Full wwPDB EM Validation Report ⓘ

Nov 30, 2022 – 01:13 pm GMT

PDB ID	:	7ZME
EMDB ID	:	EMD-14796
Title	:	CryoEM structure of mitochondrial complex I from Chaetomium thermophilum (state 2) - membrane arm
Authors	:	Laube, E.; Kuehlbrandt, W.
Deposited on	:	2022-04-19
Resolution	:	2.83 Å(reported)
Based on initial models	:	6RFQ, 6RFR

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:

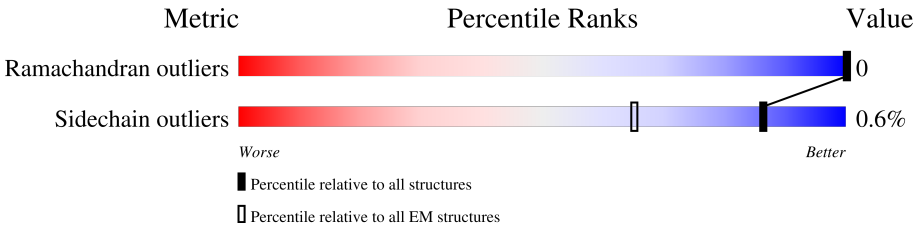
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.83 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	378	87% · 12%
2	2	571	96% ··
3	3	146	77% · 22%
4	4	542	91% 9%
5	5	679	98% ··
6	6	224	83% · 15%
7	8	86	12% 90% 10%
8	9	785	13% 87%
9	D	86	98% ··

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Mol	Chain	Length	Quality of chain
10	J	199	8% 93% 7%
11	L	89	98%
12	Q	141	60% 40%
13	R	99	99%
14	S	143	52% 48%
15	U	186	90% 9%
16	W	121	82% 18%
17	X	191	97%
18	a	815	18% 82%
19	b	94	5% 86% 14%
20	c	93	65% 35%
21	d	105	93% 7%
22	e	46	7% 80% 20%
23	g	82	94% 5%
24	i	93	8% 86% 14%
25	j	75	97%
26	n	184	10% 73% 27%

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 36964 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 NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	334	2573	1728	388	446	11	0	0

- Molecule 2 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	558	4456	2993	672	780	11	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	114	907	619	132	153	3	0	0

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	494	3904	2650	572	670	12	0	0

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	670	5272	3551	792	904	25	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	445	ARG	-	insertion	UNP G1DJA3
5	446	LEU	-	insertion	UNP G1DJA3
5	447	ALA	-	insertion	UNP G1DJA3

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Chain	Residue	Modelled	Actual	Comment	Reference
5	448	ILE	-	insertion	UNP G1DJA3
5	449	ASP	-	insertion	UNP G1DJA3
5	450	ASN	-	insertion	UNP G1DJA3
5	451	PHE	-	insertion	UNP G1DJA3
5	452	PHE	-	insertion	UNP G1DJA3
5	453	SER	-	insertion	UNP G1DJA3
5	454	ALA	-	insertion	UNP G1DJA3
5	455	GLN	-	insertion	UNP G1DJA3
5	456	ALA	-	insertion	UNP G1DJA3
5	457	ILE	-	insertion	UNP G1DJA3
5	458	LYS	-	insertion	UNP G1DJA3

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	190	Total	C	N	O	S	0	0
			1454	981	219	248	6		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	77	Total	C	N	O	S	0	0
			658	408	126	118	6		

- Molecule 8 is a protein called Subunit NDUFS5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	103	Total	C	N	O	S	0	0
			807	500	147	154	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	100	VAL	-	insertion	UNP G0SG48

- Molecule 9 is a protein called Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	85	Total	C	N	O	S	0	0
			678	432	127	115	4		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	186	Total	C	N	O	S	0	0
			1375	872	259	242	2		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	88	Total	C	N	O	S	0	0
			671	450	103	115	3		

- Molecule 12 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	85	Total	C	N	O	S	0	0
			663	418	109	135	1		

- Molecule 13 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	98	Total	C	N	O	S	0	0
			807	520	149	137	1		

- Molecule 14 is a protein called Complex I-ESSS.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	S	74	Total	C	N	O	0	0
			610	401	98	111		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	169	Total	C	N	O	S	0	0
			1365	860	254	242	9		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	99	Total	C	N	O	S	0	0
			812	519	154	137	2		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	187	Total	C	N	O	S	0	0
			1480	941	268	263	8		

- Molecule 18 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	143	Total	C	N	O	S	0	0
			1167	750	195	217	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	166	VAL	ALA	conflict	UNP G0RXU4
a	168	ALA	MET	conflict	UNP G0RXU4
a	?	-	GLU	deletion	UNP G0RXU4
a	?	-	GLY	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4

- Molecule 19 is a protein called Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	81	Total	C	N	O	S	0	0
			683	445	125	110	3		

- Molecule 20 is a protein called Subunit NDUFB3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	60	Total	C	N	O	S	0	0
			490	320	86	82	2		

- Molecule 21 is a protein called Subunit NDUFB10 of NADH-ubiquinone oxidoreductase

(Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	98	Total	C	N	O	S	0	0
			817	520	144	149	4		

- Molecule 22 is a protein called Subunit NDUFB2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	37	Total	C	N	O	S	0	0
			309	211	54	43	1		

- Molecule 23 is a protein called Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	78	Total	C	N	O	S	0	0
			610	399	105	105	1		

- Molecule 24 is a protein called Subunit NDUFB6 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	80	Total	C	N	O	S	0	0
			677	447	117	111	2		

- Molecule 25 is a protein called Subunit NDUFB4 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	73	Total	C	N	O	S	0	0
			603	391	108	101	3		

- Molecule 26 is a protein called Subunit NDUFB5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	135	Total	C	N	O	S	0	0
			1061	680	186	194	1		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP G0S086
n	2	LEU	-	insertion	UNP G0S086
n	3	ALA	-	insertion	UNP G0S086
n	4	LEU	-	insertion	UNP G0S086
n	5	ARG	-	insertion	UNP G0S086
n	6	GLN	-	insertion	UNP G0S086
n	7	ARG	-	insertion	UNP G0S086
n	8	ALA	-	insertion	UNP G0S086
n	9	ALA	-	insertion	UNP G0S086
n	10	LEU	-	insertion	UNP G0S086
n	11	LEU	-	insertion	UNP G0S086
n	12	ALA	-	insertion	UNP G0S086
n	13	ARG	-	insertion	UNP G0S086
n	14	ARG	-	insertion	UNP G0S086
n	15	VAL	-	insertion	UNP G0S086
n	16	ARG	-	insertion	UNP G0S086
n	17	PRO	-	insertion	UNP G0S086
n	18	THR	-	insertion	UNP G0S086
n	19	VAL	-	insertion	UNP G0S086
n	20	VAL	-	insertion	UNP G0S086
n	21	VAL	-	insertion	UNP G0S086
n	22	PRO	-	insertion	UNP G0S086
n	23	ARG	-	insertion	UNP G0S086
n	24	ASN	-	amidation	UNP G0S086
n	25	ALA	-	insertion	UNP G0S086
n	26	ARG	-	insertion	UNP G0S086
n	27	THR	-	insertion	UNP G0S086
n	28	TYR	-	insertion	UNP G0S086
n	29	ALA	-	insertion	UNP G0S086
n	30	SER	-	insertion	UNP G0S086
n	31	SER	-	insertion	UNP G0S086
n	32	HIS	-	insertion	UNP G0S086
n	33	ASP	-	insertion	UNP G0S086
n	34	HIS	-	insertion	UNP G0S086
n	35	ASP	-	insertion	UNP G0S086
n	36	HIS	-	insertion	UNP G0S086
n	37	HIS	-	insertion	UNP G0S086
n	38	ASP	-	insertion	UNP G0S086
n	39	HIS	-	insertion	UNP G0S086
n	40	HIS	-	insertion	UNP G0S086
n	41	HIS	-	insertion	UNP G0S086
n	42	ASP	-	insertion	UNP G0S086
n	43	HIS	-	insertion	UNP G0S086

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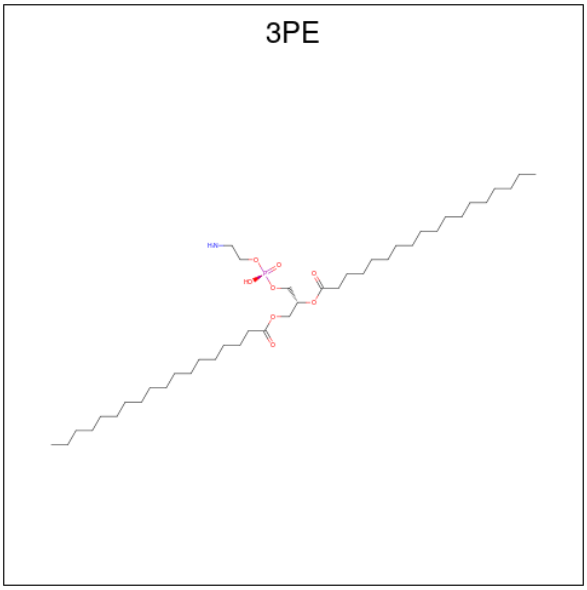
Chain	Residue	Modelled	Actual	Comment	Reference
n	44	GLY	-	insertion	UNP G0S086
n	45	HIS	-	insertion	UNP G0S086
n	46	ASN	-	insertion	UNP G0S086
n	47	VAL	-	insertion	UNP G0S086
n	48	GLU	-	insertion	UNP G0S086
n	49	GLU	-	insertion	UNP G0S086
n	50	PRO	-	insertion	UNP G0S086
n	51	LEU	-	insertion	UNP G0S086
n	52	GLY	-	insertion	UNP G0S086

- Molecule 27 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	N	O	P	0
			68	49	2	15	2	
27	1	1	Total	C	N	O	P	0
			68	49	2	15	2	
27	4	1	Total	C	N	O	P	0
			95	65	3	24	3	
27	4	1	Total	C	N	O	P	0
			95	65	3	24	3	
27	4	1	Total	C	N	O	P	0
			95	65	3	24	3	
27	5	1	Total	C	N	O	P	0
			142	102	4	32	4	

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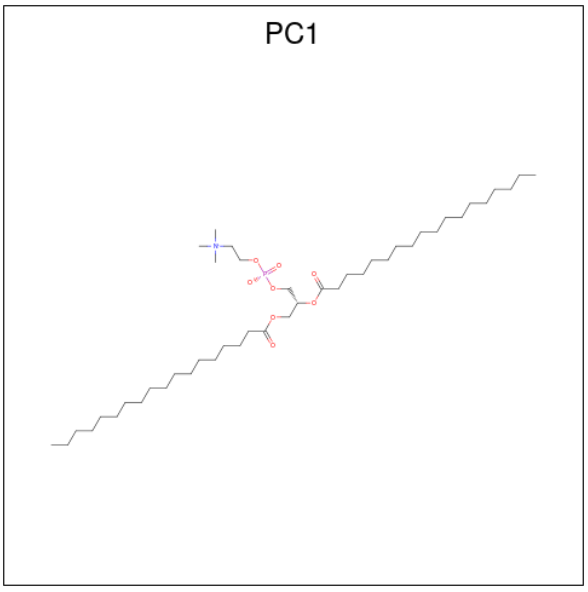
Mol	Chain	Residues	Atoms					AltConf
27	5	1	Total	C	N	O	P	0
			142	102	4	32	4	
27	5	1	Total	C	N	O	P	0
			142	102	4	32	4	
27	5	1	Total	C	N	O	P	0
			142	102	4	32	4	
27	8	1	Total	C	N	O	P	0
			36	26	1	8	1	
27	J	1	Total	C	N	O	P	0
			30	20	1	8	1	
27	W	1	Total	C	N	O	P	0
			34	24	1	8	1	
27	g	1	Total	C	N	O	P	0
			75	55	2	16	2	
27	g	1	Total	C	N	O	P	0
			75	55	2	16	2	
27	n	1	Total	C	N	O	P	0
			78	58	2	16	2	
27	n	1	Total	C	N	O	P	0
			78	58	2	16	2	

- Molecule 28 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total	C	N	O	P	0
			30	20	1	8	1	

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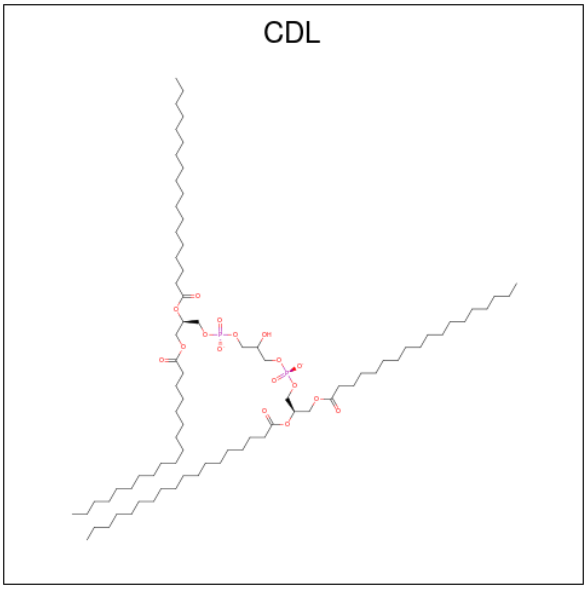
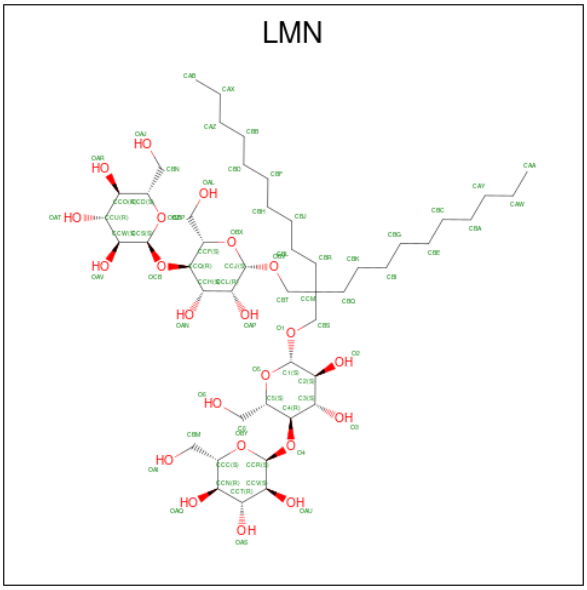
Mol	Chain	Residues	Atoms					AltConf
28	2	1	Total	C	N	O	P	0
			31	21	1	8	1	
28	3	1	Total	C	N	O	P	0
			36	26	1	8	1	
28	4	1	Total	C	N	O	P	0
			45	35	1	8	1	
28	5	1	Total	C	N	O	P	0
			86	66	2	16	2	
28	5	1	Total	C	N	O	P	0
			86	66	2	16	2	
28	n	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 29 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



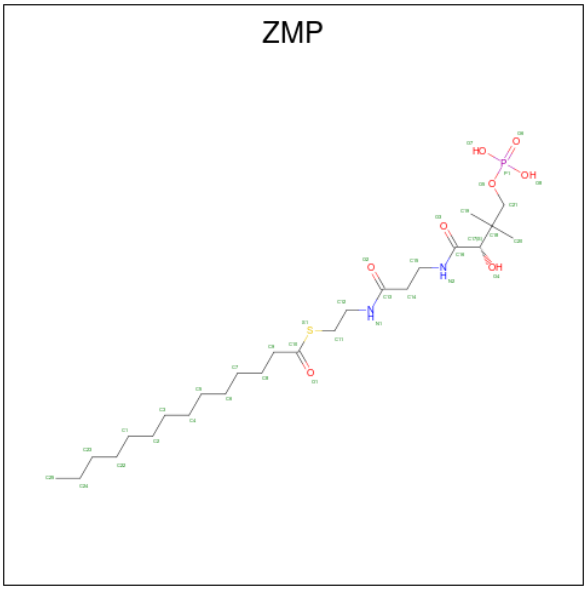
Mol	Chain	Residues	Atoms				AltConf
29	2	1	Total	C	O	P	0
			84	65	17	2	
29	4	1	Total	C	O	P	0
			86	67	17	2	
29	D	1	Total	C	O	P	0
			59	40	17	2	
29	X	1	Total	C	O	P	0
			79	60	17	2	
29	g	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 30 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: $C_{47}H_{88}O_{22}$).



Mol	Chain	Residues	Atoms			AltConf
30	2	1	Total	C	O	0
			58	41	17	
30	4	1	Total	C	O	0
			58	41	17	
30	J	1	Total	C	O	0
			69	47	22	

- Molecule 31 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
31	Q	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	1	62	Total	O	0
			62	62	
32	2	141	Total	O	0
			141	141	
32	3	24	Total	O	0
			24	24	
32	4	84	Total	O	0
			84	84	
32	5	49	Total	O	0
			49	49	
32	6	35	Total	O	0
			35	35	
32	9	19	Total	O	0
			19	19	
32	D	27	Total	O	0
			27	27	
32	J	1	Total	O	0
			1	1	
32	L	11	Total	O	0
			11	11	
32	R	4	Total	O	0
			4	4	
32	S	1	Total	O	0
			1	1	
32	U	36	Total	O	0
			36	36	
32	W	29	Total	O	0
			29	29	
32	X	45	Total	O	0
			45	45	
32	a	11	Total	O	0
			11	11	
32	b	4	Total	O	0
			4	4	
32	d	9	Total	O	0
			9	9	
32	g	10	Total	O	0
			10	10	

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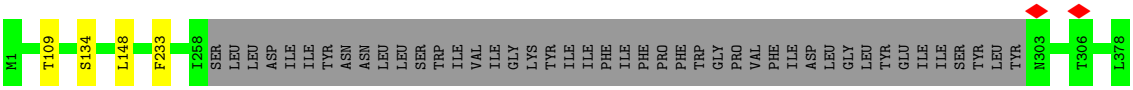
Mol	Chain	Residues	Atoms	AltConf
32	i	4	Total O 4 4	0
32	j	4	Total O 4 4	0
32	n	23	Total O 23 23	0

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.

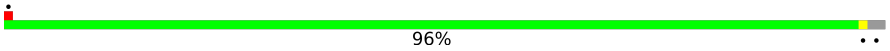
• Molecule 1: NADH-ubiquinone oxidoreductase chain 1

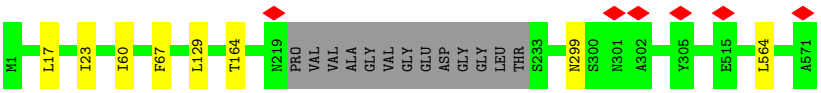
Chain 1:



• Molecule 2: NADH dehydrogenase subunit 2

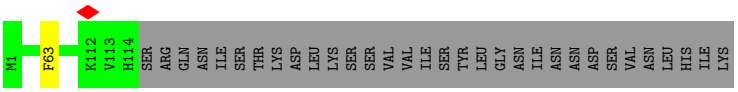
Chain 2:





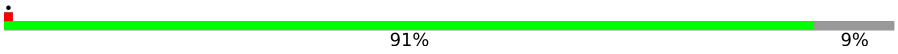
• Molecule 3: NADH-ubiquinone oxidoreductase chain 3

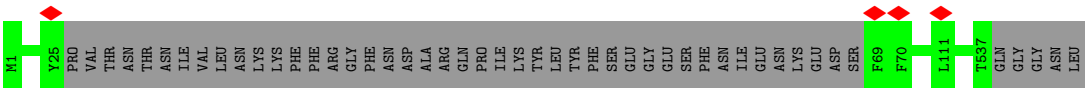
Chain 3:



• Molecule 4: NADH-ubiquinone oxidoreductase chain 4

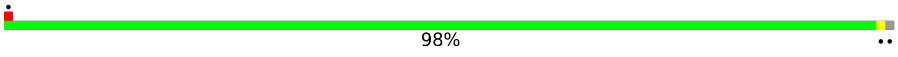
Chain 4:

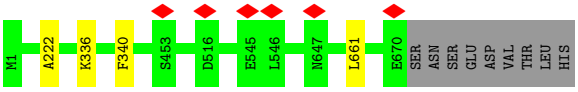




• Molecule 5: NADH-ubiquinone oxidoreductase chain 5

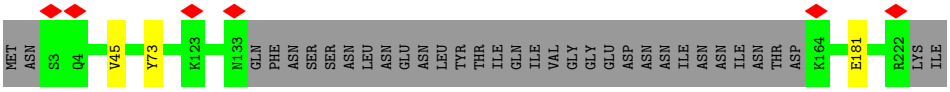
Chain 5:





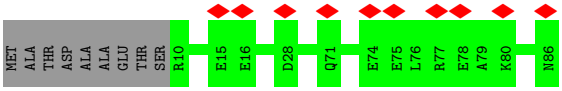
• Molecule 6: NADH-ubiquinone oxidoreductase chain 6

Chain 6:



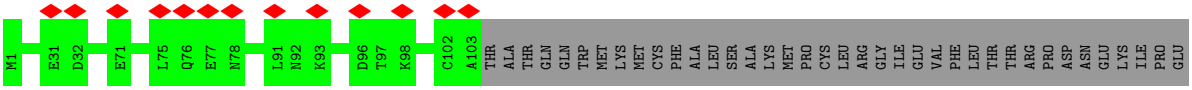
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

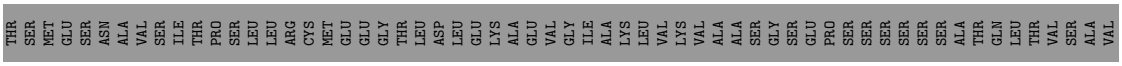
Chain 8:



• Molecule 8: Subunit NDUFS5 of NADH-ubiquinone oxidoreductase (Complex I)

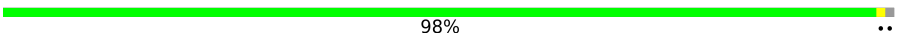
Chain 9:

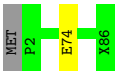




• Molecule 9: Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I)

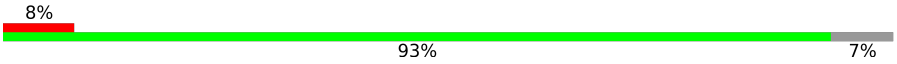
Chain D:

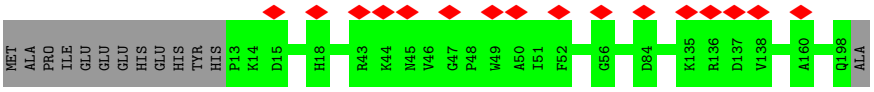




• Molecule 10: NADH-ubiquinone oxidoreductase-like protein

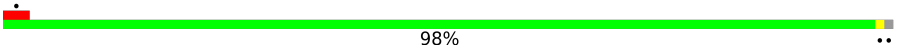
Chain J:

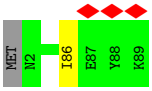




• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

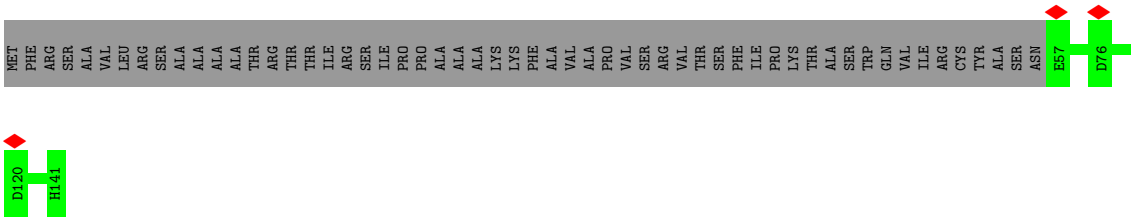
Chain L:





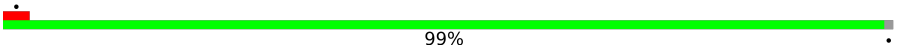
• Molecule 12: Acyl carrier protein

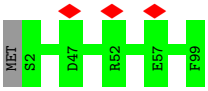
Chain Q:



• Molecule 13: Complex I-B22

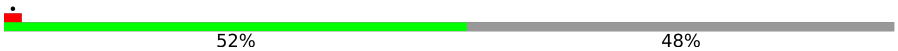
Chain R:

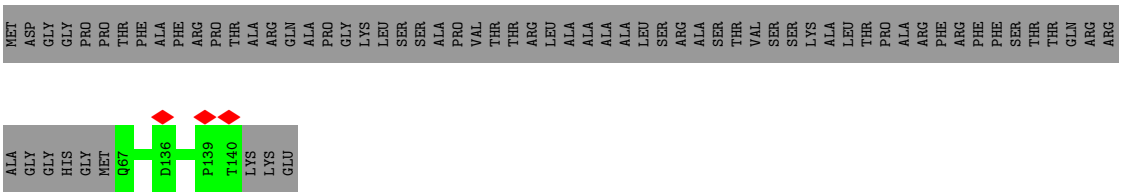




• Molecule 14: Complex I-ESSS

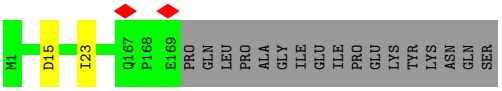
Chain S:





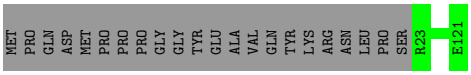
• Molecule 15: NADH-ubiquinone oxidoreductase

Chain U:



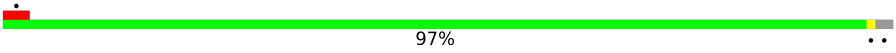
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

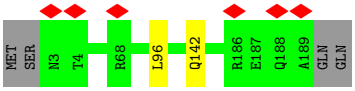
Chain W:



• Molecule 17: NADH-ubiquinone oxidoreductase-like protein

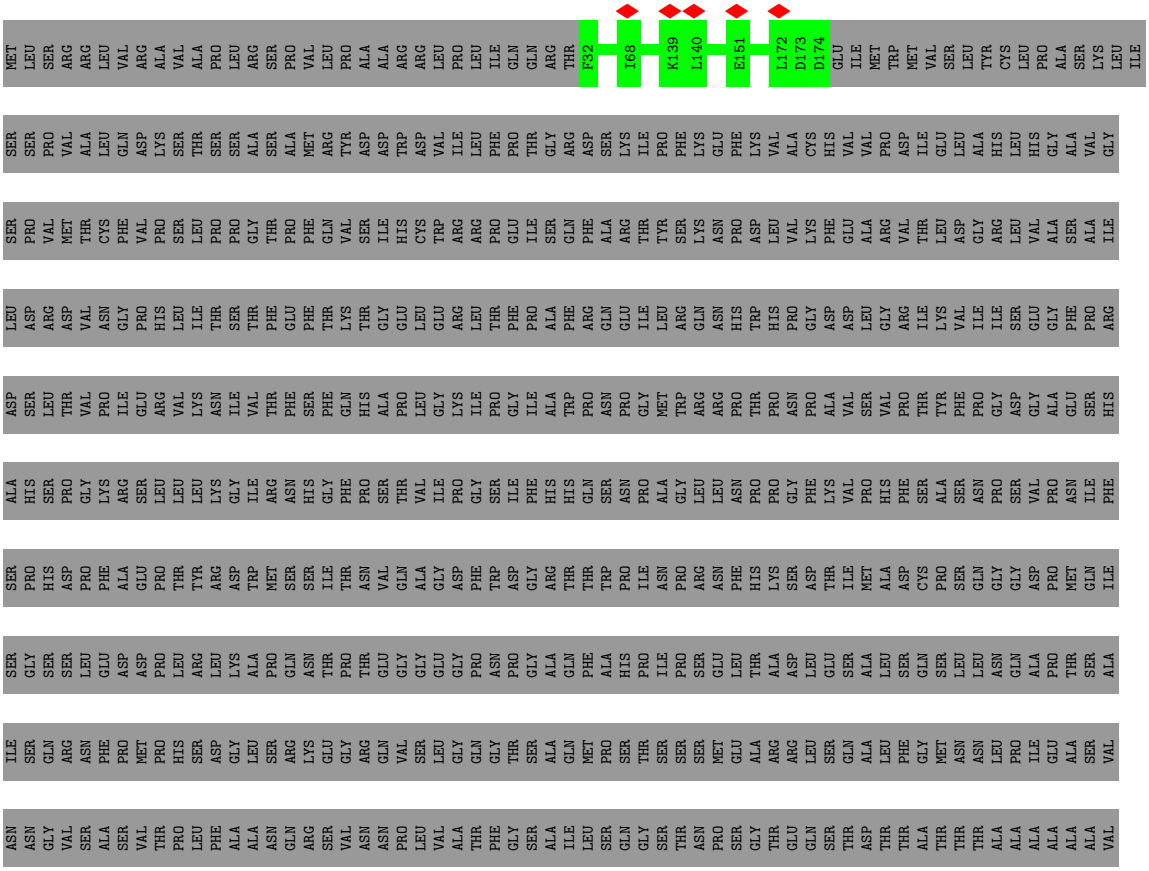
Chain X:



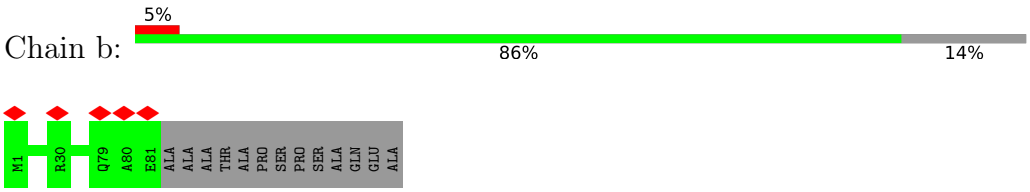


• Molecule 18: NADH dehydrogenase (Ubiquinone)-like protein

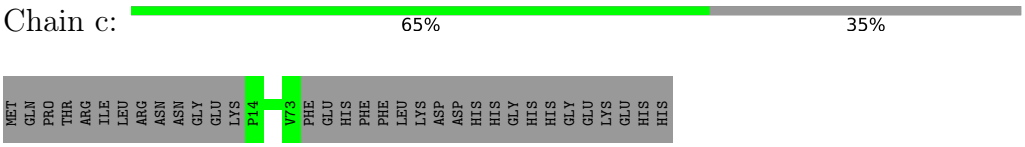
Chain a:



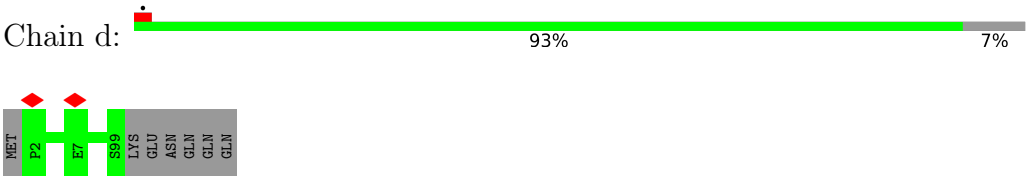
• Molecule 19: Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I)



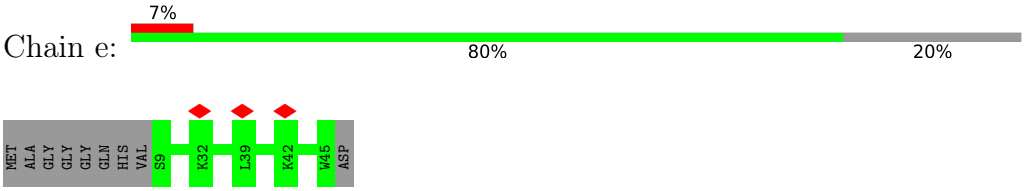
• Molecule 20: Subunit NDUFB3 of NADH-ubiquinone oxidoreductase (Complex I)



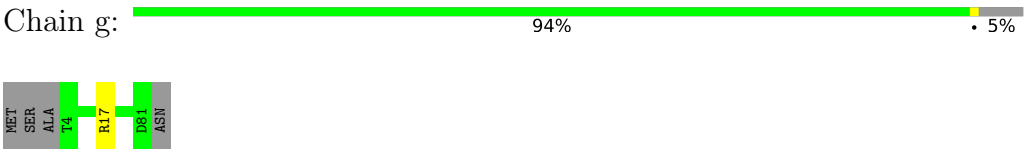
• Molecule 21: Subunit NDUFB10 of NADH-ubiquinone oxidoreductase (Complex I)



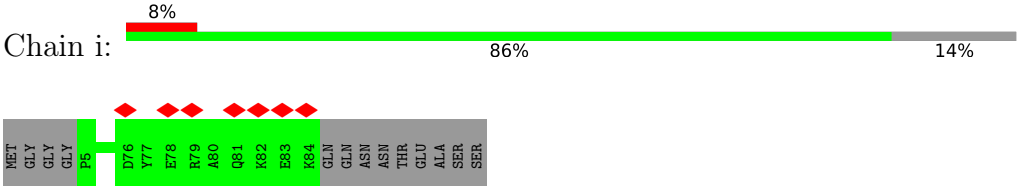
• Molecule 22: Subunit NDUFB2 of NADH-ubiquinone oxidoreductase (Complex I)



• Molecule 23: Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I)

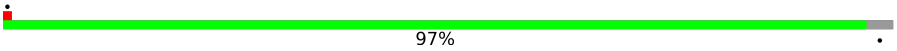


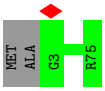
• Molecule 24: Subunit NDUFB6 of NADH-ubiquinone oxidoreductase (Complex I)



• Molecule 25: Subunit NDUFB4 of NADH-ubiquinone oxidoreductase (Complex I)

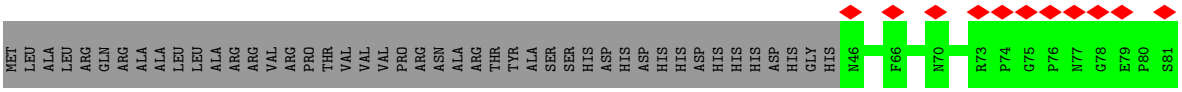
Chain j:

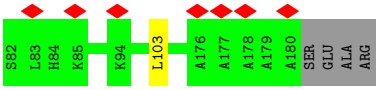




• Molecule 26: Subunit NDUFB5 of NADH-ubiquinone oxidoreductase (Complex I)

Chain n:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21989	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.226	Depositor
Minimum map value	-1.186	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.133	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	143.964, 218.457, 227.664	wwPDB
Map dimensions	272, 261, 172	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, ZMP, CDL, PC1, LMN

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	1	0.46	0/2633	0.62	0/3593
2	2	0.46	0/4562	0.61	1/6205 (0.0%)
3	3	0.43	0/934	0.56	0/1269
4	4	0.40	0/4002	0.54	0/5454
5	5	0.38	1/5414 (0.0%)	0.55	2/7371 (0.0%)
6	6	0.53	2/1481 (0.1%)	0.65	0/2020
7	8	0.27	0/671	0.43	0/896
8	9	0.40	0/824	0.56	0/1112
9	D	0.52	0/674	0.74	0/911
10	J	0.33	0/1400	0.48	0/1892
11	L	0.45	0/677	0.58	0/917
12	Q	0.28	0/673	0.47	0/913
13	R	0.33	0/832	0.48	0/1133
14	S	0.34	0/635	0.49	0/869
15	U	0.48	0/1403	0.69	0/1904
16	W	0.47	0/830	0.70	0/1120
17	X	0.50	0/1519	0.66	0/2053
18	a	0.32	0/1204	0.47	0/1632
19	b	0.29	0/701	0.40	0/939
20	c	0.28	0/509	0.45	0/691
21	d	0.35	0/835	0.47	0/1123
22	e	0.36	0/324	0.45	0/440
23	g	0.42	0/631	0.60	0/868
24	i	0.34	0/706	0.49	0/960
25	j	0.32	0/617	0.44	0/830
26	n	0.44	0/1092	0.58	0/1481
All	All	0.41	3/35783 (0.0%)	0.57	3/48596 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	45	VAL	C-N	-5.52	1.21	1.34
6	6	181	GLU	C-N	5.52	1.46	1.34
5	5	222	ALA	C-N	-5.05	1.22	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	661	LEU	CB-CG-CD2	-7.43	98.37	111.00
5	5	661	LEU	CA-CB-CG	6.20	129.56	115.30
2	2	67	PHE	CB-CA-C	5.21	120.83	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	330/378 (87%)	317 (96%)	13 (4%)	0	100	100
2	2	554/571 (97%)	545 (98%)	9 (2%)	0	100	100
3	3	112/146 (77%)	108 (96%)	4 (4%)	0	100	100
4	4	490/542 (90%)	479 (98%)	11 (2%)	0	100	100
5	5	668/679 (98%)	638 (96%)	30 (4%)	0	100	100
6	6	186/224 (83%)	178 (96%)	8 (4%)	0	100	100
7	8	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
8	9	101/785 (13%)	100 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	D	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
10	J	184/199 (92%)	179 (97%)	5 (3%)	0	100	100
11	L	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
12	Q	83/141 (59%)	83 (100%)	0	0	100	100
13	R	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
14	S	72/143 (50%)	68 (94%)	4 (6%)	0	100	100
15	U	167/186 (90%)	162 (97%)	5 (3%)	0	100	100
16	W	97/121 (80%)	97 (100%)	0	0	100	100
17	X	185/191 (97%)	182 (98%)	3 (2%)	0	100	100
18	a	141/815 (17%)	136 (96%)	5 (4%)	0	100	100
19	b	79/94 (84%)	78 (99%)	1 (1%)	0	100	100
20	c	58/93 (62%)	50 (86%)	8 (14%)	0	100	100
21	d	96/105 (91%)	92 (96%)	4 (4%)	0	100	100
22	e	35/46 (76%)	35 (100%)	0	0	100	100
23	g	76/82 (93%)	74 (97%)	2 (3%)	0	100	100
24	i	78/93 (84%)	75 (96%)	3 (4%)	0	100	100
25	j	71/75 (95%)	68 (96%)	3 (4%)	0	100	100
26	n	133/184 (72%)	129 (97%)	4 (3%)	0	100	100
All	All	4332/6253 (69%)	4198 (97%)	134 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1	284/326 (87%)	280 (99%)	4 (1%)	67	83
2	2	509/518 (98%)	502 (99%)	7 (1%)	67	83
3	3	97/128 (76%)	96 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	4	431/477 (90%)	431 (100%)	0	100 100
5	5	579/596 (97%)	577 (100%)	2 (0%)	92 96
6	6	162/203 (80%)	161 (99%)	1 (1%)	86 93
7	8	69/75 (92%)	69 (100%)	0	100 100
8	9	84/687 (12%)	84 (100%)	0	100 100
9	D	68/69 (99%)	67 (98%)	1 (2%)	65 82
10	J	126/146 (86%)	126 (100%)	0	100 100
11	L	73/76 (96%)	72 (99%)	1 (1%)	67 83
12	Q	72/119 (60%)	72 (100%)	0	100 100
13	R	87/89 (98%)	87 (100%)	0	100 100
14	S	59/111 (53%)	59 (100%)	0	100 100
15	U	149/167 (89%)	147 (99%)	2 (1%)	69 84
16	W	82/102 (80%)	82 (100%)	0	100 100
17	X	145/152 (95%)	143 (99%)	2 (1%)	67 83
18	a	123/697 (18%)	123 (100%)	0	100 100
19	b	67/74 (90%)	67 (100%)	0	100 100
20	c	47/80 (59%)	47 (100%)	0	100 100
21	d	87/94 (93%)	87 (100%)	0	100 100
22	e	29/35 (83%)	29 (100%)	0	100 100
23	g	65/69 (94%)	64 (98%)	1 (2%)	65 82
24	i	68/78 (87%)	68 (100%)	0	100 100
25	j	63/64 (98%)	63 (100%)	0	100 100
26	n	106/150 (71%)	105 (99%)	1 (1%)	78 89
All	All	3731/5382 (69%)	3708 (99%)	23 (1%)	86 93

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	109	THR
1	1	134	SER
1	1	148	LEU
1	1	233	PHE
2	2	17	LEU
2	2	23	ILE

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Mol	Chain	Res	Type
2	2	60	ILE
2	2	129	LEU
2	2	164	THR
2	2	299	ASN
2	2	564	LEU
3	3	63	PHE
5	5	336	LYS
5	5	340	PHE
6	6	73	TYR
9	D	74	GLU
11	L	86	ILE
15	U	15	ASP
15	U	23	ILE
17	X	96	LEU
17	X	142	GLN
23	g	17	ARG
26	n	103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	147	GLN
1	1	203	ASN
1	1	374	ASN
2	2	529	ASN
4	4	151	ASN
5	5	109	HIS
5	5	171	ASN
5	5	353	ASN
5	5	503	ASN
5	5	511	HIS
6	6	67	ASN
6	6	105	ASN
11	L	18	ASN
11	L	46	ASN
13	R	24	HIS
13	R	31	GLN
14	S	117	GLN
15	U	56	GLN
15	U	149	GLN
17	X	142	GLN
24	i	29	GLN

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Mol	Chain	Res	Type
26	n	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	3PE	4	603	-	32,32,50	1.05	4 (12%)	35,37,55	1.17	2 (5%)
27	3PE	1	402	-	26,26,50	0.34	0	28,30,55	0.54	0
28	PC1	4	605	-	44,44,53	1.02	4 (9%)	50,52,61	1.06	2 (4%)
27	3PE	5	702	-	39,39,50	0.30	0	42,44,55	0.36	0
27	3PE	n	201	-	38,38,50	0.99	4 (10%)	41,43,55	1.14	2 (4%)
27	3PE	5	706	-	27,27,50	1.07	3 (11%)	30,32,55	1.16	1 (3%)
28	PC1	2	603	-	30,30,53	0.34	0	36,38,61	0.37	0
29	CDL	X	201	-	78,78,99	0.31	0	84,90,111	0.40	0
30	LMN	J	202	-	72,72,72	0.16	0	96,98,98	0.29	0
27	3PE	5	703	-	31,31,50	1.08	4 (12%)	34,36,55	1.16	2 (5%)
27	3PE	5	704	-	41,41,50	0.95	4 (9%)	44,46,55	1.09	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PC1	3	201	-	35,35,53	0.34	0	41,43,61	0.39	0
27	3PE	W	201	-	33,33,50	0.31	0	34,37,55	0.40	0
29	CDL	g	101	-	55,55,99	0.35	0	61,67,111	0.55	0
30	LMN	2	602	-	60,60,72	0.20	0	78,80,98	0.54	1 (1%)
28	PC1	n	202	-	50,50,53	0.96	4 (8%)	56,58,61	1.08	2 (3%)
29	CDL	D	101	-	58,58,99	0.34	0	64,70,111	0.44	0
28	PC1	5	705	-	40,40,53	1.08	3 (7%)	46,48,61	1.14	3 (6%)
27	3PE	J	201	-	29,29,50	1.12	4 (13%)	32,34,55	1.18	2 (6%)
29	CDL	4	601	-	85,85,99	0.28	0	91,97,111	0.35	0
30	LMN	4	604	-	60,60,72	0.19	0	78,80,98	0.32	0
28	PC1	1	403	-	29,29,53	1.26	4 (13%)	35,37,61	1.25	2 (5%)
28	PC1	5	701	-	44,44,53	0.44	0	50,52,61	0.46	0
27	3PE	g	102	-	35,35,50	0.33	0	38,40,55	0.47	0
27	3PE	g	103	-	38,38,50	0.35	0	41,43,55	0.38	0
27	3PE	4	602	-	33,33,50	1.04	4 (12%)	36,38,55	1.13	2 (5%)
27	3PE	1	401	-	40,40,50	0.39	0	43,45,55	0.43	0
29	CDL	2	601	-	83,83,99	0.31	0	89,95,111	0.36	0
31	ZMP	Q	201	12	29,35,36	0.19	0	34,42,45	0.45	0
27	3PE	8	101	-	35,35,50	1.02	4 (11%)	38,40,55	1.13	2 (5%)
27	3PE	n	203	-	38,38,50	0.98	4 (10%)	41,43,55	1.12	2 (4%)
27	3PE	4	606	-	27,27,50	1.15	4 (14%)	30,32,55	1.18	2 (6%)

