wwPDB EM Validation Summary Report (i)

Nov 9, 2023 – 01:42 pm GMT

PDB ID	:	8Q1B
EMDB ID	:	EMD-18062
Title	:	III2-IV1 respiratory supercomplex from S. pombe
Authors	:	Moe, A.; Brzezinski, P.
Deposited on	:	2023-07-31
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 (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:

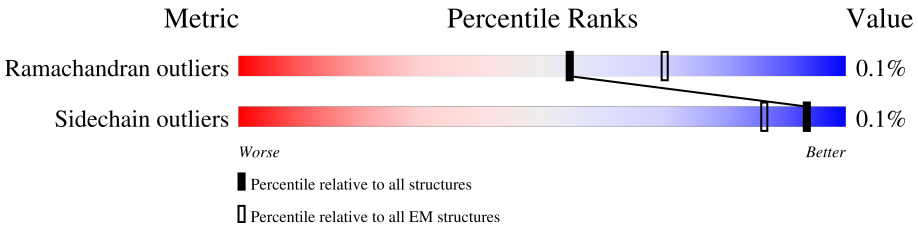
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	457	97% .
1	L	457	97% .
2	B	426	95% 5%
2	M	426	95% 5%
3	C	387	99% .
3	N	387	100%
4	D	307	80% 20%
4	O	307	80% 20%
5	E	228	. 80% 20%

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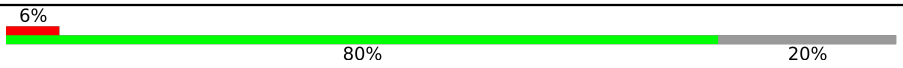
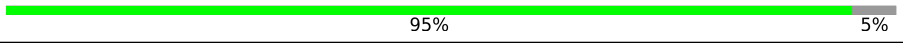
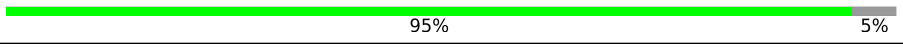
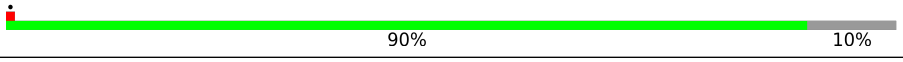
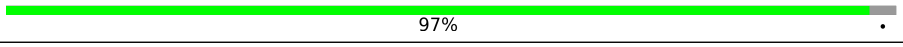
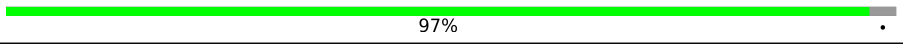
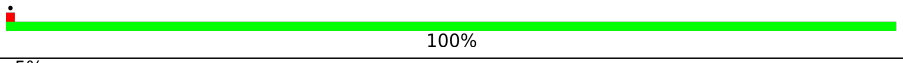
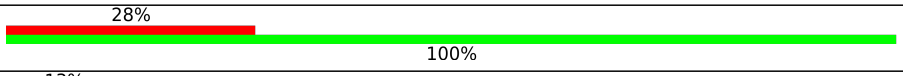
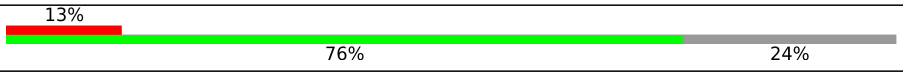
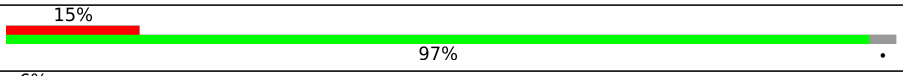
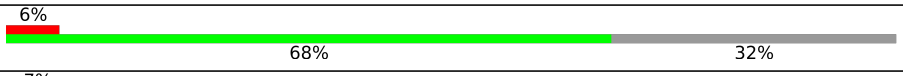
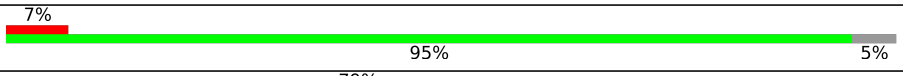
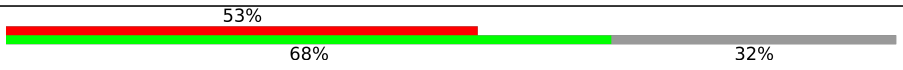
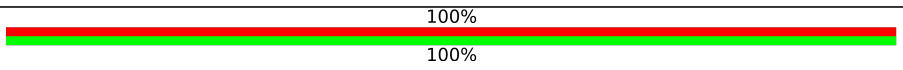
Mol	Chain	Length	Quality of chain
5	P	228	
6	F	214	
6	Q	214	
7	G	137	
7	R	137	
8	H	92	
8	S	92	
9	I	67	
9	T	67	
10	J	79	
10	U	79	
11	a	538	
12	b	248	
13	c	269	
14	d	159	
15	e	228	
16	f	140	
17	g	59	
18	h	66	
19	i	58	
20	j	86	
21	k	130	
22	l	242	
23	m	26	

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 48686 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 Probable mitochondrial-processing peptidase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	443	Total	C	N	O	S	0	0
			3449	2151	618	671	9		
1	L	443	Total	C	N	O	S	0	0
			3449	2151	618	671	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	406	Total	C	N	O	S	0	0
			3044	1943	500	596	5		
2	M	406	Total	C	N	O	S	0	0
			3043	1943	500	595	5		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	387	Total	C	N	O	S	0	0
			3101	2101	473	510	17		
3	N	387	Total	C	N	O	S	0	0
			3101	2101	473	510	17		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	245	Total	C	N	O	S	0	0
			1943	1241	336	357	9		
4	O	245	Total	C	N	O	S	0	0
			1943	1241	336	357	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	182	Total	C	N	O	S	0	0
			1384	871	240	264	9		
5	P	182	Total	C	N	O	S	0	0
			1384	871	240	264	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	66	Total	C	N	O	S	0	0
			536	334	90	104	8		
6	Q	66	Total	C	N	O	S	0	0
			536	334	90	104	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	122	Total	C	N	O	S	0	0
			1021	657	176	184	4		
7	R	122	Total	C	N	O	S	0	0
			1021	657	176	184	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	87	Total	C	N	O	S	0	0
			697	454	124	115	4		
8	S	87	Total	C	N	O	S	0	0
			698	455	124	115	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	60	Total	C	N	O	S	0	0
			497	328	82	86	1		
9	T	60	Total	C	N	O	S	0	0
			497	328	82	86	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	77	Total	C	N	O	S	0	0
			629	421	102	103	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	77	Total	C	N	O	S	0	0
			629	421	102	103	3		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	537	Total	C	N	O	S	0	0
			4212	2827	652	711	22		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	400	TYR	-	insertion	UNP P07657

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	238	Total	C	N	O	S	0	0
			1902	1242	297	354	9		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	268	Total	C	N	O	S	0	0
			2156	1452	332	365	7		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	121	Total	C	N	O	S	0	0
			922	573	160	182	7		

- Molecule 15 is a protein called Cytochrome c oxidase polypeptide 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	145	Total	C	N	O	S	0	0
			1146	728	202	212	4		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	187	GLU	-	expression tag	UNP O74988
e	188	ASN	-	expression tag	UNP O74988
e	189	LEU	-	expression tag	UNP O74988
e	190	TYR	-	expression tag	UNP O74988
e	191	PHE	-	expression tag	UNP O74988
e	192	GLN	-	expression tag	UNP O74988
e	193	GLY	-	expression tag	UNP O74988
e	194	GLY	-	expression tag	UNP O74988
e	195	GLY	-	expression tag	UNP O74988
e	196	GLY	-	expression tag	UNP O74988
e	197	GLY	-	expression tag	UNP O74988
e	198	GLY	-	expression tag	UNP O74988
e	199	SER	-	expression tag	UNP O74988
e	200	ALA	-	expression tag	UNP O74988
e	201	TRP	-	expression tag	UNP O74988
e	202	SER	-	expression tag	UNP O74988
e	203	HIS	-	expression tag	UNP O74988
e	204	PRO	-	expression tag	UNP O74988
e	205	GLN	-	expression tag	UNP O74988
e	206	PHE	-	expression tag	UNP O74988
e	207	GLU	-	expression tag	UNP O74988
e	208	LYS	-	expression tag	UNP O74988
e	209	GLY	-	expression tag	UNP O74988
e	210	GLY	-	expression tag	UNP O74988
e	211	GLY	-	expression tag	UNP O74988
e	212	SER	-	expression tag	UNP O74988
e	213	GLY	-	expression tag	UNP O74988
e	214	GLY	-	expression tag	UNP O74988
e	215	GLY	-	expression tag	UNP O74988
e	216	SER	-	expression tag	UNP O74988
e	217	GLY	-	expression tag	UNP O74988
e	218	GLY	-	expression tag	UNP O74988
e	219	SER	-	expression tag	UNP O74988
e	220	ALA	-	expression tag	UNP O74988
e	221	TRP	-	expression tag	UNP O74988
e	222	SER	-	expression tag	UNP O74988
e	223	HIS	-	expression tag	UNP O74988
e	224	PRO	-	expression tag	UNP O74988
e	225	GLN	-	expression tag	UNP O74988
e	226	PHE	-	expression tag	UNP O74988
e	227	GLU	-	expression tag	UNP O74988
e	228	LYS	-	expression tag	UNP O74988

- Molecule 16 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	100	Total	C	N	O	S	0	0
			813	520	137	154	2		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	57	Total	C	N	O	S	0	0
			457	301	78	77	1		

- Molecule 18 is a protein called Cytochrome c oxidase polypeptide VIII, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	h	45	Total	C	N	O	0	0
			363	249	57	57		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	55	Total	C	N	O	S	0	0
			445	292	77	73	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	75	Total	C	N	O	S	0	0
			636	411	107	113	5		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	88	Total	C	N	O	S	0	0
			741	480	124	136	1		

- Molecule 22 is a protein called Respiratory supercomplex factor 2 homolog C1565.01.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	l	69	Total	C	N	O	S	0	0
			550	356	95	97	2		

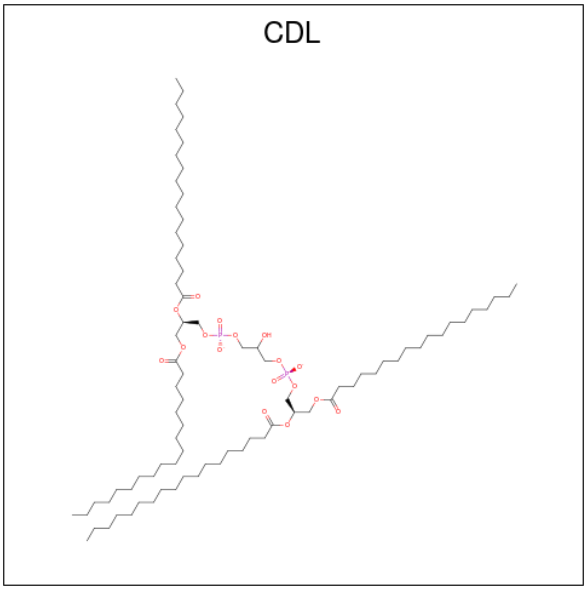
- Molecule 23 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	m	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

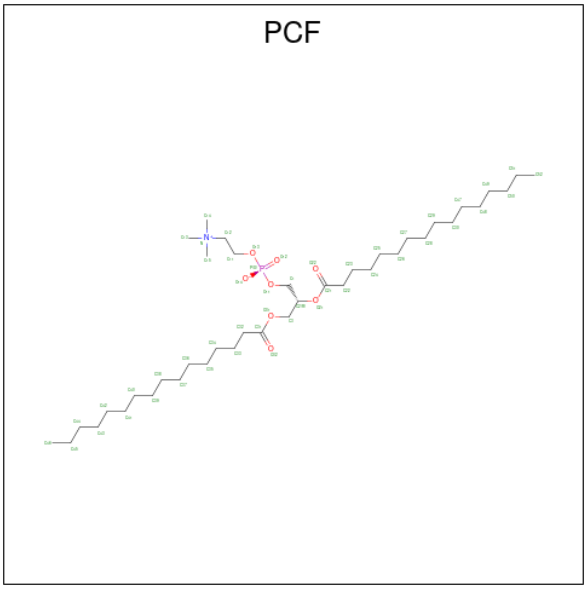
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Zn	0
			1	1	
24	L	1	Total	Zn	0
			1	1	
24	d	1	Total	Zn	0
			1	1	

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



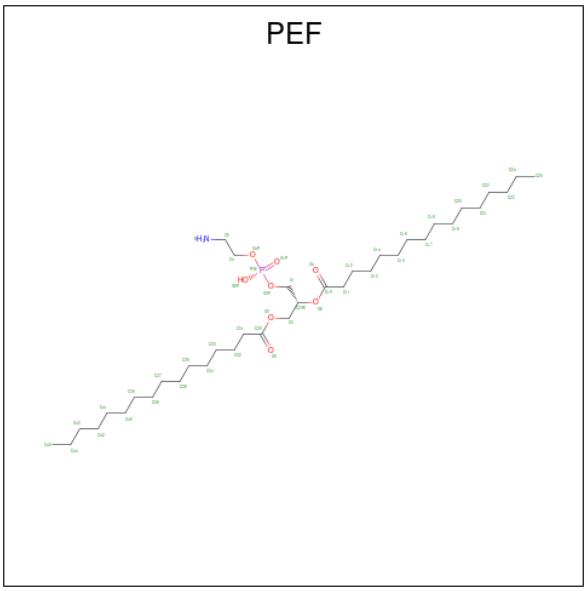
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			57	38	17	2	
25	H	1	Total	C	O	P	0
			79	60	17	2	
25	H	1	Total	C	O	P	0
			78	59	17	2	
25	L	1	Total	C	O	P	0
			57	38	17	2	
25	S	1	Total	C	O	P	0
			77	58	17	2	
25	S	1	Total	C	O	P	0
			73	54	17	2	

- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF) (formula: $C_{40}H_{80}NO_8P$).



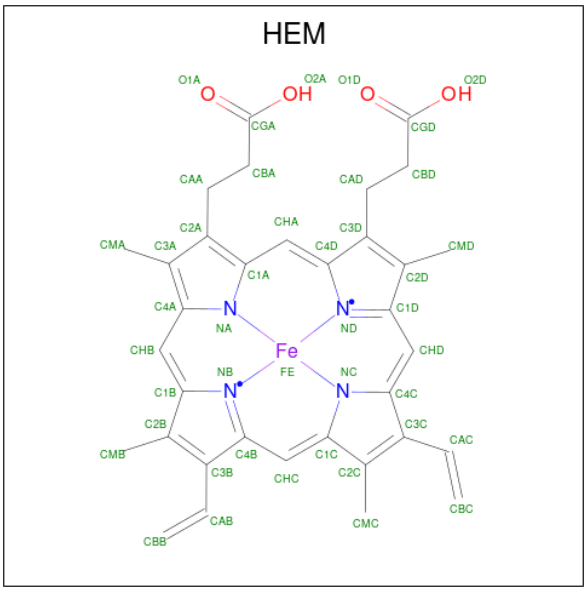
Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
26	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
26	L	1	Total	C	N	O	P	0
			50	40	1	8	1	
26	T	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 27 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



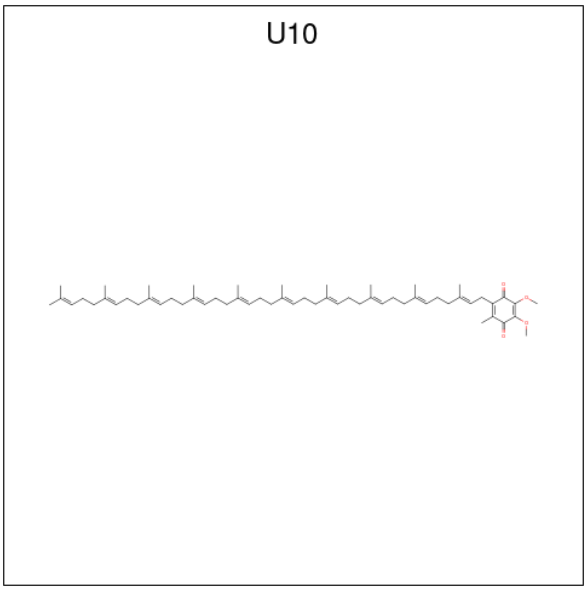
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	D	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	J	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	N	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	N	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	O	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	a	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	c	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	k	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



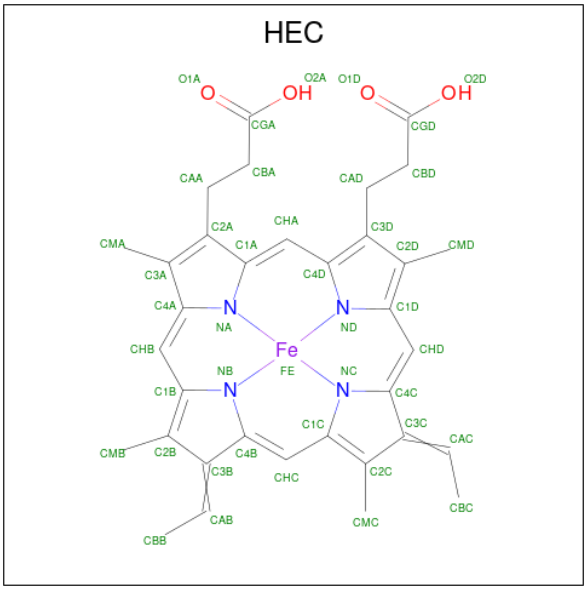
Mol	Chain	Residues	Atoms					AltConf
28	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
28	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
28	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
28	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 29 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



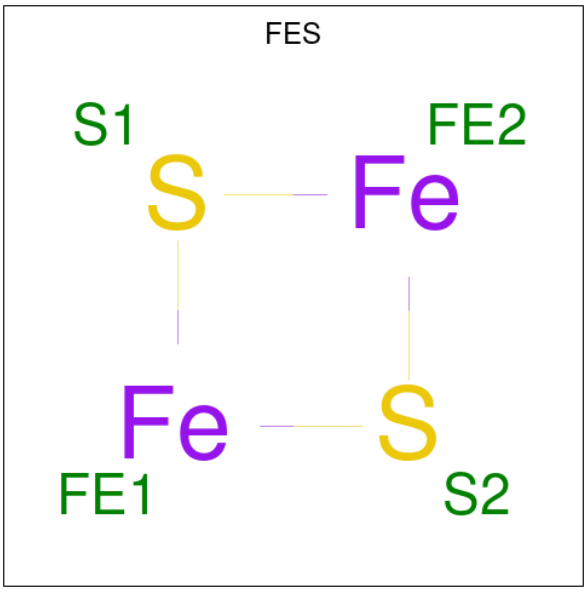
Mol	Chain	Residues	Atoms	AltConf
29	C	1	Total C O 63 59 4	0
29	N	1	Total C O 63 59 4	0

- Molecule 30 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



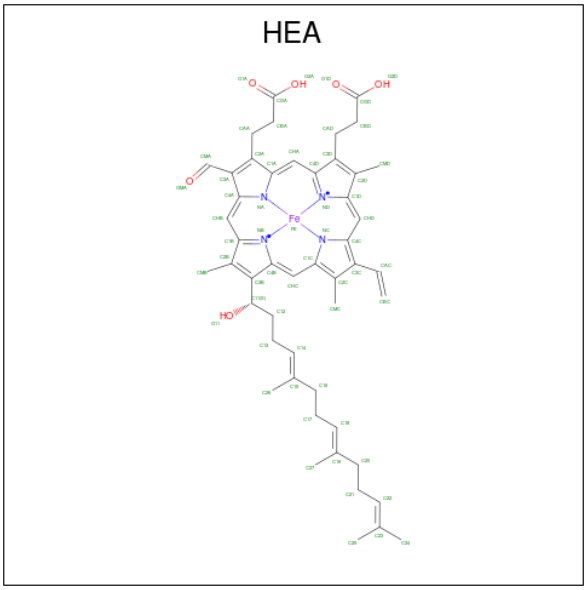
Mol	Chain	Residues	Atoms	AltConf
30	D	1	Total C Fe N O 43 34 1 4 4	0
30	O	1	Total C Fe N O 43 34 1 4 4	0

- Molecule 31 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
31	E	1	Total	Fe	S	0
			4	2	2	
31	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 32 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 33 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
33	a	1	Total Cu 1 1	0

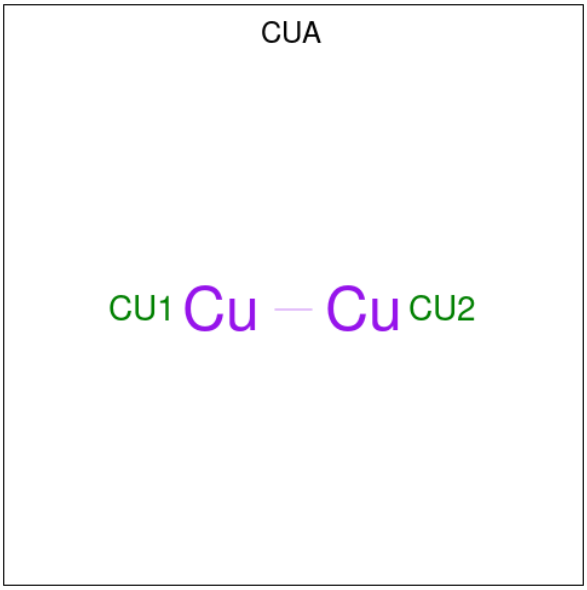
- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
34	a	1	Total Ca 1 1	0

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
35	b	1	Total Mg 1 1	0

- Molecule 36 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



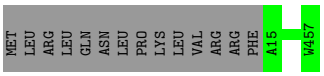
Mol	Chain	Residues	Atoms	AltConf
36	b	1	Total Cu 2 2	0

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.

