Full wwPDB EM Validation Report ⓘ

Feb 1, 2023 – 07:34 pm GMT

PDB ID	:	7R41
EMDB ID	:	EMD-14251
Title	:	Bovine complex I in the presence of IM1761092, active class i (Composite map)
Authors	:	Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on	:	2022-02-08
Resolution	:	2.30 Å(reported)

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:

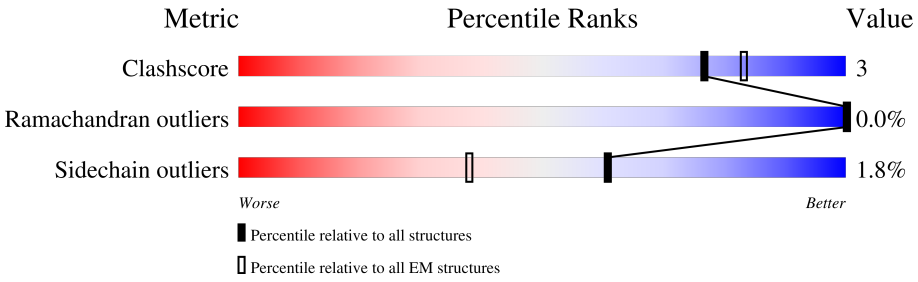
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	115	95% 5%
2	B	216	65% 6% 28%
3	C	266	74% 22%
4	D	463	85% 8% 7%
5	E	249	77% 9% 14%
6	F	464	86% 7% 7%
7	G	727	88% 6% 5%
8	H	318	90% 10%

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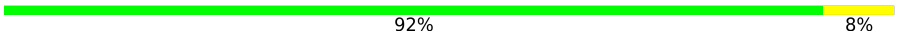
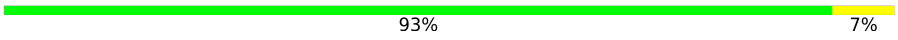
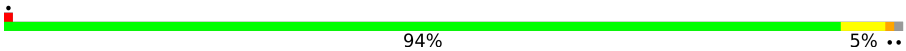
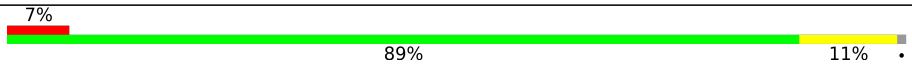
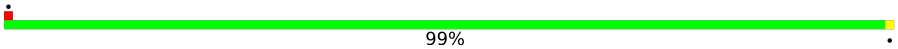
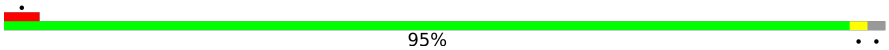
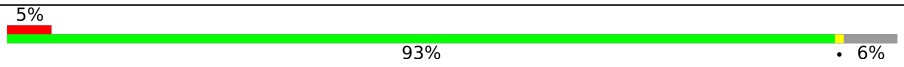
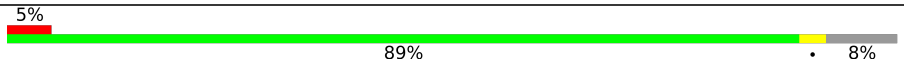
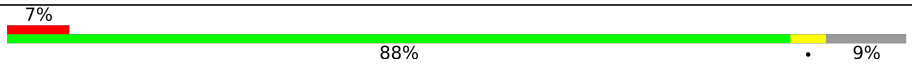
Mol	Chain	Length	Quality of chain
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	154	

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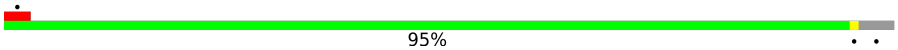
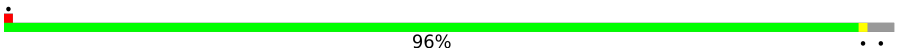
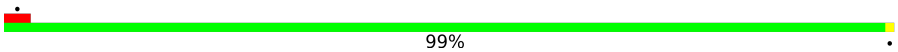
Mol	Chain	Length	Quality of chain
33	h	189	
34	i	127	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 69138 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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	115	921	622	133	159	7	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	155	1241	792	224	211	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	207	1721	1111	296	311	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	430	3459	2209	596	629	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1655	1057	277	311	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	430	Total	C	N	O	S	0	0
			3310	2086	591	613	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5279	3307	920	1013	39		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	174	Total	C	N	O	S	0	0
			1337	902	189	234	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4791	3186	736	826	43		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	341	Total	C	N	O	S	0	0
			2747	1777	486	479	5		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1016	641	181	191	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	95	Total	C	N	O	S	0	0
			730	448	137	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			677	425	126	124	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			612	393	90	124	5		
20	U	86	Total	C	N	O	S	0	0
			693	447	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			911	589	154	165	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			971	622	180	165	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1030	657	176	191	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	140	Total	C	N	O	S	0	0
			1146	737	200	200	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	82	Total	C	N	O	S	0	0
			646	422	108	114	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	48	Total	C	N	O	0	0
			405	268	69	68		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	113	Total	C	N	O	S	0	0
			945	619	161	162	3		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	97	Total	C	N	O	S	0	0
			819	518	156	139	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	52	Total	C	N	O	S	0	0
			451	296	79	75	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	98	Total	C	N	O	S	0	0
			824	529	137	154	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	102	Total	C	N	O	S	0	0
			879	579	150	149	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	67	Total	C	N	O	S	0	0
			580	381	95	103	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	79	Total	C	N	O	S	0	0
			638	418	107	111	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	155	Total	C	N	O	S	0	0
			1304	844	213	239	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	127	Total	C	N	O	0	0
			1061	681	187	193		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	172	Total	C	N	O	S	0	0
			1492	955	273	257	7		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	120	Total	C	N	O	S	0	0
			1035	645	199	183	8		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	171	Total	C	N	O	S	0	0
			1443	904	266	265	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

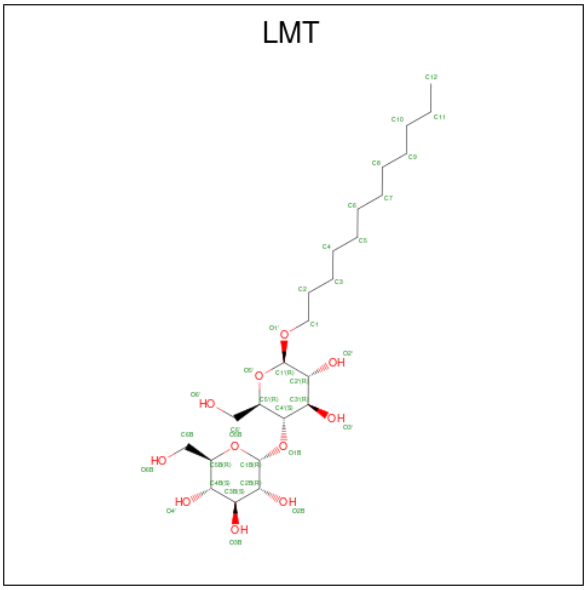
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	94	Total	C	N	O	S	0	0
			767	485	143	136	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 45 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	A	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	

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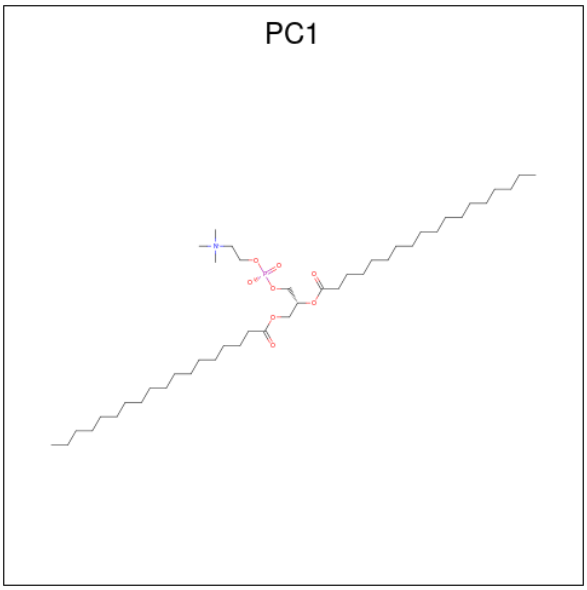
Mol	Chain	Residues	Atoms	AltConf
45	M	1	Total C O 35 24 11	0
45	M	1	Total C O 35 24 11	0
45	N	1	Total C O 35 24 11	0
45	Y	1	Total C O 35 24 11	0
45	Y	1	Total C O 35 24 11	0
45	Y	1	Total C O 35 24 11	0
45	h	1	Total C O 35 24 11	0
45	j	1	Total C O 35 24 11	0
45	l	1	Total C O 35 24 11	0

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total C N O P 21 11 1 8 1	0
46	B	1	Total C N O P 54 44 1 8 1	0

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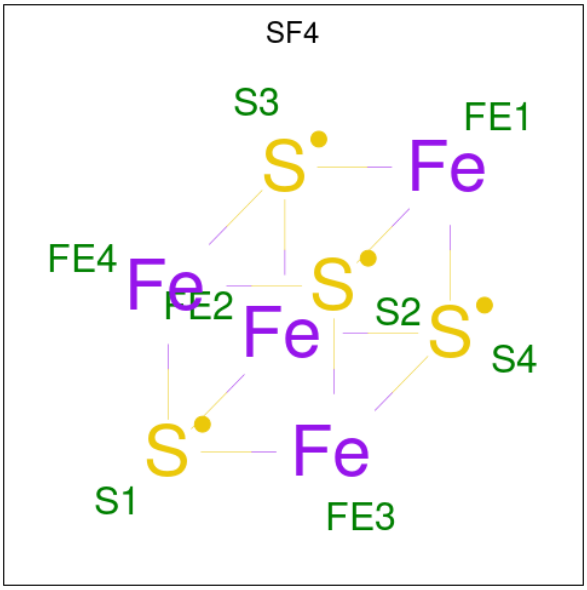
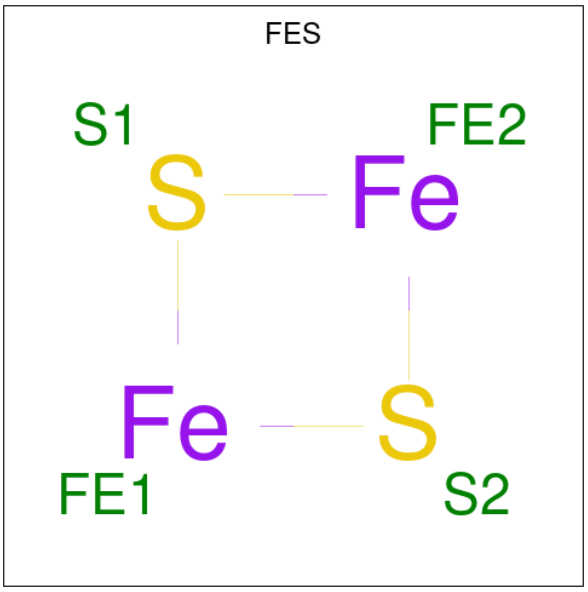
Mol	Chain	Residues	Atoms					AltConf
46	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	L	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