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	3PE	4	603	-	-	22/36/36/54	-
27	3PE	1	402	-	-	8/29/29/54	-
28	PC1	4	605	-	-	30/48/48/57	-
27	3PE	5	702	-	-	13/43/43/54	-
27	3PE	n	201	-	-	17/42/42/54	-
27	3PE	5	706	-	-	9/30/30/54	-
28	PC1	2	603	-	-	8/34/34/57	-
29	CDL	X	201	-	-	25/89/89/110	-
30	LMN	J	202	-	-	11/50/130/130	0/4/4/4
27	3PE	5	703	-	-	11/35/35/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	3PE	5	704	-	-	16/45/45/54	-
28	PC1	3	201	-	-	11/39/39/57	-
27	3PE	W	201	-	-	12/36/36/54	-
29	CDL	g	101	-	-	16/66/66/110	-
30	LMN	2	602	-	-	18/44/104/130	0/3/3/4
28	PC1	n	202	-	-	20/54/54/57	-
29	CDL	D	101	-	-	28/69/69/110	-
28	PC1	5	705	-	-	22/44/44/57	-
27	3PE	J	201	-	-	14/33/33/54	-
29	CDL	4	601	-	-	26/96/96/110	-
30	LMN	4	604	-	-	15/44/104/130	0/3/3/4
28	PC1	1	403	-	-	17/32/32/57	-
28	PC1	5	701	-	-	20/48/48/57	-
27	3PE	g	102	-	-	17/39/39/54	-
27	3PE	g	103	-	-	15/42/42/54	-
27	3PE	4	602	-	-	12/37/37/54	-
27	3PE	1	401	-	-	9/44/44/54	-
29	CDL	2	601	-	-	24/94/94/110	-
31	ZMP	Q	201	12	-	10/40/42/43	-
27	3PE	8	101	-	-	18/39/39/54	-
27	3PE	n	203	-	-	19/42/42/54	-
27	3PE	4	606	-	-	8/31/31/54	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	5	705	PC1	O21-C2	-2.69	1.39	1.46
27	n	201	3PE	O21-C2	-2.55	1.40	1.46
27	4	606	3PE	O21-C2	-2.51	1.40	1.46
27	5	704	3PE	O21-C2	-2.51	1.40	1.46
27	4	602	3PE	O21-C2	-2.50	1.40	1.46
27	5	706	3PE	O21-C2	-2.50	1.40	1.46
28	1	403	PC1	O21-C2	-2.50	1.40	1.46
27	n	203	3PE	O21-C2	-2.49	1.40	1.46
27	J	201	3PE	O21-C2	-2.48	1.40	1.46
28	n	202	PC1	O21-C2	-2.47	1.40	1.46
27	8	101	3PE	O21-C2	-2.46	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	4	605	PC1	O21-C2	-2.45	1.40	1.46
27	5	703	3PE	O31-C31	2.45	1.40	1.33
27	n	201	3PE	O31-C31	2.44	1.40	1.33
27	J	201	3PE	O31-C31	2.43	1.40	1.33
27	5	703	3PE	O21-C2	-2.42	1.40	1.46
28	5	705	PC1	O31-C31	2.42	1.40	1.33
27	n	203	3PE	O31-C31	2.41	1.40	1.33
27	4	603	3PE	O31-C31	2.41	1.40	1.33
27	4	603	3PE	O21-C2	-2.41	1.40	1.46
27	4	606	3PE	O31-C31	2.41	1.40	1.33
27	8	101	3PE	O31-C31	2.39	1.40	1.33
28	1	403	PC1	O31-C31	2.36	1.40	1.33
28	1	403	PC1	O21-C21	2.35	1.40	1.35
27	5	704	3PE	O31-C31	2.35	1.40	1.33
28	n	202	PC1	O31-C31	2.33	1.40	1.33
27	4	602	3PE	O31-C31	2.33	1.40	1.33
28	4	605	PC1	O21-C21	2.27	1.40	1.34
28	4	605	PC1	O31-C31	2.26	1.39	1.33
28	4	605	PC1	O31-C3	-2.24	1.40	1.45
27	4	602	3PE	O31-C3	-2.22	1.40	1.45
27	5	703	3PE	O21-C21	2.22	1.40	1.34
27	J	201	3PE	O21-C21	2.19	1.40	1.34
27	J	201	3PE	O31-C3	-2.16	1.40	1.45
27	8	101	3PE	O21-C21	2.16	1.40	1.34
27	n	201	3PE	O21-C21	2.16	1.40	1.34
28	n	202	PC1	O21-C21	2.15	1.40	1.34
27	5	704	3PE	O31-C3	-2.15	1.40	1.45
27	4	606	3PE	O21-C21	2.14	1.40	1.34
28	n	202	PC1	O31-C3	-2.14	1.40	1.45
27	5	706	3PE	O21-C21	2.13	1.40	1.34
27	4	603	3PE	O31-C3	-2.13	1.40	1.45
27	5	704	3PE	O21-C21	2.13	1.40	1.34
27	8	101	3PE	O31-C3	-2.13	1.40	1.45
27	5	706	3PE	O31-C3	-2.12	1.40	1.45
28	5	705	PC1	O31-C3	-2.11	1.40	1.45
27	5	703	3PE	O31-C3	-2.11	1.40	1.45
27	n	203	3PE	O21-C21	2.10	1.40	1.34
28	1	403	PC1	O31-C3	-2.09	1.40	1.45
27	n	201	3PE	O31-C3	-2.08	1.40	1.45
27	4	603	3PE	O21-C21	2.08	1.40	1.34
27	4	606	3PE	O31-C3	-2.07	1.40	1.45
27	n	203	3PE	O31-C3	-2.06	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	602	3PE	O21-C21	2.04	1.40	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	1	403	PC1	O21-C21-C22	4.87	120.05	111.09
27	n	201	3PE	O21-C21-C22	4.15	120.44	111.50
28	4	605	PC1	O21-C21-C22	4.13	120.41	111.50
28	n	202	PC1	O21-C21-C22	4.12	120.39	111.50
27	5	706	3PE	O21-C21-C22	4.12	120.37	111.50
27	n	203	3PE	O21-C21-C22	4.10	120.34	111.50
27	8	101	3PE	O21-C21-C22	4.08	120.30	111.50
27	4	603	3PE	O21-C21-C22	4.06	120.25	111.50
27	J	201	3PE	O21-C21-C22	4.03	120.19	111.50
27	5	703	3PE	O21-C21-C22	4.00	120.12	111.50
28	5	705	PC1	O21-C21-C22	3.99	120.09	111.50
27	5	704	3PE	O21-C21-C22	3.96	120.04	111.50
27	4	602	3PE	O21-C21-C22	3.95	120.01	111.50
27	4	606	3PE	O21-C21-C22	3.89	119.89	111.50
30	2	602	LMN	CBQ-CCM-CBS	-2.83	102.70	109.40
28	5	705	PC1	O31-C31-C32	2.73	120.48	111.91
28	1	403	PC1	O31-C31-C32	2.72	120.43	111.91
27	4	603	3PE	O31-C31-C32	2.70	120.39	111.91
28	4	605	PC1	O31-C31-C32	2.68	120.33	111.91
27	n	203	3PE	O31-C31-C32	2.67	120.29	111.91
27	n	201	3PE	O31-C31-C32	2.65	120.23	111.91
27	5	703	3PE	O31-C31-C32	2.61	120.10	111.91
27	8	101	3PE	O31-C31-C32	2.60	120.08	111.91
27	J	201	3PE	O31-C31-C32	2.59	120.05	111.91
27	4	606	3PE	O31-C31-C32	2.59	120.04	111.91
27	5	704	3PE	O31-C31-C32	2.56	119.95	111.91
27	4	602	3PE	O31-C31-C32	2.51	119.78	111.91
28	n	202	PC1	O31-C31-C32	2.50	119.75	111.91
28	5	705	PC1	C11-C12-N	-2.07	108.86	115.78

There are no chirality outliers.

All (521) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	1	402	3PE	C11-O13-P-O14
27	4	603	3PE	C1-O11-P-O12
27	4	603	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
27	4	603	3PE	C11-O13-P-O12
27	4	603	3PE	C11-O13-P-O14
27	4	606	3PE	C11-O13-P-O14
27	4	606	3PE	O21-C2-C3-O31
27	5	702	3PE	C11-O13-P-O14
27	5	704	3PE	C1-O11-P-O13
27	5	704	3PE	C1-O11-P-O14
27	5	704	3PE	O13-C11-C12-N
27	5	706	3PE	C1-O11-P-O12
27	5	706	3PE	C11-O13-P-O14
27	5	706	3PE	C22-C21-O21-C2
27	8	101	3PE	C11-O13-P-O11
27	8	101	3PE	C11-O13-P-O12
27	8	101	3PE	C11-O13-P-O14
27	8	101	3PE	O22-C21-O21-C2
27	8	101	3PE	C22-C21-O21-C2
27	W	201	3PE	C11-O13-P-O11
27	W	201	3PE	C2-C1-O11-P
27	W	201	3PE	O32-C31-O31-C3
27	g	102	3PE	C1-O11-P-O14
27	g	103	3PE	C2-C1-O11-P
27	g	103	3PE	C12-C11-O13-P
27	g	103	3PE	O13-C11-C12-N
27	n	201	3PE	O21-C2-C3-O31
27	n	201	3PE	O22-C21-O21-C2
27	n	201	3PE	C22-C21-O21-C2
27	n	203	3PE	C1-O11-P-O12
27	n	203	3PE	C1-O11-P-O14
27	n	203	3PE	C11-O13-P-O12
27	n	203	3PE	C11-O13-P-O14
27	n	203	3PE	O22-C21-O21-C2
28	1	403	PC1	C11-O13-P-O14
28	1	403	PC1	C1-O11-P-O12
28	1	403	PC1	C1-O11-P-O14
28	1	403	PC1	O13-C11-C12-N
28	2	603	PC1	C11-O13-P-O14
28	2	603	PC1	C1-O11-P-O14
28	2	603	PC1	C1-O11-P-O13
28	2	603	PC1	C12-C11-O13-P
28	4	605	PC1	C22-C21-O21-C2
28	5	701	PC1	C11-O13-P-O14
28	5	705	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
28	5	705	PC1	C11-O13-P-O14
28	5	705	PC1	C11-O13-P-O11
28	5	705	PC1	O13-C11-C12-N
28	n	202	PC1	C1-O11-P-O12
28	n	202	PC1	C1-O11-P-O14
28	n	202	PC1	C1-O11-P-O13
29	2	601	CDL	O1-C1-CA2-OA2
29	2	601	CDL	CA3-OA5-PA1-OA4
29	2	601	CDL	CB2-OB2-PB2-OB3
29	4	601	CDL	OA6-CA4-CA6-OA8
29	4	601	CDL	CB2-OB2-PB2-OB3
29	D	101	CDL	CA2-OA2-PA1-OA3
29	D	101	CDL	CA2-OA2-PA1-OA4
29	D	101	CDL	CA2-OA2-PA1-OA5
29	D	101	CDL	CB3-OB5-PB2-OB2
29	D	101	CDL	CB3-OB5-PB2-OB3
29	D	101	CDL	CB3-OB5-PB2-OB4
29	D	101	CDL	C51-CB5-OB6-CB4
29	g	101	CDL	OB7-CB5-OB6-CB4
29	g	101	CDL	C51-CB5-OB6-CB4
30	2	602	LMN	CBK-CBQ-CCM-CBR
30	2	602	LMN	OBX-CCJ-OBV-CBT
30	4	604	LMN	CBK-CBQ-CCM-CBR
30	4	604	LMN	CBK-CBQ-CCM-CBS
30	4	604	LMN	CBK-CBQ-CCM-CBT
30	4	604	LMN	OBV-CBT-CCM-CBQ
30	4	604	LMN	OBV-CBT-CCM-CBR
30	4	604	LMN	OBX-CCJ-OBV-CBT
31	Q	201	ZMP	O4-C17-C18-C21
31	Q	201	ZMP	C13-C14-C15-N2
28	1	403	PC1	C22-C21-O21-C2
28	1	403	PC1	O22-C21-O21-C2
27	g	103	3PE	O32-C31-O31-C3
27	g	103	3PE	C32-C31-O31-C3
27	4	603	3PE	O32-C31-O31-C3
27	J	201	3PE	O32-C31-O31-C3
27	5	706	3PE	O22-C21-O21-C2
28	4	605	PC1	O22-C21-O21-C2
29	D	101	CDL	OB7-CB5-OB6-CB4
29	X	201	CDL	OB7-CB5-OB6-CB4
27	4	603	3PE	C32-C31-O31-C3
27	n	203	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
27	J	201	3PE	C32-C31-O31-C3
27	n	203	3PE	C32-C31-O31-C3
28	4	605	PC1	C32-C31-O31-C3
28	3	201	PC1	C32-C33-C34-C35
30	4	604	LMN	CCH-CCQ-OCB-CCS
27	5	702	3PE	O22-C21-O21-C2
29	X	201	CDL	OA7-CA5-OA6-CA4
30	4	604	LMN	OBV-CBT-CCM-CBS
27	8	101	3PE	C32-C31-O31-C3
28	5	705	PC1	C32-C31-O31-C3
29	4	601	CDL	C31-CA7-OA8-CA6
27	8	101	3PE	O32-C31-O31-C3
27	1	402	3PE	C22-C21-O21-C2
27	5	702	3PE	C22-C21-O21-C2
29	D	101	CDL	C11-CA5-OA6-CA4
29	X	201	CDL	C11-CA5-OA6-CA4
29	X	201	CDL	C51-CB5-OB6-CB4
28	4	605	PC1	O32-C31-O31-C3
27	1	402	3PE	O22-C21-O21-C2
27	n	203	3PE	O32-C31-O31-C3
28	5	705	PC1	O32-C31-O31-C3
29	4	601	CDL	OA9-CA7-OA8-CA6
29	2	601	CDL	CB2-C1-CA2-OA2
29	X	201	CDL	CA7-C31-C32-C33
29	X	201	CDL	OA5-CA3-CA4-OA6
30	2	602	LMN	OBZ-CCS-OCB-CCQ
28	3	201	PC1	O21-C2-C3-O31
29	D	101	CDL	OA7-CA5-OA6-CA4
27	4	602	3PE	C21-C22-C23-C24
28	4	605	PC1	C31-C32-C33-C34
27	4	603	3PE	C31-C32-C33-C34
27	4	603	3PE	C21-C22-C23-C24
27	J	201	3PE	C21-C22-C23-C24
27	g	102	3PE	C31-C32-C33-C34
27	g	103	3PE	C21-C22-C23-C24
28	5	705	PC1	C21-C22-C23-C24
29	4	601	CDL	C54-C55-C56-C57
27	5	704	3PE	C21-C22-C23-C24
29	4	601	CDL	C51-CB5-OB6-CB4
30	4	604	LMN	CBJ-CBL-CBR-CCM
27	g	103	3PE	C22-C23-C24-C25
27	4	602	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
27	4	602	3PE	C1-O11-P-O13
27	4	603	3PE	C1-O11-P-O13
27	4	603	3PE	C11-O13-P-O11
27	J	201	3PE	C1-O11-P-O13
27	J	201	3PE	C11-O13-P-O11
27	g	103	3PE	C11-O13-P-O11
27	n	203	3PE	C1-O11-P-O13
27	n	203	3PE	C11-O13-P-O11
29	2	601	CDL	CA3-OA5-PA1-OA2
29	g	101	CDL	CA2-OA2-PA1-OA5
29	4	601	CDL	OB7-CB5-OB6-CB4
29	D	101	CDL	C71-C72-C73-C74
29	2	601	CDL	C11-CA5-OA6-CA4
27	4	603	3PE	C35-C36-C37-C38
27	4	603	3PE	C33-C34-C35-C36
27	5	702	3PE	C33-C34-C35-C36
27	4	602	3PE	O22-C21-O21-C2
29	2	601	CDL	OA7-CA5-OA6-CA4
29	2	601	CDL	CB4-CB3-OB5-PB2
29	4	601	CDL	CA4-CA3-OA5-PA1
27	5	704	3PE	C22-C23-C24-C25
29	g	101	CDL	O1-C1-CA2-OA2
27	g	102	3PE	C38-C39-C3A-C3B
28	5	701	PC1	C21-C22-C23-C24
30	2	602	LMN	C2-C1-O1-CBS
28	5	701	PC1	C22-C23-C24-C25
27	5	704	3PE	C33-C34-C35-C36
28	n	202	PC1	C23-C24-C25-C26
28	4	605	PC1	C29-C2A-C2B-C2C
28	4	605	PC1	C23-C24-C25-C26
28	5	705	PC1	C22-C23-C24-C25
28	5	705	PC1	C23-C24-C25-C26
29	X	201	CDL	C15-C16-C17-C18
30	2	602	LMN	O5-C1-O1-CBS
28	4	605	PC1	C35-C36-C37-C38
28	5	701	PC1	C2B-C2C-C2D-C2E
27	n	201	3PE	C22-C23-C24-C25
27	n	203	3PE	C36-C37-C38-C39
28	5	705	PC1	C32-C33-C34-C35
27	8	101	3PE	C27-C28-C29-C2A
28	5	705	PC1	C35-C36-C37-C38
28	4	605	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
27	5	706	3PE	C1-C2-C3-O31
27	4	602	3PE	C33-C34-C35-C36
27	4	602	3PE	C25-C26-C27-C28
28	n	202	PC1	C32-C33-C34-C35
27	g	102	3PE	C39-C3A-C3B-C3C
27	4	602	3PE	C22-C23-C24-C25
30	J	202	LMN	CBC-CBE-CBG-CBI
28	5	701	PC1	C32-C31-O31-C3
29	D	101	CDL	CB7-C71-C72-C73
27	W	201	3PE	C24-C25-C26-C27
27	n	201	3PE	C21-C22-C23-C24
29	X	201	CDL	C71-CB7-OB8-CB6
28	5	701	PC1	C31-C32-C33-C34
28	n	202	PC1	C29-C2A-C2B-C2C
27	g	102	3PE	C35-C36-C37-C38
28	5	705	PC1	C26-C27-C28-C29
27	8	101	3PE	C31-C32-C33-C34
29	4	601	CDL	CA5-C11-C12-C13
28	3	201	PC1	C22-C21-O21-C2
28	5	705	PC1	C22-C21-O21-C2
28	5	705	PC1	O11-C1-C2-O21
27	g	103	3PE	C2E-C2F-C2G-C2H
27	n	201	3PE	C23-C24-C25-C26
27	n	203	3PE	C37-C38-C39-C3A
28	1	403	PC1	C35-C36-C37-C38
27	n	203	3PE	C35-C36-C37-C38
28	4	605	PC1	C24-C25-C26-C27
30	2	602	LMN	CCL-CCJ-OBV-CBT
30	4	604	LMN	CCL-CCJ-OBV-CBT
27	5	706	3PE	O21-C2-C3-O31
29	D	101	CDL	OA6-CA4-CA6-OA8
27	1	402	3PE	C23-C24-C25-C26
27	8	101	3PE	C23-C24-C25-C26
28	n	202	PC1	C3B-C3C-C3D-C3E
27	5	703	3PE	C22-C23-C24-C25
30	2	602	LMN	OAL-CBP-CCF-OBX
28	n	202	PC1	C3D-C3E-C3F-C3G
27	W	201	3PE	C22-C21-O21-C2
27	1	402	3PE	C11-O13-P-O11
27	4	606	3PE	C11-O13-P-O11
27	5	704	3PE	C11-O13-P-O11
27	5	706	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
28	1	403	PC1	C1-O11-P-O13
28	5	705	PC1	C1-O11-P-O13
28	n	202	PC1	C11-O13-P-O11
27	W	201	3PE	C2D-C2E-C2F-C2G
28	5	705	PC1	C31-C32-C33-C34
27	5	702	3PE	C32-C31-O31-C3
29	2	601	CDL	OB5-CB3-CB4-CB6
29	X	201	CDL	OA5-CA3-CA4-CA6
29	g	101	CDL	OB5-CB3-CB4-CB6
28	5	701	PC1	C28-C29-C2A-C2B
27	5	703	3PE	C25-C26-C27-C28
28	5	705	PC1	O22-C21-O21-C2
28	4	605	PC1	C2A-C2B-C2C-C2D
27	4	606	3PE	C22-C21-O21-C2
28	5	701	PC1	O32-C31-O31-C3
30	J	202	LMN	OAI-CBM-CCC-OBY
27	4	606	3PE	C1-C2-C3-O31
28	3	201	PC1	C1-C2-C3-O31
29	X	201	CDL	CA3-CA4-CA6-OA8
27	5	702	3PE	C32-C33-C34-C35
29	X	201	CDL	C13-C14-C15-C16
27	g	102	3PE	O21-C21-C22-C23
29	2	601	CDL	C32-C31-CA7-OA8
29	4	601	CDL	C12-C11-CA5-OA6
29	g	101	CDL	CB5-C51-C52-C53
29	X	201	CDL	OB9-CB7-OB8-CB6
27	4	603	3PE	C32-C33-C34-C35
29	4	601	CDL	C71-C72-C73-C74
27	5	704	3PE	C31-C32-C33-C34
27	n	203	3PE	C3A-C3B-C3C-C3D
30	2	602	LMN	C4-C5-C6-O6
28	4	605	PC1	C36-C37-C38-C39
27	1	402	3PE	O11-C1-C2-O21
27	g	103	3PE	C2B-C2C-C2D-C2E
30	2	602	LMN	O5-C5-C6-O6
27	5	702	3PE	O32-C31-O31-C3
29	D	101	CDL	C72-C71-CB7-OB8
31	Q	201	ZMP	O4-C17-C18-C19
27	4	602	3PE	C31-C32-C33-C34
27	5	703	3PE	O31-C31-C32-C33
27	g	102	3PE	C32-C33-C34-C35
28	n	202	PC1	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
29	g	101	CDL	CB2-C1-CA2-OA2
28	3	201	PC1	O22-C21-O21-C2
28	5	701	PC1	C22-C21-O21-C2
29	D	101	CDL	C71-CB7-OB8-CB6
27	1	401	3PE	C23-C24-C25-C26
30	4	604	LMN	CAY-CBA-CBC-CBE
27	4	602	3PE	C24-C25-C26-C27
27	4	602	3PE	O11-C1-C2-C3
27	8	101	3PE	O11-C1-C2-C3
28	4	605	PC1	O11-C1-C2-C3
28	5	705	PC1	O11-C1-C2-C3
29	2	601	CDL	C18-C19-C20-C21
29	4	601	CDL	CA7-C31-C32-C33
27	W	201	3PE	O22-C21-O21-C2
28	n	202	PC1	C32-C31-O31-C3
28	4	605	PC1	C2-C1-O11-P
27	5	703	3PE	C24-C25-C26-C27
30	4	604	LMN	CCF-CCQ-OCB-CCS
27	4	603	3PE	C1-C2-C3-O31
27	5	703	3PE	C1-C2-C3-O31
27	n	201	3PE	C1-C2-C3-O31
29	D	101	CDL	CA3-CA4-CA6-OA8
27	4	603	3PE	C22-C23-C24-C25
29	g	101	CDL	C16-C17-C18-C19
28	4	605	PC1	C32-C33-C34-C35
28	4	605	PC1	C11-C12-N-C15
27	5	706	3PE	C11-O13-P-O11
30	2	602	LMN	CBE-CBG-CBI-CBK
27	8	101	3PE	O11-C1-C2-O21
29	g	101	CDL	OB5-CB3-CB4-OB6
27	5	703	3PE	C29-C2A-C2B-C2C
27	J	201	3PE	O21-C2-C3-O31
28	1	403	PC1	O31-C31-C32-C33
27	4	606	3PE	O22-C21-O21-C2
28	5	701	PC1	O22-C21-O21-C2
28	2	603	PC1	C2-C1-O11-P
29	2	601	CDL	C1-CB2-OB2-PB2
29	D	101	CDL	C1-CA2-OA2-PA1
31	Q	201	ZMP	N1-C13-C14-C15
27	5	702	3PE	C36-C37-C38-C39
27	g	102	3PE	C22-C21-O21-C2
27	g	103	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
27	4	603	3PE	O11-C1-C2-C3
27	W	201	3PE	O11-C1-C2-C3
30	J	202	LMN	C3-C4-O4-CCR
27	n	203	3PE	C32-C33-C34-C35
28	n	202	PC1	C21-C22-C23-C24
27	8	101	3PE	C33-C34-C35-C36
28	4	605	PC1	C27-C28-C29-C2A
28	5	701	PC1	C36-C37-C38-C39
28	5	701	PC1	C25-C26-C27-C28
27	J	201	3PE	C1-C2-C3-O31
27	n	201	3PE	C2-C1-O11-P
27	n	203	3PE	C2-C1-O11-P
28	1	403	PC1	C1-C2-C3-O31
29	4	601	CDL	CA3-CA4-CA6-OA8
27	4	602	3PE	O11-C1-C2-O21
27	4	603	3PE	O11-C1-C2-O21
27	4	606	3PE	O11-C1-C2-O21
27	g	102	3PE	O11-C1-C2-O21
29	2	601	CDL	OB5-CB3-CB4-OB6
28	3	201	PC1	C24-C25-C26-C27
31	Q	201	ZMP	O2-C13-C14-C15
28	n	202	PC1	O32-C31-O31-C3
29	D	101	CDL	OB9-CB7-OB8-CB6
30	J	202	LMN	C5-C4-O4-CCR
27	4	603	3PE	O21-C2-C3-O31
27	5	703	3PE	O21-C2-C3-O31
28	1	403	PC1	O21-C2-C3-O31
28	5	705	PC1	O21-C2-C3-O31
29	X	201	CDL	OA6-CA4-CA6-OA8
28	4	605	PC1	C11-C12-N-C13
30	2	602	LMN	OBV-CBT-CCM-CBR
28	5	701	PC1	C2E-C2F-C2G-C2H
28	1	403	PC1	C32-C31-O31-C3
27	5	702	3PE	C11-O13-P-O11
27	5	703	3PE	C1-O11-P-O13
27	n	201	3PE	C1-O11-P-O13
28	1	403	PC1	C11-O13-P-O11
28	2	603	PC1	C11-O13-P-O11
28	5	701	PC1	C11-O13-P-O11
29	4	601	CDL	CA3-OA5-PA1-OA2
29	X	201	CDL	CA2-OA2-PA1-OA5
27	1	401	3PE	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
28	4	605	PC1	C22-C23-C24-C25
27	1	402	3PE	C11-O13-P-O12
27	4	602	3PE	C1-O11-P-O14
27	5	704	3PE	C11-O13-P-O12
27	5	706	3PE	C1-O11-P-O14
27	J	201	3PE	C1-O11-P-O12
27	J	201	3PE	C1-O11-P-O14
27	J	201	3PE	C11-O13-P-O12
27	J	201	3PE	C11-O13-P-O14
27	W	201	3PE	C11-O13-P-O12
27	g	103	3PE	C11-O13-P-O14
27	n	201	3PE	C1-O11-P-O14
28	4	605	PC1	C11-O13-P-O12
28	5	705	PC1	C1-O11-P-O12
28	n	202	PC1	C11-O13-P-O14
29	2	601	CDL	CA3-OA5-PA1-OA3
29	g	101	CDL	CA2-OA2-PA1-OA4
28	2	603	PC1	C21-C22-C23-C24
29	2	601	CDL	CB7-C71-C72-C73
27	1	402	3PE	O11-C1-C2-C3
27	4	606	3PE	O11-C1-C2-C3
28	3	201	PC1	O11-C1-C2-C3
29	X	201	CDL	C38-C39-C40-C41
27	1	401	3PE	C24-C25-C26-C27
27	5	702	3PE	C12-C11-O13-P
27	8	101	3PE	C12-C11-O13-P
27	J	201	3PE	C12-C11-O13-P
28	5	701	PC1	C12-C11-O13-P
29	4	601	CDL	C74-C75-C76-C77
27	g	102	3PE	C37-C38-C39-C3A
27	g	102	3PE	C3C-C3D-C3E-C3F
27	g	102	3PE	O22-C21-O21-C2
30	J	202	LMN	CCW-CCS-OCB-CCQ
28	3	201	PC1	O11-C1-C2-O21
28	4	605	PC1	O11-C1-C2-O21
29	4	601	CDL	OA5-CA3-CA4-OA6
30	2	602	LMN	CBK-CBQ-CCM-CBS
28	2	603	PC1	O13-C11-C12-N
28	5	705	PC1	C1-C2-C3-O31
28	n	202	PC1	O13-C11-C12-N
28	5	701	PC1	O21-C2-C3-O31
30	J	202	LMN	OBZ-CCS-OCB-CCQ