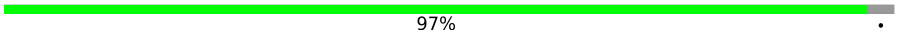
- Molecule 1: Probable mitochondrial-processing peptidase subunit beta

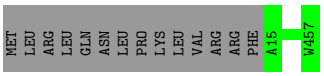
Chain A:



- Molecule 1: Probable mitochondrial-processing peptidase subunit beta

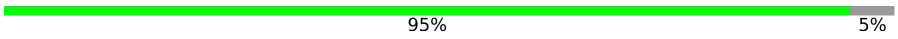
Chain L:

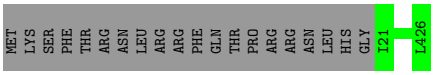




- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

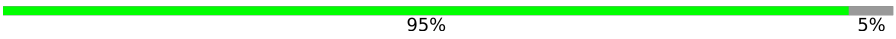
Chain B:

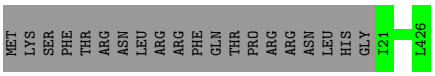




- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

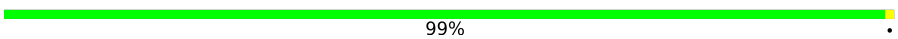
Chain M:





- Molecule 3: Cytochrome b

Chain C:



- Molecule 3: Cytochrome b

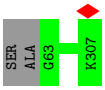
Chain N:

• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:

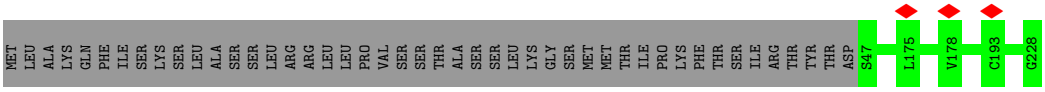
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:



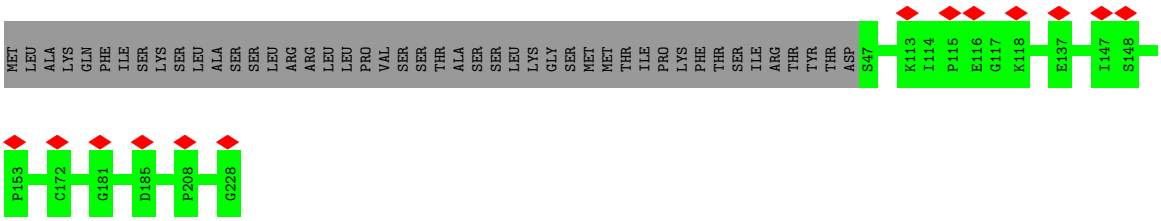
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



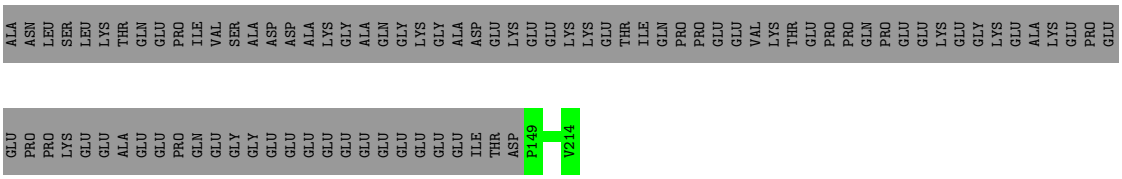
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



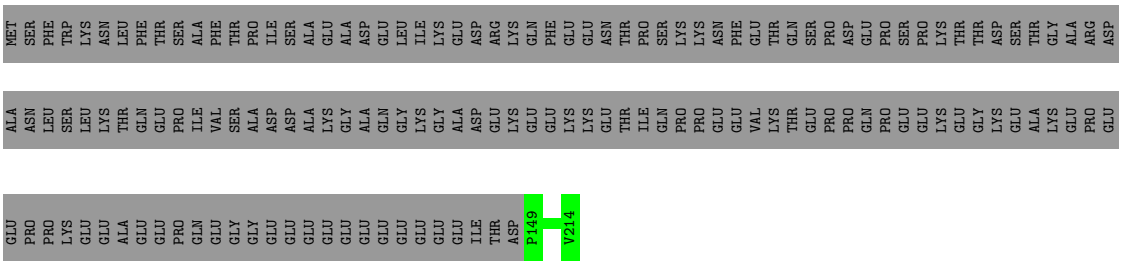
• Molecule 6: Cytochrome b-c1 complex subunit 6

Chain F:



• Molecule 6: Cytochrome b-c1 complex subunit 6

Chain Q:



• Molecule 7: Cytochrome b-c1 complex subunit 7

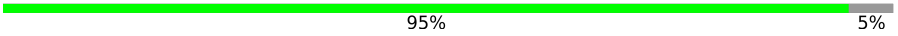
Chain G:

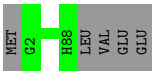
• Molecule 7: Cytochrome b-c1 complex subunit 7

Chain R:

• Molecule 8: Cytochrome b-c1 complex subunit 8

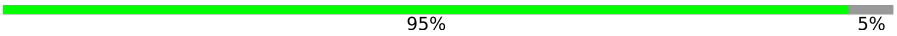
Chain H:

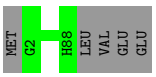




• Molecule 8: Cytochrome b-c1 complex subunit 8

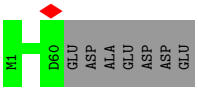
Chain S:





• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain I:

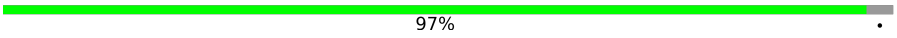


• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain T:

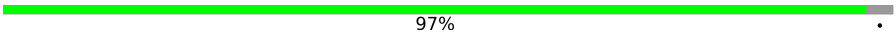
• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain J:



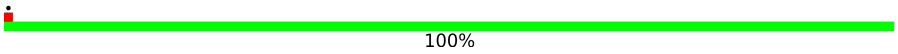
• Molecule 10: Cytochrome b-c1 complex subunit 10

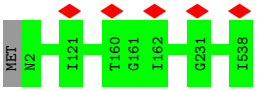
Chain U:



• Molecule 11: Cytochrome c oxidase subunit 1

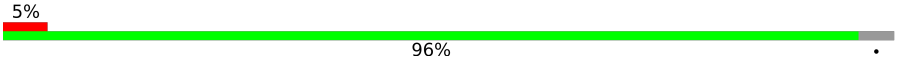
Chain a:

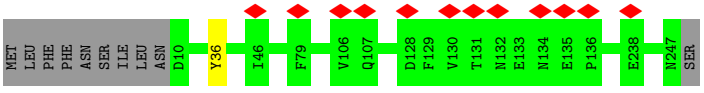




• Molecule 12: Cytochrome c oxidase subunit 2

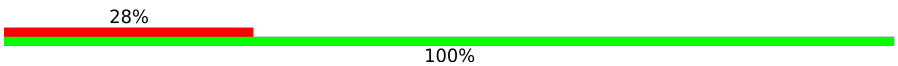
Chain b:

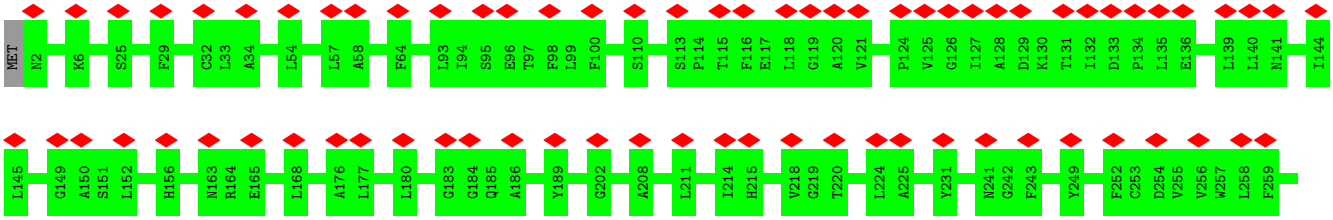


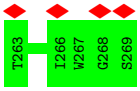


• Molecule 13: Cytochrome c oxidase subunit 3

Chain c:

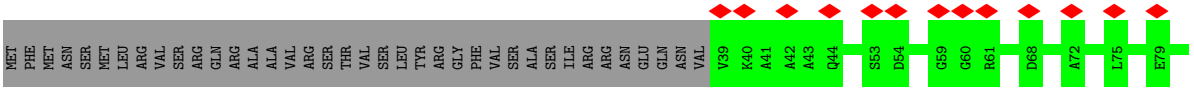


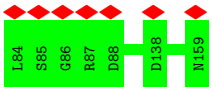




• Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial

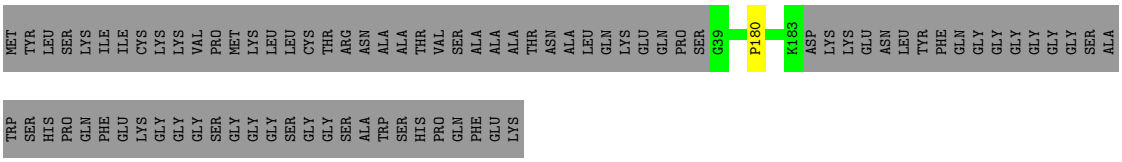
Chain d:





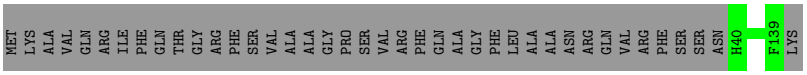
• Molecule 15: Cytochrome c oxidase polypeptide 5, mitochondrial

Chain e:



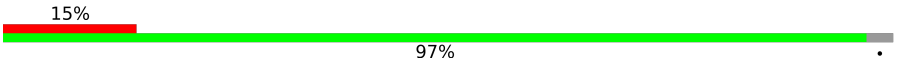
• Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

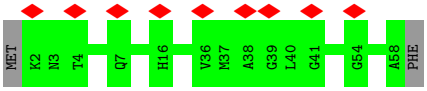
Chain f:



• Molecule 17: Cytochrome c oxidase subunit 7

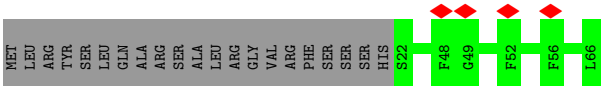
Chain g:





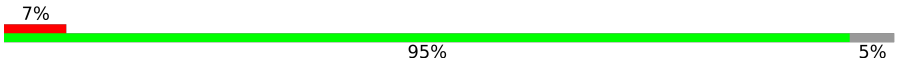
• Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

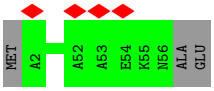
Chain h:



• Molecule 19: Cytochrome c oxidase subunit 9, mitochondrial

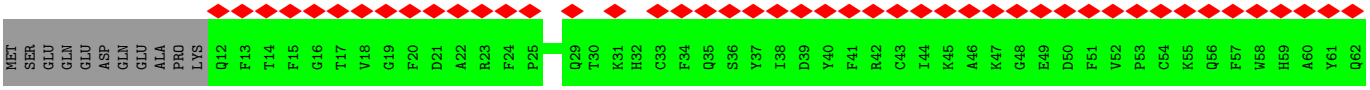
Chain i:

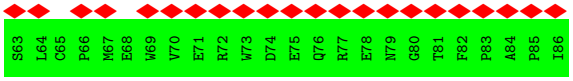




• Molecule 20: Cytochrome c oxidase subunit 12, mitochondrial

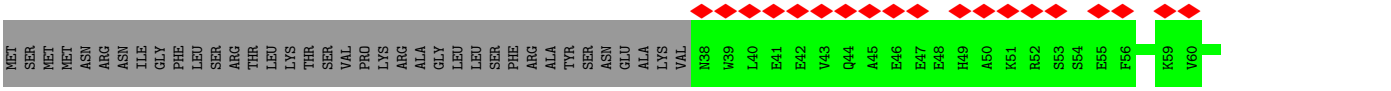
Chain j:

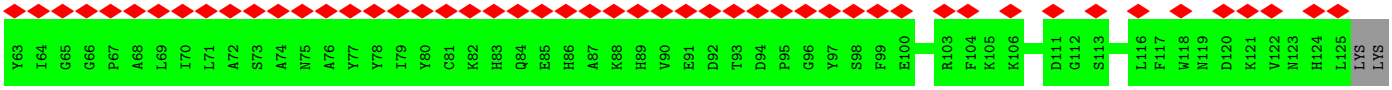




• Molecule 21: Cytochrome c oxidase subunit 13, mitochondrial

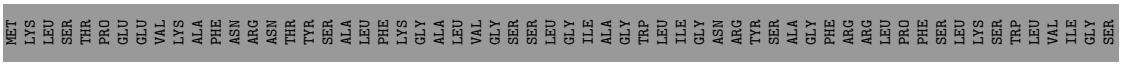
Chain k:

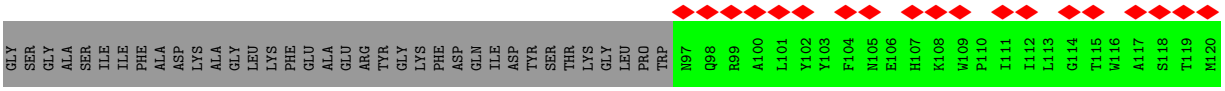


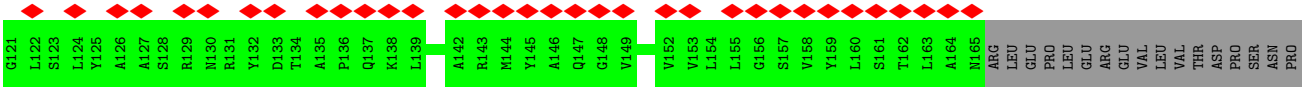


• Molecule 22: Respiratory supercomplex factor 2 homolog C1565.01

Chain l:

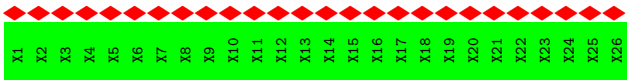






• Molecule 23: Unknown polypeptide

Chain m:


X1
X2
X3
X4
X5
X6
X7
X8
X9
X10
X11
X12
X13
X14
X15
X16
X17
X18
X19
X20
X21
X22
X23
X24
X25
X26

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125752	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 ($e^-/Å^2$)	41.0	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.727	Depositor
Minimum map value	-0.342	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	433.3568, 433.3568, 433.3568	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8464, 0.8464, 0.8464	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CUA, PEF, FES, PCF, CDL, U10, ZN, MG, HEM, CU, HEC, CA, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.23	0/3510	0.49	0/4759
1	L	0.24	0/3510	0.49	0/4759
2	B	0.25	0/3104	0.44	0/4212
2	M	0.25	0/3103	0.44	0/4212
3	C	0.27	0/3204	0.43	0/4378
3	N	0.26	0/3204	0.43	0/4378
4	D	0.25	0/2002	0.46	0/2721
4	O	0.25	0/2002	0.46	0/2721
5	E	0.28	0/1418	0.53	0/1925
5	P	0.25	0/1418	0.49	0/1925
6	F	0.30	0/547	0.51	0/731
6	Q	0.32	0/547	0.50	0/731
7	G	0.28	0/1042	0.49	0/1402
7	R	0.26	0/1042	0.48	0/1402
8	H	0.26	0/719	0.47	0/963
8	S	0.25	0/722	0.48	0/971
9	I	0.26	0/512	0.47	0/691
9	T	0.30	0/512	0.46	0/691
10	J	0.27	0/653	0.52	0/888
10	U	0.25	0/653	0.45	0/888
11	a	0.27	0/4353	0.47	0/5950
12	b	0.26	0/1953	0.49	0/2668
13	c	0.25	0/2237	0.43	0/3057
14	d	0.26	0/940	0.56	0/1270
15	e	0.49	1/1173 (0.1%)	0.51	0/1580
16	f	0.28	0/828	0.49	0/1119
17	g	0.24	0/469	0.45	0/633
18	h	0.28	0/377	0.52	0/514
19	i	0.26	0/458	0.47	0/618
20	j	0.26	0/660	0.44	0/893
21	k	0.23	0/767	0.40	0/1039
22	l	0.24	0/563	0.51	0/767

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.27	1/48202 (0.0%)	0.47	0/65456

