wwPDB EM Validation Summary Report ⓘ

Nov 20, 2024 – 06:49 pm GMT

PDB ID	:	9FU0
EMDB ID	:	EMD-50753
Title	:	CIII2/CIV respiratory chain supercomplex from Mycobacterium smegmatis
Authors	:	Kovalova, T.; Krol, S.; Gamiz-Hernandez, A.; Sjostrand, D.; Kaila, V.; Brzezinski, P.; Hogbom, M.
Deposited on	:	2024-06-25
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

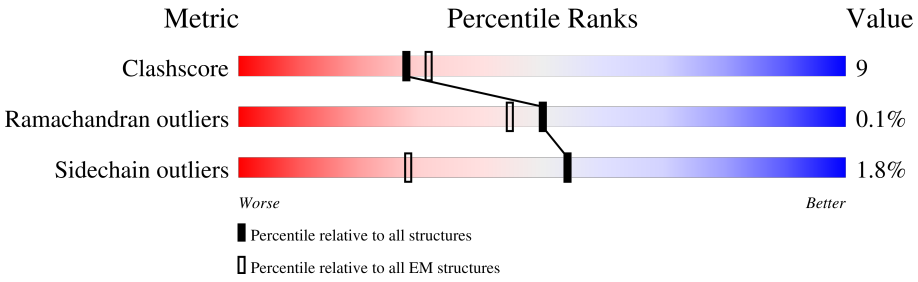
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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)
Clashscore	210492	15764
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	O	278	61% 19% 20%
2	G	408	6% 78% 13% 7%
2	M	408	82% 11% 7%
3	H	556	63% 15% 22%
3	N	556	78% 17%
4	P	100	63% 10% 27%
5	S	203	80% 11% 9%
6	T	139	83% 15%

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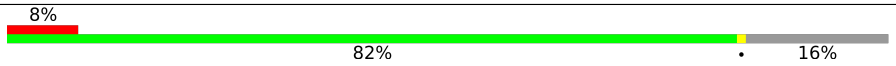
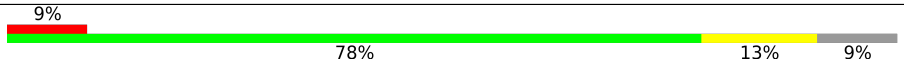
Mol	Chain	Length	Quality of chain
7	R	575	
8	Q	341	
9	U	79	
10	V	157	
11	W	186	
12	Y	236	
12	c	236	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MQ9	N	607	-	-	X	-
15	MQ9	O	304	-	-	X	-
17	FES	G	501	-	-	X	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 30643 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 bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	223	Total	C	N	O	S	0	0
			1623	1008	289	314	12		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	17	MET	-	initiating methionine	UNP A0R050
O	18	HIS	-	expression tag	UNP A0R050
O	19	HIS	-	expression tag	UNP A0R050
O	20	HIS	-	expression tag	UNP A0R050
O	21	HIS	-	expression tag	UNP A0R050
O	22	HIS	-	expression tag	UNP A0R050
O	23	HIS	-	expression tag	UNP A0R050
O	24	MET	-	expression tag	UNP A0R050
O	25	GLY	-	expression tag	UNP A0R050
O	26	SER	-	expression tag	UNP A0R050

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	380	Total	C	N	O	S	0	0
			2967	1919	502	535	11		
2	G	380	Total	C	N	O	S	0	0
			2967	1919	502	535	11		

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	533	Total	C	N	O	S	0	0
			4167	2743	707	699	18		
3	H	435	Total	C	N	O	S	0	0
			3425	2274	574	560	17		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	547	LYS	-	expression tag	UNP A0R052
N	548	LEU	-	expression tag	UNP A0R052
N	549	ASP	-	expression tag	UNP A0R052
N	550	TYR	-	expression tag	UNP A0R052
N	551	LYS	-	expression tag	UNP A0R052
N	552	ASP	-	expression tag	UNP A0R052
N	553	ASP	-	expression tag	UNP A0R052
N	554	ASP	-	expression tag	UNP A0R052
N	555	ASP	-	expression tag	UNP A0R052
N	556	LYS	-	expression tag	UNP A0R052
H	547	LYS	-	expression tag	UNP A0R052
H	548	LEU	-	expression tag	UNP A0R052
H	549	ASP	-	expression tag	UNP A0R052
H	550	TYR	-	expression tag	UNP A0R052
H	551	LYS	-	expression tag	UNP A0R052
H	552	ASP	-	expression tag	UNP A0R052
H	553	ASP	-	expression tag	UNP A0R052
H	554	ASP	-	expression tag	UNP A0R052
H	555	ASP	-	expression tag	UNP A0R052
H	556	LYS	-	expression tag	UNP A0R052

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	P	73	586	385	107	90	4	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1	MET	-	initiating methionine	UNP A0QVH4
P	2	SER	-	expression tag	UNP A0QVH4
P	3	SER	-	expression tag	UNP A0QVH4
P	4	THR	-	expression tag	UNP A0QVH4
P	5	GLN	-	expression tag	UNP A0QVH4
P	6	ASP	-	expression tag	UNP A0QVH4
P	7	ARG	-	expression tag	UNP A0QVH4
P	8	SER	-	expression tag	UNP A0QVH4
P	9	GLN	-	expression tag	UNP A0QVH4
P	10	LEU	-	expression tag	UNP A0QVH4
P	11	ASP	-	expression tag	UNP A0QVH4

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Chain	Residue	Modelled	Actual	Comment	Reference
P	12	PRO	-	expression tag	UNP A0QVH4
P	13	GLU	-	expression tag	UNP A0QVH4
P	14	GLU	-	expression tag	UNP A0QVH4
P	15	GLN	-	expression tag	UNP A0QVH4
P	16	PRO	-	expression tag	UNP A0QVH4
P	17	VAL	-	expression tag	UNP A0QVH4

- Molecule 5 is a protein called Probable cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	551	Total	C	N	O	S	0	0
			4369	2936	694	713	26		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	initiating methionine	UNP A0A2U9PNL2
R	2	VAL	-	expression tag	UNP A0A2U9PNL2
R	3	ALA	-	expression tag	UNP A0A2U9PNL2
R	4	GLU	-	expression tag	UNP A0A2U9PNL2
R	5	ALA	-	expression tag	UNP A0A2U9PNL2
R	6	PRO	-	expression tag	UNP A0A2U9PNL2
R	7	PRO	-	expression tag	UNP A0A2U9PNL2
R	8	ILE	-	expression tag	UNP A0A2U9PNL2
R	9	GLY	-	expression tag	UNP A0A2U9PNL2
R	10	GLU	-	expression tag	UNP A0A2U9PNL2
R	11	LEU	-	expression tag	UNP A0A2U9PNL2
R	12	GLU	-	expression tag	UNP A0A2U9PNL2
R	13	ALA	-	expression tag	UNP A0A2U9PNL2
R	14	ARG	-	expression tag	UNP A0A2U9PNL2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	15	ARG	-	expression tag	UNP A0A2U9PNL2
R	16	PRO	-	expression tag	UNP A0A2U9PNL2
R	17	PHE	-	expression tag	UNP A0A2U9PNL2
R	18	PRO	-	expression tag	UNP A0A2U9PNL2
R	19	GLU	-	expression tag	UNP A0A2U9PNL2
R	20	ARG	-	expression tag	UNP A0A2U9PNL2

- Molecule 8 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	299	Total	C	N	O	S	0	0
			2382	1541	396	435	10		

- Molecule 9 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	66	Total	C	N	O	S	0	0
			499	329	84	85	1		

- Molecule 10 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	143	Total	C	N	O	S	0	0
			1024	647	174	201	2		

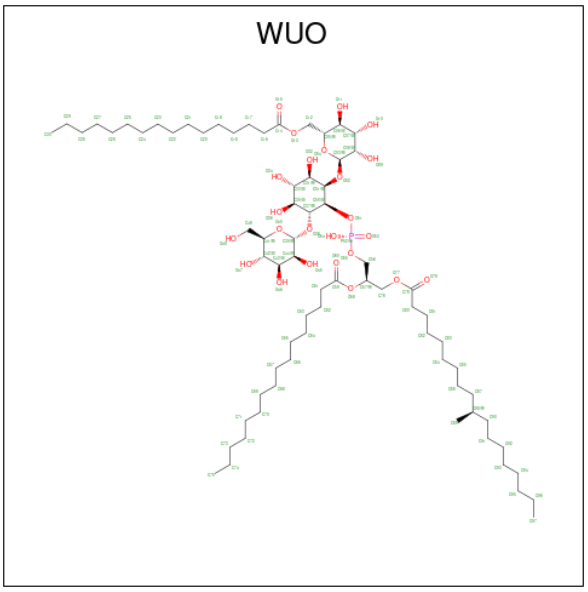
- Molecule 11 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	149	Total	C	N	O	S	0	0
			1083	670	181	231	1		

- Molecule 12 is a protein called Superoxide dismutase [Cu-Zn].

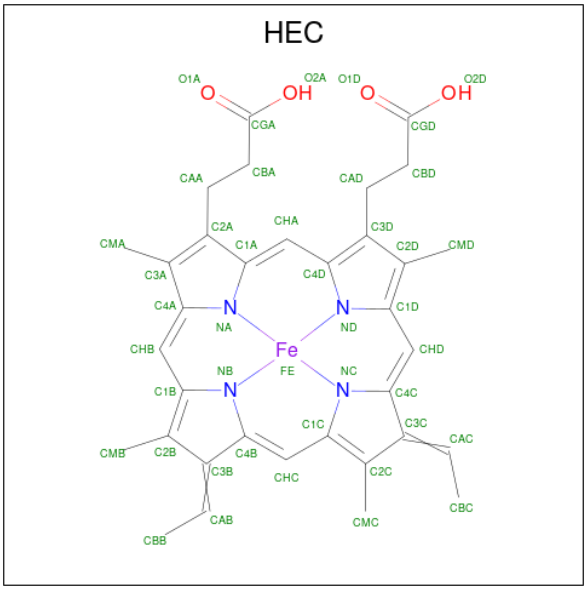
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	25	Total	C	N	O	S	0	0
			168	103	26	38	1		
12	c	25	Total	C	N	O	S	0	0
			168	103	26	38	1		

- Molecule 13 is acyl-phosphatidyl-myo-inositol dimannoside (AcPIM2) (three-letter code: WUO) (formula: $C_{72}H_{135}O_{24}P$).



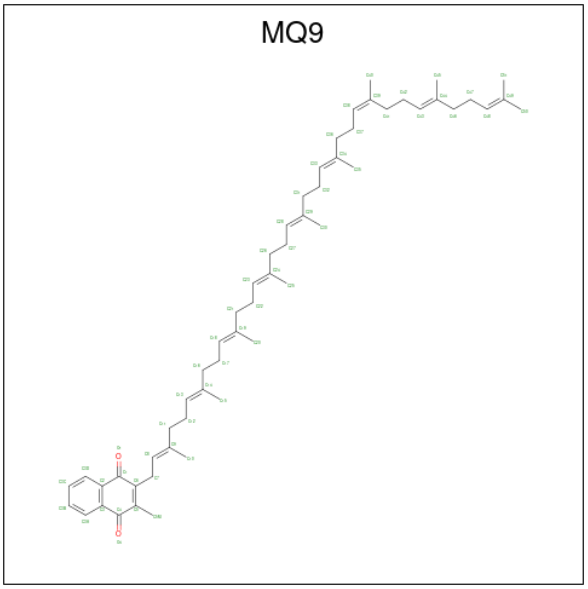
Mol	Chain	Residues	Atoms				AltConf
13	O	1	Total	C	O	P	0
			97	72	24	1	
13	P	1	Total	C	O	P	0
			97	72	24	1	

- Molecule 14 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



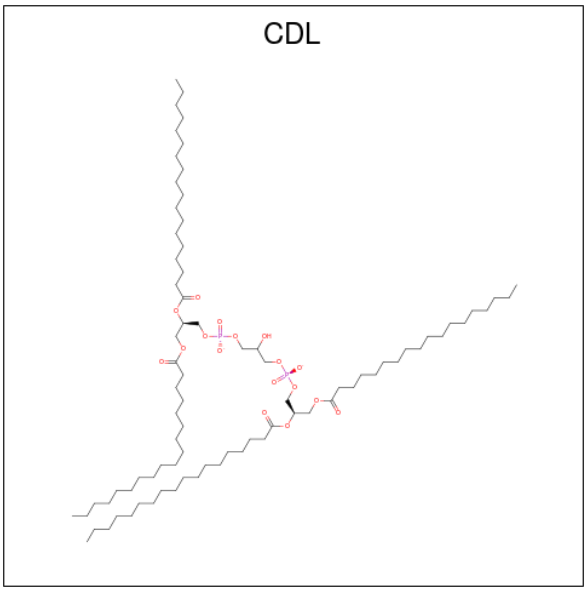
Mol	Chain	Residues	Atoms					AltConf
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 15 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



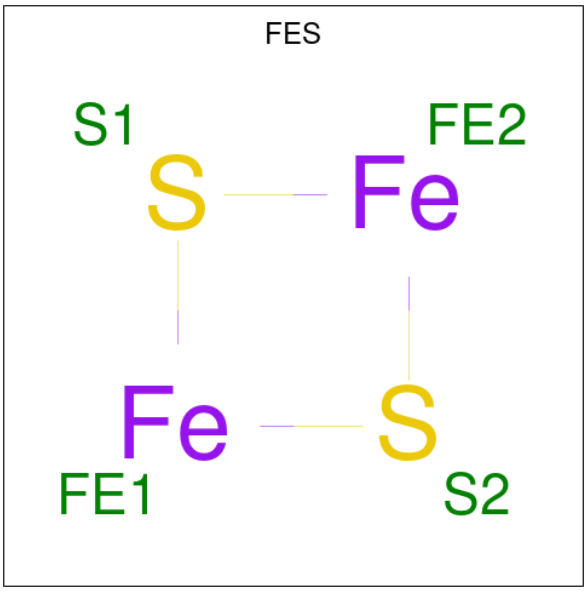
Mol	Chain	Residues	Atoms	AltConf
15	O	1	Total C O 58 56 2	0
15	N	1	Total C O 58 56 2	0
15	N	1	Total C O 58 56 2	0
15	N	1	Total C O 58 56 2	0
15	H	1	Total C O 58 56 2	0
15	H	1	Total C O 58 56 2	0

- Molecule 16 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



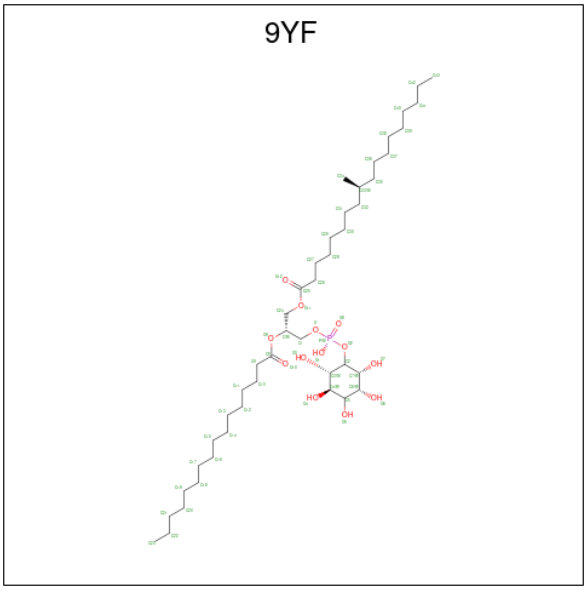
Mol	Chain	Residues	Atoms				AltConf
16	O	1	Total	C	O	P	0
			79	60	17	2	
16	N	1	Total	C	O	P	0
			74	55	17	2	
16	N	1	Total	C	O	P	0
			77	58	17	2	
16	N	1	Total	C	O	P	0
			79	60	17	2	
16	P	1	Total	C	O	P	0
			77	58	17	2	
16	R	1	Total	C	O	P	0
			77	58	17	2	
16	R	1	Total	C	O	P	0
			77	58	17	2	
16	H	1	Total	C	O	P	0
			74	55	17	2	
16	H	1	Total	C	O	P	0
			77	58	17	2	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
17	M	1	Total	Fe	S	0
			4	2	2	
17	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 18 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (three-letter code: 9YF) (formula: $C_{44}H_{85}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
18	M	1	Total	C	O	P	0
			58	44	13	1	

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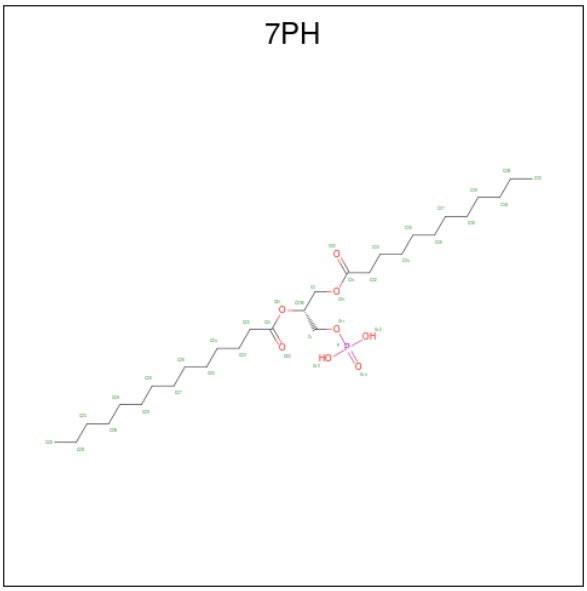
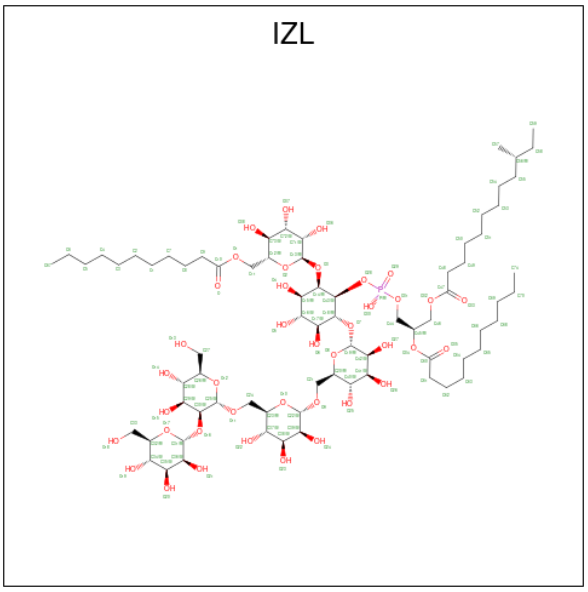
Mol	Chain	Residues	Atoms				AltConf
18	W	1	Total	C	O	P	0
			58	44	13	1	
18	G	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 19 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (three-letter code: 7PH) (formula: $C_{29}H_{57}O_8P$).



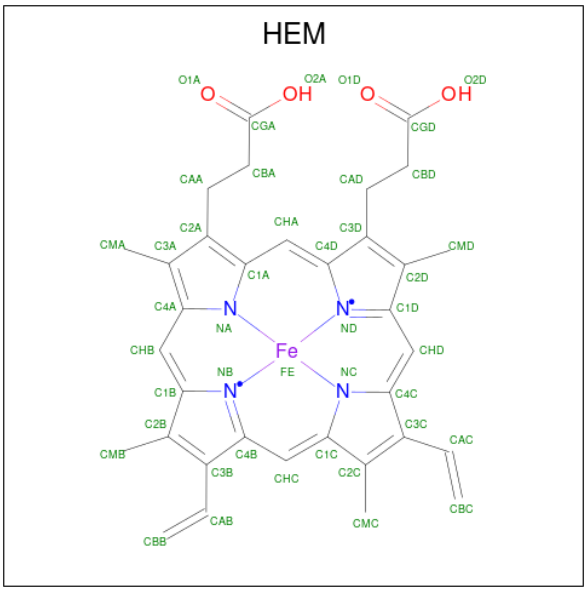
Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			38	29	8	1	
19	S	1	Total	C	O	P	0
			38	29	8	1	
19	G	1	Total	C	O	P	0
			38	29	8	1	
19	G	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 20 is [(2 {R})-3-[[(1 {S},2 {R},3 {S},4 {S},5 {R},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-[[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (three-letter code: IZL) (formula: $C_{74}H_{133}O_{39}P$).



Mol	Chain	Residues	Atoms				AltConf
20	M	1	Total	C	O	P	0
			114	74	39	1	
20	G	1	Total	C	O	P	0
			114	74	39	1	

- Molecule 21 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
21	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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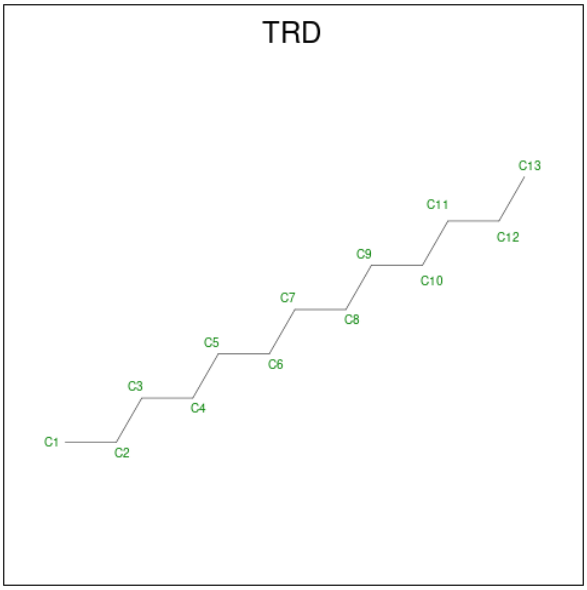
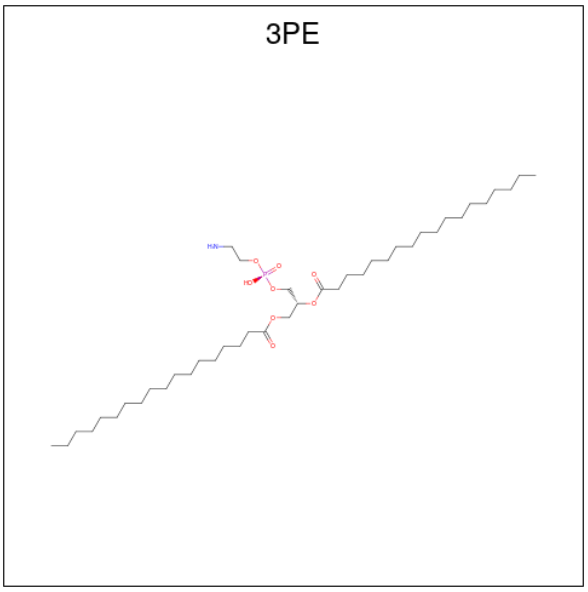
Mol	Chain	Residues	Atoms					AltConf
21	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
21	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
21	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 22 is TRIDECANE (three-letter code: TRD) (formula: $C_{13}H_{28}$).



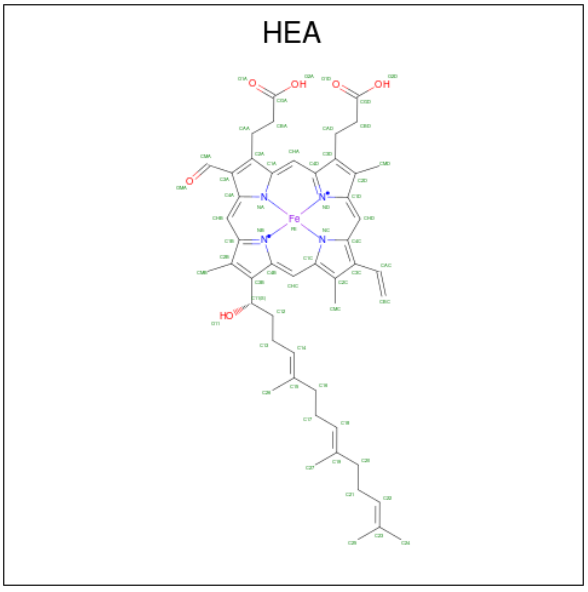
Mol	Chain	Residues	Atoms		AltConf
22	S	1	Total	C	0
			13	13	
22	T	1	Total	C	0
			13	13	
22	R	1	Total	C	0
			13	13	
22	R	1	Total	C	0
			13	13	
22	Q	1	Total	C	0
			13	13	

- Molecule 23 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
23	S	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 24 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
24	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
24	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 25 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
25	R	1	Total Cu 1 1	0
25	Q	2	Total Cu 2 2	0

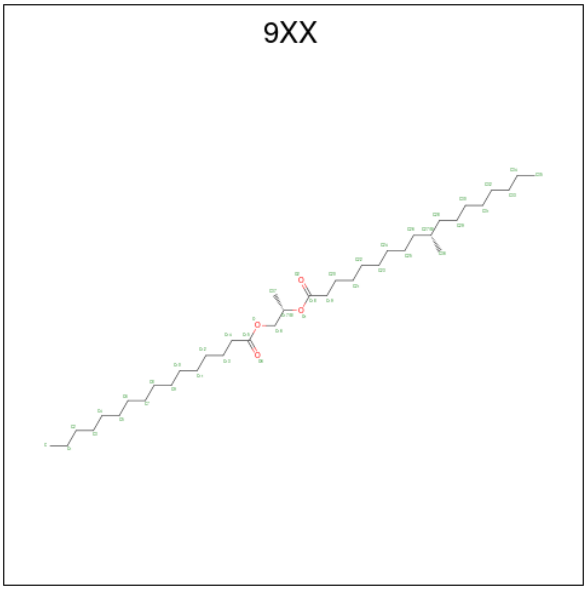
- Molecule 26 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
26	R	1	Total Ca 1 1	0

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

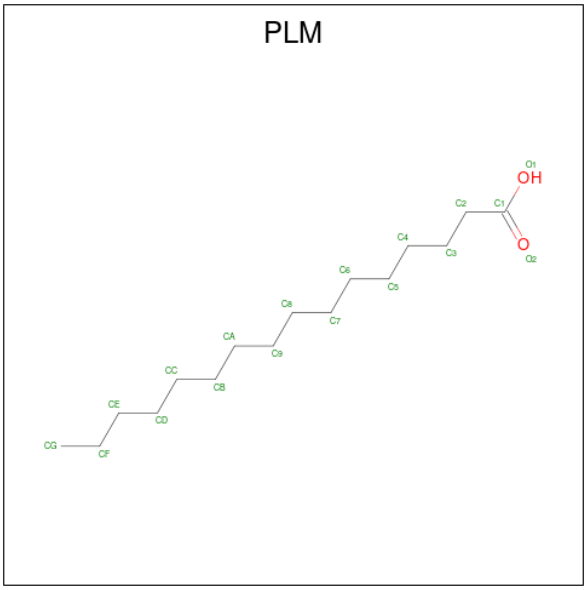
Mol	Chain	Residues	Atoms	AltConf
27	R	1	Total Mg 1 1	0

- Molecule 28 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (three-letter code: 9XX) (formula: $C_{38}H_{74}O_4$).



Mol	Chain	Residues	Atoms	AltConf
28	W	1	Total C O 42 38 4	0
28	Y	1	Total C O 32 28 4	0
28	c	1	Total C O 32 28 4	0

- Molecule 29 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms	AltConf
29	W	1	Total C O 11 10 1	0
29	Y	1	Total C O 11 10 1	0
29	c	1	Total C O 11 10 1	0

- Molecule 30 is water.