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Mol	Chain	Res	Type	Atoms
29	D	101	CDL	C13-C14-C15-C16
28	1	403	PC1	O32-C31-O31-C3
29	2	601	CDL	C24-C25-C26-C27
28	4	605	PC1	C11-C12-N-C14
29	4	601	CDL	C12-C13-C14-C15
29	X	201	CDL	C74-C75-C76-C77
29	D	101	CDL	CB6-CB4-OB6-CB5
30	J	202	LMN	OBY-CCR-O4-C4
29	D	101	CDL	CB4-CB3-OB5-PB2
27	8	101	3PE	C32-C33-C34-C35
29	X	201	CDL	C72-C73-C74-C75
30	J	202	LMN	CCV-CCR-O4-C4
27	1	401	3PE	C1-O11-P-O13
27	g	102	3PE	C1-O11-P-O13
27	g	102	3PE	C11-O13-P-O11
27	g	103	3PE	C1-O11-P-O13
27	n	201	3PE	C11-O13-P-O11
28	3	201	PC1	C11-O13-P-O11
28	4	605	PC1	C11-O13-P-O11
28	4	605	PC1	C1-O11-P-O13
29	2	601	CDL	CB2-OB2-PB2-OB5
29	4	601	CDL	CB2-OB2-PB2-OB5
29	g	101	CDL	CB2-OB2-PB2-OB5
27	n	203	3PE	C3B-C3C-C3D-C3E
29	D	101	CDL	C12-C13-C14-C15
30	J	202	LMN	CAA-CAW-CAY-CBA
29	4	601	CDL	C12-C11-CA5-OA7
29	X	201	CDL	CB4-CB6-OB8-CB7
27	5	704	3PE	C2B-C2C-C2D-C2E
28	n	202	PC1	O31-C31-C32-C33
29	4	601	CDL	C34-C35-C36-C37
27	g	103	3PE	C29-C2A-C2B-C2C
28	n	202	PC1	C39-C3A-C3B-C3C
27	g	102	3PE	O22-C21-C22-C23
29	X	201	CDL	C54-C55-C56-C57
28	5	701	PC1	C23-C24-C25-C26
31	Q	201	ZMP	C11-C12-N1-C13
28	5	705	PC1	C27-C28-C29-C2A
27	5	702	3PE	C3A-C3B-C3C-C3D
29	X	201	CDL	CB6-CB4-OB6-CB5
29	g	101	CDL	C32-C31-CA7-OA8
29	2	601	CDL	C32-C31-CA7-OA9

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Mol	Chain	Res	Type	Atoms
27	5	702	3PE	C39-C3A-C3B-C3C
27	n	203	3PE	C34-C35-C36-C37
28	1	403	PC1	C34-C35-C36-C37
27	n	203	3PE	C3C-C3D-C3E-C3F
30	J	202	LMN	CBB-CBD-CBF-CBH
31	Q	201	ZMP	C12-C11-S1-C10
27	W	201	3PE	O21-C2-C3-O31
29	g	101	CDL	OA6-CA4-CA6-OA8
27	n	201	3PE	C32-C31-O31-C3
29	D	101	CDL	CB4-CB6-OB8-CB7
28	n	202	PC1	C2D-C2E-C2F-C2G
27	n	201	3PE	C32-C33-C34-C35
27	1	401	3PE	C2C-C2D-C2E-C2F
27	5	704	3PE	C2D-C2E-C2F-C2G
27	5	704	3PE	C26-C27-C28-C29
28	4	605	PC1	C26-C27-C28-C29
27	8	101	3PE	C2-C1-O11-P
30	2	602	LMN	CBK-CBQ-CCM-CBT
29	D	101	CDL	C72-C71-CB7-OB9
27	n	201	3PE	O32-C31-O31-C3
29	2	601	CDL	CA7-C31-C32-C33
28	1	403	PC1	C33-C34-C35-C36
27	W	201	3PE	C26-C27-C28-C29
27	5	703	3PE	O32-C31-C32-C33
28	4	605	PC1	C2B-C2C-C2D-C2E
29	D	101	CDL	CA3-OA5-PA1-OA2
29	g	101	CDL	C32-C31-CA7-OA9
29	g	101	CDL	CA3-CA4-OA6-CA5
29	2	601	CDL	C17-C18-C19-C20
29	2	601	CDL	C77-C78-C79-C80
30	2	602	LMN	CCF-CCQ-OCB-CCS
27	n	201	3PE	C33-C34-C35-C36
28	1	403	PC1	O32-C31-C32-C33
27	5	702	3PE	C34-C35-C36-C37
27	g	102	3PE	O11-C1-C2-C3
29	4	601	CDL	OA5-CA3-CA4-CA6
30	2	602	LMN	OBV-CBT-CCM-CBQ
30	4	604	LMN	O1-CBS-CCM-CBQ
30	4	604	LMN	O1-CBS-CCM-CBR
30	J	202	LMN	O1-CBS-CCM-CBR
31	Q	201	ZMP	O4-C17-C18-C20
28	4	605	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
27	J	201	3PE	O31-C31-C32-C33
30	2	602	LMN	CCH-CCQ-OCB-CCS
27	g	103	3PE	C22-C21-O21-C2
29	X	201	CDL	C33-C34-C35-C36
29	X	201	CDL	C73-C74-C75-C76
30	2	602	LMN	CBC-CBE-CBG-CBI
29	2	601	CDL	C14-C15-C16-C17
27	W	201	3PE	C1-C2-C3-O31
28	5	701	PC1	C1-C2-C3-O31
27	5	704	3PE	C32-C33-C34-C35
29	4	601	CDL	CB4-CB3-OB5-PB2
29	X	201	CDL	C14-C15-C16-C17
27	1	401	3PE	C1-O11-P-O14
27	1	401	3PE	C11-O13-P-O14
27	5	703	3PE	C11-O13-P-O12
27	g	102	3PE	C11-O13-P-O14
27	n	201	3PE	C11-O13-P-O14
28	3	201	PC1	C11-O13-P-O14
28	4	605	PC1	C1-O11-P-O14
28	5	701	PC1	C11-C12-N-C15
28	n	202	PC1	C11-O13-P-O12
29	D	101	CDL	CA3-OA5-PA1-OA3
29	g	101	CDL	CB2-OB2-PB2-OB3
27	J	201	3PE	O32-C31-C32-C33
28	n	202	PC1	O11-C1-C2-C3
30	4	604	LMN	CAA-CAW-CAY-CBA
28	4	605	PC1	O22-C21-C22-C23
30	2	602	LMN	CAW-CAY-CBA-CBC
28	5	701	PC1	C27-C28-C29-C2A
27	4	603	3PE	C12-C11-O13-P
27	5	703	3PE	C12-C11-O13-P
27	5	704	3PE	C12-C11-O13-P
27	n	201	3PE	C12-C11-O13-P
28	3	201	PC1	C34-C35-C36-C37
27	5	704	3PE	O21-C21-C22-C23
27	4	603	3PE	O21-C21-C22-C23
29	2	601	CDL	C52-C51-CB5-OB6
29	4	601	CDL	C72-C71-CB7-OB8
31	Q	201	ZMP	C16-C17-C18-C21
31	Q	201	ZMP	C22-C23-C24-C25
27	1	401	3PE	O21-C21-C22-C23
27	8	101	3PE	O21-C21-C22-C23

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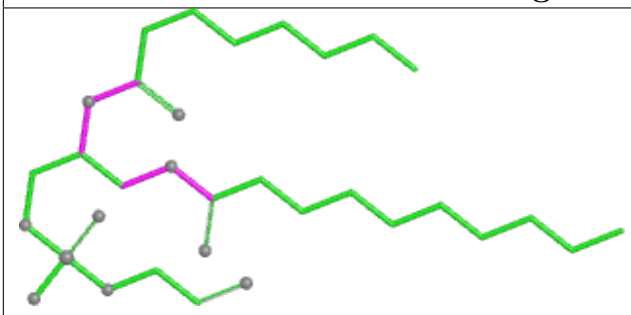
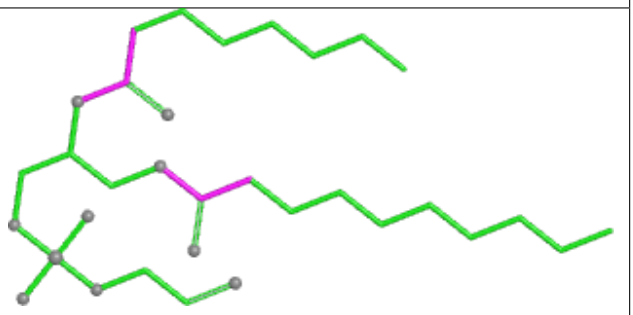
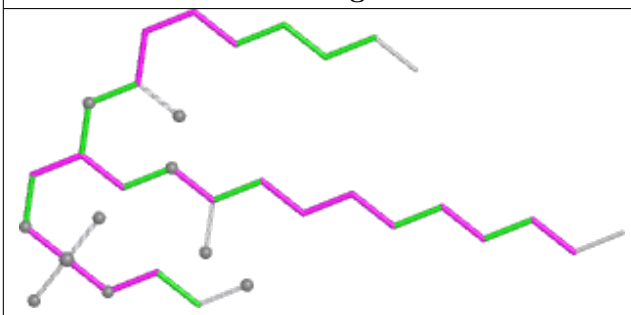
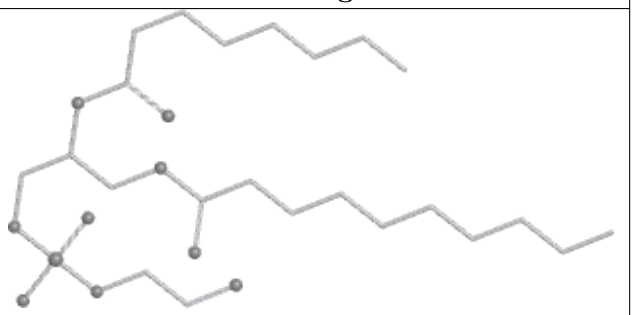
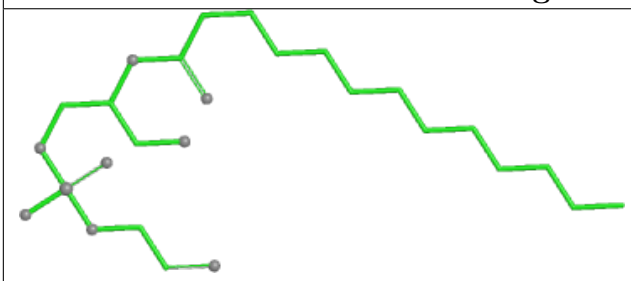
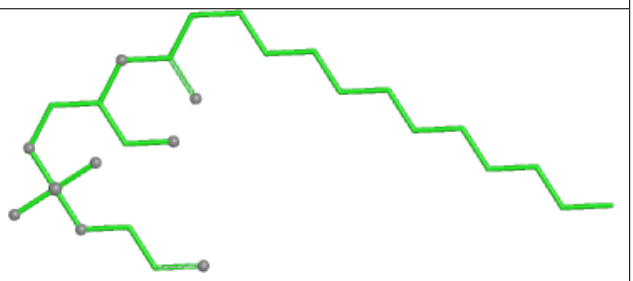
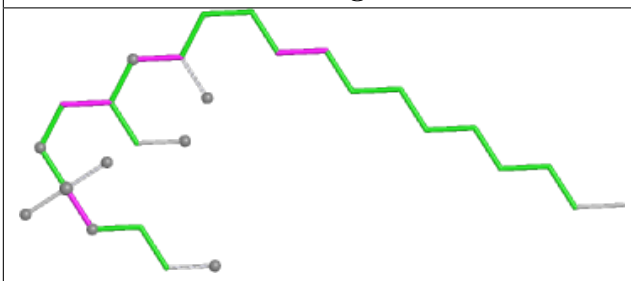
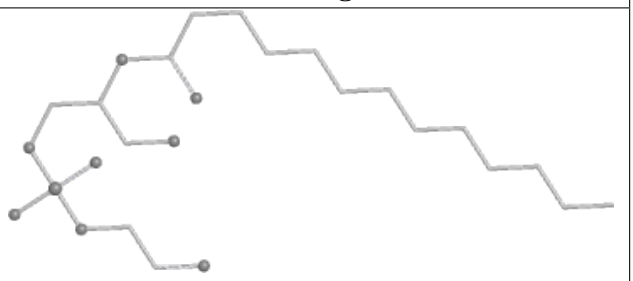
Mol	Chain	Res	Type	Atoms
29	D	101	CDL	C52-C51-CB5-OB6
27	4	603	3PE	C37-C38-C39-C3A
29	X	201	CDL	C37-C38-C39-C40
29	4	601	CDL	CB5-C51-C52-C53
27	1	401	3PE	O22-C21-C22-C23
27	5	704	3PE	O22-C21-C22-C23
29	D	101	CDL	C52-C51-CB5-OB7
28	4	605	PC1	C38-C39-C3A-C3B
29	4	601	CDL	C32-C31-CA7-OA8
27	4	603	3PE	O22-C21-C22-C23
27	8	101	3PE	O22-C21-C22-C23
29	4	601	CDL	C72-C71-CB7-OB9
29	2	601	CDL	C12-C11-CA5-OA6
29	X	201	CDL	C52-C51-CB5-OB6

There are no ring outliers.

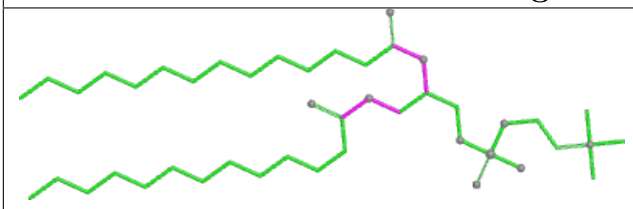
No monomer is involved in short contacts.

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

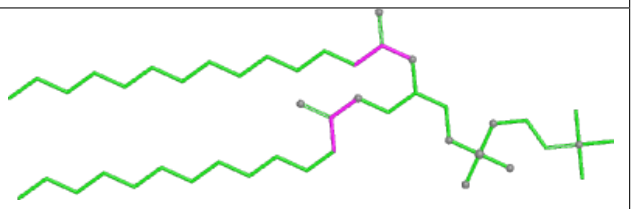
Ligand 3PE 4 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE 1 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 4 605



Bond lengths



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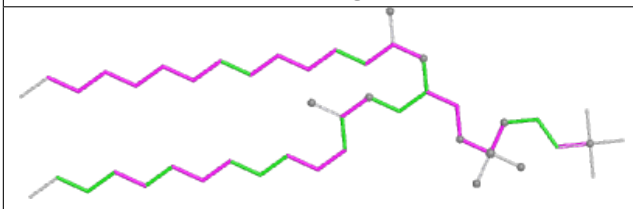

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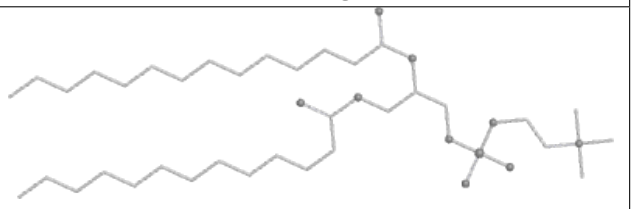
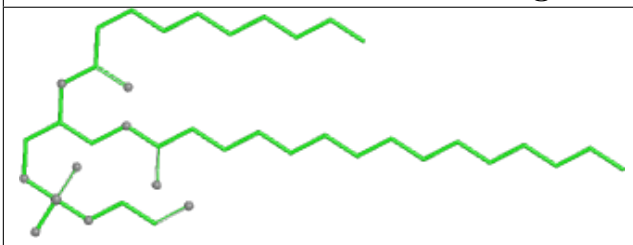


Rings

Ligand 3PE 5 702



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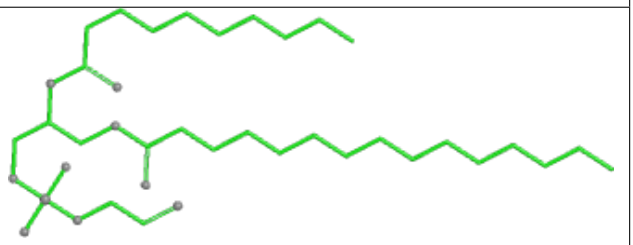

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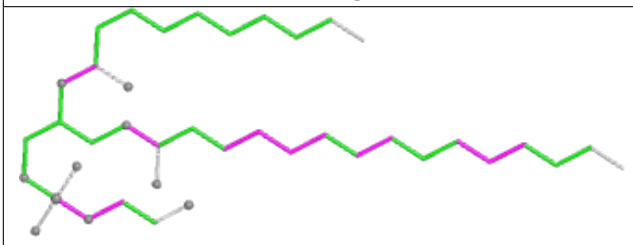

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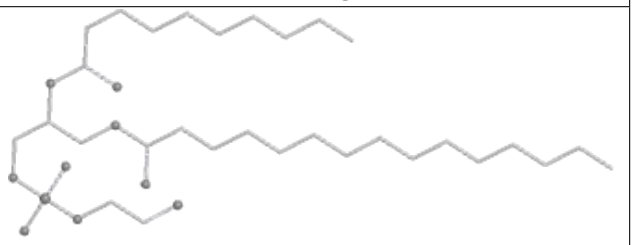
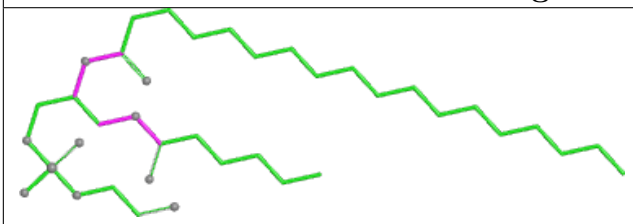


Rings

Ligand 3PE n 201



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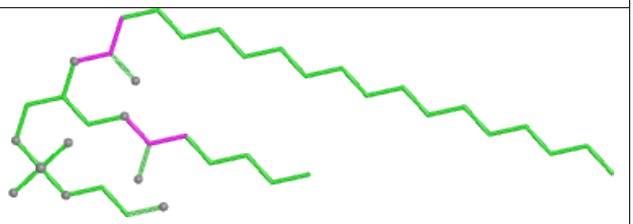

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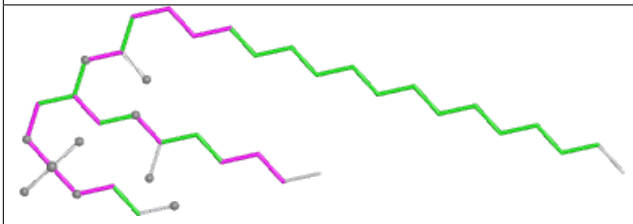

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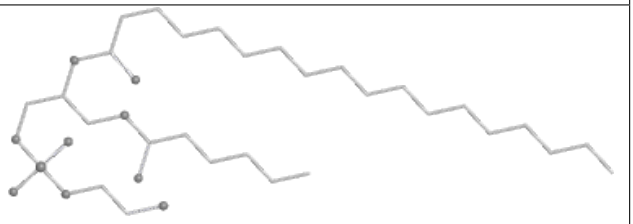
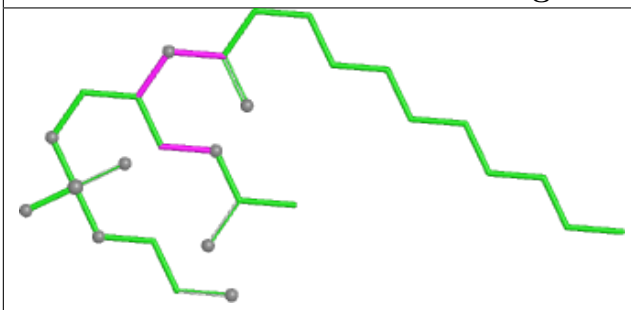


Rings

Ligand 3PE 5 706



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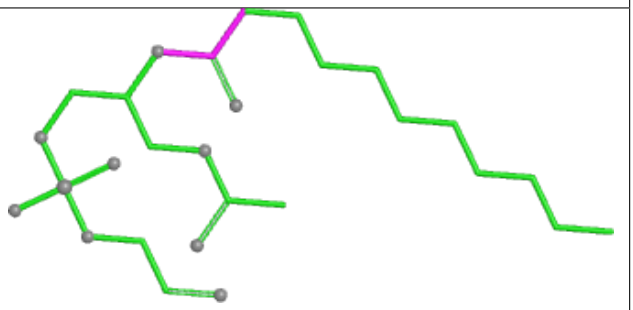

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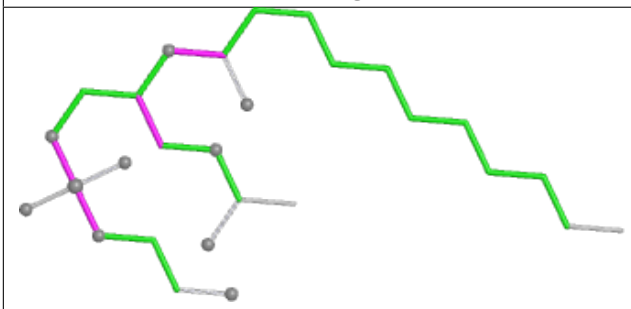

