Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:26 am GMT

PDB ID	:	6HU9
EMDB ID	:	EMD-0262
Title	:	III2-IV2 mitochondrial respiratory supercomplex from S. cerevisiae
Authors	:	Hartley, A.M.; Pinotsis, N.; Marechal, A.
Deposited on	:	2018-10-05
Resolution	:	3.35 Å(reported)
Based on initial models	:	1KYO, 1V54

This is a Full wwPDB EM Validation 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:

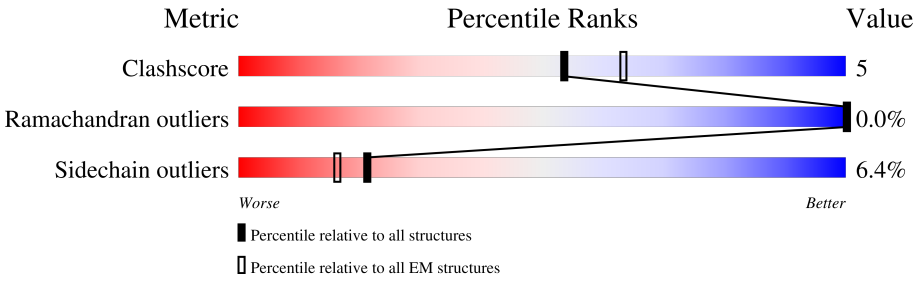
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.35 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	158937	4297
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	431	83% 16% •
1	L	431	84% 15% •
2	B	352	85% 14%
2	M	352	85% 14% •
3	C	385	79% 19% •
3	N	385	85% 13% •
4	D	248	85% 14% •
4	O	248	87% 12% •

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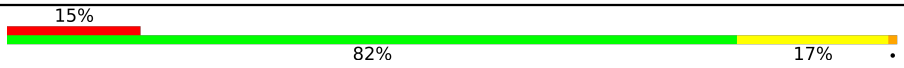
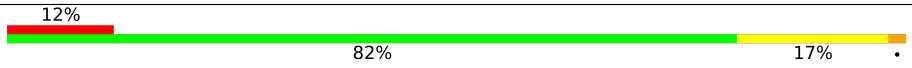
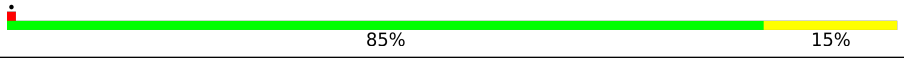
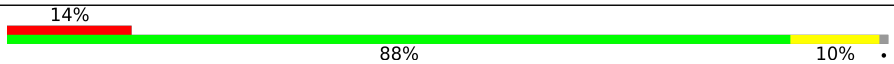
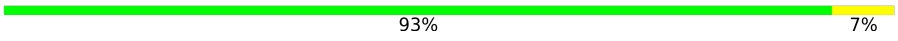
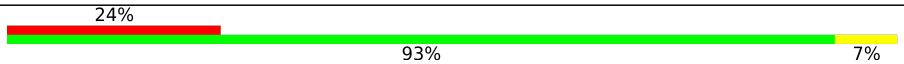
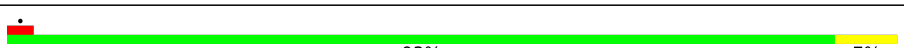
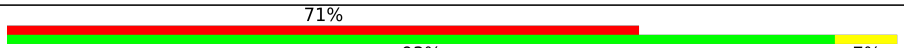
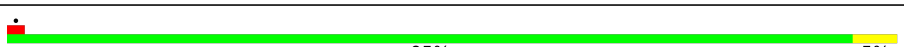
Mol	Chain	Length	Quality of chain
5	E	185	
5	P	185	
6	F	147	
6	Q	147	
7	G	127	
7	R	127	
8	H	93	
8	S	93	
9	I	66	
9	T	66	
10	J	77	
10	U	77	
11	a	534	
11	m	534	
12	b	236	
12	n	236	
13	c	269	
13	o	269	
14	d	130	
14	p	130	
15	e	133	
15	q	133	
16	f	108	
16	r	108	
17	g	59	

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Mol	Chain	Length	Quality of chain
17	s	59	76% 93% 7%
18	h	47	100%
18	t	47	32% 89% 11%
19	i	55	7% 93% 7%
19	u	55	44% 93% 7%
20	j	82	87% 84% 10% 6%
20	v	82	91% 85% 9% 6%
21	k	131	73% 79% 8% 14%
21	w	131	85% 78% 8% 14%
22	l	66	64% 5% 32%
22	x	66	23% 62% 6% 32%

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
31	HEA	a	602	X	-	-	-
31	HEA	a	603	X	-	-	-
31	HEA	m	602	X	-	-	-
31	HEA	m	603	X	-	-	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 63031 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 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		
1	L	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
2	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
3	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		
4	O	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	75	Total	C	N	O	S	0	0
			633	396	109	126	2		
6	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
7	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
8	S	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	57	Total	C	N	O	0	0
			465	310	77	78		
9	T	57	Total	C	N	O	0	0
			465	310	77	78		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	76	Total	C	N	O	S	0	0
			599	391	98	108	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	76	Total	C	N	O	S	0	0
			599	391	98	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	534	Total	C	N	O	S	0	0
			4162	2778	649	713	22		
11	m	534	Total	C	N	O	S	0	0
			4162	2778	649	713	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		
12	n	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		
13	o	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		

- 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
			913	576	151	181	5		
14	p	121	Total	C	N	O	S	0	0
			913	576	151	181	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	133	Total	C	N	O	S	0	0
			1049	663	184	198	4		
15	q	133	Total	C	N	O	S	0	0
			1049	663	184	198	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	102	Total	C	N	O	S	0	0
			851	545	137	168	1		
16	r	102	Total	C	N	O	S	0	0
			851	545	137	168	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	59	Total	C	N	O	0	0
			484	328	83	73		
17	s	59	Total	C	N	O	0	0
			484	328	83	73		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	47	Total	C	N	O	S	0	0
			383	261	62	59	1		
18	t	47	Total	C	N	O	S	0	0
			383	261	62	59	1		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	55	Total	C	N	O	S	0	0
			456	300	79	74	3		
19	u	55	Total	C	N	O	S	0	0
			456	300	79	74	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	77	Total	C	N	O	S	0	0
			642	410	109	118	5		
20	v	77	Total	C	N	O	S	0	0
			642	410	109	118	5		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 6A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	113	Total	C	N	O	S	0	0
			928	605	160	160	3		
21	w	113	Total	C	N	O	S	0	0
			928	605	160	160	3		

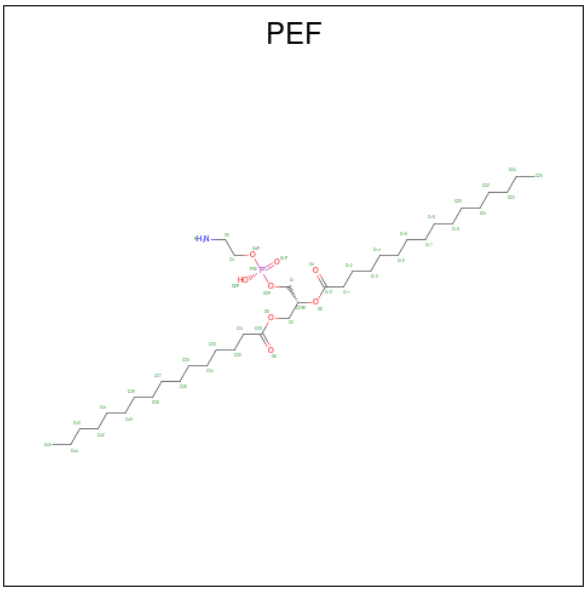
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	130	GLY	-	expression tag	UNP P32799
k	131	ALA	-	expression tag	UNP P32799
k	132	ARG	-	expression tag	UNP P32799
k	133	GLY	-	expression tag	UNP P32799
k	134	SER	-	expression tag	UNP P32799
k	135	HIS	-	expression tag	UNP P32799
k	136	HIS	-	expression tag	UNP P32799
k	137	HIS	-	expression tag	UNP P32799
k	138	HIS	-	expression tag	UNP P32799
k	139	HIS	-	expression tag	UNP P32799
k	140	HIS	-	expression tag	UNP P32799
w	130	GLY	-	expression tag	UNP P32799
w	131	ALA	-	expression tag	UNP P32799
w	132	ARG	-	expression tag	UNP P32799
w	133	GLY	-	expression tag	UNP P32799
w	134	SER	-	expression tag	UNP P32799
w	135	HIS	-	expression tag	UNP P32799
w	136	HIS	-	expression tag	UNP P32799
w	137	HIS	-	expression tag	UNP P32799
w	138	HIS	-	expression tag	UNP P32799
w	139	HIS	-	expression tag	UNP P32799
w	140	HIS	-	expression tag	UNP P32799

- Molecule 22 is a protein called Cox26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	l	45	Total	C	N	O	S	0	0
			361	238	63	59	1		
22	x	45	Total	C	N	O	S	0	0
			361	238	63	59	1		

- Molecule 23 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
23	C	1	Total	C	N	O	P	0
			75	55	2	16	2	
23	C	1	Total	C	N	O	P	0
			75	55	2	16	2	
23	D	1	Total	C	N	O	P	0
			42	32	1	8	1	
23	E	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	N	1	Total	C	N	O	P	0
			114	84	3	24	3	
23	N	1	Total	C	N	O	P	0
			114	84	3	24	3	
23	N	1	Total	C	N	O	P	0
			114	84	3	24	3	
23	O	1	Total	C	N	O	P	0
			43	33	1	8	1	
23	P	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	S	1	Total	C	N	O	P	0
			36	26	1	8	1	
23	a	1	Total	C	N	O	P	0
			113	83	3	24	3	
23	a	1	Total	C	N	O	P	0
			113	83	3	24	3	

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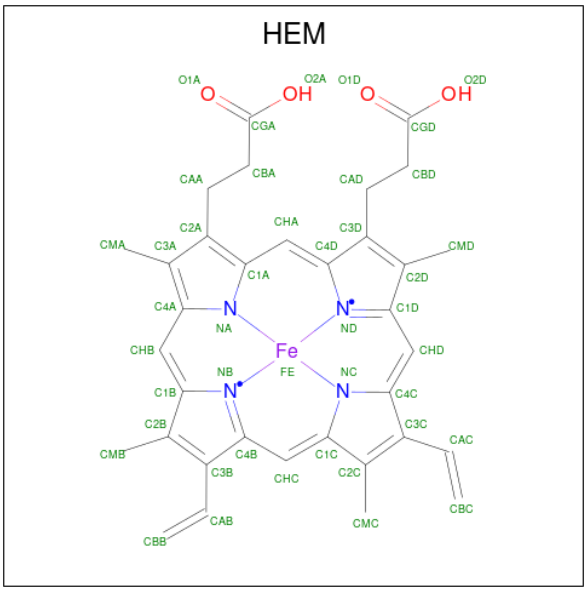
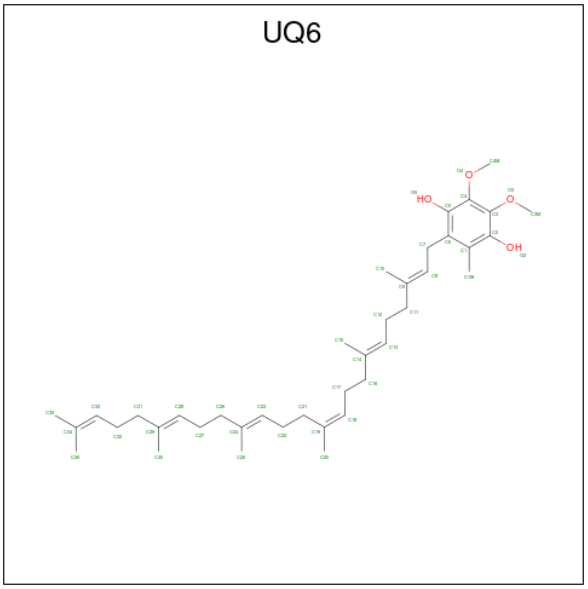
Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total	C	N	O	P	0
			113	83	3	24	3	
23	b	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	c	1	Total	C	N	O	P	0
			77	57	2	16	2	
23	c	1	Total	C	N	O	P	0
			77	57	2	16	2	
23	e	1	Total	C	N	O	P	0
			47	37	1	8	1	
23	h	1	Total	C	N	O	P	0
			47	37	1	8	1	
23	m	1	Total	C	N	O	P	0
			80	60	2	16	2	
23	m	1	Total	C	N	O	P	0
			80	60	2	16	2	
23	n	1	Total	C	N	O	P	0
			73	53	2	16	2	
23	n	1	Total	C	N	O	P	0
			73	53	2	16	2	
23	o	1	Total	C	N	O	P	0
			77	57	2	16	2	
23	o	1	Total	C	N	O	P	0
			77	57	2	16	2	
23	q	1	Total	C	N	O	P	0
			47	37	1	8	1	
23	t	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



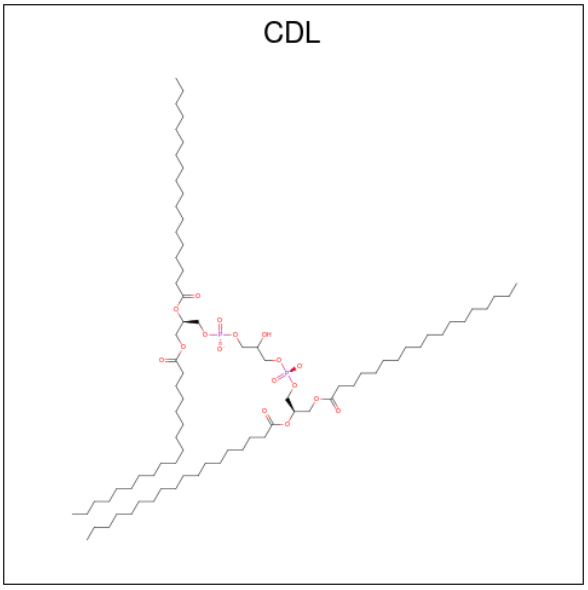
Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
24	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
24	N	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
24	N	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 25 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: $C_{39}H_{60}O_4$).



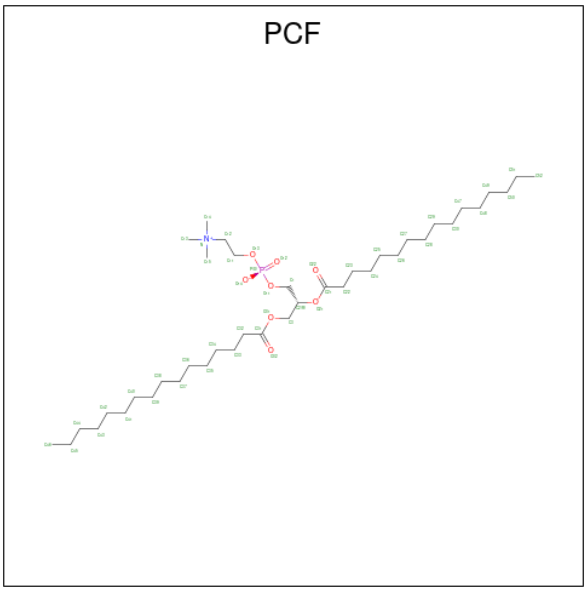
Mol	Chain	Residues	Atoms			AltConf
25	C	1	Total	C	O	1
			86	78	8	

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



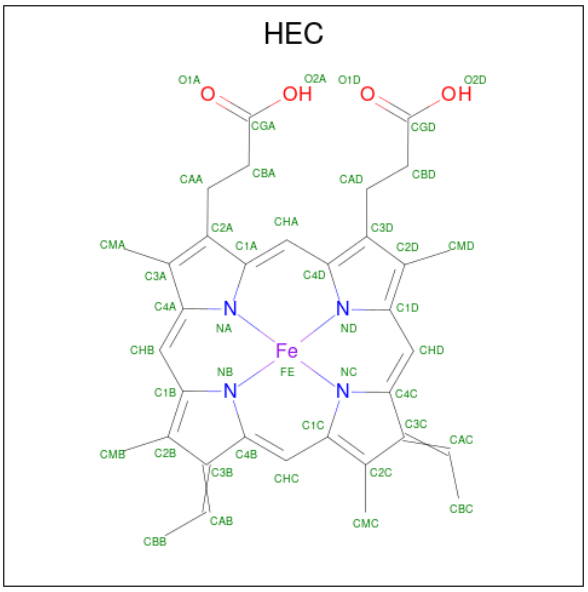
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	O	P	0
			58	39	17	2	
26	E	1	Total	C	O	P	0
			53	34	17	2	
26	H	1	Total	C	O	P	0
			137	99	34	4	
26	H	1	Total	C	O	P	0
			137	99	34	4	
26	L	1	Total	C	O	P	0
			55	36	17	2	
26	O	1	Total	C	O	P	0
			67	48	17	2	
26	P	1	Total	C	O	P	0
			48	29	17	2	
26	S	1	Total	C	O	P	0
			53	34	17	2	

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF) (formula: $C_{40}H_{80}NO_8P$).



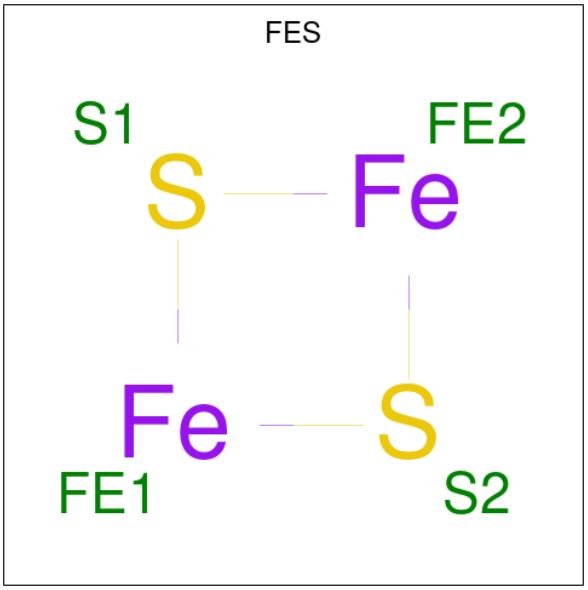
Mol	Chain	Residues	Atoms					AltConf
27	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	I	1	Total	C	N	O	P	0
			30	20	1	8	1	
27	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
27	S	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	T	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	e	1	Total	C	N	O	P	0
			36	26	1	8	1	
27	q	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 28 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

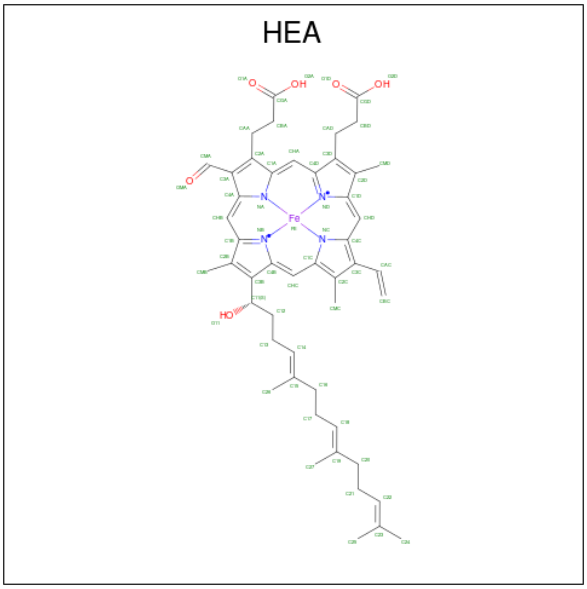


Mol	Chain	Residues	Atoms				AltConf
29	E	1	Total	Fe	S		0
			4	2	2		
29	P	1	Total	Fe	S		0
			4	2	2		

- Molecule 30 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
30	a	1	Total Cu 1 1	0
30	m	1	Total Cu 1 1	0

- Molecule 31 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms	AltConf
31	a	1	Total C Fe N O 120 98 2 8 12	0
31	a	1	Total C Fe N O 120 98 2 8 12	0
31	m	1	Total C Fe N O 120 98 2 8 12	0
31	m	1	Total C Fe N O 120 98 2 8 12	0

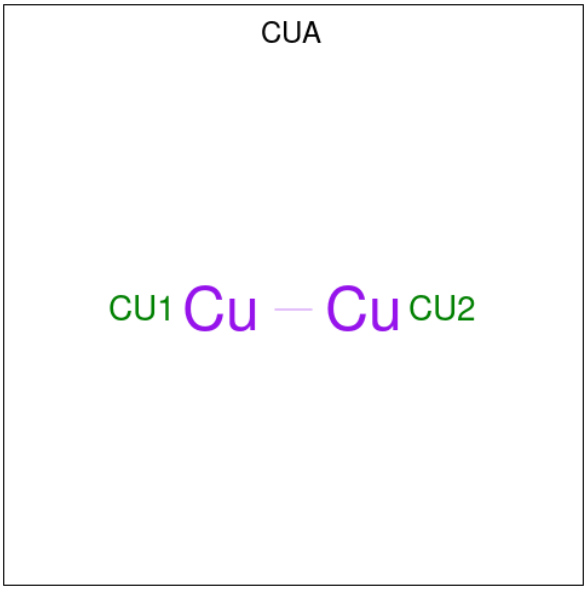
- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total Ca 1 1	0
32	m	1	Total Ca 1 1	0

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
33	a	1	Total Mg 1 1	0
33	m	1	Total Mg 1 1	0

- Molecule 34 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms	AltConf
34	b	1	Total Cu 2 2	0
34	b	1	Total Cu 2 2	0
34	n	1	Total Cu 2 2	0
34	n	1	Total Cu 2 2	0

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

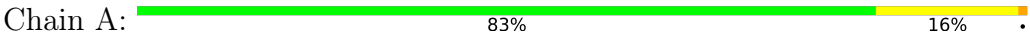
Mol	Chain	Residues	Atoms	AltConf
35	d	1	Total Zn 1 1	0
35	p	1	Total Zn 1 1	0

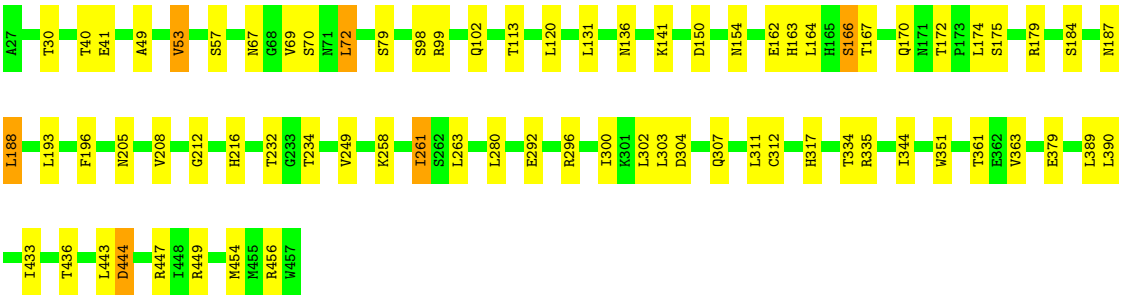
3 Residue-property plots (i)

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

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

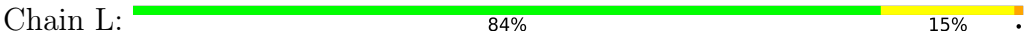
Chain A:

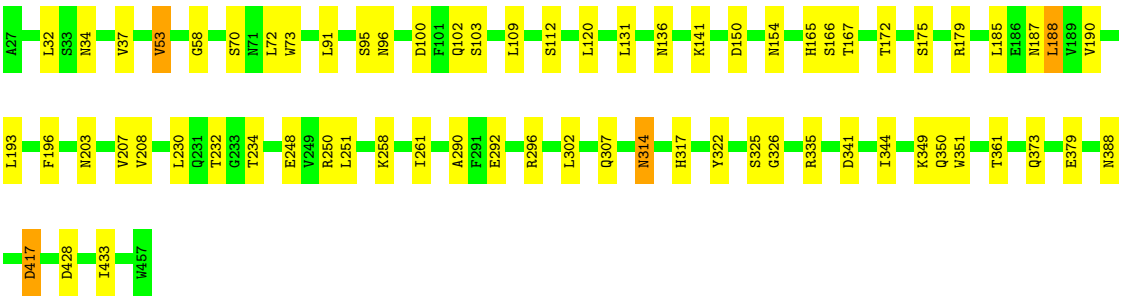




• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

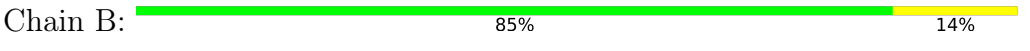
Chain L:

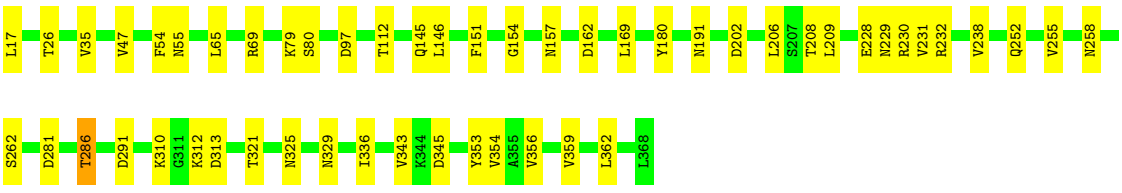




• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

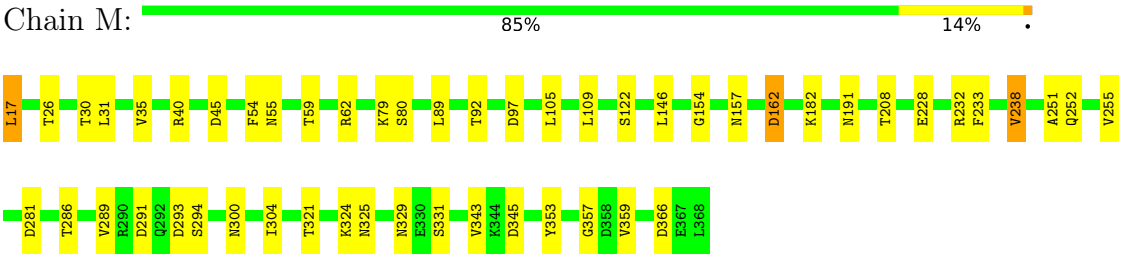
Chain B:





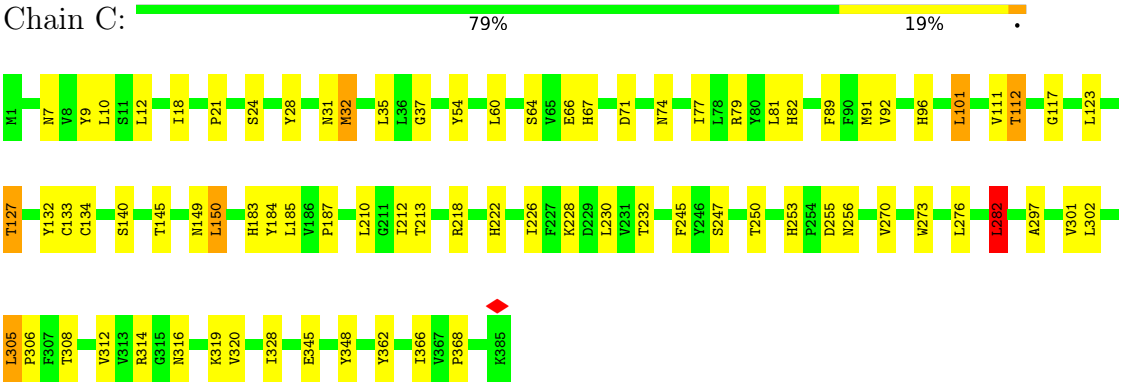
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:



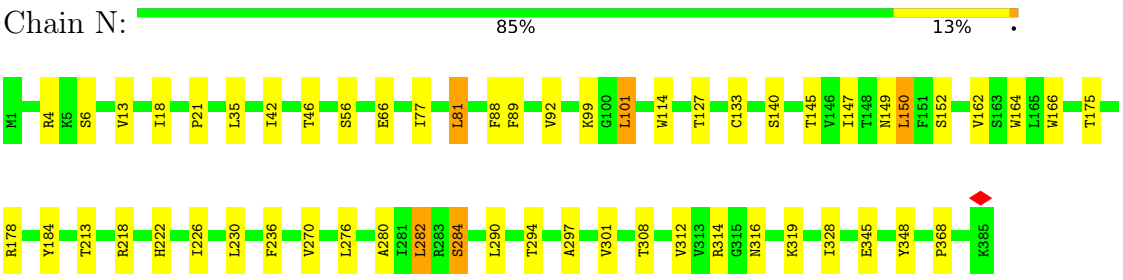
• Molecule 3: Cytochrome b

Chain C:



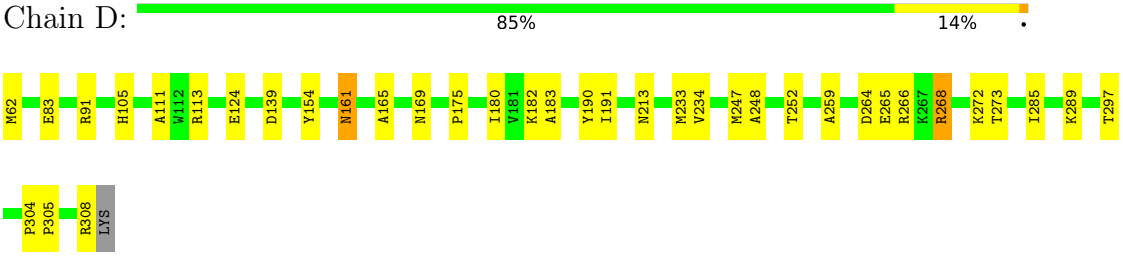
• Molecule 3: Cytochrome b

Chain N:



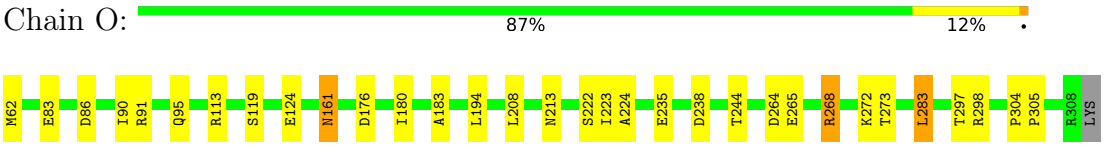
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



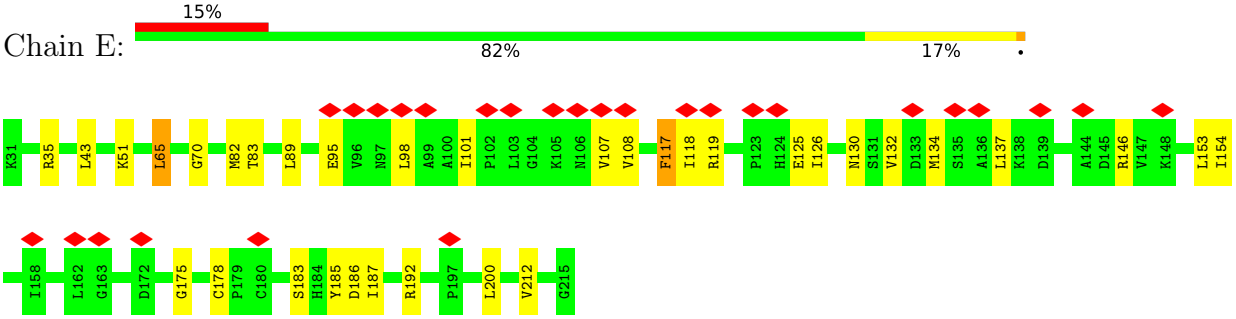
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:



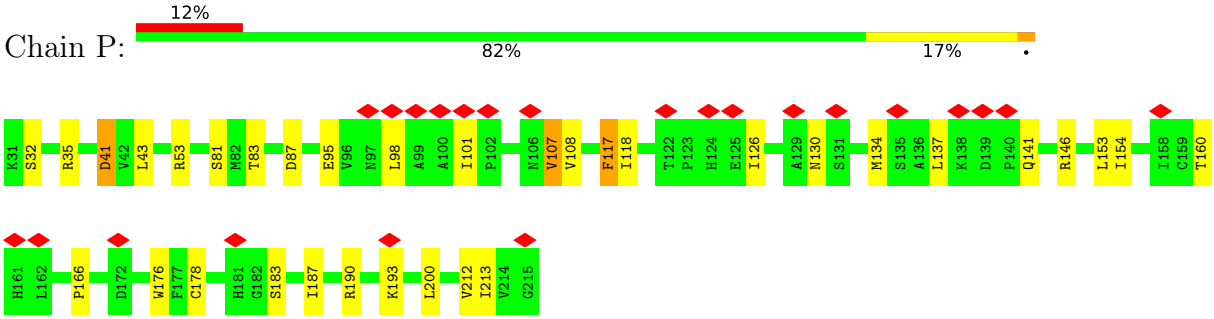
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



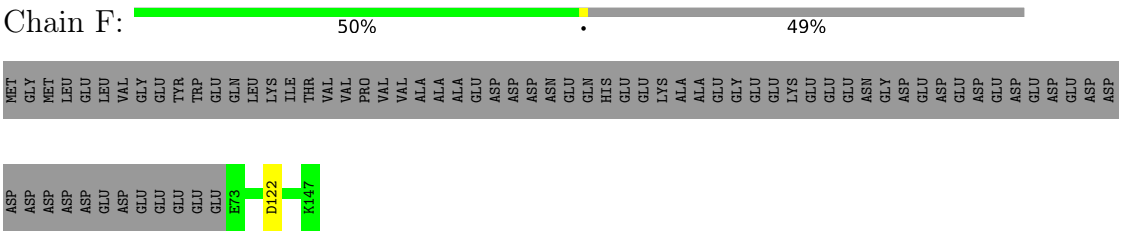
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



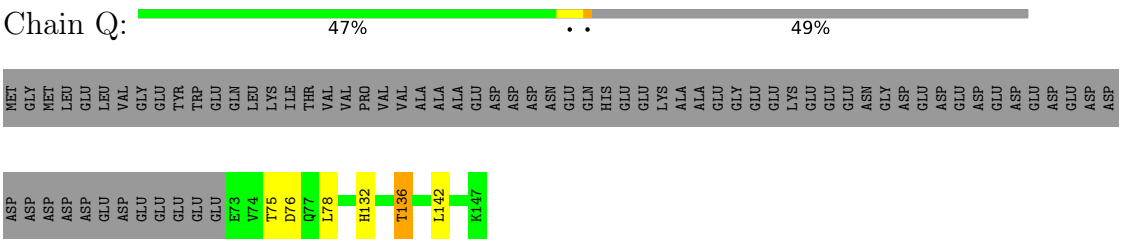
• Molecule 6: Cytochrome b-c1 complex subunit 6

Chain F:



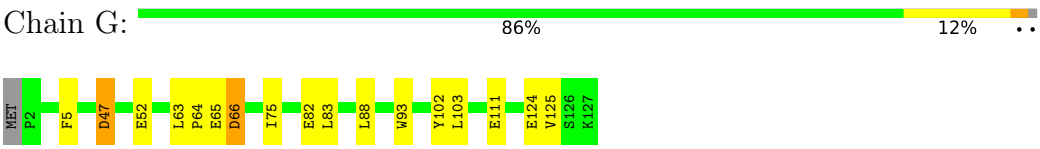
• Molecule 6: Cytochrome b-c1 complex subunit 6

Chain Q:



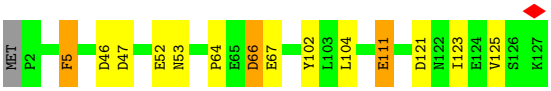
• Molecule 7: Cytochrome b-c1 complex subunit 7

Chain G:



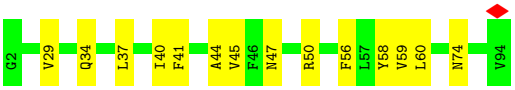
• Molecule 7: Cytochrome b-c1 complex subunit 7

Chain R:



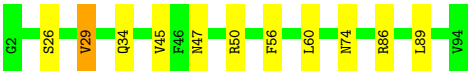
• Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H:



• Molecule 8: Cytochrome b-c1 complex subunit 8

Chain S:

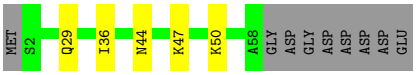


• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain I:

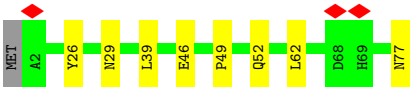
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain T:



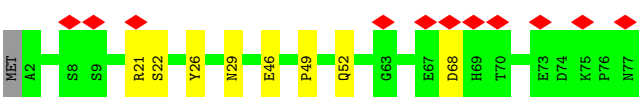
• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain J:



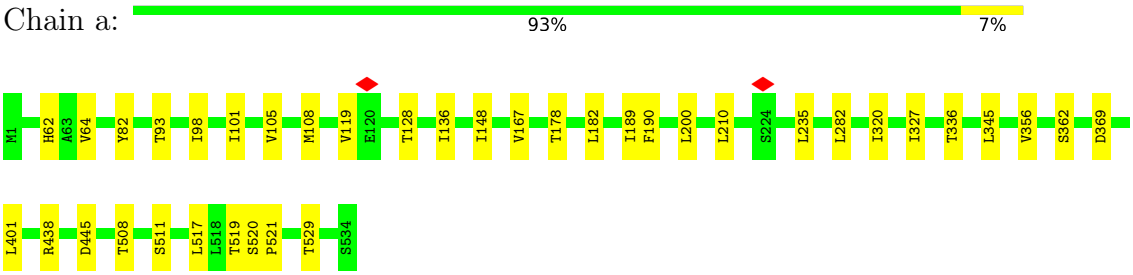
• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain U:



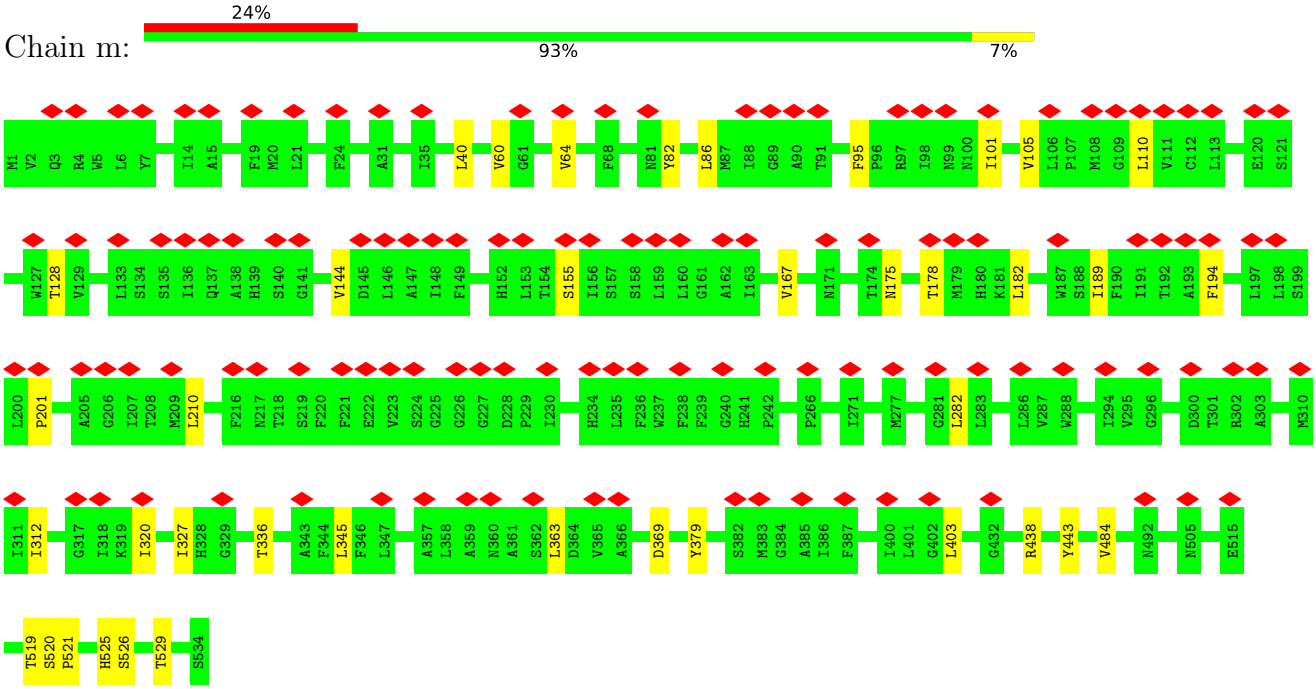
• Molecule 11: Cytochrome c oxidase subunit 1

Chain a:



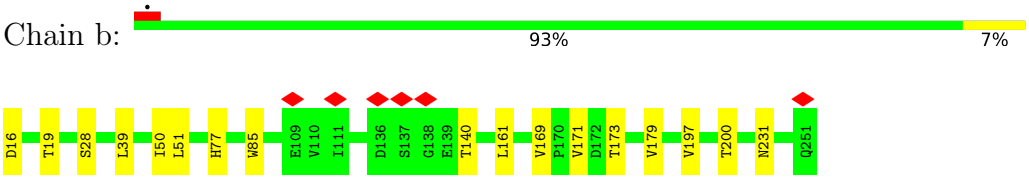
• Molecule 11: Cytochrome c oxidase subunit 1

Chain m:



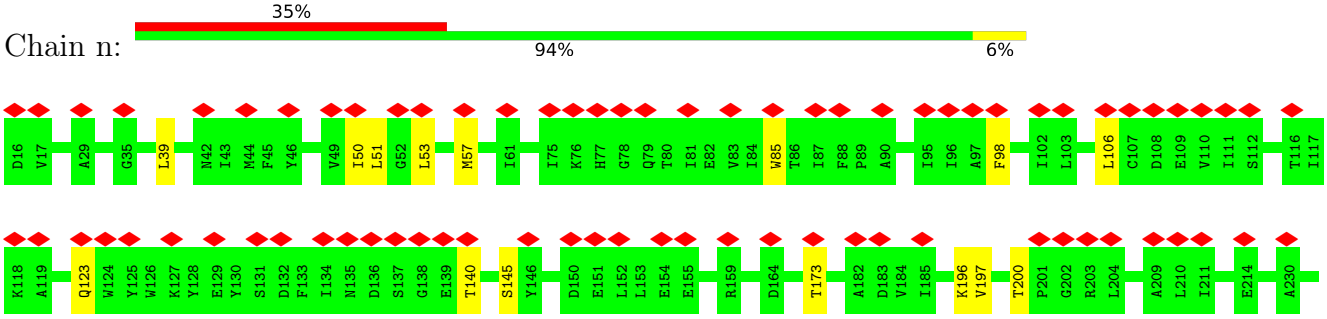
• Molecule 12: Cytochrome c oxidase subunit 2

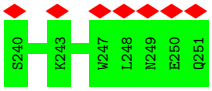
Chain b:



• Molecule 12: Cytochrome c oxidase subunit 2

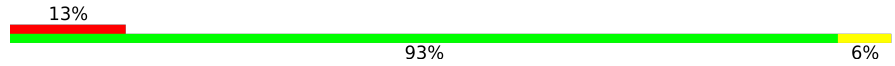
Chain n:

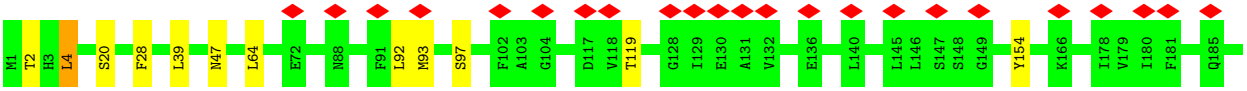


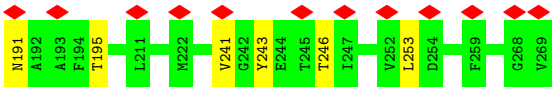


• Molecule 13: Cytochrome c oxidase subunit 3

Chain c:

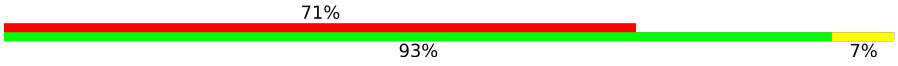


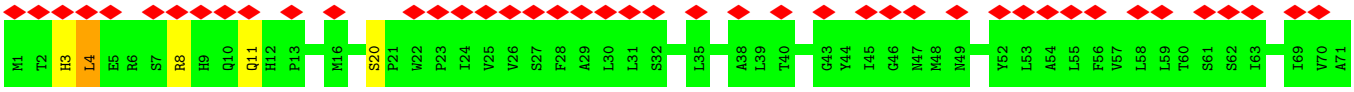


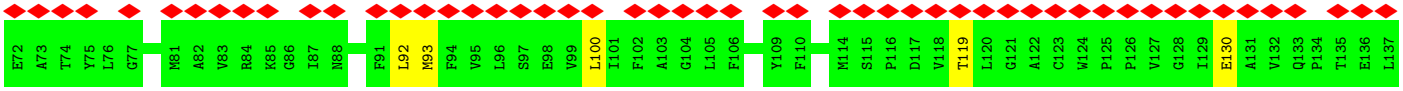


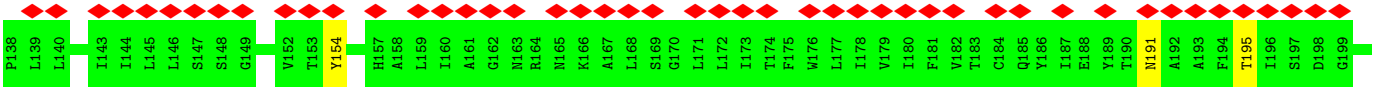
• Molecule 13: Cytochrome c oxidase subunit 3