Mol	Chain	Residues	Atoms	AltConf
30	O	42	Total O 42 42	0
30	M	37	Total O 37 37	0
30	N	68	Total O 68 68	0
30	P	9	Total O 9 9	0
30	S	6	Total O 6 6	0
30	T	10	Total O 10 10	0
30	R	53	Total O 53 53	0
30	Q	26	Total O 26 26	0

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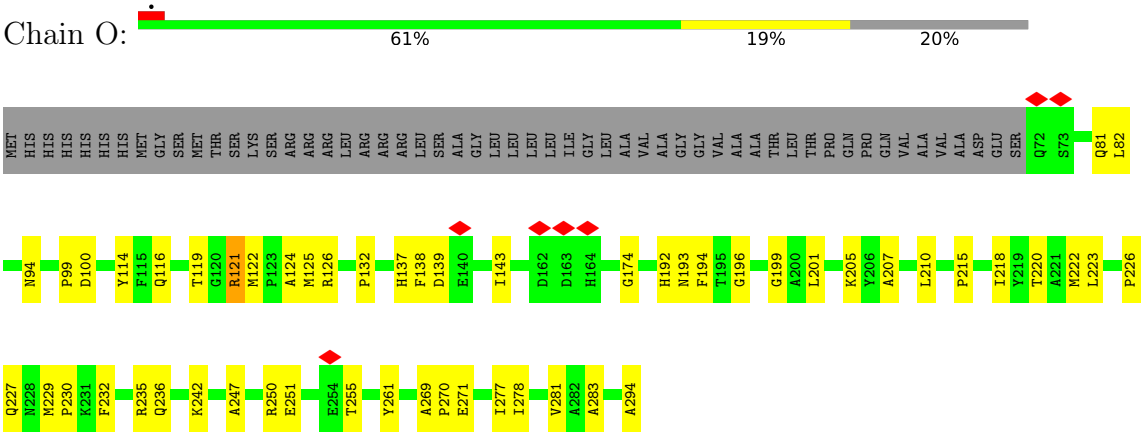
Mol	Chain	Residues	Atoms	AltConf
30	U	1	Total O 1 1	0
30	W	8	Total O 8 8	0
30	Y	1	Total O 1 1	0
30	H	12	Total O 12 12	0
30	G	10	Total O 10 10	0

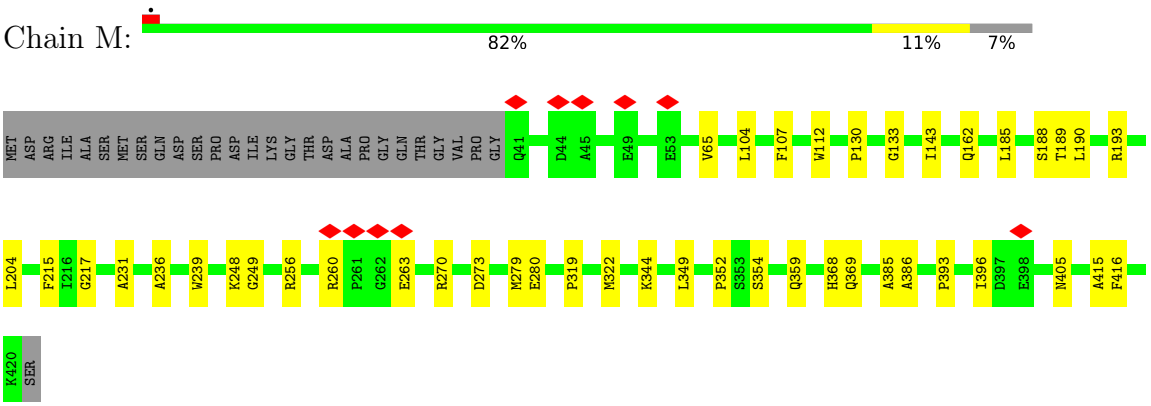
3 Residue-property plots (i)

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

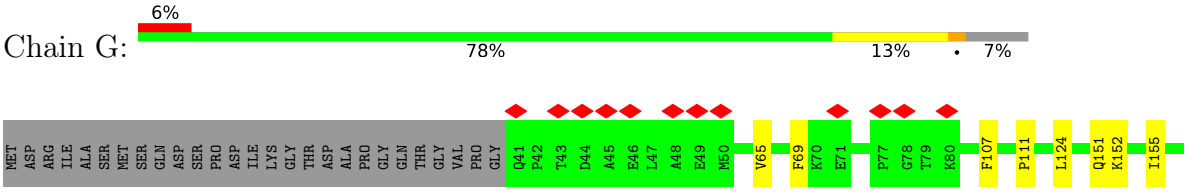
• Molecule 1: Cytochrome bc1 complex cytochrome c subunit

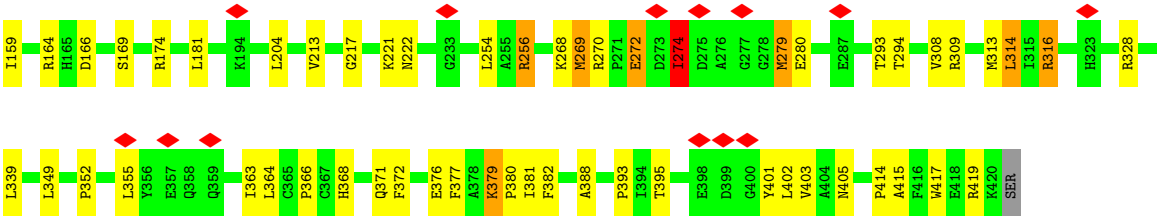


• Molecule 2: Cytochrome bc1 complex cytochrome c subunit



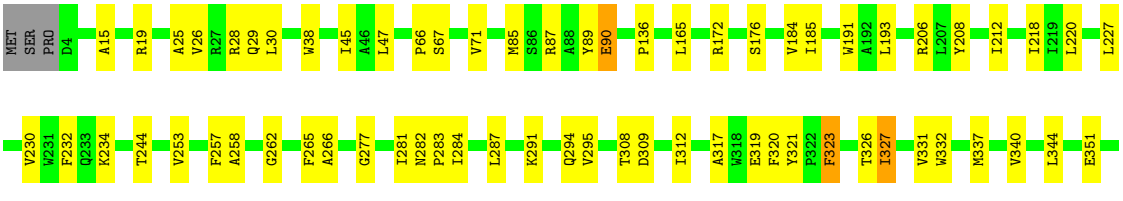
• Molecule 2: Cytochrome bc1 complex cytochrome c subunit

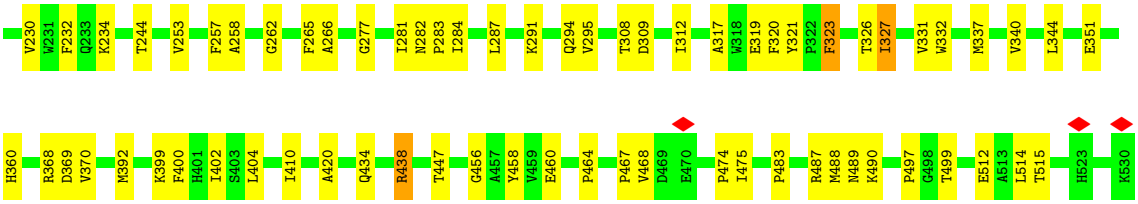


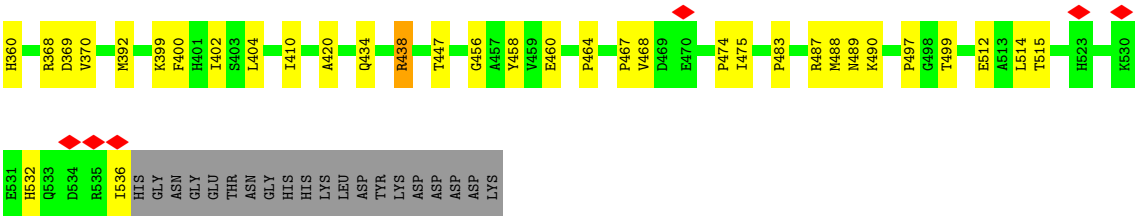


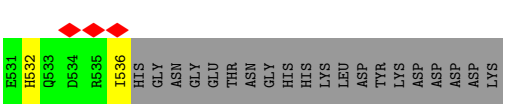
• Molecule 3: Cytochrome bc1 complex cytochrome b subunit

Chain N:



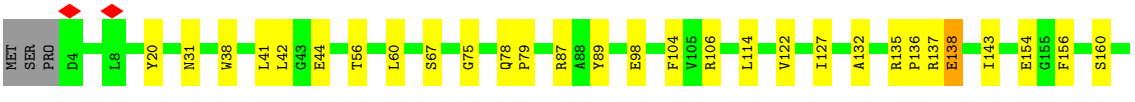


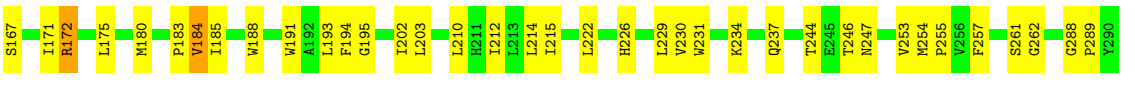


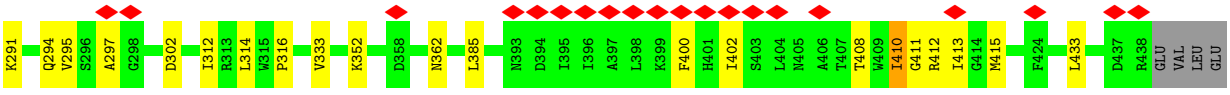


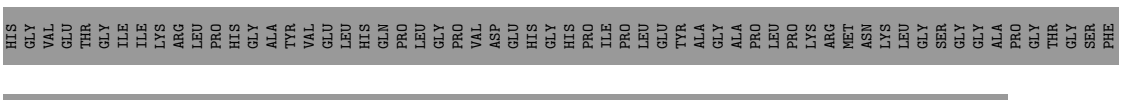
• Molecule 3: Cytochrome bc1 complex cytochrome b subunit

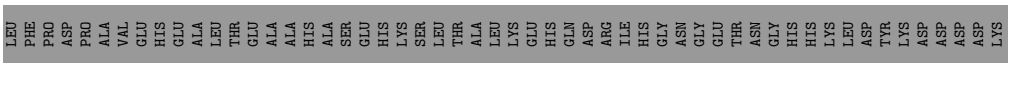
Chain H:





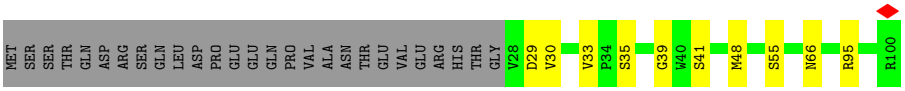




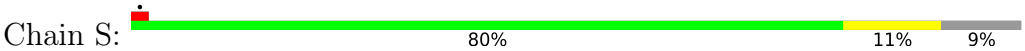


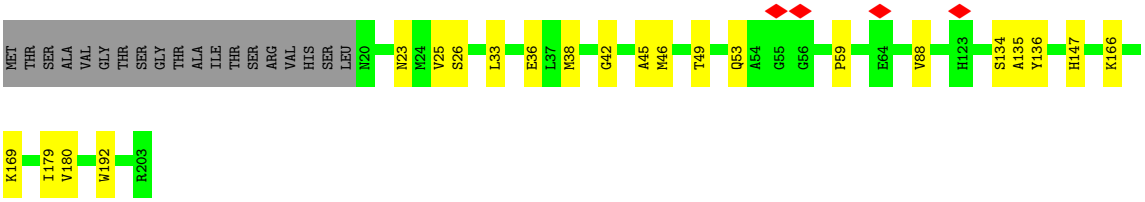
• Molecule 4: Transmembrane protein

Chain P:

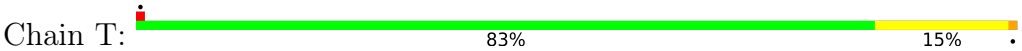


• Molecule 5: Probable cytochrome c oxidase subunit 3

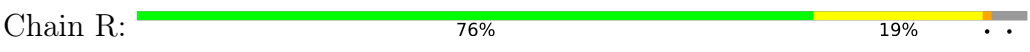


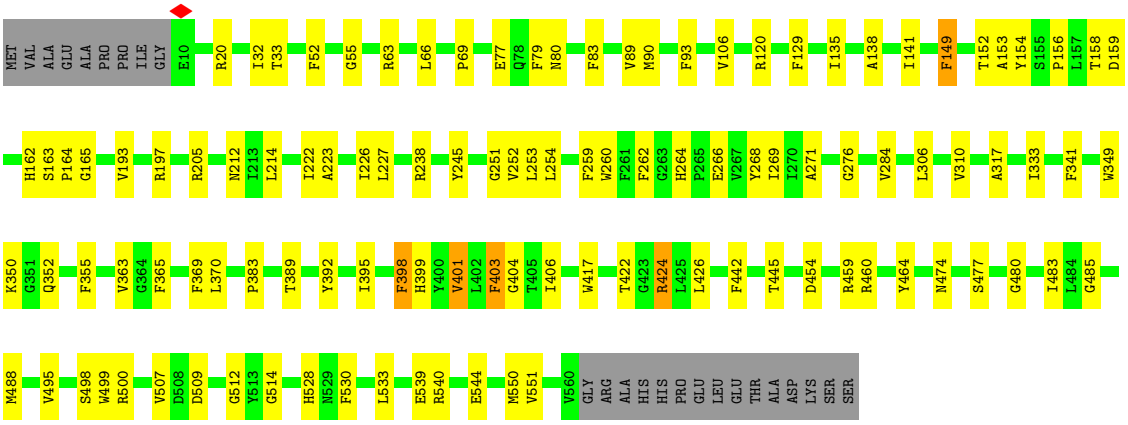


• Molecule 6: Cytochrome c oxidase polypeptide 4

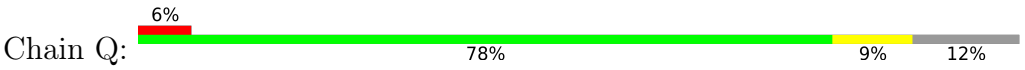


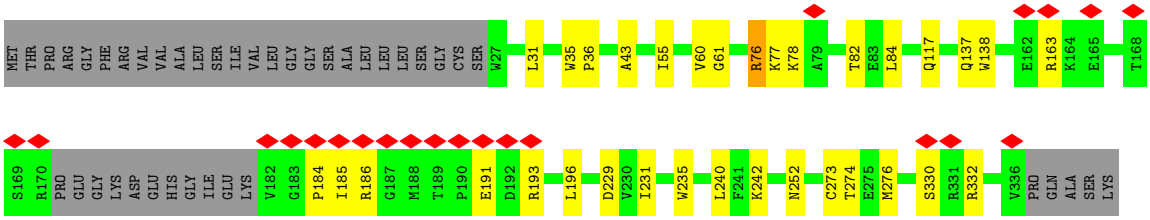
• Molecule 7: Cytochrome c oxidase subunit 1





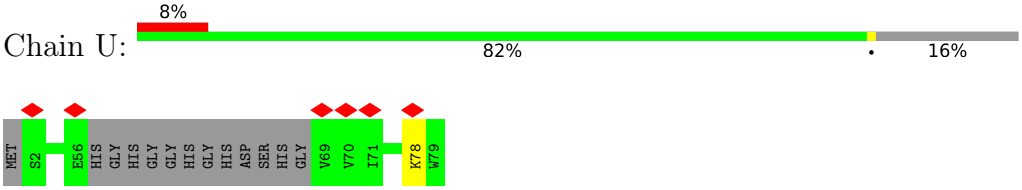
• Molecule 8: cytochrome-c oxidase





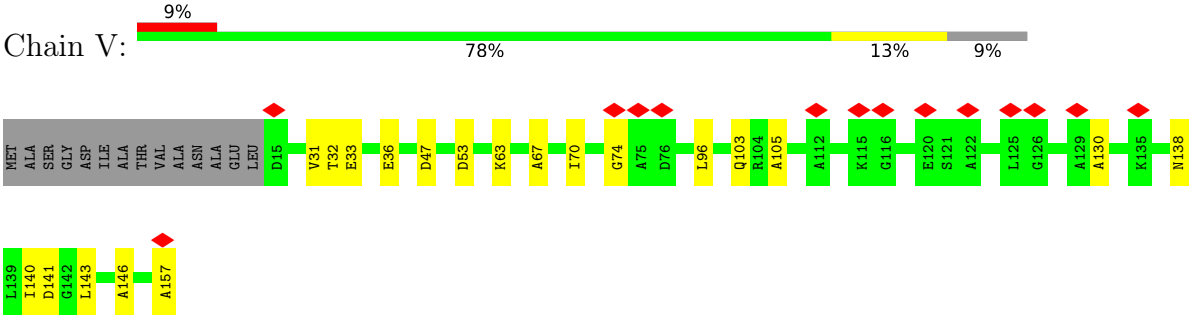
• Molecule 9: Cytochrome c oxidase subunit

Chain U:



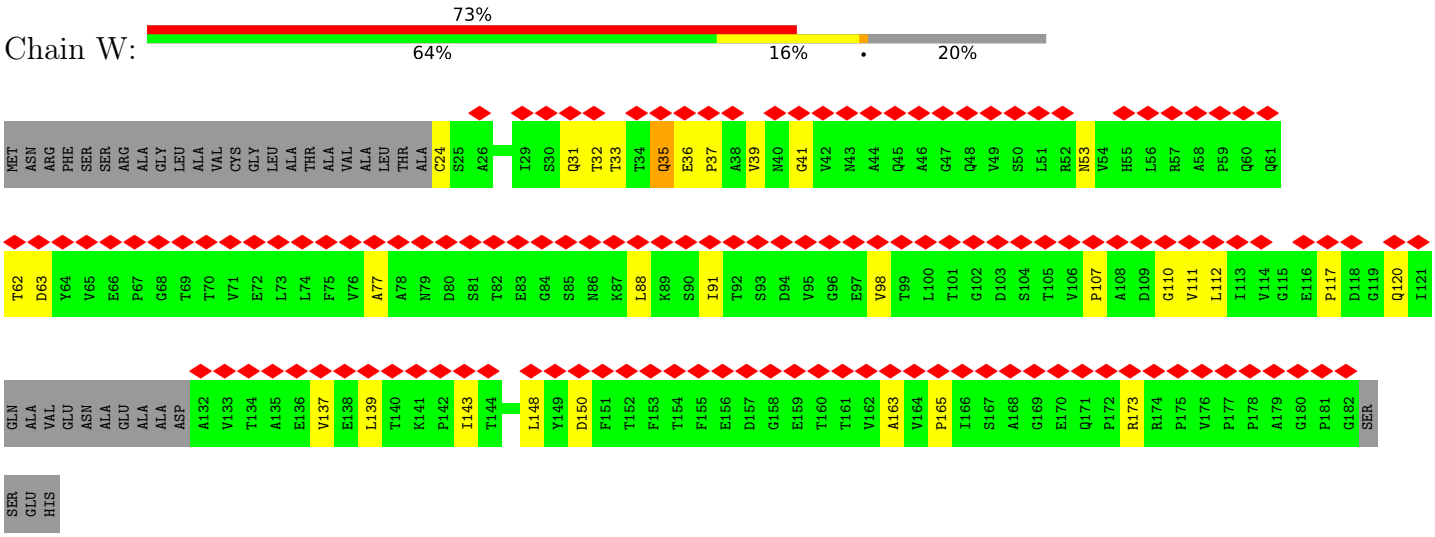
• Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain V:



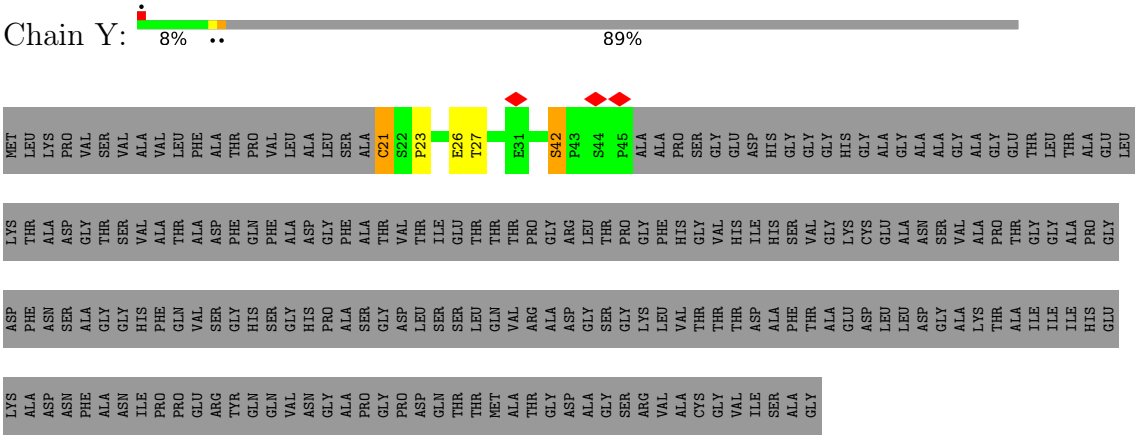
• Molecule 11: LpqE protein

Chain W:



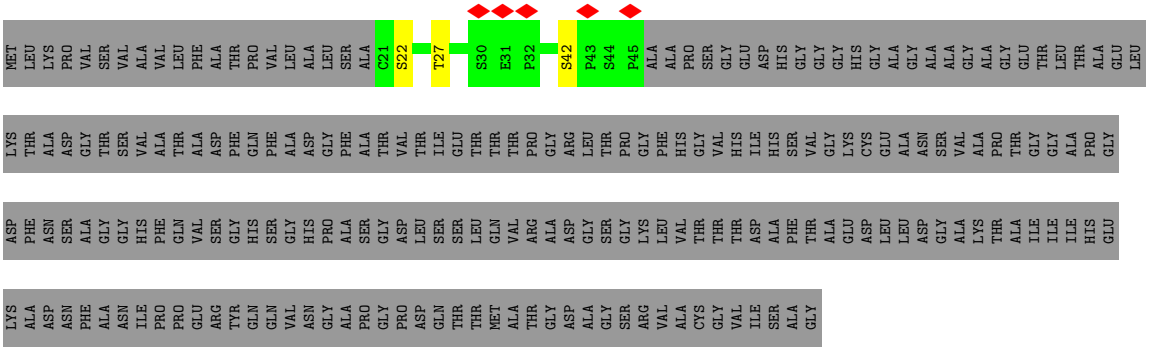
• Molecule 12: Superoxide dismutase [Cu-Zn]

Chain Y:



• Molecule 12: Superoxide dismutase [Cu-Zn]

Chain c:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.240	Depositor
Minimum map value	-0.656	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.204	Depositor
Map size (Å)	444.96, 444.96, 444.96	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, 9YF, WUO, CU, MQ9, 7PH, HEM, TRD, MG, CA, IZL, 9XX, HEA, FES, HEC, PLM, CDL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	O	0.26	0/1660	0.44	0/2250
2	G	0.32	0/3046	0.44	0/4129
2	M	0.27	0/3046	0.42	0/4129
3	H	0.31	0/3534	0.43	0/4820
3	N	0.35	0/4299	0.45	0/5862
4	P	0.24	0/606	0.38	0/825
5	S	0.25	0/1488	0.36	0/2032
6	T	0.32	0/1112	0.43	0/1524
7	R	0.33	0/4529	0.45	0/6187
8	Q	0.29	0/2447	0.46	0/3330
9	U	0.23	0/515	0.38	0/704
10	V	0.24	0/1042	0.41	0/1423
11	W	0.31	0/1100	0.46	0/1508
12	Y	0.29	0/175	0.44	0/244
12	c	0.42	0/175	0.54	0/244
All	All	0.31	0/28774	0.44	0/39211

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1623	0	1560	46	0
2	G	2967	0	2976	64	0
2	M	2967	0	2976	41	0
3	H	3425	0	3469	77	0
3	N	4167	0	4192	110	0
4	P	586	0	578	9	0
5	S	1441	0	1439	18	0
6	T	1077	0	1058	19	0
7	R	4369	0	4346	110	0
8	Q	2382	0	2335	42	0
9	U	499	0	504	1	0
10	V	1024	0	1035	13	0
11	W	1083	0	1055	31	0
12	Y	168	0	151	6	0
12	c	168	0	151	0	0
13	O	97	0	0	2	0
13	P	97	0	0	0	0
14	O	86	0	60	5	0
15	H	116	0	160	17	0
15	N	174	0	240	52	0
15	O	58	0	80	28	0
16	H	151	0	190	7	0
16	N	230	0	295	19	0
16	O	79	0	105	5	0
16	P	77	0	98	8	0
16	R	154	0	196	5	0
17	G	4	0	0	2	0
17	M	4	0	0	1	0
18	G	58	0	0	2	0
18	M	58	0	0	2	0
18	W	58	0	0	2	0
19	G	76	0	110	1	0
19	M	38	0	55	2	0
19	S	38	0	55	3	0
20	G	114	0	0	0	0
20	M	114	0	0	0	0
21	H	86	0	60	8	0
21	N	86	0	60	5	0
22	Q	13	0	28	0	0
22	R	26	0	56	0	0
22	S	13	0	28	0	0
22	T	13	0	28	0	0
23	S	32	0	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	R	120	0	108	23	0
25	Q	2	0	0	1	0
25	R	1	0	0	0	0
26	R	1	0	0	0	0
27	R	1	0	0	0	0
28	W	42	0	0	3	0
28	Y	32	0	0	1	0
28	c	32	0	0	0	0
29	W	11	0	16	3	0
29	Y	11	0	16	0	0
29	c	11	0	16	0	0
30	G	10	0	0	0	0
30	H	12	0	0	0	0
30	M	37	0	0	0	0
30	N	68	0	0	1	0
30	O	42	0	0	0	0
30	P	9	0	0	0	0
30	Q	26	0	0	0	0
30	R	53	0	0	0	0
30	S	6	0	0	0	0
30	T	10	0	0	0	0
30	U	1	0	0	0	0
30	W	8	0	0	0	0
30	Y	1	0	0	0	0
All	All	30643	0	29923	568	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 568 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:21:CYS:SG	28:Y:302:9XX:C37	2.16	1.32
3:N:337:MET:HE3	15:N:608:MQ9:H3A	1.36	1.07
11:W:36:GLU:HB3	11:W:37:PRO:HD2	1.36	1.04
7:R:550:MET:HE2	8:Q:84:LEU:HD12	1.47	0.96
15:H:605:MQ9:H261	15:H:605:MQ9:H301	1.48	0.94

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	221/278 (80%)	213 (96%)	8 (4%)	0	100	100
2	G	378/408 (93%)	358 (95%)	19 (5%)	1 (0%)	37	61
2	M	378/408 (93%)	369 (98%)	9 (2%)	0	100	100
3	H	433/556 (78%)	413 (95%)	19 (4%)	1 (0%)	44	68
3	N	531/556 (96%)	514 (97%)	16 (3%)	1 (0%)	44	68
4	P	71/100 (71%)	70 (99%)	1 (1%)	0	100	100
5	S	182/203 (90%)	182 (100%)	0	0	100	100
6	T	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
7	R	549/575 (96%)	535 (97%)	14 (3%)	0	100	100
8	Q	295/341 (86%)	284 (96%)	11 (4%)	0	100	100
9	U	62/79 (78%)	62 (100%)	0	0	100	100
10	V	141/157 (90%)	139 (99%)	2 (1%)	0	100	100
11	W	145/186 (78%)	133 (92%)	12 (8%)	0	100	100
12	Y	23/236 (10%)	21 (91%)	2 (9%)	0	100	100
12	c	23/236 (10%)	21 (91%)	2 (9%)	0	100	100
All	All	3569/4458 (80%)	3447 (97%)	119 (3%)	3 (0%)	50	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	184	VAL
3	H	184	VAL
2	G	274	ILE

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	O	163/206 (79%)	160 (98%)	3 (2%)	54 80
2	G	311/333 (93%)	300 (96%)	11 (4%)	31 60
2	M	311/333 (93%)	310 (100%)	1 (0%)	91 97
3	H	351/448 (78%)	343 (98%)	8 (2%)	45 74
3	N	428/448 (96%)	420 (98%)	8 (2%)	52 79
4	P	58/83 (70%)	58 (100%)	0	100 100
5	S	146/161 (91%)	146 (100%)	0	100 100
6	T	106/106 (100%)	102 (96%)	4 (4%)	28 56
7	R	453/471 (96%)	447 (99%)	6 (1%)	65 85
8	Q	255/288 (88%)	252 (99%)	3 (1%)	67 86
9	U	51/59 (86%)	51 (100%)	0	100 100
10	V	105/114 (92%)	105 (100%)	0	100 100
11	W	121/146 (83%)	119 (98%)	2 (2%)	56 81
12	Y	20/167 (12%)	17 (85%)	3 (15%)	2 6
12	c	20/167 (12%)	17 (85%)	3 (15%)	2 6
All	All	2899/3530 (82%)	2847 (98%)	52 (2%)	54 80

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	Y	27	THR
3	H	408	THR
12	c	22	SER
12	Y	42	SER
3	H	172	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	192	HIS
7	R	162	HIS
7	R	212	ASN
11	W	35	GLN
2	G	151	GLN

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)