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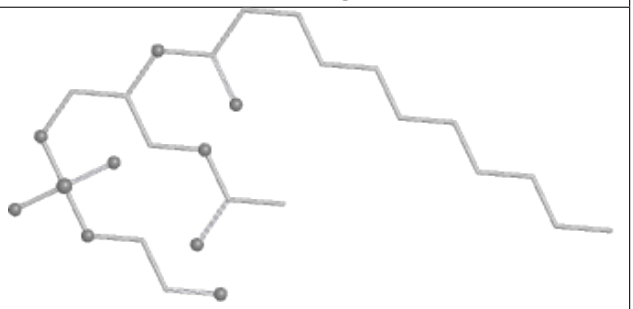
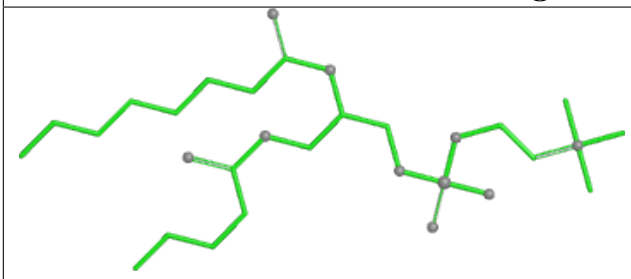


Rings

Ligand PC1 2 603



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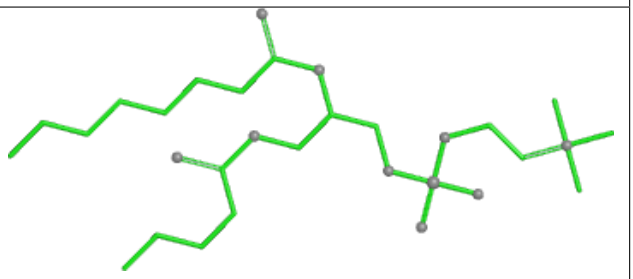

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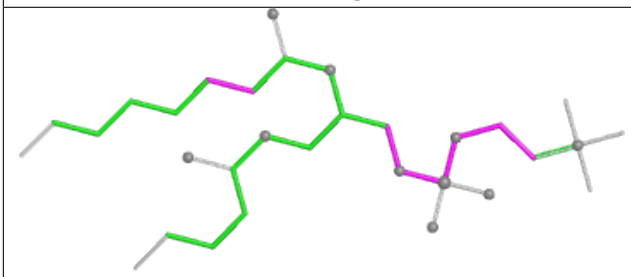

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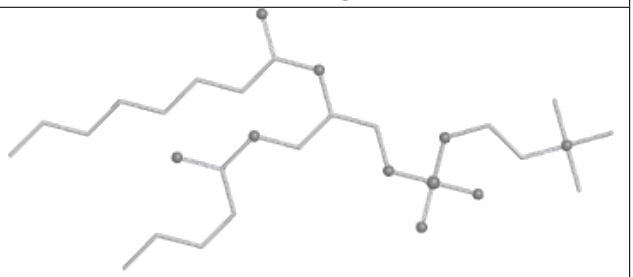
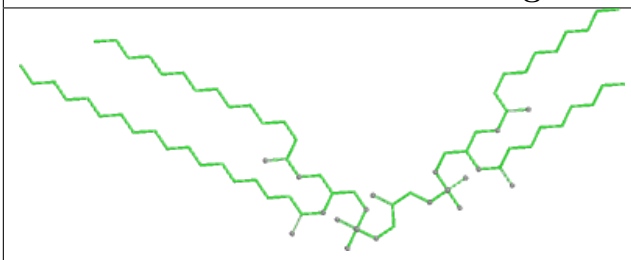


Rings

Ligand CDL X 201



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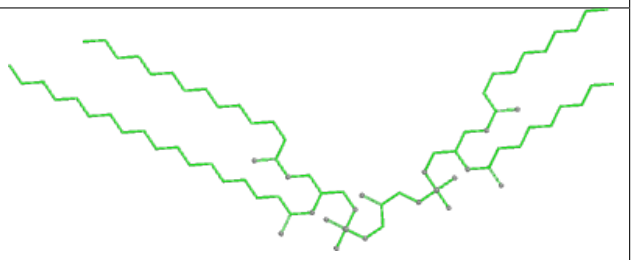

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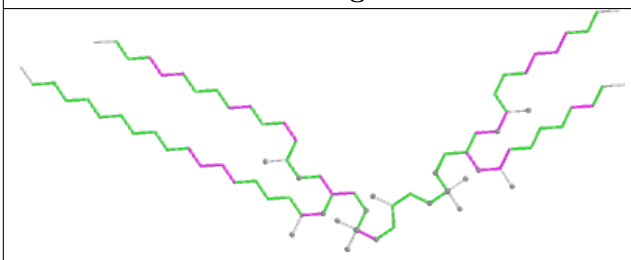

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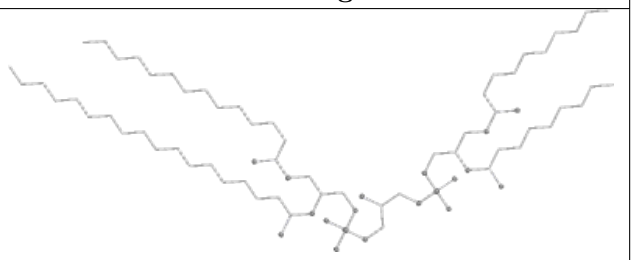
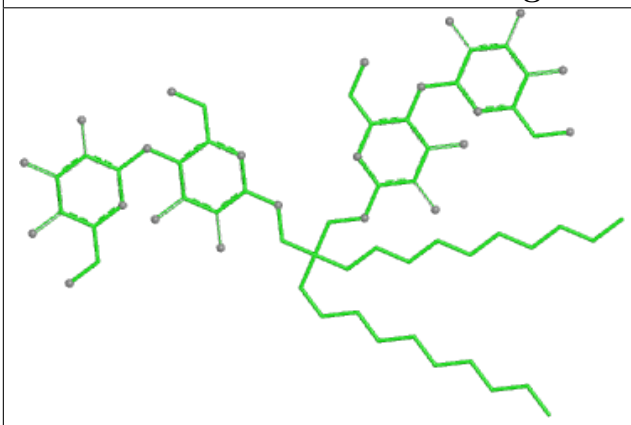


Rings

Ligand LMN J 202



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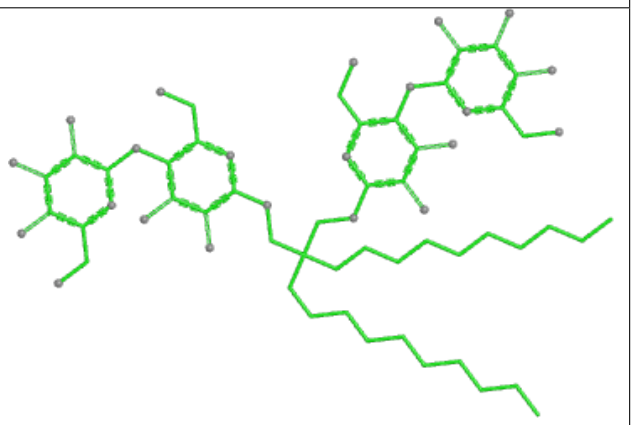

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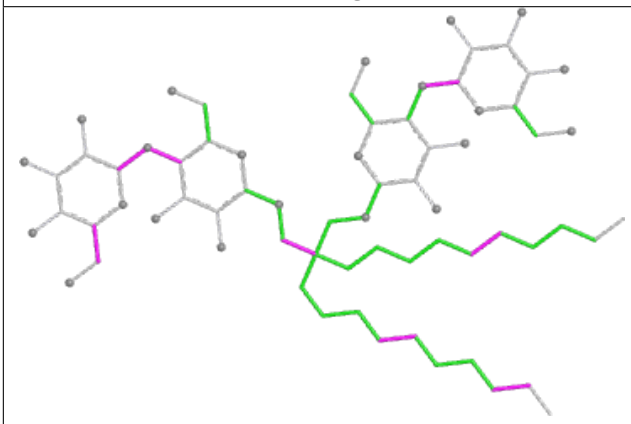

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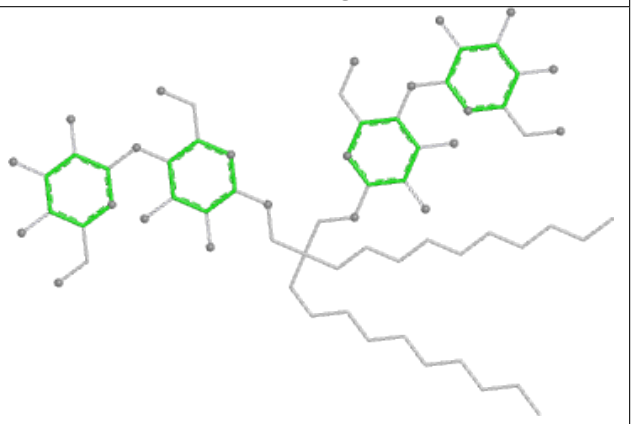
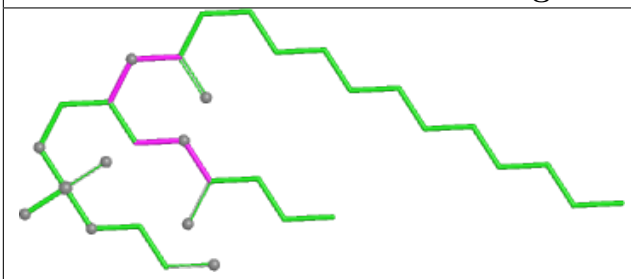
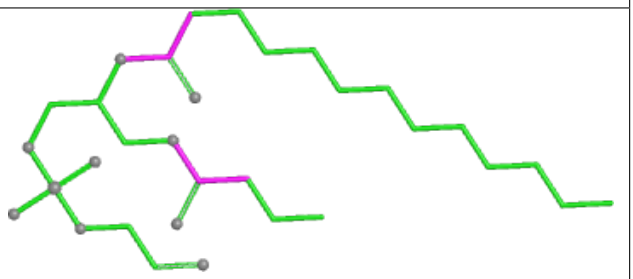
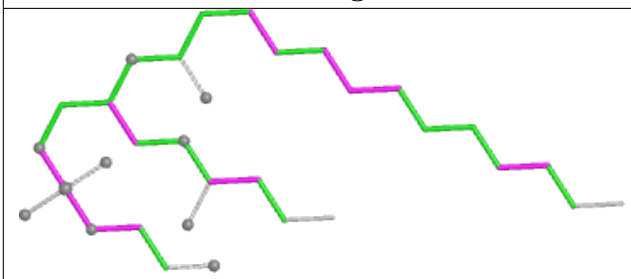
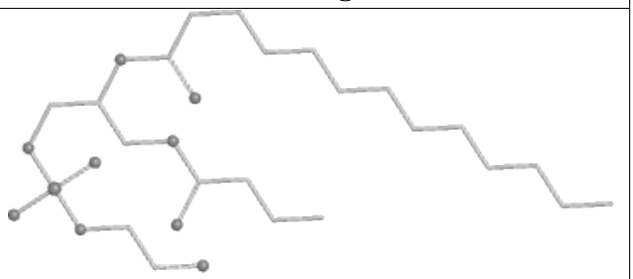


Rings

Ligand 3PE 5 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

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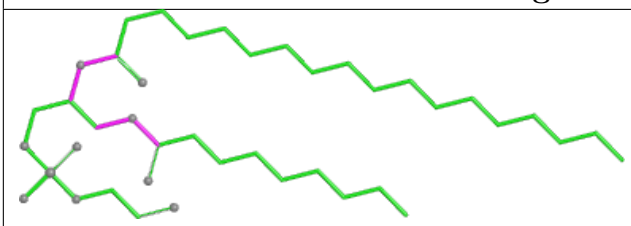
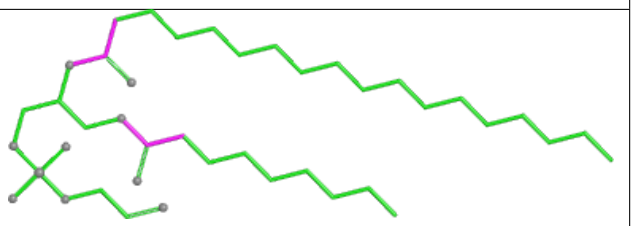
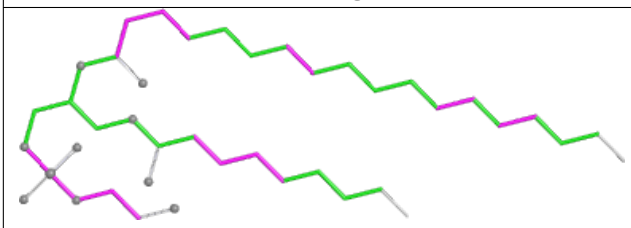
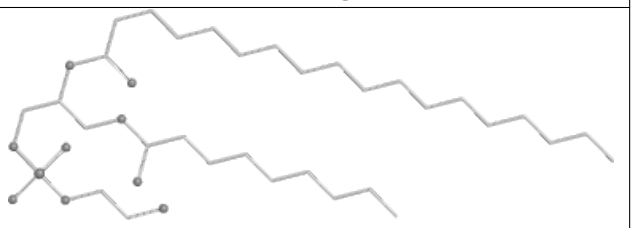
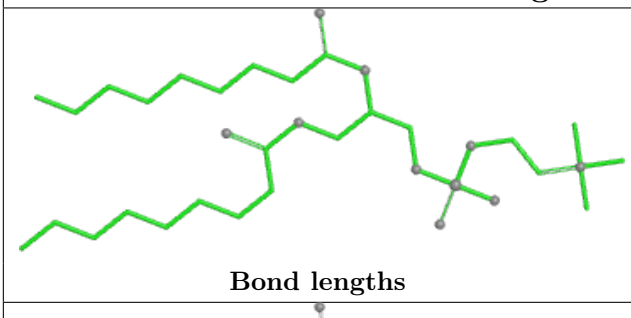
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 3 201



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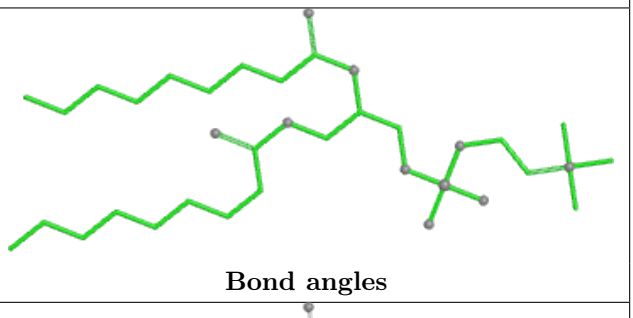
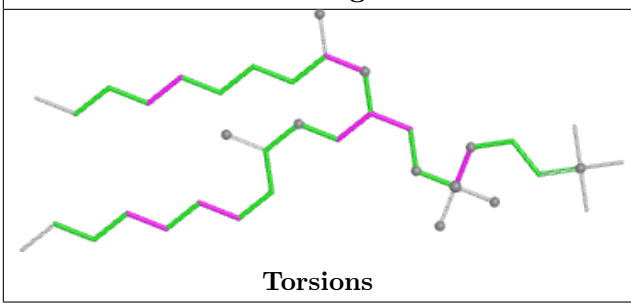
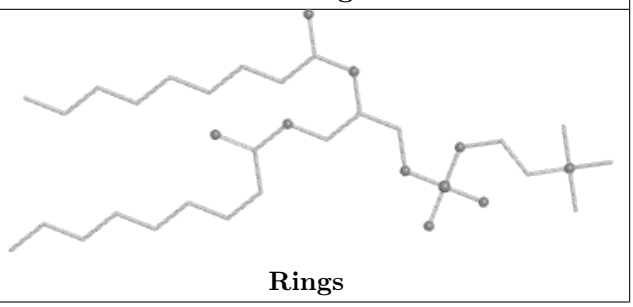


Bond angles

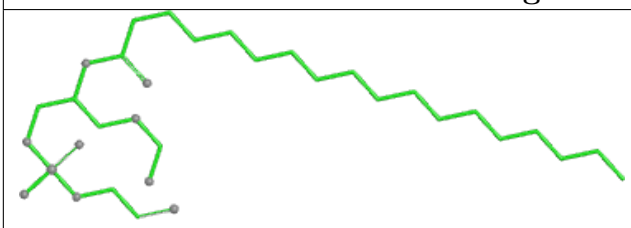


Torsions



Rings

Ligand 3PE W 201



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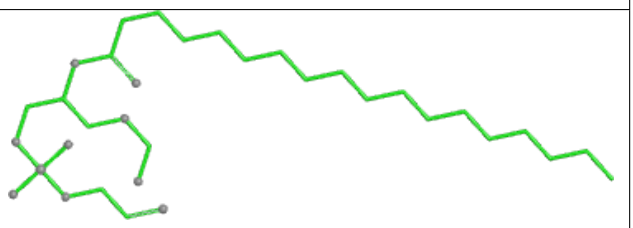

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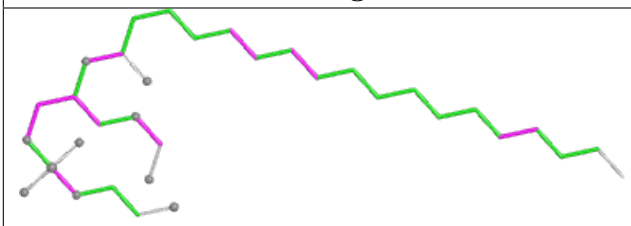

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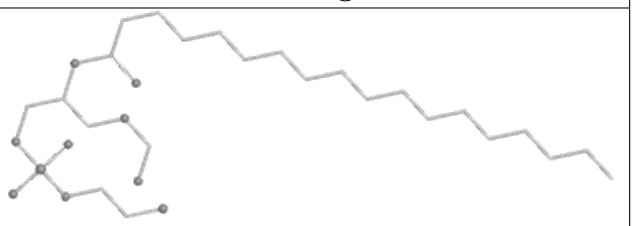
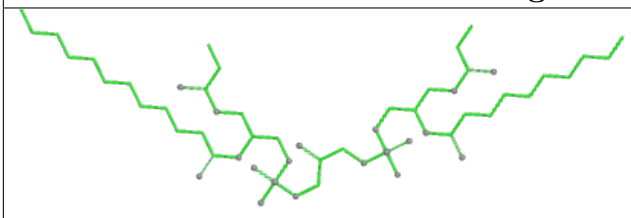


Rings

Ligand CDL g 101



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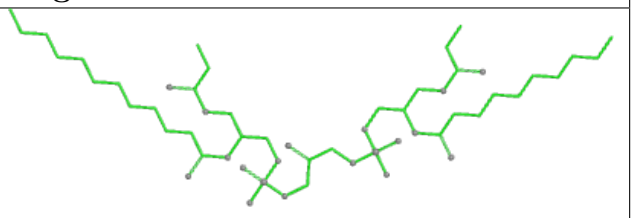

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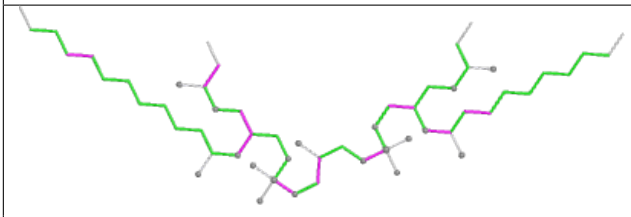