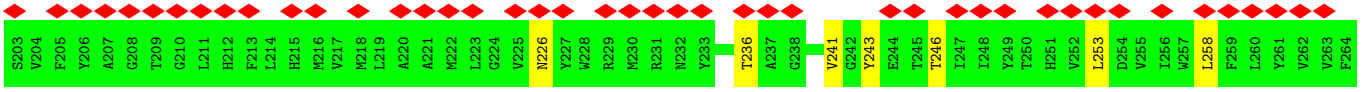
Chain o:

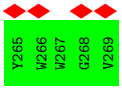






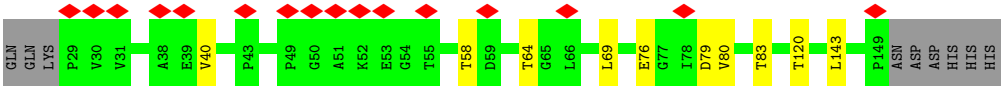






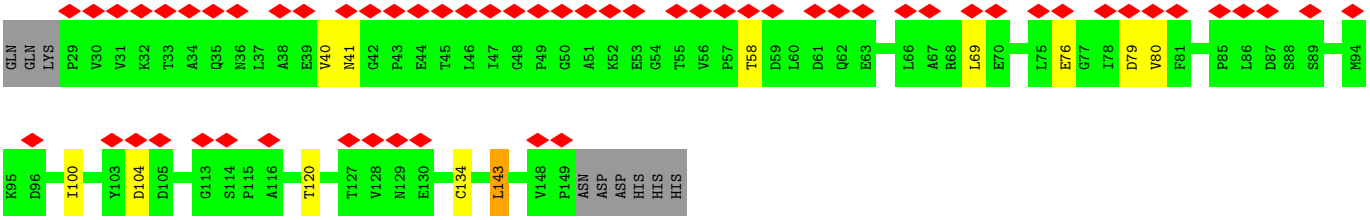
• Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial

Chain d:

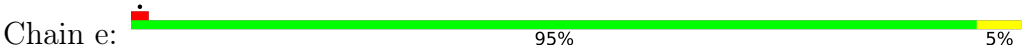


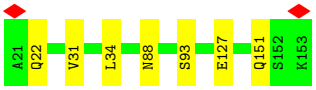
• Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial

Chain p:

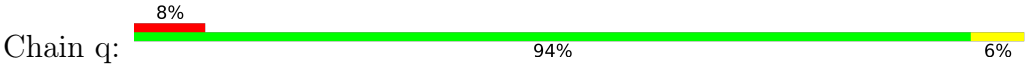


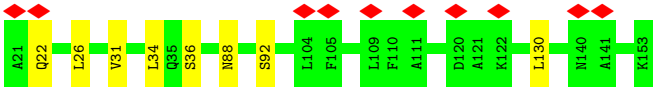
• Molecule 15: Cytochrome c oxidase polypeptide 5A, mitochondrial



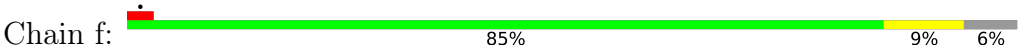


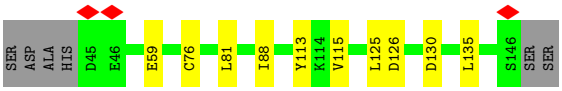
• Molecule 15: Cytochrome c oxidase polypeptide 5A, mitochondrial



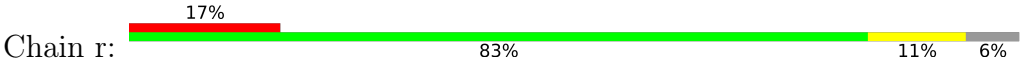


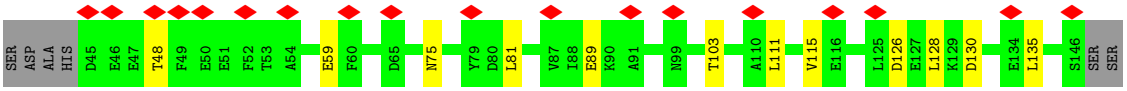
• Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial



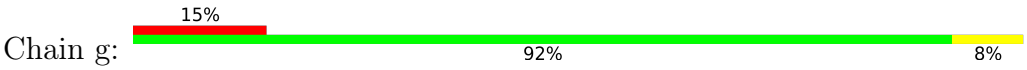


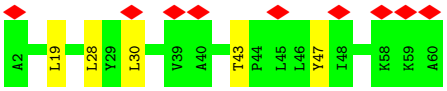
• Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial



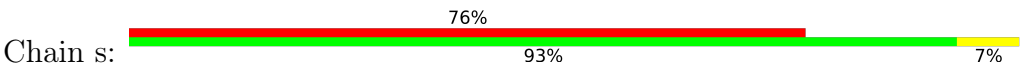


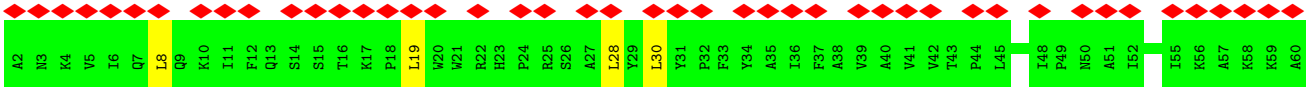
• Molecule 17: Cytochrome c oxidase subunit 7





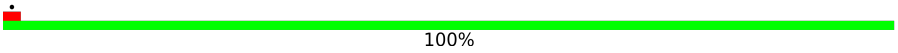
• Molecule 17: Cytochrome c oxidase subunit 7





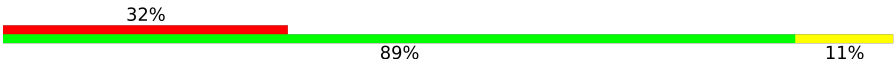
• Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

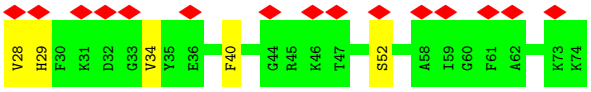
Chain h:



• Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

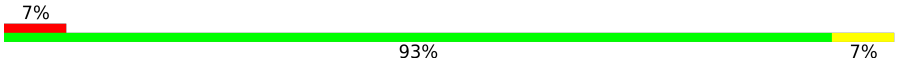
Chain t:

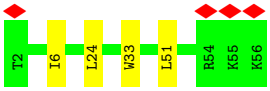




• Molecule 19: Cytochrome c oxidase subunit 7A

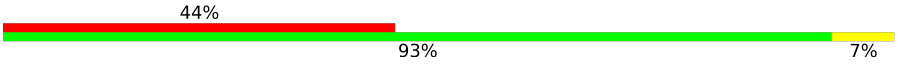
Chain i:

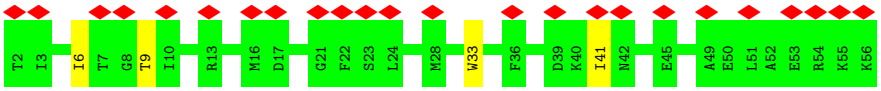




• Molecule 19: Cytochrome c oxidase subunit 7A

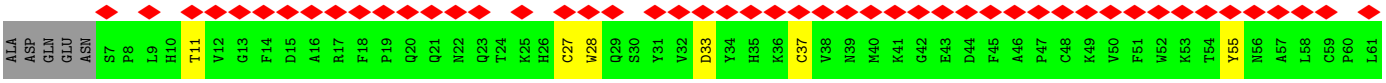
Chain u:

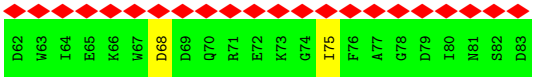




• Molecule 20: Cytochrome c oxidase subunit 6B

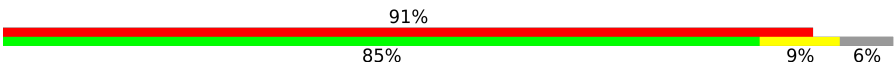
Chain j:

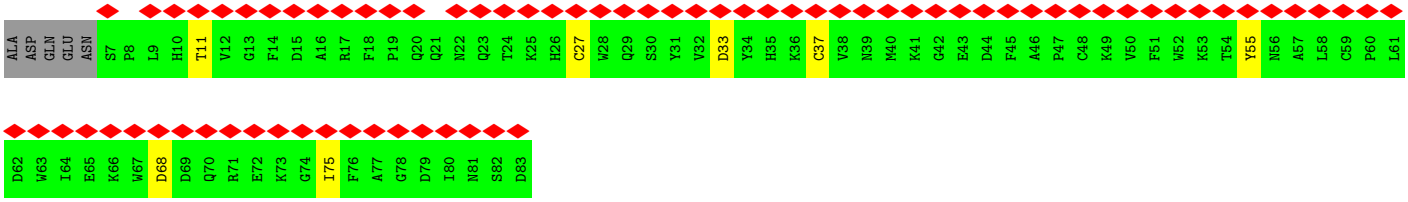




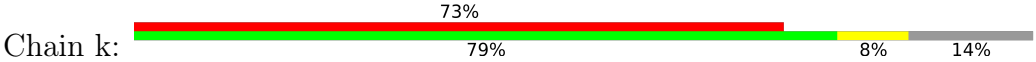
• Molecule 20: Cytochrome c oxidase subunit 6B

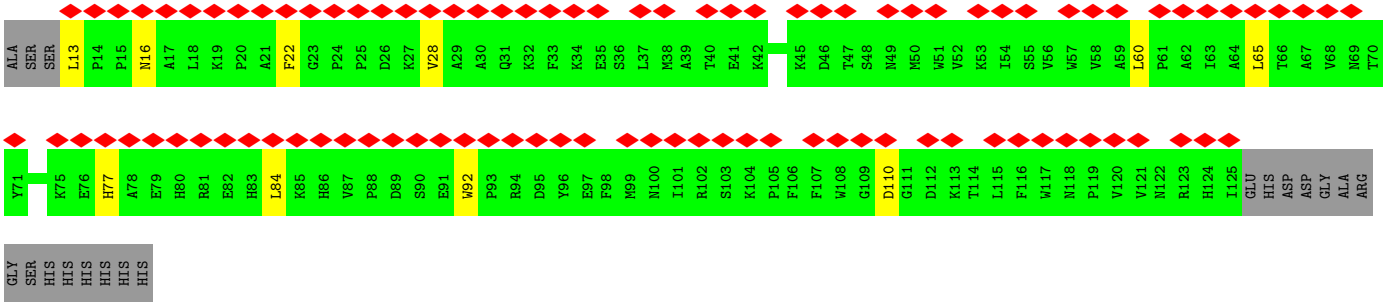
Chain v:



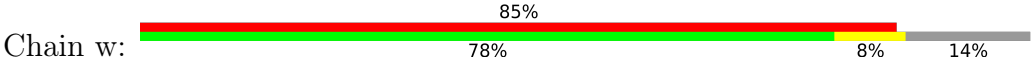


• Molecule 21: Cytochrome c oxidase subunit 6A, mitochondrial

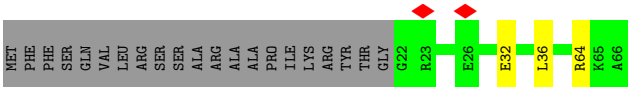




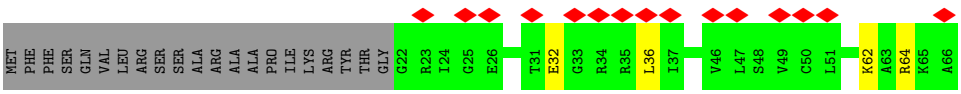
• Molecule 21: Cytochrome c oxidase subunit 6A, mitochondrial



• Molecule 22: Cox26



• Molecule 22: Cox26



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44915	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.645	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.255	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0263	Depositor
Map size (Å)	429.691, 429.691, 429.691	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3861, 1.3861, 1.3861	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, FES, CUA, CDL, PCF, HEA, CU, MG, CA, PEF, HEC, UQ6

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	0.40	0/3406	0.55	0/4615
1	L	0.41	0/3406	0.56	1/4615 (0.0%)
2	B	0.39	0/2781	0.53	0/3764
2	M	0.38	0/2781	0.52	0/3764
3	C	0.44	0/3192	0.57	1/4354 (0.0%)
3	N	0.44	0/3192	0.56	1/4354 (0.0%)
4	D	0.44	0/2012	0.49	0/2740
4	O	0.45	0/2012	0.50	0/2740
5	E	0.32	0/1444	0.50	1/1957 (0.1%)
5	P	0.32	0/1444	0.48	0/1957
6	F	0.36	0/647	0.47	0/870
6	Q	0.36	0/647	0.47	0/870
7	G	0.36	0/1040	0.52	0/1408
7	R	0.35	0/1040	0.53	0/1408
8	H	0.40	0/804	0.50	0/1088
8	S	0.42	0/804	0.47	0/1088
9	I	0.41	0/479	0.48	0/646
9	T	0.40	0/479	0.47	0/646
10	J	0.32	0/619	0.46	0/841
10	U	0.31	0/619	0.46	0/841
11	a	0.53	0/4290	0.63	1/5857 (0.0%)
11	m	0.49	0/4290	0.62	1/5857 (0.0%)
12	b	0.48	0/1941	0.62	0/2653
12	n	0.46	0/1941	0.61	0/2653
13	c	0.42	0/2218	0.55	1/3036 (0.0%)
13	o	0.42	0/2218	0.54	1/3036 (0.0%)
14	d	0.44	0/932	0.60	0/1269
14	p	0.46	0/932	0.61	1/1269 (0.1%)
15	e	0.48	0/1074	0.54	0/1451
15	q	0.46	0/1074	0.54	0/1451
16	f	0.46	0/868	0.51	0/1174
16	r	0.47	0/868	0.53	0/1174

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	g	0.40	0/500	0.57	0/681
17	s	0.38	0/500	0.58	0/681
18	h	0.53	0/397	0.50	0/533
18	t	0.43	0/397	0.49	0/533
19	i	0.40	0/468	0.49	0/626
19	u	0.39	0/468	0.51	0/626
20	j	0.30	0/664	0.49	0/899
20	v	0.28	0/664	0.47	0/899
21	k	0.29	0/962	0.46	0/1310
21	w	0.29	0/962	0.47	0/1310
22	l	0.39	0/372	0.52	0/502
22	x	0.39	0/372	0.54	0/502
All	All	0.43	0/62220	0.55	9/84548 (0.0%)

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
11	a	0	2
11	m	0	1
All	All	0	3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	65	LEU	CA-CB-CG	6.29	129.76	115.30
13	c	4	LEU	CA-CB-CG	6.25	129.67	115.30
1	L	251	LEU	CA-CB-CG	5.67	128.35	115.30
13	o	4	LEU	CA-CB-CG	5.60	128.19	115.30
3	N	282	LEU	CA-CB-CG	5.58	128.14	115.30
14	p	143	LEU	CA-CB-CG	5.55	128.07	115.30
3	C	282	LEU	CA-CB-CG	5.36	127.62	115.30
11	m	327	ILE	CG1-CB-CG2	-5.11	100.16	111.40
11	a	327	ILE	CG1-CB-CG2	-5.09	100.20	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	a	119	VAL	Peptide
11	a	520	SER	Peptide
11	m	520	SER	Peptide

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	3345	0	3323	33	0
1	L	3345	0	3323	34	0
2	B	2735	0	2774	26	0
2	M	2735	0	2774	29	0
3	C	3090	0	3129	49	0
3	N	3090	0	3129	30	0
4	D	1951	0	1875	25	0
4	O	1951	0	1875	19	0
5	E	1411	0	1386	20	0
5	P	1411	0	1386	17	0
6	F	633	0	587	1	0
6	Q	633	0	587	3	0
7	G	1019	0	1034	13	0
7	R	1019	0	1034	9	0
8	H	773	0	736	10	0
8	S	773	0	736	7	0
9	I	465	0	459	7	0
9	T	465	0	459	5	0
10	J	599	0	594	5	0
10	U	599	0	594	5	0
11	a	4162	0	4191	0	0
11	m	4162	0	4191	0	0
12	b	1889	0	1866	0	0
12	n	1889	0	1866	0	0
13	c	2146	0	2137	0	0
13	o	2146	0	2137	0	0
14	d	913	0	909	0	0
14	p	913	0	910	0	0
15	e	1049	0	1030	0	0
15	q	1049	0	1030	0	0
16	f	851	0	822	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	r	851	0	822	0	0
17	g	484	0	517	0	0
17	s	484	0	517	0	0
18	h	383	0	386	0	0
18	t	383	0	386	0	0
19	i	456	0	469	0	0
19	u	456	0	469	0	0
20	j	642	0	586	0	0
20	v	642	0	586	0	0
21	k	928	0	906	0	0
21	w	928	0	906	0	0
22	l	361	0	363	0	0
22	x	361	0	363	0	0
23	A	44	0	64	2	0
23	C	75	0	99	1	0
23	D	42	0	60	4	0
23	E	29	0	31	1	0
23	H	32	0	37	0	0
23	N	114	0	150	4	0
23	O	43	0	62	2	0
23	P	29	0	31	1	0
23	S	36	0	48	1	0
23	a	113	0	151	0	0
23	b	40	0	56	0	0
23	c	77	0	100	0	0
23	e	47	0	73	0	0
23	h	47	0	73	0	0
23	m	80	0	112	0	0
23	n	73	0	95	0	0
23	o	77	0	100	0	0
23	q	47	0	73	0	0
23	t	47	0	73	0	0
24	C	86	0	60	4	0
24	N	86	0	60	1	0
25	C	86	0	116	7	0
26	C	58	0	60	0	0
26	E	53	0	50	3	0
26	H	137	0	165	5	0
26	L	55	0	54	2	0
26	O	67	0	78	5	0
26	P	48	0	40	0	0
26	S	53	0	50	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	C	39	0	55	0	0
27	H	32	0	38	1	0
27	I	30	0	34	0	0
27	N	50	0	80	2	0
27	S	32	0	38	0	0
27	T	39	0	52	1	0
27	e	36	0	46	0	0
27	q	36	0	46	0	0
28	D	43	0	29	1	0
28	O	43	0	29	1	0
29	E	4	0	0	0	0
29	P	4	0	0	0	0
30	a	1	0	0	0	0
30	m	1	0	0	0	0
31	a	120	0	108	0	0
31	m	120	0	108	0	0
32	a	1	0	0	0	0
32	m	1	0	0	0	0
33	a	1	0	0	0	0
33	m	1	0	0	0	0
34	b	2	0	0	0	0
34	n	2	0	0	0	0
35	d	1	0	0	0	0
35	p	1	0	0	0	0
All	All	63031	0	63043	324	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 5.

All (324) 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)
2:M:325:ASN:O	2:M:329:ASN:HB2	1.84	0.77
2:B:255:VAL:HG12	2:B:321:THR:HG21	1.69	0.74
8:S:56:PHE:O	8:S:60:LEU:HB2	1.88	0.73
2:B:258:ASN:O	2:B:262:SER:HB3	1.92	0.69
1:L:317:HIS:HE1	1:L:351:TRP:HE1	1.43	0.66
1:A:258:LYS:HG2	1:A:335:ARG:HG2	1.77	0.66
2:M:255:VAL:HG12	2:M:321:THR:HG21	1.79	0.64
2:B:325:ASN:O	2:B:329:ASN:HB2	1.97	0.64
3:C:9:TYR:HB3	23:C:605:PEF:H192	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:THR:O	3:C:149:ASN:HB2	1.99	0.62
3:N:127:THR:HG21	24:N:601:HEM:HBB2	1.81	0.62
5:E:178:CYS:HB3	5:E:183:SER:HB2	1.81	0.62
3:C:316:ASN:HA	3:C:319:LYS:HD2	1.82	0.62
4:D:273:THR:HG23	23:D:402:PEF:H112	1.82	0.62
3:N:150:LEU:HD21	3:N:282:LEU:HD11	1.81	0.62
2:M:162:ASP:OD1	2:M:162:ASP:N	2.33	0.61
2:B:26:THR:OG1	2:B:191:ASN:ND2	2.34	0.61
2:B:69:ARG:NH2	7:R:121:ASP:OD1	2.34	0.60
1:L:141:LYS:NZ	1:L:185:LEU:O	2.35	0.60
4:D:165:ALA:O	4:D:169:ASN:ND2	2.33	0.60
7:G:125:VAL:HG12	1:L:361:THR:HG22	1.84	0.60
5:P:108:VAL:HG22	5:P:117:PHE:HB3	1.84	0.59
26:L:501:CDL:OB4	3:N:4:ARG:NH2	2.35	0.59
4:D:233:MET:HG3	4:D:234:VAL:HG23	1.85	0.58
3:N:316:ASN:HA	3:N:319:LYS:HD2	1.85	0.58
9:I:29:GLN:NE2	10:J:46:GLU:OE1	2.36	0.58
3:C:31:ASN:ND2	3:C:228:LYS:O	2.36	0.58
5:E:175:GLY:HA3	5:E:185:TYR:O	2.04	0.58
9:I:30:THR:HG21	10:J:62:LEU:HB3	1.85	0.58
1:L:428:ASP:O	5:P:53:ARG:NH2	2.37	0.58
4:D:297:THR:OG1	8:H:34:GLN:NE2	2.37	0.57
3:N:77:ILE:O	3:N:81:LEU:HB2	2.04	0.57
5:E:134:MET:HA	5:E:137:LEU:HD12	1.86	0.57
5:E:108:VAL:HG22	5:E:117:PHE:HB3	1.87	0.57
5:E:118:ILE:HG12	5:E:154:ILE:HG12	1.86	0.57
23:N:603:PEF:H311	23:N:603:PEF:H151	1.86	0.57
3:C:77:ILE:O	3:C:81:LEU:HB2	2.05	0.56
4:O:95:GLN:NE2	4:O:235:GLU:O	2.38	0.56
4:O:265:GLU:OE2	4:O:268:ARG:NH1	2.38	0.56
1:A:72:LEU:HB3	1:A:193:LEU:HD21	1.85	0.56
5:P:178:CYS:HB3	5:P:183:SER:HB2	1.88	0.56
7:G:47:ASP:N	7:G:47:ASP:OD1	2.37	0.56
3:C:245:PHE:O	4:D:266:ARG:NH2	2.39	0.56
4:D:308:ARG:NH2	7:G:65:GLU:OE2	2.37	0.56
23:D:402:PEF:H392	23:D:402:PEF:H332	1.87	0.56
3:N:145:THR:O	3:N:149:ASN:HB2	2.05	0.56
3:N:314:ARG:NH1	7:R:52:GLU:OE1	2.39	0.56
1:L:32:LEU:HG	1:L:37:VAL:HG22	1.88	0.56
8:H:56:PHE:O	8:H:60:LEU:HB2	2.06	0.55
1:L:150:ASP:OD1	1:L:154:ASN:ND2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:292:GLU:OE2	2:M:79:LYS:NZ	2.39	0.55
2:M:154:GLY:O	2:M:157:ASN:ND2	2.38	0.55
3:C:314:ARG:NH1	7:G:52:GLU:OE1	2.39	0.55
5:E:98:LEU:HA	5:E:101:ILE:HD12	1.88	0.55
3:N:35:LEU:HB3	3:N:92:VAL:HG11	1.89	0.55
1:A:98:SER:OG	1:A:99:ARG:N	2.39	0.55
2:B:145:GLN:OE1	2:B:229:ASN:ND2	2.40	0.55
2:M:228:GLU:HA	2:M:353:TYR:O	2.06	0.55
5:E:186:ASP:OD2	5:E:192:ARG:NH1	2.40	0.55
3:C:270:VAL:HG13	3:C:276:LEU:HD21	1.89	0.54
2:M:252:GLN:NE2	2:M:345:ASP:O	2.39	0.54
9:T:29:GLN:NE2	10:U:46:GLU:OE1	2.39	0.54
4:D:83:GLU:HA	9:I:44:ASN:HD21	1.72	0.54
2:B:162:ASP:OD2	2:M:232:ARG:NH2	2.41	0.54
2:B:232:ARG:NH1	2:M:45:ASP:OD2	2.40	0.54
2:M:26:THR:OG1	2:M:191:ASN:ND2	2.40	0.54
2:B:146:LEU:HD23	2:B:286:THR:HG22	1.89	0.54
1:A:263:LEU:HD13	1:A:433:ILE:HG12	1.90	0.54
2:M:255:VAL:HG11	2:M:343:VAL:HG21	1.89	0.54
1:A:163:HIS:HA	1:A:166:SER:HB3	1.89	0.53
1:A:261:ILE:HD12	1:A:344:ILE:HD11	1.89	0.53
1:L:317:HIS:CE1	1:L:351:TRP:HE1	2.26	0.53
5:P:134:MET:HA	5:P:137:LEU:HD12	1.88	0.53
1:L:72:LEU:HD12	1:L:188:LEU:HD23	1.91	0.53
2:M:17:LEU:N	2:M:182:LYS:O	2.42	0.53
5:P:41:ASP:N	5:P:41:ASP:OD1	2.37	0.53
4:D:161:ASN:OD1	4:D:161:ASN:N	2.42	0.53
1:A:150:ASP:OD1	1:A:154:ASN:ND2	2.42	0.53
1:A:102:GLN:HE22	1:A:196:PHE:HE2	1.56	0.52
1:A:292:GLU:OE2	2:B:79:LYS:NZ	2.42	0.52
1:A:303:LEU:O	1:A:307:GLN:HB2	2.09	0.52
3:N:230:LEU:HD13	23:N:603:PEF:H331	1.91	0.52
3:N:270:VAL:HG13	3:N:276:LEU:HD21	1.91	0.52
1:L:314:ASN:OD1	1:L:314:ASN:N	2.43	0.52
3:C:12:LEU:HD13	25:C:603[A]:UQ6:H112	1.90	0.52
1:A:141:LYS:NZ	1:A:188:LEU:O	2.41	0.52
27:N:606:PCF:H362	27:N:606:PCF:H272	1.91	0.52
3:N:21:PRO:O	3:N:218:ARG:NH2	2.42	0.52
3:C:212:ILE:HD12	7:G:75:ILE:HG12	1.92	0.52
5:E:83:THR:HG21	23:E:303:PEF:H12	1.92	0.52
3:N:280:ALA:O	3:N:284:SER:OG	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:51:ASP:N	9:I:51:ASP:OD1	2.43	0.51
2:M:40:ARG:NH1	2:M:281:ASP:OD2	2.42	0.51
3:C:67:HIS:ND1	3:C:71:ASP:OD2	2.44	0.51
4:D:289:LYS:NZ	26:H:602:CDL:OA4	2.43	0.51
8:H:40:ILE:O	8:H:44:ALA:HB2	2.10	0.51
7:R:64:PRO:HG2	7:R:67:GLU:HG3	1.93	0.51
1:A:67:ASN:O	1:A:184:SER:OG	2.29	0.51
5:P:83:THR:HG21	23:P:303:PEF:H12	1.92	0.51
5:P:43:LEU:HD21	8:S:29:VAL:HG11	1.92	0.51
1:A:131:LEU:O	1:A:136:ASN:ND2	2.44	0.51
1:A:361:THR:HG22	7:R:125:VAL:HG12	1.93	0.50
1:L:325:SER:OG	1:L:326:GLY:N	2.44	0.50
5:P:98:LEU:HA	5:P:101:ILE:HD12	1.93	0.50
2:B:55:ASN:OD1	2:B:180:TYR:OH	2.29	0.50
3:C:183:HIS:HE1	24:C:601:HEM:NB	2.08	0.50
2:B:252:GLN:NE2	2:B:345:ASP:O	2.43	0.50
3:C:111:VAL:HG13	3:C:306:PRO:HG2	1.93	0.50
6:Q:132:HIS:O	6:Q:136:THR:OG1	2.29	0.50
2:M:30:THR:HG22	2:M:92:THR:HG23	1.93	0.50
26:E:302:CDL:H342	9:I:6:LEU:HD11	1.93	0.50
4:O:83:GLU:HA	9:T:44:ASN:HD21	1.76	0.50
2:B:232:ARG:NH2	2:M:162:ASP:OD2	2.43	0.49
23:D:402:PEF:H142	5:E:70:GLY:HA3	1.92	0.49
8:H:41:PHE:HB2	27:H:604:PCF:H12	1.94	0.49
3:N:147:ILE:HA	3:N:150:LEU:HD22	1.94	0.49
5:E:126:ILE:O	5:E:130:ASN:ND2	2.45	0.49
2:M:228:GLU:HG3	2:M:353:TYR:HD2	1.77	0.49
6:Q:78:LEU:HD13	6:Q:142:LEU:HD22	1.94	0.49
3:C:60:LEU:O	3:C:64:SER:HB3	2.12	0.49
1:L:166:SER:HA	1:L:175:SER:HB2	1.92	0.49
1:L:349:LYS:HE3	26:L:501:CDL:HA22	1.94	0.49
3:C:28:TYR:HB2	26:H:601:CDL:HA32	1.94	0.49
3:C:320:VAL:HG13	8:H:58:TYR:HE1	1.78	0.49
4:O:224:ALA:HB3	28:O:401:HEC:HBD2	1.95	0.49
4:O:297:THR:OG1	8:S:34:GLN:NE2	2.41	0.49
2:B:154:GLY:O	2:B:157:ASN:ND2	2.38	0.49
3:N:345:GLU:OE2	4:O:62:MET:N	2.45	0.49
3:C:133:CYS:HA	3:C:140:SER:HB3	1.94	0.49
3:N:348:TYR:OH	8:S:74:ASN:OD1	2.31	0.49
3:C:7:ASN:HB3	3:C:10:LEU:HB2	1.93	0.49
3:C:123:LEU:O	3:C:127:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:272:LYS:HG3	9:T:36:ILE:HG21	1.93	0.49
5:E:186:ASP:OD1	5:E:186:ASP:N	2.40	0.48
7:G:88:LEU:O	7:G:93:TRP:NE1	2.42	0.48
5:P:126:ILE:O	5:P:130:ASN:ND2	2.46	0.48
3:N:42:ILE:O	3:N:46:THR:OG1	2.31	0.48
1:A:57:SER:O	1:A:102:GLN:NE2	2.45	0.48
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.32	0.48
3:C:247:SER:OG	3:C:250:THR:OG1	2.26	0.48
3:C:24:SER:HB2	7:G:83:LEU:HD12	1.95	0.48
5:E:95:GLU:HA	5:E:212:VAL:O	2.13	0.48
1:L:261:ILE:HD12	1:L:344:ILE:HD11	1.94	0.48
2:M:31:LEU:HD23	2:M:105:LEU:HD12	1.95	0.48
3:N:166:TRP:O	3:N:175:THR:OG1	2.28	0.48
1:A:444:ASP:OD1	1:A:444:ASP:N	2.39	0.48
25:C:603[B]:UQ6:H321	25:C:603[B]:UQ6:H301	1.56	0.47
1:A:57:SER:OG	1:A:205:ASN:ND2	2.41	0.47
1:A:443:LEU:HD13	1:A:447:ARG:HG2	1.96	0.47
3:C:348:TYR:OH	8:H:74:ASN:OD1	2.32	0.47
8:H:47:ASN:OD1	8:H:50:ARG:NH2	2.47	0.47
3:C:21:PRO:O	3:C:218:ARG:NH2	2.47	0.47
4:O:180:ILE:HA	4:O:183:ALA:HB3	1.96	0.47
9:I:30:THR:O	9:I:34:THR:OG1	2.31	0.47
3:N:13:VAL:HG11	23:N:605:PEF:H181	1.97	0.47
2:B:281:ASP:N	2:B:281:ASP:OD1	2.48	0.47
4:D:91:ARG:NH1	4:D:124:GLU:OE2	2.43	0.47
5:P:107:VAL:O	5:P:117:PHE:HA	2.15	0.47
10:U:22:SER:O	10:U:26:TYR:HB2	2.14	0.47
2:B:228:GLU:HA	2:B:353:TYR:O	2.15	0.47
26:O:402:CDL:O1	26:S:601:CDL:OA4	2.33	0.47
3:C:297:ALA:O	3:C:301:VAL:HB	2.14	0.47
8:H:47:ASN:ND2	26:H:602:CDL:OB3	2.43	0.47
1:L:102:GLN:HE22	1:L:196:PHE:HE2	1.61	0.47
1:L:103:SER:OG	1:L:388:ASN:ND2	2.47	0.47
1:A:296:ARG:HD2	1:A:307:GLN:HE21	1.79	0.47
2:M:233:PHE:HB3	2:M:357:GLY:HA2	1.95	0.47
4:O:283:LEU:HD22	26:O:402:CDL:H632	1.95	0.47
5:P:146:ARG:NH1	5:P:200:LEU:O	2.35	0.46
2:B:202:ASP:N	2:B:202:ASP:OD1	2.48	0.46
3:C:35:LEU:HB3	3:C:92:VAL:HG11	1.96	0.46
2:B:162:ASP:OD1	2:B:162:ASP:N	2.44	0.46
1:A:300:ILE:HG22	1:A:302:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:VAL:HG11	2:B:343:VAL:HG21	1.98	0.46
3:C:345:GLU:OE2	4:D:62:MET:N	2.48	0.46
4:D:182:LYS:HG3	4:D:259:ALA:HB1	1.96	0.46
3:C:112:THR:HB	23:N:604:PEF:H21	1.98	0.46
4:D:105:HIS:HE1	4:D:175:PRO:HD2	1.80	0.46
5:P:118:ILE:HG12	5:P:154:ILE:HG12	1.97	0.46
5:P:95:GLU:HA	5:P:212:VAL:O	2.17	0.45
8:S:47:ASN:OD1	8:S:50:ARG:NH2	2.48	0.45
25:C:603[A]:UQ6:H251	25:C:603[A]:UQ6:H272	1.70	0.45
1:A:49:ALA:HA	1:A:212:GLY:HA3	1.99	0.45
3:C:91:MET:HG3	3:C:273:TRP:HH2	1.81	0.45
9:I:23:ALA:HB2	10:J:39:LEU:HD13	1.99	0.45
1:L:131:LEU:O	1:L:136:ASN:ND2	2.49	0.45
26:O:402:CDL:OB3	8:S:47:ASN:ND2	2.48	0.45
10:U:49:PRO:HA	10:U:52:GLN:HB2	1.99	0.45
3:C:150:LEU:HD21	3:C:282:LEU:HD11	1.98	0.45
1:L:53:VAL:HG12	1:L:120:LEU:HD21	1.98	0.45
4:O:304:PRO:HA	4:O:305:PRO:HD3	1.83	0.45
1:A:312:CYS:HA	1:A:334:THR:HB	1.99	0.45
1:L:341:ASP:OD1	1:L:341:ASP:N	2.50	0.45
3:N:18:ILE:HA	3:N:222:HIS:HB2	1.98	0.45
4:O:91:ARG:NH1	4:O:124:GLU:OE2	2.37	0.45
5:P:141:GLN:OE1	5:P:146:ARG:NH2	2.45	0.45
7:R:5:PHE:N	7:R:111:GLU:OE2	2.43	0.45
25:C:603[B]:UQ6:H172	25:C:603[B]:UQ6:H151	1.70	0.45
3:C:362:TYR:HA	3:C:366:ILE:HB	1.99	0.45
5:E:132:VAL:HG21	5:E:192:ARG:HH12	1.81	0.44
3:C:32:MET:HE1	26:H:601:CDL:H322	1.98	0.44
4:D:304:PRO:HA	4:D:305:PRO:HD3	1.82	0.44
1:L:37:VAL:HB	1:L:207:VAL:HG22	1.98	0.44
1:L:248:GLU:OE1	1:L:250:ARG:NH1	2.45	0.44
2:M:79:LYS:HD2	2:M:79:LYS:HA	1.76	0.44
3:C:253:HIS:HD2	3:C:255:ASP:HB2	1.83	0.44
5:E:43:LEU:HD21	8:H:29:VAL:HG21	2.00	0.44
3:N:88:PHE:HB3	3:N:236:PHE:HE1	1.82	0.44
3:C:74:ASN:HB3	3:C:77:ILE:HD12	1.99	0.44
7:R:66:ASP:OD1	7:R:66:ASP:N	2.48	0.44
5:E:51:LYS:HG2	26:E:302:CDL:HA31	2.00	0.44
5:P:141:GLN:O	5:P:190:ARG:NE	2.50	0.44
7:G:66:ASP:OD1	7:G:66:ASP:N	2.40	0.44
10:J:49:PRO:HA	10:J:52:GLN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:O:402:CDL:H322	26:S:601:CDL:H111	1.99	0.44
2:B:310:LYS:HB2	2:B:310:LYS:HE3	1.91	0.43
7:G:63:LEU:HD12	7:G:64:PRO:HD2	1.99	0.43
1:L:417:ASP:OD1	1:L:417:ASP:N	2.51	0.43
5:E:82:MET:HB3	3:N:164:TRP:HE1	1.83	0.43
4:O:273:THR:HG23	23:O:403:PEF:H112	2.00	0.43
2:M:324:LYS:HD3	2:M:324:LYS:HA	1.88	0.43
1:A:53:VAL:HG12	1:A:120:LEU:HD21	1.99	0.43
2:B:229:ASN:O	2:B:354:VAL:HA	2.18	0.43
1:A:456:ARG:HD3	1:A:456:ARG:HA	1.92	0.43
23:A:501:PEF:H181	3:C:230:LEU:HD11	2.00	0.43
3:C:308:THR:HB	3:C:368:PRO:HG3	2.00	0.43
5:E:119:ARG:NH1	5:E:125:GLU:OE2	2.46	0.43
1:L:296:ARG:HH21	1:L:307:GLN:HE21	1.66	0.43
2:M:293:ASP:OD1	2:M:293:ASP:N	2.45	0.43
4:D:248:ALA:O	4:D:252:THR:OG1	2.30	0.43
4:O:208:LEU:HD12	4:O:208:LEU:HA	1.87	0.43
4:O:238:ASP:OD1	4:O:238:ASP:N	2.50	0.43
4:D:111:ALA:HA	4:D:154:TYR:HA	2.00	0.43
4:D:265:GLU:OE2	4:D:268:ARG:NH1	2.52	0.43
4:D:139:ASP:OD1	4:D:139:ASP:N	2.52	0.43
4:D:289:LYS:HD3	8:H:37:LEU:HD23	2.01	0.43
2:M:55:ASN:ND2	2:M:80:SER:OG	2.41	0.43
27:T:101:PCF:H142	27:T:101:PCF:H111	1.88	0.43
3:C:96:HIS:HD2	24:C:602:HEM:C1C	2.37	0.42
2:M:331:SER:O	2:M:331:SER:OG	4.37	0.42
3:N:290:LEU:O	3:N:294:THR:OG1	2.30	0.42
3:N:308:THR:HB	3:N:368:PRO:HG3	2.01	0.42
1:A:166:SER:HA	1:A:175:SER:HB2	2.01	0.42
1:A:280:LEU:HD21	1:A:363:VAL:HG13	2.01	0.42
3:N:42:ILE:HG12	23:O:403:PEF:H412	2.01	0.42
3:C:18:ILE:HA	3:C:222:HIS:HB2	2.01	0.42
3:C:127:THR:HG21	3:C:187:PRO:HG3	2.01	0.42
1:A:304:ASP:OD1	1:A:304:ASP:N	2.53	0.42
1:L:73:TRP:CD1	1:L:193:LEU:HD23	2.55	0.42
4:O:86:ASP:HA	9:T:47:LYS:HB3	2.01	0.42
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.89	0.42
5:E:146:ARG:NH1	5:E:200:LEU:O	2.44	0.42
1:L:58:GLY:N	1:L:100:ASP:O	2.51	0.42
2:M:89:LEU:HD13	2:M:109:LEU:HD11	2.02	0.42
8:S:86:ARG:HA	8:S:89:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:122:ASP:OD1	6:F:122:ASP:N	2.53	0.42
2:M:59:THR:OG1	2:M:62:ARG:O	2.34	0.42
3:C:222:HIS:HA	3:C:226:ILE:HG12	2.01	0.42
26:E:302:CDL:H521	26:E:302:CDL:H551	1.78	0.42
1:L:302:LEU:HB2	1:L:350:GLN:HG3	2.02	0.42
2:M:146:LEU:HD23	2:M:286:THR:HG22	2.01	0.42
4:O:161:ASN:OD1	4:O:161:ASN:N	2.50	0.42
3:C:54:TYR:OH	3:C:134:CYS:O	2.27	0.42
3:C:210:LEU:HD21	7:G:82:GLU:HG3	2.02	0.42
25:C:603[B]:UQ6:H172	25:C:603[B]:UQ6:H212	1.73	0.42
25:C:603[B]:UQ6:H272	25:C:603[B]:UQ6:H251	1.85	0.42
4:D:247:MET:HB2	4:D:247:MET:HE3	1.73	0.42
3:N:133:CYS:HA	3:N:140:SER:HB3	2.00	0.42
7:G:124:GLU:OE2	10:U:21:ARG:NH1	2.53	0.41
2:M:238:VAL:HA	2:M:289:VAL:O	2.19	0.41
1:A:167:THR:HG21	1:A:249:VAL:HB	2.02	0.41
4:D:272:LYS:HE2	4:D:272:LYS:HB3	1.88	0.41
1:L:290:ALA:O	1:L:296:ARG:NE	2.52	0.41
2:B:231:VAL:HB	2:B:356:VAL:HG22	2.00	0.41
4:D:180:ILE:HA	4:D:183:ALA:HB3	2.02	0.41
5:E:89:LEU:O	10:J:77:ASN:ND2	2.54	0.41
2:M:300:ASN:O	2:M:304:ILE:HG12	2.20	0.41
7:R:47:ASP:OD1	7:R:102:TYR:OH	2.30	0.41
1:A:41:GLU:HB2	1:A:390:LEU:HD22	2.02	0.41
4:D:190:TYR:OH	28:D:401:HEC:O2A	2.28	0.41
1:L:109:LEU:HD23	1:L:109:LEU:HA	1.87	0.41
3:N:101:LEU:HD12	3:N:114:TRP:HH2	1.85	0.41
4:O:283:LEU:HD13	26:O:402:CDL:H611	2.03	0.41
1:A:389:LEU:HD23	1:A:389:LEU:HA	2.46	0.41
4:D:285:ILE:HG23	26:H:602:CDL:HA31	2.02	0.41
2:B:312:LYS:HA	2:B:312:LYS:HD2	1.95	0.41
7:G:47:ASP:OD1	7:G:102:TYR:OH	2.28	0.41
1:A:40:THR:HG21	1:A:216:HIS:HA	2.03	0.41
1:L:112:SER:O	1:L:112:SER:OG	2.28	0.41
3:C:82:HIS:CE1	24:C:601:HEM:NC	2.88	0.41
1:L:72:LEU:HB3	1:L:193:LEU:HD21	2.02	0.41
3:N:226:ILE:HD13	3:N:226:ILE:HA	1.90	0.41
2:B:55:ASN:ND2	2:B:80:SER:OG	2.42	0.41
2:B:230:ARG:NH1	2:B:362:LEU:O	2.52	0.41
1:L:95:SER:OG	1:L:96:ASN:N	2.54	0.41
3:N:297:ALA:O	3:N:301:VAL:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:165:HIS:NE2	1:L:322:TYR:OH	2.40	0.40
5:P:166:PRO:HB2	5:P:176:TRP:HB3	2.04	0.40
6:Q:75:THR:OG1	6:Q:76:ASP:N	2.54	0.40
9:T:50:LYS:HB2	9:T:50:LYS:HE3	1.76	0.40
10:U:68:ASP:OD1	10:U:68:ASP:N	2.54	0.40
3:C:81:LEU:HD21	23:D:402:PEF:H362	2.03	0.40
3:C:117:GLY:C	24:C:602:HEM:HBC2	2.42	0.40
7:G:63:LEU:HD22	7:G:103:LEU:HD13	2.03	0.40
4:O:90:ILE:HG22	4:O:119:SER:HB3	2.02	0.40
5:P:193:LYS:HB3	5:P:193:LYS:HE2	1.89	0.40
23:A:501:PEF:H453	3:C:37:GLY:HA3	2.02	0.40
3:C:132:TYR:OH	3:C:256:ASN:ND2	2.54	0.40
25:C:603[B]:UQ6:H1M1	25:C:603[B]:UQ6:H103	2.03	0.40
3:N:152:SER:HB3	3:N:162:VAL:HG21	2.02	0.40
7:R:53:ASN:N	7:R:53:ASN:OD1	2.54	0.40
2:B:209:LEU:HD23	2:B:209:LEU:HA	1.94	0.40
3:C:101:LEU:HD13	3:C:305:LEU:HD21	2.02	0.40
2:M:251:ALA:O	2:M:255:VAL:HG13	2.21	0.40
27:N:606:PCF:H281	27:N:606:PCF:H252	1.89	0.40
4:O:194:LEU:HD11	4:O:223:ILE:HD12	2.03	0.40
7:R:46:ASP:HB2	7:R:102:TYR:CE1	2.57	0.40
3:C:10:LEU:HD23	3:C:10:LEU:HA	1.94	0.40
3:C:31:ASN:ND2	3:C:232:THR:OG1	2.46	0.40
4:D:191:ILE:HB	4:D:252:THR:HG23	2.04	0.40
5:E:82:MET:O	3:N:178:ARG:NH2	2.38	0.40
1:L:258:LYS:HG2	1:L:335:ARG:HG2	2.02	0.40
1:L:349:LYS:HD3	1:L:349:LYS:HA	1.91	0.40
23:S:602:PEF:H361	23:S:602:PEF:H331	1.79	0.40

