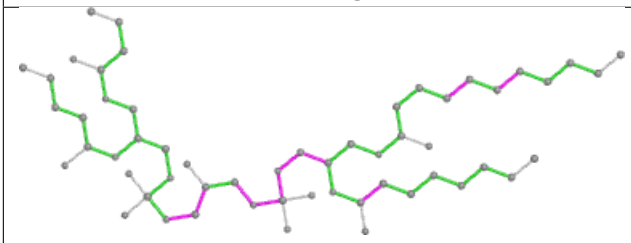
Ligand CDL Ag 102



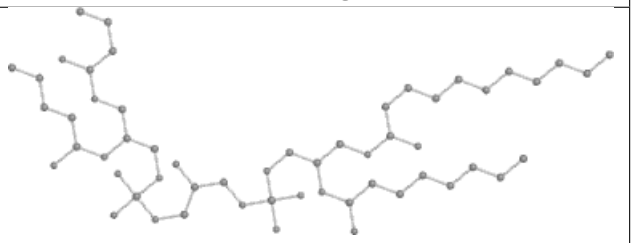
Bond lengths



Bond angles

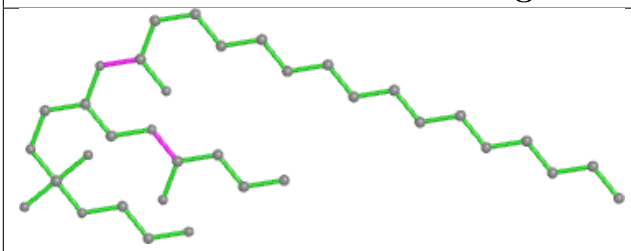


Torsions



Rings

Ligand 3PE AC 404



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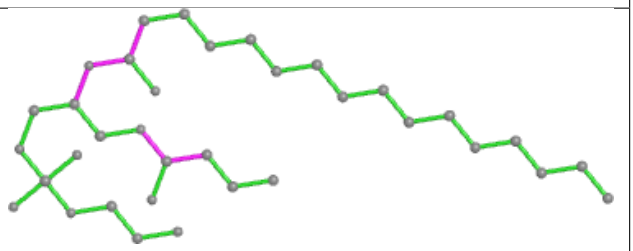
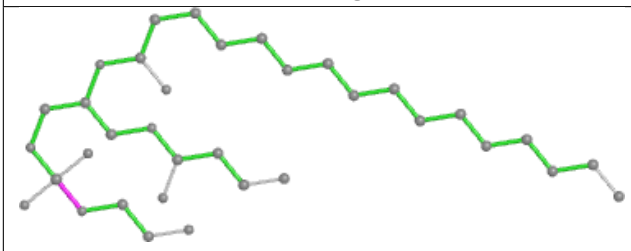


Bond angles



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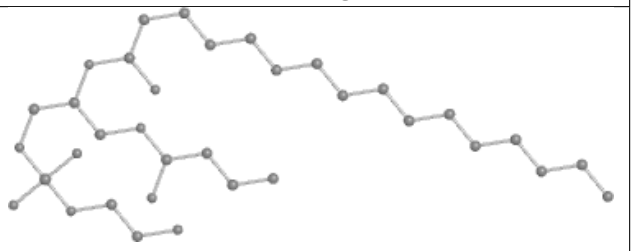
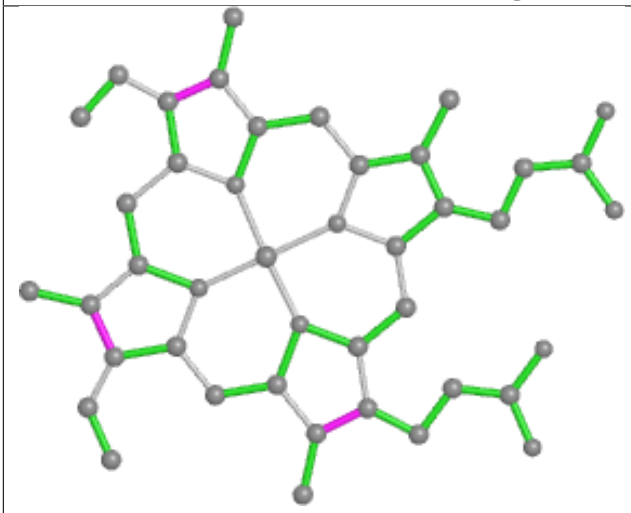


Rings

Ligand HEC AD 401



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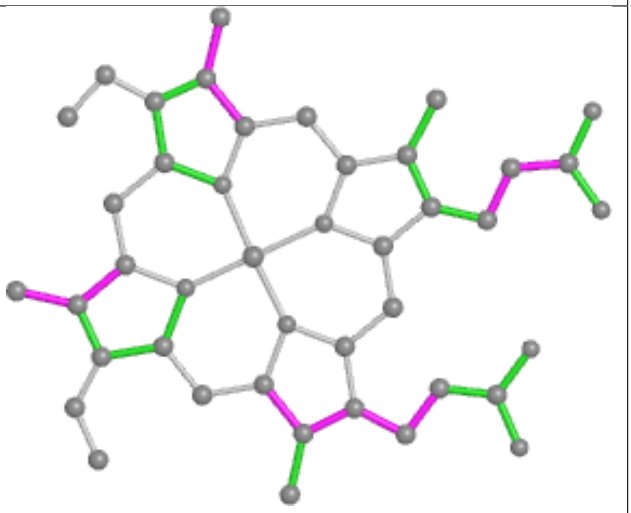
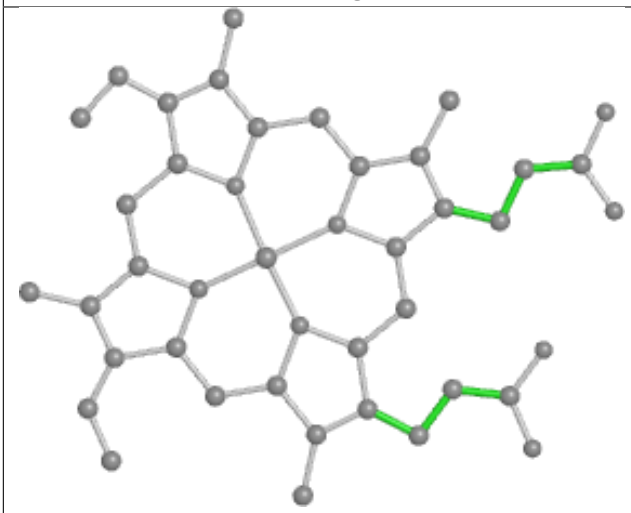


Bond angles



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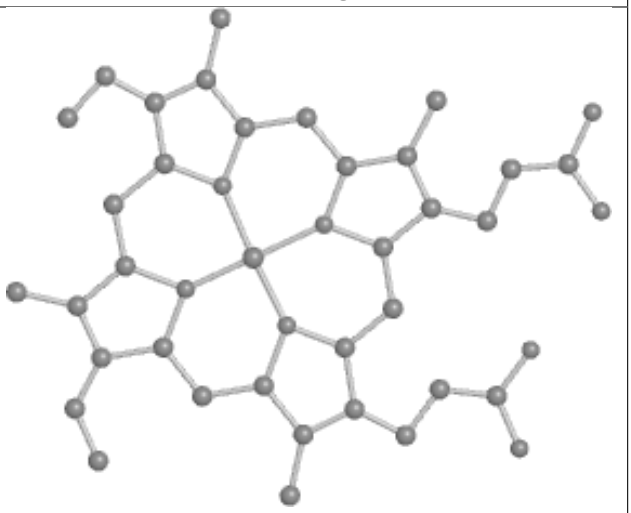
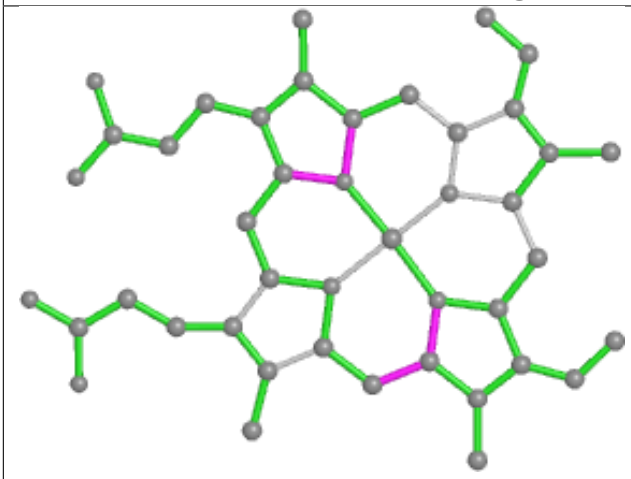


Rings

Ligand HEM Ac 401



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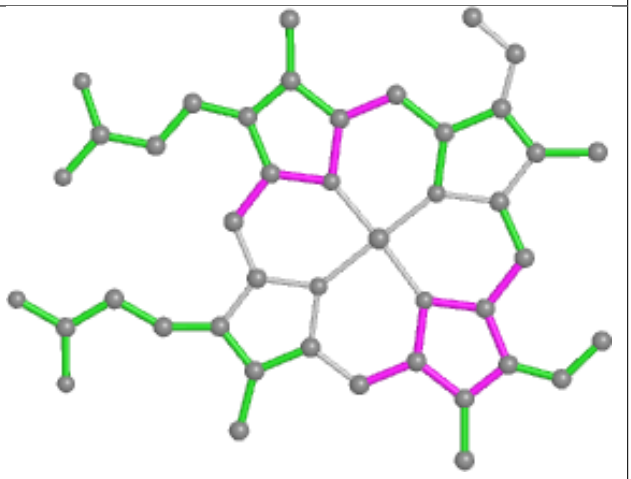
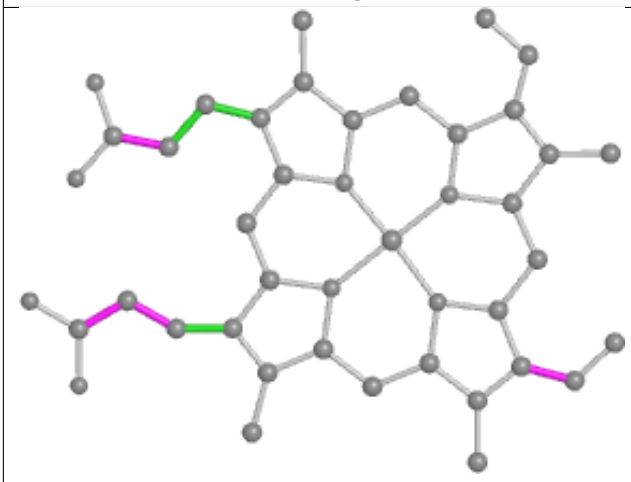
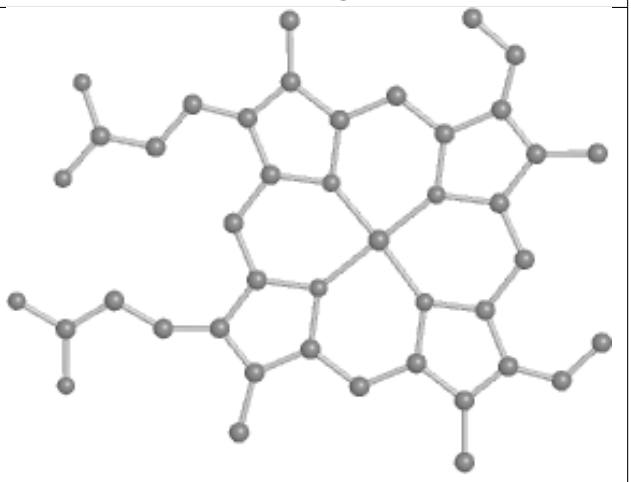