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	e	180	PRO	N-CD	14.46	1.68	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	112	ARG	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/457 (96%)	424 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	441/457 (96%)	425 (96%)	16 (4%)	0	100	100
2	B	404/426 (95%)	393 (97%)	11 (3%)	0	100	100
2	M	404/426 (95%)	386 (96%)	18 (4%)	0	100	100
3	C	385/387 (100%)	367 (95%)	18 (5%)	0	100	100
3	N	385/387 (100%)	370 (96%)	15 (4%)	0	100	100
4	D	243/307 (79%)	232 (96%)	11 (4%)	0	100	100
4	O	243/307 (79%)	231 (95%)	12 (5%)	0	100	100
5	E	180/228 (79%)	172 (96%)	8 (4%)	0	100	100
5	P	180/228 (79%)	172 (96%)	8 (4%)	0	100	100
6	F	64/214 (30%)	63 (98%)	1 (2%)	0	100	100
6	Q	64/214 (30%)	60 (94%)	4 (6%)	0	100	100
7	G	120/137 (88%)	115 (96%)	3 (2%)	2 (2%)	9	34
7	R	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
8	H	84/92 (91%)	79 (94%)	5 (6%)	0	100	100
8	S	85/92 (92%)	79 (93%)	6 (7%)	0	100	100
9	I	58/67 (87%)	54 (93%)	4 (7%)	0	100	100
9	T	58/67 (87%)	55 (95%)	2 (3%)	1 (2%)	9	34
10	J	75/79 (95%)	67 (89%)	8 (11%)	0	100	100
10	U	75/79 (95%)	66 (88%)	9 (12%)	0	100	100
11	a	535/538 (99%)	514 (96%)	21 (4%)	0	100	100
12	b	236/248 (95%)	221 (94%)	15 (6%)	0	100	100
13	c	266/269 (99%)	257 (97%)	9 (3%)	0	100	100
14	d	119/159 (75%)	114 (96%)	5 (4%)	0	100	100
15	e	143/228 (63%)	131 (92%)	12 (8%)	0	100	100
16	f	98/140 (70%)	91 (93%)	7 (7%)	0	100	100
17	g	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
18	h	43/66 (65%)	37 (86%)	6 (14%)	0	100	100
19	i	53/58 (91%)	53 (100%)	0	0	100	100
20	j	73/86 (85%)	69 (94%)	4 (6%)	0	100	100
21	k	86/130 (66%)	81 (94%)	5 (6%)	0	100	100
22	l	67/242 (28%)	64 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5883/7011 (84%)	5614 (95%)	266 (4%)	3 (0%)	54 82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	114	ALA
7	G	113	GLU
9	T	9	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	368/382 (96%)	368 (100%)	0	100 100
1	L	368/382 (96%)	368 (100%)	0	100 100
2	B	333/352 (95%)	333 (100%)	0	100 100
2	M	333/352 (95%)	333 (100%)	0	100 100
3	C	335/335 (100%)	333 (99%)	2 (1%)	86 94
3	N	335/335 (100%)	335 (100%)	0	100 100
4	D	206/258 (80%)	206 (100%)	0	100 100
4	O	206/258 (80%)	206 (100%)	0	100 100
5	E	148/190 (78%)	148 (100%)	0	100 100
5	P	148/190 (78%)	148 (100%)	0	100 100
6	F	61/191 (32%)	61 (100%)	0	100 100
6	Q	61/191 (32%)	61 (100%)	0	100 100
7	G	112/123 (91%)	112 (100%)	0	100 100
7	R	112/123 (91%)	112 (100%)	0	100 100
8	H	67/73 (92%)	67 (100%)	0	100 100
8	S	68/73 (93%)	68 (100%)	0	100 100
9	I	52/58 (90%)	52 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	T	52/58 (90%)	52 (100%)	0	100	100
10	J	68/70 (97%)	68 (100%)	0	100	100
10	U	68/70 (97%)	68 (100%)	0	100	100
11	a	452/453 (100%)	452 (100%)	0	100	100
12	b	213/223 (96%)	212 (100%)	1 (0%)	88	94
13	c	226/227 (100%)	226 (100%)	0	100	100
14	d	101/135 (75%)	101 (100%)	0	100	100
15	e	119/180 (66%)	119 (100%)	0	100	100
16	f	90/121 (74%)	90 (100%)	0	100	100
17	g	47/49 (96%)	47 (100%)	0	100	100
18	h	41/59 (70%)	41 (100%)	0	100	100
19	i	44/46 (96%)	44 (100%)	0	100	100
20	j	67/77 (87%)	67 (100%)	0	100	100
21	k	76/113 (67%)	76 (100%)	0	100	100
22	l	57/203 (28%)	57 (100%)	0	100	100
All	All	5034/5950 (85%)	5031 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	132	TYR
3	C	184	TYR
12	b	36	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	256	HIS
7	G	11	GLN
13	c	185	GLN
5	P	174	HIS
4	D	213	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 6 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
36	CUA	b	303	12	0,1,1	-	-	-		
25	CDL	L	502	-	56,56,99	0.39	0	62,68,111	0.26	0
27	PEF	A	504	-	46,46,46	0.90	4 (8%)	49,51,51	1.13	2 (4%)
27	PEF	c	301	-	46,46,46	0.90	4 (8%)	49,51,51	1.06	2 (4%)
28	HEM	C	401	3	41,50,50	1.45	3 (7%)	45,82,82	1.37	6 (13%)
32	HEA	a	602	11	57,67,67	1.31	5 (8%)	61,103,103	1.52	13 (21%)
27	PEF	k	201	-	46,46,46	0.91	3 (6%)	49,51,51	1.09	2 (4%)
28	HEM	C	402	3	41,50,50	1.44	4 (9%)	45,82,82	1.38	6 (13%)
28	HEM	N	401	3	41,50,50	1.44	3 (7%)	45,82,82	1.36	7 (15%)
27	PEF	a	605	-	46,46,46	0.91	4 (8%)	49,51,51	1.09	2 (4%)
32	HEA	a	601	11	57,67,67	1.29	5 (8%)	61,103,103	1.53	11 (18%)
27	PEF	D	402	-	46,46,46	0.90	4 (8%)	49,51,51	1.05	2 (4%)
27	PEF	N	405	-	46,46,46	0.91	4 (8%)	49,51,51	1.12	2 (4%)
25	CDL	A	502	-	56,56,99	0.39	0	62,68,111	0.26	0
25	CDL	H	101	-	78,78,99	0.33	0	84,90,111	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	FES	E	301	5	0,4,4	-	-	-		
27	PEF	O	402	-	46,46,46	0.89	4 (8%)	49,51,51	1.12	2 (4%)
28	HEM	N	402	3	41,50,50	1.45	3 (7%)	45,82,82	1.44	7 (15%)
29	U10	N	403	-	63,63,63	2.70	17 (26%)	76,79,79	1.75	22 (28%)
30	HEC	O	401	4	32,50,50	2.16	3 (9%)	24,82,82	1.50	3 (12%)
27	PEF	N	404	-	46,46,46	0.89	4 (8%)	49,51,51	1.13	2 (4%)
29	U10	C	403	-	63,63,63	2.71	17 (26%)	76,79,79	1.71	20 (26%)
30	HEC	D	401	4	32,50,50	2.20	3 (9%)	24,82,82	1.41	4 (16%)
27	PEF	b	302	-	46,46,46	0.90	4 (8%)	49,51,51	1.07	2 (4%)
25	CDL	S	102	-	72,72,99	0.35	0	78,84,111	0.22	0
27	PEF	J	101	-	46,46,46	0.91	4 (8%)	49,51,51	1.12	2 (4%)
26	PCF	A	503	1	49,49,49	1.11	3 (6%)	55,57,57	1.01	2 (3%)
26	PCF	L	503	-	49,49,49	1.10	3 (6%)	55,57,57	1.07	2 (3%)
26	PCF	A	505	-	49,49,49	1.10	4 (8%)	55,57,57	1.08	2 (3%)
31	FES	P	301	5	0,4,4	-	-	-		
25	CDL	H	102	-	77,77,99	0.34	0	83,89,111	0.22	0
26	PCF	T	101	-	49,49,49	1.10	4 (8%)	55,57,57	1.05	2 (3%)
25	CDL	S	101	-	76,76,99	0.34	0	82,88,111	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CDL	L	502	-	-	42/67/67/110	-
27	PEF	A	504	-	-	17/50/50/50	-
27	PEF	c	301	-	-	16/50/50/50	-
28	HEM	C	401	3	-	1/12/54/54	-
32	HEA	a	602	11	-	7/32/76/76	-
27	PEF	k	201	-	-	22/50/50/50	-
28	HEM	C	402	3	-	1/12/54/54	-
28	HEM	N	401	3	-	3/12/54/54	-
27	PEF	a	605	-	-	24/50/50/50	-
32	HEA	a	601	11	-	5/32/76/76	-
27	PEF	D	402	-	-	25/50/50/50	-
27	PEF	N	405	-	-	16/50/50/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CDL	A	502	-	-	43/67/67/110	-
25	CDL	H	101	-	-	58/89/89/110	-
31	FES	E	301	5	-	-	0/1/1/1
27	PEF	O	402	-	-	19/50/50/50	-
28	HEM	N	402	3	-	3/12/54/54	-
29	U10	N	403	-	-	27/63/87/87	0/1/1/1
30	HEC	O	401	4	-	0/10/54/54	-
27	PEF	N	404	-	-	20/50/50/50	-
29	U10	C	403	-	-	26/63/87/87	0/1/1/1
30	HEC	D	401	4	-	0/10/54/54	-
27	PEF	b	302	-	-	21/50/50/50	-
25	CDL	S	102	-	-	46/83/83/110	-
27	PEF	J	101	-	-	22/50/50/50	-
26	PCF	A	503	1	-	18/53/53/53	-
26	PCF	L	503	-	-	18/53/53/53	-
26	PCF	A	505	-	-	17/53/53/53	-
31	FES	P	301	5	-	-	0/1/1/1
25	CDL	H	102	-	-	55/88/88/110	-
26	PCF	T	101	-	-	15/53/53/53	-
25	CDL	S	101	-	-	59/87/87/110	-

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	401	HEC	C2B-C3B	-6.54	1.33	1.40
30	D	401	HEC	C3C-C2C	-6.19	1.34	1.40
30	O	401	HEC	C3C-C2C	-6.16	1.34	1.40
30	O	401	HEC	C2B-C3B	-6.16	1.34	1.40
29	N	403	U10	C13-C14	6.12	1.47	1.33

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	L	503	PCF	O21-C21-C22	4.20	120.55	111.50
29	N	403	U10	C7-C8-C9	-4.17	119.85	126.79
27	N	404	PEF	O2-C10-C11	4.10	120.33	111.50
32	a	601	HEA	CBA-CAA-C2A	4.07	119.47	112.60
26	A	505	PCF	O21-C21-C22	4.00	120.12	111.50

There are no chirality outliers.

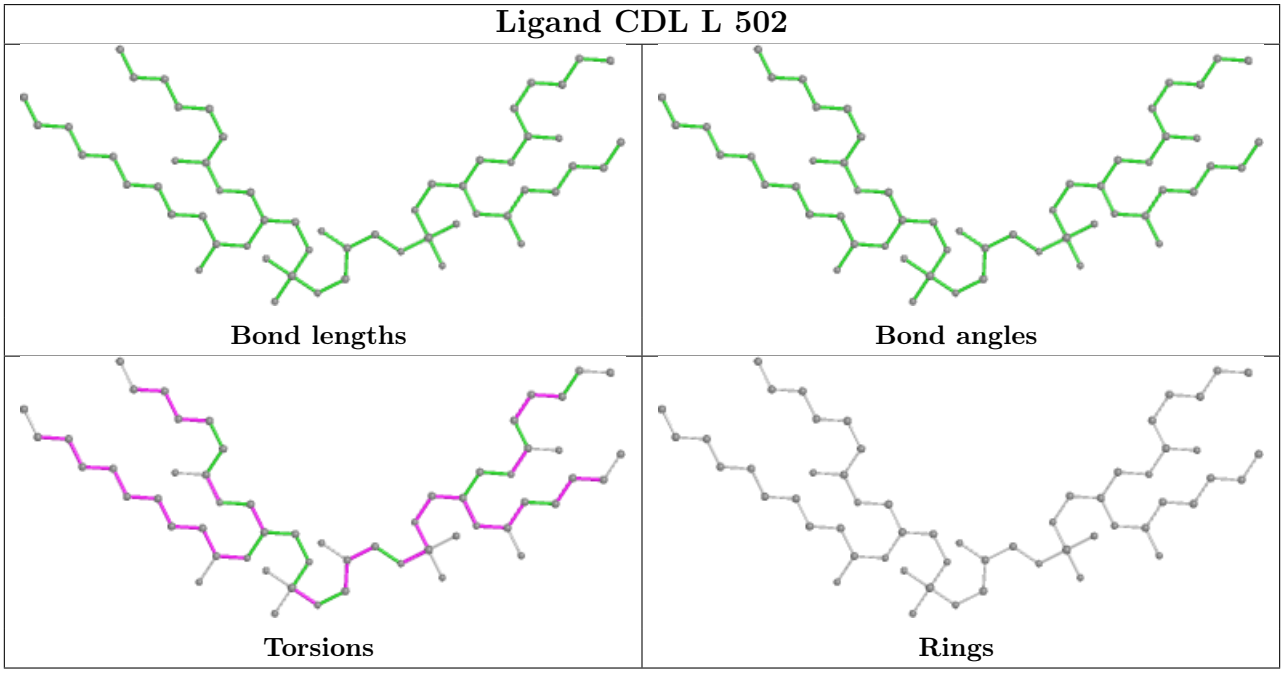
5 of 646 torsion outliers are listed below:

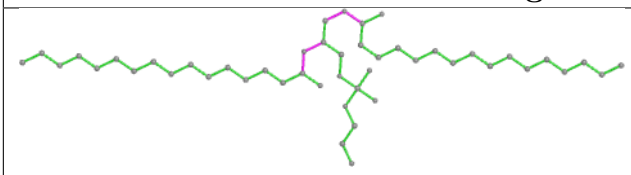
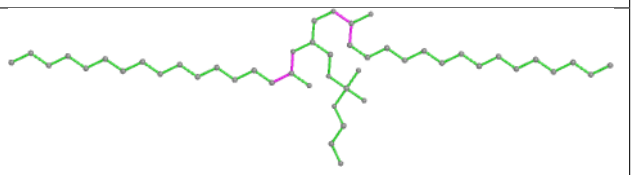
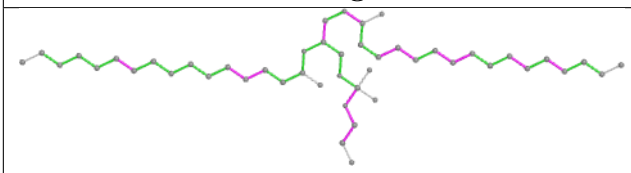
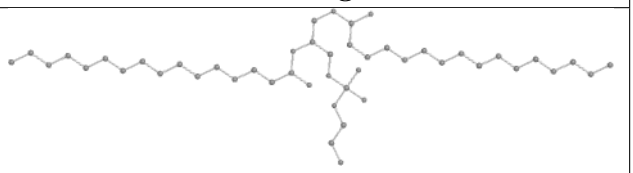
Mol	Chain	Res	Type	Atoms
25	A	502	CDL	CA2-OA2-PA1-OA3
25	A	502	CDL	CA2-OA2-PA1-OA4
25	A	502	CDL	CA2-OA2-PA1-OA5
25	A	502	CDL	CB2-OB2-PB2-OB3
25	H	101	CDL	O1-C1-CB2-OB2

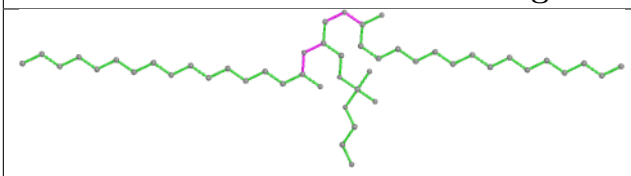
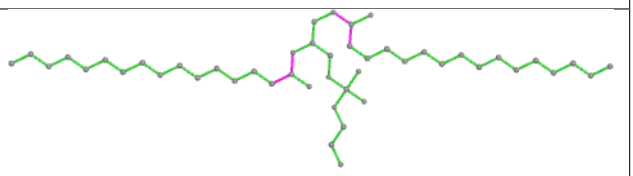
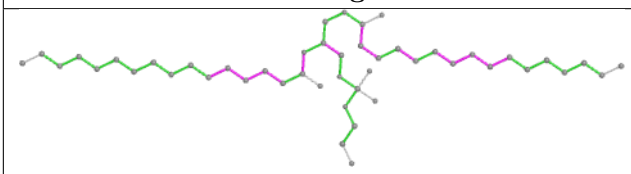
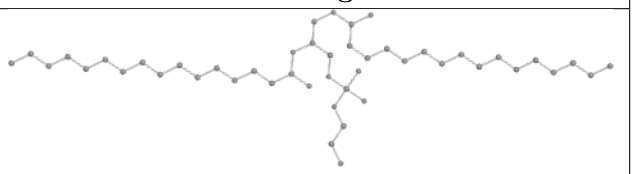
There are no ring outliers.

No monomer is involved in short contacts.

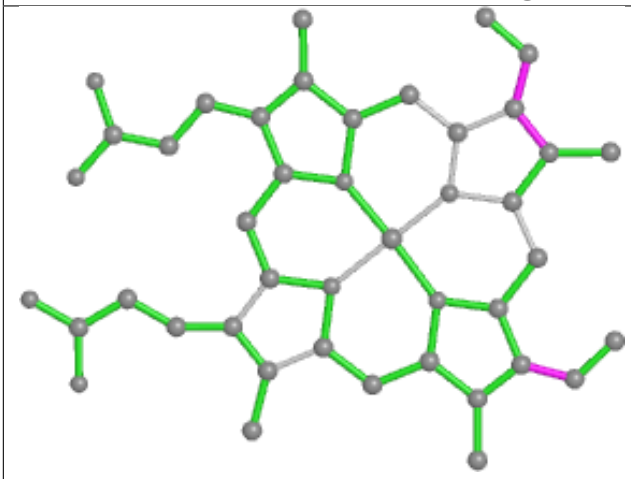
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



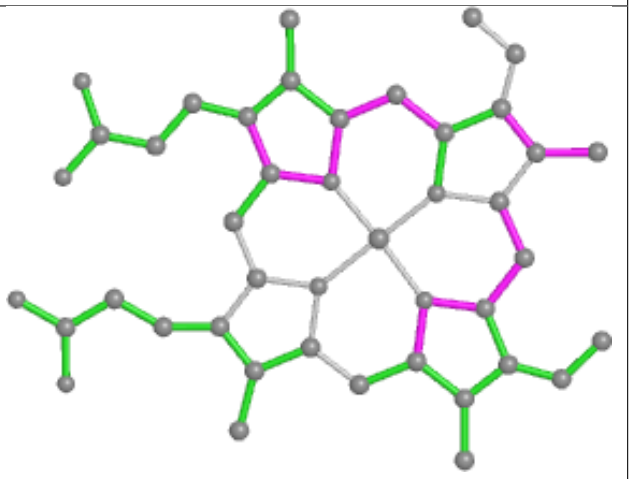
Ligand PEF A 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEF c 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