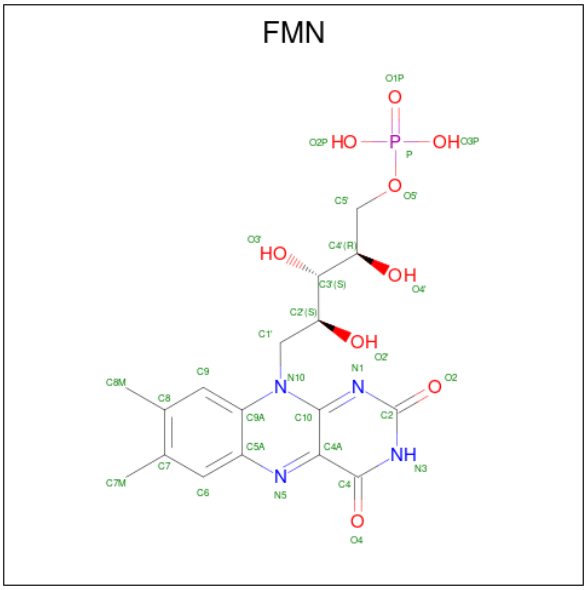
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
48	E	1	Total	Fe	S	0
			4	2	2	
48	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

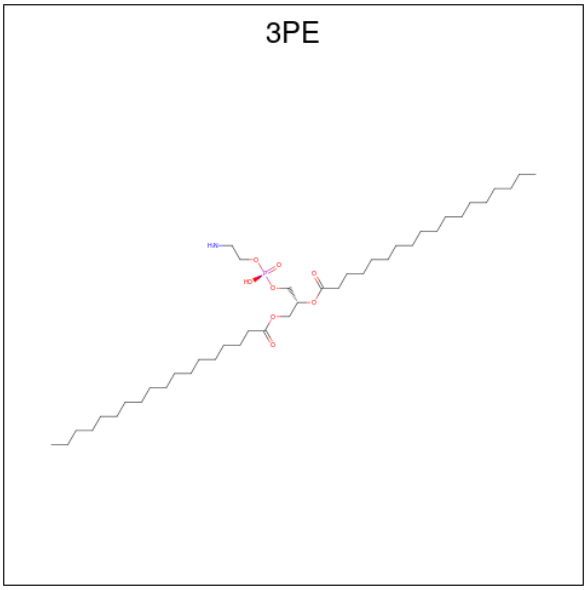


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
50	G	1	Total K 1 1	0

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
51	H	1	Total C N O P 44 34 1 8 1	0
51	H	1	Total C N O P 34 24 1 8 1	0
51	I	1	Total C N O P 51 41 1 8 1	0
51	L	1	Total C N O P 49 39 1 8 1	0
51	L	1	Total C N O P 45 35 1 8 1	0
51	M	1	Total C N O P 46 36 1 8 1	0
51	M	1	Total C N O P 51 41 1 8 1	0
51	N	1	Total C N O P 51 41 1 8 1	0
51	N	1	Total C N O P 41 31 1 8 1	0
51	N	1	Total C N O P 29 19 1 8 1	0

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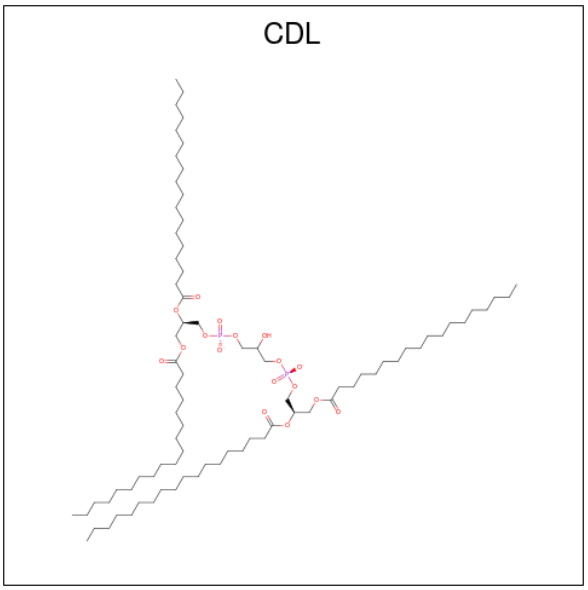
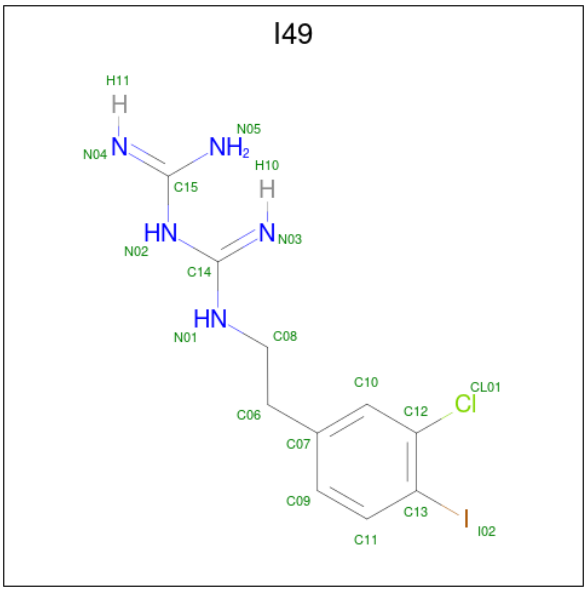
Mol	Chain	Residues	Atoms					AltConf
51	P	1	Total	C	N	O	P	0
			37	27	1	8	1	
51	X	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
51	d	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



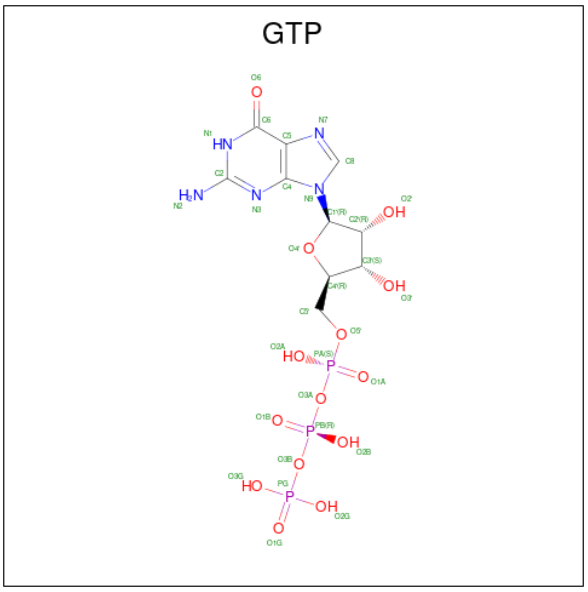
Mol	Chain	Residues	Atoms				AltConf
52	J	1	Total	C	O	P	0
			62	43	17	2	
52	K	1	Total	C	O	P	0
			71	52	17	2	
52	L	1	Total	C	O	P	0
			69	50	17	2	
52	h	1	Total	C	O	P	0
			67	48	17	2	
52	q	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 53 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (three-letter code: I49) (formula: $C_{10}H_{13}ClIN_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
53	N	1	Total	C	Cl	I	N	0
			17	10	1	1	5	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

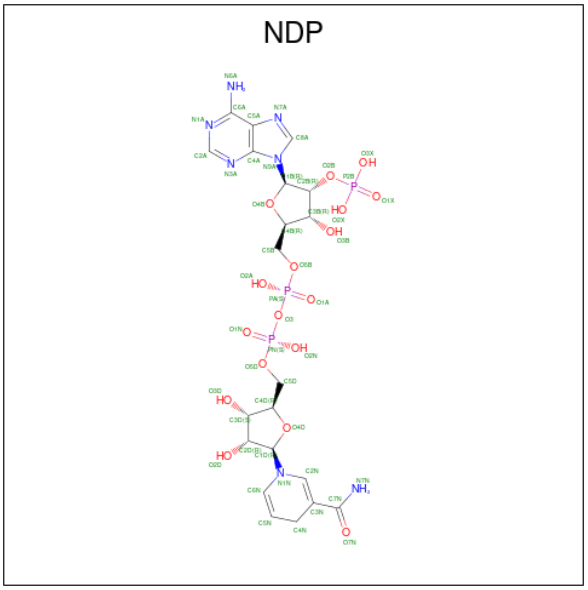


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	O	1	Total	Mg	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

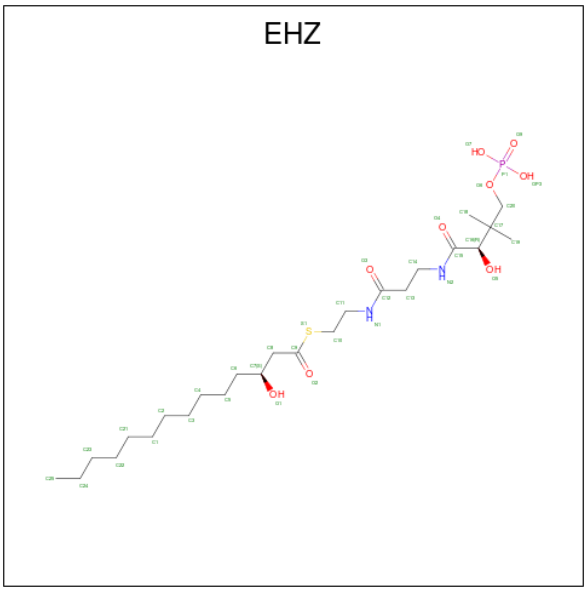


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

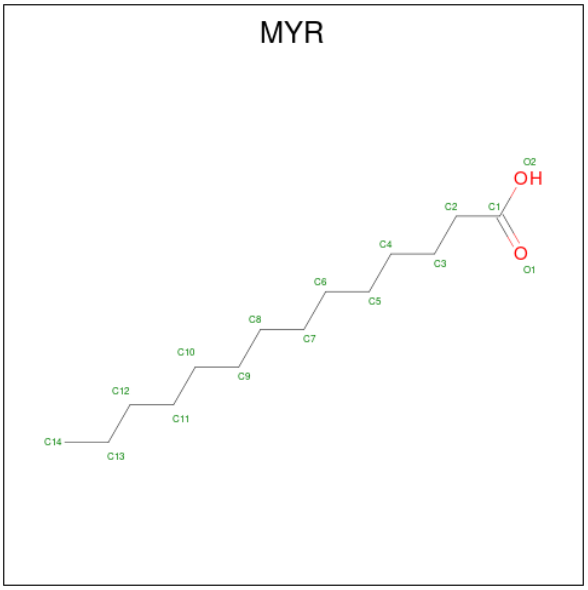
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- Molecule 58 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