Of 53 ligands modelled in this entry, 5 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	IZL	G	503	-	119,119,119	1.75	33 (27%)	161,163,163	1.31	17 (10%)
16	CDL	P	301	-	76,76,99	1.38	11 (14%)	82,88,111	1.10	4 (4%)
28	9XX	W	202	-	41,41,41	0.98	4 (9%)	44,44,44	1.26	2 (4%)
24	HEA	R	603	7	57,67,67	2.08	17 (29%)	61,103,103	2.26	20 (32%)
15	MQ9	H	606	-	59,59,59	0.35	0	72,75,75	0.31	0
13	WUO	O	301	-	99,99,99	1.62	11 (11%)	123,125,125	1.30	13 (10%)
15	MQ9	O	304	-	59,59,59	0.36	0	72,75,75	0.32	0
18	9YF	W	201	-	58,58,58	1.40	5 (8%)	69,71,71	1.07	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	TRD	Q	403	-	12,12,12	0.09	0	11,11,11	0.05	0
16	CDL	N	603	-	73,73,99	0.30	0	79,85,111	0.35	0
17	FES	M	501	2	0,4,4	-	-	-		
16	CDL	H	602	-	73,73,99	0.30	0	79,85,111	0.35	0
15	MQ9	N	607	-	59,59,59	0.35	0	72,75,75	0.31	0
16	CDL	R	605	-	76,76,99	0.29	0	82,88,111	0.34	0
16	CDL	N	605	-	78,78,99	0.29	0	84,90,111	0.34	0
28	9XX	c	302	-	31,31,41	1.10	4 (12%)	34,34,44	1.40	4 (11%)
20	IZL	M	504	-	119,119,119	1.75	29 (24%)	161,163,163	1.31	17 (10%)
22	TRD	T	201	-	12,12,12	0.29	0	11,11,11	0.85	0
21	HEM	H	604	3	41,50,50	1.47	4 (9%)	45,82,82	1.40	7 (15%)
22	TRD	S	502	-	12,12,12	0.29	0	11,11,11	0.86	0
13	WUO	P	302	-	99,99,99	1.59	9 (9%)	123,125,125	1.30	15 (12%)
22	TRD	R	608	-	12,12,12	0.09	0	11,11,11	0.05	0
23	3PE	S	503	-	31,31,50	1.07	4 (12%)	34,36,55	1.12	2 (5%)
16	CDL	H	603	-	76,76,99	0.29	0	82,88,111	0.34	0
28	9XX	Y	302	-	31,31,41	1.10	4 (12%)	34,34,44	1.40	4 (11%)
21	HEM	N	602	3	41,50,50	1.46	5 (12%)	45,82,82	1.37	6 (13%)
29	PLM	Y	301	-	10,10,17	0.65	0	9,9,17	0.54	0
16	CDL	N	604	-	76,76,99	0.29	0	82,88,111	0.34	0
19	7PH	G	504	-	37,37,37	0.95	4 (10%)	41,42,42	1.15	2 (4%)
15	MQ9	H	605	-	59,59,59	0.35	0	72,75,75	0.31	0
19	7PH	G	505	-	37,37,37	0.96	4 (10%)	41,42,42	1.11	2 (4%)
17	FES	G	501	2	0,4,4	-	-	-		
22	TRD	R	607	-	12,12,12	0.09	0	11,11,11	0.05	0
18	9YF	M	502	-	58,58,58	1.38	4 (6%)	69,71,71	1.08	3 (4%)
16	CDL	R	601	-	76,76,99	1.38	11 (14%)	82,88,111	1.13	4 (4%)
29	PLM	W	203	-	10,10,17	0.64	0	9,9,17	0.54	0
24	HEA	R	602	-	57,67,67	1.85	15 (26%)	61,103,103	2.62	27 (44%)
21	HEM	N	606	3	41,50,50	1.47	5 (12%)	45,82,82	1.28	5 (11%)
15	MQ9	N	601	-	59,59,59	0.35	0	72,75,75	0.32	0
21	HEM	H	601	3	41,50,50	1.53	3 (7%)	45,82,82	1.51	5 (11%)
19	7PH	S	501	-	37,37,37	0.30	0	41,42,42	0.34	0
19	7PH	M	503	-	37,37,37	0.96	4 (10%)	41,42,42	1.15	2 (4%)
14	HEC	O	302	1	32,50,50	2.16	3 (9%)	24,82,82	1.46	3 (12%)
16	CDL	O	305	-	78,78,99	0.29	0	84,90,111	0.34	0
18	9YF	G	502	-	58,58,58	1.40	5 (8%)	69,71,71	1.07	3 (4%)
14	HEC	O	303	1	32,50,50	2.17	4 (12%)	24,82,82	1.45	3 (12%)
15	MQ9	N	608	-	59,59,59	0.35	0	72,75,75	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	PLM	c	301	-	10,10,17	0.64	0	9,9,17	0.54	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
20	IZL	G	503	-	-	38/84/208/208	0/6/6/6
16	CDL	P	301	-	-	50/87/87/110	-
28	9XX	W	202	-	-	13/43/43/43	-
24	HEA	R	603	7	-	16/32/76/76	-
15	MQ9	H	606	-	-	32/53/73/73	0/2/2/2
13	WUO	O	301	-	-	33/84/148/148	0/3/3/3
15	MQ9	O	304	-	-	25/53/73/73	0/2/2/2
18	9YF	W	201	-	-	31/54/78/78	0/1/1/1
22	TRD	Q	403	-	-	0/10/10/10	-
16	CDL	N	603	-	-	47/84/84/110	-
17	FES	M	501	2	-	-	0/1/1/1
16	CDL	H	602	-	-	36/84/84/110	-
15	MQ9	N	607	-	-	36/53/73/73	0/2/2/2
16	CDL	R	605	-	-	47/87/87/110	-
16	CDL	N	605	-	-	52/89/89/110	-
28	9XX	c	302	-	-	9/33/33/43	-
20	IZL	M	504	-	-	38/84/208/208	0/6/6/6
22	TRD	T	201	-	-	1/10/10/10	-
21	HEM	H	604	3	-	2/12/54/54	-
22	TRD	S	502	-	-	1/10/10/10	-
13	WUO	P	302	-	-	40/84/148/148	0/3/3/3
22	TRD	R	608	-	-	1/10/10/10	-
23	3PE	S	503	-	-	14/35/35/54	-
16	CDL	H	603	-	-	43/87/87/110	-
28	9XX	Y	302	-	-	9/33/33/43	-
21	HEM	N	602	3	-	1/12/54/54	-
29	PLM	Y	301	-	-	0/7/8/15	-
16	CDL	N	604	-	-	41/87/87/110	-
19	7PH	G	504	-	-	18/39/39/39	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	MQ9	H	605	-	-	23/53/73/73	0/2/2/2
19	7PH	G	505	-	-	12/39/39/39	-
17	FES	G	501	2	-	-	0/1/1/1
22	TRD	R	607	-	-	0/10/10/10	-
18	9YF	M	502	-	-	32/54/78/78	0/1/1/1
16	CDL	R	601	-	-	55/87/87/110	-
29	PLM	W	203	-	-	0/7/8/15	-
24	HEA	R	602	-	-	6/32/76/76	-
21	HEM	N	606	3	-	5/12/54/54	-
15	MQ9	N	601	-	-	8/53/73/73	0/2/2/2
21	HEM	H	601	3	-	2/12/54/54	-
19	7PH	S	501	-	-	11/39/39/39	-
19	7PH	M	503	-	-	12/39/39/39	-
14	HEC	O	302	1	-	0/10/54/54	-
16	CDL	O	305	-	-	39/89/89/110	-
18	9YF	G	502	-	-	32/54/78/78	0/1/1/1
14	HEC	O	303	1	-	3/10/54/54	-
15	MQ9	N	608	-	-	29/53/73/73	0/2/2/2
29	PLM	c	301	-	-	0/7/8/15	-

The worst 5 of 202 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	301	WUO	P52-O51	6.60	1.77	1.60
13	P	302	WUO	P52-O51	6.51	1.77	1.60
14	O	302	HEC	C3C-C2C	-6.18	1.34	1.40
14	O	303	HEC	C3C-C2C	-6.12	1.34	1.40
14	O	303	HEC	C2B-C3B	-6.11	1.34	1.40

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	602	HEA	C3D-C4D-ND	6.54	116.69	110.36
24	R	602	HEA	C13-C12-C11	-5.68	105.81	114.35
24	R	603	HEA	C2B-C1B-NB	5.59	116.58	109.88
24	R	602	HEA	CBA-CAA-C2A	-5.55	103.25	112.60
20	M	504	IZL	O10-C23-C24	5.39	117.55	106.67

There are no chirality outliers.

5 of 943 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	P	302	WUO	C06-C05-C12-O13
13	P	302	WUO	O55-C56-C57-O58
14	O	303	HEC	C3D-CAD-CBD-CGD
15	O	304	MQ9	C1-C6-C7-C8
15	O	304	MQ9	C7-C8-C9-C10

There are no ring outliers.

35 monomers are involved in 197 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	P	301	CDL	8	0
28	W	202	9XX	3	0
24	R	603	HEA	9	0
15	H	606	MQ9	5	0
13	O	301	WUO	2	0
15	O	304	MQ9	28	0
18	W	201	9YF	2	0
16	N	603	CDL	13	0
17	M	501	FES	1	0
16	H	602	CDL	3	0
15	N	607	MQ9	27	0
16	R	605	CDL	3	0
16	N	605	CDL	3	0
21	H	604	HEM	4	0
16	H	603	CDL	4	0
28	Y	302	9XX	1	0
21	N	602	HEM	2	0
16	N	604	CDL	4	0
15	H	605	MQ9	12	0
19	G	505	7PH	1	0
17	G	501	FES	2	0
18	M	502	9YF	2	0
16	R	601	CDL	2	0
29	W	203	PLM	3	0
24	R	602	HEA	14	0
21	N	606	HEM	3	0
15	N	601	MQ9	5	0
21	H	601	HEM	4	0
19	S	501	7PH	3	0
19	M	503	7PH	2	0
14	O	302	HEC	3	0

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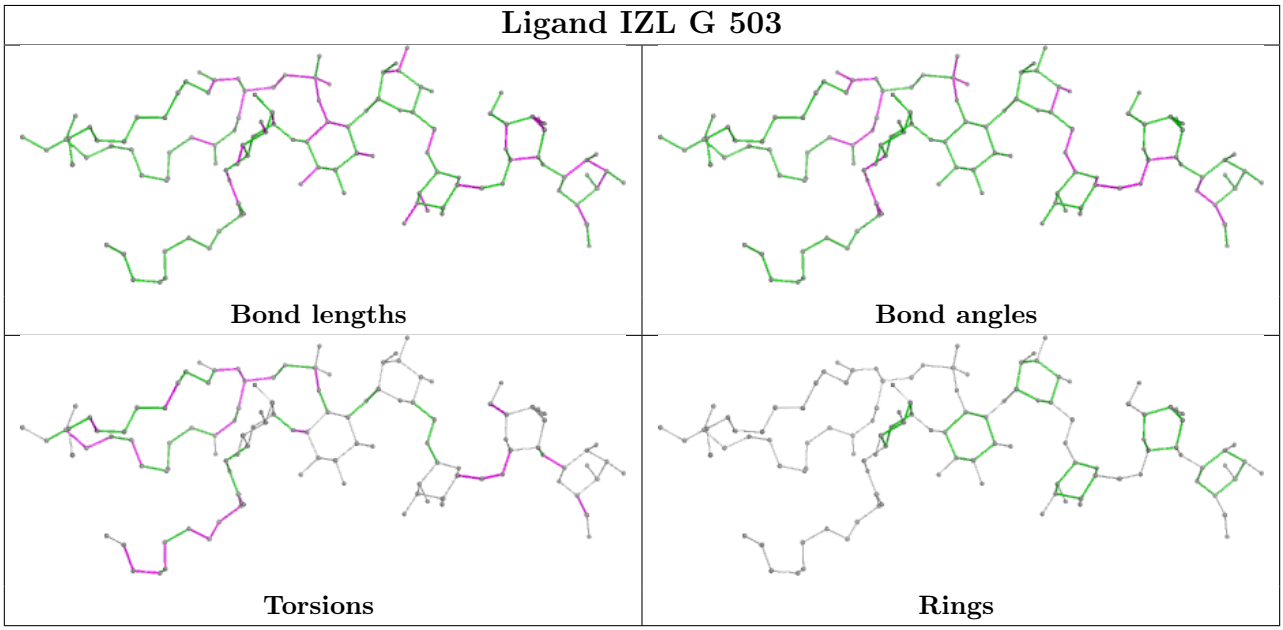
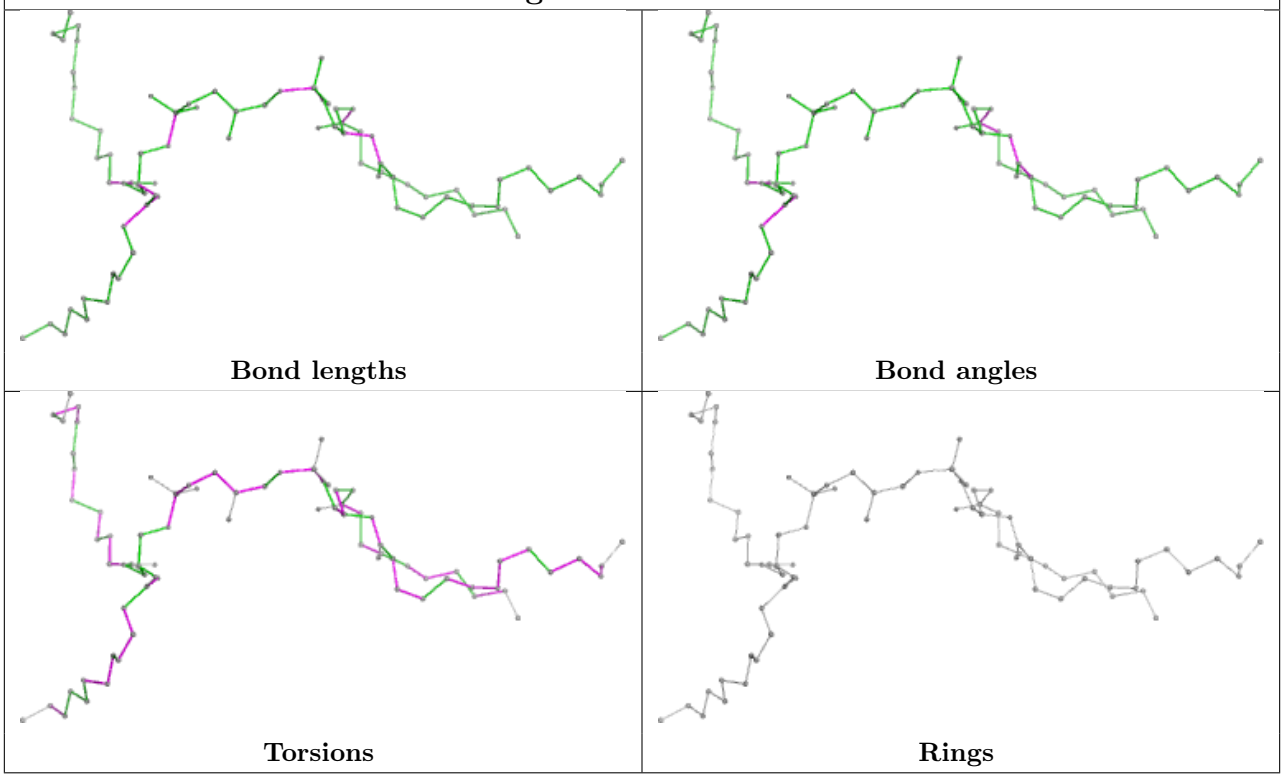
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	O	305	CDL	5	0
18	G	502	9YF	2	0
14	O	303	HEC	2	0
15	N	608	MQ9	20	0

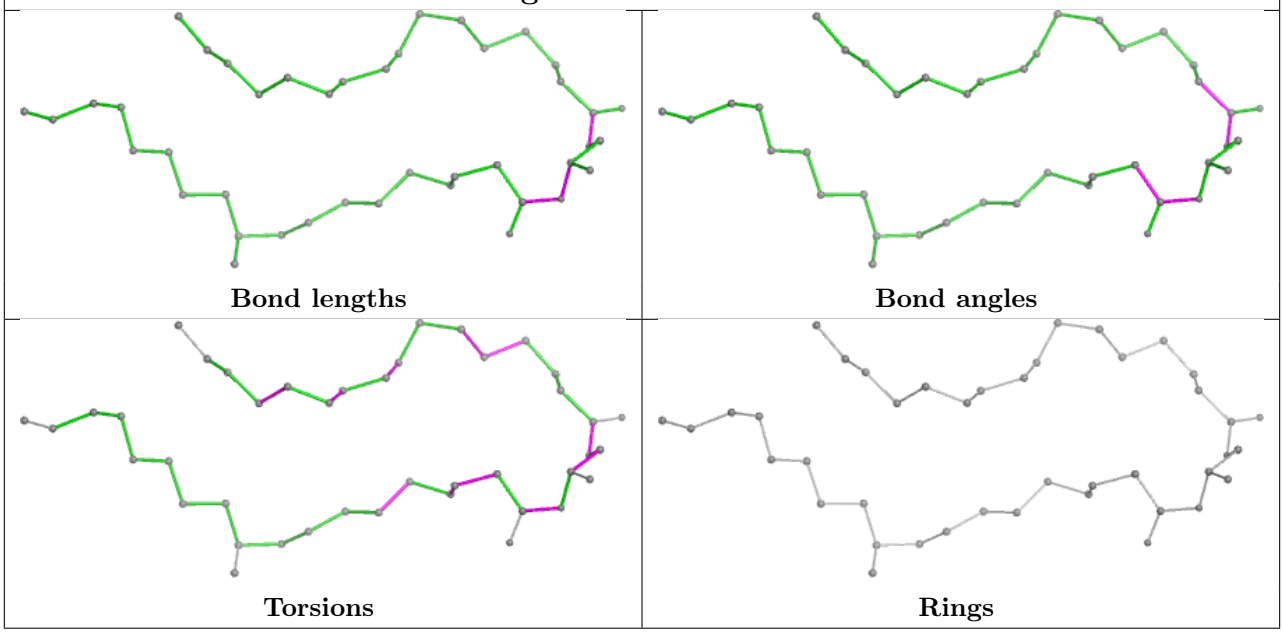
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