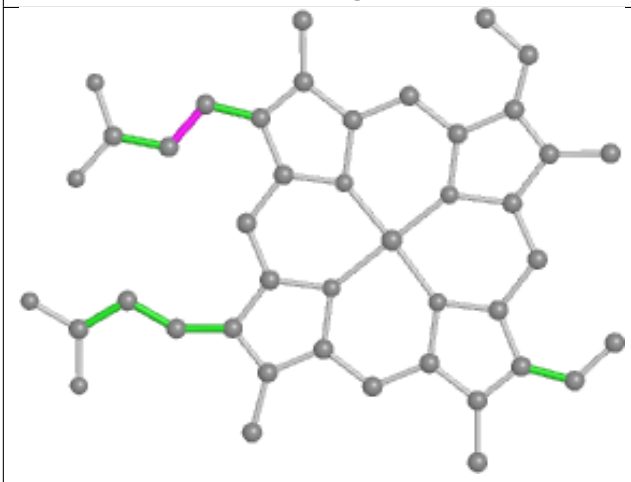
Ligand HEM C 401



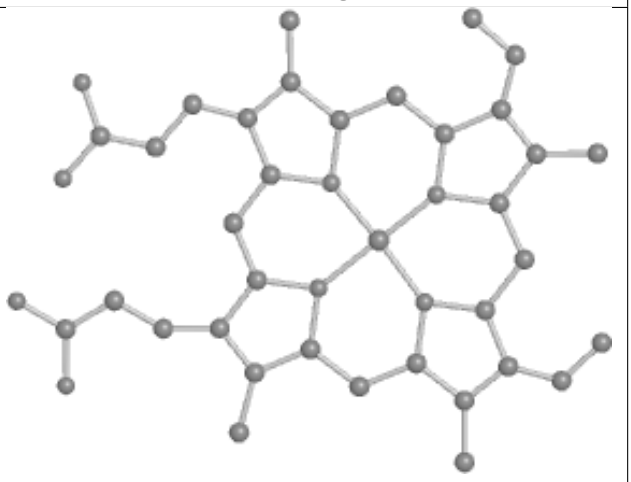
Bond lengths



Bond angles

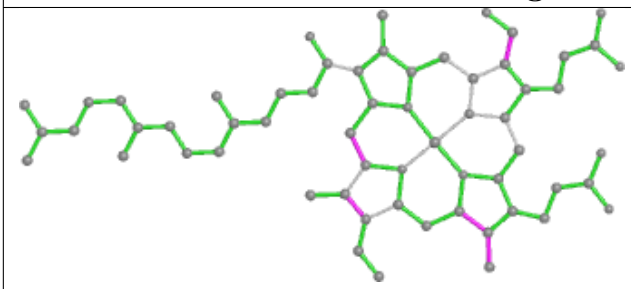


Torsions

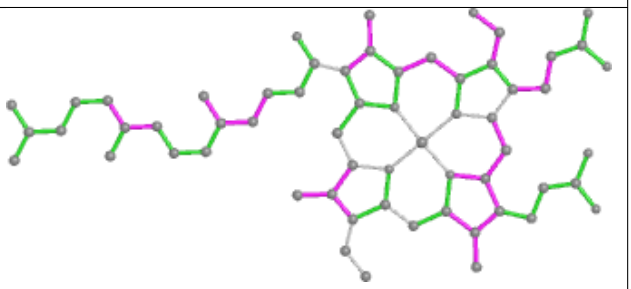


Rings

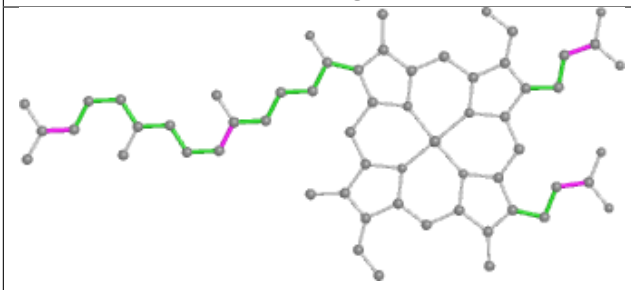
Ligand HEA a 602



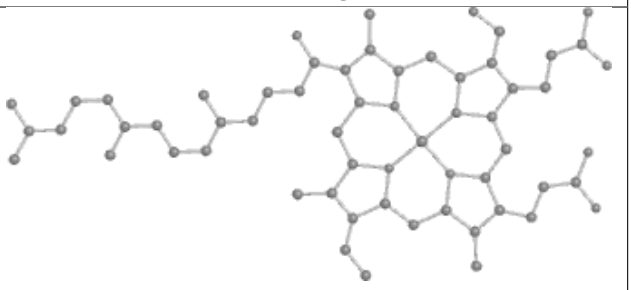
Bond lengths



Bond angles

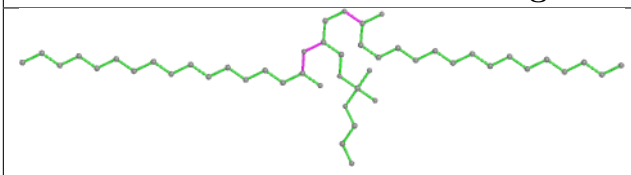


Torsions

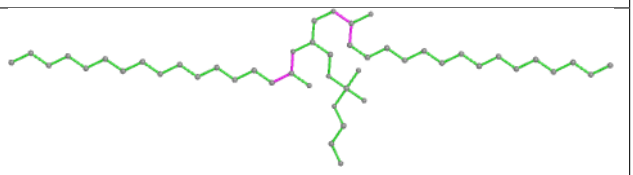


Rings

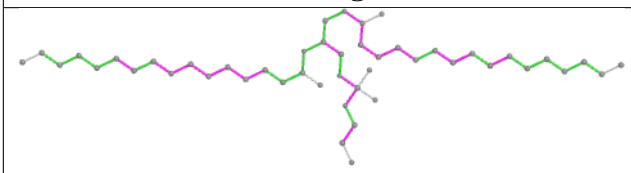
Ligand PEF k 201



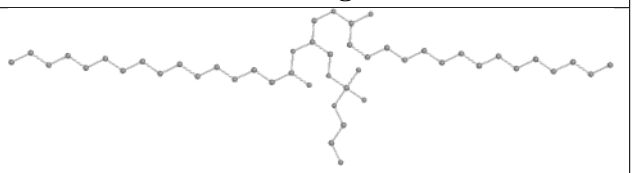
Bond lengths



Bond angles

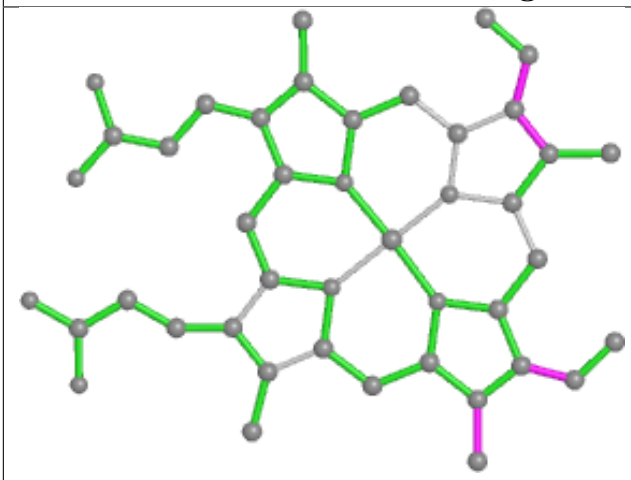


Torsions



Rings

Ligand HEM C 402



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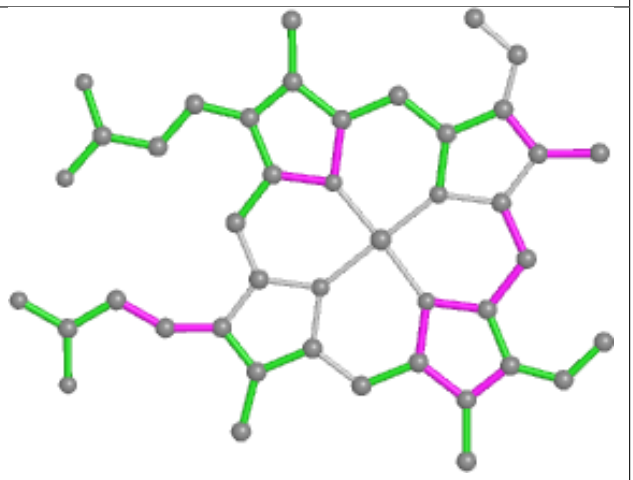
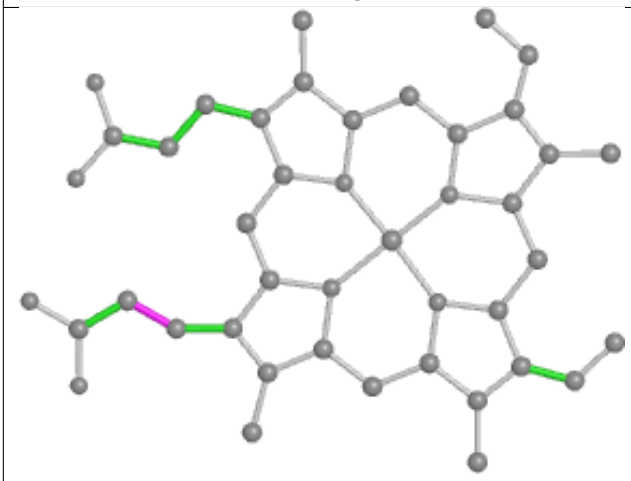
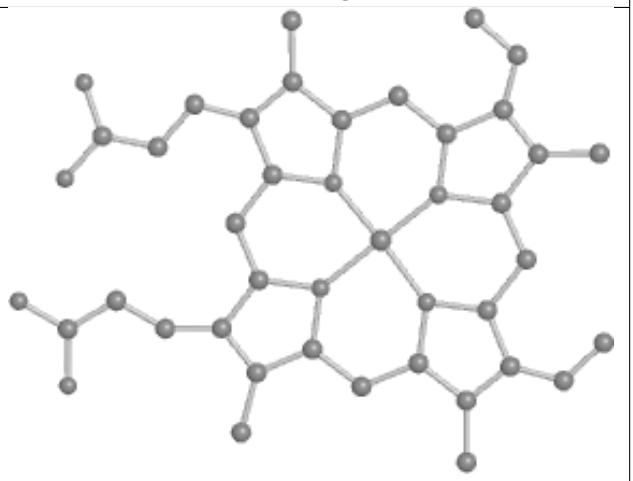


Bond angles

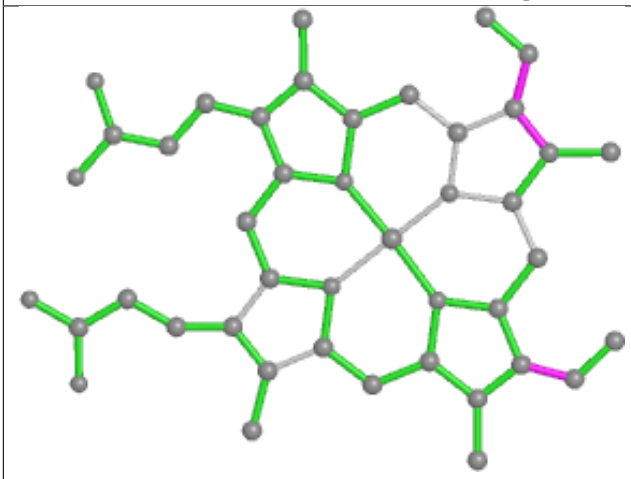


Torsions

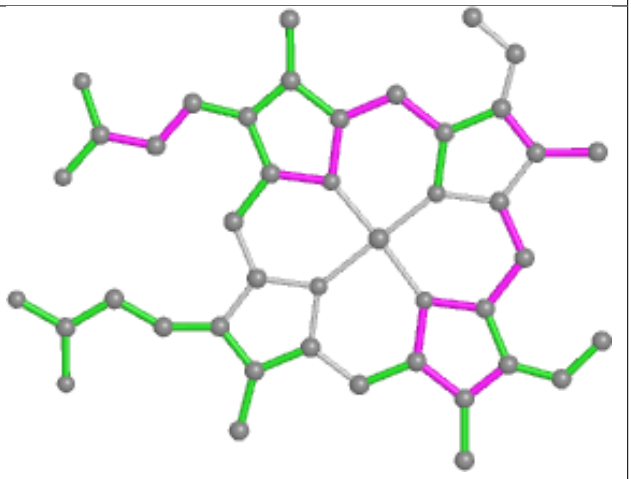


Rings

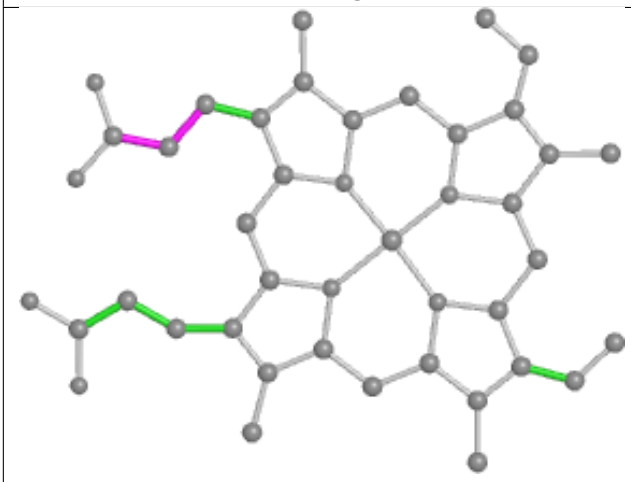
Ligand HEM N 401



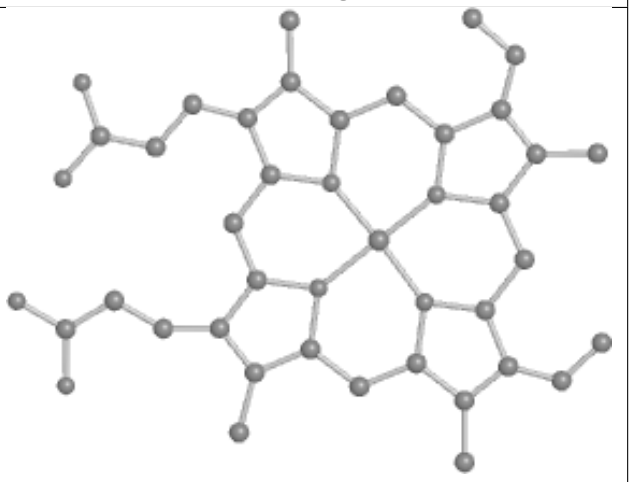
Bond lengths



Bond angles

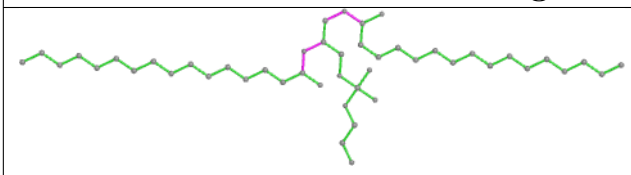


Torsions

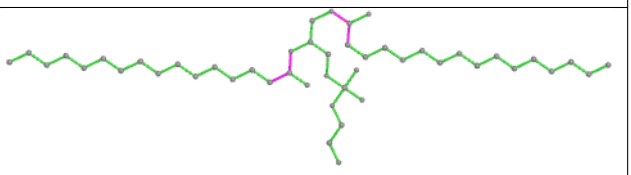


Rings

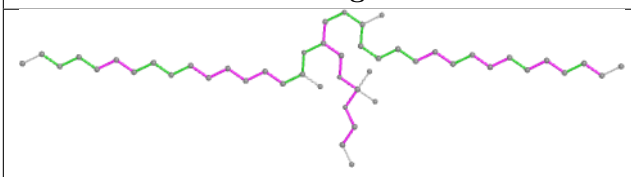
Ligand PEF a 605



Bond lengths



Bond angles



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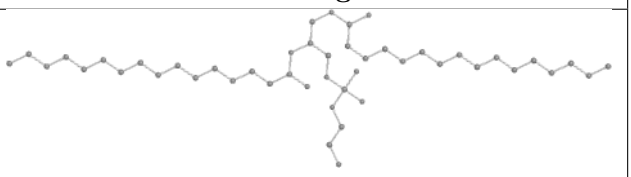
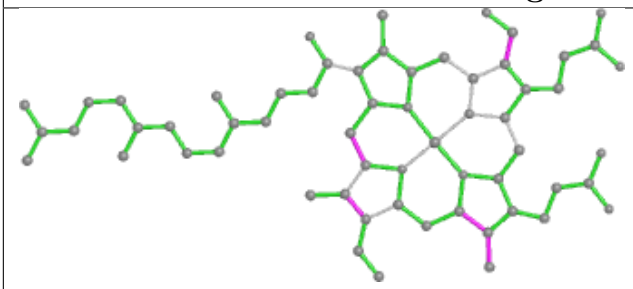
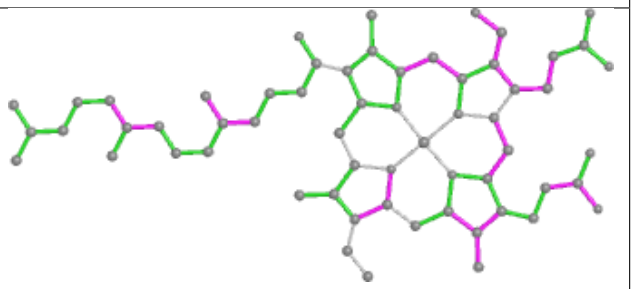


Rings

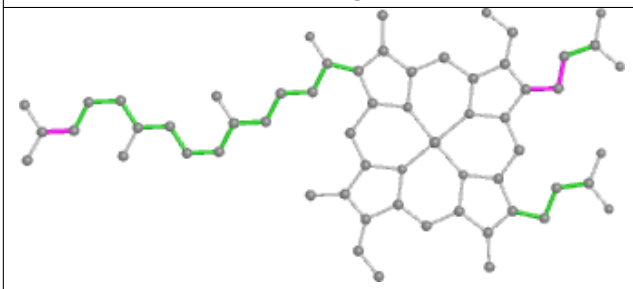
Ligand HEA a 601



Bond lengths



Bond angles



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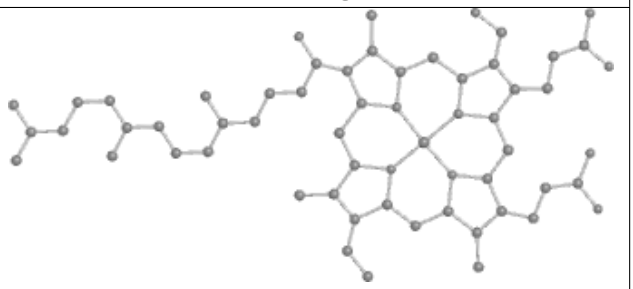
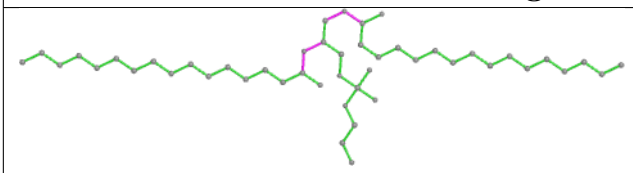
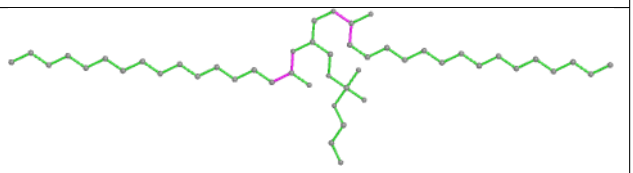


