wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 09:35 PM JST

PDB ID	:	5XTE / pdb_00005xte
EMDB ID	:	EMD-6774
Title	:	Cryo-EM structure of human respiratory complex III (cytochrome bc1 complex)
Authors	:	Gu, J.; Wu, M.; Yang, M.
Deposited on	:	2017-06-19
Resolution	:	3.40 Å(reported)

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

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

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

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

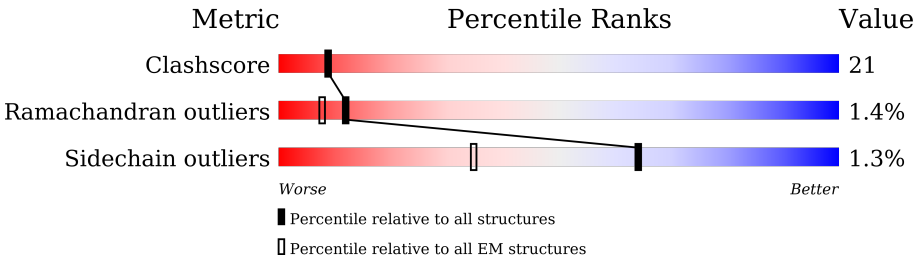
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	81	26% 65% 27% 7%
1	N	81	27% 75% 23% .
2	B	57	95% 49% 46% 5%
2	O	57	98% 51% 40% 9%
3	C	196	60% 69% 29% .
3	P	196	53% 64% 35% .
4	D	62	29% 76% 24%
4	Q	62	32% 61% 39%

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Mol	Chain	Length	Quality of chain
5	E	75	45% 68% 28%
5	R	75	36% 73% 24%
6	F	106	12% 56% 34% 10%
6	S	106	10% 63% 37%
7	G	51	24% 73% 27%
7	T	51	43% 65% 31%
8	H	241	12% 72% 27%
8	U	241	10% 70% 29%
9	J	378	67% 33%
9	V	378	61% 37%
10	K	419	12% 61% 37%
10	W	419	13% 65% 33%
11	L	446	16% 63% 36%
11	Y	446	18% 64% 34%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CDL	G	101	-	-	X	-
12	CDL	L	502	-	-	X	-
13	FES	C	301	-	-	X	-
13	FES	P	301	-	-	X	-
14	PEE	H	401	-	-	X	-
14	PEE	L	503	-	-	X	-
14	PEE	U	401	-	-	X	-
14	PEE	V	403	-	-	X	-
14	PEE	Y	502	-	-	X	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 34492 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	81	Total	C	N	O	S	0	0
			694	450	126	117	1		
1	N	81	Total	C	N	O	S	0	0
			687	444	126	116	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	57	Total	C	N	O	S	0	0
			413	261	75	76	1		
2	O	57	Total	C	N	O	S	0	0
			409	259	74	75	1		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		
3	P	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	62	Total	C	N	O	S	0	0
			509	332	87	89	1		
4	Q	62	Total	C	N	O	S	0	0
			509	332	87	89	1		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	74	Total	C	N	O	S	0	0
			580	351	108	116	5		
5	R	74	Total	C	N	O	S	0	0
			580	351	108	116	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	106	Total	C	N	O	S	0	0
			921	589	162	168	2		
6	S	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	51	Total	C	N	O	0	0
			425	287	72	66		
7	T	51	Total	C	N	O	0	0
			425	287	72	66		

- Molecule 8 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		
8	U	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

- Molecule 9 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		
9	V	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	419	Total	C	N	O	S	0	0
			3159	1986	553	610	10		

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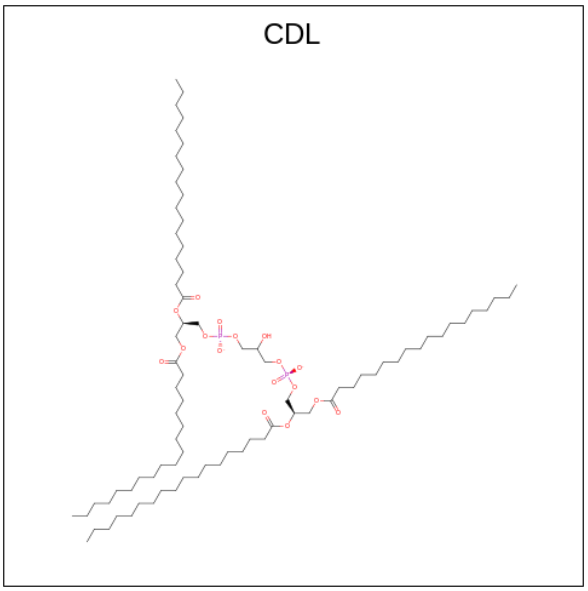
Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	419	Total	C	N	O	S	0	0
			3162	1989	553	610	10		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		
11	Y	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O	P	0
			64	45	17	2	
12	G	1	Total	C	O	P	0
			64	45	17	2	
12	H	1	Total	C	O	P	0
			64	45	17	2	
12	J	1	Total	C	O	P	0
			64	45	17	2	
12	J	1	Total	C	O	P	0
			64	45	17	2	
12	L	1	Total	C	O	P	0
			64	45	17	2	

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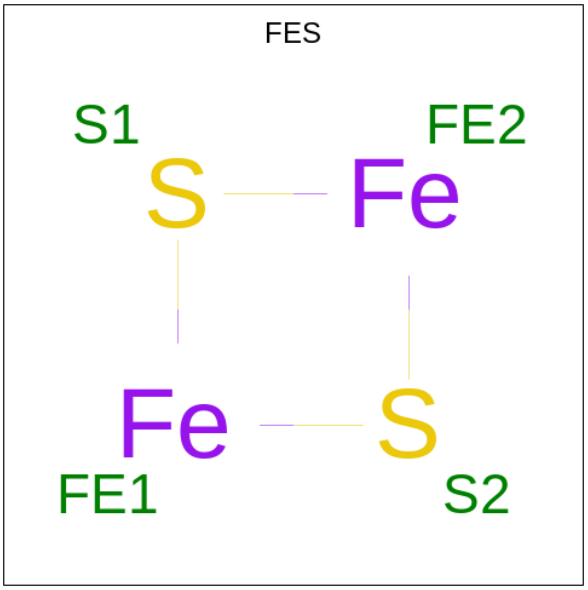
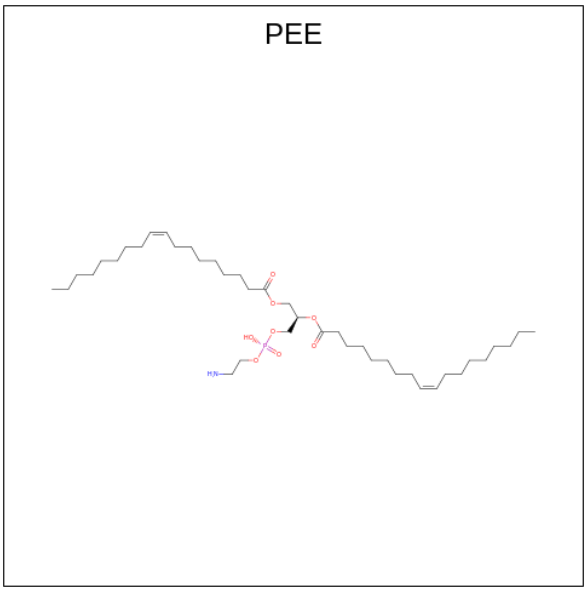
Mol	Chain	Residues	Atoms				AltConf
12	N	1	Total	C	O	P	0
			64	45	17	2	
12	U	1	Total	C	O	P	0
			64	45	17	2	
12	Y	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



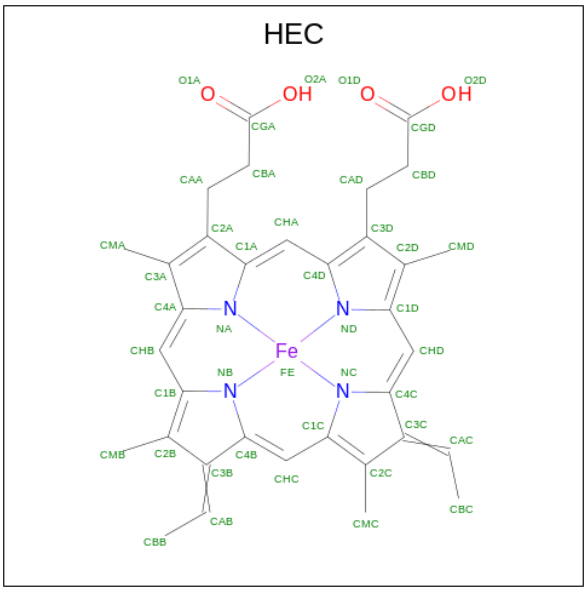
Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	Fe	S	0
			4	2	2	
13	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 14 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



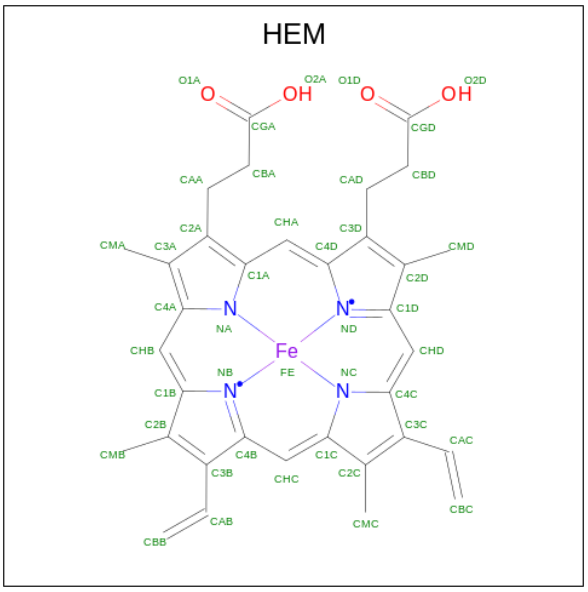
Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total	C	N	O	P	0
			49	39	1	8	1	
14	J	1	Total	C	N	O	P	0
			49	39	1	8	1	
14	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
14	U	1	Total	C	N	O	P	0
			41	31	1	8	1	
14	V	1	Total	C	N	O	P	0
			49	39	1	8	1	
14	Y	1	Total	C	N	O	P	0
			49	39	1	8	1	

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



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

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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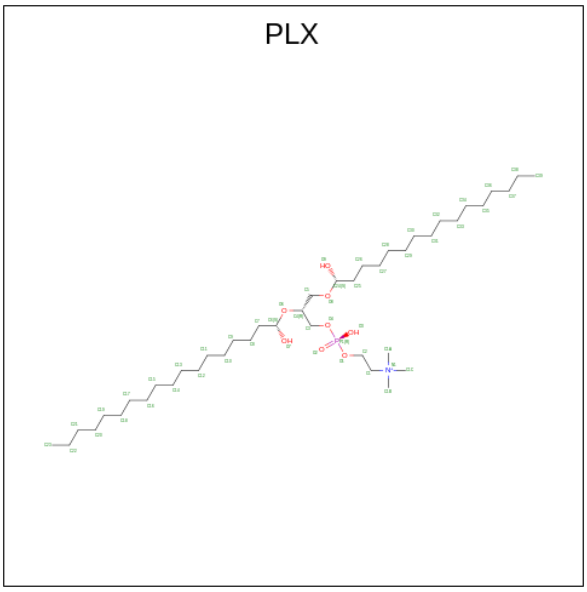
Mol	Chain	Residues	Atoms					AltConf
16	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 17 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).



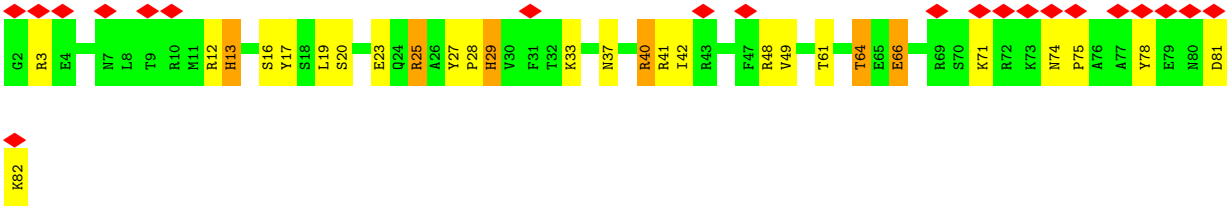
Mol	Chain	Residues	Atoms					AltConf
17	L	1	Total	C	N	O	P	0
			52	42	1	8	1	
17	Q	1	Total	C	N	O	P	0
			52	42	1	8	1	
17	T	1	Total	C	N	O	P	0
			52	42	1	8	1	

3 Residue-property plots (i)

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

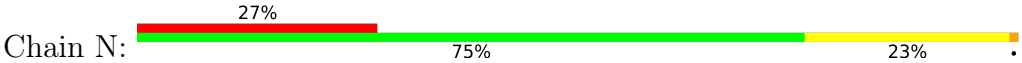
• Molecule 1: Cytochrome b-c1 complex subunit 8

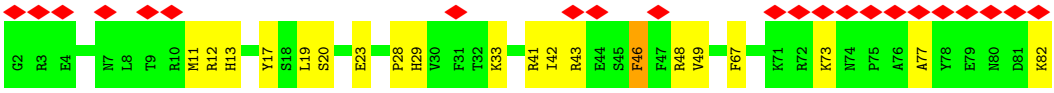
Chain A:



• Molecule 1: Cytochrome b-c1 complex subunit 8

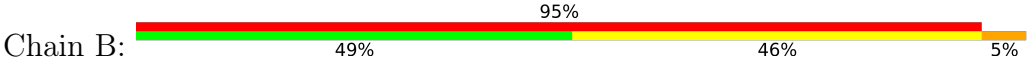
Chain N:





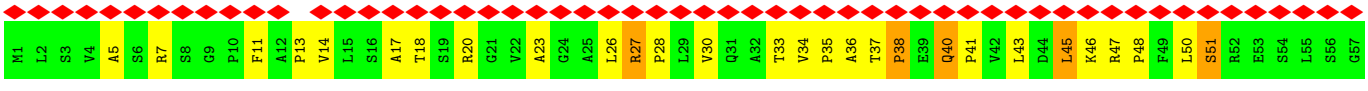
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain B:



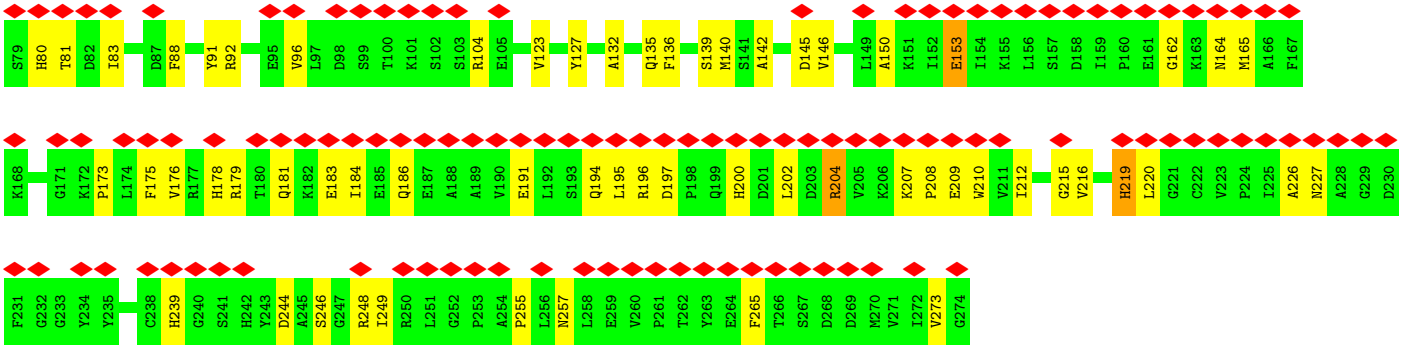
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain O:



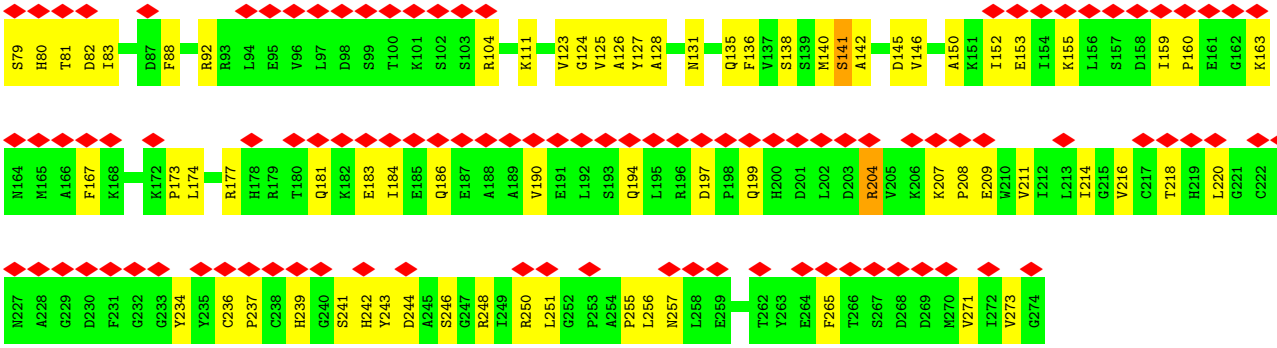
• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain C:



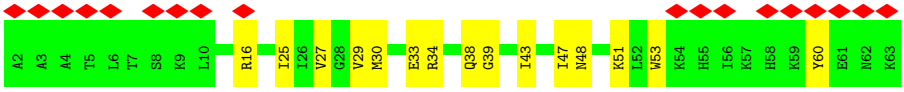
• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



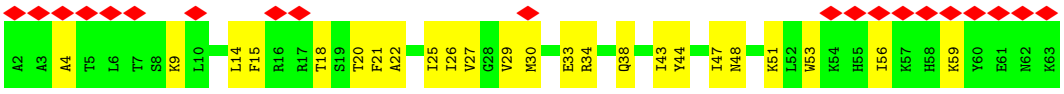
• Molecule 4: Cytochrome b-c1 complex subunit 9

Chain D:



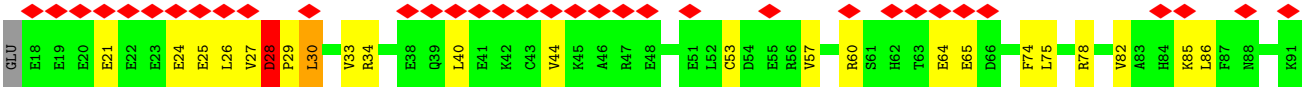
• Molecule 4: Cytochrome b-c1 complex subunit 9

Chain Q:



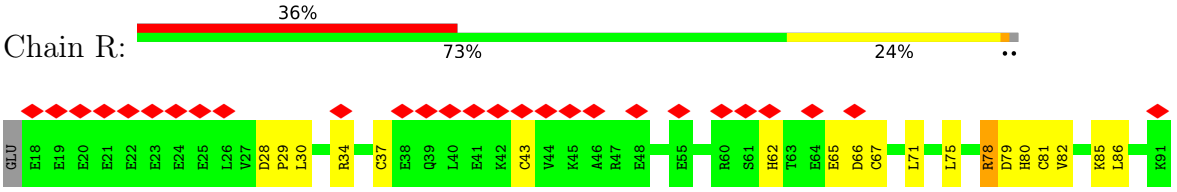
• Molecule 5: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain E:



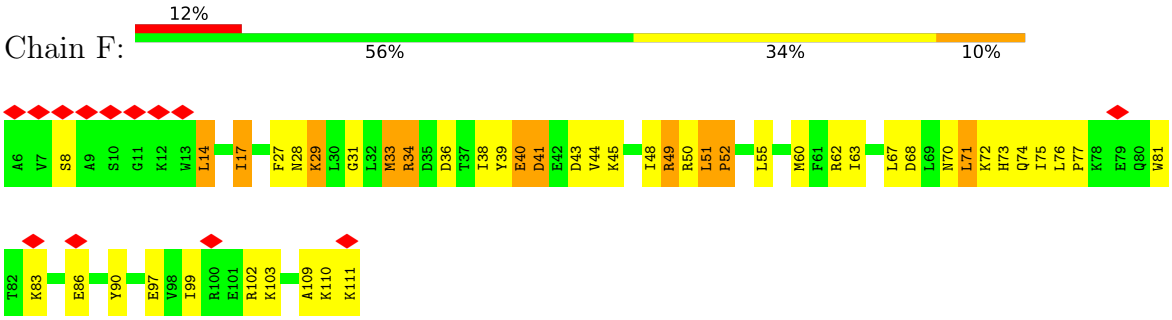
• Molecule 5: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain R:



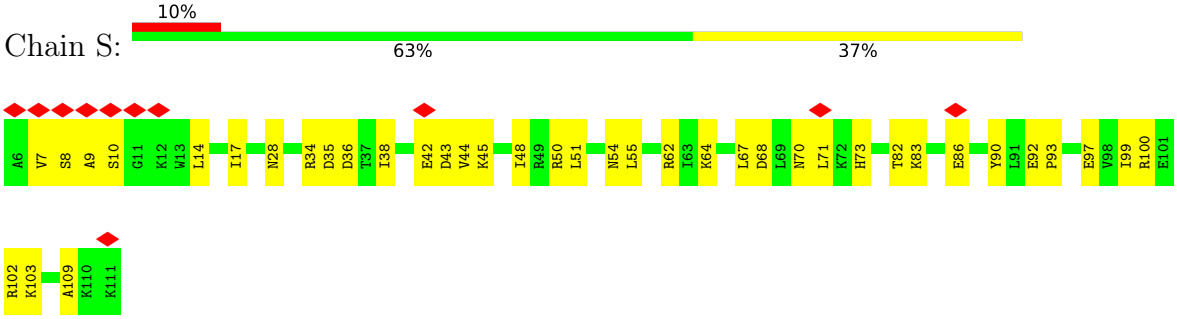
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:



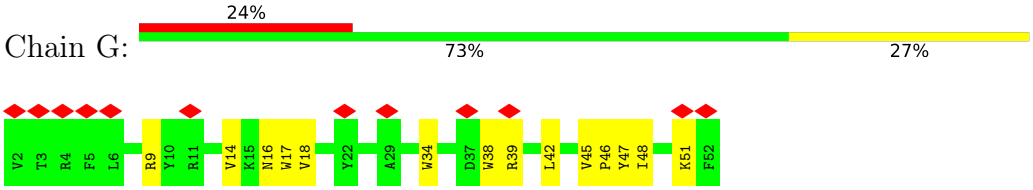
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain S:



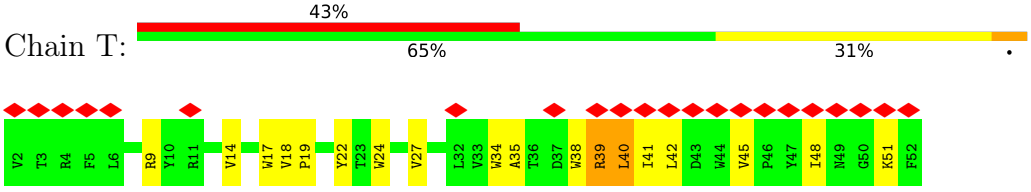
• Molecule 7: Cytochrome b-c1 complex subunit 10

Chain G:



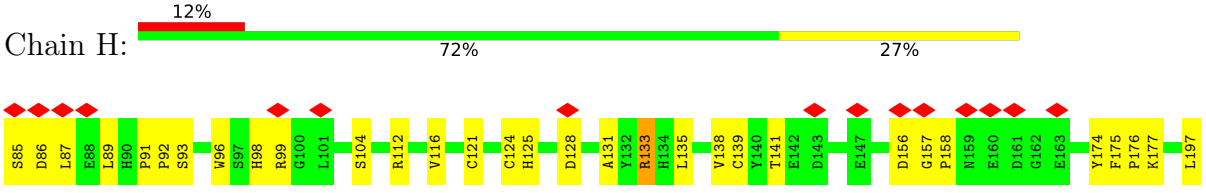
• Molecule 7: Cytochrome b-c1 complex subunit 10

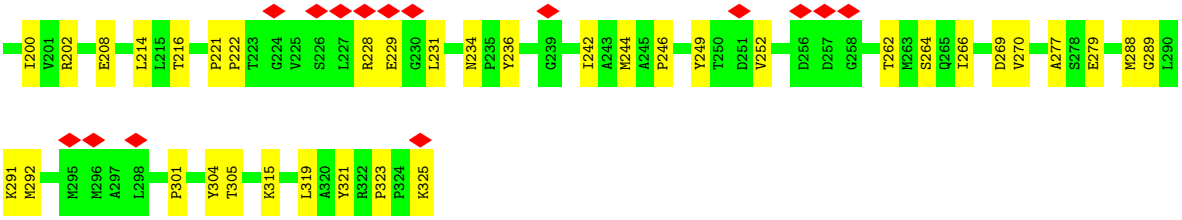
Chain T:



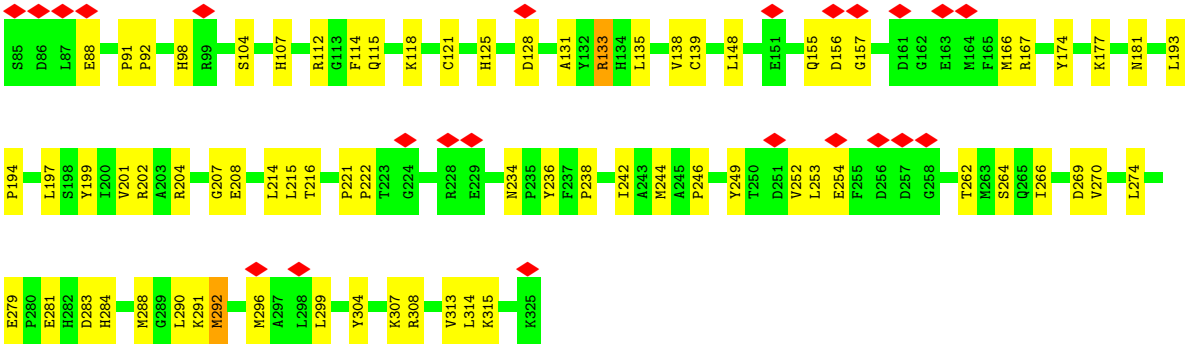
• Molecule 8: Cytochrome c1, heme protein, mitochondrial

Chain H:

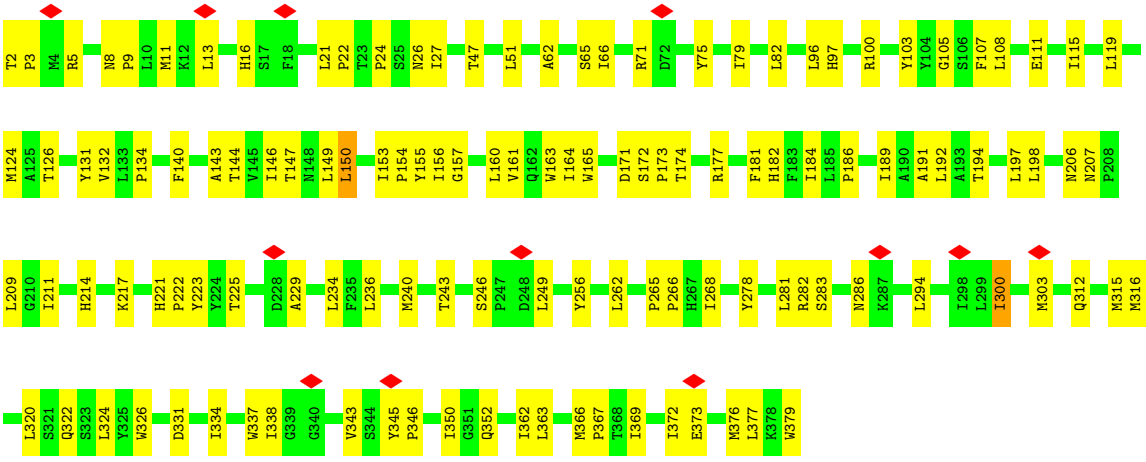




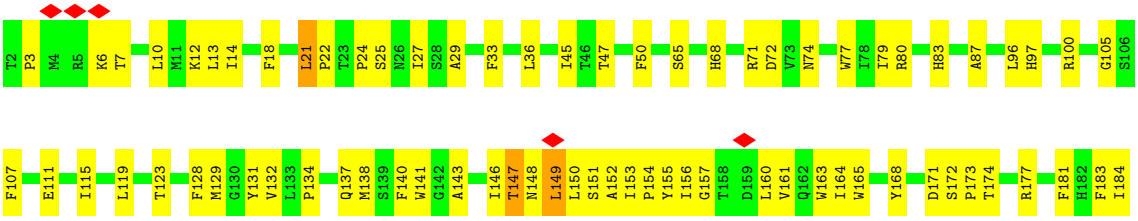
• Molecule 8: Cytochrome c1, heme protein, mitochondrial

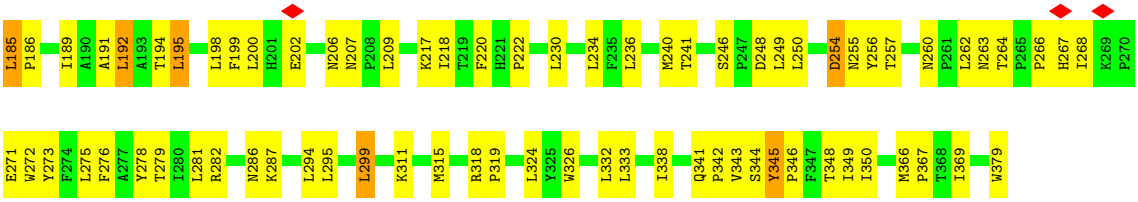


• Molecule 9: Cytochrome b



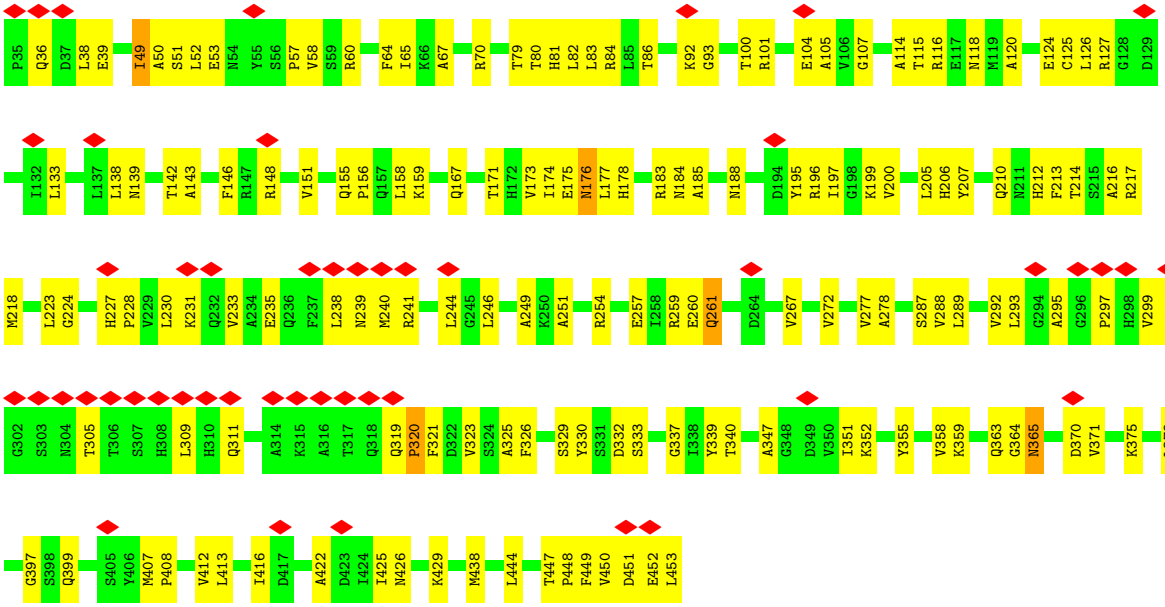
• Molecule 9: Cytochrome b





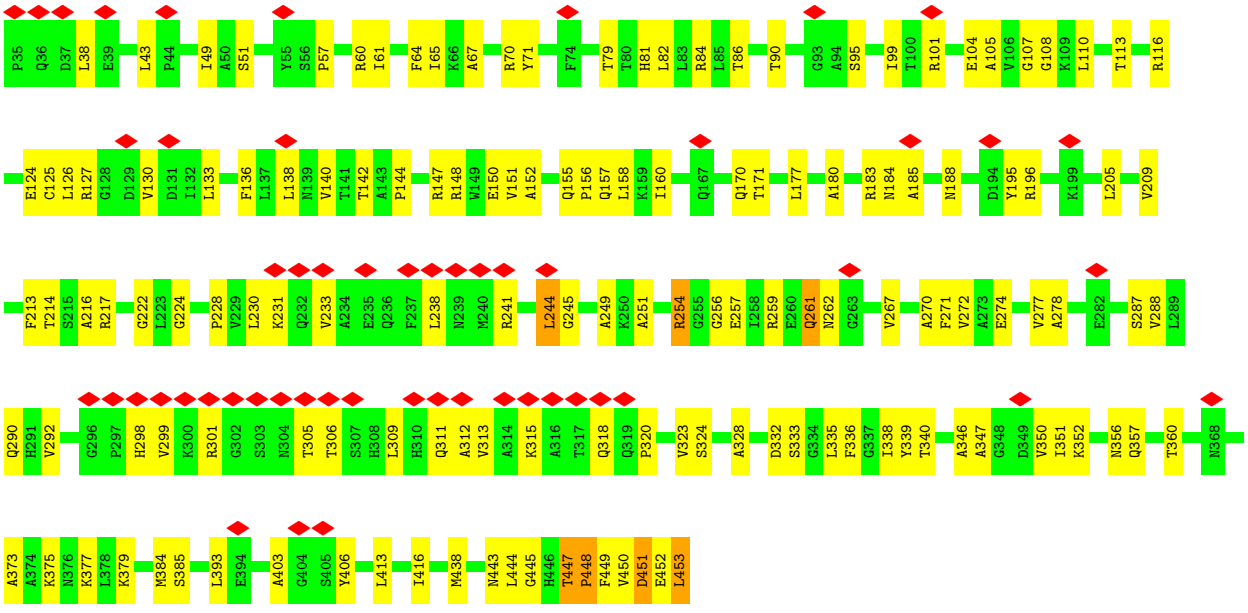
• Molecule 10: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain K:



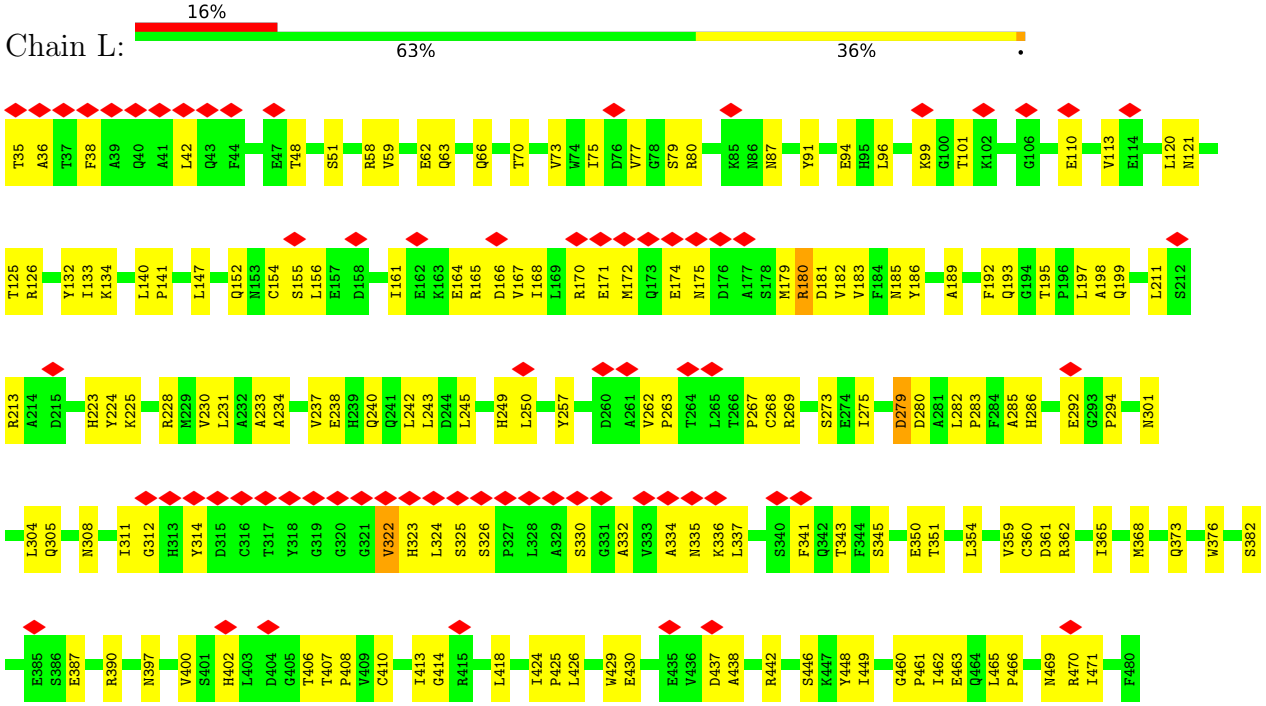
• Molecule 10: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain W:



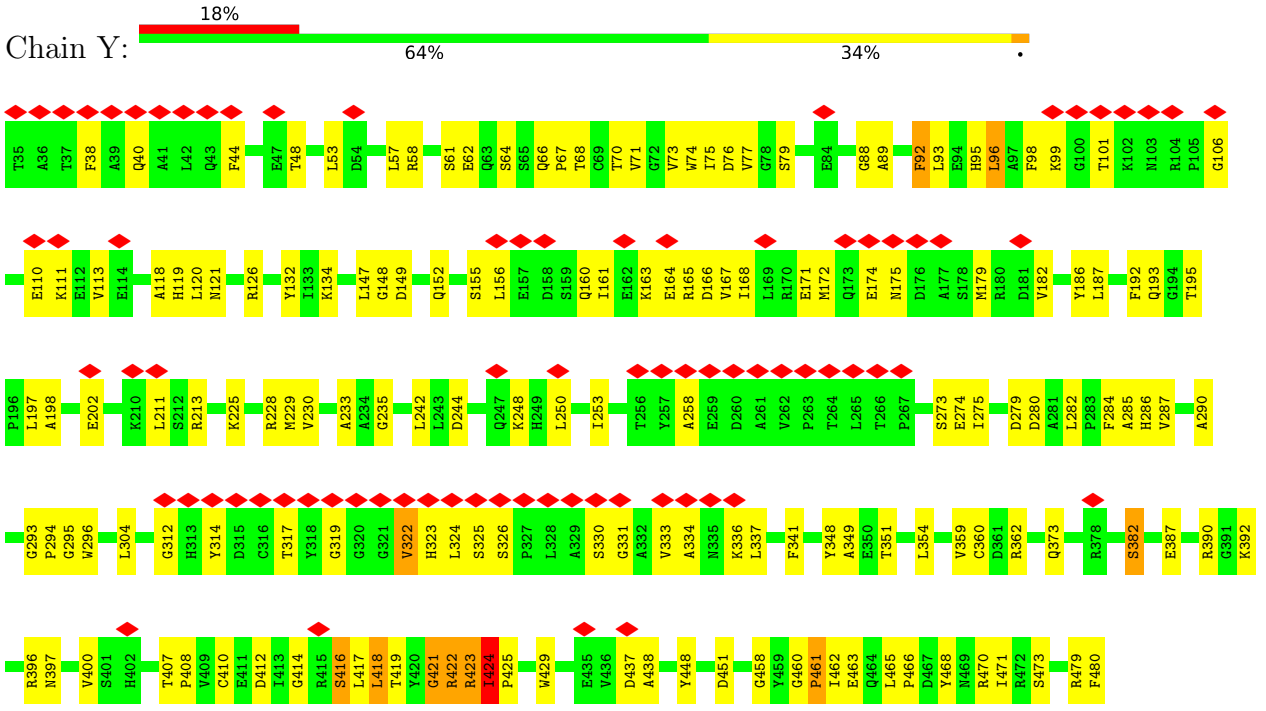
• Molecule 11: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:



• Molecule 11: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.339	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0783	Depositor
Map size (Å)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, PEE, HEM, CDL, PLX, FES

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	0.31	0/715	0.48	0/964
1	N	0.27	0/707	0.49	0/953
2	B	0.23	0/421	0.60	1/574 (0.2%)
2	O	0.25	0/417	0.61	1/569 (0.2%)
3	C	0.24	0/1554	0.43	0/2104
3	P	0.23	0/1554	0.42	0/2104
4	D	0.26	0/521	0.42	0/699
4	Q	0.27	0/521	0.43	0/699
5	E	0.35	0/587	0.54	1/789 (0.1%)
5	R	0.27	0/587	0.46	0/789
6	F	0.42	1/942 (0.1%)	0.52	1/1263 (0.1%)
6	S	0.27	0/942	0.44	0/1263
7	G	0.27	0/442	0.48	0/608
7	T	0.28	0/442	0.49	0/608
8	H	0.26	0/1983	0.46	0/2691
8	U	0.27	0/1983	0.45	0/2691
9	J	0.31	1/3108 (0.0%)	0.52	1/4254 (0.0%)
9	V	0.34	1/3108 (0.0%)	0.54	3/4254 (0.1%)
10	K	0.27	0/3217	0.49	0/4361
10	W	0.29	1/3220 (0.0%)	0.48	1/4365 (0.0%)
11	L	0.27	0/3527	0.47	0/4788
11	Y	0.29	1/3527 (0.0%)	0.50	2/4788 (0.0%)
All	All	0.29	5/34025 (0.0%)	0.49	11/46178 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	W	448	PRO	N-CD	5.33	1.55	1.47
9	J	154	PRO	N-CD	5.18	1.55	1.47
9	V	154	PRO	N-CD	5.18	1.55	1.47
11	Y	425	PRO	N-CD	5.12	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	52	PRO	N-CD	5.04	1.54	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	28	ASP	C-N-CD	6.17	141.36	128.40
9	V	345	TYR	C-N-CD	5.81	140.59	128.40
9	V	153	ILE	C-N-CD	5.76	140.50	128.40
9	J	153	ILE	C-N-CD	5.75	140.48	128.40
6	F	51	LEU	C-N-CD	5.68	140.34	128.40

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	694	0	683	47	0
1	N	687	0	676	25	0
2	B	413	0	438	26	0
2	O	409	0	432	27	0
3	C	1521	0	1505	55	0
3	P	1521	0	1505	61	0
4	D	509	0	511	15	0
4	Q	509	0	511	24	0
5	E	580	0	526	51	0
5	R	580	0	526	34	0
6	F	921	0	909	70	0
6	S	921	0	910	29	0
7	G	425	0	422	15	0
7	T	425	0	422	30	0
8	H	1924	0	1874	59	0
8	U	1924	0	1874	80	0
9	J	3009	0	3065	108	0
9	V	3009	0	3065	167	0
10	K	3159	0	3130	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	W	3162	0	3139	125	0
11	L	3453	0	3370	142	0
11	Y	3453	0	3368	160	0
12	A	64	0	72	3	0
12	G	64	0	72	28	0
12	H	64	0	72	6	0
12	J	128	0	144	23	0
12	L	64	0	72	22	0
12	N	64	0	72	8	0
12	U	64	0	72	12	0
12	Y	64	0	72	4	0
13	C	4	0	0	3	0
13	P	4	0	0	2	0
14	H	49	0	75	32	0
14	J	49	0	75	8	0
14	L	49	0	75	37	0
14	U	41	0	56	25	0
14	V	49	0	75	23	0
14	Y	49	0	75	21	0
15	H	43	0	32	5	0
15	U	43	0	32	8	0
16	J	86	0	60	7	0
16	V	86	0	60	13	0
17	L	52	0	88	4	0
17	Q	52	0	88	7	0
17	T	52	0	88	3	0
All	All	34492	0	34388	1416	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 21.

The worst 5 of 1416 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)
11:Y:296:TRP:CD1	11:Y:419:THR:CG2	1.74	1.61
6:F:29:LYS:CD	6:F:75:ILE:HD11	1.30	1.58
12:J:405:CDL:H112	14:Y:502:PEE:C45	1.18	1.58
6:F:29:LYS:CG	6:F:75:ILE:HD11	1.16	1.54
11:Y:296:TRP:CD1	11:Y:419:THR:HG23	0.99	1.51

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	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	4 22
1	N	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	10 33
2	B	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	1 10
2	O	55/57 (96%)	43 (78%)	6 (11%)	6 (11%)	0 3
3	C	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	4 22
3	P	194/196 (99%)	178 (92%)	13 (7%)	3 (2%)	8 30
4	D	60/62 (97%)	57 (95%)	3 (5%)	0	100 100
4	Q	60/62 (97%)	55 (92%)	5 (8%)	0	100 100
5	E	72/75 (96%)	65 (90%)	5 (7%)	2 (3%)	4 20
5	R	72/75 (96%)	69 (96%)	2 (3%)	1 (1%)	9 31
6	F	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	13 39
6	S	104/106 (98%)	102 (98%)	2 (2%)	0	100 100
7	G	49/51 (96%)	48 (98%)	1 (2%)	0	100 100
7	T	49/51 (96%)	47 (96%)	2 (4%)	0	100 100
8	H	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	16 44
8	U	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	16 44
9	J	376/378 (100%)	363 (96%)	10 (3%)	3 (1%)	16 44
9	V	376/378 (100%)	359 (96%)	14 (4%)	3 (1%)	16 44
10	K	417/419 (100%)	390 (94%)	22 (5%)	5 (1%)	11 35
10	W	417/419 (100%)	397 (95%)	15 (4%)	5 (1%)	11 35
11	L	444/446 (100%)	405 (91%)	33 (7%)	6 (1%)	9 31
11	Y	444/446 (100%)	413 (93%)	24 (5%)	7 (2%)	8 29
All	All	4178/4224 (99%)	3911 (94%)	210 (5%)	57 (1%)	12 31

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	268	ILE
10	K	241	ARG
2	O	23	ALA
3	P	141	SER
11	Y	424	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	74/74 (100%)	68 (92%)	6 (8%)	9 31
1	N	73/74 (99%)	73 (100%)	0	100 100
2	B	46/46 (100%)	46 (100%)	0	100 100
2	O	45/46 (98%)	45 (100%)	0	100 100
3	C	166/166 (100%)	166 (100%)	0	100 100
3	P	166/166 (100%)	166 (100%)	0	100 100
4	D	52/52 (100%)	52 (100%)	0	100 100
4	Q	52/52 (100%)	52 (100%)	0	100 100
5	E	61/72 (85%)	59 (97%)	2 (3%)	33 58
5	R	61/72 (85%)	59 (97%)	2 (3%)	33 58
6	F	95/95 (100%)	84 (88%)	11 (12%)	4 17
6	S	95/95 (100%)	95 (100%)	0	100 100
7	G	42/42 (100%)	42 (100%)	0	100 100
7	T	42/42 (100%)	40 (95%)	2 (5%)	21 48
8	H	207/207 (100%)	207 (100%)	0	100 100
8	U	207/207 (100%)	206 (100%)	1 (0%)	86 91
9	J	330/330 (100%)	327 (99%)	3 (1%)	75 86
9	V	330/330 (100%)	322 (98%)	8 (2%)	44 66
10	K	334/335 (100%)	331 (99%)	3 (1%)	75 86
10	W	335/335 (100%)	332 (99%)	3 (1%)	75 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	367/367 (100%)	367 (100%)	0	100	100
11	Y	367/367 (100%)	361 (98%)	6 (2%)	58	75
All	All	3547/3572 (99%)	3500 (99%)	47 (1%)	64	78

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	T	40	LEU
9	V	195	LEU
8	U	292	MET
9	V	183	PHE
9	V	345	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
11	L	308	ASN
11	Y	223	HIS
6	S	73	HIS
11	Y	152	GLN
10	W	310	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)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	PLX	T	101	-	51,51,51	0.76	1 (1%)	55,59,59	0.60	1 (1%)
12	CDL	L	502	-	63,63,99	1.24	5 (7%)	69,75,111	1.05	4 (5%)
15	HEC	H	402	8	32,50,50	2.23	3 (9%)	24,82,82	1.35	1 (4%)
16	HEM	J	402	9	41,50,50	1.90	6 (14%)	45,82,82	1.58	9 (20%)
17	PLX	Q	101	-	51,51,51	0.77	1 (1%)	55,59,59	0.61	2 (3%)
14	PEE	V	403	-	48,48,50	1.34	4 (8%)	51,53,55	1.04	2 (3%)
17	PLX	L	501	-	51,51,51	0.77	1 (1%)	55,59,59	0.63	1 (1%)
12	CDL	Y	501	-	63,63,99	1.24	5 (7%)	69,75,111	1.01	4 (5%)
16	HEM	J	401	9	41,50,50	1.92	6 (14%)	45,82,82	1.60	5 (11%)
12	CDL	U	403	-	63,63,99	1.25	6 (9%)	69,75,111	1.04	4 (5%)
15	HEC	U	402	8	32,50,50	2.27	3 (9%)	24,82,82	1.39	2 (8%)
12	CDL	H	403	-	63,63,99	1.25	5 (7%)	69,75,111	1.03	4 (5%)
14	PEE	U	401	-	40,40,50	1.46	4 (10%)	43,45,55	0.95	3 (6%)
14	PEE	Y	502	-	48,48,50	1.39	4 (8%)	51,53,55	0.96	2 (3%)
14	PEE	J	403	-	48,48,50	1.33	4 (8%)	51,53,55	0.99	2 (3%)
14	PEE	H	401	-	48,48,50	1.35	4 (8%)	51,53,55	0.95	2 (3%)
14	PEE	L	503	-	48,48,50	1.38	4 (8%)	51,53,55	0.92	2 (3%)
13	FES	C	301	3	0,4,4	-	-	-		
16	HEM	V	402	9	41,50,50	1.90	6 (14%)	45,82,82	1.60	8 (17%)
12	CDL	N	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.02	4 (5%)
12	CDL	J	404	-	63,63,99	1.24	5 (7%)	69,75,111	1.02	4 (5%)
12	CDL	G	101	-	63,63,99	1.15	4 (6%)	69,75,111	1.16	6 (8%)
12	CDL	J	405	-	63,63,99	1.13	4 (6%)	69,75,111	1.22	5 (7%)
16	HEM	V	401	9	41,50,50	1.97	5 (12%)	45,82,82	1.54	5 (11%)
13	FES	P	301	3	0,4,4	-	-	-		
12	CDL	A	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PLX	T	101	-	-	23/55/55/55	-
12	CDL	L	502	-	-	43/74/74/110	-
15	HEC	H	402	8	-	2/10/54/54	-
16	HEM	J	402	9	-	2/12/54/54	-
17	PLX	Q	101	-	-	25/55/55/55	-
14	PEE	V	403	-	-	30/52/52/54	-
17	PLX	L	501	-	-	23/55/55/55	-
12	CDL	Y	501	-	-	36/74/74/110	-
16	HEM	J	401	9	-	1/12/54/54	-
12	CDL	U	403	-	-	48/74/74/110	-
15	HEC	U	402	8	-	0/10/54/54	-
12	CDL	H	403	-	-	42/74/74/110	-
14	PEE	U	401	-	-	17/44/44/54	-
14	PEE	Y	502	-	-	20/52/52/54	-
14	PEE	J	403	-	-	20/52/52/54	-
14	PEE	H	401	-	-	27/52/52/54	-
14	PEE	L	503	-	-	22/52/52/54	-
13	FES	C	301	3	-	-	0/1/1/1
16	HEM	V	402	9	-	4/12/54/54	-
12	CDL	N	101	-	-	40/74/74/110	-
12	CDL	J	404	-	-	33/74/74/110	-
12	CDL	G	101	-	-	38/74/74/110	-
12	CDL	J	405	-	-	28/74/74/110	-
16	HEM	V	401	9	-	3/12/54/54	-
13	FES	P	301	3	-	-	0/1/1/1
12	CDL	A	101	-	-	35/74/74/110	-

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	402	HEM	C3D-C2D	7.86	1.53	1.36
16	J	401	HEM	C3D-C2D	7.85	1.53	1.36
16	J	402	HEM	C3D-C2D	7.83	1.53	1.36
16	V	401	HEM	C3D-C2D	7.75	1.53	1.36
15	U	402	HEC	C3C-C2C	-6.96	1.33	1.40

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	402	HEM	C4D-ND-C1D	6.17	111.44	105.07
16	J	401	HEM	C4D-ND-C1D	6.12	111.40	105.07
16	J	402	HEM	C4D-ND-C1D	6.04	111.31	105.07
16	V	401	HEM	C4D-ND-C1D	5.31	110.56	105.07
14	Y	502	PEE	O2-C10-C11	4.31	120.78	111.50

There are no chirality outliers.

5 of 562 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	101	CDL	O1-C1-CB2-OB2
12	A	101	CDL	CB2-OB2-PB2-OB4
12	A	101	CDL	CB2-OB2-PB2-OB5
12	G	101	CDL	OA9-CA7-OA8-CA6
12	G	101	CDL	CB2-OB2-PB2-OB4

There are no ring outliers.