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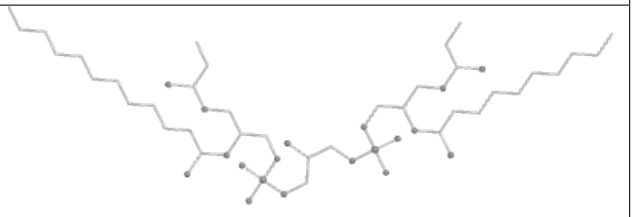
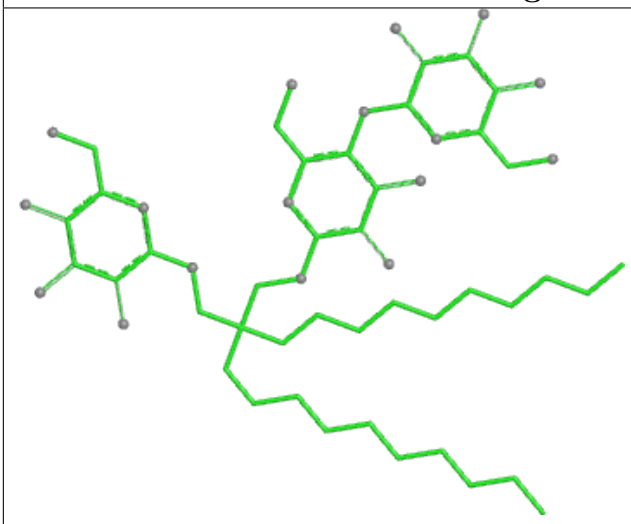
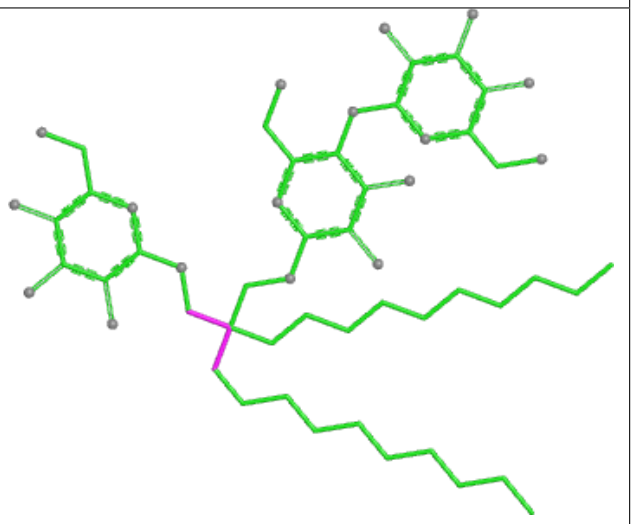
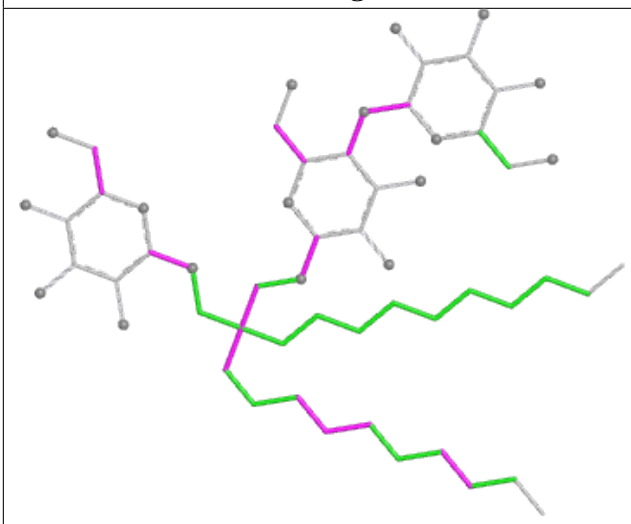
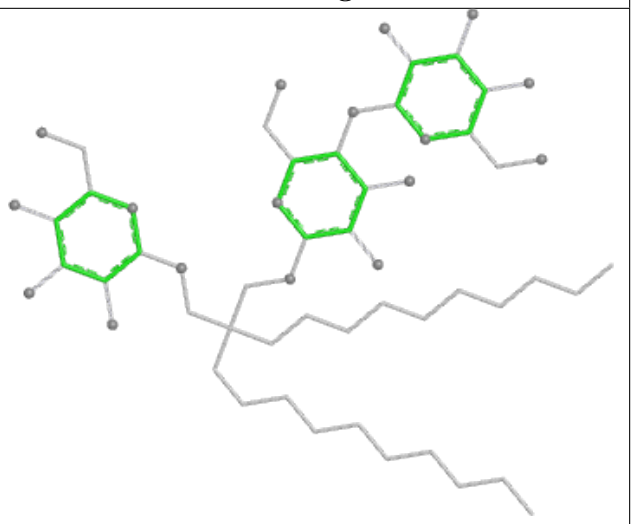
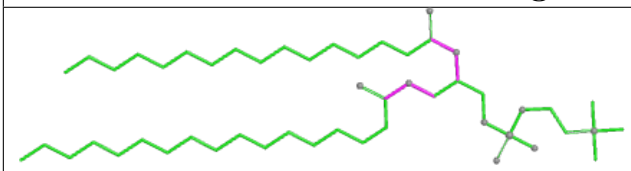
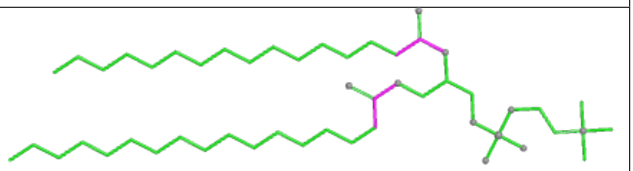
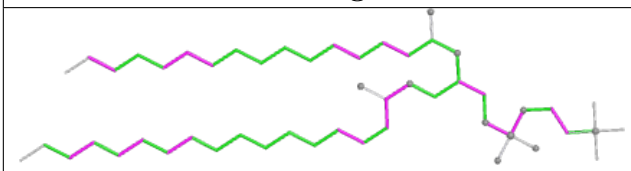
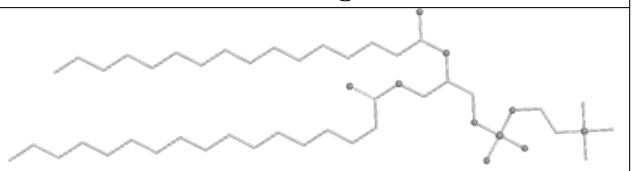
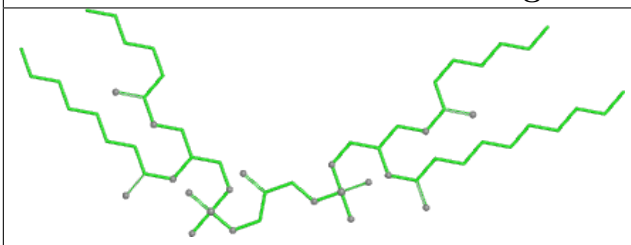
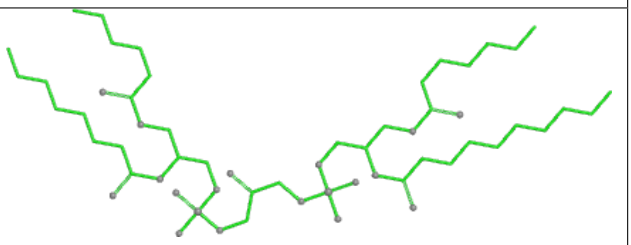
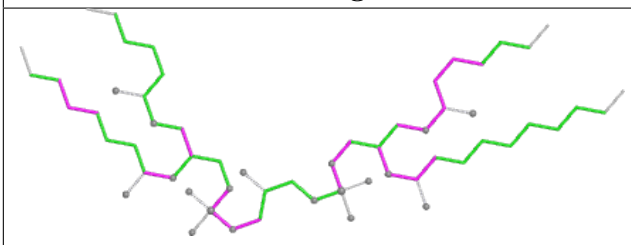
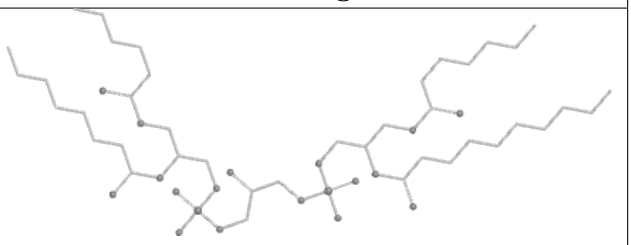
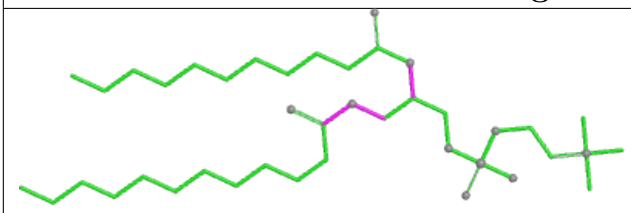
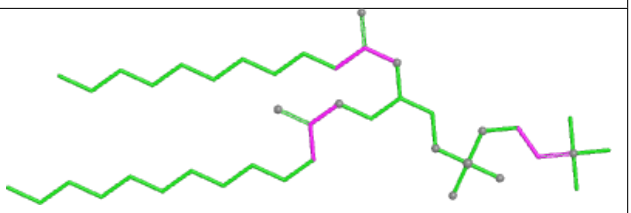
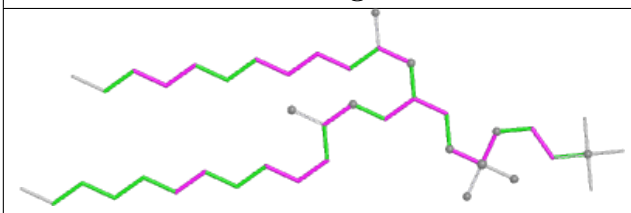
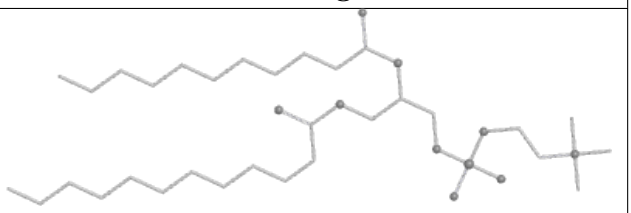


Rings

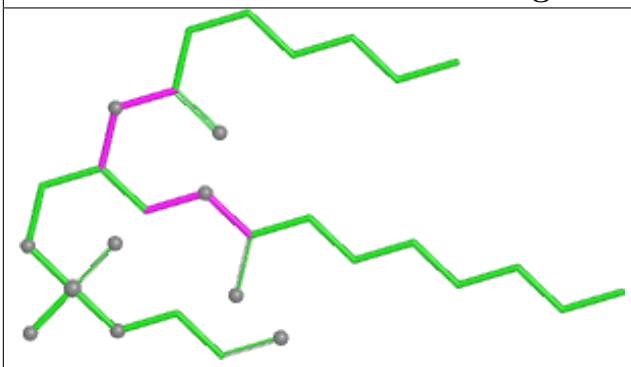
Ligand LMN 2 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 n 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

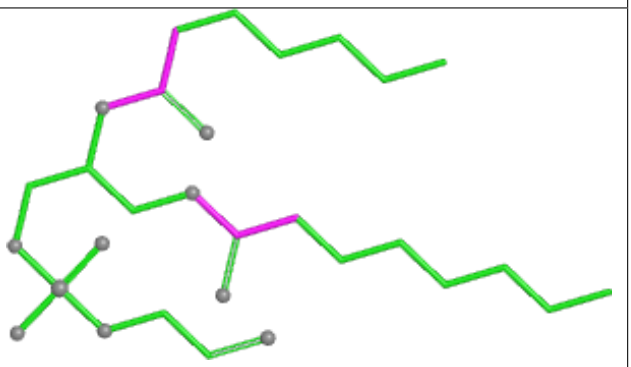
Ligand CDL D 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 5 705	
 Bond lengths	 Bond angles
 Torsions	 Rings

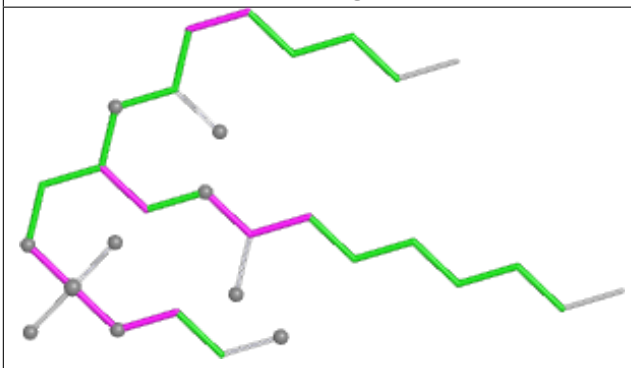
Ligand 3PE J 201



Bond lengths



Bond angles



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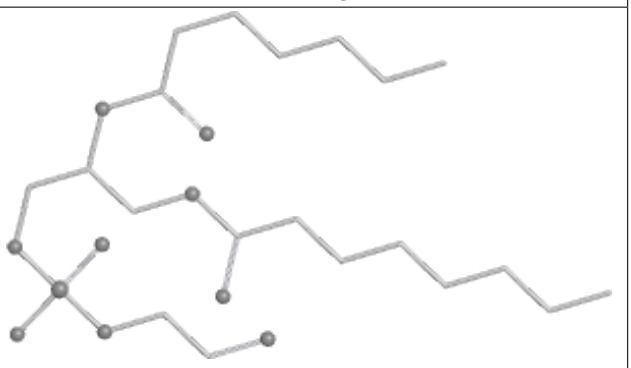
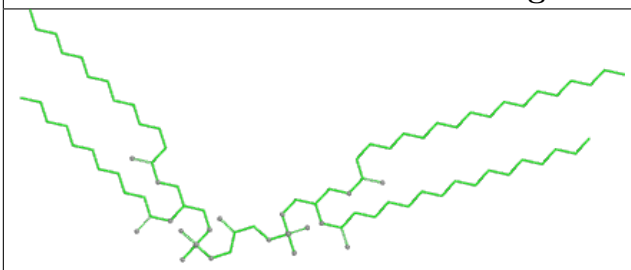
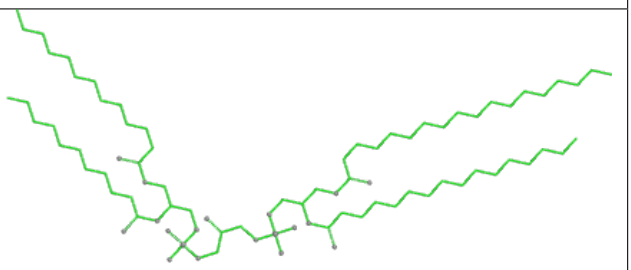


Rings

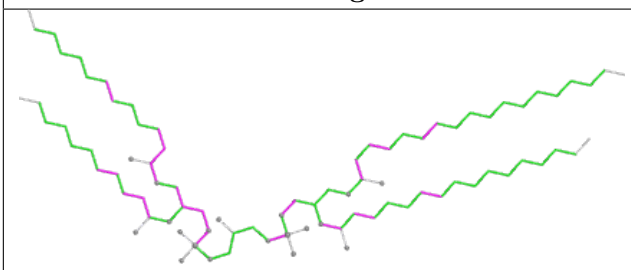
Ligand CDL 4 601



Bond lengths



Bond angles



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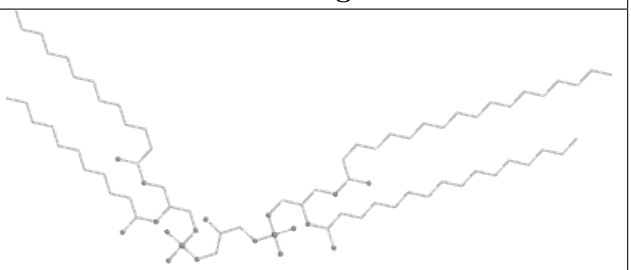
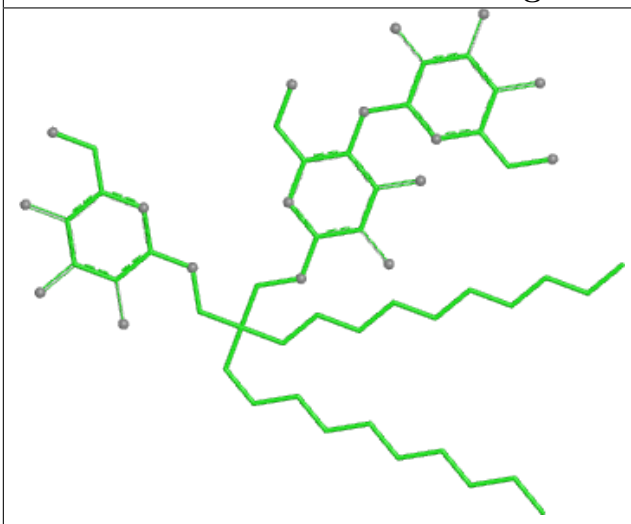


Rings

Ligand LMN 4 604



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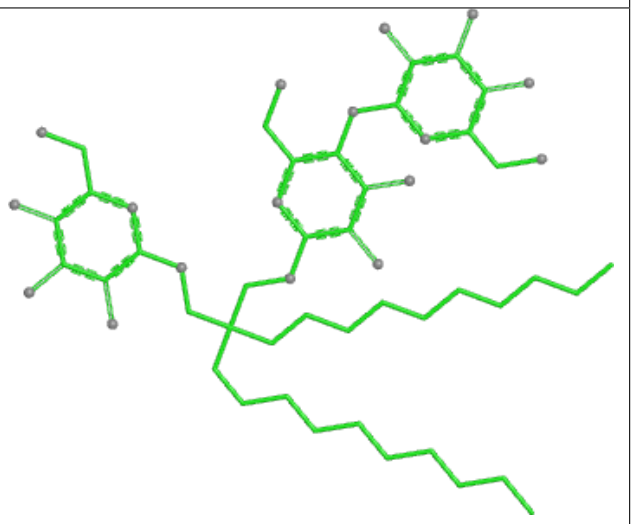

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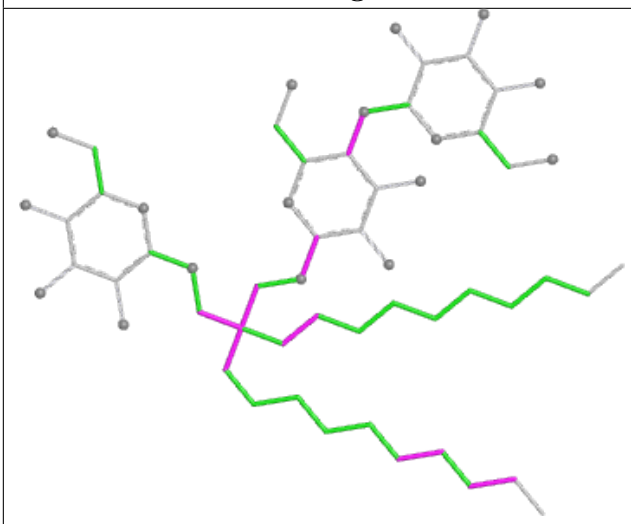

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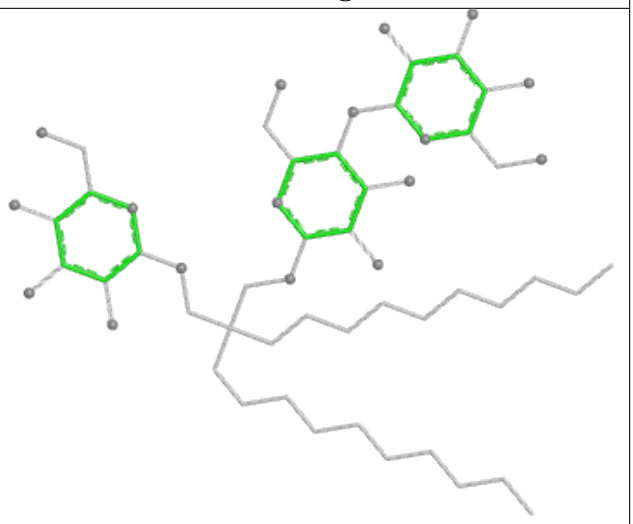
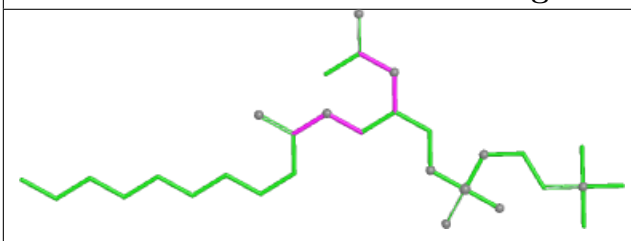


Rings

Ligand PC1 1 403



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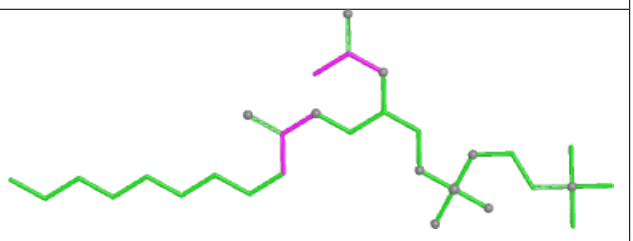

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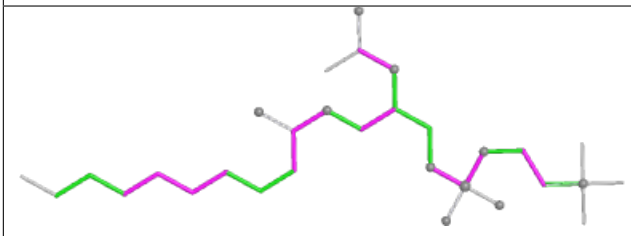

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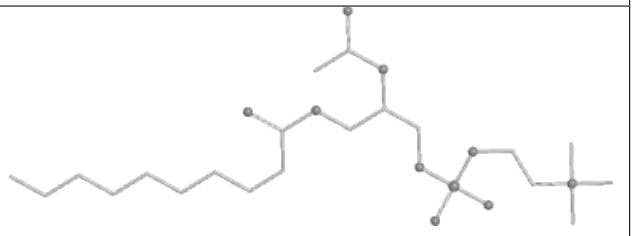
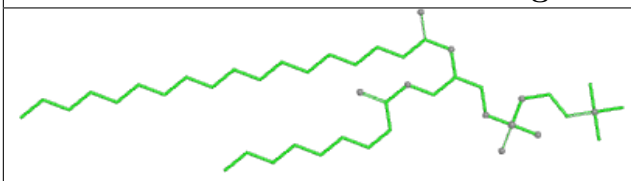


Rings

Ligand PC1 5 701



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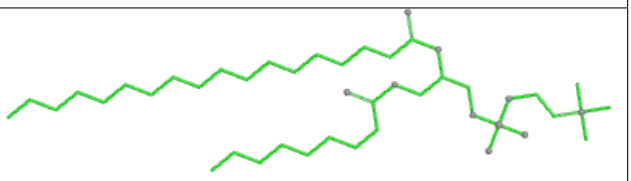
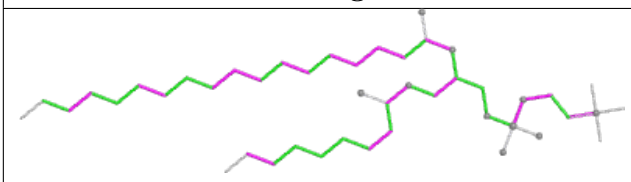


Bond angles



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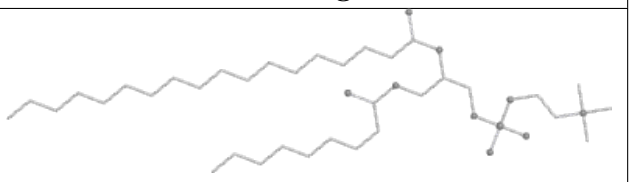
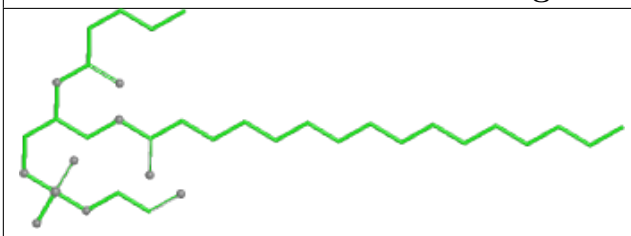


Rings

Ligand 3PE g 102



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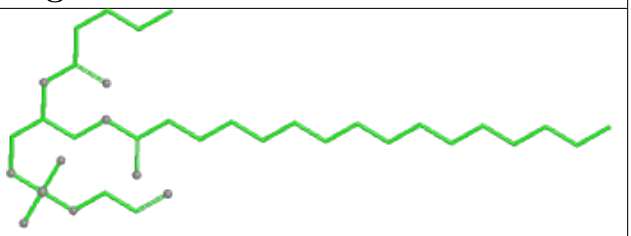
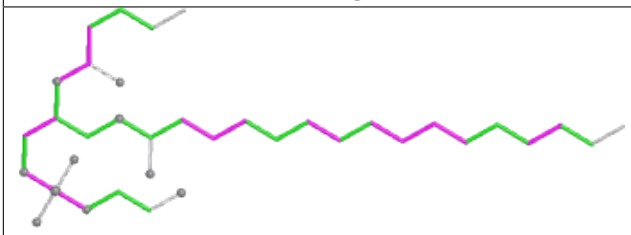


Bond angles



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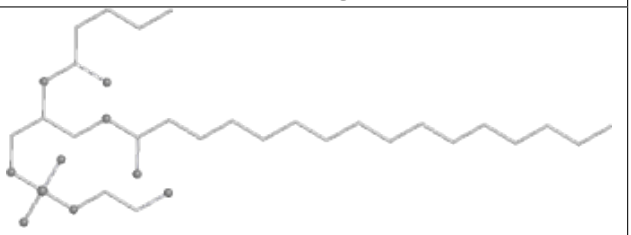
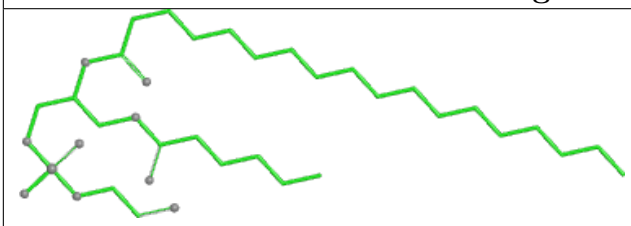
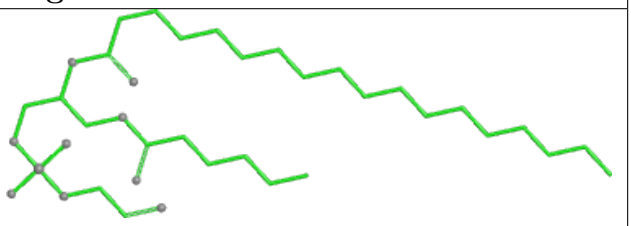


Rings

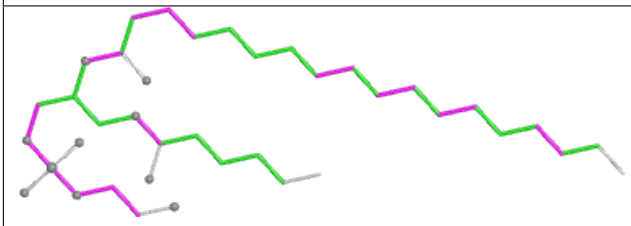
Ligand 3PE g 103



Bond lengths



Bond angles



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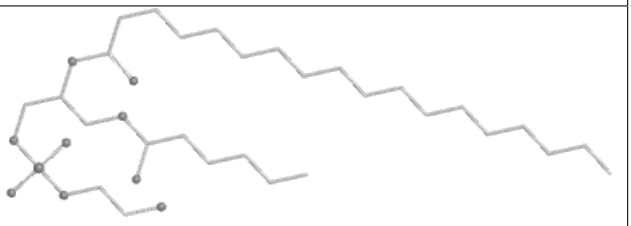
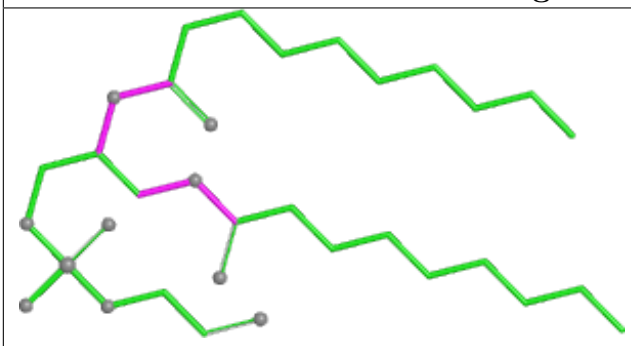
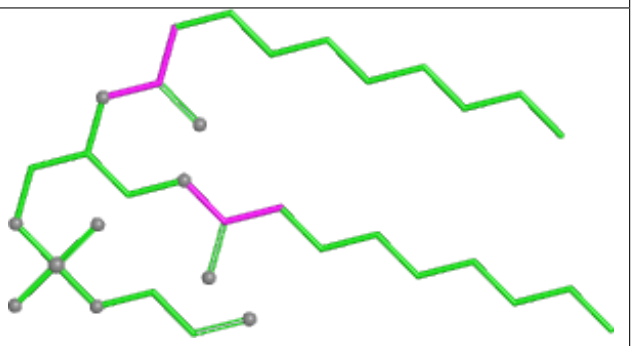