Rings

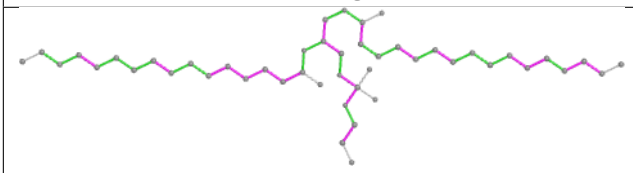
Ligand PEF D 402



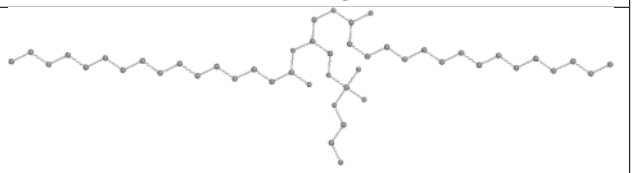
Bond lengths



Bond angles

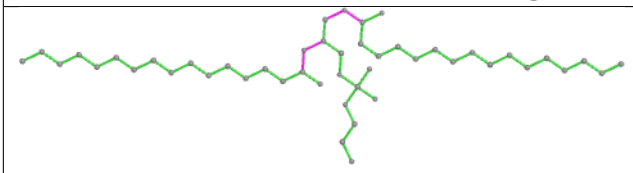


Torsions

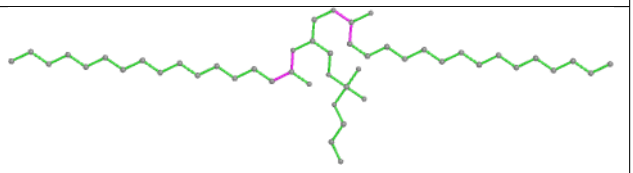


Rings

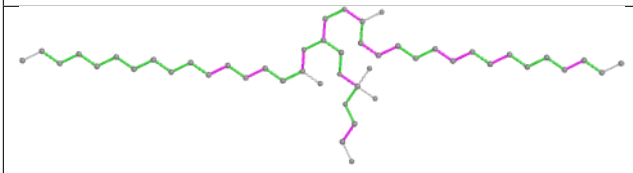
Ligand PEF N 405



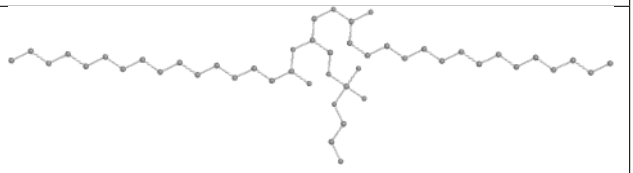
Bond lengths



Bond angles

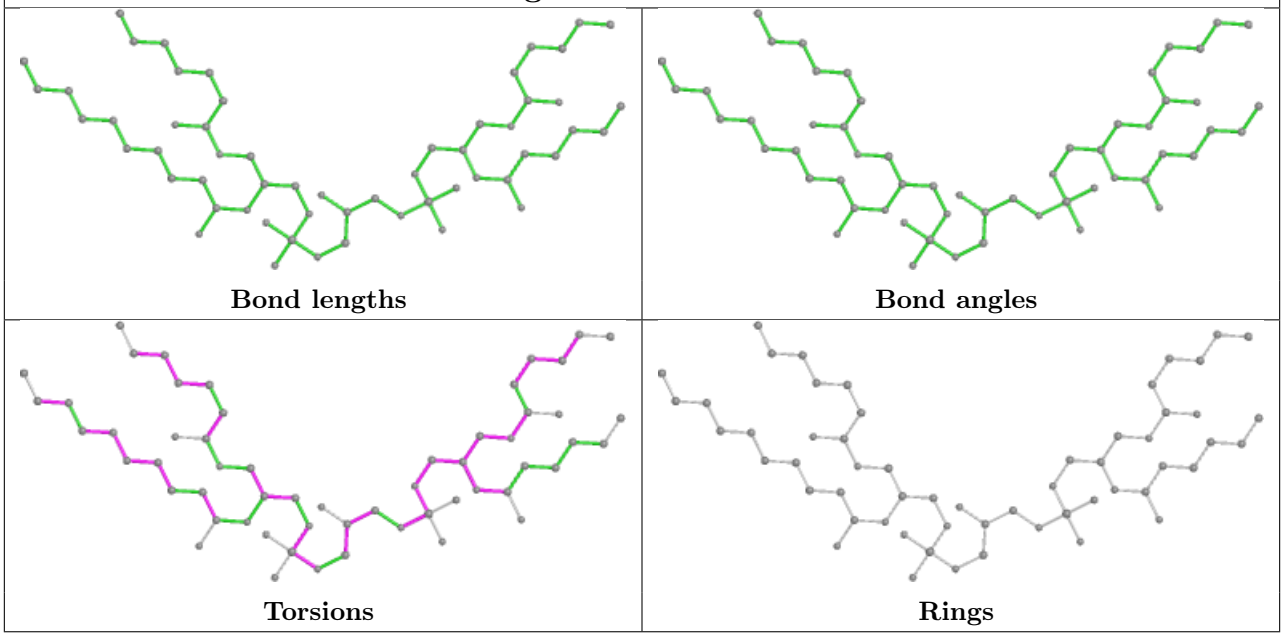


Torsions

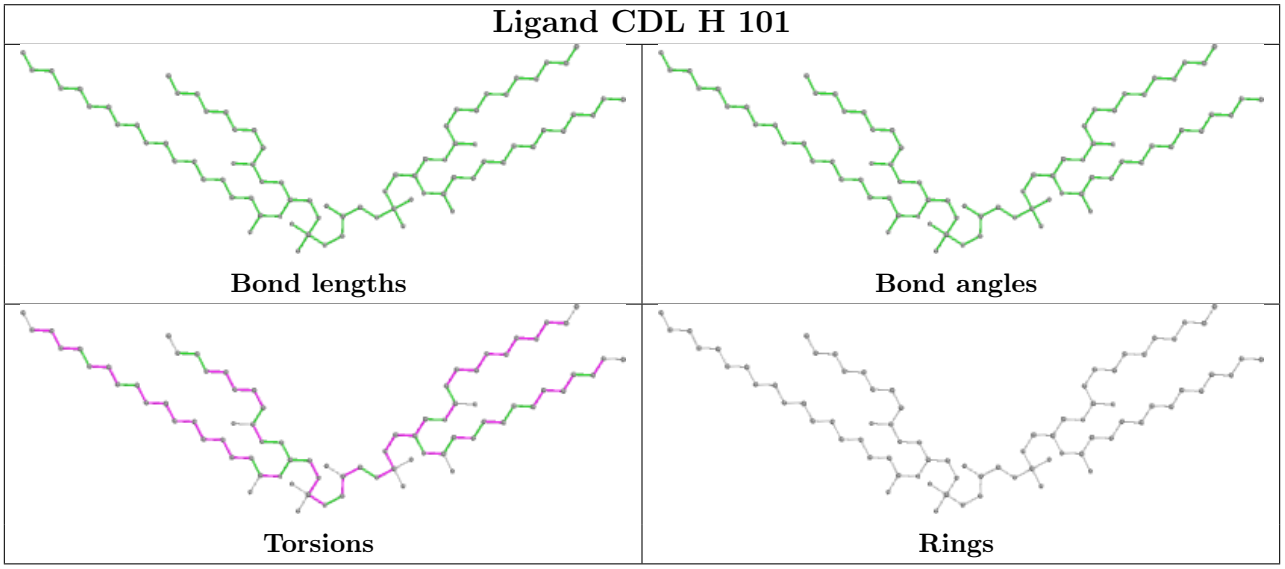


Rings

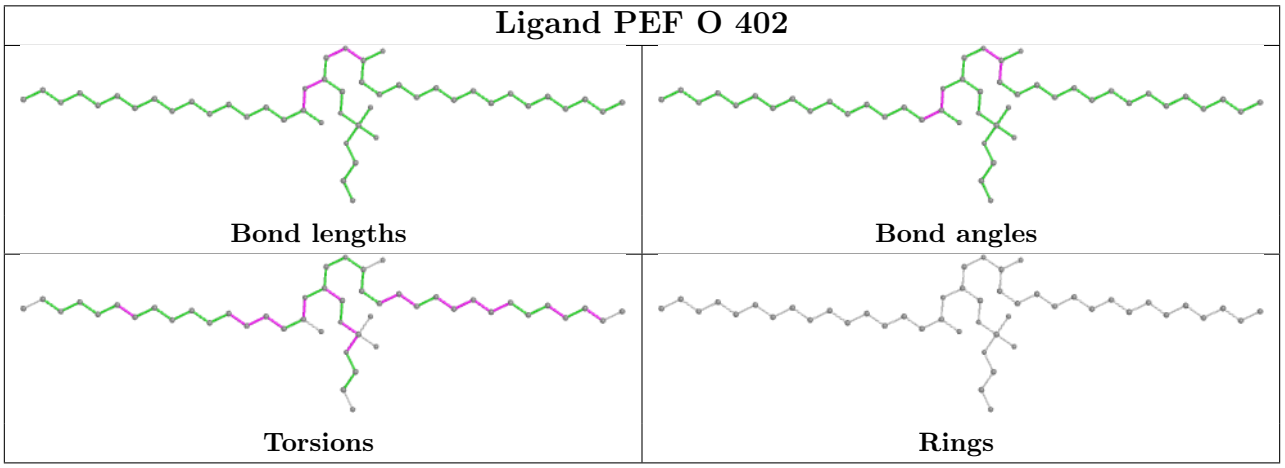
Ligand CDL A 502



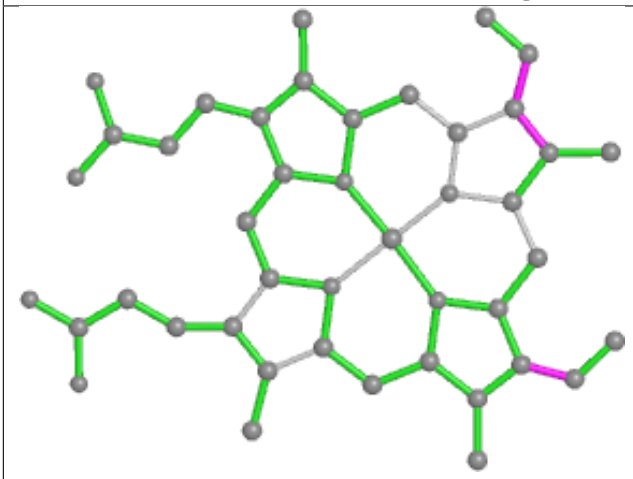
Ligand CDL H 101



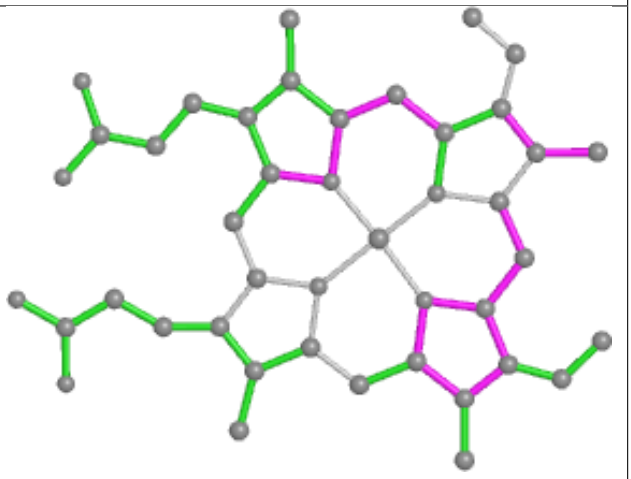
Ligand PEF O 402



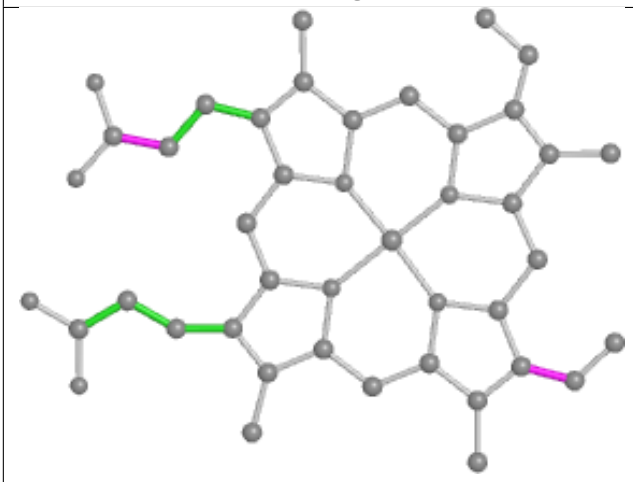
Ligand HEM N 402



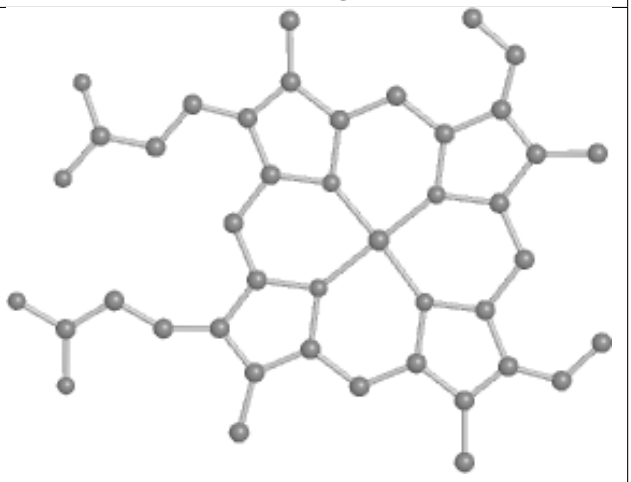
Bond lengths



Bond angles

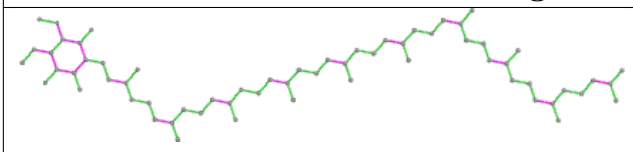


Torsions

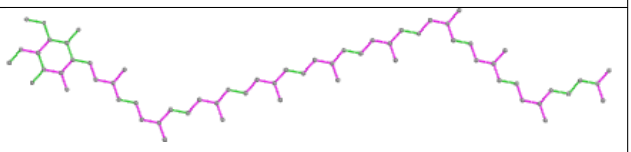


Rings

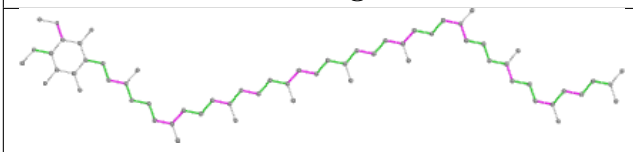
Ligand U10 N 403



Bond lengths



Bond angles



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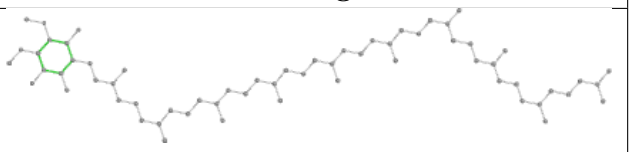
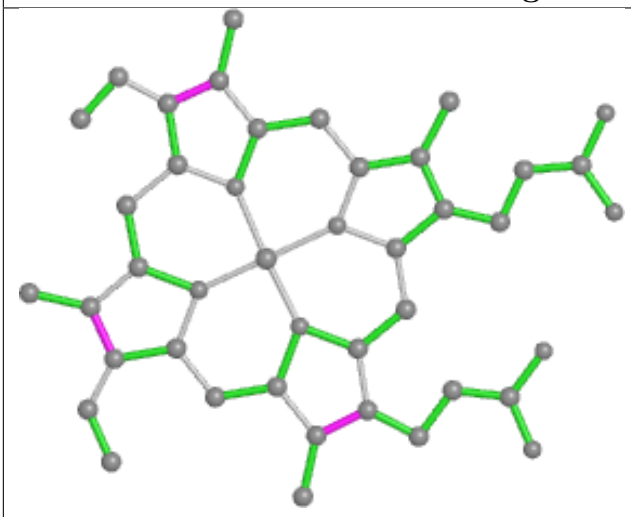
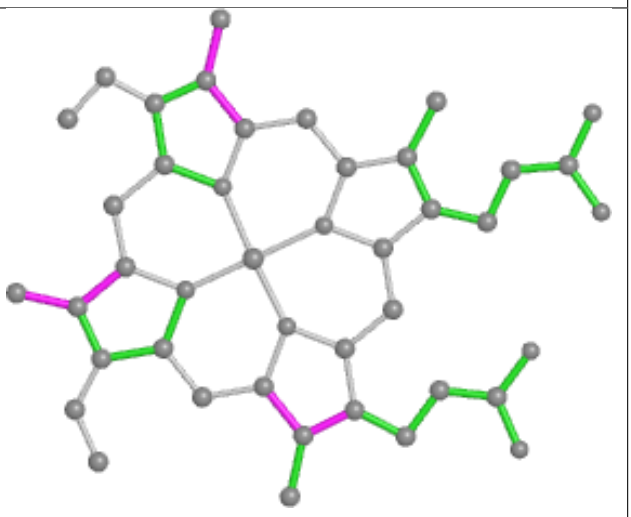


