wwPDB EM Validation Summary Report (i)

Aug 25, 2026 – 03:40 am BST

PDB ID	:	9FTZ / pdb_00009ftz
EMDB ID	:	EMD-50752
Title	:	CIII2/CIV respiratory supercomplex from Mycobacterium smegmatis with lansoprazole sulfide
Authors	:	Kovalova, T.; Krol, S.; Gamiz-Hernandez, A.; Sjostrand, D.; Kaila, V.; Brzezinski, P.; Hogbom, M.
Deposited on	:	2024-06-25
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

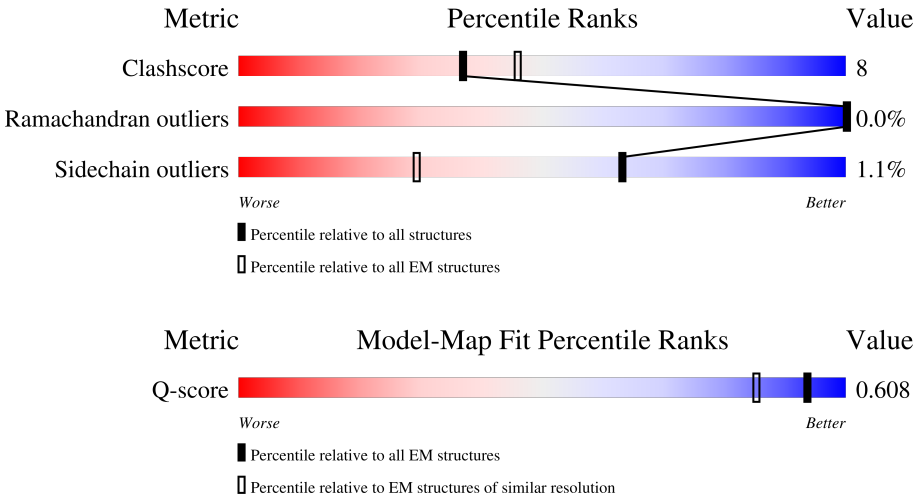
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	69% 9% 20%
2	G	408	86% 7% 7%
2	M	408	85% 8% 7%
3	H	556	63% 14% 22%

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Mol	Chain	Length	Quality of chain
3	N	556	79% 16%
4	P	100	64% 9% 27%
5	S	203	81% 10% 9%
6	T	139	88% 11%
7	R	575	79% 16%
8	Q	341	74% 14% 12%
9	U	79	76% 8% 16%
10	V	157	73% 17% 9%
11	W	186	20% 68% 12% 20%
12	Y	236	9% 89%
12	c	236	10% 89%

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	HEC	O	303	X	-	-	-
15	HEC	O	304	X	-	-	-

2 Entry composition (i)

There are 31 unique types of molecules in this entry. The entry contains 30674 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		

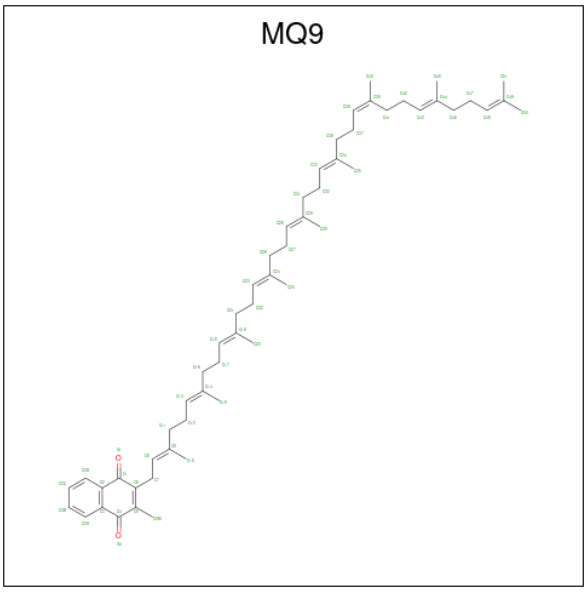
- Molecule 11 is a protein called LpqE protein.

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].

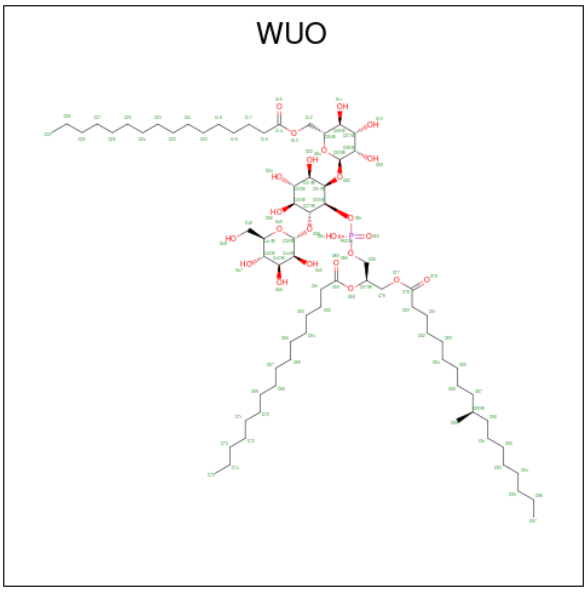
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	25	Total	C	N	O	S	0	0
			168	103	26	38	1		
12	c	25	Total	C	N	O	S	0	0
			168	103	26	38	1		

- Molecule 13 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



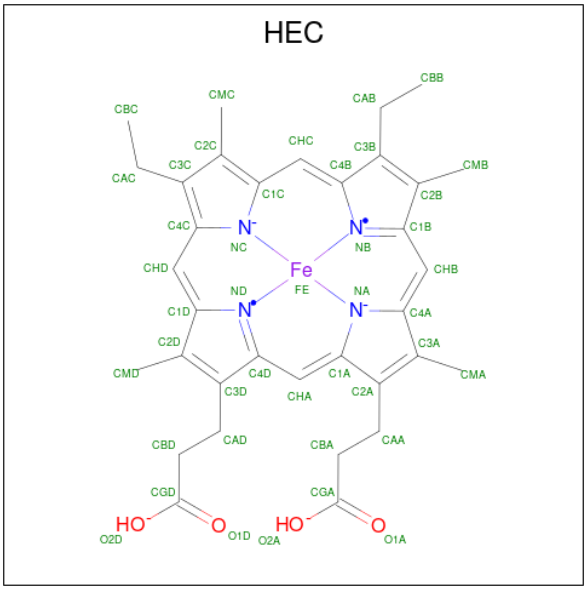
Mol	Chain	Residues	Atoms	AltConf
13	O	1	Total C O 58 56 2	0
13	O	1	Total C O 58 56 2	0
13	N	1	Total C O 58 56 2	0
13	H	1	Total C O 58 56 2	0
13	H	1	Total C O 58 56 2	0

- Molecule 14 is acyl-phosphatidyl-myo-inositol dimannoside (AcPIM2) (CCD ID: WUO) (formula: $C_{72}H_{135}O_{24}P$).



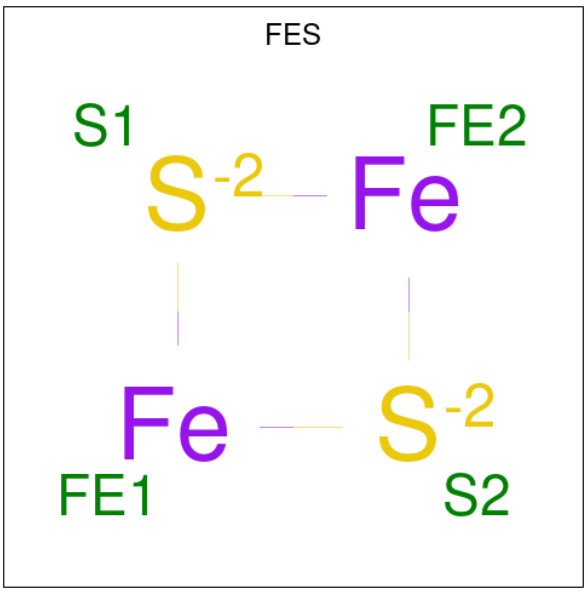
Mol	Chain	Residues	Atoms				AltConf
14	O	1	Total 97	C 72	O 24	P 1	0
14	P	1	Total 97	C 72	O 24	P 1	0

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



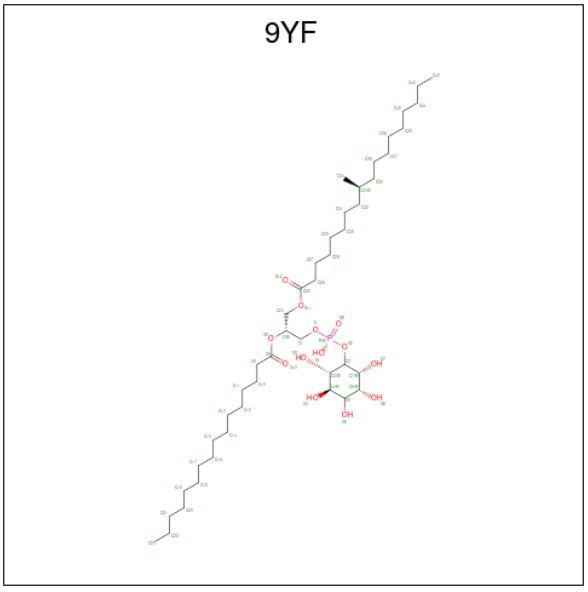
Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total 43	C 34	Fe 1	N 4	O 4	0
15	O	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



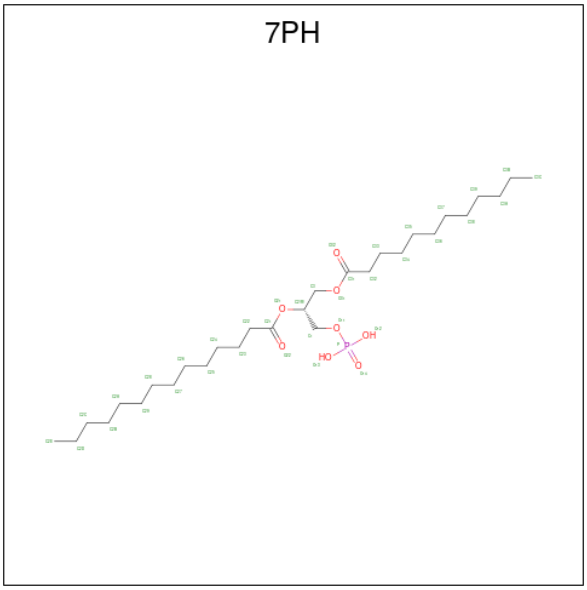
Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	Fe	S	0
			4	2	2	
16	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 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 (CCD ID: 9YF) (formula: $C_{44}H_{85}O_{13}P$).



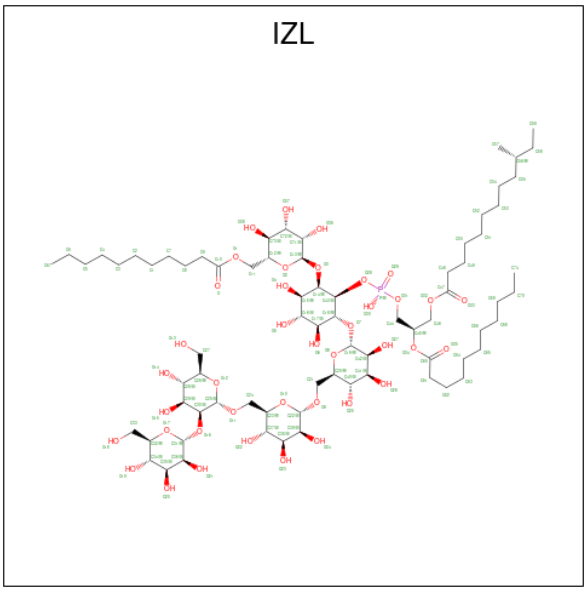
Mol	Chain	Residues	Atoms				AltConf
17	M	1	Total	C	O	P	0
			58	44	13	1	
17	W	1	Total	C	O	P	0
			58	44	13	1	
17	G	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 18 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: $C_{29}H_{57}O_8P$).



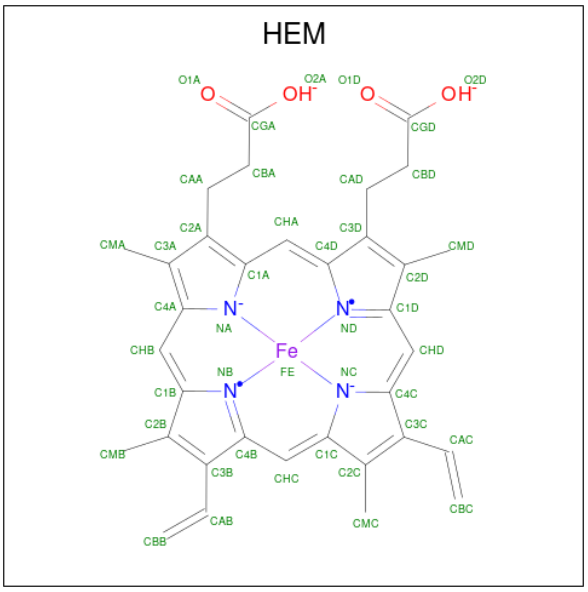
Mol	Chain	Residues	Atoms				AltConf
18	M	1	Total	C	O	P	0
			38	29	8	1	
18	S	1	Total	C	O	P	0
			38	29	8	1	
18	G	1	Total	C	O	P	0
			38	29	8	1	
18	G	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 19 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 (CCD ID: IZL) (formula: $C_{74}H_{133}O_{39}P$).



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

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



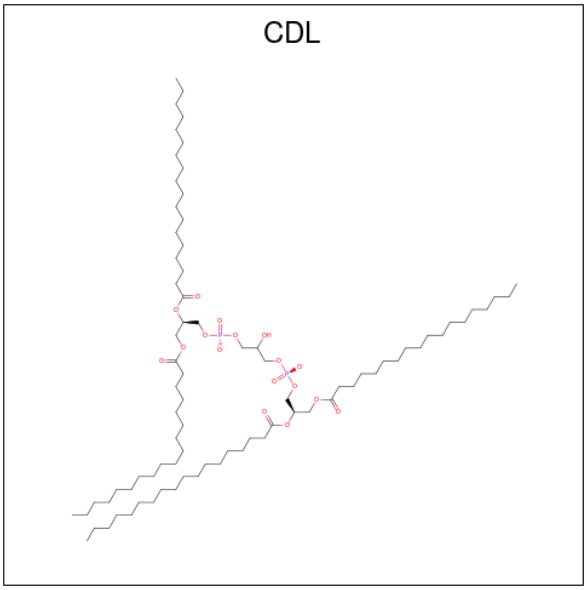
Mol	Chain	Residues	Atoms					AltConf
20	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 21 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



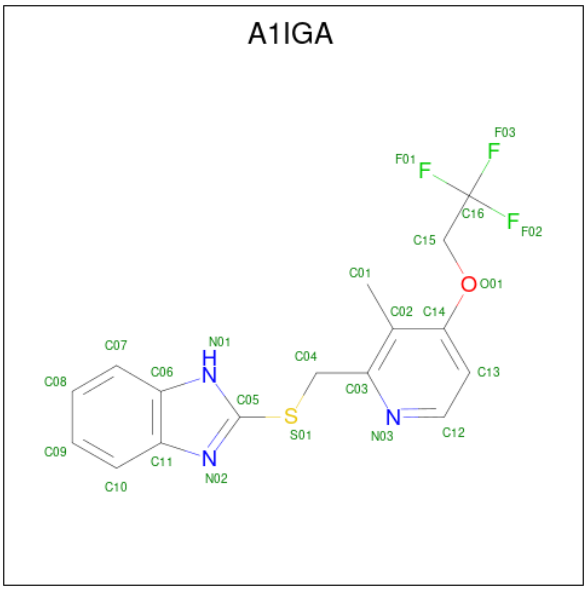
Mol	Chain	Residues	Atoms				AltConf
21	N	1	Total	C	O	P	0
			77	58	17	2	
21	N	1	Total	C	O	P	0
			79	60	17	2	
21	N	1	Total	C	O	P	0
			79	60	17	2	
21	P	1	Total	C	O	P	0
			77	58	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	H	1	Total	C	O	P	0
			74	55	17	2	
21	H	1	Total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

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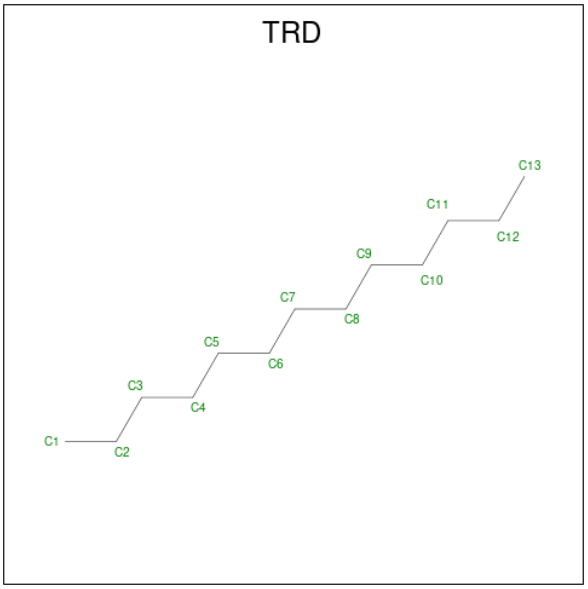
Mol	Chain	Residues	Atoms				AltConf
21	H	1	Total	C	O	P	0
			77	58	17	2	

- Molecule 22 is Lansoprazole sulfide (CCD ID: A1IGA) (formula: $C_{16}H_{14}F_3N_3OS$) (labeled as "Ligand of Interest" by depositor).



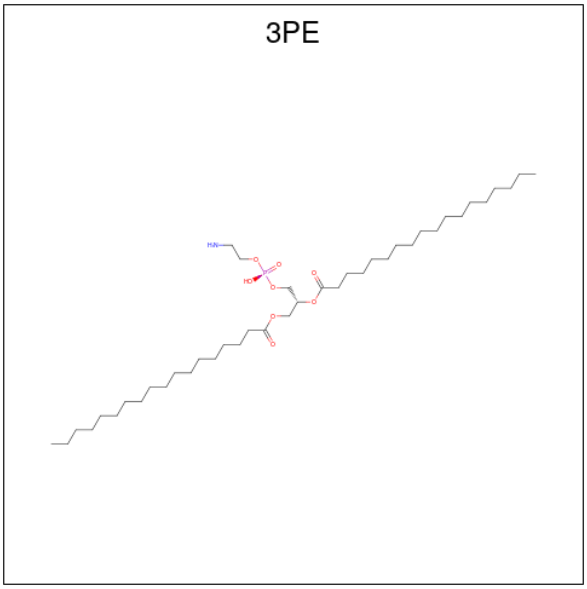
Mol	Chain	Residues	Atoms						AltConf
22	N	1	Total	C	F	N	O	S	0
			24	16	3	3	1	1	

- Molecule 23 is TRIDECANE (CCD ID: TRD) (formula: $C_{13}H_{28}$).



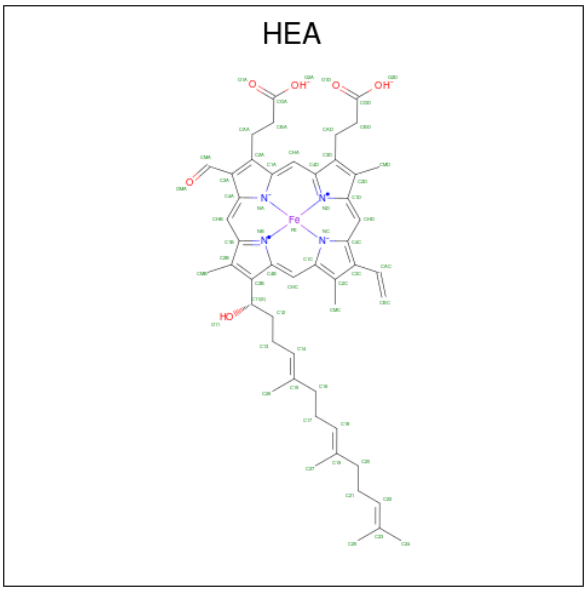
Mol	Chain	Residues	Atoms	AltConf
23	S	1	Total C 13 13	0
23	T	1	Total C 13 13	0
23	R	1	Total C 13 13	0
23	R	1	Total C 13 13	0
23	Q	1	Total C 13 13	0

- Molecule 24 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



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

- Molecule 25 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

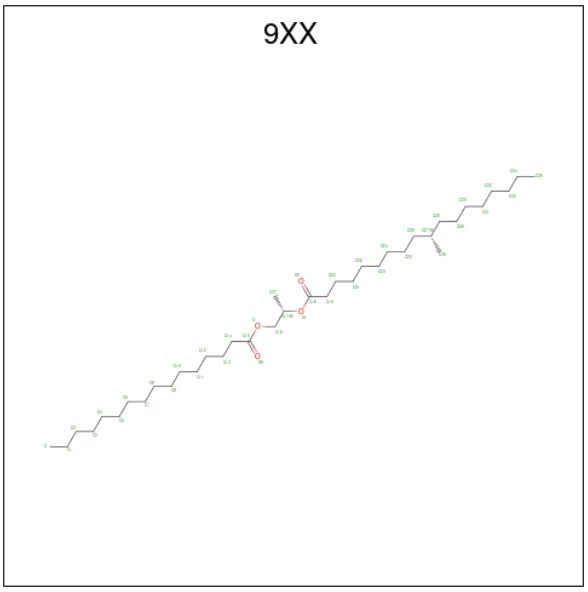
- Molecule 26 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

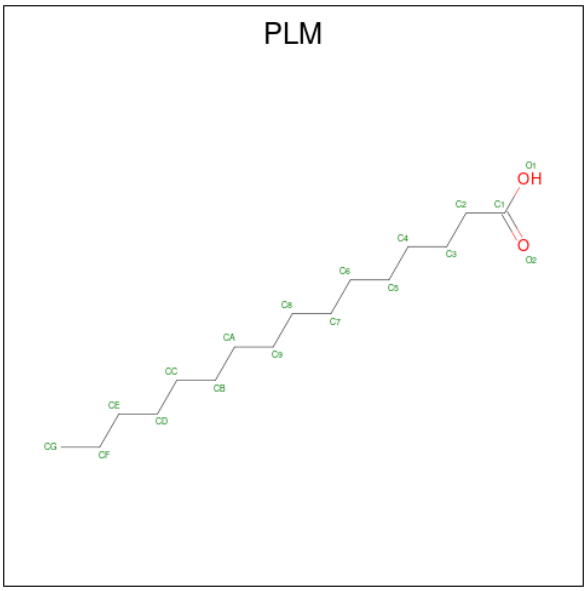


Mol	Chain	Residues	Atoms	AltConf
28	R	1	Total C O 42 38 4	0
28	Y	1	Total C O 32 28 4	0
28	c	1	Total C O 32 28 4	0

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 30 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



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

- Molecule 31 is water.

Mol	Chain	Residues	Atoms	AltConf
31	O	50	Total O 50 50	0
31	M	51	Total O 51 51	0
31	N	78	Total O 78 78	0
31	P	8	Total O 8 8	0
31	S	10	Total O 10 10	0
31	T	9	Total O 9 9	0
31	R	67	Total O 67 67	0
31	Q	44	Total O 44 44	0
31	V	3	Total O 3 3	0

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Mol	Chain	Residues	Atoms	AltConf
31	W	2	Total O 2 2	0
31	Y	2	Total O 2 2	0
31	H	13	Total O 13 13	0
31	G	11	Total O 11 11	0

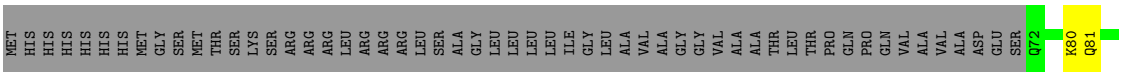
3 Residue-property plots (i)

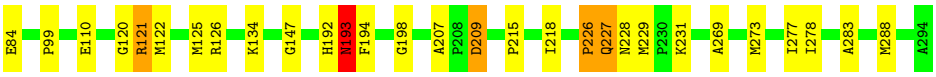
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

Chain O:



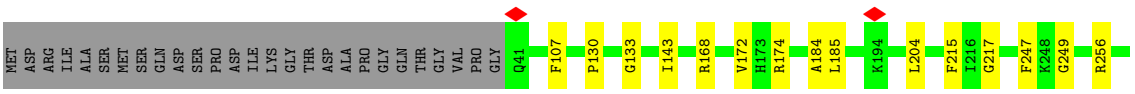


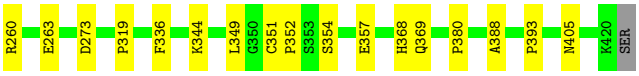


• Molecule 2: Cytochrome bc1 complex cytochrome c subunit

Chain M:



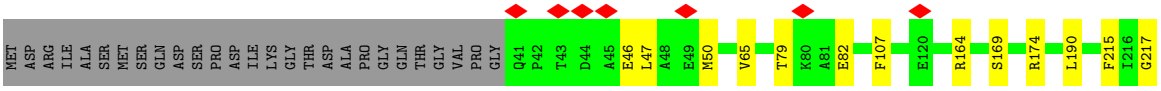


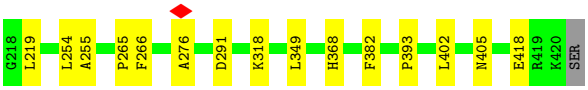


• Molecule 2: Cytochrome bc1 complex cytochrome c subunit

Chain G:



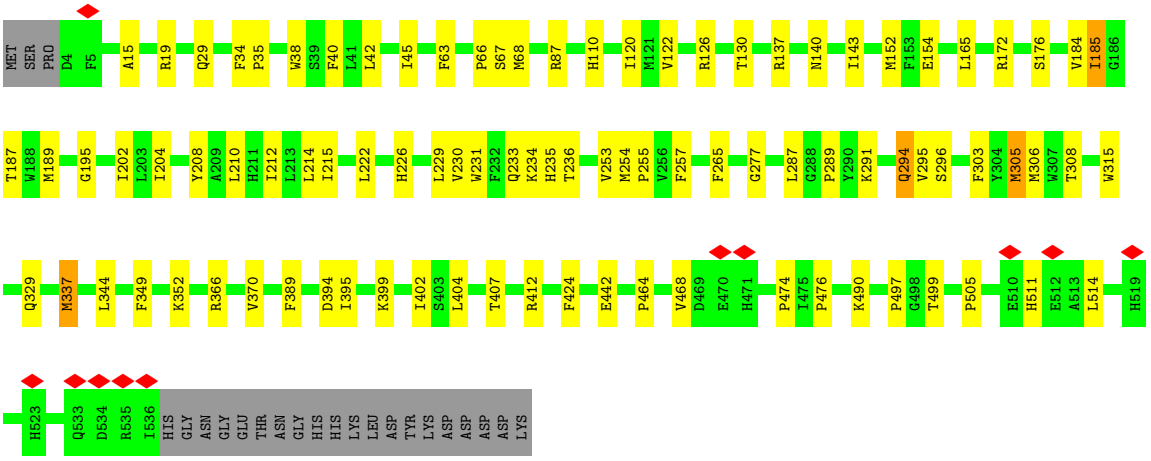




• Molecule 3: Cytochrome bc1 complex cytochrome b subunit

Chain N:

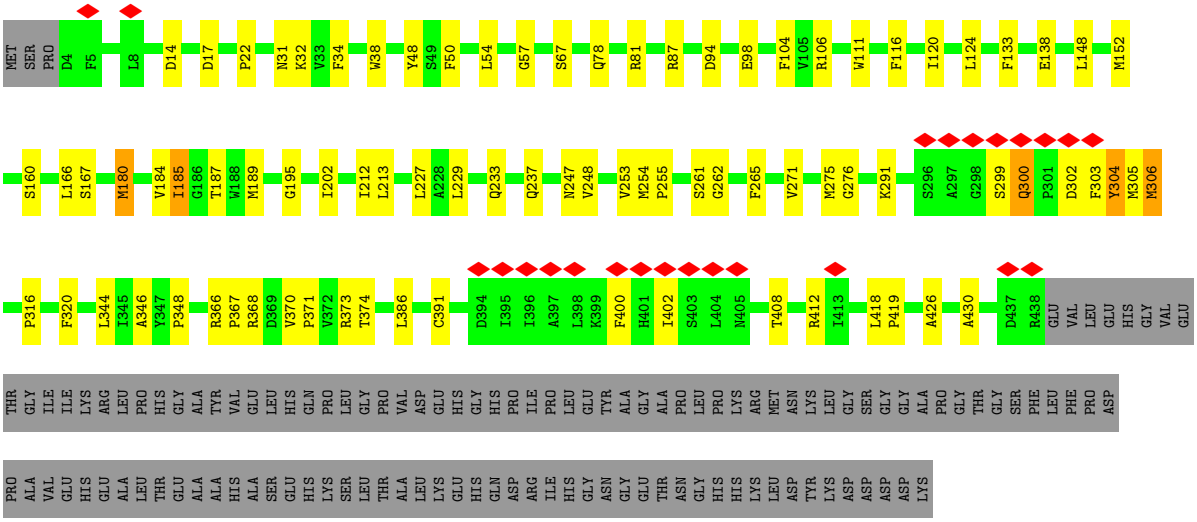




• Molecule 3: Cytochrome bc1 complex cytochrome b subunit

Chain H:

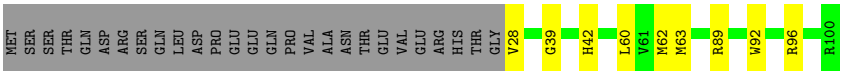




• Molecule 4: Transmembrane protein

Chain P:

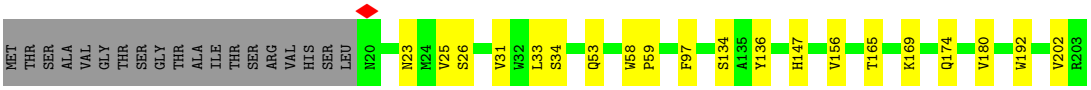




• Molecule 5: Probable cytochrome c oxidase subunit 3

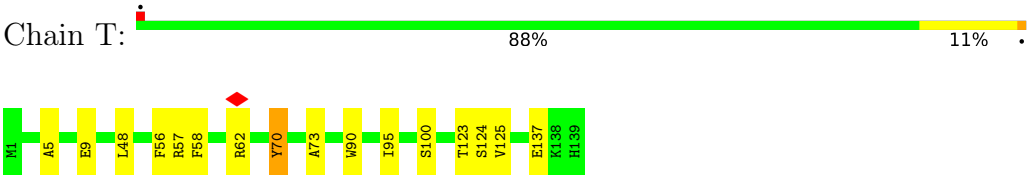
Chain S:





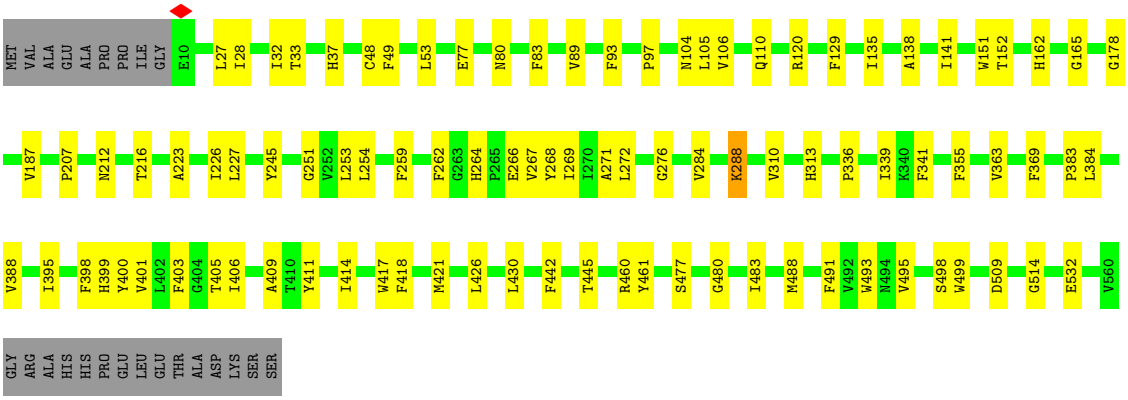
• Molecule 6: Cytochrome c oxidase polypeptide 4

Chain T:



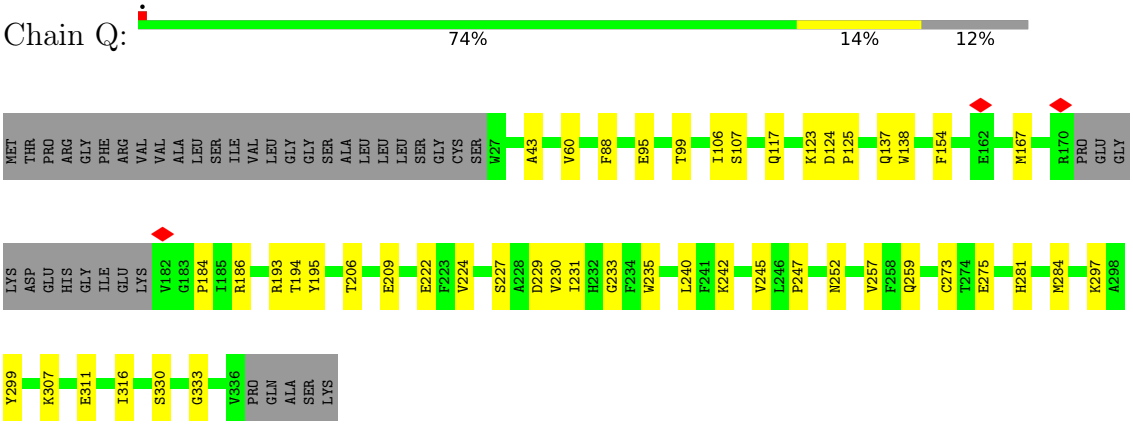
• Molecule 7: Cytochrome c oxidase subunit 1

Chain R:



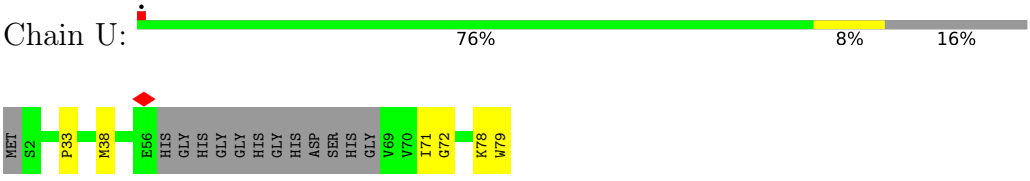
• Molecule 8: cytochrome-c oxidase

Chain Q:



• Molecule 9: Cytochrome c oxidase subunit

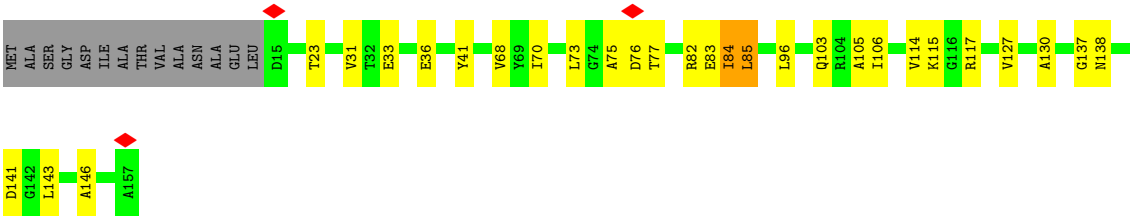
Chain U:



• Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain V:

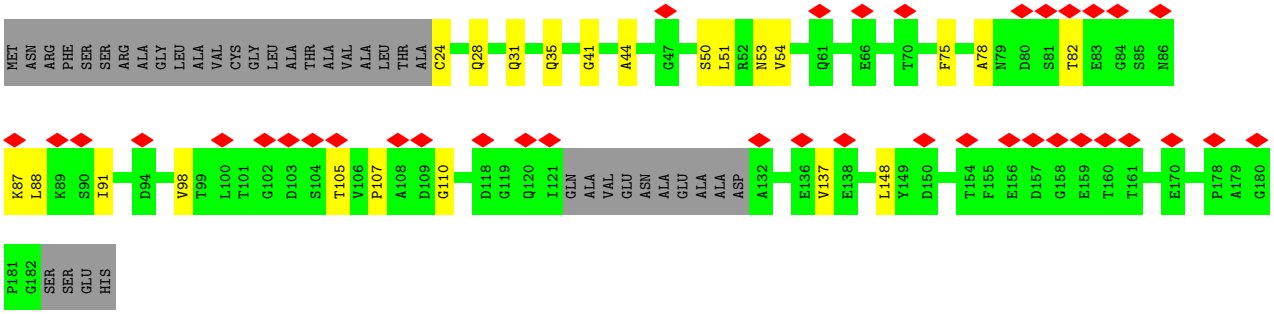




• Molecule 11: LpqE protein

Chain W:

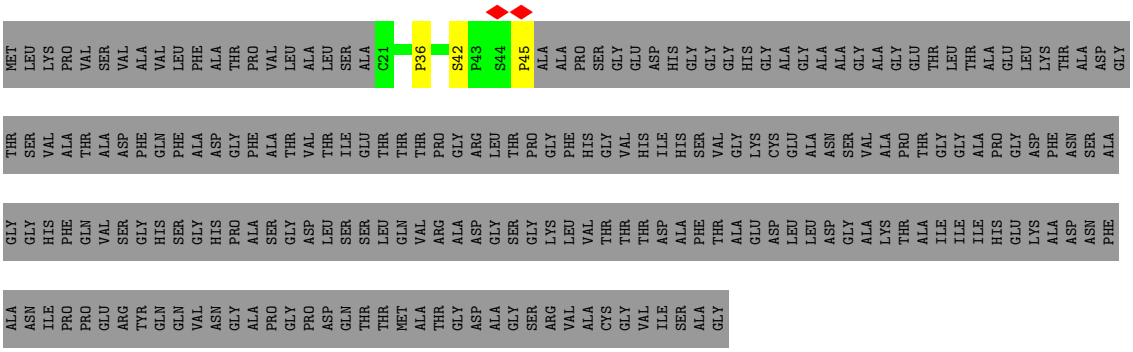




• Molecule 12: Superoxide dismutase [Cu-Zn]

Chain Y:

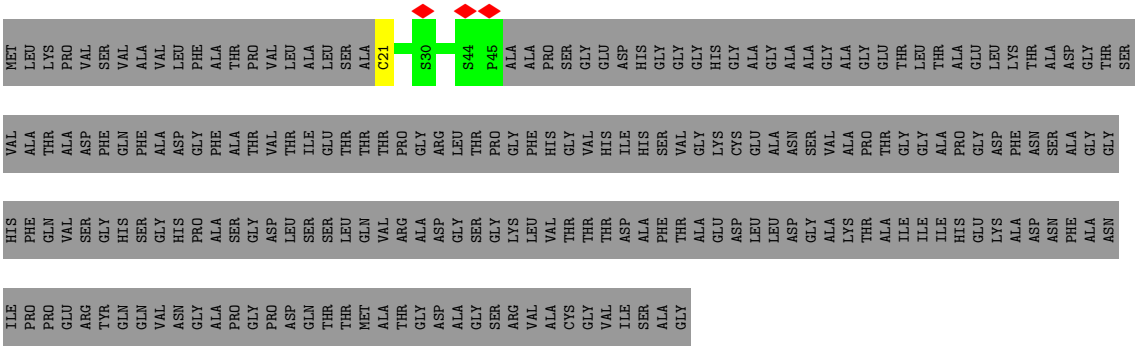




• Molecule 12: Superoxide dismutase [Cu-Zn]

Chain c:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100396	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	1.166	Depositor
Minimum map value	-0.628	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.176	Depositor
Map size (Å)	447.12, 447.12, 447.12	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, HEM, CA, PLM, HEC, 9YF, CU, MQ9, 9XX, 7PH, WUO, A1IGA, 3PE, TRD, CDL, FES, IZL, HEA

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	0.48	2/1660 (0.1%)	0.65	4/2250 (0.2%)
2	G	0.18	0/3046	0.32	0/4129
2	M	0.19	0/3046	0.34	0/4129
3	H	0.32	0/3534	0.46	0/4820
3	N	0.34	1/4299 (0.0%)	0.46	0/5862
4	P	0.14	0/606	0.26	0/825
5	S	0.11	0/1488	0.28	0/2032
6	T	0.22	0/1112	0.34	0/1524
7	R	0.25	0/4529	0.40	0/6187
8	Q	0.28	0/2447	0.41	0/3330
9	U	0.48	0/515	0.48	0/704
10	V	0.44	0/1042	0.65	1/1423 (0.1%)
11	W	0.15	0/1100	0.37	0/1508
12	Y	0.11	0/175	0.30	0/244
12	c	0.09	0/175	0.27	0/244
All	All	0.29	3/28774 (0.0%)	0.42	5/39211 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	236	THR	C-O	-5.37	1.17	1.23
1	O	226	PRO	C-O	-5.12	1.18	1.23
1	O	192	HIS	CE1-NE2	-5.07	1.27	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	192	HIS	CA-C-O	-7.96	109.66	119.28
10	V	75	ALA	N-CA-C	-5.65	106.43	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	192	HIS	CA-CB-CG	-5.64	108.16	113.80
1	O	193	ASN	CA-CB-CG	5.39	117.99	112.60
1	O	209	ASP	CA-C-O	-5.03	115.66	121.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	31	0
2	G	2967	0	2976	25	0
2	M	2967	0	2976	33	0
3	H	3425	0	3469	69	0
3	N	4167	0	4192	82	0
4	P	586	0	578	7	0
5	S	1441	0	1439	17	0
6	T	1077	0	1058	12	0
7	R	4369	0	4346	74	0
8	Q	2382	0	2335	38	0
9	U	499	0	504	6	0
10	V	1024	0	1035	26	0
11	W	1083	0	1055	14	0
12	Y	168	0	150	3	0
12	c	168	0	151	6	0
13	H	116	0	160	12	0
13	N	58	0	80	17	0
13	O	116	0	160	16	0
14	O	97	0	0	3	0
14	P	97	0	0	3	0
15	O	86	0	60	6	0
16	G	4	0	0	1	0
16	M	4	0	0	1	0
17	G	58	0	0	0	0
17	M	58	0	0	0	0
17	W	58	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	G	76	0	110	2	0
18	M	38	0	55	1	0
18	S	38	0	55	1	0
19	G	114	0	0	0	0
19	M	114	0	0	0	0
20	H	86	0	60	17	0
20	N	86	0	60	13	0
21	H	225	0	282	14	0
21	N	235	0	308	8	0
21	P	77	0	98	11	0
21	R	154	0	196	12	0
22	N	24	0	0	0	0
23	Q	13	0	28	0	0
23	R	26	0	56	0	0
23	S	13	0	28	1	0
23	T	13	0	28	0	0
24	S	32	0	38	0	0
25	R	120	0	108	20	0
26	Q	2	0	0	0	0
26	R	1	0	0	0	0
27	R	1	0	0	0	0
28	R	42	0	0	1	0
28	Y	32	0	0	0	0
28	c	32	0	0	6	0
29	R	1	0	0	0	0
30	W	11	0	16	1	0
30	Y	11	0	16	0	0
30	c	11	0	16	2	0
31	G	11	0	0	0	0
31	H	13	0	0	0	0
31	M	51	0	0	0	0
31	N	78	0	0	2	0
31	O	50	0	0	1	0
31	P	8	0	0	0	0
31	Q	44	0	0	0	0
31	R	67	0	0	1	0
31	S	10	0	0	0	0
31	T	9	0	0	0	0
31	V	3	0	0	0	0
31	W	2	0	0	0	0
31	Y	2	0	0	0	0
All	All	30674	0	29842	458	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 8.

The worst 5 of 458 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:c:21:CYS:N	30:c:301:PLM:O2	1.81	1.14
7:R:406:ILE:HD11	25:R:603:HEA:HAC	1.15	1.12
1:O:273:MET:HG3	14:O:302:WUO:C89	1.93	0.98
21:P:301:CDL:H532	21:P:301:CDL:H742	1.44	0.97
25:R:603:HEA:HBD2	25:R:603:HEA:HHA	1.48	0.93

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%)	211 (96%)	10 (4%)	0	100	100
2	G	378/408 (93%)	365 (97%)	13 (3%)	0	100	100
2	M	378/408 (93%)	370 (98%)	8 (2%)	0	100	100
3	H	433/556 (78%)	422 (98%)	10 (2%)	1 (0%)	43	66
3	N	531/556 (96%)	518 (98%)	13 (2%)	0	100	100
4	P	71/100 (71%)	70 (99%)	1 (1%)	0	100	100
5	S	182/203 (90%)	181 (100%)	1 (0%)	0	100	100
6	T	137/139 (99%)	134 (98%)	3 (2%)	0	100	100
7	R	549/575 (96%)	544 (99%)	5 (1%)	0	100	100
8	Q	295/341 (86%)	287 (97%)	8 (3%)	0	100	100
9	U	62/79 (78%)	62 (100%)	0	0	100	100
10	V	141/157 (90%)	137 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	W	145/186 (78%)	132 (91%)	13 (9%)	0	100	100
12	Y	23/236 (10%)	20 (87%)	3 (13%)	0	100	100
12	c	23/236 (10%)	22 (96%)	1 (4%)	0	100	100
All	All	3569/4458 (80%)	3475 (97%)	93 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	184	VAL

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%)	159 (98%)	4 (2%)	42	69
2	G	311/333 (93%)	311 (100%)	0	100	100
2	M	311/333 (93%)	311 (100%)	0	100	100
3	H	351/448 (78%)	339 (97%)	12 (3%)	32	60
3	N	428/448 (96%)	422 (99%)	6 (1%)	59	81
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%)	105 (99%)	1 (1%)	70	87
7	R	453/471 (96%)	451 (100%)	2 (0%)	84	93
8	Q	255/288 (88%)	253 (99%)	2 (1%)	73	88
9	U	51/59 (86%)	50 (98%)	1 (2%)	48	74
10	V	105/114 (92%)	100 (95%)	5 (5%)	23	47
11	W	121/146 (83%)	121 (100%)	0	100	100
12	Y	20/167 (12%)	20 (100%)	0	100	100
12	c	20/167 (12%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2899/3530 (82%)	2866 (99%)	33 (1%)	63 84

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	303	PHE
3	H	304	TYR
3	H	374	THR
7	R	288	LYS
7	R	129	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
8	Q	302	GLN
3	H	29	GLN
2	G	180	ASN
3	H	300	GLN
3	N	140	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)

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	$\#\|Z\| > 2$
19	IZL	M	504	-	119,119,119	1.75	30 (25%)	161,163,163	1.31	18 (11%)
30	PLM	Y	301	12	10,10,17	0.79	0	9,9,17	0.60	0
20	HEM	H	602	3	50,50,50	1.89	14 (28%)	66,82,82	1.85	21 (31%)
18	7PH	G	505	-	37,37,37	0.96	4 (10%)	41,42,42	1.11	2 (4%)
23	TRD	T	201	-	12,12,12	0.09	0	11,11,11	0.05	0
17	9YF	G	502	-	58,58,58	1.39	5 (8%)	69,71,71	1.07	3 (4%)
13	MQ9	H	606	-	59,59,59	0.35	0	72,75,75	0.32	0
28	9XX	Y	302	12	31,31,41	1.25	2 (6%)	34,34,44	1.12	4 (11%)
21	CDL	H	603	-	73,73,99	0.30	0	79,85,111	0.35	0
22	A1IGA	N	604	-	26,26,26	2.33	7 (26%)	37,37,37	2.51	13 (35%)
24	3PE	S	503	-	31,31,50	0.33	0	34,36,55	0.38	0
25	HEA	R	602	7	66,67,67	2.27	25 (37%)	78,103,103	2.56	33 (42%)
28	9XX	R	609	-	41,41,41	1.14	2 (4%)	44,44,44	0.96	4 (9%)
16	FES	G	501	2	0,4,4	-	-	-		
21	CDL	P	301	-	76,76,99	0.40	0	82,88,111	0.52	0
17	9YF	M	502	-	58,58,58	1.38	5 (8%)	69,71,71	1.08	3 (4%)
21	CDL	N	603	-	78,78,99	0.29	0	84,90,111	0.34	0
15	HEC	O	304	1	50,50,50	1.38	6 (12%)	68,82,82	1.18	7 (10%)
18	7PH	S	501	-	37,37,37	0.30	0	41,42,42	0.34	0
28	9XX	c	302	-	31,31,41	1.25	2 (6%)	34,34,44	1.09	4 (11%)
21	CDL	H	601	-	73,73,99	0.30	0	79,85,111	0.35	0
23	TRD	S	502	-	12,12,12	0.09	0	11,11,11	0.06	0
16	FES	M	501	2	0,4,4	-	-	-		
21	CDL	N	607	-	78,78,99	0.29	0	84,90,111	0.35	0
21	CDL	R	605	-	76,76,99	0.29	0	82,88,111	0.34	0
13	MQ9	N	606	-	59,59,59	0.34	0	72,75,75	0.31	0
15	HEC	O	303	1	50,50,50	1.44	4 (8%)	68,82,82	1.41	12 (17%)
18	7PH	M	503	-	37,37,37	0.30	0	41,42,42	0.34	0
19	IZL	G	503	-	119,119,119	1.75	30 (25%)	161,163,163	1.31	18 (11%)
20	HEM	N	605	3	50,50,50	2.05	19 (38%)	66,82,82	1.74	16 (24%)
23	TRD	R	608	-	12,12,12	0.09	0	11,11,11	0.05	0
21	CDL	R	601	-	76,76,99	0.29	0	82,88,111	0.34	0
25	HEA	R	603	7	66,67,67	2.60	23 (34%)	78,103,103	2.23	34 (43%)
14	WUO	P	302	-	99,99,99	1.61	10 (10%)	123,125,125	1.30	12 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	WUO	O	302	-	99,99,99	1.60	10 (10%)	123,125,125	1.29	12 (9%)
21	CDL	N	602	-	76,76,99	0.29	0	82,88,111	0.34	0
23	TRD	R	607	-	12,12,12	0.09	0	11,11,11	0.06	0
23	TRD	Q	403	-	12,12,12	0.09	0	11,11,11	0.06	0
30	PLM	W	202	-	10,10,17	0.78	0	9,9,17	0.60	0
18	7PH	G	504	-	37,37,37	0.95	4 (10%)	41,42,42	1.14	2 (4%)
13	MQ9	H	607	-	59,59,59	0.35	0	72,75,75	0.31	0
21	CDL	H	604	-	76,76,99	0.30	0	82,88,111	0.34	0
20	HEM	N	601	3	50,50,50	1.96	15 (30%)	66,82,82	1.96	14 (21%)
17	9YF	W	201	-	58,58,58	1.40	5 (8%)	69,71,71	1.08	3 (4%)
30	PLM	c	301	-	10,10,17	0.41	0	9,9,17	0.45	0
13	MQ9	O	301	-	59,59,59	0.36	0	72,75,75	0.32	0
20	HEM	H	605	3	50,50,50	2.05	18 (36%)	66,82,82	1.98	20 (30%)
13	MQ9	O	305	-	59,59,59	0.48	0	72,75,75	0.41	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
19	IZL	M	504	-	-	38/84/208/208	0/6/6/6
30	PLM	Y	301	12	-	0/7/8/15	-
20	HEM	H	602	3	-	4/14/54/54	-
18	7PH	G	505	-	-	11/39/39/39	-
23	TRD	T	201	-	-	1/10/10/10	-
17	9YF	G	502	-	-	28/54/78/78	0/1/1/1
13	MQ9	H	606	-	-	21/53/73/73	0/2/2/2
28	9XX	Y	302	12	-	11/33/33/43	-
21	CDL	H	603	-	-	41/84/84/110	-
22	A1IGA	N	604	-	-	8/11/11/11	0/3/3/3
24	3PE	S	503	-	-	14/35/35/54	-
25	HEA	R	602	7	-	12/36/76/76	-
28	9XX	R	609	-	-	24/43/43/43	-
16	FES	G	501	2	-	-	0/1/1/1
21	CDL	P	301	-	-	47/87/87/110	-
17	9YF	M	502	-	-	28/54/78/78	0/1/1/1
21	CDL	N	603	-	-	53/89/89/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEC	O	304	1	1/1/3/7	5/14/54/54	-
18	7PH	S	501	-	-	13/39/39/39	-
28	9XX	c	302	-	-	16/33/33/43	-
21	CDL	H	601	-	-	37/84/84/110	-
23	TRD	S	502	-	-	2/10/10/10	-
16	FES	M	501	2	-	-	0/1/1/1
21	CDL	N	607	-	-	48/89/89/110	-
21	CDL	R	605	-	-	42/87/87/110	-
13	MQ9	N	606	-	-	27/53/73/73	0/2/2/2
15	HEC	O	303	1	1/1/3/7	4/14/54/54	-
18	7PH	M	503	-	-	16/39/39/39	-
19	IZL	G	503	-	-	38/84/208/208	0/6/6/6
20	HEM	N	605	3	-	8/14/54/54	-
23	TRD	R	608	-	-	2/10/10/10	-
21	CDL	R	601	-	-	53/87/87/110	-
25	HEA	R	603	7	-	16/36/76/76	-
14	WUO	P	302	-	-	42/84/148/148	0/3/3/3
14	WUO	O	302	-	-	29/84/148/148	0/3/3/3
21	CDL	N	602	-	-	51/87/87/110	-
23	TRD	R	607	-	-	1/10/10/10	-
23	TRD	Q	403	-	-	1/10/10/10	-
30	PLM	W	202	-	-	1/7/8/15	-
18	7PH	G	504	-	-	10/39/39/39	-
13	MQ9	H	607	-	-	28/53/73/73	0/2/2/2
21	CDL	H	604	-	-	41/87/87/110	-
20	HEM	N	601	3	-	7/14/54/54	-
17	9YF	W	201	-	-	33/54/78/78	0/1/1/1
30	PLM	c	301	-	-	0/7/8/15	-
13	MQ9	O	301	-	-	9/53/73/73	0/2/2/2
20	HEM	H	605	3	-	8/14/54/54	-
13	MQ9	O	305	-	-	20/53/73/73	0/2/2/2

The worst 5 of 240 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	603	HEA	FE-NB	7.08	2.16	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	O	302	WUO	P52-O51	6.61	1.77	1.60
14	P	302	WUO	P52-O51	6.60	1.77	1.60
20	H	602	HEM	FE-NB	6.37	2.14	1.94
25	R	603	HEA	FE-NC	6.22	2.16	1.95

The worst 5 of 255 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	604	A1IGA	C04-S01-C05	8.63	118.18	100.12
25	R	602	HEA	C3C-C4C-NC	7.22	114.69	110.25
20	N	601	HEM	CHC-C4B-NB	6.97	131.99	124.42
25	R	602	HEA	C3D-C4D-ND	5.97	116.14	110.36
22	N	604	A1IGA	C03-C04-S01	5.40	120.23	109.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	O	303	HEC	NA
15	O	304	HEC	NA

5 of 949 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	O	301	MQ9	C18-C19-C21-C22
13	O	301	MQ9	C20-C19-C21-C22
13	O	305	MQ9	C12-C13-C14-C15
13	O	305	MQ9	C12-C13-C14-C16
13	O	305	MQ9	C22-C23-C24-C25

There are no ring outliers.

