wwPDB EM Validation Summary Report (i)

Apr 8, 2025 – 07:33 am BST

PDB ID	:	9GY6 / pdb_00009gy6
EMDB ID	:	EMD-51689
Title	:	Mycobacterial cytochrome bc1:aa3 with inhibitor
Authors	:	lamers, M.H.; Verma, A.K.
Deposited on	:	2024-10-01
Resolution	:	3.10 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:

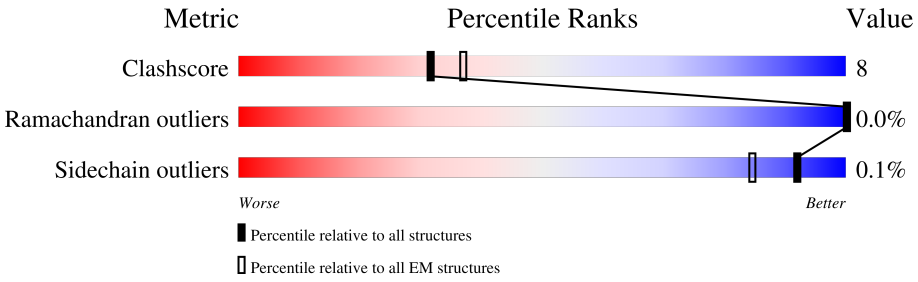
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.10 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	A	421	79% 10% 10%
1	M	421	75% 14% 10%
2	B	546	81% 16%
2	N	546	81% 16%
3	C	268	68% 15% 17%
3	O	268	70% 13% 17%
4	D	84	67% 21% 12%
4	P	84	5% 69% 19% 12%

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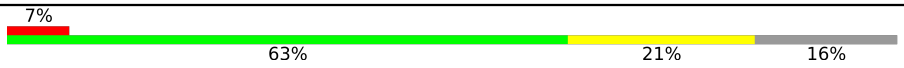
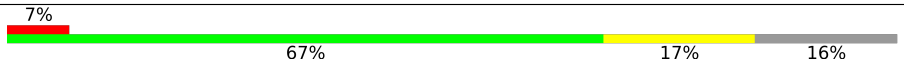
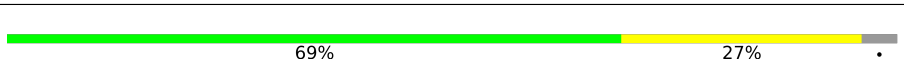
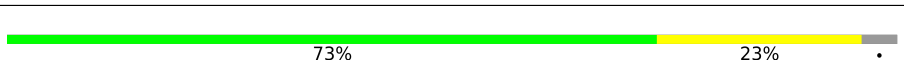
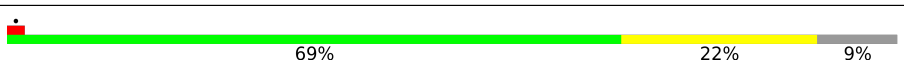
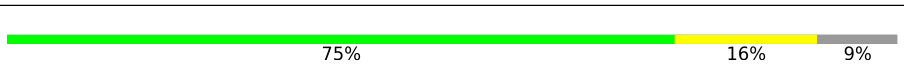
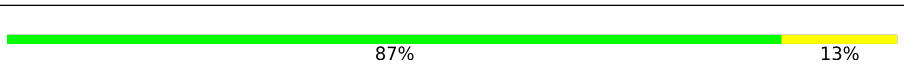
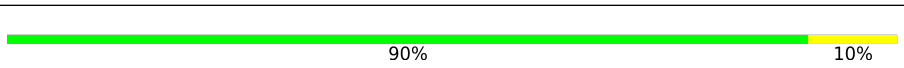
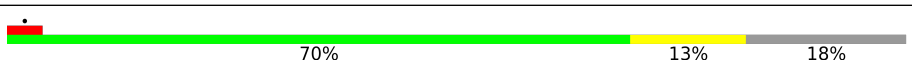
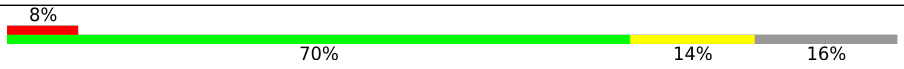
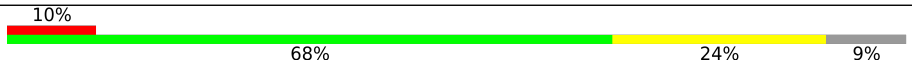
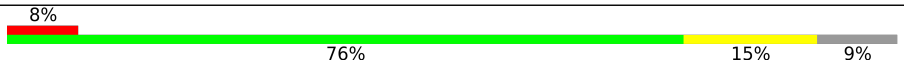
Mol	Chain	Length	Quality of chain
5	E	341	
5	Q	341	
6	F	575	
6	R	575	
7	G	203	
7	S	203	
8	H	139	
8	T	139	
9	I	79	
9	U	79	
10	J	157	
10	V	157	
11	L	236	
11	X	236	

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 43307 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 Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	377	Total	C	N	O	S	0	0
			2947	1907	498	531	11		
1	M	377	Total	C	N	O	S	0	0
			2942	1904	496	531	11		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0R051
A	2	ASP	-	expression tag	UNP A0R051
A	3	TYR	-	expression tag	UNP A0R051
A	4	ARG	-	expression tag	UNP A0R051
A	5	ASN	-	expression tag	UNP A0R051
A	6	GLY	-	expression tag	UNP A0R051
A	7	GLY	-	expression tag	UNP A0R051
A	8	ARG	-	expression tag	UNP A0R051
A	9	HIS	-	expression tag	UNP A0R051
A	10	ARG	-	expression tag	UNP A0R051
A	11	CYS	-	expression tag	UNP A0R051
A	12	GLY	-	expression tag	UNP A0R051
A	13	HIS	-	expression tag	UNP A0R051
A	14	VAL	-	expression tag	UNP A0R051
M	1	MET	-	initiating methionine	UNP A0R051
M	2	ASP	-	expression tag	UNP A0R051
M	3	TYR	-	expression tag	UNP A0R051
M	4	ARG	-	expression tag	UNP A0R051
M	5	ASN	-	expression tag	UNP A0R051
M	6	GLY	-	expression tag	UNP A0R051
M	7	GLY	-	expression tag	UNP A0R051
M	8	ARG	-	expression tag	UNP A0R051
M	9	HIS	-	expression tag	UNP A0R051
M	10	ARG	-	expression tag	UNP A0R051
M	11	CYS	-	expression tag	UNP A0R051
M	12	GLY	-	expression tag	UNP A0R051

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Chain	Residue	Modelled	Actual	Comment	Reference
M	13	HIS	-	expression tag	UNP A0R051
M	14	VAL	-	expression tag	UNP A0R051

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	531	Total	C	N	O	S	0	0
			4153	2734	705	696	18		
2	N	534	Total	C	N	O	S	0	0
			4176	2747	710	701	18		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	156	TYR	PHE	engineered mutation	UNP A0R052
B	182	MET	ILE	engineered mutation	UNP A0R052
B	189	LEU	MET	engineered mutation	UNP A0R052
B	309	GLU	ASP	engineered mutation	UNP A0R052
B	312	ALA	ILE	engineered mutation	UNP A0R052
N	156	TYR	PHE	engineered mutation	UNP A0R052
N	182	MET	ILE	engineered mutation	UNP A0R052
N	189	LEU	MET	engineered mutation	UNP A0R052
N	309	GLU	ASP	engineered mutation	UNP A0R052
N	312	ALA	ILE	engineered mutation	UNP A0R052

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

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

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	74	Total	C	N	O	S	0	0
			590	387	108	91	4		
4	P	74	Total	C	N	O	S	0	0
			590	387	108	91	4		

- Molecule 5 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	285	Total	C	N	O	S	0	0
			2271	1472	375	415	9		
5	Q	285	Total	C	N	O	S	0	0
			2271	1472	375	415	9		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	551	Total	C	N	O	S	0	0
			4364	2933	694	711	26		
6	R	551	Total	C	N	O	S	0	0
			4364	2933	694	711	26		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	initiating methionine	UNP A0A2U9PNL2
F	2	VAL	-	expression tag	UNP A0A2U9PNL2
F	3	ALA	-	expression tag	UNP A0A2U9PNL2
F	4	GLU	-	expression tag	UNP A0A2U9PNL2
F	5	ALA	-	expression tag	UNP A0A2U9PNL2
F	6	PRO	-	expression tag	UNP A0A2U9PNL2
F	7	PRO	-	expression tag	UNP A0A2U9PNL2
F	8	ILE	-	expression tag	UNP A0A2U9PNL2
F	9	GLY	-	expression tag	UNP A0A2U9PNL2
F	10	GLU	-	expression tag	UNP A0A2U9PNL2
F	11	LEU	-	expression tag	UNP A0A2U9PNL2
F	12	GLU	-	expression tag	UNP A0A2U9PNL2
F	13	ALA	-	expression tag	UNP A0A2U9PNL2
F	14	ARG	-	expression tag	UNP A0A2U9PNL2
F	15	ARG	-	expression tag	UNP A0A2U9PNL2
F	16	PRO	-	expression tag	UNP A0A2U9PNL2
F	17	PHE	-	expression tag	UNP A0A2U9PNL2
F	18	PRO	-	expression tag	UNP A0A2U9PNL2
F	19	GLU	-	expression tag	UNP A0A2U9PNL2
F	20	ARG	-	expression tag	UNP A0A2U9PNL2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 7 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	185	Total	C	N	O	S	0	0
			1449	973	230	239	7		
7	S	185	Total	C	N	O	S	0	0
			1449	973	230	239	7		

- Molecule 8 is a protein called Cytochrome c oxidase polypeptide 4.

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

- Molecule 9 is a protein called Secreted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	65	Total	C	N	O	S	0	0
			490	324	83	82	1		
9	U	66	Total	C	N	O	S	0	0
			498	329	84	83	2		

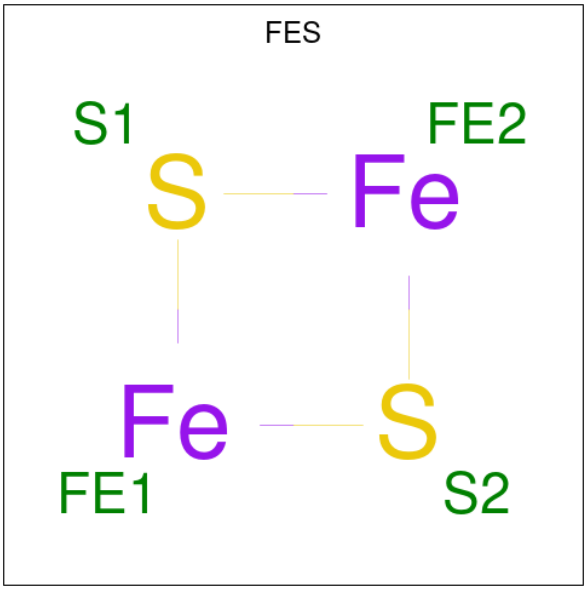
- Molecule 10 is a protein called DUF5130 domain-containing protein.

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

- Molecule 11 is a protein called Superoxide dismutase [Cu-Zn].

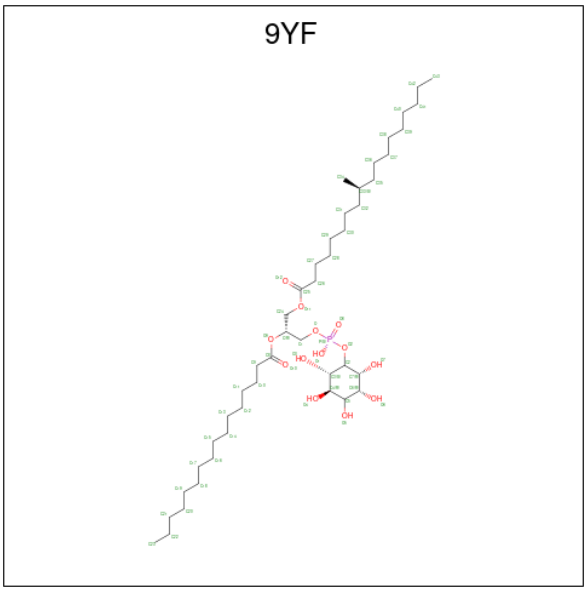
Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	28	Total	C	N	O	S	0	0
			185	113	29	42	1		
11	X	28	Total	C	N	O	S	0	0
			185	113	29	42	1		

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



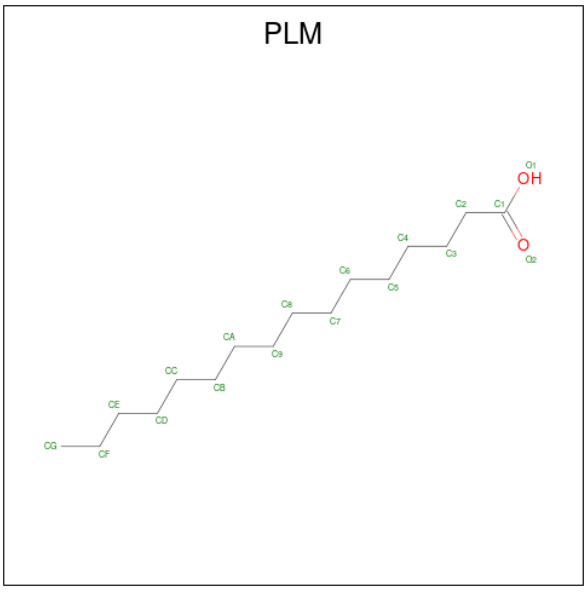
Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	Fe	S	0
			4	2	2	
12	M	1	Total	Fe	S	0
			4	2	2	

- Molecule 13 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: $C_{44}H_{85}O_{13}P$).



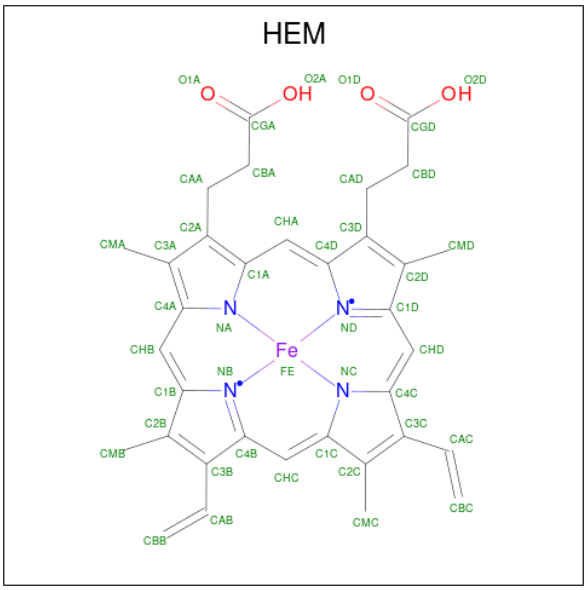
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			58	44	13	1	
13	C	1	Total	C	O	P	0
			58	44	13	1	
13	M	1	Total	C	O	P	0
			58	44	13	1	
13	O	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 14 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



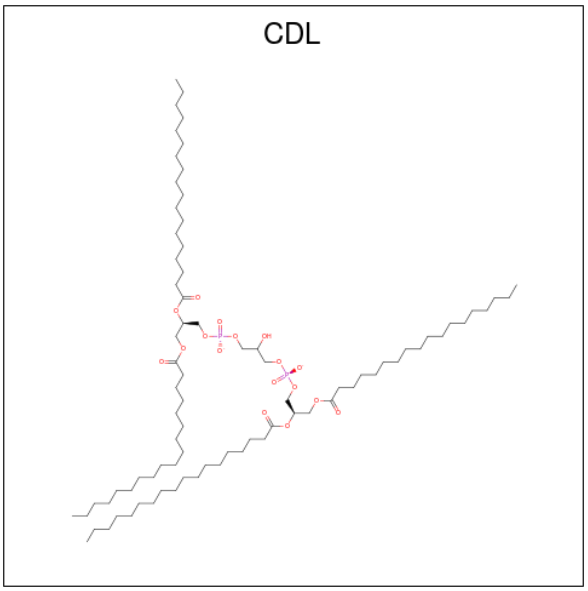
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			17	16	1	
14	G	1	Total	C	O	0
			17	16	1	
14	M	1	Total	C	O	0
			17	16	1	
14	T	1	Total	C	O	0
			17	16	1	

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
15	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	N	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
15	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



Mol	Chain	Residues	Atoms				AltConf
16	B	1	Total	C	O	P	0
			74	55	17	2	
16	B	1	Total	C	O	P	0
			77	58	17	2	
16	B	1	Total	C	O	P	0
			79	60	17	2	
16	C	1	Total	C	O	P	0
			79	60	17	2	
16	D	1	Total	C	O	P	0
			88	69	17	2	
16	D	1	Total	C	O	P	0
			95	76	17	2	
16	F	1	Total	C	O	P	0
			76	57	17	2	
16	F	1	Total	C	O	P	0
			81	62	17	2	
16	M	1	Total	C	O	P	0
			74	55	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	N	1	Total	C	O	P	0
			79	60	17	2	
16	P	1	Total	C	O	P	0
			88	69	17	2	

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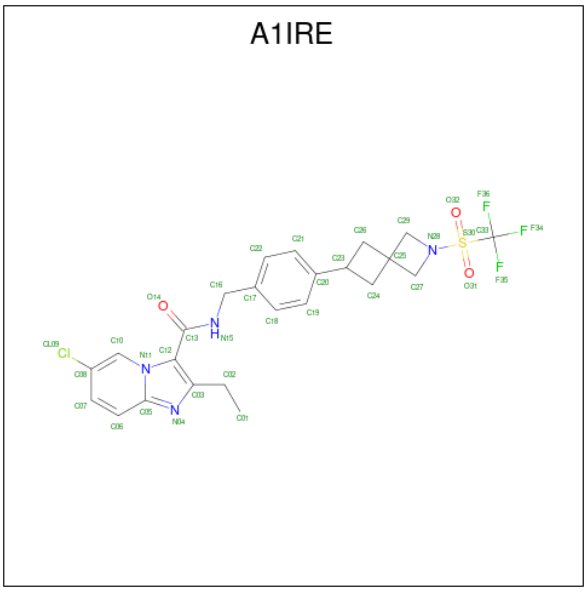
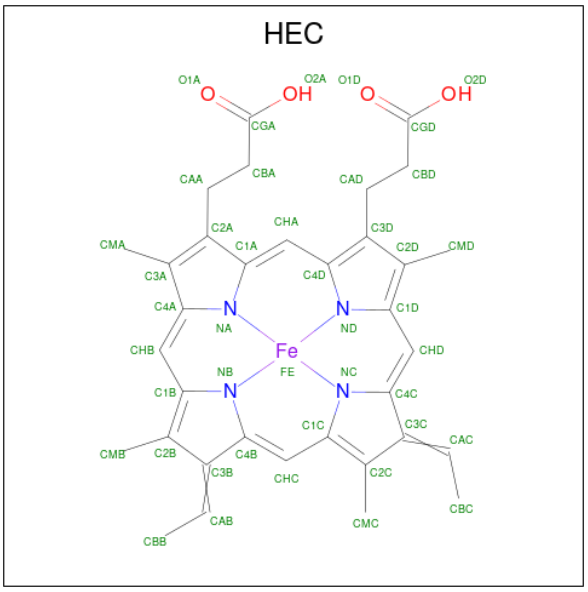
Mol	Chain	Residues	Atoms				AltConf
16	P	1	Total	C	O	P	0
			95	76	17	2	
16	R	1	Total	C	O	P	0
			76	57	17	2	
16	R	1	Total	C	O	P	0
			81	62	17	2	

- Molecule 17 is 6-chloranyl-2-ethyl-N-[[4-[2-(trifluoromethylsulfonyl)-2-azaspiro[3.3]heptan-6-yl]phenyl]methyl]imidazo[1,2-a]pyridine-3-carboxamide (CCD ID: A1IRE) (formula: $C_{24}H_{24}ClF_3N_4O_3S$).



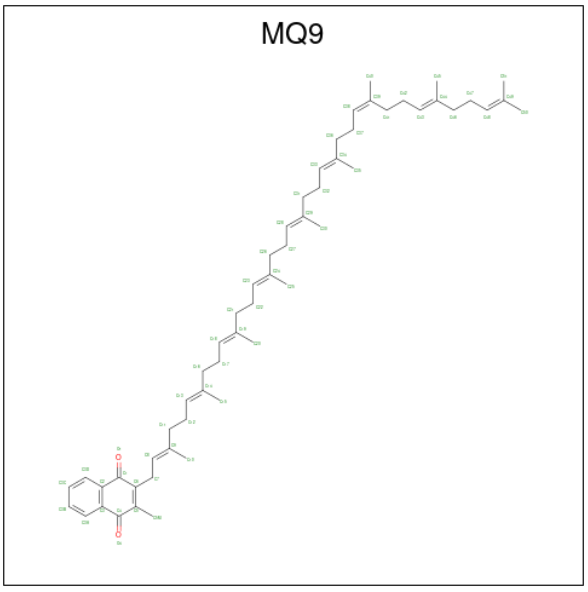
Mol	Chain	Residues	Atoms							AltConf
17	B	1	Total	C	Cl	F	N	O	S	0
			36	24	1	3	4	3	1	
17	N	1	Total	C	Cl	F	N	O	S	0
			36	24	1	3	4	3	1	

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



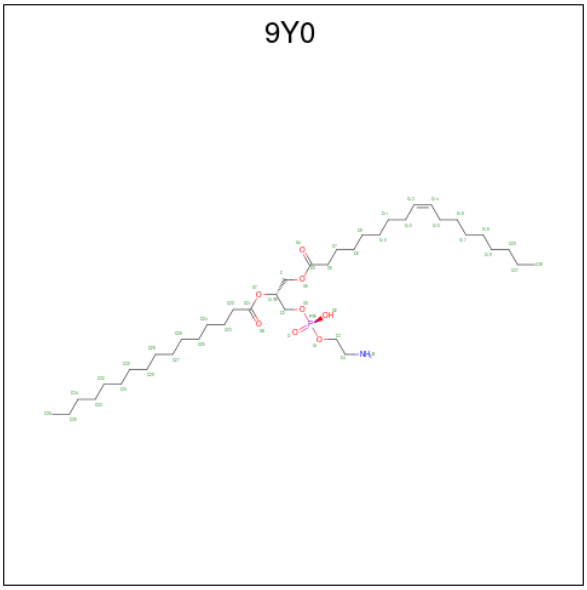
Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 19 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).



Mol	Chain	Residues	Atoms	AltConf
19	C	1	Total C O 58 56 2	0
19	O	1	Total C O 58 56 2	0

- Molecule 20 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: $C_{39}H_{76}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
20	D	1	Total C N O P 41 31 1 8 1	0
20	G	1	Total C N O P 43 33 1 8 1	0
20	P	1	Total C N O P 41 31 1 8 1	0
20	S	1	Total C N O P 43 33 1 8 1	0

- Molecule 21 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
21	E	2	Total Cu 2 2	0
21	F	2	Total Cu 2 2	0
21	Q	2	Total Cu 2 2	0

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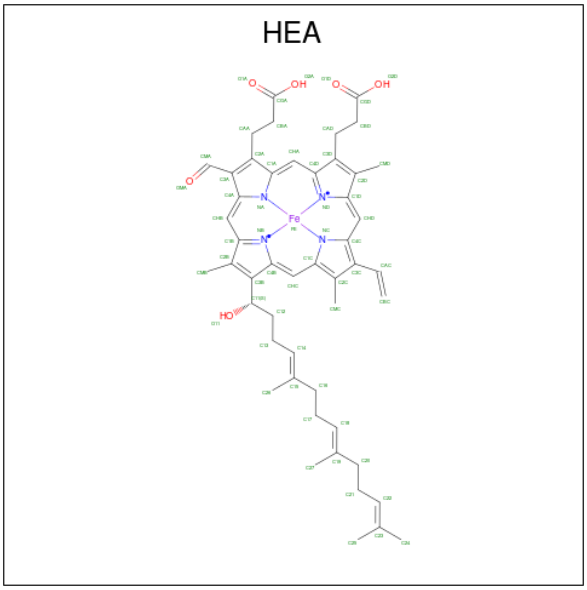
Mol	Chain	Residues	Atoms	AltConf
21	R	2	Total Cu 2 2	0

- Molecule 22 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

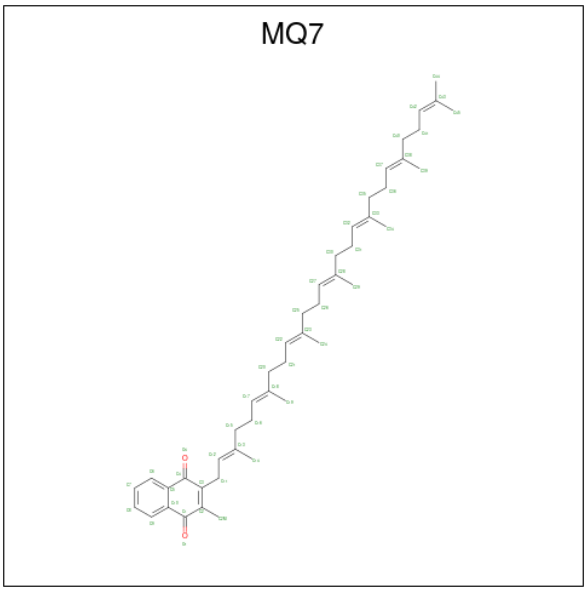


Mol	Chain	Residues	Atoms	AltConf
22	F	1	Total C Fe N O 60 49 1 4 6	0
22	F	1	Total C Fe N O 60 49 1 4 6	0
22	R	1	Total C Fe N O 60 49 1 4 6	0
22	R	1	Total C Fe N O 60 49 1 4 6	0

- Molecule 23 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
23	F	1	Total Ca 1 1	0
23	R	1	Total Ca 1 1	0

- Molecule 24 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



Mol	Chain	Residues	Atoms	AltConf
24	H	1	Total C O 48 46 2	0
24	O	1	Total C O 48 46 2	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	AltConf
25	A	25	Total O 25 25	0
25	B	45	Total O 45 45	0
25	C	10	Total O 10 10	0
25	D	4	Total O 4 4	0
25	E	8	Total O 8 8	0
25	F	25	Total O 25 25	0
25	G	1	Total O 1 1	0
25	H	5	Total O 5 5	0
25	J	1	Total O 1 1	0
25	L	1	Total O 1 1	0

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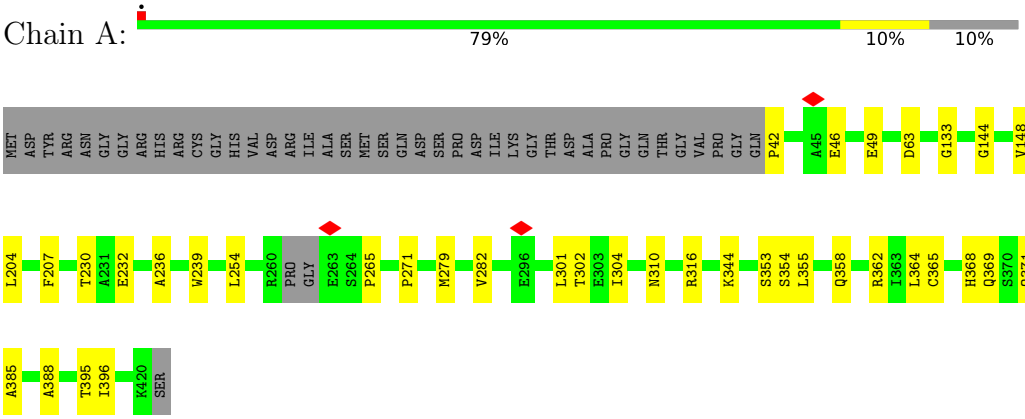
Mol	Chain	Residues	Atoms	AltConf
25	M	21	Total O 21 21	0
25	N	43	Total O 43 43	0
25	O	2	Total O 2 2	0
25	P	3	Total O 3 3	0
25	Q	1	Total O 1 1	0
25	R	11	Total O 11 11	0
25	S	2	Total O 2 2	0
25	T	2	Total O 2 2	0
25	U	1	Total O 1 1	0

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.

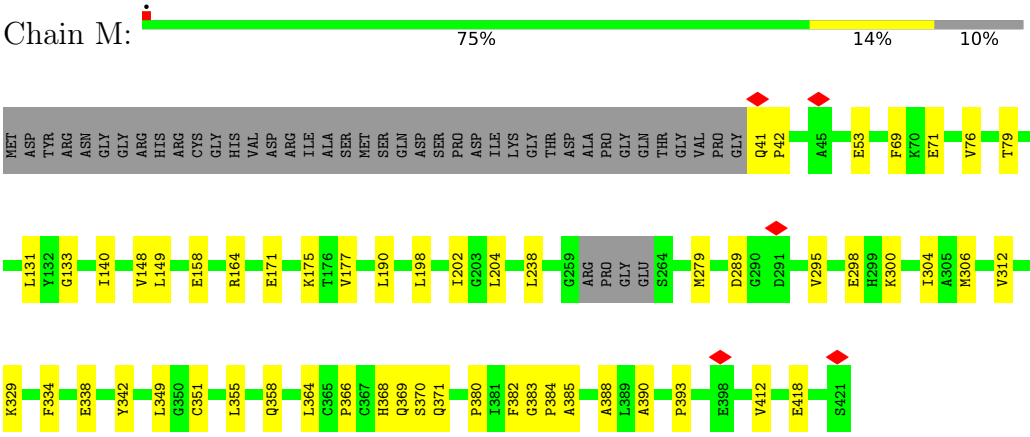
• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain A:



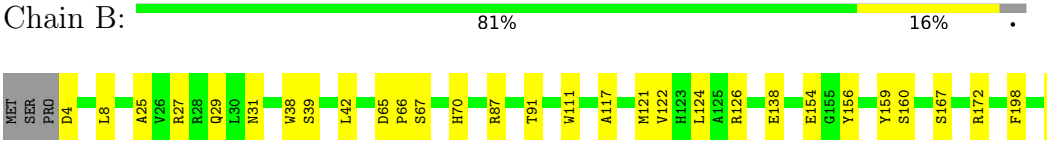
• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

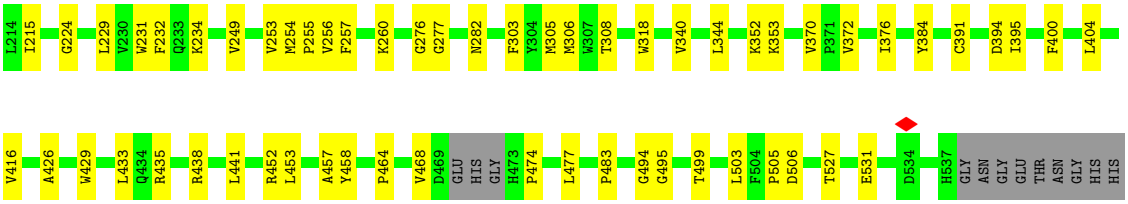
Chain M:



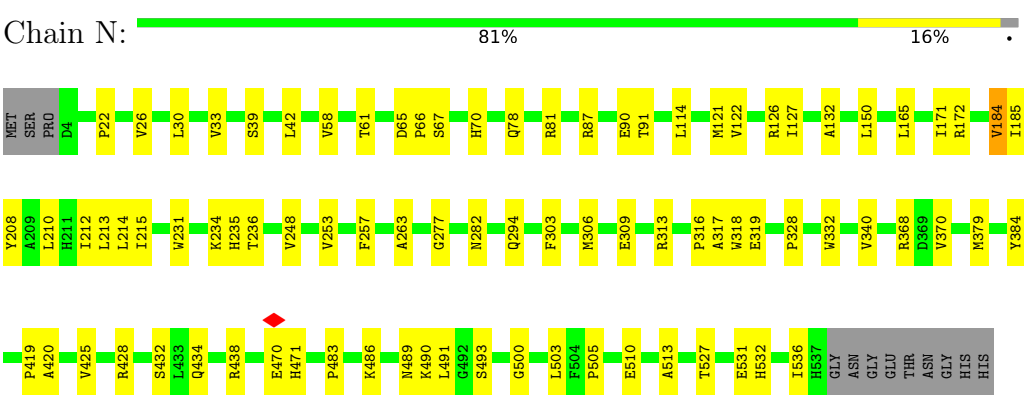
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain B:

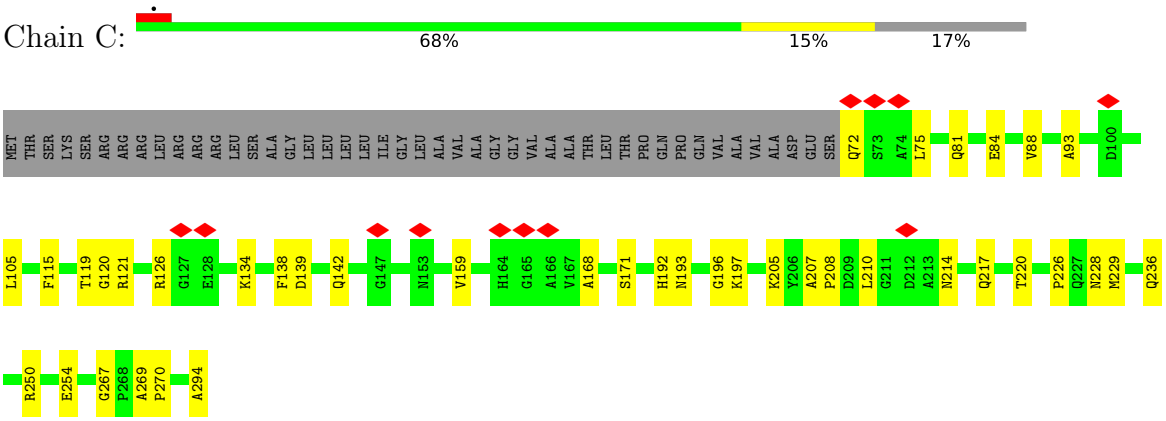




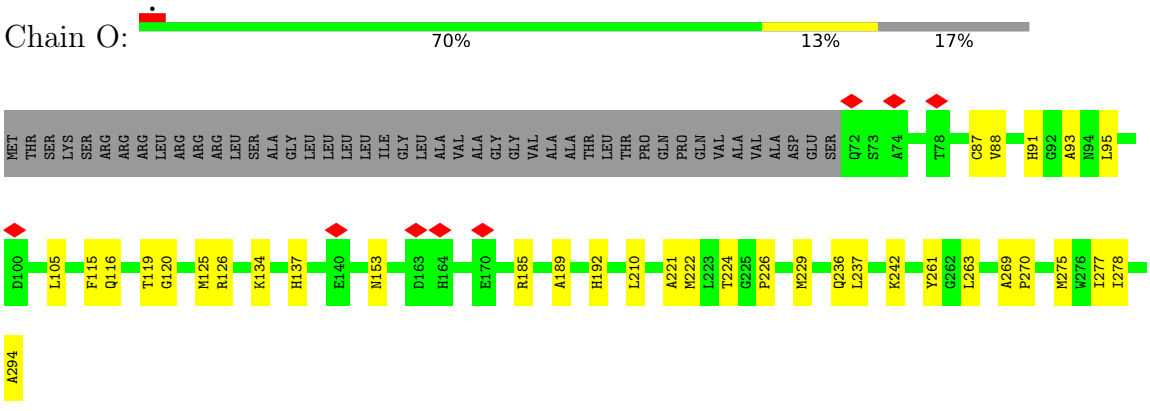
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit



• Molecule 3: Cytochrome bc1 complex cytochrome c subunit

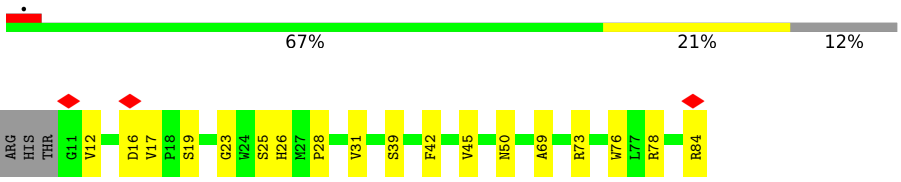


• Molecule 3: Cytochrome bc1 complex cytochrome c subunit



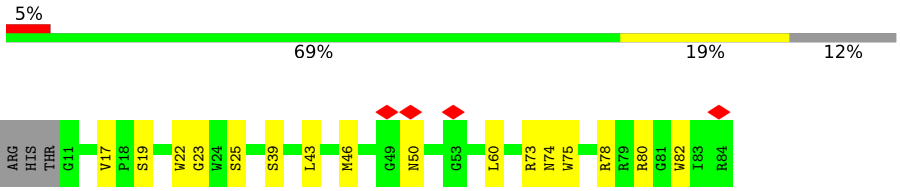
• Molecule 4: Transmembrane protein

Chain D:



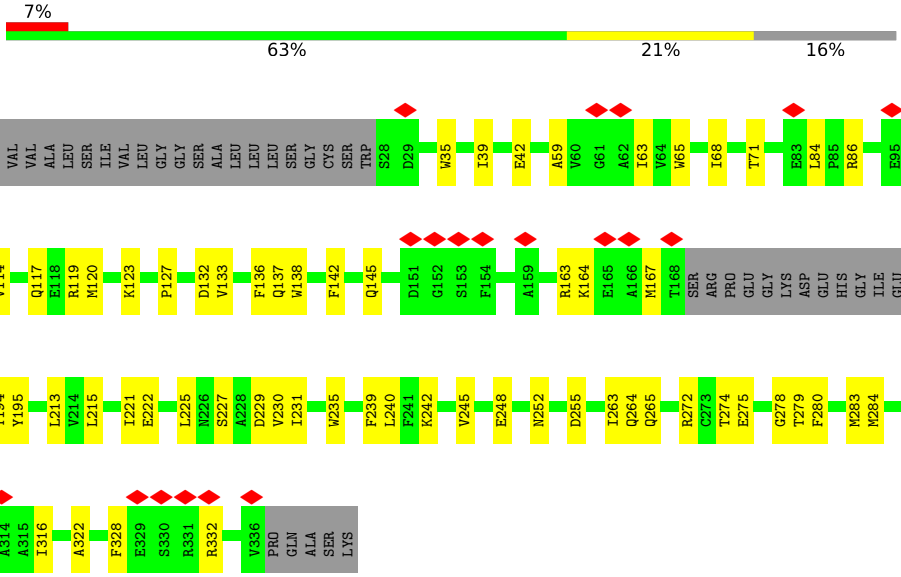
• Molecule 4: Transmembrane protein

Chain P:



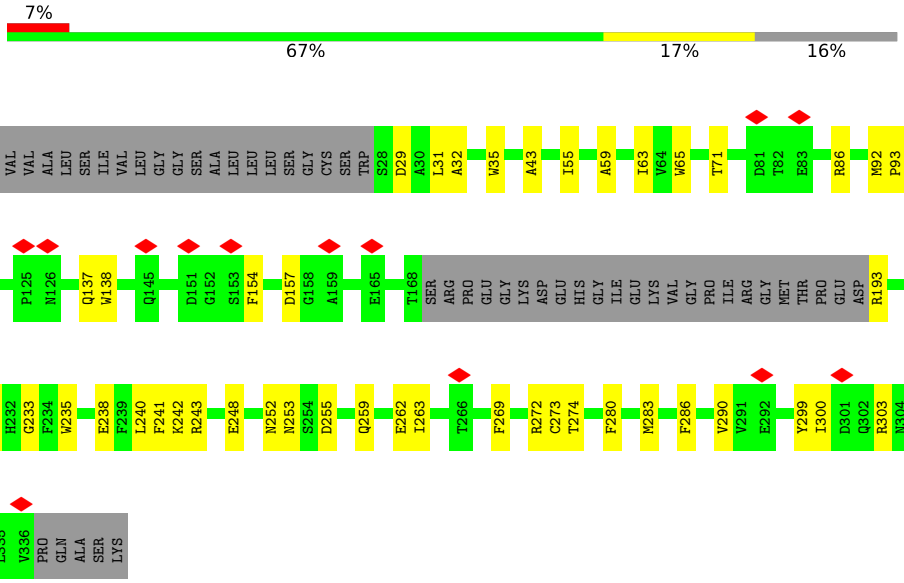
• Molecule 5: Cytochrome c oxidase subunit 2

Chain E:



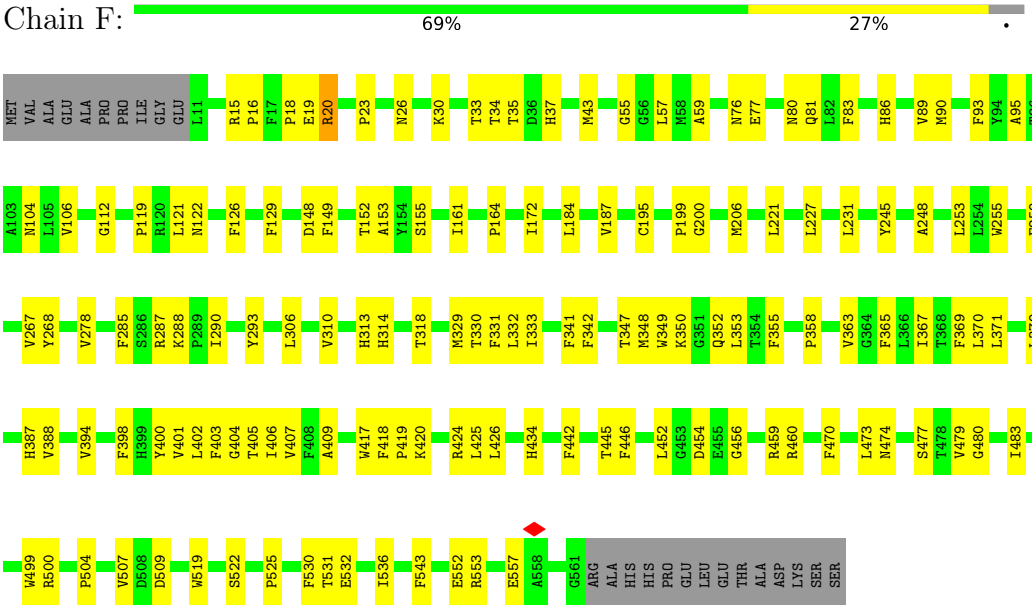
• Molecule 5: Cytochrome c oxidase subunit 2

Chain Q:



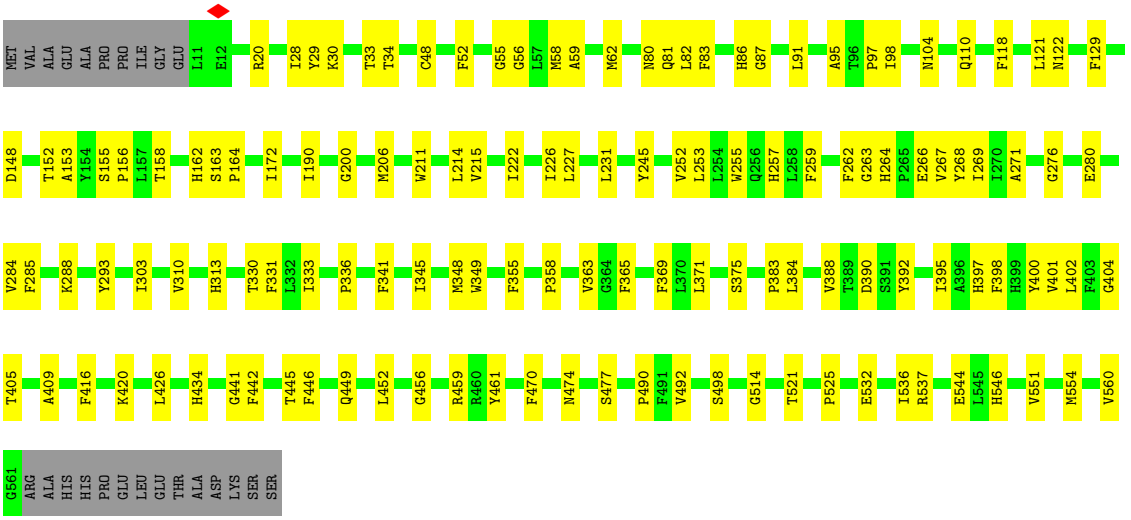
• Molecule 6: Cytochrome c oxidase subunit 1

Chain F:



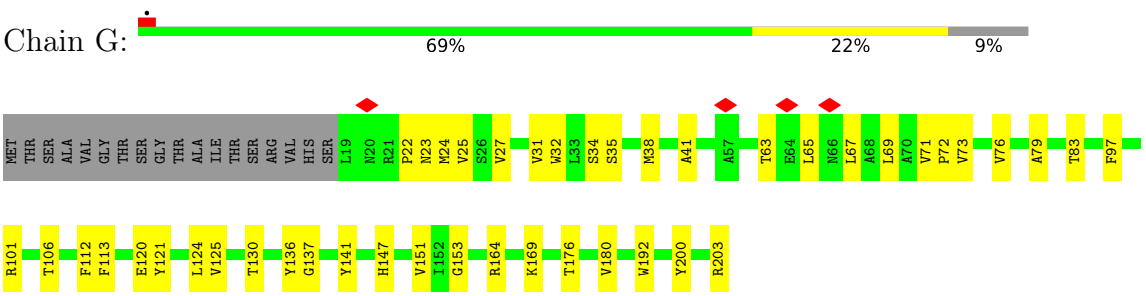
• Molecule 6: Cytochrome c oxidase subunit 1

Chain R:



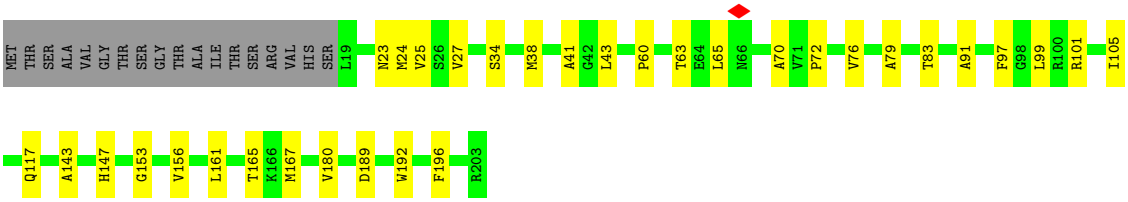
• Molecule 7: Cytochrome c oxidase subunit 3

Chain G:



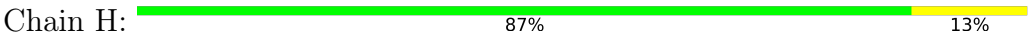
• Molecule 7: Cytochrome c oxidase subunit 3

Chain S:



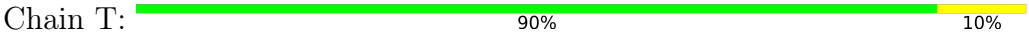
• Molecule 8: Cytochrome c oxidase polypeptide 4

Chain H:



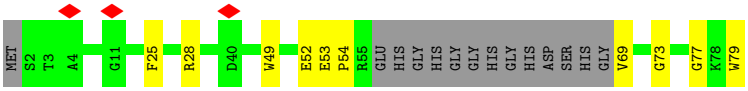
• Molecule 8: Cytochrome c oxidase polypeptide 4

Chain T:



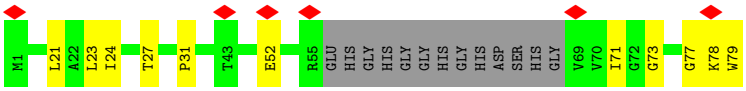
• Molecule 9: Secreted protein

Chain I:



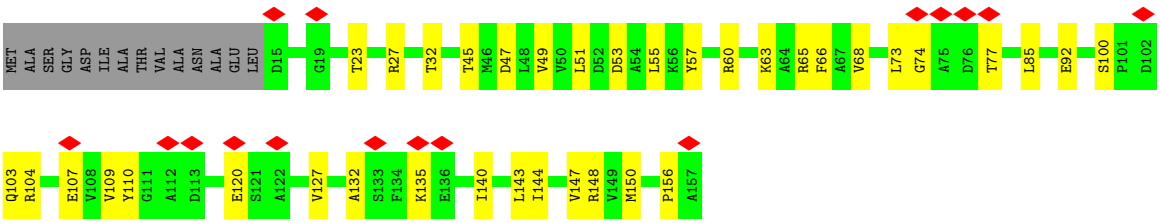
• Molecule 9: Secreted protein

Chain U:



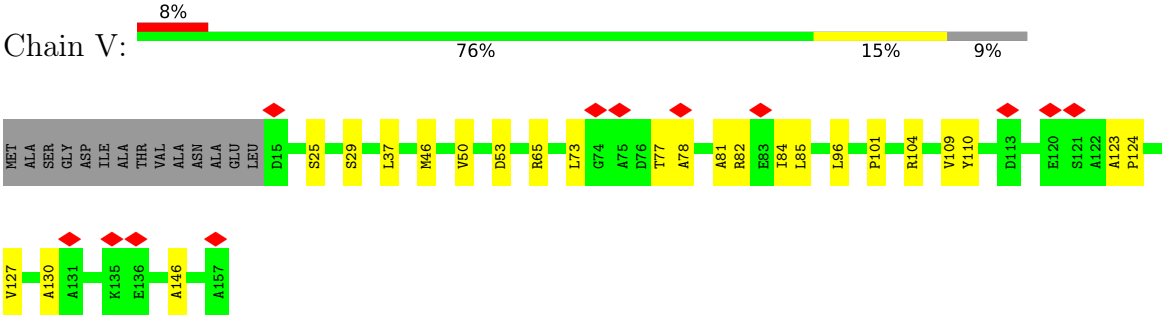
• Molecule 10: DUF5130 domain-containing protein

Chain J:



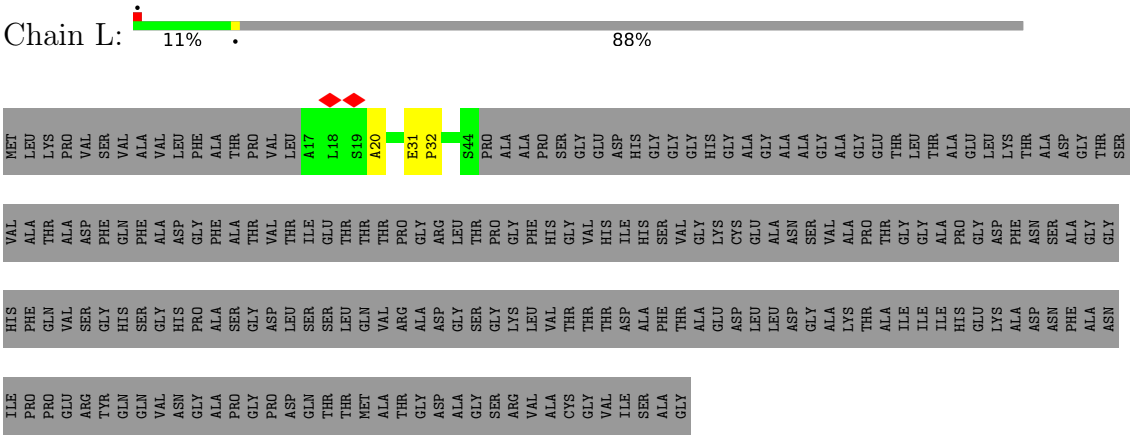
• Molecule 10: DUF5130 domain-containing protein

Chain V:



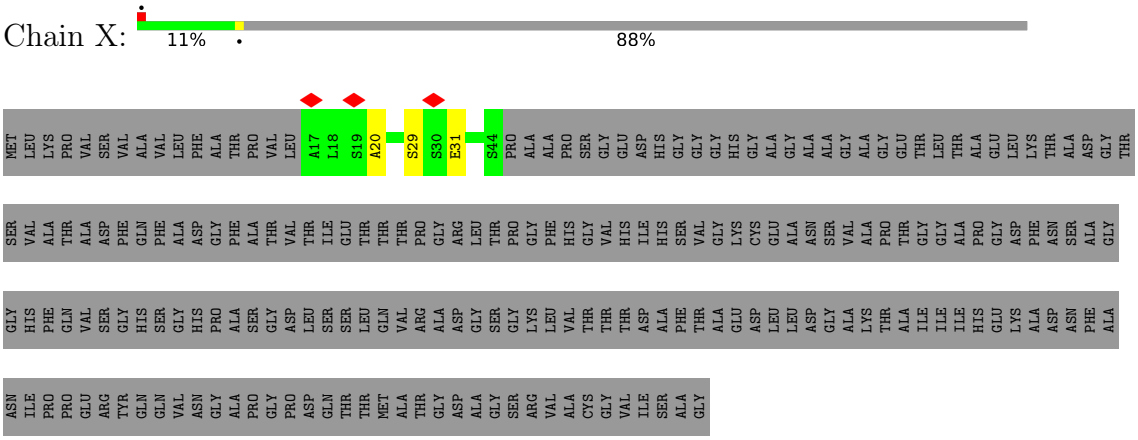
• Molecule 11: Superoxide dismutase [Cu-Zn]

Chain L:



• Molecule 11: Superoxide dismutase [Cu-Zn]

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	351.12003, 351.12003, 351.12003	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8360001, 0.8360001, 0.8360001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MQ7, A1IRE, CDL, 9Y0, FES, CU, HEA, MQ9, 9YF, HEM, PLM, CA, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/3024	0.43	0/4096
1	M	0.27	0/3019	0.44	0/4091
2	B	0.28	0/4284	0.42	0/5841
2	N	0.28	0/4309	0.43	0/5876
3	C	0.28	0/1660	0.46	0/2250
3	O	0.27	0/1660	0.46	0/2250
4	D	0.24	0/610	0.39	0/830
4	P	0.23	0/610	0.40	0/830
5	E	0.28	0/2332	0.47	0/3173
5	Q	0.27	0/2332	0.45	0/3173
6	F	0.29	0/4524	0.46	0/6180
6	R	0.30	0/4524	0.46	0/6180
7	G	0.30	0/1496	0.44	0/2043
7	S	0.31	0/1496	0.44	0/2043
8	H	0.30	0/1112	0.47	0/1524
8	T	0.27	0/1112	0.45	0/1524
9	I	0.26	0/506	0.49	0/692
9	U	0.25	0/514	0.50	0/702
10	J	0.27	0/1042	0.46	0/1423
10	V	0.27	0/1042	0.45	0/1423
11	L	0.25	0/191	0.48	0/265
11	X	0.24	0/191	0.48	0/265
All	All	0.28	0/41590	0.45	0/56674

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 (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	A	2947	0	2958	29	0
1	M	2942	0	2951	44	0
2	B	4153	0	4176	67	0
2	N	4176	0	4195	69	0
3	C	1623	0	1560	33	0
3	O	1623	0	1560	29	0
4	D	590	0	581	14	0
4	P	590	0	581	14	0
5	E	2271	0	2228	59	0
5	Q	2271	0	2228	43	0
6	F	4364	0	4343	124	0
6	R	4364	0	4343	109	0
7	G	1449	0	1450	38	0
7	S	1449	0	1450	27	0
8	H	1077	0	1058	14	0
8	T	1077	0	1058	13	0
9	I	490	0	498	11	0
9	U	498	0	510	11	0
10	J	1024	0	1035	30	0
10	V	1024	0	1035	20	0
11	L	185	0	170	3	0
11	X	185	0	170	3	0
12	A	4	0	0	1	0
12	M	4	0	0	1	0
13	A	58	0	0	0	0
13	C	58	0	0	1	0
13	M	58	0	0	0	0
13	O	58	0	0	0	0
14	A	17	0	31	0	0
14	G	17	0	31	1	0
14	M	17	0	31	1	0
14	T	17	0	31	4	0
15	B	85	0	57	5	0
15	N	85	0	57	5	0
16	B	230	0	294	13	0
16	C	79	0	105	3	0
16	D	183	0	269	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	F	157	0	205	15	0
16	M	74	0	92	6	0
16	N	309	0	400	12	0
16	P	183	0	269	11	0
16	R	157	0	208	6	0
17	B	36	0	0	0	0
17	N	36	0	0	1	0
18	C	86	0	60	2	0
18	O	86	0	60	2	0
19	C	58	0	80	7	0
19	O	58	0	80	7	0
20	D	41	0	0	0	0
20	G	43	0	0	0	0
20	P	41	0	0	1	0
20	S	43	0	0	0	0
21	E	2	0	0	0	0
21	F	2	0	0	0	0
21	Q	2	0	0	0	0
21	R	2	0	0	0	0
22	F	120	0	108	19	0
22	R	120	0	108	12	0
23	F	1	0	0	0	0
23	R	1	0	0	0	0
24	H	48	0	64	2	0
24	O	48	0	64	2	0
25	A	25	0	0	0	0
25	B	45	0	0	0	0
25	C	10	0	0	0	0
25	D	4	0	0	0	0
25	E	8	0	0	0	0
25	F	25	0	0	2	0
25	G	1	0	0	0	0
25	H	5	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	21	0	0	0	0
25	N	43	0	0	1	0
25	O	2	0	0	0	0
25	P	3	0	0	0	0
25	Q	1	0	0	0	0
25	R	11	0	0	0	0
25	S	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	2	0	0	0	0
25	U	1	0	0	0	0
All	All	43307	0	42842	730	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 730 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)
6:F:406:ILE:HD11	22:F:602:HEA:HBC2	1.31	1.07
6:F:406:ILE:HD11	22:F:602:HEA:CBC	1.91	0.99
6:F:402:LEU:HD13	22:F:602:HEA:HAC	1.45	0.98
6:F:406:ILE:CD1	22:F:602:HEA:HBC2	2.02	0.89
1:A:133:GLY:HA3	2:B:277:GLY:HA3	1.63	0.80

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	A	373/421 (89%)	362 (97%)	11 (3%)	0	100	100
1	M	373/421 (89%)	362 (97%)	11 (3%)	0	100	100
2	B	527/546 (96%)	508 (96%)	19 (4%)	0	100	100
2	N	532/546 (97%)	513 (96%)	18 (3%)	1 (0%)	44	74
3	C	221/268 (82%)	210 (95%)	11 (5%)	0	100	100
3	O	221/268 (82%)	210 (95%)	11 (5%)	0	100	100
4	D	72/84 (86%)	71 (99%)	1 (1%)	0	100	100
4	P	72/84 (86%)	70 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	281/341 (82%)	267 (95%)	14 (5%)	0	100	100
5	Q	281/341 (82%)	269 (96%)	12 (4%)	0	100	100
6	F	549/575 (96%)	536 (98%)	13 (2%)	0	100	100
6	R	549/575 (96%)	528 (96%)	21 (4%)	0	100	100
7	G	183/203 (90%)	182 (100%)	1 (0%)	0	100	100
7	S	183/203 (90%)	180 (98%)	3 (2%)	0	100	100
8	H	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
8	T	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
9	I	61/79 (77%)	58 (95%)	3 (5%)	0	100	100
9	U	62/79 (78%)	57 (92%)	5 (8%)	0	100	100
10	J	141/157 (90%)	138 (98%)	3 (2%)	0	100	100
10	V	141/157 (90%)	138 (98%)	3 (2%)	0	100	100
11	L	26/236 (11%)	25 (96%)	1 (4%)	0	100	100
11	X	26/236 (11%)	24 (92%)	2 (8%)	0	100	100
All	All	5148/6098 (84%)	4974 (97%)	173 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	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	A	309/343 (90%)	309 (100%)	0	100	100
1	M	309/343 (90%)	309 (100%)	0	100	100
2	B	426/437 (98%)	425 (100%)	1 (0%)	92	96
2	N	428/437 (98%)	428 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	163/197 (83%)	162 (99%)	1 (1%)	84 91
3	O	163/197 (83%)	163 (100%)	0	100 100
4	D	58/67 (87%)	58 (100%)	0	100 100
4	P	58/67 (87%)	58 (100%)	0	100 100
5	E	243/288 (84%)	243 (100%)	0	100 100
5	Q	243/288 (84%)	243 (100%)	0	100 100
6	F	452/471 (96%)	451 (100%)	1 (0%)	92 96
6	R	452/471 (96%)	452 (100%)	0	100 100
7	G	147/161 (91%)	147 (100%)	0	100 100
7	S	147/161 (91%)	145 (99%)	2 (1%)	62 81
8	H	106/106 (100%)	106 (100%)	0	100 100
8	T	106/106 (100%)	106 (100%)	0	100 100
9	I	50/59 (85%)	50 (100%)	0	100 100
9	U	51/59 (86%)	51 (100%)	0	100 100
10	J	105/114 (92%)	105 (100%)	0	100 100
10	V	105/114 (92%)	105 (100%)	0	100 100
11	L	21/167 (13%)	21 (100%)	0	100 100
11	X	21/167 (13%)	21 (100%)	0	100 100
All	All	4163/4820 (86%)	4158 (100%)	5 (0%)	92 97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	353	LYS
3	C	126	ARG
6	F	20	ARG
7	S	23	ASN
7	S	189	ASP

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

Mol	Chain	Res	Type
2	B	519	HIS
6	F	434	HIS
7	G	23	ASN

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Mol	Chain	Res	Type
3	O	153	ASN
6	R	387	HIS

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 59 ligands modelled in this entry, 10 are monoatomic - leaving 49 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	$\#\|Z\| > 2$
16	CDL	P	101	-	87,87,99	1.30	10 (11%)	93,99,111	1.10	5 (5%)
16	CDL	N	605	-	78,78,99	1.34	9 (11%)	84,90,111	1.11	4 (4%)
17	A1IRE	B	606	-	37,40,40	2.40	12 (32%)	47,63,63	4.17	16 (34%)
22	HEA	R	601	6	57,67,67	2.05	17 (29%)	61,103,103	2.49	28 (45%)
15	HEM	B	601	2	41,49,50	1.27	3 (7%)	46,81,82	1.33	6 (13%)
20	9Y0	S	301	-	42,42,48	0.94	4 (9%)	44,47,53	1.11	2 (4%)
16	CDL	B	605	-	78,78,99	1.33	10 (12%)	84,90,111	1.14	4 (4%)
13	9YF	M	502	-	58,58,58	0.88	4 (6%)	69,71,71	1.17	5 (7%)
18	HEC	C	301	3	32,50,50	2.17	3 (9%)	24,82,82	1.56	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CDL	C	305	-	78,78,99	1.35	11 (14%)	84,90,111	1.13	4 (4%)
24	MQ7	O	301	-	49,49,49	1.69	5 (10%)	60,63,63	1.63	15 (25%)
18	HEC	C	302	3	32,50,50	2.18	3 (9%)	24,82,82	1.49	3 (12%)
16	CDL	N	607	-	78,78,99	1.34	11 (14%)	84,90,111	1.14	4 (4%)
19	MQ9	C	304	-	59,59,59	1.55	5 (8%)	72,75,75	1.63	20 (27%)
18	HEC	O	302	3	32,50,50	2.15	3 (9%)	24,82,82	1.66	6 (25%)
16	CDL	M	503	-	73,73,99	1.41	12 (16%)	79,85,111	1.17	5 (6%)
14	PLM	A	503	-	16,16,17	0.52	0	15,15,17	0.42	0
16	CDL	F	605	-	75,75,99	1.38	10 (13%)	81,87,111	1.15	4 (4%)
19	MQ9	O	305	-	59,59,59	1.56	5 (8%)	72,75,75	1.63	20 (27%)
20	9Y0	G	301	-	42,42,48	0.95	4 (9%)	44,47,53	1.07	2 (4%)
24	MQ7	H	201	-	49,49,49	1.72	5 (10%)	60,63,63	1.62	14 (23%)
14	PLM	M	504	-	16,16,17	0.52	0	15,15,17	0.44	0
20	9Y0	D	102	-	40,40,48	0.95	4 (10%)	43,45,53	1.10	2 (4%)
16	CDL	B	603	-	73,73,99	1.38	10 (13%)	79,85,111	1.17	4 (5%)
16	CDL	R	605	-	75,75,99	1.38	11 (14%)	81,87,111	1.13	4 (4%)
12	FES	A	501	1	0,4,4	-	-	-		
16	CDL	P	103	-	94,94,99	1.29	11 (11%)	100,106,111	1.09	4 (4%)
16	CDL	R	606	-	80,80,99	1.34	9 (11%)	86,92,111	1.06	4 (4%)
13	9YF	C	303	-	58,58,58	0.87	4 (6%)	69,71,71	1.02	2 (2%)
22	HEA	F	602	6	57,67,67	2.17	19 (33%)	61,103,103	2.40	27 (44%)
22	HEA	F	601	-	57,67,67	2.06	16 (28%)	61,103,103	2.43	25 (40%)
13	9YF	A	502	-	58,58,58	0.87	4 (6%)	69,71,71	1.12	6 (8%)
14	PLM	T	201	-	16,16,17	0.54	0	15,15,17	0.43	0
12	FES	M	501	1	0,4,4	-	-	-		
16	CDL	D	101	-	87,87,99	1.30	10 (11%)	93,99,111	1.11	4 (4%)
16	CDL	D	103	-	94,94,99	1.29	9 (9%)	100,106,111	1.09	4 (4%)
16	CDL	N	603	-	73,73,99	1.38	10 (13%)	79,85,111	1.12	4 (5%)
16	CDL	N	604	-	76,76,99	1.35	10 (13%)	82,88,111	1.17	4 (4%)
15	HEM	N	602	2	41,50,50	1.45	4 (9%)	45,82,82	1.35	8 (17%)
18	HEC	O	303	3	32,50,50	2.19	3 (9%)	24,82,82	1.45	3 (12%)
20	9Y0	P	102	-	40,40,48	0.96	2 (5%)	43,45,53	1.03	2 (4%)
15	HEM	N	601	2	41,49,50	1.27	3 (7%)	46,81,82	1.35	7 (15%)
22	HEA	R	602	6	57,67,67	2.11	18 (31%)	61,103,103	2.39	26 (42%)
13	9YF	O	304	-	58,58,58	0.87	4 (6%)	69,71,71	1.07	3 (4%)
14	PLM	G	302	-	16,16,17	0.53	0	15,15,17	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	A1IRE	N	606	-	37,40,40	2.42	12 (32%)	47,63,63	4.30	14 (29%)
16	CDL	F	606	-	80,80,99	1.34	10 (12%)	86,92,111	1.08	4 (4%)
15	HEM	B	602	2	41,50,50	1.45	3 (7%)	45,82,82	1.30	6 (13%)
16	CDL	B	604	-	76,76,99	1.36	10 (13%)	82,88,111	1.16	4 (4%)

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
16	CDL	P	101	-	-	59/98/98/110	-
16	CDL	N	605	-	-	53/89/89/110	-
17	A1IRE	B	606	-	-	15/24/50/50	0/5/5/5
22	HEA	R	601	6	-	5/32/76/76	-
15	HEM	B	601	2	-	2/12/52/54	-
20	9Y0	S	301	-	-	19/46/46/52	-
16	CDL	B	605	-	-	51/89/89/110	-
13	9YF	M	502	-	-	23/54/78/78	0/1/1/1
18	HEC	C	301	3	-	2/10/54/54	-
16	CDL	C	305	-	-	47/89/89/110	-
24	MQ7	O	301	-	-	11/41/61/61	0/2/2/2
18	HEC	C	302	3	-	5/10/54/54	-
16	CDL	N	607	-	-	59/89/89/110	-
19	MQ9	C	304	-	-	17/53/73/73	0/2/2/2
18	HEC	O	302	3	-	1/10/54/54	-
16	CDL	M	503	-	-	41/84/84/110	-
14	PLM	A	503	-	-	1/13/14/15	-
16	CDL	F	605	-	-	46/86/86/110	-
19	MQ9	O	305	-	-	22/53/73/73	0/2/2/2
20	9Y0	G	301	-	-	22/46/46/52	-
24	MQ7	H	201	-	-	12/41/61/61	0/2/2/2
14	PLM	M	504	-	-	5/13/14/15	-
20	9Y0	D	102	-	-	21/44/44/52	-
16	CDL	B	603	-	-	42/84/84/110	-
16	CDL	R	605	-	-	42/86/86/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CDL	P	103	-	-	63/105/105/110	-
16	CDL	R	606	-	-	56/91/91/110	-
22	HEA	F	602	6	-	9/32/76/76	-
13	9YF	C	303	-	-	34/54/78/78	0/1/1/1
12	FES	A	501	1	-	-	0/1/1/1
22	HEA	F	601	-	-	5/32/76/76	-
13	9YF	A	502	-	-	26/54/78/78	0/1/1/1
12	FES	M	501	1	-	-	0/1/1/1
14	PLM	T	201	-	-	6/13/14/15	-
20	9Y0	P	102	-	-	22/44/44/52	-
16	CDL	D	101	-	-	54/98/98/110	-
16	CDL	D	103	-	-	62/105/105/110	-
16	CDL	N	603	-	-	38/84/84/110	-
16	CDL	N	604	-	-	44/87/87/110	-
15	HEM	N	602	2	-	1/12/54/54	-
18	HEC	O	303	3	-	1/10/54/54	-
22	HEA	R	602	6	-	6/32/76/76	-
15	HEM	N	601	2	-	4/12/52/54	-
13	9YF	O	304	-	-	36/54/78/78	0/1/1/1
14	PLM	G	302	-	-	4/13/14/15	-
17	A1IRE	N	606	-	-	13/24/50/50	0/5/5/5
16	CDL	F	606	-	-	44/91/91/110	-
15	HEM	B	602	2	-	2/12/54/54	-
16	CDL	B	604	-	-	43/87/87/110	-

The worst 5 of 342 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	H	201	MQ7	C3-C2	7.74	1.49	1.35
19	O	305	MQ9	C6-C5	7.42	1.48	1.35
24	O	301	MQ7	C3-C2	7.41	1.48	1.35
19	C	304	MQ9	C6-C5	7.40	1.48	1.35
17	N	606	A1IRE	S30-N28	6.76	1.71	1.59

The worst 5 of 341 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	606	A1IRE	C26-C25-C29	16.41	169.33	120.79
17	B	606	A1IRE	C26-C25-C29	16.28	168.93	120.79
17	N	606	A1IRE	O32-S30-O31	-10.50	100.97	120.87
17	B	606	A1IRE	O32-S30-O31	-10.13	101.67	120.87
17	N	606	A1IRE	C24-C23-C20	-8.79	105.47	119.33

There are no chirality outliers.