Rings

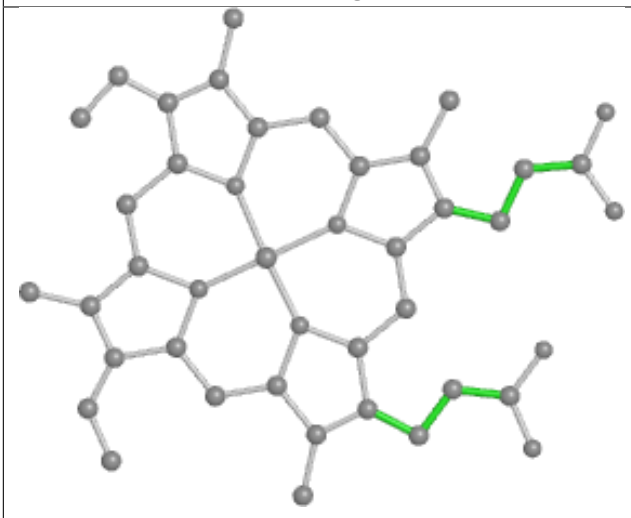
Ligand HEC O 401



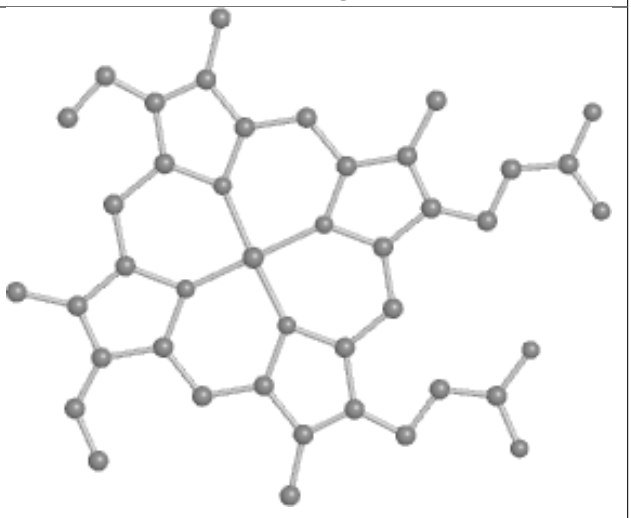
Bond lengths



Bond angles

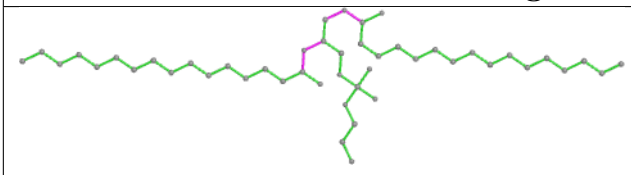


Torsions

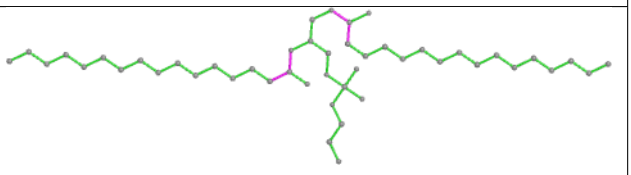


Rings

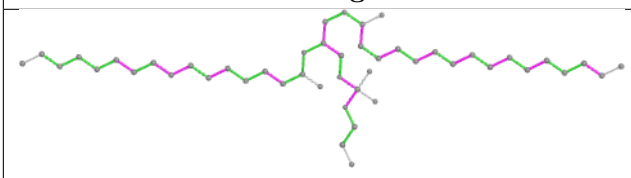
Ligand PEF N 404



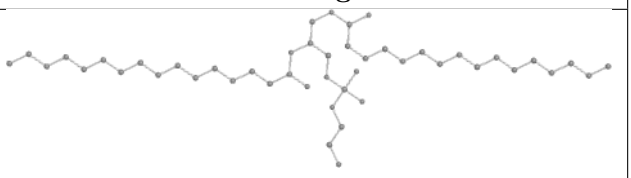
Bond lengths



Bond angles

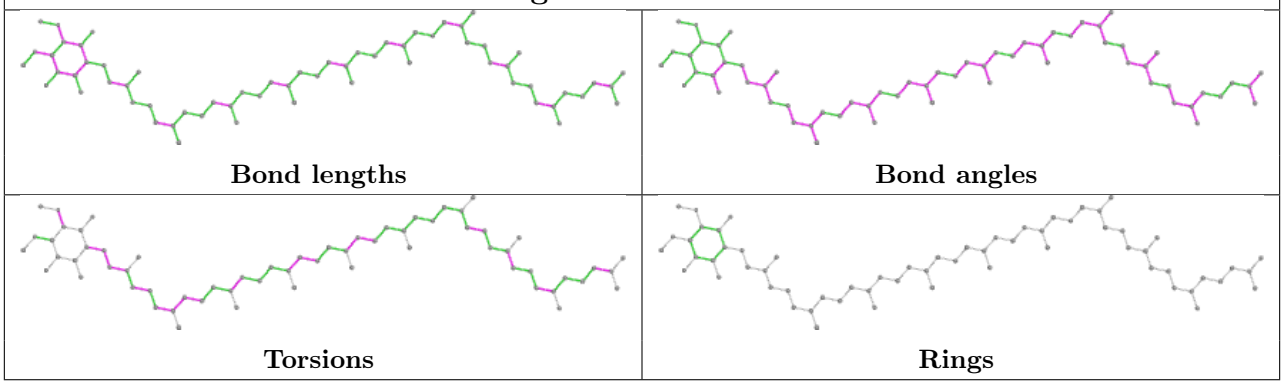


Torsions

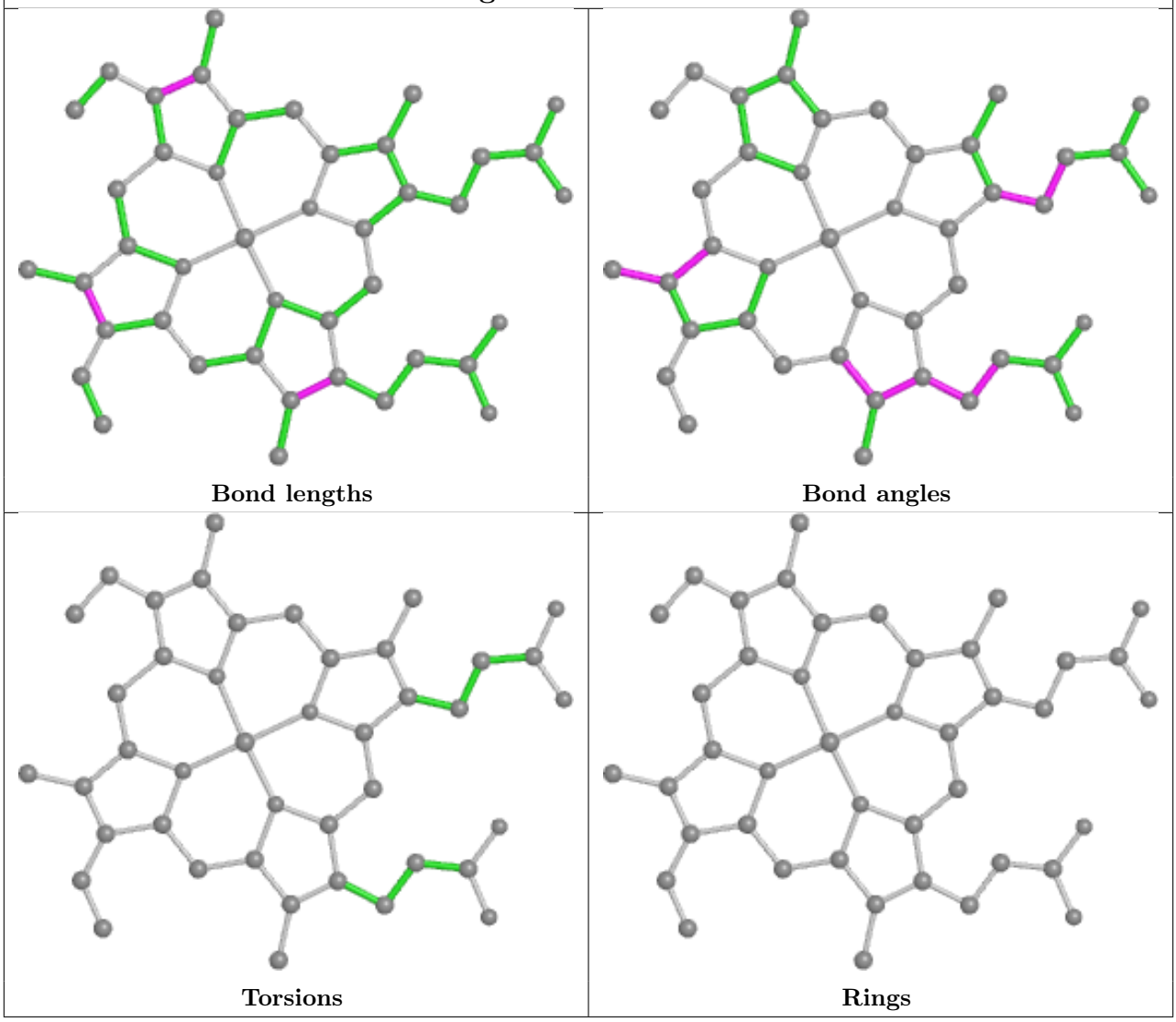


Rings

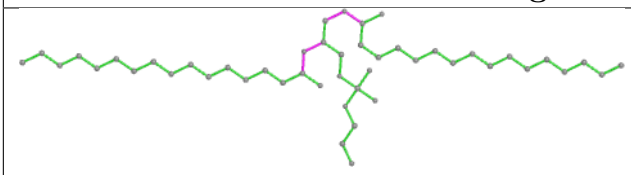
Ligand U10 C 403



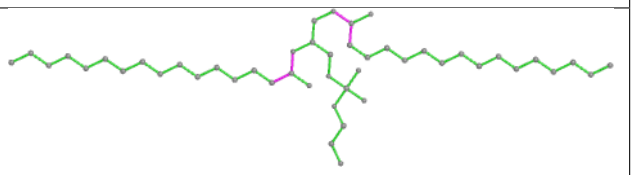
Ligand HEC D 401



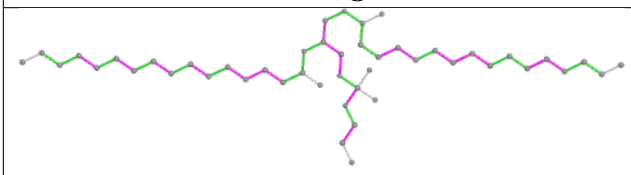
Ligand PEF b 302



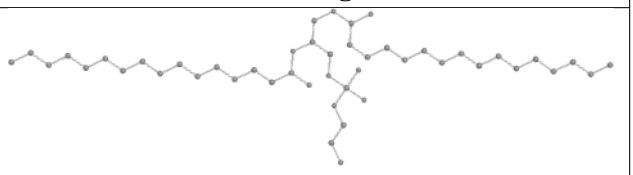
Bond lengths



Bond angles

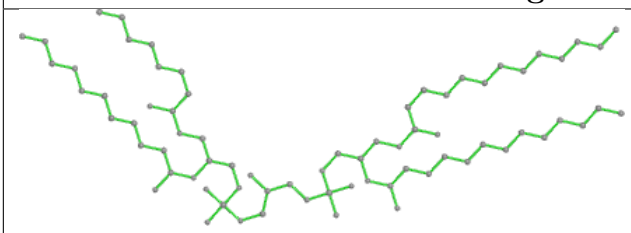


Torsions

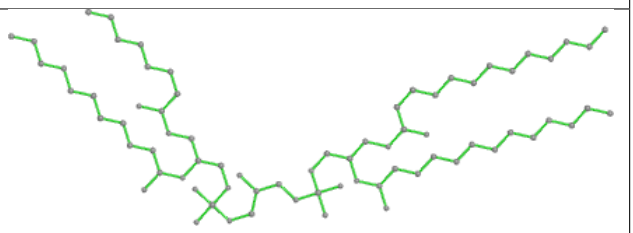


Rings

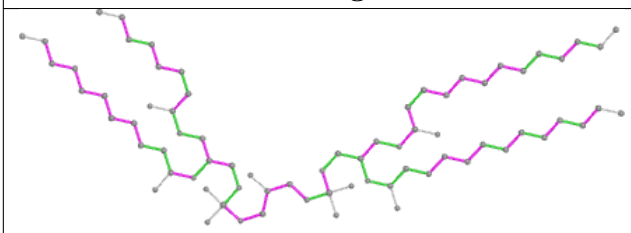
Ligand CDL S 102



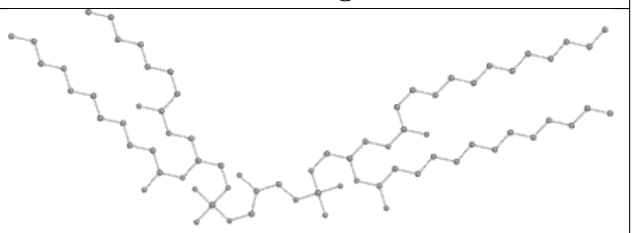
Bond lengths



Bond angles

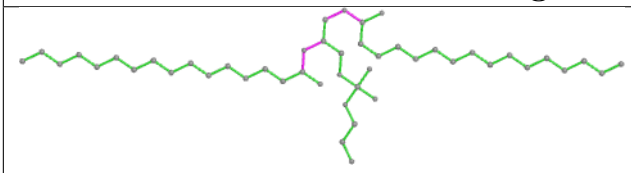


Torsions

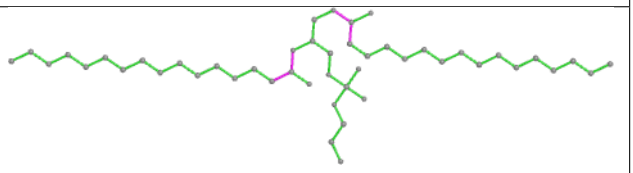


Rings

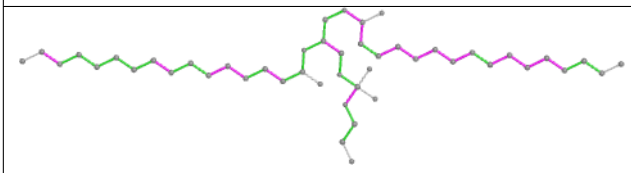
Ligand PEF J 101



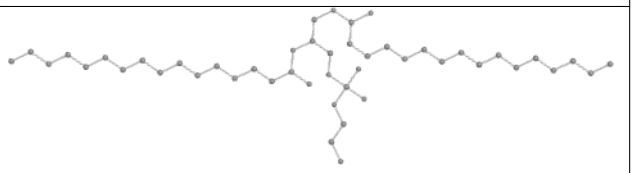
Bond lengths



Bond angles

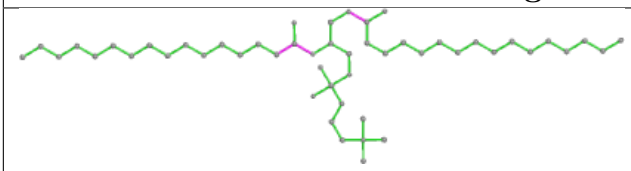


Torsions

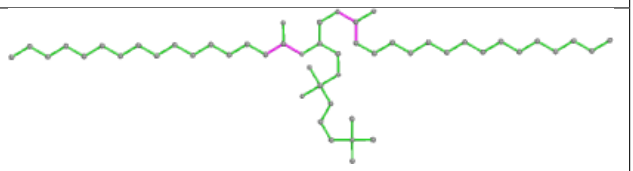


Rings

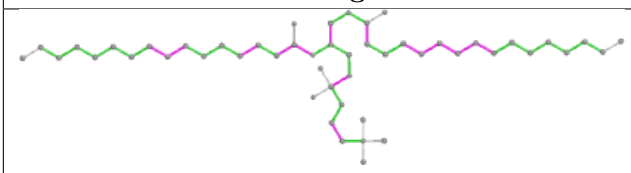
Ligand PCF A 503



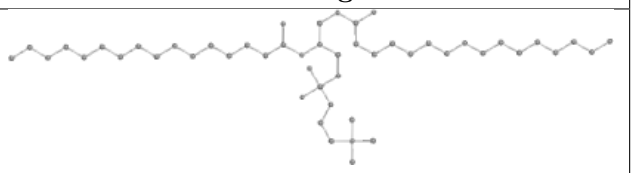
Bond lengths



Bond angles

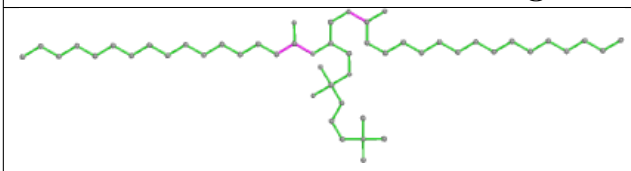


Torsions

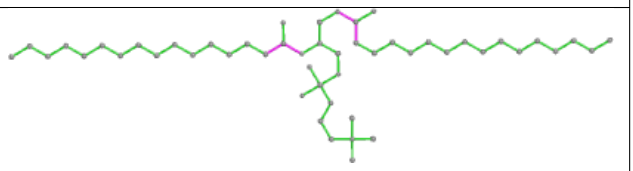


Rings

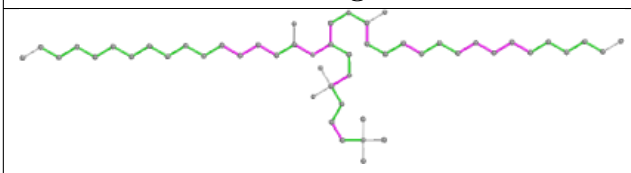
Ligand PCF L 503



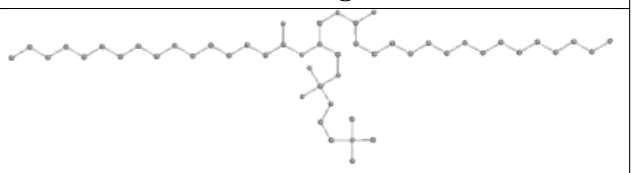
Bond lengths



Bond angles

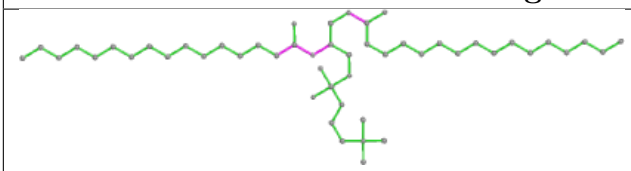


Torsions

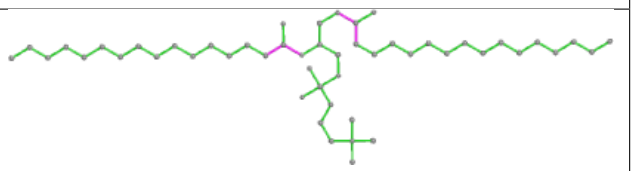


Rings

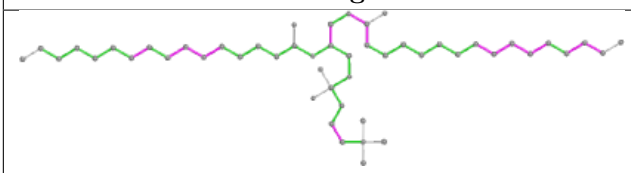
Ligand PCF A 505



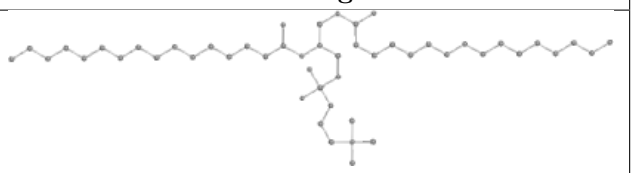
Bond lengths



Bond angles

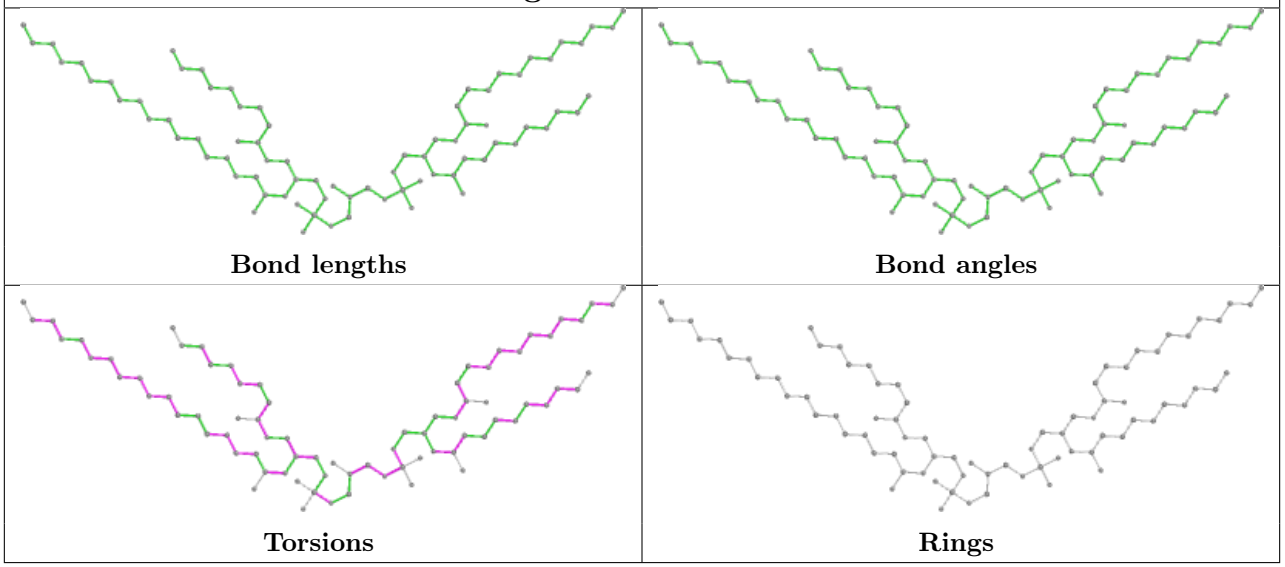


Torsions

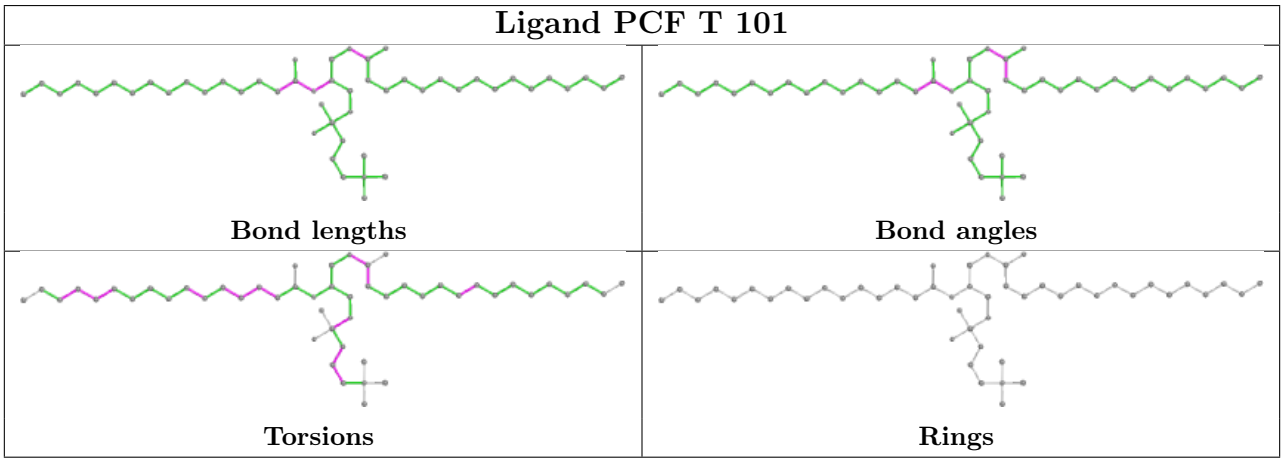


Rings

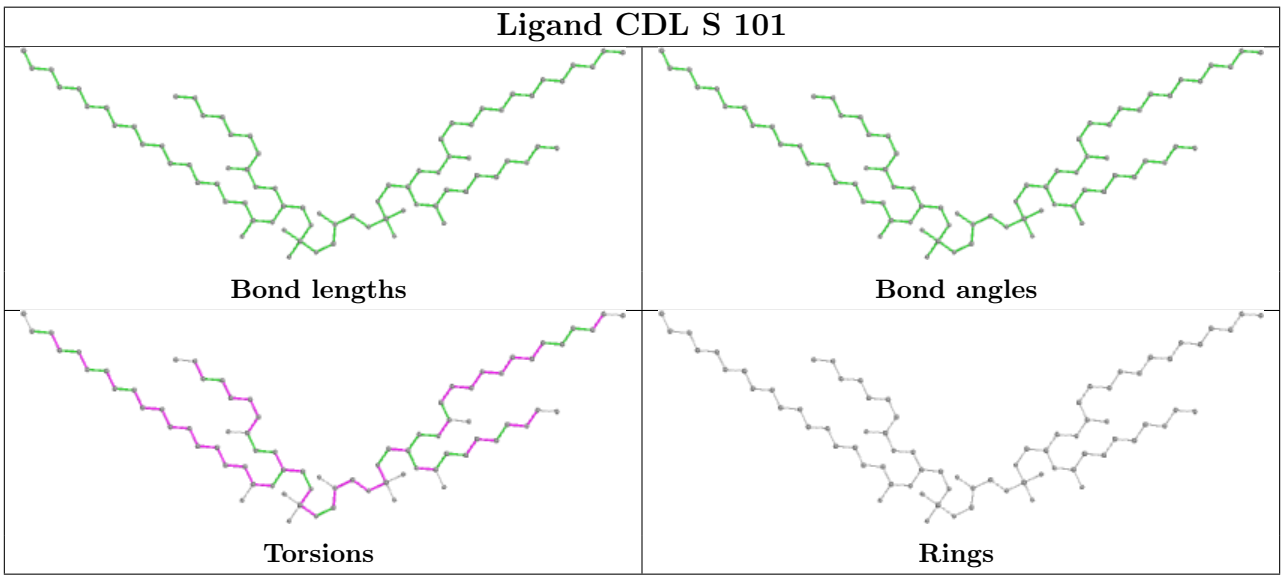
Ligand CDL H 102



Ligand PCF T 101



Ligand CDL S 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.