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	429/431 (100%)	409 (95%)	20 (5%)	0	100	100
1	L	429/431 (100%)	411 (96%)	18 (4%)	0	100	100
2	B	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
2	M	350/352 (99%)	333 (95%)	17 (5%)	0	100	100
3	C	383/385 (100%)	371 (97%)	12 (3%)	0	100	100
3	N	383/385 (100%)	371 (97%)	12 (3%)	0	100	100
4	D	245/248 (99%)	239 (98%)	6 (2%)	0	100	100
4	O	245/248 (99%)	240 (98%)	5 (2%)	0	100	100
5	E	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
5	P	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
6	F	73/147 (50%)	72 (99%)	1 (1%)	0	100	100
6	Q	73/147 (50%)	70 (96%)	3 (4%)	0	100	100
7	G	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
7	R	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
8	H	91/93 (98%)	88 (97%)	3 (3%)	0	100	100
8	S	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
9	I	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
9	T	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
10	J	74/77 (96%)	73 (99%)	1 (1%)	0	100	100
10	U	74/77 (96%)	71 (96%)	3 (4%)	0	100	100
11	a	532/534 (100%)	502 (94%)	29 (6%)	1 (0%)	47	78
11	m	532/534 (100%)	506 (95%)	25 (5%)	1 (0%)	47	78
12	b	234/236 (99%)	223 (95%)	11 (5%)	0	100	100
12	n	234/236 (99%)	222 (95%)	12 (5%)	0	100	100
13	c	267/269 (99%)	259 (97%)	8 (3%)	0	100	100
13	o	267/269 (99%)	258 (97%)	9 (3%)	0	100	100
14	d	119/130 (92%)	104 (87%)	15 (13%)	0	100	100
14	p	119/130 (92%)	105 (88%)	14 (12%)	0	100	100
15	e	131/133 (98%)	123 (94%)	7 (5%)	1 (1%)	19	53
15	q	131/133 (98%)	119 (91%)	12 (9%)	0	100	100
16	f	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
16	r	100/108 (93%)	98 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	g	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
17	s	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
18	h	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
18	t	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
19	i	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
19	u	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
20	j	75/82 (92%)	68 (91%)	7 (9%)	0	100	100
20	v	75/82 (92%)	69 (92%)	6 (8%)	0	100	100
21	k	111/131 (85%)	102 (92%)	9 (8%)	0	100	100
21	w	111/131 (85%)	106 (96%)	5 (4%)	0	100	100
22	l	43/66 (65%)	42 (98%)	1 (2%)	0	100	100
22	x	43/66 (65%)	42 (98%)	1 (2%)	0	100	100
All	All	7548/7922 (95%)	7217 (96%)	328 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	e	151	GLN
11	a	521	PRO
11	m	521	PRO

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	370/370 (100%)	345 (93%)	25 (7%)	16	46
1	L	370/370 (100%)	350 (95%)	20 (5%)	22	54
2	B	301/301 (100%)	284 (94%)	17 (6%)	21	53
2	M	301/301 (100%)	289 (96%)	12 (4%)	31	62
3	C	338/338 (100%)	322 (95%)	16 (5%)	26	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	338/338 (100%)	325 (96%)	13 (4%)	33	63
4	D	205/206 (100%)	200 (98%)	5 (2%)	49	74
4	O	205/206 (100%)	195 (95%)	10 (5%)	25	57
5	E	151/151 (100%)	145 (96%)	6 (4%)	31	62
5	P	151/151 (100%)	140 (93%)	11 (7%)	14	43
6	F	68/131 (52%)	68 (100%)	0	100	100
6	Q	68/131 (52%)	67 (98%)	1 (2%)	65	82
7	G	110/111 (99%)	106 (96%)	4 (4%)	35	64
7	R	110/111 (99%)	105 (96%)	5 (4%)	27	59
8	H	77/77 (100%)	75 (97%)	2 (3%)	46	73
8	S	77/77 (100%)	74 (96%)	3 (4%)	32	62
9	I	47/54 (87%)	44 (94%)	3 (6%)	17	48
9	T	47/54 (87%)	47 (100%)	0	100	100
10	J	65/66 (98%)	63 (97%)	2 (3%)	40	69
10	U	65/66 (98%)	64 (98%)	1 (2%)	65	82
11	a	447/447 (100%)	413 (92%)	34 (8%)	13	41
11	m	447/447 (100%)	411 (92%)	36 (8%)	11	38
12	b	209/209 (100%)	192 (92%)	17 (8%)	11	38
12	n	209/209 (100%)	194 (93%)	15 (7%)	14	44
13	c	228/228 (100%)	210 (92%)	18 (8%)	12	40
13	o	228/228 (100%)	208 (91%)	20 (9%)	10	34
14	d	102/111 (92%)	92 (90%)	10 (10%)	8	30
14	p	102/111 (92%)	90 (88%)	12 (12%)	5	21
15	e	110/110 (100%)	104 (94%)	6 (6%)	21	53
15	q	110/110 (100%)	102 (93%)	8 (7%)	14	43
16	f	91/96 (95%)	81 (89%)	10 (11%)	6	24
16	r	91/96 (95%)	79 (87%)	12 (13%)	4	17
17	g	50/50 (100%)	45 (90%)	5 (10%)	7	29
17	s	50/50 (100%)	46 (92%)	4 (8%)	12	39
18	h	39/39 (100%)	39 (100%)	0	100	100
18	t	39/39 (100%)	34 (87%)	5 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	i	46/46 (100%)	42 (91%)	4 (9%)	10 35
19	u	46/46 (100%)	42 (91%)	4 (9%)	10 35
20	j	69/73 (94%)	61 (88%)	8 (12%)	5 21
20	v	69/73 (94%)	62 (90%)	7 (10%)	7 28
21	k	99/113 (88%)	89 (90%)	10 (10%)	7 28
21	w	99/113 (88%)	88 (89%)	11 (11%)	6 24
22	l	36/53 (68%)	33 (92%)	3 (8%)	11 37
22	x	36/53 (68%)	32 (89%)	4 (11%)	6 24
All	All	6516/6760 (96%)	6097 (94%)	419 (6%)	21 48

All (419) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	53	VAL
1	A	69	VAL
1	A	70	SER
1	A	72	LEU
1	A	79	SER
1	A	113	THR
1	A	162	GLU
1	A	164	LEU
1	A	166	SER
1	A	170	GLN
1	A	172	THR
1	A	179	ARG
1	A	187	ASN
1	A	188	LEU
1	A	208	VAL
1	A	232	THR
1	A	234	THR
1	A	261	ILE
1	A	311	LEU
1	A	379	GLU
1	A	436	THR
1	A	444	ASP
1	A	449	ARG
1	A	454	MET
2	B	17	LEU

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Mol	Chain	Res	Type
2	B	35	VAL
2	B	47	VAL
2	B	54	PHE
2	B	65	LEU
2	B	97	ASP
2	B	112	THR
2	B	151	PHE
2	B	169	LEU
2	B	206	LEU
2	B	208	THR
2	B	238	VAL
2	B	286	THR
2	B	291	ASP
2	B	313	ASP
2	B	336	ILE
2	B	359	VAL
3	C	32	MET
3	C	66	GLU
3	C	79	ARG
3	C	89	PHE
3	C	101	LEU
3	C	112	THR
3	C	127	THR
3	C	150	LEU
3	C	184	TYR
3	C	185	LEU
3	C	213	THR
3	C	282	LEU
3	C	302	LEU
3	C	305	LEU
3	C	312	VAL
3	C	328	ILE
4	D	113	ARG
4	D	161	ASN
4	D	213	ASN
4	D	264	ASP
4	D	268	ARG
5	E	35	ARG
5	E	65	LEU
5	E	107	VAL
5	E	117	PHE
5	E	153	LEU

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Mol	Chain	Res	Type
5	E	187	ILE
7	G	5	PHE
7	G	47	ASP
7	G	66	ASP
7	G	111	GLU
8	H	45	VAL
8	H	59	VAL
9	I	6	LEU
9	I	34	THR
9	I	51	ASP
10	J	26	TYR
10	J	29	ASN
1	L	34	ASN
1	L	53	VAL
1	L	70	SER
1	L	91	LEU
1	L	167	THR
1	L	172	THR
1	L	179	ARG
1	L	187	ASN
1	L	188	LEU
1	L	190	VAL
1	L	203	ASN
1	L	208	VAL
1	L	230	LEU
1	L	232	THR
1	L	234	THR
1	L	314	ASN
1	L	373	GLN
1	L	379	GLU
1	L	417	ASP
1	L	433	ILE
2	M	17	LEU
2	M	35	VAL
2	M	54	PHE
2	M	97	ASP
2	M	122	SER
2	M	162	ASP
2	M	208	THR
2	M	238	VAL
2	M	291	ASP
2	M	294	SER

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Mol	Chain	Res	Type
2	M	359	VAL
2	M	366	ASP
3	N	6	SER
3	N	56	SER
3	N	66	GLU
3	N	81	LEU
3	N	89	PHE
3	N	99	LYS
3	N	101	LEU
3	N	150	LEU
3	N	184	TYR
3	N	213	THR
3	N	284	SER
3	N	312	VAL
3	N	328	ILE
4	O	113	ARG
4	O	161	ASN
4	O	176	ASP
4	O	213	ASN
4	O	222	SER
4	O	244	THR
4	O	264	ASP
4	O	268	ARG
4	O	283	LEU
4	O	298	ARG
5	P	32	SER
5	P	35	ARG
5	P	41	ASP
5	P	81	SER
5	P	87	ASP
5	P	107	VAL
5	P	117	PHE
5	P	153	LEU
5	P	160	THR
5	P	187	ILE
5	P	213	ILE
6	Q	136	THR
7	R	5	PHE
7	R	66	ASP
7	R	104	LEU
7	R	111	GLU
7	R	123	ILE

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Mol	Chain	Res	Type
8	S	26	SER
8	S	29	VAL
8	S	45	VAL
10	U	29	ASN
11	a	62	HIS
11	a	64	VAL
11	a	82	TYR
11	a	93	THR
11	a	98	ILE
11	a	101	ILE
11	a	105	VAL
11	a	108	MET
11	a	128	THR
11	a	136	ILE
11	a	148	ILE
11	a	167	VAL
11	a	178	THR
11	a	182	LEU
11	a	189	ILE
11	a	190	PHE
11	a	200	LEU
11	a	210	LEU
11	a	235	LEU
11	a	282	LEU
11	a	320	ILE
11	a	336	THR
11	a	345	LEU
11	a	356	VAL
11	a	362	SER
11	a	369	ASP
11	a	401	LEU
11	a	438	ARG
11	a	445	ASP
11	a	508	THR
11	a	511	SER
11	a	517	LEU
11	a	519	THR
11	a	529	THR
12	b	16	ASP
12	b	19	THR
12	b	28	SER
12	b	39	LEU

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Mol	Chain	Res	Type
12	b	50	ILE
12	b	51	LEU
12	b	77	HIS
12	b	85	TRP
12	b	140	THR
12	b	161	LEU
12	b	169	VAL
12	b	171	VAL
12	b	173	THR
12	b	179	VAL
12	b	197	VAL
12	b	200	THR
12	b	231	ASN
13	c	2	THR
13	c	4	LEU
13	c	20	SER
13	c	28	PHE
13	c	39	LEU
13	c	47	ASN
13	c	64	LEU
13	c	92	LEU
13	c	93	MET
13	c	97	SER
13	c	119	THR
13	c	154	TYR
13	c	191	ASN
13	c	195	THR
13	c	241	VAL
13	c	243	TYR
13	c	246	THR
13	c	253	LEU
14	d	40	VAL
14	d	58	THR
14	d	64	THR
14	d	69	LEU
14	d	76	GLU
14	d	79	ASP
14	d	80	VAL
14	d	83	THR
14	d	120	THR
14	d	143	LEU
15	e	22	GLN

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Mol	Chain	Res	Type
15	e	31	VAL
15	e	34	LEU
15	e	88	ASN
15	e	93	SER
15	e	127	GLU
16	f	59	GLU
16	f	76	CYS
16	f	81	LEU
16	f	88	ILE
16	f	113	TYR
16	f	115	VAL
16	f	125	LEU
16	f	126	ASP
16	f	130	ASP
16	f	135	LEU
17	g	19	LEU
17	g	28	LEU
17	g	30	LEU
17	g	43	THR
17	g	47	TYR
19	i	6	ILE
19	i	24	LEU
19	i	33	TRP
19	i	51	LEU
20	j	11	THR
20	j	27	CYS
20	j	28	TRP
20	j	33	ASP
20	j	37	CYS
20	j	55	TYR
20	j	68	ASP
20	j	75	ILE
21	k	13	LEU
21	k	16	ASN
21	k	22	PHE
21	k	28	VAL
21	k	60	LEU
21	k	65	LEU
21	k	77	HIS
21	k	84	LEU
21	k	92	TRP
21	k	110	ASP

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Mol	Chain	Res	Type
22	l	32	GLU
22	l	36	LEU
22	l	64	ARG
11	m	40	LEU
11	m	60	VAL
11	m	64	VAL
11	m	82	TYR
11	m	86	LEU
11	m	95	PHE
11	m	101	ILE
11	m	105	VAL
11	m	110	LEU
11	m	128	THR
11	m	144	VAL
11	m	155	SER
11	m	167	VAL
11	m	175	ASN
11	m	178	THR
11	m	182	LEU
11	m	189	ILE
11	m	194	PHE
11	m	201	PRO
11	m	210	LEU
11	m	282	LEU
11	m	312	ILE
11	m	320	ILE
11	m	336	THR
11	m	345	LEU
11	m	363	LEU
11	m	369	ASP
11	m	379	TYR
11	m	403	LEU
11	m	438	ARG
11	m	443	TYR
11	m	484	VAL
11	m	519	THR
11	m	525	HIS
11	m	526	SER
11	m	529	THR
12	n	39	LEU
12	n	50	ILE
12	n	51	LEU

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Mol	Chain	Res	Type
12	n	53	LEU
12	n	57	MET
12	n	85	TRP
12	n	98	PHE
12	n	106	LEU
12	n	123	GLN
12	n	140	THR
12	n	145	SER
12	n	173	THR
12	n	196	LYS
12	n	197	VAL
12	n	200	THR
13	o	3	HIS
13	o	4	LEU
13	o	8	ARG
13	o	11	GLN
13	o	20	SER
13	o	92	LEU
13	o	93	MET
13	o	100	LEU
13	o	119	THR
13	o	130	GLU
13	o	154	TYR
13	o	191	ASN
13	o	195	THR
13	o	226	ASN
13	o	236	THR
13	o	241	VAL
13	o	243	TYR
13	o	246	THR
13	o	253	LEU
13	o	258	LEU
14	p	40	VAL
14	p	41	ASN
14	p	58	THR
14	p	69	LEU
14	p	76	GLU
14	p	79	ASP
14	p	80	VAL
14	p	100	ILE
14	p	104	ASP
14	p	120	THR

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Mol	Chain	Res	Type
14	p	134	CYS
14	p	143	LEU
15	q	22	GLN
15	q	26	LEU
15	q	31	VAL
15	q	34	LEU
15	q	36	SER
15	q	88	ASN
15	q	92	SER
15	q	130	LEU
16	r	48	THR
16	r	59	GLU
16	r	75	ASN
16	r	81	LEU
16	r	89	GLU
16	r	103	THR
16	r	111	LEU
16	r	115	VAL
16	r	126	ASP
16	r	128	LEU
16	r	130	ASP
16	r	135	LEU
17	s	8	LEU
17	s	19	LEU
17	s	28	LEU
17	s	30	LEU
18	t	28	VAL
18	t	29	HIS
18	t	34	VAL
18	t	40	PHE
18	t	52	SER
19	u	6	ILE
19	u	9	THR
19	u	33	TRP
19	u	41	ILE
20	v	11	THR
20	v	27	CYS
20	v	33	ASP
20	v	37	CYS
20	v	55	TYR
20	v	68	ASP
20	v	75	ILE

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Mol	Chain	Res	Type
21	w	13	LEU
21	w	16	ASN
21	w	22	PHE
21	w	45	LYS
21	w	52	VAL
21	w	53	LYS
21	w	60	LEU
21	w	65	LEU
21	w	84	LEU
21	w	92	TRP
21	w	122	ASN
22	x	32	GLU
22	x	36	LEU
22	x	62	LYS
22	x	64	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	43	ASN
1	A	170	GLN
1	A	171	ASN
1	A	187	ASN
1	A	199	ASN
1	A	305	ASN
1	A	317	HIS
1	A	388	ASN
2	B	58	ASN
2	B	103	ASN
3	C	43	GLN
3	C	253	HIS
3	C	256	ASN
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
5	E	130	ASN
5	E	184	HIS
8	H	34	GLN
8	H	43	ASN
9	I	44	ASN
10	J	29	ASN

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Mol	Chain	Res	Type
1	L	42	HIS
1	L	75	ASN
1	L	171	ASN
1	L	187	ASN
1	L	199	ASN
1	L	307	GLN
1	L	317	HIS
1	L	350	GLN
1	L	388	ASN
2	M	170	GLN
3	N	43	GLN
4	O	127	ASN
5	P	130	ASN
9	T	44	ASN
11	a	257	HIS
11	a	399	GLN
11	a	478	ASN
11	a	482	ASN
11	a	528	ASN
12	b	157	GLN
12	b	249	ASN
13	c	10	GLN
13	c	239	HIS
14	d	35	GLN
15	e	125	ASN
15	e	149	GLN
16	f	70	GLN
16	f	75	ASN
18	h	53	HIS
19	i	42	ASN
20	j	10	HIS
21	k	49	ASN
11	m	257	HIS
11	m	451	ASN
11	m	482	ASN
12	n	157	GLN
12	n	249	ASN
14	p	35	GLN
14	p	62	GLN
18	t	53	HIS
19	u	42	ASN
20	v	20	GLN

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Mol	Chain	Res	Type
20	v	29	GLN
20	v	39	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 70 ligands modelled in this entry, 8 are monoatomic and 4 are modelled with single atom - leaving 58 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	$\#\|Z\| > 2$
27	PCF	q	202	-	35,35,49	1.12	2 (5%)	41,43,57	1.17	4 (9%)
26	CDL	O	402	-	66,66,99	1.10	4 (6%)	72,78,111	1.19	6 (8%)
23	PEF	t	101	-	46,46,46	0.94	2 (4%)	49,51,51	1.14	3 (6%)
23	PEF	N	604	-	42,42,46	0.95	2 (4%)	45,47,51	0.95	3 (6%)
25	UQ6	C	603[B]	-	43,43,43	2.08	6 (13%)	51,55,55	1.55	12 (23%)
23	PEF	C	605	-	38,38,46	1.04	2 (5%)	41,43,51	1.00	3 (7%)
23	PEF	o	302	-	40,40,46	1.04	2 (5%)	43,45,51	1.12	3 (6%)
24	HEM	N	602	3	41,50,50	1.42	6 (14%)	45,82,82	1.92	13 (28%)
23	PEF	c	301	-	35,35,46	1.07	2 (5%)	38,40,51	1.11	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	PEF	A	501	-	43,43,46	0.97	2 (4%)	46,48,51	1.05	3 (6%)
23	PEF	m	606	-	46,46,46	0.95	2 (4%)	49,51,51	1.02	2 (4%)
27	PCF	N	606	-	49,49,49	0.93	3 (6%)	55,57,57	1.03	4 (7%)
31	HEA	m	602	11	57,67,67	1.90	15 (26%)	61,103,103	2.68	33 (54%)
23	PEF	N	605	-	30,30,46	1.17	2 (6%)	33,35,51	1.24	4 (12%)
23	PEF	q	201	-	46,46,46	0.95	2 (4%)	49,51,51	1.11	4 (8%)
28	HEC	O	401	4	32,50,50	2.00	10 (31%)	24,82,82	1.87	5 (20%)
24	HEM	N	601	3	41,50,50	1.40	5 (12%)	45,82,82	1.96	11 (24%)
26	CDL	H	601	-	65,65,99	1.12	4 (6%)	71,77,111	1.21	7 (9%)
26	CDL	H	602	-	70,70,99	1.05	4 (5%)	76,82,111	1.25	5 (6%)
29	FES	P	301	5	0,4,4	-	-	-		
23	PEF	h	101	-	46,46,46	0.90	2 (4%)	49,51,51	1.03	3 (6%)
23	PEF	H	603	-	31,31,46	1.16	2 (6%)	34,36,51	1.28	4 (11%)
26	CDL	S	601	-	52,52,99	1.24	4 (7%)	58,64,111	1.40	8 (13%)
28	HEC	D	401	4	32,50,50	2.18	12 (37%)	24,82,82	2.28	9 (37%)
29	FES	E	301	5	0,4,4	-	-	-		
26	CDL	C	604	-	57,57,99	1.17	4 (7%)	63,69,111	1.36	8 (12%)
27	PCF	H	604	-	31,31,49	1.17	2 (6%)	37,39,57	1.08	2 (5%)
26	CDL	E	302	-	52,52,99	1.22	4 (7%)	58,64,111	1.36	8 (13%)
23	PEF	S	602	-	35,35,46	1.07	2 (5%)	38,40,51	1.10	4 (10%)
31	HEA	m	603	11	57,67,67	1.90	16 (28%)	61,103,103	2.41	26 (42%)
27	PCF	I	101	-	29,29,49	1.26	2 (6%)	35,37,57	1.17	2 (5%)
23	PEF	N	603	-	39,39,46	1.00	2 (5%)	42,44,51	1.20	3 (7%)
23	PEF	b	303	-	39,39,46	1.02	2 (5%)	42,44,51	1.03	2 (4%)
23	PEF	C	606	-	35,35,46	1.08	2 (5%)	38,40,51	1.15	3 (7%)
23	PEF	P	303	-	28,28,46	1.20	2 (7%)	31,33,51	1.28	4 (12%)
31	HEA	a	602	11	57,67,67	1.91	13 (22%)	61,103,103	2.74	33 (54%)
23	PEF	n	304	-	32,32,46	1.10	2 (6%)	35,37,51	1.42	4 (11%)
23	PEF	a	606	-	46,46,46	0.94	2 (4%)	49,51,51	1.08	3 (6%)
26	CDL	L	501	-	54,54,99	1.15	4 (7%)	60,66,111	1.21	5 (8%)
23	PEF	a	607	-	32,32,46	1.10	2 (6%)	35,37,51	1.35	4 (11%)
23	PEF	D	402	-	41,41,46	1.03	2 (4%)	44,46,51	1.07	3 (6%)
27	PCF	e	202	-	35,35,49	1.14	2 (5%)	41,43,57	1.13	3 (7%)
23	PEF	c	302	-	40,40,46	1.02	2 (5%)	43,45,51	1.19	3 (6%)
24	HEM	C	601	3	41,50,50	1.41	6 (14%)	45,82,82	2.07	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CDL	P	302	-	47,47,99	1.29	4 (8%)	53,59,111	1.51	10 (18%)
27	PCF	S	603	-	31,31,49	1.18	2 (6%)	37,39,57	1.23	3 (8%)
23	PEF	O	403	-	42,42,46	0.98	2 (4%)	45,47,51	1.08	4 (8%)
23	PEF	a	608	-	32,32,46	1.10	2 (6%)	35,37,51	1.25	4 (11%)
23	PEF	e	201	-	46,46,46	0.93	2 (4%)	49,51,51	1.11	4 (8%)
24	HEM	C	602	3	41,50,50	1.45	6 (14%)	45,82,82	1.81	12 (26%)
23	PEF	E	303	-	28,28,46	1.21	2 (7%)	31,33,51	1.26	2 (6%)
27	PCF	T	101	-	38,38,49	1.13	2 (5%)	44,46,57	1.16	2 (4%)
25	UQ6	C	603[A]	-	43,43,43	2.05	6 (13%)	51,55,55	1.46	11 (21%)
23	PEF	m	607	-	32,32,46	1.09	2 (6%)	35,37,51	1.25	4 (11%)
27	PCF	C	607	-	38,38,49	1.12	2 (5%)	44,46,57	1.06	2 (4%)
23	PEF	o	301	-	35,35,46	1.08	2 (5%)	38,40,51	1.17	3 (7%)
31	HEA	a	603	11	57,67,67	1.90	16 (28%)	61,103,103	2.45	27 (44%)
23	PEF	n	303	-	39,39,46	1.03	2 (5%)	42,44,51	1.06	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PCF	q	202	-	-	11/39/39/53	-
26	CDL	O	402	-	-	24/77/77/110	-
23	PEF	t	101	-	-	18/50/50/50	-
23	PEF	N	604	-	-	21/46/46/50	-
25	UQ6	C	603[B]	-	-	13/39/39/39	0/1/1/1
23	PEF	C	605	-	-	9/42/42/50	-
23	PEF	o	302	-	-	10/44/44/50	-
24	HEM	N	602	3	-	4/12/54/54	-
23	PEF	c	301	-	-	9/39/39/50	-
23	PEF	A	501	-	-	12/47/47/50	-
31	HEA	m	602	11	2/2/7/16	10/32/76/76	-
23	PEF	m	606	-	-	10/50/50/50	-
27	PCF	N	606	-	-	19/53/53/53	-
23	PEF	N	605	-	-	18/34/34/50	-
23	PEF	q	201	-	-	20/50/50/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	HEC	O	401	4	-	0/10/54/54	-
24	HEM	N	601	3	-	8/12/54/54	-
26	CDL	H	601	-	-	20/76/76/110	-
26	CDL	H	602	-	-	25/81/81/110	-
29	FES	P	301	5	-	-	0/1/1/1
23	PEF	h	101	-	-	19/50/50/50	-
23	PEF	H	603	-	-	6/35/35/50	-
26	CDL	S	601	-	-	14/63/63/110	-
28	HEC	D	401	4	-	2/10/54/54	-
29	FES	E	301	5	-	-	0/1/1/1
26	CDL	C	604	-	-	18/68/68/110	-
27	PCF	H	604	-	-	14/35/35/53	-
26	CDL	E	302	-	-	23/63/63/110	-
31	HEA	m	603	11	2/2/7/16	2/32/76/76	-
23	PEF	S	602	-	-	11/39/39/50	-
27	PCF	I	101	-	-	14/33/33/53	-
23	PEF	N	603	-	-	16/43/43/50	-
23	PEF	b	303	-	-	16/43/43/50	-
23	PEF	C	606	-	-	11/39/39/50	-
23	PEF	P	303	-	-	9/32/32/50	-
31	HEA	a	602	11	2/2/7/16	7/32/76/76	-
23	PEF	n	304	-	-	17/36/36/50	-
23	PEF	a	606	-	-	10/50/50/50	-
26	CDL	L	501	-	-	24/64/64/110	-
23	PEF	a	607	-	-	12/36/36/50	-
23	PEF	D	402	-	-	16/45/45/50	-
27	PCF	e	202	-	-	13/39/39/53	-
23	PEF	c	302	-	-	9/44/44/50	-
24	HEM	C	601	3	-	8/12/54/54	-
26	CDL	P	302	-	-	21/58/58/110	-
27	PCF	S	603	-	-	13/35/35/53	-
23	PEF	O	403	-	-	13/46/46/50	-
23	PEF	a	608	-	-	9/36/36/50	-
23	PEF	e	201	-	-	18/50/50/50	-
24	HEM	C	602	3	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PEF	E	303	-	-	15/32/32/50	-
27	PCF	T	101	-	-	15/42/42/53	-
25	UQ6	C	603[A]	-	-	9/39/39/39	0/1/1/1
23	PEF	m	607	-	-	6/36/36/50	-
27	PCF	C	607	-	-	10/42/42/53	-
23	PEF	o	301	-	-	10/39/39/50	-
31	HEA	a	603	11	2/2/7/16	7/32/76/76	-
23	PEF	n	303	-	-	18/43/43/50	-

All (222) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	401	HEC	C2B-C3B	6.77	1.47	1.40
25	C	603[B]	UQ6	C5-C4	6.24	1.49	1.39
25	C	603[A]	UQ6	C2-C3	6.03	1.49	1.39
25	C	603[B]	UQ6	C2-C3	6.03	1.49	1.39
25	C	603[A]	UQ6	C5-C6	5.89	1.49	1.40
25	C	603[B]	UQ6	C5-C6	5.88	1.49	1.40
25	C	603[A]	UQ6	C5-C4	5.78	1.48	1.39
25	C	603[B]	UQ6	C6-C1	5.38	1.49	1.40
25	C	603[A]	UQ6	C6-C1	5.37	1.49	1.40
28	O	401	HEC	C3C-C2C	5.11	1.46	1.40
31	m	603	HEA	C3B-C2B	4.97	1.45	1.34
31	a	602	HEA	CHC-C4B	4.82	1.47	1.35
31	a	603	HEA	C3B-C2B	4.81	1.45	1.34
28	D	401	HEC	C3C-C2C	4.77	1.45	1.40
25	C	603[B]	UQ6	C4-C3	4.76	1.49	1.39
31	a	603	HEA	CHD-C1D	4.75	1.47	1.35
31	m	603	HEA	CHD-C1D	4.71	1.47	1.35
31	a	603	HEA	C3D-C2D	4.63	1.46	1.36
25	C	603[A]	UQ6	C4-C3	4.62	1.49	1.39
31	a	602	HEA	C3B-C2B	4.62	1.45	1.34
31	m	602	HEA	CHC-C4B	4.60	1.46	1.35
31	a	602	HEA	C3C-C2C	4.57	1.46	1.40
31	m	602	HEA	CHD-C1D	4.54	1.46	1.35
31	m	603	HEA	C3D-C2D	4.47	1.46	1.36
25	C	603[A]	UQ6	C2-C1	4.46	1.49	1.40
31	m	602	HEA	C3D-C2D	4.46	1.46	1.36
28	O	401	HEC	C2B-C3B	4.44	1.45	1.40
23	o	302	PEF	O3-C30	4.42	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	m	602	HEA	C3B-C2B	4.38	1.44	1.34
27	T	101	PCF	O31-C31	4.38	1.46	1.33
31	m	603	HEA	C3A-C2A	4.37	1.46	1.40
23	c	302	PEF	O3-C30	4.37	1.46	1.33
27	I	101	PCF	O31-C31	4.35	1.46	1.33
26	C	604	CDL	OA8-CA7	4.30	1.45	1.33
31	a	602	HEA	CHD-C1D	4.29	1.46	1.35
23	D	402	PEF	O3-C30	4.28	1.45	1.33
31	a	602	HEA	C3D-C2D	4.28	1.45	1.36
27	C	607	PCF	O21-C21	4.28	1.46	1.34
27	e	202	PCF	O31-C31	4.27	1.45	1.33
23	P	303	PEF	O3-C30	4.26	1.45	1.33
26	S	601	CDL	OA6-CA5	4.26	1.46	1.34
23	N	605	PEF	O3-C30	4.25	1.45	1.33
23	C	605	PEF	O2-C10	4.25	1.46	1.34
26	L	501	CDL	OB6-CB5	4.23	1.46	1.34
31	a	603	HEA	C3A-C2A	4.22	1.46	1.40
31	m	602	HEA	C3A-C2A	4.21	1.46	1.40
23	H	603	PEF	O3-C30	4.21	1.45	1.33
23	E	303	PEF	O2-C10	4.20	1.46	1.34
25	C	603[B]	UQ6	C2-C1	4.19	1.48	1.40
26	H	601	CDL	OA6-CA5	4.17	1.46	1.34
26	L	501	CDL	OB8-CB7	4.17	1.45	1.33
27	q	202	PCF	O31-C31	4.17	1.45	1.33
23	c	301	PEF	O3-C30	4.17	1.45	1.33
23	o	301	PEF	O3-C30	4.16	1.45	1.33
23	C	606	PEF	O3-C30	4.16	1.45	1.33
23	N	604	PEF	O2-C10	4.16	1.46	1.34
23	n	303	PEF	O3-C30	4.15	1.45	1.33
23	m	606	PEF	O3-C30	4.15	1.45	1.33
23	a	606	PEF	O2-C10	4.14	1.46	1.34
26	H	601	CDL	OB6-CB5	4.14	1.46	1.34
23	q	201	PEF	O2-C10	4.14	1.46	1.34
27	H	604	PCF	O31-C31	4.14	1.45	1.33
23	n	304	PEF	O3-C30	4.13	1.45	1.33
23	H	603	PEF	O2-C10	4.13	1.46	1.34
23	n	303	PEF	O2-C10	4.13	1.45	1.34
31	a	603	HEA	CHC-C4B	4.12	1.45	1.35
23	D	402	PEF	O2-C10	4.11	1.45	1.34
31	m	603	HEA	CHC-C4B	4.11	1.45	1.35
23	m	606	PEF	O2-C10	4.11	1.45	1.34
26	E	302	CDL	OB8-CB7	4.10	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	O	403	PEF	O2-C10	4.10	1.45	1.34
23	E	303	PEF	O3-C30	4.10	1.45	1.33
23	b	303	PEF	O3-C30	4.10	1.45	1.33
26	S	601	CDL	OB6-CB5	4.09	1.45	1.34
23	b	303	PEF	O2-C10	4.08	1.45	1.34
27	C	607	PCF	O31-C31	4.08	1.45	1.33
26	H	601	CDL	OA8-CA7	4.07	1.45	1.33
26	C	604	CDL	OB8-CB7	4.07	1.45	1.33
26	P	302	CDL	OB8-CB7	4.06	1.45	1.33
26	S	601	CDL	OA8-CA7	4.06	1.45	1.33
23	o	301	PEF	O2-C10	4.06	1.45	1.34
26	H	602	CDL	OA6-CA5	4.06	1.45	1.34
26	O	402	CDL	OA8-CA7	4.05	1.45	1.33
26	L	501	CDL	OA6-CA5	4.05	1.45	1.34
23	S	602	PEF	O2-C10	4.05	1.45	1.34
23	q	201	PEF	O3-C30	4.05	1.45	1.33
23	C	605	PEF	O3-C30	4.04	1.45	1.33
24	C	602	HEM	C1B-NB	-4.03	1.33	1.40
27	S	603	PCF	O31-C31	4.03	1.45	1.33
26	O	402	CDL	OA6-CA5	4.03	1.45	1.34
23	S	602	PEF	O3-C30	4.03	1.45	1.33
23	e	201	PEF	O3-C30	4.03	1.45	1.33
26	O	402	CDL	OB6-CB5	4.03	1.45	1.34
26	O	402	CDL	OB8-CB7	4.02	1.45	1.33
23	t	101	PEF	O2-C10	4.02	1.45	1.34
23	A	501	PEF	O2-C10	4.02	1.45	1.34
26	E	302	CDL	OA8-CA7	4.02	1.45	1.33
23	N	605	PEF	O2-C10	4.02	1.45	1.34
26	P	302	CDL	OA6-CA5	4.01	1.45	1.34
31	m	602	HEA	C3C-C2C	4.00	1.45	1.40
26	P	302	CDL	OA8-CA7	4.00	1.45	1.33
23	a	606	PEF	O3-C30	3.99	1.45	1.33
27	S	603	PCF	O21-C21	3.99	1.45	1.34
23	O	403	PEF	O3-C30	3.99	1.45	1.33
23	o	302	PEF	O2-C10	3.98	1.45	1.34
23	t	101	PEF	O3-C30	3.98	1.45	1.33
23	e	201	PEF	O2-C10	3.97	1.45	1.34
26	H	601	CDL	OB8-CB7	3.97	1.44	1.33
23	A	501	PEF	O3-C30	3.96	1.44	1.33
26	H	602	CDL	OA8-CA7	3.96	1.44	1.33
23	m	607	PEF	O2-C10	3.95	1.45	1.34
24	N	602	HEM	C1B-NB	-3.95	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	301	PEF	O2-C10	3.95	1.45	1.34
23	N	603	PEF	O3-C30	3.95	1.44	1.33
23	a	608	PEF	O3-C30	3.94	1.44	1.33
23	C	606	PEF	O2-C10	3.94	1.45	1.34
23	a	608	PEF	O2-C10	3.94	1.45	1.34
27	N	606	PCF	O31-C31	3.94	1.44	1.33
23	a	607	PEF	O3-C30	3.93	1.44	1.33
26	H	602	CDL	OB8-CB7	3.93	1.44	1.33
23	a	607	PEF	O2-C10	3.92	1.45	1.34
27	T	101	PCF	O21-C21	3.92	1.45	1.34
26	C	604	CDL	OA6-CA5	3.92	1.45	1.34
26	E	302	CDL	OA6-CA5	3.92	1.45	1.34
26	P	302	CDL	OB6-CB5	3.91	1.45	1.34
23	N	603	PEF	O2-C10	3.90	1.45	1.34
23	c	302	PEF	O2-C10	3.89	1.45	1.34
23	P	303	PEF	O2-C10	3.89	1.45	1.34
26	E	302	CDL	OB6-CB5	3.87	1.45	1.34
23	h	101	PEF	O2-C10	3.87	1.45	1.34
27	I	101	PCF	O21-C21	3.86	1.45	1.34
27	e	202	PCF	O21-C21	3.85	1.45	1.34
26	S	601	CDL	OB8-CB7	3.84	1.44	1.33
28	D	401	HEC	C3C-C4C	3.83	1.50	1.43
26	C	604	CDL	OB6-CB5	3.82	1.45	1.34
31	a	602	HEA	C3A-C2A	3.82	1.45	1.40
23	m	607	PEF	O3-C30	3.81	1.44	1.33
23	N	604	PEF	O3-C30	3.80	1.44	1.33
27	H	604	PCF	O21-C21	3.79	1.45	1.34
24	N	602	HEM	C4D-ND	-3.76	1.33	1.40
31	a	603	HEA	C3C-C2C	3.74	1.45	1.40
27	q	202	PCF	O21-C21	3.74	1.44	1.34
24	C	602	HEM	C4D-ND	-3.72	1.33	1.40
23	n	304	PEF	O2-C10	3.69	1.44	1.34
23	h	101	PEF	O3-C30	3.65	1.44	1.33
26	H	602	CDL	OB6-CB5	3.64	1.44	1.34
31	a	602	HEA	C1D-ND	-3.63	1.34	1.40
27	N	606	PCF	O21-C21	3.62	1.44	1.34
31	m	603	HEA	C3C-C2C	3.62	1.45	1.40
28	O	401	HEC	C3C-C4C	3.51	1.49	1.43
31	m	602	HEA	C1D-ND	-3.38	1.34	1.40
28	O	401	HEC	C4B-C3B	3.37	1.49	1.43
24	N	601	HEM	C1B-NB	-3.37	1.34	1.40
31	a	603	HEA	C4B-NB	-3.30	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	601	HEM	C1B-NB	-3.30	1.34	1.40
31	m	603	HEA	C4B-NB	-3.25	1.34	1.40
31	a	603	HEA	C1D-ND	-3.24	1.34	1.40
28	D	401	HEC	C3D-C2D	3.18	1.47	1.37
31	m	603	HEA	C1D-ND	-3.15	1.34	1.40
28	O	401	HEC	C3D-C2D	3.02	1.46	1.37
28	D	401	HEC	C2A-C3A	3.00	1.46	1.37
24	N	601	HEM	C4D-ND	-2.99	1.35	1.40
24	C	601	HEM	C4D-ND	-2.94	1.35	1.40
28	O	401	HEC	C2A-C3A	2.92	1.46	1.37
31	m	602	HEA	C4B-NB	-2.91	1.35	1.40
31	a	602	HEA	FE-ND	2.87	2.11	1.96
24	N	601	HEM	FE-NB	2.84	2.10	1.96
31	m	603	HEA	FE-NB	2.84	2.10	1.96
31	a	602	HEA	C4B-NB	-2.82	1.35	1.40
31	a	603	HEA	FE-NB	2.79	2.10	1.96
31	a	603	HEA	FE-ND	2.79	2.10	1.96
31	m	602	HEA	FE-ND	2.78	2.10	1.96
31	m	602	HEA	C4B-C3B	2.77	1.49	1.44
24	C	601	HEM	FE-NB	2.77	2.10	1.96
31	m	602	HEA	FE-NB	2.76	2.10	1.96
31	a	602	HEA	FE-NB	2.74	2.10	1.96
31	m	603	HEA	FE-ND	2.73	2.10	1.96
24	C	602	HEM	FE-NB	2.73	2.10	1.96
24	C	601	HEM	C1D-ND	-2.72	1.33	1.38
24	N	602	HEM	FE-NB	2.72	2.10	1.96
28	D	401	HEC	C1D-CHD	2.70	1.48	1.41
31	a	602	HEA	C4B-C3B	2.67	1.49	1.44
24	C	602	HEM	C1D-ND	-2.60	1.33	1.38
28	D	401	HEC	C2A-C1A	2.50	1.48	1.42
26	L	501	CDL	OA8-CA7	2.49	1.45	1.33
24	N	601	HEM	C1D-ND	-2.46	1.33	1.38
28	O	401	HEC	C2A-C1A	2.46	1.48	1.42
31	a	602	HEA	C1C-CHC	2.44	1.47	1.41
28	D	401	HEC	C4B-C3B	2.41	1.47	1.43
24	C	602	HEM	C4B-NB	-2.39	1.33	1.38
31	a	602	HEA	C1B-NB	-2.37	1.33	1.38
31	m	602	HEA	C1B-NB	-2.37	1.33	1.38
28	O	401	HEC	C1C-CHC	2.34	1.47	1.41
24	C	601	HEM	C4B-NB	-2.33	1.34	1.38
31	m	603	HEA	C4D-ND	-2.31	1.34	1.38
28	O	401	HEC	C1D-CHD	2.28	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	601	HEM	C4B-NB	-2.28	1.34	1.38
28	D	401	HEC	C3A-C4A	2.25	1.47	1.42
31	a	603	HEA	C2A-C1A	2.25	1.47	1.42
31	a	603	HEA	C4C-CHD	2.25	1.47	1.41
24	N	602	HEM	C4B-NB	-2.24	1.34	1.38
28	D	401	HEC	C4D-CHA	2.24	1.47	1.41
31	m	602	HEA	C2A-C1A	2.23	1.47	1.42
31	a	603	HEA	C4D-ND	-2.23	1.34	1.38
24	N	602	HEM	C1D-ND	-2.23	1.34	1.38
28	D	401	HEC	C1B-CHB	2.23	1.47	1.41
31	a	603	HEA	C1B-NB	-2.20	1.34	1.38
31	m	603	HEA	C2A-C1A	2.17	1.47	1.42
28	O	401	HEC	C4D-CHA	2.17	1.47	1.41
31	m	602	HEA	C1C-CHC	2.17	1.47	1.41
31	a	603	HEA	C4B-C3B	2.16	1.48	1.44
24	N	602	HEM	FE-ND	-2.15	1.86	1.96
24	C	602	HEM	FE-ND	-2.14	1.86	1.96
31	m	603	HEA	C4B-C3B	2.13	1.48	1.44
31	a	603	HEA	C1D-C2D	2.08	1.48	1.44
28	D	401	HEC	C1C-CHC	2.08	1.46	1.41
31	m	602	HEA	C4C-CHD	2.07	1.46	1.41
31	m	603	HEA	C1D-C2D	2.07	1.48	1.44
31	m	603	HEA	C4C-CHD	2.07	1.46	1.41
27	N	606	PCF	O21-C2	-2.02	1.41	1.46
24	C	601	HEM	FE-ND	-2.02	1.86	1.96
31	m	603	HEA	C1B-NB	-2.02	1.34	1.38