Rings

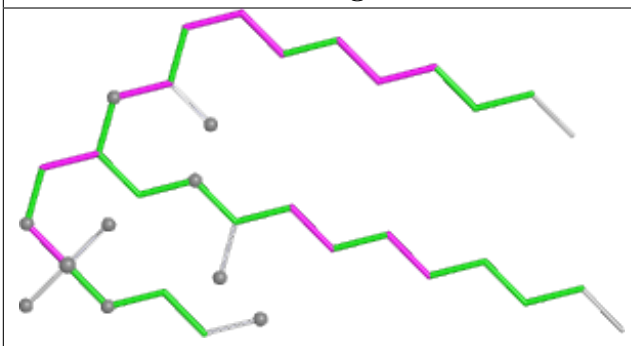
Ligand 3PE 4 602



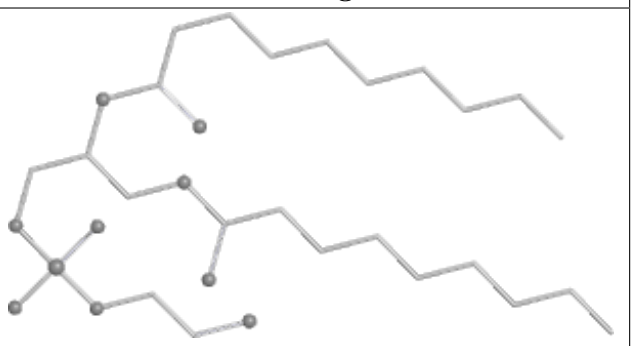
Bond lengths



Bond angles

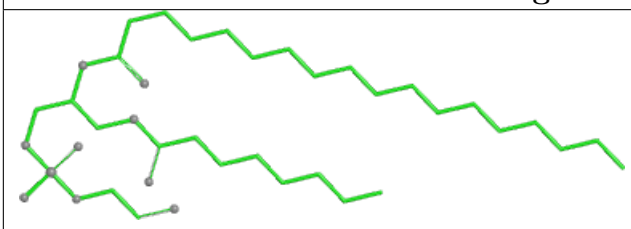


Torsions

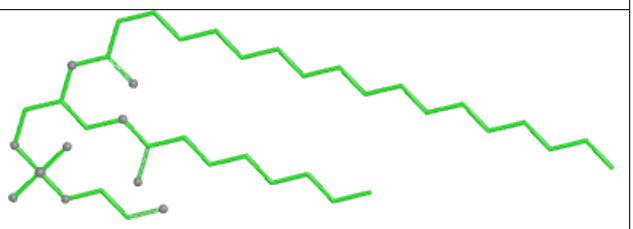


Rings

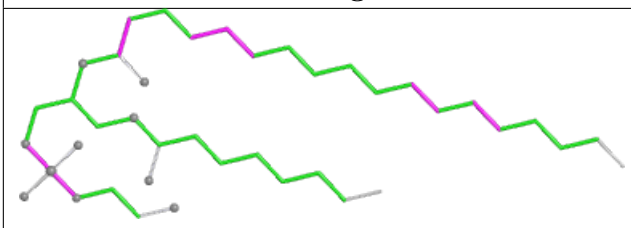
Ligand 3PE 1 401



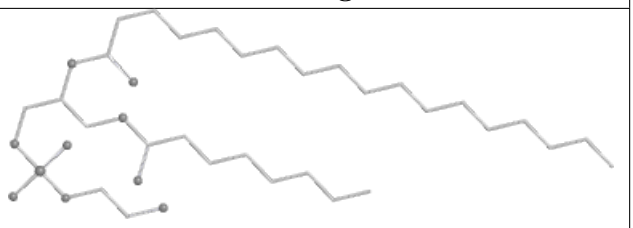
Bond lengths



Bond angles

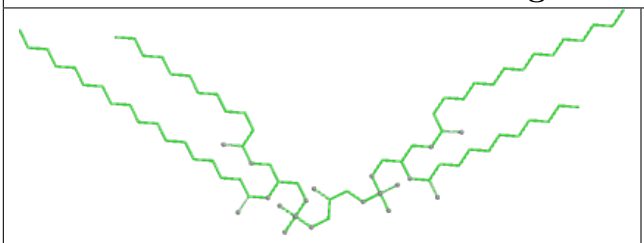


Torsions

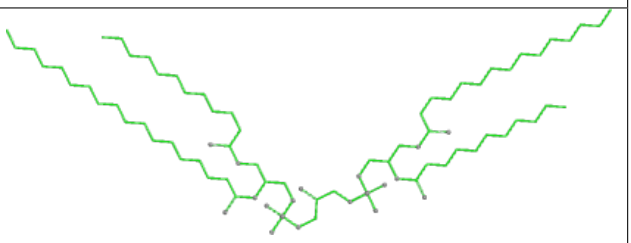


Rings

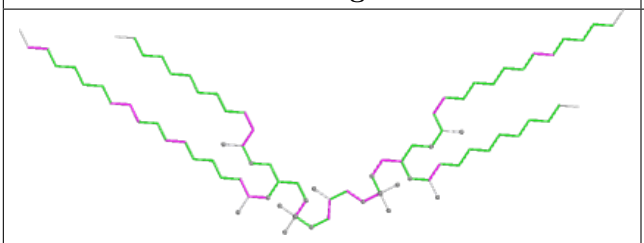
Ligand CDL 2 601



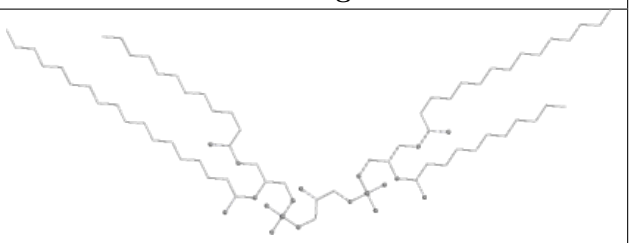
Bond lengths



Bond angles

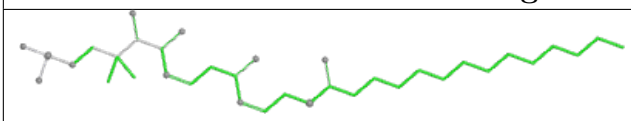


Torsions

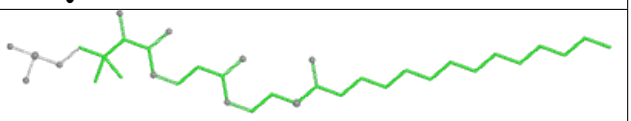


Rings

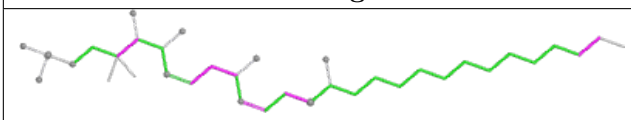
Ligand ZMP Q 201



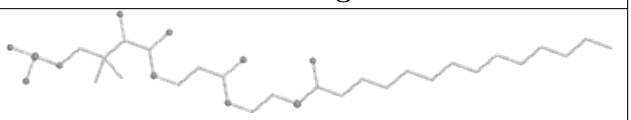
Bond lengths



Bond angles

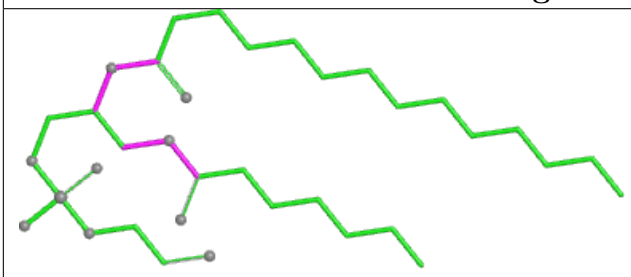


Torsions

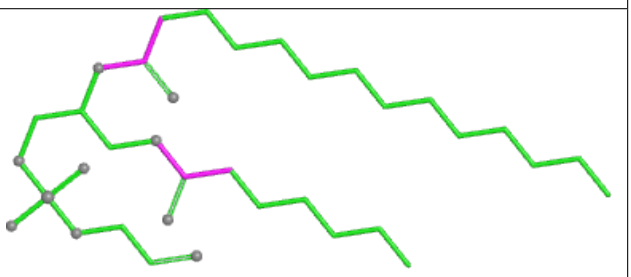


Rings

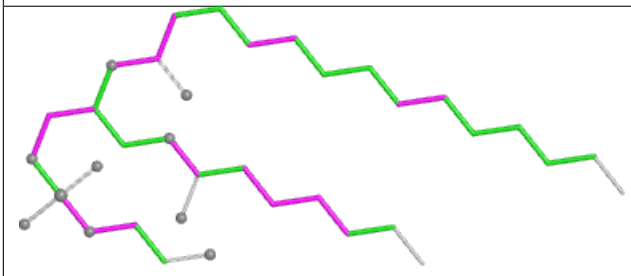
Ligand 3PE 8 101



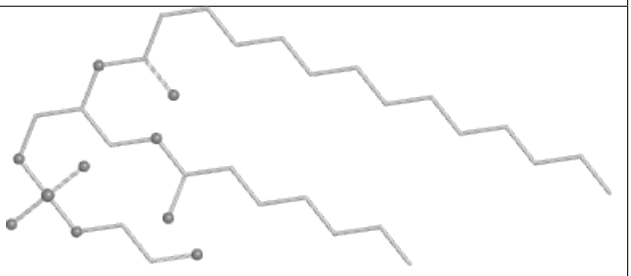
Bond lengths



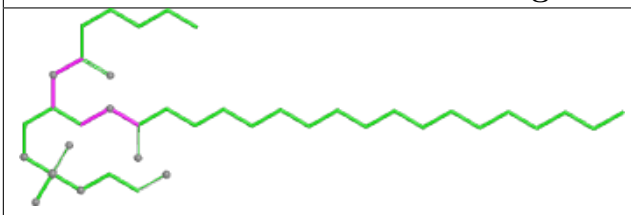
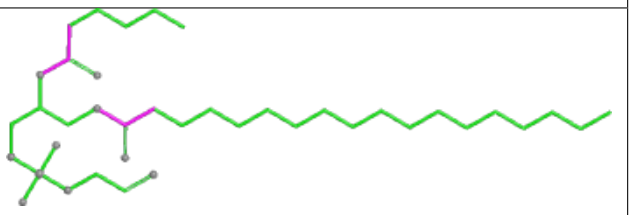
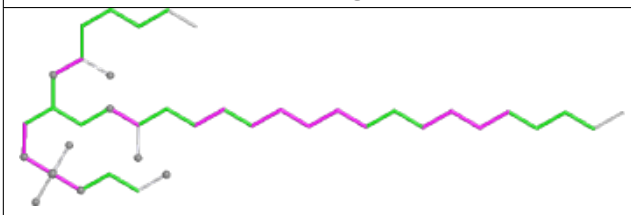
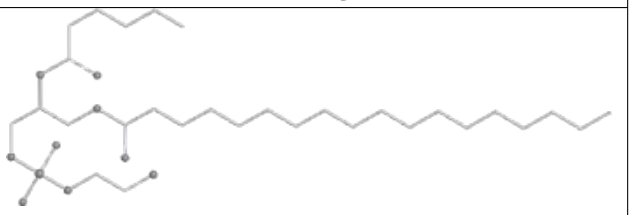
Bond angles

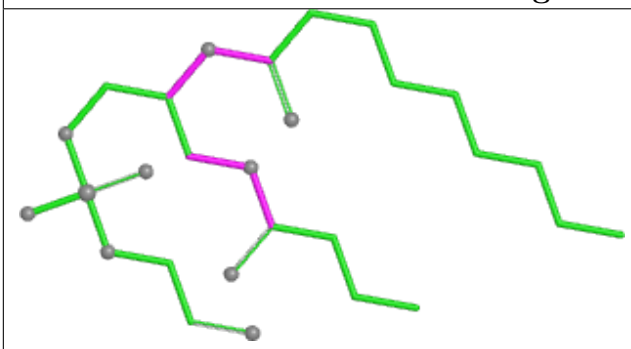
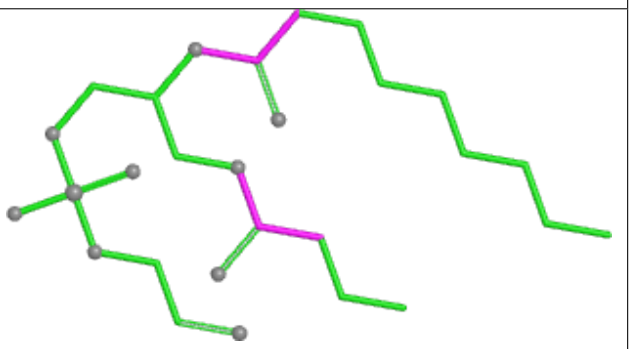
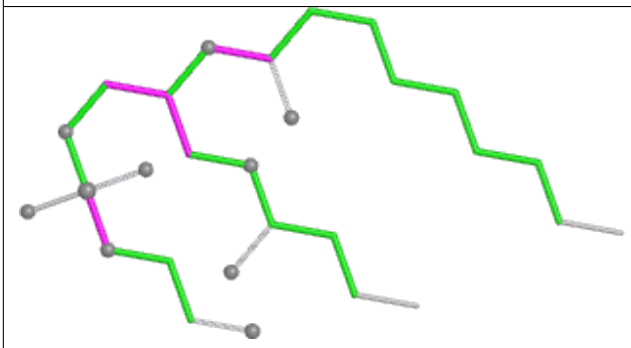
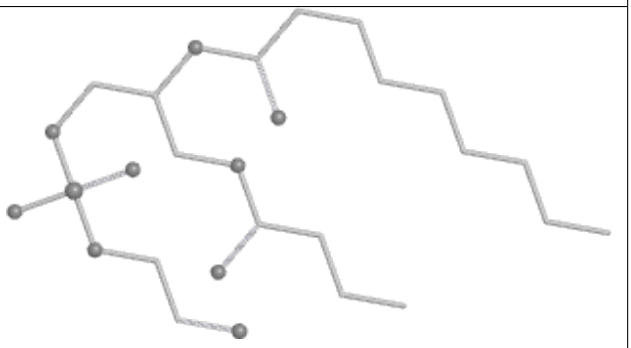


Torsions



Rings

Ligand 3PE n 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE 4 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

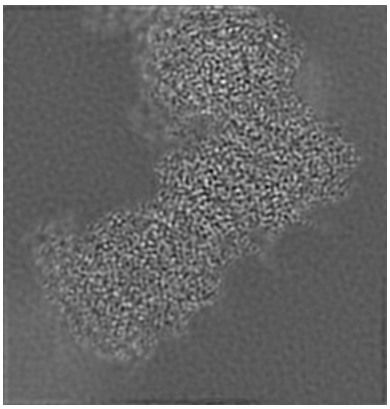
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14796. These allow visual inspection of the internal detail of the map and identification of artifacts.

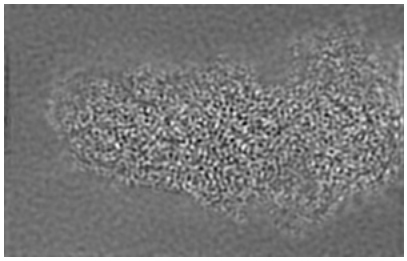
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

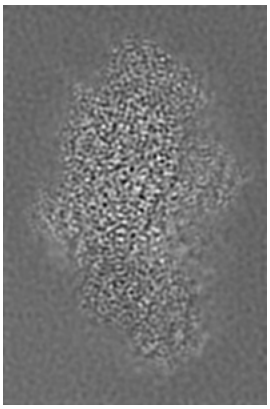
6.1.1 Primary map



X

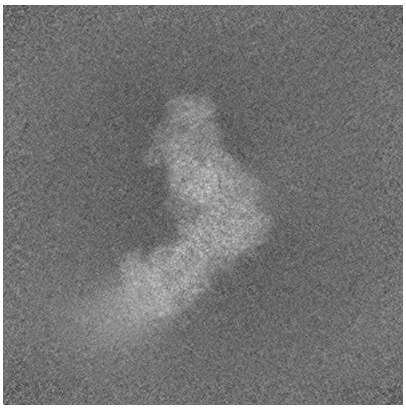


Y

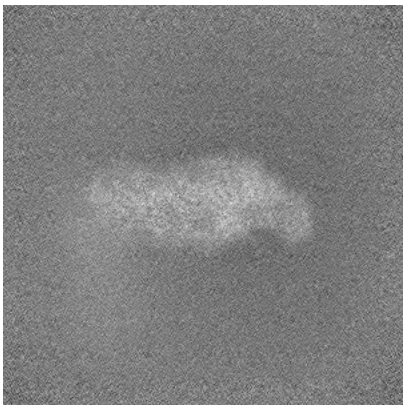


Z

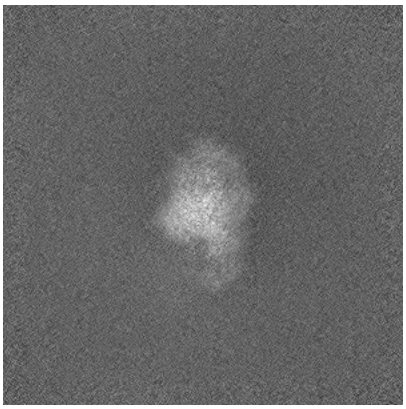
6.1.2 Raw map



X



Y

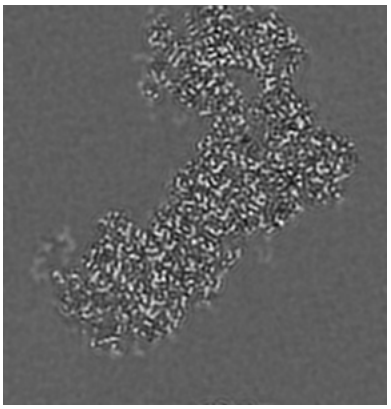


Z

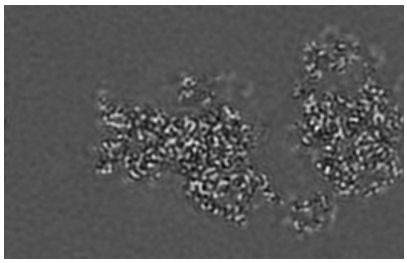
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

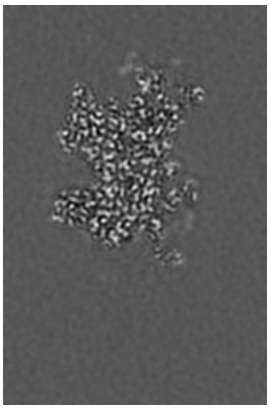
6.2.1 Primary map



X Index: 86

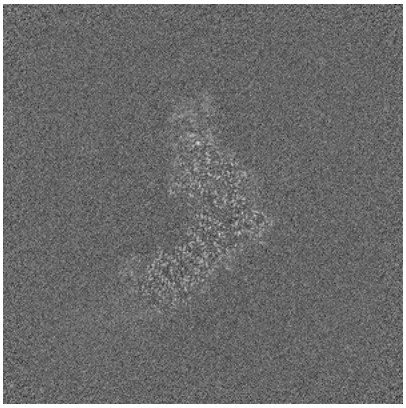


Y Index: 130

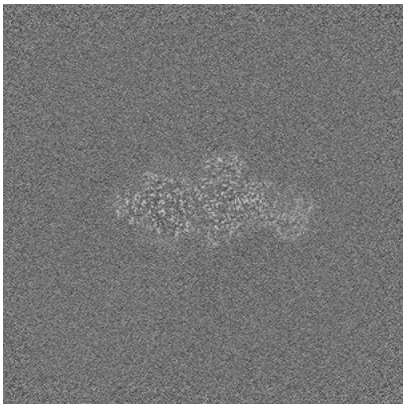


Z Index: 136

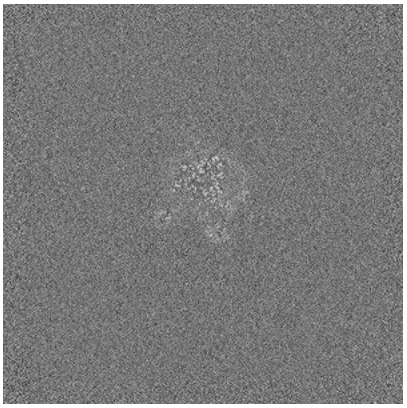
6.2.2 Raw map



X Index: 294



Y Index: 294

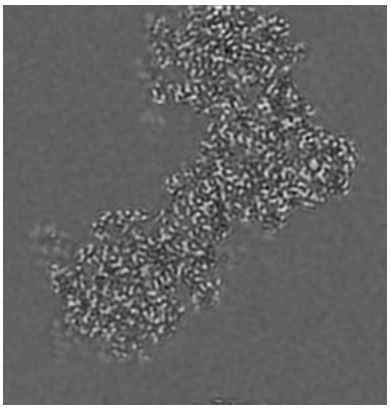


Z Index: 294

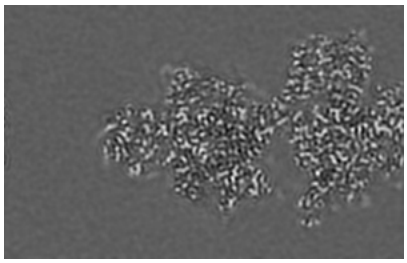
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

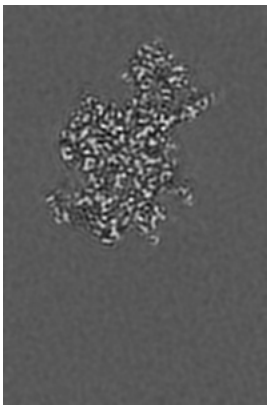
6.3.1 Primary map



X Index: 92

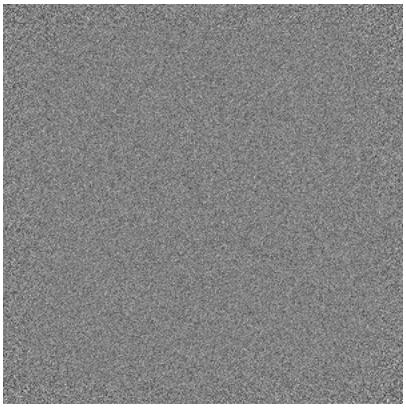


Y Index: 140

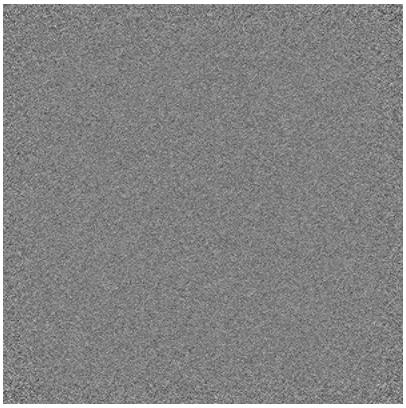


Z Index: 145

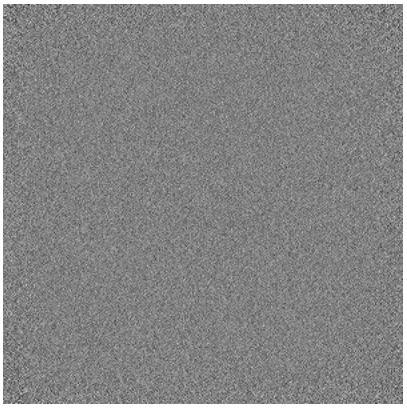
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