36 monomers are involved in 165 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	H	602	HEM	9	0
18	G	505	7PH	1	0
13	H	606	MQ9	9	0
21	H	603	CDL	4	0
25	R	602	HEA	3	0
28	R	609	9XX	1	0
16	G	501	FES	1	0
21	P	301	CDL	11	0

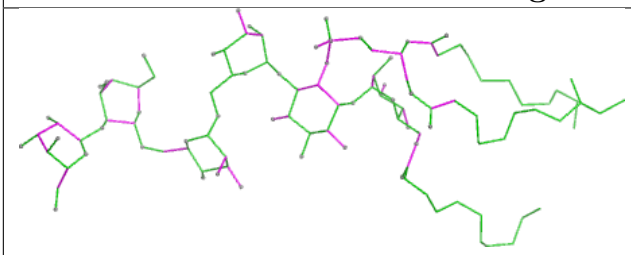
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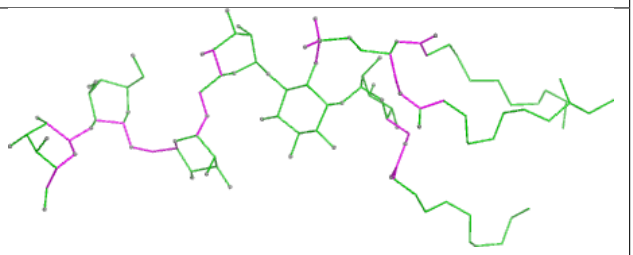
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	N	603	CDL	1	0
15	O	304	HEC	1	0
18	S	501	7PH	1	0
28	c	302	9XX	6	0
21	H	601	CDL	4	0
23	S	502	TRD	1	0
16	M	501	FES	1	0
21	N	607	CDL	2	0
21	R	605	CDL	9	0
13	N	606	MQ9	17	0
15	O	303	HEC	5	0
18	M	503	7PH	1	0
20	N	605	HEM	7	0
21	R	601	CDL	3	0
25	R	603	HEA	17	0
14	P	302	WUO	3	0
14	O	302	WUO	3	0
21	N	602	CDL	5	0
30	W	202	PLM	1	0
18	G	504	7PH	1	0
13	H	607	MQ9	3	0
21	H	604	CDL	8	0
20	N	601	HEM	6	0
17	W	201	9YF	1	0
30	c	301	PLM	2	0
13	O	301	MQ9	4	0
20	H	605	HEM	8	0
13	O	305	MQ9	12	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.