5 of 1196 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	502	9YF	C1-O-P-O1
13	A	502	9YF	C1-O-P-O8
13	A	502	9YF	O9-C-C1-O
13	C	303	9YF	C2-O2-P-O
13	C	303	9YF	C1-O-P-O1

There are no ring outliers.

40 monomers are involved in 149 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	P	101	CDL	6	0
16	N	605	CDL	5	0
22	R	601	HEA	5	0
15	B	601	HEM	2	0
16	B	605	CDL	5	0
16	C	305	CDL	3	0
24	O	301	MQ7	2	0
18	C	302	HEC	2	0
16	N	607	CDL	4	0
19	C	304	MQ9	7	0
18	O	302	HEC	1	0
16	M	503	CDL	6	0
16	F	605	CDL	6	0
19	O	305	MQ9	7	0
24	H	201	MQ7	2	0
14	M	504	PLM	1	0
16	B	603	CDL	5	0
16	R	605	CDL	3	0
12	A	501	FES	1	0
16	P	103	CDL	5	0
16	R	606	CDL	3	0
13	C	303	9YF	1	0

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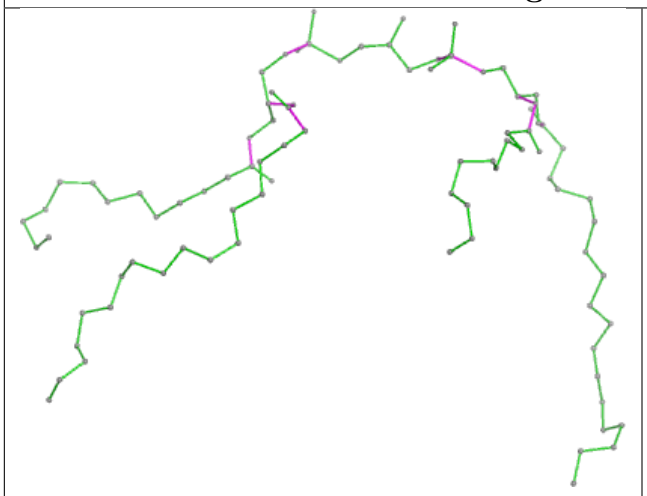
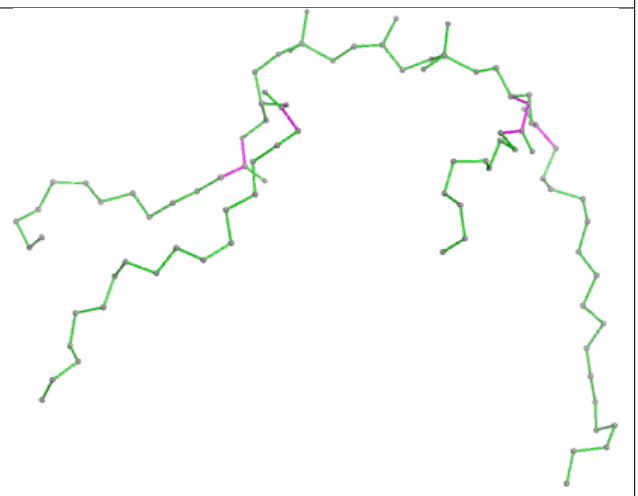
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	602	HEA	14	0
22	F	601	HEA	5	0
14	T	201	PLM	4	0
12	M	501	FES	1	0
16	D	101	CDL	7	0
16	D	103	CDL	12	0
16	N	603	CDL	3	0
16	N	604	CDL	2	0
15	N	602	HEM	3	0
18	O	303	HEC	1	0
20	P	102	9Y0	1	0
15	N	601	HEM	2	0
22	R	602	HEA	7	0
14	G	302	PLM	1	0
17	N	606	A1IRE	1	0
16	F	606	CDL	9	0
15	B	602	HEM	3	0
16	B	604	CDL	4	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.

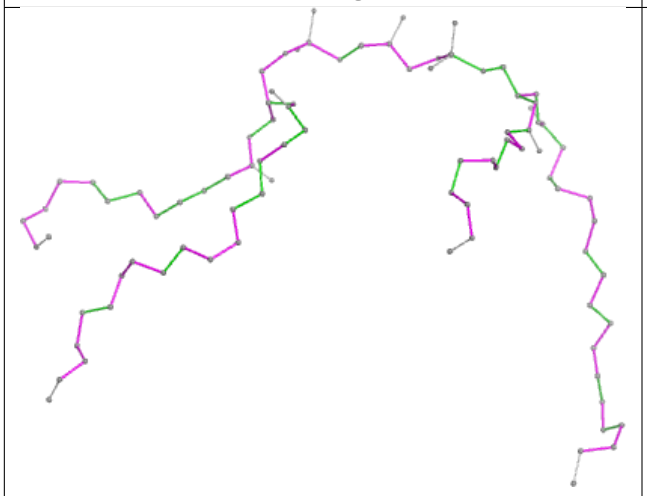
Ligand CDL P 101



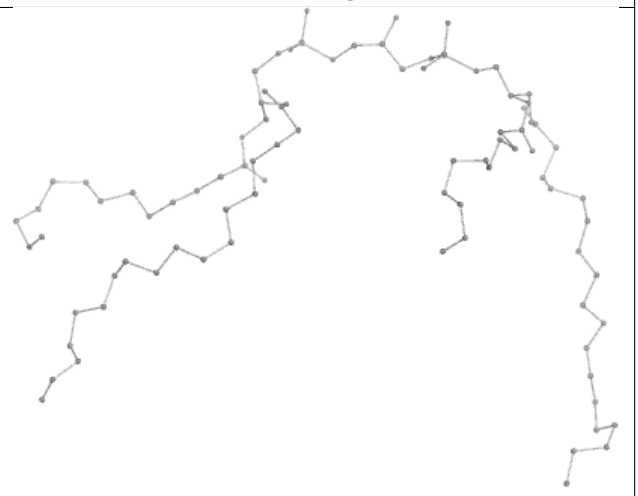
Bond lengths



Bond angles

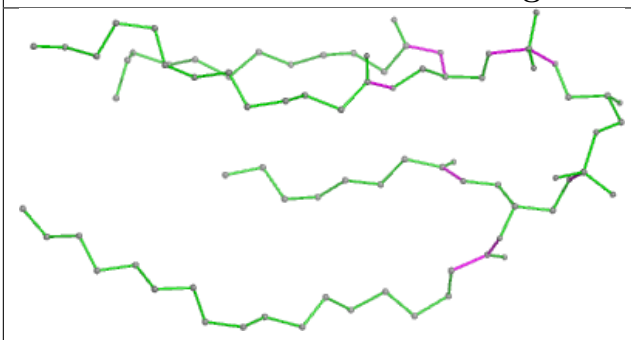


Torsions

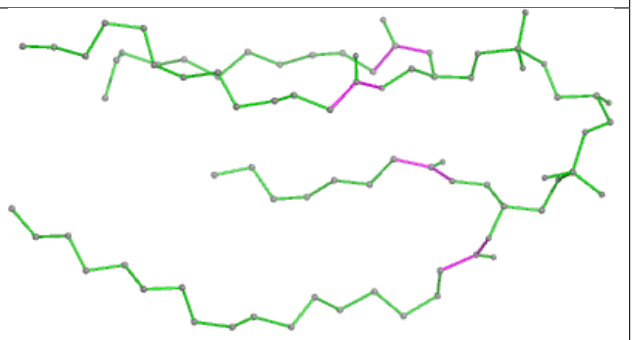


Rings

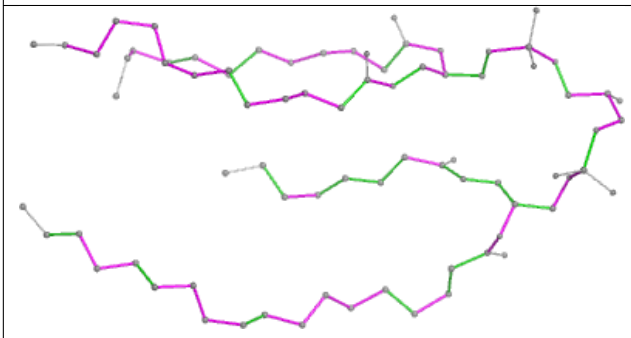
Ligand CDL N 605



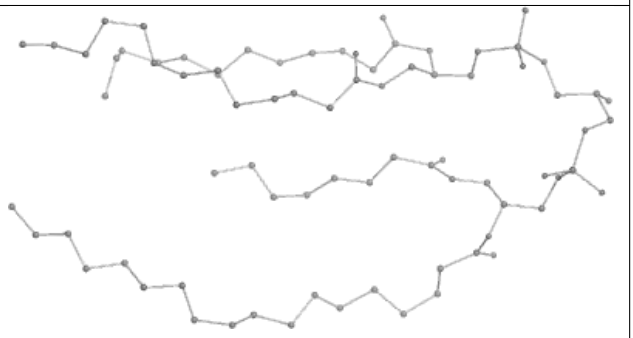
Bond lengths



Bond angles

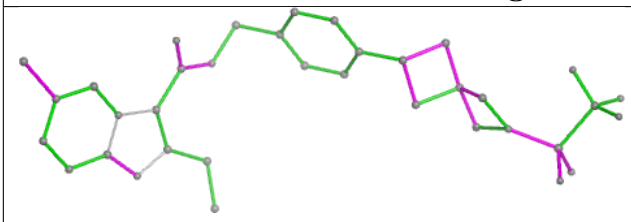


Torsions



Rings

Ligand A1IRE B 606



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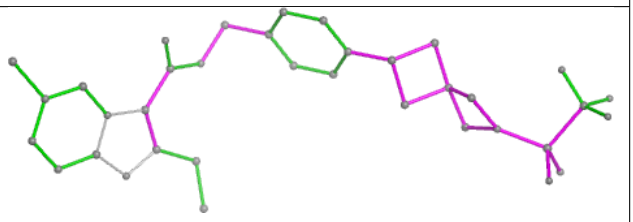
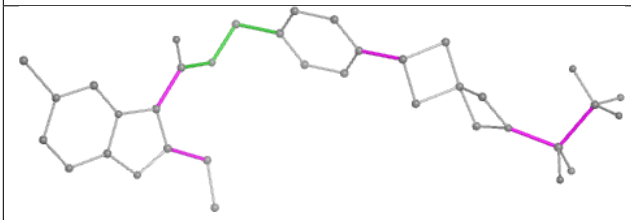
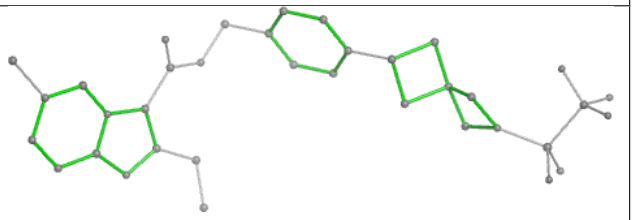


Bond angles

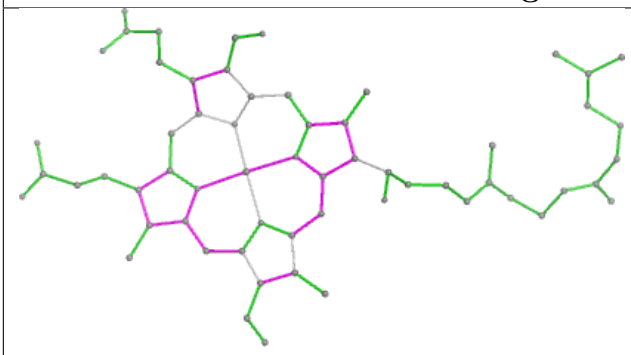


Torsions



Rings

Ligand HEA R 601



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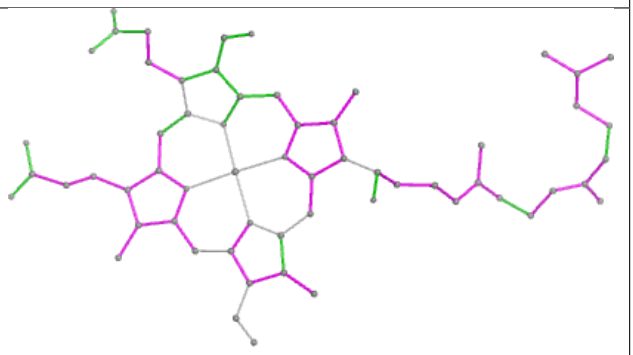
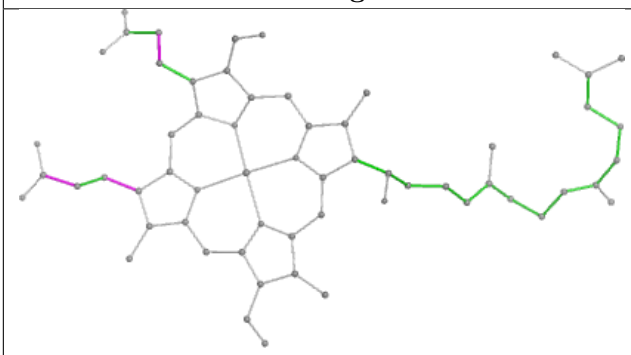
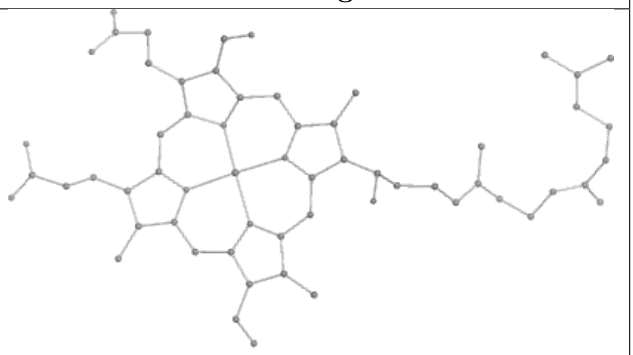


Bond angles

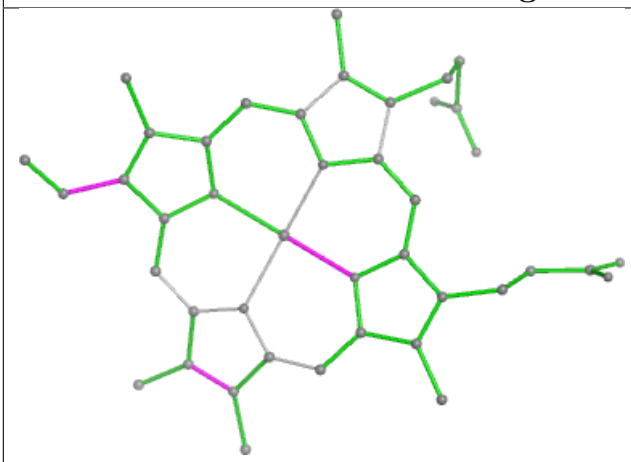


Torsions



Rings

Ligand HEM B 601



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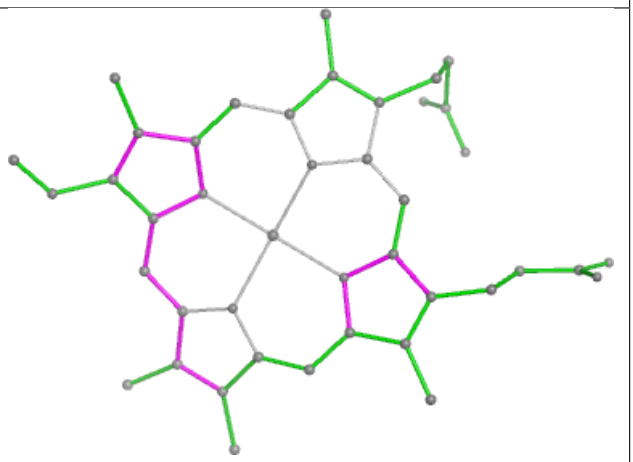
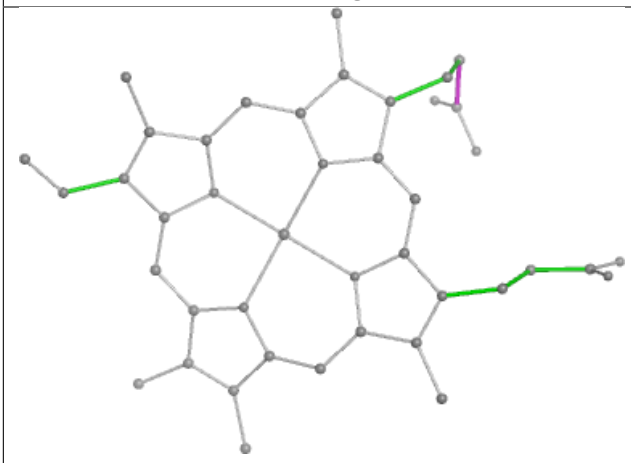


Bond angles



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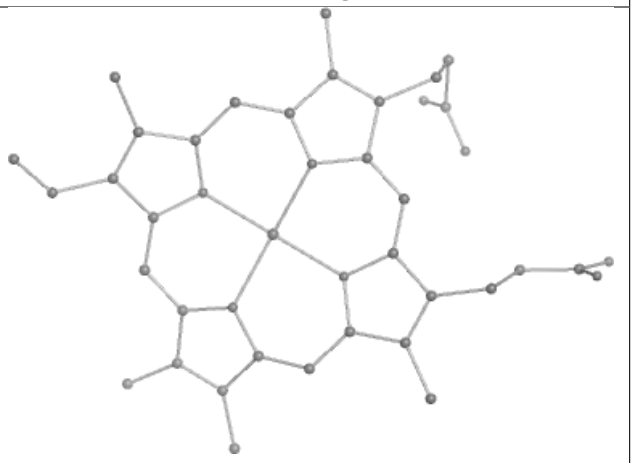
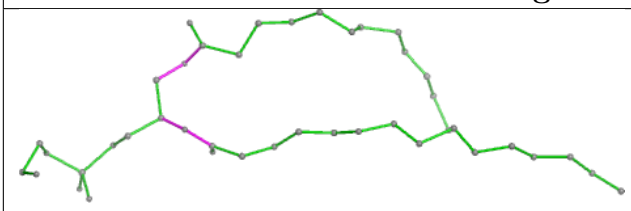


Rings

Ligand 9Y0 S 301



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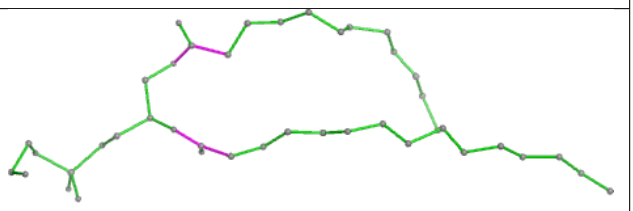
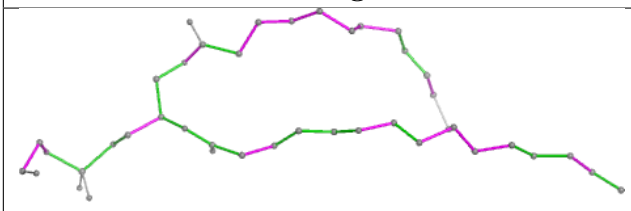


Bond angles



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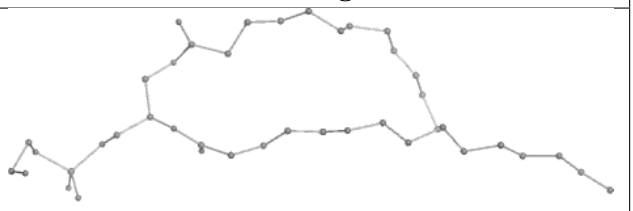
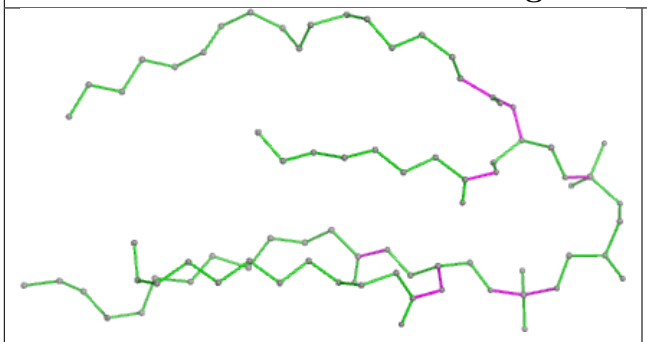


Rings

Ligand CDL B 605



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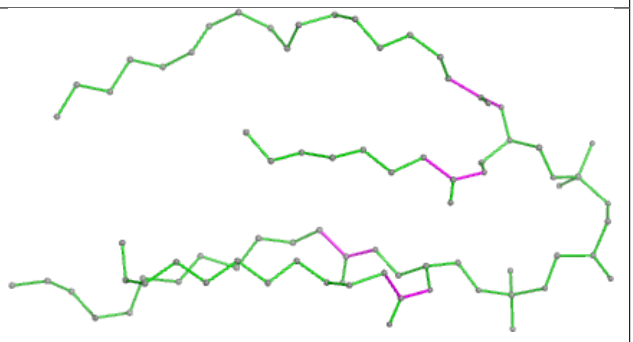
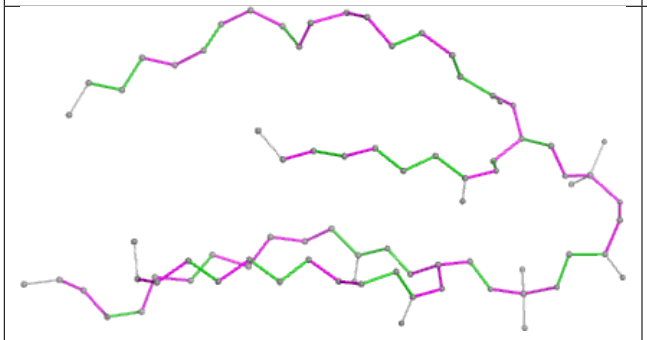
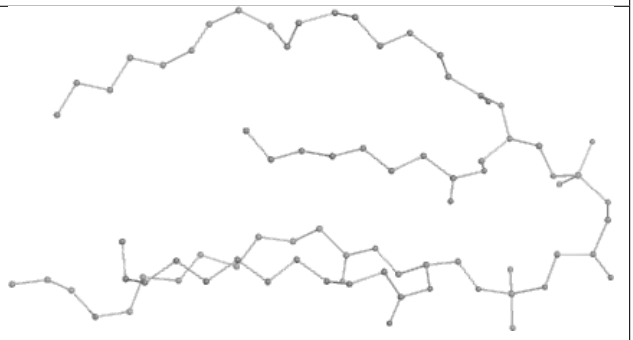


Bond angles

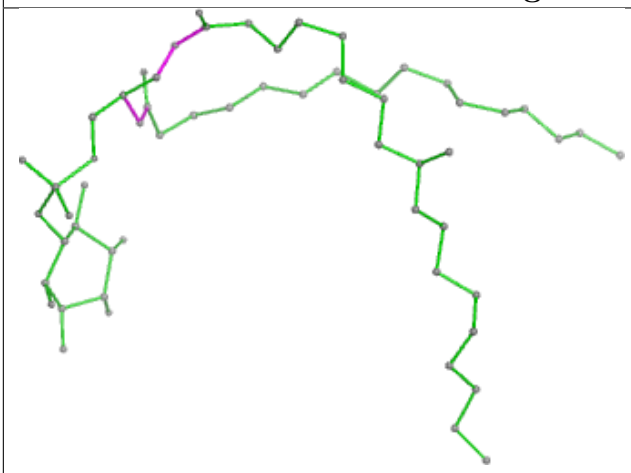


Torsions



Rings

Ligand 9YF M 502



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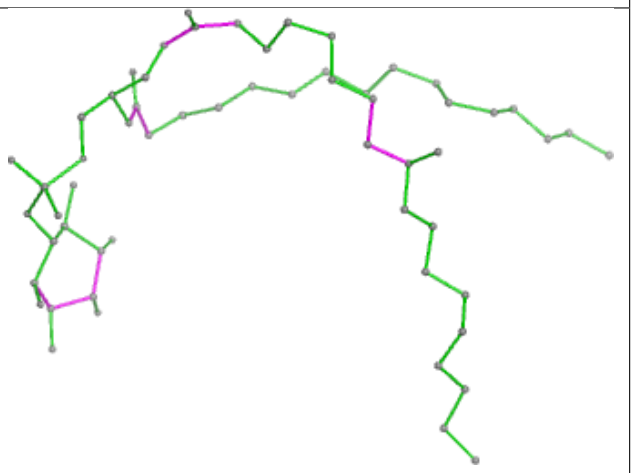
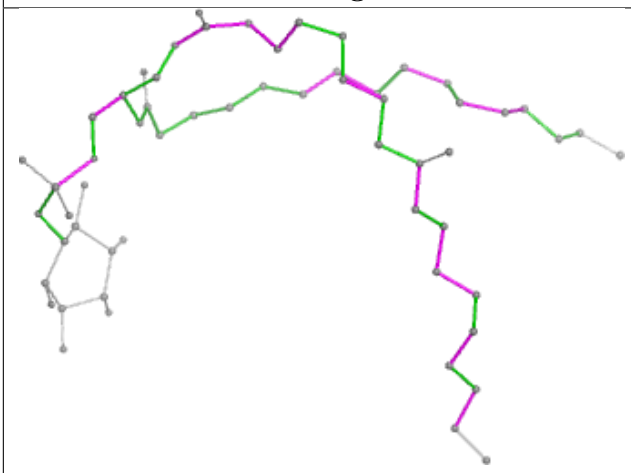
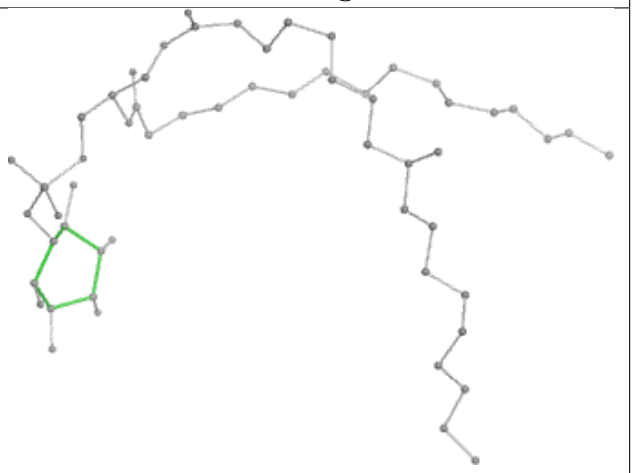


Bond angles

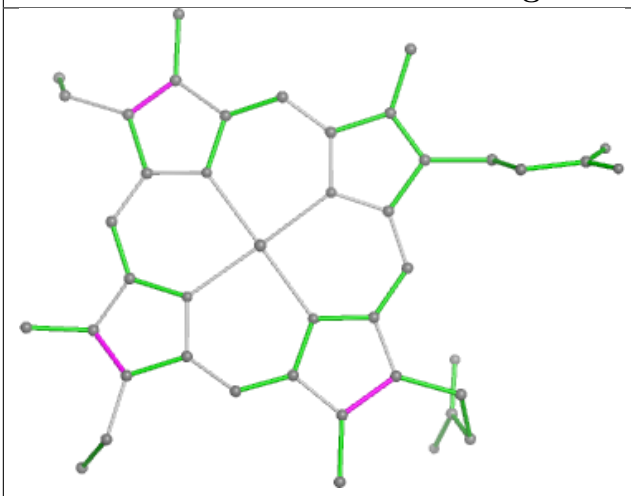


Torsions



Rings

Ligand HEC C 301



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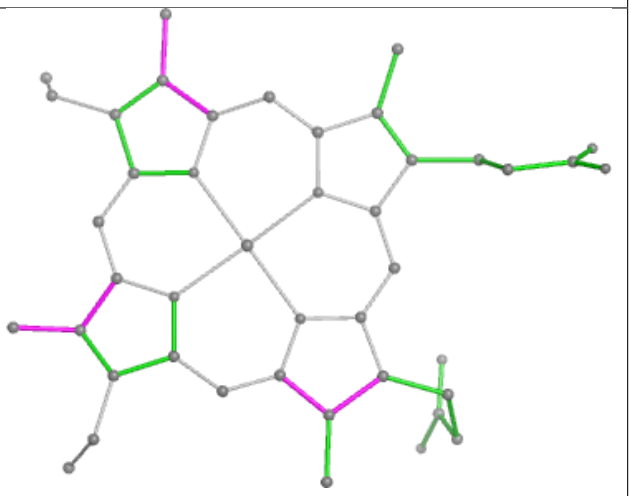
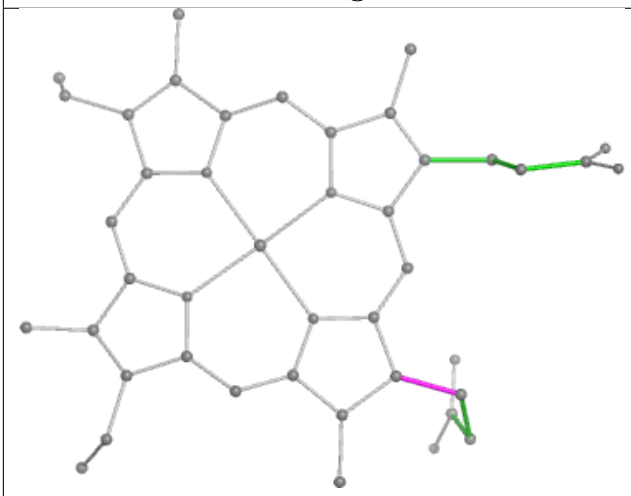
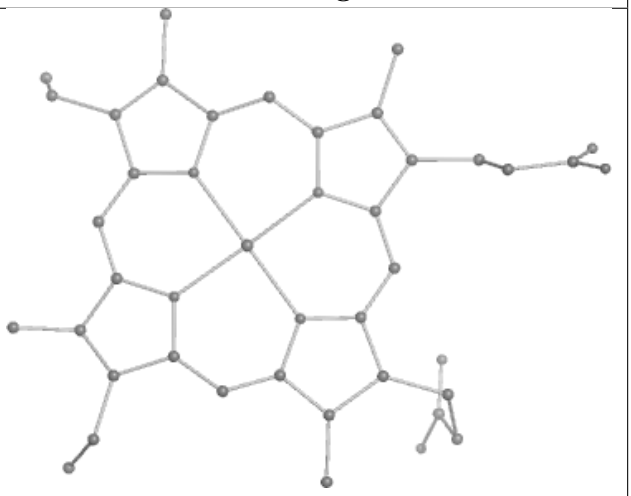