All (371) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	602	HEA	C3D-C4D-ND	7.17	117.30	110.36
31	a	603	HEA	C3D-C4D-ND	7.17	117.30	110.36
28	D	401	HEC	CMB-C2B-C3B	7.12	134.19	125.82
31	m	602	HEA	C3D-C4D-ND	6.94	117.07	110.36
31	m	603	HEA	C3D-C4D-ND	6.79	116.93	110.36
31	a	602	HEA	CBA-CAA-C2A	-6.66	101.38	112.60
31	m	603	HEA	C3B-C4B-NB	5.91	116.84	109.84
31	m	602	HEA	C2B-C1B-NB	5.84	116.88	109.88
31	m	602	HEA	C13-C12-C11	-5.69	105.80	114.35
31	a	602	HEA	C2D-C1D-ND	5.65	116.53	109.84
31	a	603	HEA	C2B-C1B-NB	5.64	116.64	109.88
24	C	601	HEM	CAD-C3D-C4D	5.63	134.50	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	O	401	HEC	C1D-C2D-C3D	-5.59	103.11	107.00
31	a	603	HEA	C3B-C4B-NB	5.54	116.41	109.84
31	a	602	HEA	C13-C12-C11	-5.45	106.17	114.35
31	a	602	HEA	C2B-C1B-NB	5.20	116.11	109.88
31	m	603	HEA	C2D-C1D-ND	5.09	115.87	109.84
31	m	603	HEA	C2B-C1B-NB	5.02	115.89	109.88
24	N	601	HEM	CAD-C3D-C4D	5.01	133.41	124.66
31	m	602	HEA	C2D-C1D-ND	5.00	115.77	109.84
31	a	603	HEA	C2D-C1D-ND	4.96	115.72	109.84
24	C	601	HEM	CHC-C4B-NB	4.94	129.79	124.43
24	N	602	HEM	CHC-C4B-NB	4.90	129.76	124.43
28	D	401	HEC	C1D-C2D-C3D	-4.85	103.62	107.00
31	m	602	HEA	C3B-C4B-NB	4.82	115.56	109.84
23	a	607	PEF	O2-C10-C11	4.80	121.84	111.50
24	C	601	HEM	CHD-C1D-ND	4.68	129.51	124.43
24	N	601	HEM	CHC-C4B-NB	4.65	129.48	124.43
31	a	602	HEA	C26-C15-C16	4.58	122.97	115.27
31	m	602	HEA	C26-C15-C16	4.57	122.97	115.27
24	N	602	HEM	CHD-C1D-ND	4.57	129.40	124.43
26	P	302	CDL	OB6-CB5-C51	4.55	121.31	111.50
23	E	303	PEF	O2-C10-C11	4.55	121.30	111.50
23	n	304	PEF	O2-C10-C11	4.45	121.10	111.50
26	P	302	CDL	OA6-CA5-C11	4.42	121.04	111.50
24	C	602	HEM	CHC-C4B-NB	4.42	129.23	124.43
26	C	604	CDL	OB6-CB5-C51	4.41	121.01	111.50
23	N	605	PEF	O2-C10-C11	4.39	120.96	111.50
23	N	603	PEF	O2-C10-C11	4.37	120.92	111.50
31	a	602	HEA	C3B-C4B-NB	4.37	115.02	109.84
23	n	304	PEF	C2-O2-C10	-4.31	107.19	117.79
31	m	602	HEA	CAD-C3D-C4D	4.31	132.18	124.66
23	a	608	PEF	O2-C10-C11	4.30	120.77	111.50
31	a	602	HEA	C3C-C4C-NC	4.29	114.76	109.21
31	m	603	HEA	C1D-C2D-C3D	-4.26	102.47	106.96
23	t	101	PEF	O2-C10-C11	4.26	120.68	111.50
26	O	402	CDL	OA6-CA5-C11	4.24	120.64	111.50
23	q	201	PEF	O2-C10-C11	4.22	120.60	111.50
23	a	606	PEF	O2-C10-C11	4.18	120.51	111.50
26	H	602	CDL	OA6-CA5-C11	4.16	120.47	111.50
24	C	601	HEM	C1B-NB-C4B	4.15	109.36	105.07
25	C	603[B]	UQ6	C25-C24-C26	4.15	122.25	115.27
26	C	604	CDL	OA6-CA5-C11	4.15	120.44	111.50
23	o	301	PEF	O2-C10-C11	4.14	120.42	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	H	602	CDL	OB6-CB5-C51	4.13	120.40	111.50
27	C	607	PCF	O21-C21-C22	4.12	120.39	111.50
31	m	602	HEA	CBA-CAA-C2A	-4.11	105.68	112.60
26	S	601	CDL	OB6-CB5-C51	4.10	120.33	111.50
24	C	601	HEM	CAD-C3D-C2D	-4.06	120.31	127.88
26	H	601	CDL	OA6-CA5-C11	4.04	120.21	111.50
23	m	607	PEF	O2-C10-C11	4.03	120.19	111.50
23	e	201	PEF	O2-C10-C11	4.03	120.19	111.50
24	C	602	HEM	CHD-C1D-ND	4.03	128.80	124.43
23	H	603	PEF	O2-C10-C11	3.95	120.02	111.50
23	c	302	PEF	O2-C10-C11	3.95	120.02	111.50
23	m	606	PEF	O2-C10-C11	3.92	119.94	111.50
26	H	601	CDL	OB6-CB5-C51	3.91	119.92	111.50
23	P	303	PEF	O2-C10-C11	3.88	119.87	111.50
26	L	501	CDL	OA6-CA5-C11	3.88	119.87	111.50
26	O	402	CDL	OB6-CB5-C51	3.87	119.83	111.50
26	S	601	CDL	OA6-CA5-C11	3.85	119.80	111.50
31	m	602	HEA	C4D-C3D-C2D	-3.85	101.29	106.90
24	N	601	HEM	C1B-NB-C4B	3.84	109.04	105.07
31	m	602	HEA	C3C-C4C-NC	3.84	114.17	109.21
31	a	603	HEA	C1D-C2D-C3D	-3.83	102.93	106.96
23	c	301	PEF	O2-C10-C11	3.83	119.75	111.50
27	S	603	PCF	C3-C2-C1	-3.79	102.83	111.79
26	E	302	CDL	OB6-CB5-C51	3.78	119.64	111.50
23	C	606	PEF	O2-C10-C11	3.77	119.62	111.50
31	a	603	HEA	C13-C12-C11	-3.75	108.72	114.35
26	E	302	CDL	OA6-CA5-C11	3.74	119.56	111.50
27	I	101	PCF	O21-C21-C22	3.74	119.55	111.50
31	a	602	HEA	C4D-C3D-C2D	-3.73	101.45	106.90
23	o	302	PEF	O2-C10-C11	3.73	119.54	111.50
23	n	303	PEF	O2-C10-C11	3.73	119.54	111.50
31	a	602	HEA	C1D-C2D-C3D	-3.72	103.05	106.96
25	C	603[A]	UQ6	C6-C7-C8	-3.71	106.29	112.17
26	L	501	CDL	OB6-CB5-C51	3.70	119.47	111.50
27	q	202	PCF	O21-C21-C22	3.68	119.44	111.50
24	N	601	HEM	CHD-C1D-ND	3.68	128.43	124.43
23	O	403	PEF	O2-C10-C11	3.65	119.36	111.50
31	m	603	HEA	CMB-C2B-C1B	3.64	130.59	125.04
28	O	401	HEC	CMB-C2B-C3B	3.63	130.08	125.82
31	a	603	HEA	C4D-C3D-C2D	-3.62	101.62	106.90
27	e	202	PCF	O21-C21-C22	3.61	119.29	111.50
24	N	601	HEM	CHB-C1B-NB	3.61	128.84	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	m	602	HEA	CAD-CBD-CGD	-3.60	105.86	113.60
24	C	601	HEM	CHB-C1B-NB	3.59	128.82	124.38
23	S	602	PEF	O2-C10-C11	3.59	119.23	111.50
25	C	603[A]	UQ6	C25-C24-C26	3.58	121.30	115.27
24	C	602	HEM	CHB-C1B-NB	3.56	128.78	124.38
24	N	602	HEM	C1B-NB-C4B	3.54	108.73	105.07
27	H	604	PCF	O21-C21-C22	3.53	119.10	111.50
31	a	603	HEA	C1B-C2B-C3B	-3.52	102.59	106.80
31	m	603	HEA	C3C-C4C-NC	3.51	113.75	109.21
31	a	602	HEA	CMC-C2C-C3C	3.51	131.25	124.68
23	C	605	PEF	O2-C10-C11	3.51	119.06	111.50
27	S	603	PCF	O21-C21-C22	3.50	119.04	111.50
25	C	603[B]	UQ6	C30-C29-C31	3.49	121.14	115.27
24	C	601	HEM	CHD-C1D-C2D	-3.48	119.54	124.98
27	T	101	PCF	O21-C21-C22	3.48	119.00	111.50
31	a	603	HEA	CMB-C2B-C1B	3.43	130.26	125.04
31	a	603	HEA	CMC-C2C-C3C	3.43	131.09	124.68
23	D	402	PEF	O2-C10-C11	3.41	118.86	111.50
23	A	501	PEF	O2-C10-C11	3.41	118.86	111.50
24	C	602	HEM	CHA-C4D-ND	3.39	128.57	124.38
26	H	602	CDL	OB8-CB7-C71	3.38	120.24	111.38
24	N	602	HEM	CHA-C4D-ND	3.36	128.53	124.38
23	H	603	PEF	O3-C30-C31	3.35	122.41	111.91
24	C	601	HEM	CBD-CAD-C3D	3.34	121.92	112.63
31	m	603	HEA	C4B-C3B-C2B	-3.32	101.74	107.41
26	C	604	CDL	OB8-CB7-C71	3.31	122.31	111.91
24	N	602	HEM	CHB-C1B-NB	3.31	128.47	124.38
31	a	602	HEA	C1D-ND-C4D	-3.31	101.66	105.07
24	N	601	HEM	CAD-C3D-C2D	-3.30	121.73	127.88
31	m	602	HEA	C1D-C2D-C3D	-3.30	103.49	106.96
23	h	101	PEF	O2-C10-C11	3.28	118.58	111.50
23	b	303	PEF	O2-C10-C11	3.28	118.57	111.50
31	m	603	HEA	C13-C12-C11	-3.28	109.42	114.35
26	P	302	CDL	CB4-OB6-CB5	-3.27	109.75	117.79
24	C	602	HEM	C1B-NB-C4B	3.26	108.44	105.07
31	a	603	HEA	C3C-C4C-NC	3.24	113.40	109.21
28	D	401	HEC	CMC-C2C-C3C	3.22	129.61	125.82
24	N	601	HEM	CBD-CAD-C3D	3.20	121.53	112.63
23	a	607	PEF	C2-O2-C10	-3.20	109.92	117.79
26	S	601	CDL	CB2-C1-CA2	-3.20	103.38	112.79
23	m	607	PEF	O3-C30-C31	3.20	121.94	111.91
31	m	603	HEA	C4D-C3D-C2D	-3.19	102.25	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	601	HEM	CBA-CAA-C2A	-3.18	107.19	112.62
23	e	201	PEF	C2-O2-C10	-3.17	109.99	117.79
27	N	606	PCF	O21-C21-C22	3.15	118.29	111.50
31	m	602	HEA	CHA-C4D-ND	-3.13	121.03	124.43
27	T	101	PCF	O31-C31-C32	3.13	121.72	111.91
31	m	602	HEA	CMC-C2C-C3C	3.12	130.52	124.68
31	a	602	HEA	C27-C19-C20	3.12	120.53	115.27
23	a	608	PEF	O3-C30-C31	3.12	121.70	111.91
26	E	302	CDL	OA8-CA7-C31	3.12	121.69	111.91
23	D	402	PEF	O3-C30-C31	3.09	121.62	111.91
31	a	602	HEA	CAD-C3D-C4D	3.07	130.03	124.66
31	m	602	HEA	C4B-C3B-C2B	-3.07	102.17	107.41
27	I	101	PCF	O31-C31-C32	3.04	121.46	111.91
26	C	604	CDL	CB4-OB6-CB5	-3.04	110.30	117.79
24	N	602	HEM	CAD-CBD-CGD	-3.04	107.06	113.60
31	m	603	HEA	C1B-C2B-C3B	-3.04	103.17	106.80
23	P	303	PEF	O3-C30-C31	3.04	121.44	111.91
31	a	603	HEA	C4B-C3B-C2B	-3.04	102.22	107.41
31	m	602	HEA	C1B-C2B-C3B	-3.03	103.18	106.80
23	t	101	PEF	O3-C30-C31	3.02	121.38	111.91
31	a	602	HEA	C4B-C3B-C2B	-3.01	102.28	107.41
31	m	603	HEA	CMC-C2C-C3C	2.99	130.27	124.68
23	c	302	PEF	C2-O2-C10	-2.98	110.45	117.79
26	P	302	CDL	CA4-OA6-CA5	-2.96	110.50	117.79
31	m	602	HEA	C27-C19-C20	2.96	120.25	115.27
27	N	606	PCF	C2-O21-C21	-2.96	110.51	117.79
26	P	302	CDL	OA8-CA7-C31	2.95	121.16	111.91
31	m	603	HEA	CBA-CAA-C2A	-2.93	107.67	112.60
31	m	603	HEA	C27-C19-C20	2.93	120.19	115.27
23	O	403	PEF	O3-C30-C31	2.92	121.06	111.91
26	E	302	CDL	CB4-OB6-CB5	-2.89	110.67	117.79
26	S	601	CDL	OB8-CB7-C71	2.88	120.94	111.91
31	a	602	HEA	C12-C13-C14	-2.87	104.64	112.23
23	o	301	PEF	O3-C30-C31	2.87	120.92	111.91
26	E	302	CDL	OB8-CB7-C71	2.87	120.91	111.91
26	H	601	CDL	OA8-CA7-C31	2.87	120.91	111.91
24	N	602	HEM	CHD-C1D-C2D	-2.85	120.53	124.98
31	a	603	HEA	C4B-NB-C1B	-2.84	102.14	105.07
26	P	302	CDL	OB8-CB7-C71	2.84	120.82	111.91
23	C	606	PEF	O3-C30-C31	2.83	120.79	111.91
23	h	101	PEF	O3-C30-C31	2.81	120.74	111.91
23	a	606	PEF	O3-C30-C31	2.81	120.72	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	N	604	PEF	O2-C10-C11	2.81	117.55	111.50
27	C	607	PCF	O31-C31-C32	2.81	120.72	111.91
28	O	401	HEC	CAA-CBA-CGA	-2.80	105.90	113.76
31	a	602	HEA	C1B-C2B-C3B	-2.80	103.46	106.80
25	C	603[B]	UQ6	C15-C14-C16	2.78	119.95	115.27
23	N	603	PEF	O3-C30-C31	2.78	120.63	111.91
31	m	602	HEA	C4B-NB-C1B	-2.78	102.20	105.07
24	C	602	HEM	C4B-C3B-C2B	-2.78	104.91	107.11
26	H	602	CDL	OA8-CA7-C31	2.77	120.61	111.91
23	A	501	PEF	C2-O2-C10	-2.77	110.97	117.79
23	c	302	PEF	O3-C30-C31	2.76	120.58	111.91
23	n	304	PEF	O3-C30-C31	2.76	120.56	111.91
25	C	603[A]	UQ6	C30-C29-C31	2.75	119.89	115.27
23	b	303	PEF	O3-C30-C31	2.74	120.52	111.91
25	C	603[B]	UQ6	C20-C19-C21	2.74	119.88	115.27
27	e	202	PCF	O31-C31-C32	2.74	120.50	111.91
31	a	602	HEA	CHA-C4D-ND	-2.73	121.46	124.43
23	q	201	PEF	C2-O2-C10	-2.73	111.07	117.79
26	C	604	CDL	OA8-CA7-C31	2.72	120.44	111.91
23	h	101	PEF	O3-C30-O5	-2.72	116.73	123.59
26	O	402	CDL	OA8-CA7-C31	2.72	120.43	111.91
23	e	201	PEF	O3-C30-C31	2.71	120.40	111.91
23	c	301	PEF	O3-C30-C31	2.70	120.39	111.91
23	m	606	PEF	O3-C30-C31	2.70	120.39	111.91
31	m	602	HEA	C17-C18-C19	-2.70	121.16	127.66
26	S	601	CDL	OA8-CA7-C31	2.70	120.38	111.91
23	D	402	PEF	C2-O2-C10	-2.70	111.15	117.79
31	a	603	HEA	C26-C15-C16	2.70	119.81	115.27
23	S	602	PEF	O3-C30-C31	2.69	120.35	111.91
27	S	603	PCF	O31-C31-C32	2.68	120.31	111.91
23	P	303	PEF	C2-O2-C10	-2.67	111.21	117.79
31	a	603	HEA	CAD-CBD-CGD	-2.66	107.88	113.60
31	a	602	HEA	C17-C18-C19	-2.66	121.27	127.66
27	q	202	PCF	O31-C31-C32	2.63	120.18	111.91
27	q	202	PCF	C2-O21-C21	-2.63	111.32	117.79
31	m	603	HEA	C4B-NB-C1B	-2.63	102.36	105.07
23	o	302	PEF	C2-O2-C10	-2.63	111.33	117.79
31	a	603	HEA	CHA-C4D-C3D	-2.62	120.98	124.84
31	m	602	HEA	C1D-ND-C4D	-2.62	102.36	105.07
23	N	605	PEF	C2-O2-C10	-2.62	111.34	117.79
26	S	601	CDL	CB4-OB6-CB5	-2.61	111.36	117.79
31	m	602	HEA	C12-C13-C14	-2.61	105.34	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	m	603	HEA	CHA-C4D-C3D	-2.61	121.01	124.84
27	H	604	PCF	O31-C31-C32	2.60	120.08	111.91
31	a	603	HEA	CBA-CAA-C2A	-2.60	108.22	112.60
27	N	606	PCF	O31-C31-C32	2.60	120.07	111.91
24	N	602	HEM	C4B-C3B-C2B	-2.60	105.05	107.11
31	a	602	HEA	OMA-CMA-C3A	-2.59	119.26	124.91
25	C	603[B]	UQ6	C3M-O3-C3	2.59	121.87	114.78
31	m	602	HEA	CHB-C1B-C2B	-2.58	120.94	124.98
23	N	604	PEF	O3-C30-C31	2.58	120.01	111.91
23	N	603	PEF	C2-O2-C10	-2.58	111.44	117.79
23	q	201	PEF	O3-C30-C31	2.58	120.00	111.91
28	D	401	HEC	CAA-CBA-CGA	-2.58	106.53	113.76
25	C	603[A]	UQ6	C20-C19-C21	2.56	119.58	115.27
31	a	603	HEA	C1D-ND-C4D	-2.56	102.43	105.07
24	C	602	HEM	CHD-C1D-C2D	-2.55	120.99	124.98
23	m	607	PEF	O3-C30-O5	-2.54	117.17	123.59
23	a	607	PEF	O2-C10-O4	-2.54	117.57	123.70
31	m	603	HEA	C1D-ND-C4D	-2.53	102.46	105.07
31	a	603	HEA	C13-C14-C15	-2.53	121.57	127.66
25	C	603[B]	UQ6	C7-C8-C9	-2.53	123.32	127.24
23	O	403	PEF	C2-O2-C10	-2.53	111.57	117.79
25	C	603[A]	UQ6	C17-C18-C19	-2.52	121.58	127.66
31	a	602	HEA	C25-C23-C24	2.52	120.17	114.60
31	m	603	HEA	CHB-C1B-NB	-2.52	121.70	124.43
25	C	603[B]	UQ6	C12-C13-C14	-2.51	121.61	127.66
31	a	603	HEA	CHA-C4D-ND	-2.51	121.70	124.43
31	a	603	HEA	C27-C19-C20	2.51	119.49	115.27
26	L	501	CDL	CB4-OB6-CB5	-2.48	111.67	117.79
25	C	603[B]	UQ6	C25-C24-C23	-2.46	117.36	123.68
31	m	602	HEA	C21-C20-C19	-2.46	104.89	112.98
31	a	602	HEA	CHA-C4D-C3D	-2.45	121.23	124.84
26	C	604	CDL	OB6-CB5-OB7	-2.45	117.79	123.70
26	E	302	CDL	CA4-OA6-CA5	-2.45	111.77	117.79
28	O	401	HEC	CMA-C3A-C2A	2.44	129.54	124.94
26	L	501	CDL	OB8-CB7-C71	2.43	119.54	111.91
23	A	501	PEF	O3-C30-C31	2.43	119.52	111.91
23	n	303	PEF	O3-C30-C31	2.43	119.52	111.91
31	m	603	HEA	C13-C14-C15	-2.40	121.87	127.66
23	N	604	PEF	O3-C30-O5	-2.40	117.54	123.59
31	a	603	HEA	CHB-C1B-C2B	-2.40	121.23	124.98
23	t	101	PEF	O3-C30-O5	-2.39	117.55	123.59
31	m	602	HEA	CMD-C2D-C1D	2.37	128.65	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	402	CDL	CA6-CA4-CA3	-2.37	106.17	111.79
31	a	602	HEA	C21-C20-C19	-2.37	105.17	112.98
26	L	501	CDL	CA4-OA6-CA5	-2.37	111.96	117.79
23	n	304	PEF	O2-C10-O4	-2.37	117.98	123.70
31	m	602	HEA	CMB-C2B-C1B	2.36	128.64	125.04
24	C	601	HEM	CBA-CAA-C2A	-2.36	108.60	112.62
26	E	302	CDL	OA8-CA7-OA9	-2.35	117.65	123.59
23	E	303	PEF	O3-C30-C31	2.35	119.29	111.91
24	N	601	HEM	CHD-C1D-C2D	-2.35	121.30	124.98
26	C	604	CDL	OB8-CB7-OB9	-2.34	117.67	123.59
24	C	602	HEM	CMB-C2B-C1B	-2.34	121.48	125.04
26	C	604	CDL	CA4-OA6-CA5	-2.34	112.04	117.79
23	o	302	PEF	O3-C30-C31	2.33	119.23	111.91
23	S	602	PEF	O3-C30-O5	-2.33	117.70	123.59
24	N	602	HEM	C4D-ND-C1D	2.33	107.48	105.07
24	C	602	HEM	CHB-C1B-C2B	-2.33	120.28	126.72
25	C	603[B]	UQ6	C27-C28-C29	-2.33	122.06	127.66
24	N	601	HEM	CHA-C4D-ND	2.32	127.24	124.38
24	N	602	HEM	CBD-CAD-C3D	-2.32	106.19	112.63
25	C	603[B]	UQ6	C10-C9-C11	2.31	119.16	115.27
25	C	603[A]	UQ6	C30-C29-C28	-2.29	117.81	123.68
31	m	603	HEA	C25-C23-C24	2.29	119.65	114.60
26	H	601	CDL	OB8-CB7-C71	2.28	119.07	111.91
26	P	302	CDL	OA8-CA7-OA9	-2.28	117.83	123.59
31	m	603	HEA	CAD-CBD-CGD	-2.26	108.74	113.60
23	a	607	PEF	O3-C30-C31	2.25	118.96	111.91
25	C	603[A]	UQ6	C3M-O3-C3	2.24	120.92	114.78
28	D	401	HEC	C3B-C4B-NB	2.24	115.17	110.94
25	C	603[A]	UQ6	C25-C24-C23	-2.24	117.94	123.68
23	a	608	PEF	C2-O2-C10	-2.23	112.30	117.79
26	H	601	CDL	CA4-OA6-CA5	-2.23	112.31	117.79
31	m	603	HEA	CMD-C2D-C1D	2.22	128.42	125.04
23	H	603	PEF	O3-C30-O5	-2.22	118.00	123.59
31	a	602	HEA	CMD-C2D-C1D	2.22	128.41	125.04
31	a	602	HEA	CAD-CBD-CGD	-2.22	108.84	113.60
31	m	602	HEA	CBD-CAD-C3D	2.21	118.78	112.63
23	N	605	PEF	O3-C30-C31	2.21	118.85	111.91
23	a	608	PEF	O3-C30-O5	-2.21	118.01	123.59
28	O	401	HEC	CMC-C2C-C3C	2.21	128.42	125.82
31	a	602	HEA	CMB-C2B-C1B	2.21	128.40	125.04
31	m	603	HEA	CHA-C4D-ND	-2.20	122.04	124.43
31	a	602	HEA	C13-C14-C15	-2.20	122.36	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	601	CDL	OB8-CB7-OB9	-2.20	118.04	123.59
31	m	602	HEA	C25-C23-C24	2.20	119.46	114.60
31	a	603	HEA	CAA-CBA-CGA	-2.20	107.60	113.76
26	H	601	CDL	CB2-C1-CA2	-2.20	106.32	112.79
24	N	602	HEM	CMA-C3A-C4A	-2.19	125.09	128.46
23	a	606	PEF	C2-O2-C10	-2.19	112.39	117.79
27	q	202	PCF	C23-C22-C21	-2.19	105.65	113.62
31	m	602	HEA	C13-C14-C15	-2.19	122.39	127.66
25	C	603[B]	UQ6	C17-C18-C19	-2.18	122.40	127.66
26	E	302	CDL	OB8-CB7-OB9	-2.18	118.08	123.59
24	C	602	HEM	C4D-ND-C1D	2.18	107.32	105.07
28	D	401	HEC	CMA-C3A-C2A	2.18	129.05	124.94
24	C	602	HEM	CHA-C4D-C3D	-2.17	121.25	125.33
28	D	401	HEC	CMB-C2B-C1B	-2.17	125.13	128.46
31	m	602	HEA	C16-C15-C14	-2.16	116.74	121.12
31	m	603	HEA	CHD-C1D-C2D	-2.16	120.74	126.72
31	a	603	HEA	CHB-C1B-NB	-2.15	122.09	124.43
23	N	605	PEF	O2-C10-O4	-2.15	118.50	123.70
31	m	603	HEA	CMB-C2B-C3B	-2.15	126.24	130.34
23	C	606	PEF	O3-C30-O5	-2.15	118.17	123.59
23	q	201	PEF	O2-C10-O4	-2.14	118.53	123.70
23	m	607	PEF	C2-O2-C10	-2.14	112.53	117.79
26	P	302	CDL	OB8-CB7-OB9	-2.14	118.20	123.59
25	C	603[A]	UQ6	C12-C13-C14	-2.13	122.53	127.66
31	m	602	HEA	CHD-C1D-C2D	-2.13	120.83	126.72
24	C	602	HEM	CAD-CBD-CGD	-2.13	109.03	113.60
24	N	602	HEM	CHB-C1B-C2B	-2.12	120.86	126.72
31	a	602	HEA	C21-C22-C23	-2.11	120.53	127.75
31	a	603	HEA	CMD-C2D-C1D	2.11	128.25	125.04
31	m	602	HEA	CHC-C4B-NB	-2.10	121.78	124.38
31	a	602	HEA	C16-C15-C14	-2.10	116.87	121.12
31	a	602	HEA	CHB-C1B-C2B	-2.10	121.70	124.98
31	m	602	HEA	CHB-C1B-NB	-2.09	122.16	124.43
31	a	602	HEA	CHB-C1B-NB	-2.09	122.16	124.43
27	e	202	PCF	C3-C2-C1	-2.09	106.84	111.79
28	D	401	HEC	C2B-C3B-C4B	-2.09	104.09	106.35
26	H	602	CDL	OB6-CB5-OB7	-2.09	118.65	123.70
31	a	603	HEA	CHD-C1D-C2D	-2.09	120.95	126.72
26	H	601	CDL	CA6-CA4-CA3	-2.08	106.86	111.79
25	C	603[B]	UQ6	C36-C34-C35	2.08	119.20	114.60
23	C	605	PEF	C32-C31-C30	-2.07	106.08	113.62
25	C	603[A]	UQ6	C15-C14-C16	2.07	118.75	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	601	HEM	CHB-C1B-C2B	-2.07	121.00	126.72
26	P	302	CDL	OA6-CA5-OA7	-2.06	118.72	123.70
31	a	603	HEA	C25-C23-C24	2.06	119.16	114.60
26	P	302	CDL	OB6-CB5-OB7	-2.06	118.72	123.70
31	m	603	HEA	CAA-CBA-CGA	-2.06	107.99	113.76
23	e	201	PEF	O2-C10-O4	-2.06	118.73	123.70
31	a	602	HEA	O1A-CGA-CBA	-2.05	116.49	123.08
24	N	602	HEM	CMB-C2B-C1B	-2.05	121.92	125.04
25	C	603[A]	UQ6	C4M-O4-C4	2.04	120.37	114.78
27	N	606	PCF	O14-P-O12	2.03	122.26	112.24
31	a	602	HEA	CHD-C1D-C2D	-2.03	121.12	126.72
26	S	601	CDL	OA4-PA1-OA3	2.02	122.23	112.24
26	O	402	CDL	CB6-CB4-CB3	-2.02	107.01	111.79
23	C	605	PEF	O3-C30-C31	2.01	118.23	111.91
23	o	301	PEF	O3-C30-O5	-2.01	118.51	123.59
23	O	403	PEF	O3-C30-O5	-2.01	118.51	123.59
31	m	602	HEA	CHA-C4D-C3D	-2.01	121.88	124.84
24	C	601	HEM	CHB-C1B-C2B	-2.01	121.16	126.72
26	O	402	CDL	OA4-PA1-OA3	2.01	122.18	112.24
23	P	303	PEF	O3-C30-O5	-2.01	118.53	123.59
28	D	401	HEC	CBD-CAD-C3D	-2.01	109.19	112.62
23	S	602	PEF	C2-O2-C10	-2.01	112.85	117.79
23	H	603	PEF	C2-O2-C10	-2.01	112.85	117.79

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	a	602	HEA	NB
31	a	602	HEA	ND
31	a	603	HEA	NB
31	a	603	HEA	ND
31	m	602	HEA	NB
31	m	602	HEA	ND
31	m	603	HEA	NB
31	m	603	HEA	ND