Bond angles

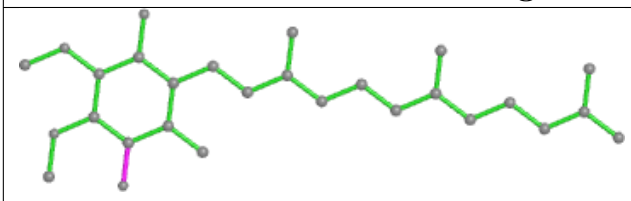


Torsions

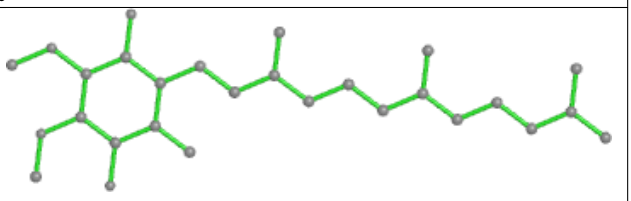


Rings

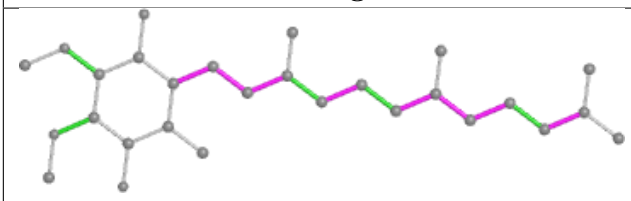
Ligand UQ6 Ac 405



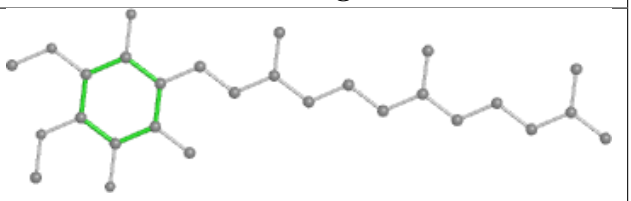
Bond lengths



Bond angles

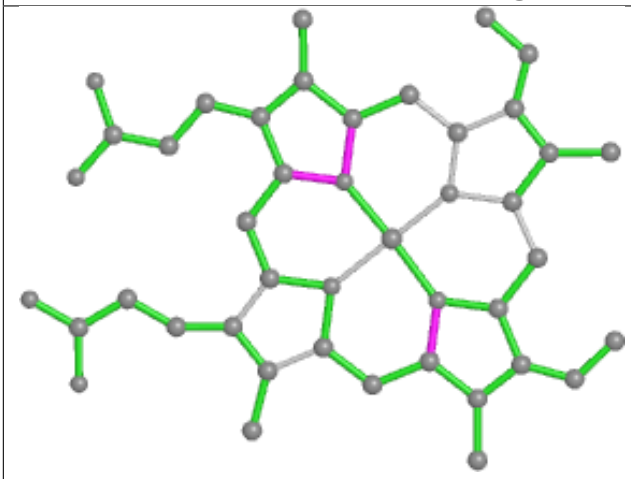


Torsions

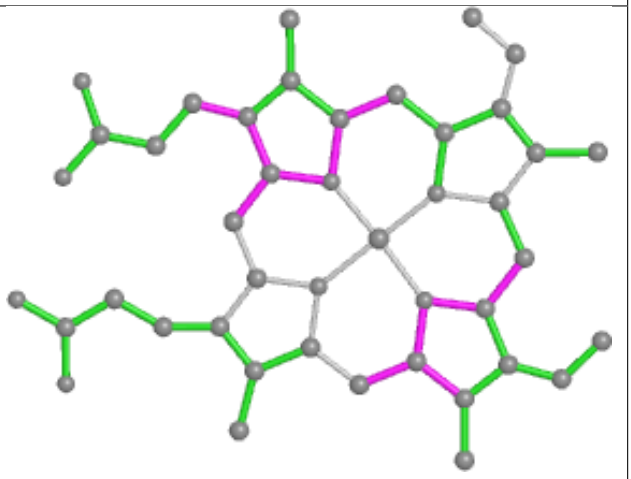


Rings

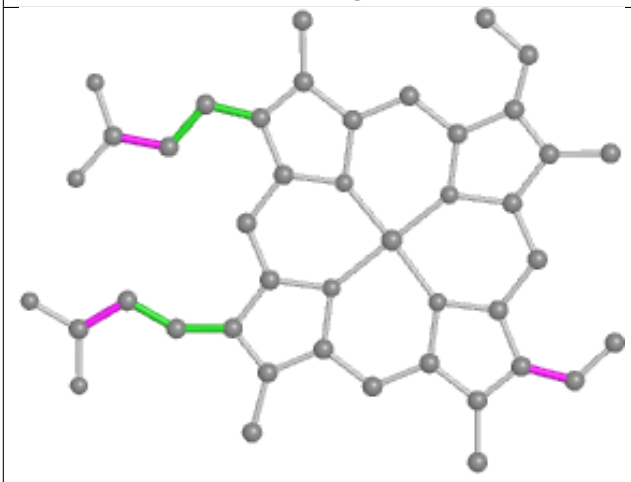
Ligand HEM Ac 402



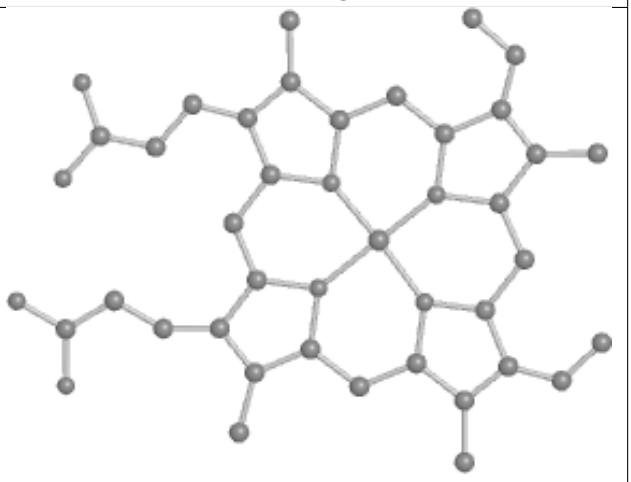
Bond lengths



Bond angles

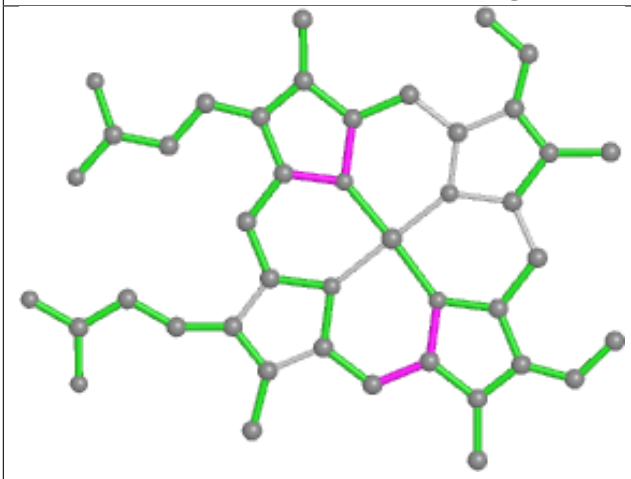


Torsions



Rings

Ligand HEM AC 402



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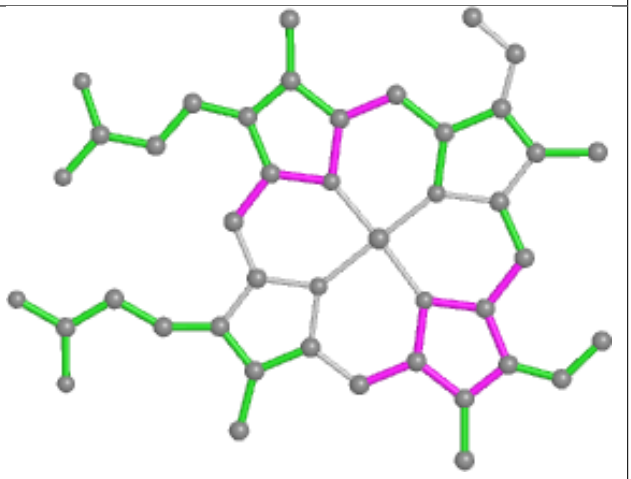
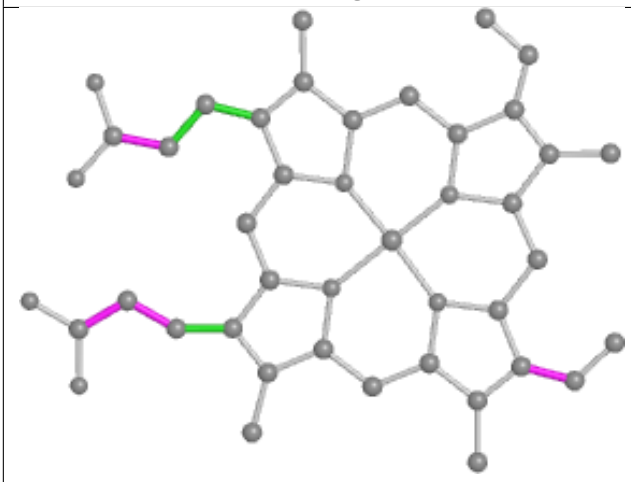
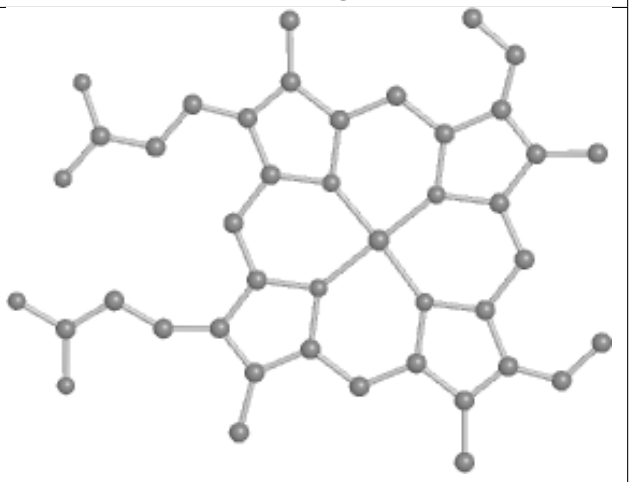