26 monomers are involved in 276 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	101	PLX	3	0
12	L	502	CDL	22	0
15	H	402	HEC	5	0
16	J	402	HEM	4	0
17	Q	101	PLX	7	0
14	V	403	PEE	23	0
17	L	501	PLX	4	0
12	Y	501	CDL	4	0
16	J	401	HEM	3	0
12	U	403	CDL	12	0
15	U	402	HEC	8	0
12	H	403	CDL	6	0
14	U	401	PEE	25	0
14	Y	502	PEE	21	0
14	J	403	PEE	8	0
14	H	401	PEE	32	0
14	L	503	PEE	37	0
13	C	301	FES	3	0
16	V	402	HEM	6	0
12	N	101	CDL	8	0
12	J	404	CDL	6	0
12	G	101	CDL	28	0

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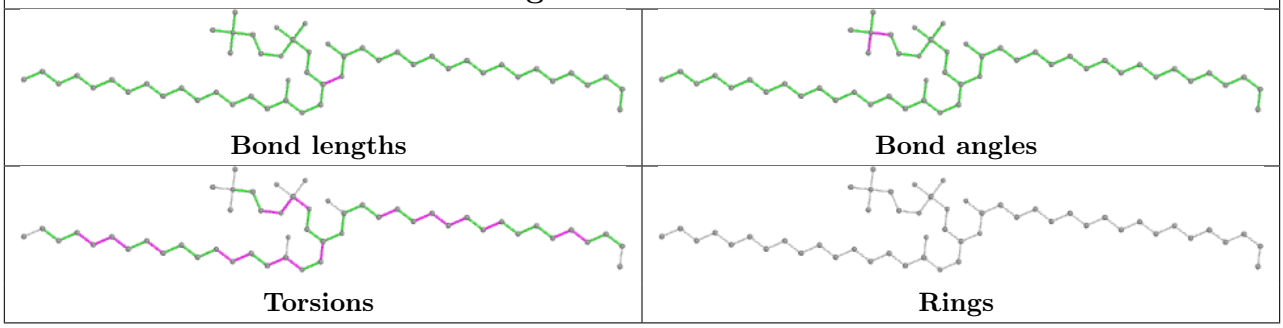
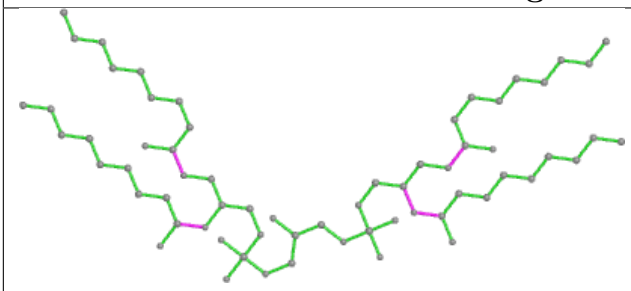
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	J	405	CDL	17	0
16	V	401	HEM	7	0
13	P	301	FES	2	0
12	A	101	CDL	3	0

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.

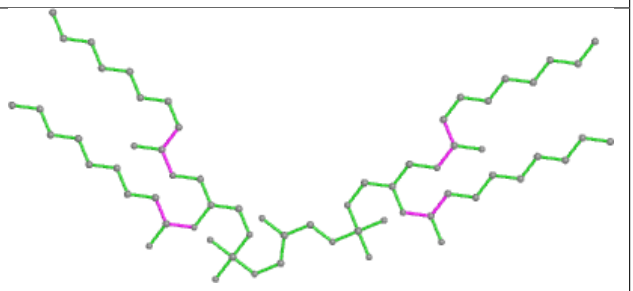
Ligand PLX T 101



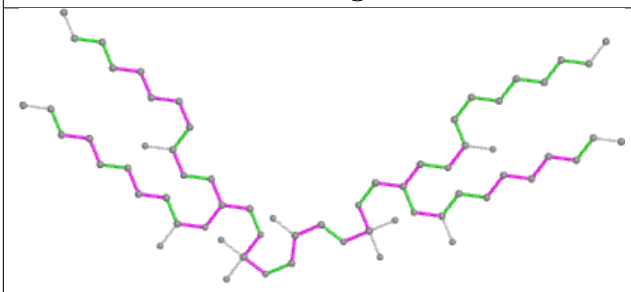
Ligand CDL L 502



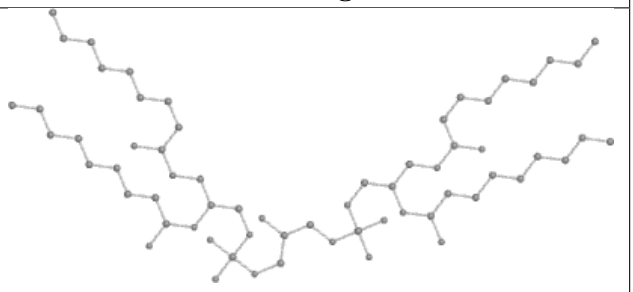
Bond lengths



Bond angles

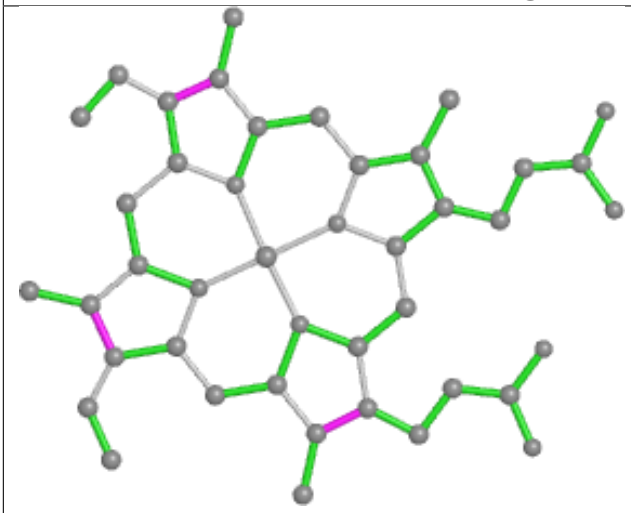


Torsions

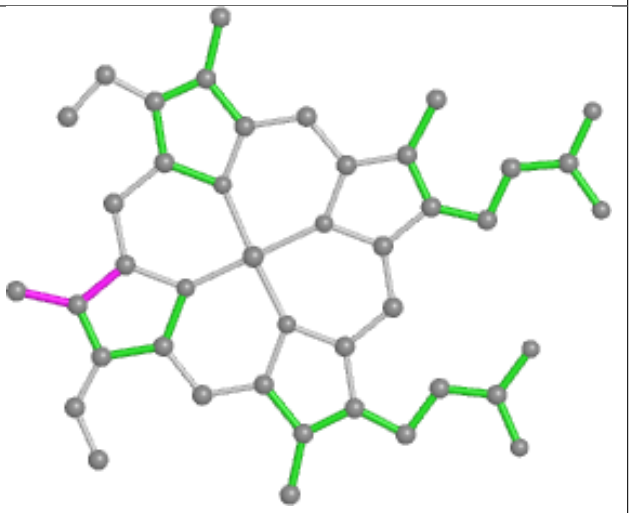


Rings

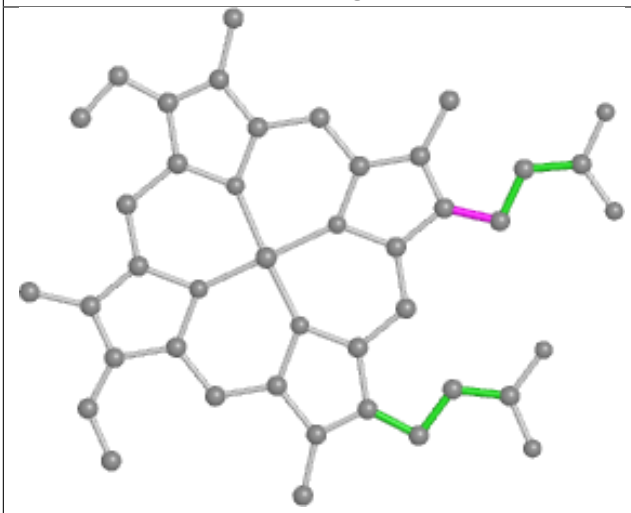
Ligand HEC H 402



Bond lengths



Bond angles



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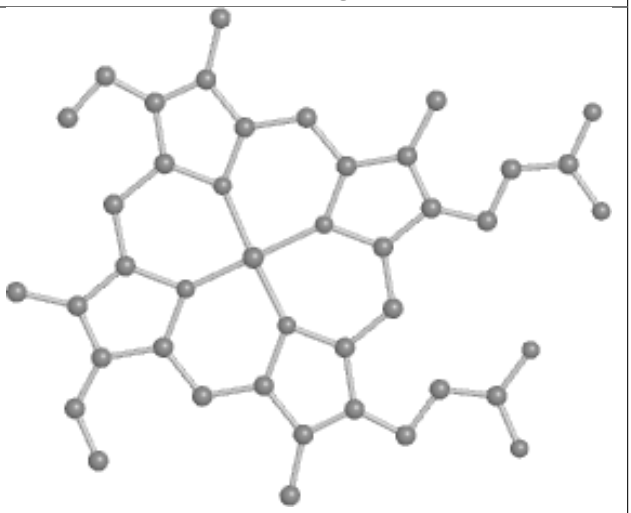
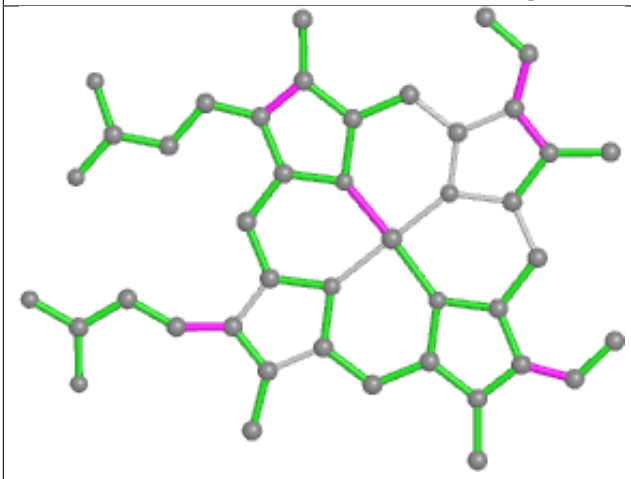
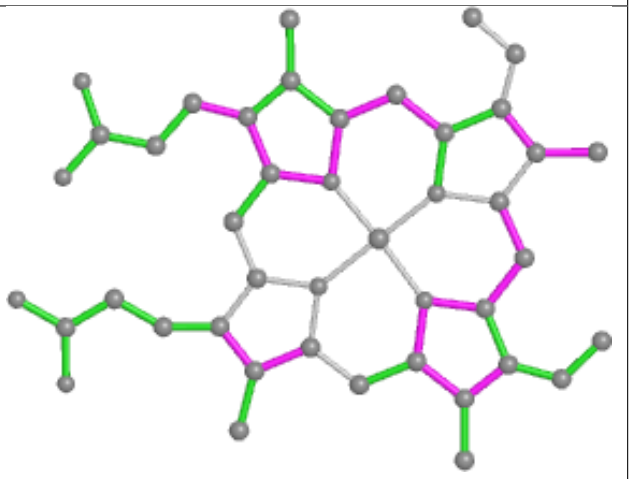


Rings

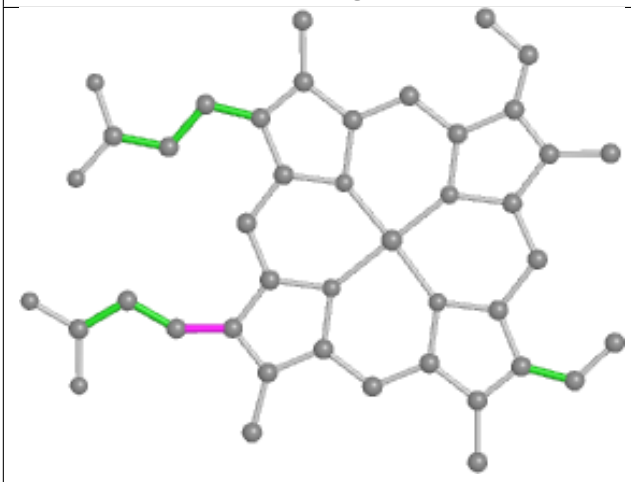
Ligand HEM J 402



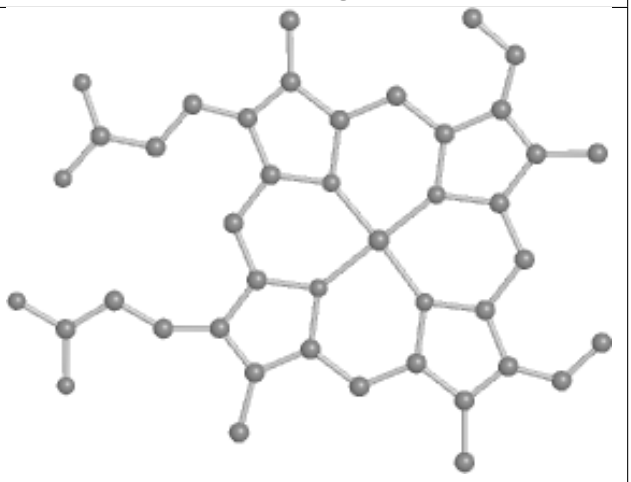
Bond lengths



Bond angles

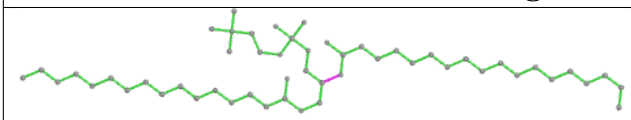


Torsions



Rings

Ligand PLX Q 101



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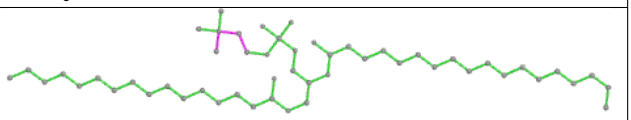
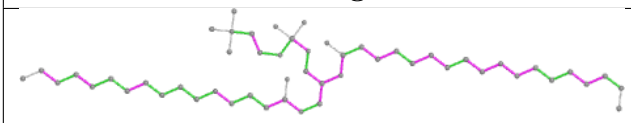
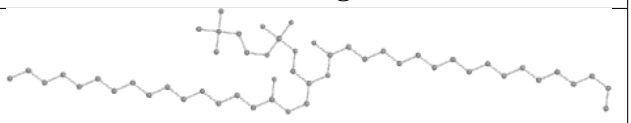


Bond angles

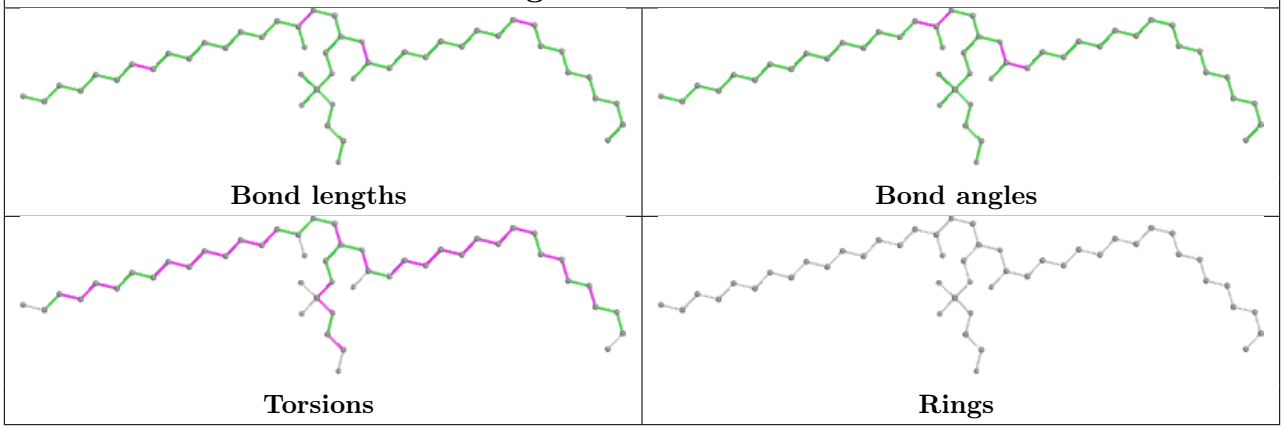


Torsions



Rings

Ligand PEE V 403



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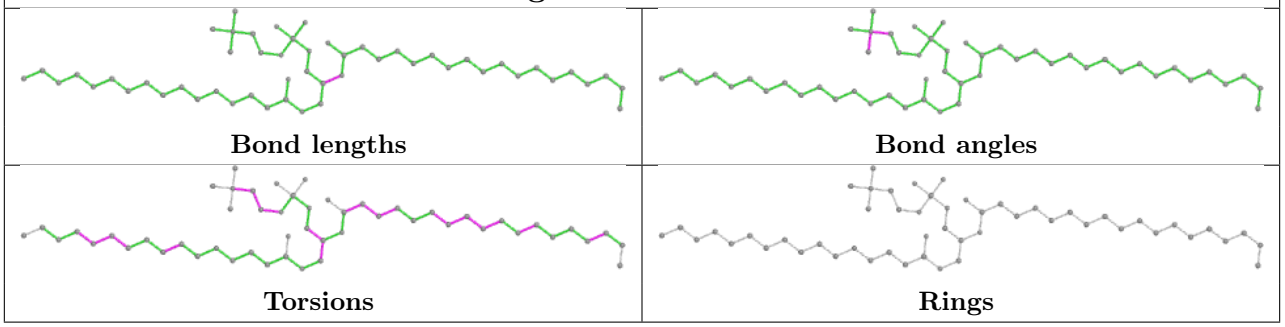
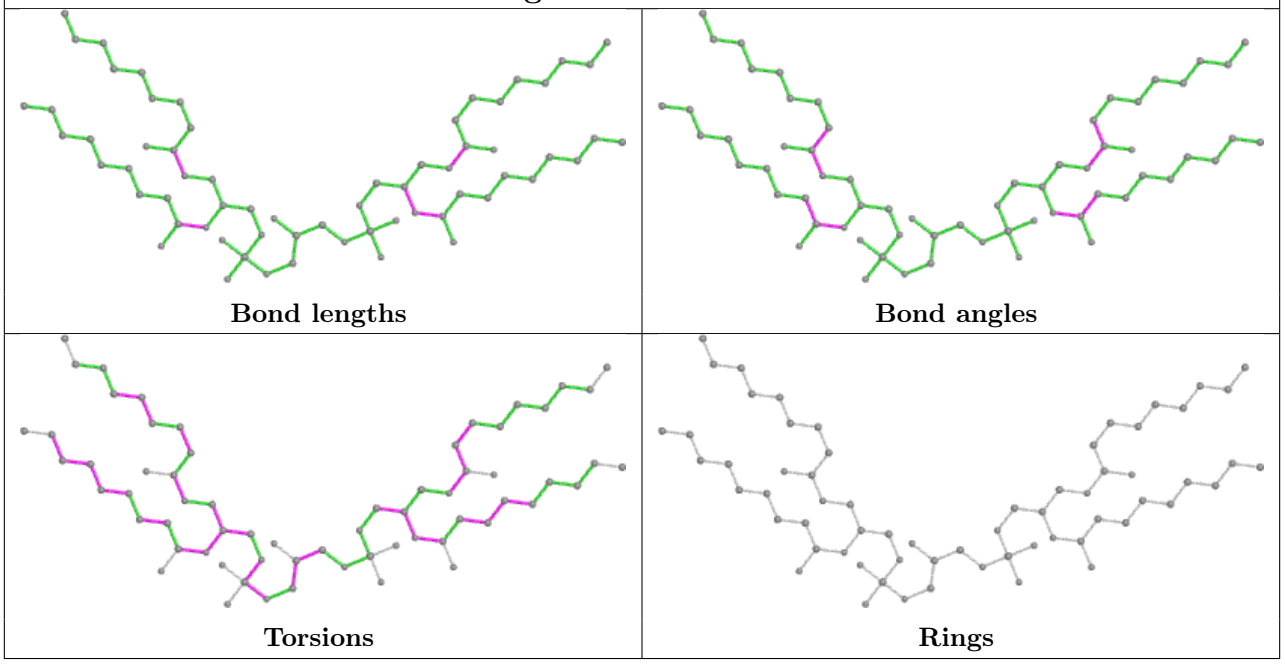