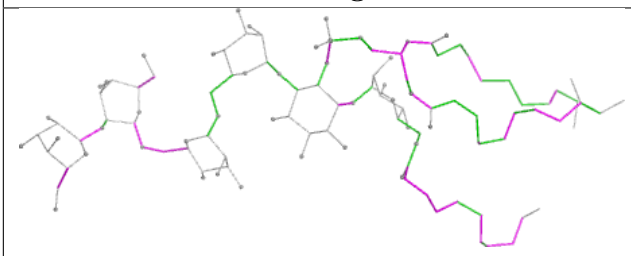
Ligand IZL M 504



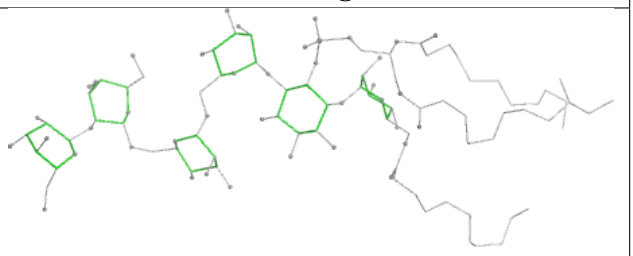
Bond lengths



Bond angles

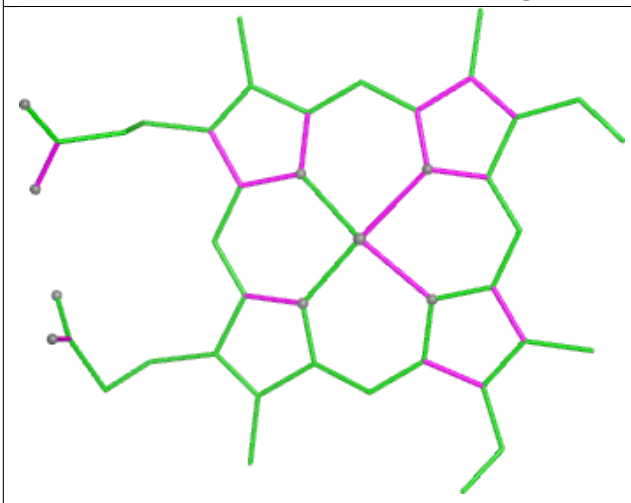


Torsions

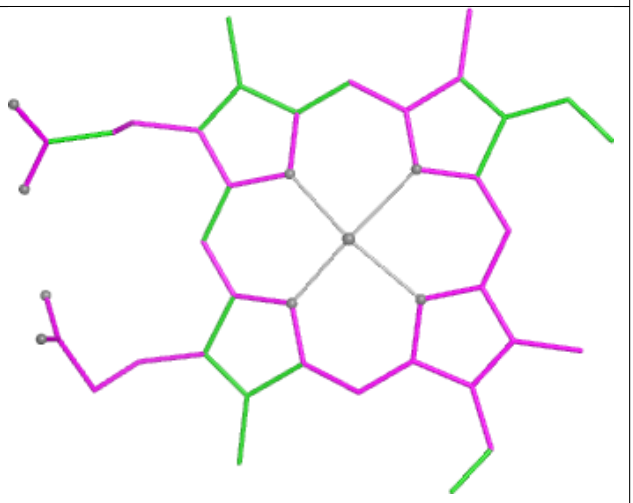


Rings

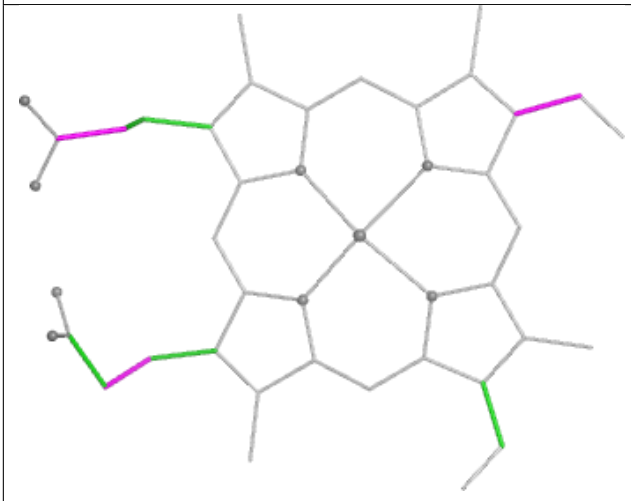
Ligand HEM H 602



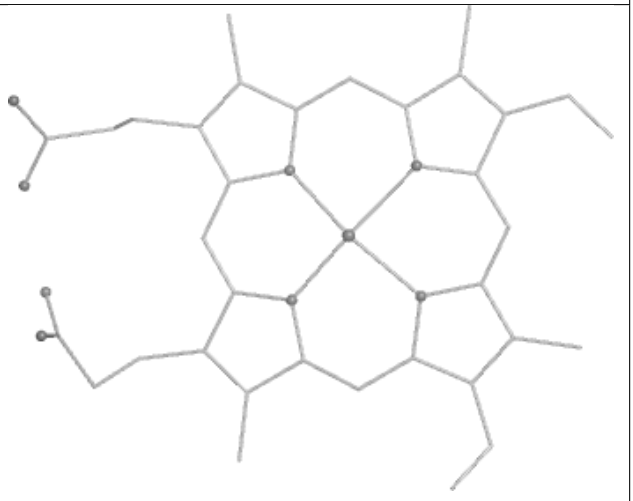
Bond lengths



Bond angles

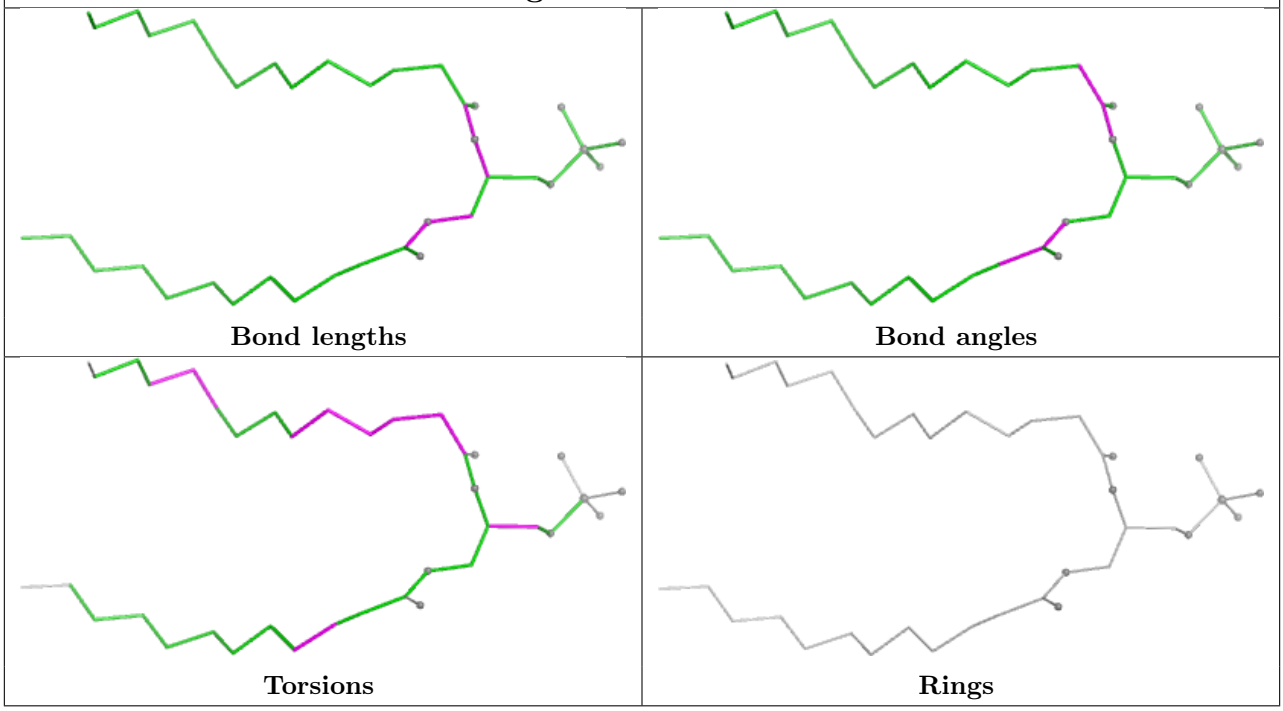


Torsions

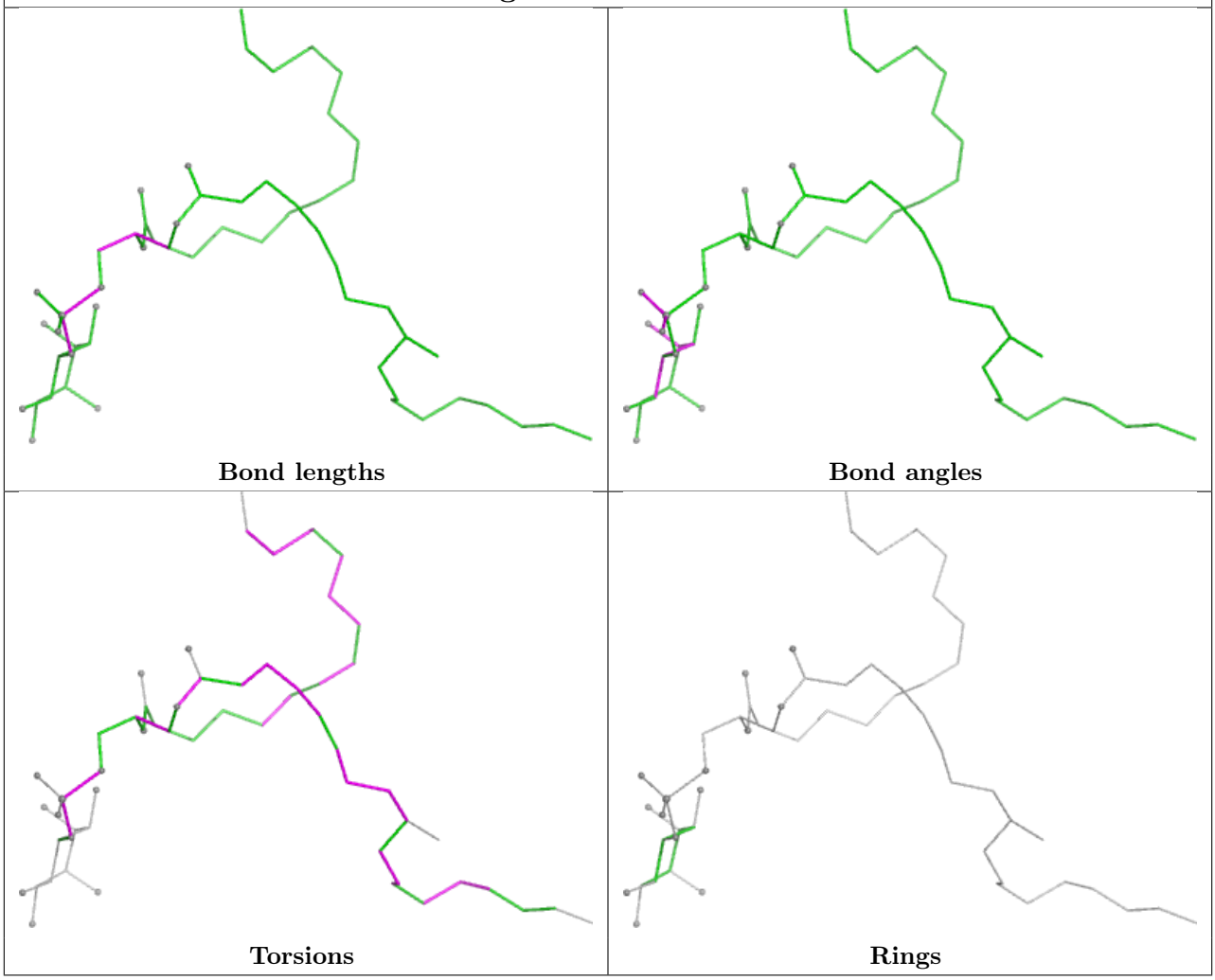


Rings

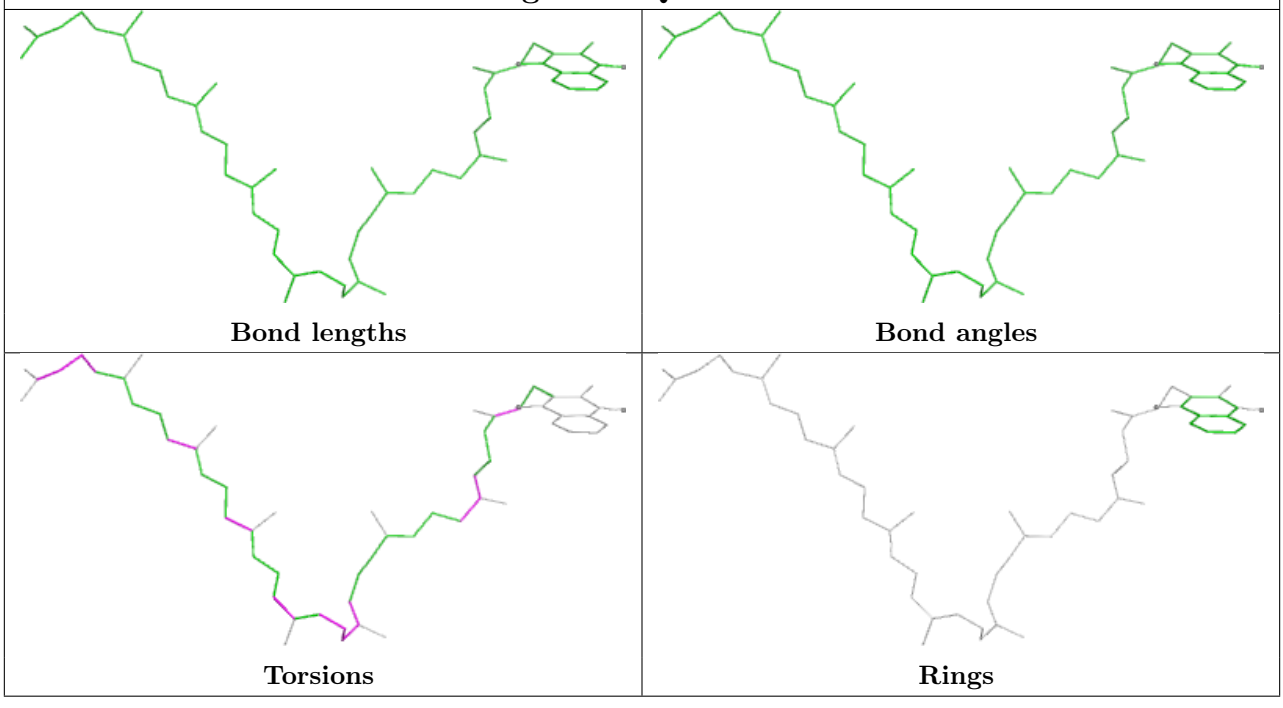
Ligand 7PH G 505



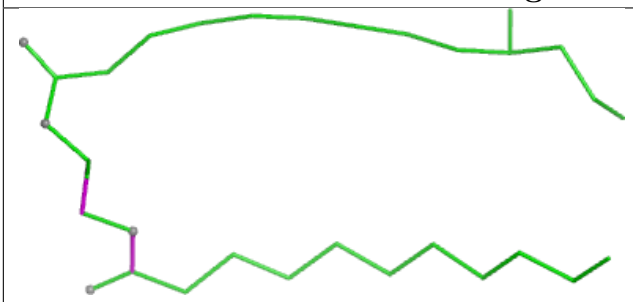
Ligand 9YF G 502



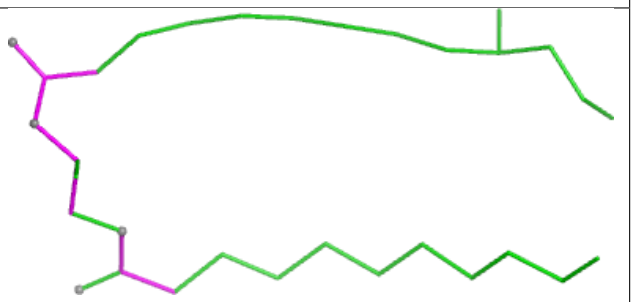
Ligand MQ9 H 606



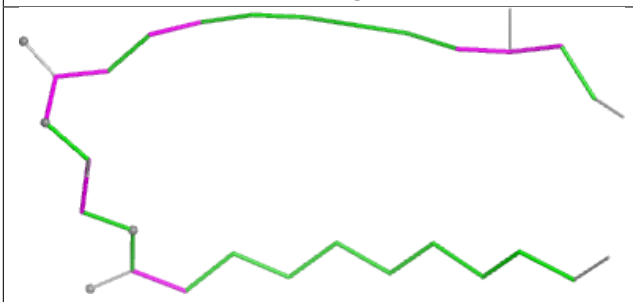
Ligand 9XX Y 302



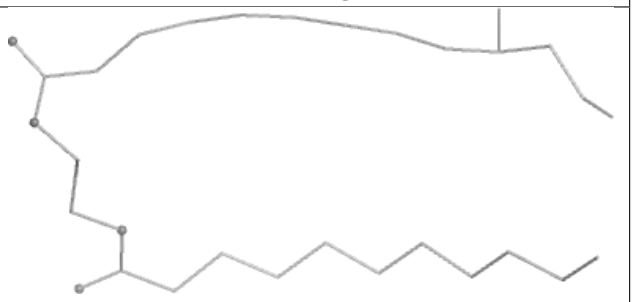
Bond lengths



Bond angles

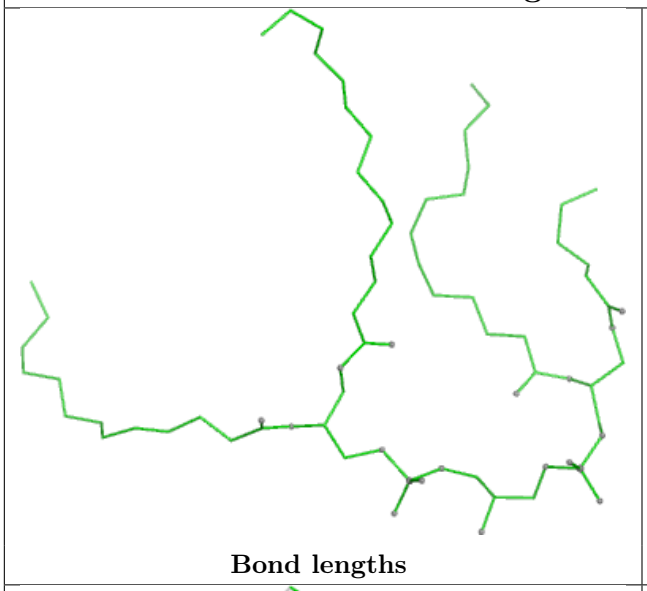


Torsions

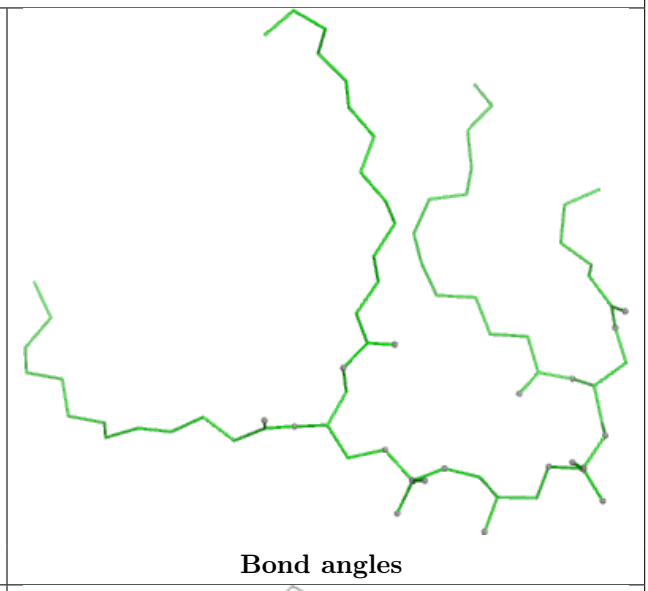


Rings

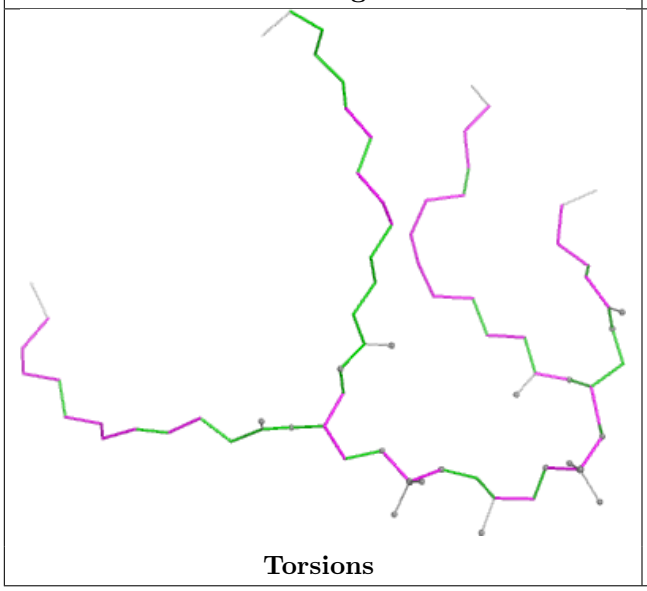
Ligand CDL H 603



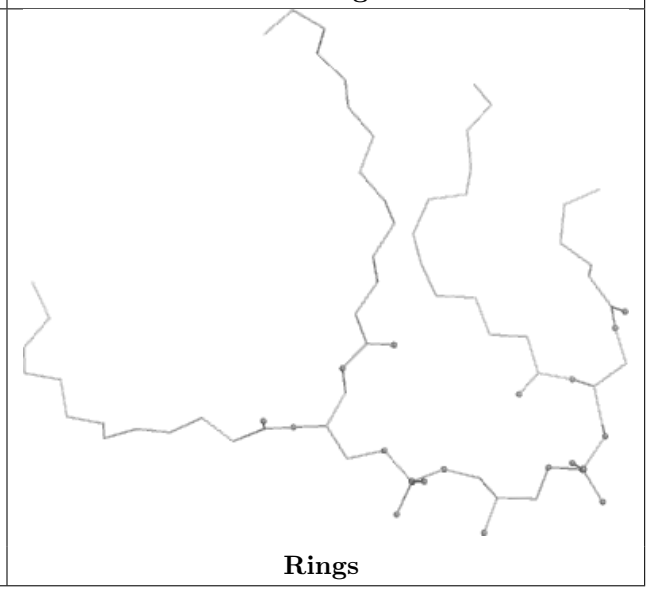
Bond lengths



Bond angles

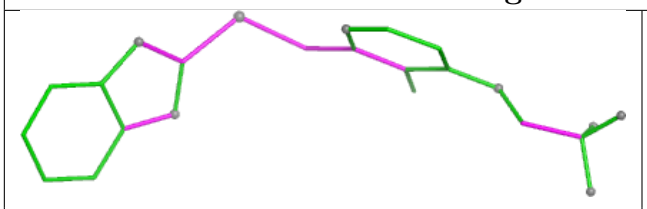


Torsions

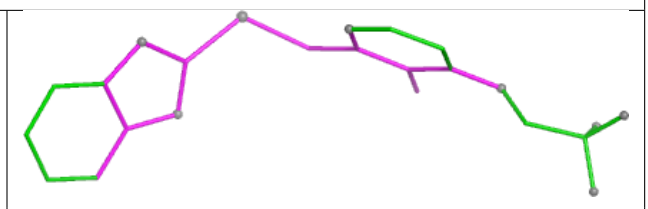


Rings

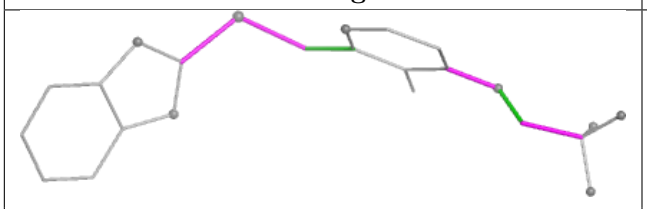
Ligand A1IGA N 604



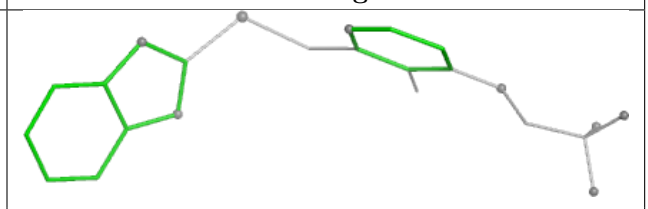
Bond lengths



Bond angles

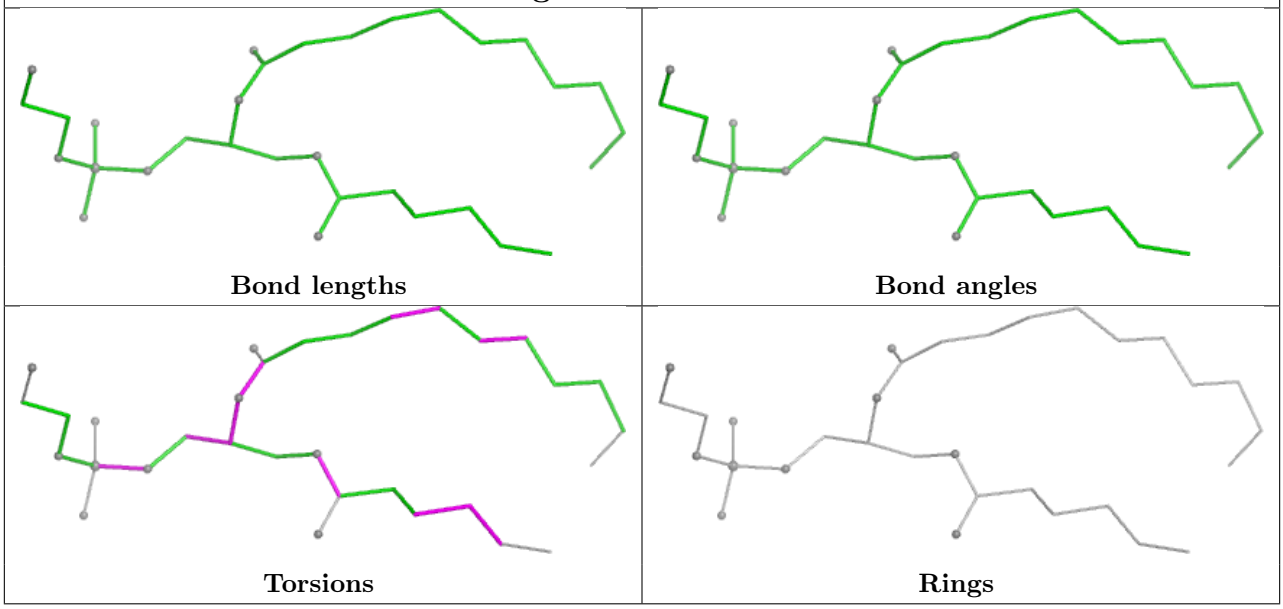


Torsions

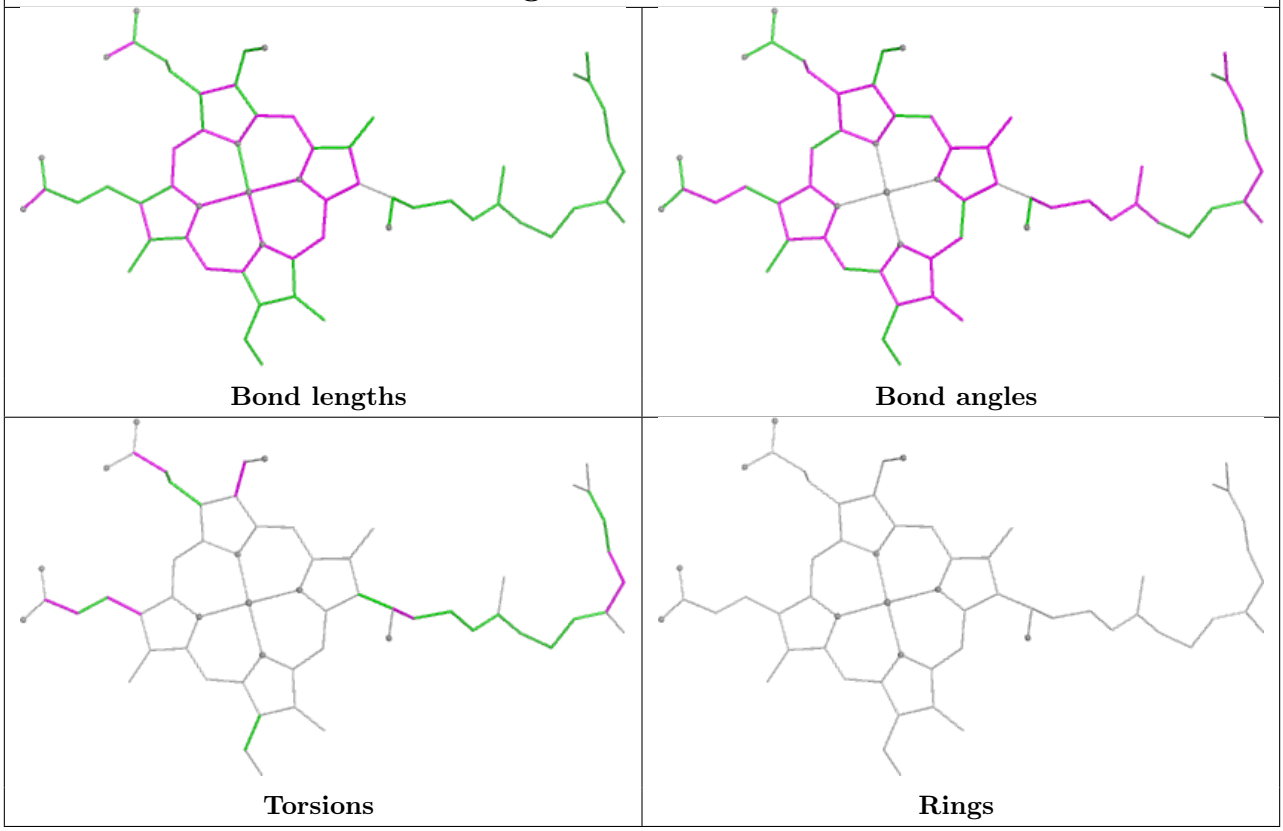


Rings

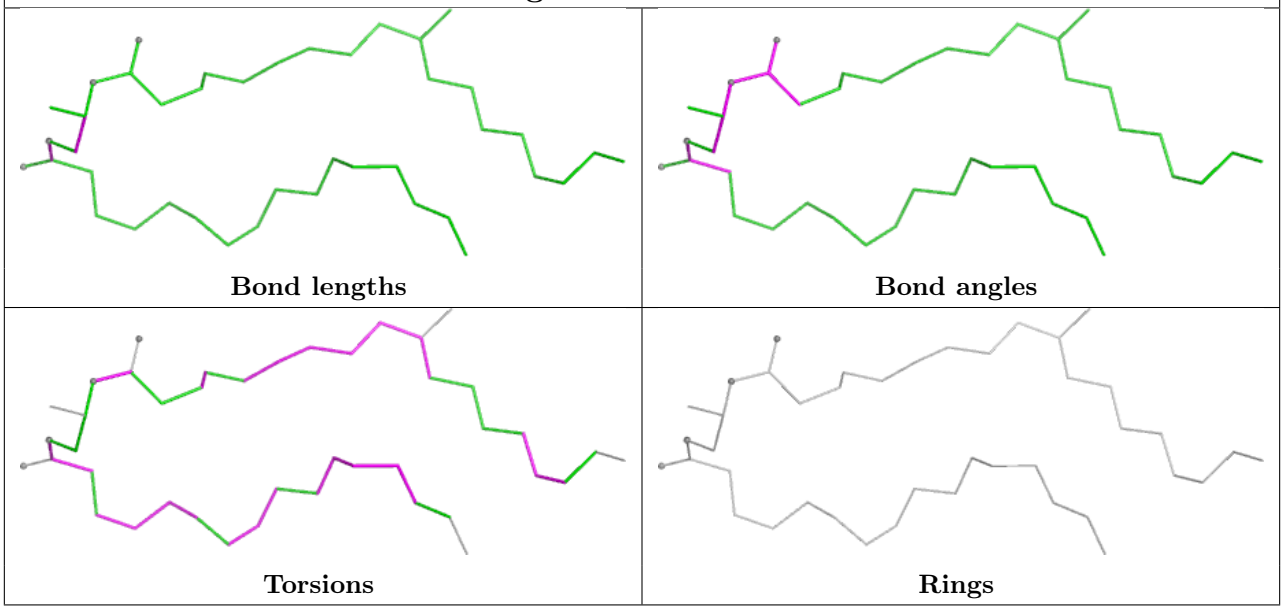
Ligand 3PE S 503



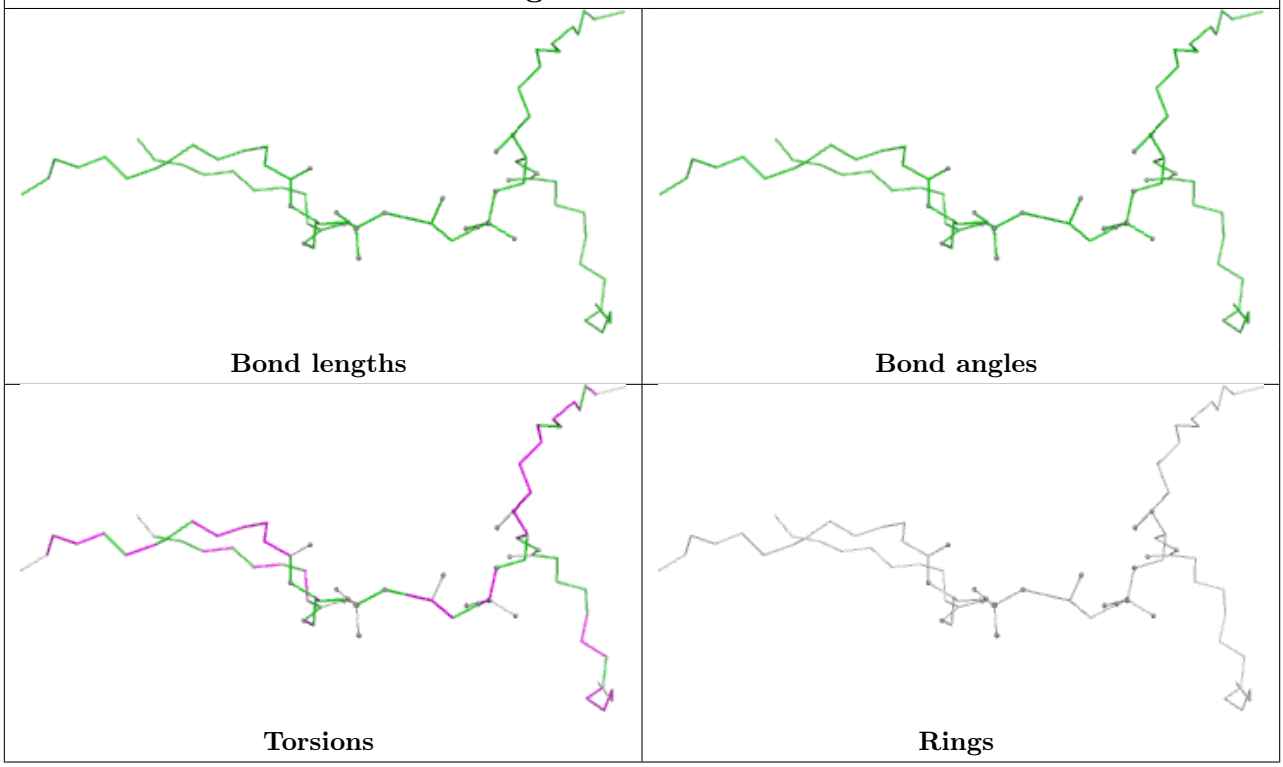
Ligand HEA R 602



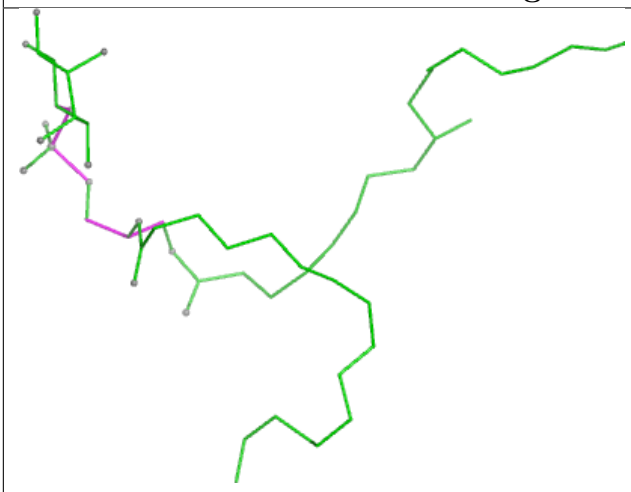
Ligand 9XX R 609



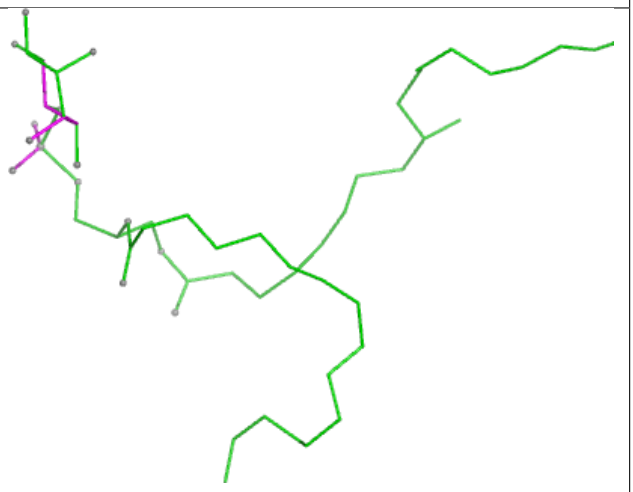
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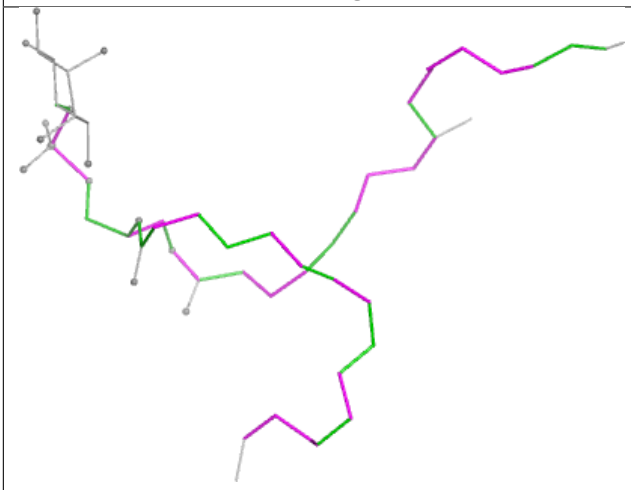
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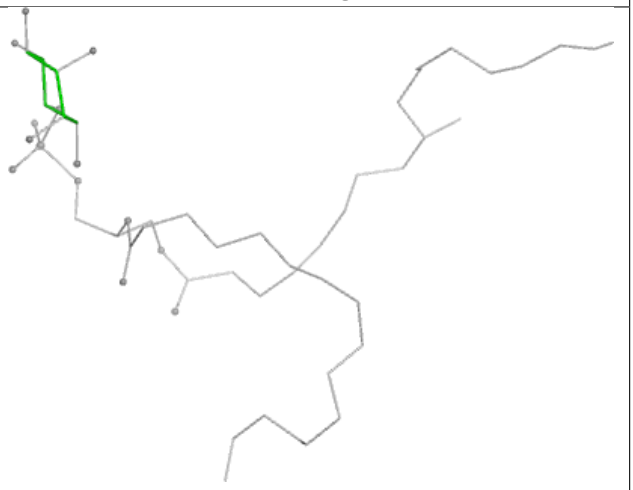
Bond lengths



Bond angles

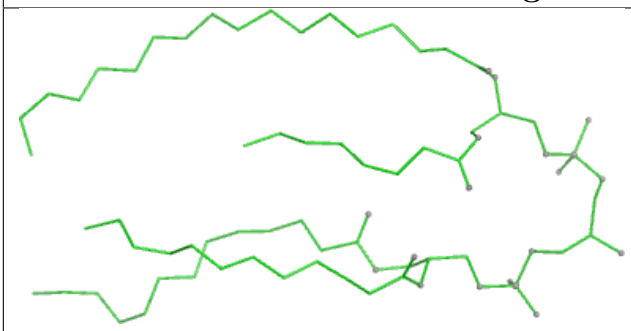


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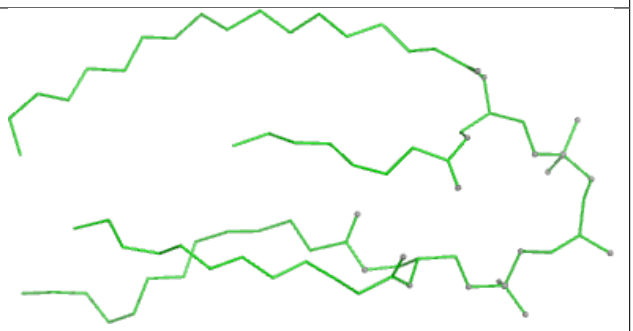


Rings

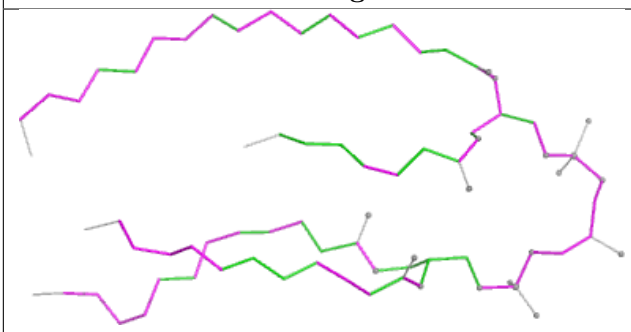
Ligand CDL N 603



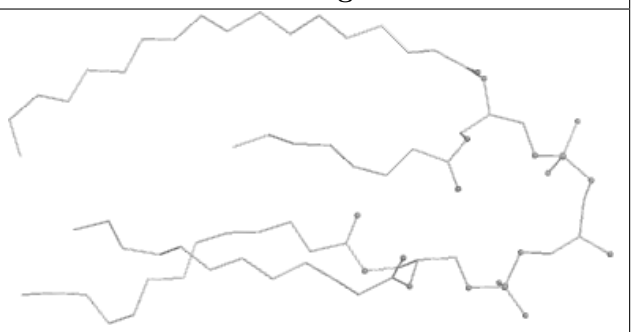
Bond lengths



Bond angles

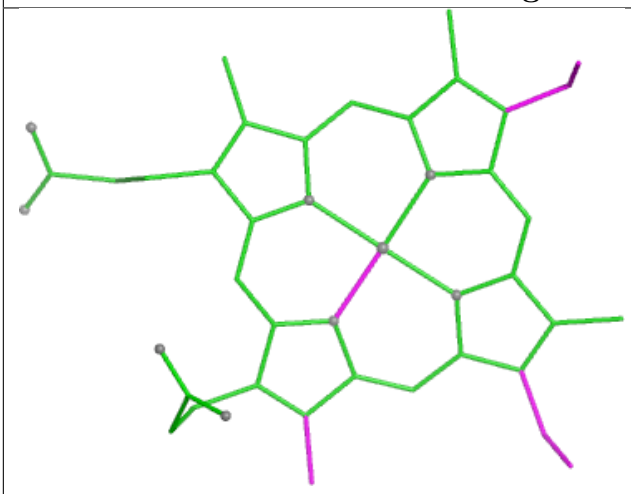


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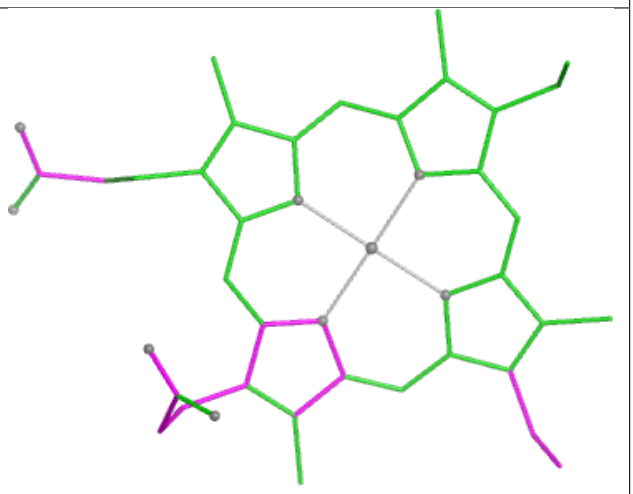


Rings

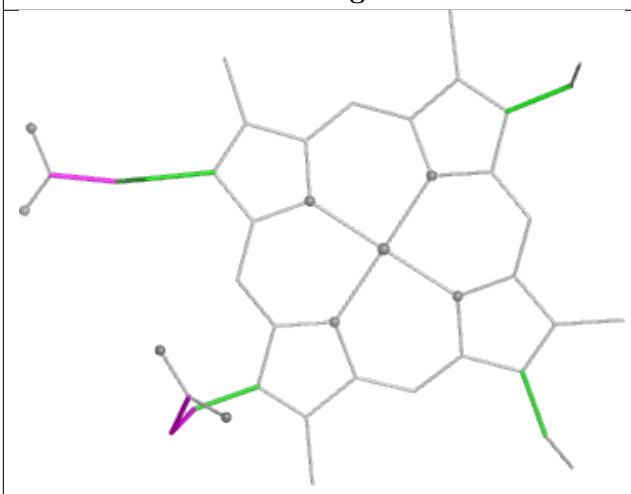
Ligand HEC O 304



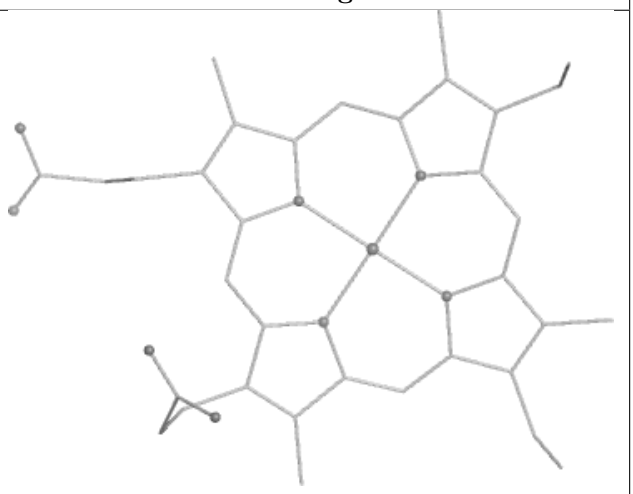
Bond lengths



Bond angles

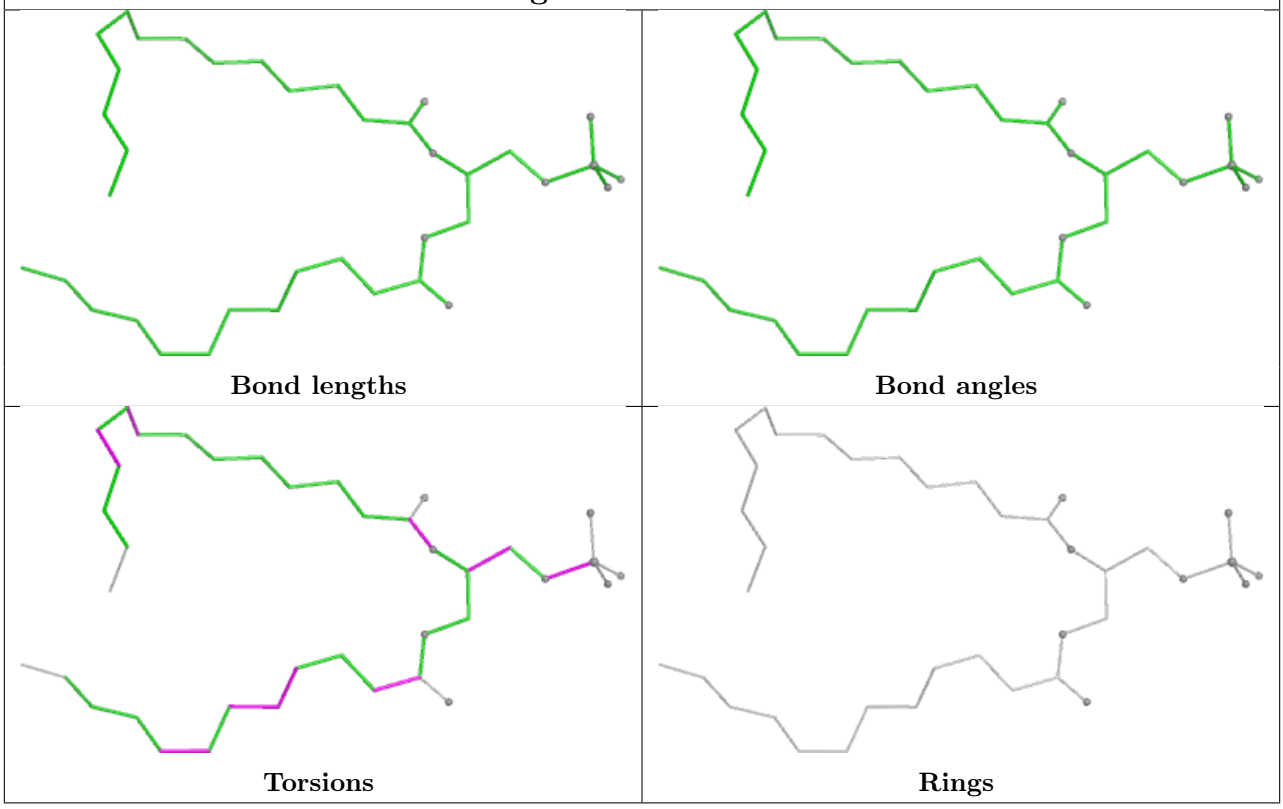


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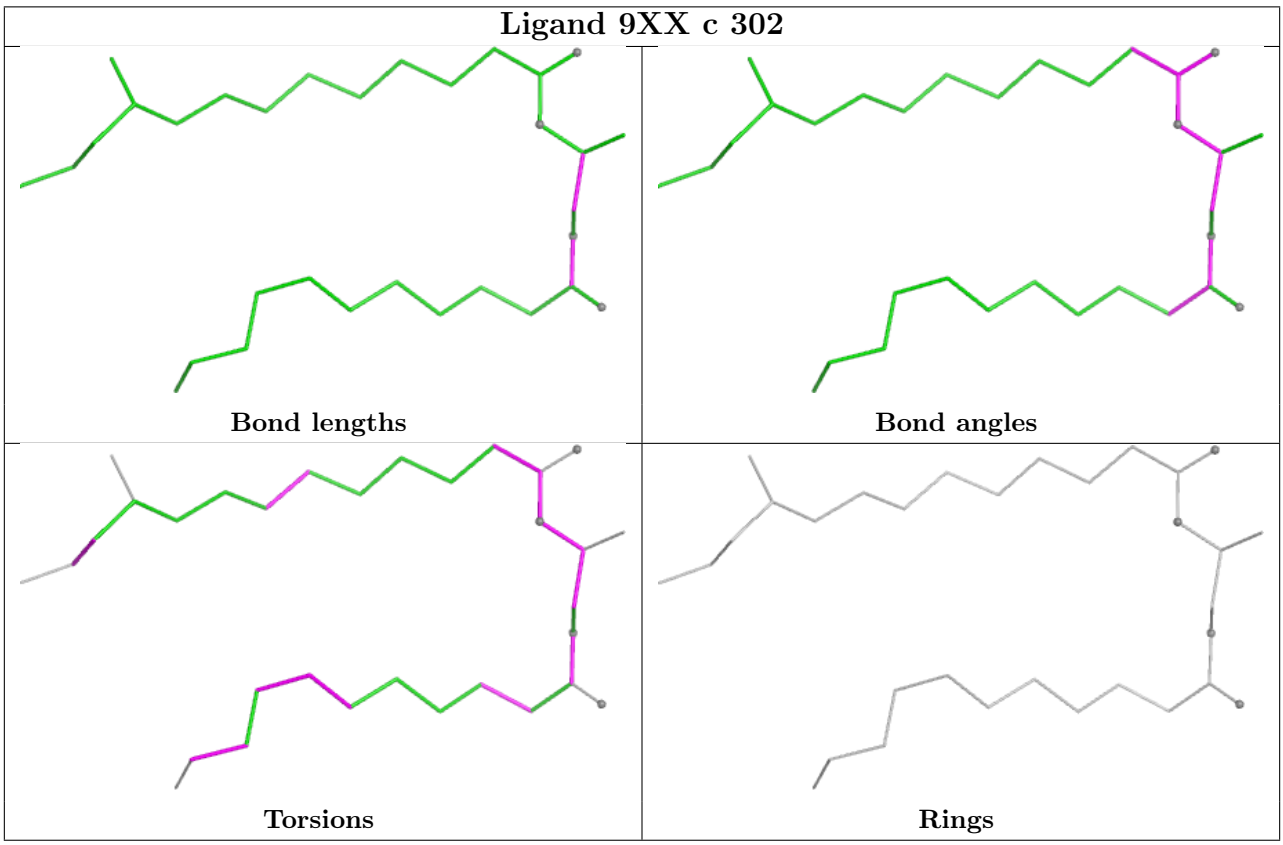