Mol	Chain	Residues	Atoms						AltConf
58	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 59 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
59	o	1	Total	C	O	0
			6	5	1	

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	A	21	Total O 21 21	0
60	B	62	Total O 62 62	0
60	C	83	Total O 83 83	0
60	D	155	Total O 155 155	0
60	E	13	Total O 13 13	0
60	F	59	Total O 59 59	0
60	G	183	Total O 183 183	0
60	H	61	Total O 61 61	0
60	I	91	Total O 91 91	0
60	J	21	Total O 21 21	0
60	K	15	Total O 15 15	0
60	L	31	Total O 31 31	0
60	M	49	Total O 49 49	0
60	N	49	Total O 49 49	0
60	O	21	Total O 21 21	0
60	P	58	Total O 58 58	0
60	Q	59	Total O 59 59	0
60	R	39	Total O 39 39	0
60	S	2	Total O 2 2	0
60	V	15	Total O 15 15	0
60	W	10	Total O 10 10	0
60	X	23	Total O 23 23	0

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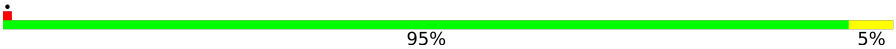
Mol	Chain	Residues	Atoms	AltConf
60	Y	3	Total O 3 3	0
60	Z	24	Total O 24 24	0
60	a	11	Total O 11 11	0
60	b	7	Total O 7 7	0
60	d	9	Total O 9 9	0
60	e	15	Total O 15 15	0
60	f	1	Total O 1 1	0
60	g	4	Total O 4 4	0
60	h	15	Total O 15 15	0
60	i	2	Total O 2 2	0
60	j	1	Total O 1 1	0
60	k	2	Total O 2 2	0
60	l	3	Total O 3 3	0
60	m	7	Total O 7 7	0
60	n	9	Total O 9 9	0
60	p	10	Total O 10 10	0
60	q	35	Total O 35 35	0
60	r	25	Total O 25 25	0
60	s	4	Total O 4 4	0

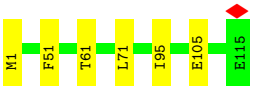
3 Residue-property plots (i)

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 3

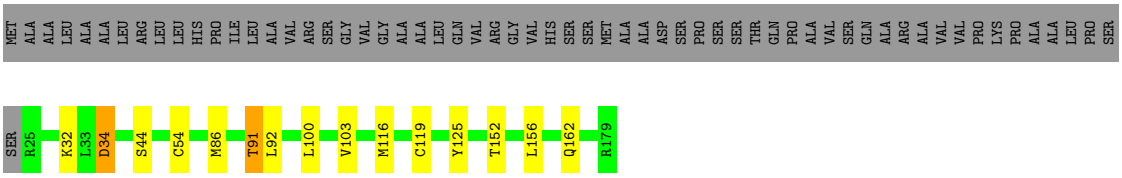
Chain A:





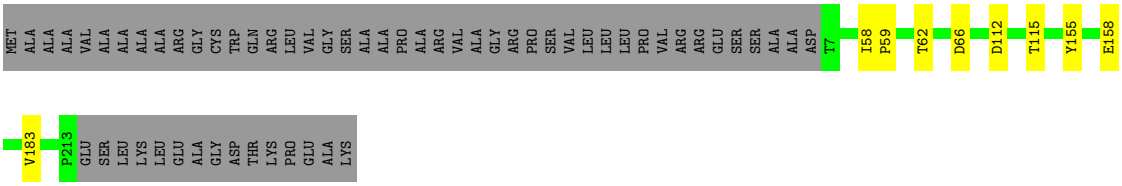
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:



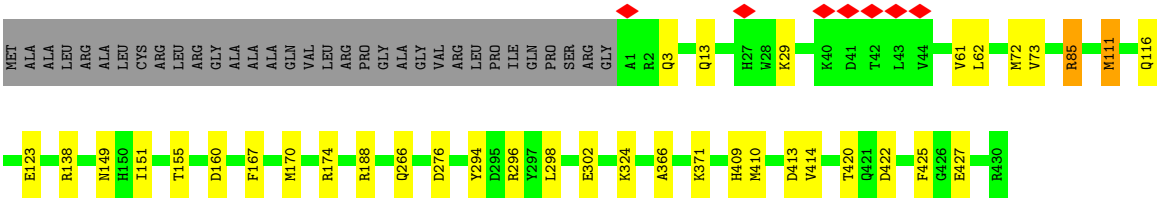
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:



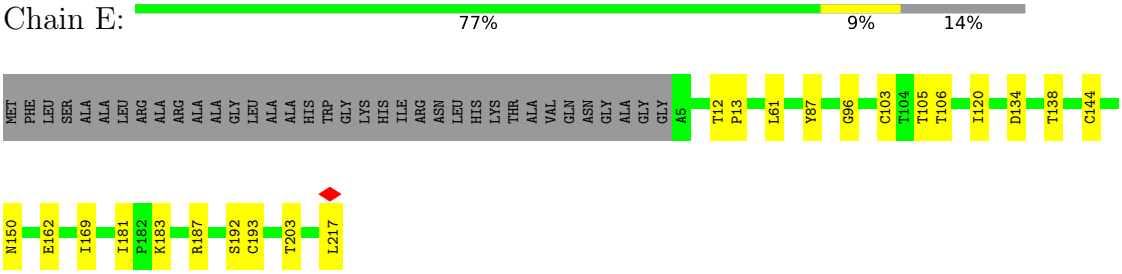
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:



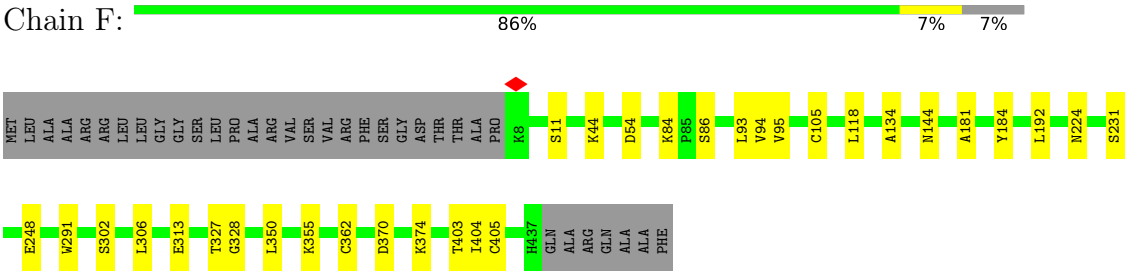
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



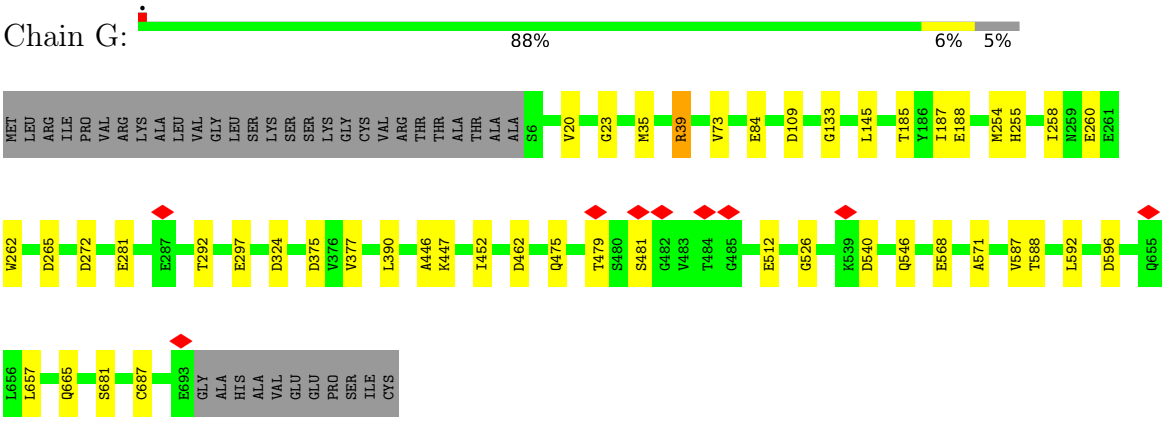
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:



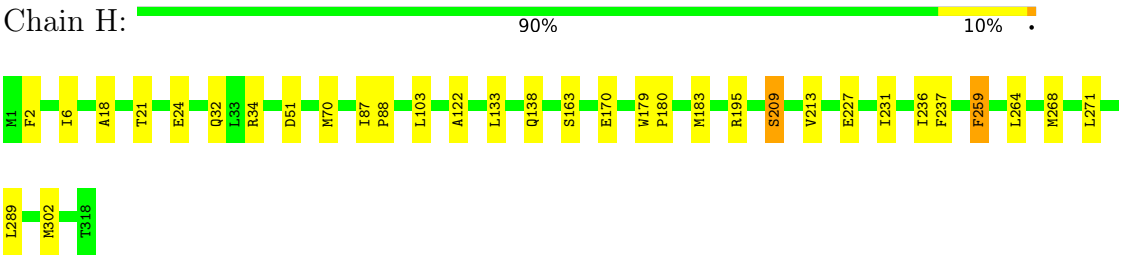
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:



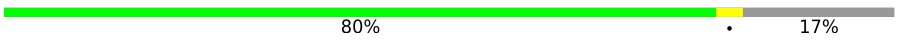
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



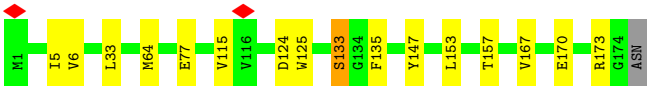
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:

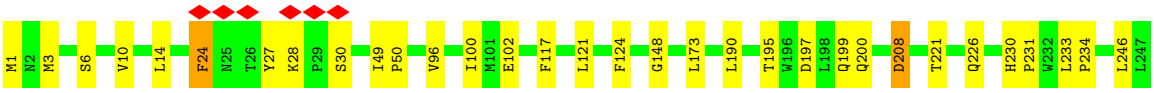


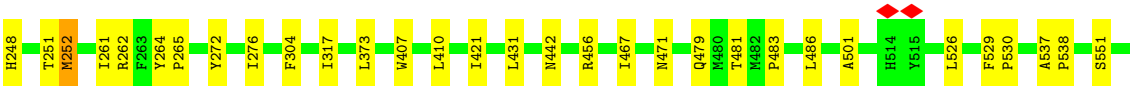
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

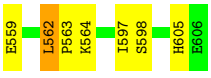
Chain K:

• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:





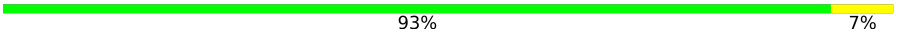


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:

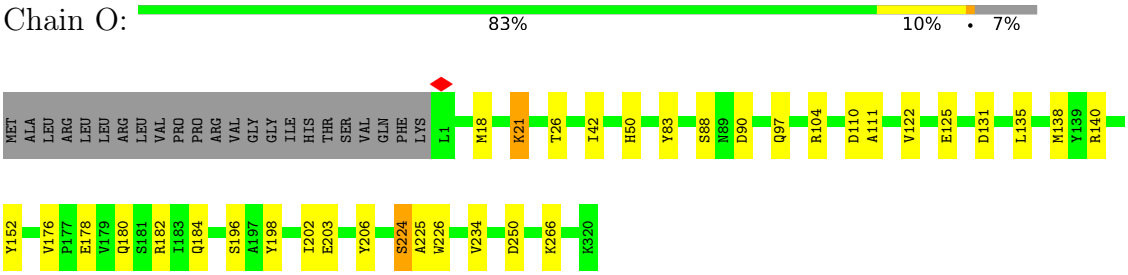
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



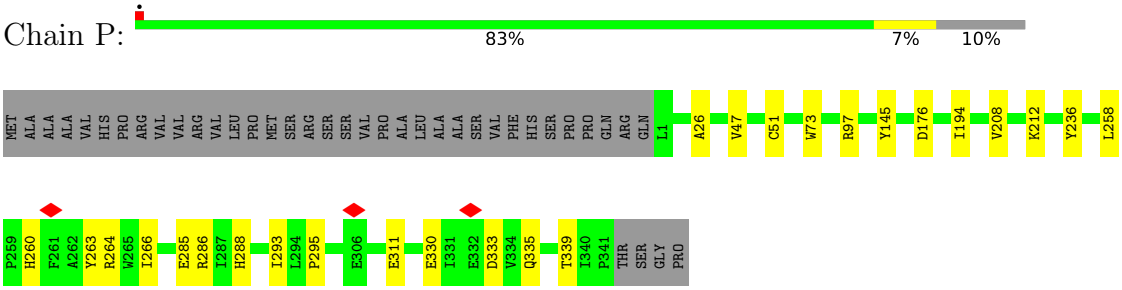
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



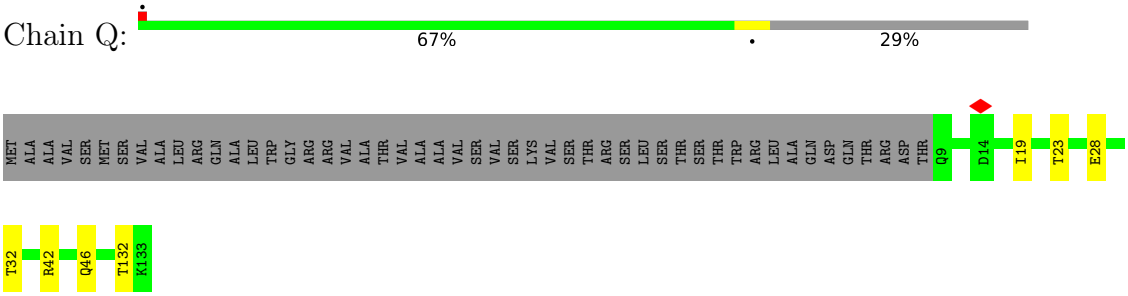
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



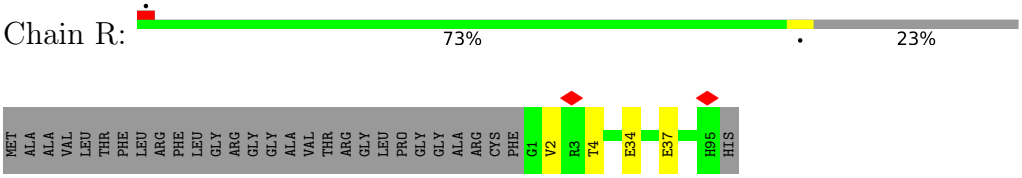
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



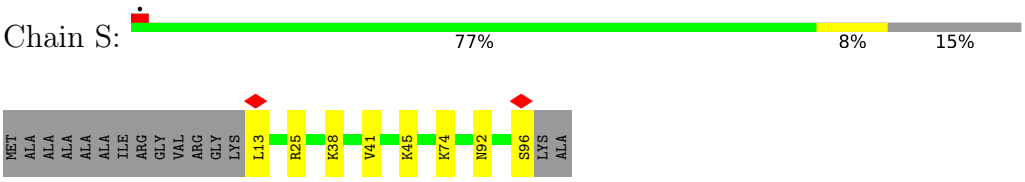
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:

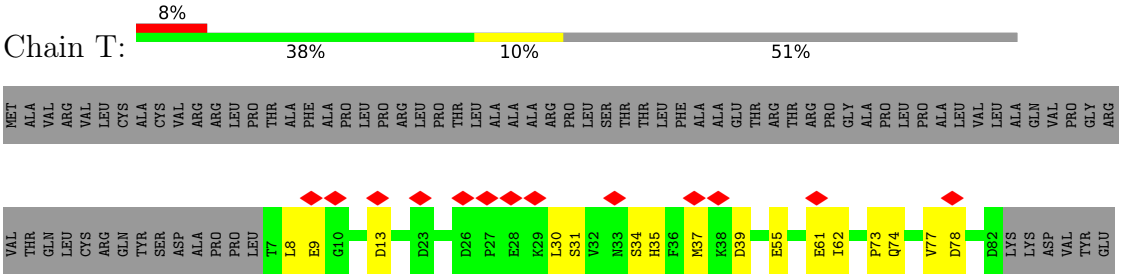


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

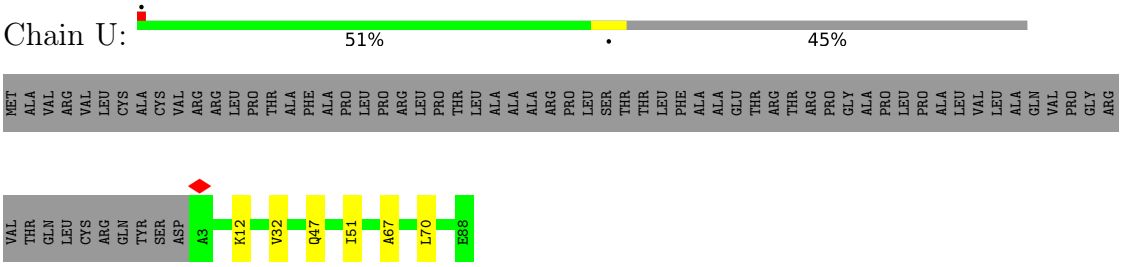
Chain S:



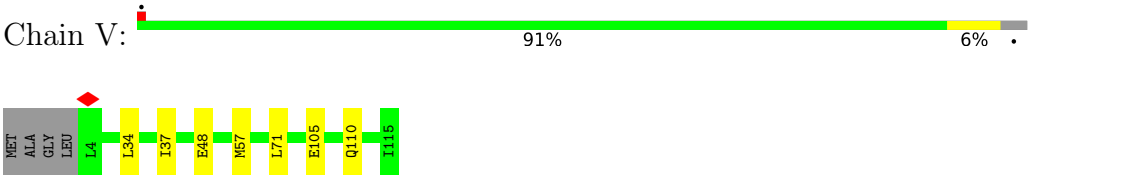
• Molecule 20: Acyl carrier protein, mitochondrial



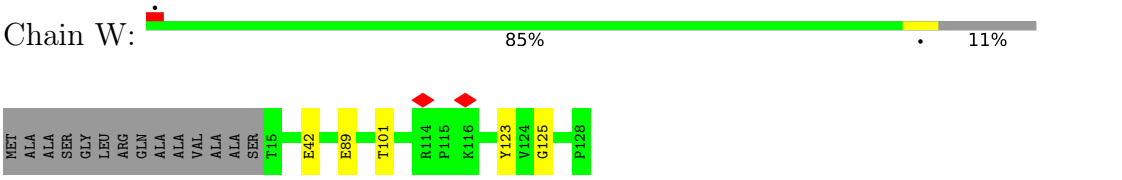
• Molecule 20: Acyl carrier protein, mitochondrial



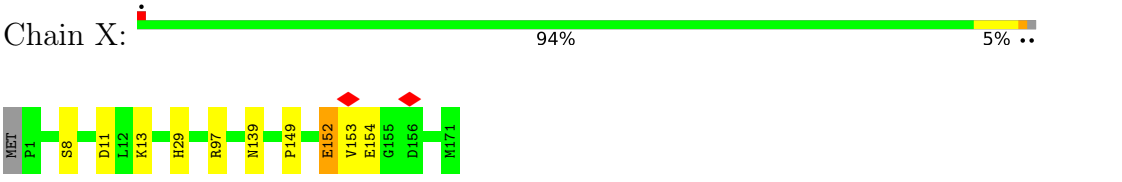
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



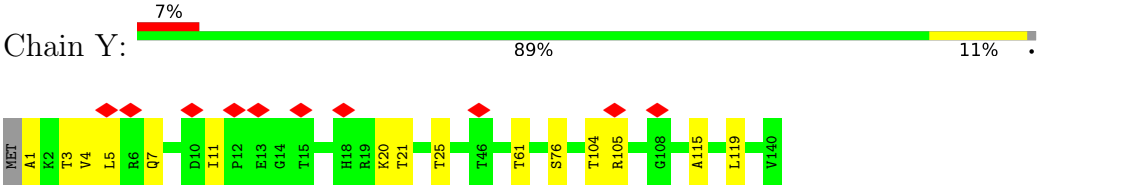
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

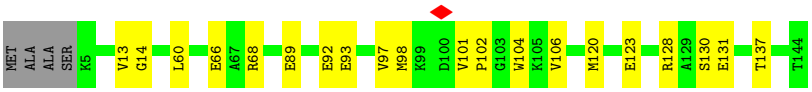


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



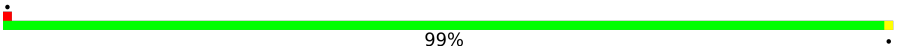
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



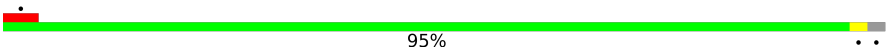
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

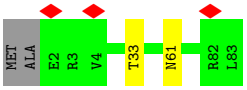
Chain a:



• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

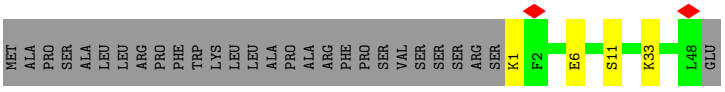
Chain b:





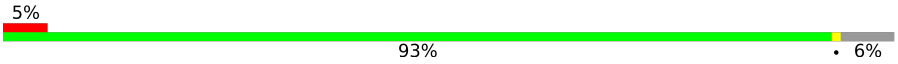
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