Bond angles

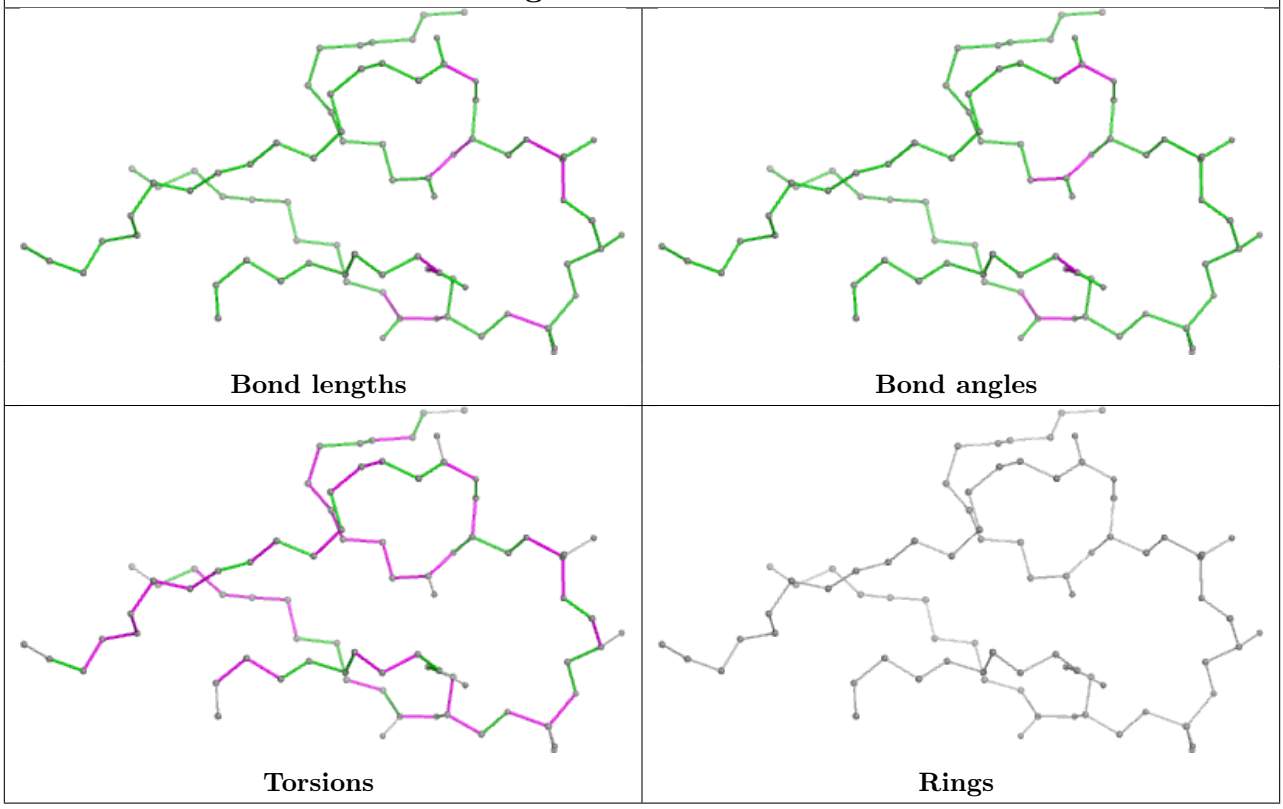


Torsions

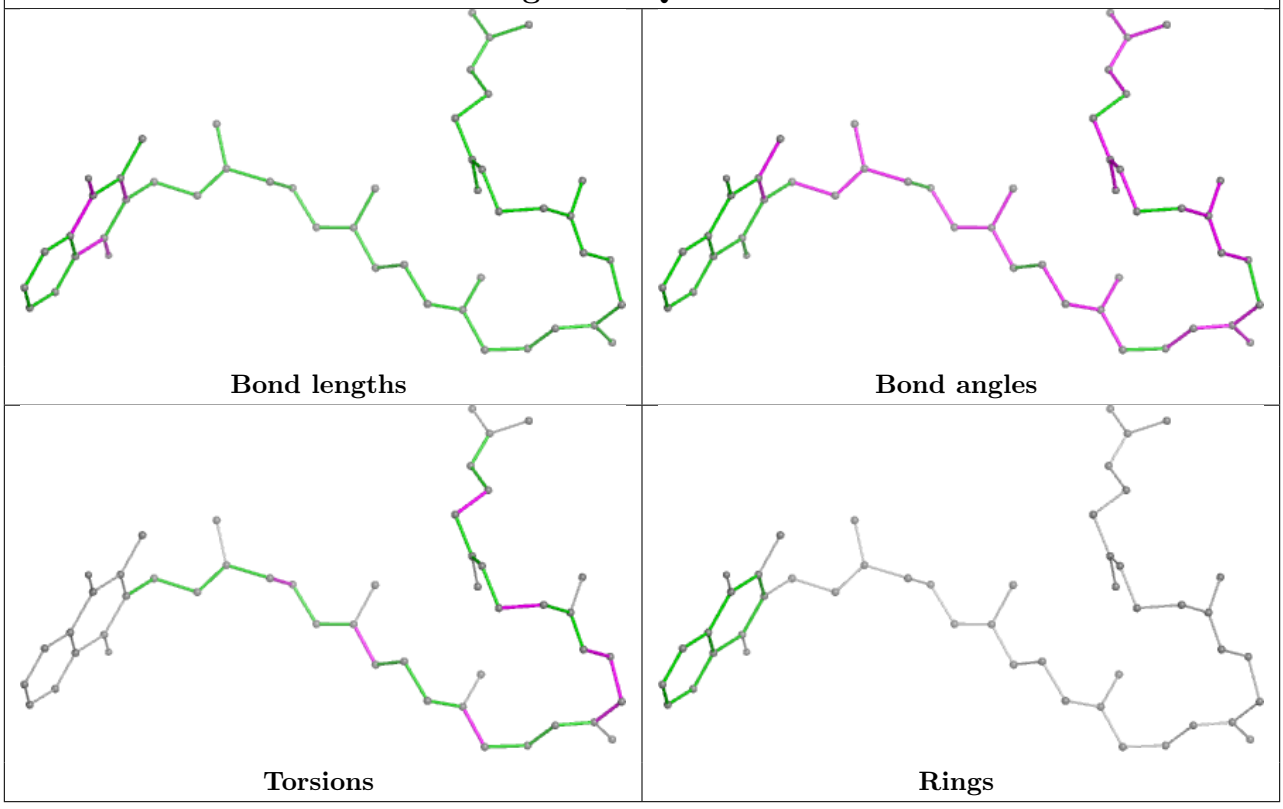


Rings

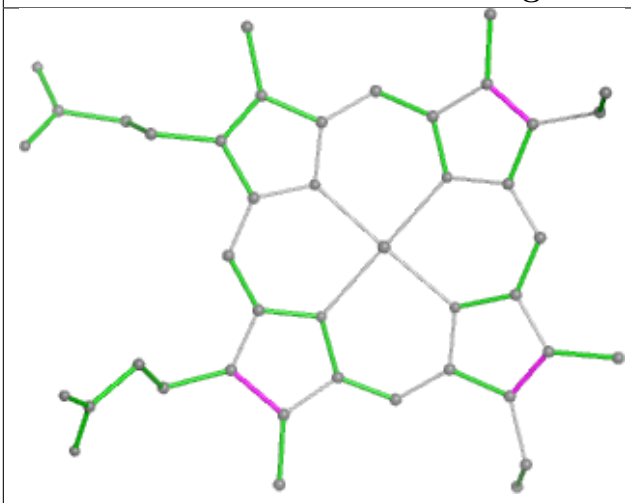
Ligand CDL C 305



Ligand MQ7 O 301



Ligand HEC C 302



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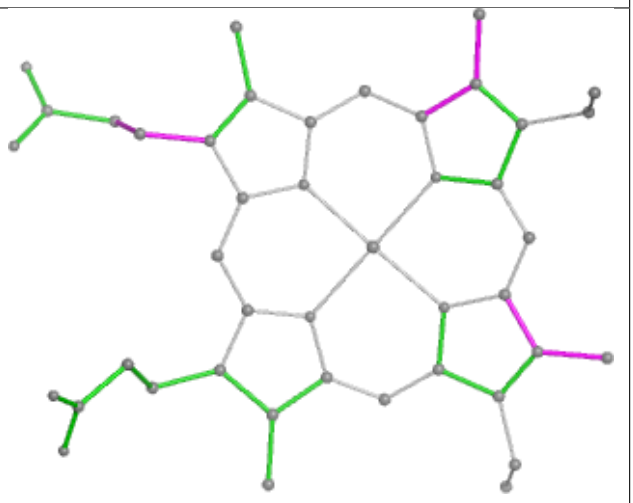
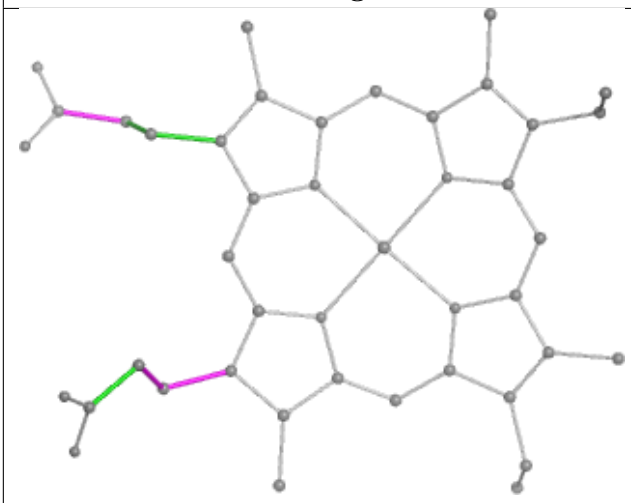
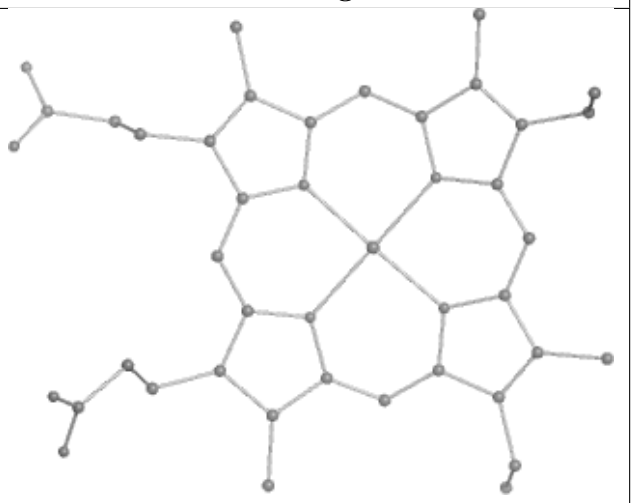


Bond angles

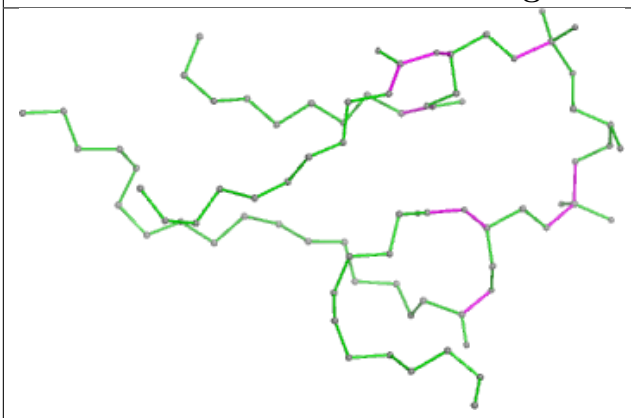


Torsions



Rings

Ligand CDL N 607



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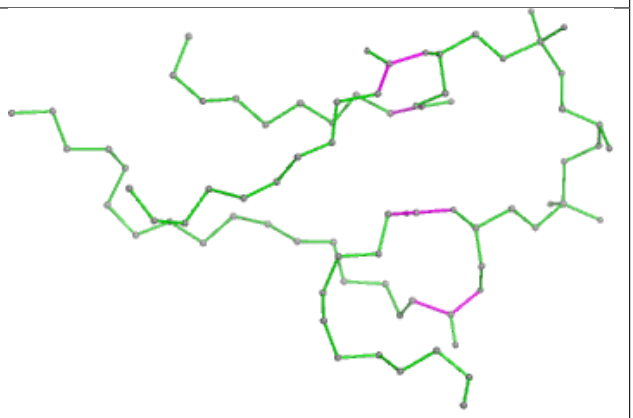
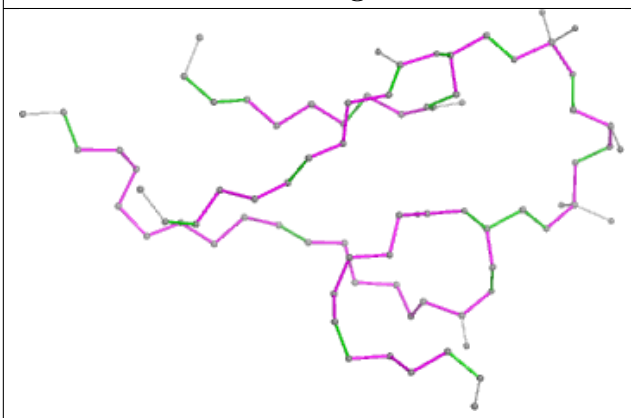
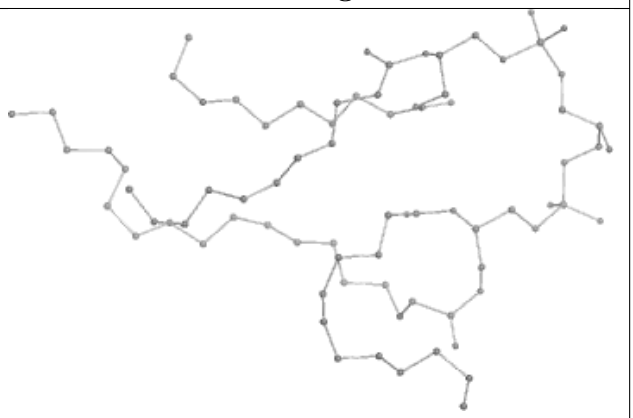


Bond angles

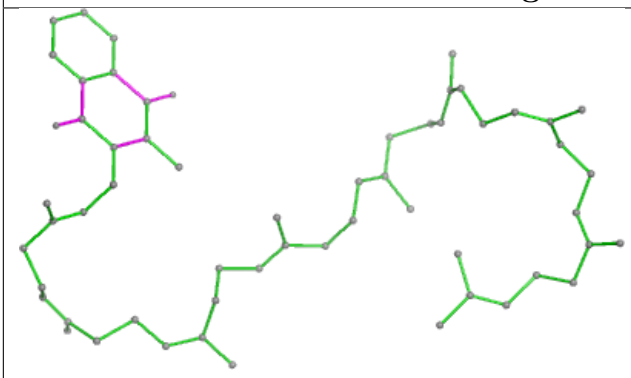


Torsions



Rings

Ligand MQ9 C 304



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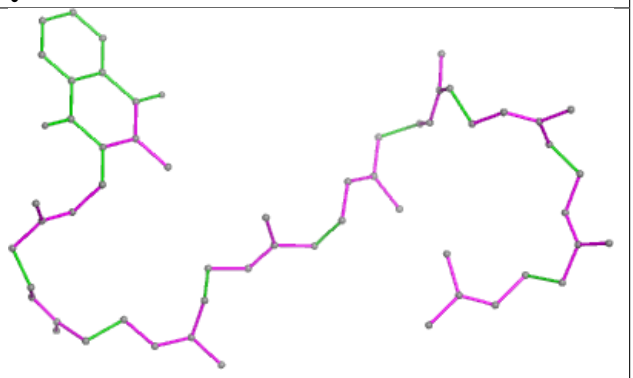
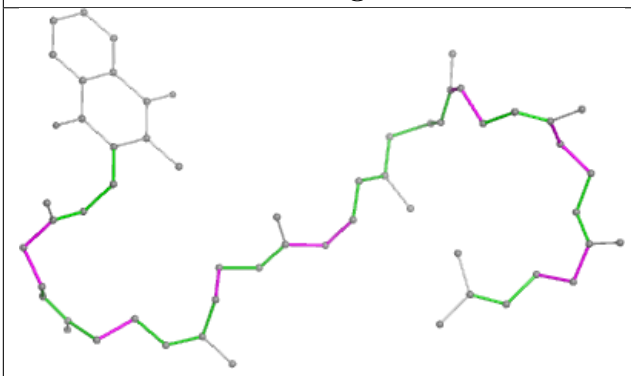
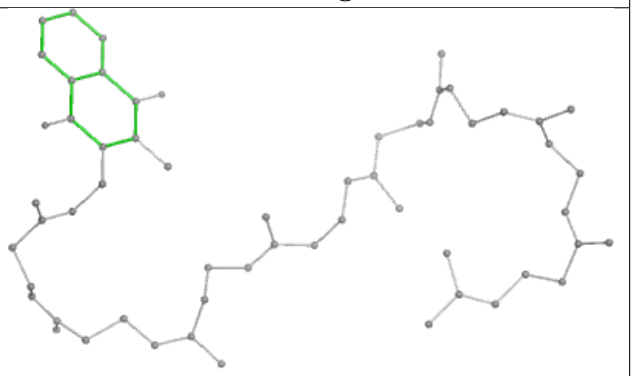


Bond angles

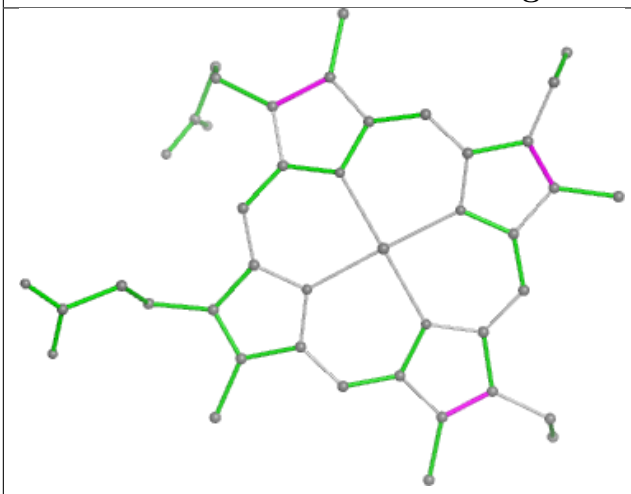


Torsions



Rings

Ligand HEC O 302



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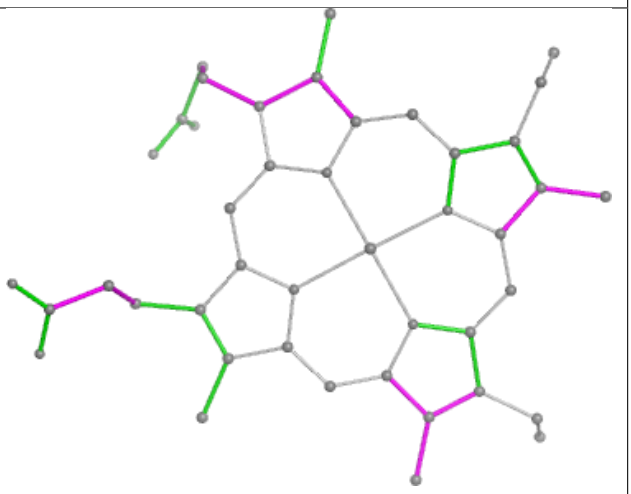
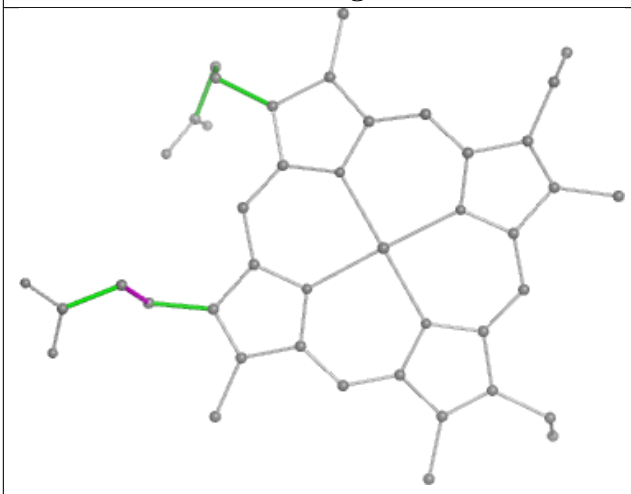
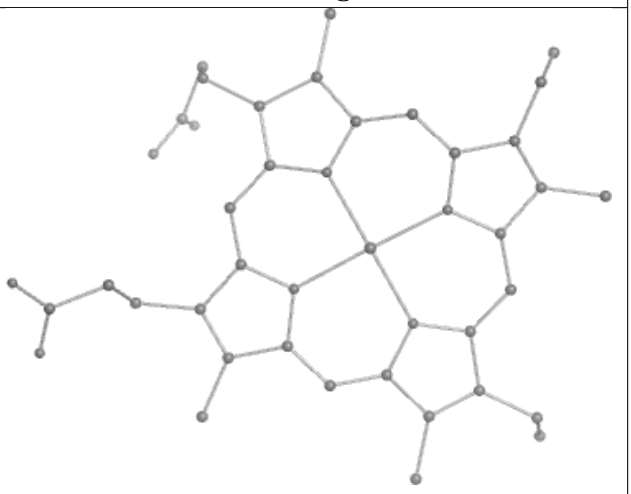


Bond angles

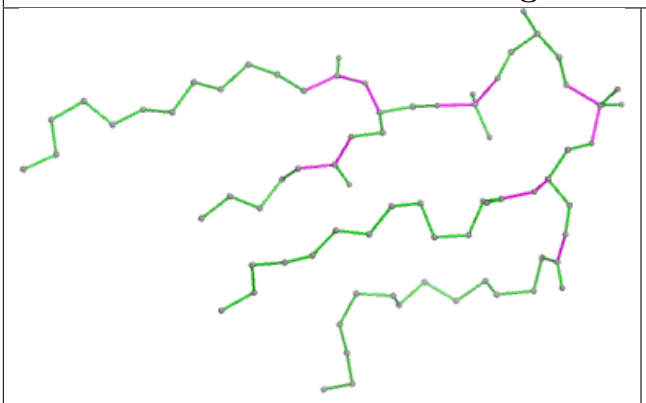


Torsions



Rings

Ligand CDL M 503



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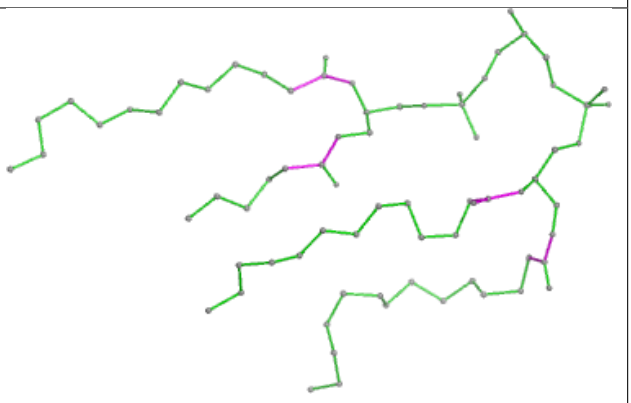
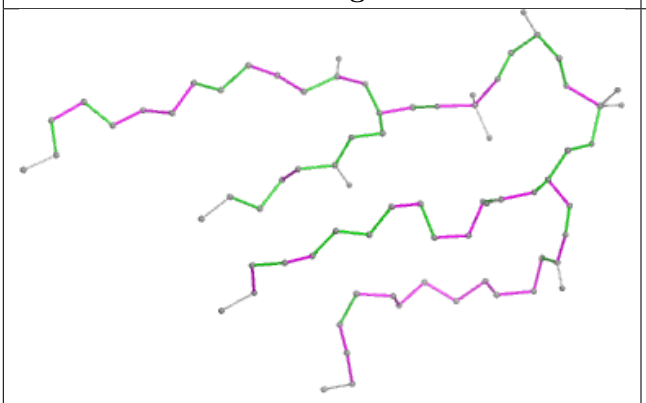
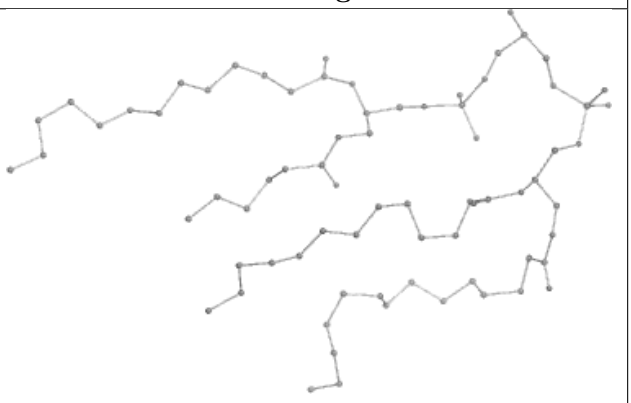


Bond angles

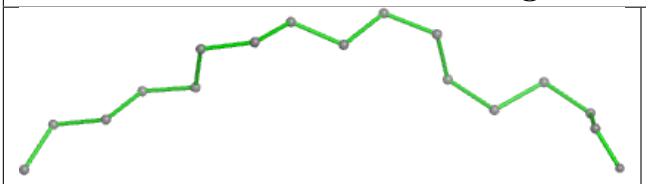


Torsions

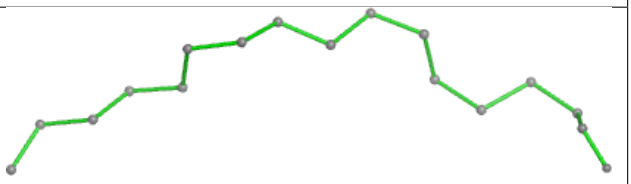


Rings

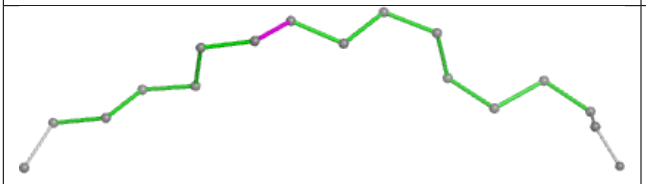
Ligand PLM A 503



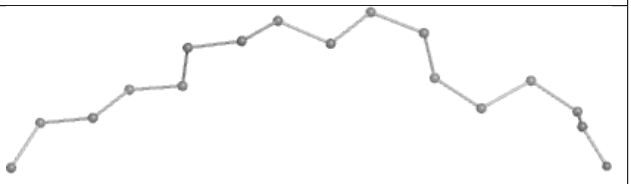
Bond lengths



Bond angles

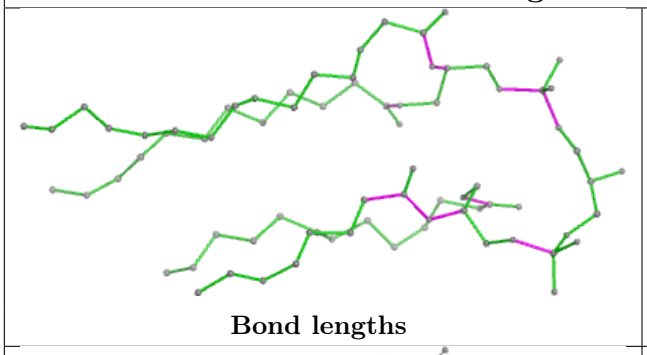


Torsions



Rings

Ligand CDL F 605



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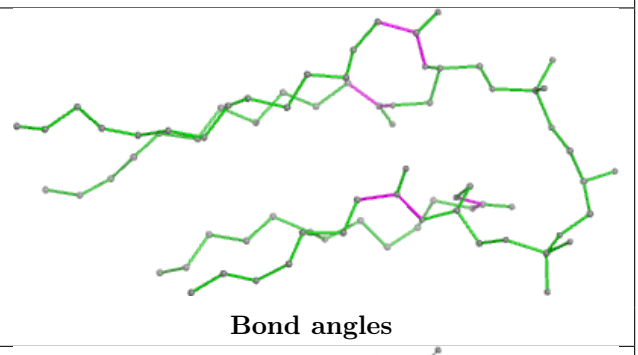
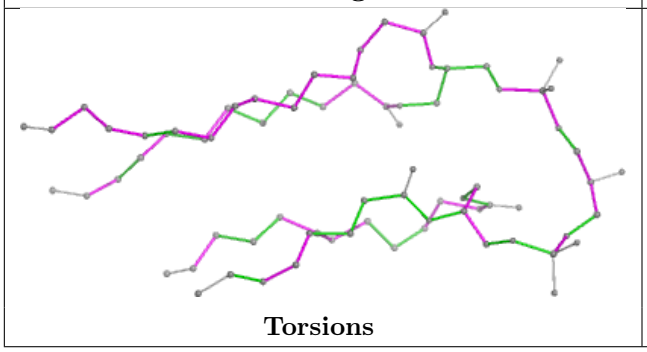
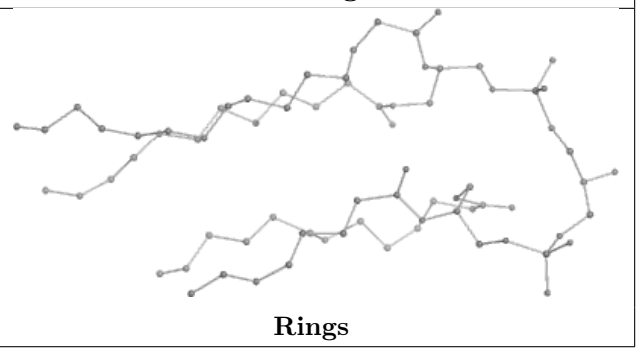


Bond angles

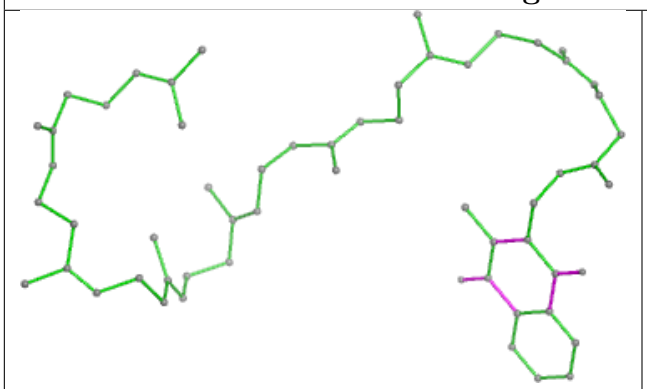


Torsions



Rings

Ligand MQ9 O 305



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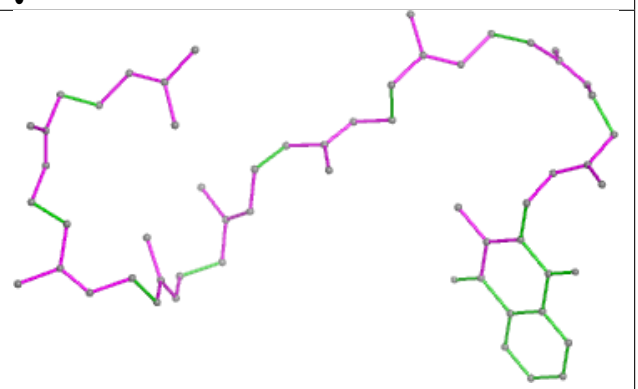
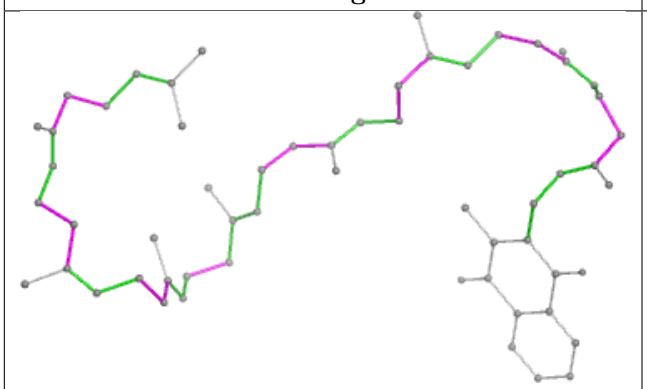
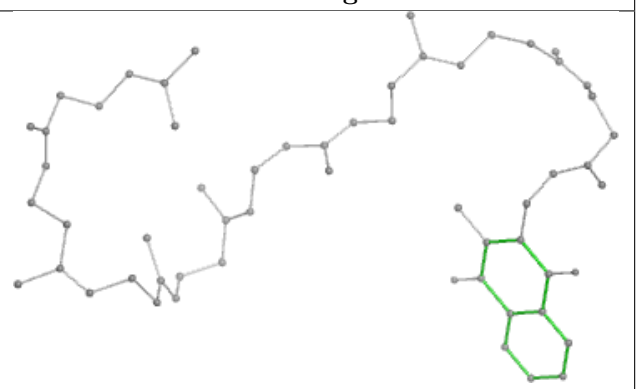