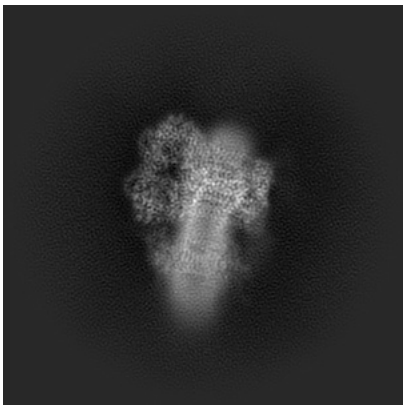
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18062. These allow visual inspection of the internal detail of the map and identification of artifacts.

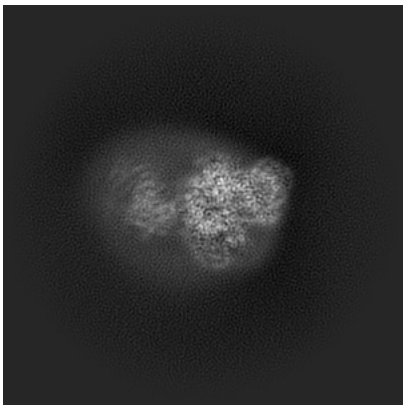
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

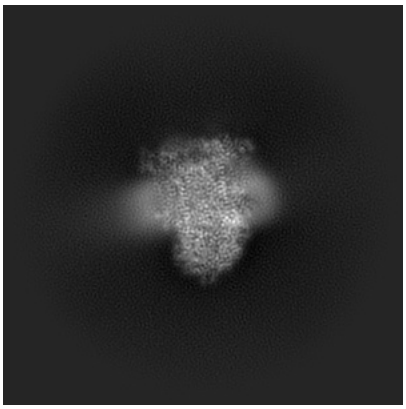
6.1.1 Primary map



X

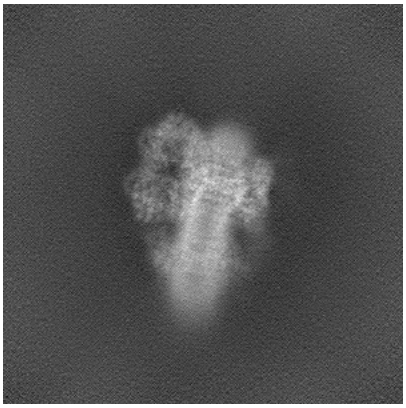


Y

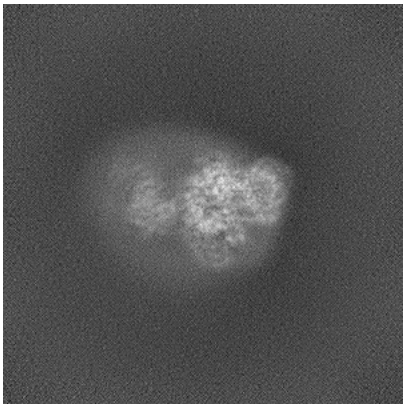


Z

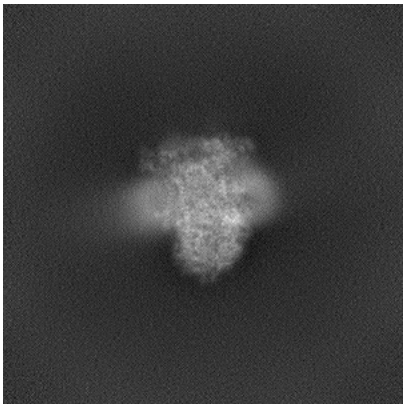
6.1.2 Raw map



X



Y

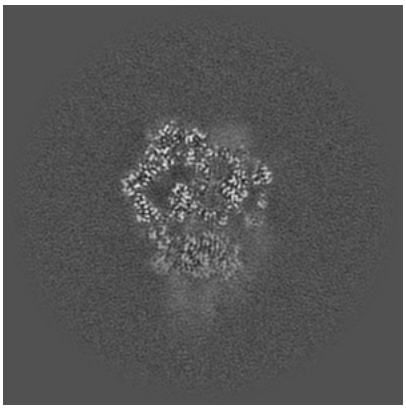


Z

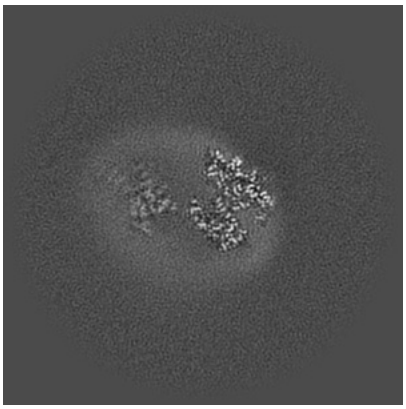
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

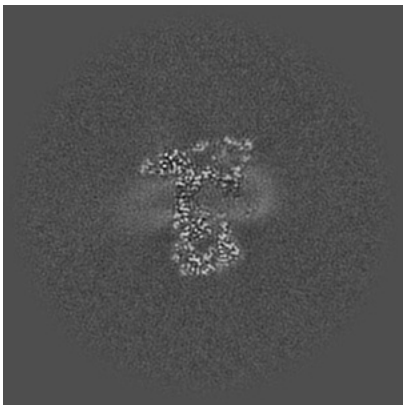
6.2.1 Primary map



X Index: 256

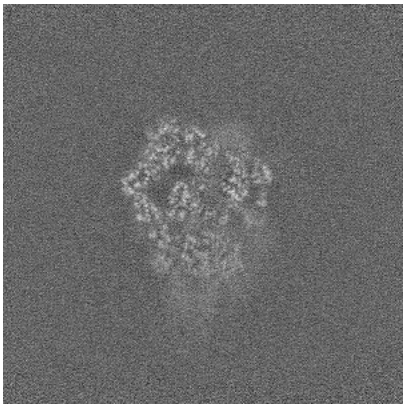


Y Index: 256

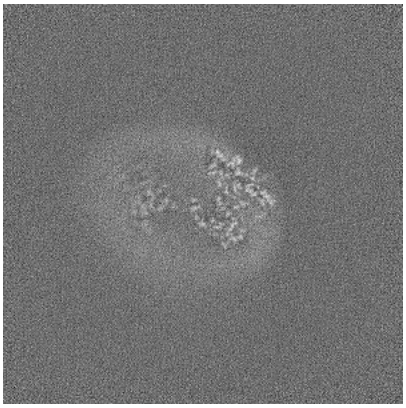


Z Index: 256

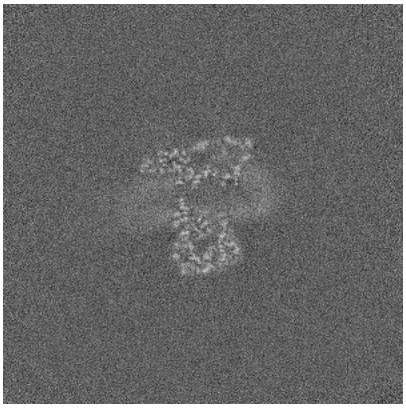
6.2.2 Raw map



X Index: 256



Y Index: 256

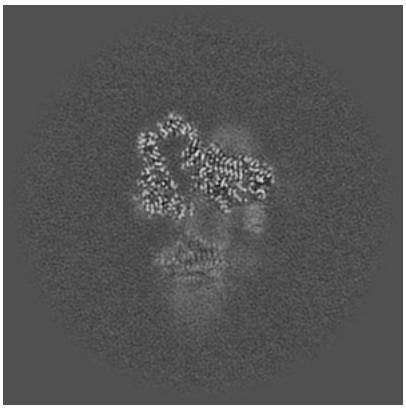


Z Index: 256

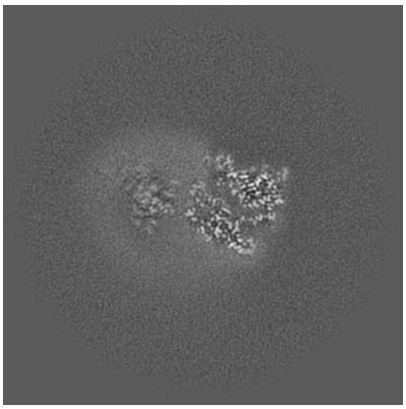
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

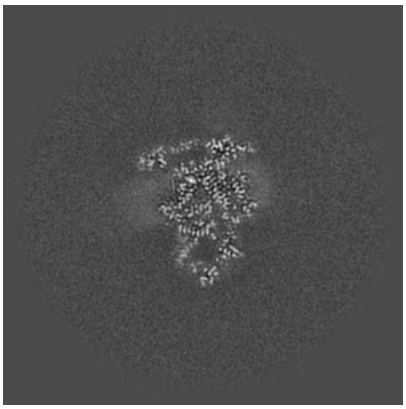
6.3.1 Primary map



X Index: 280

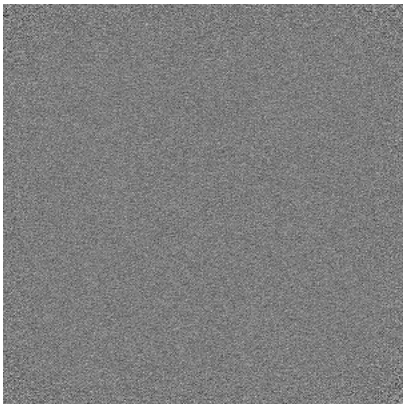


Y Index: 242

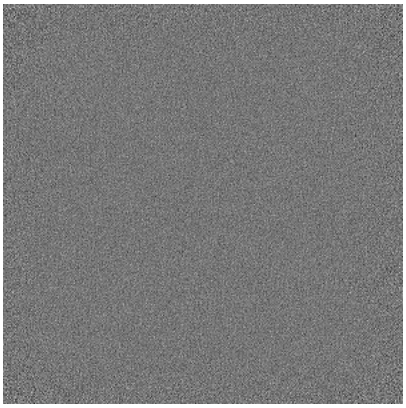


Z Index: 275

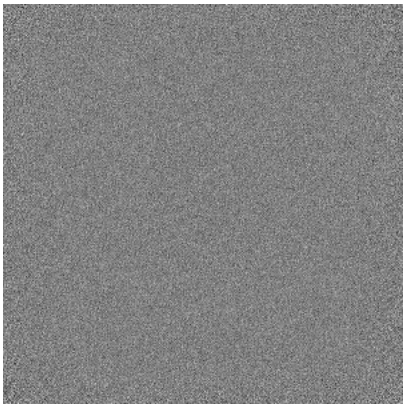
6.3.2 Raw map



X Index: 0



Y Index: 0

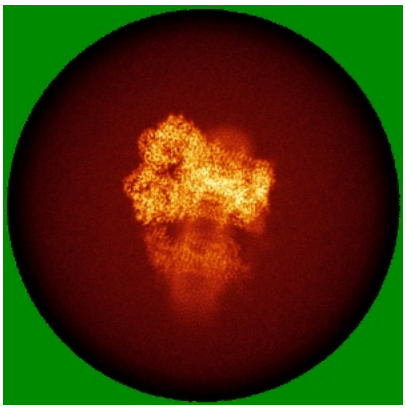


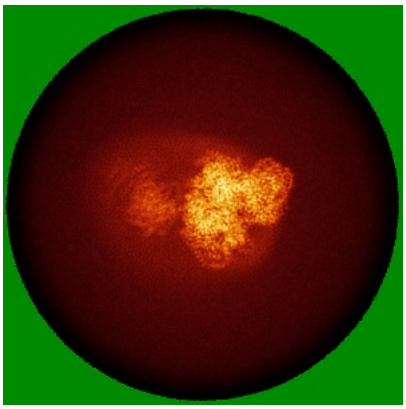
Z Index: 511

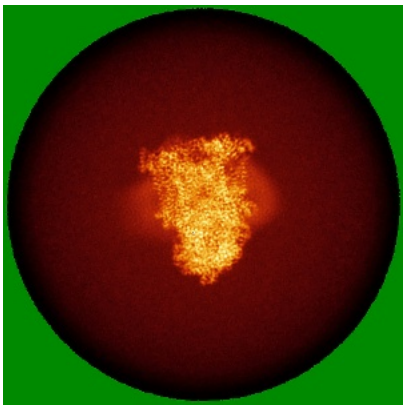
The images above show the largest variance slices of the map in three orthogonal directions.

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

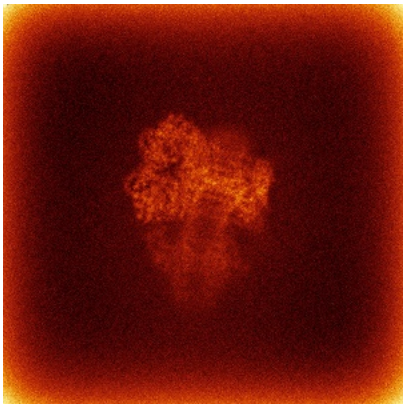
6.4.1 Primary map

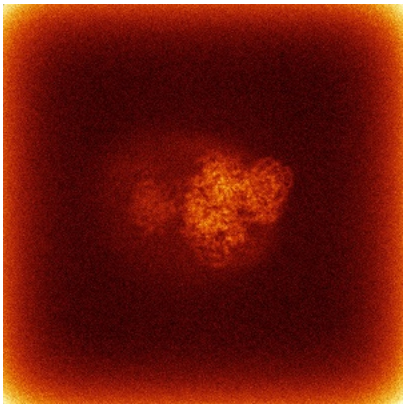

X

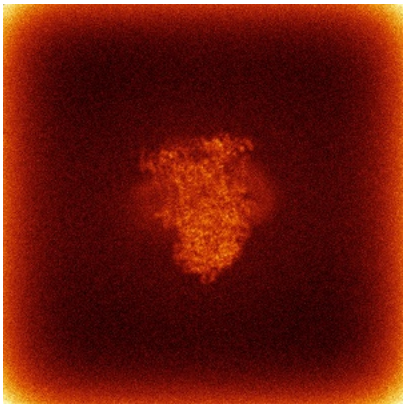

Y


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.

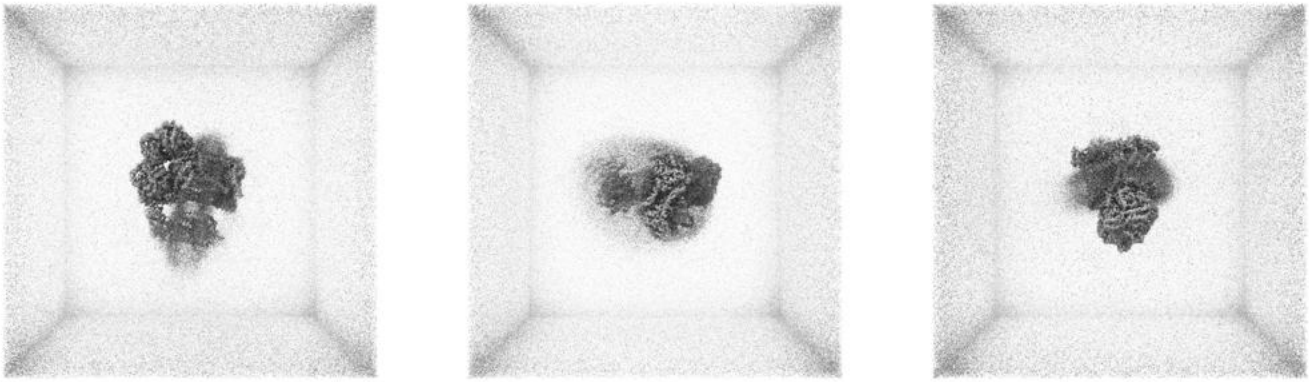
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

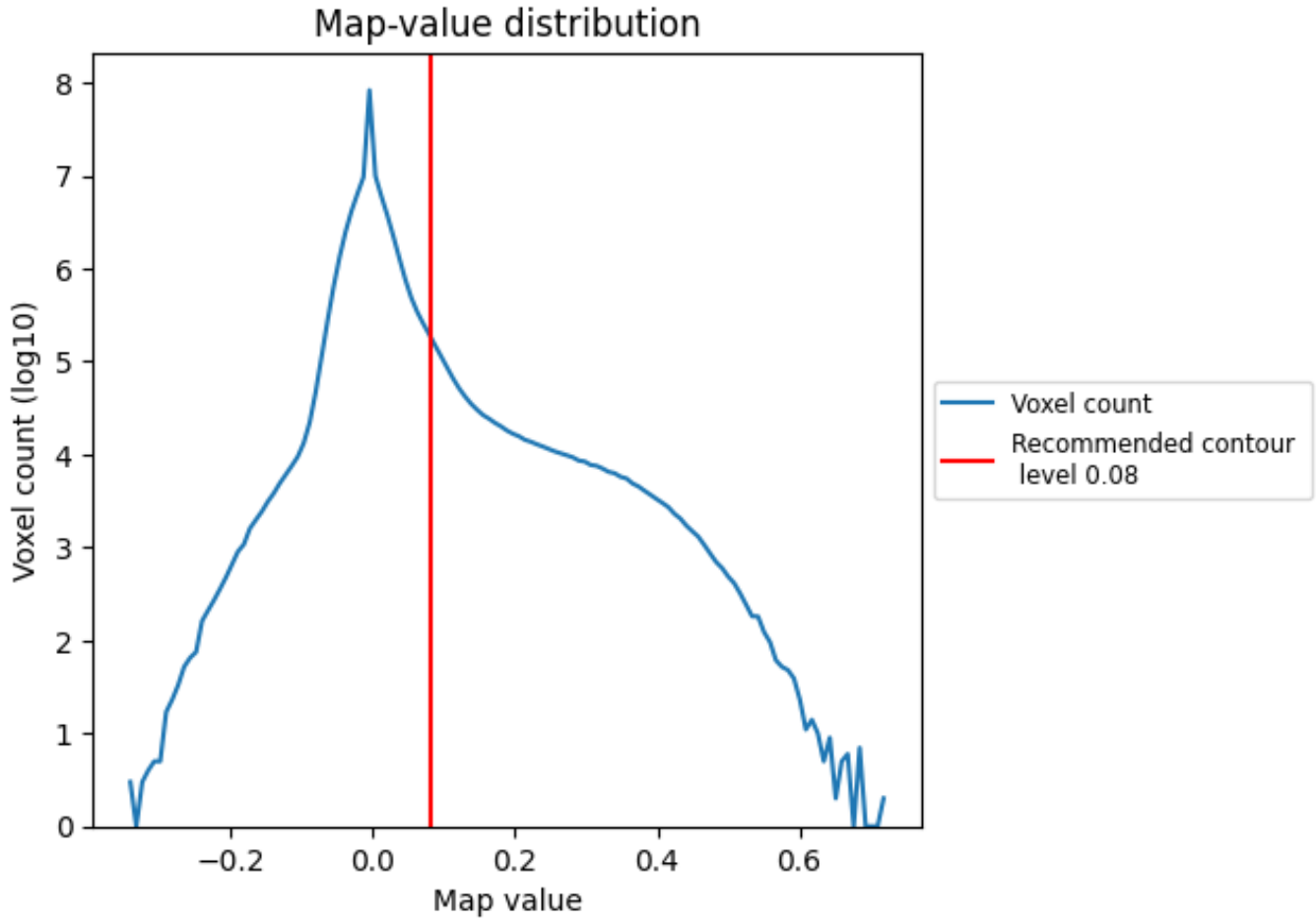
6.6 Mask visualisation (i)

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

7 Map analysis

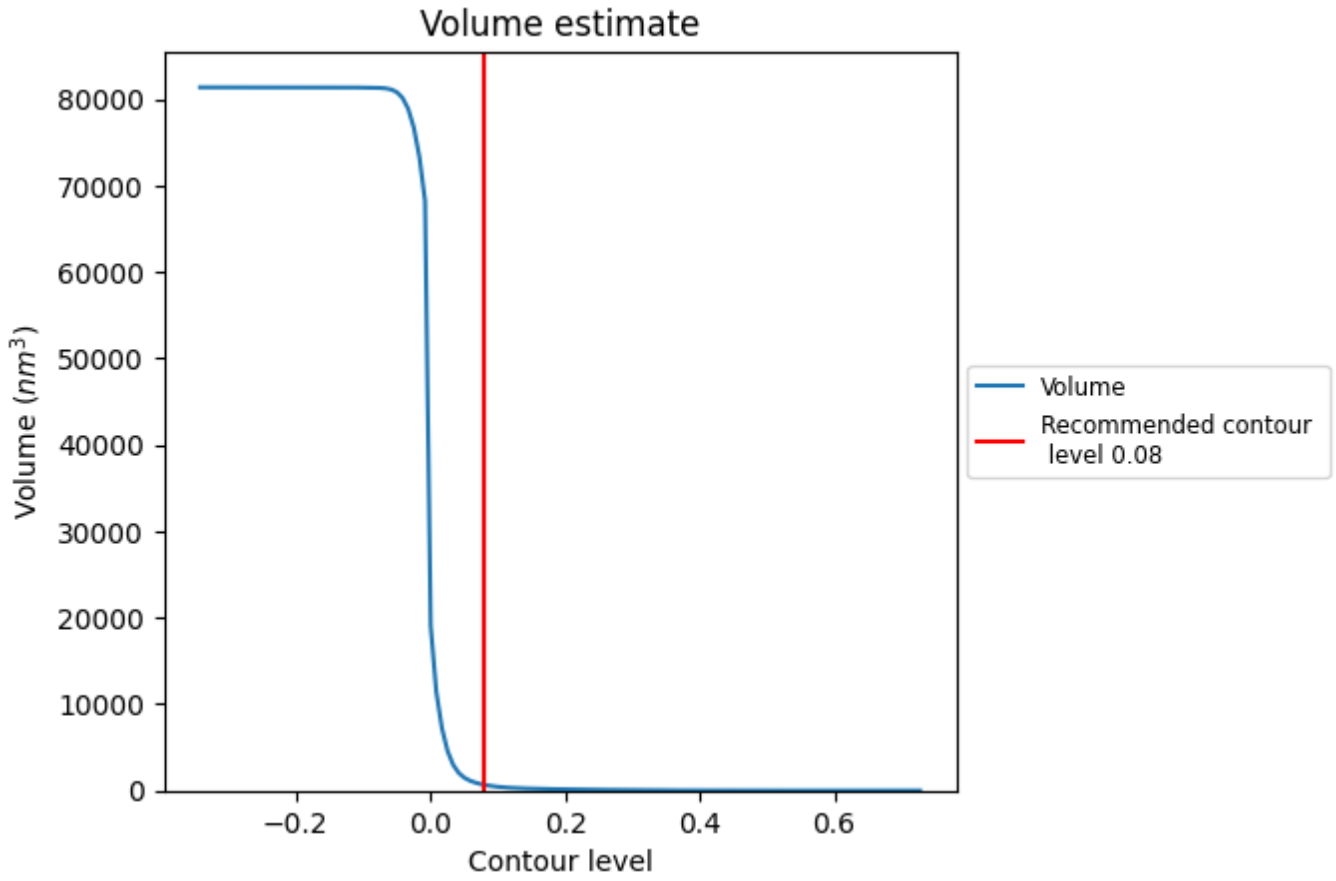
This section contains the results of statistical analysis of the map.