Ligand CDL Y 501



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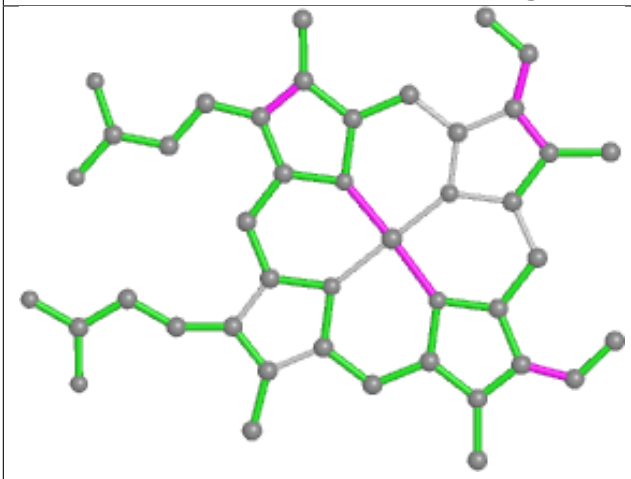

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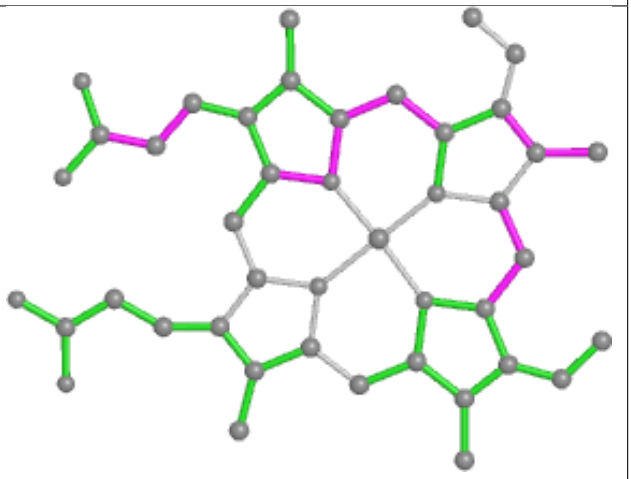

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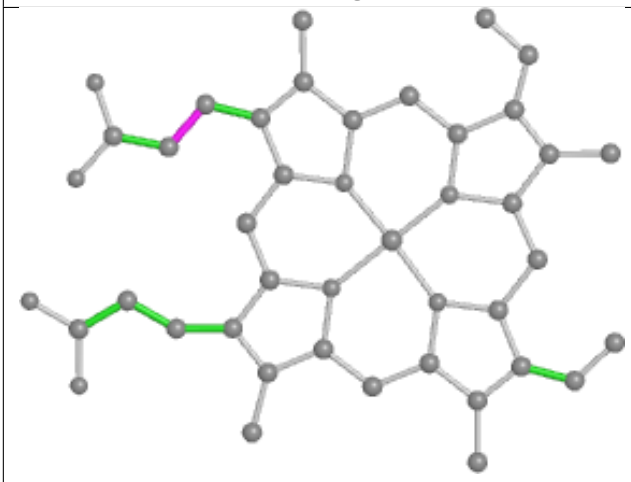

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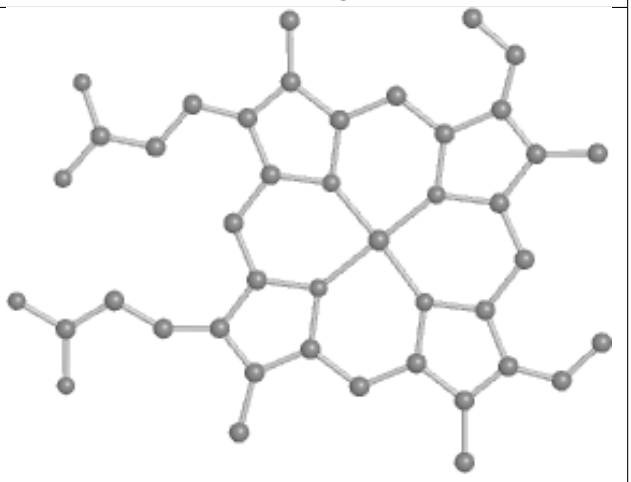
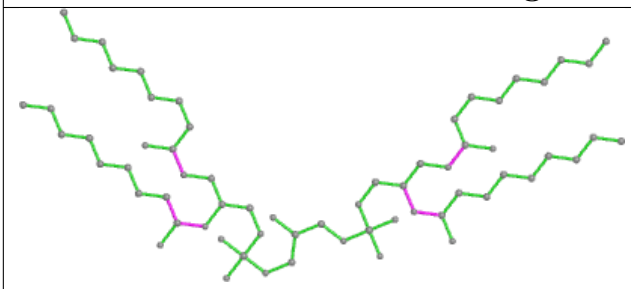


Rings

Ligand CDL U 403



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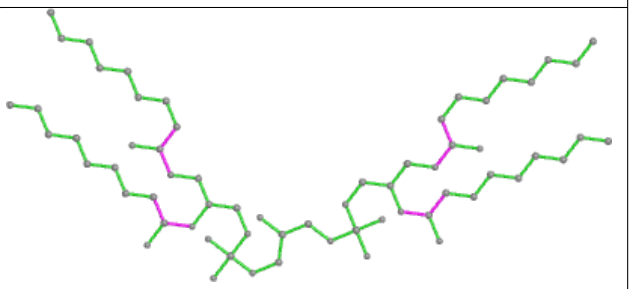

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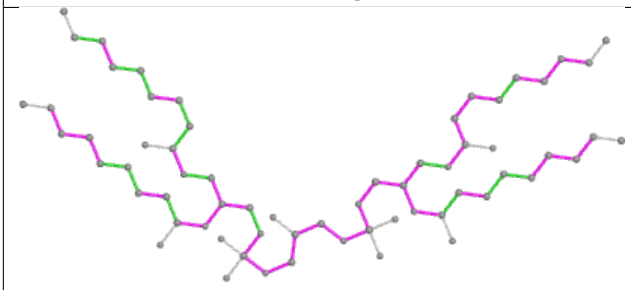

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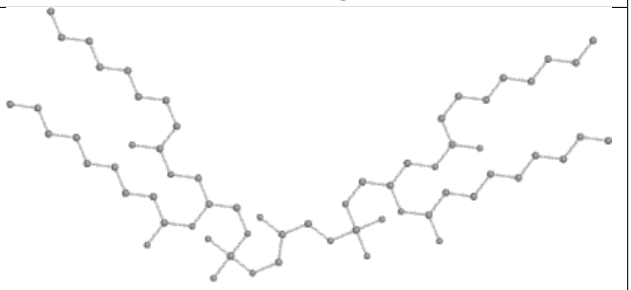
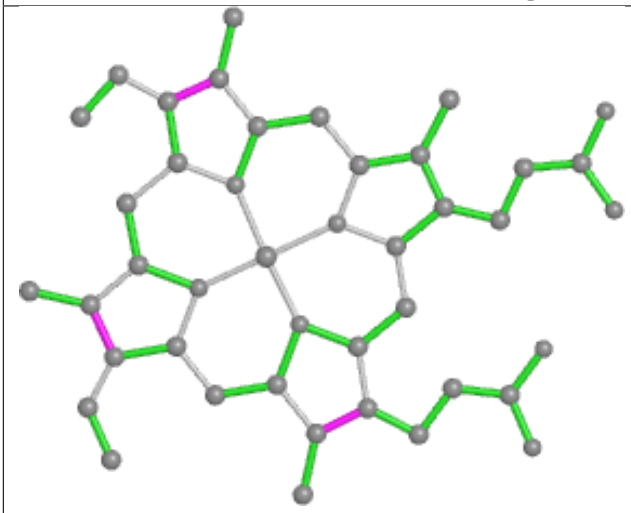


Rings

Ligand HEC U 402



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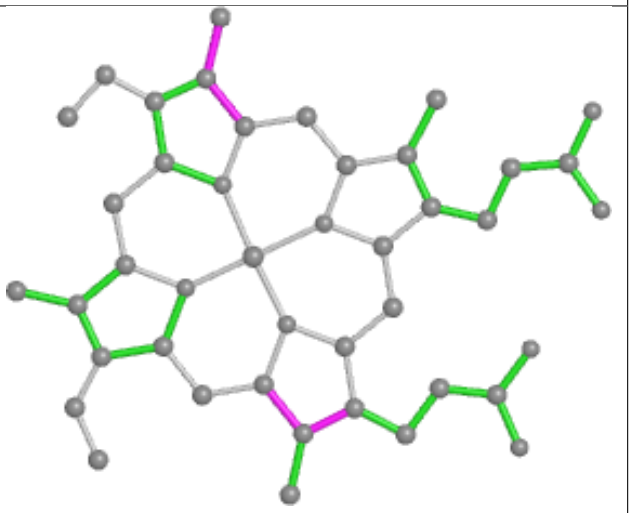
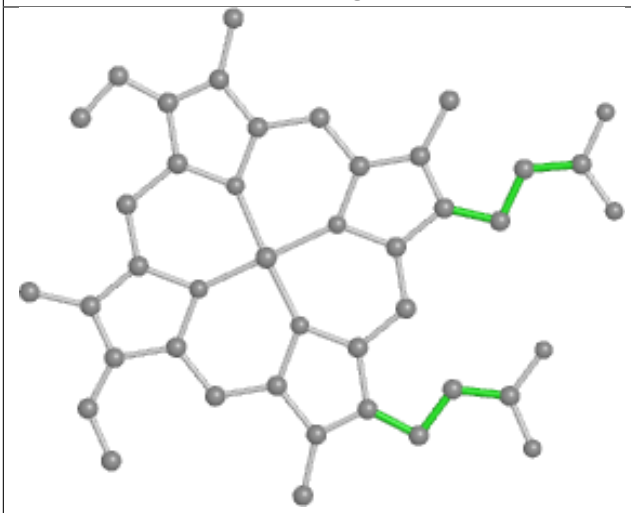
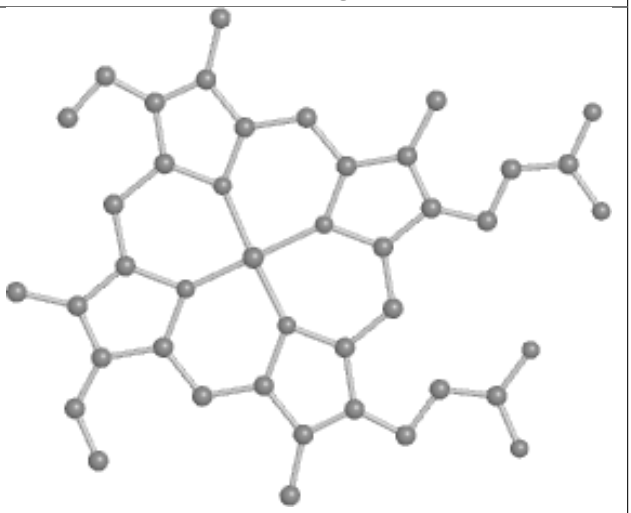


Bond angles

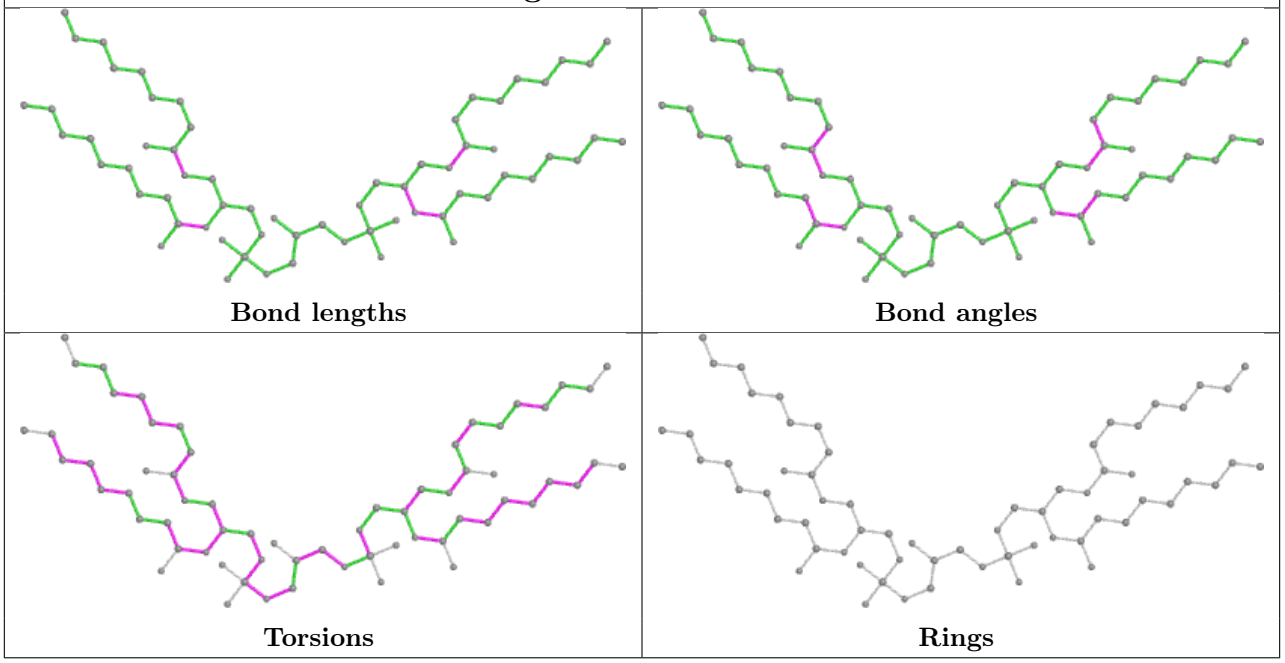


Torsions



Rings

Ligand CDL H 403



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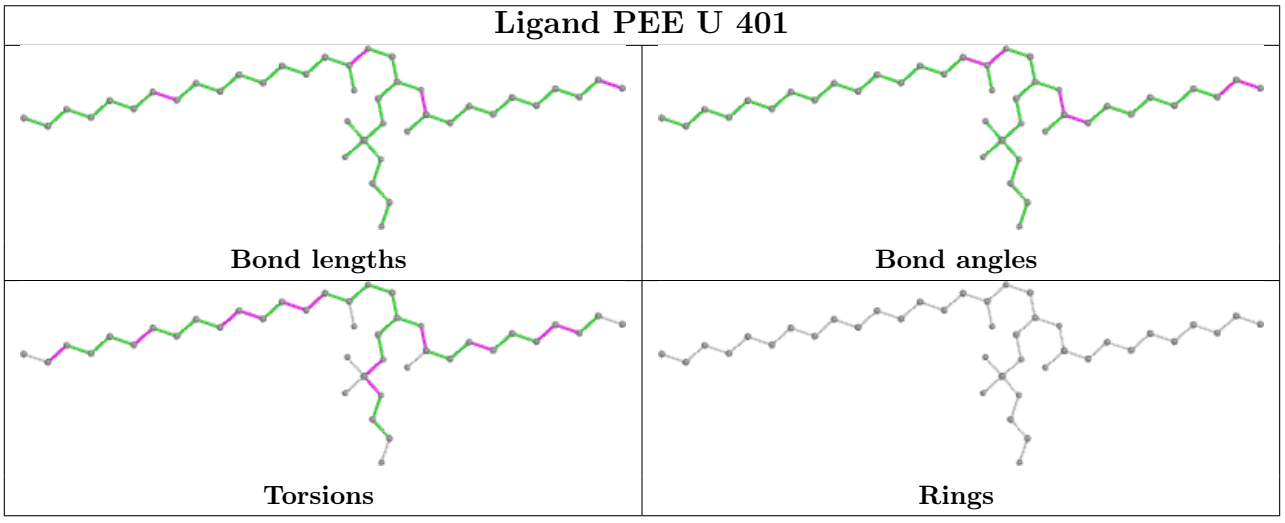
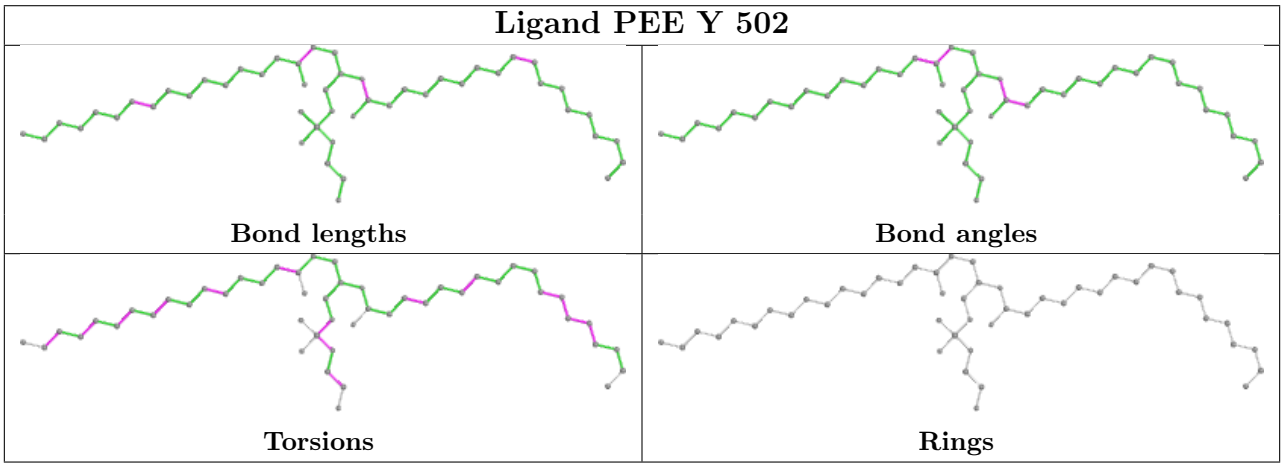