Bond angles

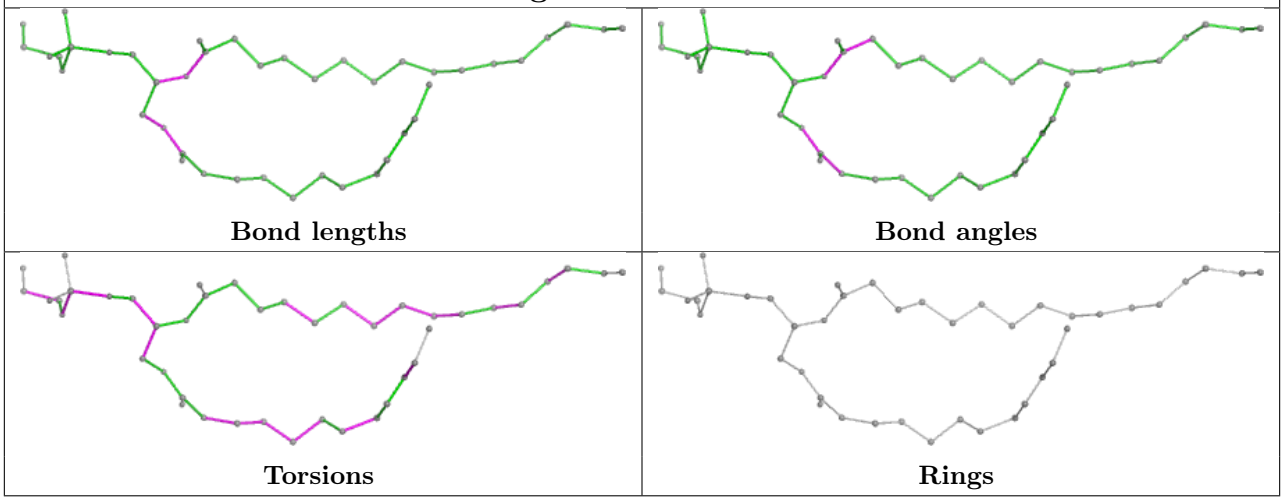


Torsions

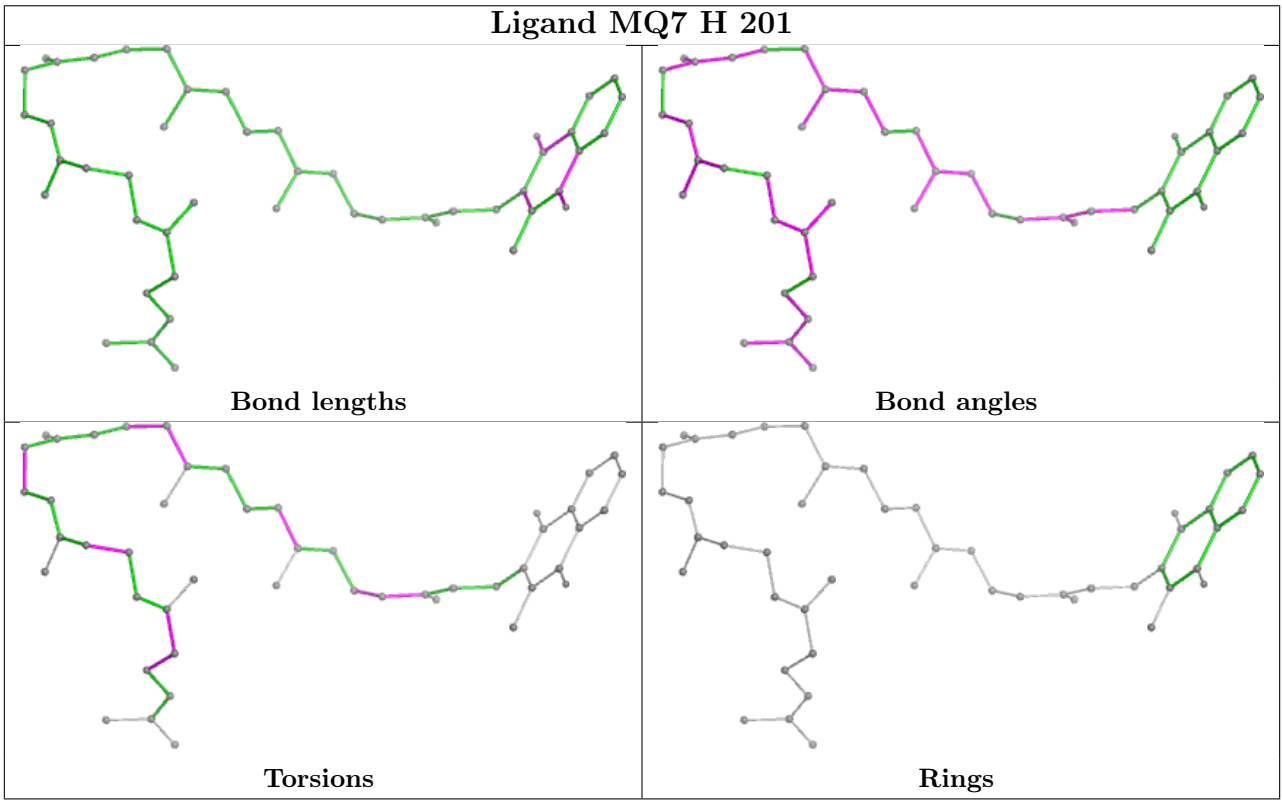


Rings

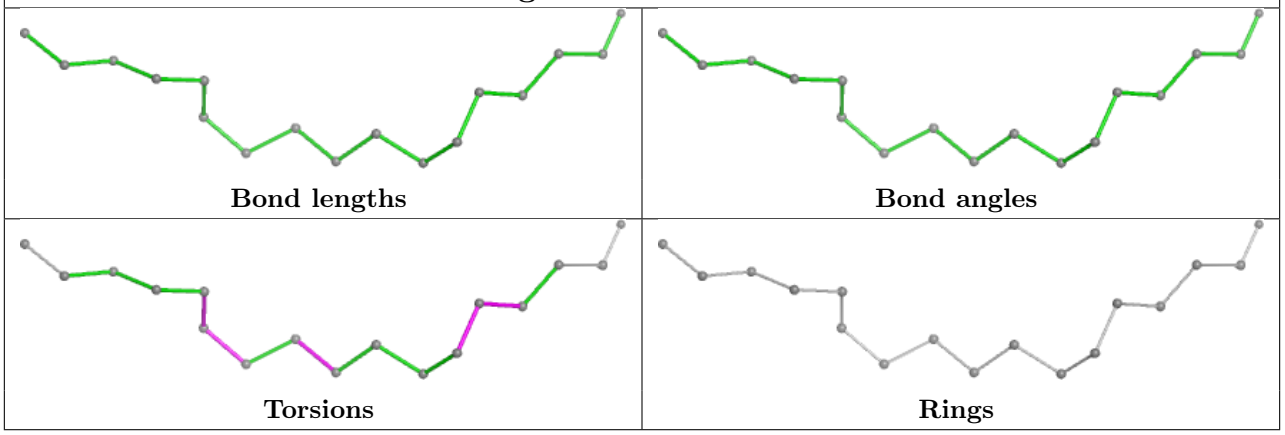
Ligand 9Y0 G 301



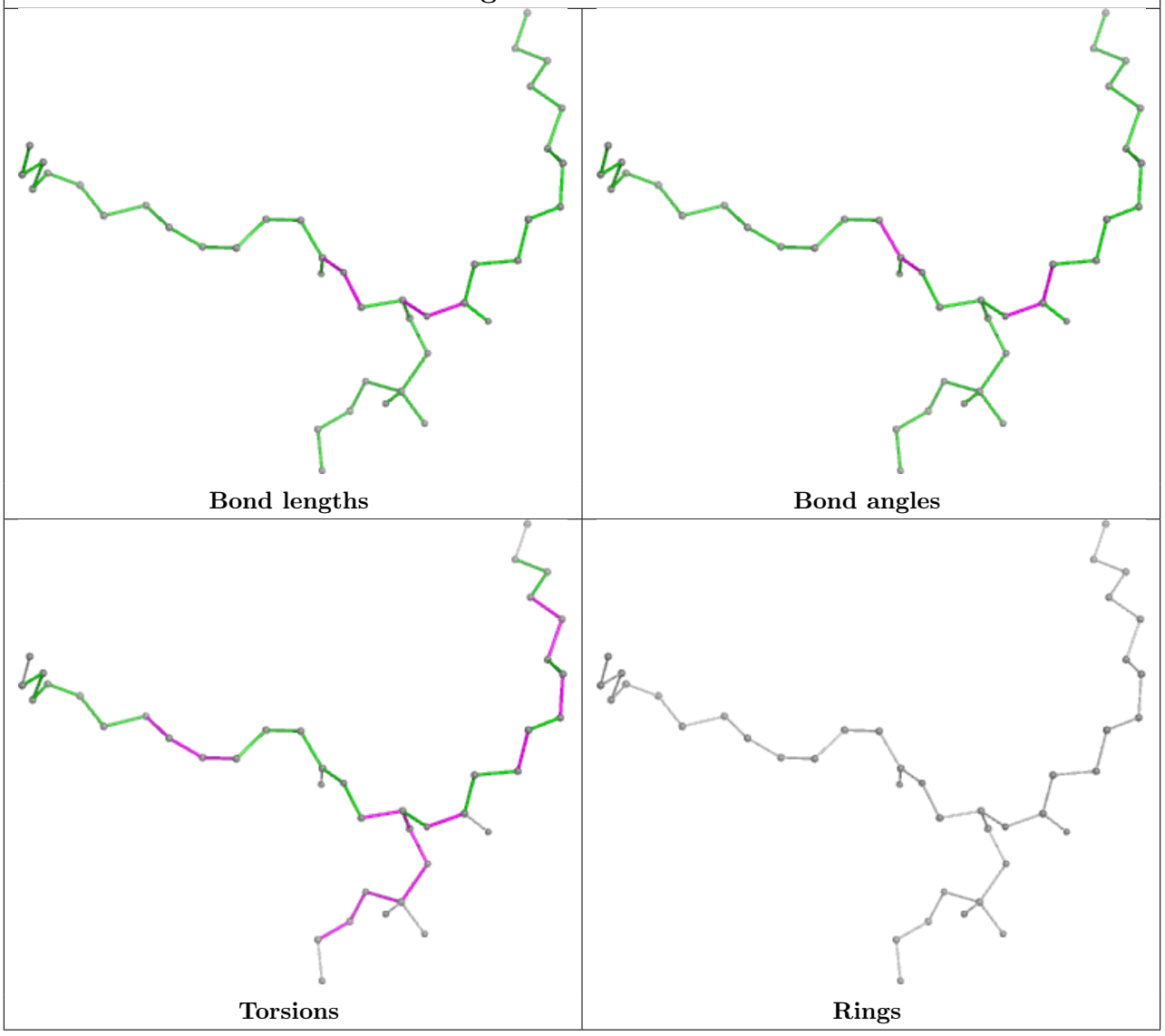
Ligand MQ7 H 201



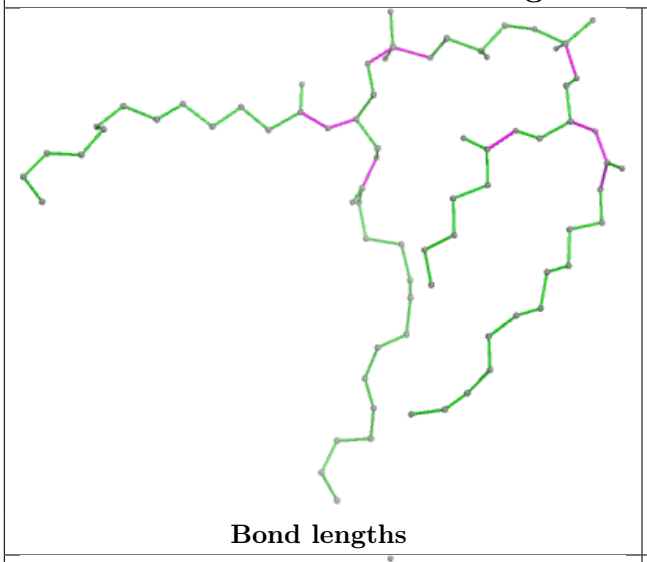
Ligand PLM M 504



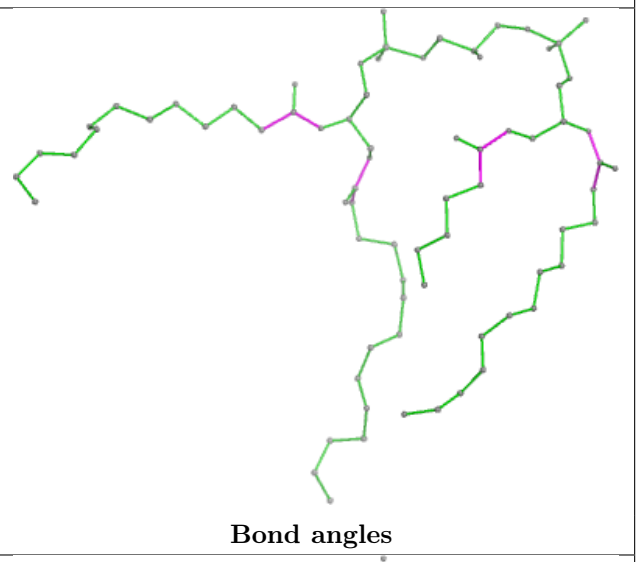
Ligand 9Y0 D 102



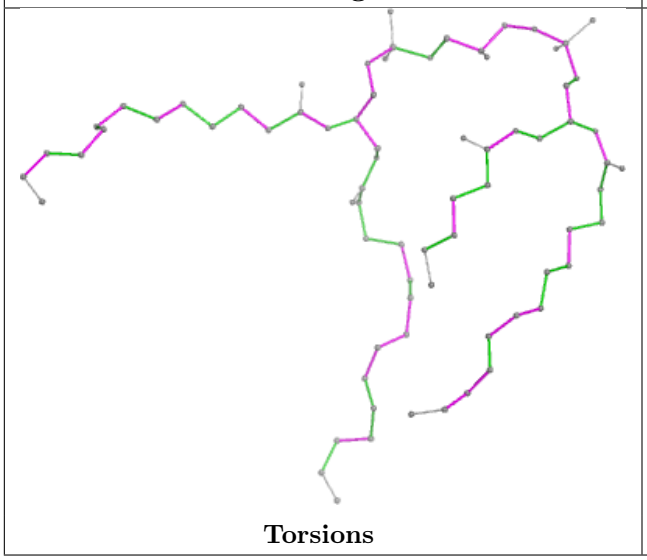
Ligand CDL B 603



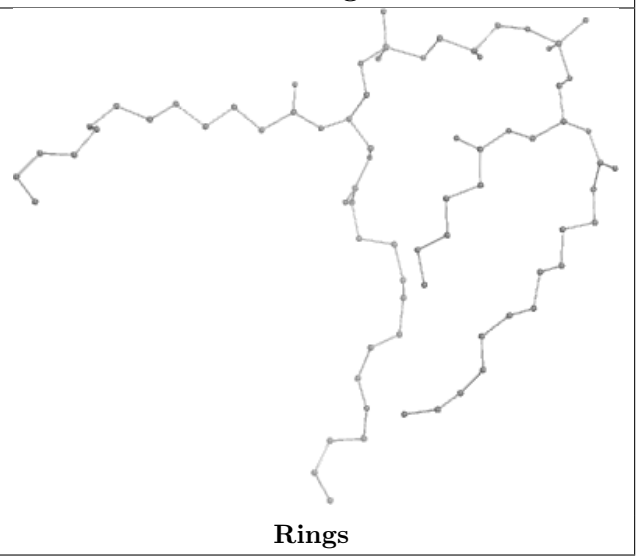
Bond lengths



Bond angles

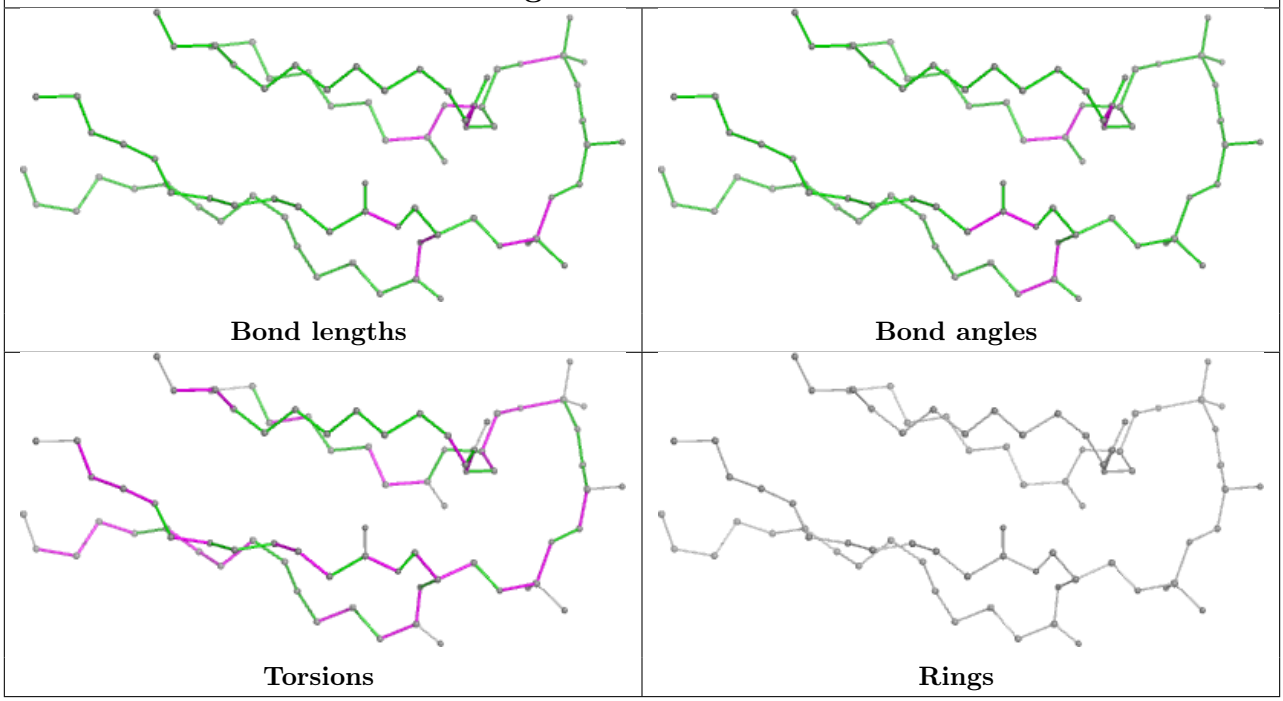


Torsions

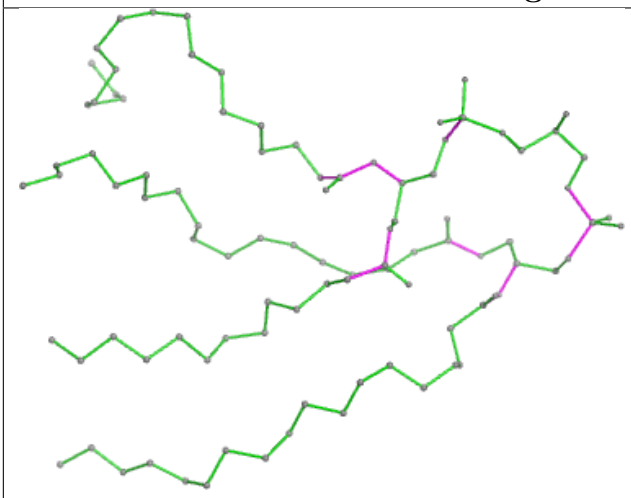


Rings

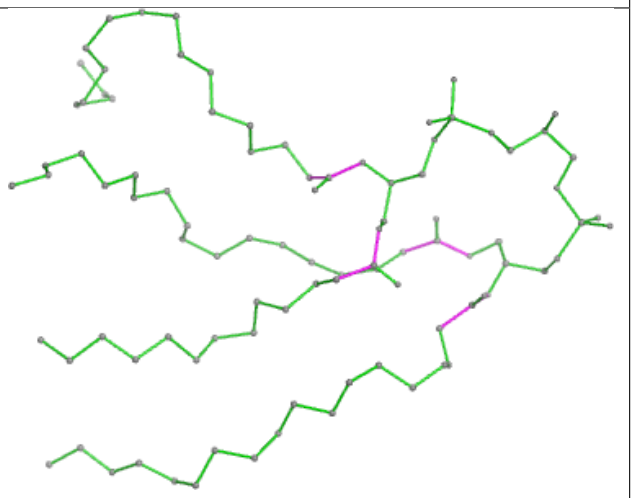
Ligand CDL R 605



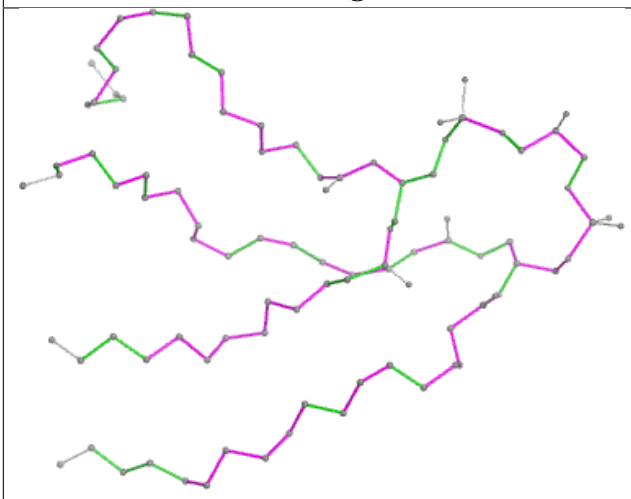
Ligand CDL P 103



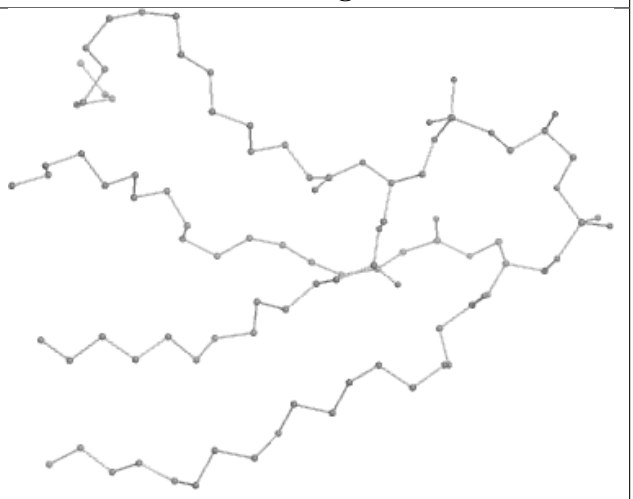
Bond lengths



Bond angles

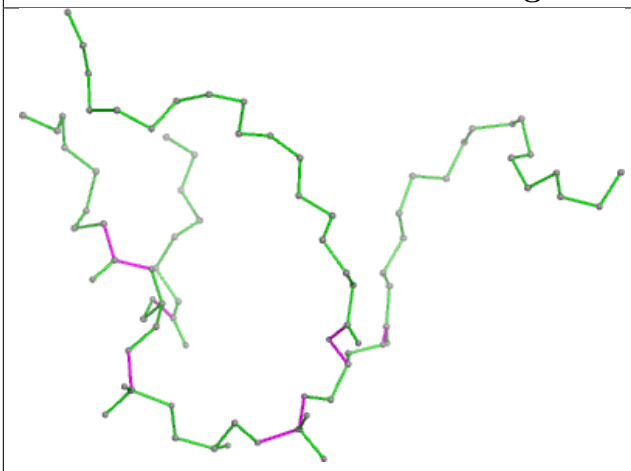


Torsions

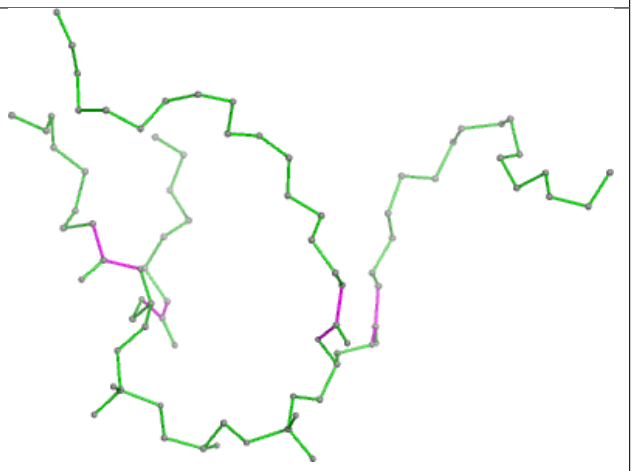


Rings

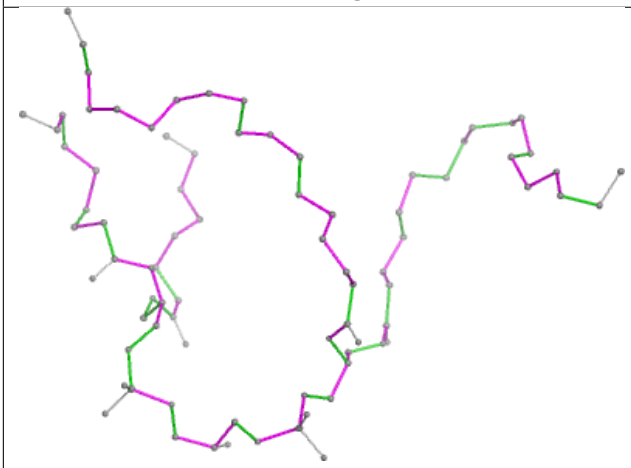
Ligand CDL R 606



Bond lengths



Bond angles



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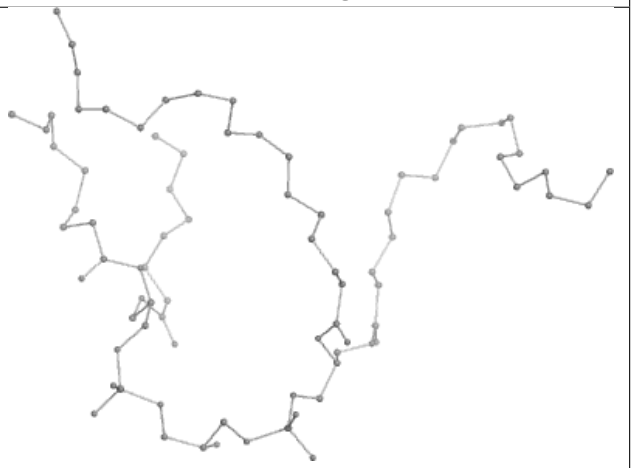
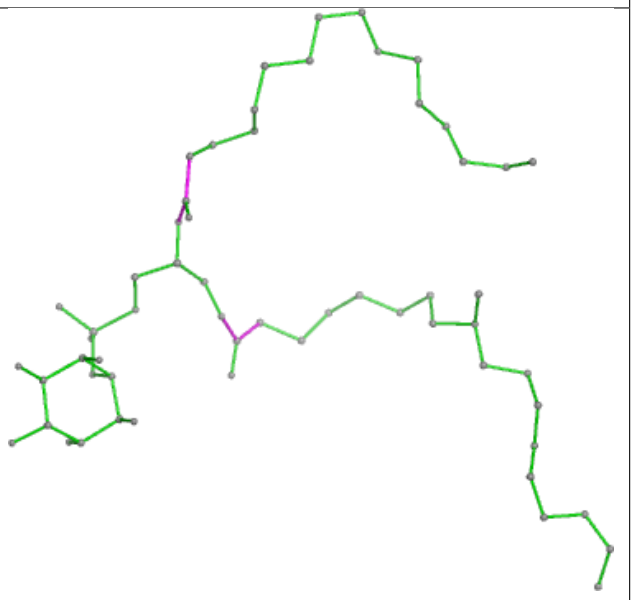


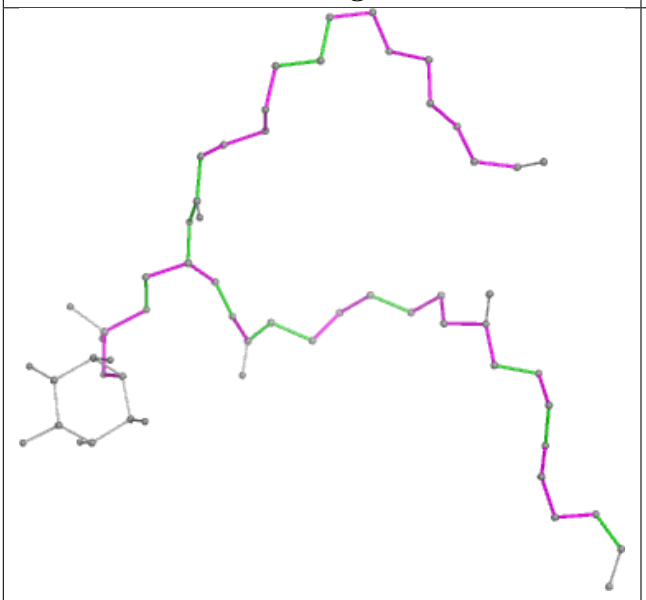
Rings

Ligand 9YF C 303

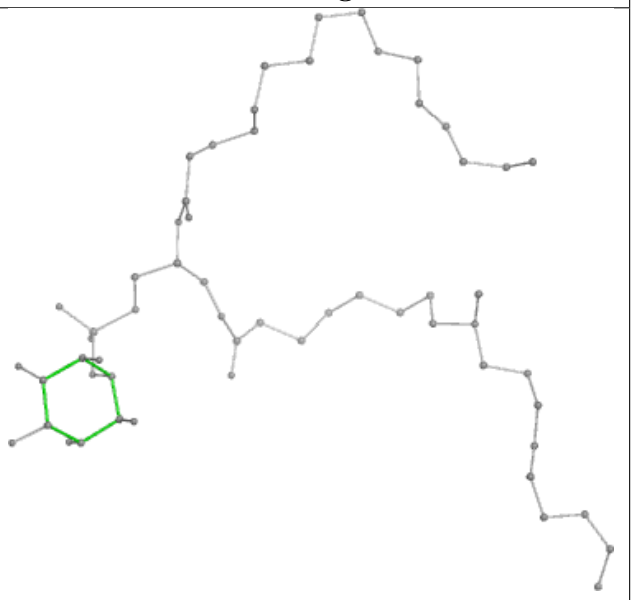
Bond lengths



Bond angles

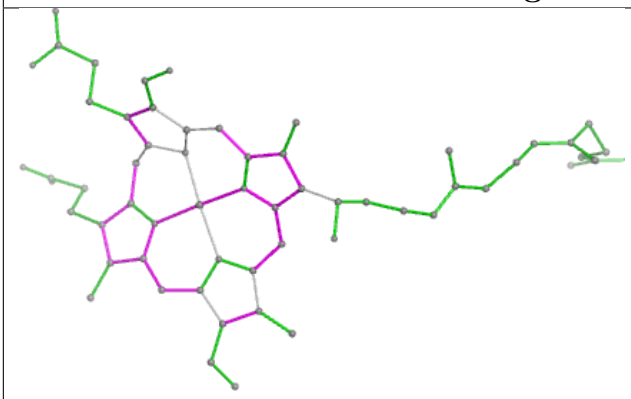


Torsions

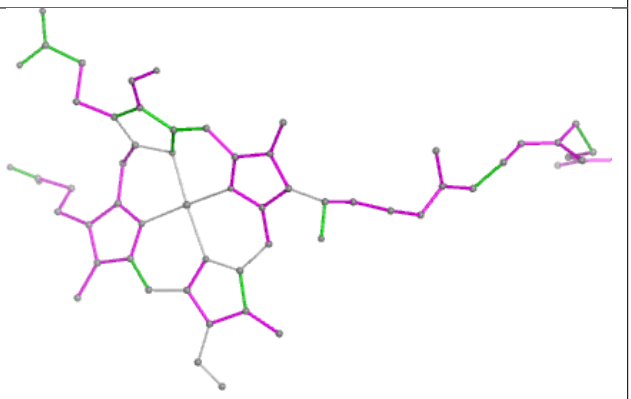


Rings

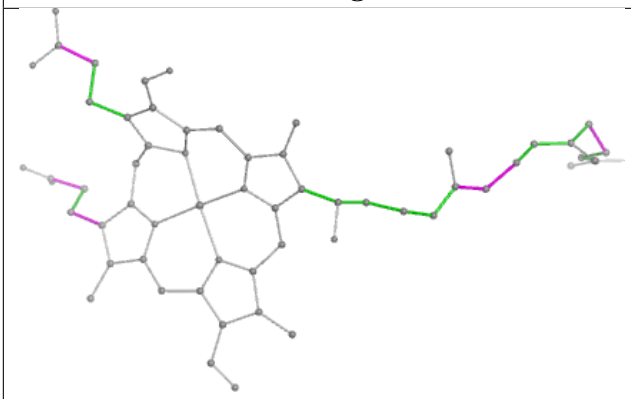
Ligand HEA F 602



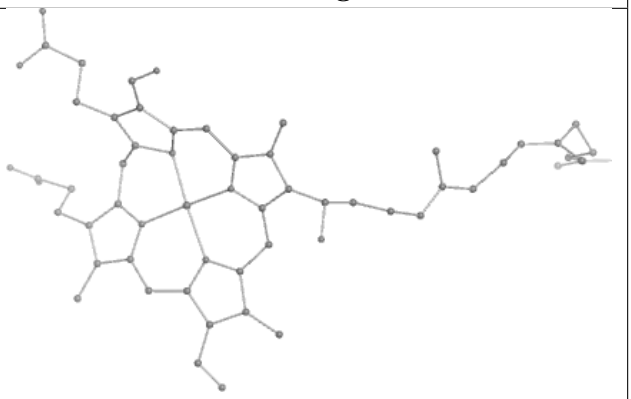
Bond lengths



Bond angles

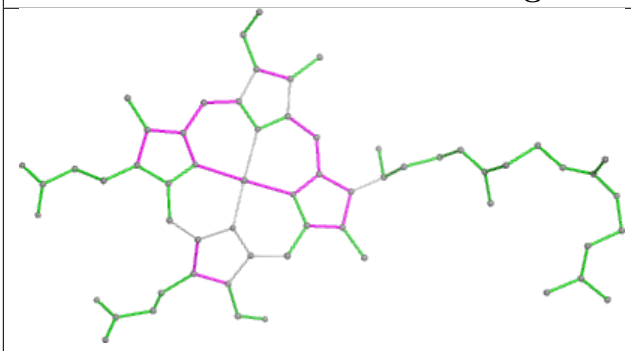


Torsions



Rings

Ligand HEA F 601



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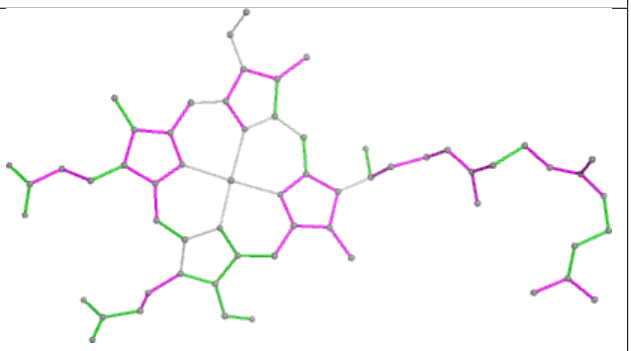
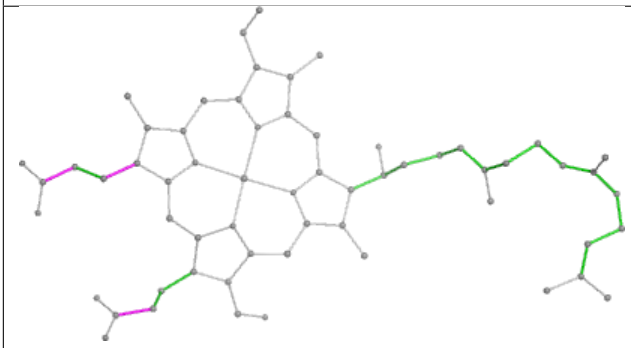