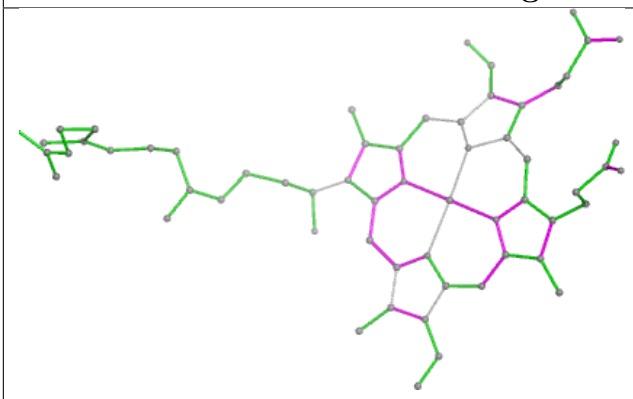
Ligand CDL P 301



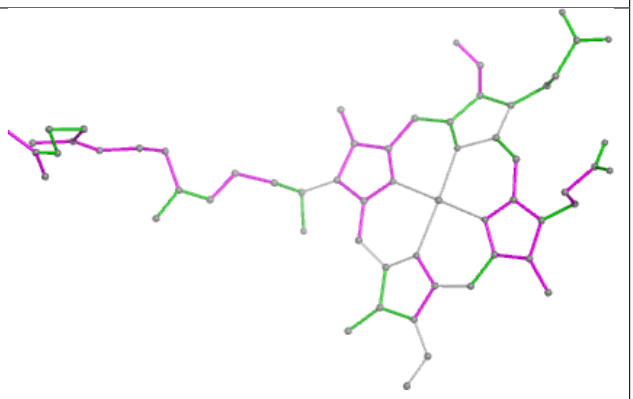
Ligand 9XX W 202



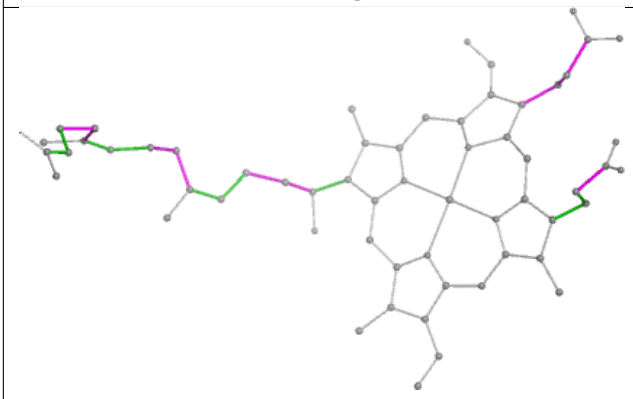
Ligand HEA R 603



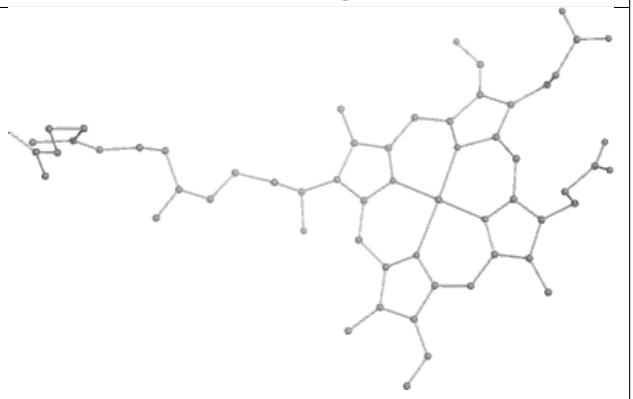
Bond lengths



Bond angles

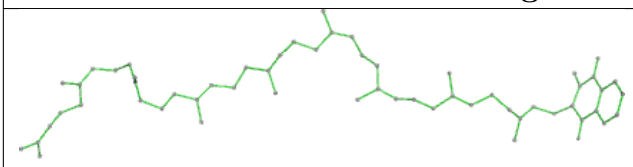


Torsions

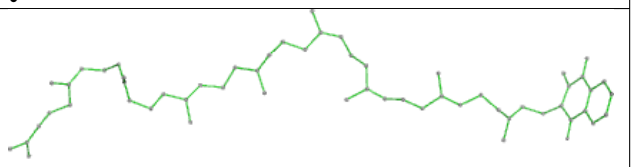


Rings

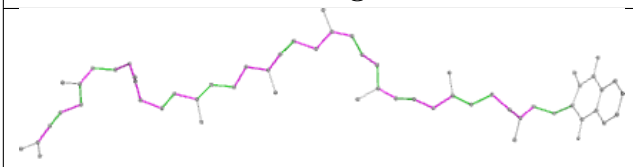
Ligand MQ9 H 606



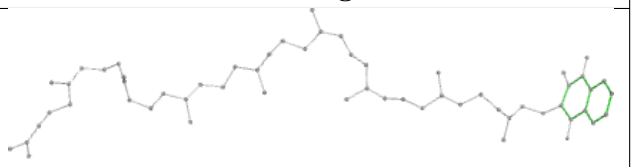
Bond lengths



Bond angles

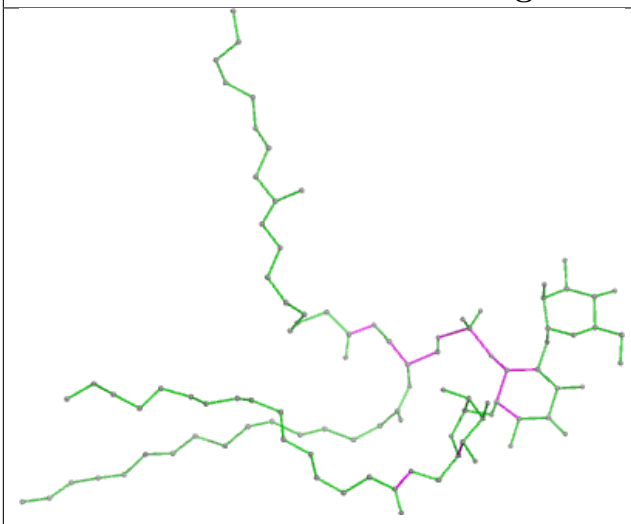


Torsions

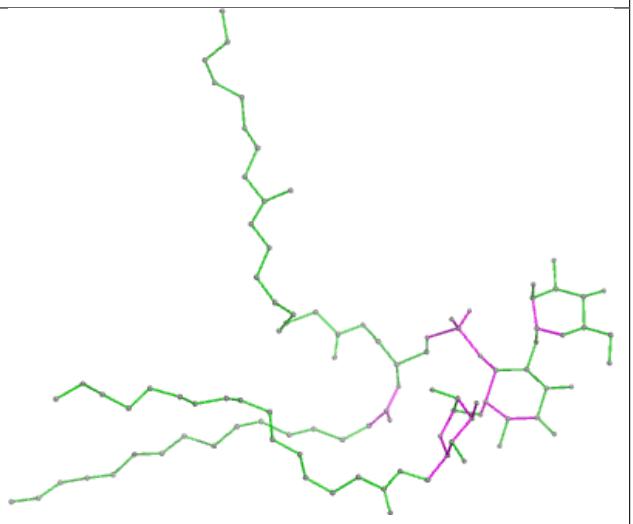


Rings

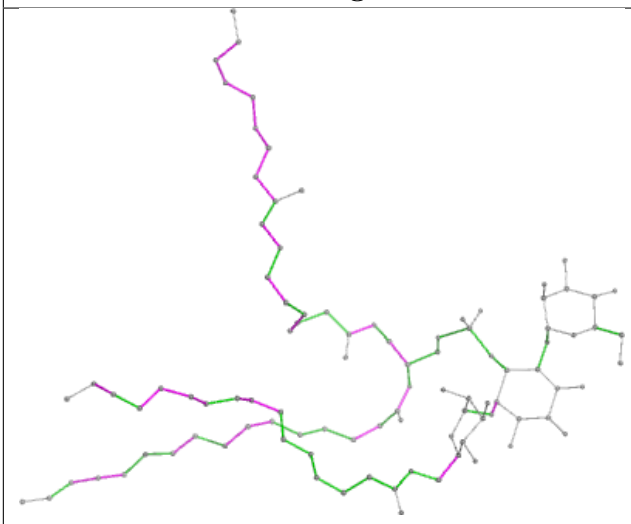
Ligand WUO O 301



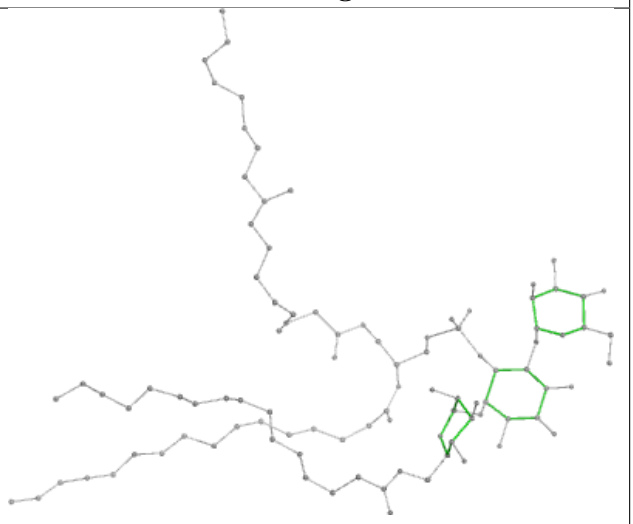
Bond lengths



Bond angles

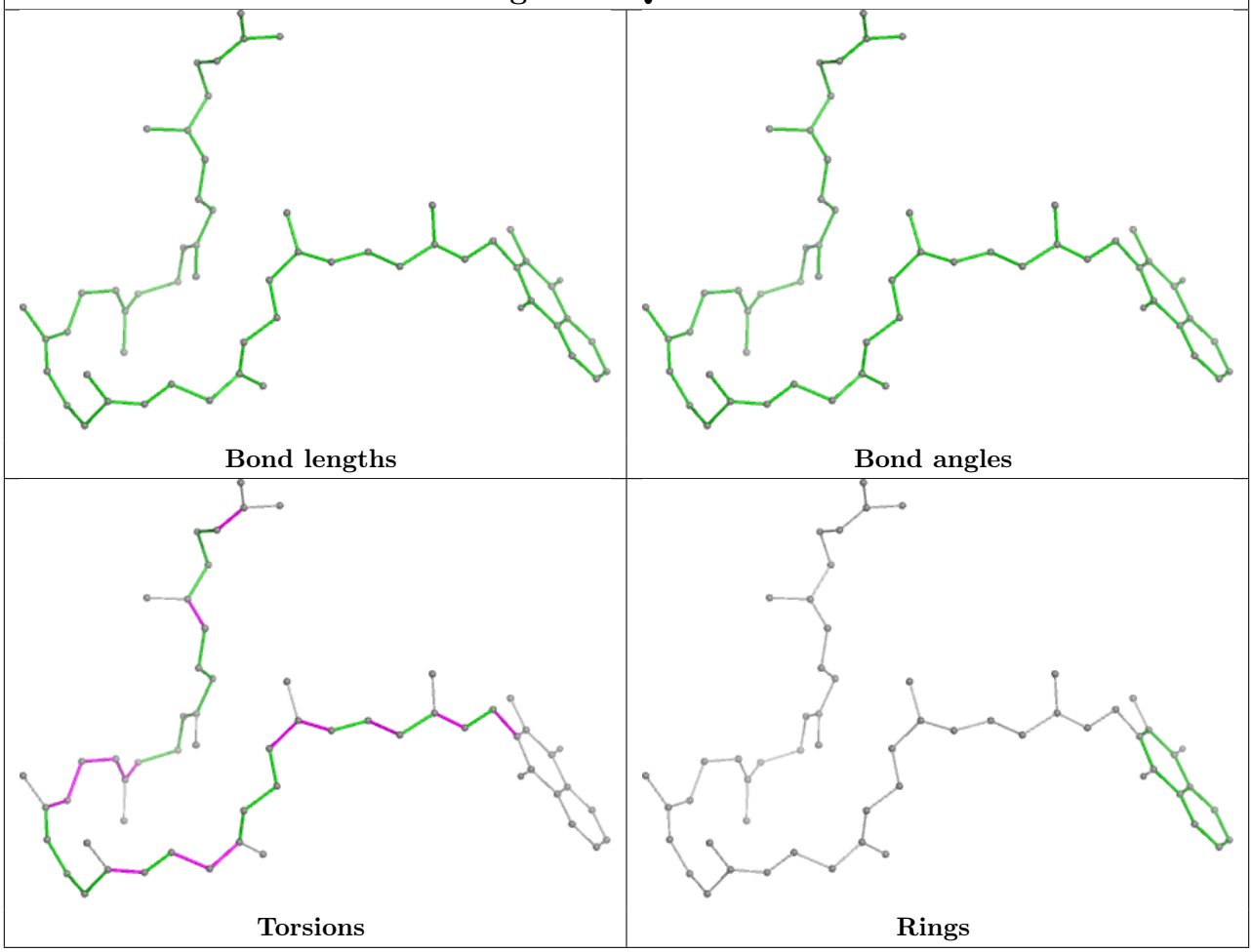


Torsions

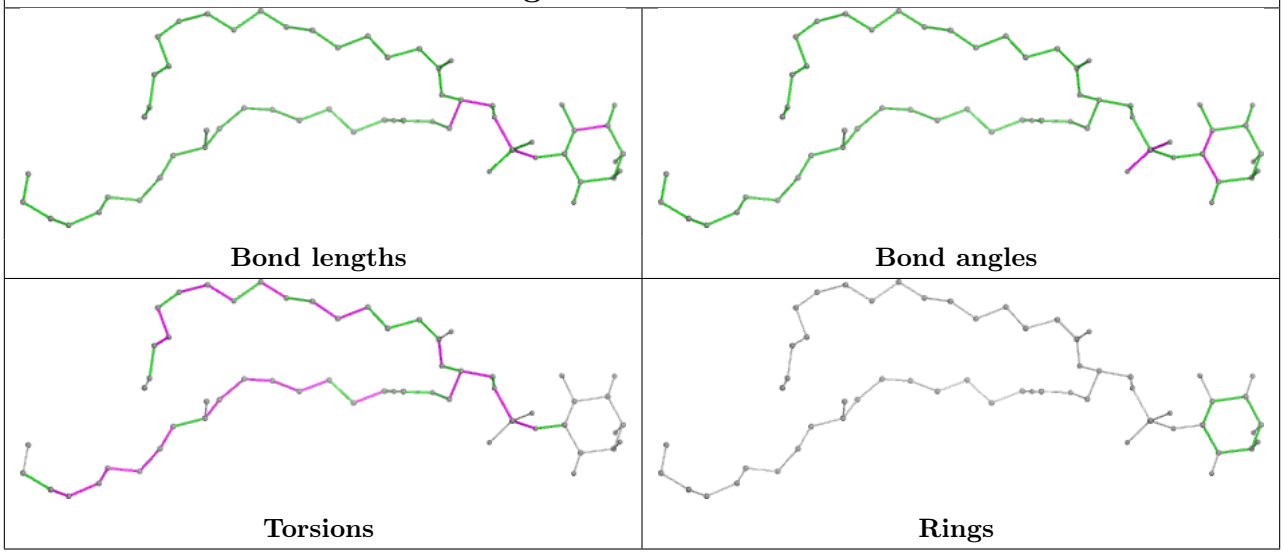


Rings

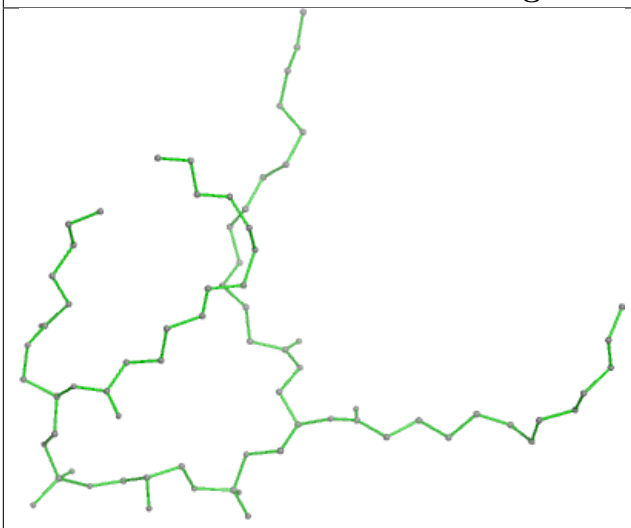
Ligand MQ9 O 304



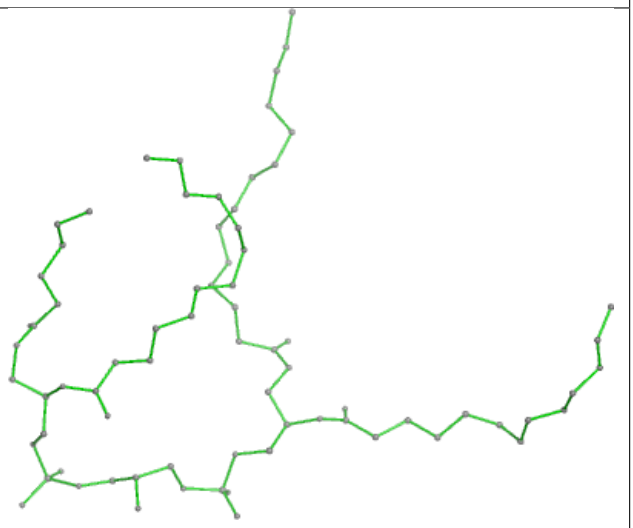
Ligand 9YF W 201



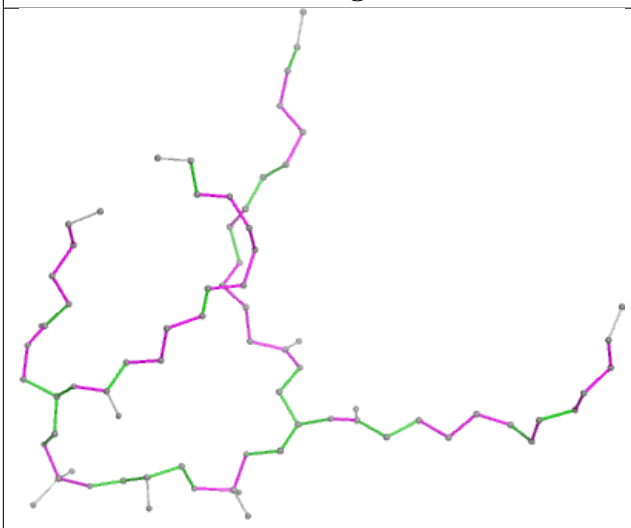
Ligand CDL N 603



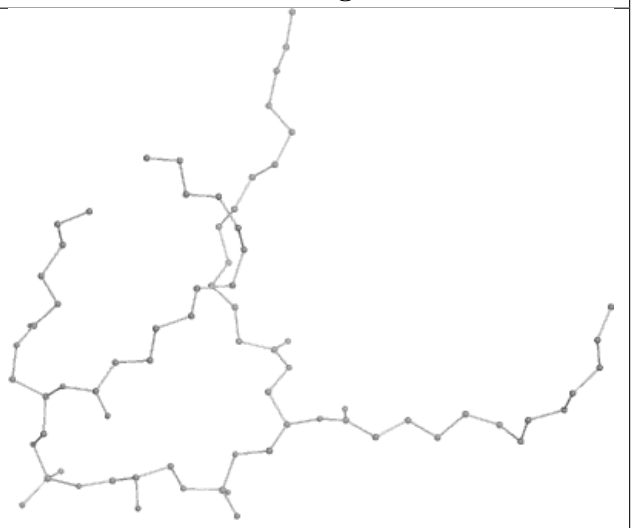
Bond lengths



Bond angles

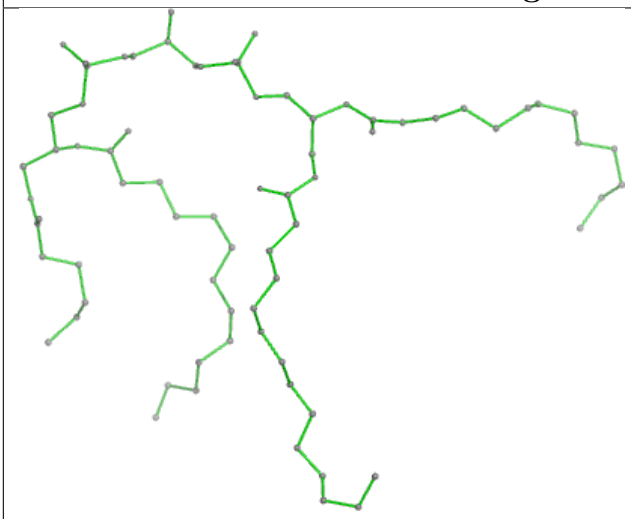


Torsions



Rings

Ligand CDL H 602



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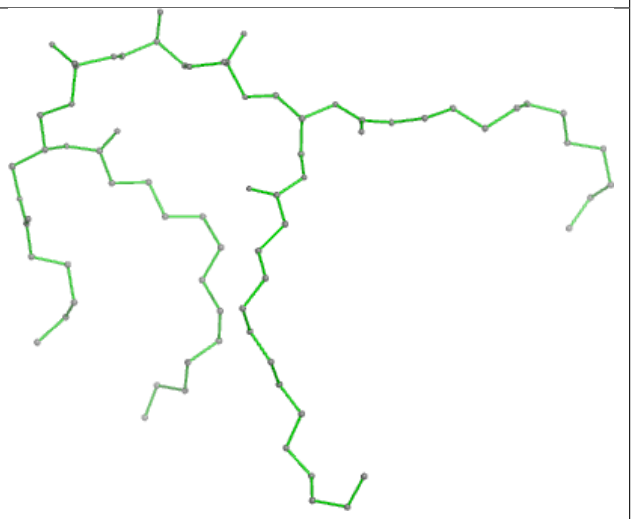
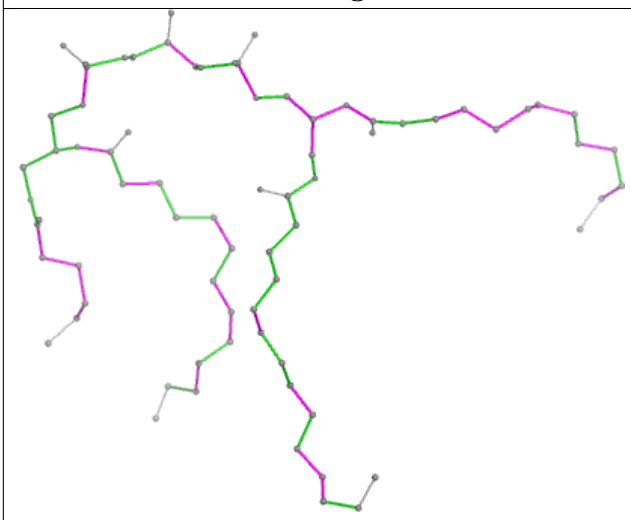


Bond angles



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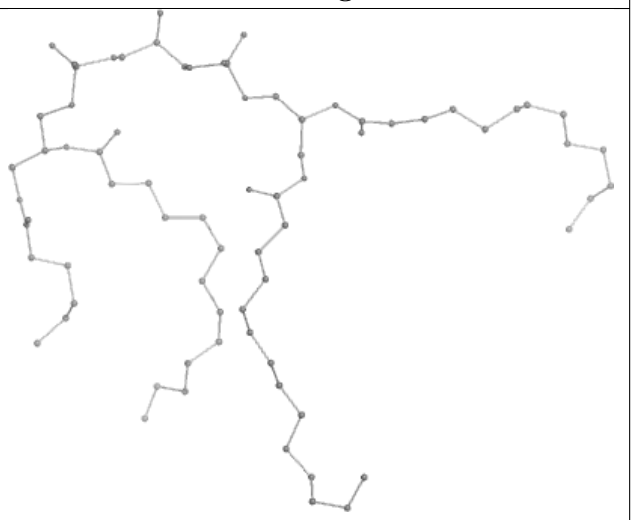
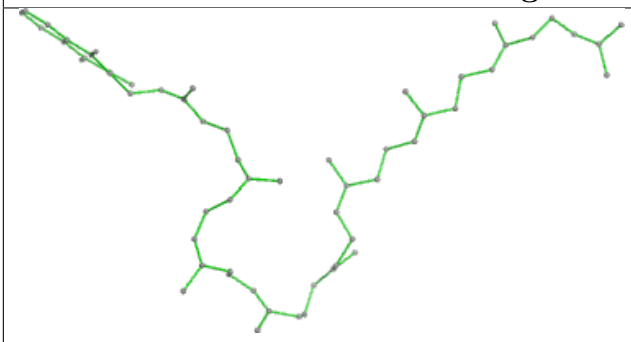


Rings

Ligand MQ9 N 607



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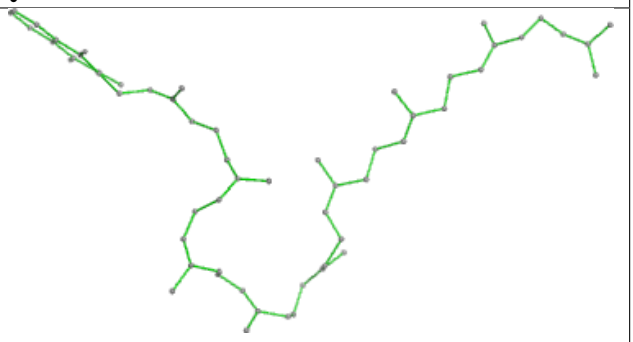
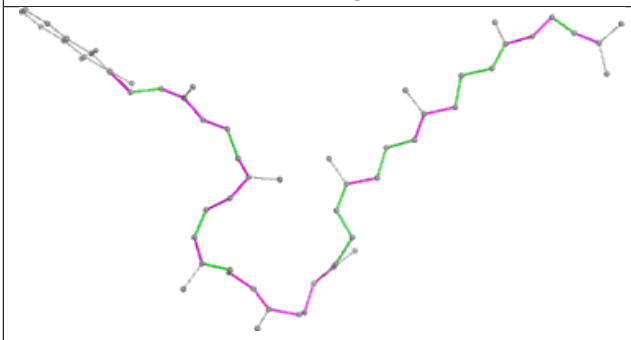


Bond angles



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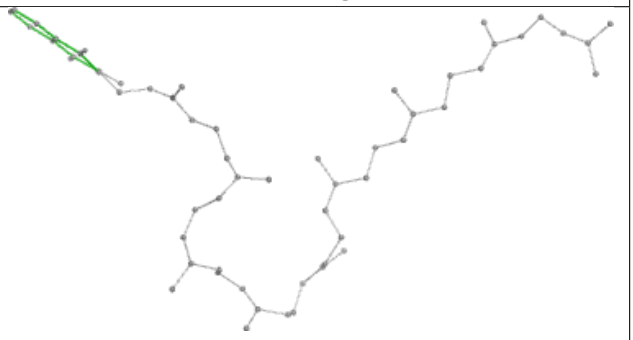
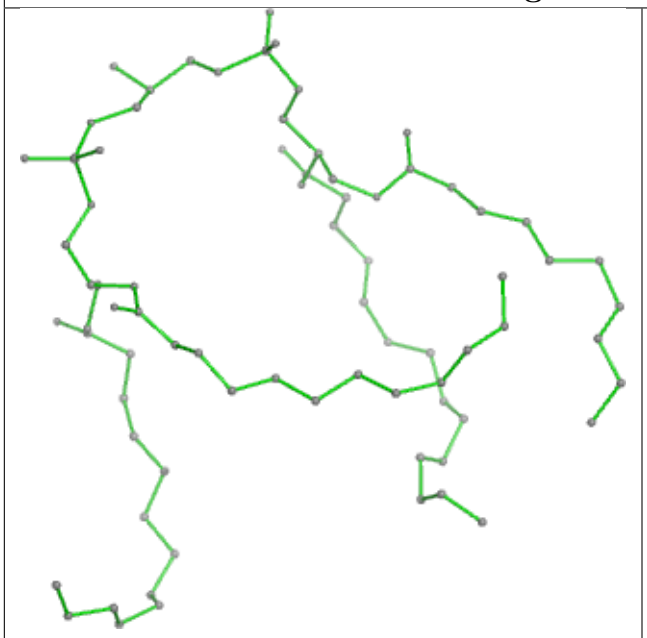


Rings

Ligand CDL R 605



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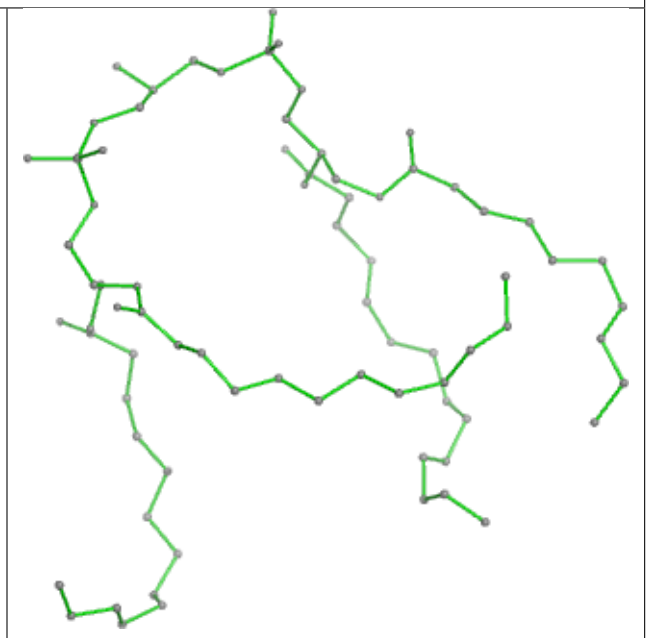
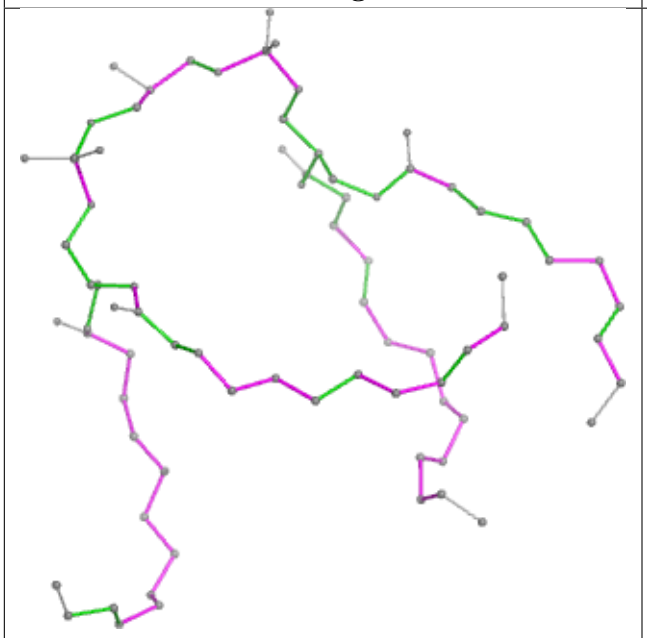
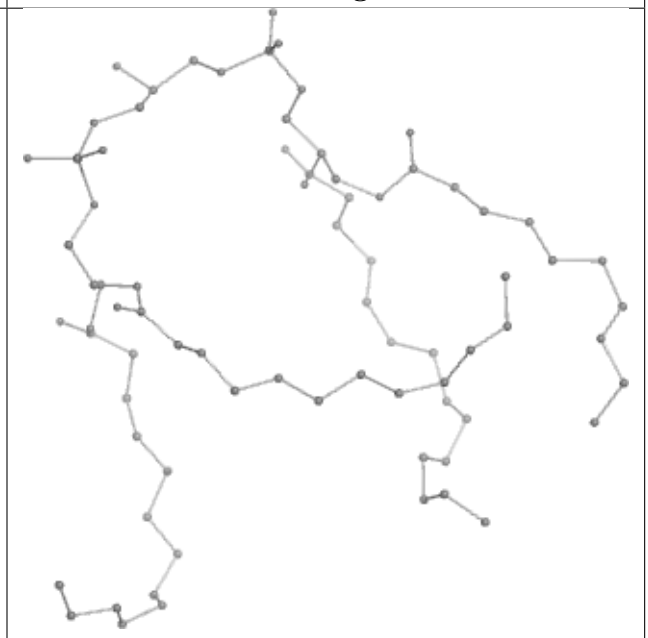


Bond angles

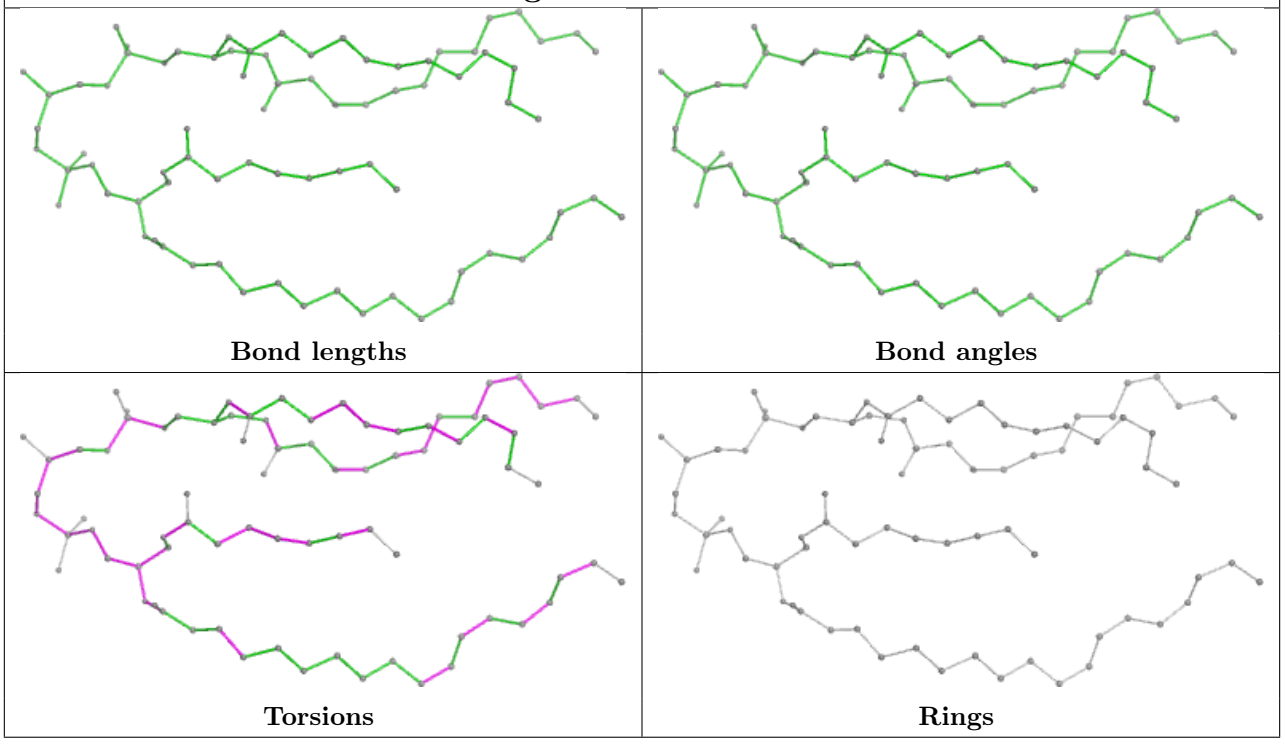


Torsions

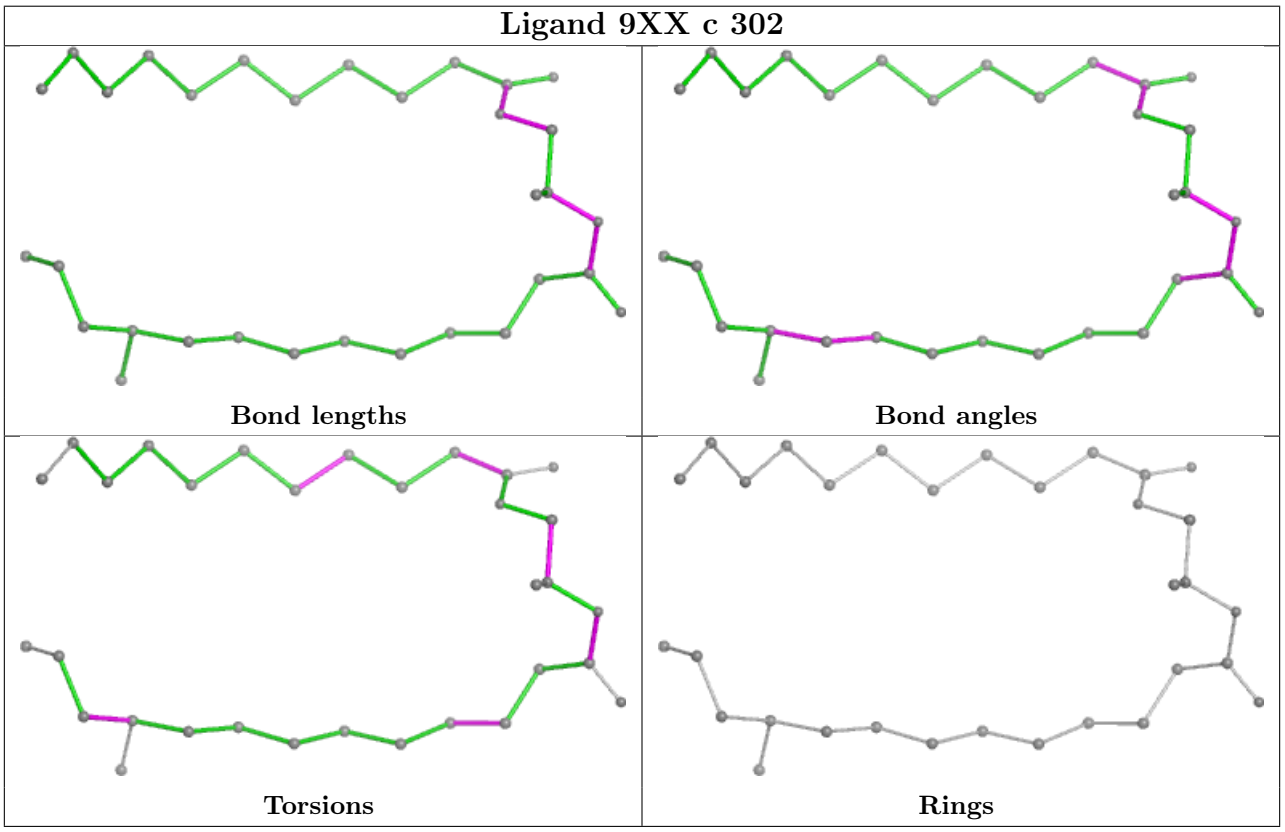


Rings

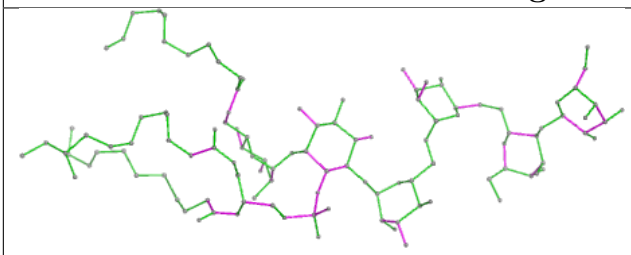
Ligand CDL N 605



Ligand 9XX c 302



Ligand IZL M 504



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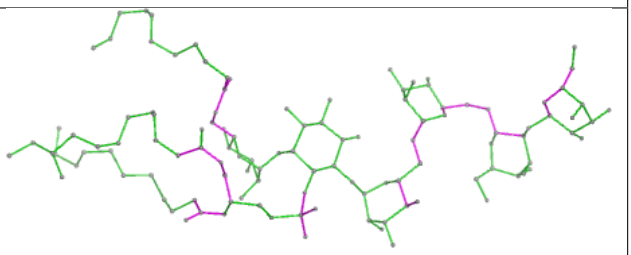
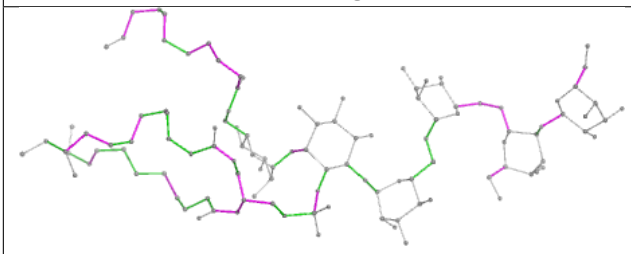


Bond angles



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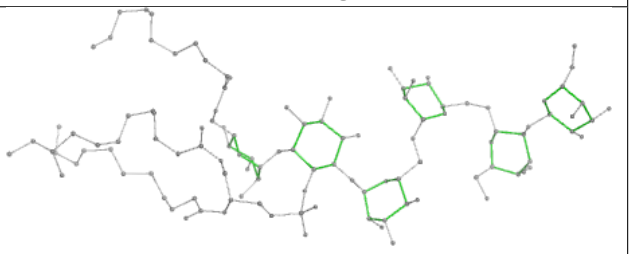
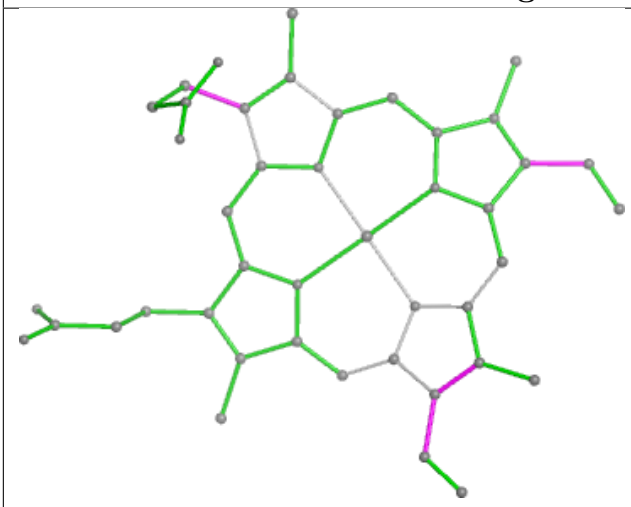