Rings

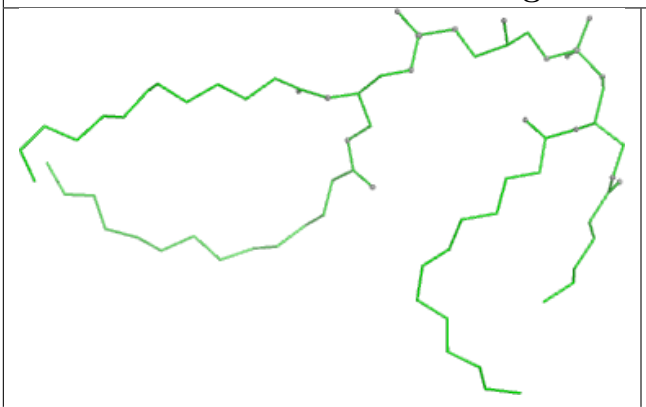
Ligand 7PH S 501



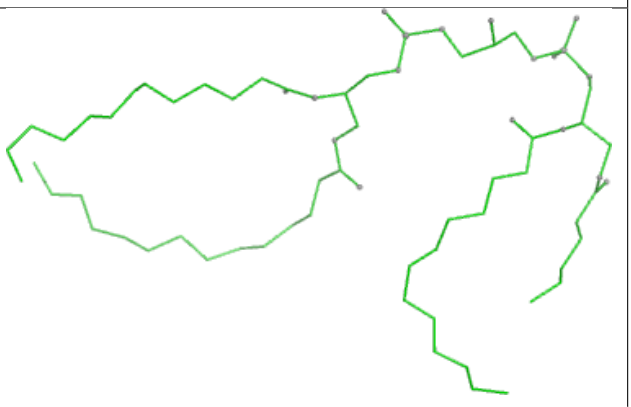
Ligand 9XX c 302



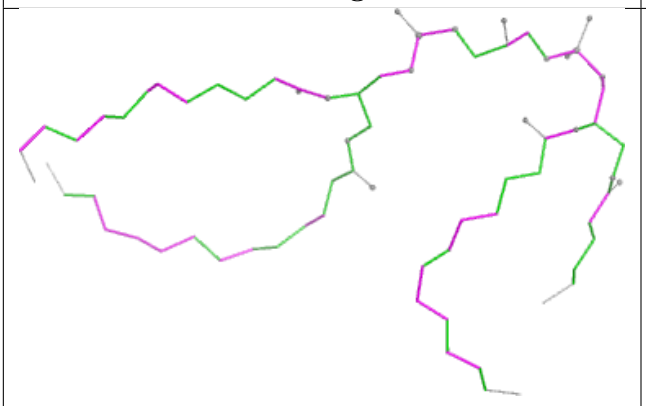
Ligand CDL H 601



Bond lengths



Bond angles

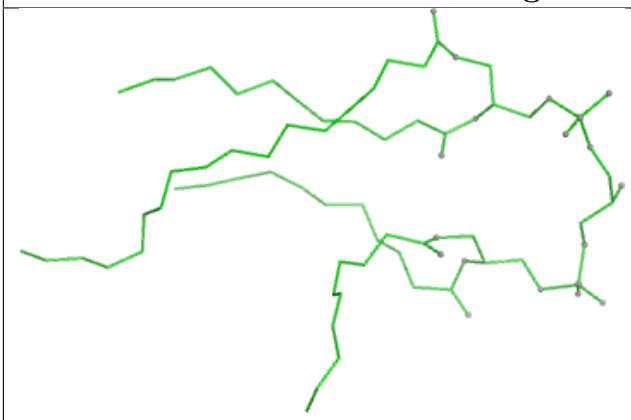


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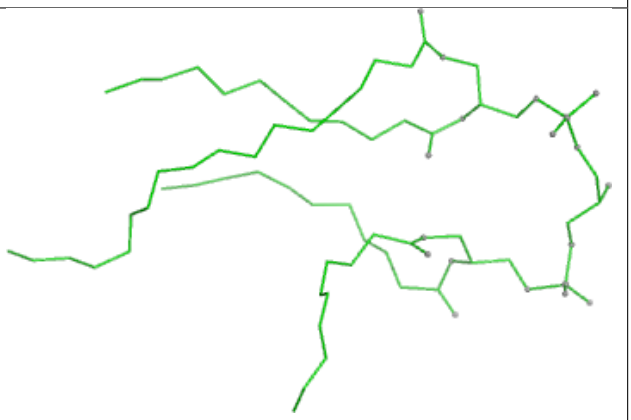


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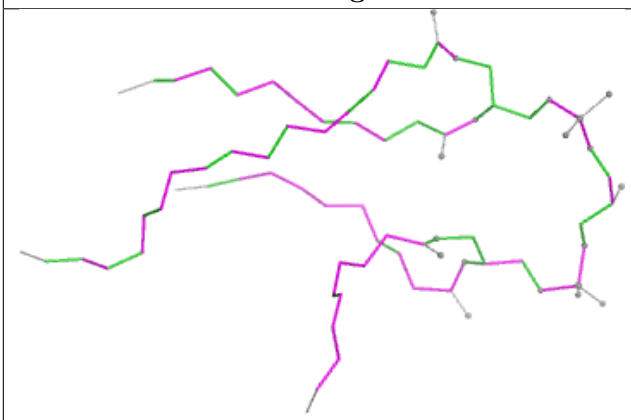
Ligand CDL N 607



Bond lengths



Bond angles

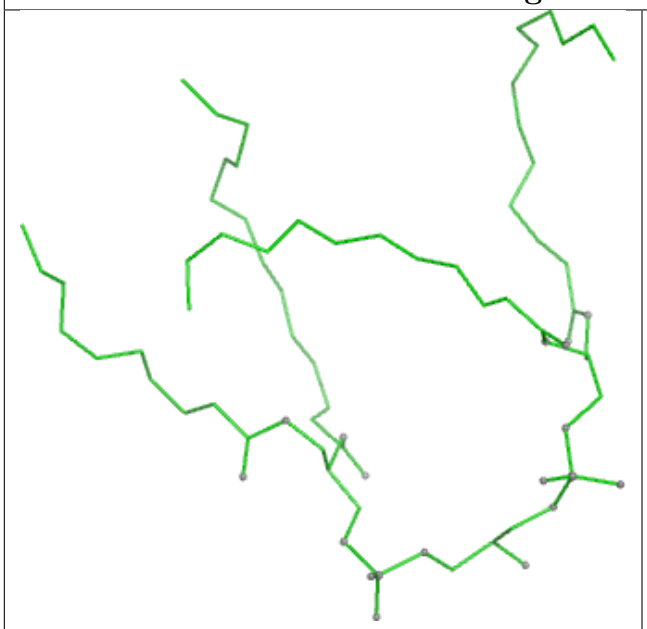


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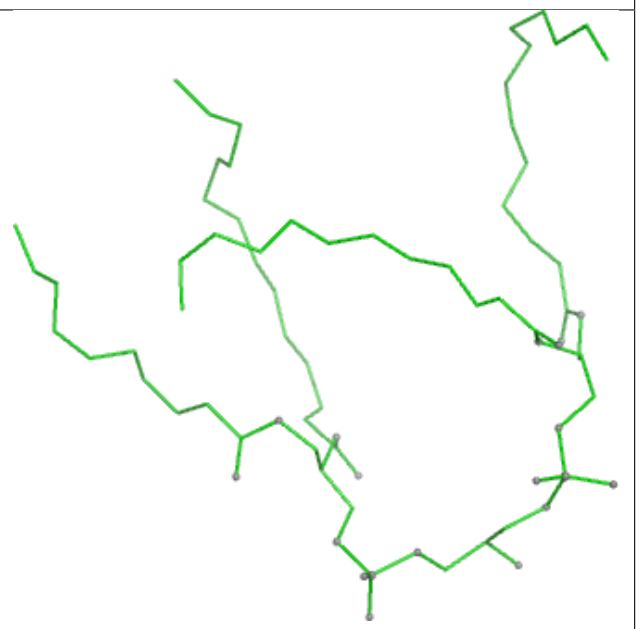


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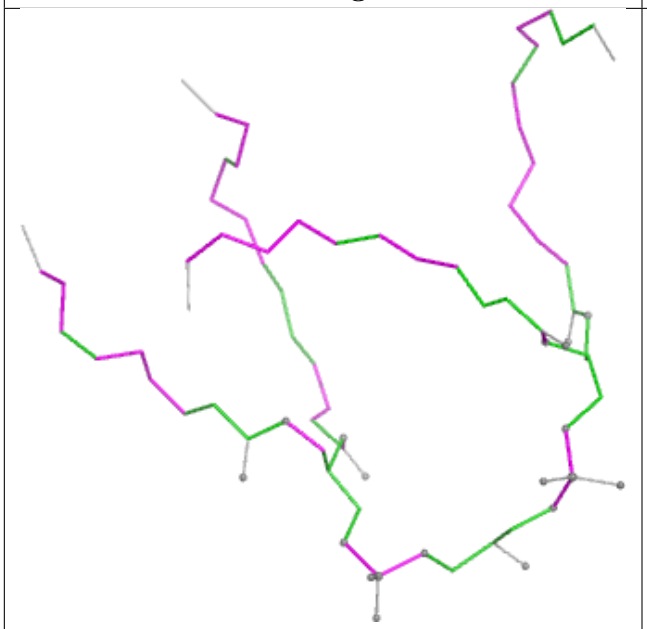
Ligand CDL R 605



Bond lengths



Bond angles

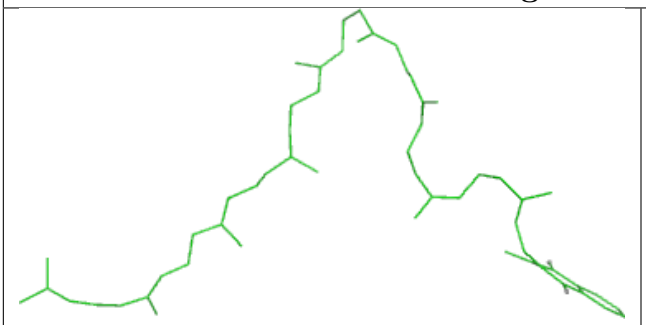


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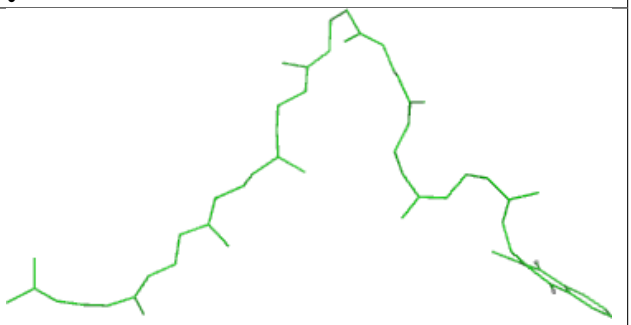


Rings

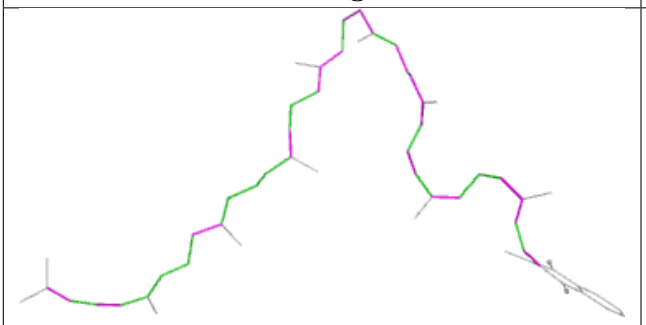
Ligand MQ9 N 606



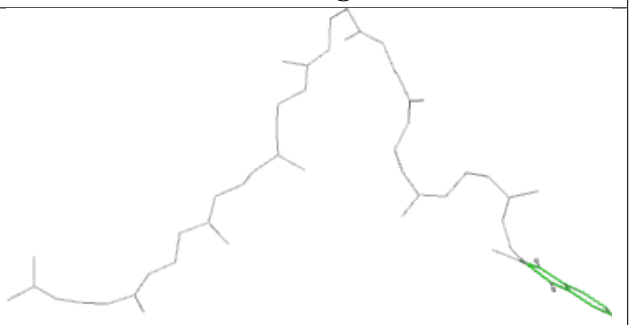
Bond lengths



Bond angles

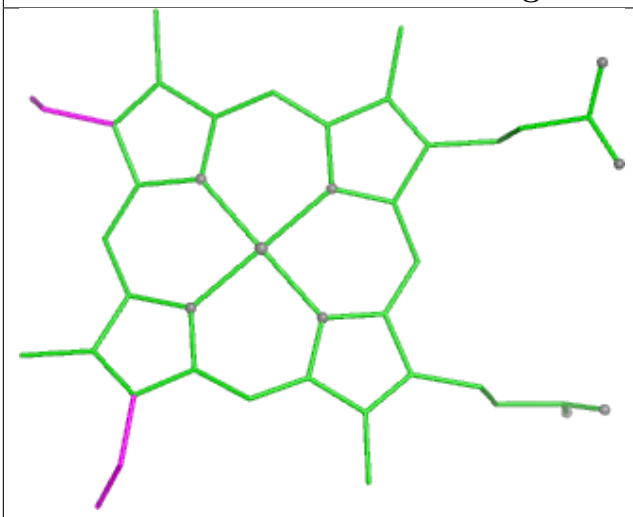


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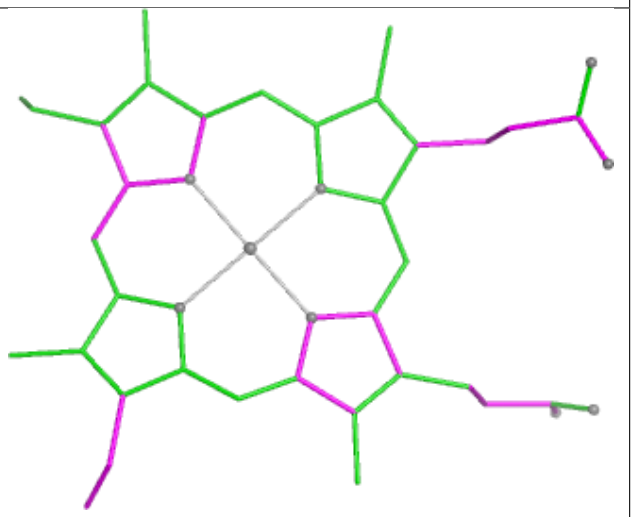


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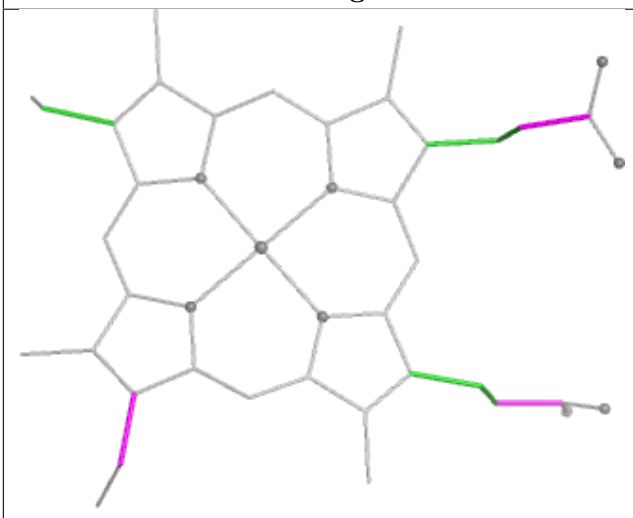
Ligand HEC O 303



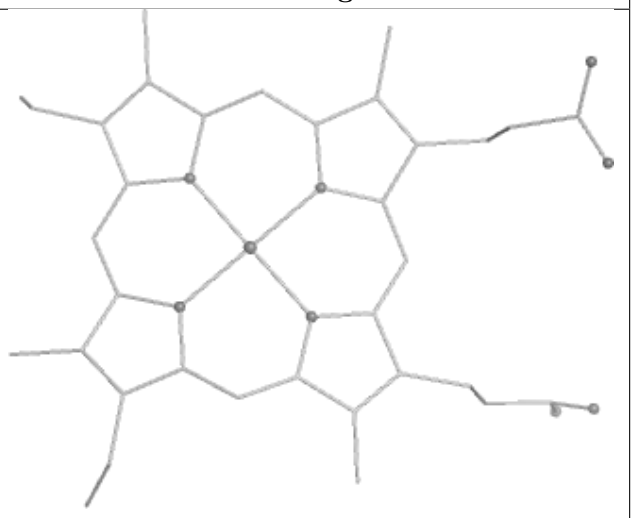
Bond lengths



Bond angles

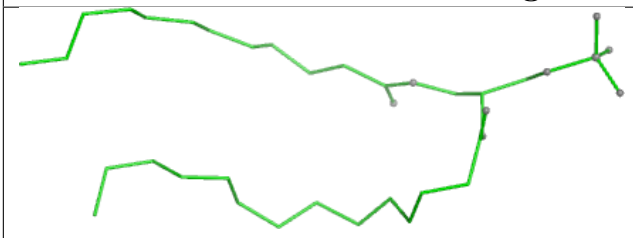


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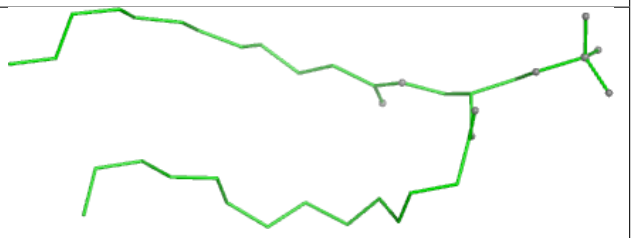


Rings

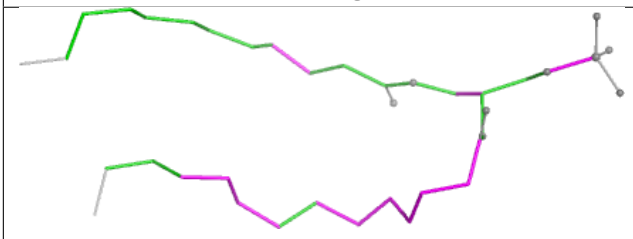
Ligand 7PH M 503



Bond lengths



Bond angles

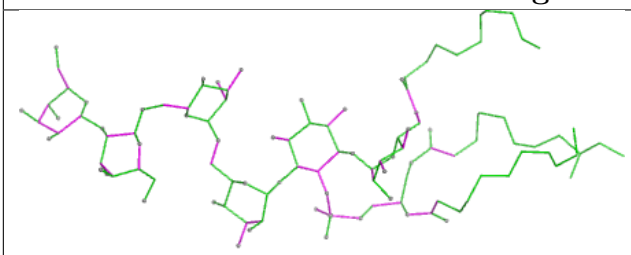


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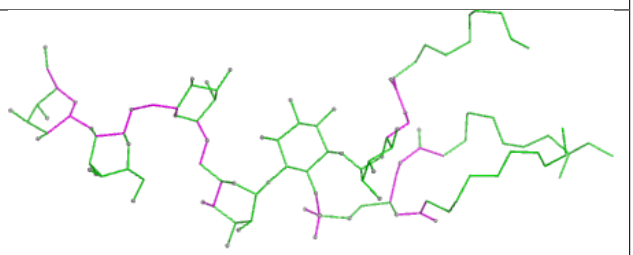


Rings

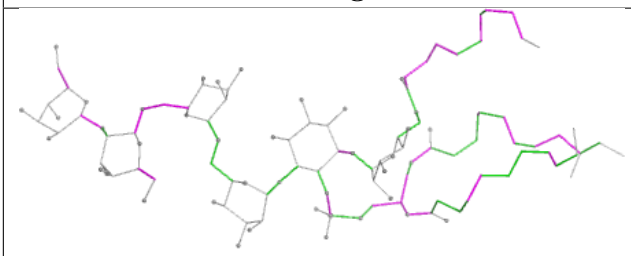
Ligand IZL G 503



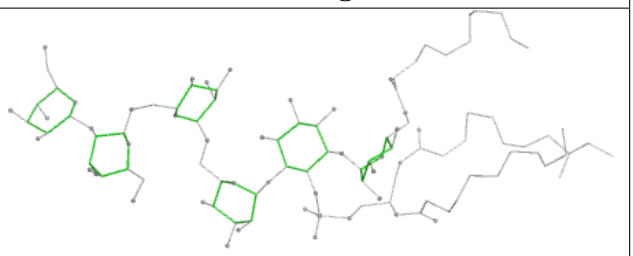
Bond lengths



Bond angles

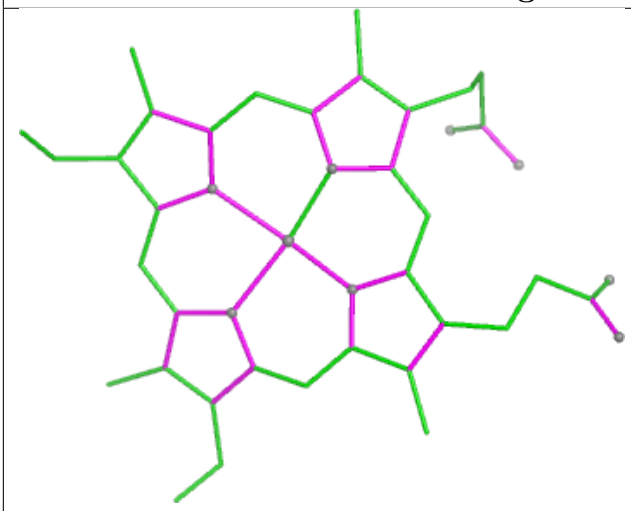


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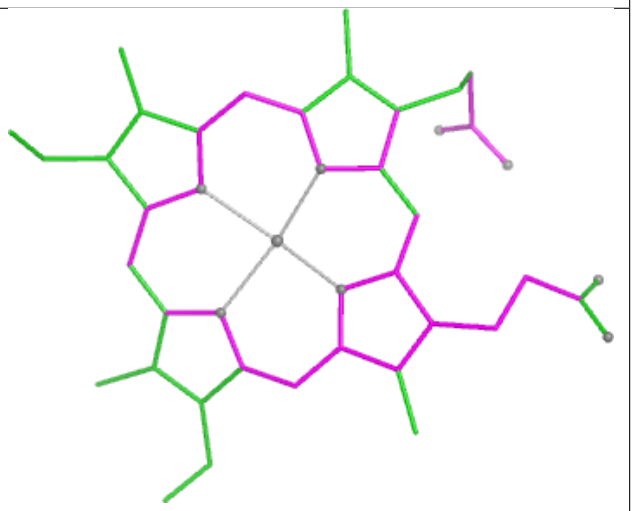


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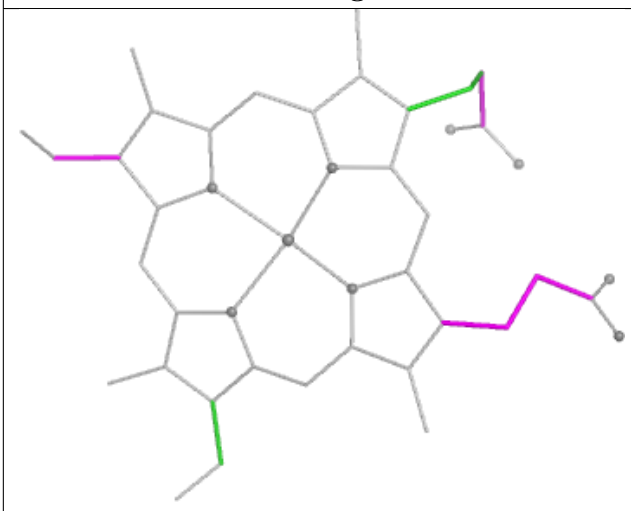
Ligand HEM N 605