Bond angles



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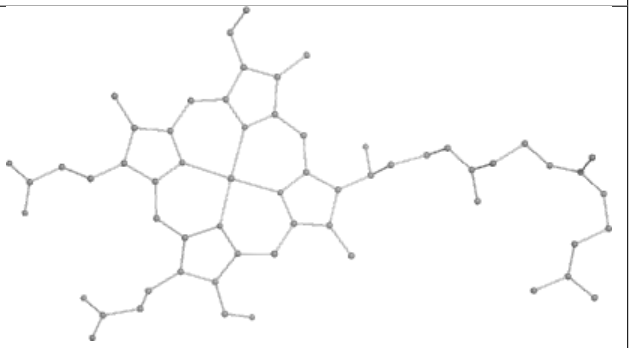
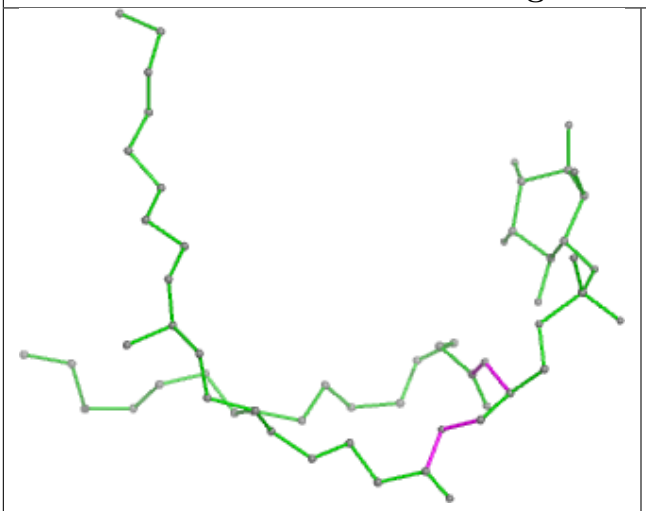


Rings

Ligand 9YF A 502



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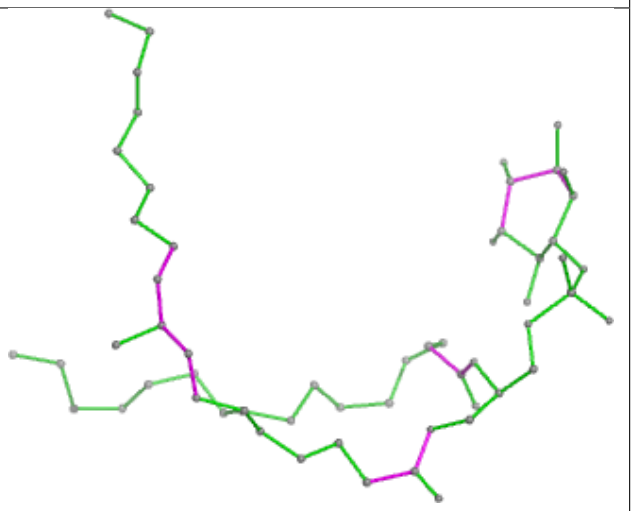
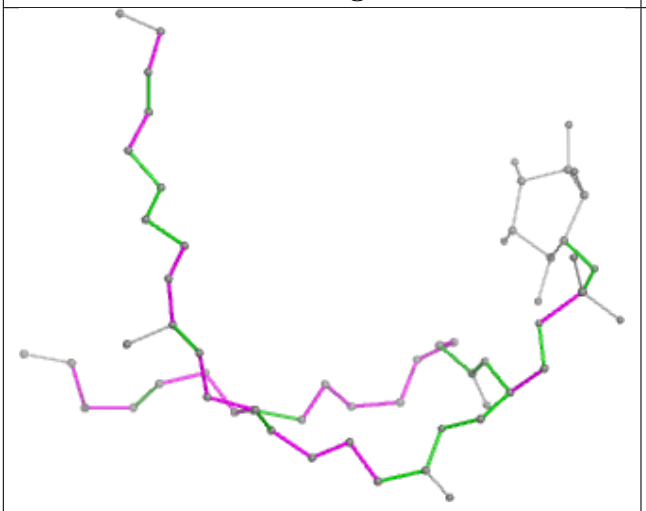


Bond angles



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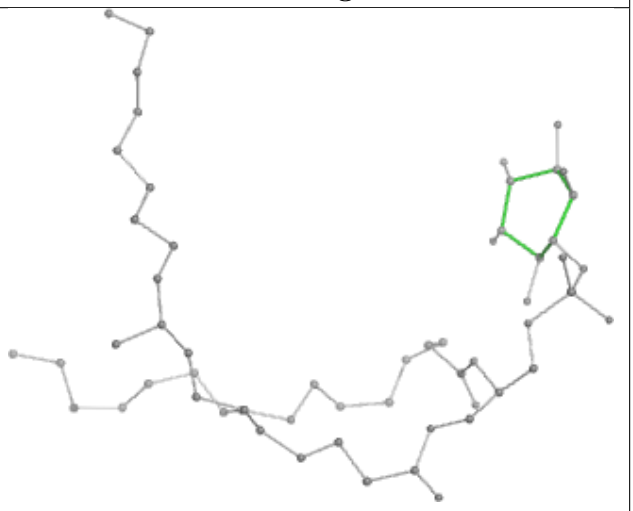
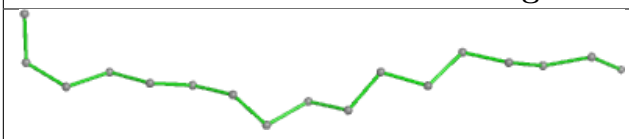


Rings

Ligand PLM T 201



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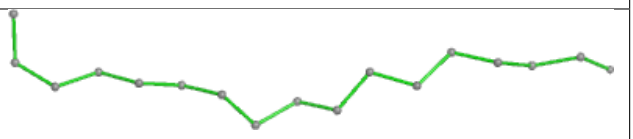
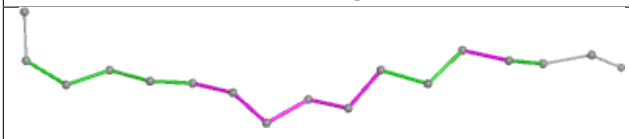


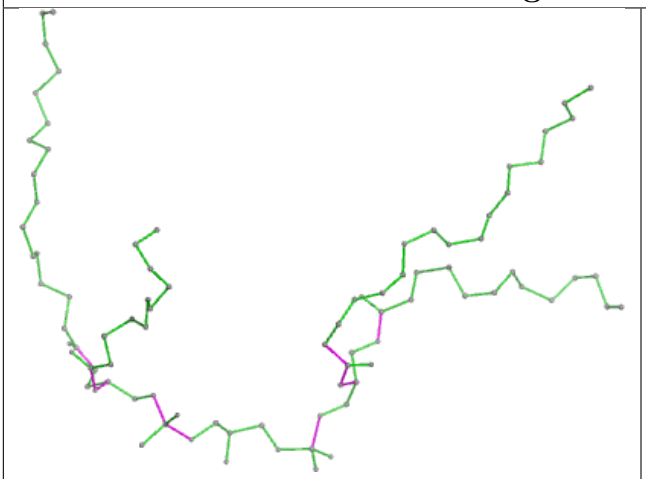
Bond angles



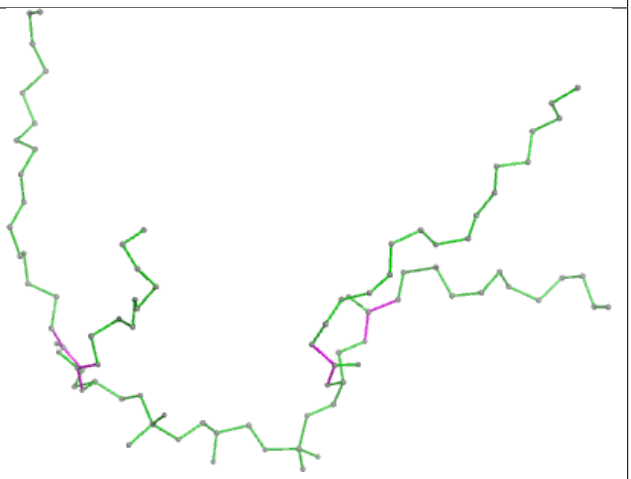
Torsions

Rings

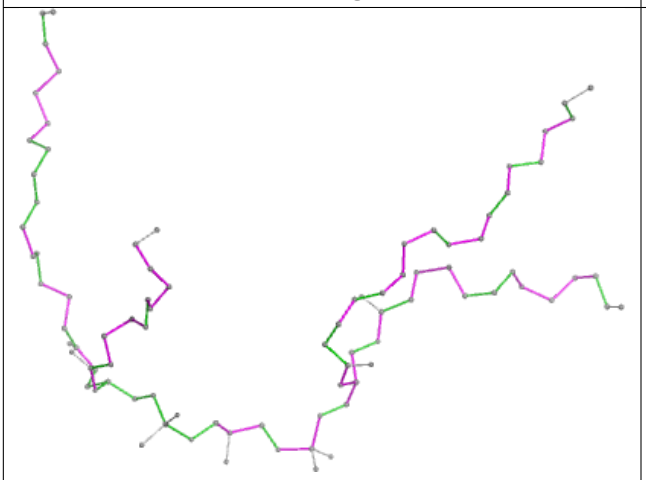
Ligand CDL D 101



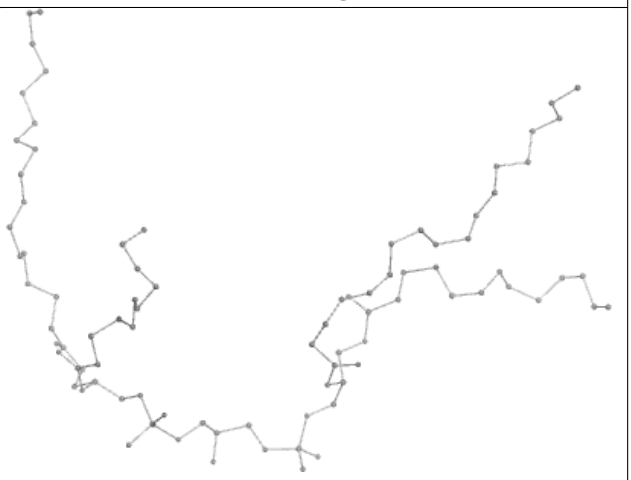
Bond lengths



Bond angles

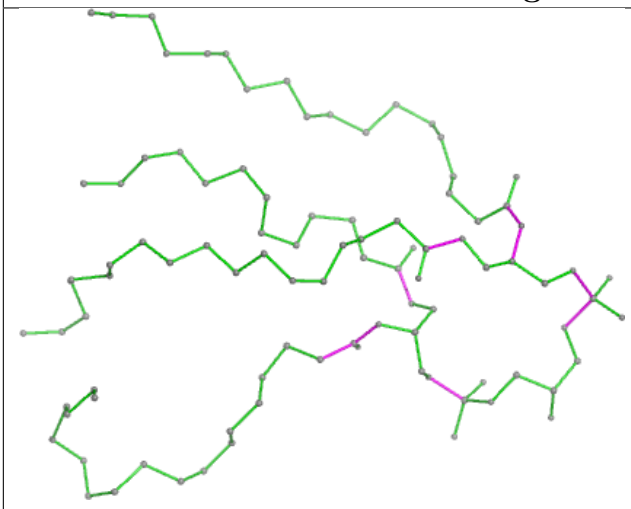


Torsions



Rings

Ligand CDL D 103



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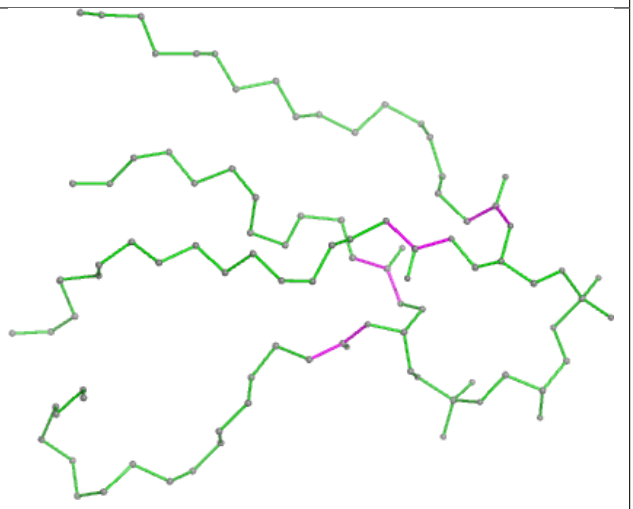
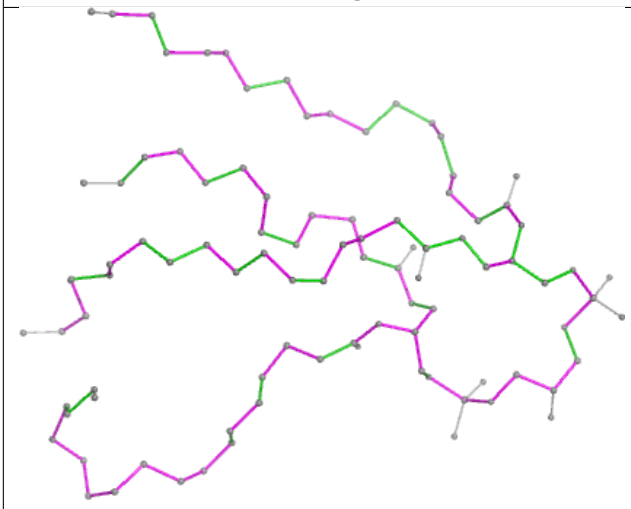
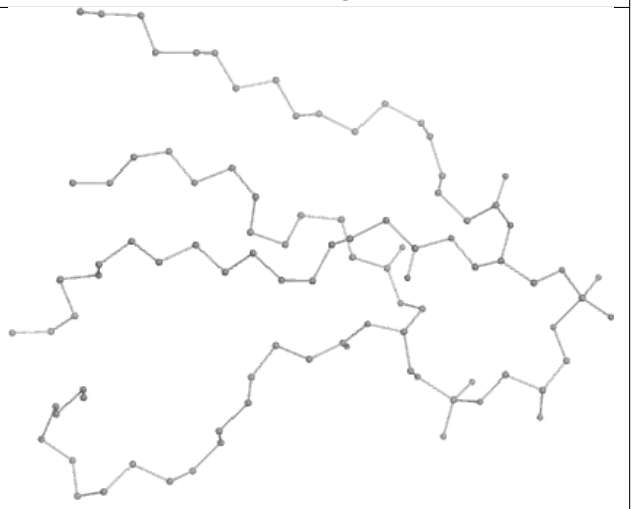