Rings

Ligand HEM H 604



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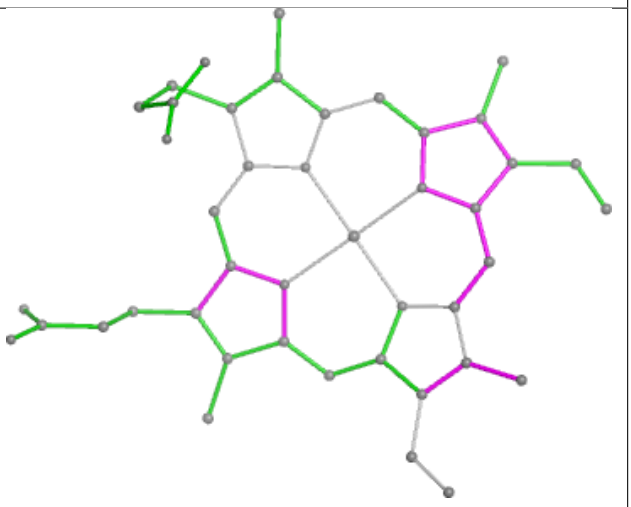
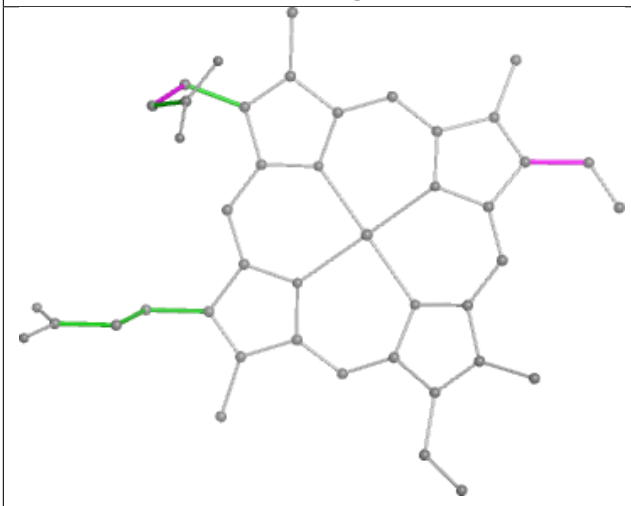


Bond angles



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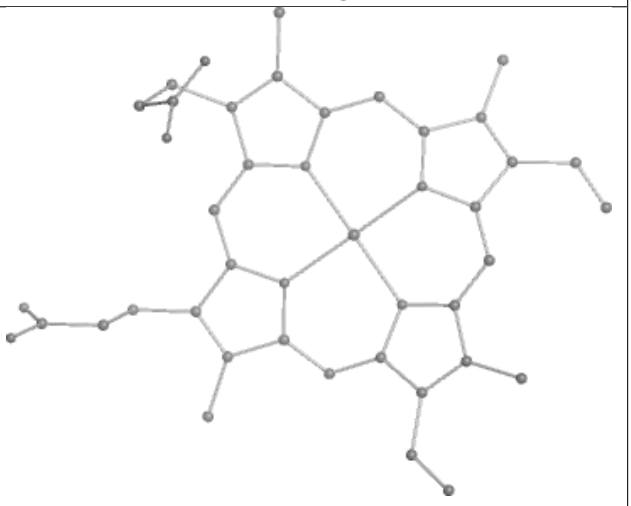
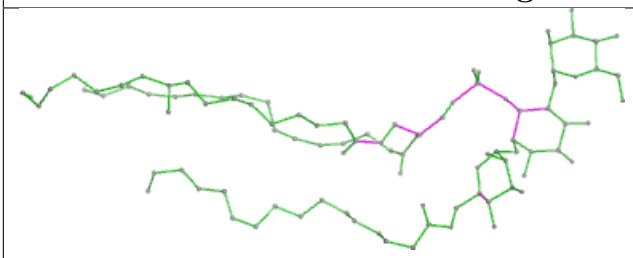


Rings

Ligand WUO P 302



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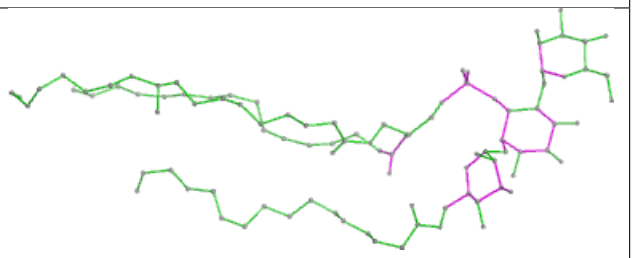
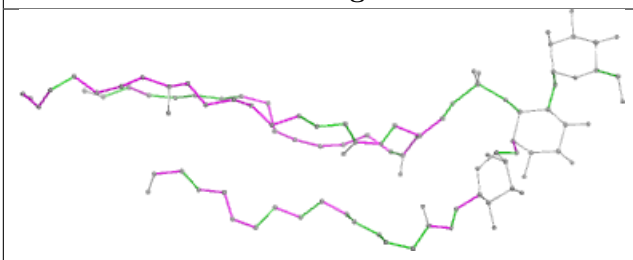


Bond angles



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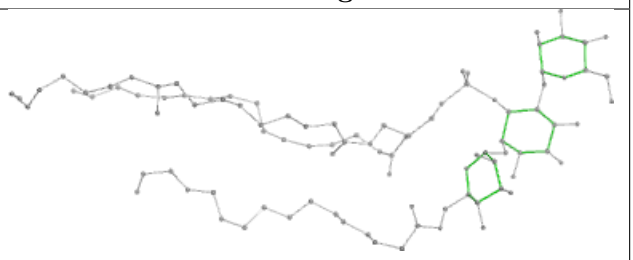
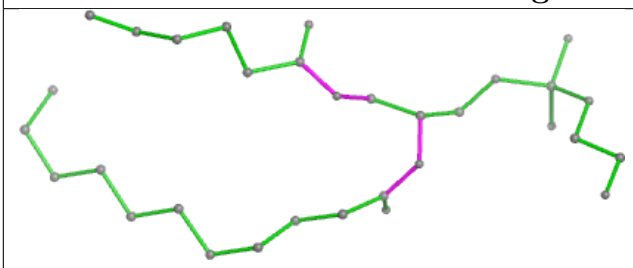


Rings

Ligand 3PE S 503



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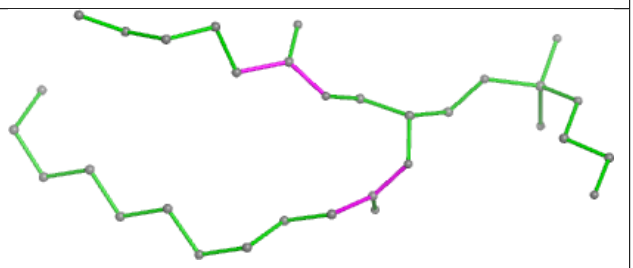
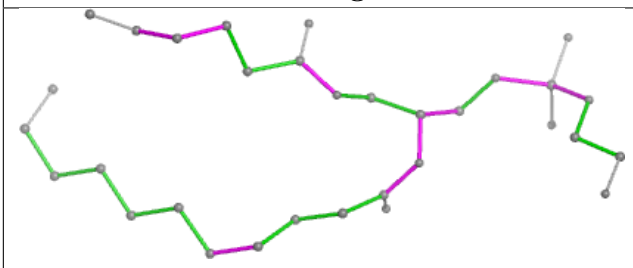
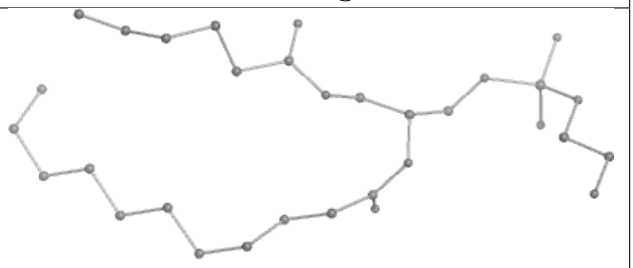


Bond angles

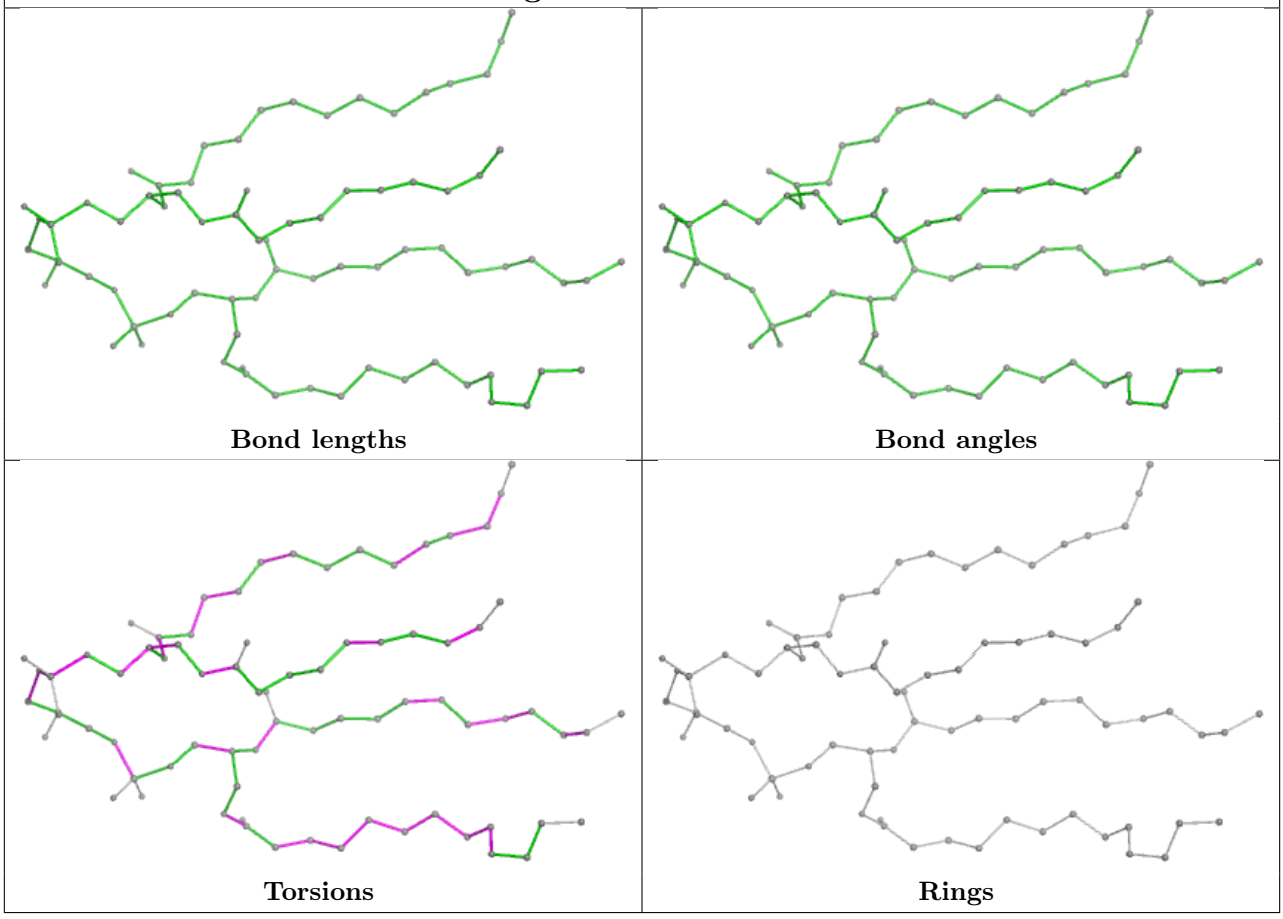


Torsions

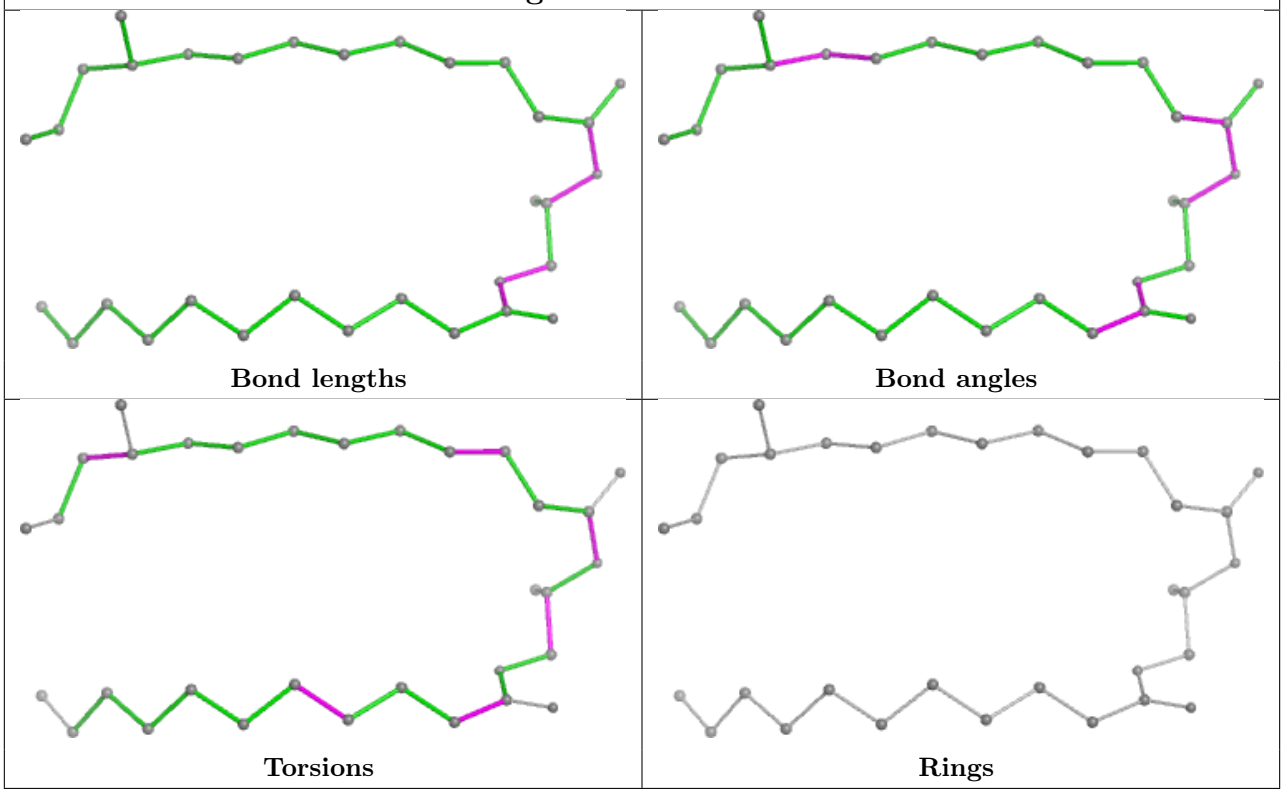


Rings

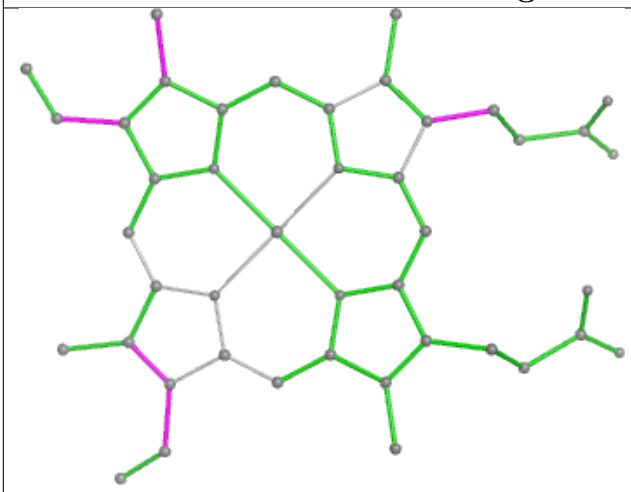
Ligand CDL H 603



Ligand 9XX Y 302



Ligand HEM N 602



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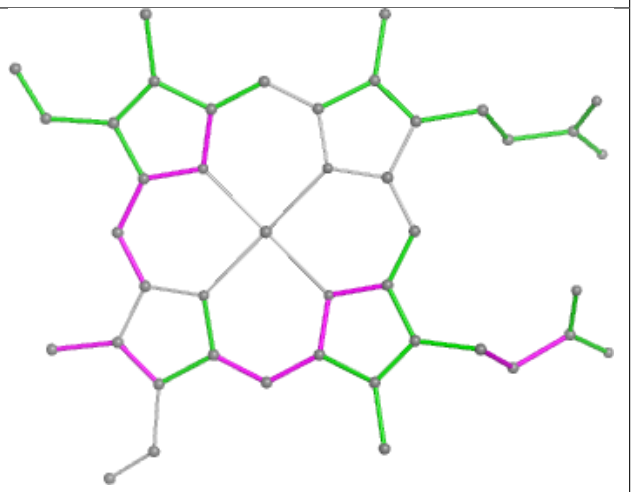
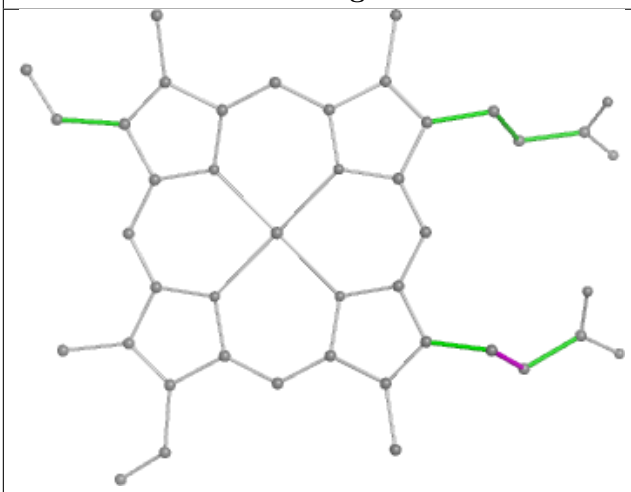


Bond angles



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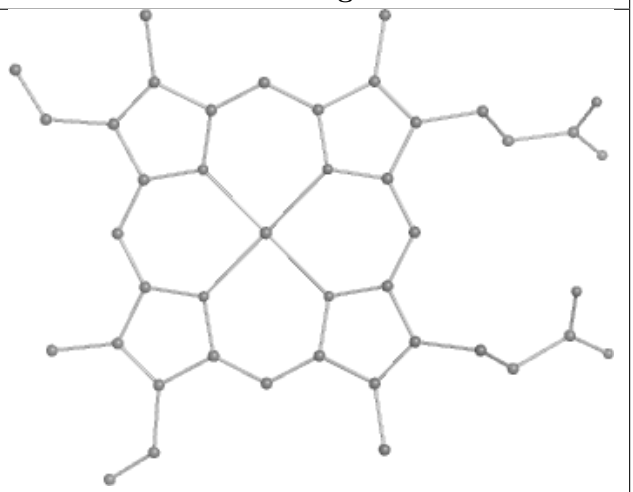
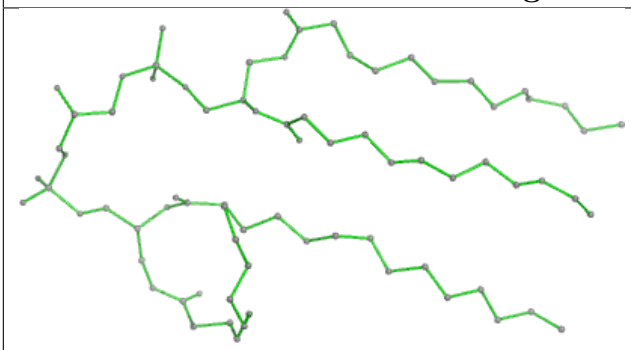


Rings

Ligand CDL N 604



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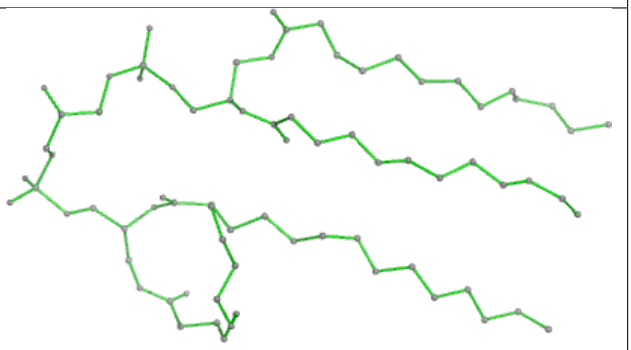
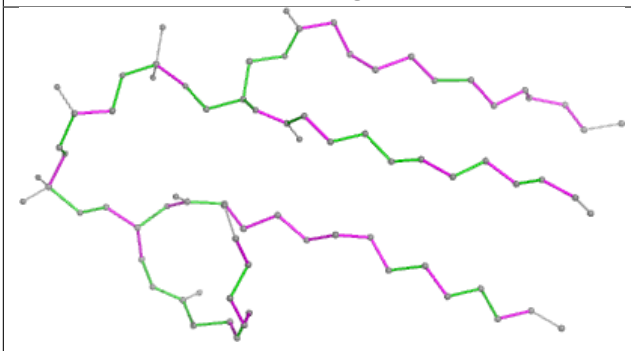


Bond angles



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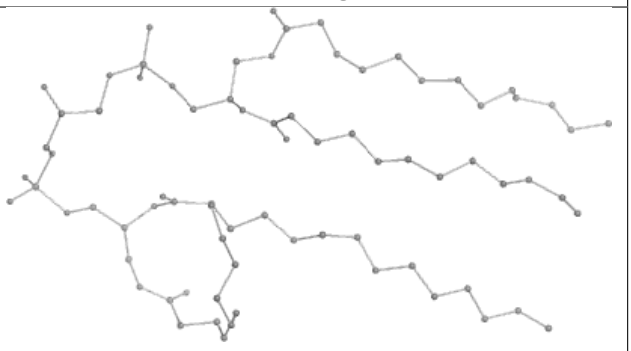
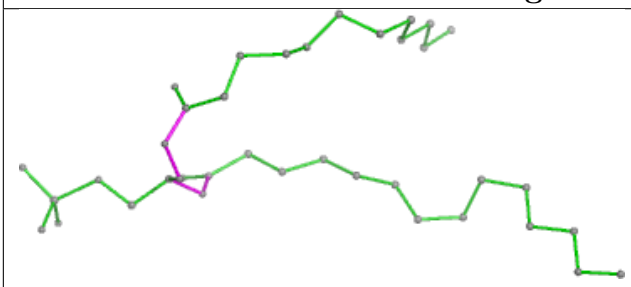


Rings

Ligand 7PH G 504



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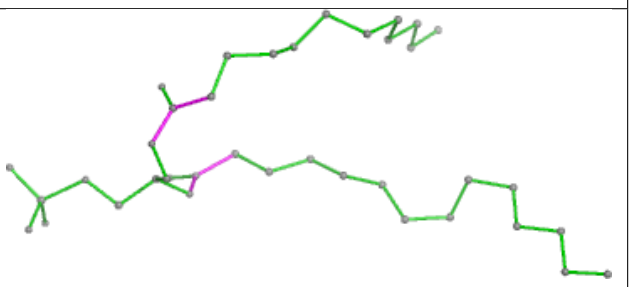
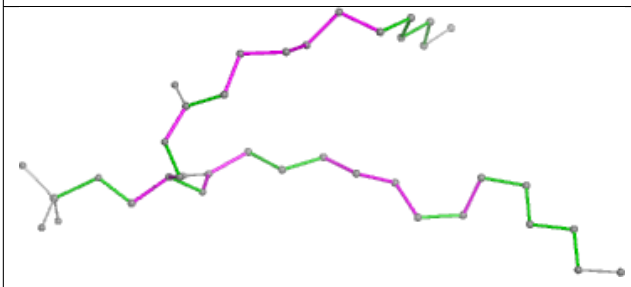


Bond angles



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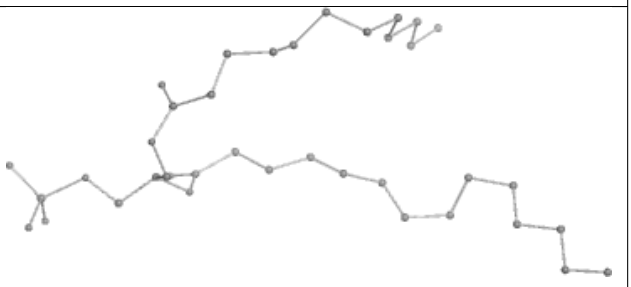
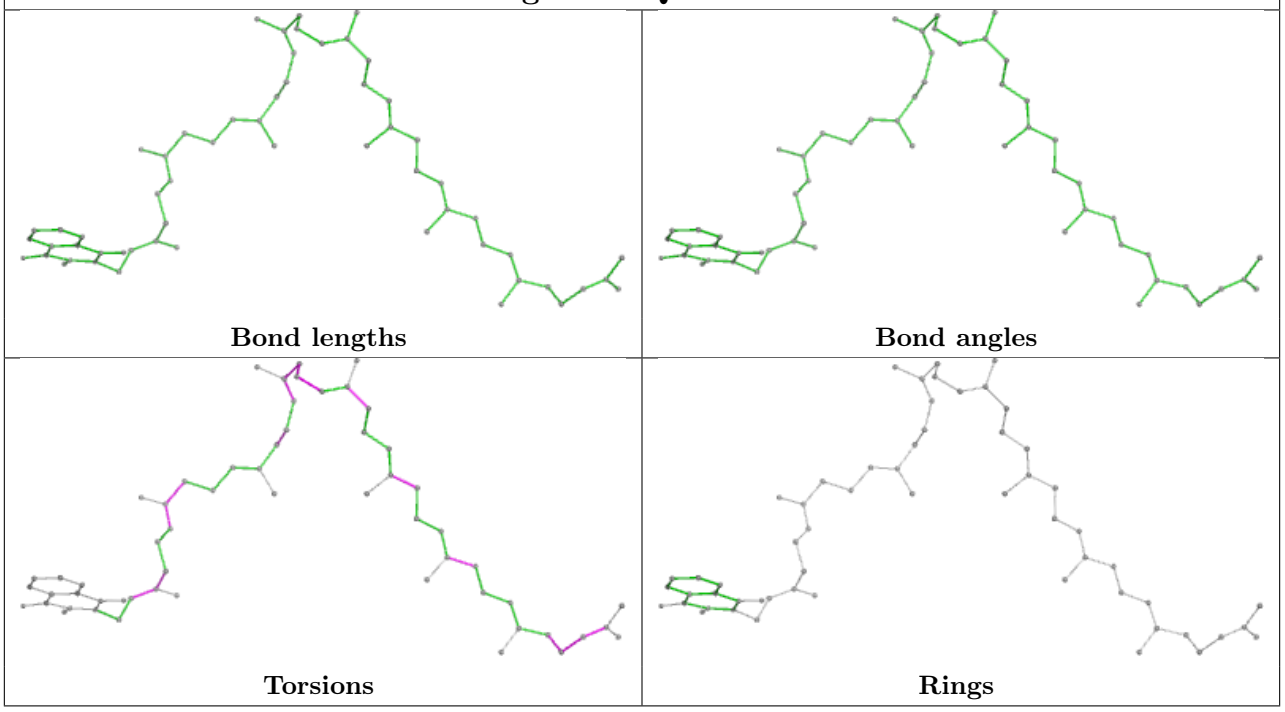
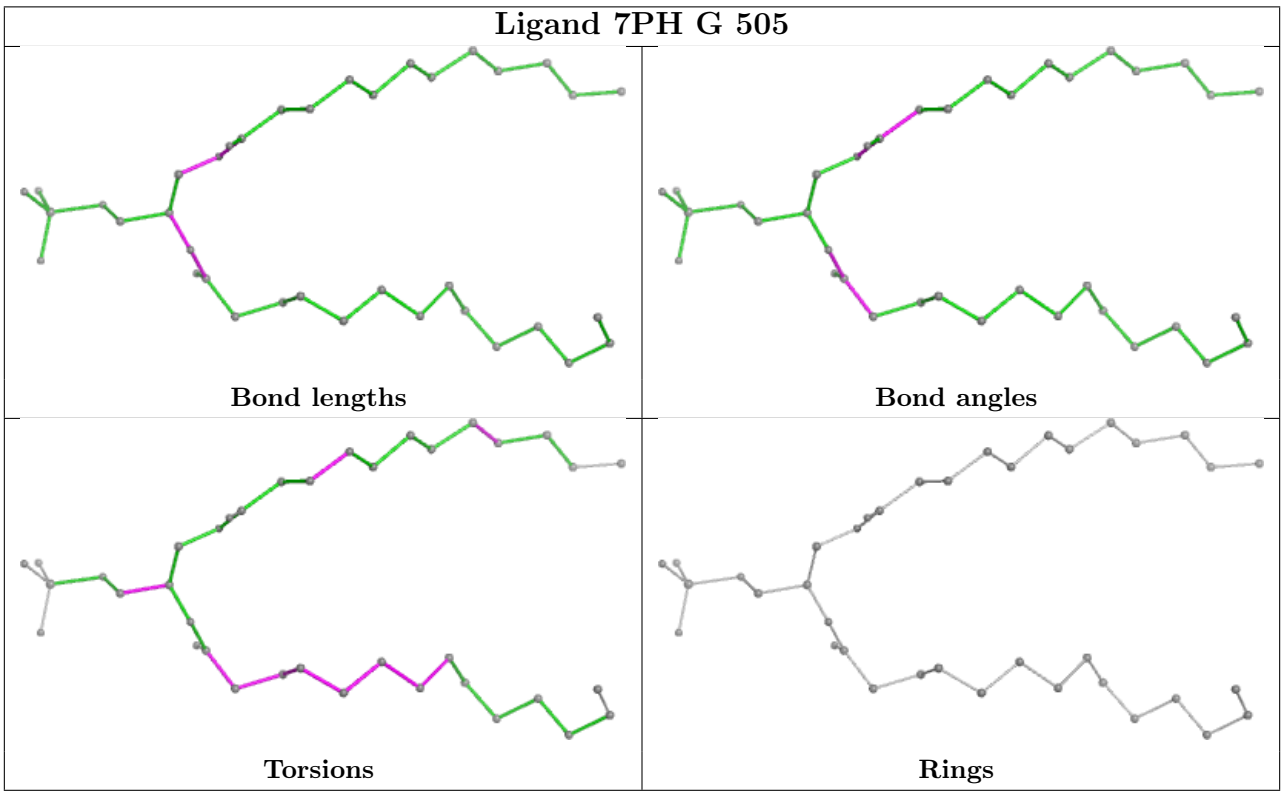