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.

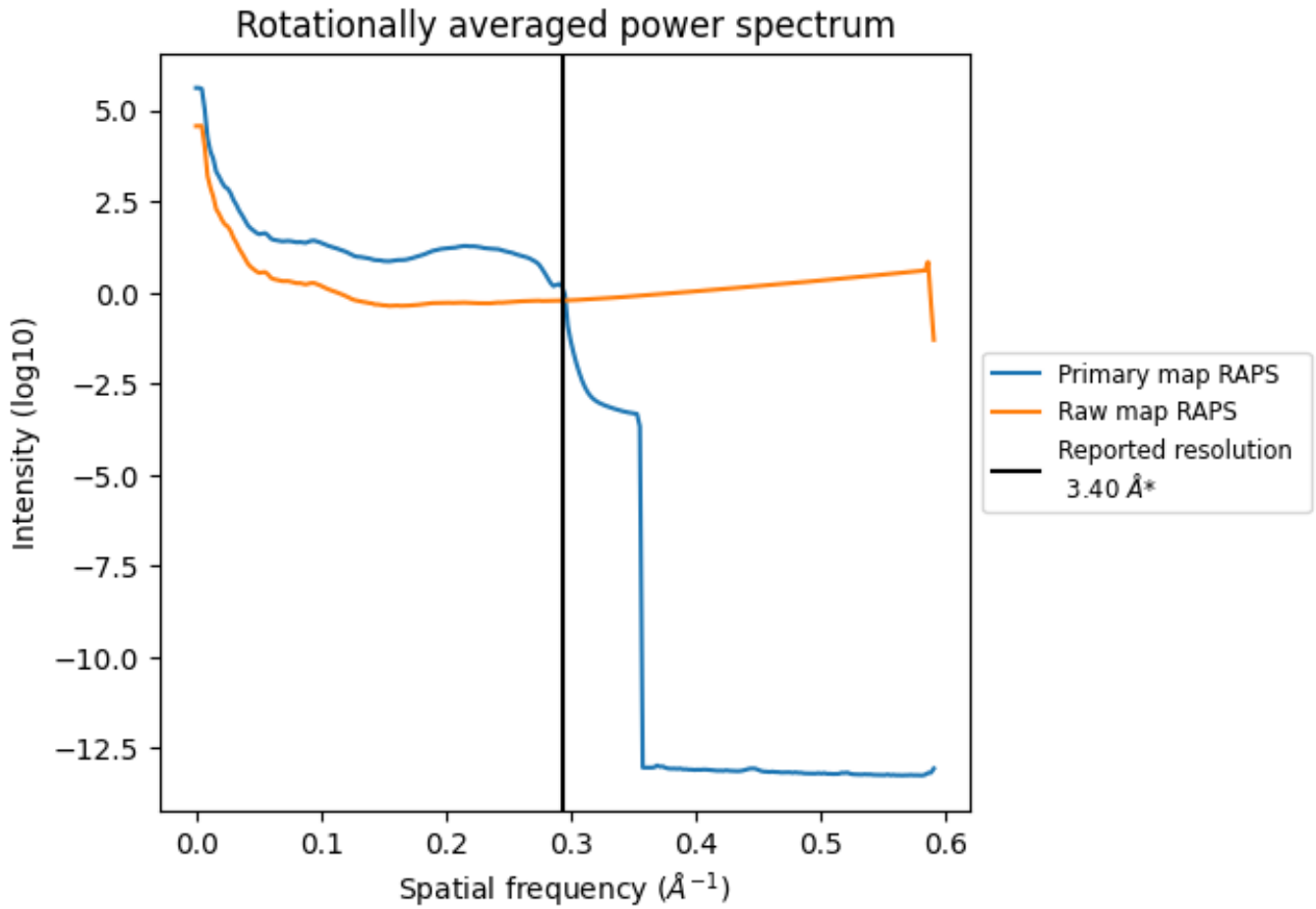
7.2 Volume estimate (i)



The volume at the recommended contour level is 667 nm^3; this corresponds to an approximate mass of 602 kDa.

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

7.3 Rotationally averaged power spectrum (i)

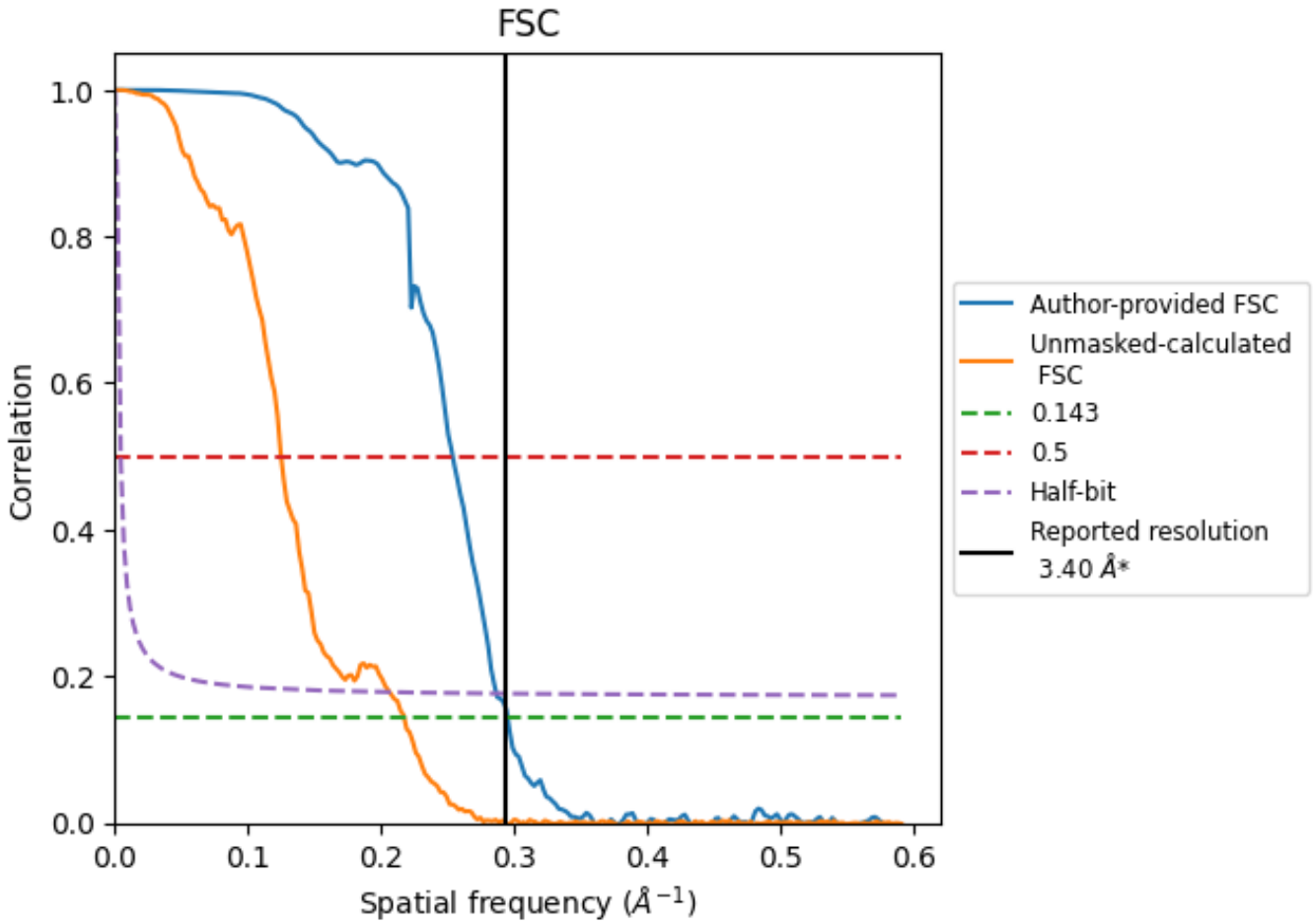


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



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

8.2 Resolution estimates (i)

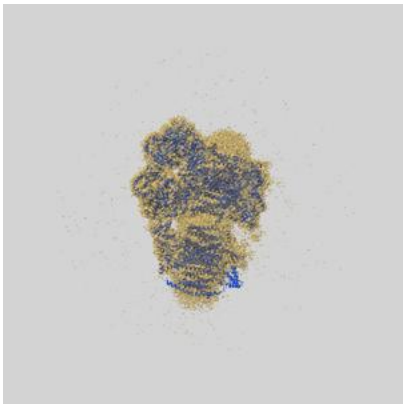
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.94	3.49
Unmasked-calculated*	4.60	8.01	4.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.60 differs from the reported value 3.4 by more than 10 %

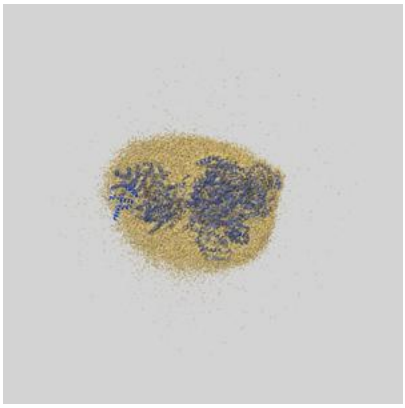
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18062 and PDB model 8Q1B. Per-residue inclusion information can be found in section 3 on page 16.

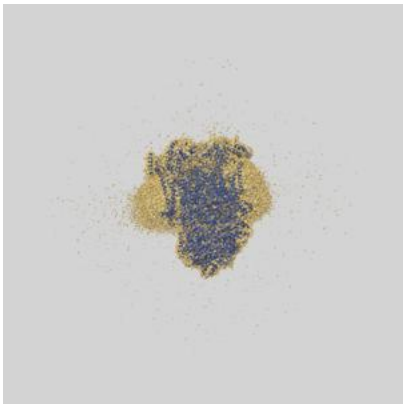
9.1 Map-model overlay



X



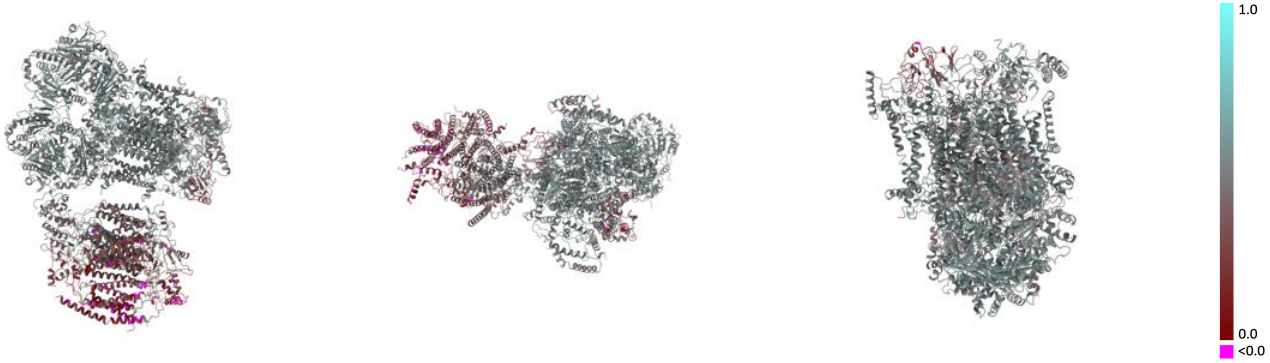
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

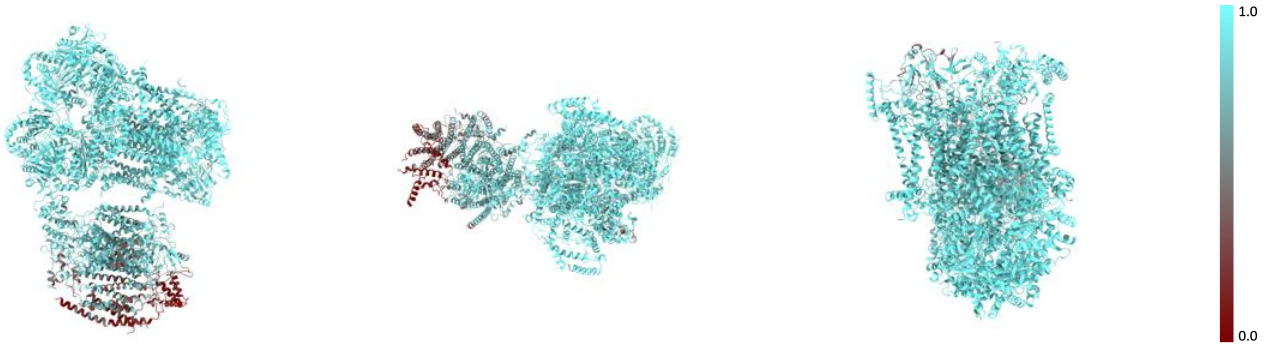
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

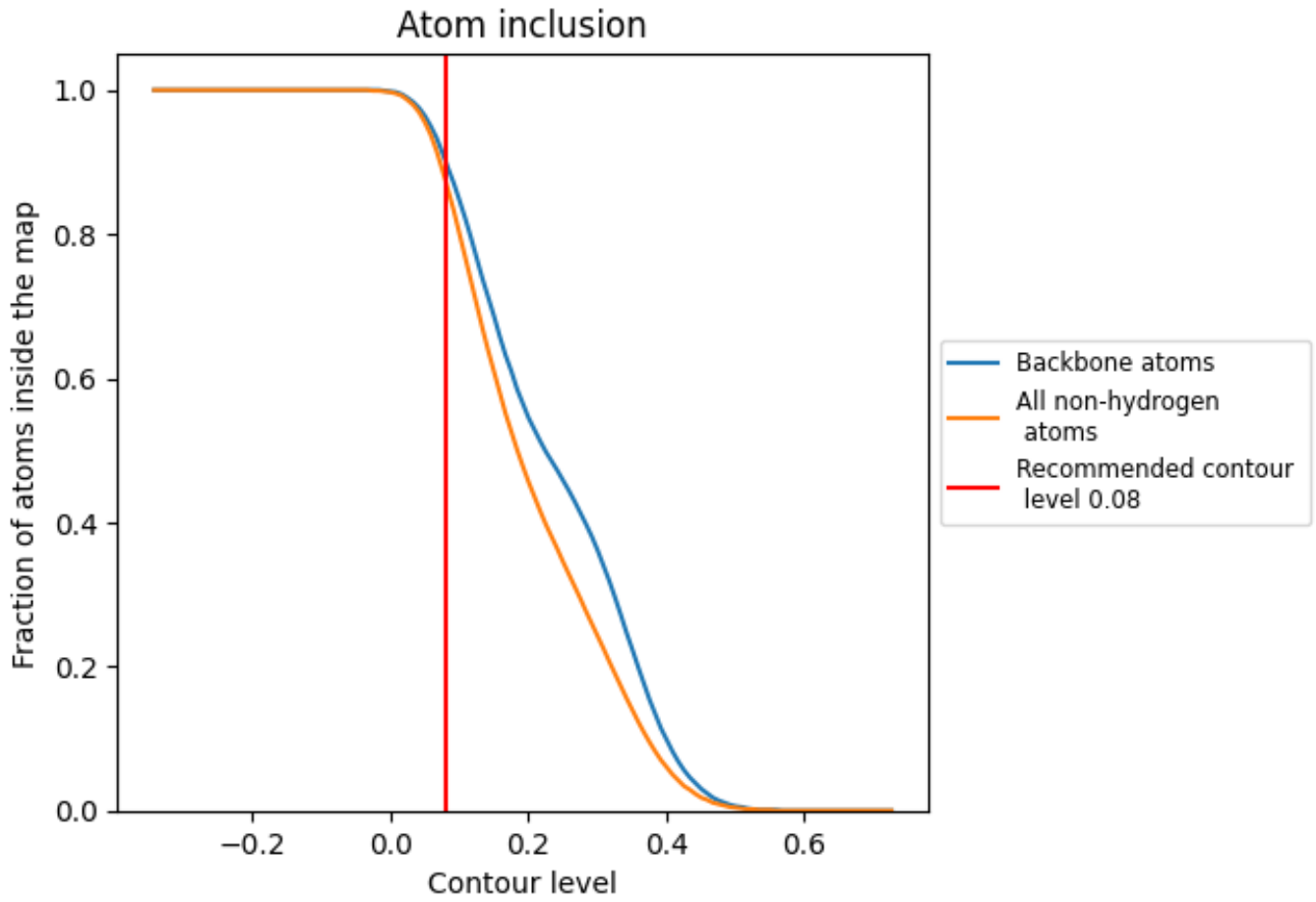
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8760	0.4600
A	0.9660	0.5260
B	0.9830	0.5310
C	0.9570	0.5290
D	0.9730	0.5290
E	0.9000	0.3990
F	0.9340	0.4650
G	0.9680	0.5160
H	0.9700	0.5360
I	0.9440	0.5070
J	0.9340	0.5040
L	0.9670	0.5230
M	0.9810	0.5330
N	0.9460	0.5300
O	0.9720	0.5360
P	0.7930	0.3470
Q	0.9420	0.4530
R	0.9680	0.5280
S	0.9800	0.5400
T	0.9360	0.5040
U	0.9490	0.4940
a	0.8450	0.4010
b	0.7870	0.3750
c	0.5790	0.2470
d	0.7080	0.3410
e	0.9020	0.4490
f	0.8810	0.3920
g	0.6650	0.2740
h	0.7820	0.3390
i	0.7920	0.3760
j	0.1370	0.2290
k	0.2460	0.2410
l	0.2720	0.1770
m	0.0230	0.1830