Ligand PEE Y 502



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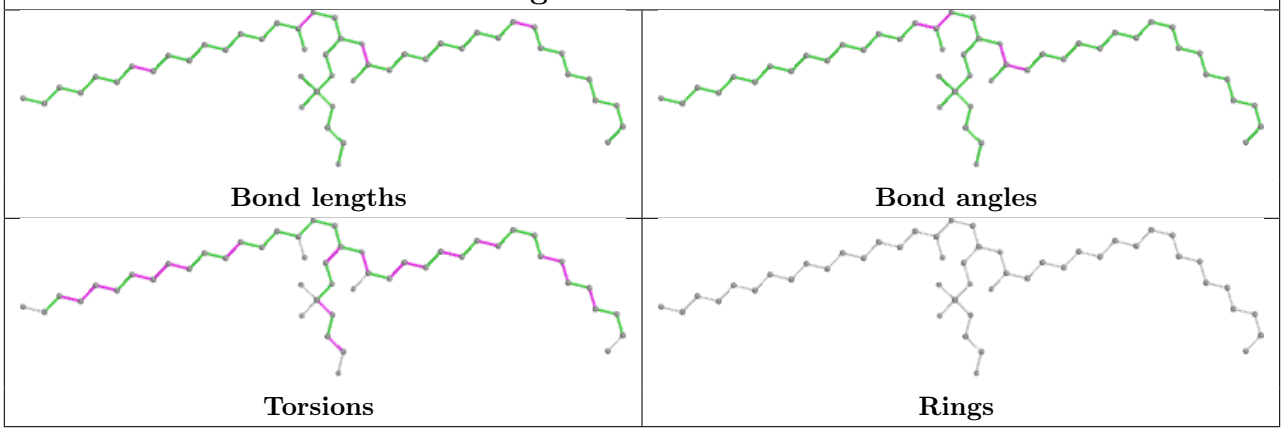

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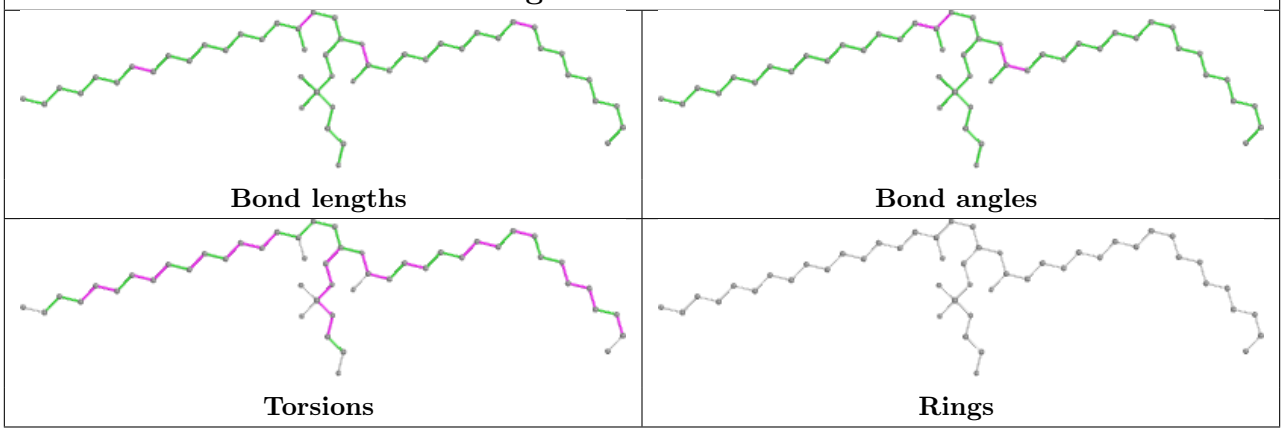

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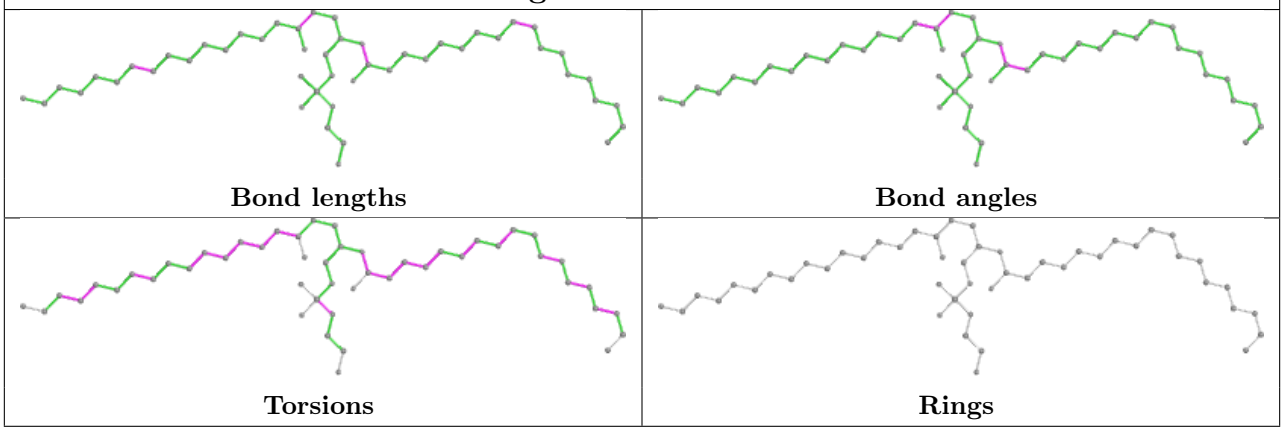
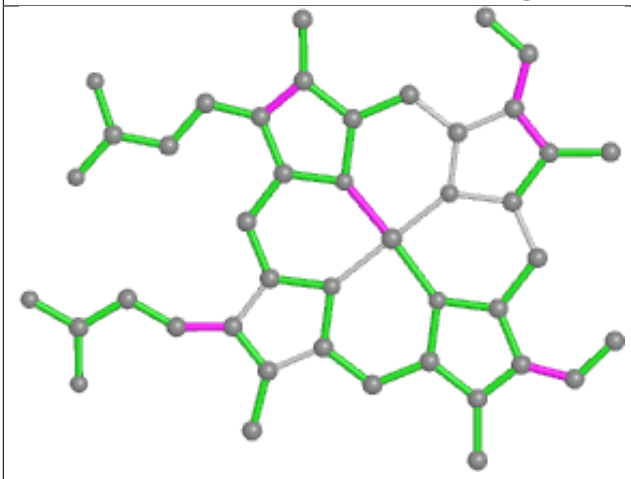
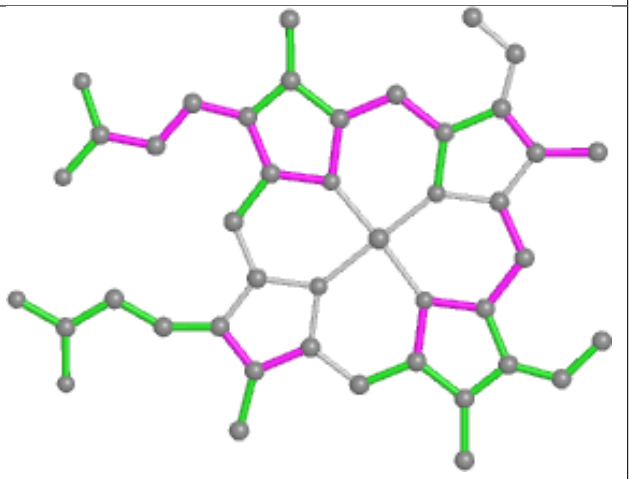


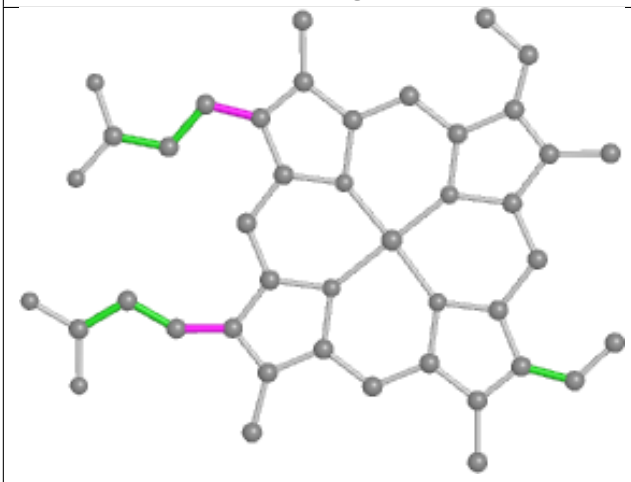
Ligand HEM V 402



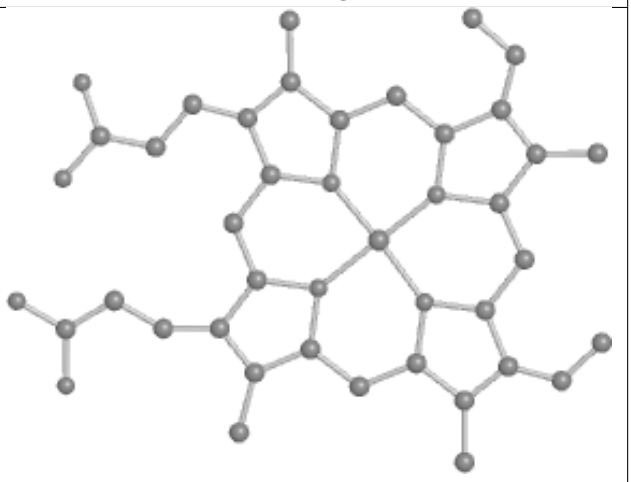
Bond lengths



Bond angles

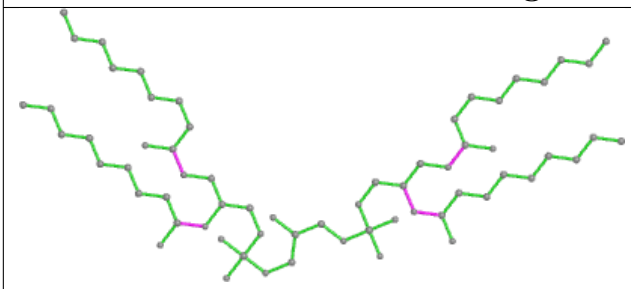


Torsions



Rings

Ligand CDL N 101



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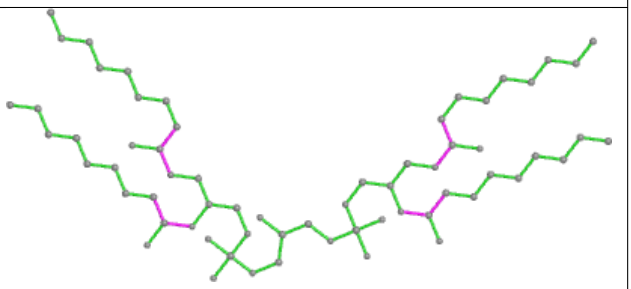
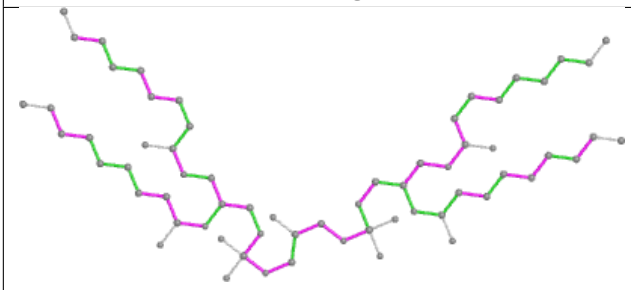
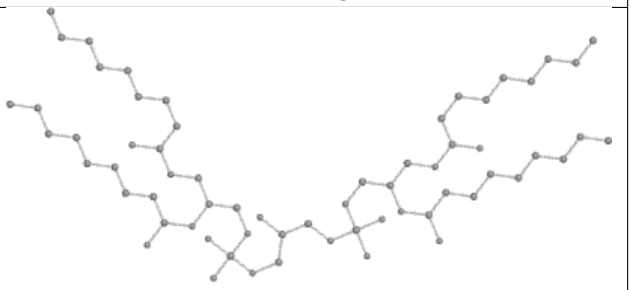