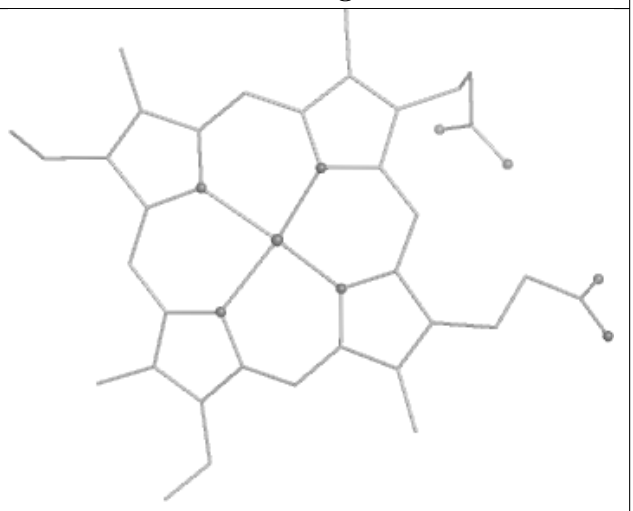
Bond lengths



Bond angles

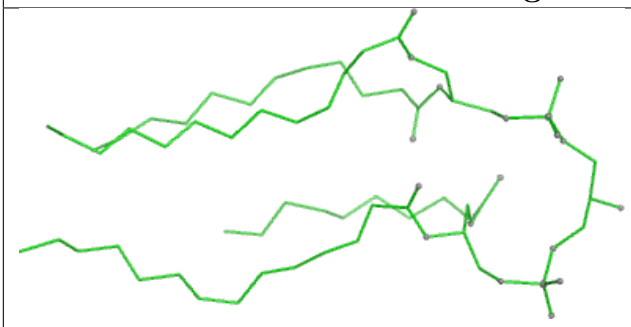


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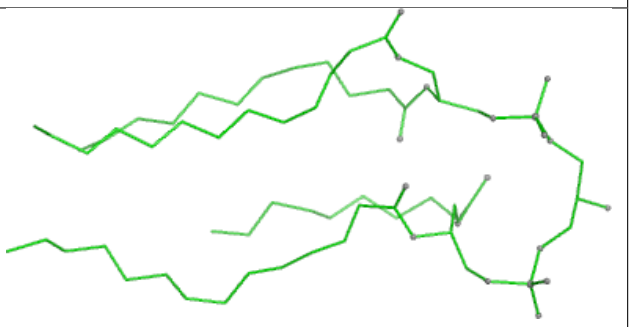


Rings

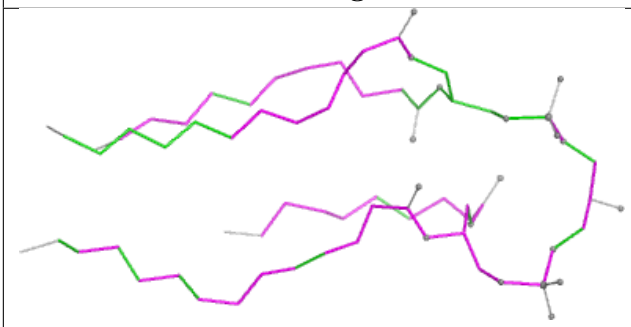
Ligand CDL R 601



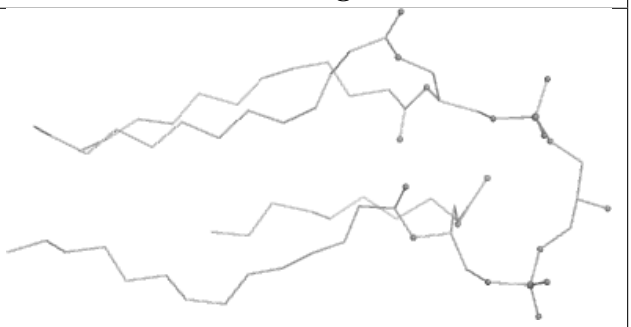
Bond lengths



Bond angles

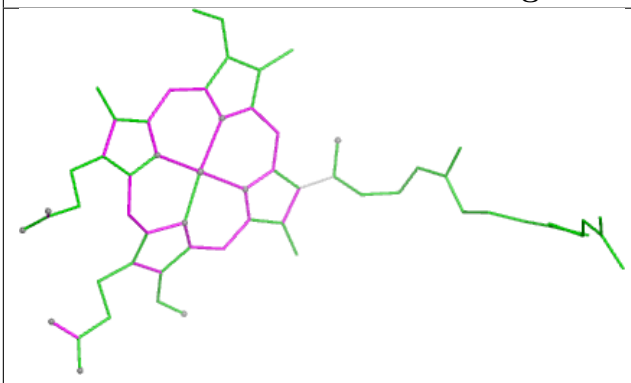


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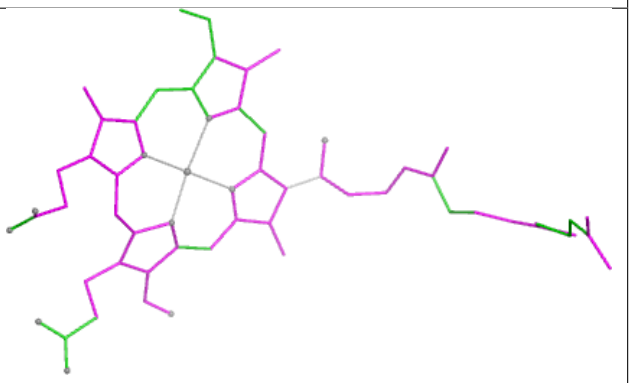


Rings

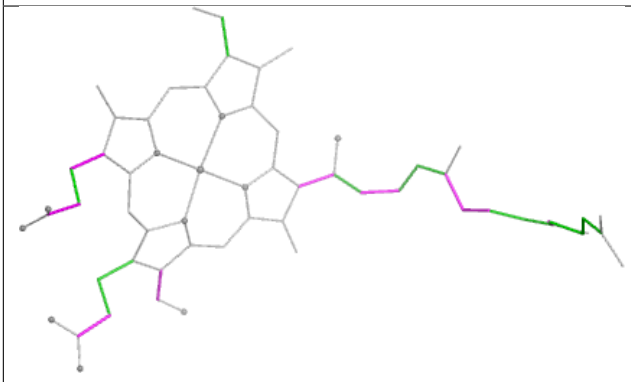
Ligand HEA R 603



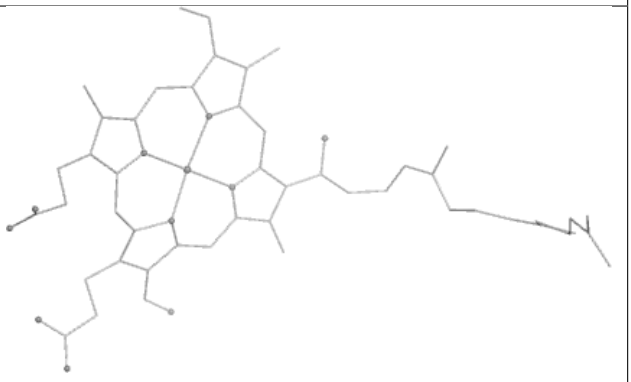
Bond lengths



Bond angles

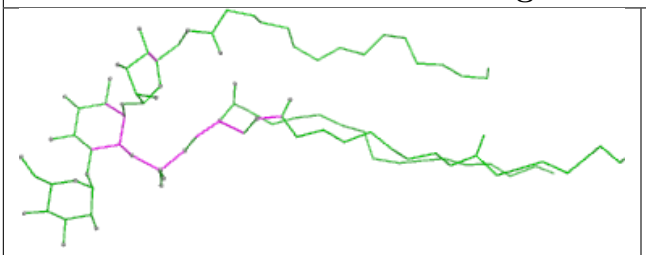


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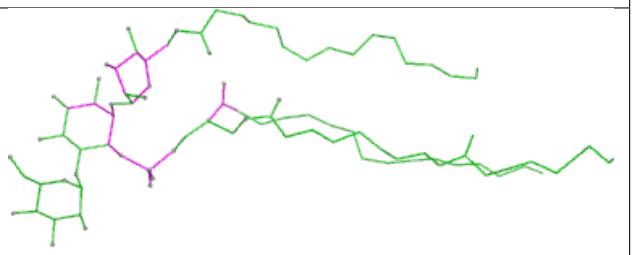