Rings

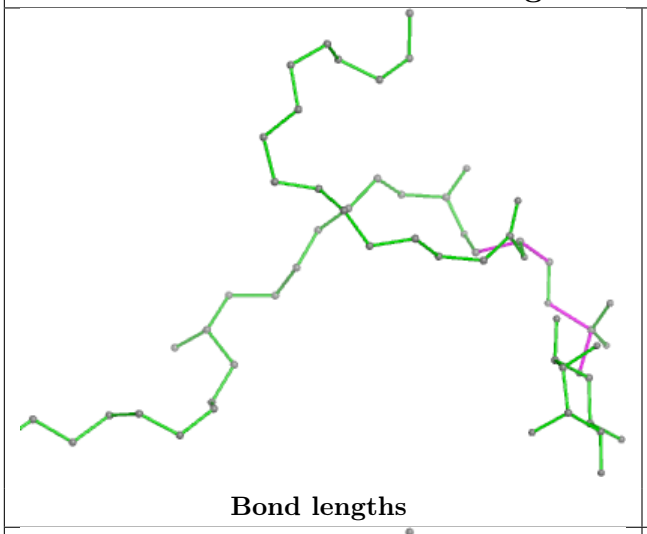
Ligand MQ9 H 605



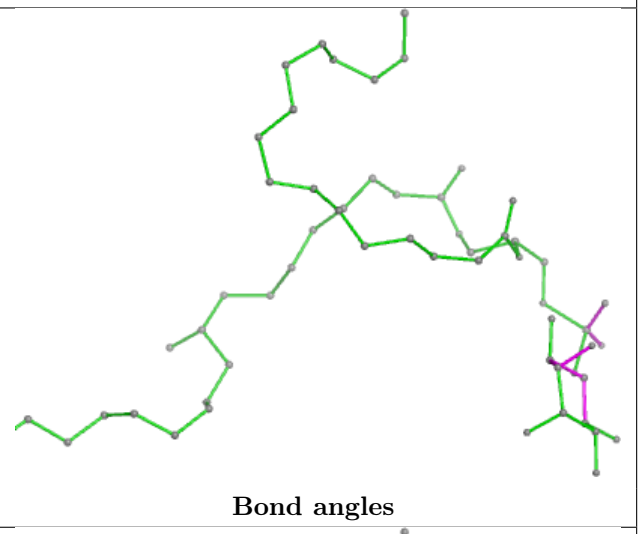
Ligand 7PH G 505



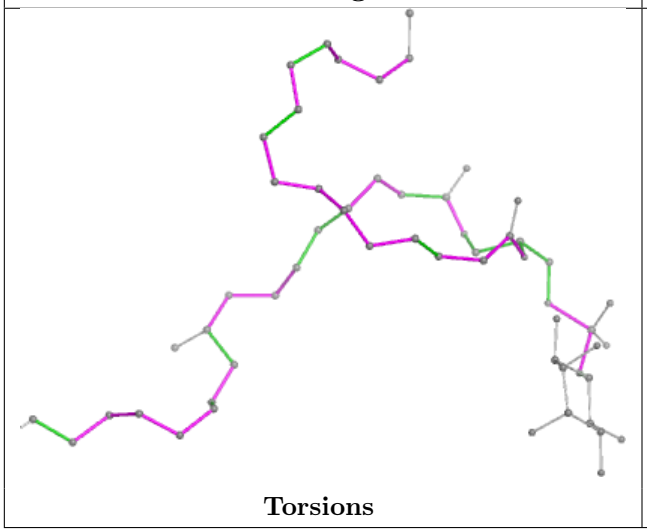
Ligand 9YF M 502



Bond lengths



Bond angles



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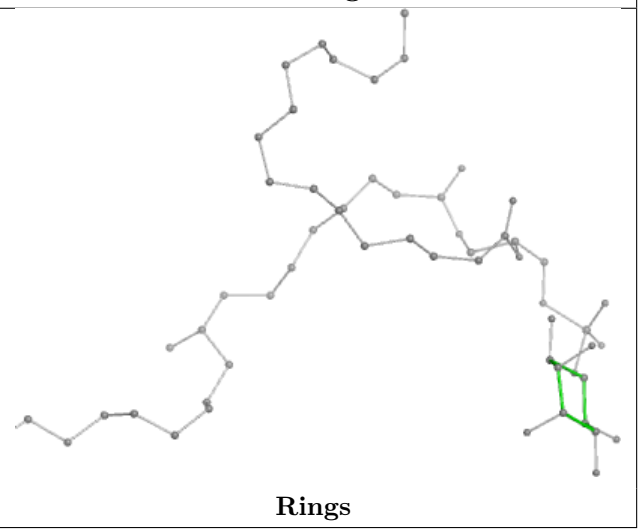
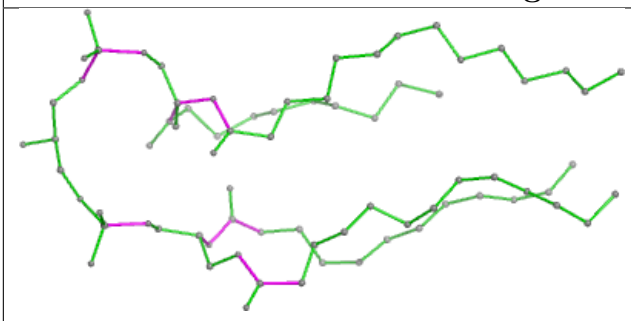
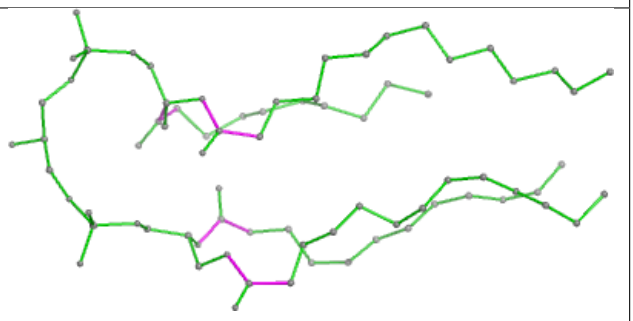