Bond angles

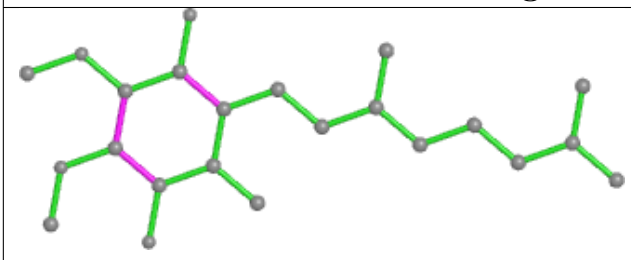


Torsions

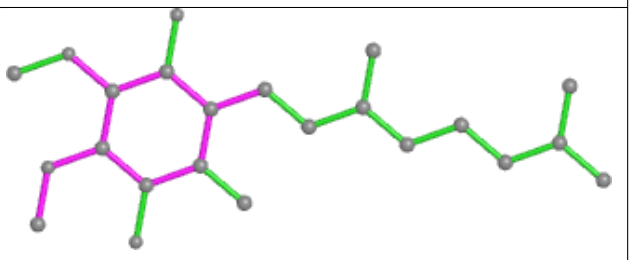


Rings

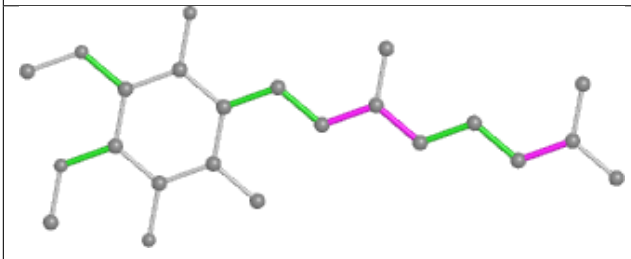
Ligand U10 Ac 404



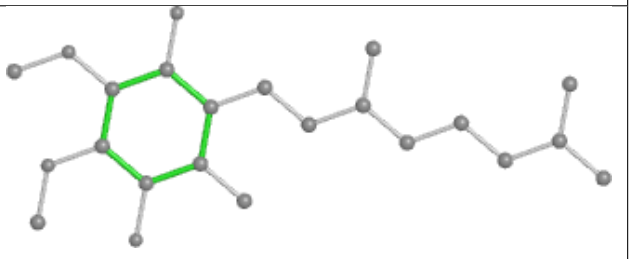
Bond lengths



Bond angles

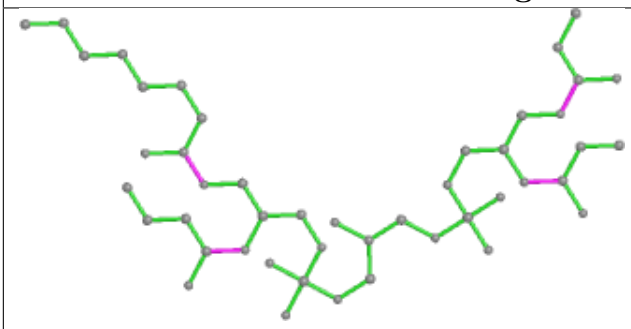


Torsions

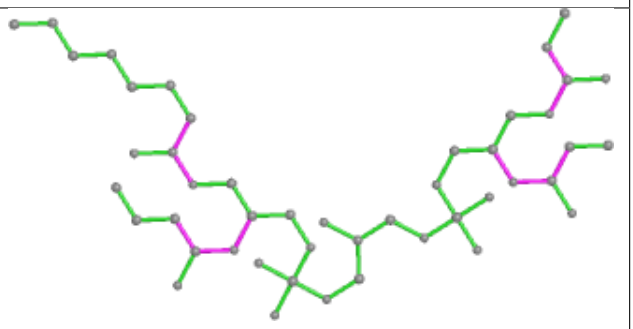


Rings

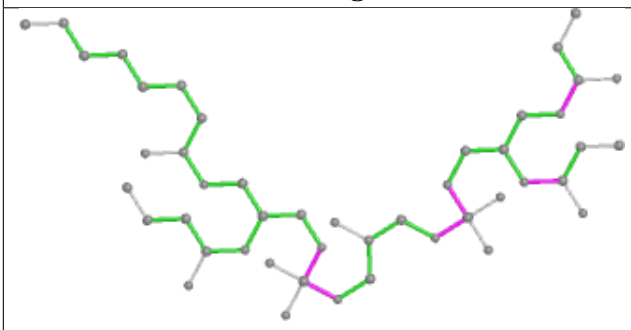
Ligand CDL Aa 502



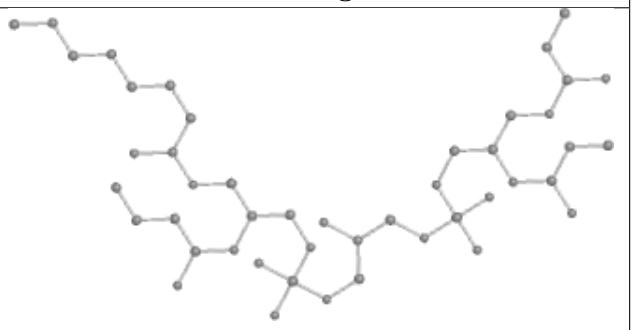
Bond lengths



Bond angles

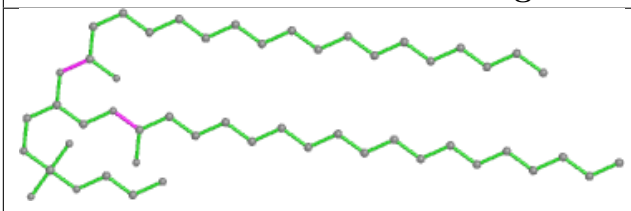


Torsions

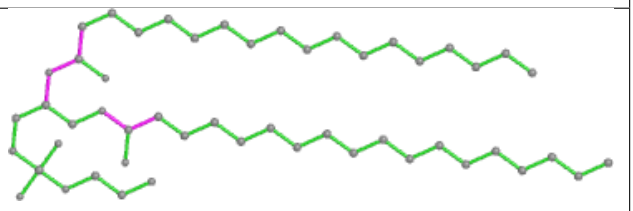


Rings

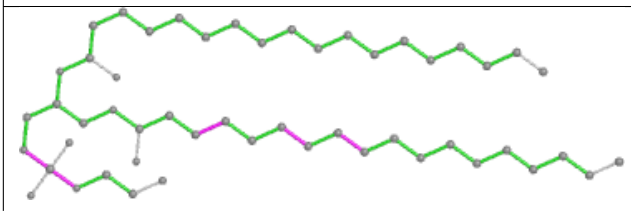
Ligand 3PE AG 103



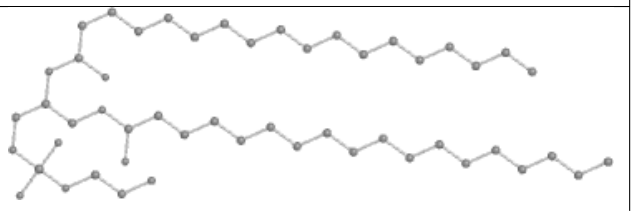
Bond lengths



Bond angles

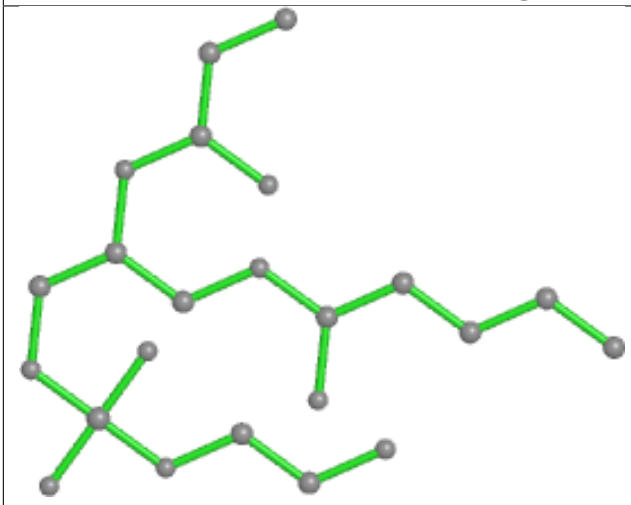


Torsions

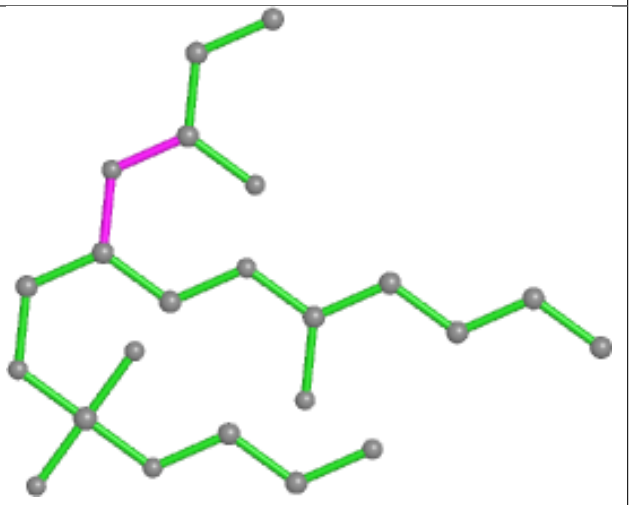


Rings

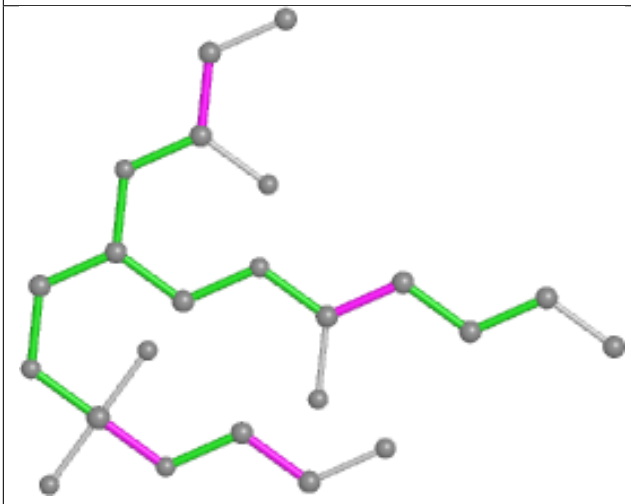
Ligand 3PE AC 401



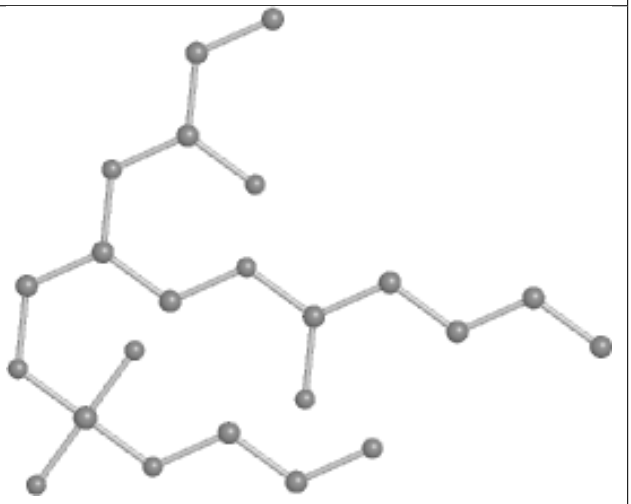
Bond lengths



Bond angles

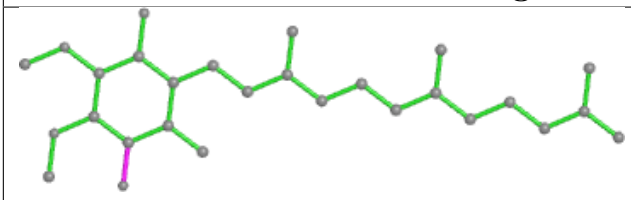


Torsions

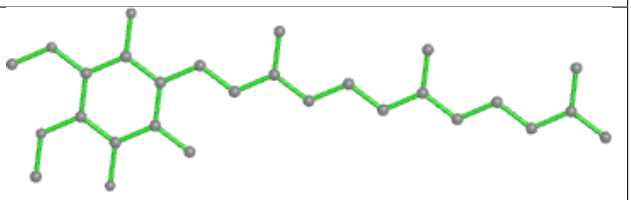


Rings

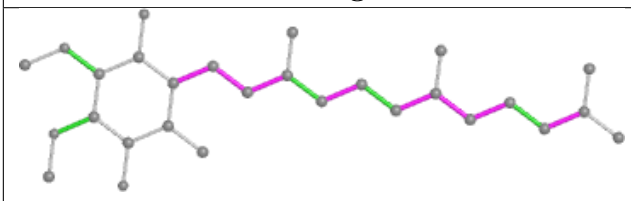