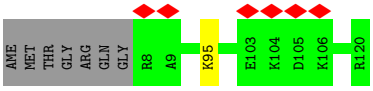
Chain c:



• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

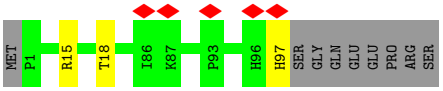
Chain d:





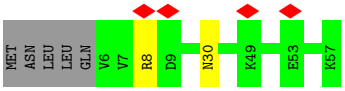
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



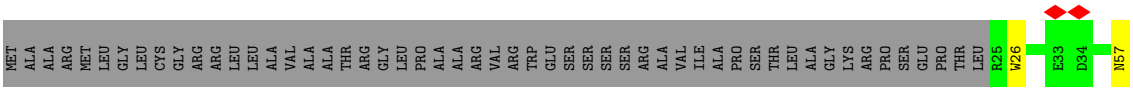
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:



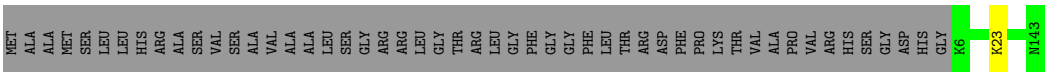
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



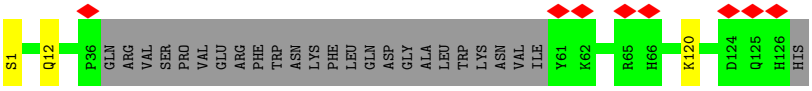
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:

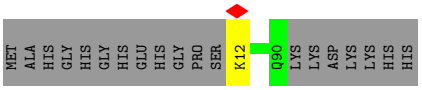


• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:

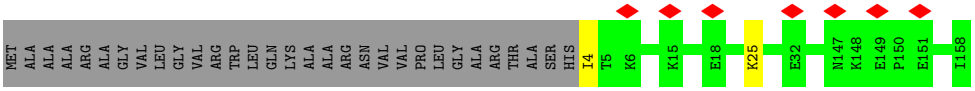
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



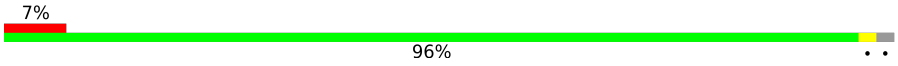
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

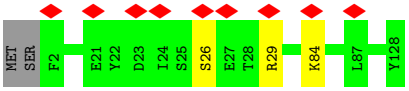
Chain l:



• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

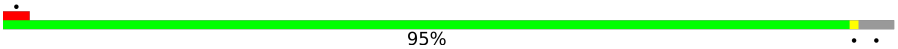
Chain m:

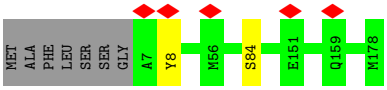




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

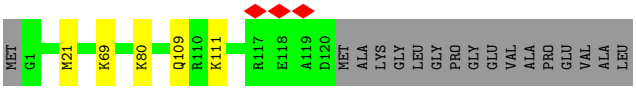
Chain n:





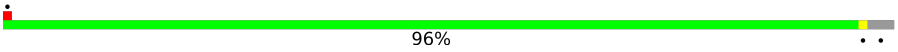
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

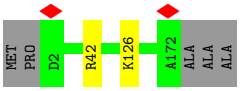
Chain o:



• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

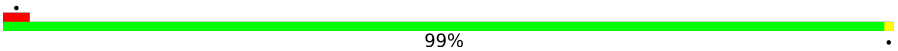
Chain p:

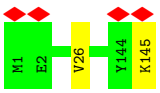




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

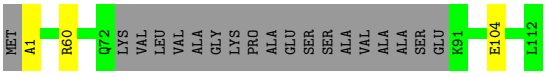
Chain q:





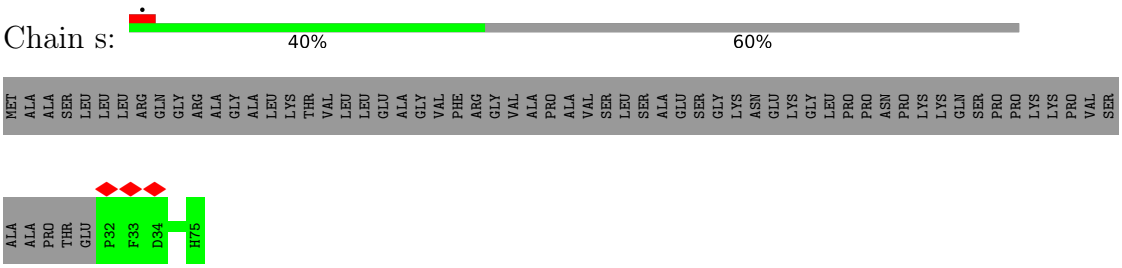
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48367	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	34.153	Depositor
Minimum map value	-13.918	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.021	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, LMT, SAC, FES, NDP, MG, PC1, FMN, AYA, EHZ, 2MR, SF4, CDL, K, I49, ZN, 3PE, GTP, MYR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.32	0/936	0.42	0/1281
2	B	0.42	0/1272	0.46	0/1720
3	C	0.37	0/1772	0.46	0/2413
4	D	0.37	0/3537	0.45	0/4794
5	E	0.34	0/1695	0.46	0/2307
6	F	0.35	0/3384	0.45	0/4572
7	G	0.34	0/5367	0.46	0/7274
8	H	0.35	0/2571	0.44	0/3513
9	I	0.38	0/1445	0.48	0/1956
10	J	0.34	0/1362	0.43	0/1848
11	K	0.29	0/745	0.43	0/1008
12	L	0.33	0/4908	0.42	0/6679
13	M	0.34	0/3738	0.43	0/5097
14	N	0.32	0/2792	0.44	0/3800
15	O	0.35	0/2651	0.42	0/3587
16	P	0.34	0/2824	0.45	0/3831
17	Q	0.33	0/1039	0.46	0/1404
18	R	0.38	0/742	0.46	0/999
19	S	0.31	0/688	0.46	0/927
20	T	0.30	0/621	0.41	0/837
20	U	0.37	0/705	0.43	0/952
21	V	0.31	0/931	0.38	0/1261
22	W	0.32	0/995	0.42	0/1337
23	X	0.32	0/1439	0.42	0/1942
24	Y	0.28	0/1042	0.44	0/1414
25	Z	0.34	0/1175	0.45	0/1584
26	a	0.35	0/584	0.44	0/786
27	b	0.31	0/667	0.43	0/916
28	c	0.33	0/418	0.37	0/567
29	d	0.38	0/975	0.40	0/1319
30	e	0.32	0/840	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
31	f	0.32	0/464	0.43	0/626
32	g	0.35	0/850	0.39	0/1154
33	h	0.35	0/1188	0.41	0/1607
34	i	0.34	0/900	0.44	0/1224
35	j	0.34	0/607	0.39	0/833
36	k	0.34	0/657	0.42	0/887
37	l	0.35	0/1358	0.42	0/1858
38	m	0.34	0/1088	0.42	0/1472
39	n	0.37	0/1545	0.40	0/2092
40	o	0.36	0/1060	0.42	0/1420
41	p	0.36	0/1476	0.41	0/1990
42	q	0.35	0/1250	0.45	0/1698
43	r	0.35	0/780	0.45	0/1056
44	s	0.31	0/383	0.41	0/518
All	All	0.34	0/67466	0.44	0/91483