Rings

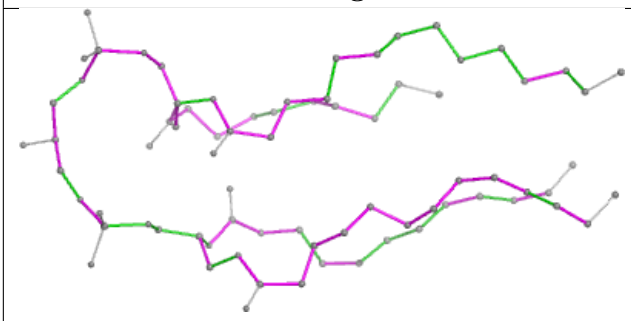
Ligand CDL R 601



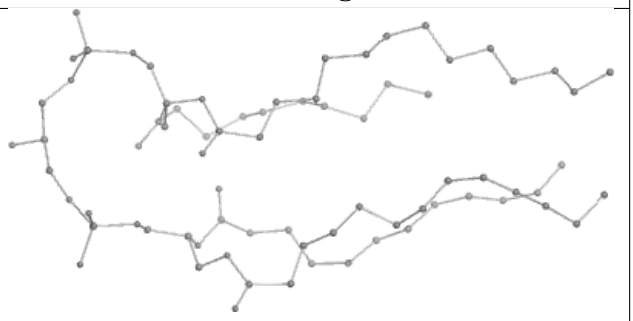
Bond lengths



Bond angles

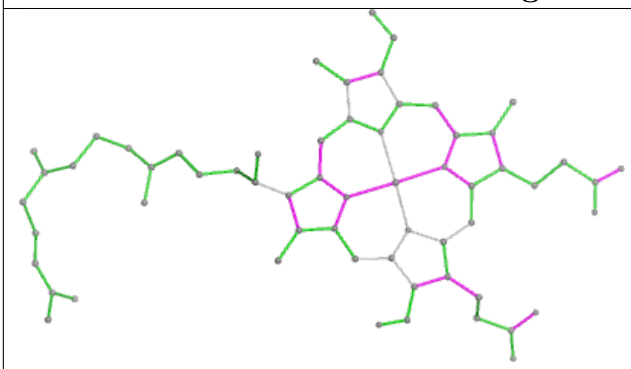


Torsions

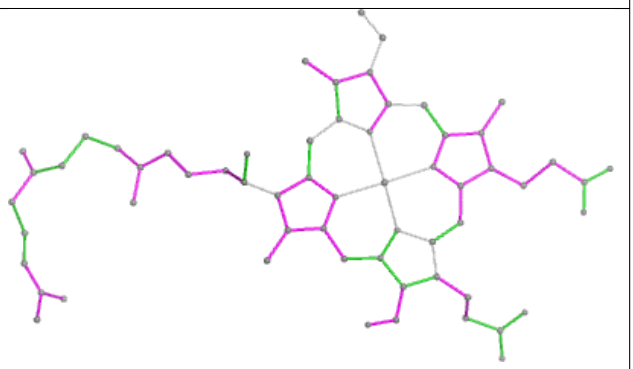


Rings

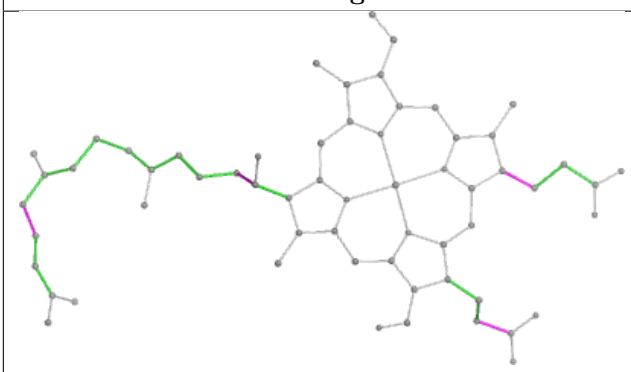
Ligand HEA R 602



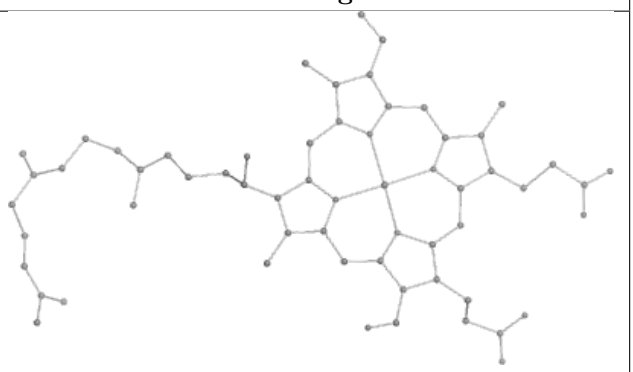
Bond lengths



Bond angles

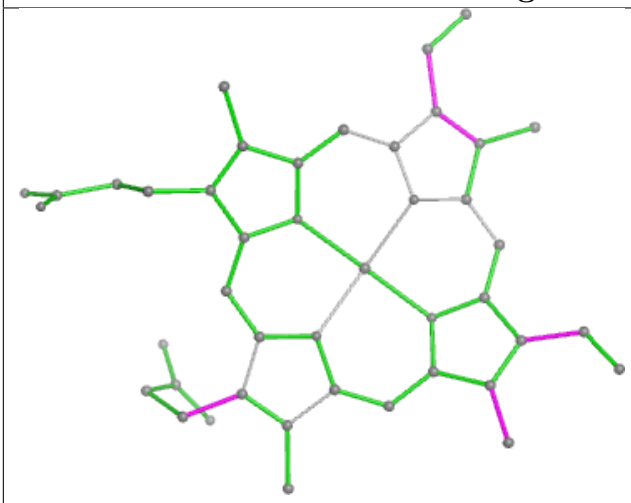


Torsions

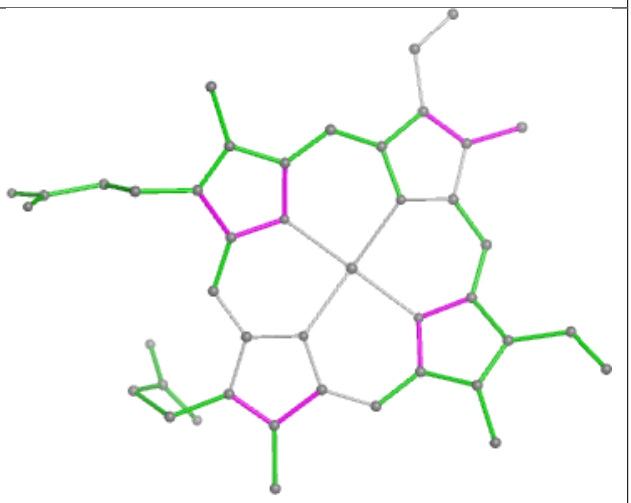


Rings

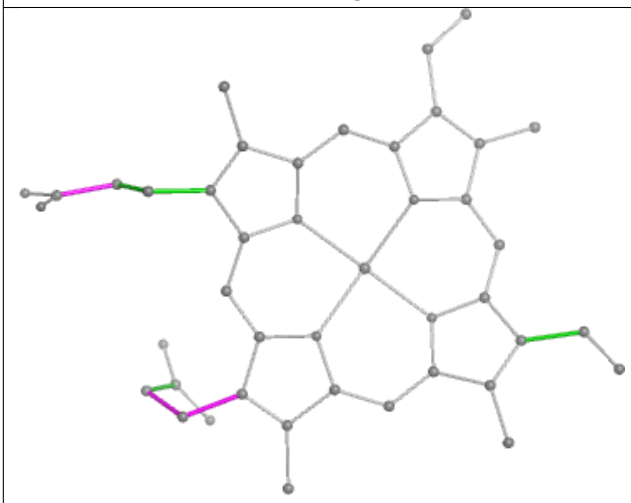
Ligand HEM N 606



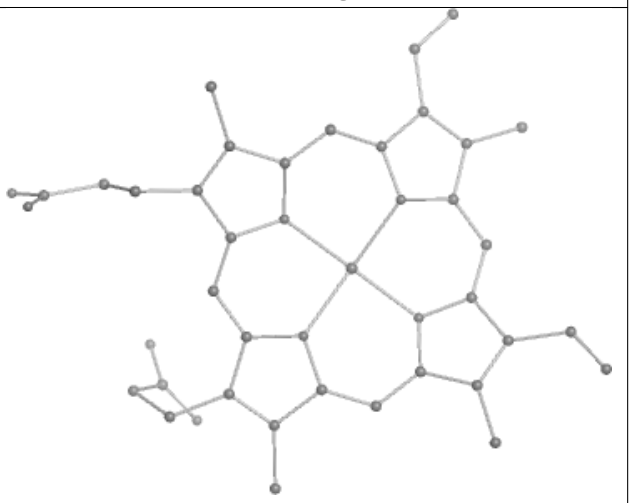
Bond lengths



Bond angles

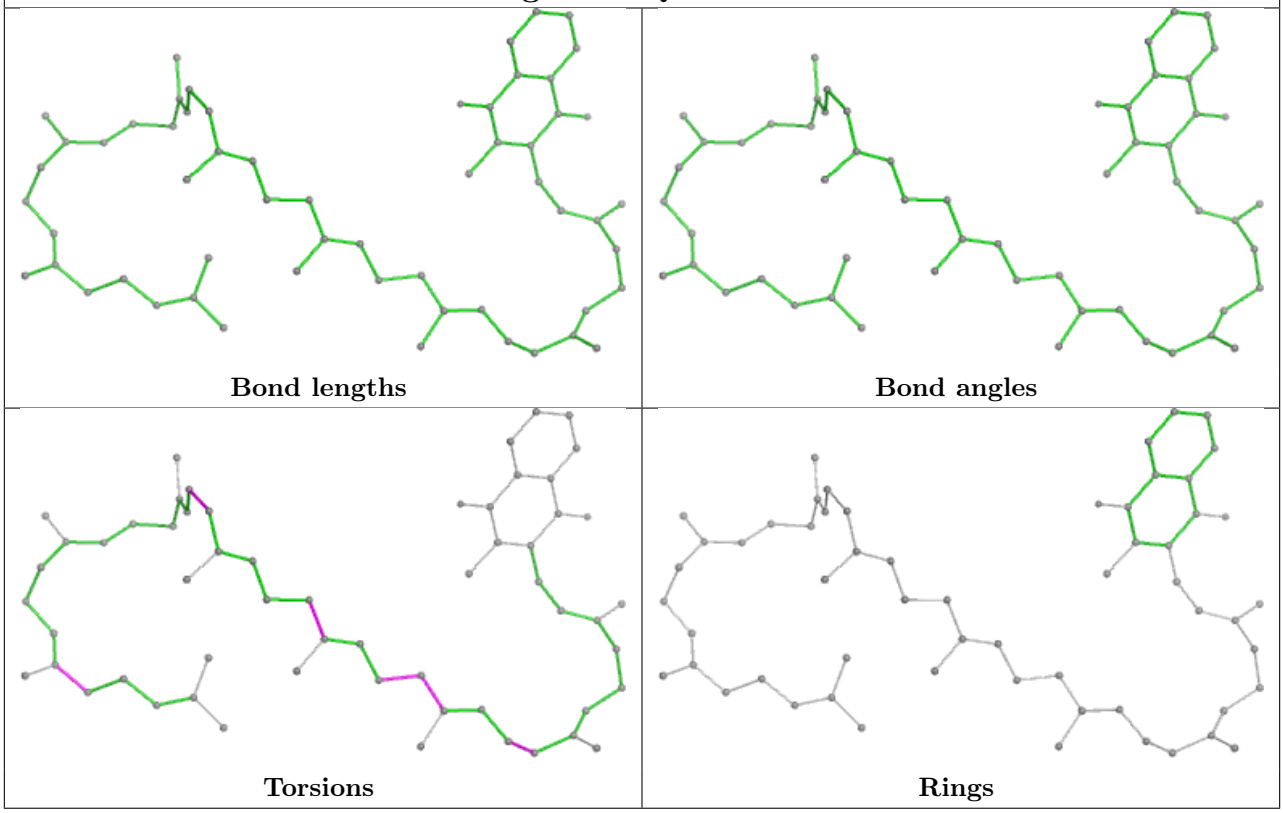


Torsions

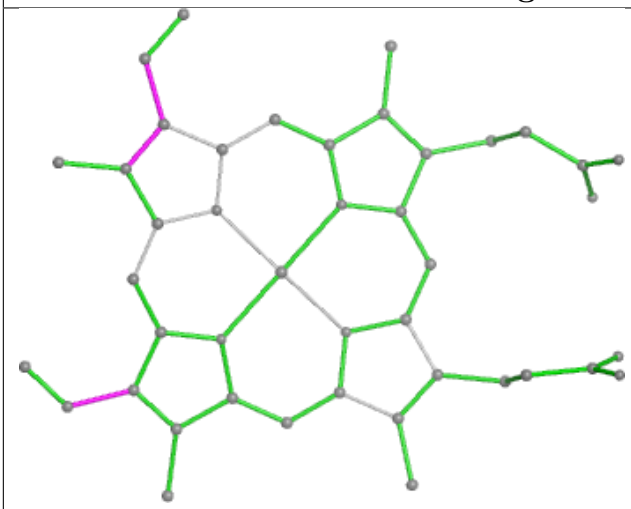


Rings

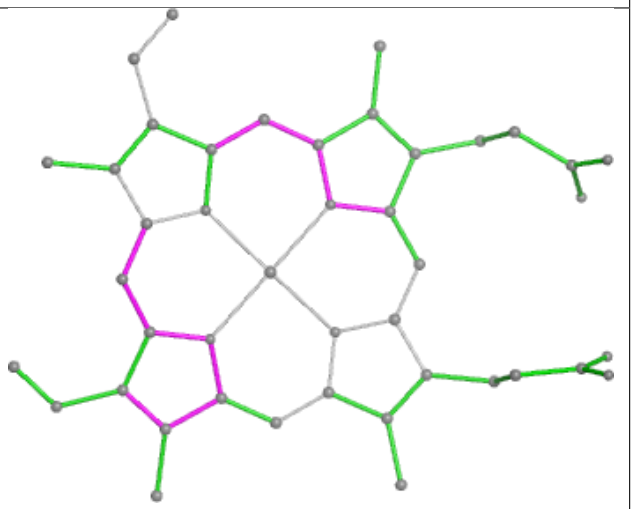
Ligand MQ9 N 601



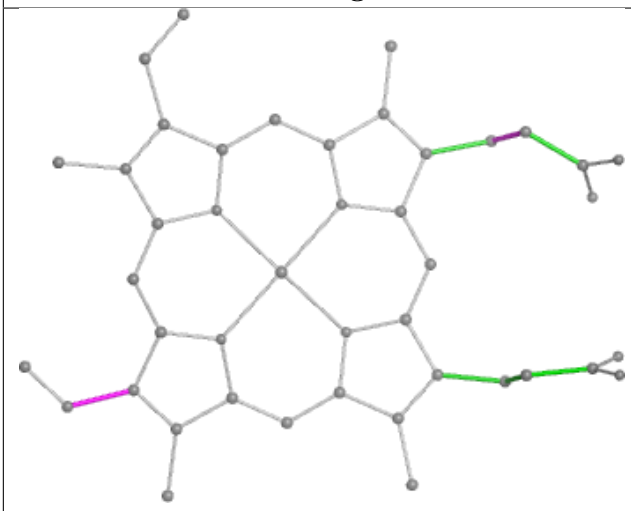
Ligand HEM H 601



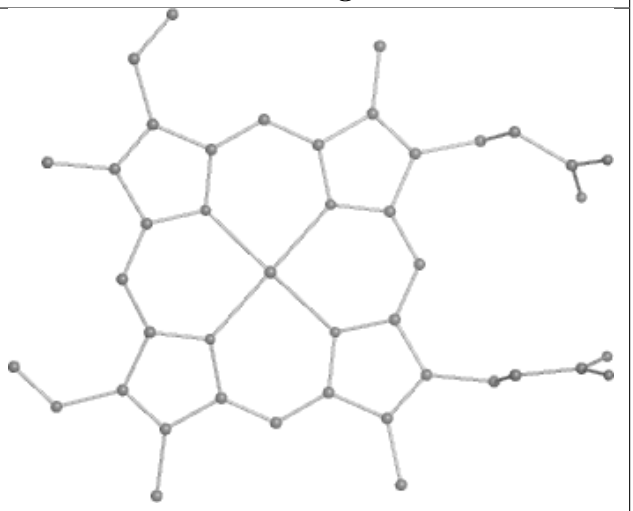
Bond lengths



Bond angles

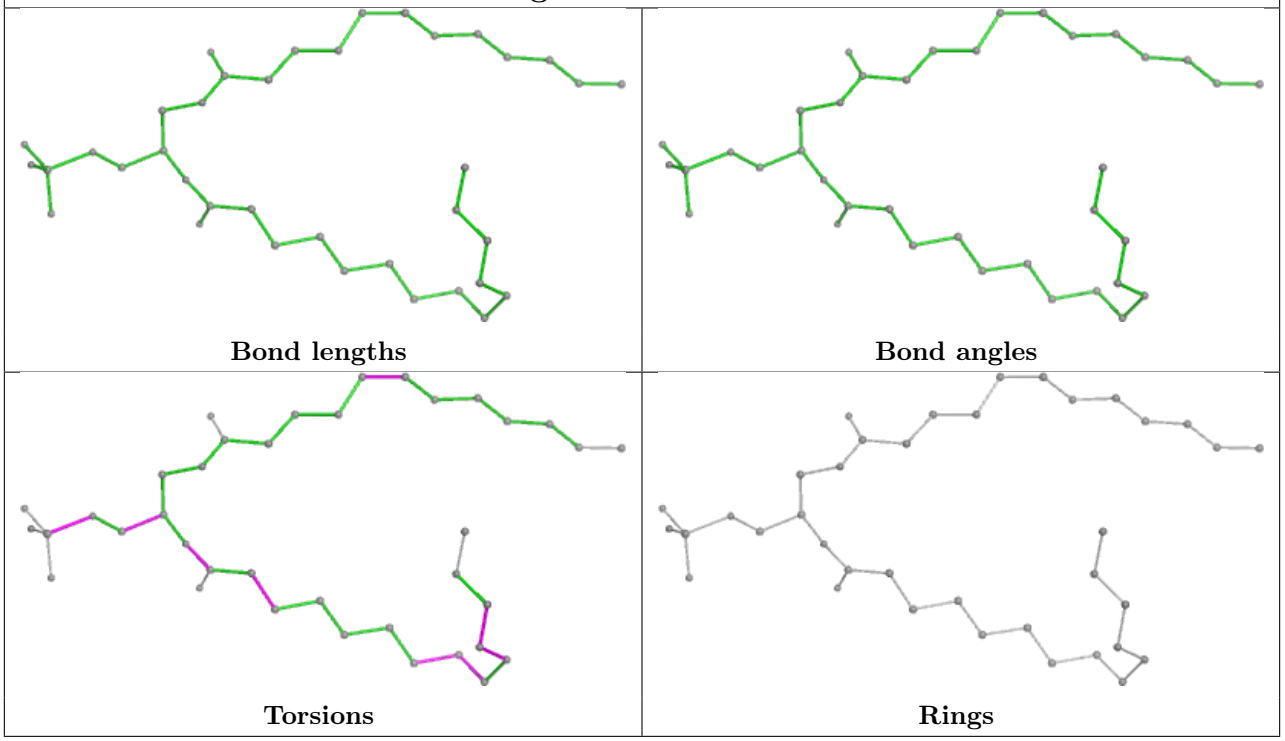


Torsions

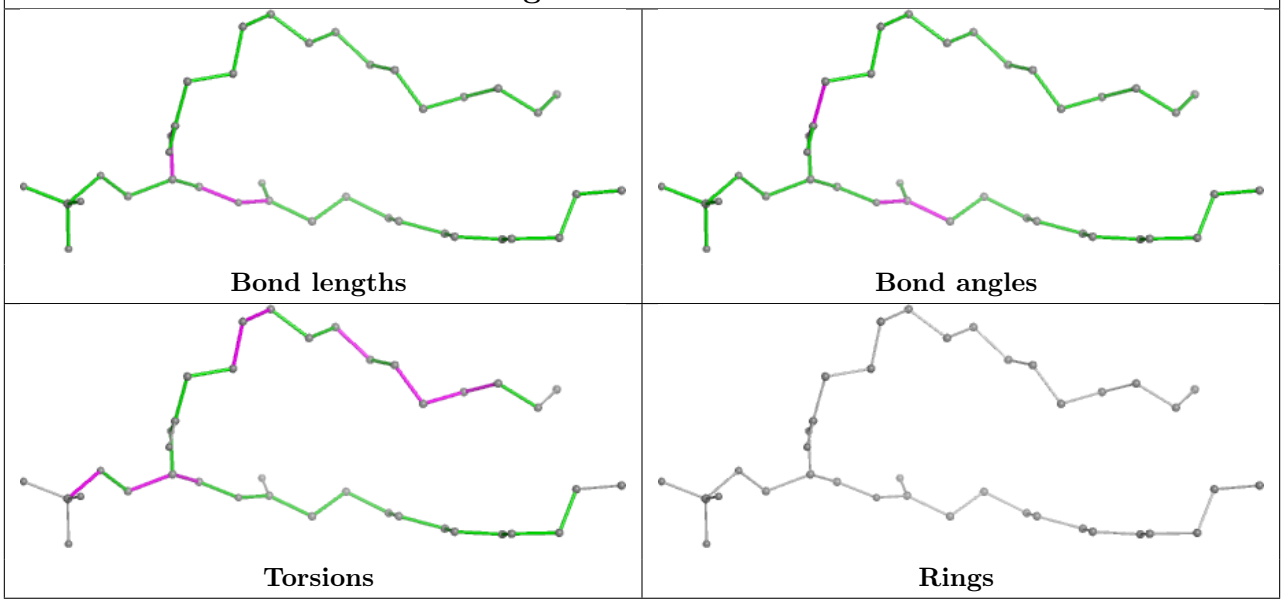


Rings

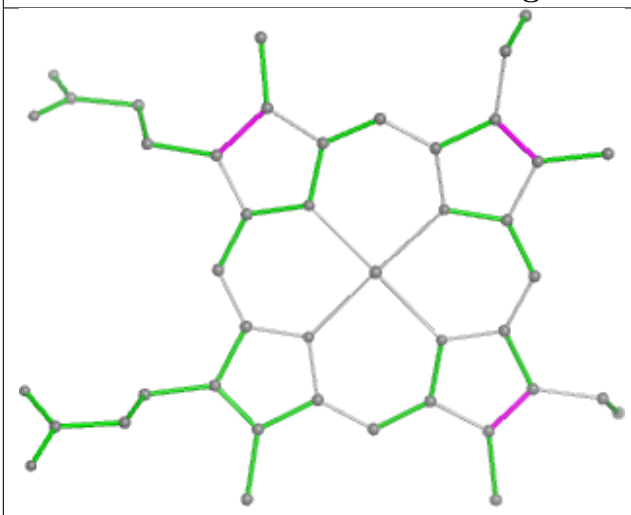
Ligand 7PH S 501



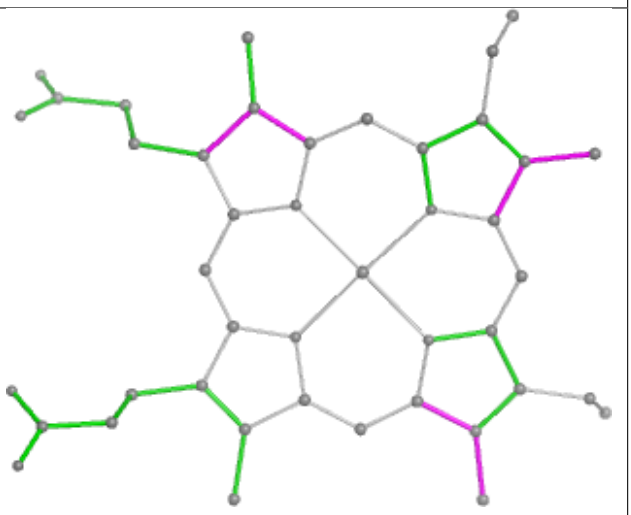
Ligand 7PH M 503



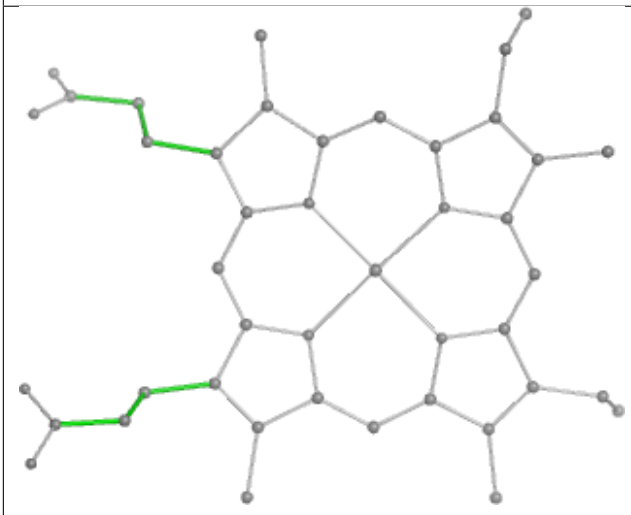
Ligand HEC O 302



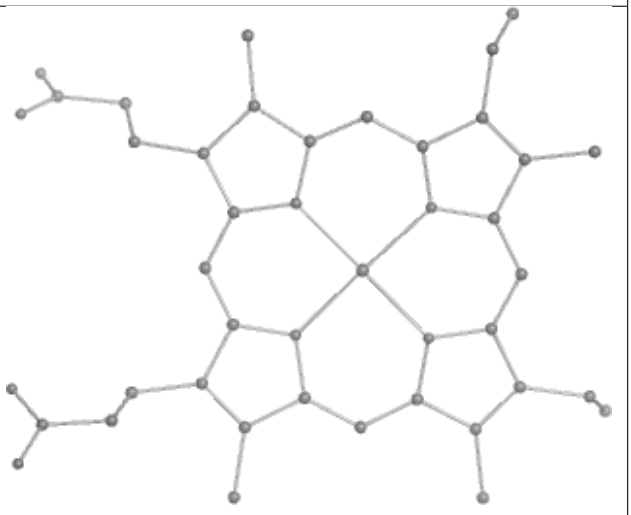
Bond lengths



Bond angles

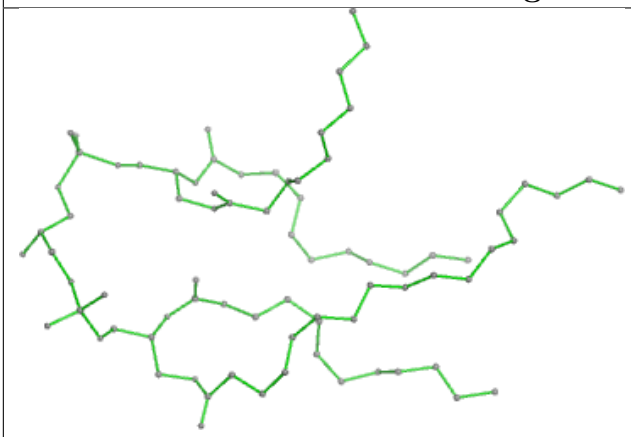


Torsions

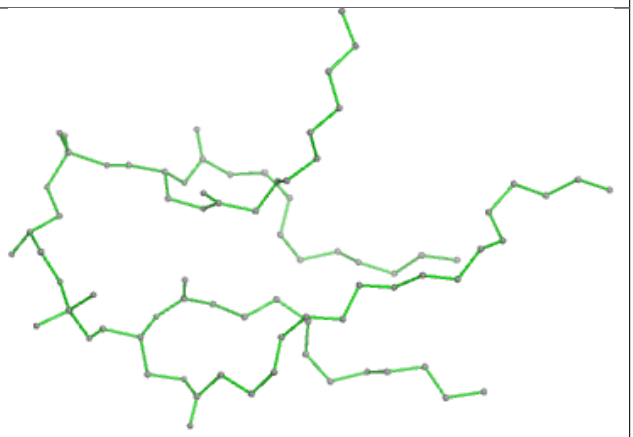


Rings

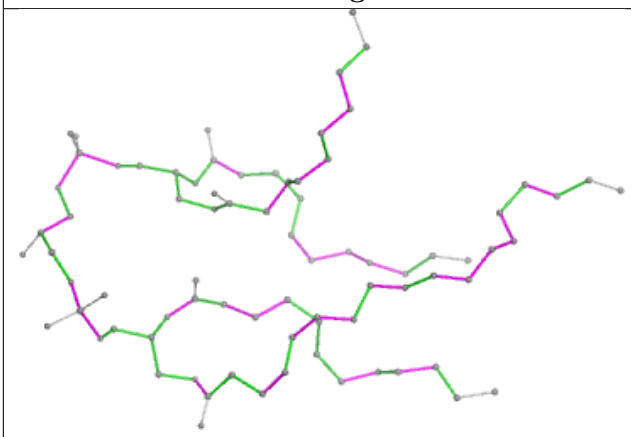
Ligand CDL O 305



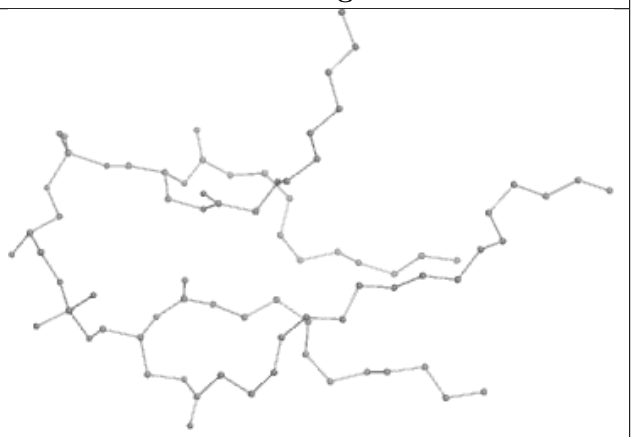
Bond lengths



Bond angles

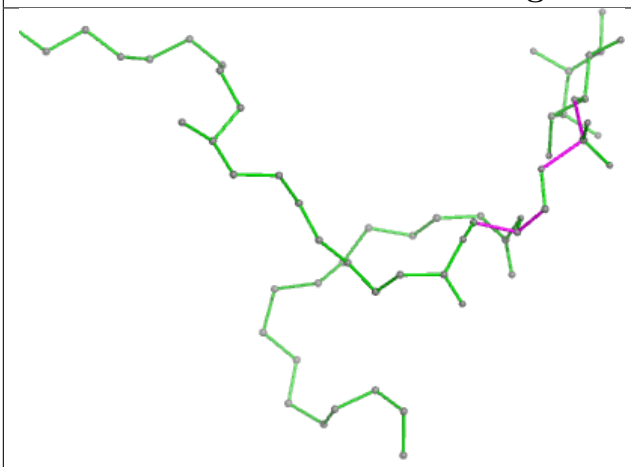


Torsions

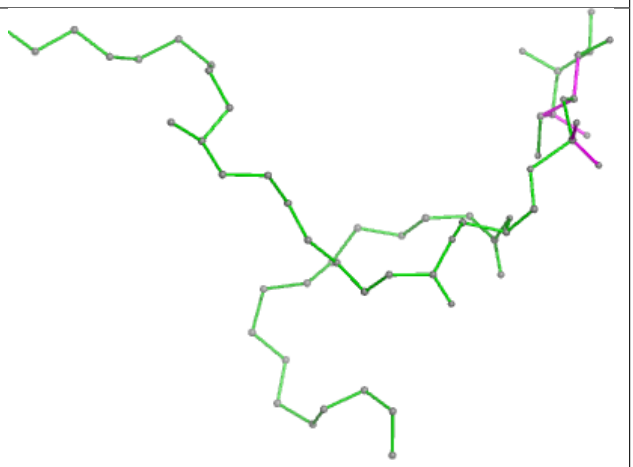


Rings

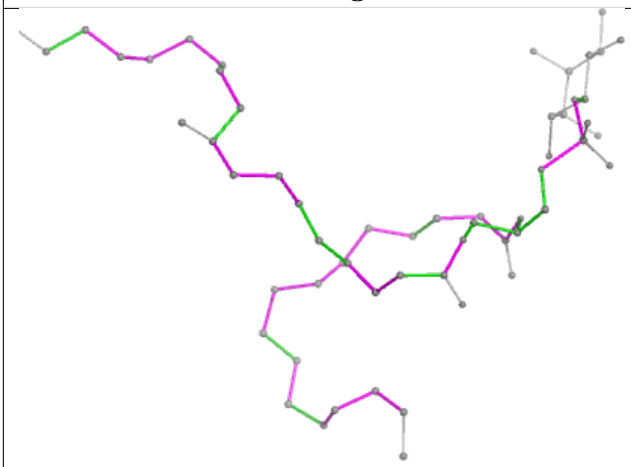
Ligand 9YF G 502



Bond lengths



Bond angles



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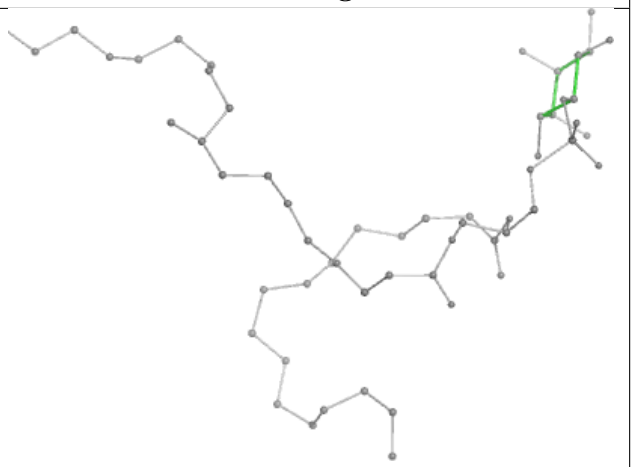
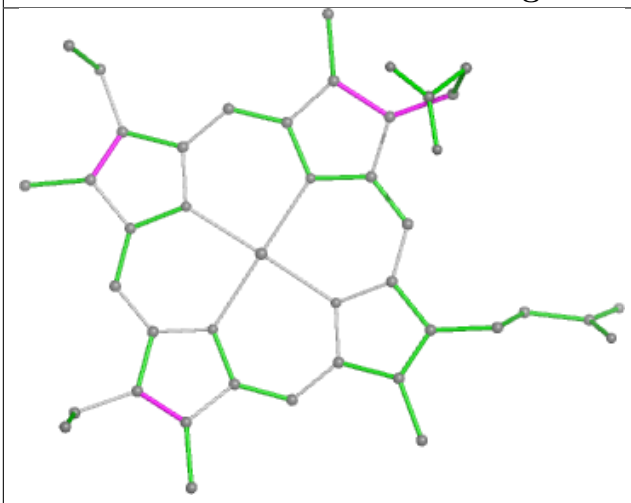
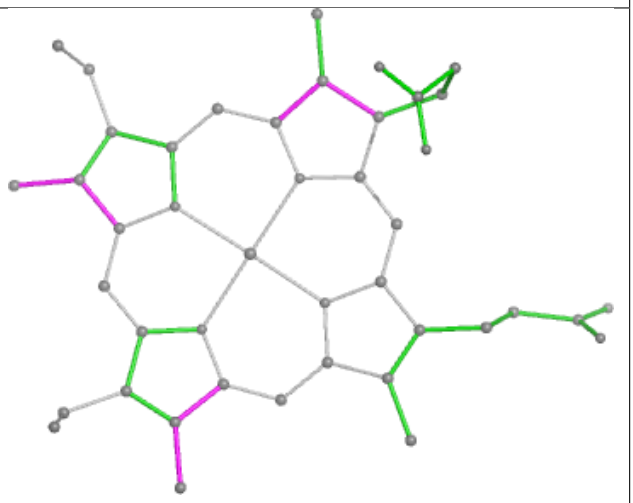


Rings

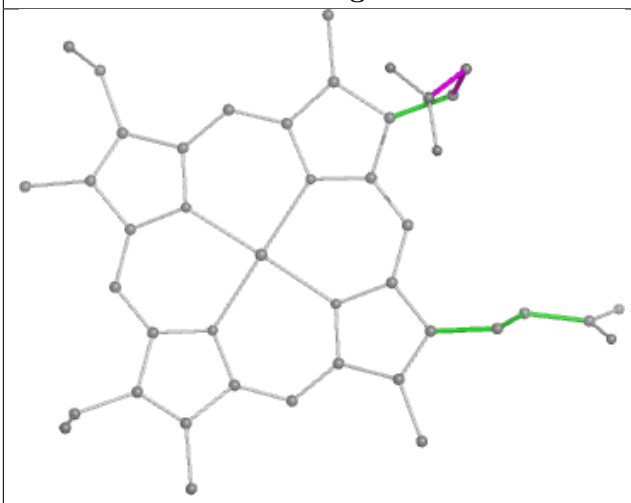
Ligand HEC O 303



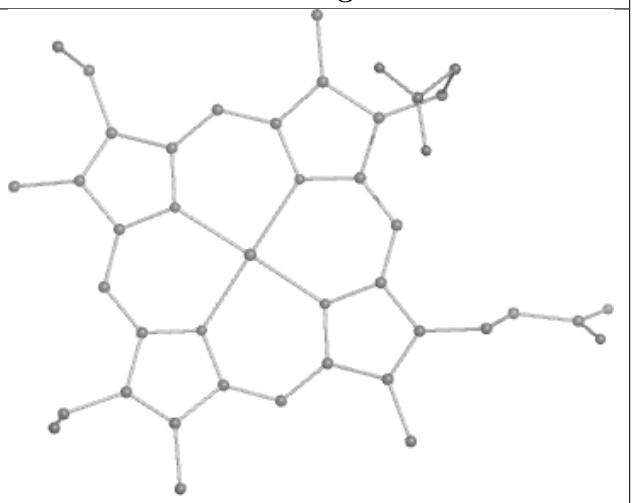
Bond lengths



Bond angles

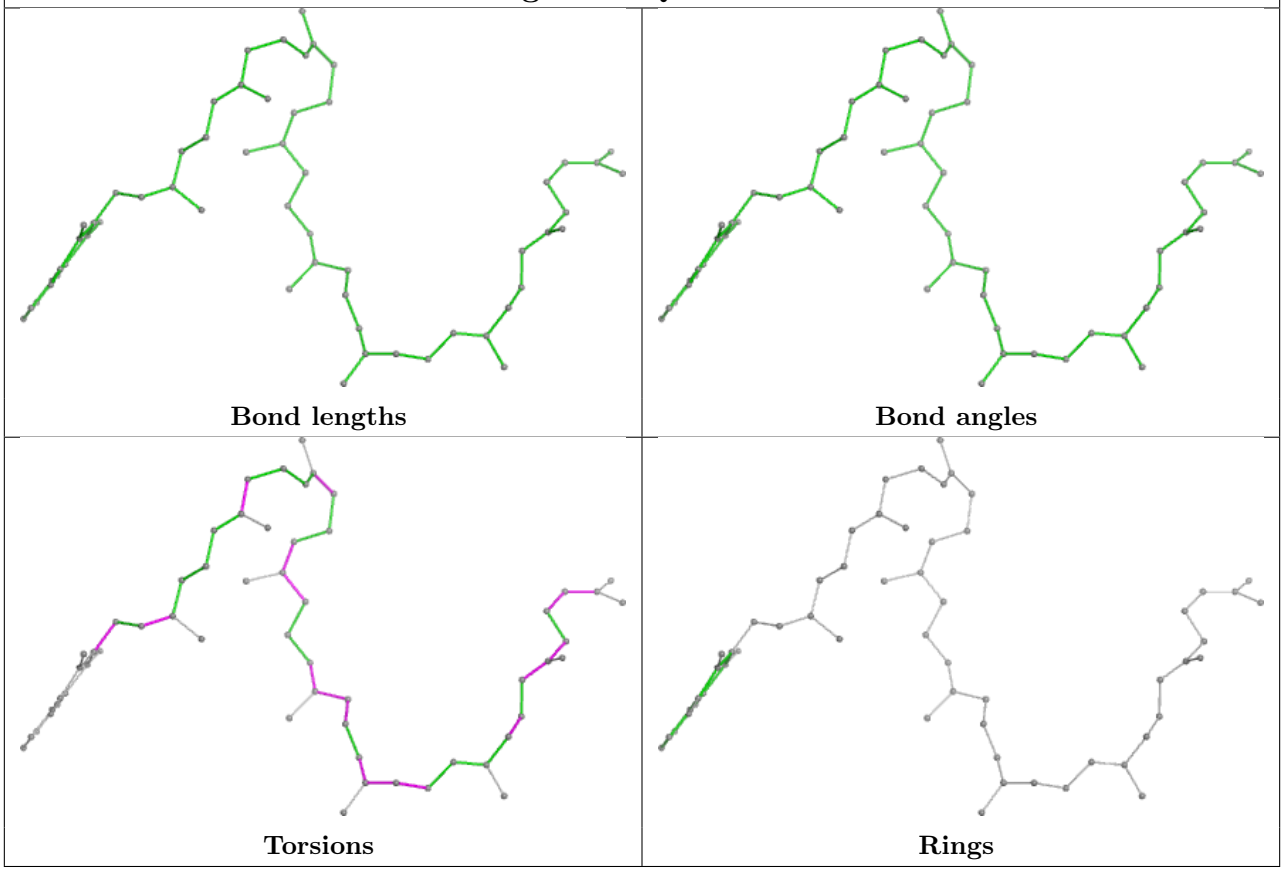


Torsions



Rings

Ligand MQ9 N 608



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.

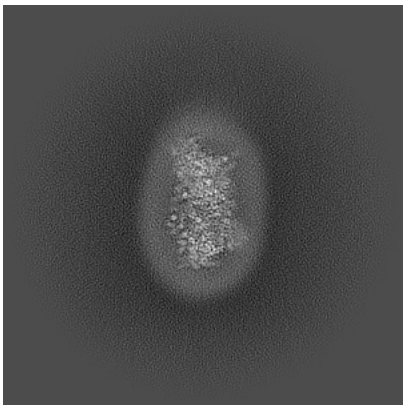
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50753. These allow visual inspection of the internal detail of the map and identification of artifacts.

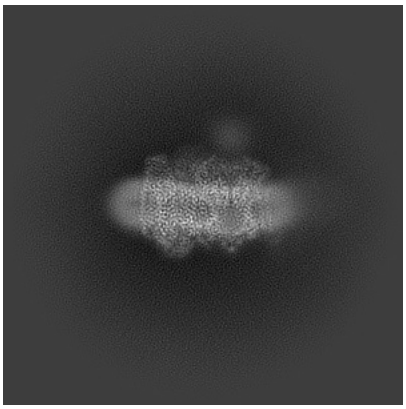
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

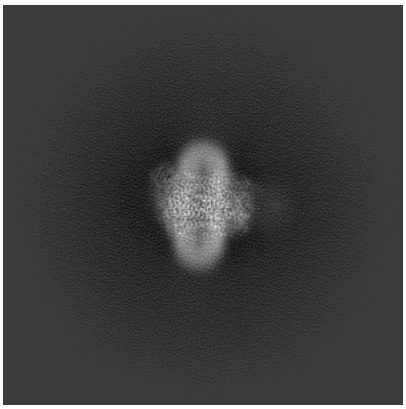
6.1.1 Primary map



X

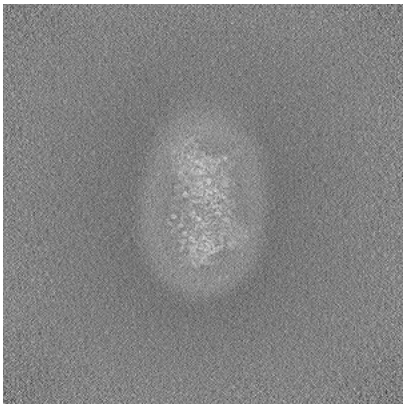


Y

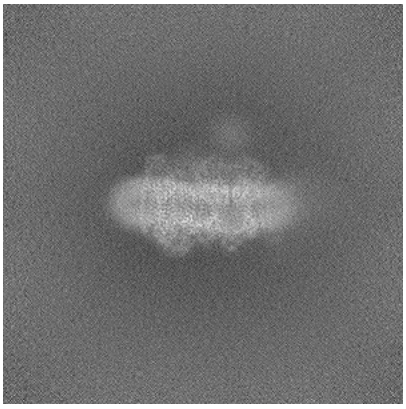


Z

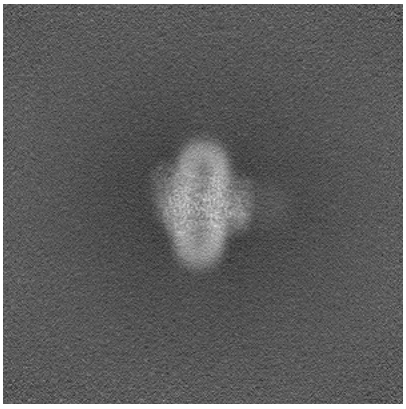
6.1.2 Raw map



X



Y

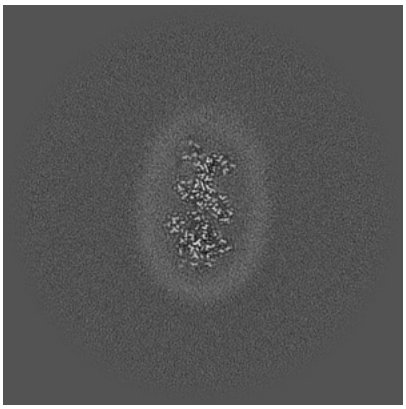


Z

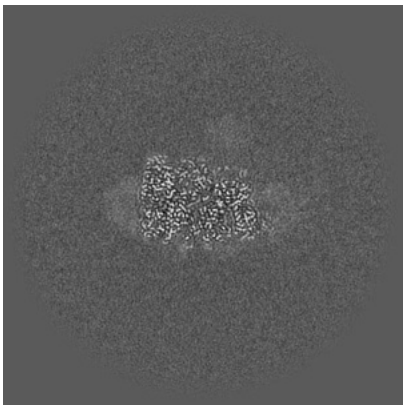
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

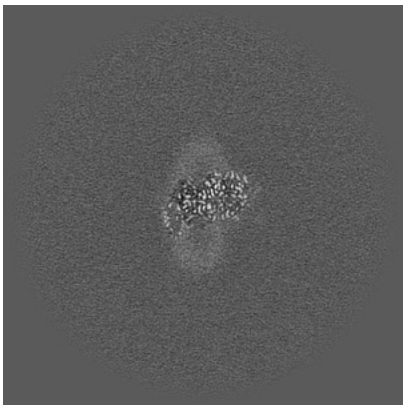
6.2.1 Primary map



X Index: 270

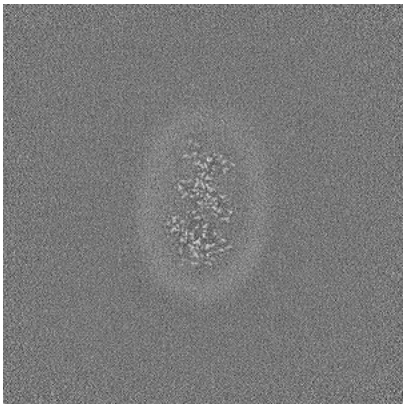


Y Index: 270

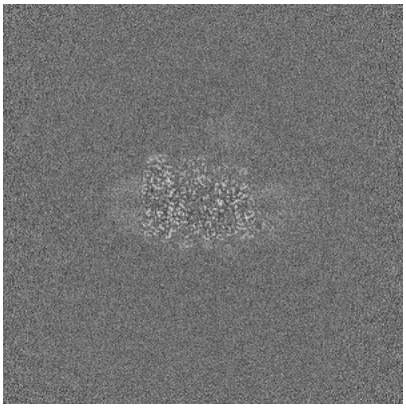


Z Index: 270

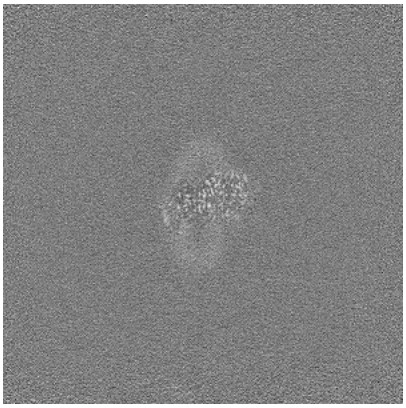
6.2.2 Raw map



X Index: 270



Y Index: 270

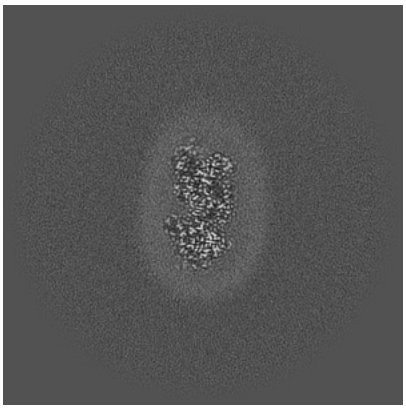


Z Index: 270

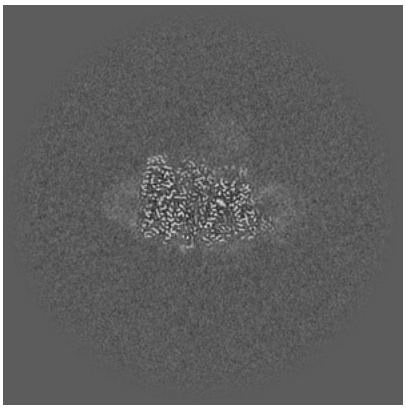
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

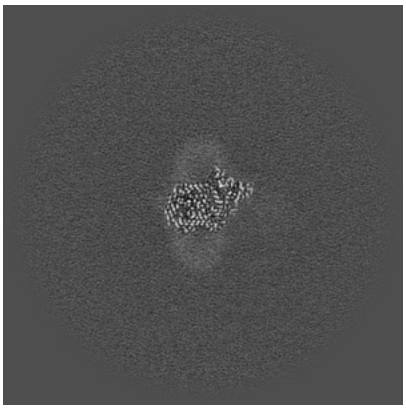
6.3.1 Primary map



X Index: 279

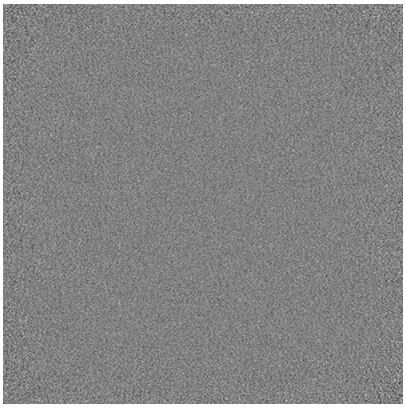


Y Index: 269

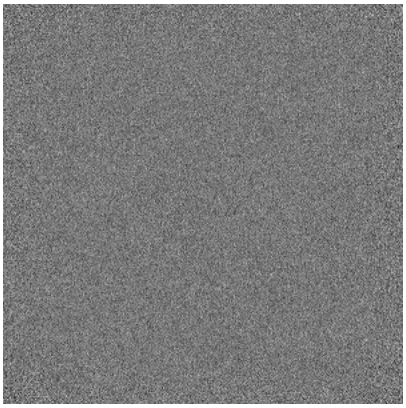


Z Index: 283

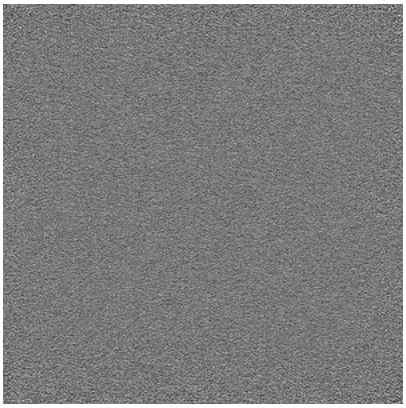
6.3.2 Raw map



X Index: 0



Y Index: 0

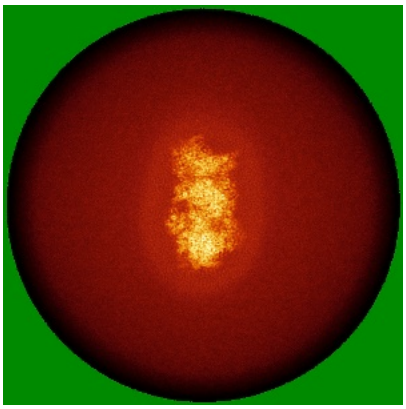


Z Index: 539

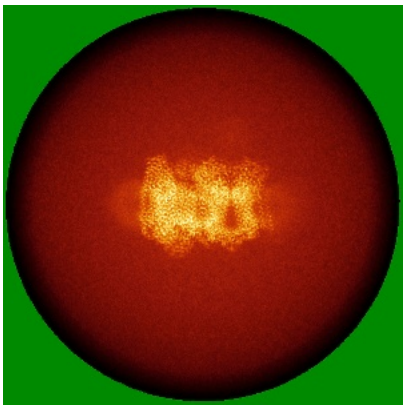
The images above show the largest variance slices of the map in three orthogonal directions.