Ligand UQ6 AC 406



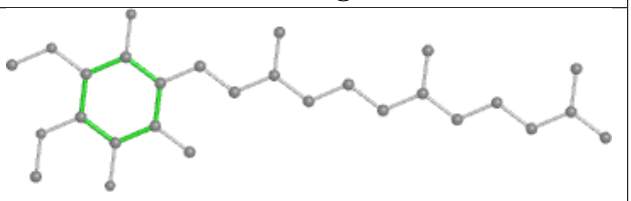
Bond lengths



Bond angles

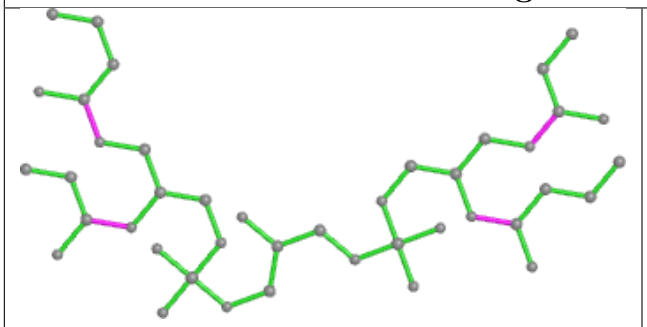


Torsions

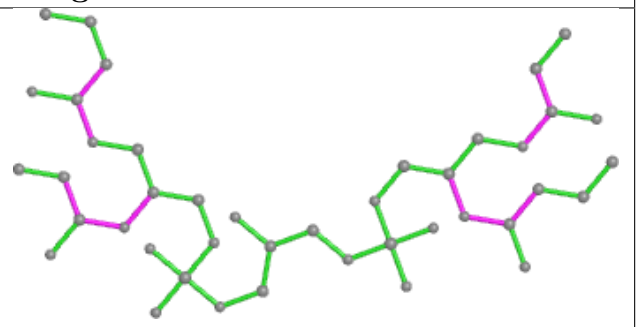


Rings

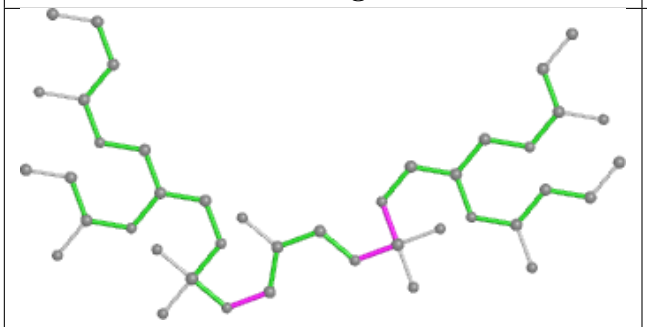
Ligand CDL Ag 101



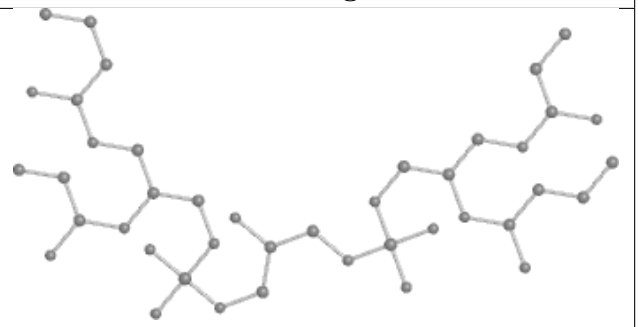
Bond lengths



Bond angles

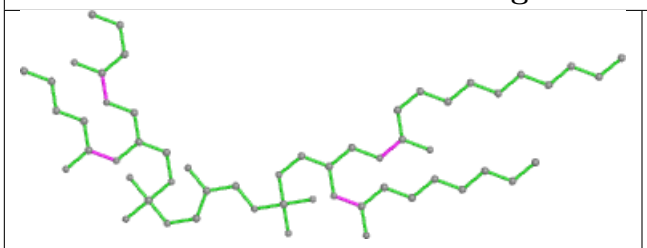


Torsions

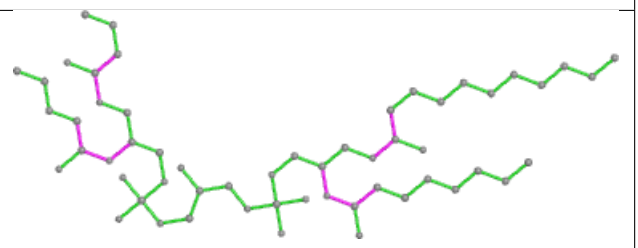


Rings

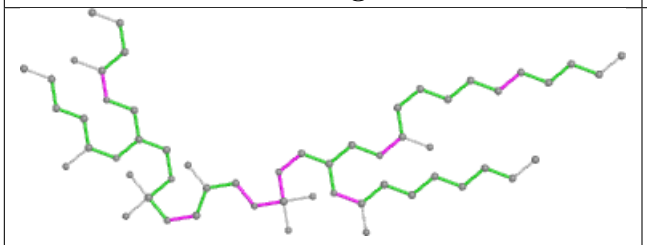
Ligand CDL AG 102



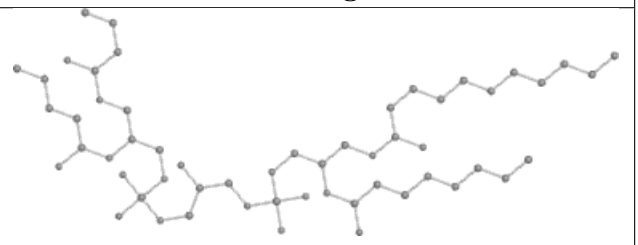
Bond lengths



Bond angles

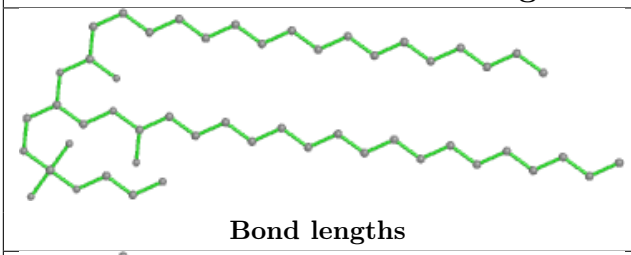


Torsions

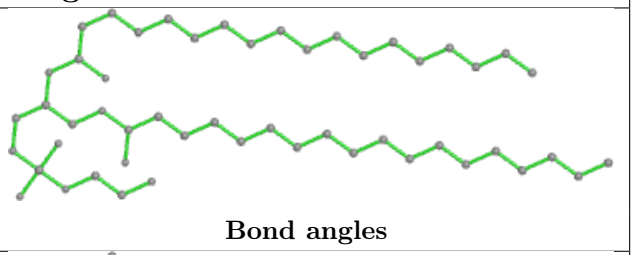


Rings

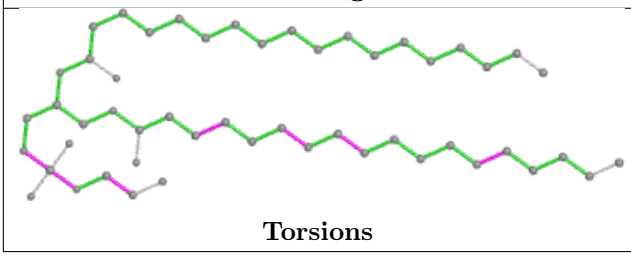
Ligand 3PE Ag 103



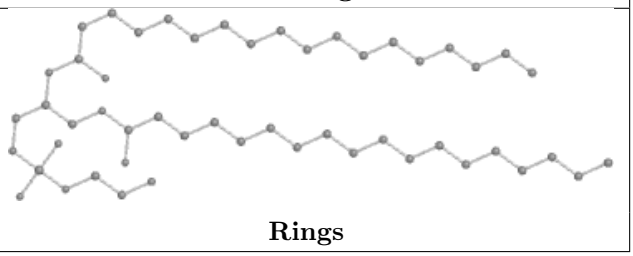
Bond lengths



Bond angles

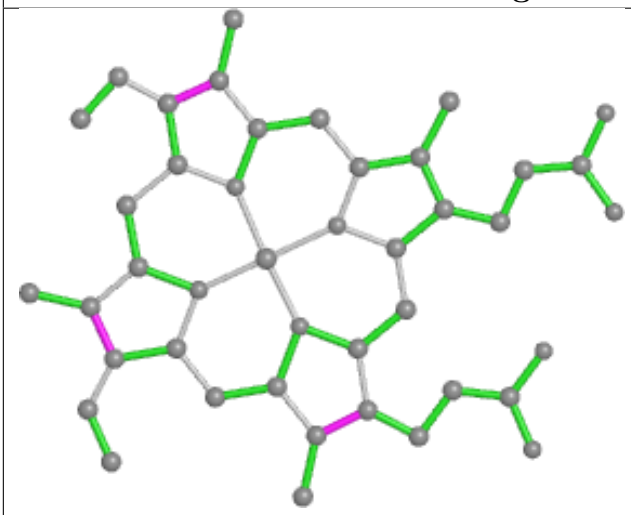


Torsions

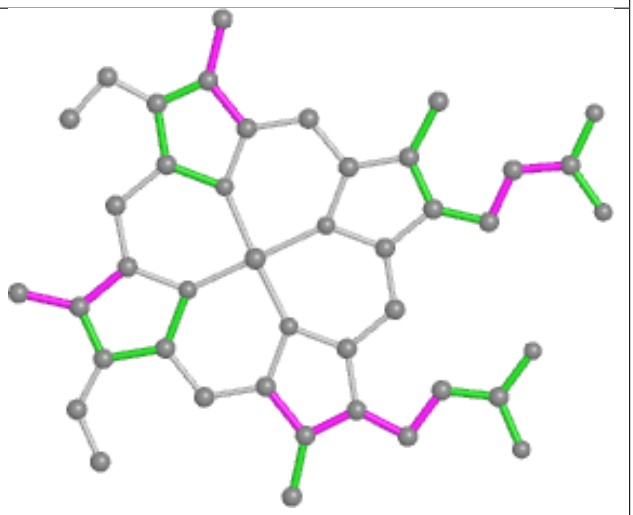


Rings

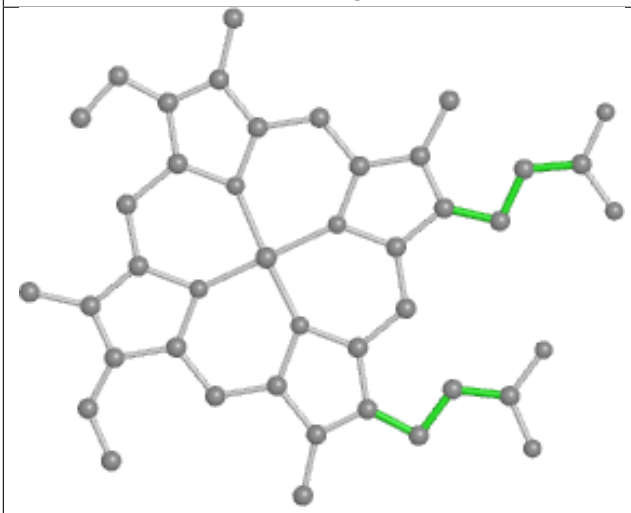
Ligand HEC Ad 401



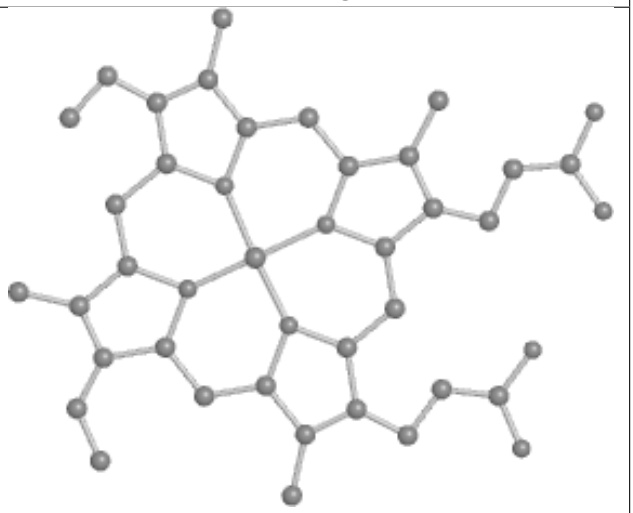
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