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	4	0
2	B	1241	0	1251	9	0
3	C	1721	0	1675	7	0
4	D	3459	0	3404	25	0
5	E	1655	0	1661	13	0
6	F	3310	0	3266	16	0
7	G	5279	0	5301	26	0
8	H	2509	0	2621	20	0
9	I	1414	0	1370	5	0
10	J	1337	0	1346	15	0
11	K	745	0	785	5	0
12	L	4791	0	4942	43	0
13	M	3654	0	3852	21	0
14	N	2733	0	2912	17	0
15	O	2589	0	2566	19	0
16	P	2747	0	2766	16	0
17	Q	1016	0	1014	4	0
18	R	730	0	707	1	0
19	S	677	0	688	3	0
20	T	612	0	604	10	0
20	U	693	0	688	3	0
21	V	911	0	950	7	0
22	W	971	0	989	4	0
23	X	1402	0	1383	8	0
24	Y	1030	0	1039	7	0
25	Z	1146	0	1146	14	0
26	a	569	0	568	0	0
27	b	646	0	654	0	0
28	c	405	0	409	0	0
29	d	945	0	932	0	0
30	e	819	0	821	0	0
31	f	451	0	453	0	0
32	g	824	0	772	0	0
33	h	1154	0	1168	0	0
34	i	879	0	892	0	0
35	j	580	0	519	0	0
36	k	638	0	621	0	0
37	l	1304	0	1203	0	0
38	m	1061	0	1059	0	0
39	n	1492	0	1438	0	0
40	o	1035	0	1003	0	0
41	p	1443	0	1415	0	0
42	q	1209	0	1182	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	r	767	0	776	0	0
44	s	371	0	344	0	0
45	A	70	0	92	1	0
45	J	35	0	46	1	0
45	L	105	0	138	1	0
45	M	105	0	138	4	0
45	N	35	0	46	0	0
45	Y	105	0	138	4	0
45	h	35	0	46	0	0
45	j	35	0	46	0	0
45	l	35	0	46	0	0
46	A	21	0	18	1	0
46	B	89	0	132	2	0
46	L	49	0	75	0	0
47	B	8	0	0	1	0
47	F	8	0	0	1	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	2	0
50	G	1	0	0	0	0
51	H	78	0	112	1	0
51	I	51	0	82	0	0
51	L	94	0	142	0	0
51	M	97	0	151	4	0
51	N	121	0	170	2	0
51	P	37	0	48	0	0
51	X	51	0	82	4	0
51	Y	35	0	44	0	0
51	d	51	0	82	0	0
52	J	62	0	68	1	0
52	K	71	0	86	0	0
52	L	69	0	82	0	0
52	h	67	0	81	0	0
52	q	76	0	96	0	0
53	N	17	0	0	1	0
54	O	32	0	12	3	0
55	O	1	0	0	0	0
56	P	48	0	26	1	0
57	R	1	0	0	0	0
58	T	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	U	37	0	0	0	0
59	o	6	0	6	0	0
60	A	21	0	0	0	0
60	B	62	0	0	2	0
60	C	83	0	0	3	0
60	D	155	0	0	9	0
60	E	13	0	0	1	0
60	F	59	0	0	3	0
60	G	183	0	0	7	0
60	H	61	0	0	2	0
60	I	91	0	0	3	0
60	J	21	0	0	1	0
60	K	15	0	0	0	0
60	L	31	0	0	2	0
60	M	49	0	0	3	0
60	N	49	0	0	3	0
60	O	21	0	0	2	0
60	P	58	0	0	1	0
60	Q	59	0	0	1	0
60	R	39	0	0	0	0
60	S	2	0	0	0	0
60	V	15	0	0	2	0
60	W	10	0	0	1	0
60	X	23	0	0	3	0
60	Y	3	0	0	0	0
60	Z	24	0	0	2	0
60	a	11	0	0	0	0
60	b	7	0	0	0	0
60	d	9	0	0	0	0
60	e	15	0	0	0	0
60	f	1	0	0	0	0
60	g	4	0	0	0	0
60	h	15	0	0	0	0
60	i	2	0	0	0	0
60	j	1	0	0	0	0
60	k	2	0	0	0	0
60	l	3	0	0	0	0
60	m	7	0	0	0	0
60	n	9	0	0	0	0
60	p	10	0	0	0	0
60	q	35	0	0	0	0
60	r	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	s	4	0	0	0	0
All	All	69138	0	68457	313	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (313) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:479:GLN:NE2	12:L:481:THR:O	2.08	0.87
16:P:51:CYS:O	60:P:601:HOH:O	1.96	0.83
21:V:105:GLU:O	60:V:201:HOH:O	1.94	0.83
4:D:72:MET:SD	60:D:653:HOH:O	2.35	0.82
2:B:44:SER:OG	8:H:51:ASP:OD1	1.97	0.82
9:I:43:ARG:O	60:I:301:HOH:O	1.97	0.82
15:O:83:TYR:HH	54:O:401:GTP:HO3'	1.19	0.81
6:F:306:LEU:O	60:F:601:HOH:O	1.98	0.81
12:L:562:LEU:HD13	45:M:602:LMT:H123	1.62	0.81
45:A:302:LMT:H3O2	45:A:302:LMT:H2O1	1.25	0.81
6:F:144:ASN:OD1	60:F:602:HOH:O	1.99	0.80
53:N:1305:I49:N05	60:N:1403:HOH:O	2.15	0.79
5:E:61:LEU:O	60:E:401:HOH:O	1.99	0.79
23:X:139:ASN:OD1	60:X:501:HOH:O	2.00	0.79
3:C:158:GLU:OE2	60:C:301:HOH:O	2.01	0.79
4:D:427:GLU:OE1	60:D:501:HOH:O	1.99	0.78
15:O:88:SER:OG	15:O:90:ASP:OD1	2.01	0.78
52:J:701:CDL:OB4	60:J:801:HOH:O	2.03	0.77
7:G:265:ASP:OD2	60:G:901:HOH:O	2.03	0.75
3:C:155:TYR:O	60:C:302:HOH:O	2.05	0.75
12:L:190:LEU:O	60:L:801:HOH:O	2.04	0.75
25:Z:66:GLU:OE1	60:Z:201:HOH:O	2.04	0.75
2:B:162:GLN:OE1	9:I:140:SER:OG	2.05	0.74
17:Q:132:THR:O	60:Q:201:HOH:O	2.04	0.74
15:O:110:ASP:O	60:O:501:HOH:O	2.05	0.74
23:X:149:PRO:O	60:X:502:HOH:O	2.04	0.74
13:M:173:SER:OG	60:M:701:HOH:O	2.05	0.73
12:L:197:ASP:OD1	60:L:802:HOH:O	2.07	0.73
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.21	0.73
2:B:34:ASP:OD1	60:B:302:HOH:O	2.06	0.72
4:D:266:GLN:OE1	60:D:502:HOH:O	2.08	0.71
6:F:370:ASP:OD2	60:F:603:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:175:TYR:O	60:I:302:HOH:O	2.07	0.71
14:N:308:THR:O	60:N:1401:HOH:O	2.09	0.70
45:Y:801:LMT:O5B	45:Y:801:LMT:O6'	2.06	0.70
7:G:665:GLN:OE1	60:G:903:HOH:O	2.10	0.69
13:M:81:GLN:OE1	60:M:702:HOH:O	2.09	0.69
4:D:422:ASP:OD2	60:D:503:HOH:O	2.10	0.69
7:G:109:ASP:OD2	60:G:902:HOH:O	2.09	0.69
3:C:66:ASP:OD2	60:C:303:HOH:O	2.08	0.69
6:F:291:TRP:NE1	6:F:313:GLU:OE1	2.26	0.69
9:I:124:GLU:OE2	60:I:303:HOH:O	2.11	0.68
12:L:562:LEU:HD13	45:M:602:LMT:C12	2.24	0.68
20:T:35:HIS:N	20:T:39:ASP:OD2	2.26	0.68
51:H:401:3PE:O14	60:H:502:HOH:O	2.12	0.68
4:D:3:GLN:NE2	13:M:137:GLY:O	2.26	0.67
21:V:110:GLN:OE1	60:V:202:HOH:O	2.12	0.67
14:N:289:ASN:OD1	60:N:1402:HOH:O	2.11	0.67
19:S:13:LEU:HD12	19:S:13:LEU:O	1.95	0.67
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.32	0.65
14:N:128:LEU:O	14:N:132:THR:OG1	2.13	0.65
23:X:29:HIS:ND1	60:X:503:HOH:O	2.30	0.64
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.80	0.64
20:T:9:GLU:OE2	20:T:9:GLU:N	2.31	0.63
14:N:162:ILE:HD13	14:N:282:MET:HG2	1.81	0.62
12:L:173:LEU:HD12	13:M:405:LEU:HD21	1.80	0.62
13:M:306:PRO:HA	13:M:458:LEU:HD22	1.81	0.62
1:A:61:THR:HG21	1:A:105:GLU:OE2	2.01	0.61
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.30	0.61
3:C:183:VAL:O	22:W:101:THR:OG1	2.16	0.61
7:G:475:GLN:O	7:G:479:THR:HG23	2.02	0.60
23:X:152:GLU:OE1	23:X:153:VAL:N	2.34	0.60
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.84	0.60
12:L:102:GLU:OE2	12:L:456:ARG:NH2	2.34	0.60
45:J:702:LMT:O3'	45:J:702:LMT:O2B	2.17	0.59
10:J:124:ASP:OD2	11:K:4:VAL:HB	2.02	0.59
10:J:115:VAL:HG23	10:J:115:VAL:O	2.02	0.59
45:Y:804:LMT:O6'	45:Y:804:LMT:O4'	2.18	0.59
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.84	0.58
10:J:153:LEU:O	10:J:157:THR:HG23	2.03	0.58
10:J:77:GLU:OE2	10:J:77:GLU:N	2.36	0.58
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.38	0.58
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:42:ILE:HD11	15:O:234:VAL:HG11	1.85	0.57
18:R:2:VAL:HG11	18:R:37:GLU:OE2	2.04	0.57
1:A:51:PHE:CD1	8:H:133:LEU:HD13	2.38	0.57
4:D:302:GLU:OE1	60:D:504:HOH:O	2.17	0.57
16:P:330:GLU:N	16:P:333:ASP:OD2	2.37	0.57
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.15	0.57
46:B:202:PC1:O12	60:B:303:HOH:O	2.18	0.57
16:P:311:GLU:OE1	16:P:311:GLU:N	2.39	0.56
24:Y:21:THR:O	24:Y:25:THR:OG1	2.18	0.56
24:Y:61:THR:HG21	45:Y:804:LMT:H6D	1.86	0.56
2:B:54:CYS:HB2	47:B:201:SF4:S1	2.46	0.56
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.88	0.56
23:X:8:SER:N	23:X:11:ASP:OD2	2.39	0.56
12:L:6:SER:O	12:L:10:VAL:HG13	2.05	0.56
16:P:194:ILE:HD12	16:P:288:HIS:ND1	2.21	0.56
20:T:55:GLU:HG2	20:T:62:ILE:HD13	1.87	0.56
15:O:50:HIS:NE2	15:O:125:GLU:OE2	2.38	0.55
12:L:467:ILE:O	12:L:471:ASN:ND2	2.34	0.55
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.89	0.55
8:H:163:SER:OG	60:H:503:HOH:O	2.18	0.55
46:A:303:PC1:O13	46:A:303:PC1:H132	2.06	0.54
7:G:596:ASP:OD2	60:G:905:HOH:O	2.18	0.54
15:O:138:MET:CE	54:O:401:GTP:HN21	2.21	0.54
24:Y:11:ILE:O	24:Y:20:LYS:NZ	2.32	0.54
10:J:170:GLU:OE2	10:J:173:ARG:NH1	2.38	0.54
25:Z:93:GLU:O	25:Z:97:VAL:HG23	2.07	0.54
16:P:26:ALA:HB3	16:P:47:VAL:HG13	1.90	0.53
25:Z:98:MET:CE	25:Z:101:VAL:HG21	2.39	0.53
15:O:97:GLN:NE2	15:O:131:ASP:OD1	2.42	0.53
13:M:293:HIS:ND1	60:M:704:HOH:O	2.34	0.53
7:G:272:ASP:OD1	7:G:681:SER:OG	2.17	0.53
51:X:401:3PE:H3I1	51:X:401:3PE:H261	1.91	0.52
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.42	0.52
7:G:23:GLY:O	60:G:906:HOH:O	2.19	0.52
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.90	0.52
25:Z:68:ARG:NH1	60:Z:202:HOH:O	2.42	0.52
7:G:375:ASP:OD2	7:G:446:ALA:HB1	2.09	0.52
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.39	0.52
14:N:242:VAL:HG11	51:N:1301:3PE:H332	1.92	0.52
1:A:71:LEU:O	10:J:147:TYR:OH	2.20	0.52
23:X:8:SER:OG	23:X:11:ASP:OD2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.91	0.51
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.45	0.51
2:B:91:THR:HA	2:B:119:CYS:HB3	1.91	0.51
8:H:18:ALA:O	8:H:21:THR:OG1	2.23	0.51
4:D:111:MET:H	4:D:111:MET:HE2	1.76	0.51
6:F:224:ASN:ND2	49:F:501:FMN:O2	2.41	0.51
12:L:564:LYS:NZ	45:M:602:LMT:O6B	2.33	0.51
20:T:61:GLU:C	20:T:62:ILE:HD12	2.31	0.50
3:C:58:ILE:O	3:C:62:THR:OG1	2.23	0.50
21:V:57:MET:HE2	21:V:71:LEU:HD23	1.92	0.50
16:P:293:ILE:HG22	16:P:295:PRO:HD3	1.93	0.50
20:T:62:ILE:HD12	20:T:62:ILE:N	2.27	0.50
25:Z:98:MET:HE3	25:Z:101:VAL:HG21	1.93	0.50
19:S:92:ASN:O	19:S:96:SER:N	2.44	0.50
12:L:28:LYS:O	12:L:30:SER:N	2.44	0.50
5:E:183:LYS:O	5:E:187:ARG:NH1	2.45	0.49
23:X:97:ARG:HD2	25:Z:60:LEU:HD13	1.93	0.49
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.94	0.49
25:Z:98:MET:HE2	25:Z:104:TRP:CD2	2.48	0.49
4:D:13:GLN:O	60:D:506:HOH:O	2.20	0.48
6:F:374:LYS:NZ	7:G:133:GLY:O	2.46	0.48
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.95	0.48
13:M:217:PRO:O	13:M:221:VAL:HG23	2.13	0.48
12:L:233:LEU:HB3	12:L:234:PRO:HD3	1.95	0.48
12:L:562:LEU:CB	12:L:563:PRO:CD	2.91	0.48
14:N:342:MET:O	14:N:345:VAL:HG22	2.13	0.48
51:M:601:3PE:H3C2	14:N:284:ILE:HG21	1.96	0.48
9:I:75:GLU:O	9:I:105:ARG:NH1	2.46	0.48
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.96	0.48
20:T:8:LEU:HD23	20:T:8:LEU:O	2.12	0.48
10:J:133:SER:O	10:J:133:SER:OG	2.32	0.48
3:C:112:ASP:OD1	3:C:115:THR:OG1	2.17	0.48
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.96	0.48
8:H:236:ILE:HG23	8:H:259:PHE:CE1	2.49	0.48
22:W:125:GLY:O	60:W:201:HOH:O	2.20	0.48
24:Y:104:THR:HG22	24:Y:104:THR:O	2.13	0.47
16:P:208:VAL:HG12	16:P:212:LYS:HD2	1.96	0.47
5:E:181:ILE:HG23	5:E:181:ILE:O	2.13	0.47
4:D:366:ALA:O	60:D:505:HOH:O	2.20	0.47
20:U:12:LYS:HD2	20:U:32:VAL:HG11	1.96	0.47
46:B:203:PC1:O13	46:B:203:PC1:H133	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:100:MET:O	14:N:104:MET:HG3	2.14	0.47
20:U:47:GLN:NE2	20:U:70:LEU:O	2.48	0.47
13:M:135:ARG:NH1	14:N:301:THR:O	2.48	0.47
15:O:104:ARG:NH2	54:O:401:GTP:O6	2.48	0.47
12:L:559:GLU:HG2	13:M:214:LEU:HD13	1.96	0.46
10:J:125:TRP:HB2	25:Z:137:THR:HG21	1.97	0.46
7:G:540:ASP:OD1	7:G:540:ASP:N	2.45	0.46
12:L:421:ILE:HA	12:L:501:ALA:HB2	1.97	0.46
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.95	0.46
15:O:224:SER:OG	15:O:225:ALA:N	2.46	0.46
12:L:264:TYR:N	12:L:265:PRO:CD	2.79	0.46
51:M:605:3PE:H2I3	51:X:401:3PE:H3F2	1.97	0.46
7:G:255:HIS:CD2	7:G:258:ILE:HD12	2.51	0.46
12:L:230:HIS:N	12:L:231:PRO:CD	2.78	0.46
10:J:157:THR:HG21	11:K:62:ILE:HD12	1.98	0.46
15:O:21:LYS:O	15:O:21:LYS:NZ	2.40	0.46
22:W:42:GLU:OE2	22:W:42:GLU:HA	2.16	0.46
6:F:184:TYR:CE2	49:F:501:FMN:HM73	2.51	0.45