All (720) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	501	PEF	O4P-C4-C5-N
23	A	501	PEF	C11-C10-O2-C2
23	A	501	PEF	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
23	A	501	PEF	C4-O4P-P-O1P
23	A	501	PEF	C4-O4P-P-O2P
23	A	501	PEF	C4-O4P-P-O3P
23	C	605	PEF	O4P-C4-C5-N
23	C	605	PEF	C1-O3P-P-O2P
23	C	606	PEF	C1-O3P-P-O2P
23	D	402	PEF	C11-C10-O2-C2
23	E	303	PEF	O4-C10-O2-C2
23	E	303	PEF	C1-O3P-P-O1P
23	E	303	PEF	C4-O4P-P-O1P
23	E	303	PEF	C4-O4P-P-O2P
23	E	303	PEF	C4-O4P-P-O3P
23	H	603	PEF	C1-O3P-P-O1P
23	H	603	PEF	C1-O3P-P-O2P
23	H	603	PEF	C1-O3P-P-O4P
23	N	603	PEF	C1-O3P-P-O2P
23	N	603	PEF	C4-O4P-P-O1P
23	N	603	PEF	C4-O4P-P-O2P
23	N	603	PEF	C4-O4P-P-O3P
23	N	604	PEF	O4P-C4-C5-N
23	N	604	PEF	C4-O4P-P-O2P
23	N	605	PEF	O2-C2-C3-O3
23	N	605	PEF	C4-O4P-P-O1P
23	N	605	PEF	C4-O4P-P-O2P
23	N	605	PEF	C4-O4P-P-O3P
23	O	403	PEF	C1-O3P-P-O1P
23	O	403	PEF	C1-O3P-P-O4P
23	P	303	PEF	O4P-C4-C5-N
23	P	303	PEF	C11-C10-O2-C2
23	S	602	PEF	C1-O3P-P-O1P
23	a	607	PEF	O4P-C4-C5-N
23	a	607	PEF	C1-O3P-P-O1P
23	a	607	PEF	C1-O3P-P-O2P
23	a	607	PEF	C1-O3P-P-O4P
23	a	607	PEF	C4-O4P-P-O1P
23	a	607	PEF	C4-O4P-P-O2P
23	a	607	PEF	C4-O4P-P-O3P
23	a	608	PEF	C1-O3P-P-O4P
23	a	608	PEF	C4-O4P-P-O1P
23	a	608	PEF	C4-O4P-P-O2P
23	a	608	PEF	C4-O4P-P-O3P
23	b	303	PEF	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
23	c	302	PEF	C1-O3P-P-O2P
23	c	302	PEF	C4-O4P-P-O1P
23	c	302	PEF	C4-O4P-P-O3P
23	e	201	PEF	C11-C10-O2-C2
23	e	201	PEF	O4-C10-O2-C2
23	e	201	PEF	C1-O3P-P-O2P
23	m	606	PEF	C4-O4P-P-O2P
23	m	607	PEF	C1-O3P-P-O4P
23	m	607	PEF	C4-O4P-P-O2P
23	n	303	PEF	C4-O4P-P-O1P
23	n	303	PEF	C4-O4P-P-O3P
23	n	304	PEF	C1-O3P-P-O1P
23	n	304	PEF	C1-O3P-P-O2P
23	n	304	PEF	C1-O3P-P-O4P
23	o	301	PEF	C1-O3P-P-O2P
23	o	301	PEF	C4-O4P-P-O1P
23	o	302	PEF	C1-O3P-P-O2P
23	o	302	PEF	C4-O4P-P-O1P
23	o	302	PEF	C4-O4P-P-O3P
23	q	201	PEF	C11-C10-O2-C2
23	q	201	PEF	C1-O3P-P-O2P
23	q	201	PEF	C4-O4P-P-O1P
23	q	201	PEF	C4-O4P-P-O2P
23	q	201	PEF	C4-O4P-P-O3P
23	t	101	PEF	C1-O3P-P-O1P
23	t	101	PEF	C1-O3P-P-O4P
24	C	601	HEM	C2B-C3B-CAB-CBB
24	C	601	HEM	C2D-C3D-CAD-CBD
24	N	601	HEM	C2B-C3B-CAB-CBB
24	N	601	HEM	C4B-C3B-CAB-CBB
25	C	603[A]	UQ6	C29-C31-C32-C33
25	C	603[B]	UQ6	C12-C11-C9-C10
25	C	603[B]	UQ6	C19-C21-C22-C23
25	C	603[B]	UQ6	C29-C31-C32-C33
26	C	604	CDL	CA2-OA2-PA1-OA4
26	C	604	CDL	CA3-OA5-PA1-OA2
26	C	604	CDL	CA3-OA5-PA1-OA3
26	C	604	CDL	CA3-OA5-PA1-OA4
26	C	604	CDL	CB3-OB5-PB2-OB3
26	C	604	CDL	C51-CB5-OB6-CB4
26	E	302	CDL	CA2-C1-CB2-OB2
26	E	302	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
26	E	302	CDL	CA3-OA5-PA1-OA3
26	E	302	CDL	CA3-OA5-PA1-OA4
26	E	302	CDL	C11-CA5-OA6-CA4
26	E	302	CDL	CB3-OB5-PB2-OB3
26	E	302	CDL	CB3-OB5-PB2-OB4
26	H	601	CDL	CA3-OA5-PA1-OA3
26	H	601	CDL	CB2-OB2-PB2-OB3
26	H	602	CDL	CA2-OA2-PA1-OA4
26	H	602	CDL	CB3-OB5-PB2-OB2
26	H	602	CDL	CB3-OB5-PB2-OB3
26	H	602	CDL	CB3-OB5-PB2-OB4
26	H	602	CDL	C51-CB5-OB6-CB4
26	L	501	CDL	CA2-OA2-PA1-OA3
26	L	501	CDL	CA2-OA2-PA1-OA4
26	L	501	CDL	CA3-OA5-PA1-OA2
26	L	501	CDL	CA3-OA5-PA1-OA3
26	L	501	CDL	CA3-OA5-PA1-OA4
26	L	501	CDL	CB3-OB5-PB2-OB4
26	L	501	CDL	OB5-CB3-CB4-OB6
26	L	501	CDL	OB6-CB4-CB6-OB8
26	O	402	CDL	CA3-OA5-PA1-OA2
26	O	402	CDL	CB2-OB2-PB2-OB3
26	O	402	CDL	CB2-OB2-PB2-OB4
26	O	402	CDL	CB2-OB2-PB2-OB5
26	P	302	CDL	O1-C1-CA2-OA2
26	P	302	CDL	CB2-OB2-PB2-OB3
26	P	302	CDL	CB3-OB5-PB2-OB4
26	P	302	CDL	CB4-CB3-OB5-PB2
26	S	601	CDL	O1-C1-CA2-OA2
26	S	601	CDL	CA2-OA2-PA1-OA3
27	C	607	PCF	C11-O13-P-O11
27	C	607	PCF	C11-O13-P-O12
27	C	607	PCF	C11-O13-P-O14
27	H	604	PCF	C1-O11-P-O12
27	H	604	PCF	C11-O13-P-O11
27	H	604	PCF	C11-O13-P-O12
27	I	101	PCF	C11-O13-P-O12
27	N	606	PCF	C1-O11-P-O12
27	S	603	PCF	C11-O13-P-O12
27	S	603	PCF	O11-C1-C2-O21
27	T	101	PCF	C1-O11-P-O14
31	a	602	HEA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	a	602	HEA	C15-C16-C17-C18
31	m	602	HEA	C11-C12-C13-C14
31	m	602	HEA	C15-C16-C17-C18
26	O	402	CDL	OB9-CB7-OB8-CB6
27	I	101	PCF	O32-C31-O31-C3
26	O	402	CDL	C71-CB7-OB8-CB6
27	I	101	PCF	C32-C31-O31-C3
27	T	101	PCF	O32-C31-O31-C3
23	A	501	PEF	O4-C10-O2-C2
23	D	402	PEF	O4-C10-O2-C2
23	P	303	PEF	O4-C10-O2-C2
23	q	201	PEF	O4-C10-O2-C2
26	C	604	CDL	OB7-CB5-OB6-CB4
26	E	302	CDL	OA7-CA5-OA6-CA4
26	H	602	CDL	OB7-CB5-OB6-CB4
23	E	303	PEF	C11-C10-O2-C2
26	P	302	CDL	C11-CA5-OA6-CA4
25	C	603[A]	UQ6	C20-C19-C21-C22
25	C	603[B]	UQ6	C12-C11-C9-C8
27	T	101	PCF	C32-C31-O31-C3
24	C	601	HEM	C4D-C3D-CAD-CBD
23	N	605	PEF	O4-C10-O2-C2
26	E	302	CDL	O1-C1-CB2-OB2
26	H	602	CDL	O1-C1-CB2-OB2
26	S	601	CDL	O1-C1-CB2-OB2
23	t	101	PEF	C31-C30-O3-C3
27	S	603	PCF	C32-C31-O31-C3
27	S	603	PCF	O32-C31-O31-C3
23	N	605	PEF	C11-C10-O2-C2
26	E	302	CDL	C51-CB5-OB6-CB4
26	P	302	CDL	OA7-CA5-OA6-CA4
25	C	603[A]	UQ6	C25-C24-C26-C27
25	C	603[B]	UQ6	C25-C24-C26-C27
25	C	603[B]	UQ6	C30-C29-C31-C32
31	a	602	HEA	C26-C15-C16-C17
31	m	602	HEA	C26-C15-C16-C17
25	C	603[A]	UQ6	C23-C24-C26-C27
25	C	603[B]	UQ6	C23-C24-C26-C27
25	C	603[B]	UQ6	C28-C29-C31-C32
31	a	602	HEA	C14-C15-C16-C17
31	m	602	HEA	C14-C15-C16-C17
23	t	101	PEF	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
25	C	603[A]	UQ6	C9-C11-C12-C13
25	C	603[A]	UQ6	C19-C21-C22-C23
26	H	602	CDL	CA2-C1-CB2-OB2
26	P	302	CDL	CB2-C1-CA2-OA2
26	S	601	CDL	CB2-C1-CA2-OA2
26	S	601	CDL	CA2-C1-CB2-OB2
27	H	604	PCF	C11-C12-N-C14
27	H	604	PCF	C11-C12-N-C15
26	L	501	CDL	C71-CB7-OB8-CB6
23	m	607	PEF	O2-C2-C3-O3
26	E	302	CDL	OB7-CB5-OB6-CB4
26	O	402	CDL	CA7-C31-C32-C33
23	N	605	PEF	C31-C30-O3-C3
23	h	101	PEF	C31-C30-O3-C3
23	N	604	PEF	C10-C11-C12-C13
23	O	403	PEF	C10-C11-C12-C13
23	N	603	PEF	C10-C11-C12-C13
23	a	606	PEF	C30-C31-C32-C33
23	m	606	PEF	C30-C31-C32-C33
23	n	304	PEF	C30-C31-C32-C33
26	C	604	CDL	CA5-C11-C12-C13
26	H	601	CDL	CA7-C31-C32-C33
26	H	601	CDL	CB5-C51-C52-C53
26	P	302	CDL	CB5-C51-C52-C53
27	N	606	PCF	C31-C32-C33-C34
26	H	601	CDL	CA5-C11-C12-C13
27	q	202	PCF	C21-C22-C23-C24
23	c	302	PEF	C11-C10-O2-C2
26	L	501	CDL	OB9-CB7-OB8-CB6
23	N	605	PEF	O5-C30-O3-C3
25	C	603[B]	UQ6	C9-C11-C12-C13
23	N	603	PEF	C30-C31-C32-C33
23	O	403	PEF	C30-C31-C32-C33
27	I	101	PCF	C21-C22-C23-C24
24	N	601	HEM	C4D-C3D-CAD-CBD
23	N	604	PEF	C11-C10-O2-C2
23	o	302	PEF	C11-C10-O2-C2
26	P	302	CDL	C51-CB5-OB6-CB4
23	A	501	PEF	C1-O3P-P-O4P
23	C	605	PEF	C1-O3P-P-O4P
23	C	606	PEF	C4-O4P-P-O3P
23	D	402	PEF	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
23	H	603	PEF	C4-O4P-P-O3P
23	N	603	PEF	C1-O3P-P-O4P
23	N	605	PEF	C1-O3P-P-O4P
23	S	602	PEF	C4-O4P-P-O3P
23	b	303	PEF	C1-O3P-P-O4P
23	c	302	PEF	C1-O3P-P-O4P
23	e	201	PEF	C1-O3P-P-O4P
23	h	101	PEF	C1-O3P-P-O4P
23	m	607	PEF	C4-O4P-P-O3P
23	n	303	PEF	C1-O3P-P-O4P
23	n	304	PEF	C4-O4P-P-O3P
23	o	301	PEF	C1-O3P-P-O4P
23	o	302	PEF	C1-O3P-P-O4P
23	q	201	PEF	C1-O3P-P-O4P
26	C	604	CDL	CA2-OA2-PA1-OA5
26	E	302	CDL	CB3-OB5-PB2-OB2
26	H	602	CDL	CA2-OA2-PA1-OA5
26	L	501	CDL	CA2-OA2-PA1-OA5
26	L	501	CDL	CB3-OB5-PB2-OB2
26	O	402	CDL	CB3-OB5-PB2-OB2
26	P	302	CDL	CB3-OB5-PB2-OB2
27	T	101	PCF	C1-O11-P-O13
23	o	301	PEF	C30-C31-C32-C33
23	N	604	PEF	O4-C10-O2-C2
23	c	302	PEF	O4-C10-O2-C2
25	C	603[B]	UQ6	C15-C14-C16-C17
25	C	603[A]	UQ6	C18-C19-C21-C22
27	e	202	PCF	C11-C12-N-C13
23	h	101	PEF	C37-C38-C39-C40
27	N	606	PCF	C47-C48-C49-C50
24	N	601	HEM	C2D-C3D-CAD-CBD
23	N	603	PEF	C33-C34-C35-C36
23	C	605	PEF	O4-C10-O2-C2
23	o	302	PEF	O4-C10-O2-C2
26	P	302	CDL	OB7-CB5-OB6-CB4
23	S	602	PEF	C36-C37-C38-C39
23	h	101	PEF	C31-C32-C33-C34
27	C	607	PCF	C24-C25-C26-C27
27	e	202	PCF	C34-C35-C36-C37
23	n	303	PEF	C21-C22-C23-C24
27	e	202	PCF	C22-C23-C24-C25
23	e	201	PEF	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
23	m	606	PEF	C37-C38-C39-C40
23	q	201	PEF	C38-C39-C40-C41
23	t	101	PEF	C31-C32-C33-C34
26	H	601	CDL	C71-C72-C73-C74
23	N	605	PEF	C11-C12-C13-C14
27	H	604	PCF	C31-C32-C33-C34
23	A	501	PEF	C34-C35-C36-C37
23	N	604	PEF	C14-C15-C16-C17
23	N	604	PEF	C21-C22-C23-C24
23	h	101	PEF	C19-C20-C21-C22
23	h	101	PEF	O5-C30-O3-C3
23	N	604	PEF	C33-C34-C35-C36
23	C	605	PEF	C11-C10-O2-C2
23	t	101	PEF	C37-C38-C39-C40
26	H	601	CDL	C36-C37-C38-C39
26	H	602	CDL	C58-C59-C60-C61
26	L	501	CDL	CB5-C51-C52-C53
27	C	607	PCF	C21-C22-C23-C24
27	q	202	PCF	C31-C32-C33-C34
23	N	603	PEF	C15-C16-C17-C18
23	N	604	PEF	C13-C14-C15-C16
23	a	607	PEF	C33-C34-C35-C36
23	o	301	PEF	O3P-C1-C2-C3
23	C	605	PEF	C13-C14-C15-C16
23	C	606	PEF	C11-C12-C13-C14
23	O	403	PEF	C32-C33-C34-C35
27	e	202	PCF	C23-C24-C25-C26
23	D	402	PEF	O4P-C4-C5-N
26	O	402	CDL	C12-C13-C14-C15
23	q	201	PEF	C33-C34-C35-C36
23	C	605	PEF	C15-C16-C17-C18
23	D	402	PEF	C15-C16-C17-C18
23	o	301	PEF	C10-C11-C12-C13
27	N	606	PCF	C22-C21-O21-C2
23	O	403	PEF	C40-C41-C42-C43
23	n	303	PEF	C12-C13-C14-C15
27	S	603	PCF	C22-C23-C24-C25
27	T	101	PCF	C21-C22-C23-C24
27	H	604	PCF	C11-C12-N-C13
27	T	101	PCF	C11-C12-N-C13
27	T	101	PCF	C11-C12-N-C14
27	e	202	PCF	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
27	e	202	PCF	C11-C12-N-C15
23	c	301	PEF	C31-C32-C33-C34
23	t	101	PEF	C30-C31-C32-C33
23	N	603	PEF	C12-C13-C14-C15
23	O	403	PEF	O4-C10-O2-C2
23	q	201	PEF	C31-C30-O3-C3
26	H	601	CDL	C31-CA7-OA8-CA6
23	S	602	PEF	C32-C33-C34-C35
26	E	302	CDL	CB7-C71-C72-C73
23	m	606	PEF	C39-C40-C41-C42
25	C	603[A]	UQ6	C24-C26-C27-C28
23	N	604	PEF	C32-C33-C34-C35
23	e	201	PEF	C10-C11-C12-C13
23	N	603	PEF	C11-C10-O2-C2
23	O	403	PEF	C11-C10-O2-C2
23	a	607	PEF	C11-C10-O2-C2
23	n	304	PEF	C11-C10-O2-C2
26	S	601	CDL	C51-CB5-OB6-CB4
24	C	601	HEM	C4B-C3B-CAB-CBB
23	N	603	PEF	O4-C10-O2-C2
23	n	304	PEF	O4-C10-O2-C2
26	S	601	CDL	OB7-CB5-OB6-CB4
27	N	606	PCF	O22-C21-O21-C2
23	P	303	PEF	O2-C2-C3-O3
27	H	604	PCF	O21-C2-C3-O31
23	a	606	PEF	C38-C39-C40-C41
27	I	101	PCF	C11-C12-N-C14
27	I	101	PCF	C11-C12-N-C15
27	T	101	PCF	C11-C12-N-C15
25	C	603[B]	UQ6	C13-C14-C16-C17
23	e	201	PEF	C37-C38-C39-C40
23	q	201	PEF	C10-C11-C12-C13
23	a	606	PEF	C32-C33-C34-C35
23	h	101	PEF	C15-C16-C17-C18
23	a	607	PEF	O4-C10-O2-C2
23	E	303	PEF	C1-O3P-P-O4P
23	N	604	PEF	C4-O4P-P-O3P
23	m	606	PEF	C4-O4P-P-O3P
26	H	601	CDL	CA3-OA5-PA1-OA2
23	C	606	PEF	C30-C31-C32-C33
26	L	501	CDL	OA5-CA3-CA4-CA6
26	O	402	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
26	P	302	CDL	OB5-CB3-CB4-CB6
27	S	603	PCF	O11-C1-C2-C3
23	n	303	PEF	C32-C33-C34-C35
23	S	602	PEF	C30-C31-C32-C33
23	t	101	PEF	C11-C12-C13-C14
23	c	302	PEF	C31-C32-C33-C34
23	t	101	PEF	C12-C13-C14-C15
27	q	202	PCF	C23-C24-C25-C26
26	S	601	CDL	C11-CA5-OA6-CA4
23	E	303	PEF	C1-C2-C3-O3
23	P	303	PEF	C1-C2-C3-O3
23	m	607	PEF	C1-C2-C3-O3
26	C	604	CDL	CB3-CB4-CB6-OB8
26	H	602	CDL	CB3-CB4-CB6-OB8
27	T	101	PCF	C1-C2-C3-O31
23	q	201	PEF	O5-C30-O3-C3
26	H	601	CDL	OA9-CA7-OA8-CA6
23	N	604	PEF	C34-C35-C36-C37
23	h	101	PEF	C16-C17-C18-C19
25	C	603[B]	UQ6	C24-C26-C27-C28
23	P	303	PEF	C31-C32-C33-C34
23	O	403	PEF	C16-C17-C18-C19
23	N	605	PEF	C16-C17-C18-C19
27	N	606	PCF	C37-C38-C39-C40
23	P	303	PEF	C13-C14-C15-C16
23	t	101	PEF	C19-C20-C21-C22
26	H	602	CDL	C31-CA7-OA8-CA6
26	S	601	CDL	OB5-CB3-CB4-OB6
26	H	602	CDL	C31-C32-C33-C34
26	H	602	CDL	OA9-CA7-OA8-CA6
23	m	606	PEF	C32-C33-C34-C35
23	E	303	PEF	O2-C2-C3-O3
27	T	101	PCF	C34-C35-C36-C37
27	q	202	PCF	C22-C21-O21-C2
23	a	608	PEF	C31-C32-C33-C34
27	C	607	PCF	C23-C24-C25-C26
27	I	101	PCF	C11-C12-N-C13
23	b	303	PEF	O3P-C1-C2-C3
23	t	101	PEF	O3P-C1-C2-C3
26	C	604	CDL	OA5-CA3-CA4-CA6
26	L	501	CDL	OB5-CB3-CB4-CB6
27	I	101	PCF	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	b	303	PEF	C18-C19-C20-C21
26	L	501	CDL	CA5-C11-C12-C13
23	N	603	PEF	O4P-C4-C5-N
23	m	606	PEF	C38-C39-C40-C41
23	o	301	PEF	C31-C32-C33-C34
23	n	304	PEF	C33-C34-C35-C36
26	H	602	CDL	C33-C34-C35-C36
23	c	301	PEF	C30-C31-C32-C33
27	N	606	PCF	C21-C22-C23-C24
26	H	602	CDL	C60-C61-C62-C63
23	D	402	PEF	C37-C38-C39-C40
23	n	304	PEF	C31-C32-C33-C34
23	O	403	PEF	C39-C40-C41-C42
23	q	201	PEF	C37-C38-C39-C40
23	S	602	PEF	C1-C2-C3-O3
23	e	201	PEF	C1-C2-C3-O3
26	L	501	CDL	CB3-CB4-CB6-OB8
26	P	302	CDL	CA3-CA4-CA6-OA8
27	H	604	PCF	C1-C2-C3-O31
26	S	601	CDL	OA7-CA5-OA6-CA4
31	m	602	HEA	C2D-C3D-CAD-CBD
27	e	202	PCF	C24-C25-C26-C27
23	S	602	PEF	C1-O3P-P-O4P
23	c	301	PEF	C4-O4P-P-O3P
23	e	201	PEF	C4-O4P-P-O3P
26	H	601	CDL	CA2-OA2-PA1-OA5
26	H	601	CDL	CB2-OB2-PB2-OB5
23	N	604	PEF	O3P-C1-C2-O2
23	o	301	PEF	O3P-C1-C2-O2
27	I	101	PCF	O11-C1-C2-O21
26	H	601	CDL	C71-CB7-OB8-CB6
26	O	402	CDL	C11-C12-C13-C14
23	C	606	PEF	O2-C2-C3-O3
26	C	604	CDL	OB6-CB4-CB6-OB8
26	L	501	CDL	OA6-CA4-CA6-OA8
23	e	201	PEF	C42-C43-C44-C45
23	N	604	PEF	C19-C20-C21-C22
23	c	302	PEF	C32-C33-C34-C35
27	I	101	PCF	C22-C23-C24-C25
26	P	302	CDL	C1-CB2-OB2-PB2
23	h	101	PEF	C21-C22-C23-C24
26	O	402	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
26	H	602	CDL	C52-C53-C54-C55
23	D	402	PEF	O3P-C1-C2-C3
23	a	608	PEF	O3P-C1-C2-C3
23	h	101	PEF	O3P-C1-C2-C3
26	E	302	CDL	OA5-CA3-CA4-CA6
23	a	606	PEF	C37-C38-C39-C40
23	e	201	PEF	C17-C18-C19-C20
26	C	604	CDL	CB7-C71-C72-C73
26	E	302	CDL	C71-CB7-OB8-CB6
27	N	606	PCF	C32-C31-O31-C3
23	N	604	PEF	C3-C2-O2-C10
23	A	501	PEF	C1-C2-C3-O3
23	C	606	PEF	C1-C2-C3-O3
23	N	605	PEF	C1-C2-C3-O3
23	b	303	PEF	C1-C2-C3-O3
26	O	402	CDL	CA3-CA4-CA6-OA8
27	N	606	PCF	C1-C2-C3-O31
23	A	501	PEF	C41-C42-C43-C44
23	D	402	PEF	O3P-C1-C2-O2
23	b	303	PEF	O3P-C1-C2-O2
23	c	301	PEF	O3P-C1-C2-O2
23	h	101	PEF	O3P-C1-C2-O2
23	n	303	PEF	O3P-C1-C2-O2
26	C	604	CDL	OA5-CA3-CA4-OA6
26	P	302	CDL	OB5-CB3-CB4-OB6
27	H	604	PCF	O11-C1-C2-O21
27	N	606	PCF	O11-C1-C2-O21
23	N	603	PEF	C32-C33-C34-C35
23	n	303	PEF	C17-C18-C19-C20
26	O	402	CDL	OA7-CA5-OA6-CA4
27	N	606	PCF	O32-C31-O31-C3
23	S	602	PEF	O2-C2-C3-O3
23	b	303	PEF	O2-C2-C3-O3
26	H	602	CDL	OB6-CB4-CB6-OB8
27	I	101	PCF	O21-C2-C3-O31
23	a	606	PEF	C11-C12-C13-C14
27	q	202	PCF	O22-C21-O21-C2
23	A	501	PEF	C37-C38-C39-C40
23	D	402	PEF	C11-C12-C13-C14
26	L	501	CDL	C11-C12-C13-C14
23	o	301	PEF	C17-C18-C19-C20
23	h	101	PEF	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	E	302	CDL	CB5-C51-C52-C53
23	O	403	PEF	C41-C42-C43-C44
23	C	606	PEF	C1-O3P-P-O4P
23	t	101	PEF	C4-O4P-P-O3P
26	P	302	CDL	CB2-OB2-PB2-OB5
26	S	601	CDL	CA2-OA2-PA1-OA5
27	I	101	PCF	C11-O13-P-O11
26	H	602	CDL	C15-C16-C17-C18
23	n	303	PEF	C15-C16-C17-C18
23	E	303	PEF	C2-C1-O3P-P
23	m	606	PEF	C14-C15-C16-C17
27	T	101	PCF	C33-C34-C35-C36
23	C	605	PEF	C1-O3P-P-O1P
23	C	606	PEF	C1-O3P-P-O1P
23	C	606	PEF	C4-O4P-P-O1P
23	D	402	PEF	C1-O3P-P-O1P
23	E	303	PEF	C1-O3P-P-O2P
23	H	603	PEF	C4-O4P-P-O1P
23	N	604	PEF	C4-O4P-P-O1P
23	N	605	PEF	C1-O3P-P-O1P
23	S	602	PEF	C1-O3P-P-O2P
23	S	602	PEF	C4-O4P-P-O1P
23	a	608	PEF	C1-O3P-P-O2P
23	b	303	PEF	C1-O3P-P-O1P
23	e	201	PEF	C1-O3P-P-O1P
23	h	101	PEF	C1-O3P-P-O1P
23	m	606	PEF	C4-O4P-P-O1P
23	m	607	PEF	C1-O3P-P-O1P
23	n	303	PEF	C1-O3P-P-O1P
23	n	304	PEF	C4-O4P-P-O1P
23	q	201	PEF	C1-O3P-P-O1P
26	H	601	CDL	CA2-OA2-PA1-OA4
26	H	601	CDL	CA3-OA5-PA1-OA4
26	H	601	CDL	CB2-OB2-PB2-OB4
26	O	402	CDL	CA3-OA5-PA1-OA4
26	O	402	CDL	CB3-OB5-PB2-OB3
27	I	101	PCF	C11-O13-P-O14
27	N	606	PCF	C11-C12-N-C14
27	T	101	PCF	C1-O11-P-O12
23	N	605	PEF	C10-C11-C12-C13
23	n	304	PEF	C31-C30-O3-C3
23	c	301	PEF	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	H	602	CDL	OB5-CB3-CB4-CB6
26	S	601	CDL	OB5-CB3-CB4-CB6
27	H	604	PCF	O11-C1-C2-C3
27	N	606	PCF	O11-C1-C2-C3
26	H	601	CDL	OB9-CB7-OB8-CB6
31	a	602	HEA	O11-C11-C12-C13
31	m	602	HEA	O11-C11-C12-C13
23	b	303	PEF	C21-C22-C23-C24
23	a	608	PEF	O3P-C1-C2-O2
23	t	101	PEF	O3P-C1-C2-O2
26	E	302	CDL	OA5-CA3-CA4-OA6
26	H	602	CDL	OA5-CA3-CA4-OA6
26	H	602	CDL	OB5-CB3-CB4-OB6
26	L	501	CDL	OA5-CA3-CA4-OA6
27	e	202	PCF	C31-C32-C33-C34
26	E	302	CDL	OB9-CB7-OB8-CB6
23	N	604	PEF	C36-C37-C38-C39
27	q	202	PCF	C11-C12-N-C13
23	a	607	PEF	C32-C33-C34-C35
27	C	607	PCF	O13-C11-C12-N
27	I	101	PCF	C1-C2-C3-O31
27	T	101	PCF	O21-C2-C3-O31
23	b	303	PEF	C19-C20-C21-C22
23	e	201	PEF	C20-C21-C22-C23
27	q	202	PCF	C22-C23-C24-C25
23	n	304	PEF	O5-C30-O3-C3
27	N	606	PCF	C11-C12-N-C13
27	N	606	PCF	C11-C12-N-C15
26	O	402	CDL	C72-C73-C74-C75
26	L	501	CDL	O1-C1-CB2-OB2
23	a	606	PEF	C39-C40-C41-C42
23	n	304	PEF	C35-C36-C37-C38
23	C	605	PEF	C3-C2-O2-C10
23	n	303	PEF	O5-C30-O3-C3
26	H	601	CDL	C14-C15-C16-C17
23	t	101	PEF	C38-C39-C40-C41
26	O	402	CDL	OA5-CA3-CA4-OA6
27	q	202	PCF	C11-C12-N-C15
31	m	602	HEA	C4D-C3D-CAD-CBD
23	h	101	PEF	C11-C12-C13-C14
26	E	302	CDL	C31-C32-C33-C34
23	a	607	PEF	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
23	n	303	PEF	O2-C2-C3-O3
26	O	402	CDL	OA6-CA4-CA6-OA8
26	P	302	CDL	OA6-CA4-CA6-OA8
23	D	402	PEF	C4-O4P-P-O3P
23	b	303	PEF	C4-O4P-P-O3P
23	c	301	PEF	C1-O3P-P-O4P
23	h	101	PEF	C4-O4P-P-O3P
23	o	301	PEF	C4-O4P-P-O3P
26	C	604	CDL	CB3-OB5-PB2-OB2
26	E	302	CDL	CA2-OA2-PA1-OA5
26	P	302	CDL	CA3-OA5-PA1-OA2
27	S	603	PCF	C1-O11-P-O13
26	O	402	CDL	C62-C63-C64-C65
26	L	501	CDL	CA3-CA4-CA6-OA8
23	n	303	PEF	C18-C19-C20-C21
23	o	302	PEF	C32-C33-C34-C35
26	H	602	CDL	C54-C55-C56-C57
27	S	603	PCF	C11-C12-N-C13
26	E	302	CDL	C52-C51-CB5-OB6
23	D	402	PEF	C12-C13-C14-C15
23	c	301	PEF	C31-C30-O3-C3
23	n	303	PEF	C31-C30-O3-C3
23	h	101	PEF	C13-C14-C15-C16
23	t	101	PEF	C35-C36-C37-C38
23	O	403	PEF	C34-C35-C36-C37
23	q	201	PEF	C11-C12-C13-C14
24	N	602	HEM	CAD-CBD-CGD-O1D
23	c	302	PEF	C33-C34-C35-C36
26	H	602	CDL	C14-C15-C16-C17
26	O	402	CDL	CB5-C51-C52-C53
23	N	604	PEF	C15-C16-C17-C18
23	P	303	PEF	C30-C31-C32-C33
27	S	603	PCF	C31-C32-C33-C34
23	n	304	PEF	C34-C35-C36-C37
27	e	202	PCF	C25-C26-C27-C28
24	C	601	HEM	CAD-CBD-CGD-O1D
24	C	602	HEM	CAD-CBD-CGD-O1D
24	C	602	HEM	CAD-CBD-CGD-O2D
23	q	201	PEF	C1-C2-C3-O3
27	S	603	PCF	C1-C2-C3-O31
23	a	606	PEF	C14-C15-C16-C17
23	a	606	PEF	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
26	L	501	CDL	C71-C72-C73-C74
31	a	603	HEA	CAA-CBA-CGA-O2A
23	O	403	PEF	C13-C14-C15-C16
23	t	101	PEF	C15-C16-C17-C18
31	m	602	HEA	CAA-CBA-CGA-O1A
23	E	303	PEF	C31-C30-O3-C3
27	S	603	PCF	C11-C12-N-C14
27	q	202	PCF	C11-C12-N-C14
26	O	402	CDL	C34-C35-C36-C37
23	t	101	PEF	C13-C14-C15-C16
24	C	601	HEM	CAA-CBA-CGA-O1A
31	a	603	HEA	CAA-CBA-CGA-O1A
23	N	604	PEF	C20-C21-C22-C23
23	b	303	PEF	O4-C10-O2-C2
23	n	303	PEF	O3P-C1-C2-C3
26	H	602	CDL	OA5-CA3-CA4-CA6
23	q	201	PEF	C30-C31-C32-C33
24	C	601	HEM	CAA-CBA-CGA-O2A
27	T	101	PCF	C25-C26-C27-C28
26	L	501	CDL	C53-C54-C55-C56
23	h	101	PEF	C35-C36-C37-C38
24	N	602	HEM	CAD-CBD-CGD-O2D
31	m	602	HEA	CAA-CBA-CGA-O2A
23	c	301	PEF	O5-C30-O3-C3
24	C	601	HEM	CAD-CBD-CGD-O2D
23	q	201	PEF	C18-C19-C20-C21
23	S	602	PEF	C41-C42-C43-C44
24	N	601	HEM	CAD-CBD-CGD-O2D
23	C	606	PEF	C18-C19-C20-C21
31	a	603	HEA	CAD-CBD-CGD-O2D
23	C	606	PEF	C15-C16-C17-C18
23	D	402	PEF	C35-C36-C37-C38
24	C	602	HEM	CAA-CBA-CGA-O2A
24	N	602	HEM	CAA-CBA-CGA-O2A
24	N	601	HEM	CAD-CBD-CGD-O1D
25	C	603[B]	UQ6	C14-C16-C17-C18
24	N	601	HEM	CAA-CBA-CGA-O2A
23	e	201	PEF	O4P-C4-C5-N
23	o	302	PEF	C16-C17-C18-C19
23	D	402	PEF	O3-C30-C31-C32
26	P	302	CDL	CA5-C11-C12-C13
23	n	304	PEF	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	a	603	HEA	C26-C15-C16-C17
31	m	603	HEA	C26-C15-C16-C17
23	n	304	PEF	C12-C13-C14-C15
23	q	201	PEF	C20-C21-C22-C23
27	H	604	PCF	C24-C25-C26-C27
31	a	602	HEA	CAA-CBA-CGA-O1A
23	E	303	PEF	C12-C13-C14-C15
27	N	606	PCF	C35-C36-C37-C38
27	S	603	PCF	C11-C12-N-C15
24	N	601	HEM	CAA-CBA-CGA-O1A
23	E	303	PEF	O5-C30-O3-C3
23	n	303	PEF	O2-C10-C11-C12
23	c	301	PEF	C14-C15-C16-C17
28	D	401	HEC	CAD-CBD-CGD-O2D
31	a	603	HEA	CAD-CBD-CGD-O1D
27	e	202	PCF	C1-C2-C3-O31
23	b	303	PEF	O2-C10-C11-C12
27	H	604	PCF	O31-C31-C32-C33
24	C	602	HEM	CAA-CBA-CGA-O1A
23	e	201	PEF	C13-C14-C15-C16
23	h	101	PEF	O3-C30-C31-C32
24	N	602	HEM	CAA-CBA-CGA-O1A
26	C	604	CDL	C52-C53-C54-C55
26	O	402	CDL	OB6-CB4-CB6-OB8
27	N	606	PCF	O21-C2-C3-O31
27	T	101	PCF	C31-C32-C33-C34
31	a	602	HEA	CAA-CBA-CGA-O2A
27	N	606	PCF	O21-C21-C22-C23
28	D	401	HEC	CAD-CBD-CGD-O1D
23	b	303	PEF	C11-C10-O2-C2
23	N	603	PEF	O2-C10-C11-C12
23	e	201	PEF	C21-C22-C23-C24
23	m	606	PEF	O4-C10-O2-C2
23	N	604	PEF	C12-C13-C14-C15
23	b	303	PEF	C13-C14-C15-C16
23	N	605	PEF	C15-C16-C17-C18
23	D	402	PEF	C30-C31-C32-C33
23	b	303	PEF	O4-C10-C11-C12
27	H	604	PCF	O32-C31-C32-C33
26	H	601	CDL	C72-C73-C74-C75
23	q	201	PEF	C13-C14-C15-C16
25	C	603[A]	UQ6	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
23	H	603	PEF	C34-C35-C36-C37
23	e	201	PEF	C31-C30-O3-C3
23	n	303	PEF	O4-C10-C11-C12
27	q	202	PCF	C1-C2-C3-O31
23	h	101	PEF	O5-C30-C31-C32
23	N	605	PEF	O2-C10-C11-C12
26	O	402	CDL	C1-CA2-OA2-PA1
23	o	302	PEF	C31-C32-C33-C34
31	a	603	HEA	C14-C15-C16-C17
26	E	302	CDL	C53-C54-C55-C56
31	m	602	HEA	CAD-CBD-CGD-O2D
23	a	606	PEF	C4-O4P-P-O1P
26	E	302	CDL	CA2-OA2-PA1-OA3
26	P	302	CDL	CB2-OB2-PB2-OB4
27	S	603	PCF	C1-O11-P-O12
27	e	202	PCF	C11-O13-P-O12
23	P	303	PEF	O3P-C1-C2-C3
26	C	604	CDL	OB5-CB3-CB4-CB6
26	P	302	CDL	C52-C53-C54-C55
23	E	303	PEF	O4P-C4-C5-N
23	n	304	PEF	O4P-C4-C5-N
27	N	606	PCF	O22-C21-C22-C23
23	N	605	PEF	C31-C32-C33-C34
26	C	604	CDL	C51-C52-C53-C54
23	o	302	PEF	C5-C4-O4P-P
27	C	607	PCF	C12-C11-O13-P
31	a	603	HEA	C3B-C11-C12-C13
23	N	604	PEF	C30-C31-C32-C33
27	e	202	PCF	O31-C31-C32-C33
23	a	606	PEF	C40-C41-C42-C43
26	S	601	CDL	C72-C71-CB7-OB9
31	m	603	HEA	CAA-CBA-CGA-O1A
23	D	402	PEF	C38-C39-C40-C41
23	n	303	PEF	C31-C32-C33-C34
26	S	601	CDL	C72-C71-CB7-OB8
26	H	601	CDL	C32-C33-C34-C35
27	C	607	PCF	C30-C47-C48-C49
23	e	201	PEF	O5-C30-O3-C3
23	N	603	PEF	O4-C10-C11-C12
23	N	605	PEF	O4-C10-C11-C12
27	C	607	PCF	O31-C31-C32-C33
23	a	608	PEF	C32-C33-C34-C35

Continued on next page...

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Mol	Chain	Res	Type	Atoms
27	e	202	PCF	O32-C31-C32-C33
23	t	101	PEF	O3-C30-C31-C32
27	q	202	PCF	O31-C31-C32-C33

There are no ring outliers.

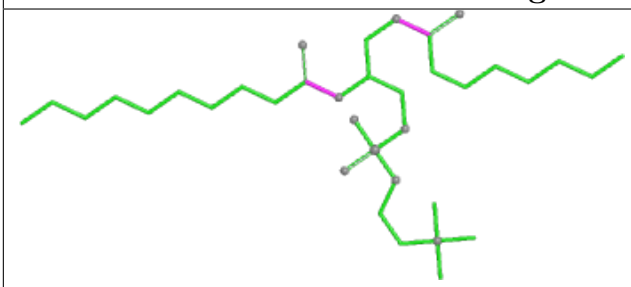
26 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	O	402	CDL	5	0
23	N	604	PEF	1	0
25	C	603[B]	UQ6	5	0
23	C	605	PEF	1	0
23	A	501	PEF	2	0
27	N	606	PCF	2	0
23	N	605	PEF	1	0
28	O	401	HEC	1	0
24	N	601	HEM	1	0
26	H	601	CDL	2	0
26	H	602	CDL	3	0
26	S	601	CDL	2	0
28	D	401	HEC	1	0
27	H	604	PCF	1	0
26	E	302	CDL	3	0
23	S	602	PEF	1	0
23	N	603	PEF	2	0
23	P	303	PEF	1	0
26	L	501	CDL	2	0
23	D	402	PEF	4	0
24	C	601	HEM	2	0
23	O	403	PEF	2	0
24	C	602	HEM	2	0
23	E	303	PEF	1	0
27	T	101	PCF	1	0
25	C	603[A]	UQ6	2	0

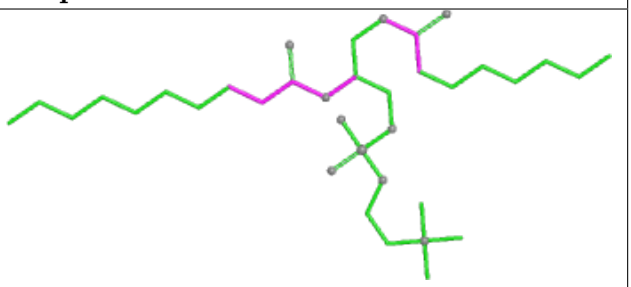
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

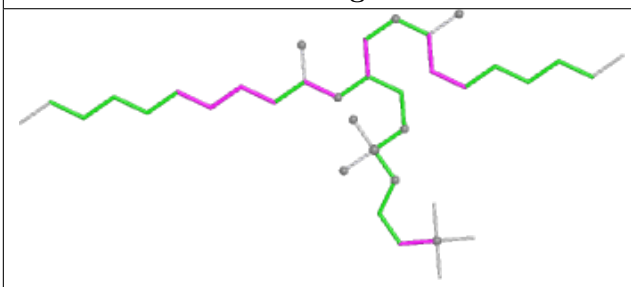
Ligand PCF q 202



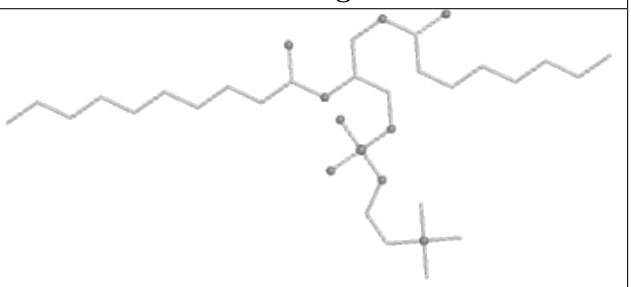
Bond lengths



Bond angles

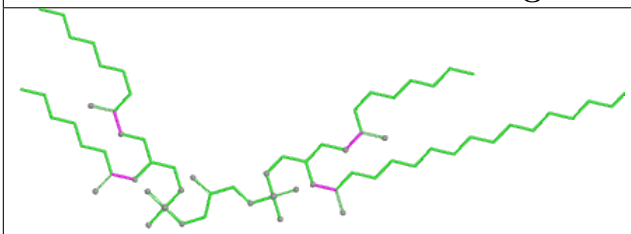


Torsions

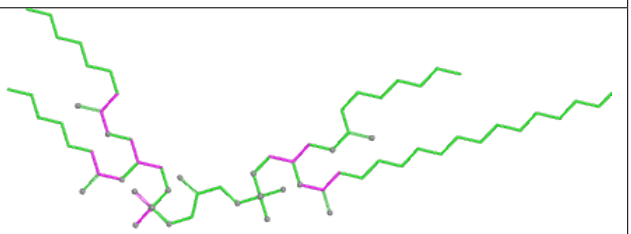


Rings

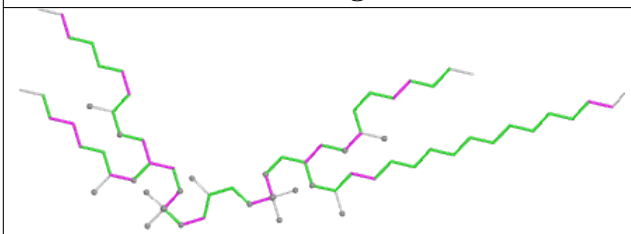
Ligand CDL O 402



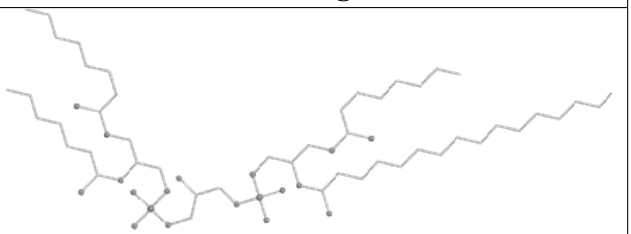
Bond lengths



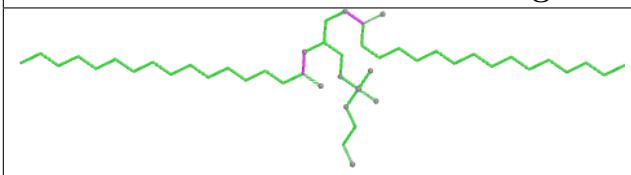
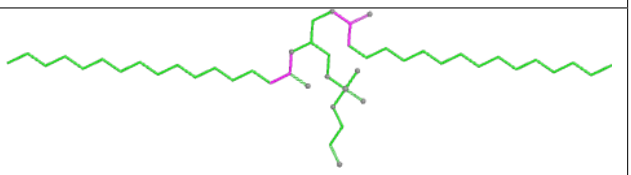
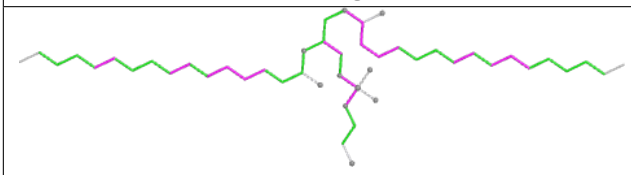
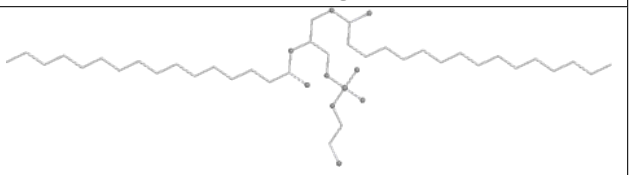
Bond angles

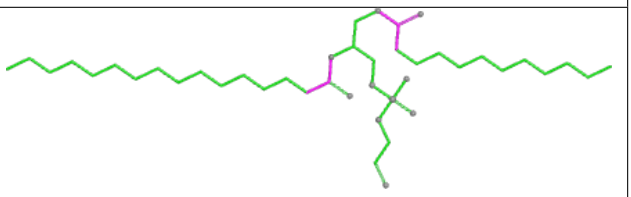
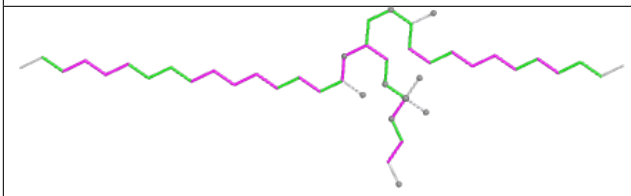
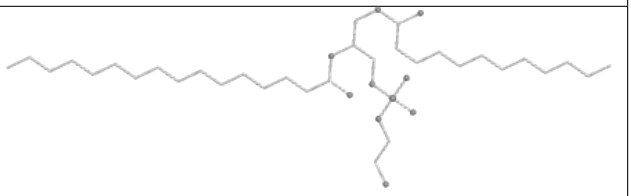


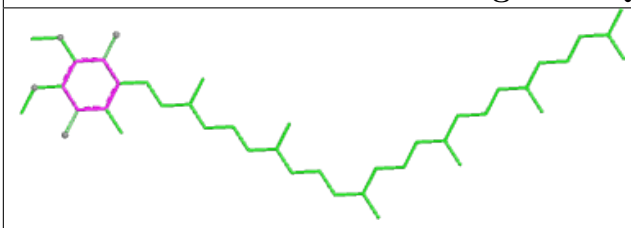
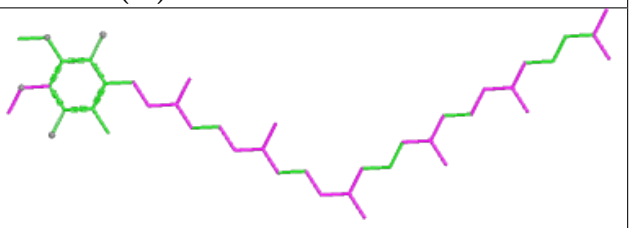
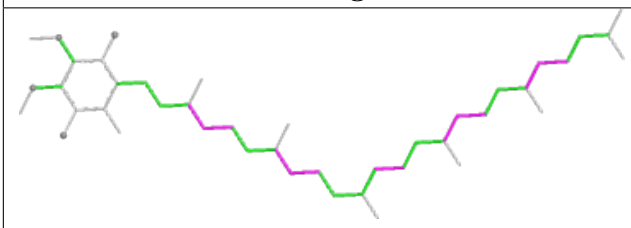
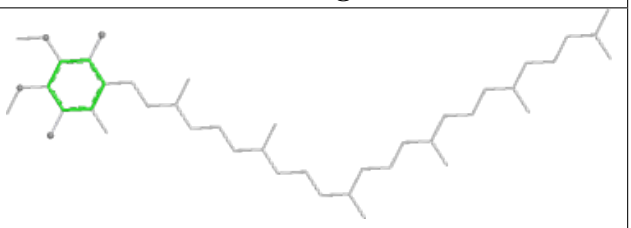
Torsions



Rings

Ligand PEF t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF N 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ6 C 603 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

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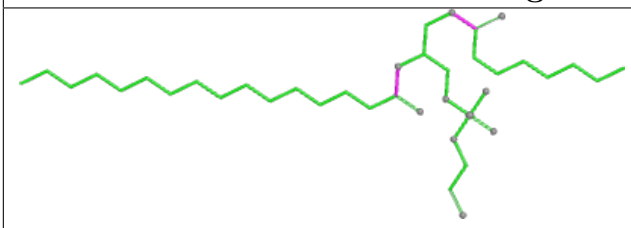
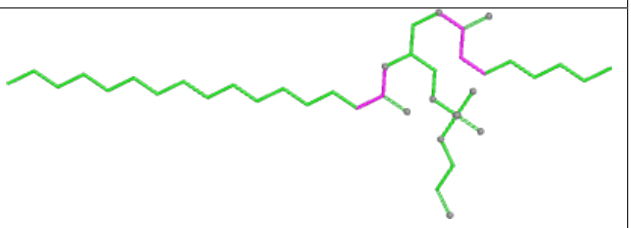
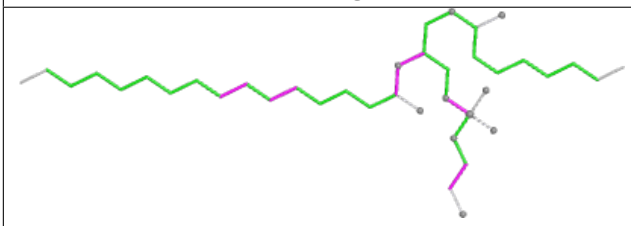
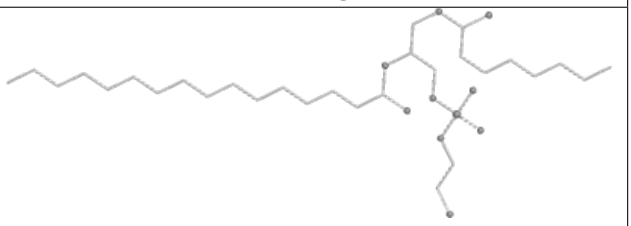
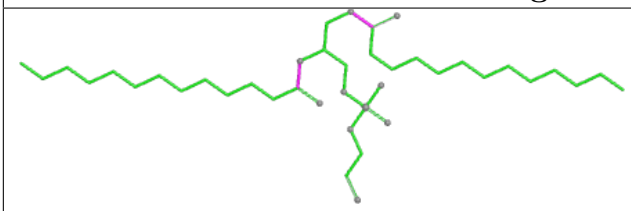
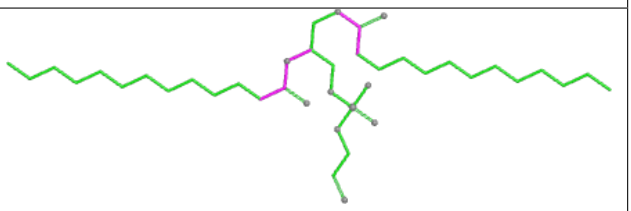
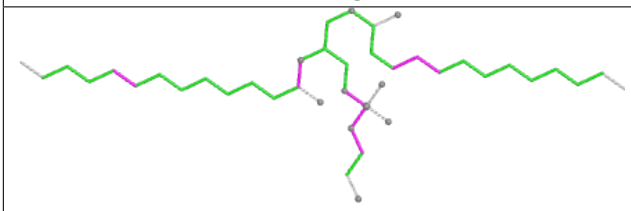
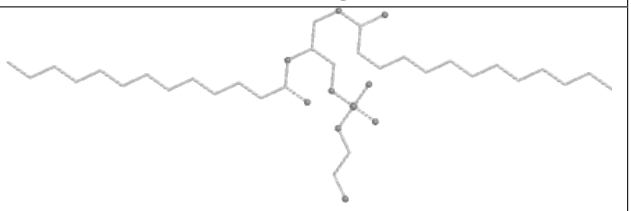
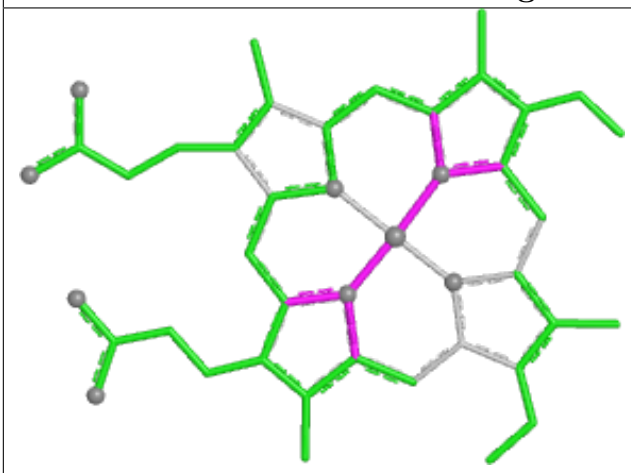
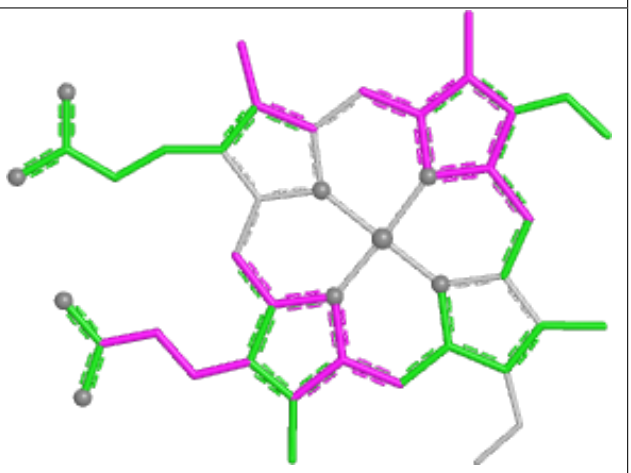
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEF o 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

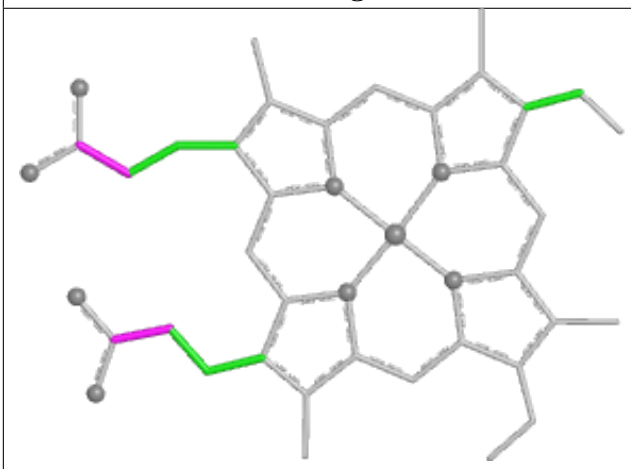
Ligand HEM N 602



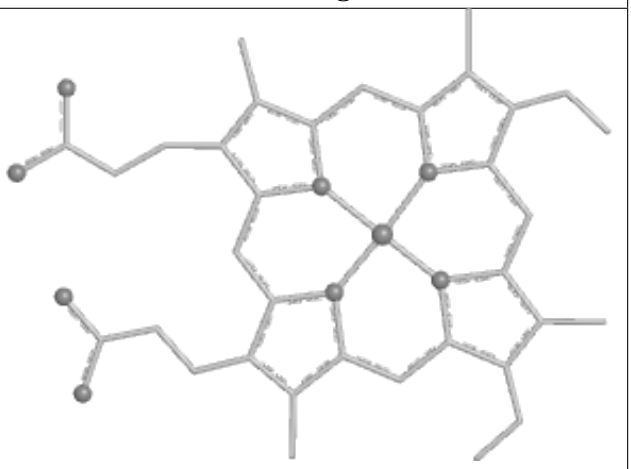
Bond lengths



Bond angles

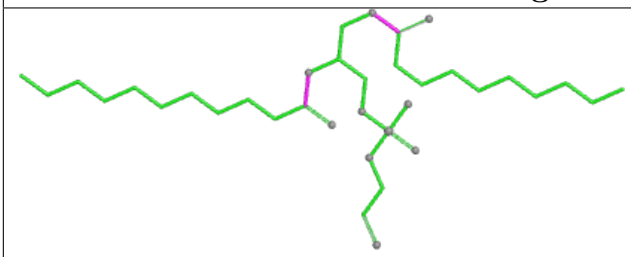


Torsions

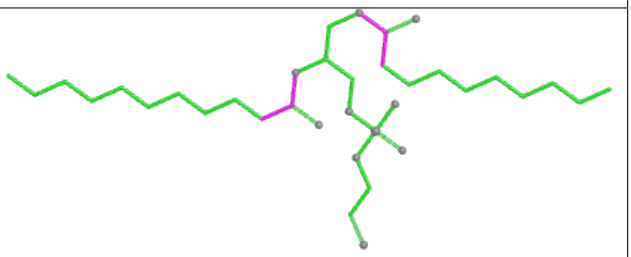


Rings

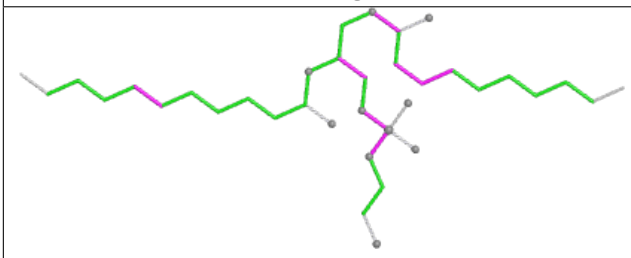
Ligand PEF c 301



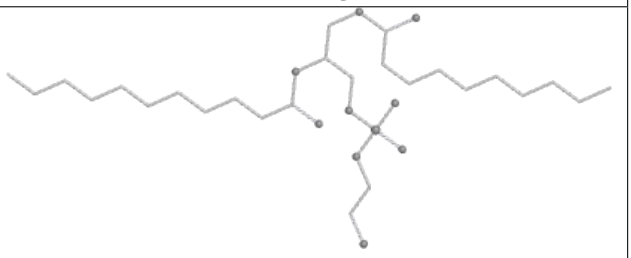
Bond lengths



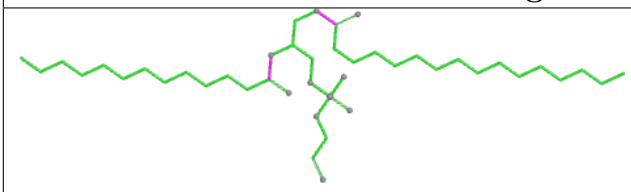
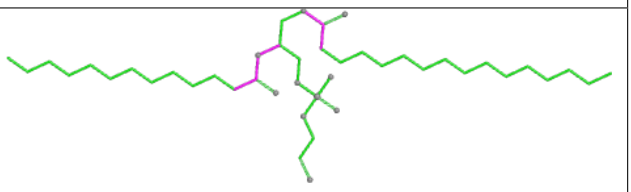
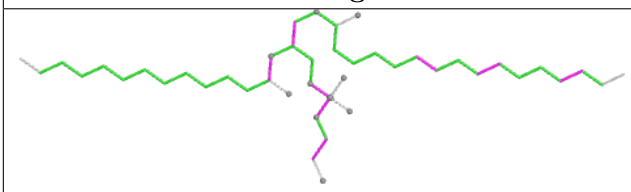
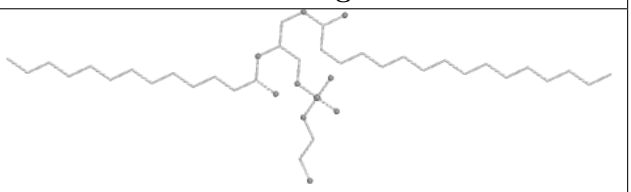
Bond angles

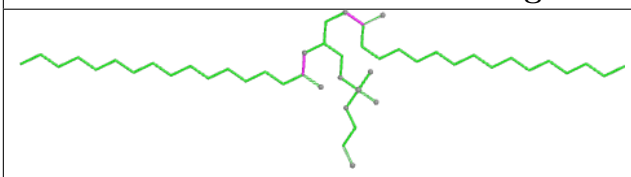
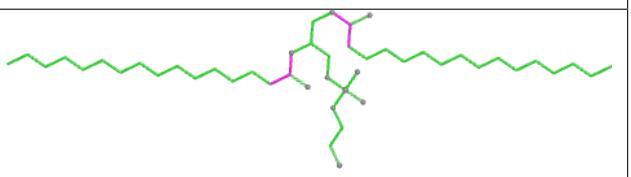
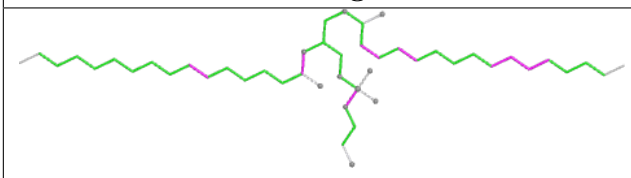
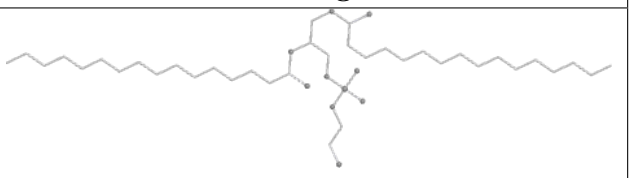


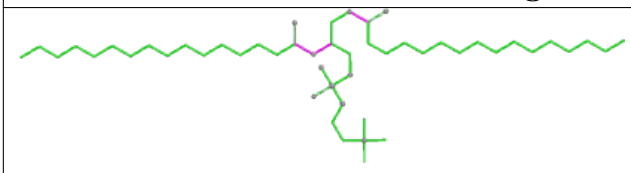
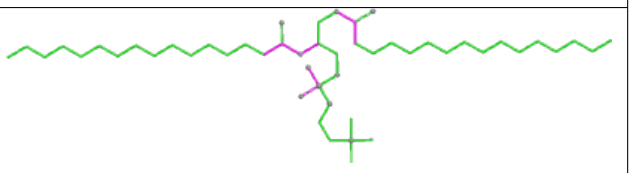
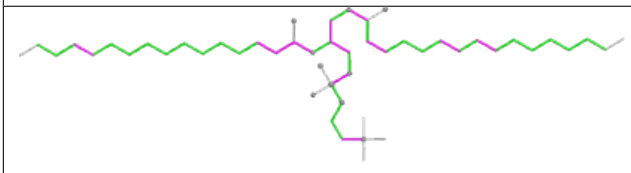
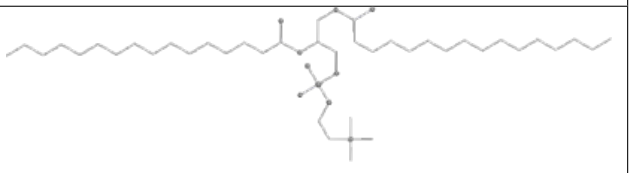
Torsions