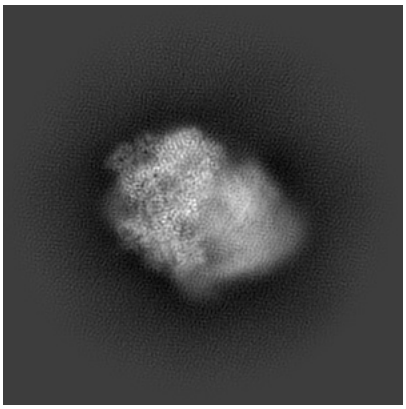
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35316. These allow visual inspection of the internal detail of the map and identification of artifacts.

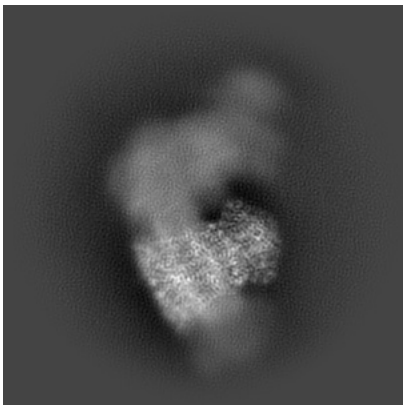
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

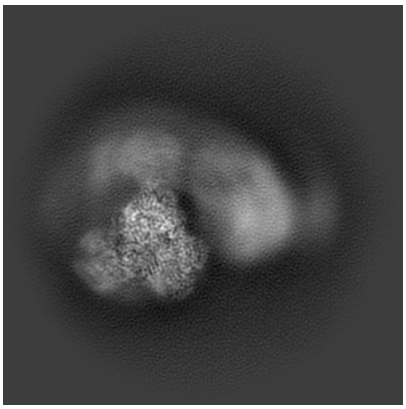
6.1.1 Primary map



X

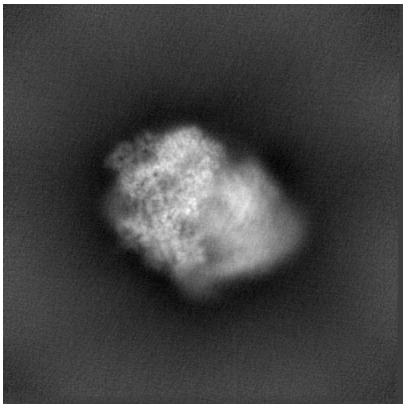


Y

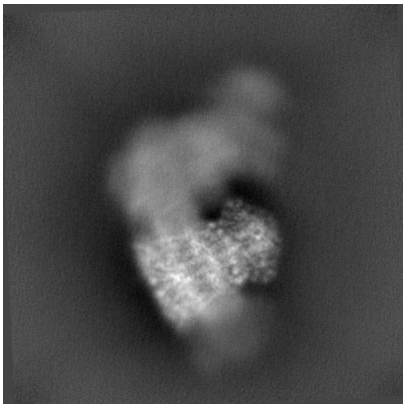


Z

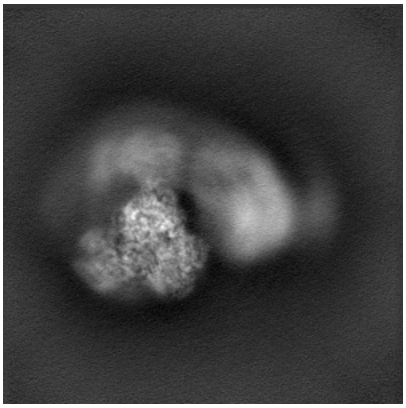
6.1.2 Raw map



X



Y

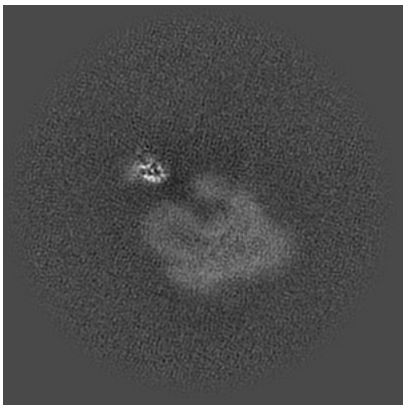


Z

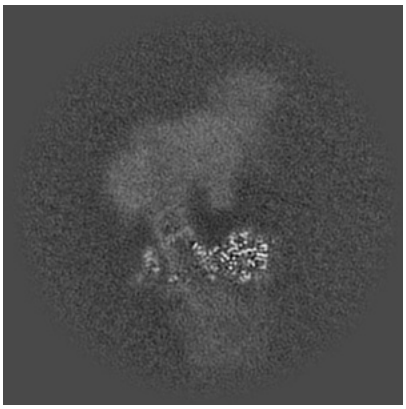
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

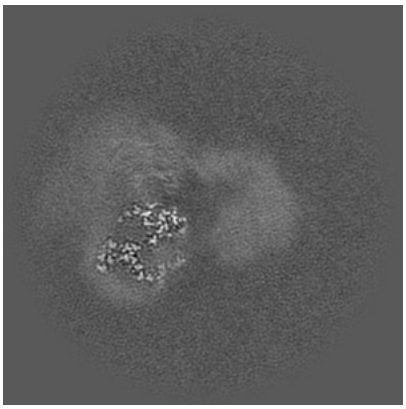
6.2.1 Primary map



X Index: 192

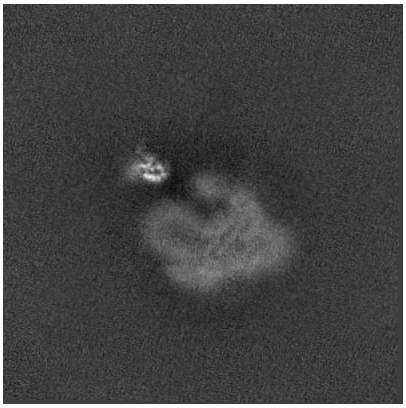


Y Index: 192

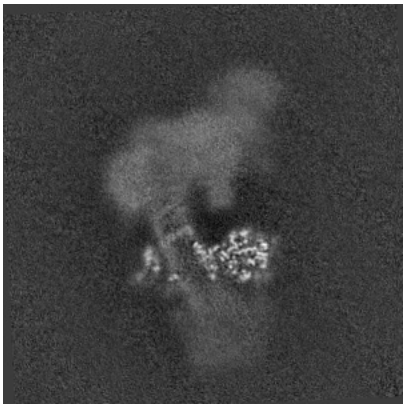


Z Index: 192

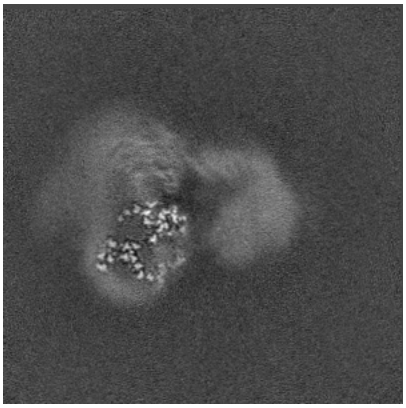
6.2.2 Raw map



X Index: 192



Y Index: 192

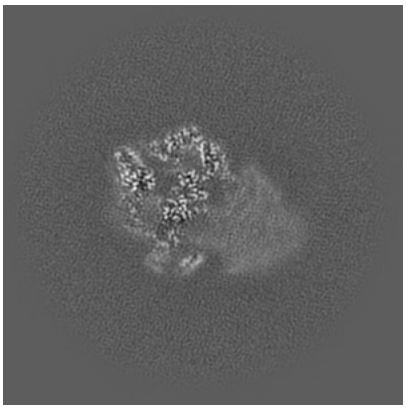


Z Index: 192

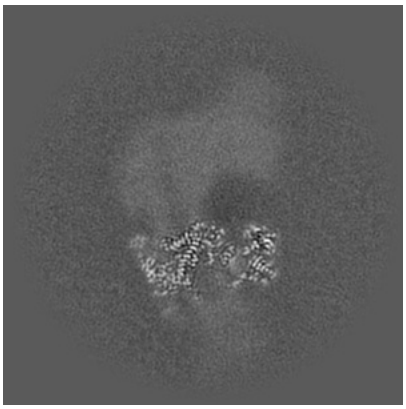
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