Bond angles

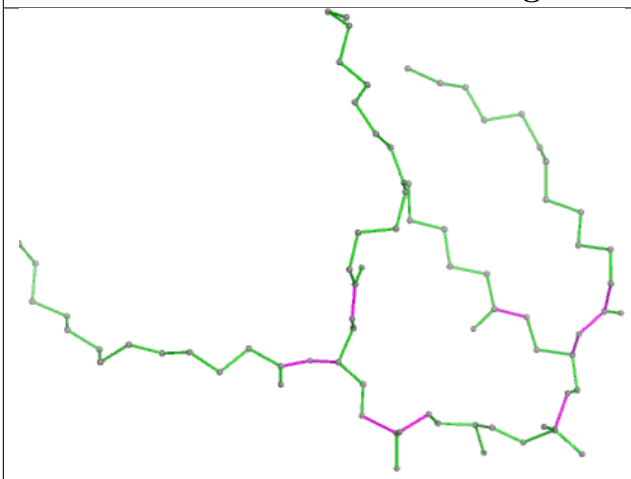


Torsions

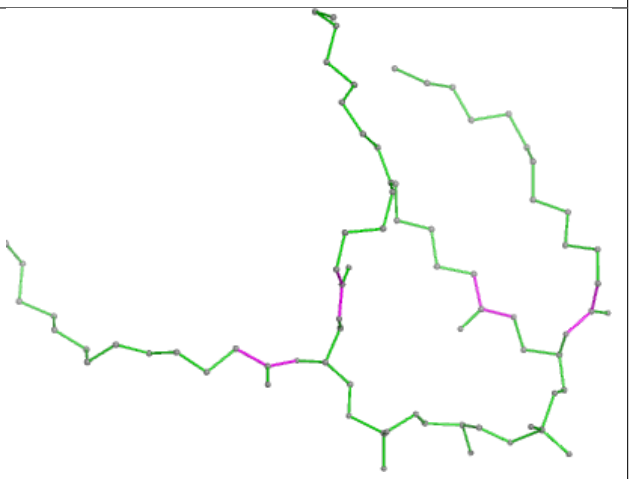


Rings

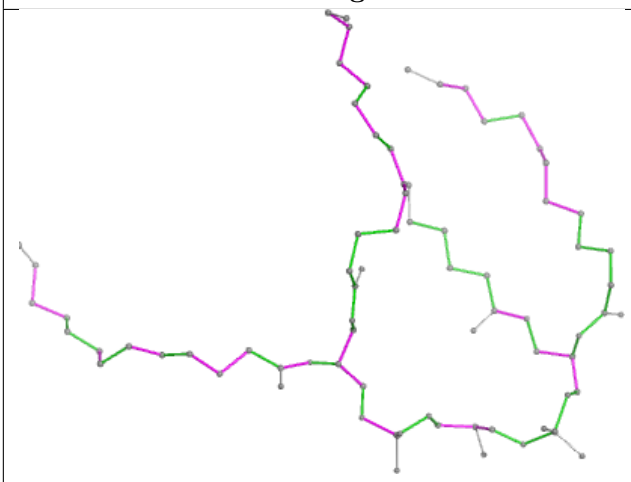
Ligand CDL N 603



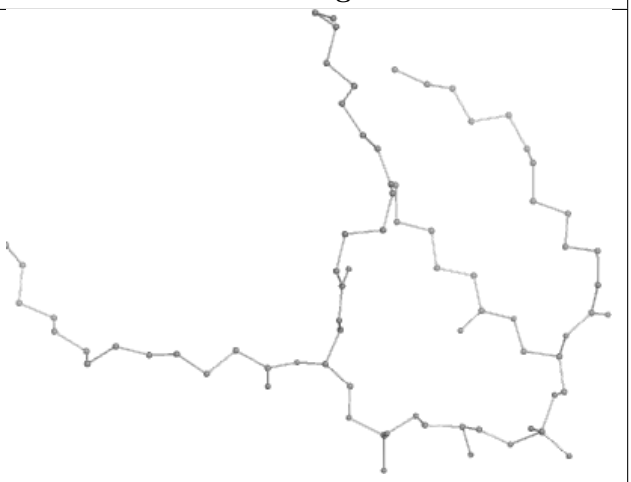
Bond lengths



Bond angles

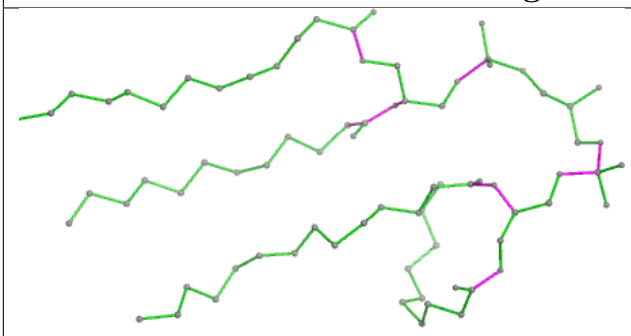


Torsions

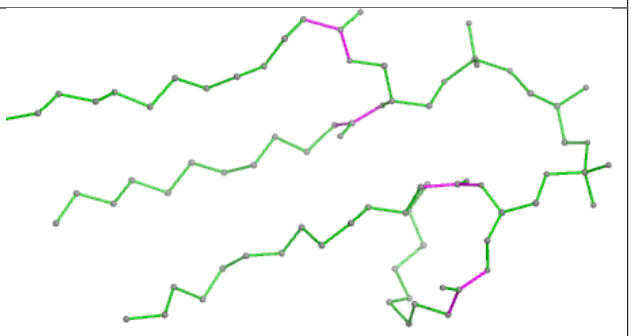


Rings

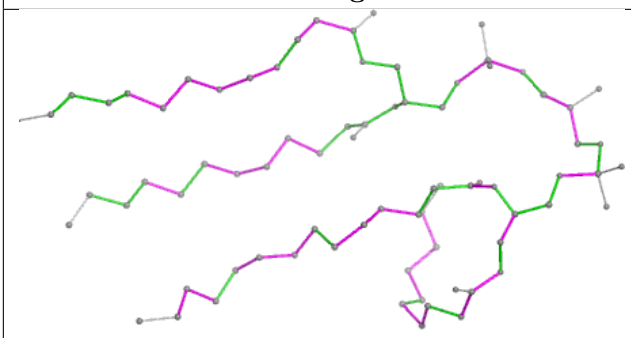
Ligand CDL N 604



Bond lengths



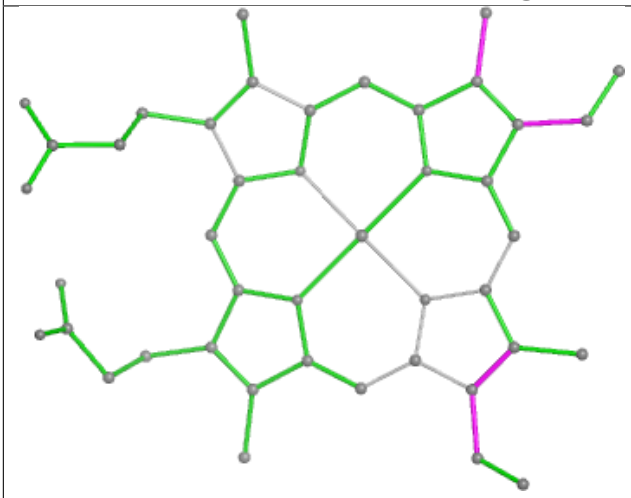
Bond angles



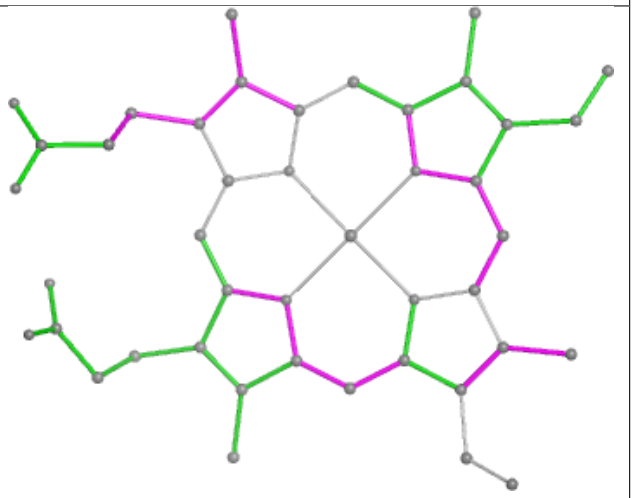
Torsions

Rings

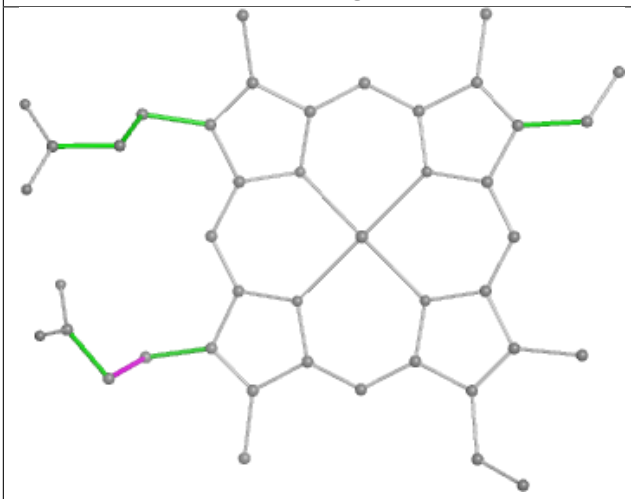
Ligand HEM N 602



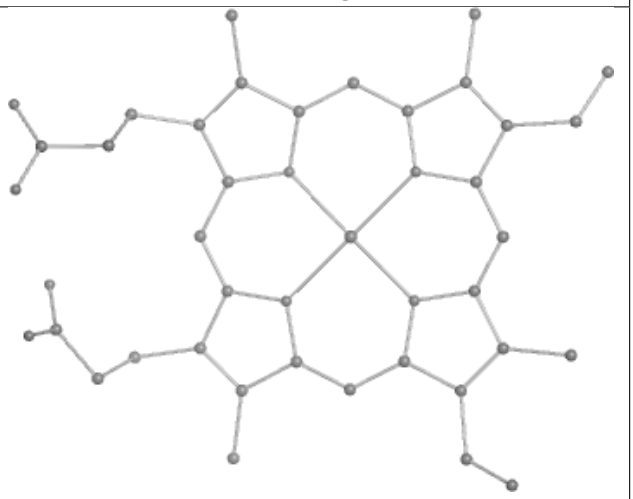
Bond lengths



Bond angles

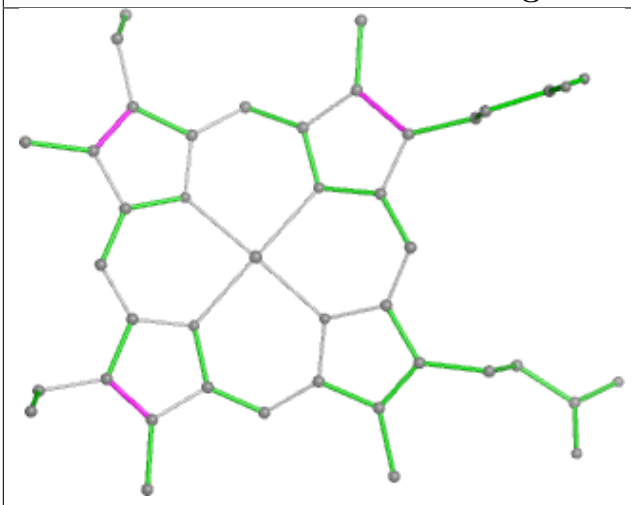


Torsions

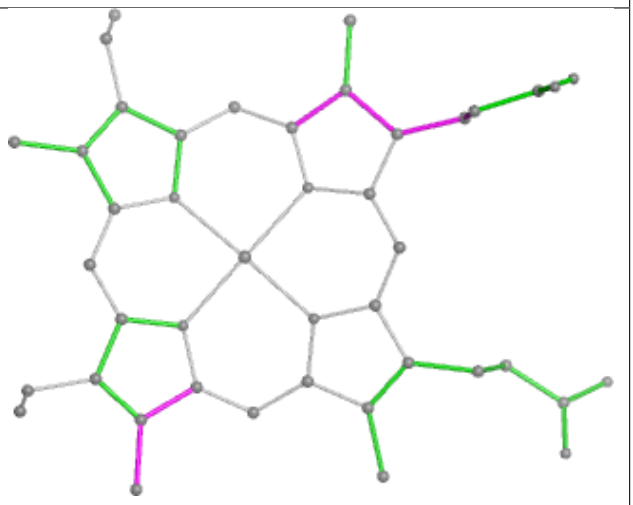


Rings

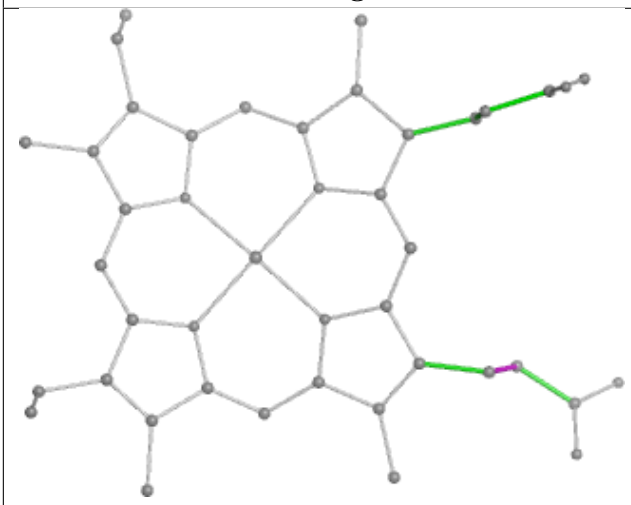
Ligand HEC O 303



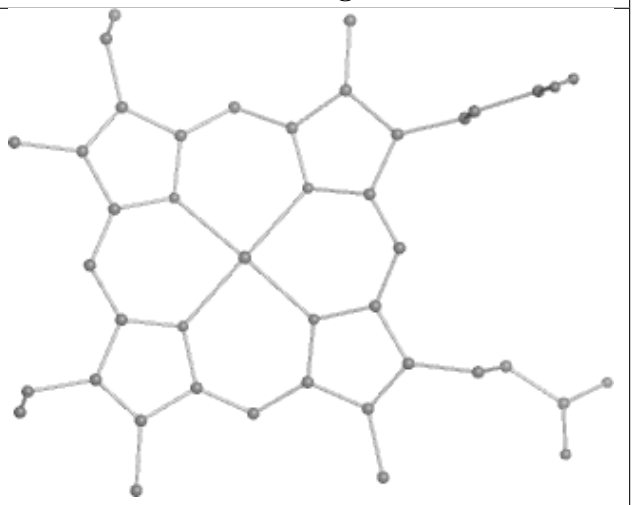
Bond lengths



Bond angles

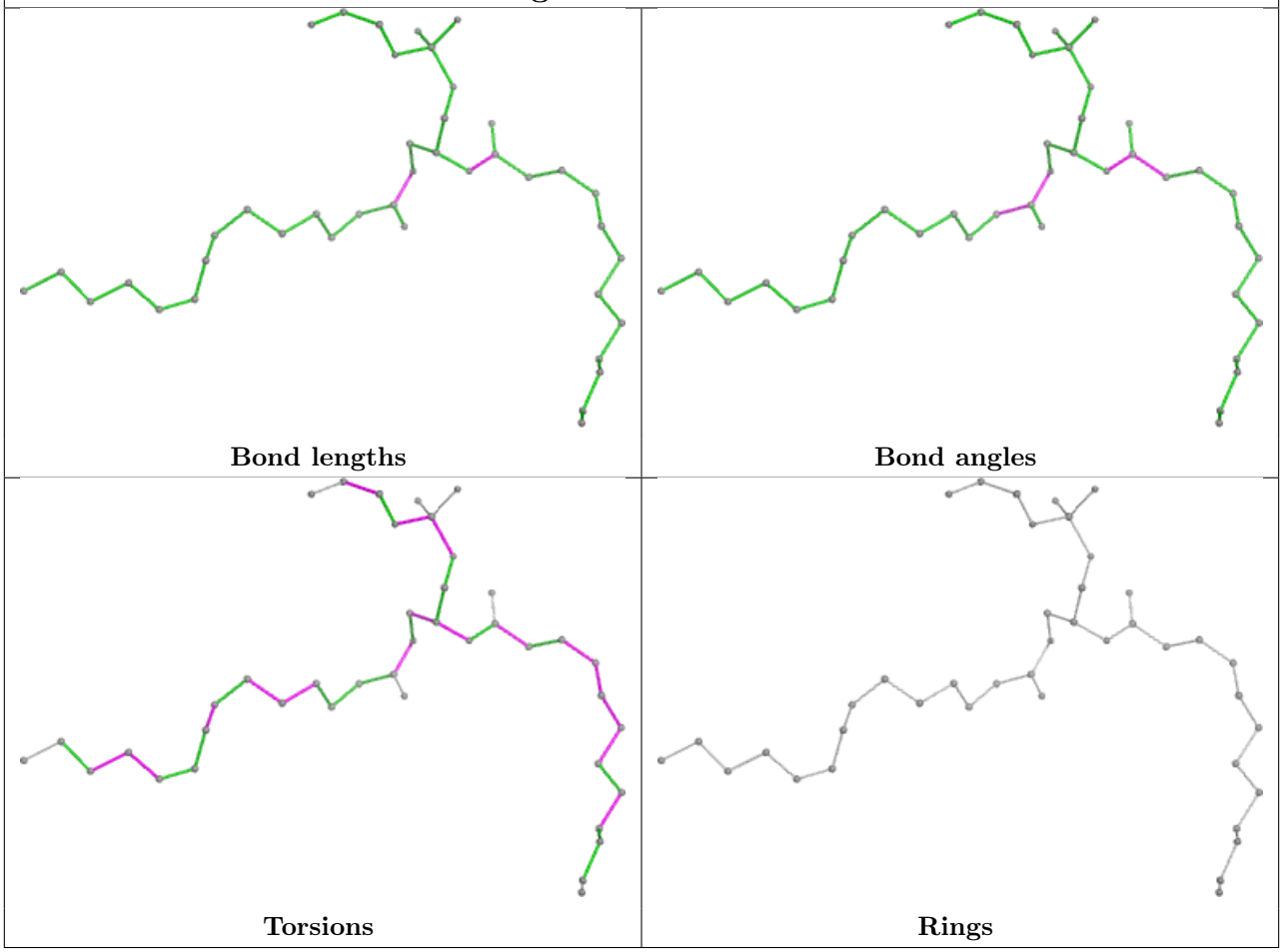


Torsions

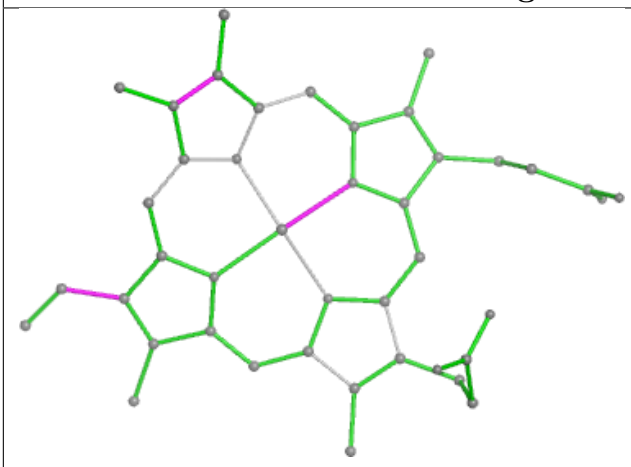


Rings

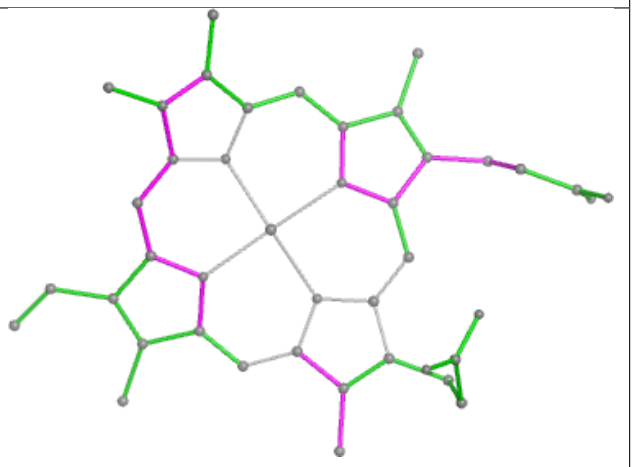
Ligand 9Y0 P 102



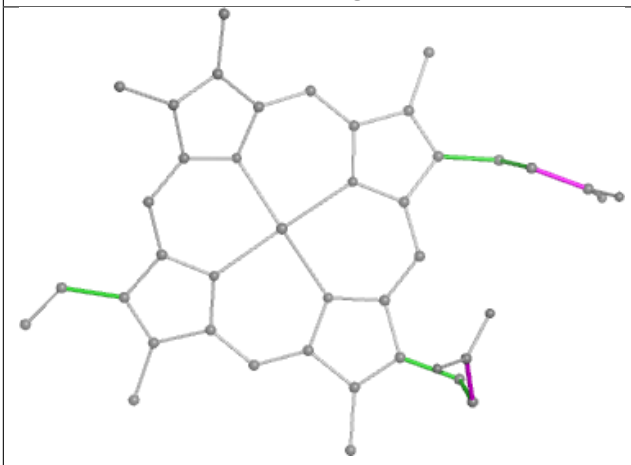
Ligand HEM N 601



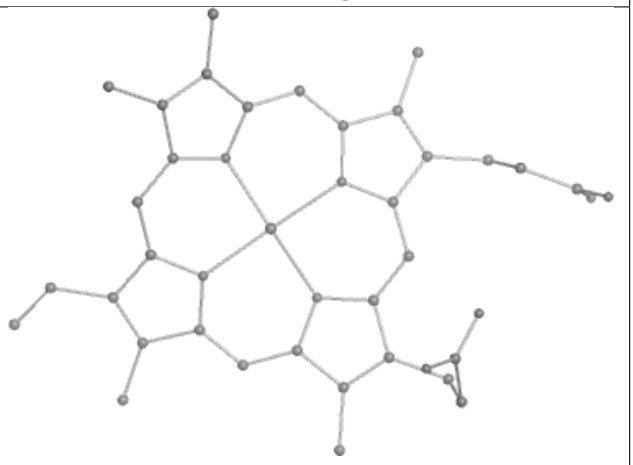
Bond lengths



Bond angles

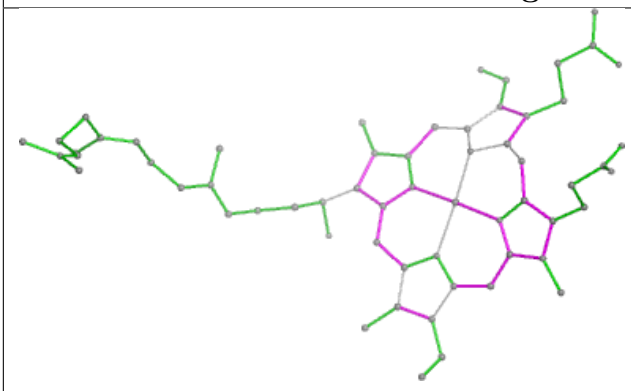


Torsions

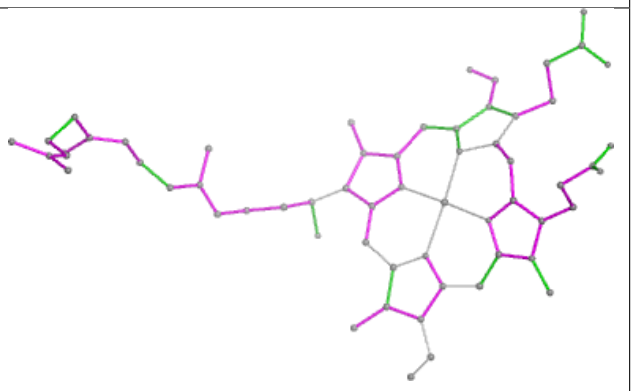


Rings

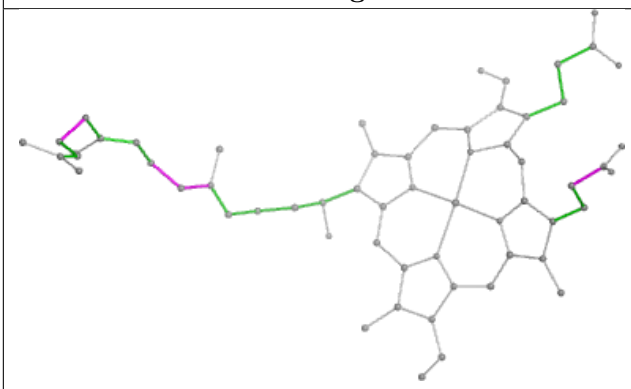
Ligand HEA R 602



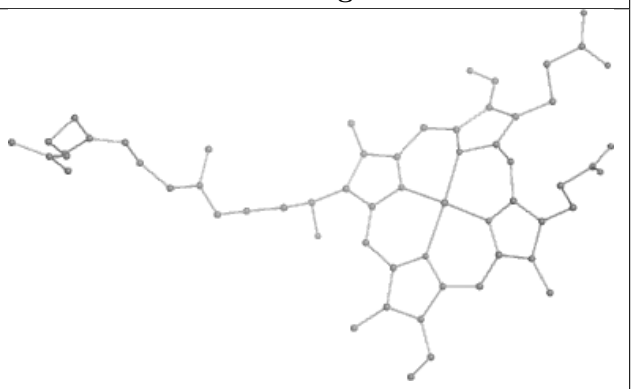
Bond lengths



Bond angles

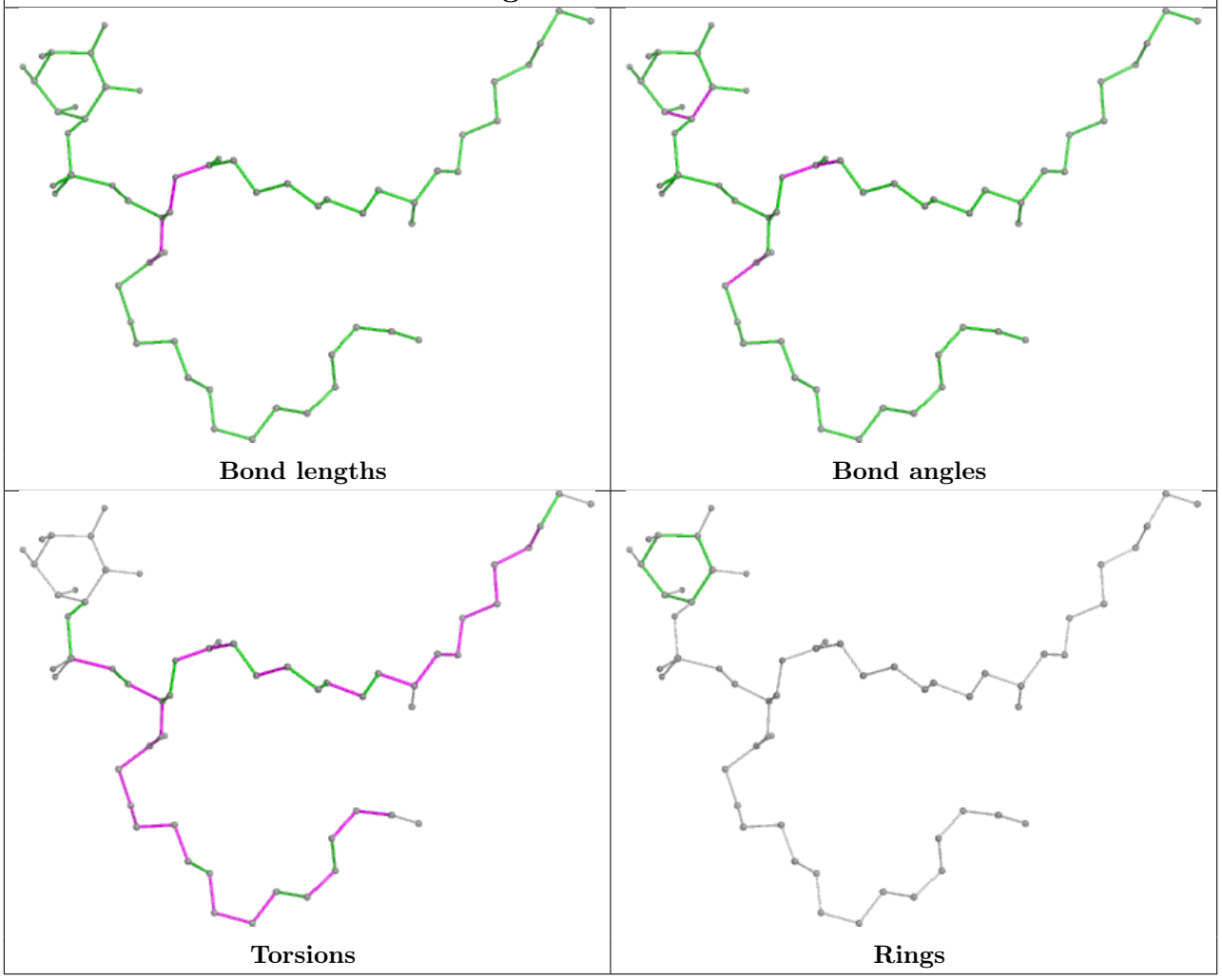


Torsions

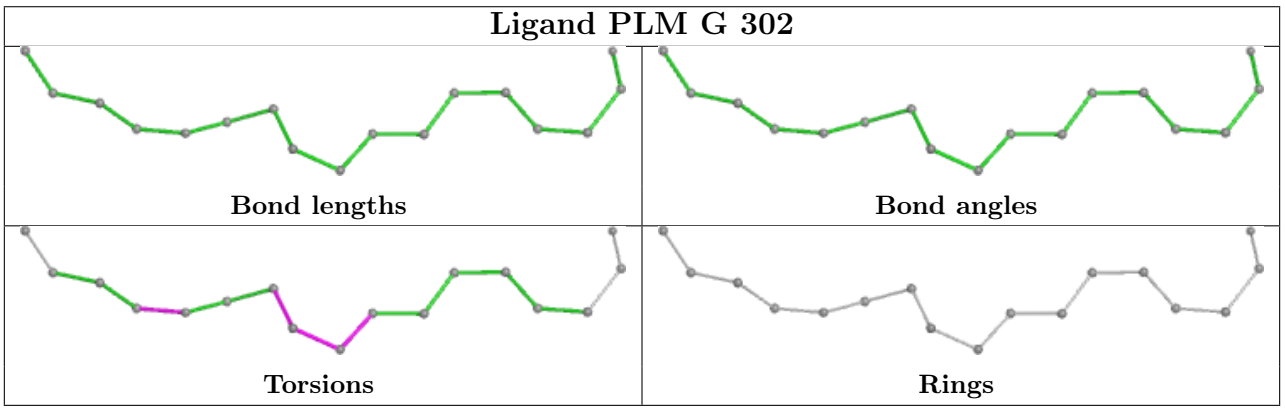


Rings

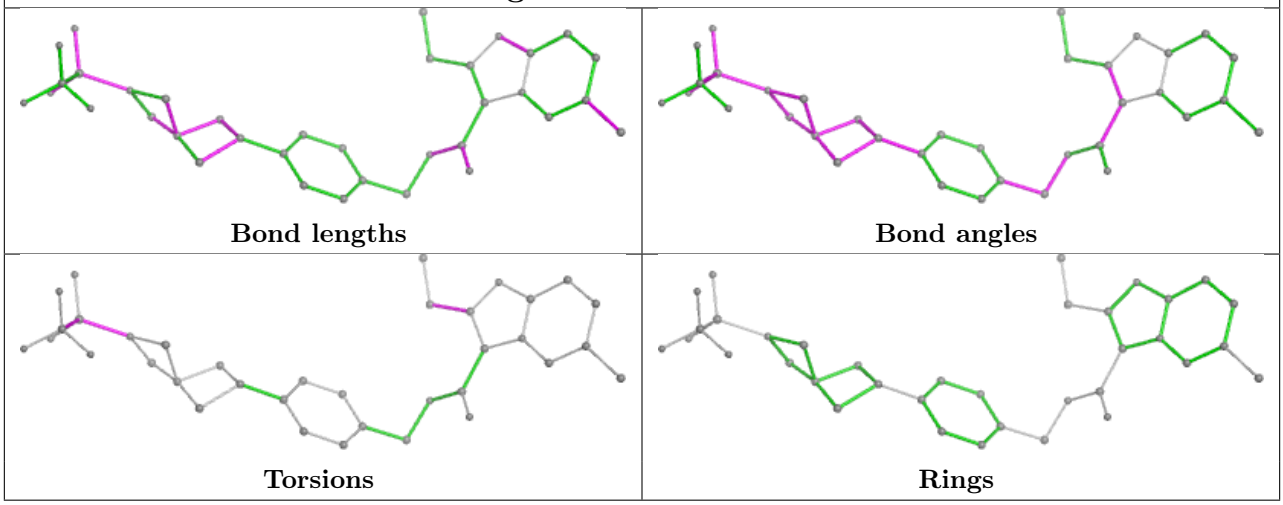
Ligand 9YF O 304



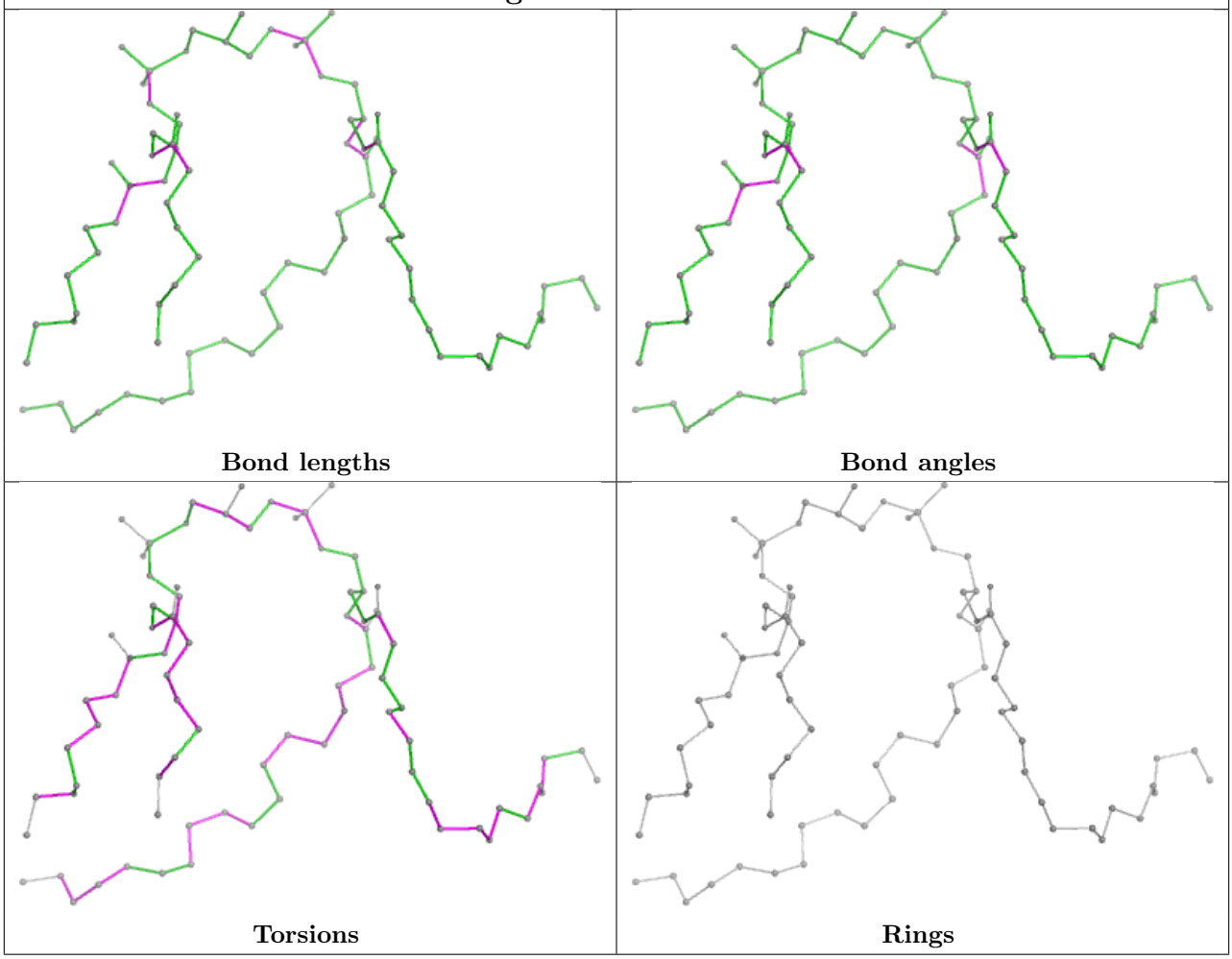
Ligand PLM G 302



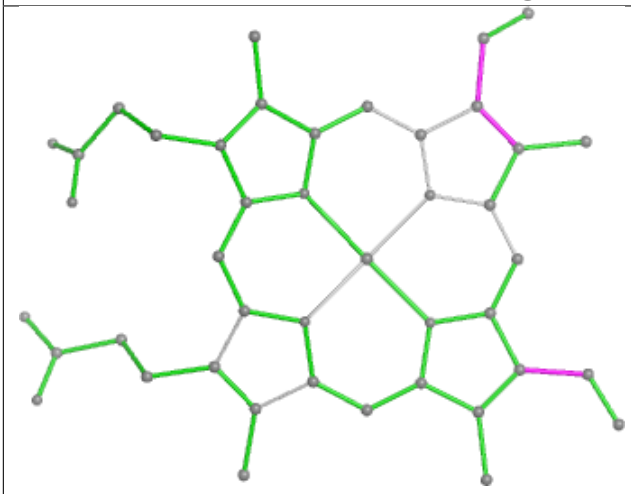
Ligand A1IRE N 606



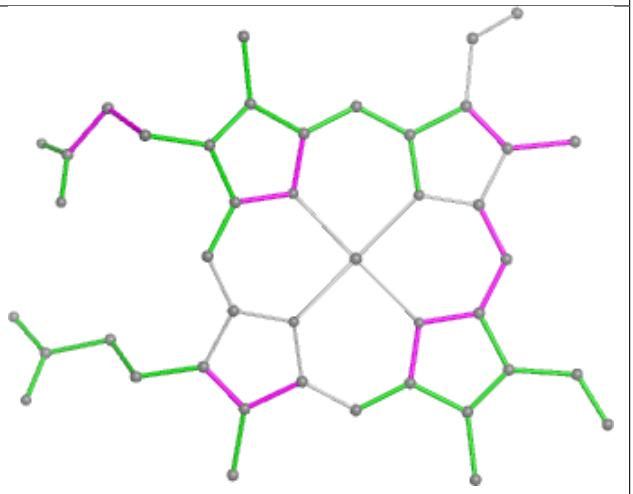
Ligand CDL F 606



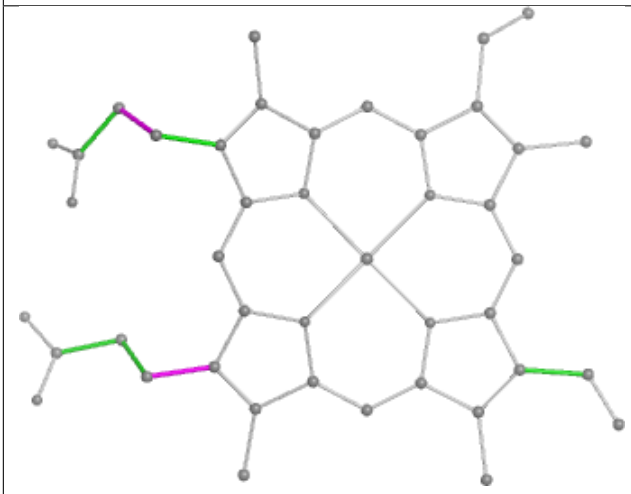
Ligand HEM B 602



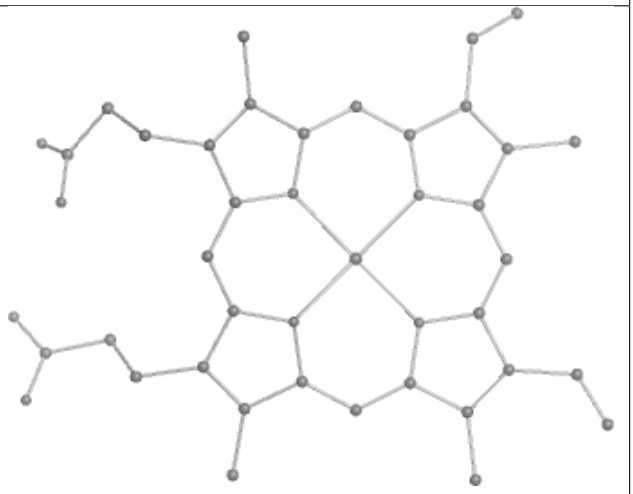
Bond lengths



Bond angles

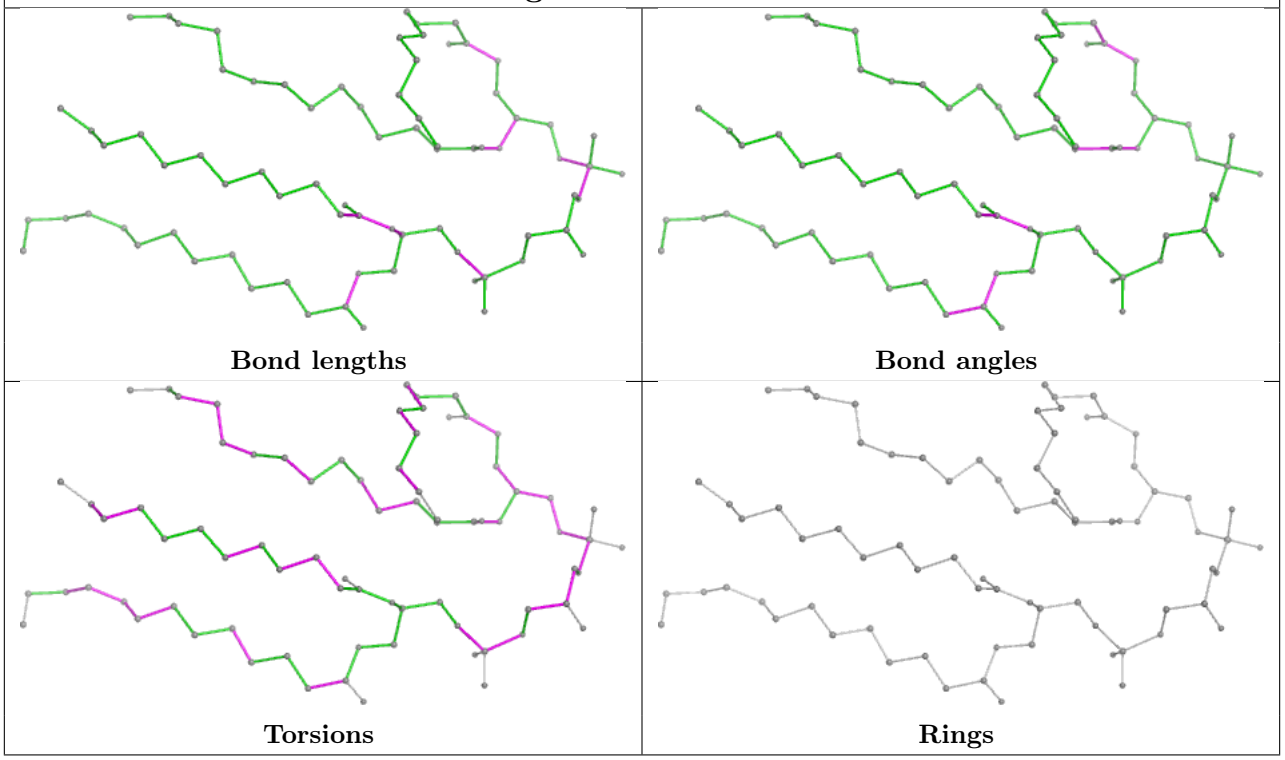


Torsions



Rings

Ligand CDL B 604



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.

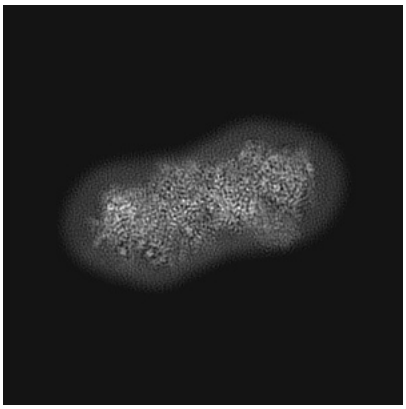
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51689. These allow visual inspection of the internal detail of the map and identification of artifacts.

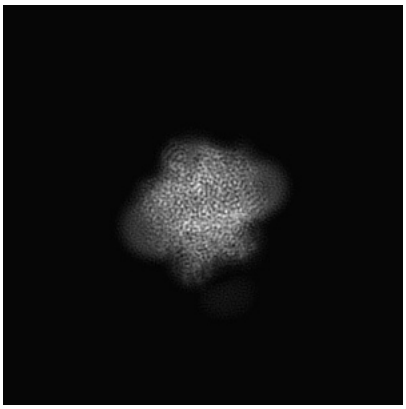
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

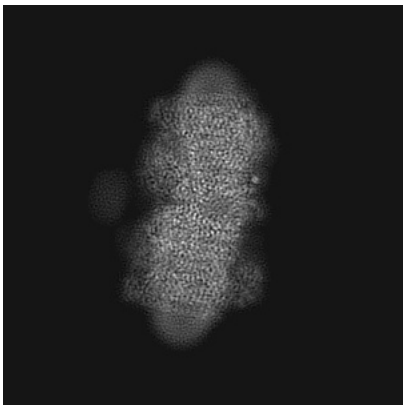
6.1.1 Primary map



X

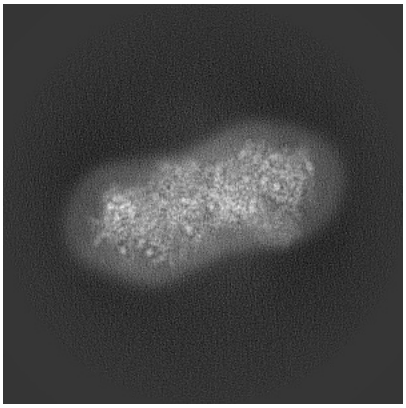


Y

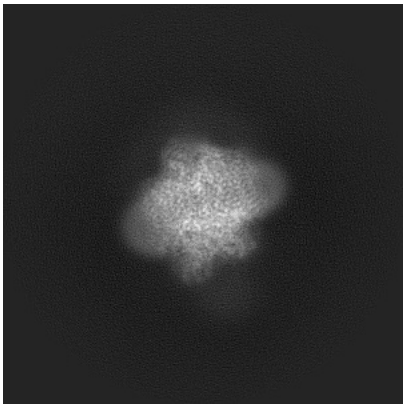


Z

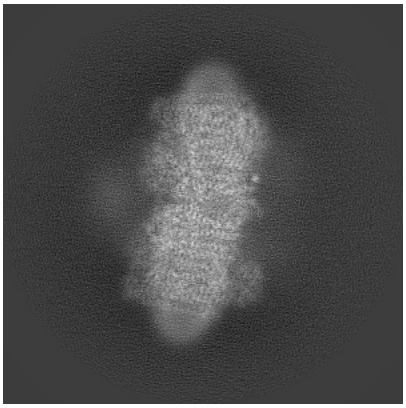
6.1.2 Raw map



X



Y

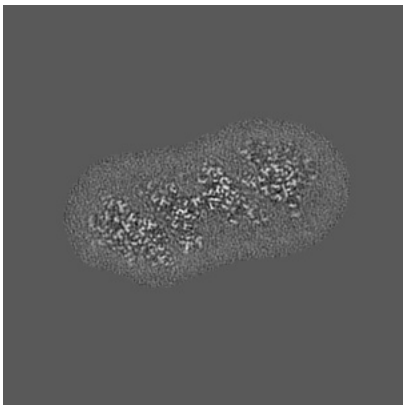


Z

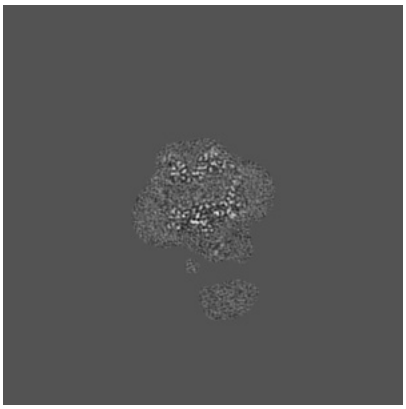
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