7:G:281:GLU:HG2	7:G:592:LEU:HD12	1.98	0.45
7:G:588:THR:OG1	60:G:904:HOH:O	2.13	0.45
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.51	0.45
7:G:185:THR:O	7:G:187:ILE:N	2.49	0.45
12:L:208:ASP:CG	12:L:208:ASP:O	2.55	0.45
20:U:51:ILE:HG21	20:U:67:ALA:HB1	1.99	0.45
8:H:264:LEU:O	8:H:268:MET:HG2	2.15	0.45
2:B:86:MET:CE	2:B:103:VAL:HG23	2.46	0.45
5:E:12:THR:HG23	5:E:13:PRO:HD2	1.99	0.45
11:K:37:MET:HG2	11:K:67:ALA:HB2	1.99	0.45
12:L:529:PHE:HB3	12:L:530:PRO:HD3	1.99	0.45
5:E:217:LEU:HD22	6:F:44:LYS:CE	2.47	0.45
20:T:74:GLN:NE2	20:T:78:ASP:OD2	2.45	0.45
7:G:377:VAL:HG13	7:G:452:ILE:HD12	1.99	0.45
8:H:170:GLU:OE2	23:X:97:ARG:NH1	2.48	0.45
8:H:179:TRP:N	8:H:180:PRO:CD	2.80	0.45
12:L:233:LEU:HD11	12:L:248:HIS:NE2	2.31	0.45
12:L:597:ILE:HD12	12:L:598:SER:N	2.32	0.45
12:L:562:LEU:HB2	12:L:563:PRO:CD	2.47	0.45
5:E:134:ASP:OD1	5:E:134:ASP:N	2.40	0.44
13:M:413:MET:HA	13:M:413:MET:HE2	1.99	0.44
4:D:151:ILE:HG21	4:D:174:ARG:HG3	2.00	0.44
12:L:246:LEU:O	12:L:251:THR:OG1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:178:GLU:OE1	15:O:178:GLU:HA	2.17	0.44
2:B:152:THR:HG22	4:D:188:ARG:HD3	1.99	0.44
12:L:483:PRO:HD2	12:L:486:LEU:HD12	1.98	0.44
13:M:12:MET:HB2	13:M:13:PRO:HD3	1.99	0.44
15:O:198:TYR:CE2	15:O:202:ILE:HD11	2.53	0.44
15:O:26:THR:HG21	60:O:507:HOH:O	2.18	0.44
16:P:335:GLN:CD	16:P:335:GLN:H	2.21	0.44
4:D:160:ASP:OD2	60:D:507:HOH:O	2.21	0.44
8:H:32:GLN:OE1	8:H:34:ARG:NH1	2.50	0.44
12:L:148:GLY:HA2	12:L:252:MET:HE3	1.98	0.44
16:P:194:ILE:HD12	16:P:288:HIS:CE1	2.52	0.44
21:V:34:LEU:HD13	21:V:48:GLU:HG3	1.99	0.44
21:V:34:LEU:HD23	21:V:37:ILE:HD12	1.99	0.44
7:G:39:ARG:NH1	60:G:914:HOH:O	2.37	0.44
7:G:254:MET:HA	7:G:260:GLU:O	2.18	0.44
13:M:126:LEU:HD21	13:M:153:THR:HG21	2.00	0.44
10:J:33:LEU:HD23	10:J:64:MET:SD	2.57	0.44
14:N:337:LEU:HD23	51:X:401:3PE:H391	1.98	0.44
15:O:21:LYS:O	15:O:21:LYS:HG2	2.18	0.44
25:Z:131:GLU:OE2	25:Z:131:GLU:HA	2.18	0.44
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.18	0.43
20:T:30:LEU:HD12	20:T:34:SER:OG	2.18	0.43
21:V:57:MET:CE	21:V:71:LEU:HD23	2.48	0.43
7:G:462:ASP:HB3	7:G:657:LEU:HD13	2.00	0.43
16:P:258:LEU:HD21	16:P:266:ILE:CD1	2.48	0.43
16:P:260:HIS:NE2	16:P:285:GLU:OE1	2.40	0.43
12:L:27:TYR:HA	45:L:706:LMT:O2'	2.18	0.43
4:D:296:ARG:HH21	4:D:420:THR:HG21	1.84	0.43
5:E:96:GLY:N	5:E:138:THR:OG1	2.43	0.43
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.53	0.43
4:D:151:ILE:HG23	4:D:170:MET:HB3	2.01	0.43
12:L:10:VAL:O	12:L:14:LEU:HB2	2.19	0.43
5:E:105:THR:HG22	5:E:106:THR:H	1.83	0.43
7:G:20:VAL:HG21	7:G:73:VAL:HG21	2.00	0.43
13:M:191:SER:OG	51:M:601:3PE:O22	2.37	0.43
12:L:442:ASN:ND2	12:L:442:ASN:O	2.52	0.43
16:P:236:TYR:CE2	16:P:339:THR:HG22	2.53	0.43
45:Y:801:LMT:H6'	45:Y:801:LMT:C1B	2.25	0.43
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.01	0.43
7:G:568:GLU:HA	7:G:587:VAL:O	2.19	0.43
11:K:8:ILE:HG22	11:K:43:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:41:VAL:O	19:S:45:LYS:HG2	2.18	0.43
7:G:297:GLU:HG3	22:W:123:TYR:CZ	2.54	0.43
12:L:407:TRP:CZ3	12:L:410:LEU:HD23	2.54	0.43
4:D:324:LYS:NZ	60:D:511:HOH:O	2.34	0.42
5:E:120:ILE:HD11	5:E:169:ILE:HG12	2.01	0.42
10:J:170:GLU:OE1	10:J:173:ARG:NH2	2.49	0.42
13:M:379:LEU:O	13:M:383:MET:HG2	2.19	0.42
25:Z:120:MET:HG2	25:Z:123:GLU:OE2	2.19	0.42
4:D:73:VAL:HG21	4:D:414:VAL:HG21	2.00	0.42
7:G:145:LEU:HD21	7:G:687:CYS:SG	2.58	0.42
20:T:73:PRO:O	20:T:77:VAL:HG23	2.18	0.42
8:H:87:ILE:N	8:H:88:PRO:CD	2.82	0.42
8:H:87:ILE:HG12	8:H:88:PRO:HD3	2.01	0.42
13:M:452:LYS:HA	13:M:455:LEU:HD12	2.02	0.42
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.52	0.42
24:Y:115:ALA:O	24:Y:119:LEU:HD12	2.19	0.42
12:L:272:TYR:CZ	12:L:276:ILE:HD11	2.54	0.42
15:O:110:ASP:OD1	15:O:266:LYS:NZ	2.38	0.42
4:D:294:TYR:CE2	4:D:298:LEU:HD11	2.55	0.42
20:T:8:LEU:HD23	20:T:8:LEU:C	2.40	0.42
8:H:70:MET:HB3	8:H:122:ALA:HB2	2.01	0.42
13:M:243:MET:HB3	13:M:301:ILE:HG21	2.02	0.42
4:D:409:HIS:HB3	4:D:413:ASP:HB2	2.02	0.42
5:E:87:TYR:HB3	6:F:181:ALA:O	2.19	0.42
6:F:327:THR:OG1	6:F:328:GLY:N	2.53	0.42
6:F:362:CYS:HB3	6:F:404:ILE:HD12	2.02	0.42
8:H:195:ARG:HD3	8:H:231:ILE:HD11	2.02	0.42
12:L:96:VAL:HG12	12:L:100:ILE:HD12	2.00	0.42
21:V:57:MET:HE1	21:V:71:LEU:HA	2.02	0.42
5:E:192:SER:OG	5:E:193:CYS:N	2.52	0.41
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.02	0.41
8:H:179:TRP:O	8:H:183:MET:HG3	2.20	0.41
12:L:597:ILE:HD12	12:L:597:ILE:C	2.41	0.41
10:J:5:ILE:HG23	10:J:6:VAL:N	2.36	0.41
7:G:526:GLY:N	7:G:546:GLN:O	2.51	0.41
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.55	0.41
10:J:33:LEU:HD23	10:J:64:MET:CE	2.51	0.41
51:M:601:3PE:H2I1	45:M:602:LMT:H111	2.03	0.41
8:H:209:SER:HB3	8:H:213:VAL:HA	2.03	0.41
16:P:97:ARG:NH2	56:P:501:NDP:O2X	2.51	0.41
25:Z:13:VAL:HG13	25:Z:14:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:3:THR:O	24:Y:7:GLN:HG3	2.21	0.41
2:B:92:LEU:HD13	2:B:100:LEU:HD13	2.03	0.41
4:D:72:MET:SD	4:D:410:MET:HG2	2.61	0.41
12:L:261:ILE:HG13	12:L:317:ILE:HD11	2.03	0.41
13:M:66:LEU:HD11	13:M:111:THR:HG23	2.02	0.41
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.03	0.41
14:N:96:MET:O	14:N:100:MET:HG3	2.20	0.41
25:Z:89:GLU:OE2	25:Z:128:ARG:NH2	2.54	0.41
6:F:403:THR:HB	47:F:502:SF4:S4	2.61	0.41
8:H:227:GLU:HA	8:H:227:GLU:OE1	2.21	0.41
10:J:125:TRP:CB	25:Z:137:THR:HG21	2.51	0.41
11:K:19:LEU:HD22	11:K:36:MET:HE3	2.03	0.41
12:L:605:HIS:HB2	14:N:93:MET:SD	2.61	0.41
13:M:76:MET:SD	13:M:230:VAL:HB	2.61	0.41
14:N:146:PHE:N	14:N:147:PRO:CD	2.84	0.41
14:N:307:SER:OG	14:N:308:THR:N	2.54	0.41
5:E:103:CYS:SG	5:E:144:CYS:HA	2.61	0.41
12:L:230:HIS:N	12:L:231:PRO:HD3	2.36	0.41
16:P:176:ASP:C	16:P:176:ASP:OD1	2.60	0.41
6:F:93:LEU:O	6:F:134:ALA:HA	2.21	0.40
15:O:176:VAL:HG23	15:O:203:GLU:OE1	2.21	0.40
2:B:116:MET:HG3	2:B:156:LEU:HD13	2.02	0.40
12:L:24:PHE:CD1	12:L:24:PHE:N	2.88	0.40
15:O:180:GLN:O	15:O:184:GLN:HG2	2.21	0.40
12:L:195:THR:HG21	12:L:200:GLN:HB3	2.04	0.40
16:P:258:LEU:HD21	16:P:266:ILE:HD12	2.02	0.40
25:Z:92:GLU:OE1	25:Z:92:GLU:HA	2.22	0.40
4:D:62:LEU:HB2	4:D:425:PHE:CZ	2.56	0.40
4:D:155:THR:HB	4:D:167:PHE:HA	2.04	0.40
4:D:371:LYS:HG2	4:D:422:ASP:OD2	2.21	0.40
12:L:373:LEU:HD23	12:L:431:LEU:HD11	2.02	0.40
16:P:145:TYR:CD1	16:P:286:ARG:HD3	2.56	0.40
4:D:123:GLU:OE1	4:D:138:ARG:NH2	2.53	0.40
51:N:1301:3PE:H3H2	51:X:401:3PE:H3I3	2.02	0.40
24:Y:3:THR:CG2	24:Y:4:VAL:N	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
2	B	153/216 (71%)	146 (95%)	7 (5%)	0	100	100
3	C	205/266 (77%)	200 (98%)	5 (2%)	0	100	100
4	D	427/463 (92%)	415 (97%)	12 (3%)	0	100	100
5	E	211/249 (85%)	206 (98%)	5 (2%)	0	100	100
6	F	428/464 (92%)	420 (98%)	8 (2%)	0	100	100
7	G	686/727 (94%)	668 (97%)	18 (3%)	0	100	100
8	H	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
9	I	174/212 (82%)	169 (97%)	5 (3%)	0	100	100
10	J	172/175 (98%)	161 (94%)	11 (6%)	0	100	100
11	K	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
12	L	604/606 (100%)	580 (96%)	23 (4%)	1 (0%)	47	58
13	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	313 (98%)	5 (2%)	0	100	100
16	P	339/380 (89%)	332 (98%)	7 (2%)	0	100	100
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	93/124 (75%)	90 (97%)	3 (3%)	0	100	100
19	S	82/99 (83%)	80 (98%)	2 (2%)	0	100	100
20	T	74/156 (47%)	73 (99%)	1 (1%)	0	100	100
20	U	84/156 (54%)	83 (99%)	1 (1%)	0	100	100
21	V	110/116 (95%)	109 (99%)	1 (1%)	0	100	100
22	W	112/128 (88%)	109 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	168 (99%)	1 (1%)	0	100	100
24	Y	138/141 (98%)	134 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	138/144 (96%)	135 (98%)	2 (1%)	1 (1%)	22	26
26	a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
27	b	80/84 (95%)	76 (95%)	4 (5%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100
29	d	111/120 (92%)	110 (99%)	1 (1%)	0	100	100
30	e	95/106 (90%)	93 (98%)	2 (2%)	0	100	100
31	f	50/57 (88%)	49 (98%)	1 (2%)	0	100	100
32	g	96/154 (62%)	91 (95%)	5 (5%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	98/127 (77%)	95 (97%)	3 (3%)	0	100	100
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	77/98 (79%)	76 (99%)	1 (1%)	0	100	100
37	l	153/186 (82%)	149 (97%)	4 (3%)	0	100	100
38	m	125/129 (97%)	121 (97%)	4 (3%)	0	100	100
39	n	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
40	o	118/137 (86%)	113 (96%)	5 (4%)	0	100	100
41	p	169/176 (96%)	167 (99%)	2 (1%)	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
All	All	8099/9212 (88%)	7899 (98%)	198 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
25	Z	102	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	100 (100%)	0	100	100
2	B	131/175 (75%)	127 (97%)	4 (3%)	40	55
3	C	188/228 (82%)	188 (100%)	0	100	100
4	D	370/392 (94%)	367 (99%)	3 (1%)	81	91
5	E	183/205 (89%)	182 (100%)	1 (0%)	88	95
6	F	344/368 (94%)	335 (97%)	9 (3%)	46	63
7	G	578/608 (95%)	570 (99%)	8 (1%)	67	81
8	H	274/274 (100%)	268 (98%)	6 (2%)	52	69
9	I	151/175 (86%)	150 (99%)	1 (1%)	84	92
10	J	140/141 (99%)	138 (99%)	2 (1%)	67	81
11	K	85/85 (100%)	82 (96%)	3 (4%)	36	50
12	L	531/533 (100%)	523 (98%)	8 (2%)	65	79
13	M	412/412 (100%)	404 (98%)	8 (2%)	57	73
14	N	315/315 (100%)	312 (99%)	3 (1%)	76	87
15	O	283/303 (93%)	274 (97%)	9 (3%)	39	54
16	P	295/327 (90%)	292 (99%)	3 (1%)	76	87
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	78/97 (80%)	76 (97%)	2 (3%)	46	63
19	S	75/82 (92%)	72 (96%)	3 (4%)	31	44
20	T	70/135 (52%)	67 (96%)	3 (4%)	29	40
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	107/114 (94%)	106 (99%)	1 (1%)	78	89
23	X	154/155 (99%)	151 (98%)	3 (2%)	57	73
24	Y	101/102 (99%)	98 (97%)	3 (3%)	41	57
25	Z	119/121 (98%)	117 (98%)	2 (2%)	60	76
26	a	59/59 (100%)	58 (98%)	1 (2%)	60	76
27	b	71/72 (99%)	69 (97%)	2 (3%)	43	60
28	c	44/68 (65%)	40 (91%)	4 (9%)	9	11
29	d	101/105 (96%)	100 (99%)	1 (1%)	76	87
30	e	88/96 (92%)	85 (97%)	3 (3%)	37	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	f	49/54 (91%)	47 (96%)	2 (4%)	30 43
32	g	89/131 (68%)	82 (92%)	7 (8%)	12 15
33	h	121/158 (77%)	120 (99%)	1 (1%)	81 91
34	i	97/120 (81%)	95 (98%)	2 (2%)	53 70
35	j	61/84 (73%)	57 (93%)	4 (7%)	16 22
36	k	61/76 (80%)	60 (98%)	1 (2%)	62 78
37	l	139/159 (87%)	137 (99%)	2 (1%)	67 81
38	m	113/115 (98%)	110 (97%)	3 (3%)	44 61
39	n	156/161 (97%)	154 (99%)	2 (1%)	69 82
40	o	109/120 (91%)	104 (95%)	5 (5%)	27 38
41	p	155/157 (99%)	153 (99%)	2 (1%)	69 82
42	q	131/131 (100%)	129 (98%)	2 (2%)	65 79
43	r	84/97 (87%)	82 (98%)	2 (2%)	49 66
44	s	43/92 (47%)	43 (100%)	0	100 100
All	All	7146/7892 (90%)	7015 (98%)	131 (2%)	61 75