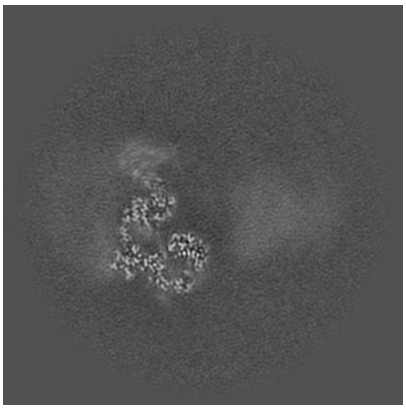
6.3.1 Primary map



X Index: 148

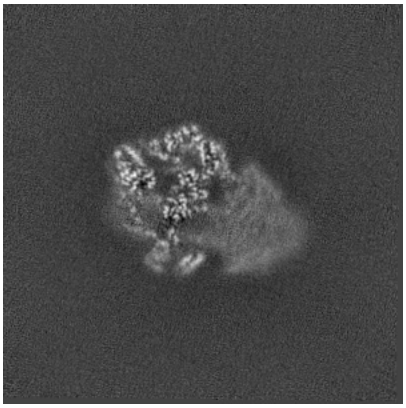


Y Index: 168

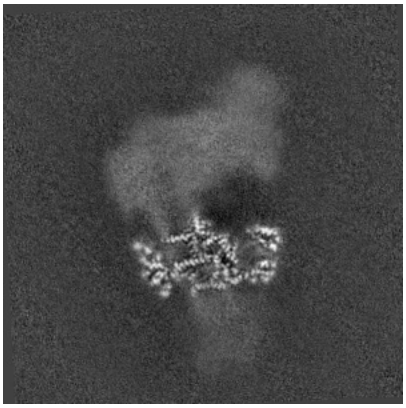


Z Index: 223

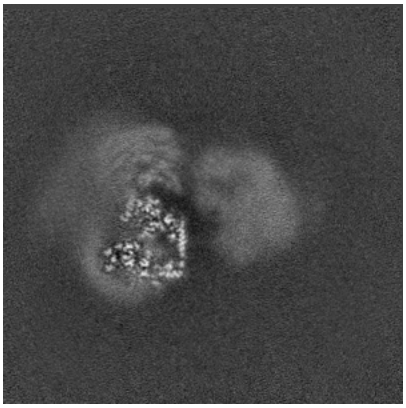
6.3.2 Raw map



X Index: 148



Y Index: 177

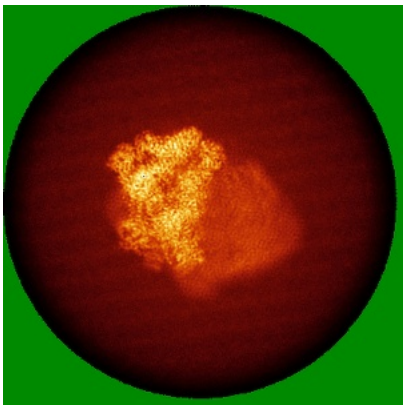


Z Index: 200

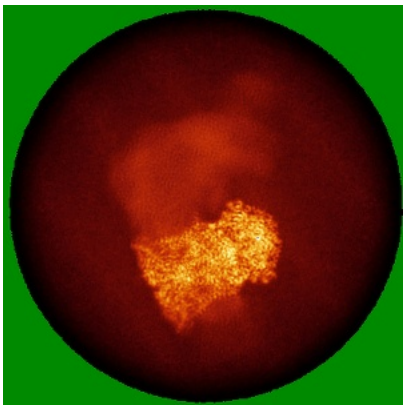
The images above show the largest variance slices of the map in three orthogonal directions.

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

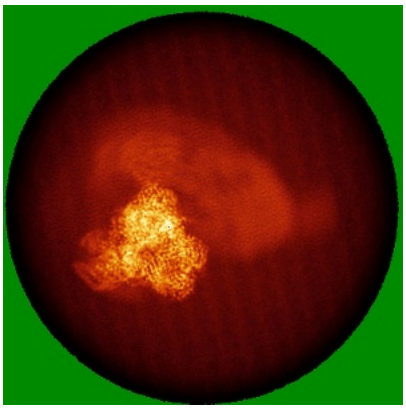
6.4.1 Primary map



X

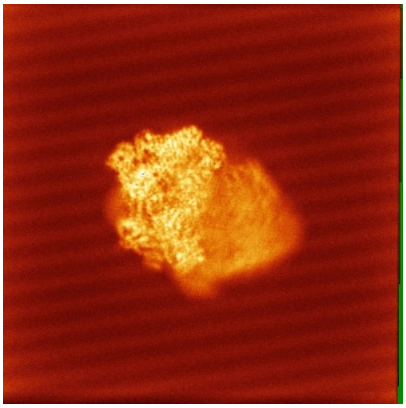


Y

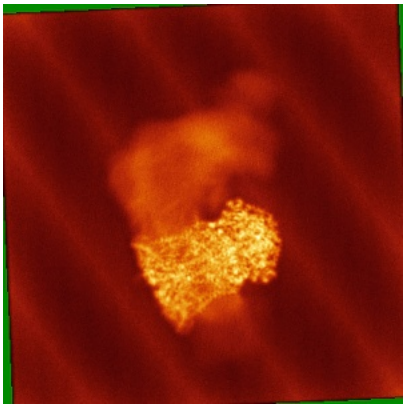


Z

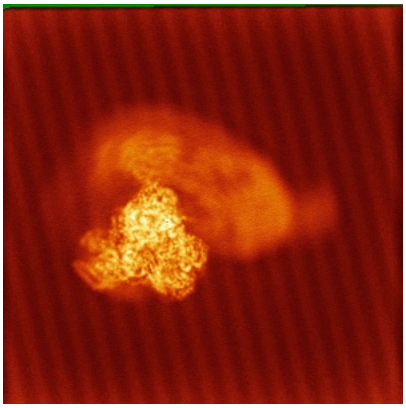
6.4.2 Raw map



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.

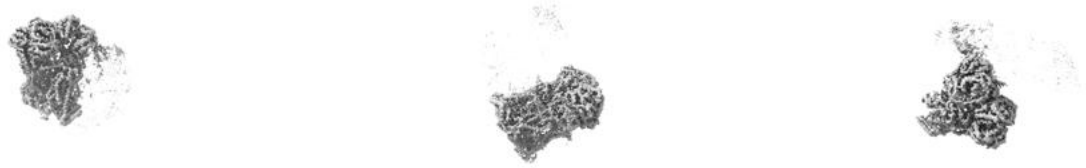
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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)

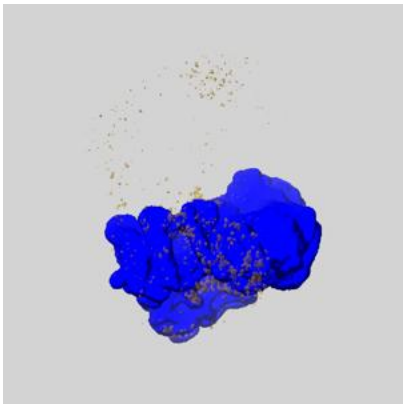
This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

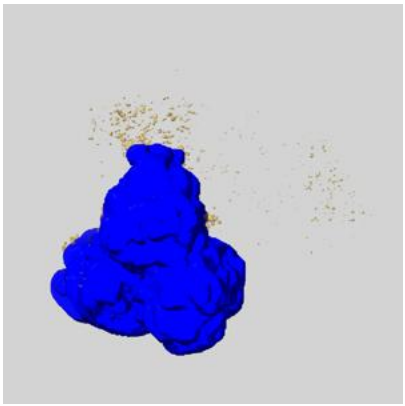
- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_35316_msk_1.map (i)