Rings

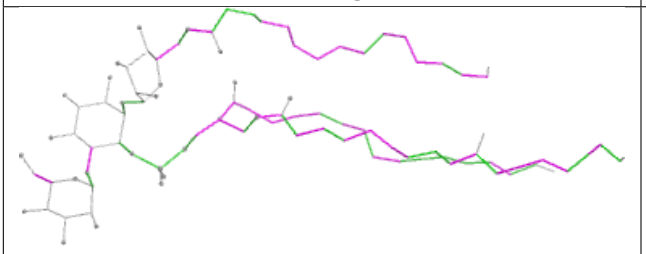
Ligand WUO P 302



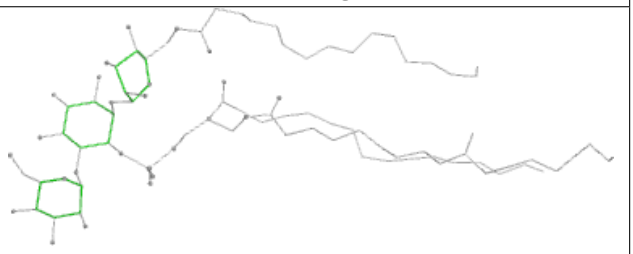
Bond lengths



Bond angles

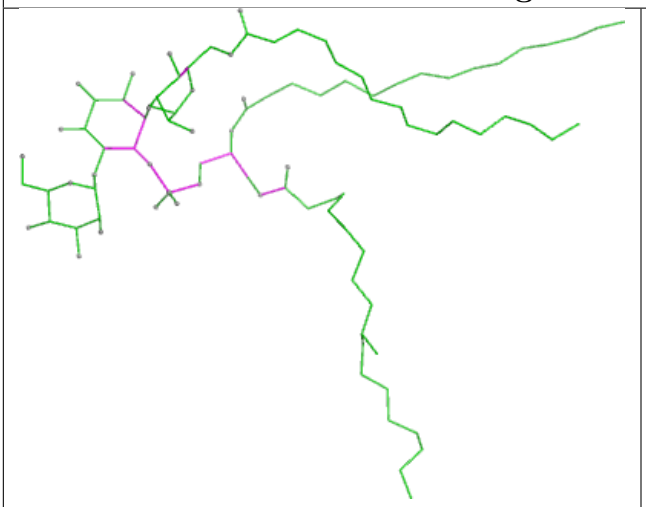


Torsions

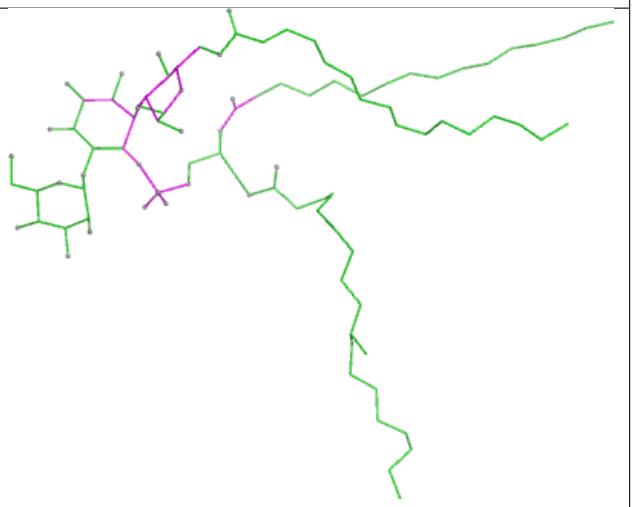


Rings

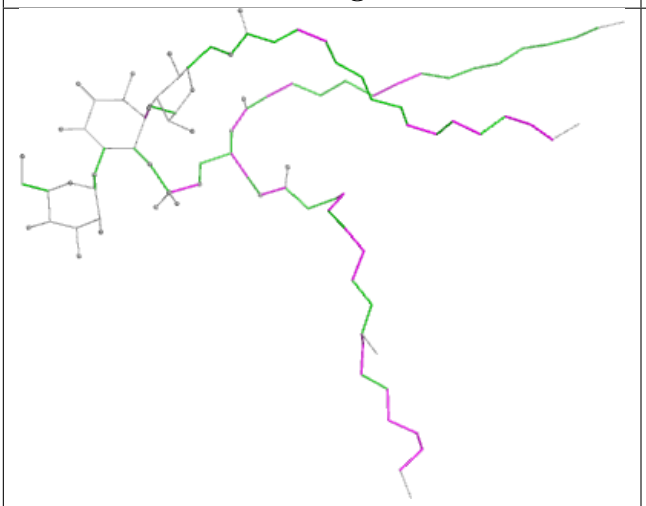
Ligand WUO O 302



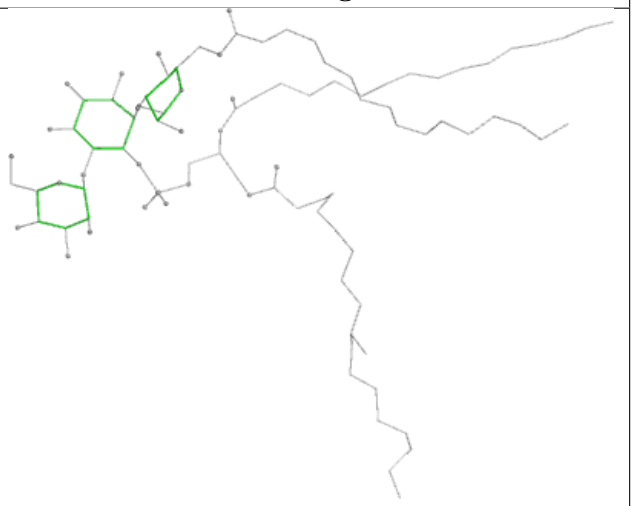
Bond lengths



Bond angles

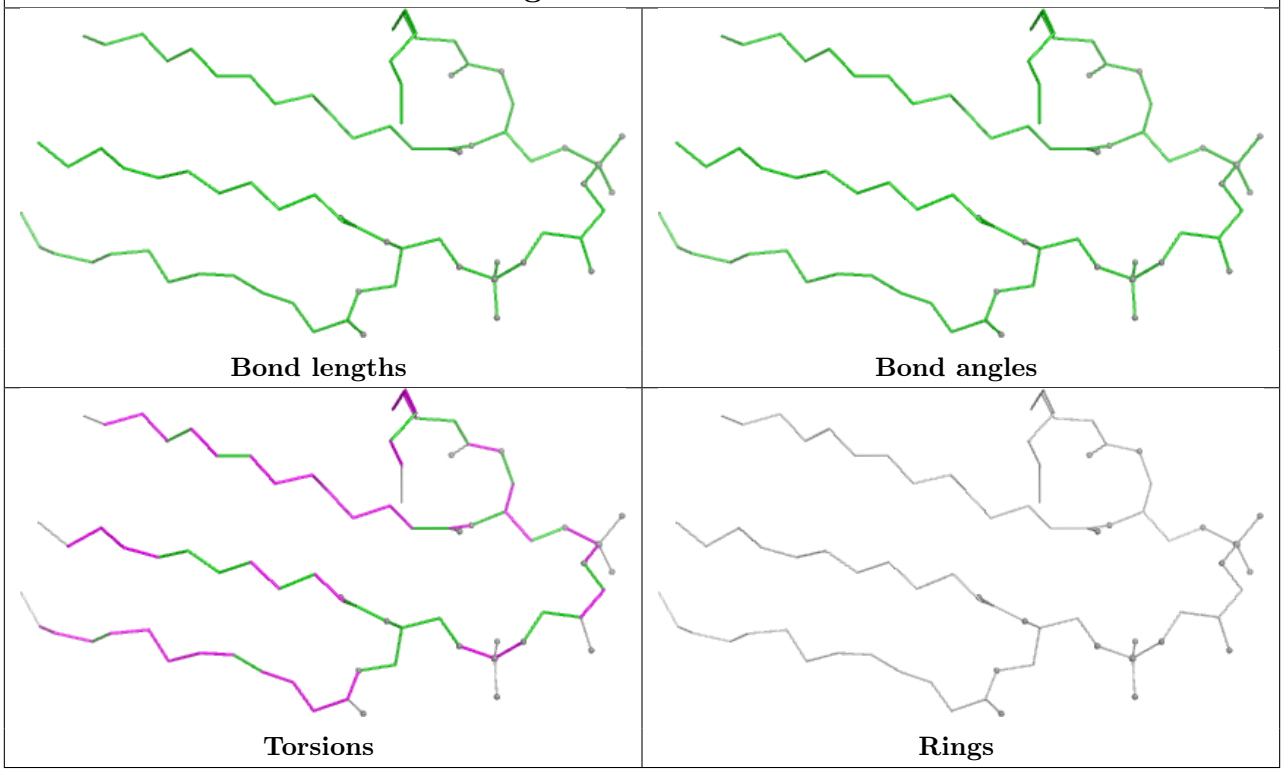


Torsions

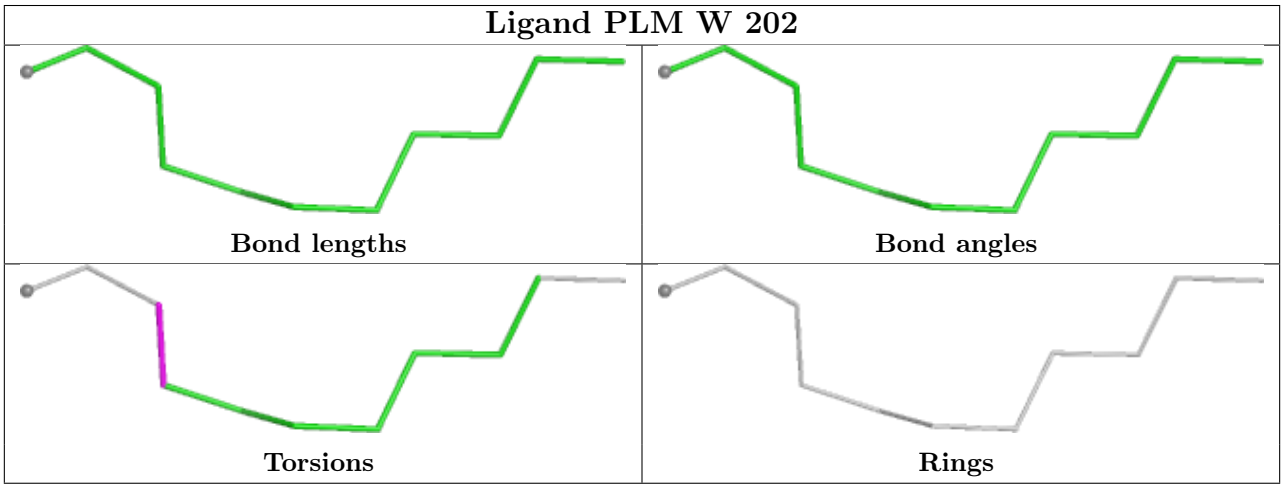


Rings

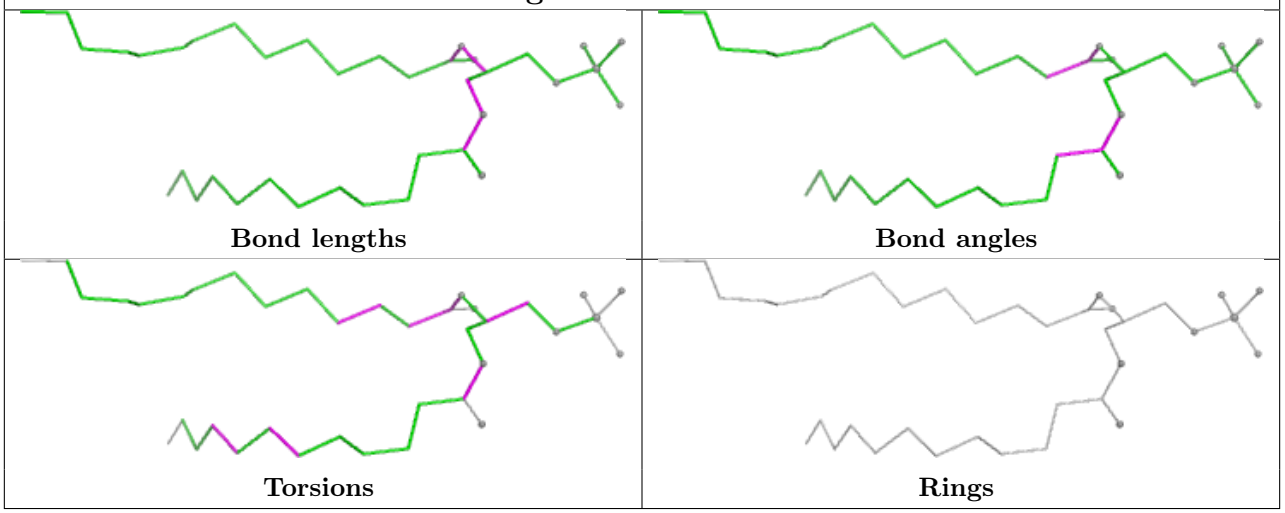
Ligand CDL N 602



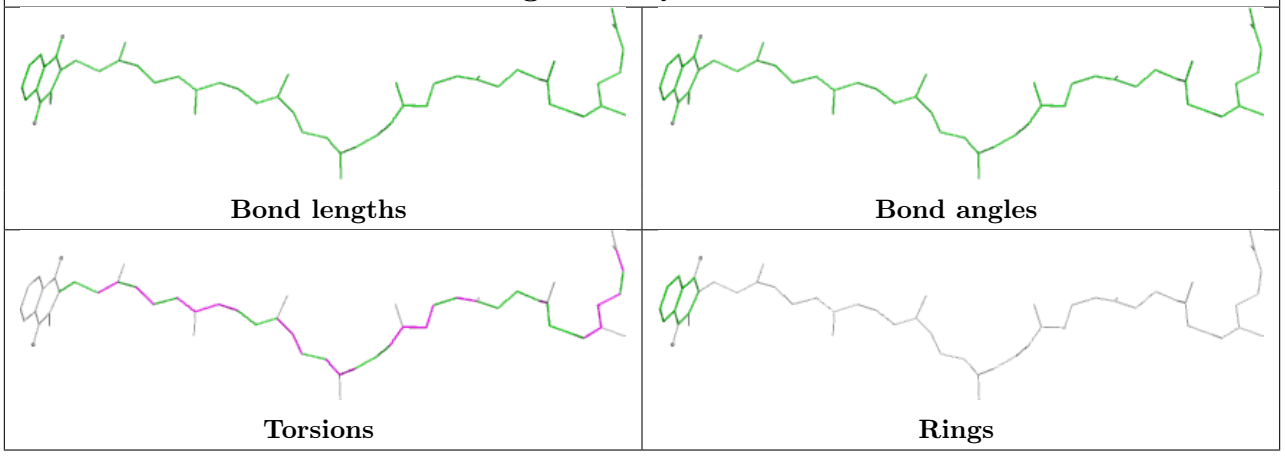
Ligand PLM W 202



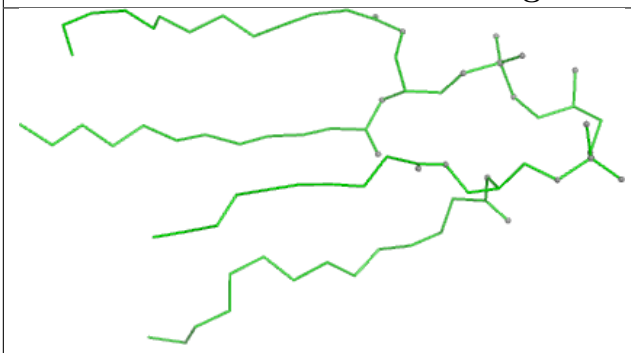
Ligand 7PH G 504



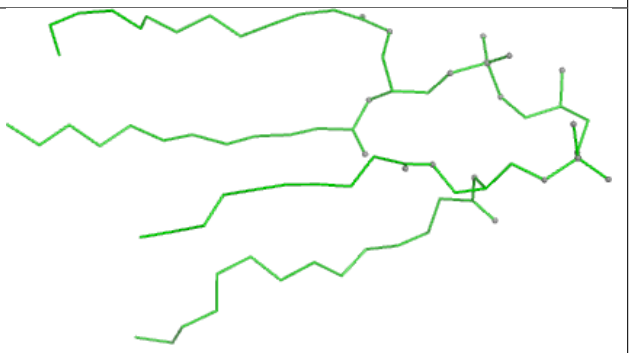
Ligand MQ9 H 607



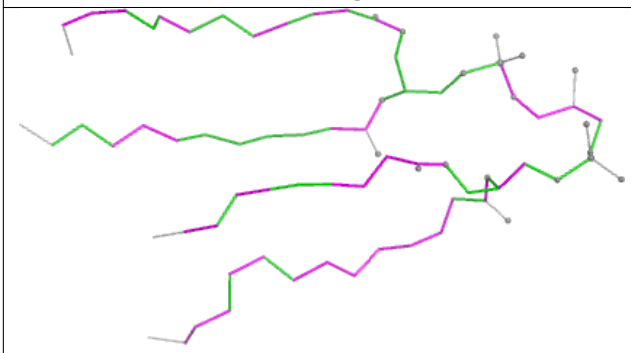
Ligand CDL H 604



Bond lengths



Bond angles

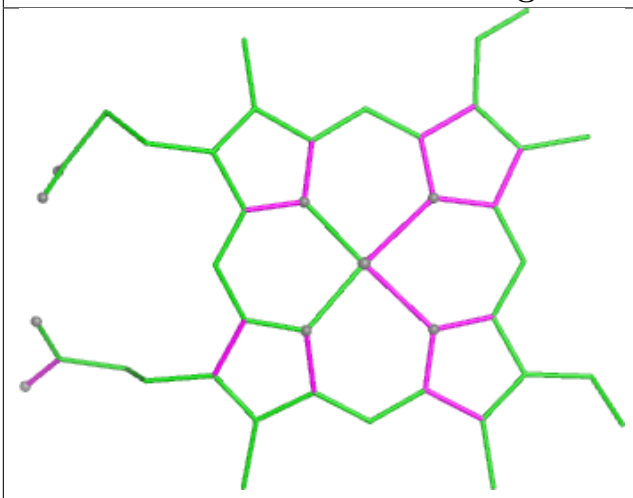


Torsions

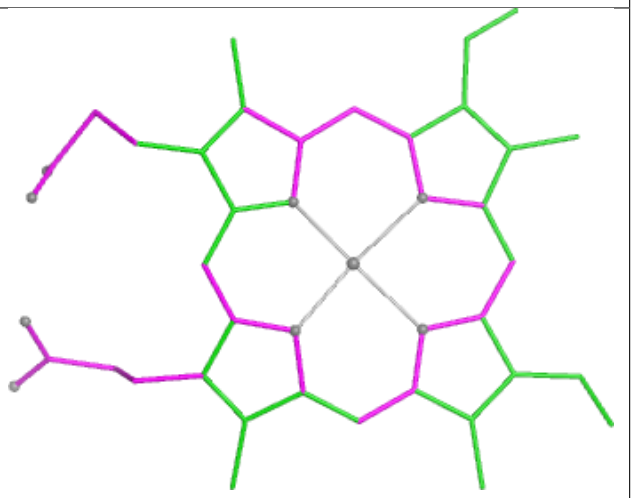


Rings

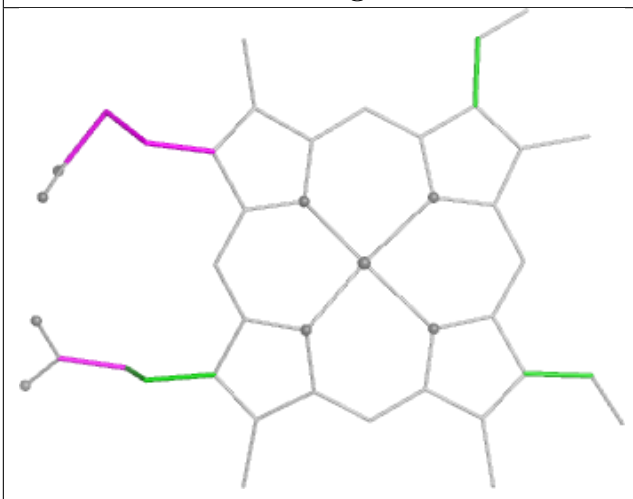
Ligand HEM N 601



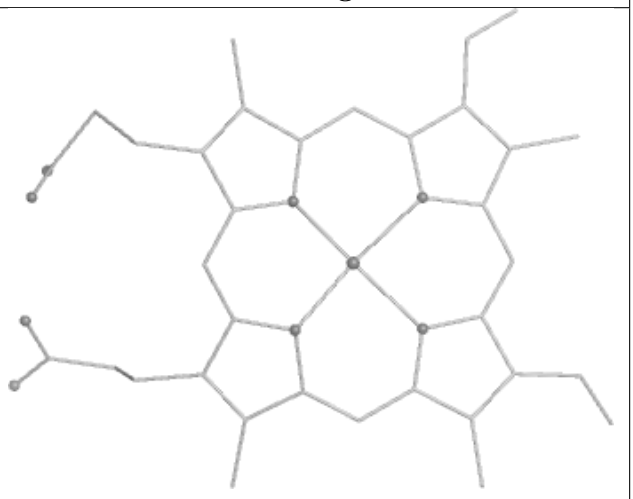
Bond lengths



Bond angles

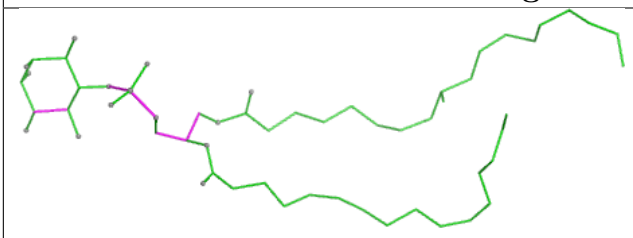


Torsions

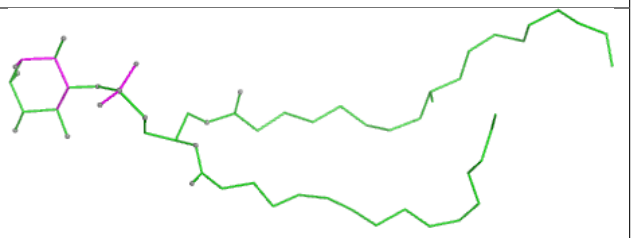


Rings

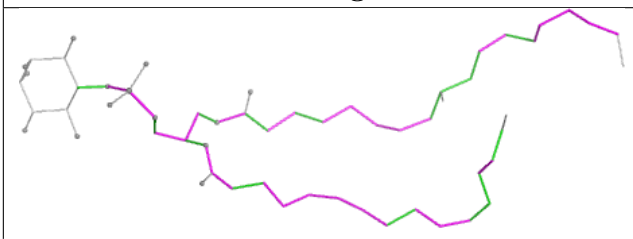
Ligand 9YF W 201



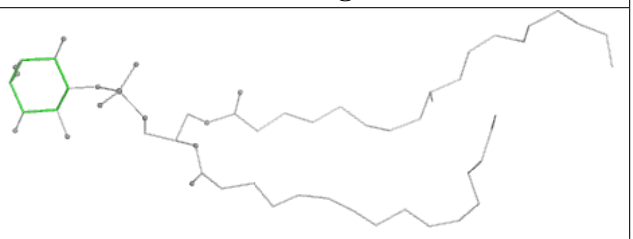
Bond lengths



Bond angles

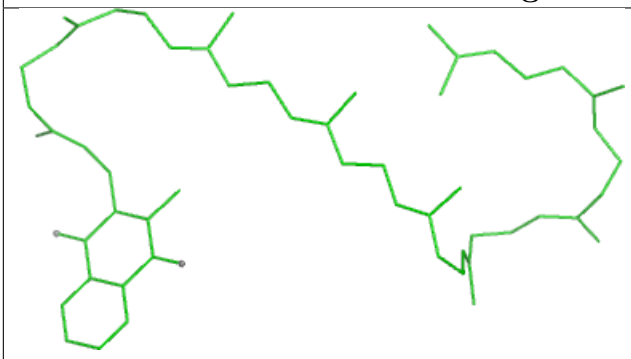


Torsions

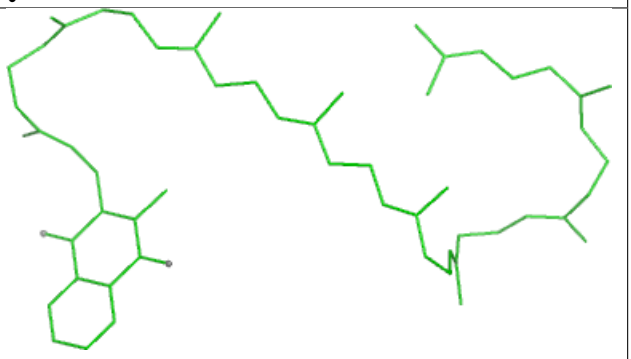


Rings

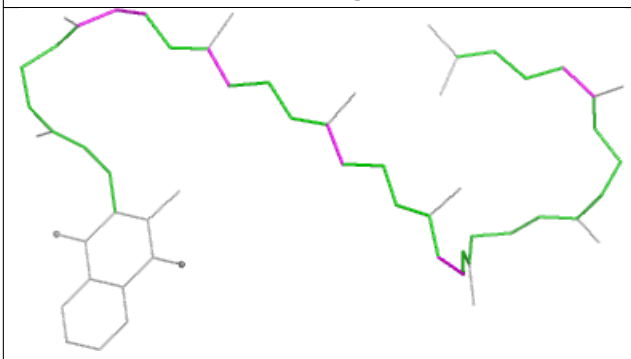
Ligand MQ9 O 301



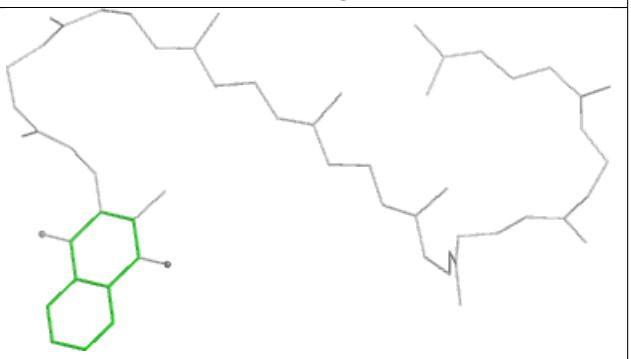
Bond lengths



Bond angles

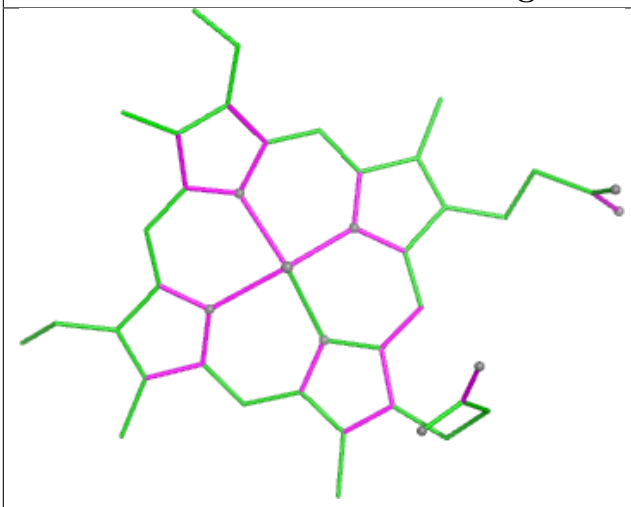


Torsions

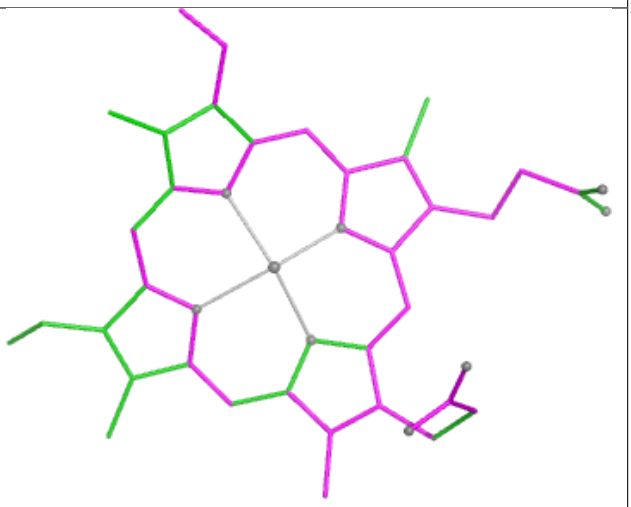


Rings

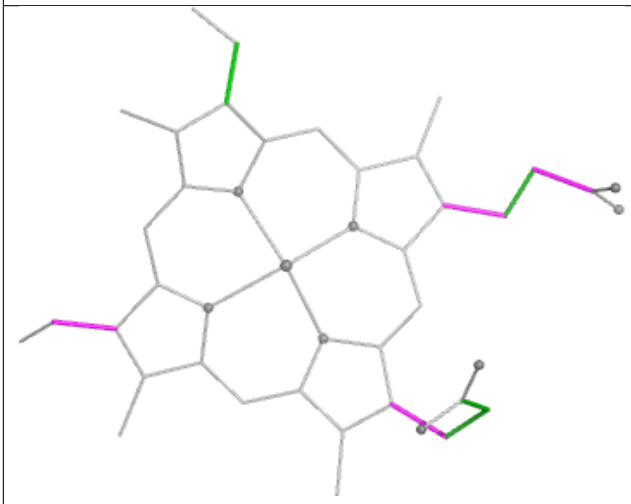
Ligand HEM H 605



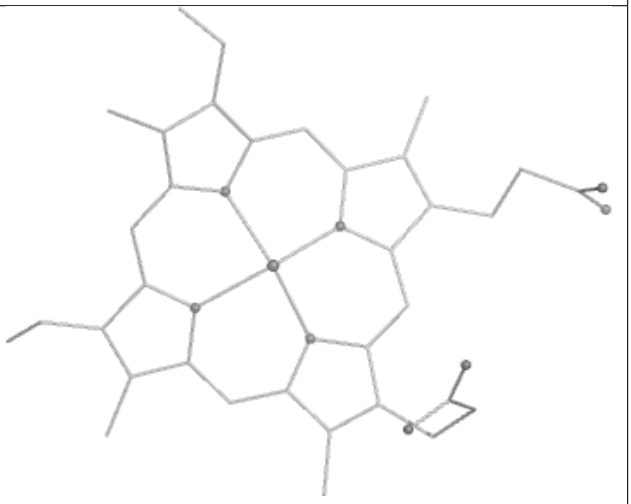
Bond lengths



Bond angles

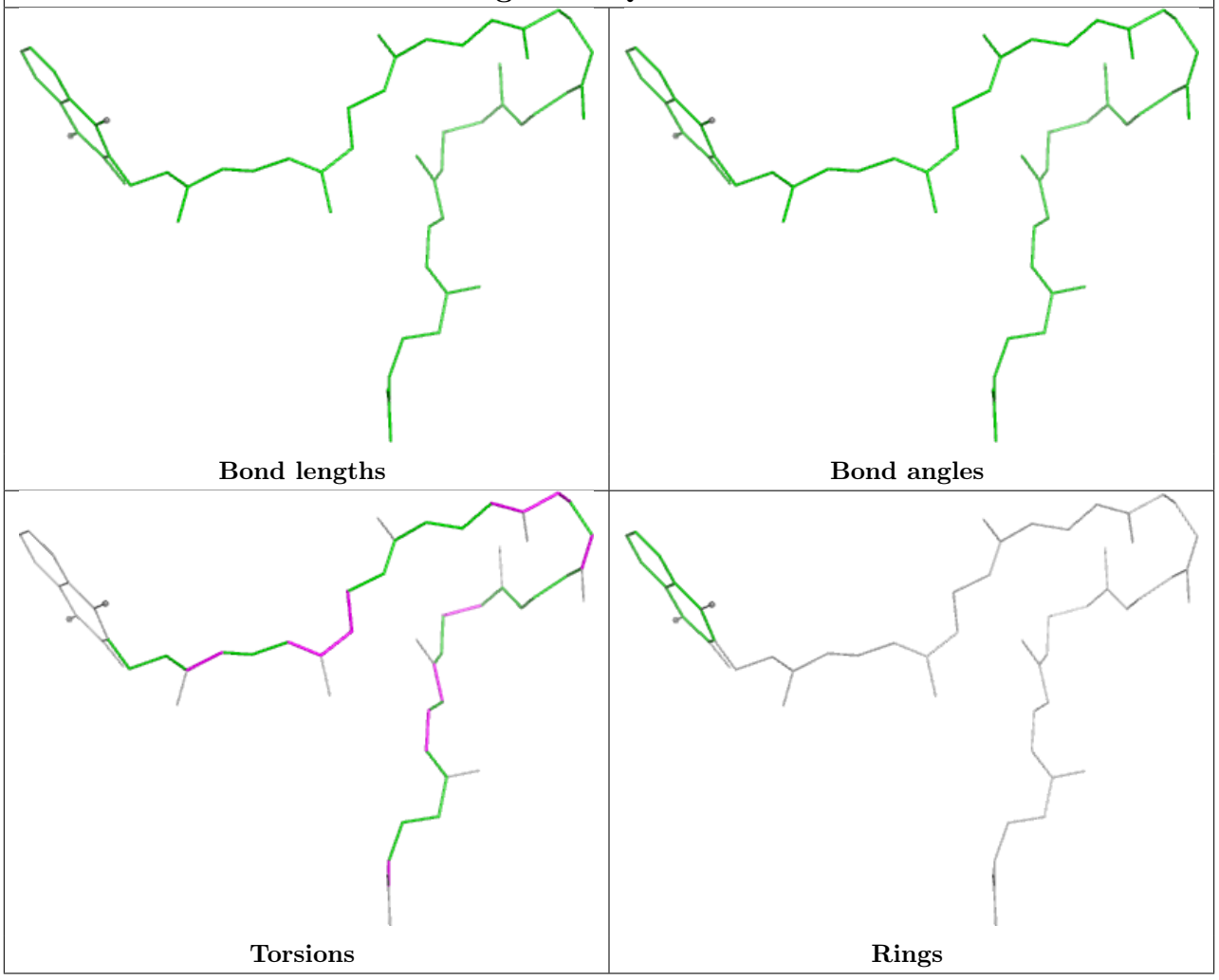


Torsions



Rings

Ligand MQ9 O 305



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.

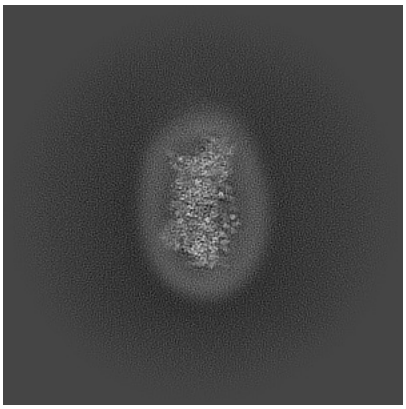
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50752. These allow visual inspection of the internal detail of the map and identification of artifacts.

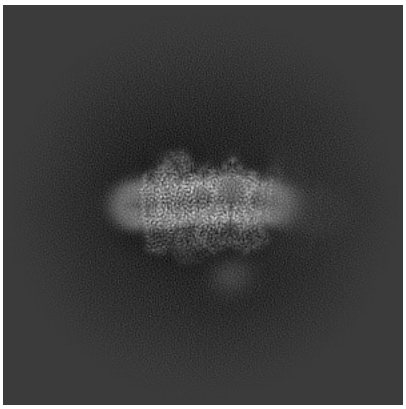
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

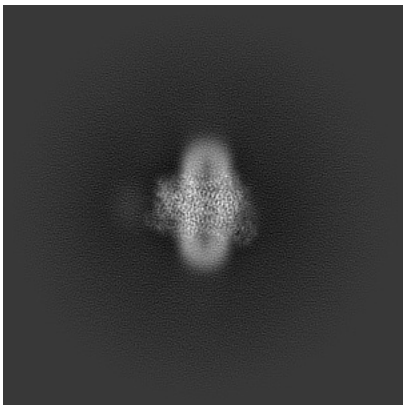
6.1.1 Primary map



X

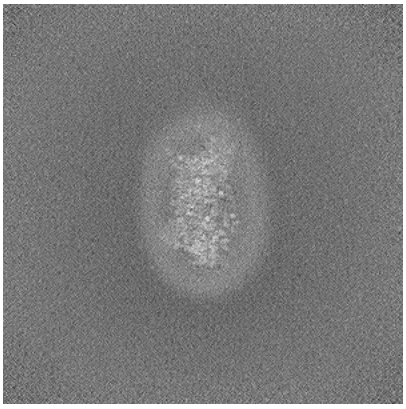


Y

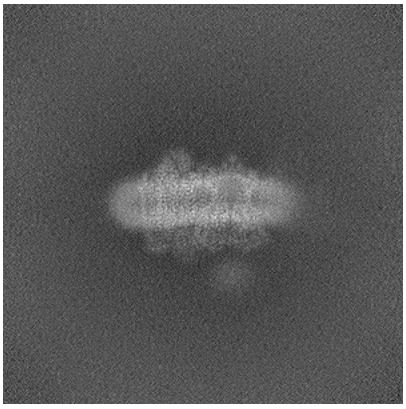


Z

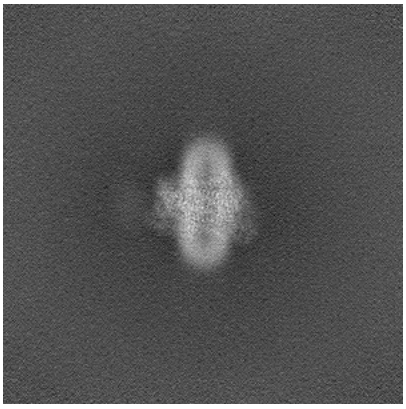
6.1.2 Raw map



X



Y

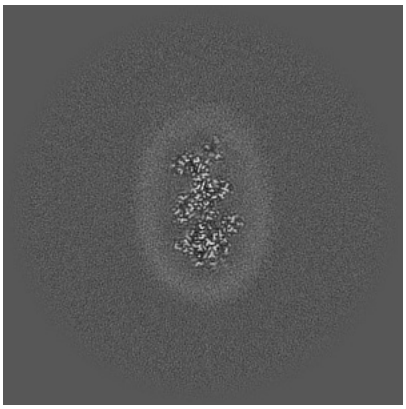


Z

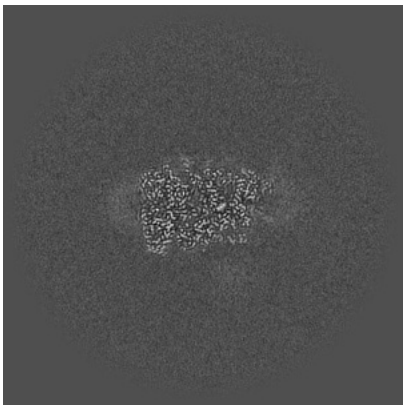
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

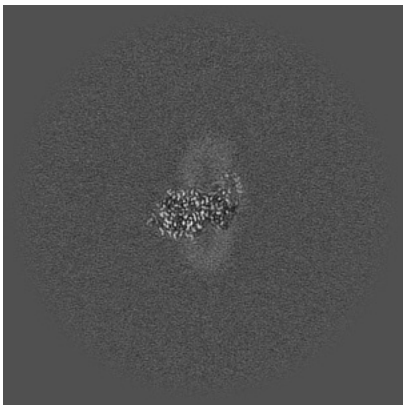
6.2.1 Primary map



X Index: 270

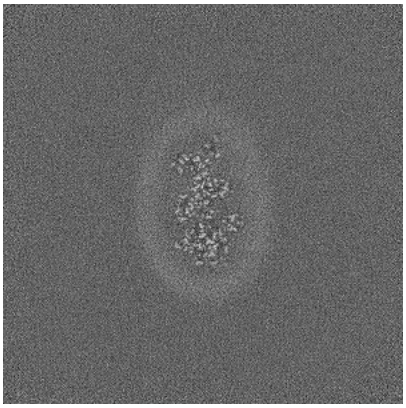


Y Index: 270

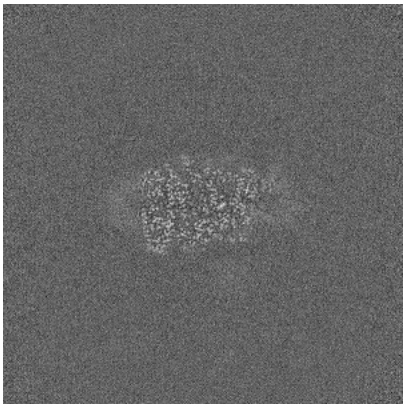


Z Index: 270

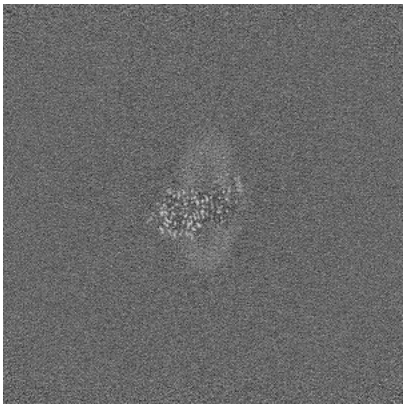
6.2.2 Raw map



X Index: 270



Y Index: 270

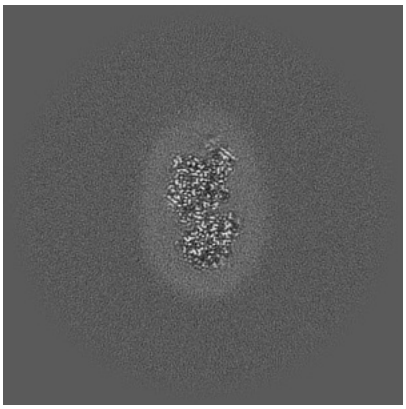


Z Index: 270

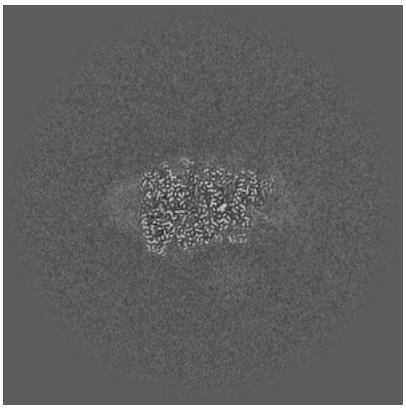
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

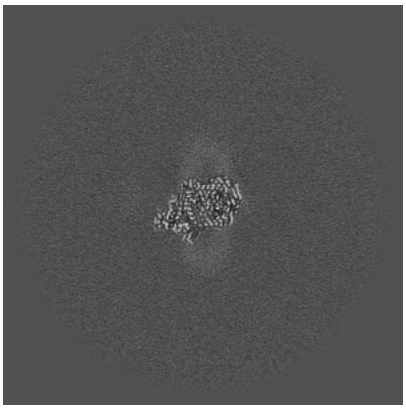
6.3.1 Primary map



X Index: 255

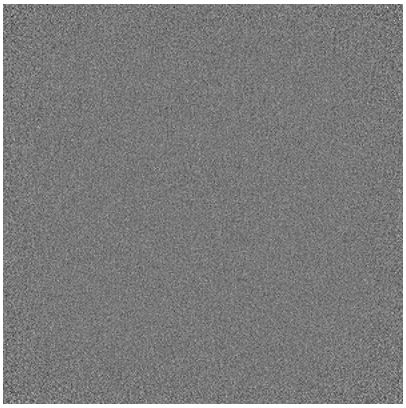


Y Index: 271

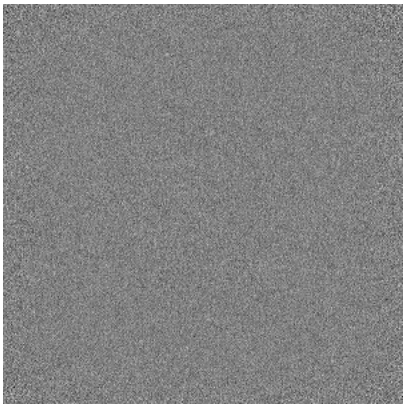


Z Index: 283

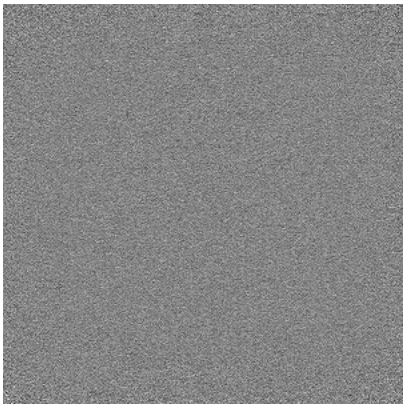
6.3.2 Raw map



X Index: 0



Y Index: 0

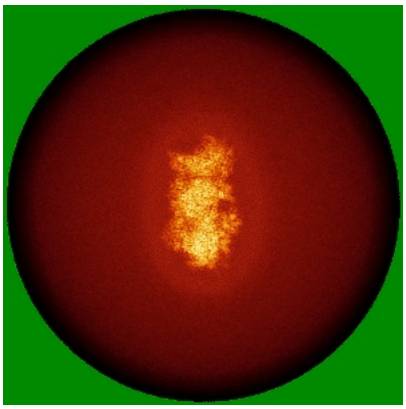


Z Index: 539

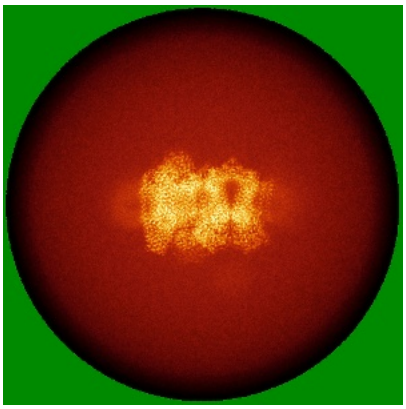
The images above show the largest variance slices of the map in three orthogonal directions.