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

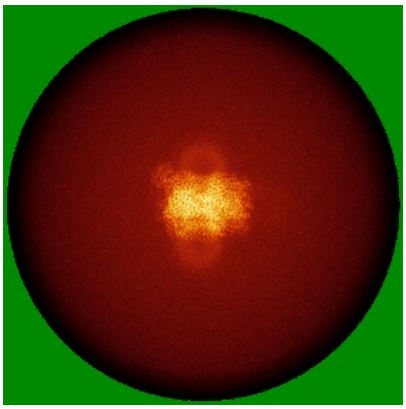
6.4.1 Primary map



X

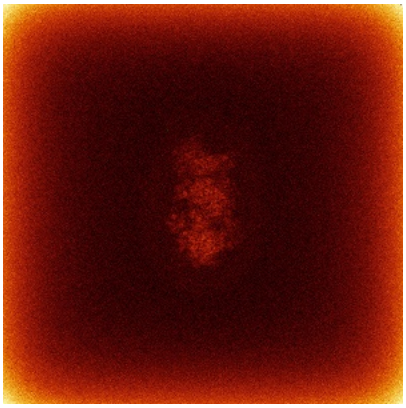


Y

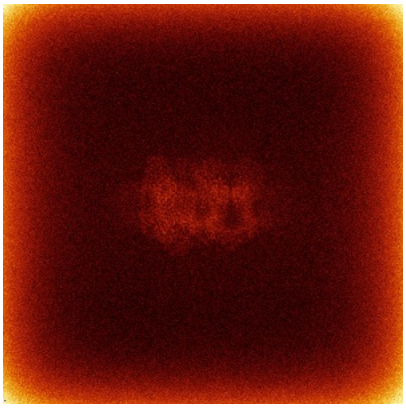


Z

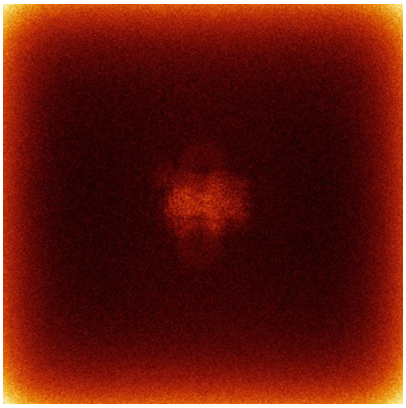
6.4.2 Raw map



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 0.204. 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.

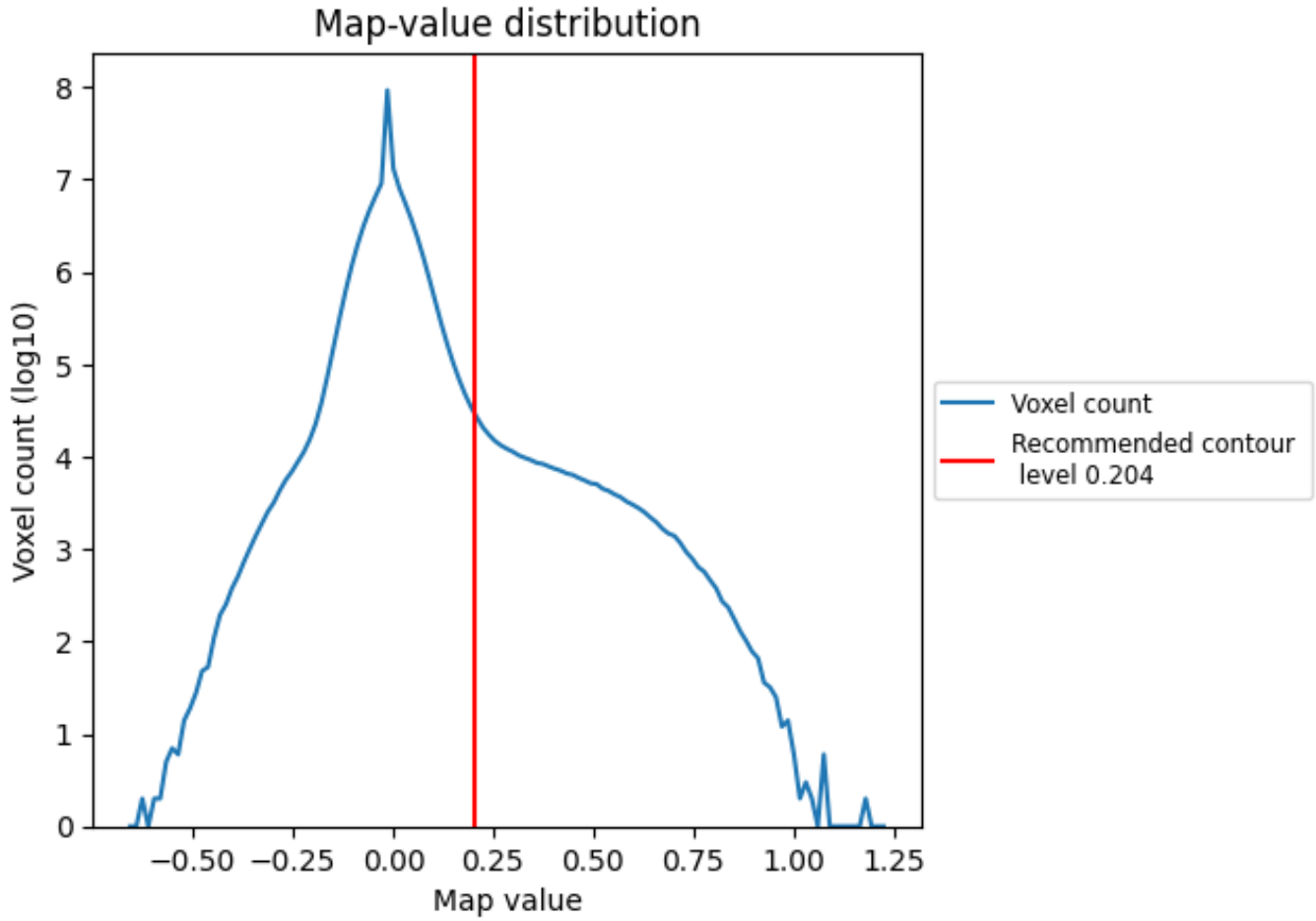
6.6 Mask visualisation (i)

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

7 Map analysis

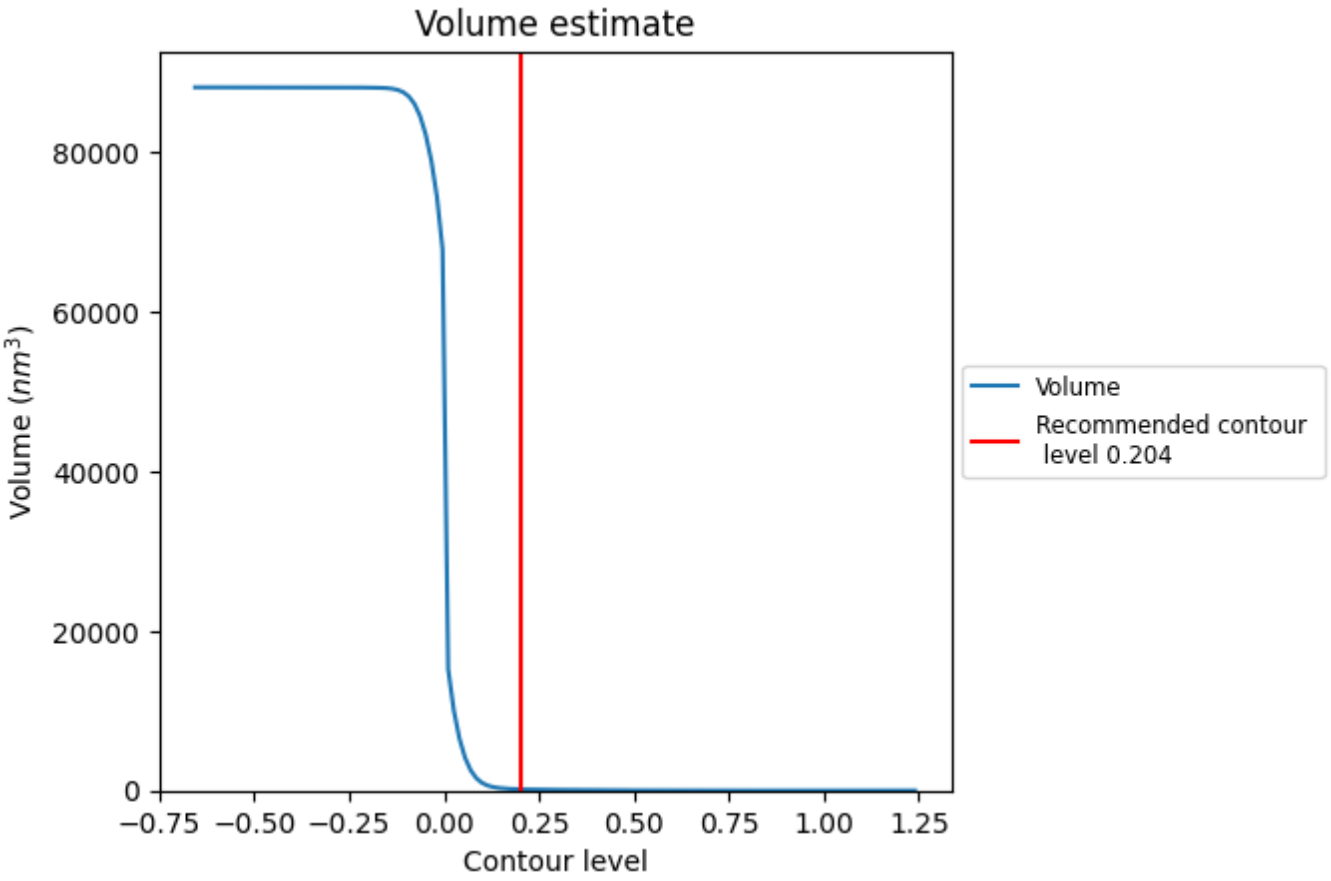
This section contains the results of statistical analysis of the map.

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.

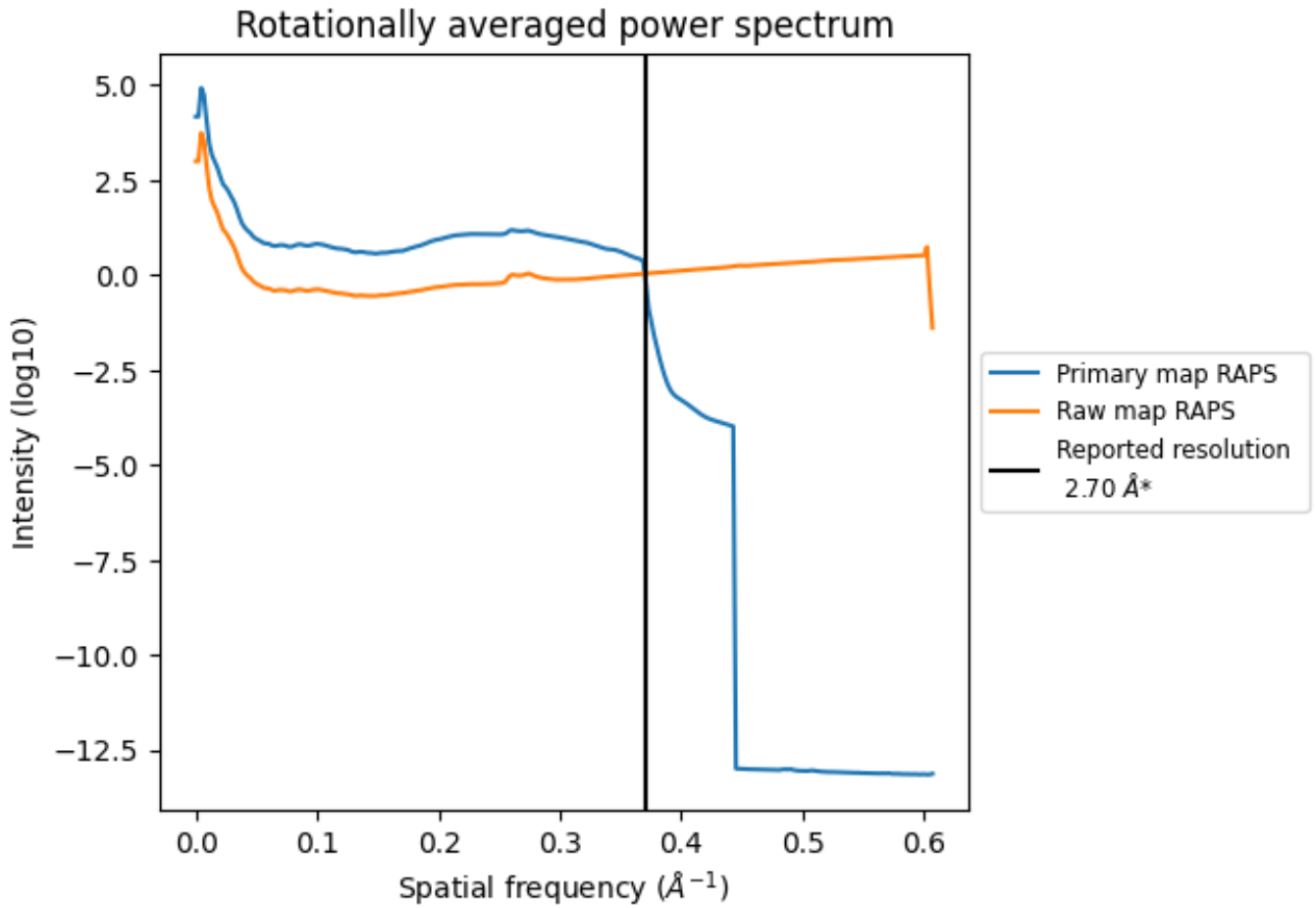
7.2 Volume estimate (i)



The volume at the recommended contour level is 154 nm^3; this corresponds to an approximate mass of 139 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)

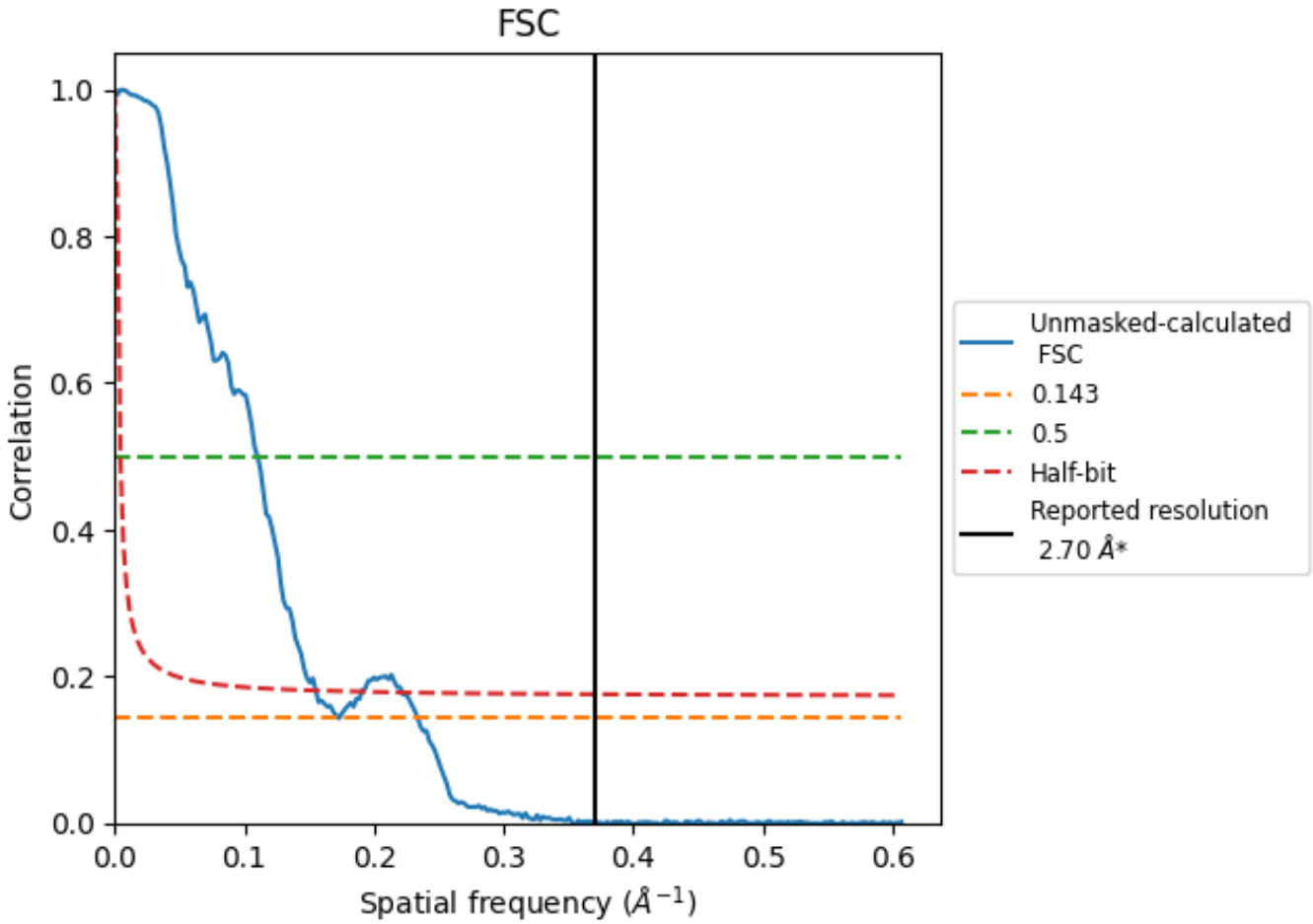


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

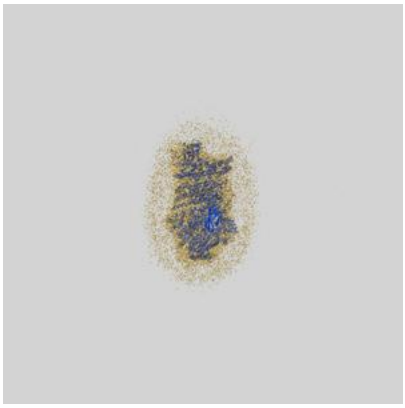
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.79	9.08	6.45

*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 5.79 differs from the reported value 2.7 by more than 10 %

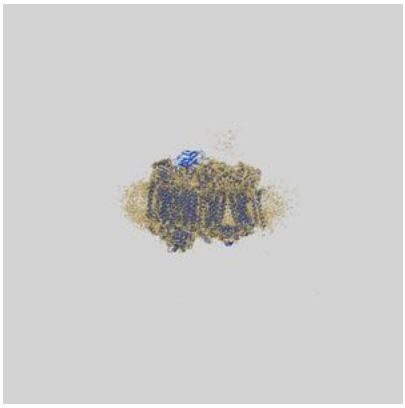
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50753 and PDB model 9FU0. Per-residue inclusion information can be found in section 3 on page 19.

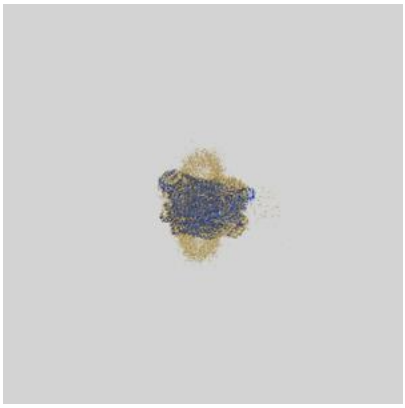
9.1 Map-model overlay



X



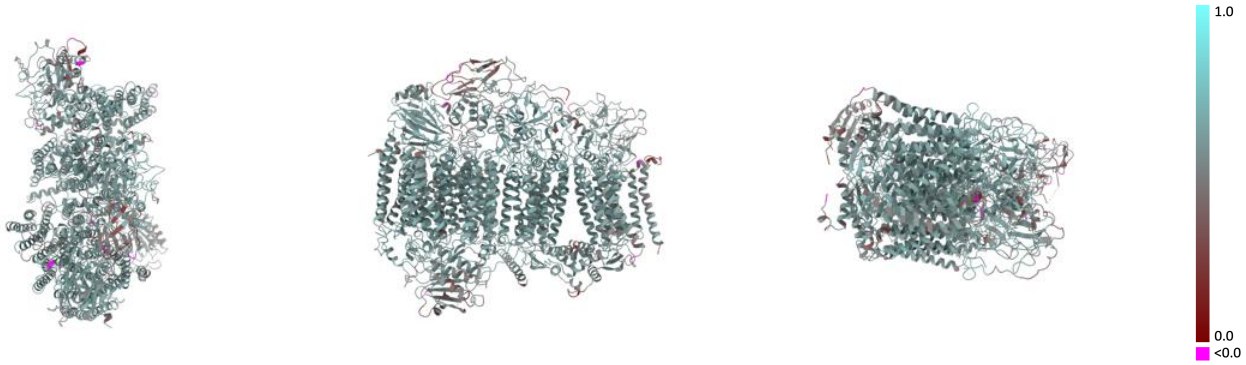
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.204 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.

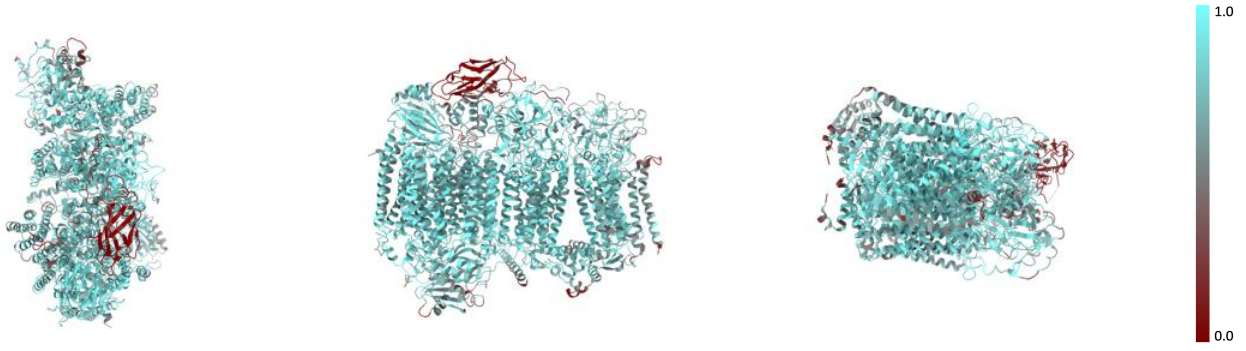
9.2 Q-score mapped to coordinate model (i)



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.

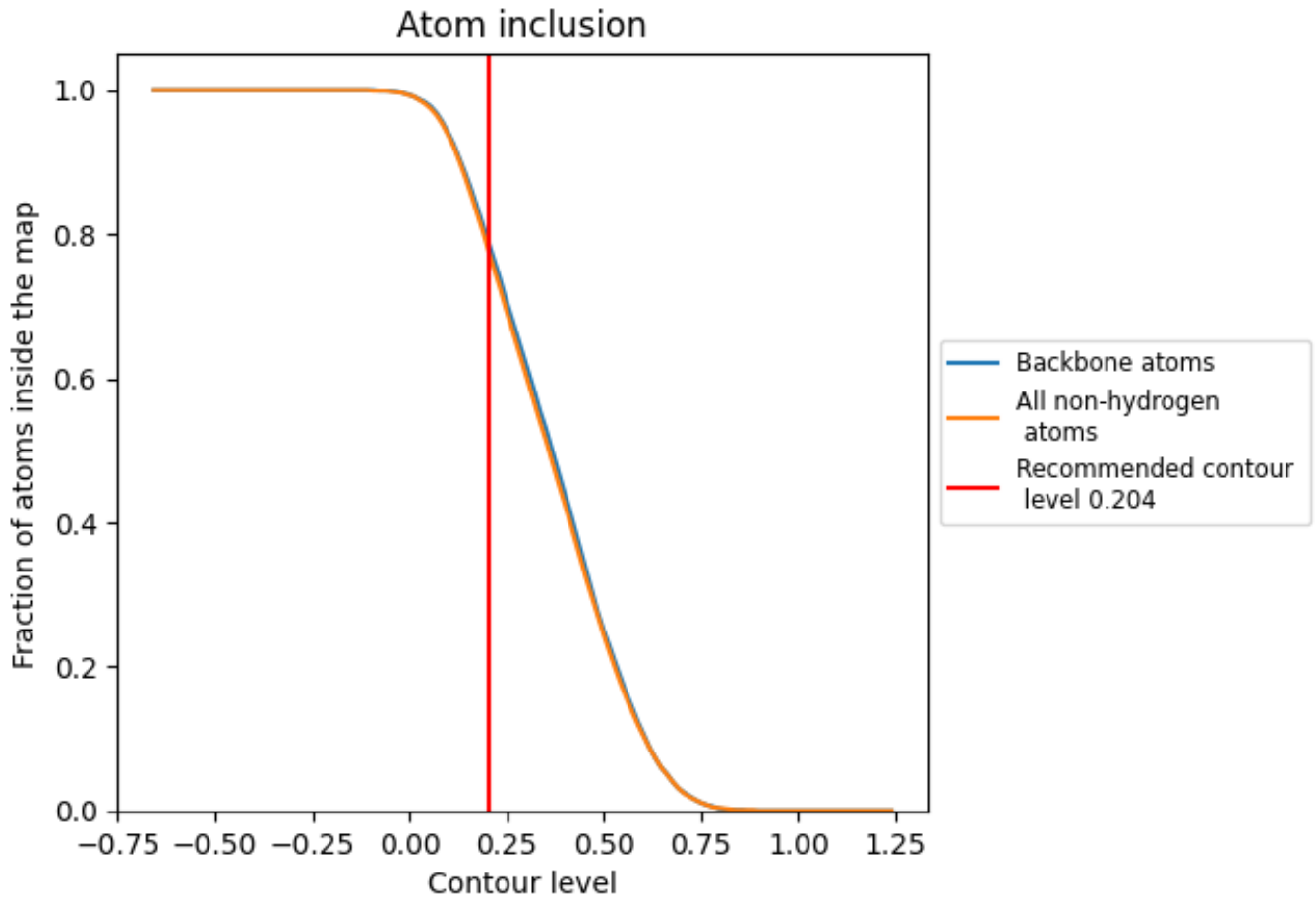
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.204).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7760	0.5730
G	0.7270	0.5410
H	0.7760	0.5700
M	0.8130	0.5820
N	0.8610	0.6080
O	0.7620	0.5800
P	0.7690	0.5750
Q	0.7730	0.5660
R	0.8930	0.6130
S	0.8190	0.5940
T	0.8590	0.6060
U	0.7210	0.5300
V	0.7060	0.5250
W	0.1560	0.4220
Y	0.6140	0.4480
c	0.4860	0.3980