X



Y

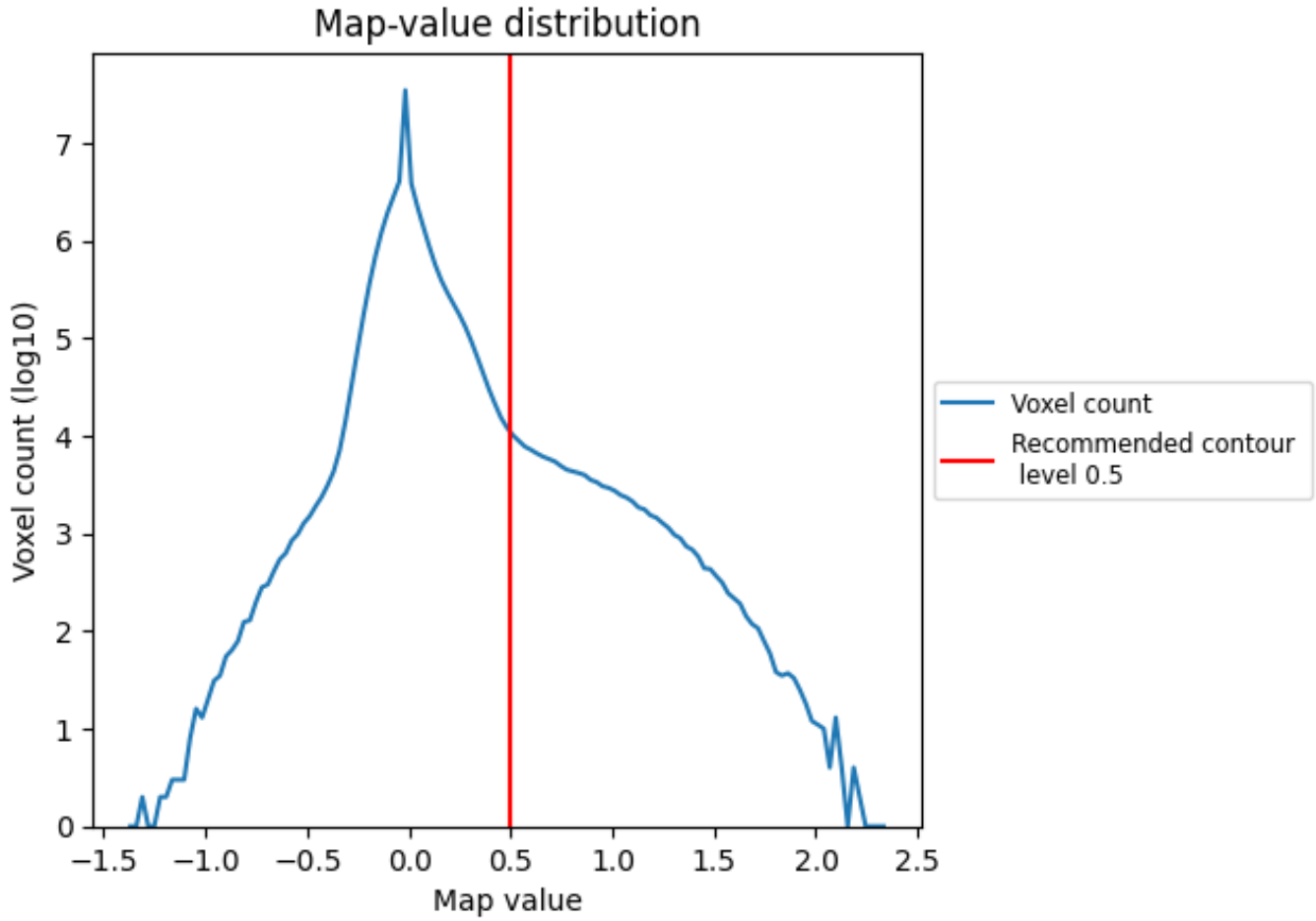


Z

7 Map analysis

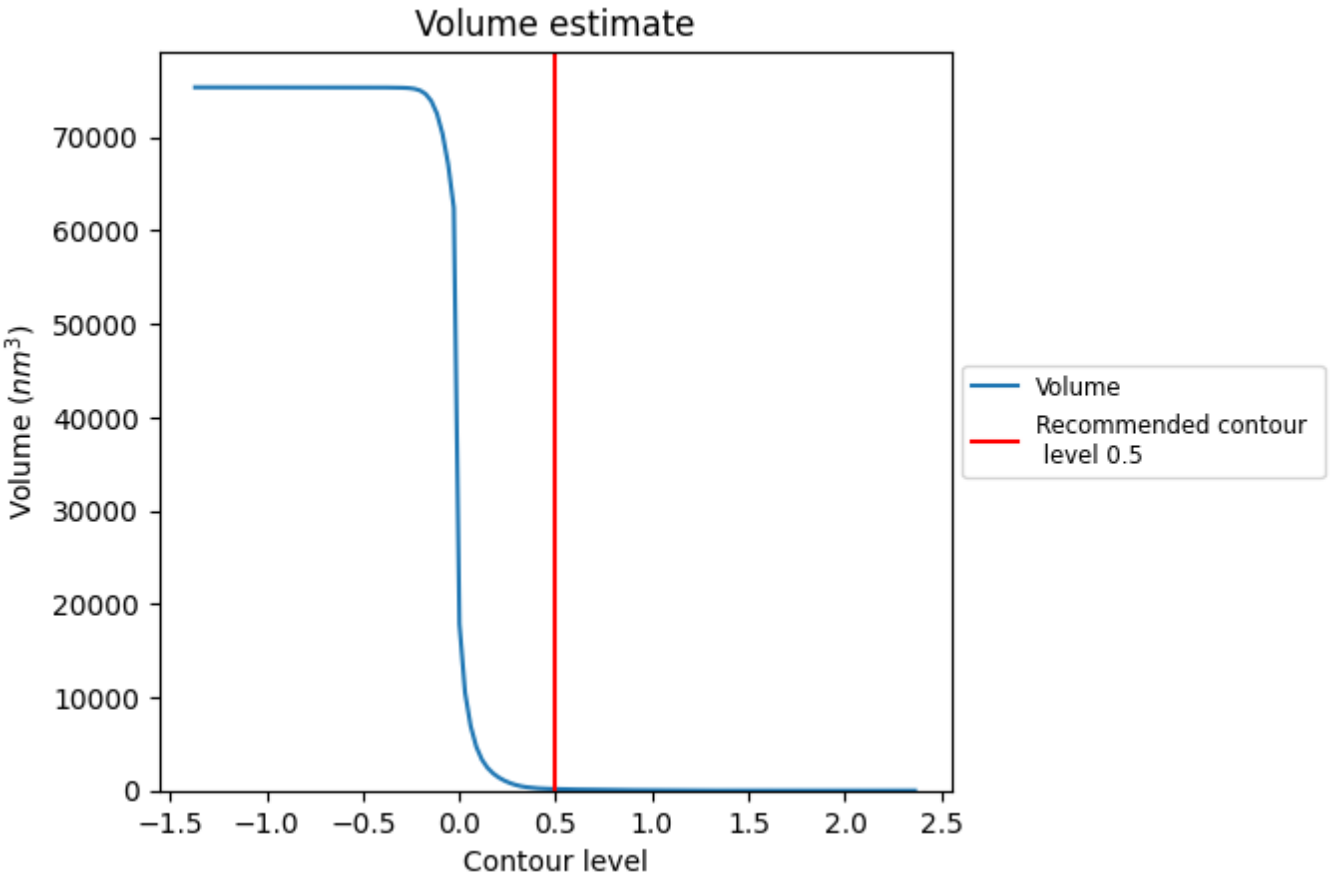
This section contains the results of statistical analysis of the map.

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.

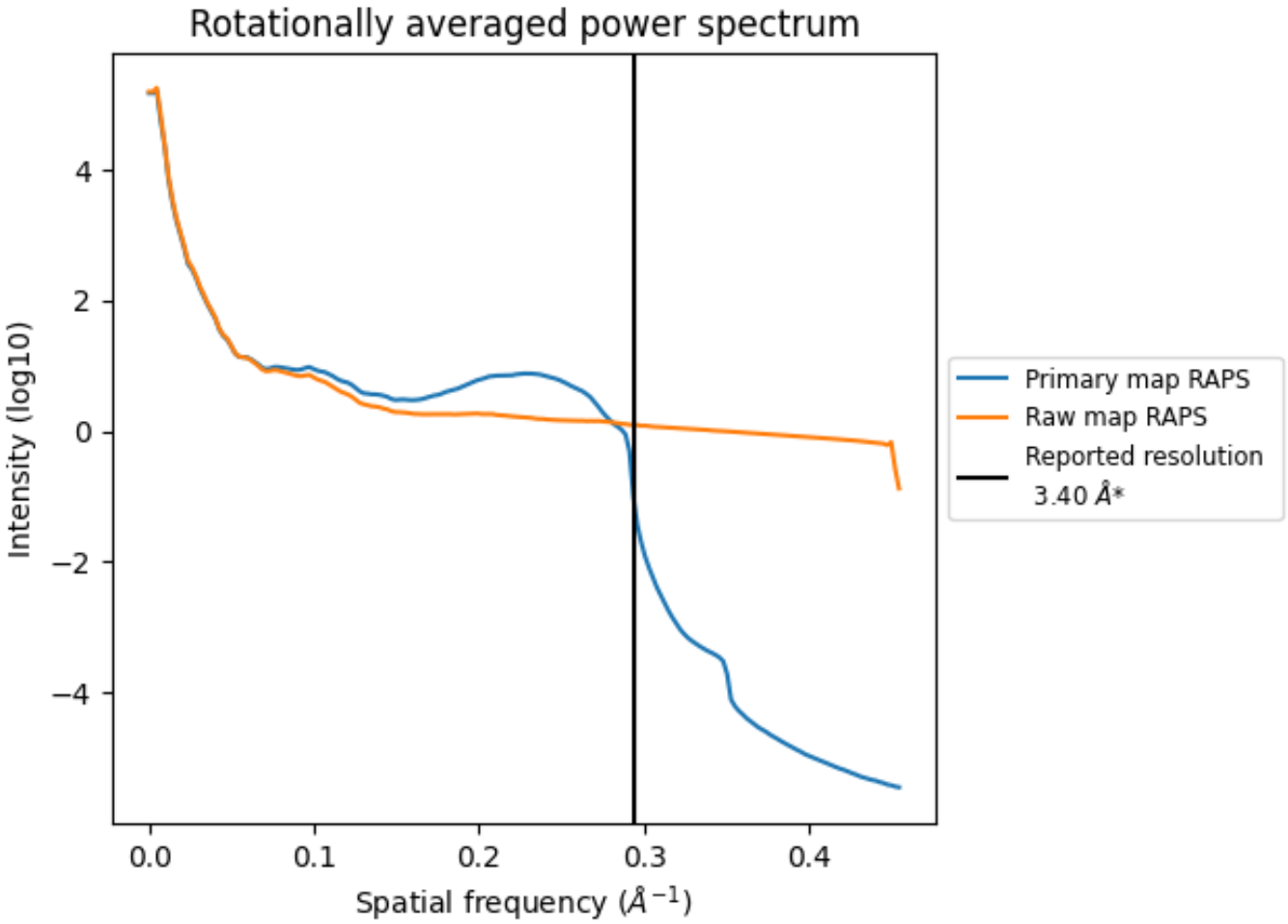
7.2 Volume estimate



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

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

7.3 Rotationally averaged power spectrum (i)

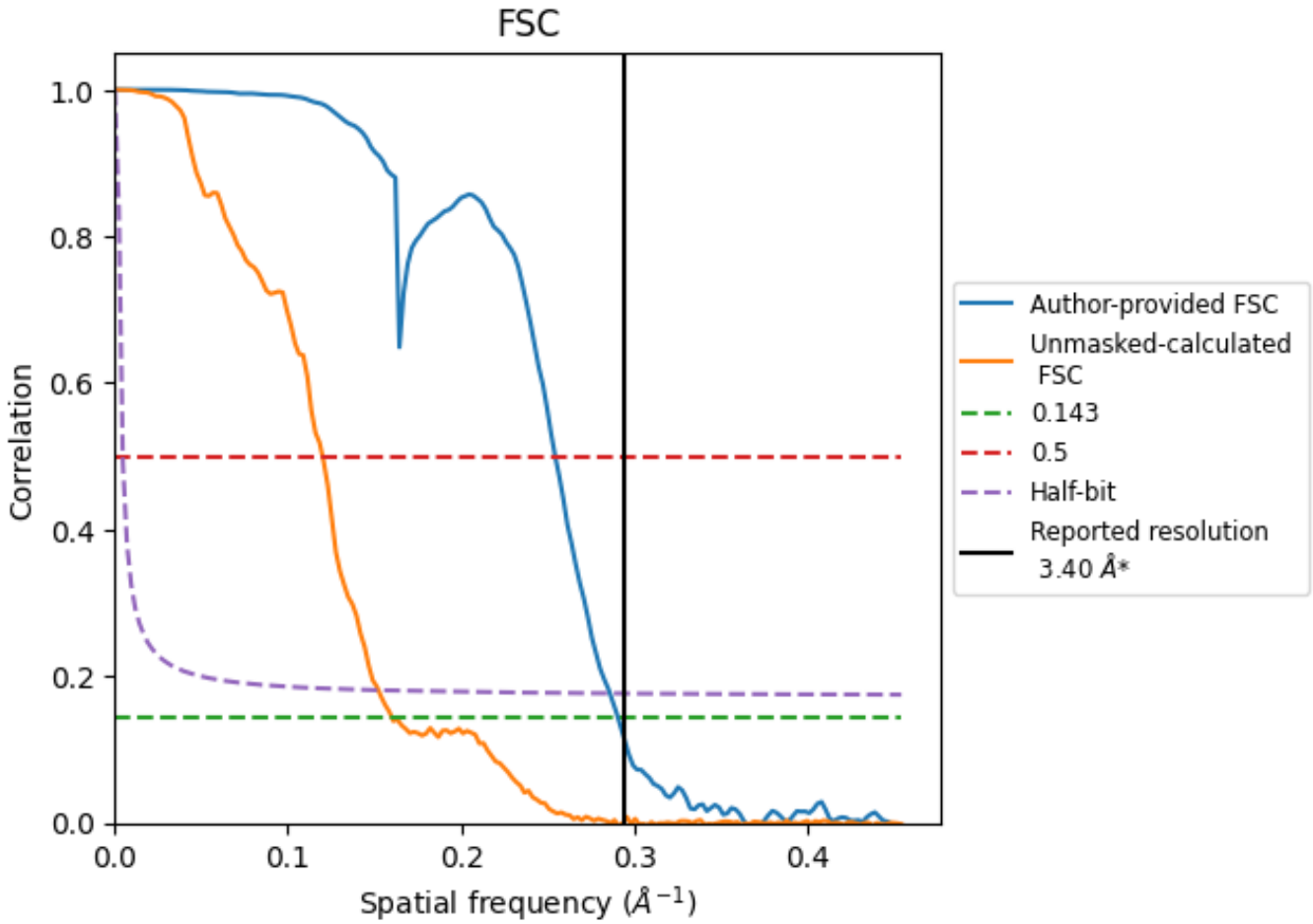


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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)