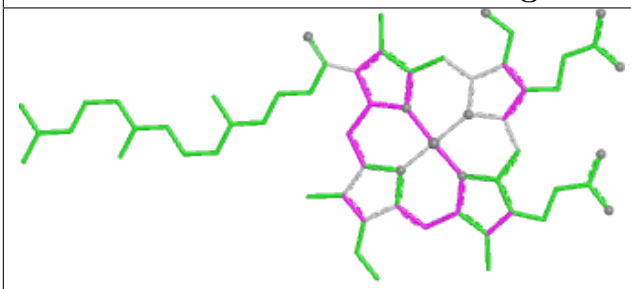
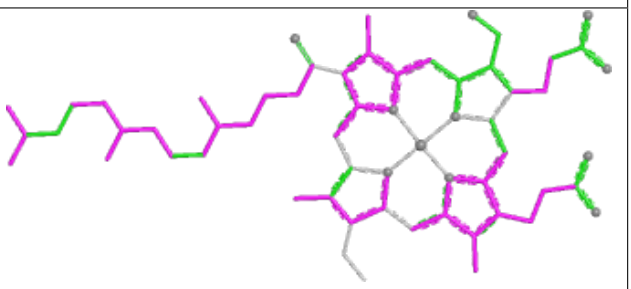
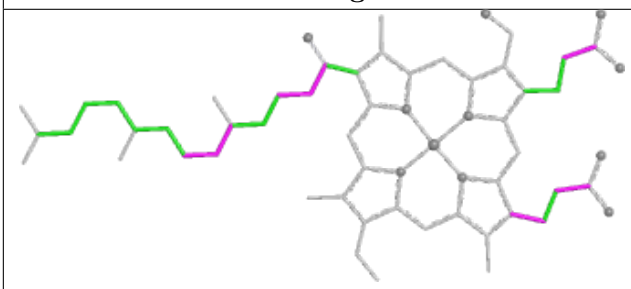
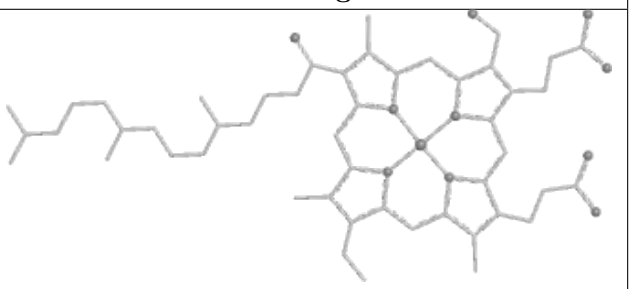


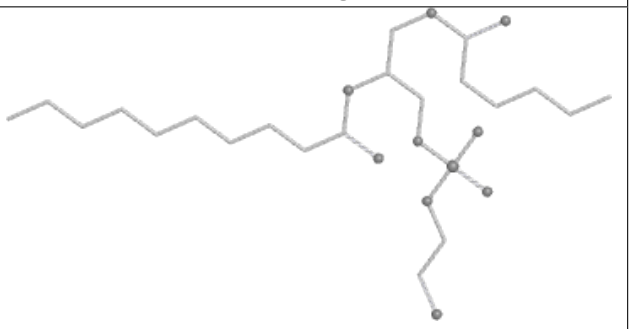
Rings

Ligand PEF A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF m 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCF N 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA m 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF N 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

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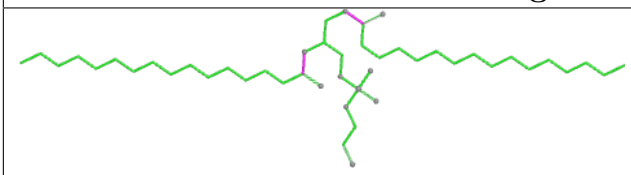
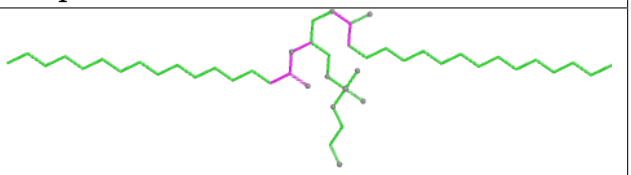
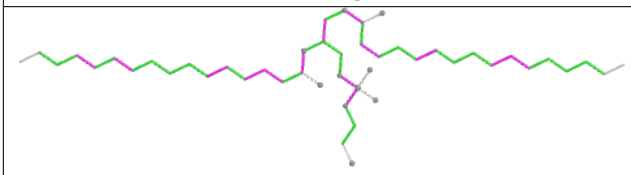
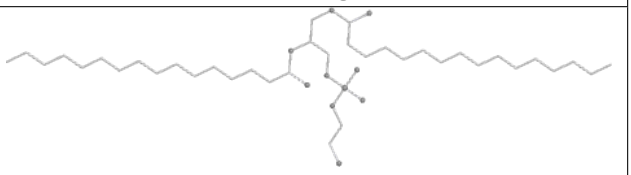
 Bond lengths	 Bond angles
 Torsions	 Rings

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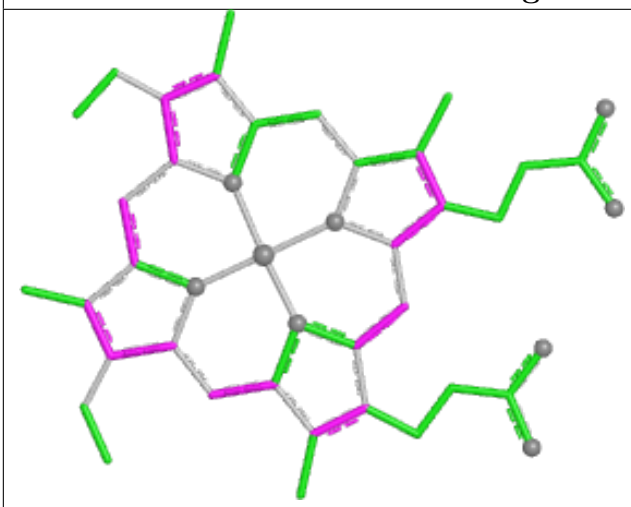
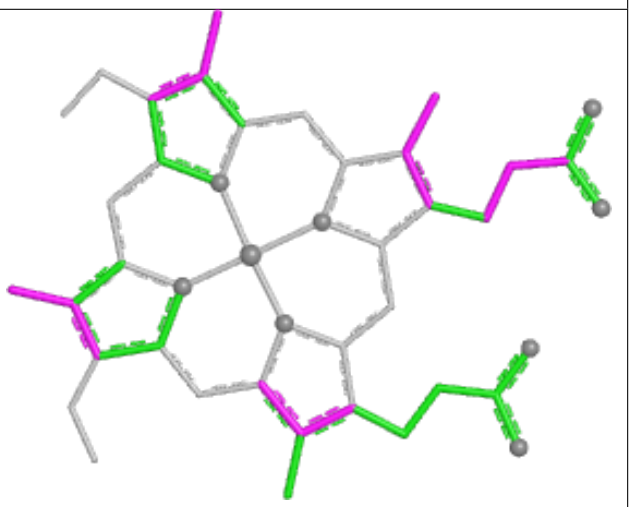
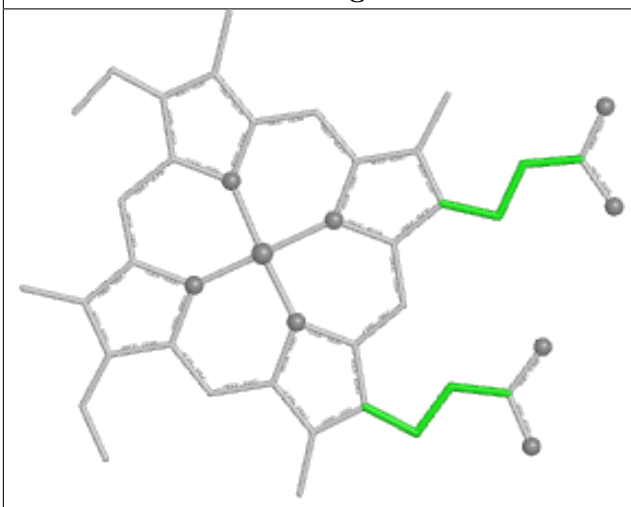
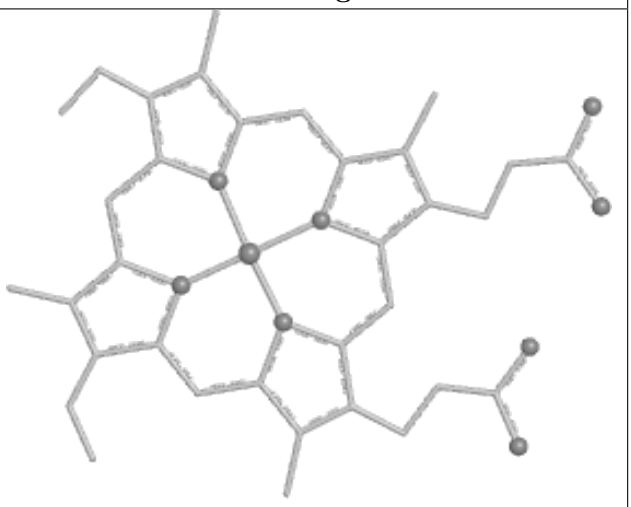
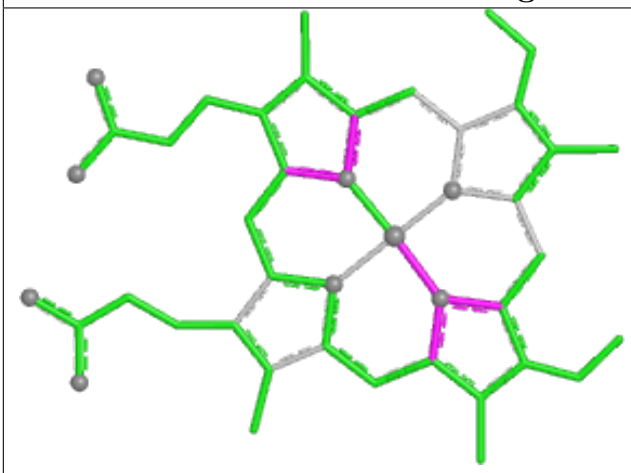
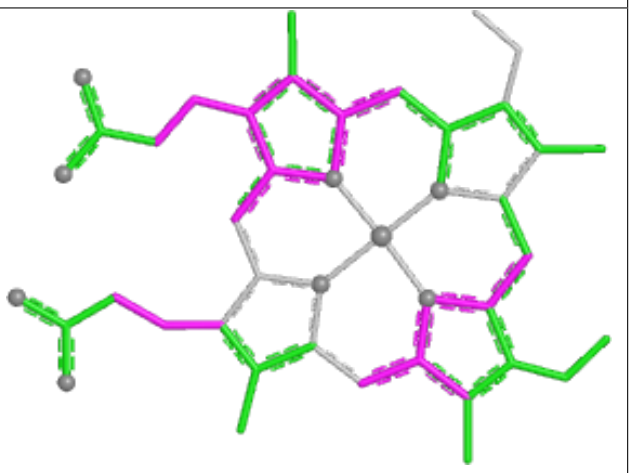
 Bond lengths	 Bond angles
 Torsions	 Rings

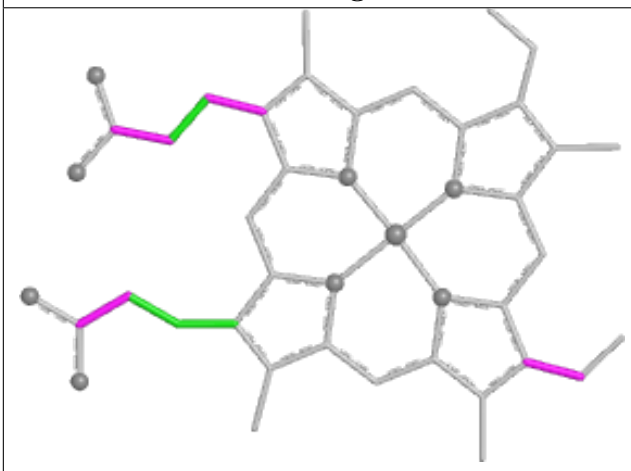
Ligand HEM N 601



Bond lengths



Bond angles



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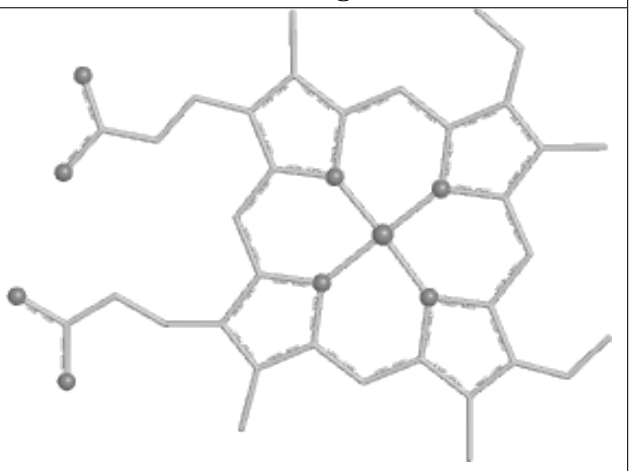
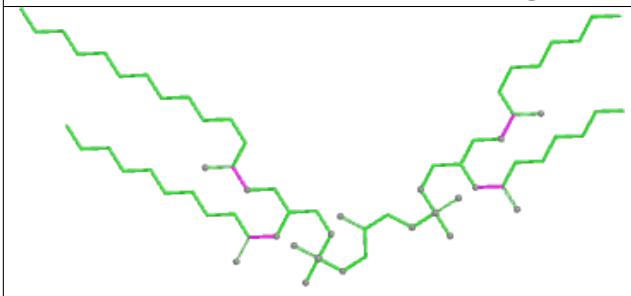


Rings

Ligand CDL H 601



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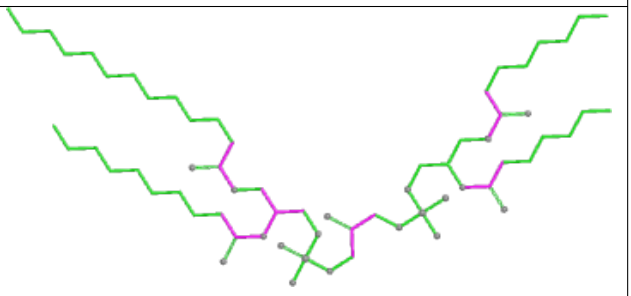
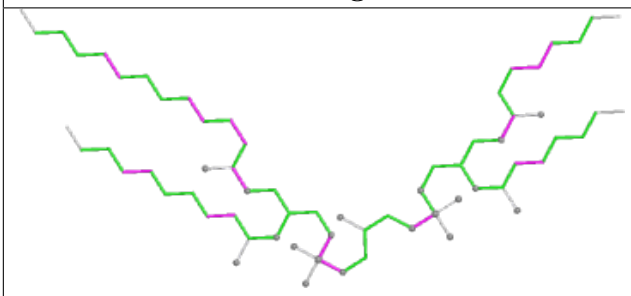


Bond angles



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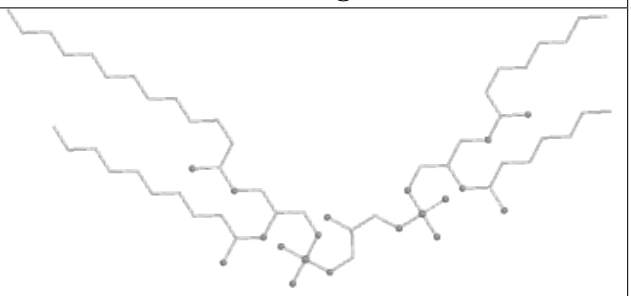

Rings

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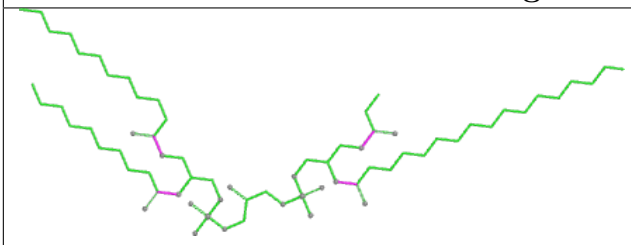
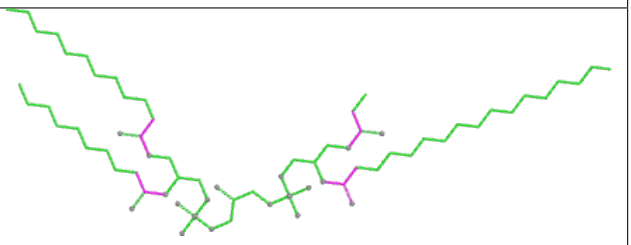
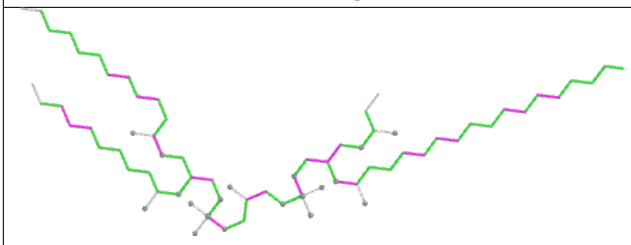
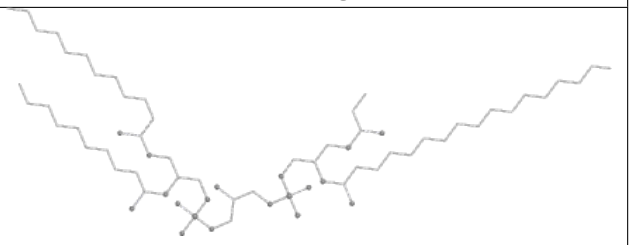
 Bond lengths	 Bond angles
 Torsions	 Rings

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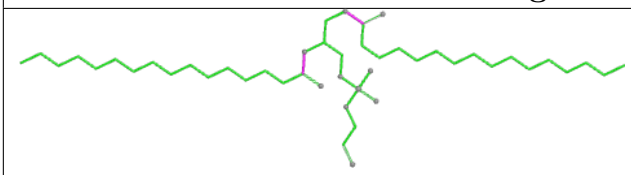
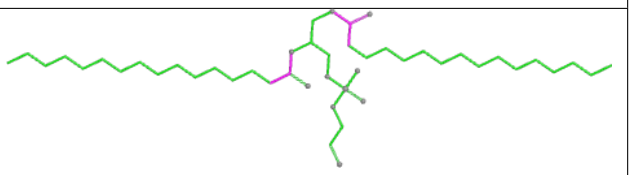
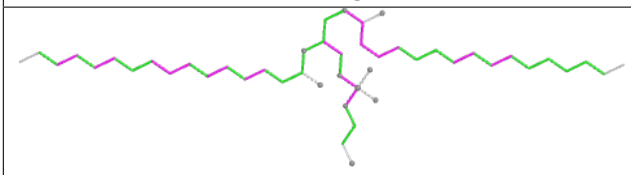
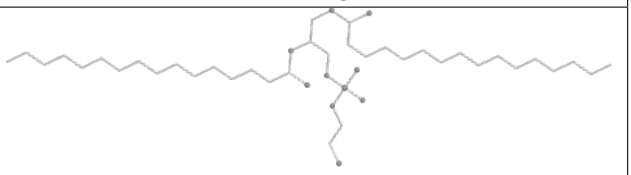
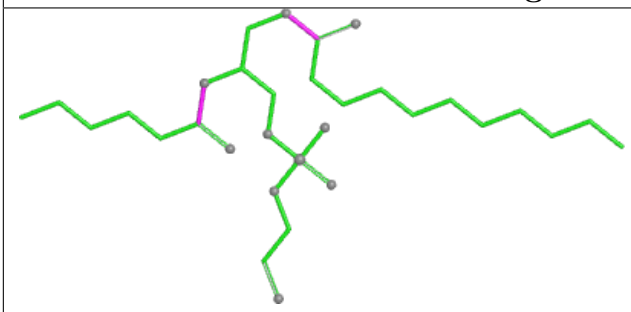
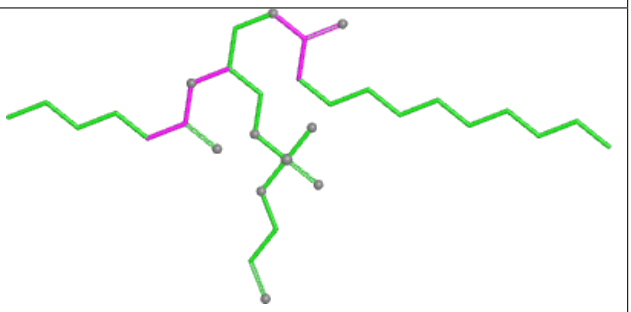
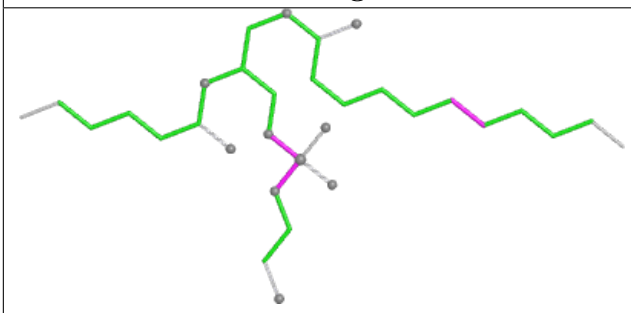
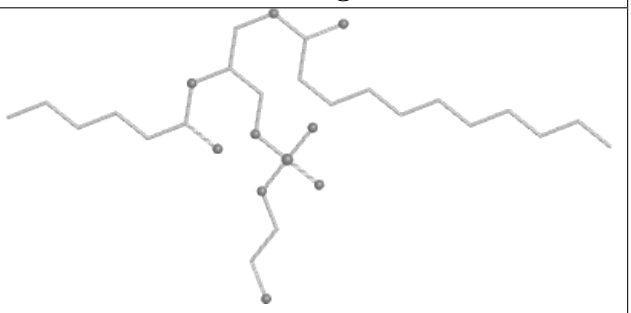
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF H 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

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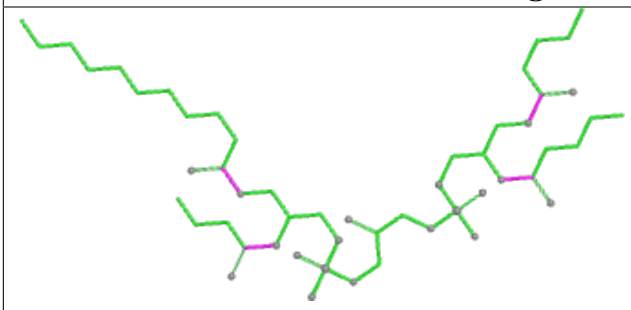
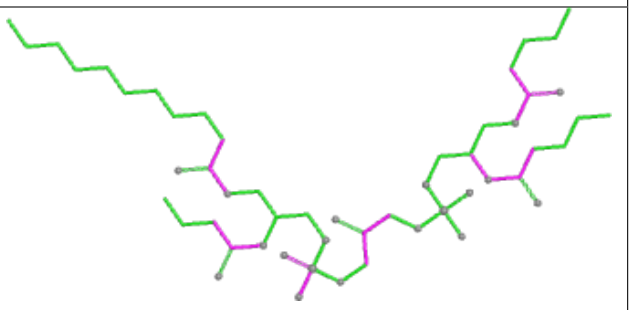
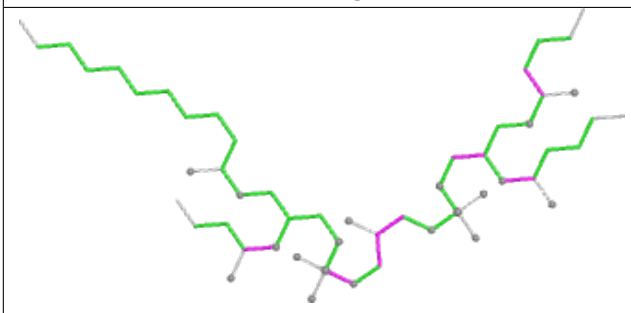
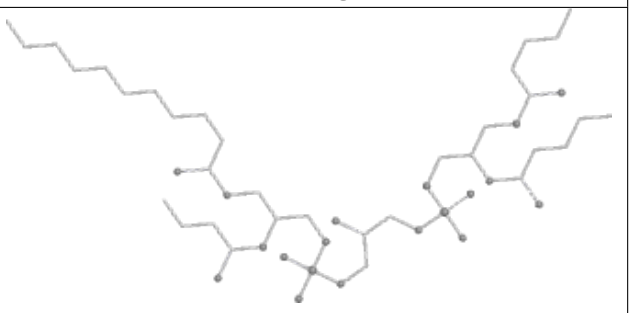
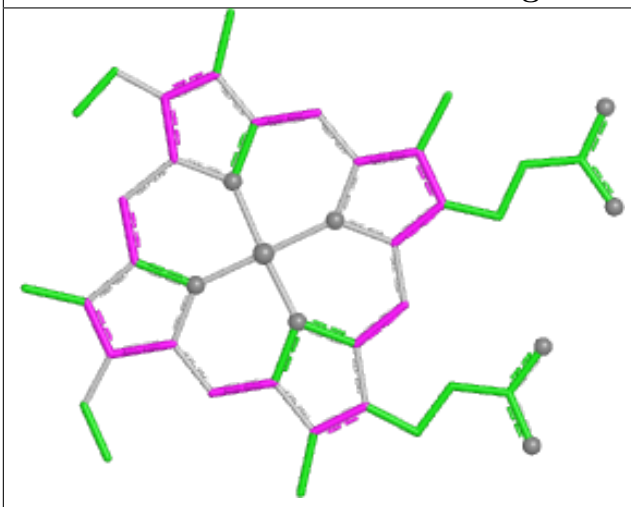
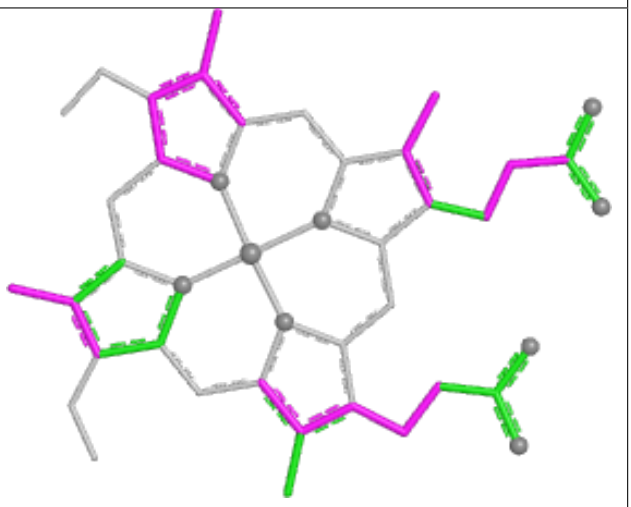
 Bond lengths	 Bond angles
 Torsions	 Rings

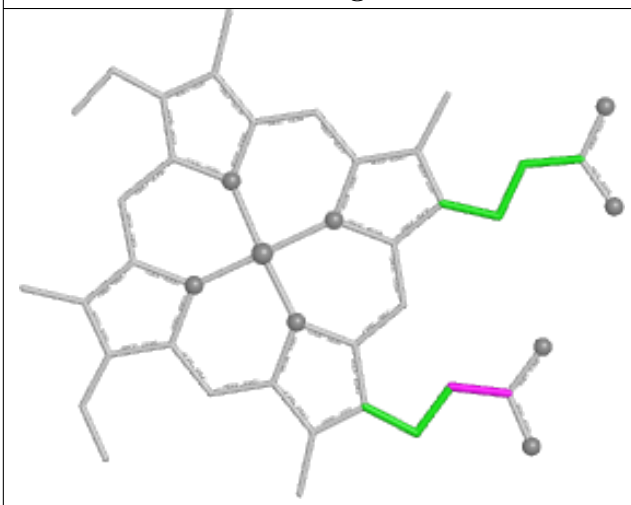
Ligand HEC D 401



Bond lengths



Bond angles



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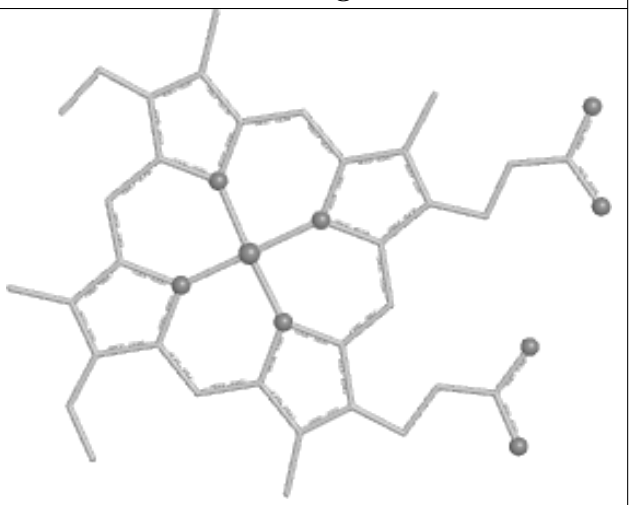
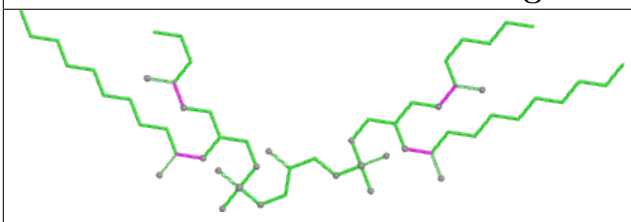


Rings

Ligand CDL C 604



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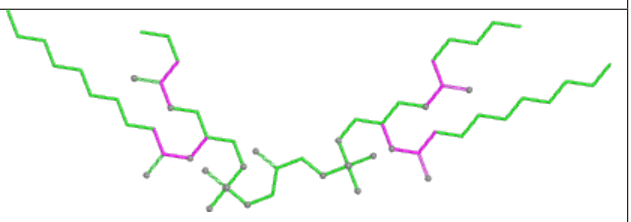
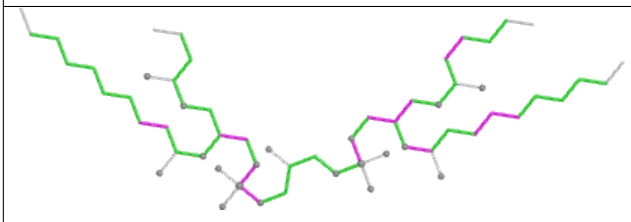


Bond angles



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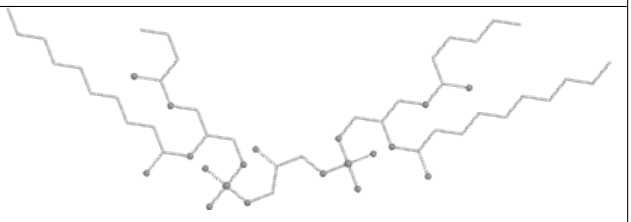
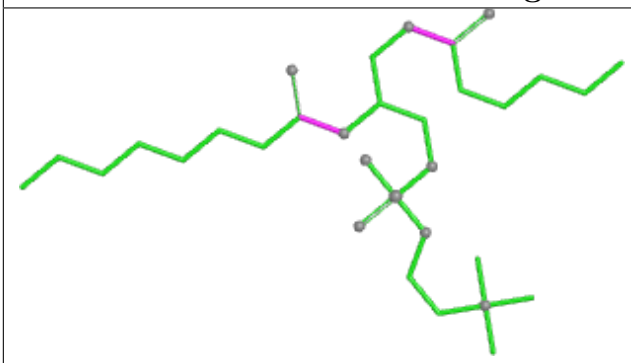


Rings

Ligand PCF H 604



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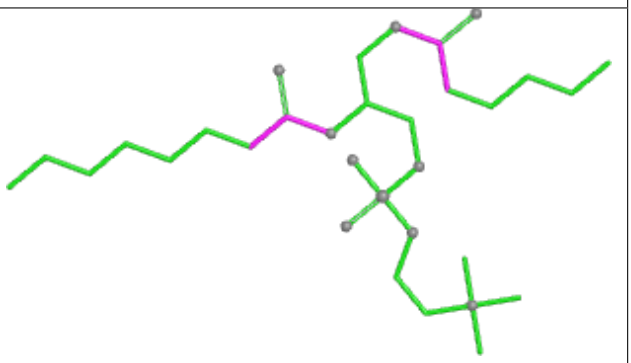
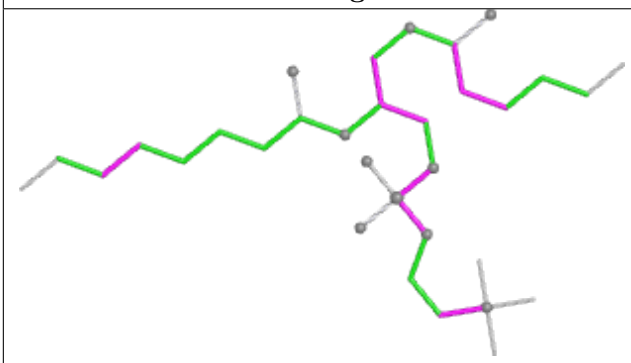


Bond angles



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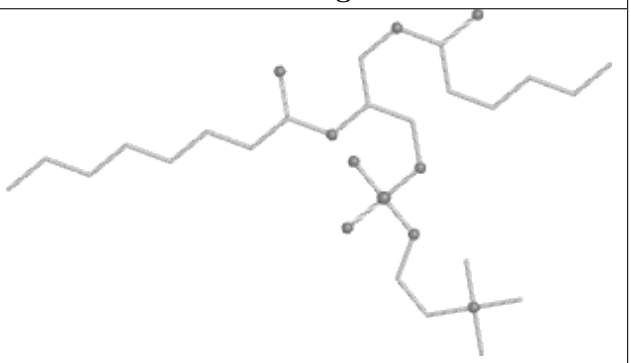
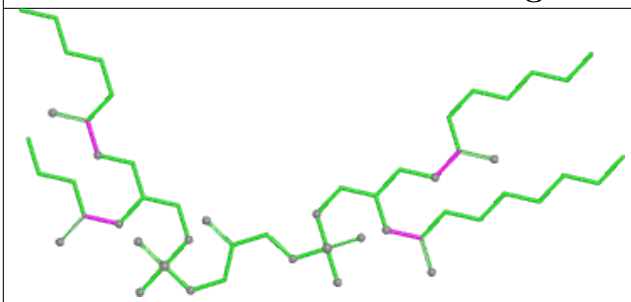
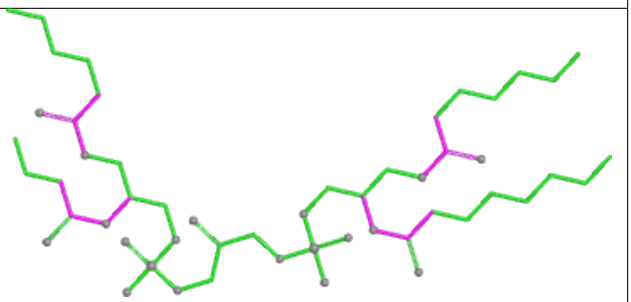


Rings

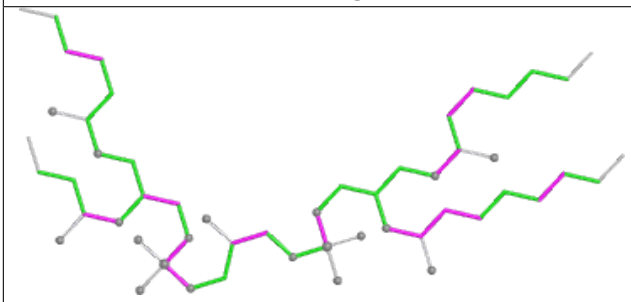
Ligand CDL E 302



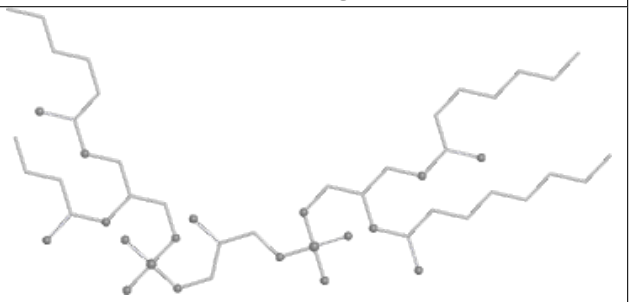
Bond lengths



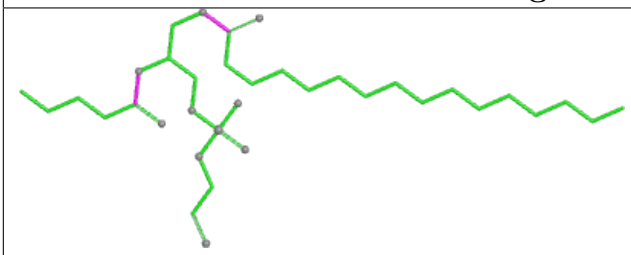
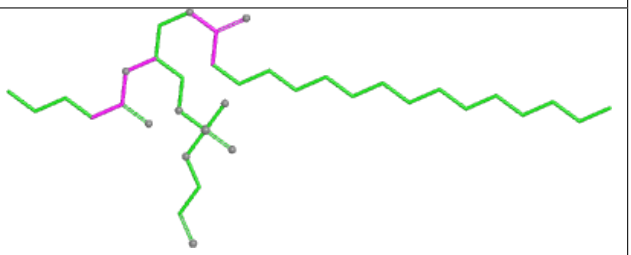
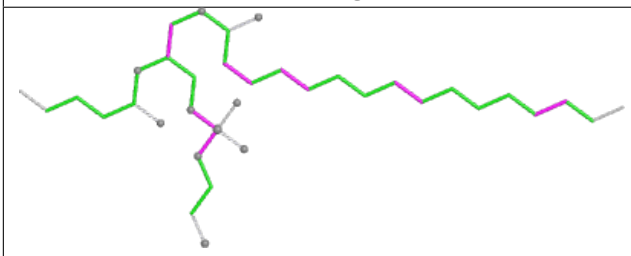
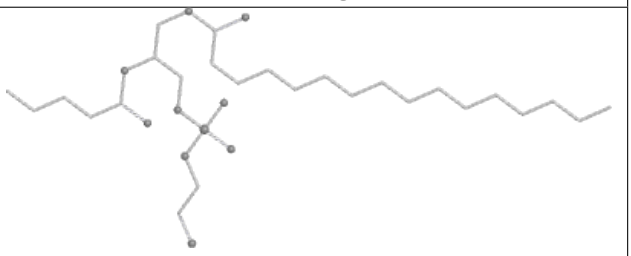
Bond angles

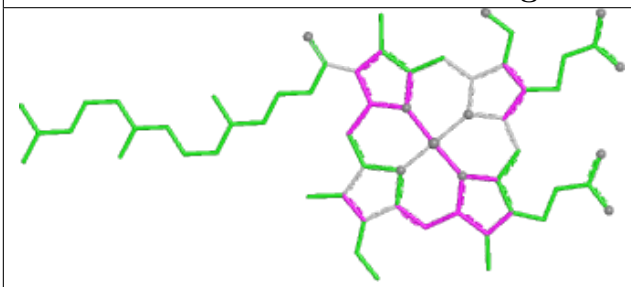
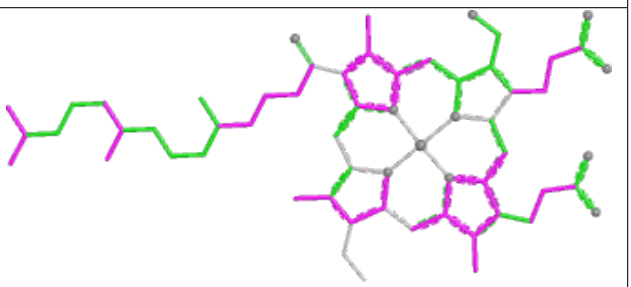
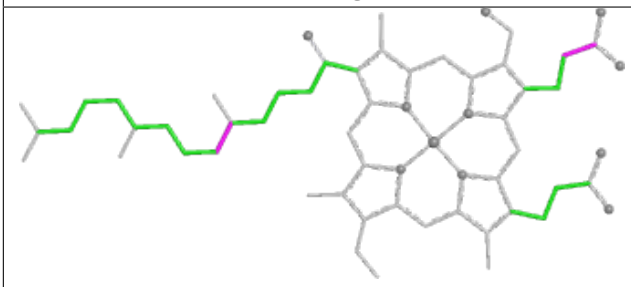
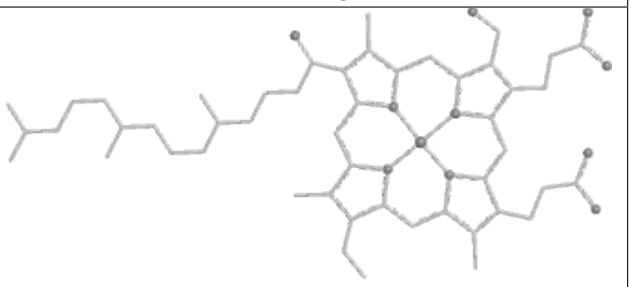


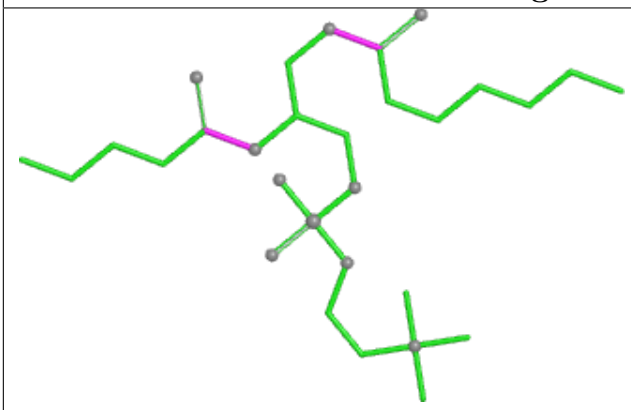
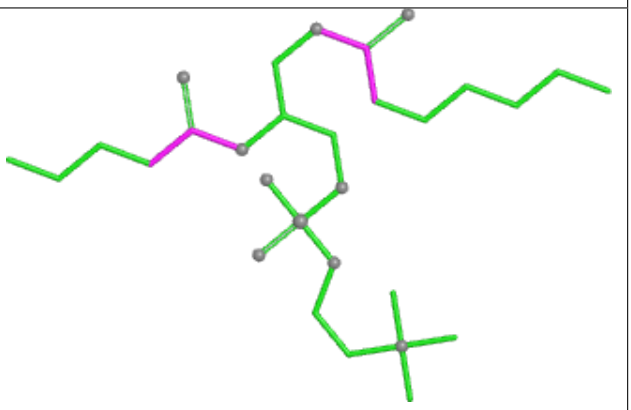
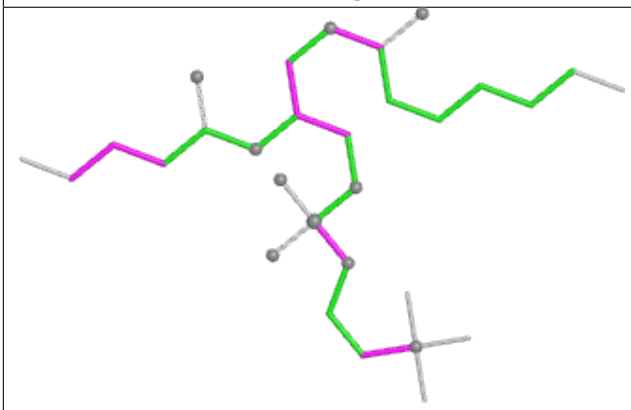
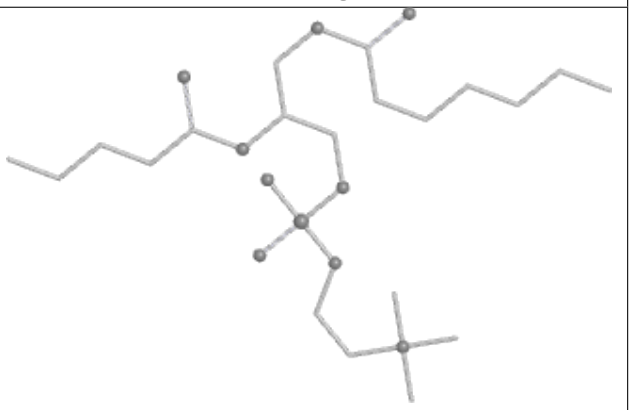
Torsions

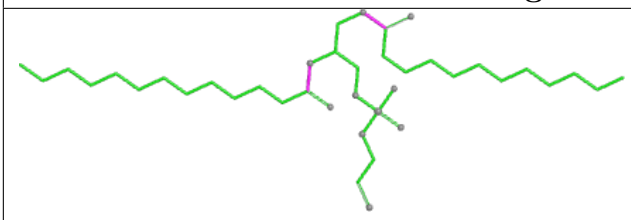
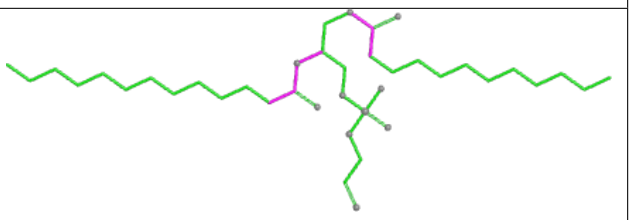
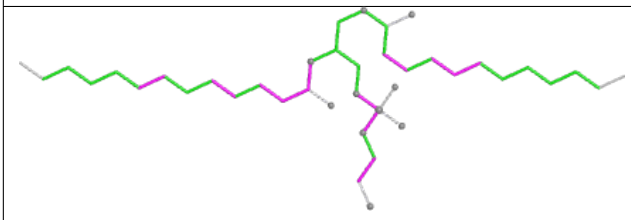
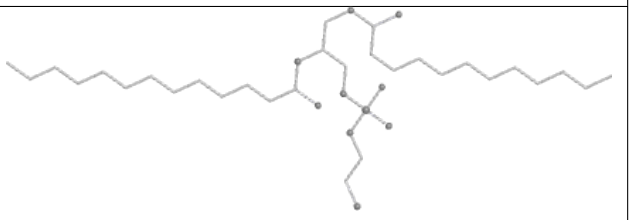