Bond angles

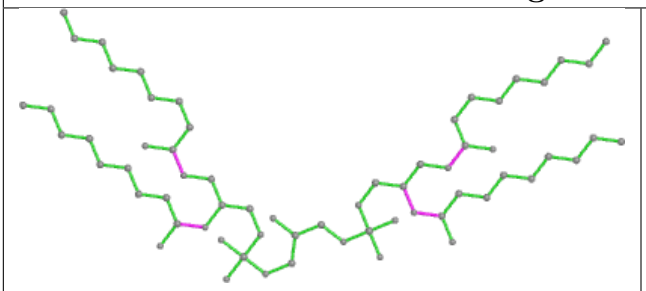


Torsions

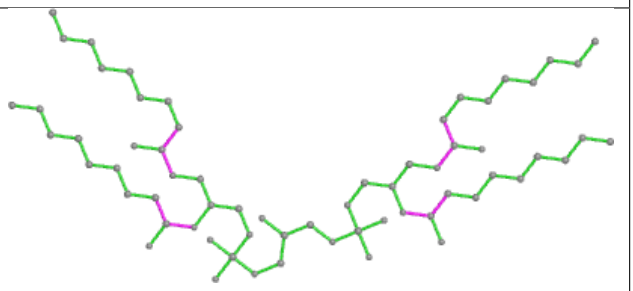


Rings

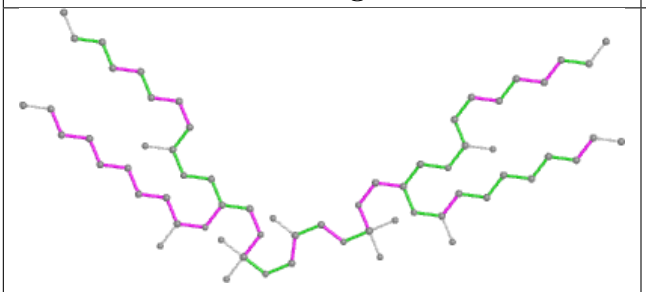
Ligand CDL J 404



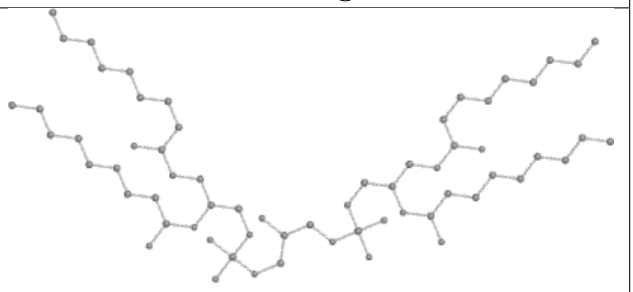
Bond lengths



Bond angles

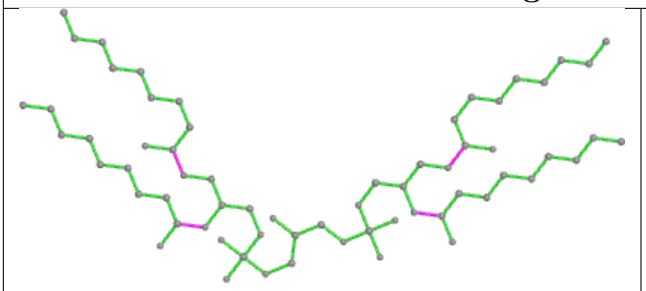


Torsions

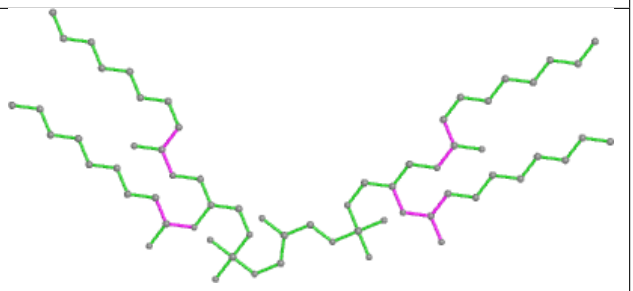


Rings

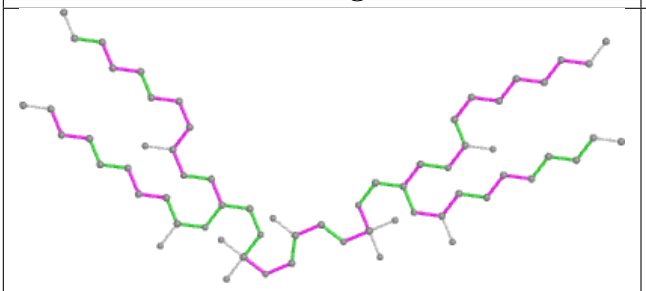
Ligand CDL G 101



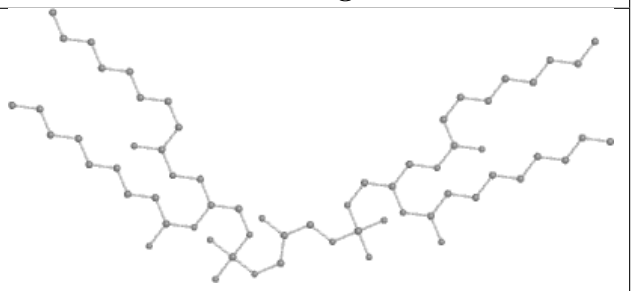
Bond lengths



Bond angles

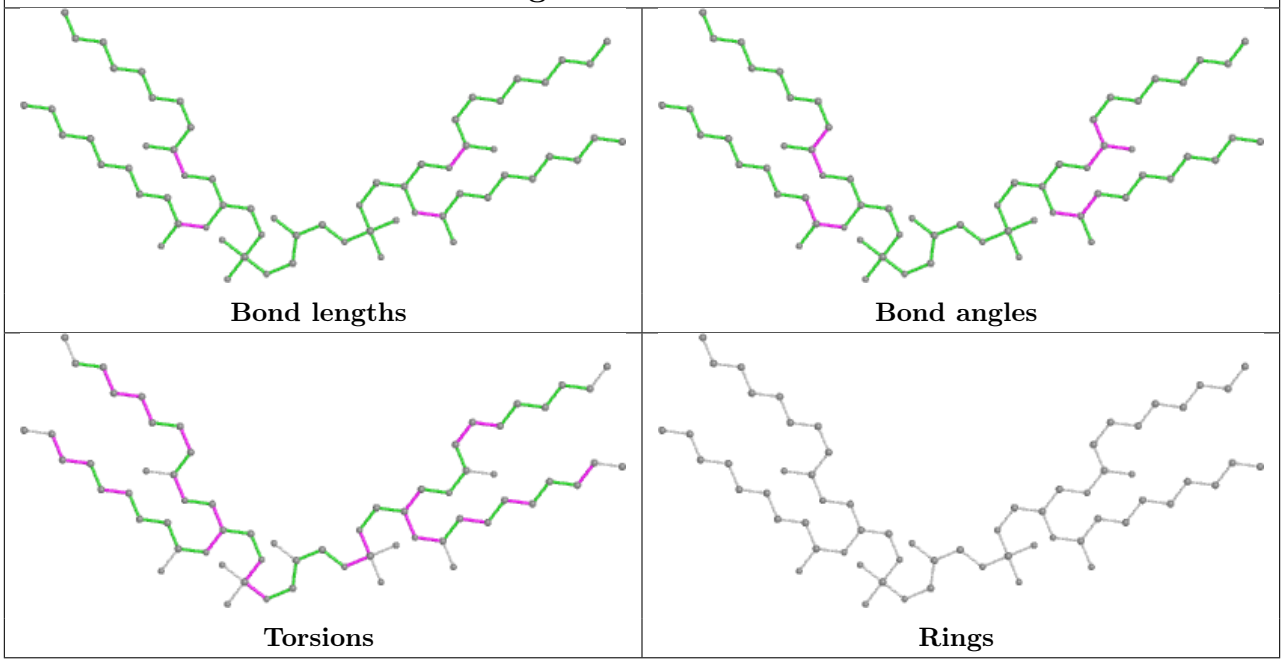


Torsions

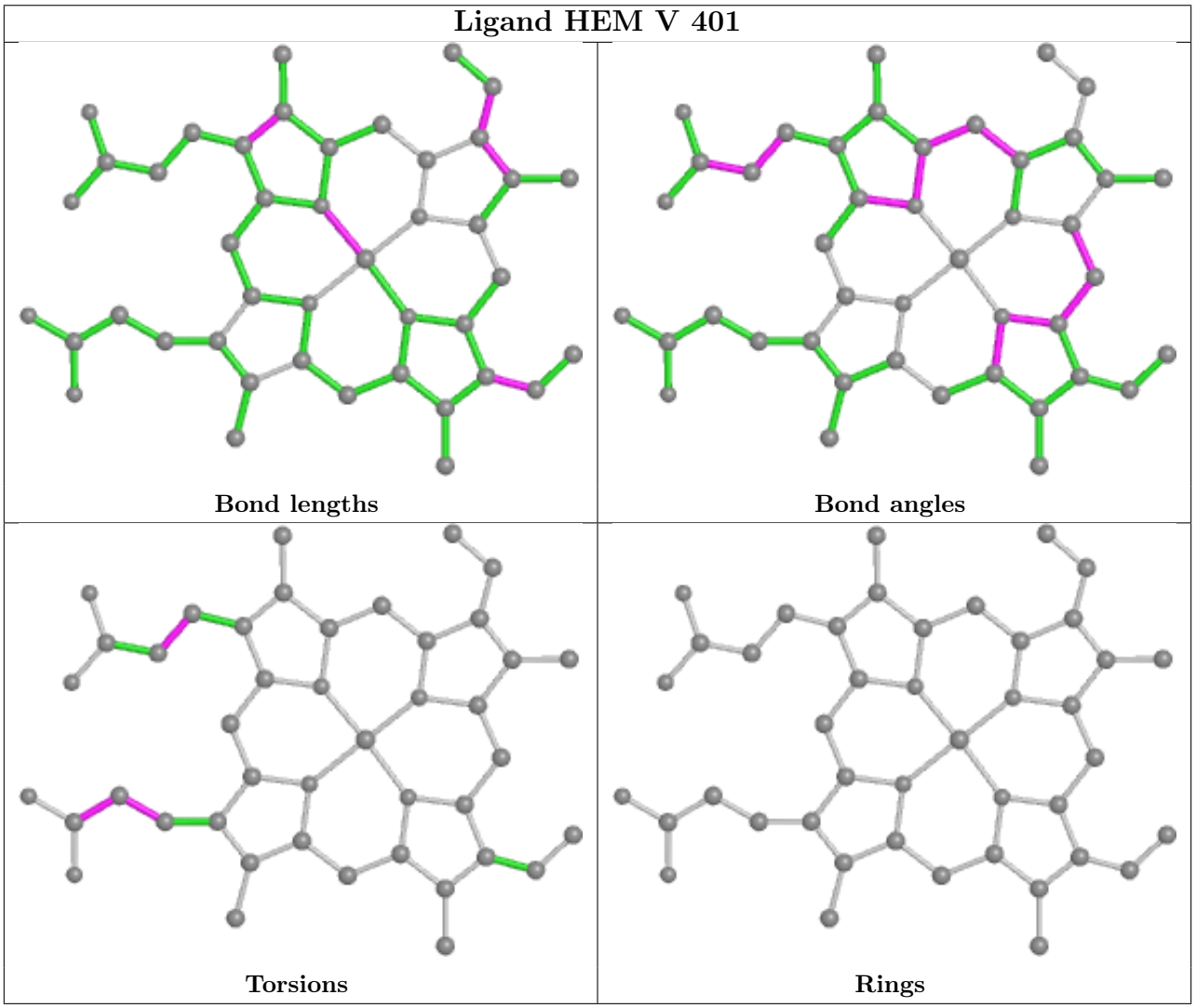


Rings

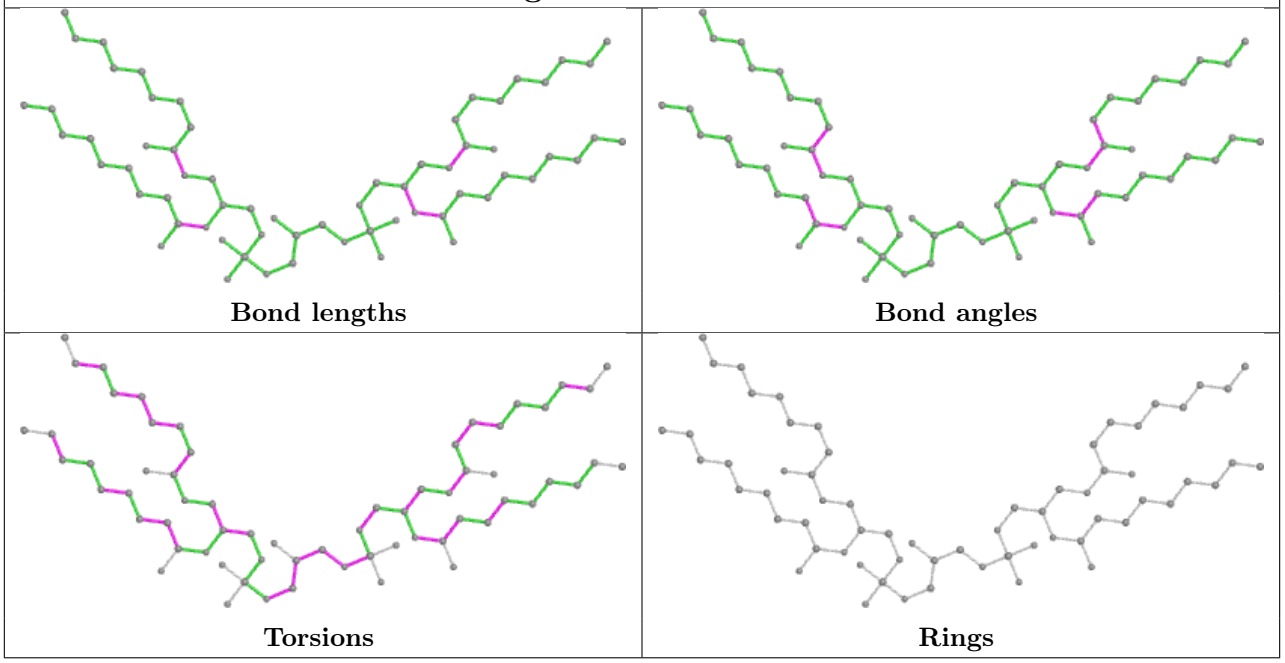
Ligand CDL J 405



Ligand HEM V 401



Ligand CDL A 101



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.

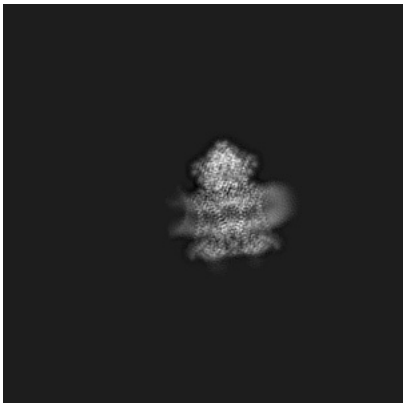
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6774. These allow visual inspection of the internal detail of the map and identification of artifacts.

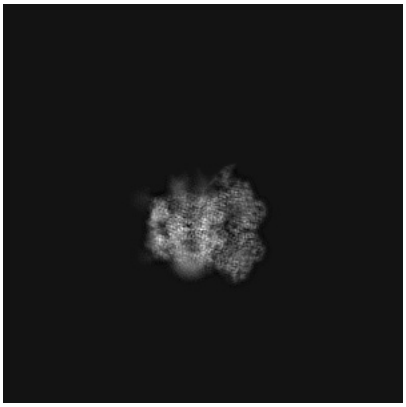
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

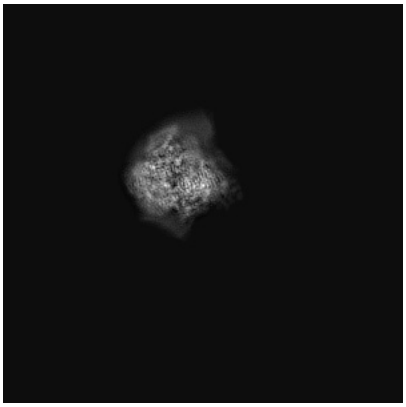
6.1.1 Primary map



X



Y

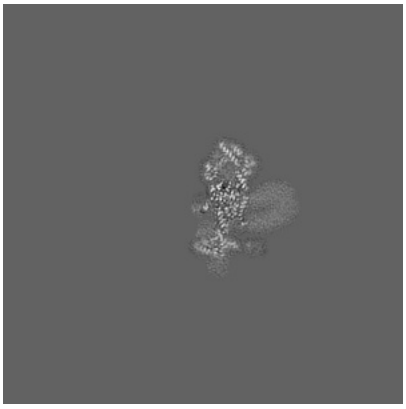


Z

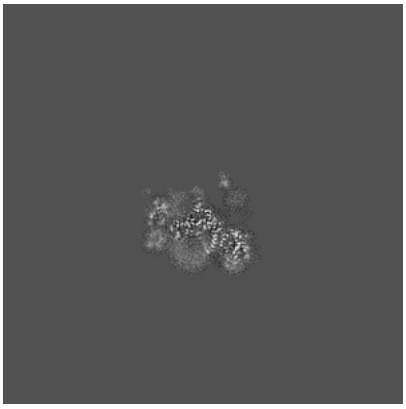
The images above show the map projected in three orthogonal directions.

6.2 Central slices

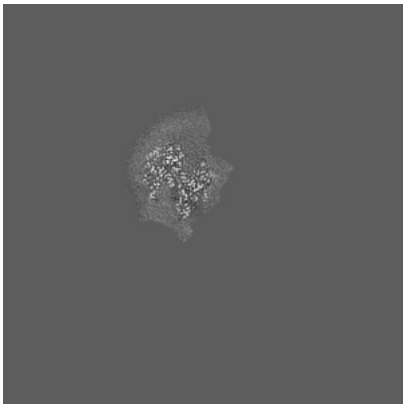
6.2.1 Primary map



X Index: 240



Y Index: 240

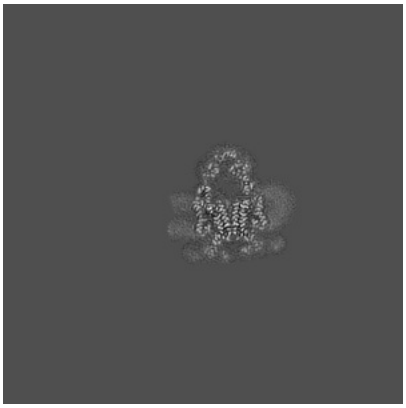


Z Index: 240

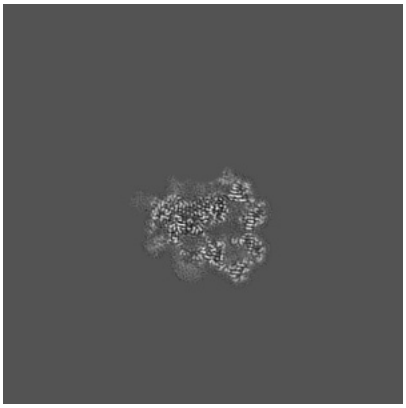
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

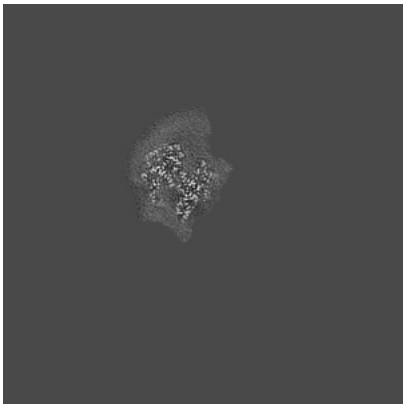
6.3.1 Primary map



X Index: 209



Y Index: 263

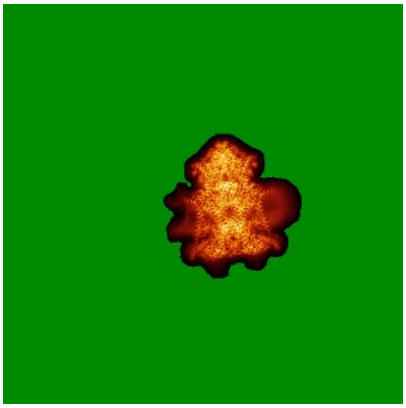


Z Index: 241

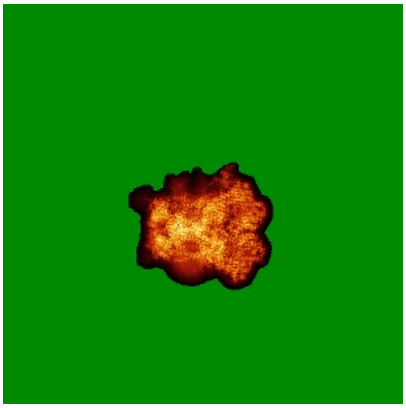
The images above show the largest variance slices of the map in three orthogonal directions.

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

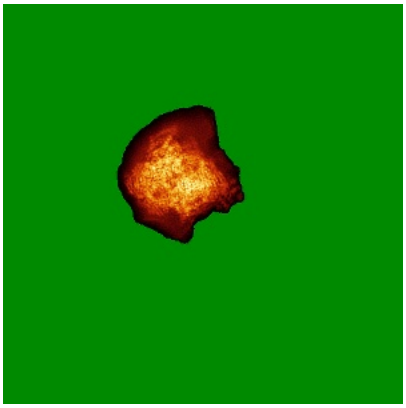
6.4.1 Primary map



X



Y



Z

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 0.0783. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

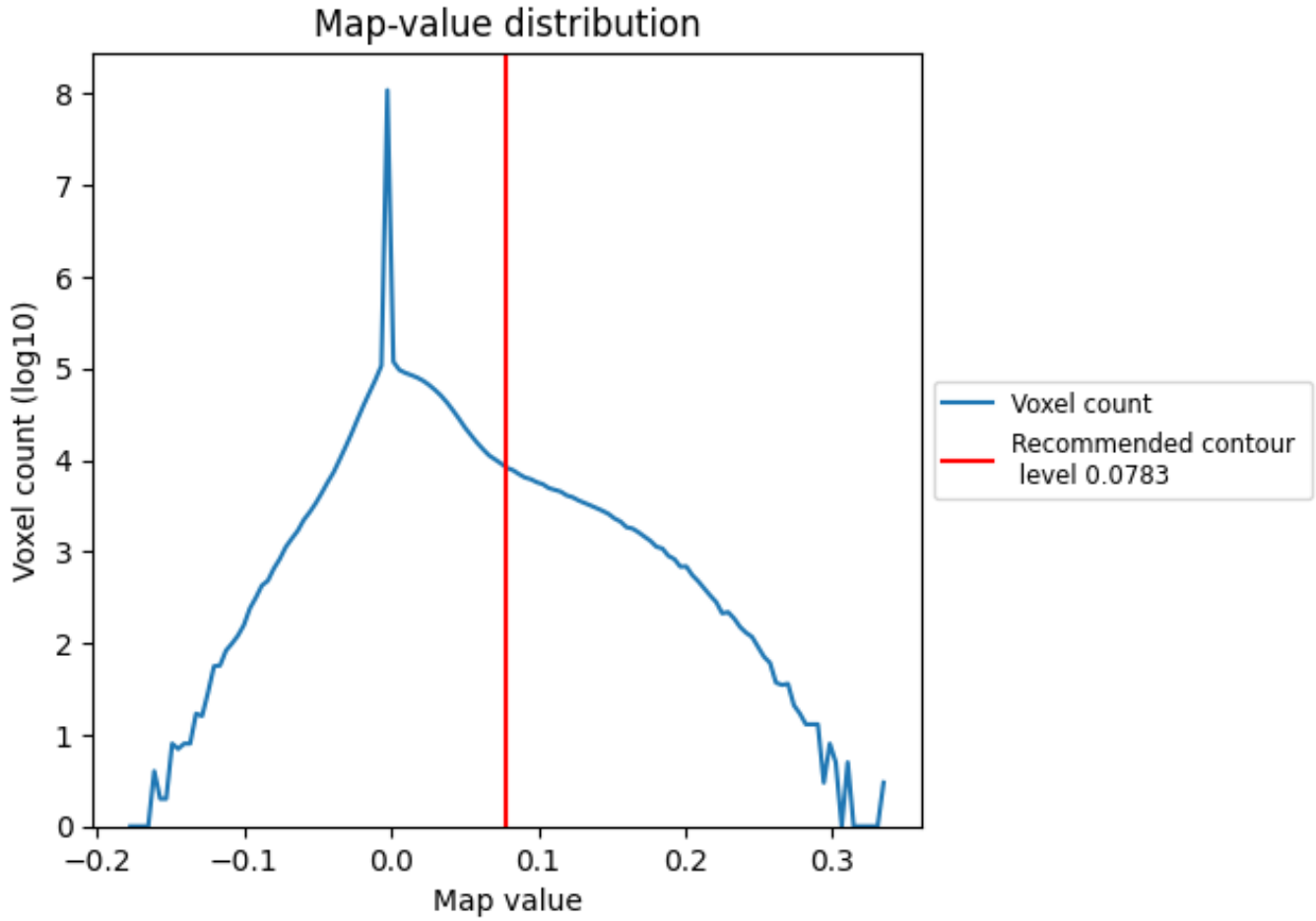
6.6 Mask visualisation (i)