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

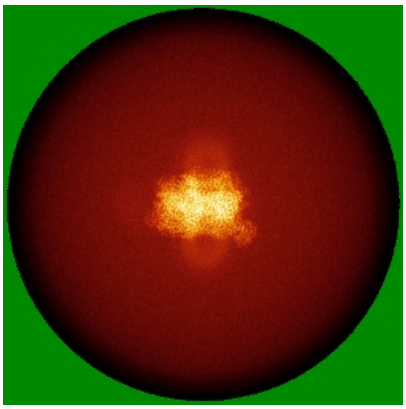
6.4.1 Primary map



X

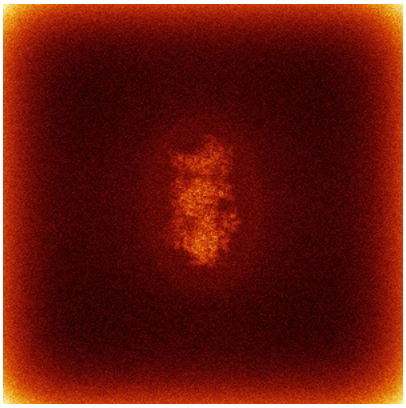


Y

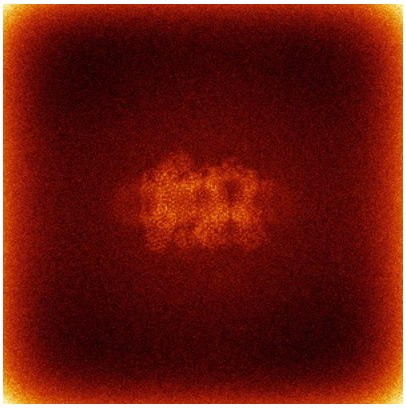


Z

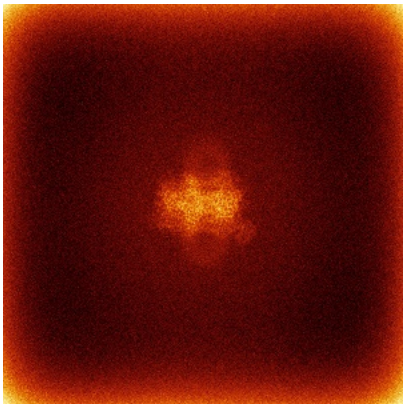
6.4.2 Raw map



X



Y

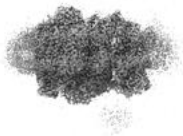
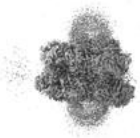


Z

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)

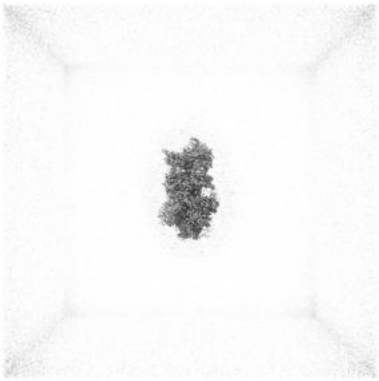
6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.176. 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.

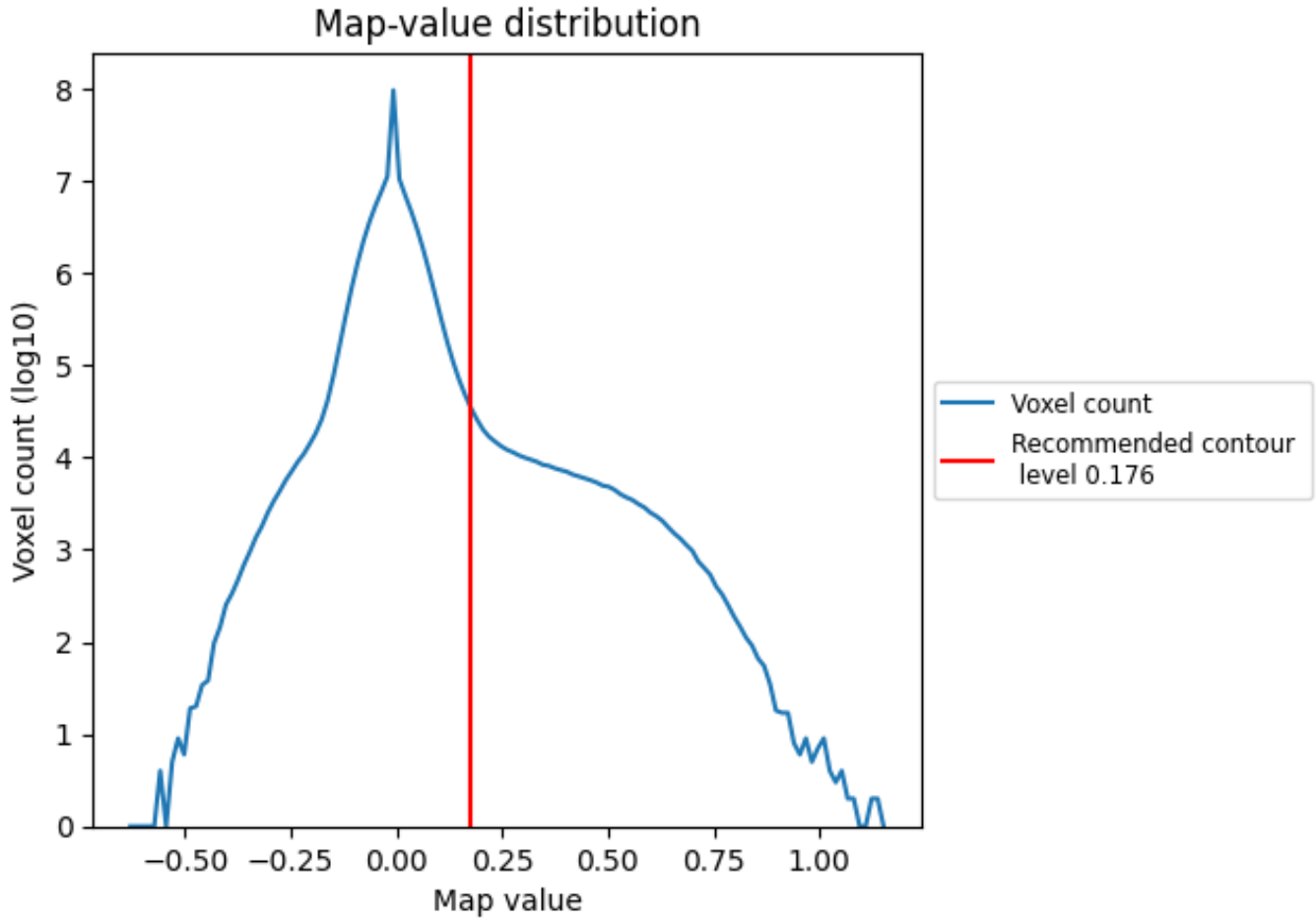
6.6 Mask visualisation (i)

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

7 Map analysis

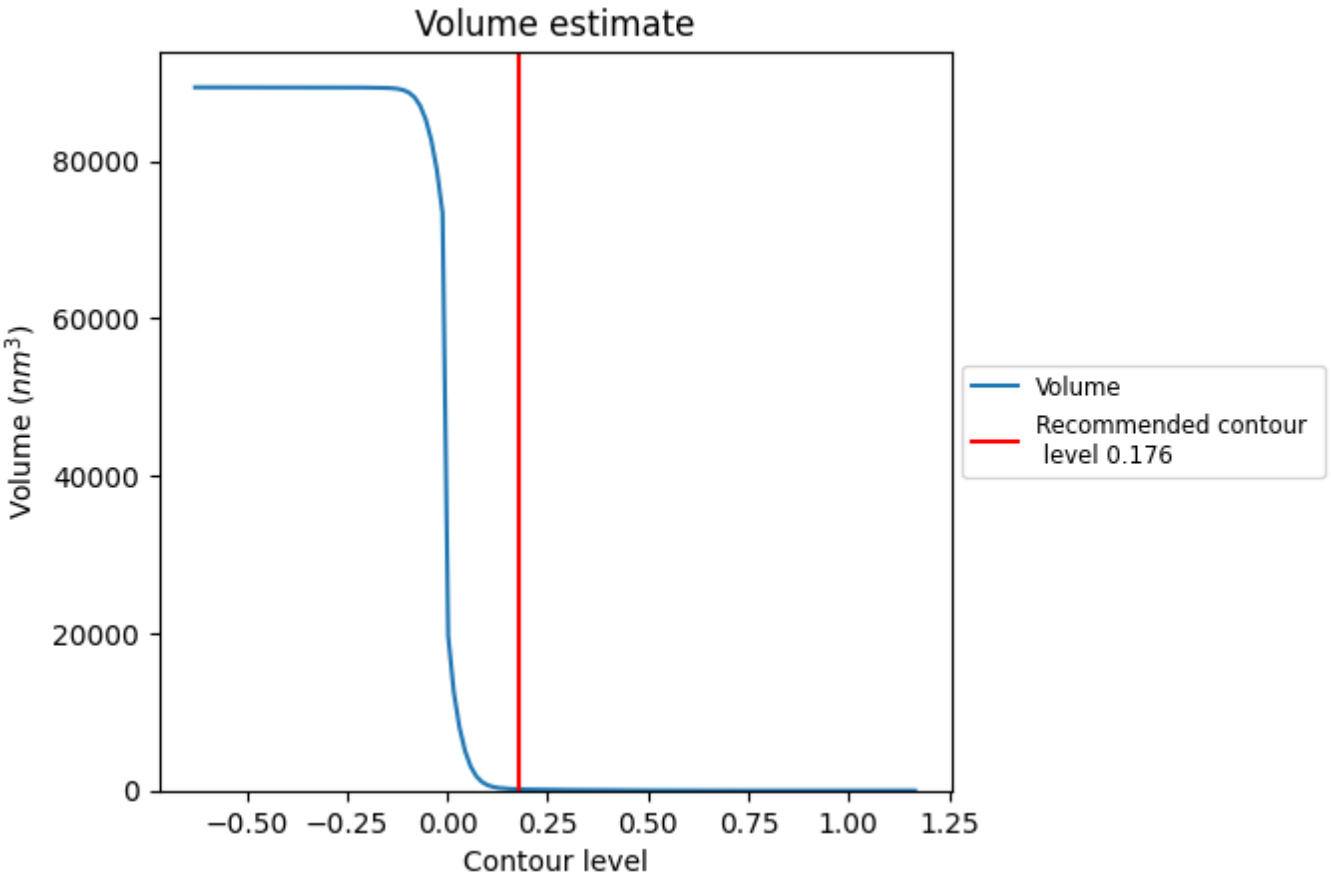
This section contains the results of statistical analysis of the map.

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.

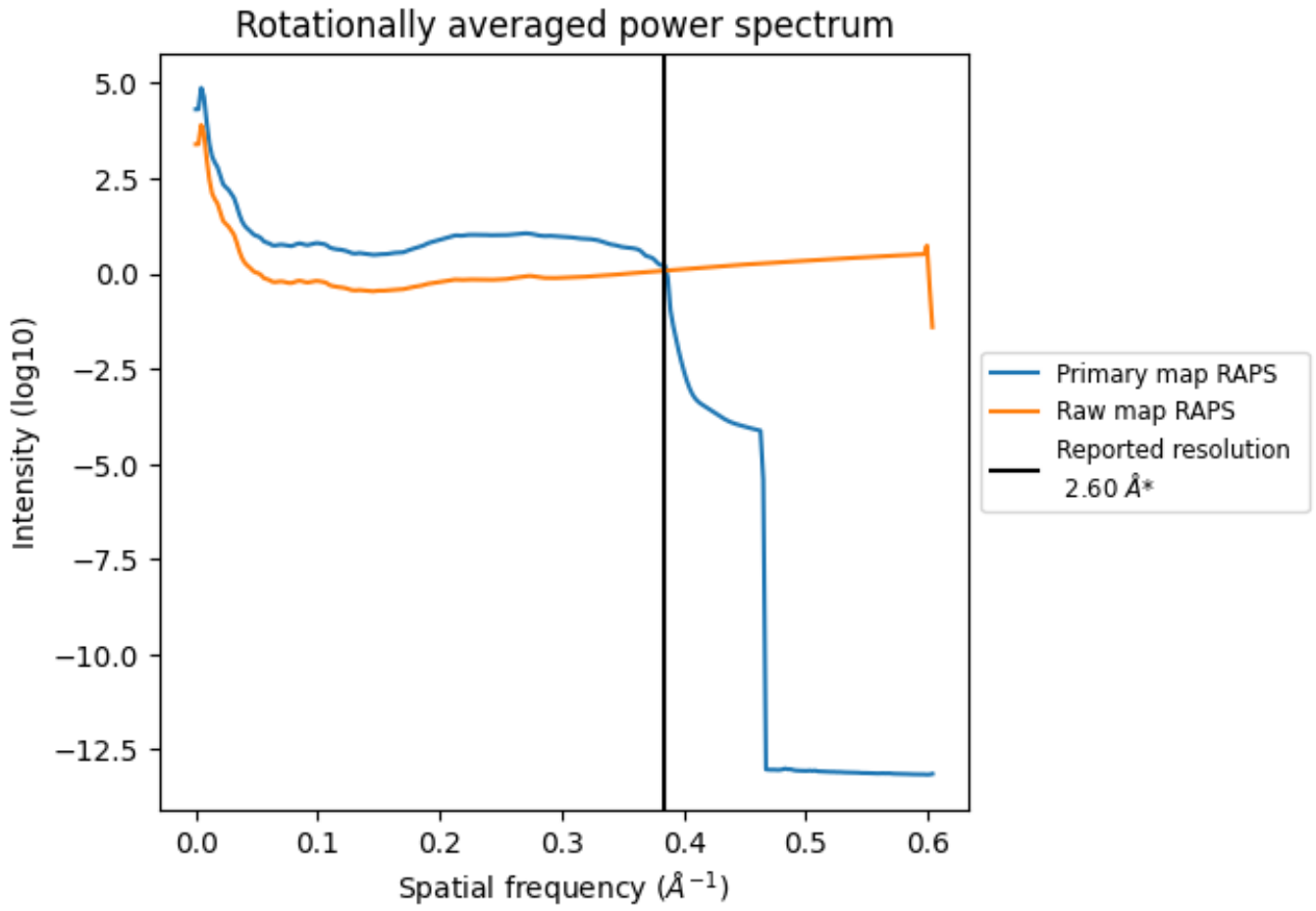
7.2 Volume estimate (i)



The volume at the recommended contour level is 174 nm^3; this corresponds to an approximate mass of 158 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)

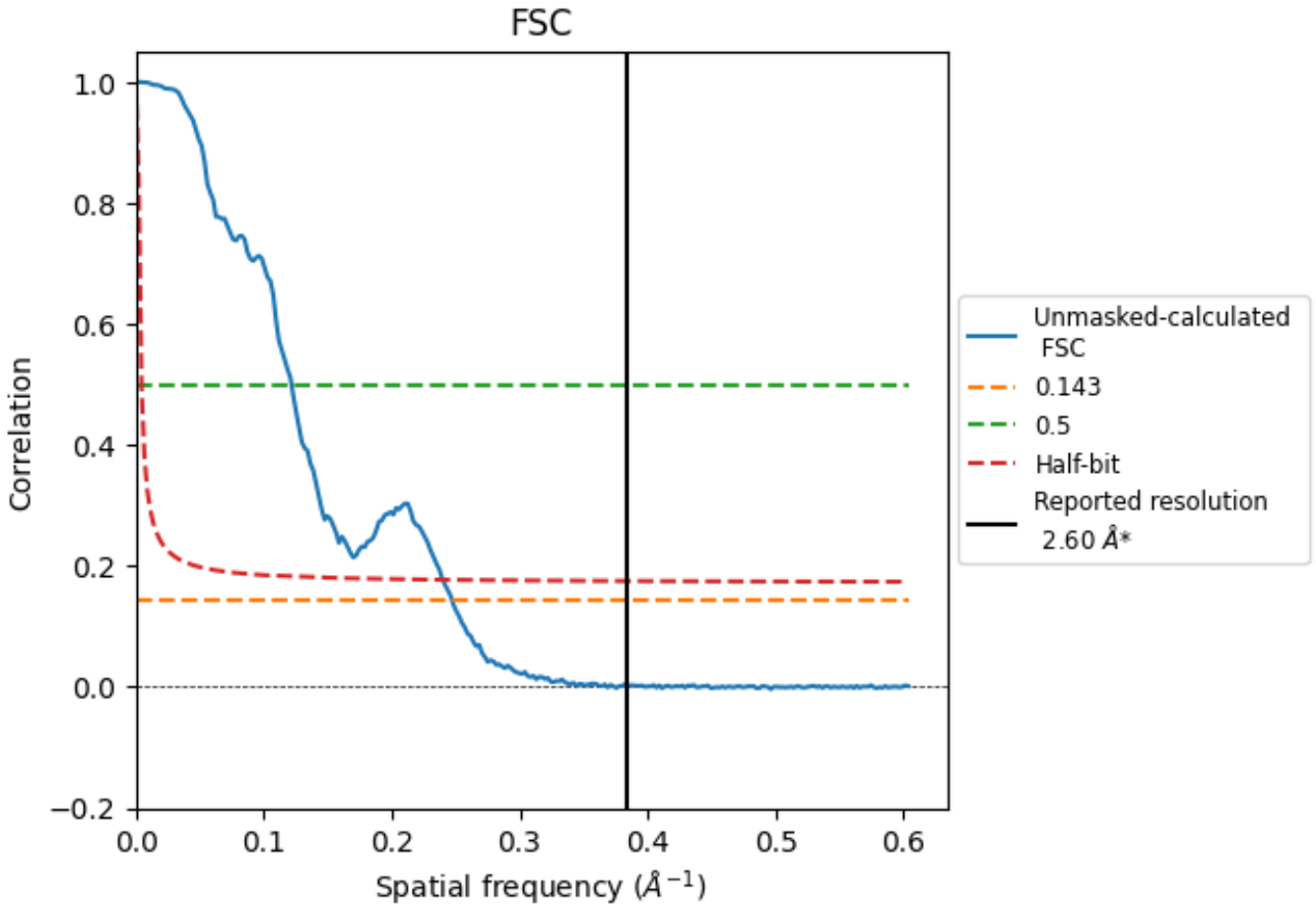


*Reported resolution corresponds to spatial frequency of 0.385 $Å^{-1}$

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

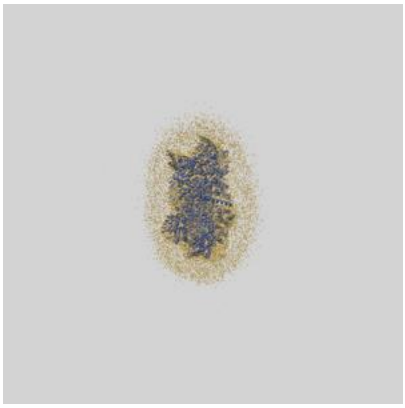
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	8.22	4.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 2.6 by more than 10 %

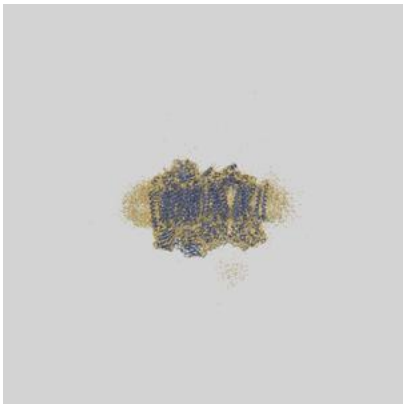
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50752 and PDB model 9FTZ. Per-residue inclusion information can be found in section 3 on page 20.

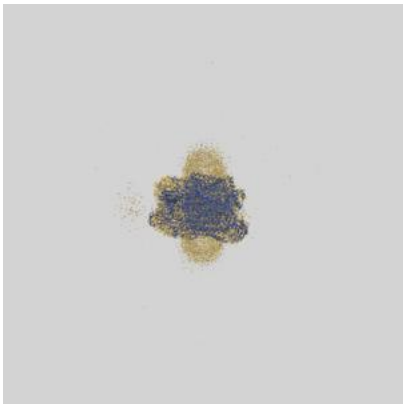
9.1 Map-model overlay



X



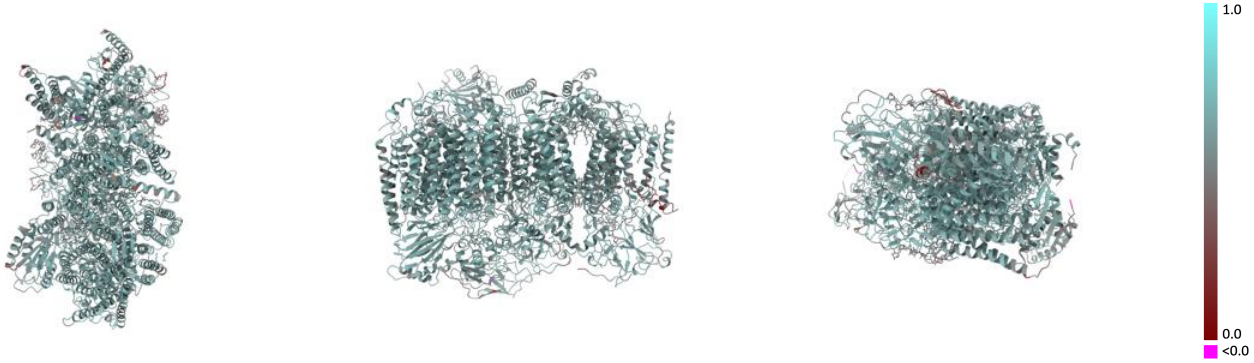
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.176 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.

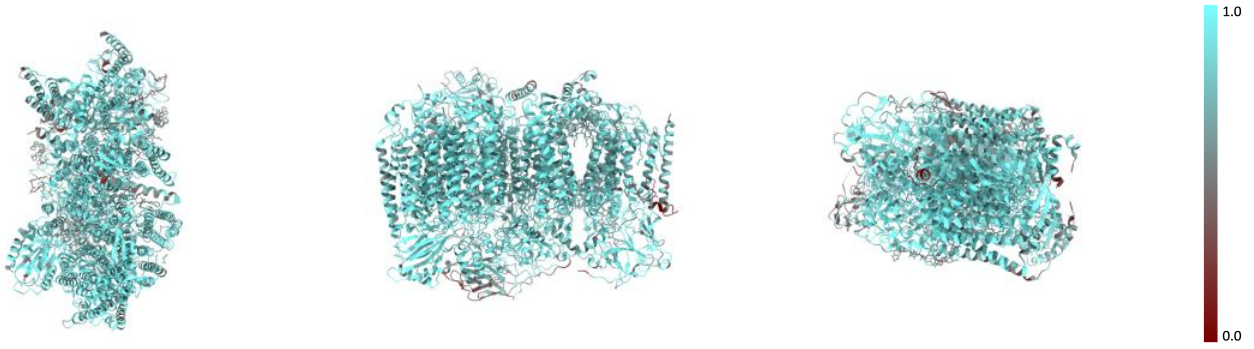
9.2 Q-score mapped to coordinate model (i)



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.

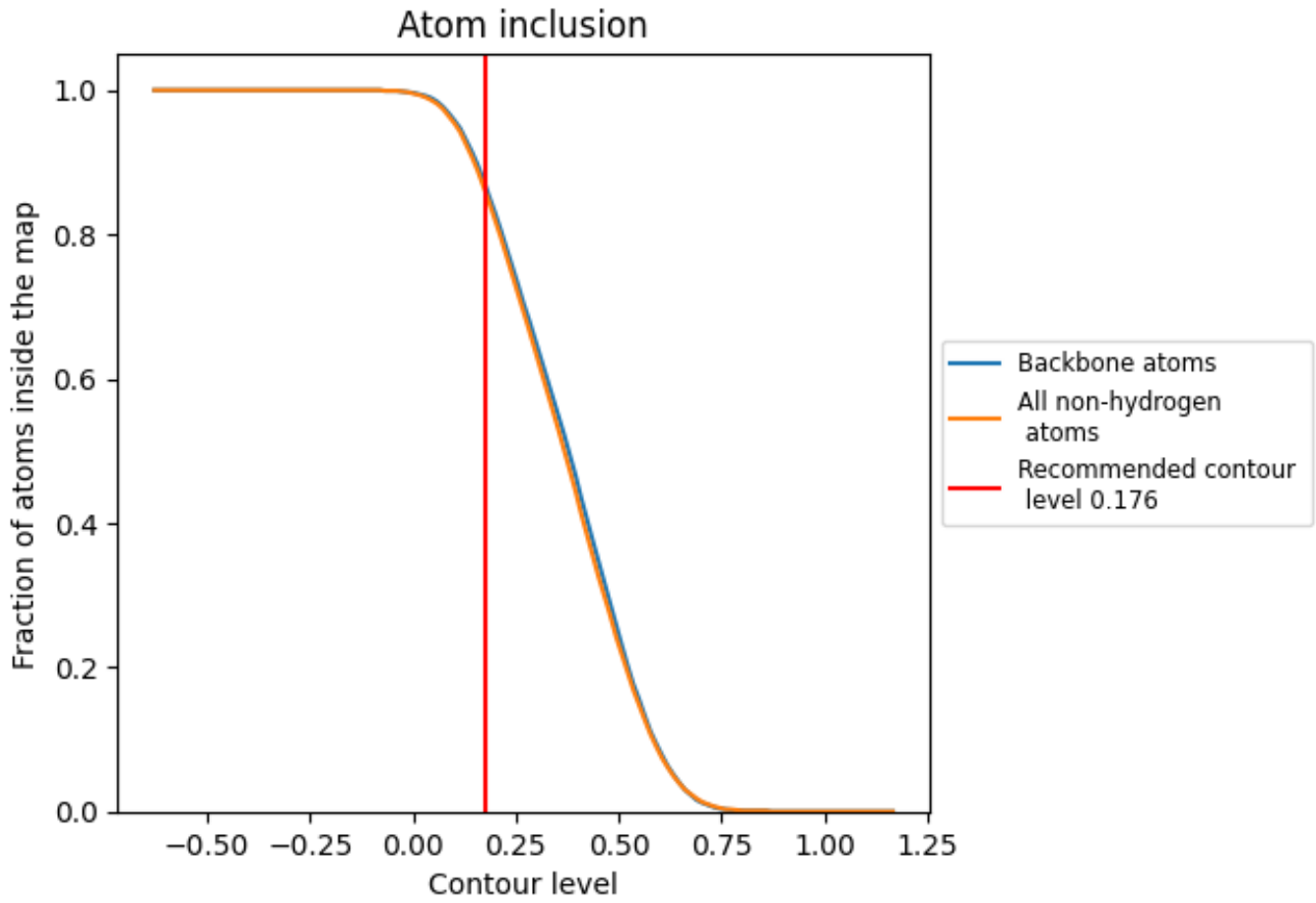
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.176).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.176) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8590	0.6080
G	0.8170	0.5840
H	0.8320	0.5930
M	0.8750	0.6110
N	0.9070	0.6320
O	0.8950	0.6260
P	0.8530	0.6170
Q	0.8670	0.6050
R	0.9280	0.6360
S	0.8760	0.6200
T	0.8780	0.6130
U	0.8230	0.5720
V	0.8340	0.5880
W	0.5750	0.5390
Y	0.7380	0.5430
c	0.6240	0.4640