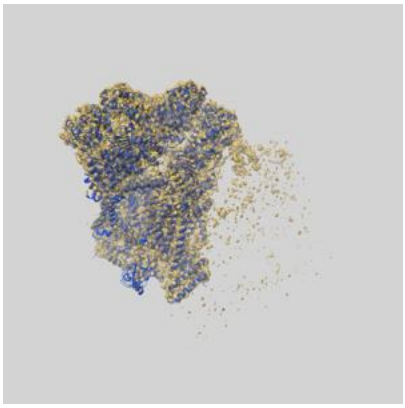
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.44	3.93	3.50
Unmasked-calculated*	6.24	8.33	6.57

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

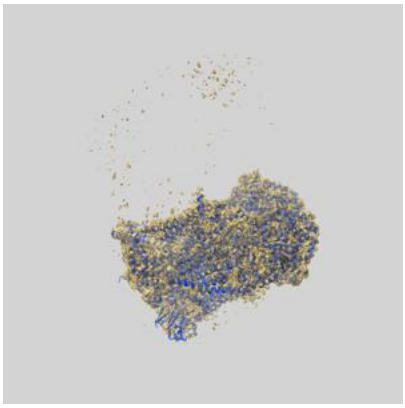
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35316 and PDB model 8IAR. Per-residue inclusion information can be found in section 3 on page 11.

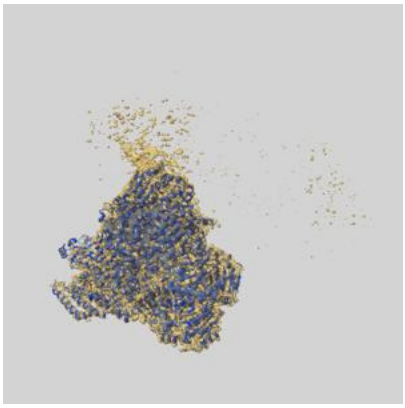
9.1 Map-model overlay



X



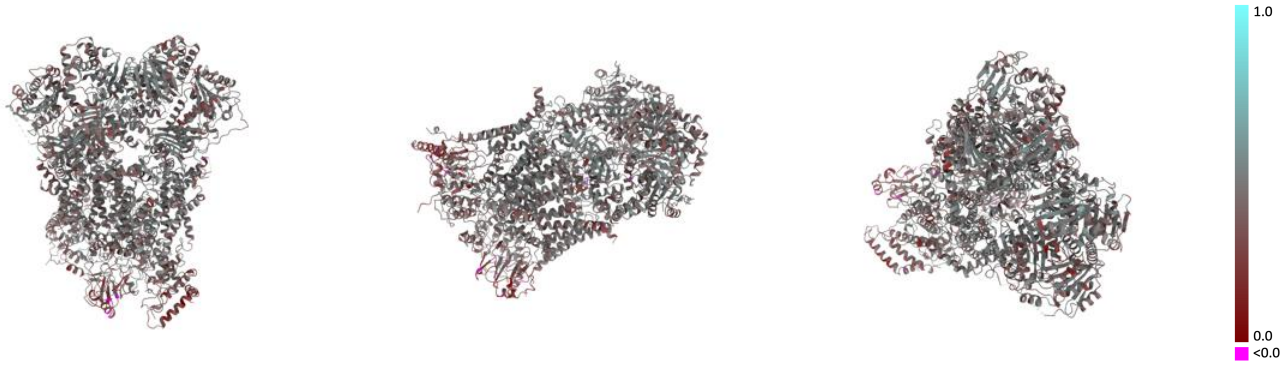
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

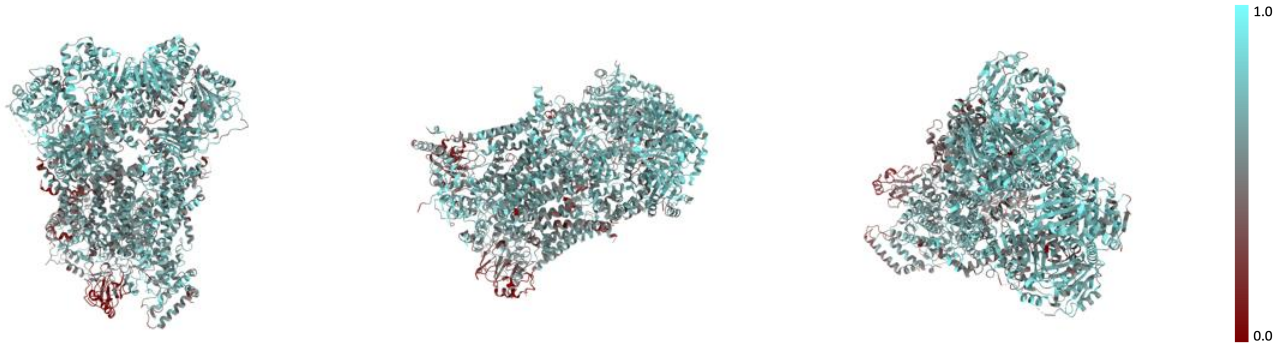
9.2 Q-score mapped to coordinate model (i)



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.

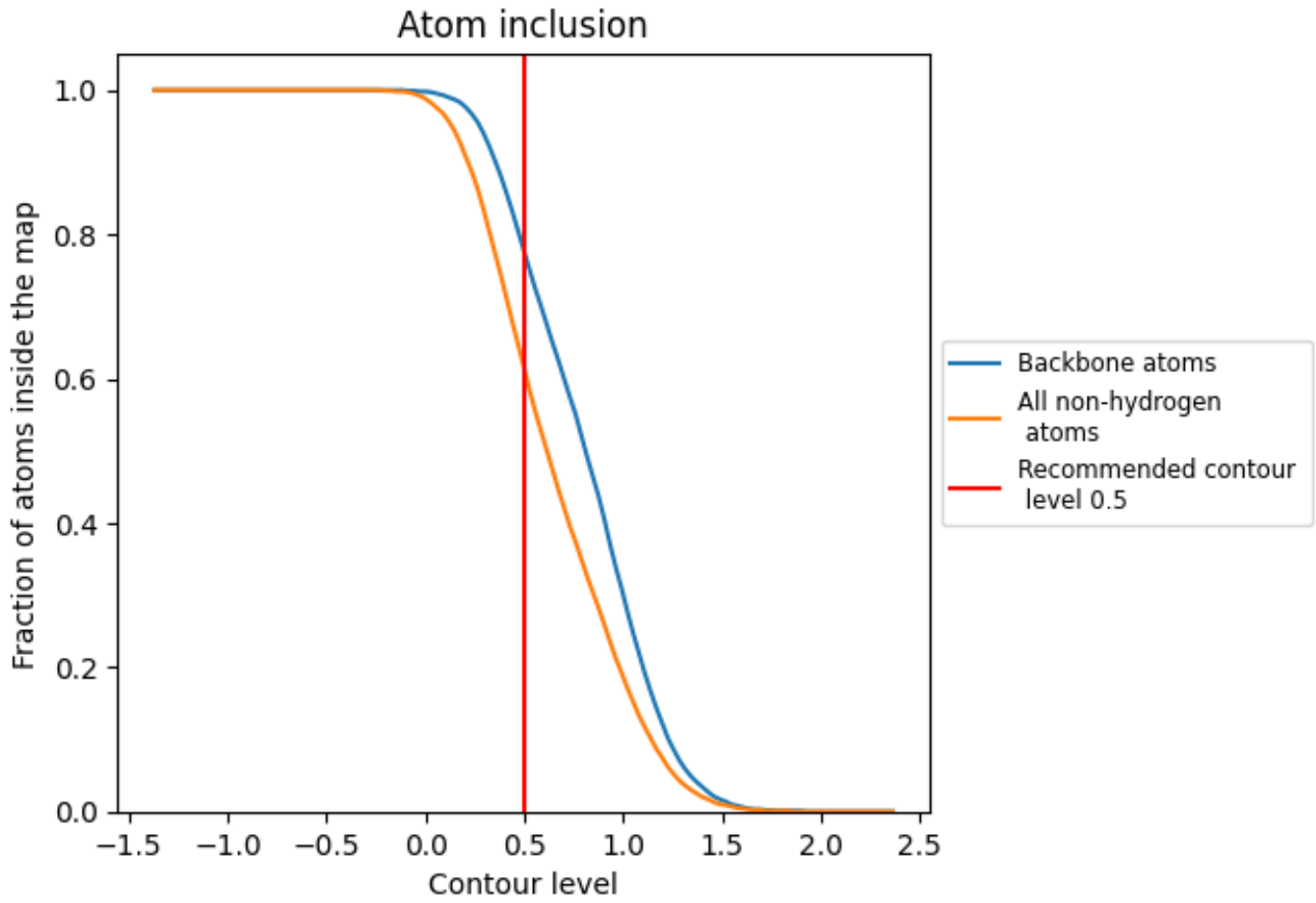
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6140	0.4210
AA	0.6930	0.4360
AB	0.6970	0.4430
AC	0.6340	0.4390
AD	0.6420	0.4110
AE	0.3000	0.3300
AF	0.6890	0.4360
AG	0.5460	0.4300
AH	0.4600	0.3000
AI	0.2990	0.4200
AJ	0.4040	0.4060
AK	0.2680	0.4070
Aa	0.6650	0.4410
Ab	0.7140	0.4410
Ac	0.6520	0.4510
Ad	0.6810	0.4290
Ae	0.3660	0.3230
Af	0.6890	0.4560
Ag	0.6160	0.4490
Ah	0.5440	0.3010
Ai	0.2490	0.3150
Aj	0.4970	0.3930
Ak	0.3720	0.3750