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

7 Map analysis

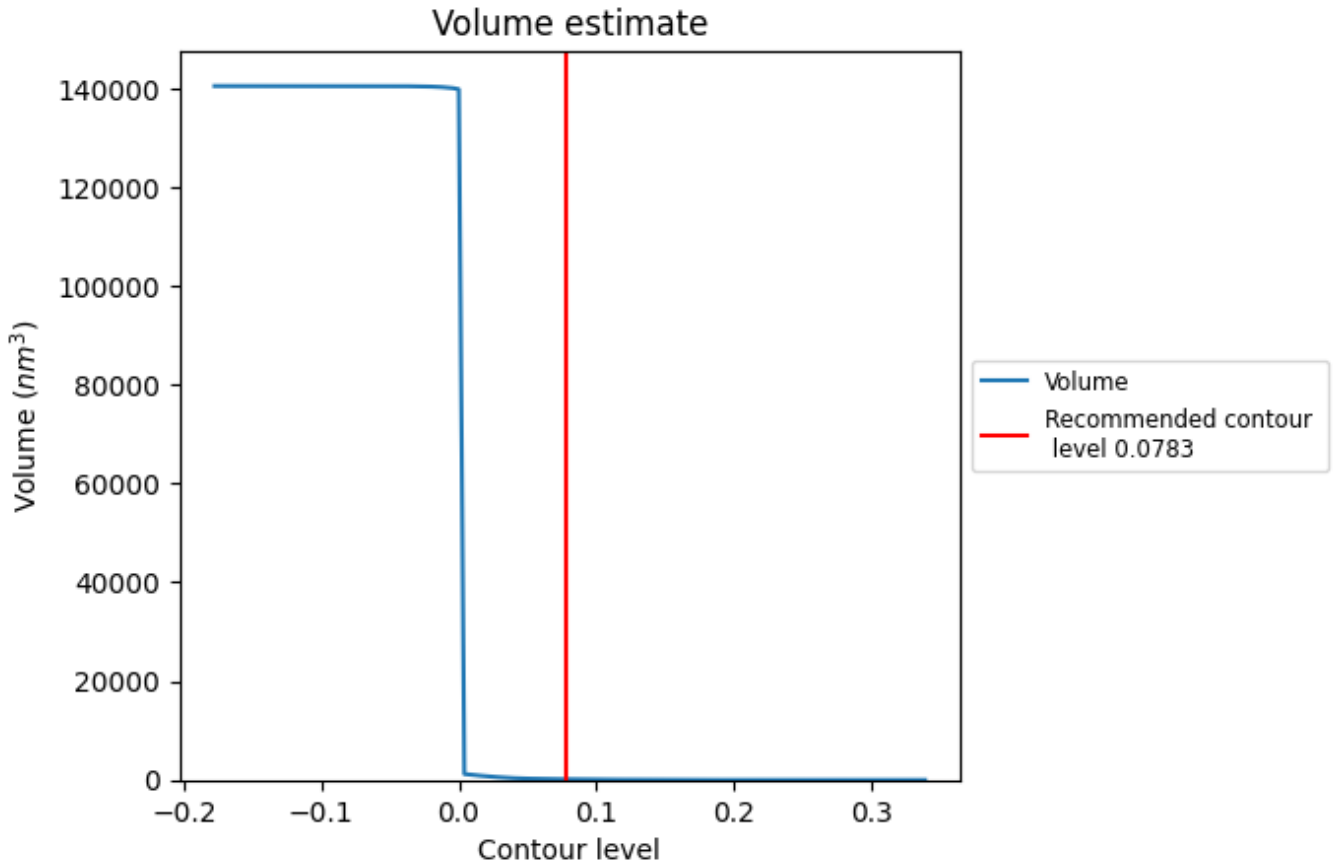
This section contains the results of statistical analysis of the map.

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.

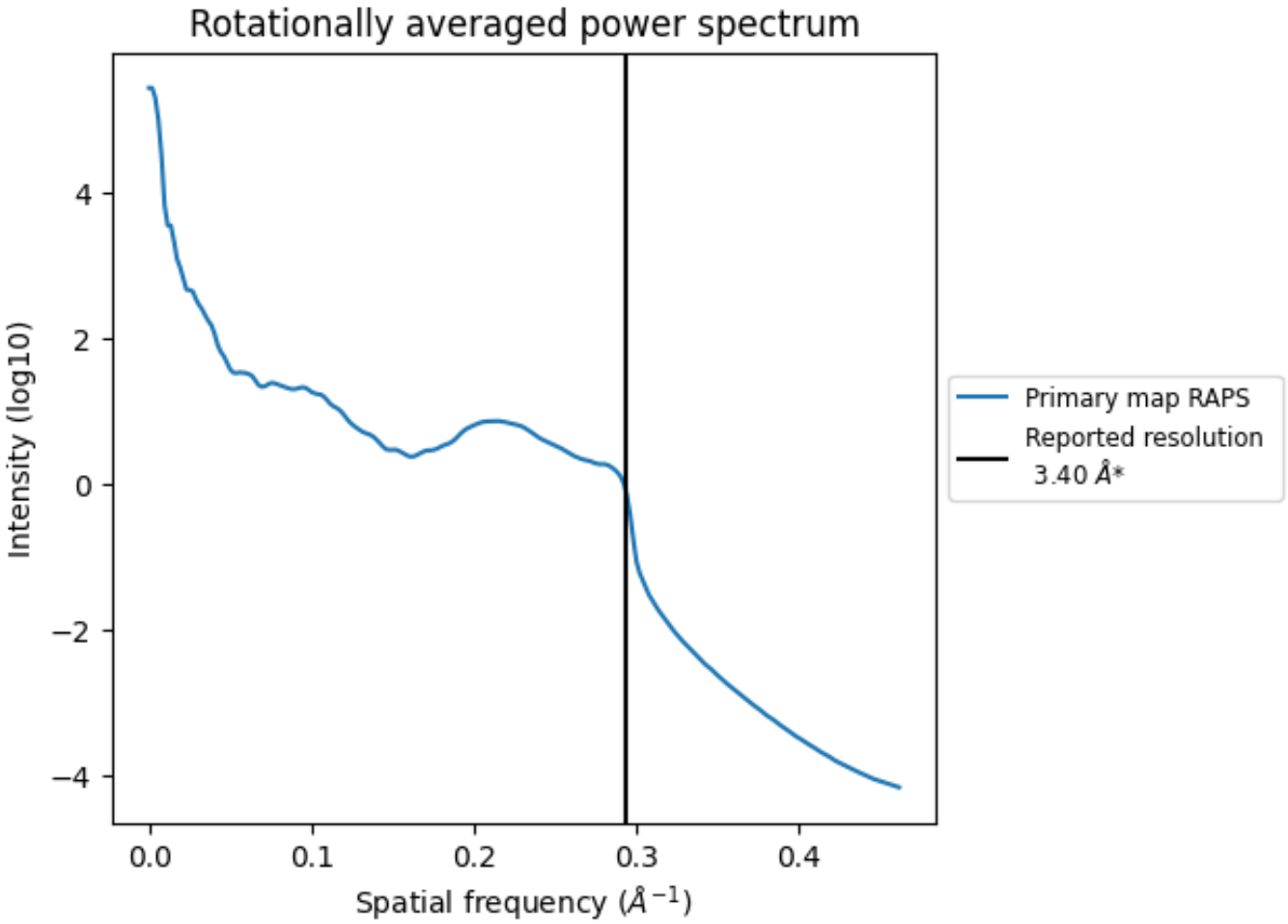
7.2 Volume estimate (i)



The volume at the recommended contour level is 139 nm^3; this corresponds to an approximate mass of 126 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

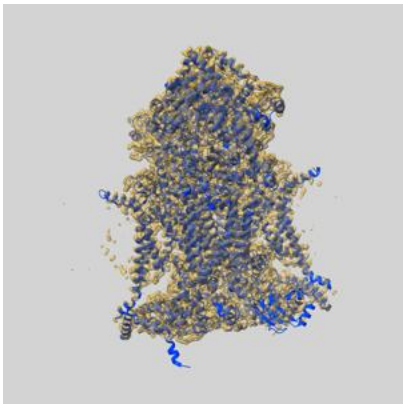
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

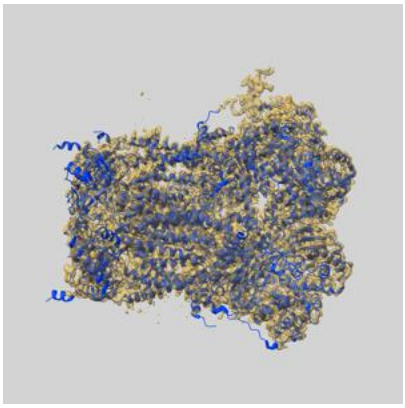
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6774 and PDB model 5XTE. Per-residue inclusion information can be found in section 3 on page 11.

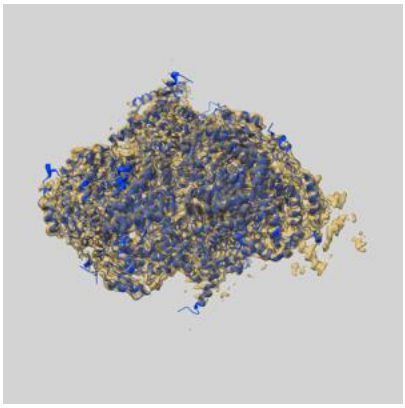
9.1 Map-model overlay



X



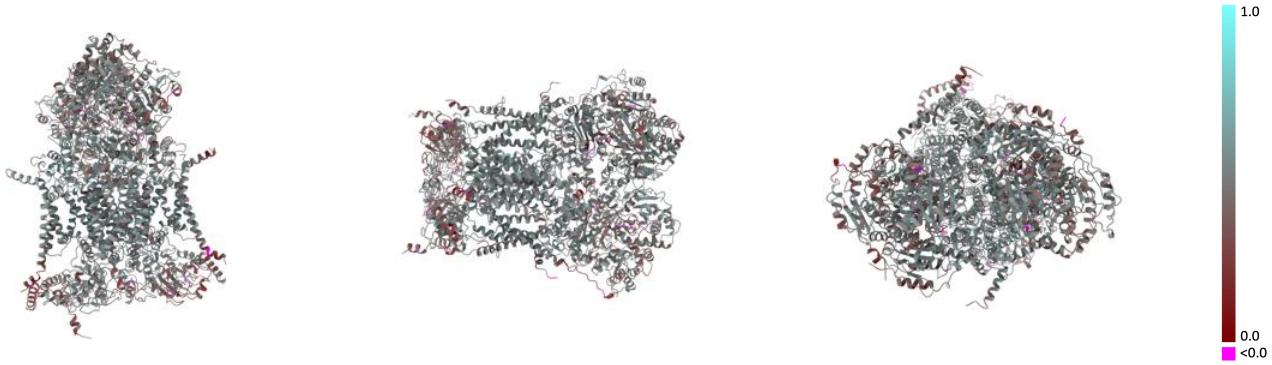
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0783 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.

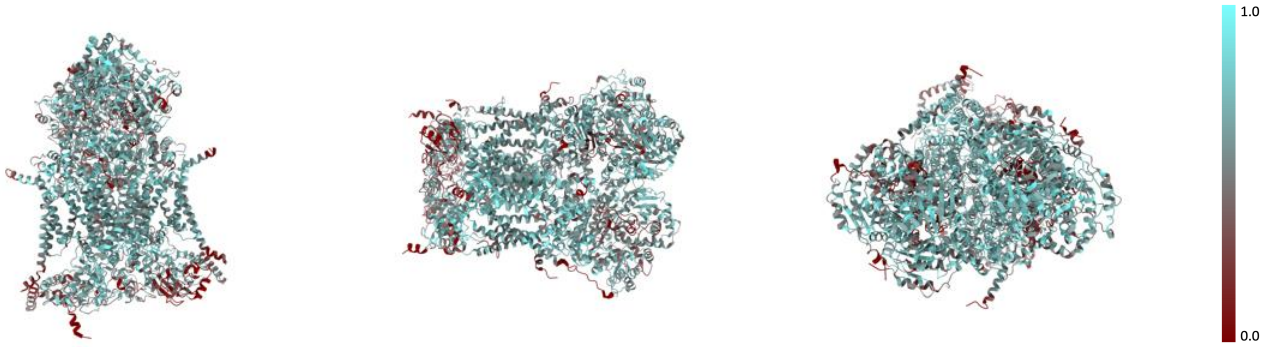
9.2 Q-score mapped to coordinate model



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.

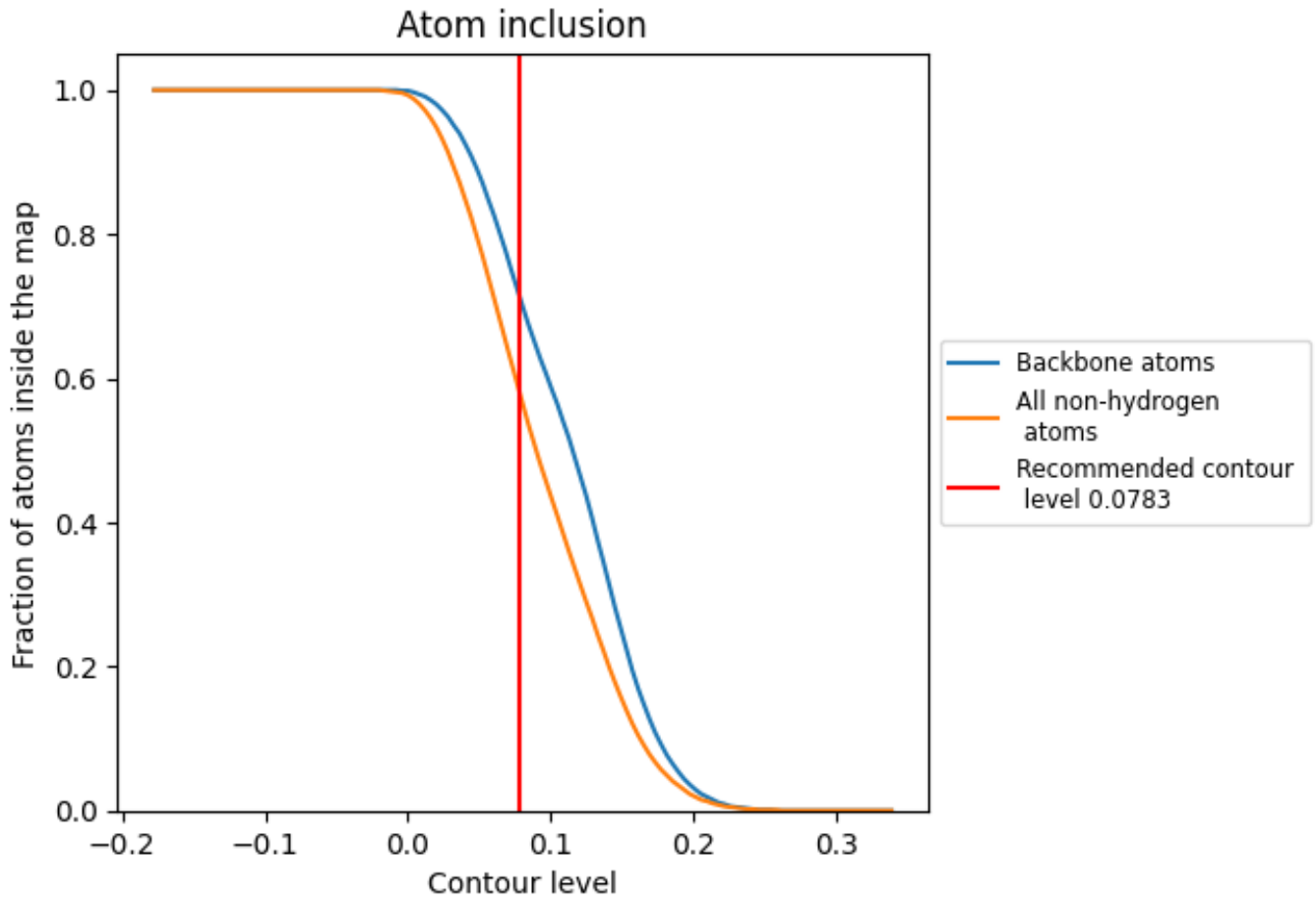
9.3 Atom inclusion mapped to coordinate model



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 (0.0783).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0783) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5810	0.4640
A	0.5490	0.4510
B	0.0270	0.2470
C	0.3410	0.4050
D	0.4730	0.4470
E	0.4310	0.3710
F	0.6540	0.5240
G	0.4860	0.4840
H	0.6230	0.4850
J	0.6690	0.5210
K	0.6410	0.4730
L	0.6080	0.4590
N	0.5500	0.4560
O	0.0150	0.2100
P	0.3710	0.4030
Q	0.4570	0.4190
R	0.5020	0.4050
S	0.6660	0.4810
T	0.3970	0.4610
U	0.6620	0.4890
V	0.7120	0.5160
W	0.6300	0.4750
Y	0.5910	0.4470