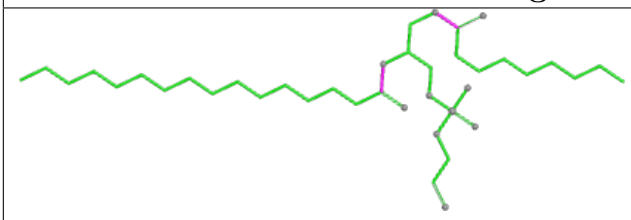
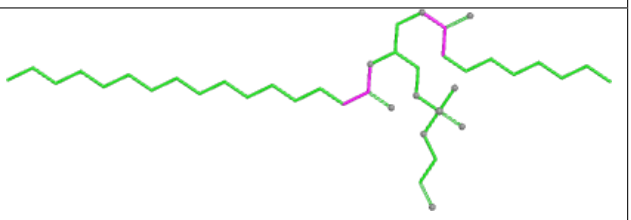
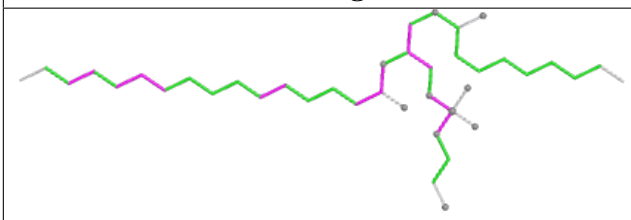
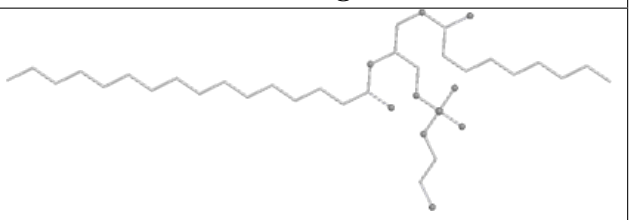
Rings

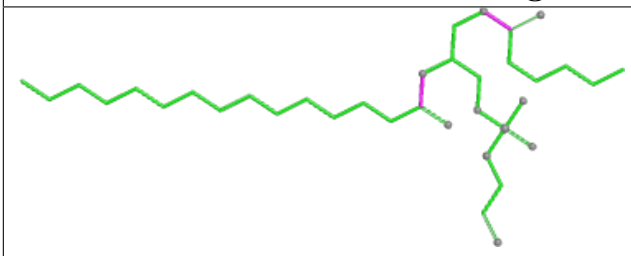
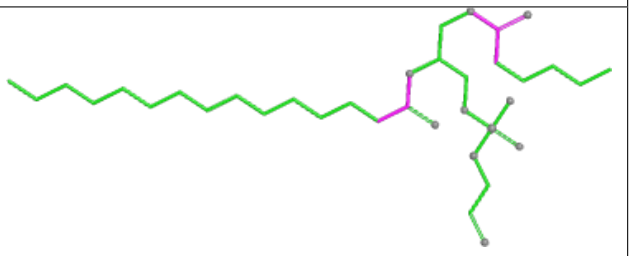
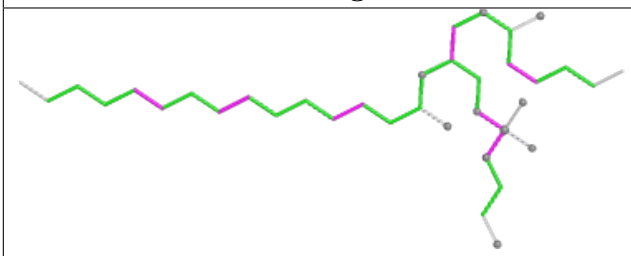
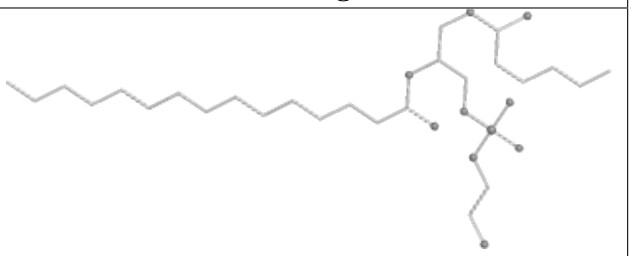
Ligand PEF S 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA m 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

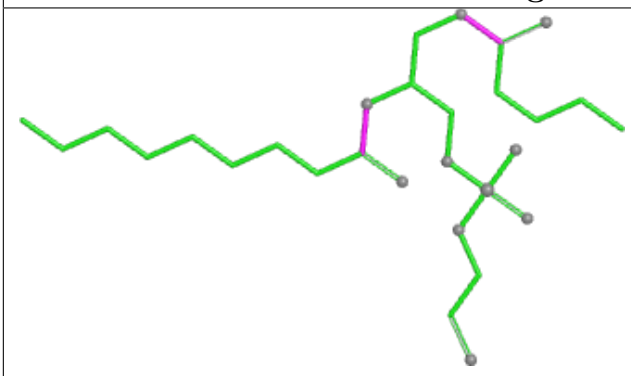
Ligand PCF I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF N 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

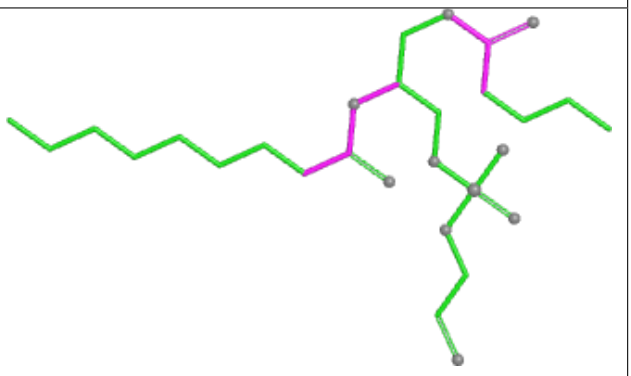
Ligand PEF b 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF C 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF P 303

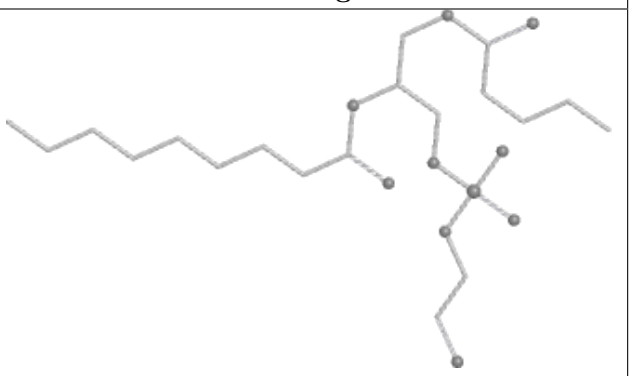


Bond lengths



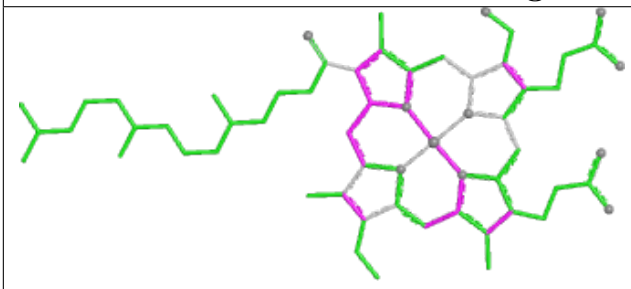
Bond angles

Torsions

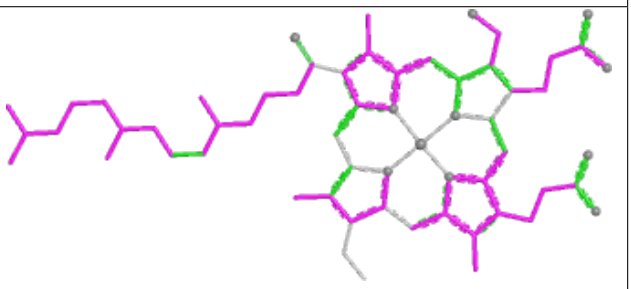


Rings

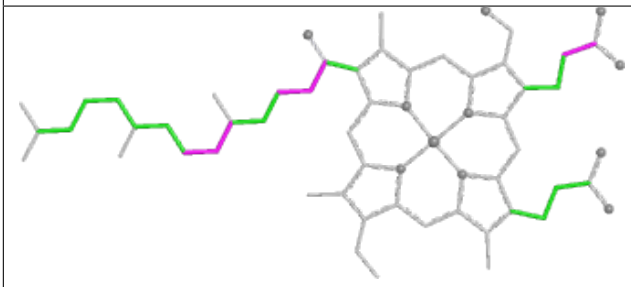
Ligand HEA a 602



Bond lengths



Bond angles



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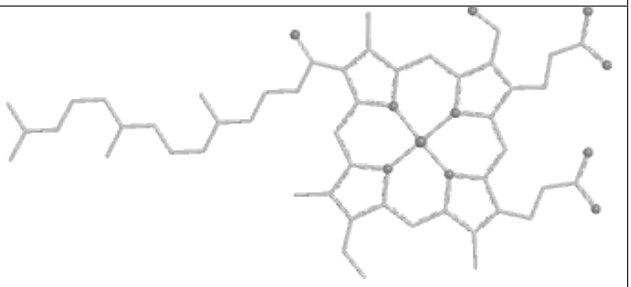
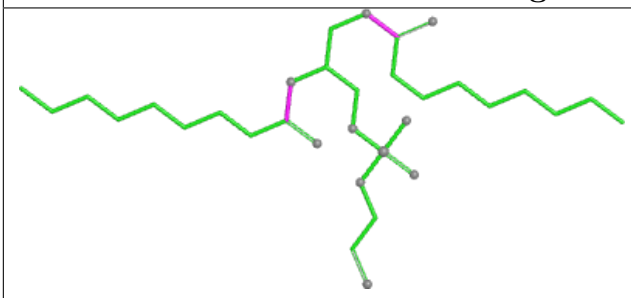


Rings

Ligand PEF n 304



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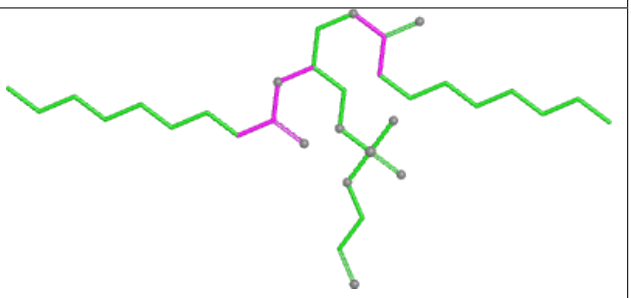
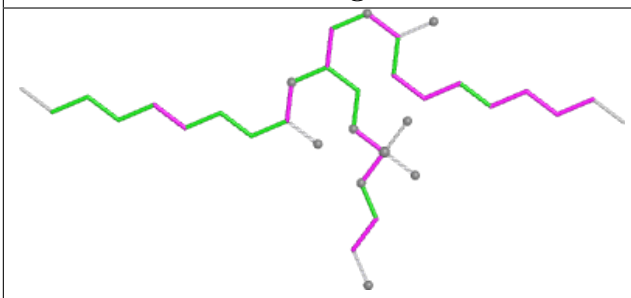


Bond angles



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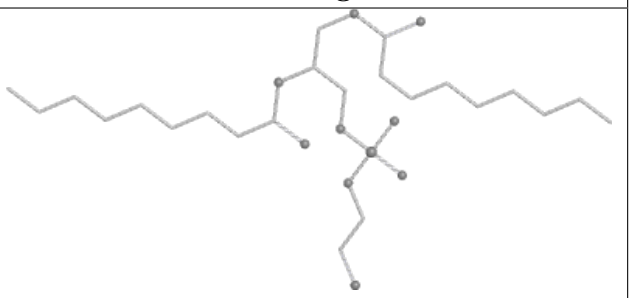

Rings

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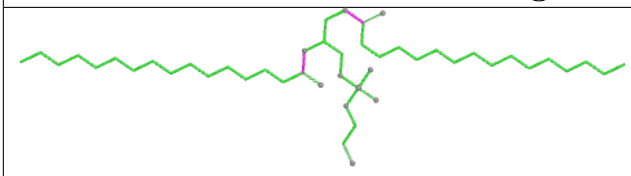

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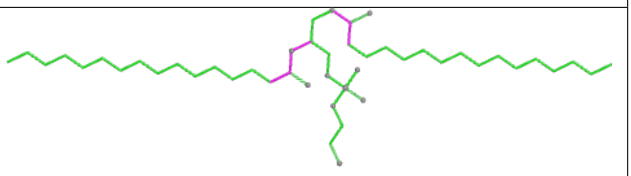
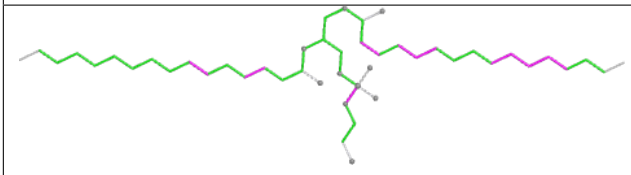


Bond angles



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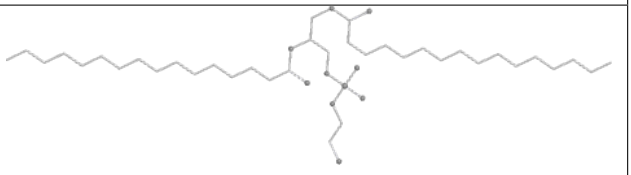
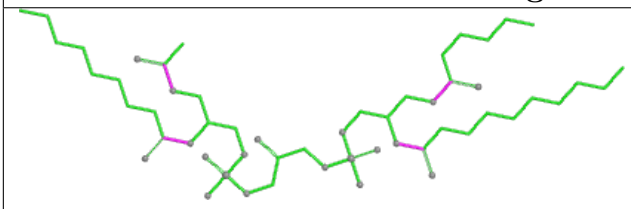
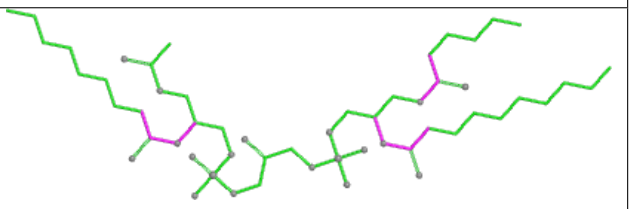


Rings

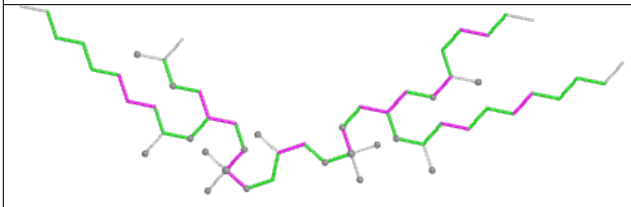
Ligand CDL L 501



Bond lengths



Bond angles



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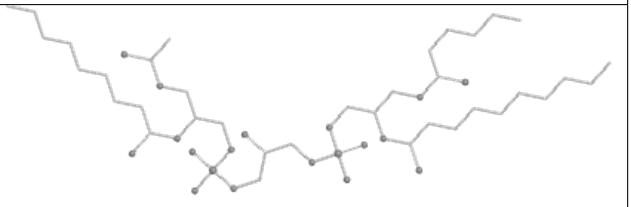
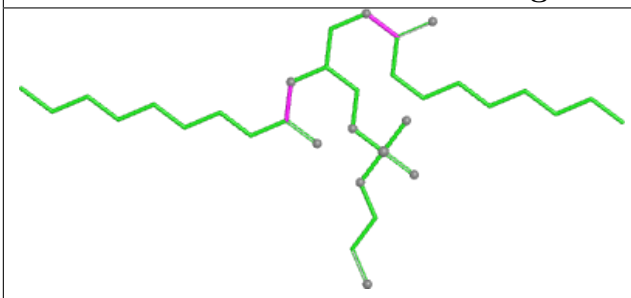
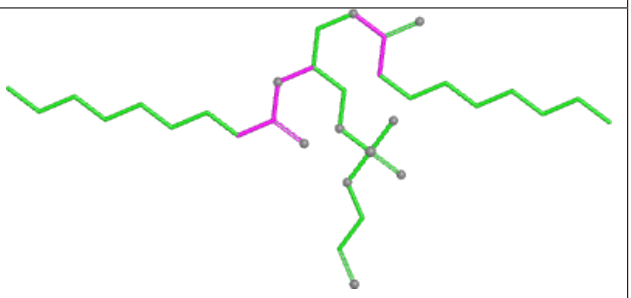
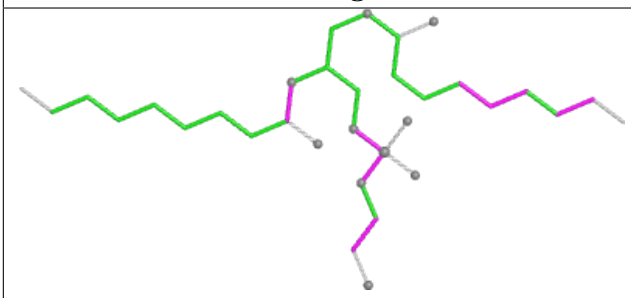
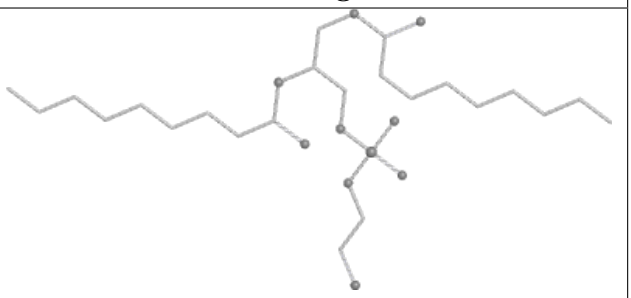
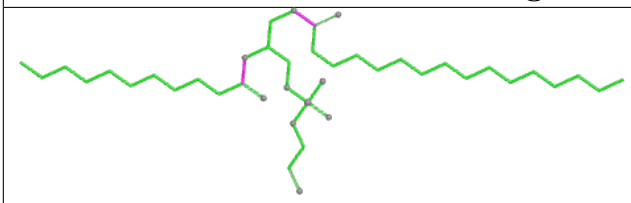
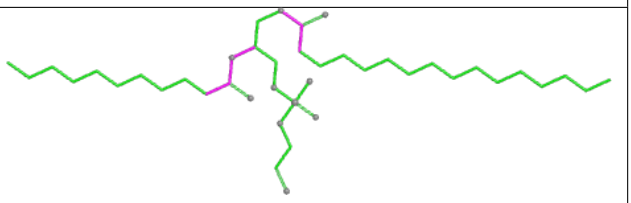
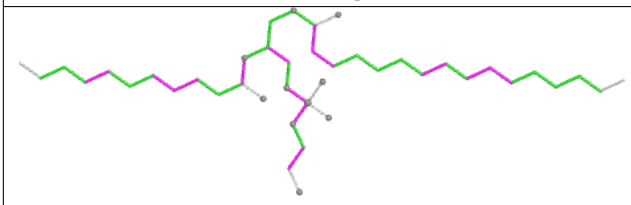
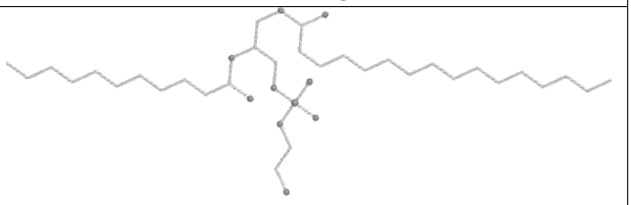
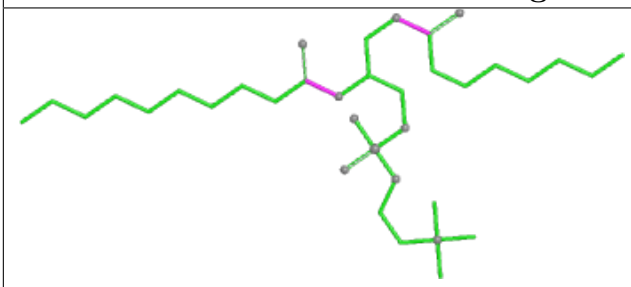
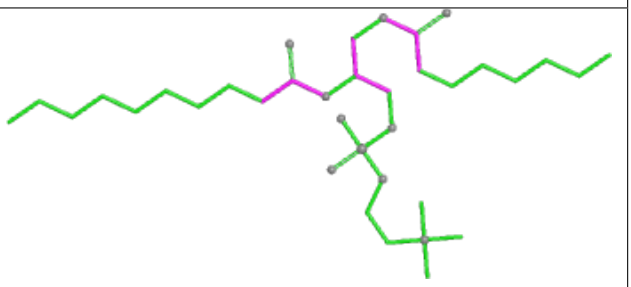
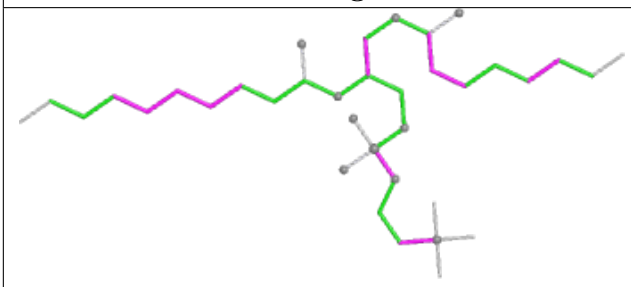
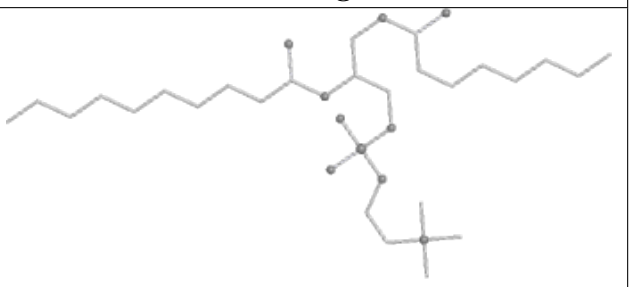
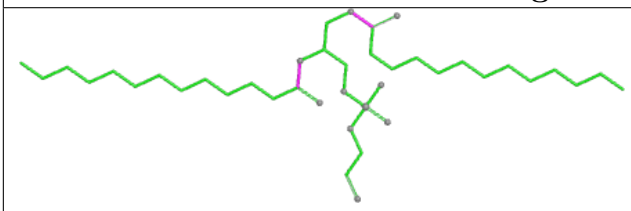
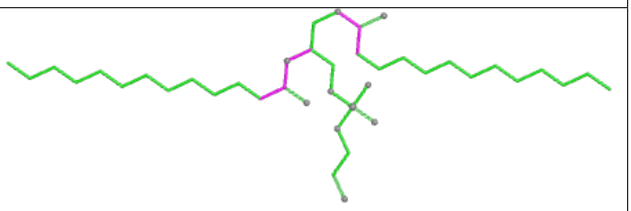
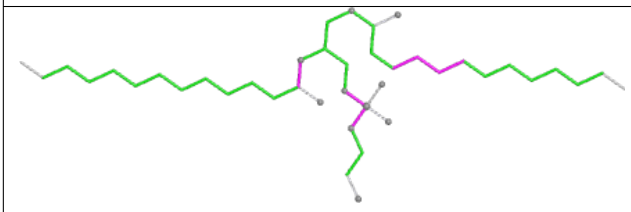
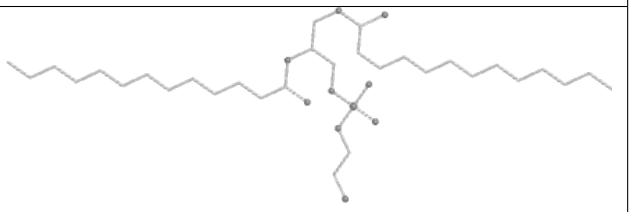


Rings

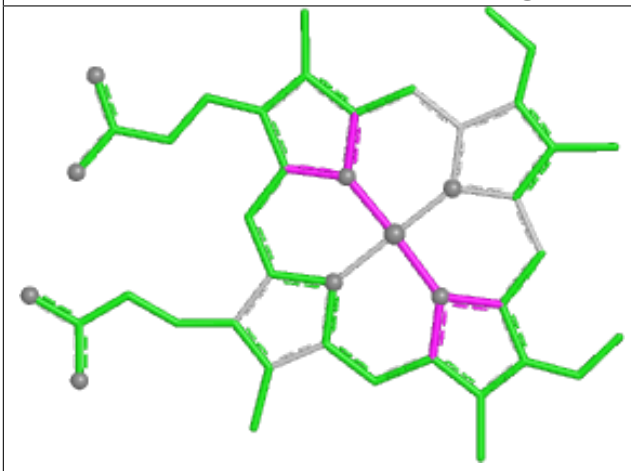
Ligand PEF a 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF D 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

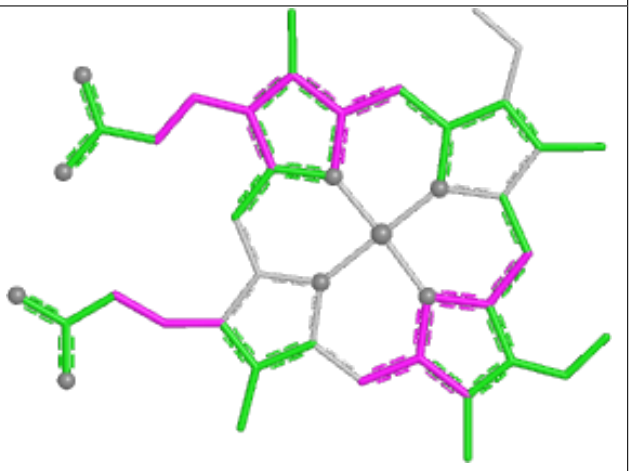
Ligand PCF e 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEF c 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

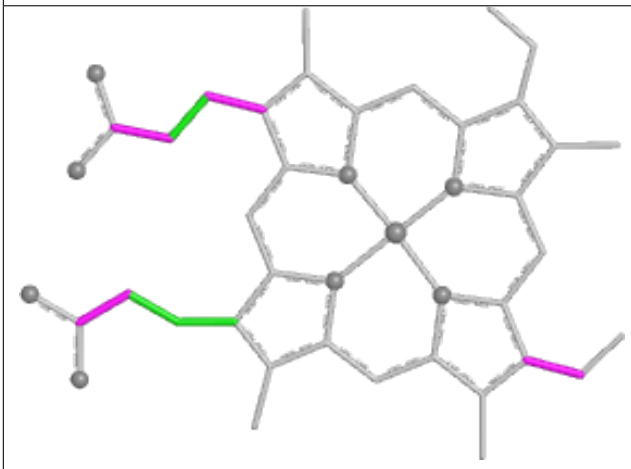
Ligand HEM C 601



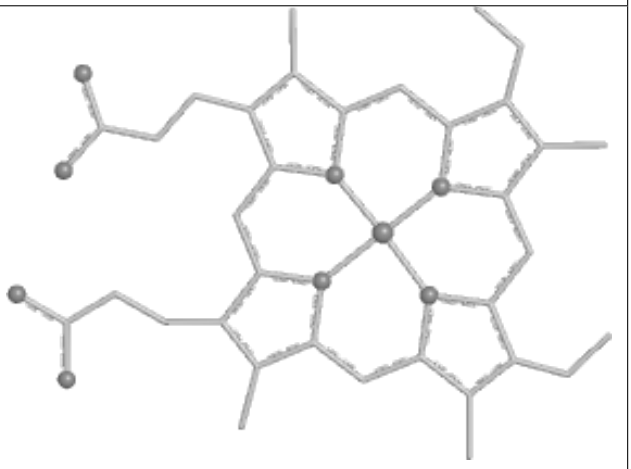
Bond lengths



Bond angles

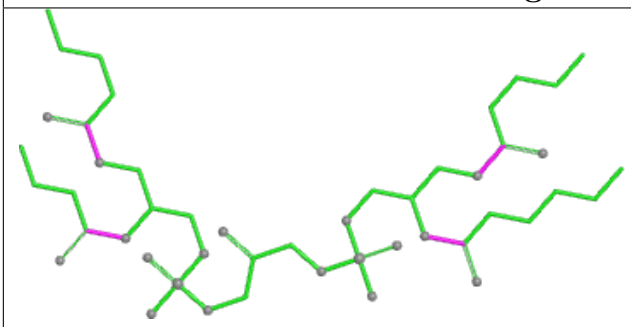


Torsions

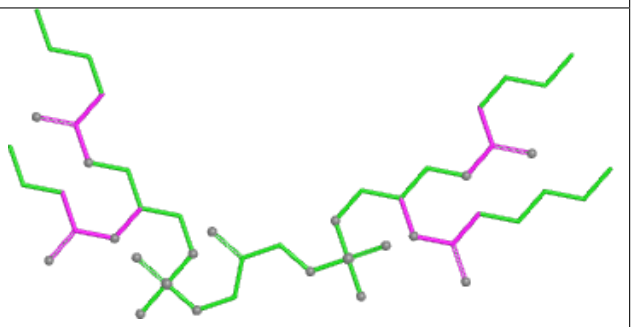


Rings

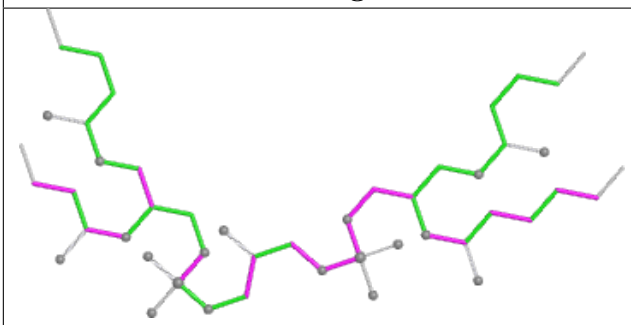
Ligand CDL P 302



Bond lengths



Bond angles



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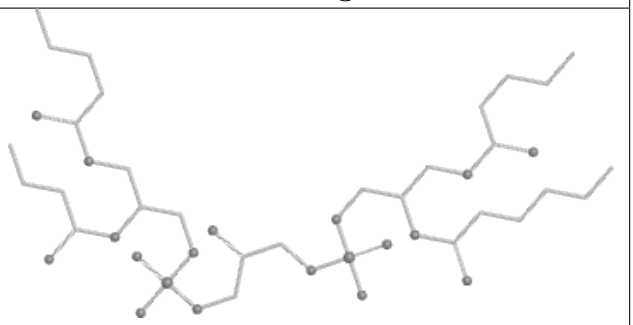
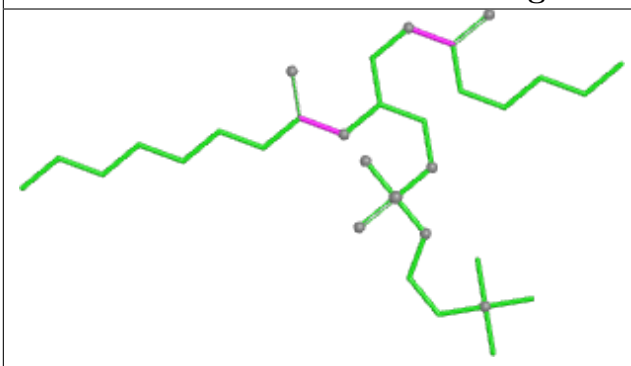
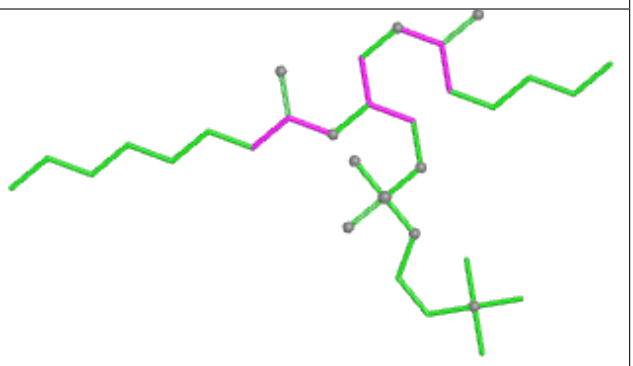


Rings

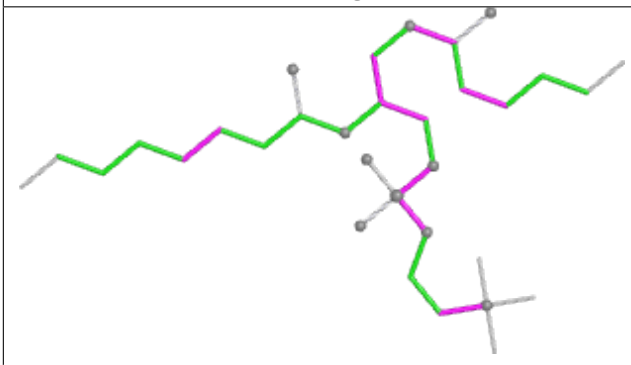
Ligand PCF S 603



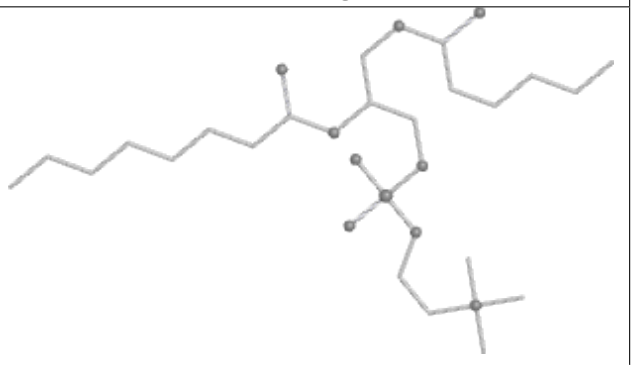
Bond lengths



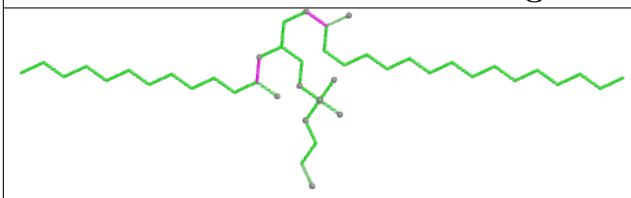
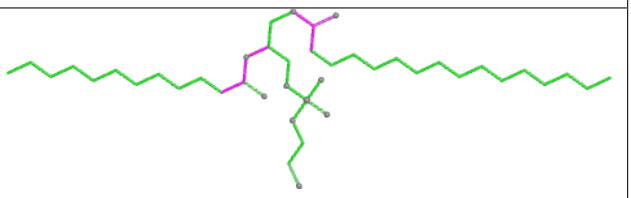
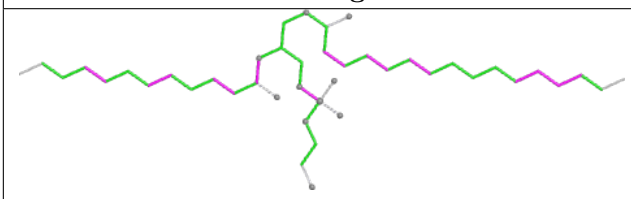
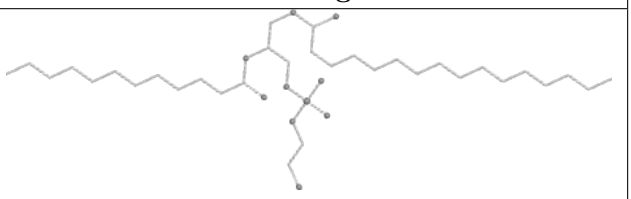
Bond angles

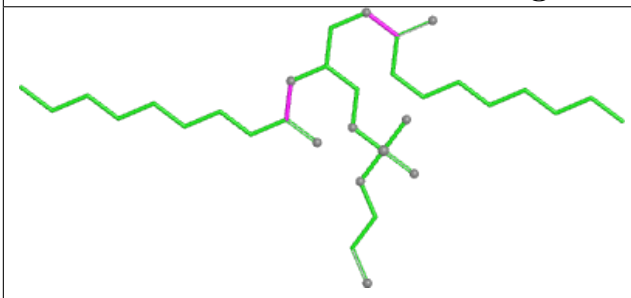
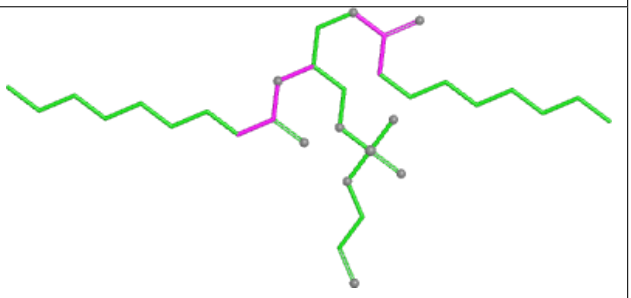
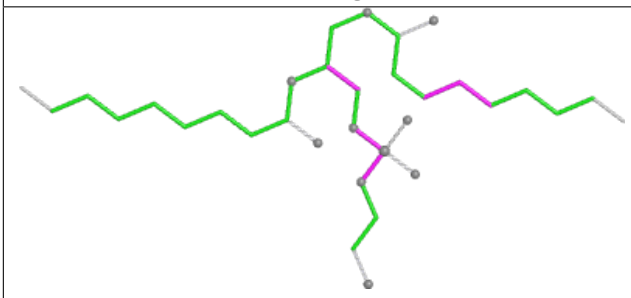
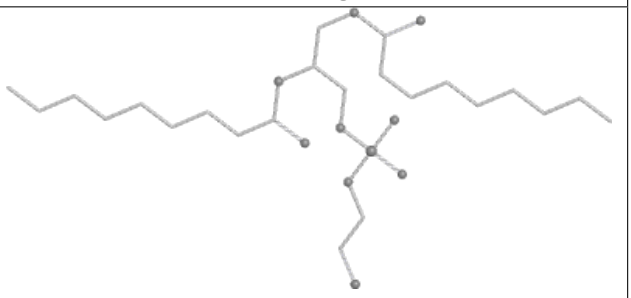


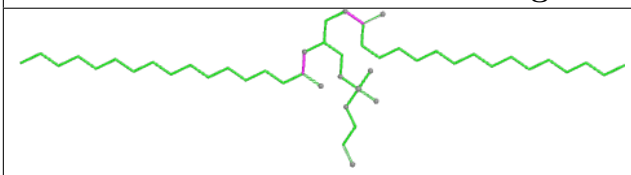
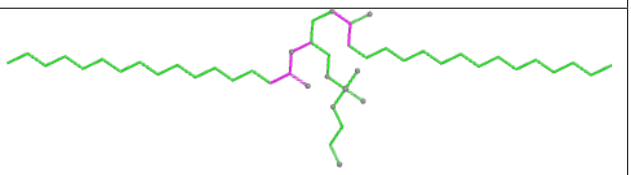
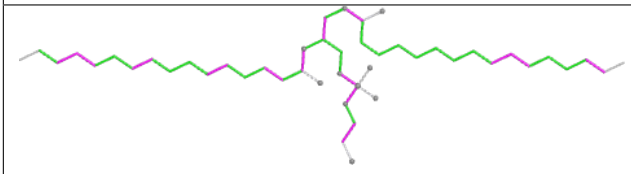
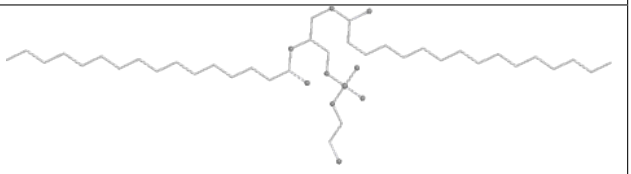
Torsions



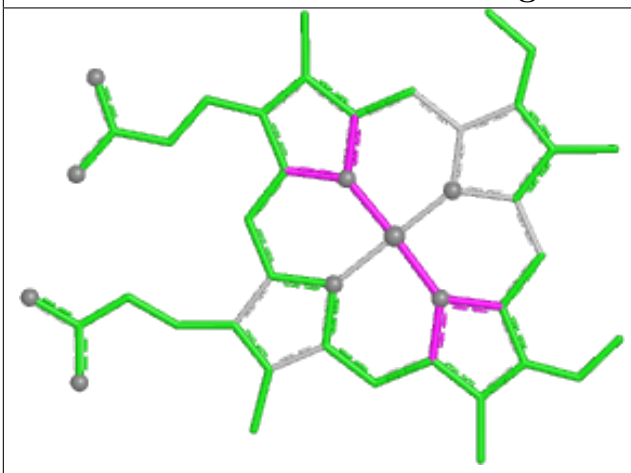
Rings

Ligand PEF O 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

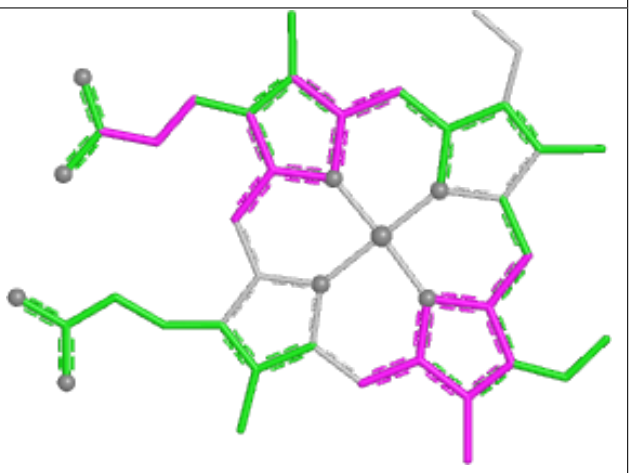
Ligand PEF a 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF e 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

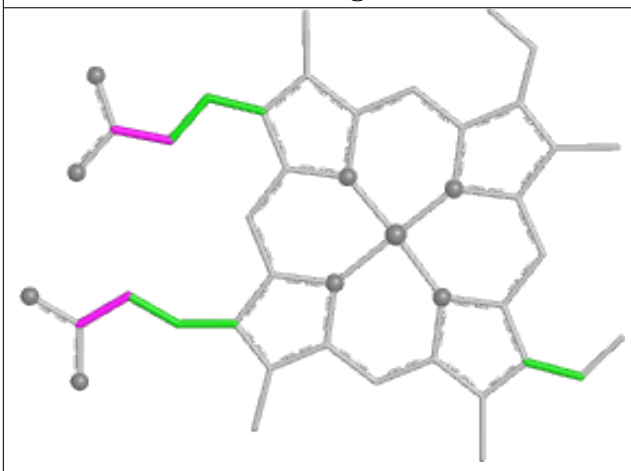
Ligand HEM C 602



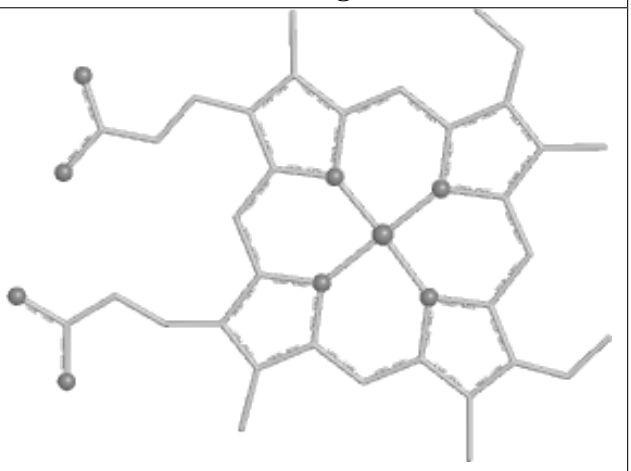
Bond lengths



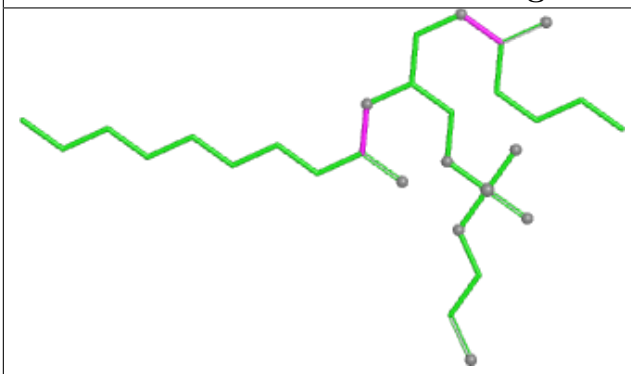
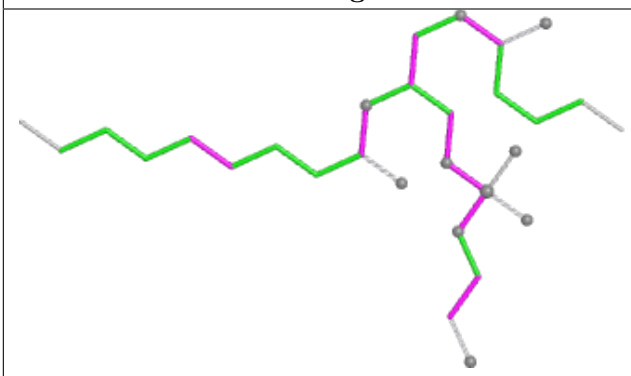
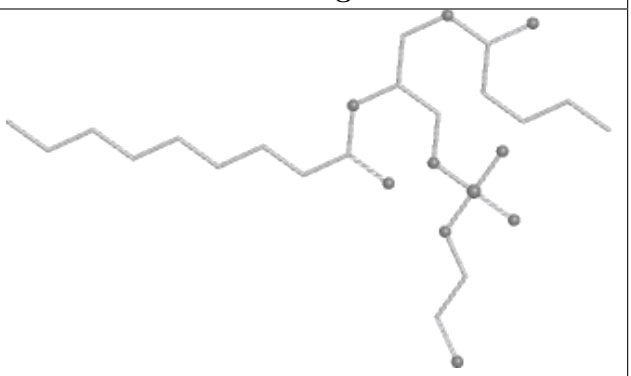
Bond angles