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

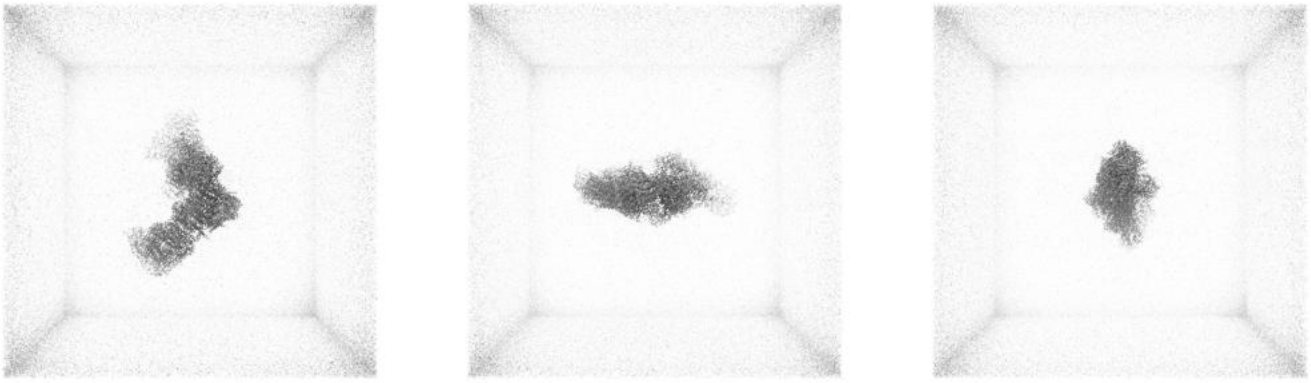
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

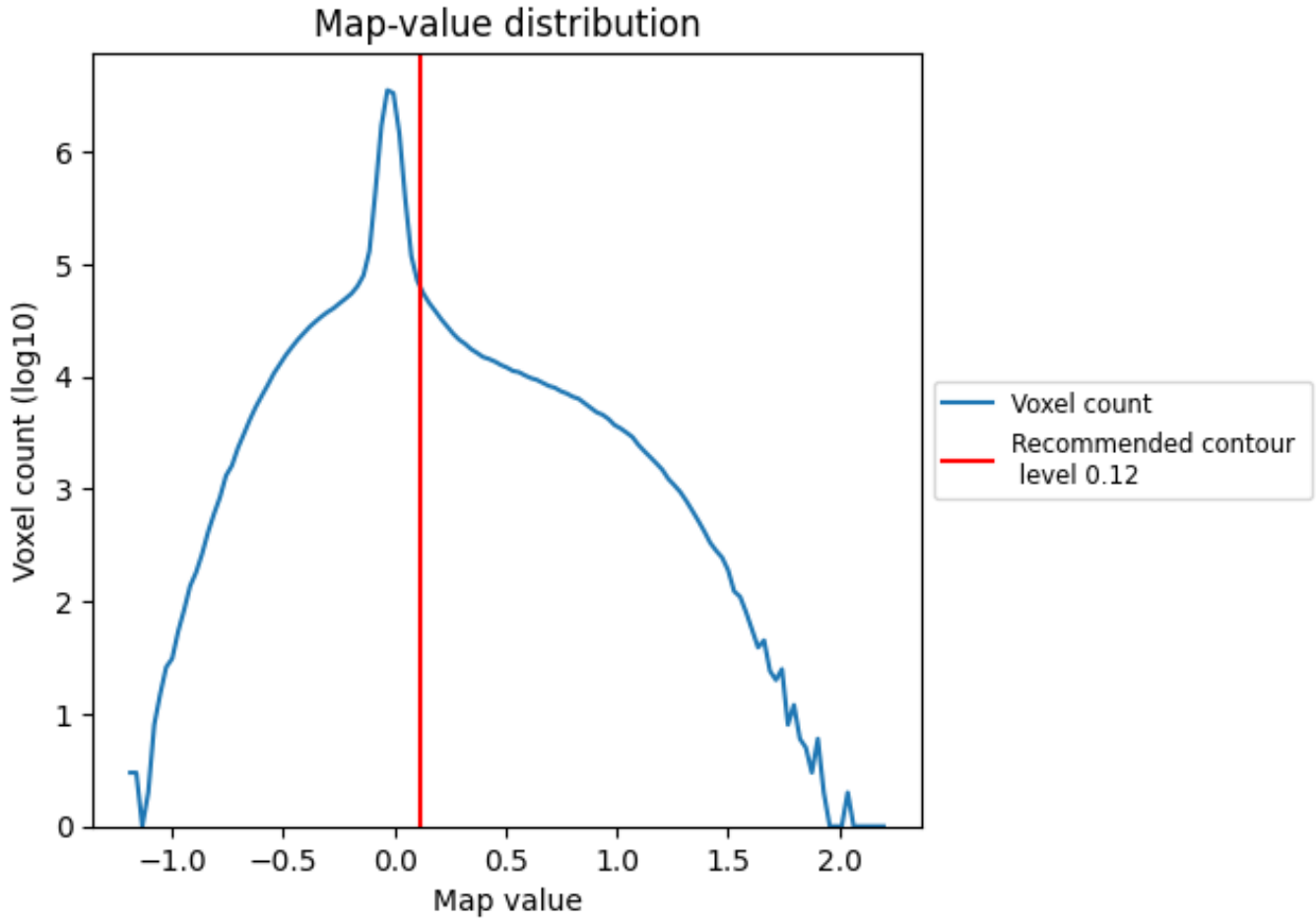
6.5 Mask visualisation (i)

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

7 Map analysis

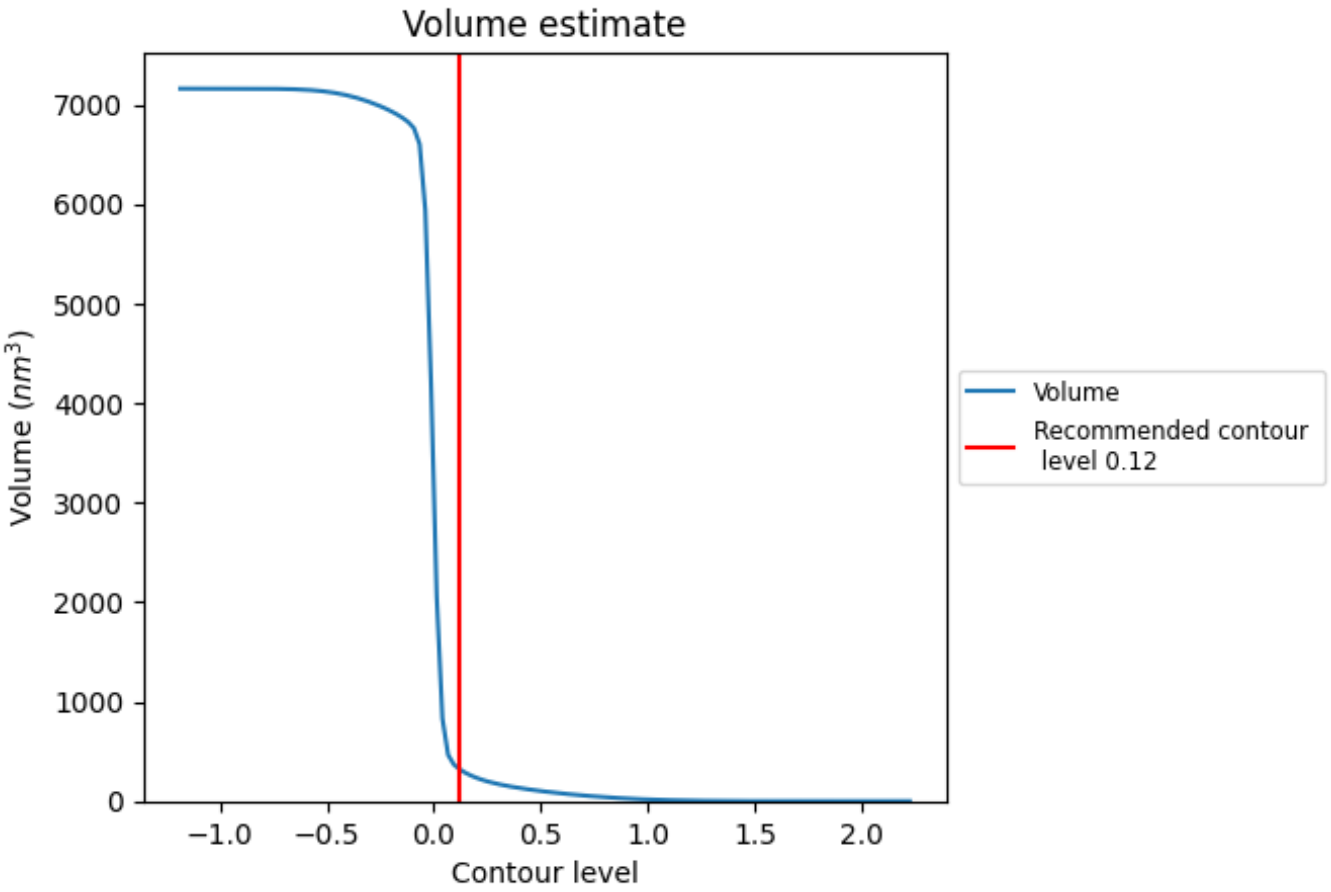
This section contains the results of statistical analysis of the map.

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 (i)



The volume at the recommended contour level is 320 nm^3; this corresponds to an approximate mass of 289 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.

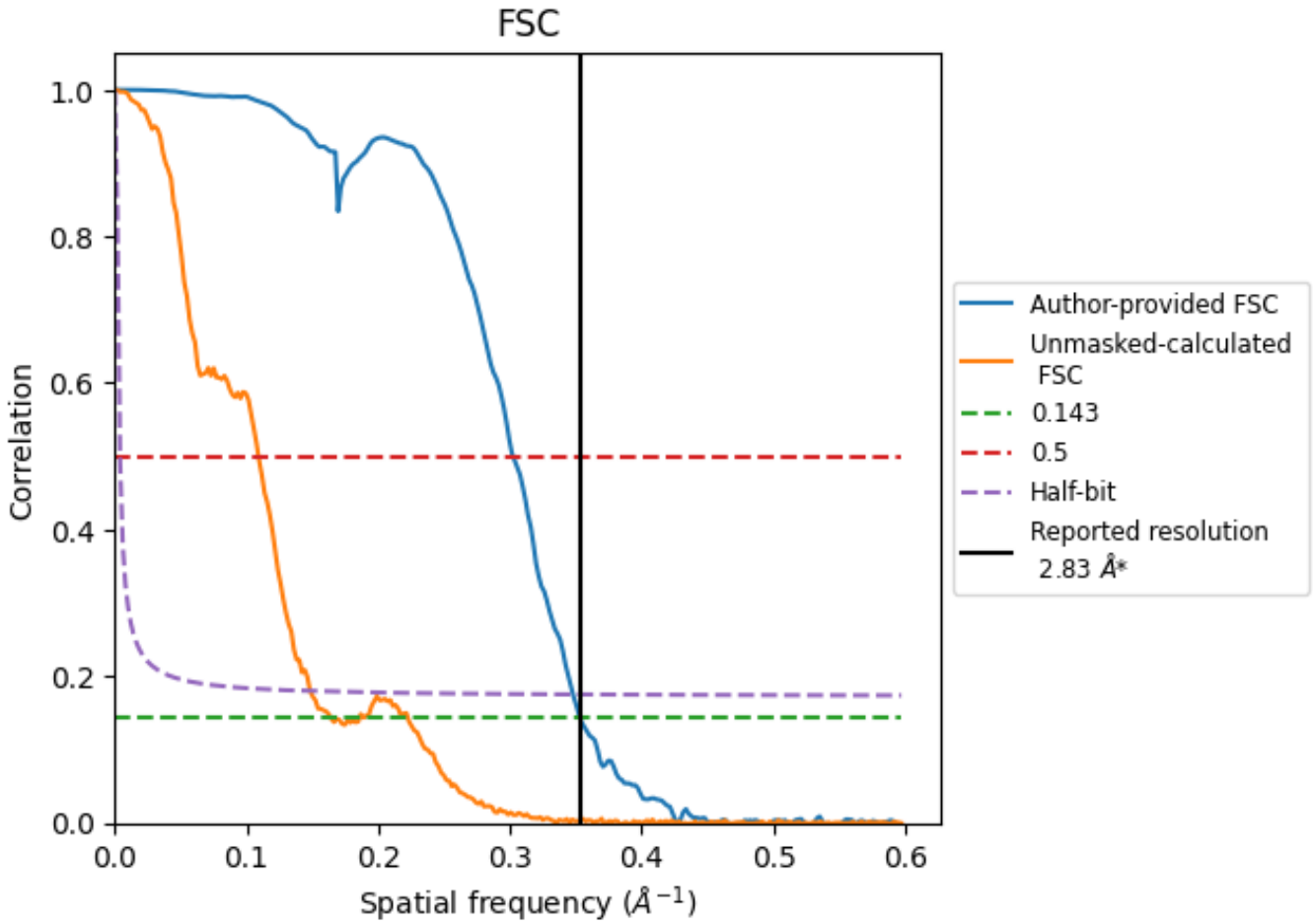
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.353 Å^{-1}

8.2 Resolution estimates (i)

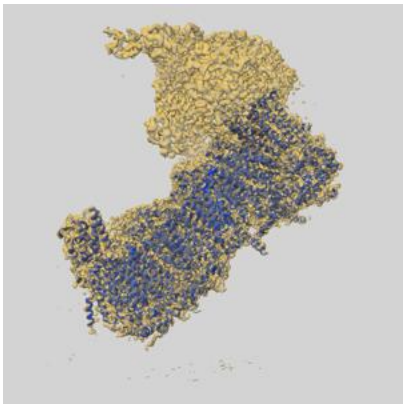
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.31	2.87
Unmasked-calculated*	6.09	9.16	6.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.09 differs from the reported value 2.83 by more than 10 %

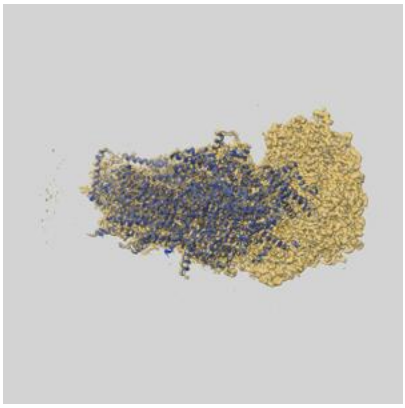
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14796 and PDB model 7ZME. Per-residue inclusion information can be found in section 3 on page 16.

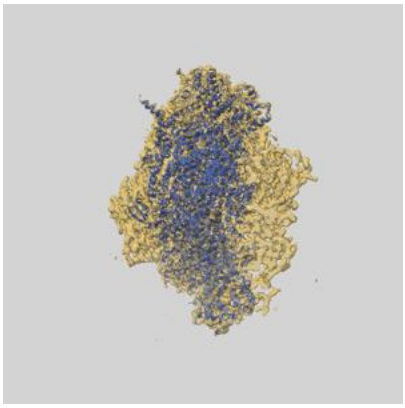
9.1 Map-model overlay



X



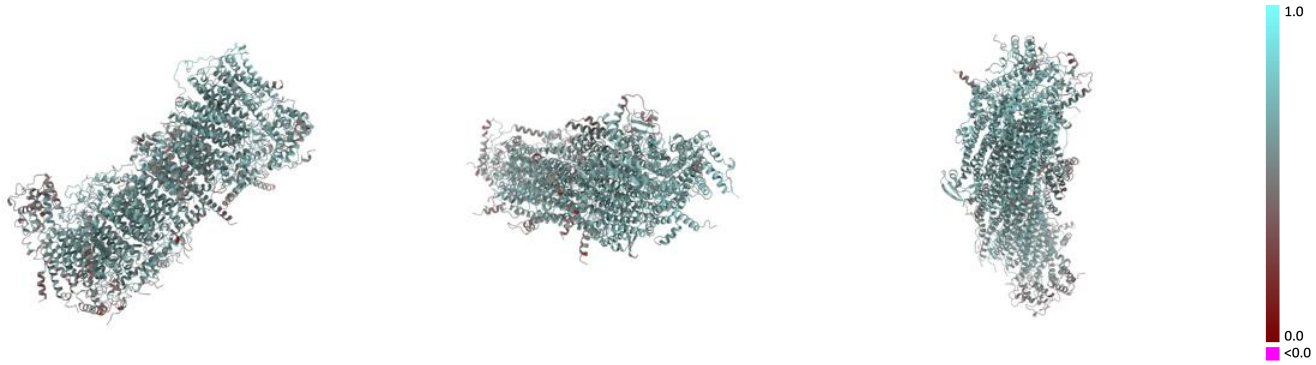
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

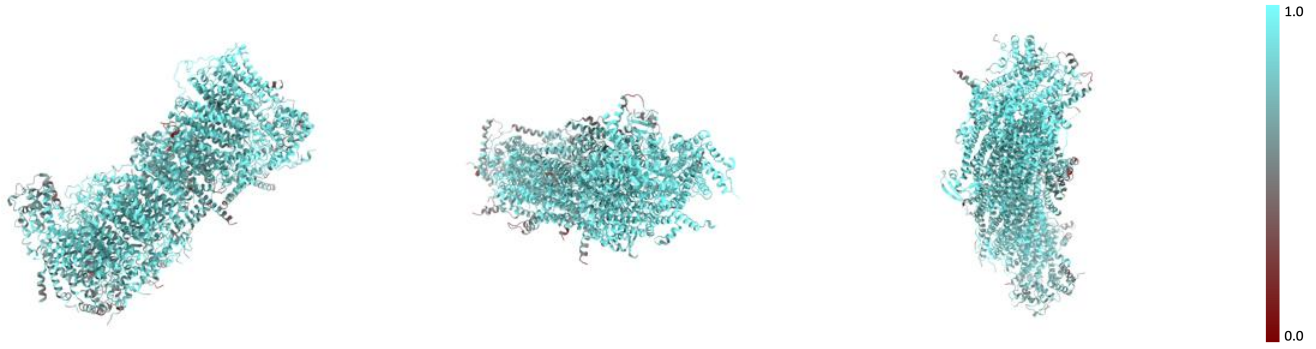
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

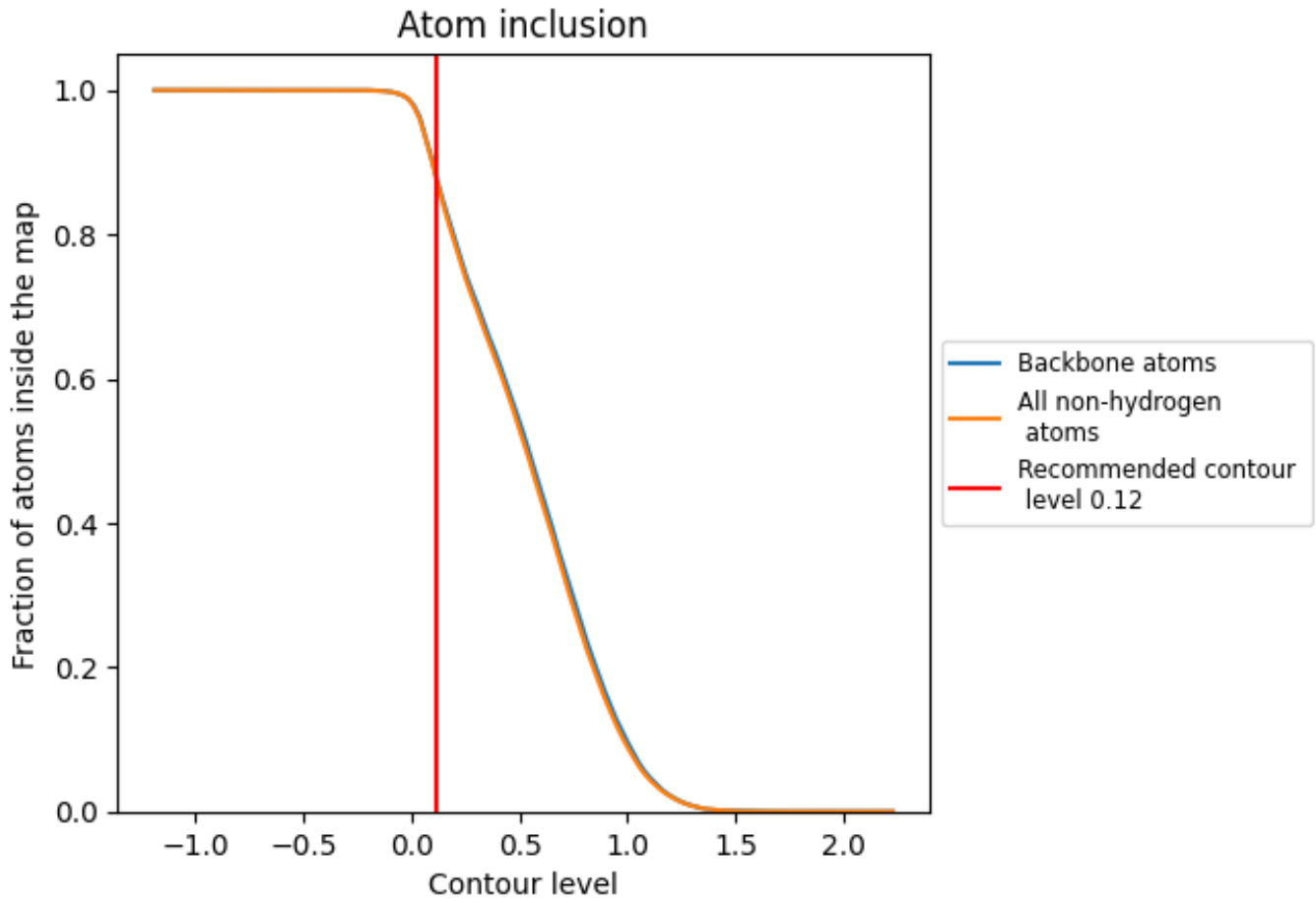
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8726	0.5960
1	0.9563	0.6450
2	0.9400	0.6410
3	0.9261	0.6270
4	0.9264	0.6290
5	0.9002	0.6030
6	0.8994	0.6080
8	0.6256	0.4540
9	0.8035	0.5620
D	0.9374	0.6340
J	0.6965	0.5030
L	0.9335	0.6310
Q	0.6465	0.4580
R	0.7839	0.5400
S	0.8514	0.5740
U	0.9220	0.6120
W	0.9005	0.6230
X	0.9160	0.6160
a	0.8090	0.5430
b	0.8452	0.5780
c	0.7230	0.4780
d	0.8654	0.5840
e	0.7400	0.5080
g	0.9015	0.5920
i	0.7918	0.5460
j	0.8998	0.5970
n	0.7104	0.5340