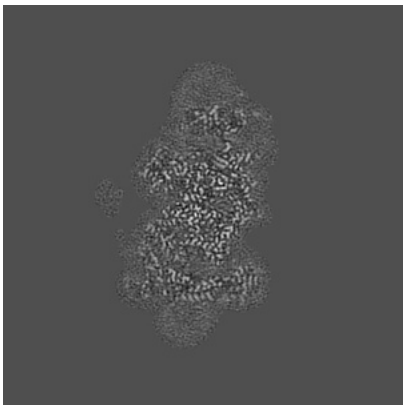
6.2.1 Primary map



X Index: 210

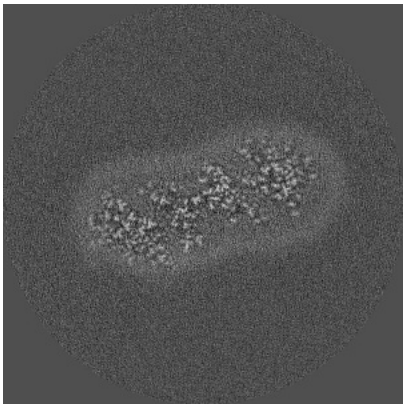


Y Index: 210

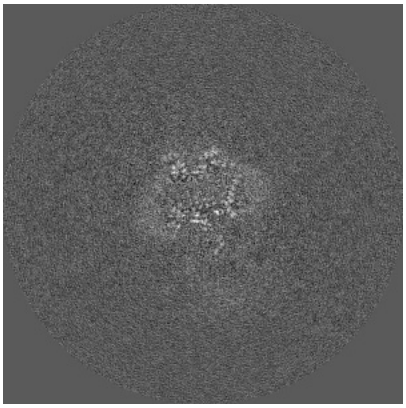


Z Index: 210

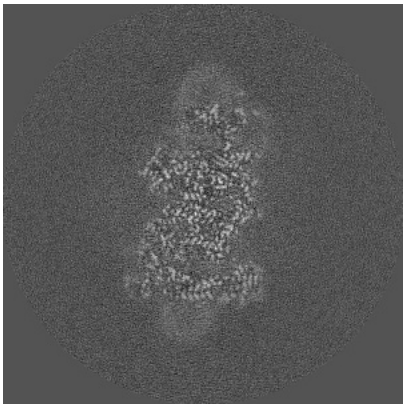
6.2.2 Raw map



X Index: 210



Y Index: 210

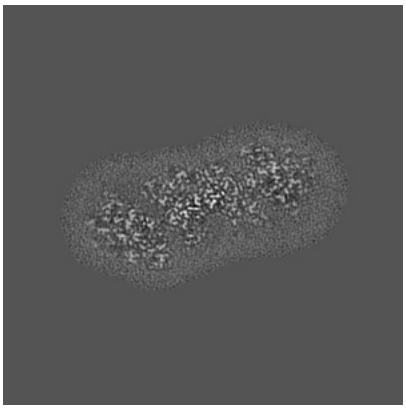


Z Index: 210

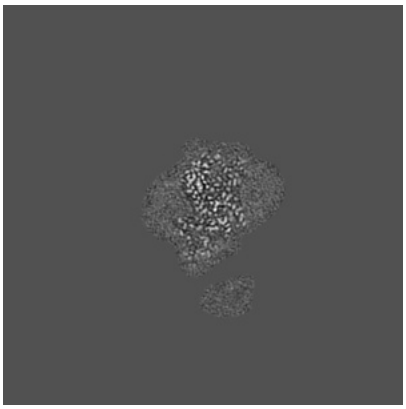
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

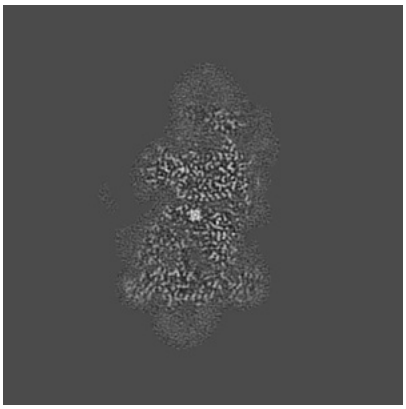
6.3.1 Primary map



X Index: 204

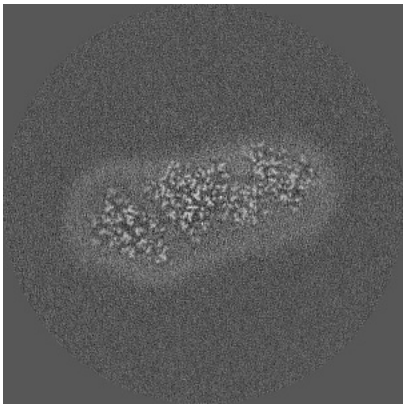


Y Index: 230

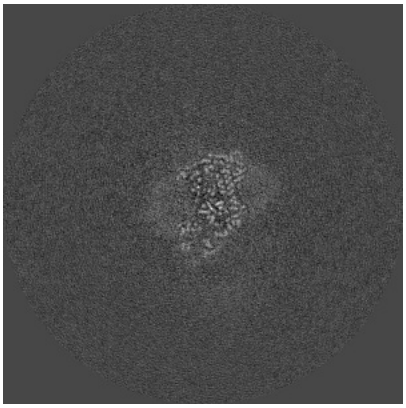


Z Index: 206

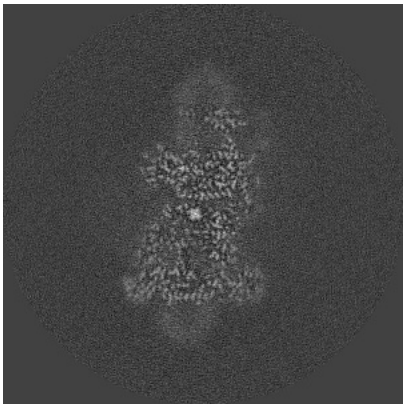
6.3.2 Raw map



X Index: 199



Y Index: 225

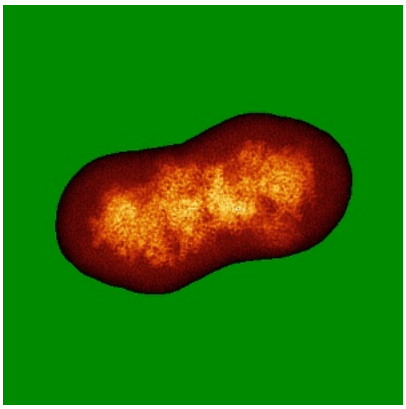


Z Index: 206

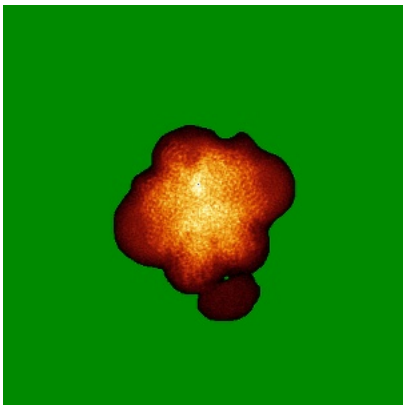
The images above show the largest variance slices of the map in three orthogonal directions.

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

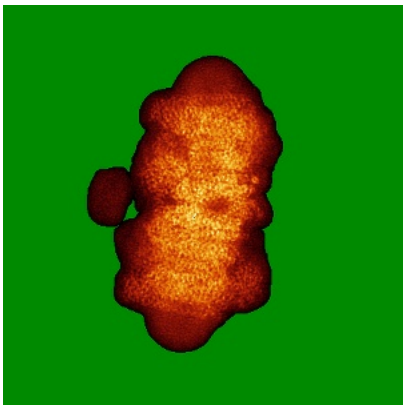
6.4.1 Primary map



X

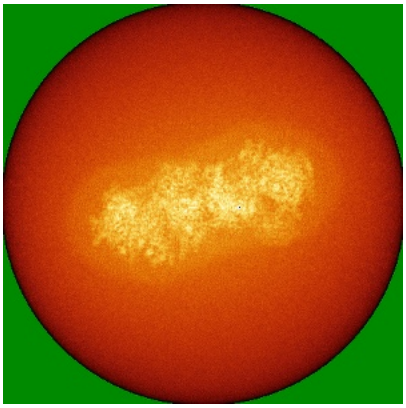


Y

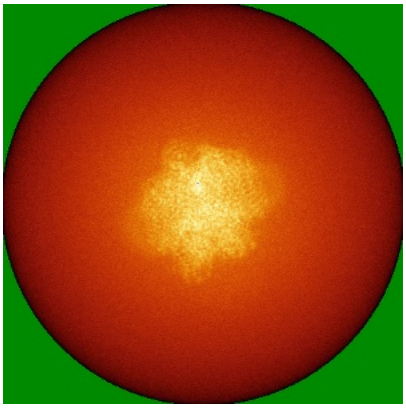


Z

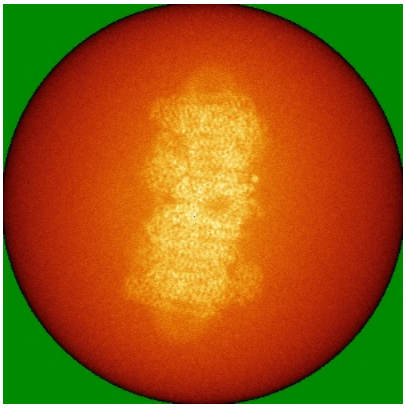
6.4.2 Raw map



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.

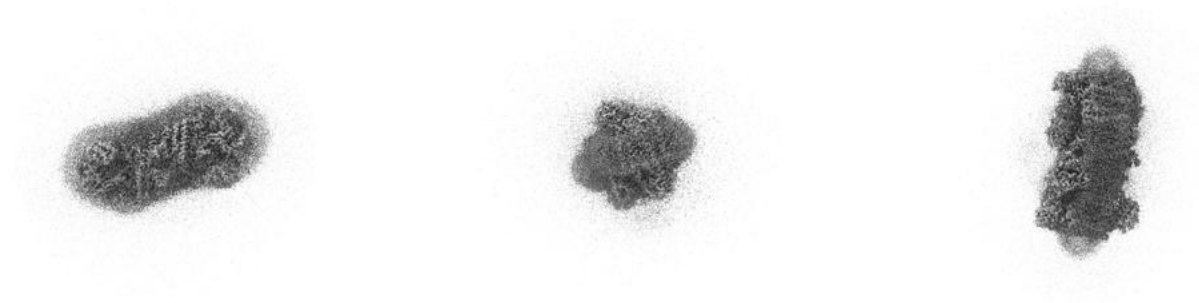
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. 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.

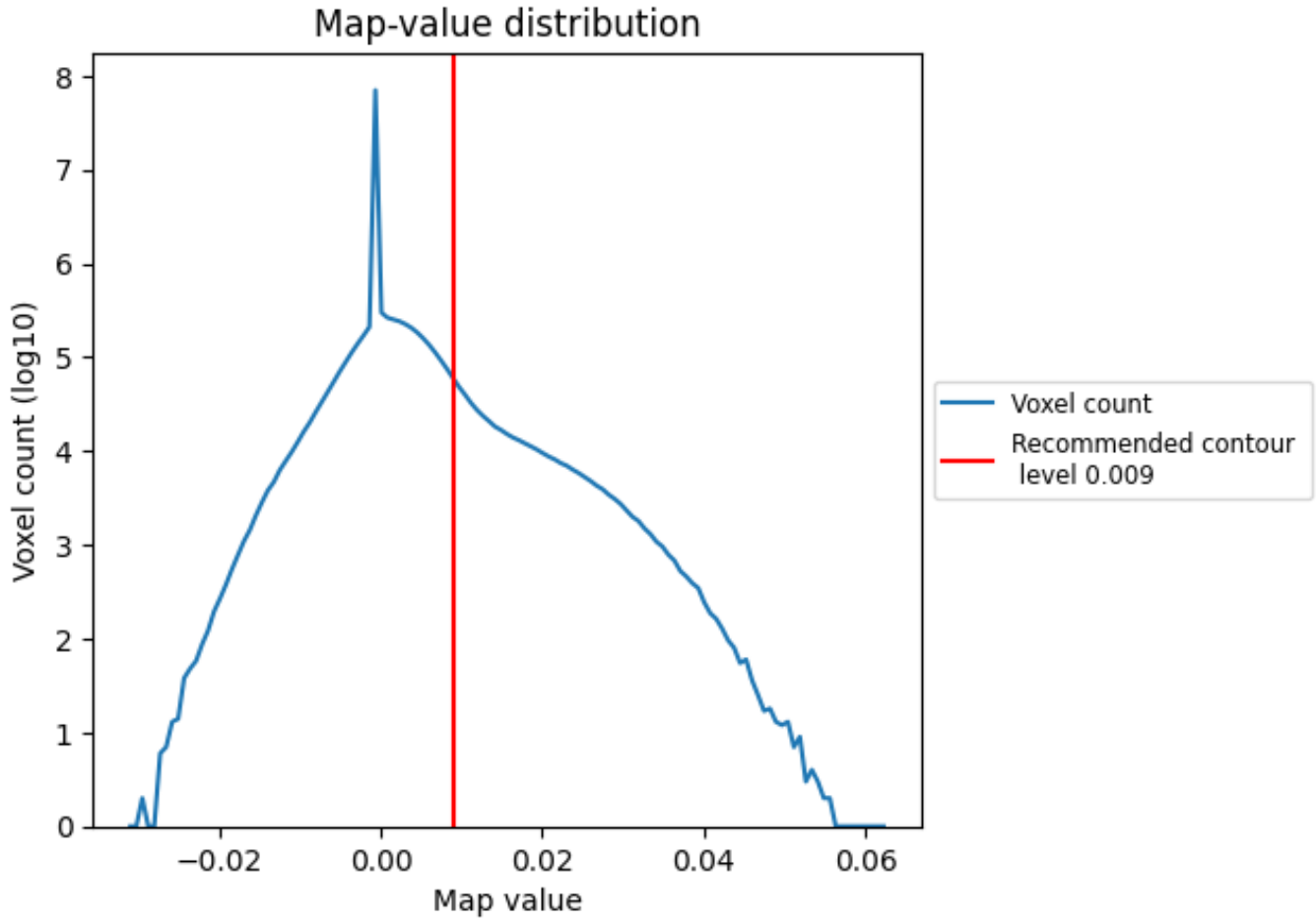
6.6 Mask visualisation (i)

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

7 Map analysis

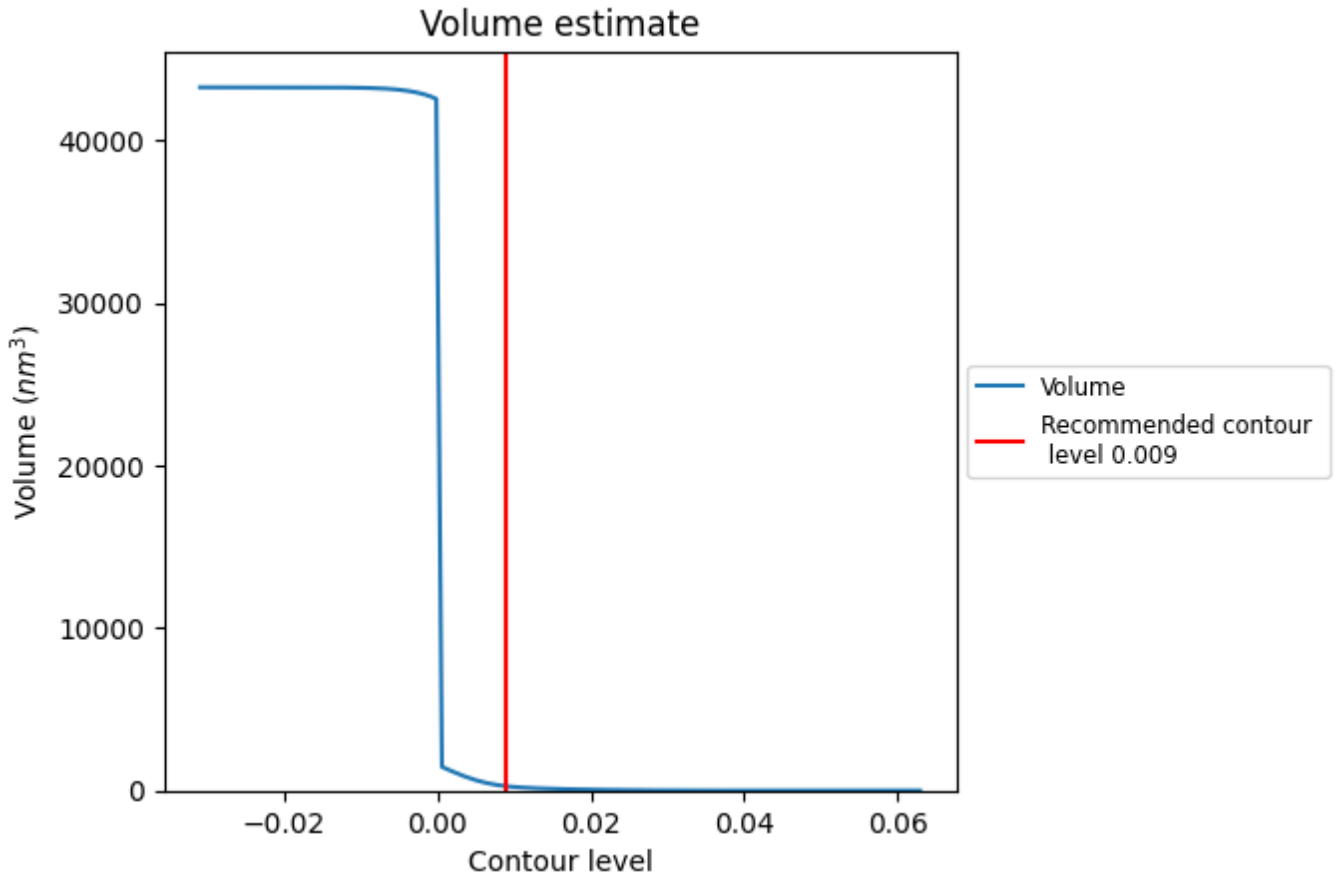
This section contains the results of statistical analysis of the map.

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.

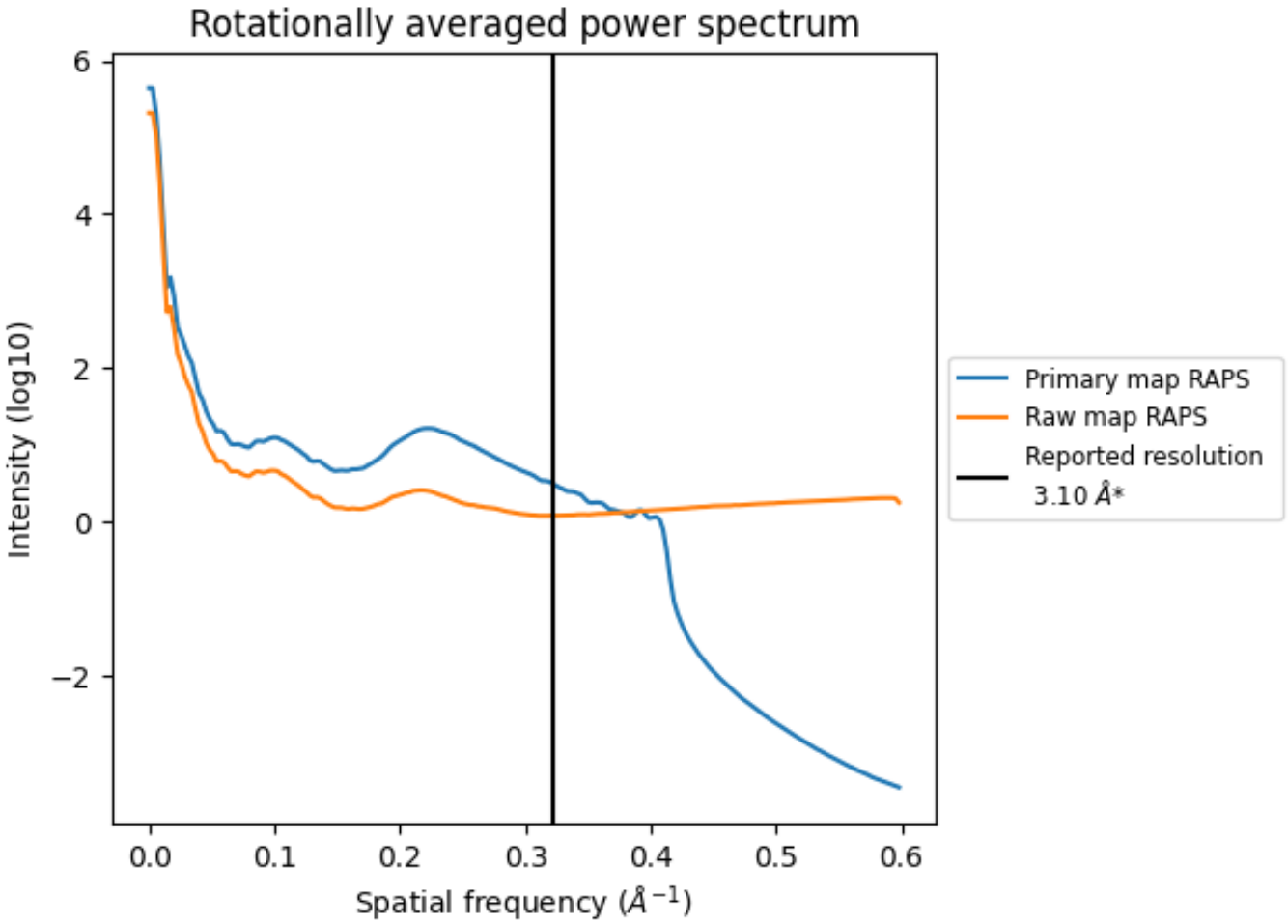
7.2 Volume estimate (i)



The volume at the recommended contour level is 268 nm^3; this corresponds to an approximate mass of 242 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)

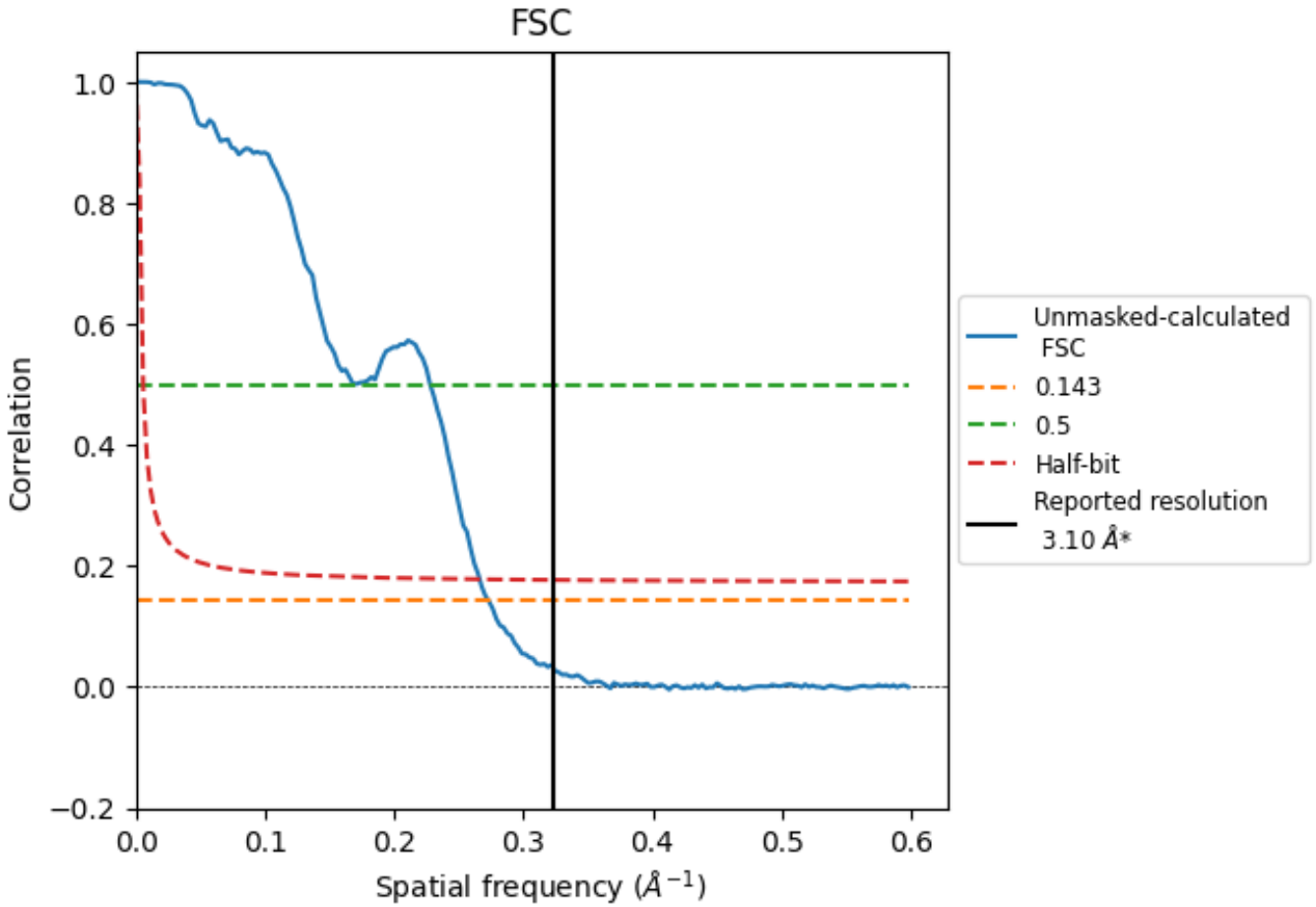


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 $Å^{-1}$

8.2 Resolution estimates (i)

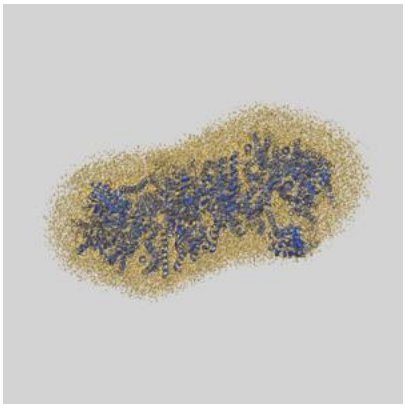
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.39	3.76

*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 3.66 differs from the reported value 3.1 by more than 10 %

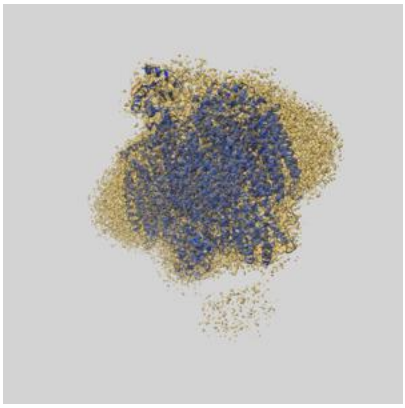
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51689 and PDB model 9GY6. Per-residue inclusion information can be found in section 3 on page 18.

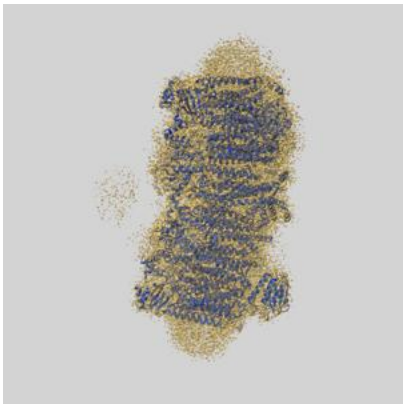
9.1 Map-model overlay



X



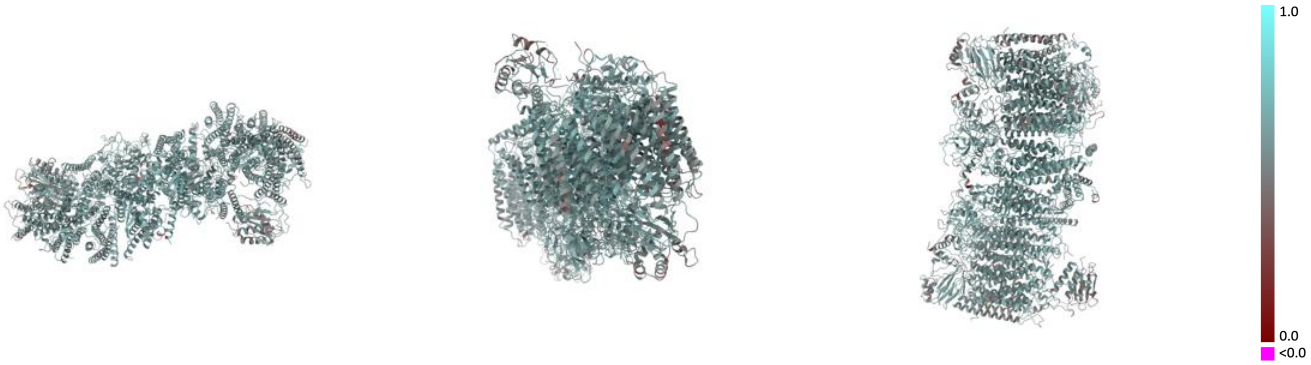
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

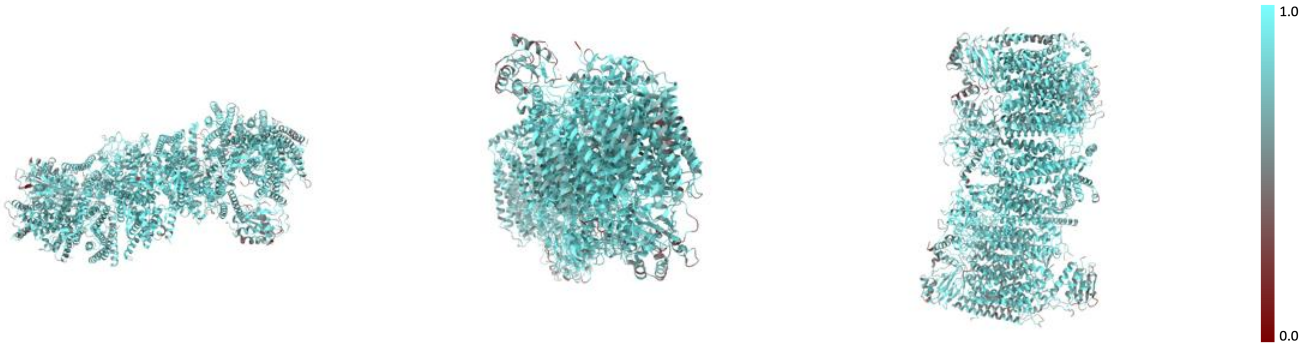
9.2 Q-score mapped to coordinate model



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.

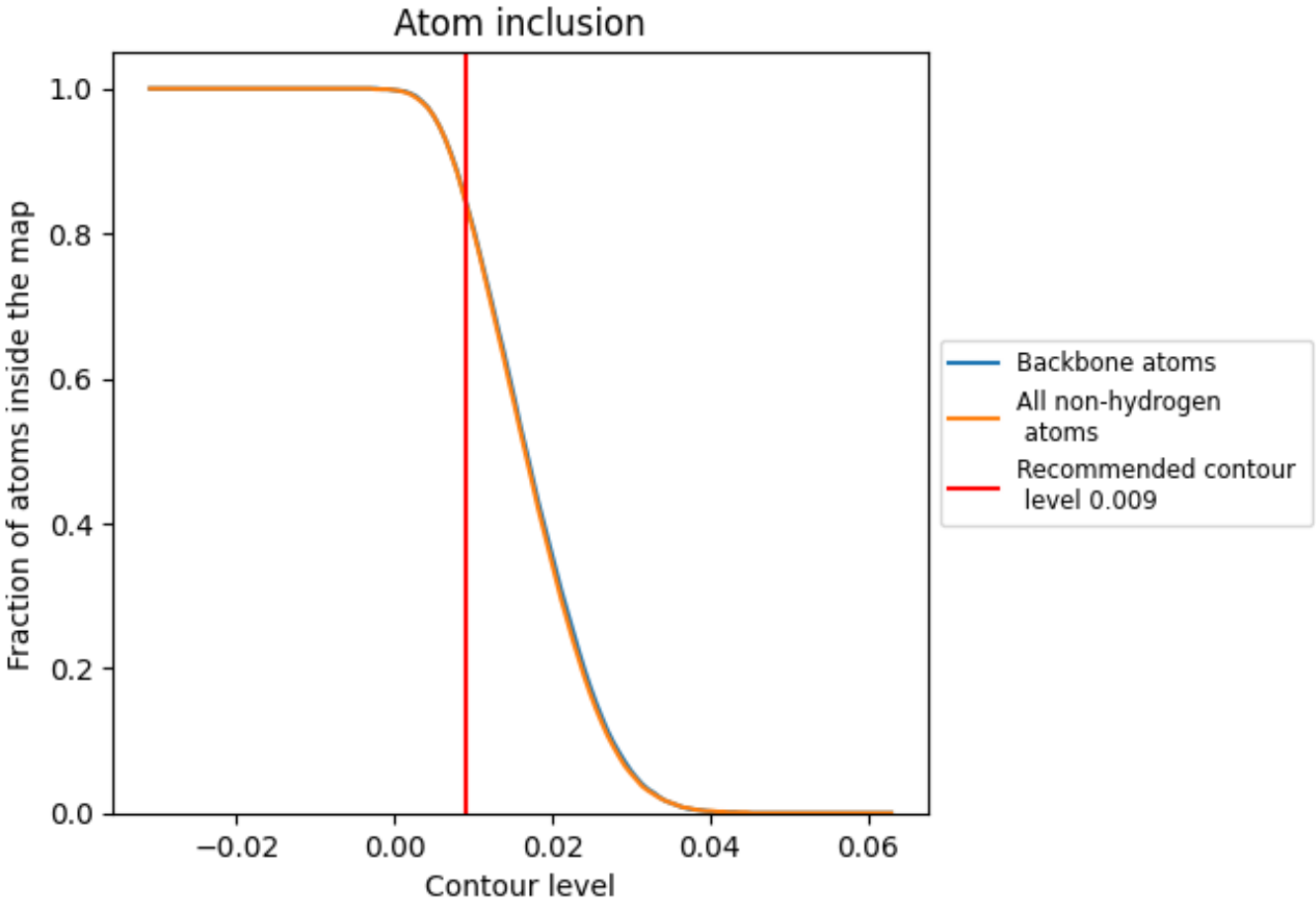
9.3 Atom inclusion mapped to coordinate model



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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8440	0.5920
A	0.8950	0.6120
B	0.9240	0.6310
C	0.8130	0.5800
D	0.7510	0.5750
E	0.7310	0.5460
F	0.8890	0.6030
G	0.8380	0.5810
H	0.8240	0.5900
I	0.7140	0.5200
J	0.7010	0.5140
L	0.7660	0.5490
M	0.8730	0.6080
N	0.9180	0.6270
O	0.7950	0.5790
P	0.7360	0.5710
Q	0.7310	0.5410
R	0.8980	0.6040
S	0.8580	0.5840
T	0.8450	0.5870
U	0.7000	0.5330
V	0.7110	0.5240
X	0.7010	0.5420