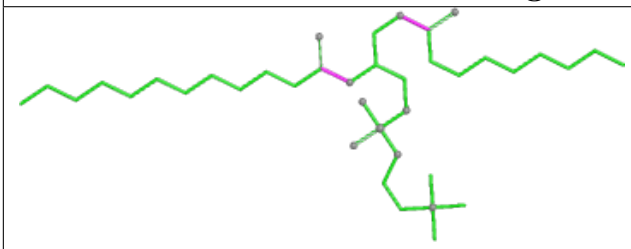
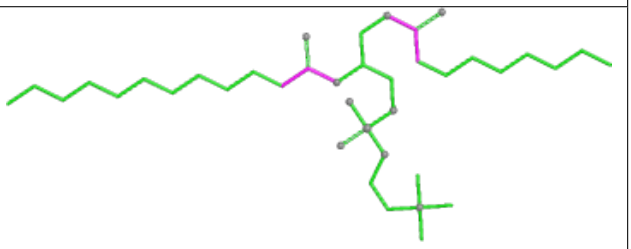
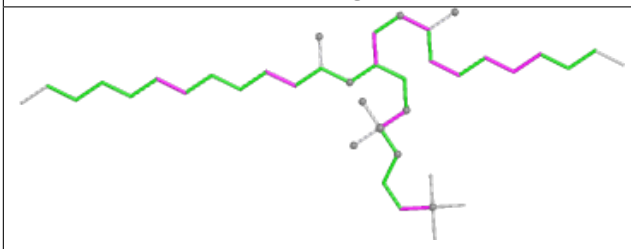
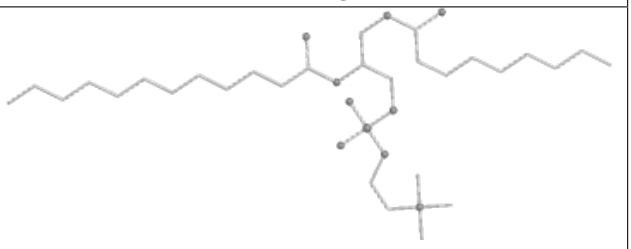


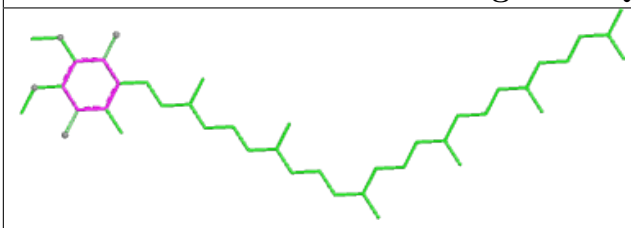
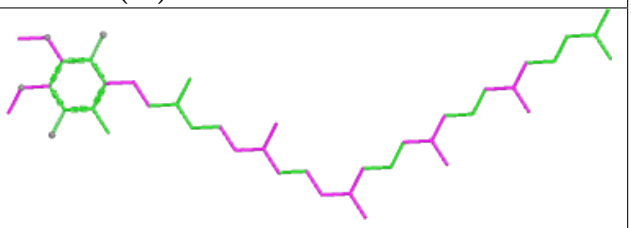
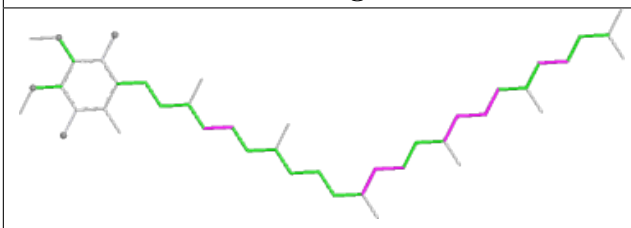
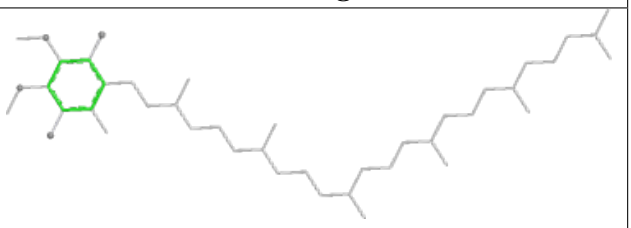
Torsions

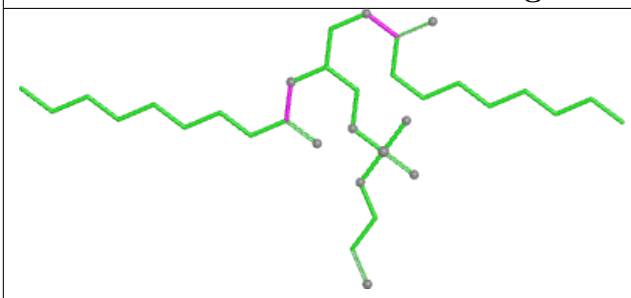
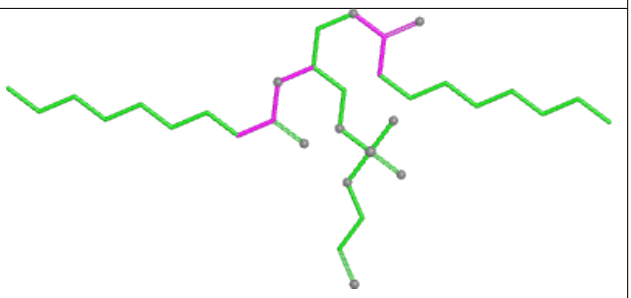
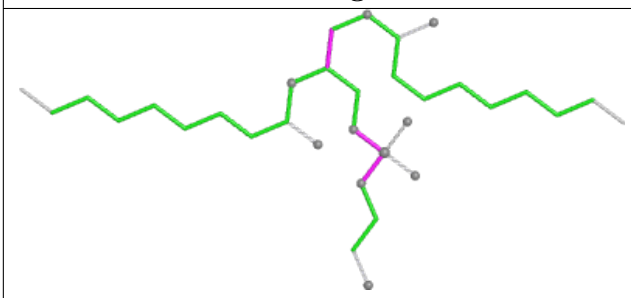
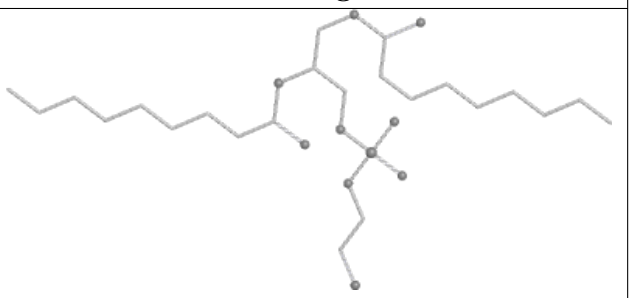


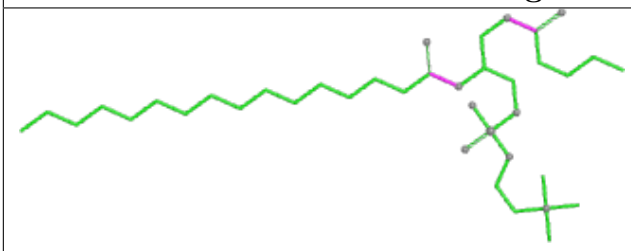
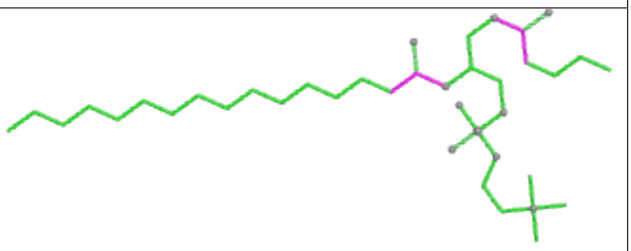
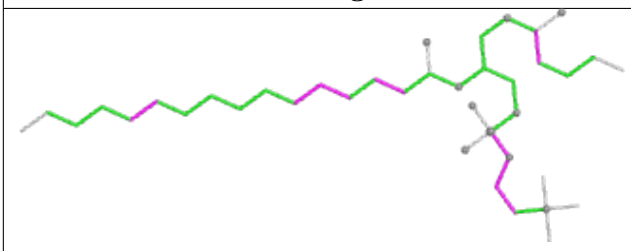
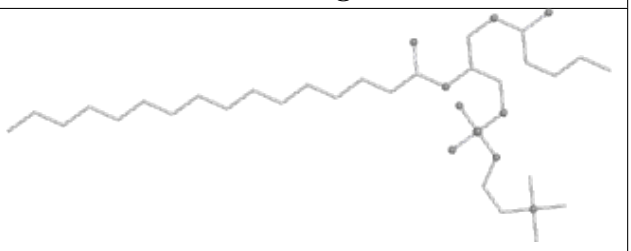
Rings

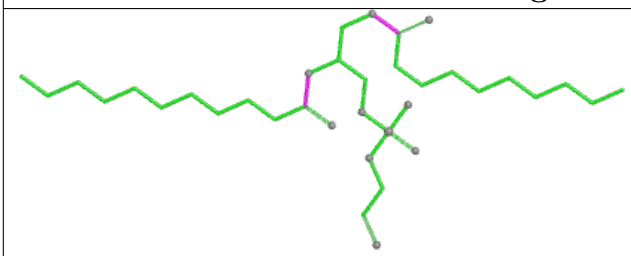
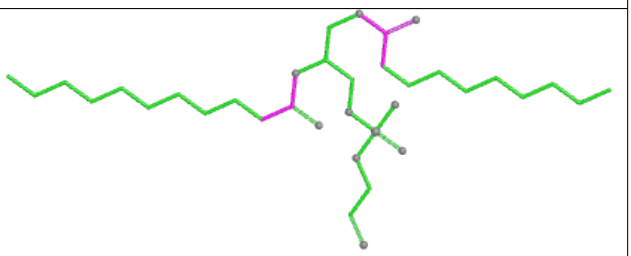
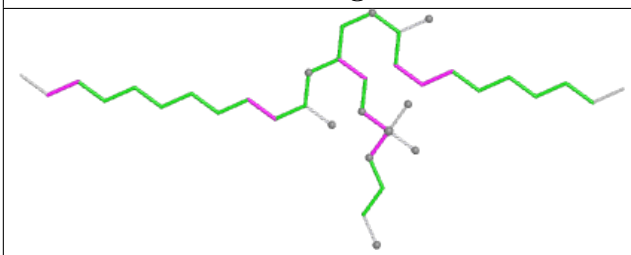
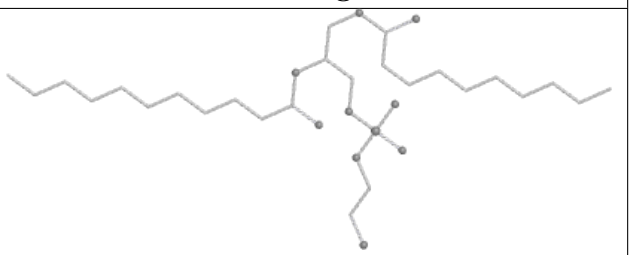
Ligand PEF E 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCF T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

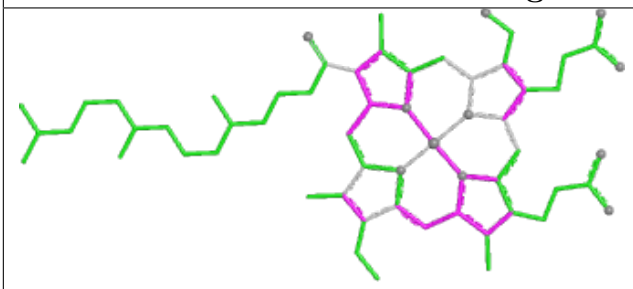
Ligand UQ6 C 603 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF m 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

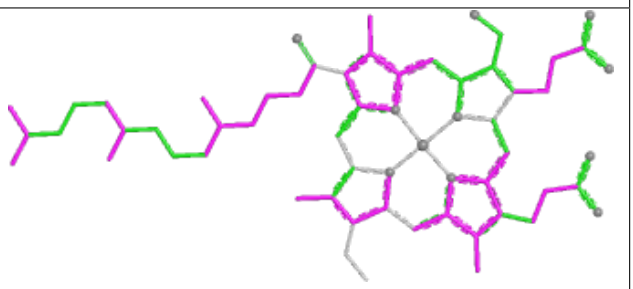
Ligand PCF C 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF o 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

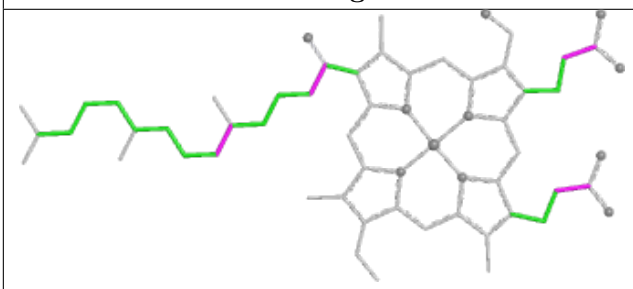
Ligand HEA a 603



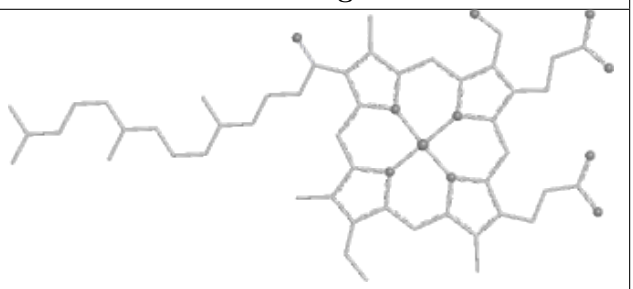
Bond lengths



Bond angles

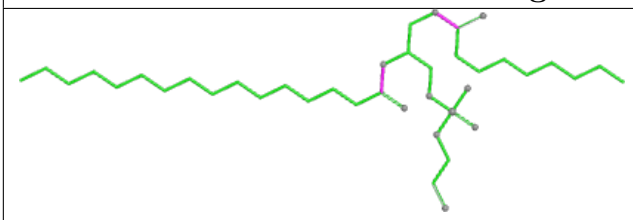


Torsions

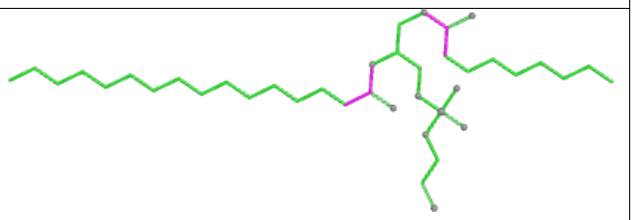


Rings

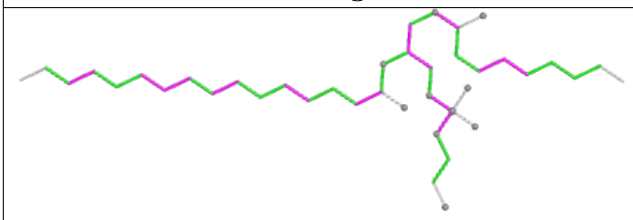
Ligand PEF n 303



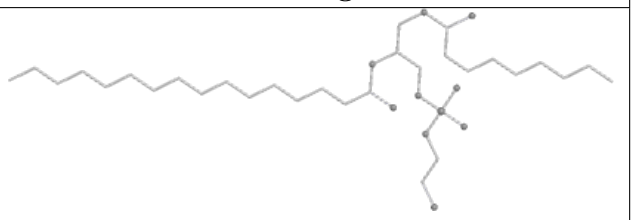
Bond lengths



Bond angles



Torsions



Rings

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.

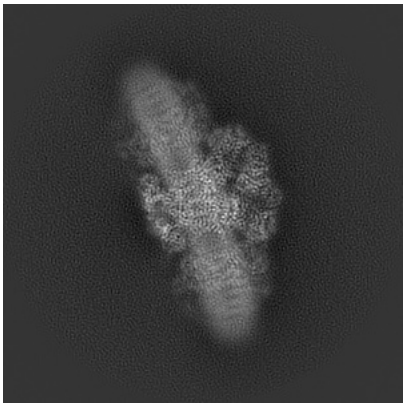
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0262. These allow visual inspection of the internal detail of the map and identification of artifacts.

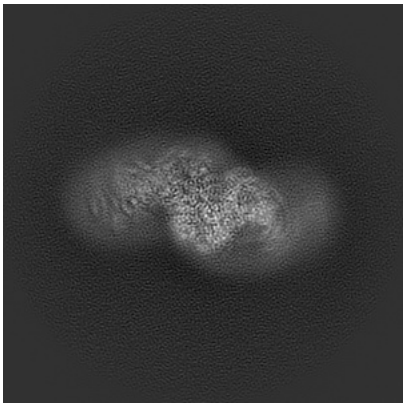
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

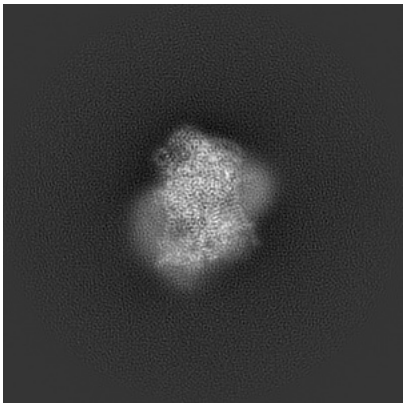
6.1.1 Primary map



X



Y

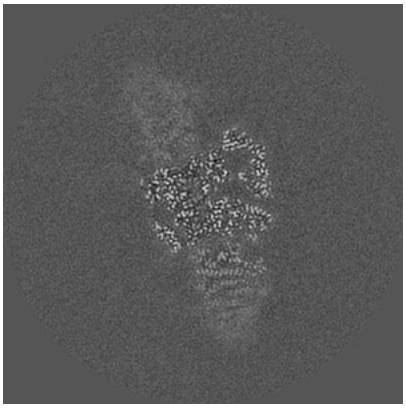


Z

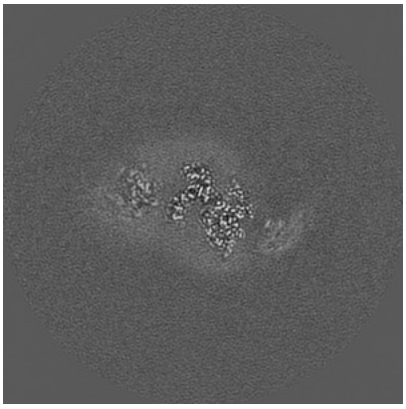
The images above show the map projected in three orthogonal directions.

6.2 Central slices

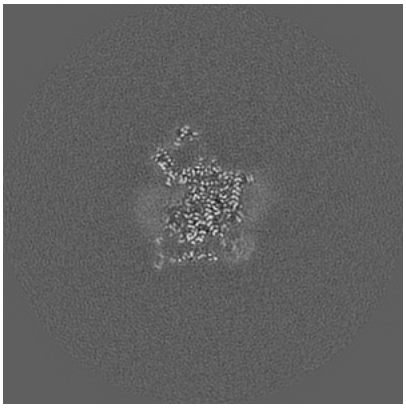
6.2.1 Primary map



X Index: 155



Y Index: 155

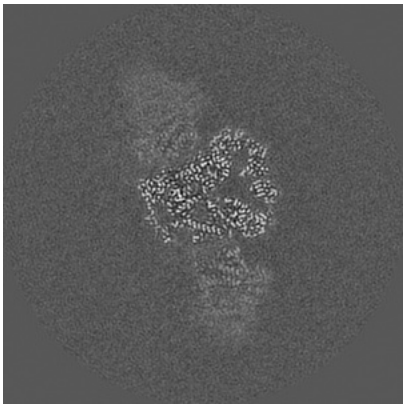


Z Index: 155

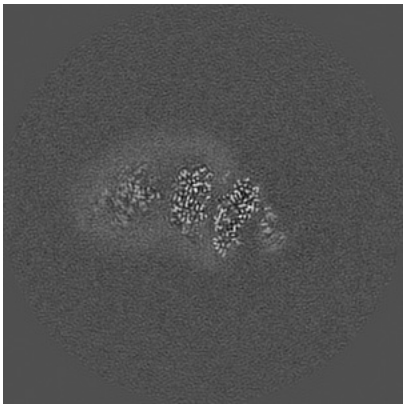
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

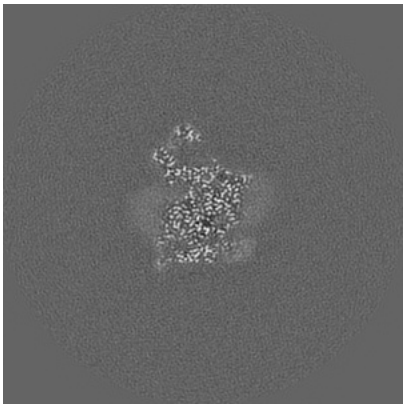
6.3.1 Primary map



X Index: 151



Y Index: 163



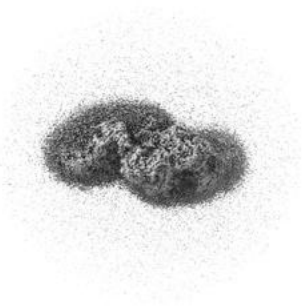
Z Index: 157

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

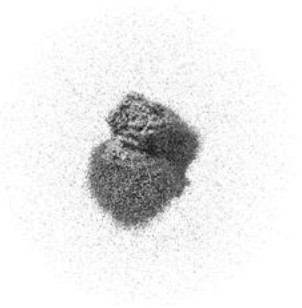
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0263. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

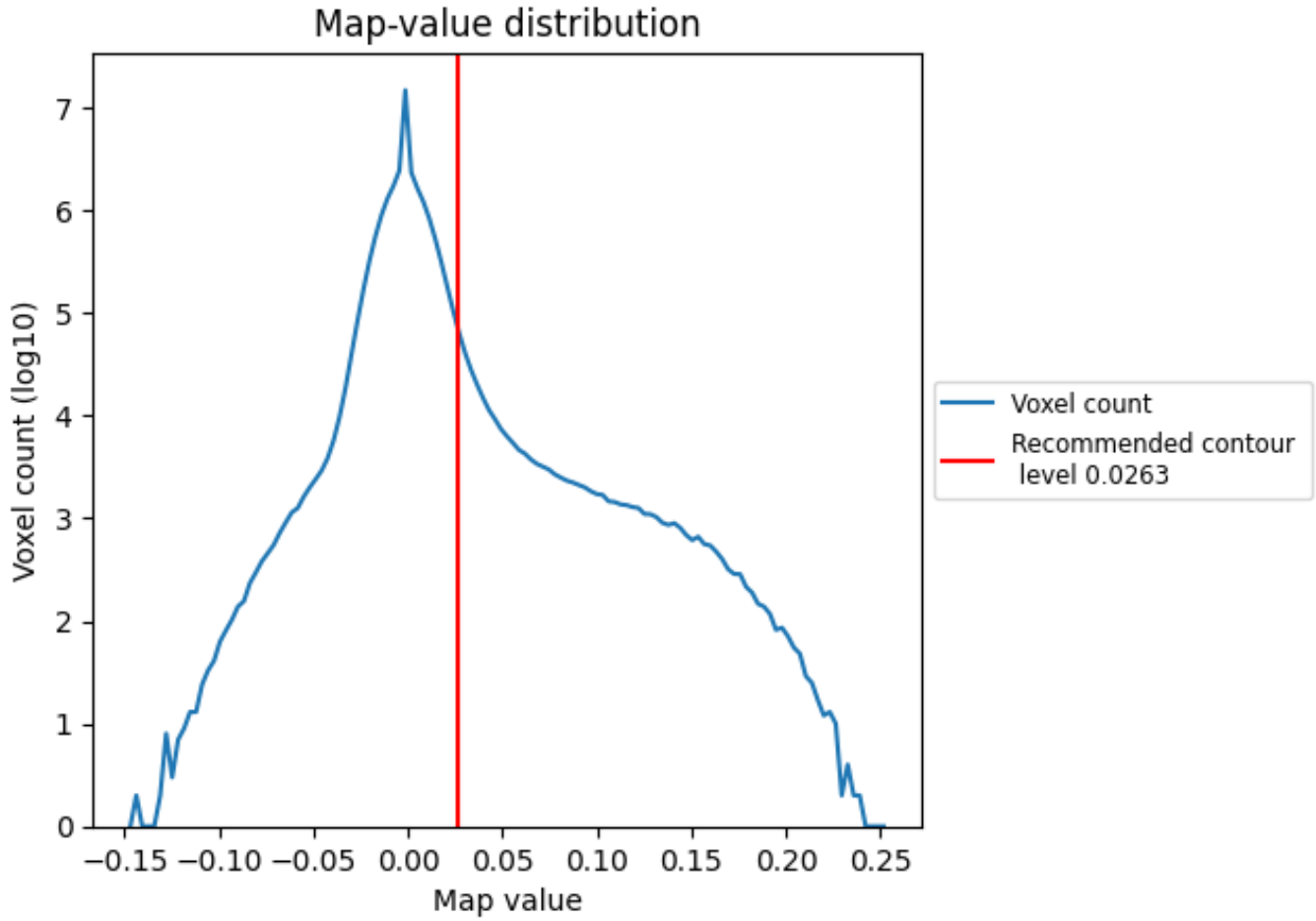
6.5 Mask visualisation (i)

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

7 Map analysis

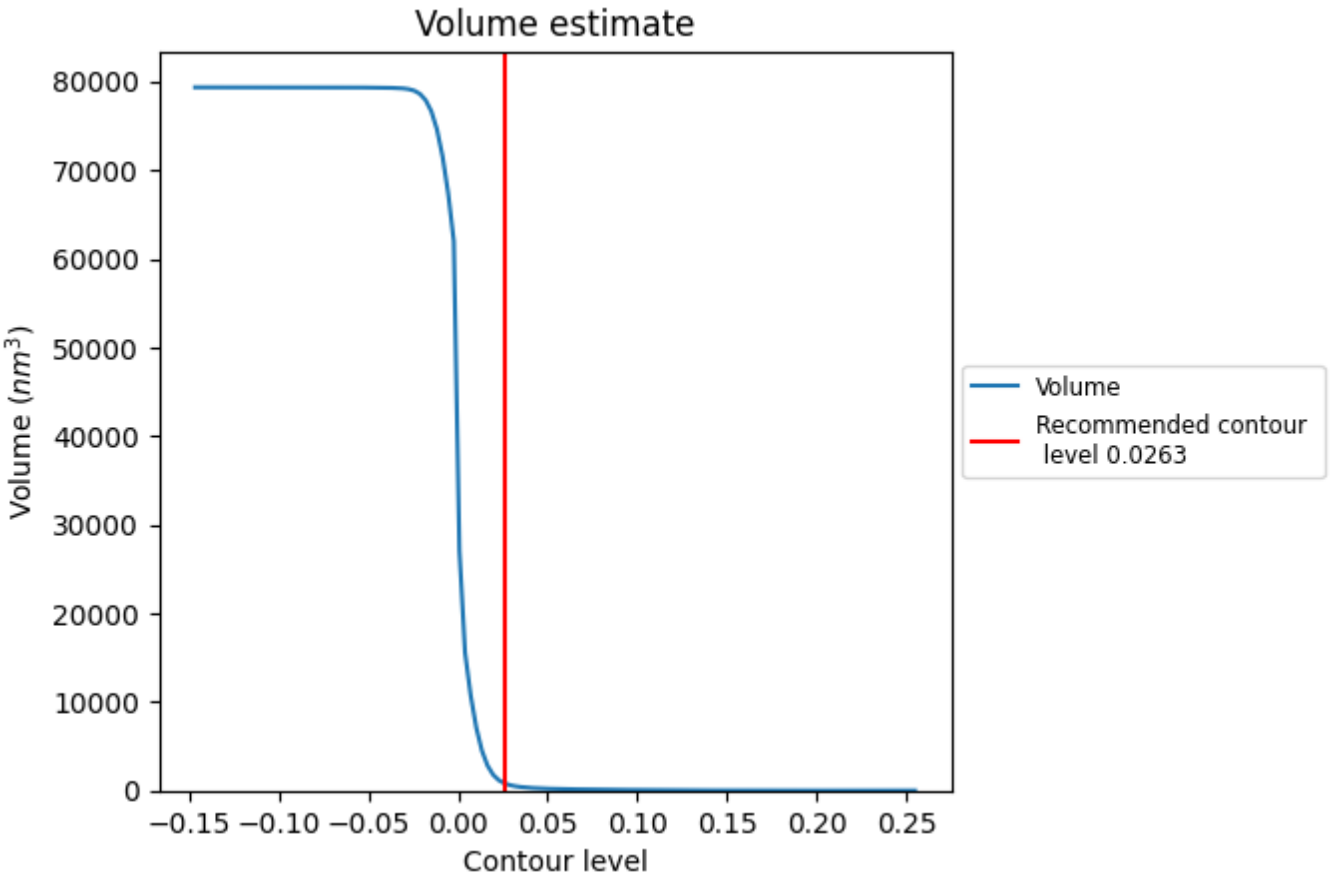
This section contains the results of statistical analysis of the map.

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.

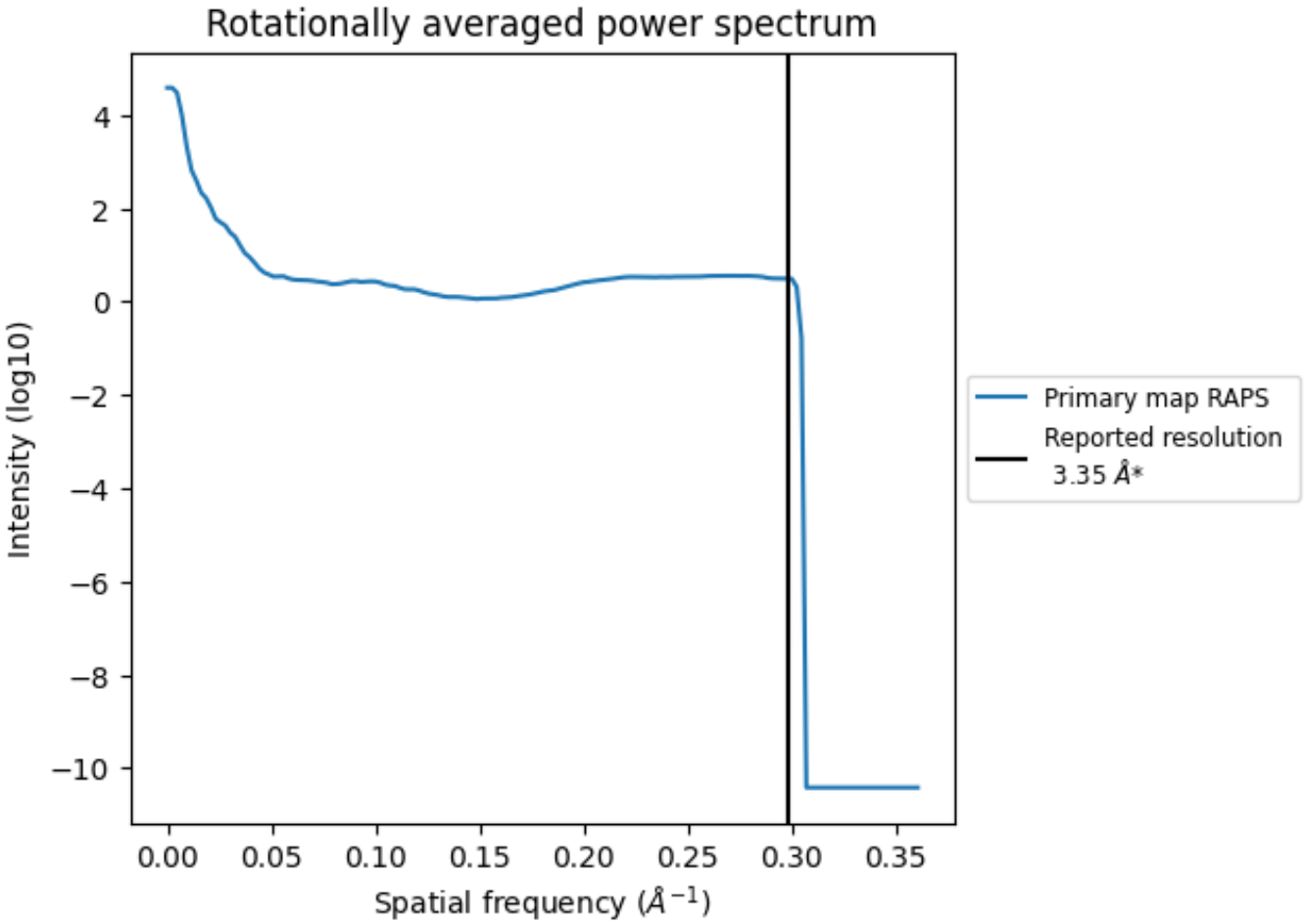
7.2 Volume estimate



The volume at the recommended contour level is 786 nm^3; this corresponds to an approximate mass of 710 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)

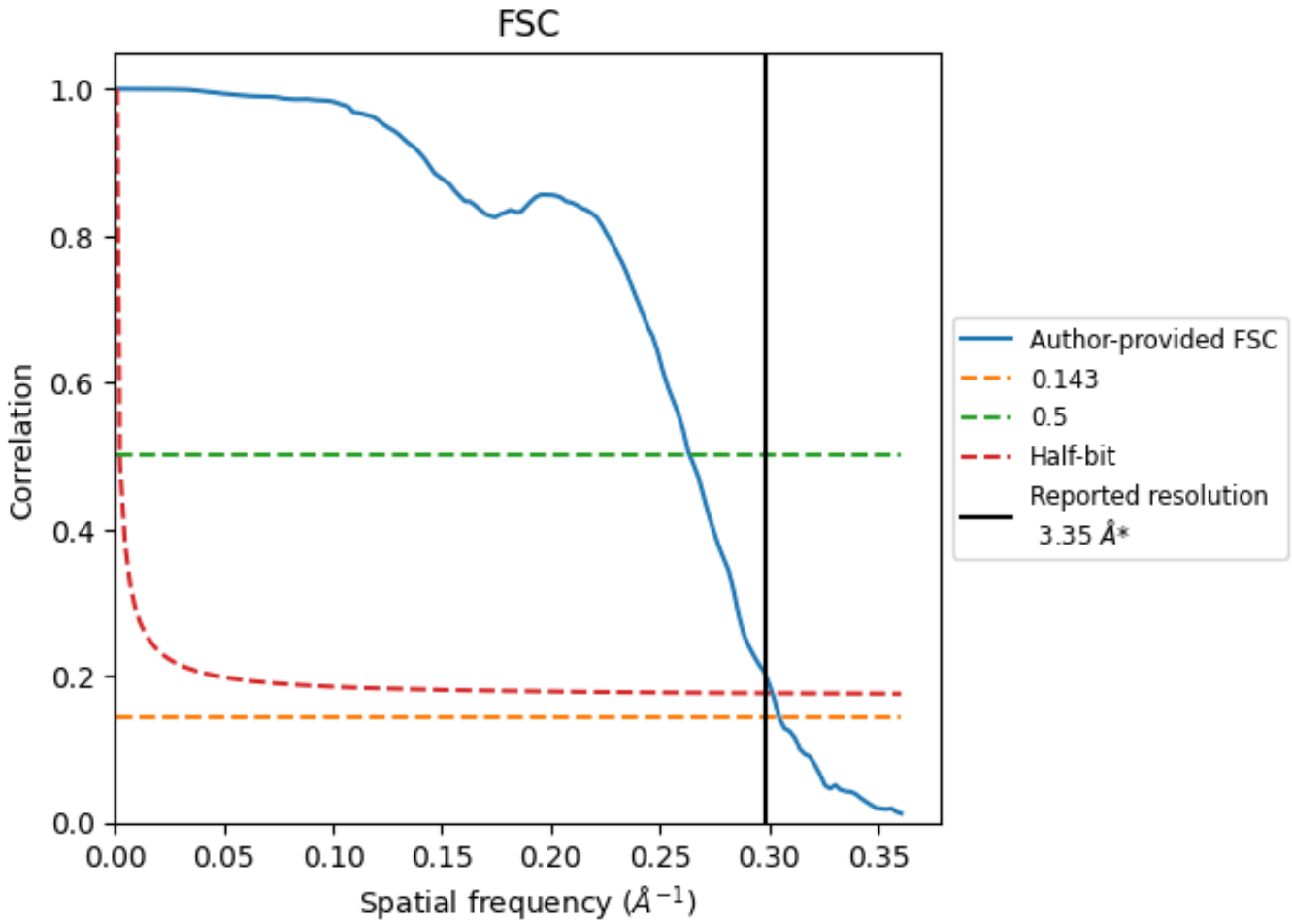


*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

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 0.299 Å^{-1}

8.2 Resolution estimates (i)

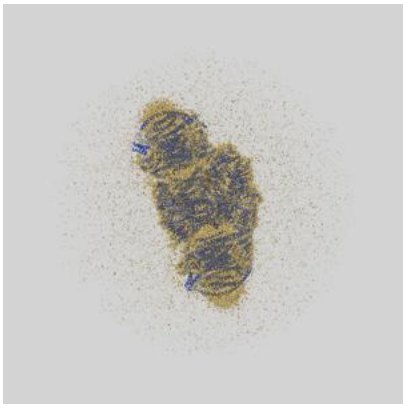
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.35	-
Author-provided FSC curve	3.28	3.79	3.32
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 3.79 differs from the reported value 3.35 by more than 10 %

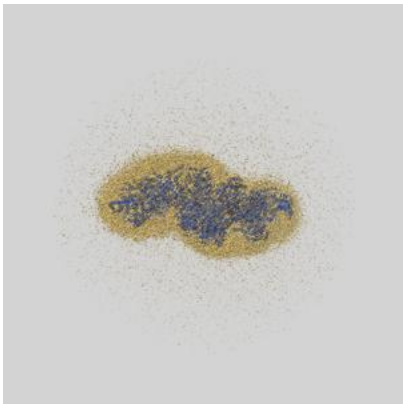
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0262 and PDB model 6HU9. Per-residue inclusion information can be found in section 3 on page 18.

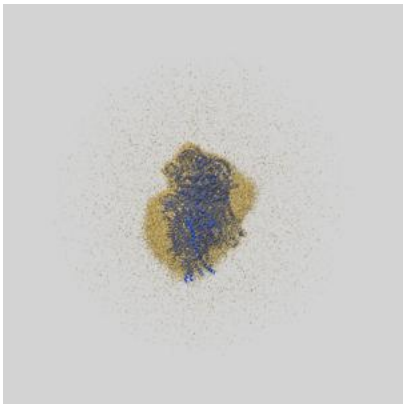
9.1 Map-model overlay



X



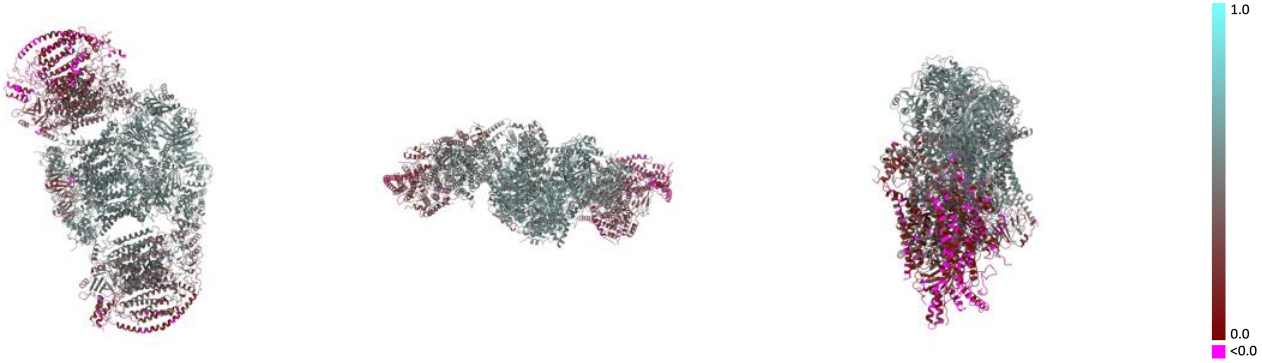
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0263 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.

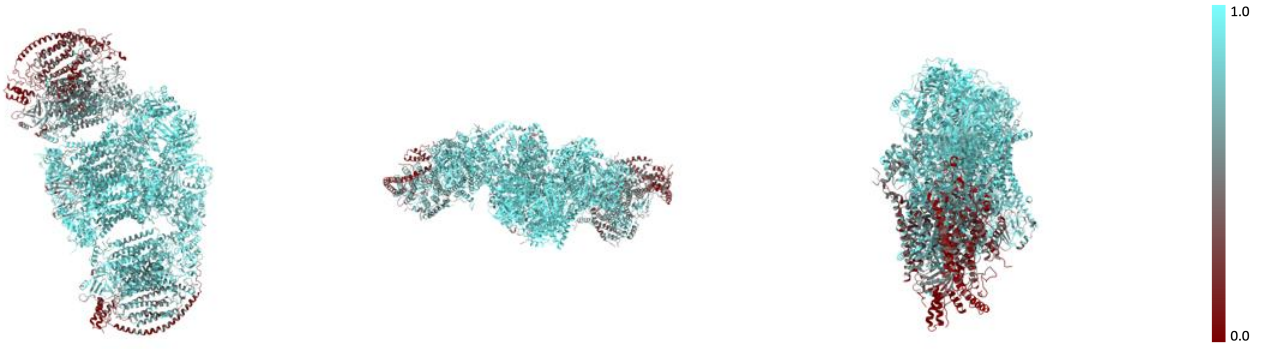
9.2 Q-score mapped to coordinate model



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.

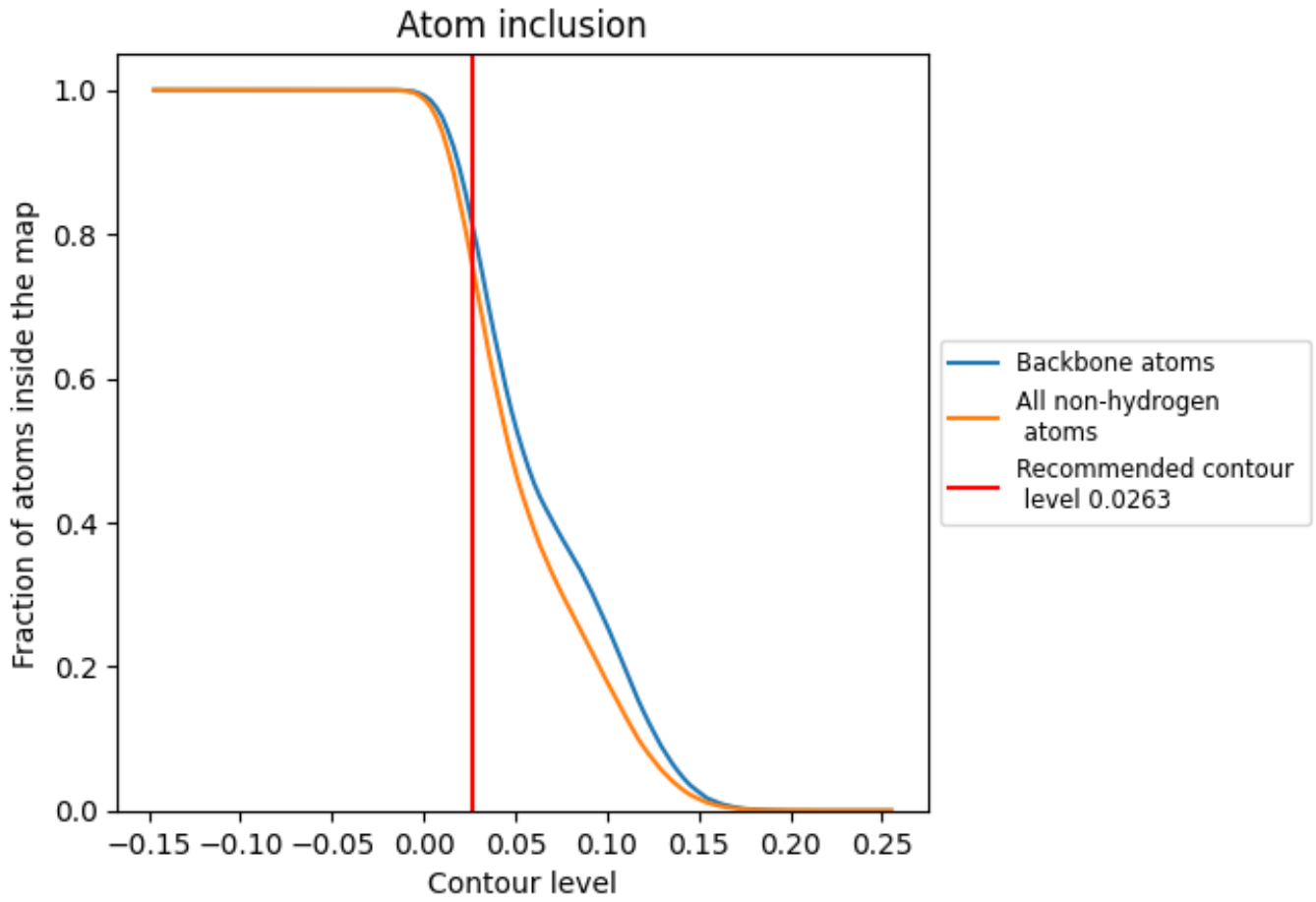
9.3 Atom inclusion mapped to coordinate model



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 (0.0263).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 76% 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 (0.0263) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.4310
A	0.9394	0.5540
B	0.9328	0.5540
C	0.9367	0.5660
D	0.9467	0.5650
E	0.7464	0.3780
F	0.8974	0.5060
G	0.9238	0.5490
H	0.9328	0.5640
I	0.9199	0.5460
J	0.7610	0.4780
L	0.9387	0.5520
M	0.9302	0.5520
N	0.9445	0.5730
O	0.9445	0.5670
P	0.7517	0.3860
Q	0.8990	0.5040
R	0.9299	0.5520
S	0.9427	0.5620
T	0.9234	0.5450
U	0.7017	0.4510
a	0.8467	0.4880
b	0.8146	0.4450
c	0.6394	0.3240
d	0.7344	0.3770
e	0.8489	0.4970
f	0.8424	0.4330
g	0.6695	0.3190
h	0.7718	0.4330
i	0.7630	0.3980
j	0.1157	0.1890
k	0.1895	0.1450
l	0.7708	0.4200
m	0.5872	0.2920
n	0.5126	0.2370

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
o	0.2805	0.1300
p	0.4111	0.1980
q	0.7113	0.3710
r	0.6161	0.2490
s	0.2648	0.1390
t	0.4894	0.2530
u	0.4876	0.1720
v	0.0428	0.0320
w	0.0712	0.0140
x	0.5129	0.2290