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	32	LYS
2	B	34	ASP
2	B	91	THR
2	B	125	TYR
4	D	29	LYS
4	D	61	VAL
4	D	111	MET
5	E	203	THR
6	F	11	SER
6	F	54	ASP
6	F	84	LYS
6	F	86	SER
6	F	105	CYS
6	F	231	SER
6	F	248	GLU
6	F	355	LYS
6	F	405	CYS
7	G	35	MET

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Mol	Chain	Res	Type
7	G	39	ARG
7	G	84	GLU
7	G	188	GLU
7	G	292	THR
7	G	447	LYS
7	G	481	SER
7	G	512	GLU
8	H	103	LEU
8	H	138	GLN
8	H	209	SER
8	H	237	PHE
8	H	259	PHE
8	H	289	LEU
9	I	1	THR
10	J	133	SER
10	J	135	PHE
11	K	46	LEU
11	K	52	HIS
11	K	53	PHE
12	L	3	MET
12	L	24	PHE
12	L	124	PHE
12	L	199	GLN
12	L	208	ASP
12	L	252	MET
12	L	262	ARG
12	L	551	SER
13	M	57	PHE
13	M	72	LEU
13	M	80	SER
13	M	114	GLU
13	M	116	ILE
13	M	393	ILE
13	M	406	TYR
13	M	427	SER
14	N	204	ASN
14	N	223	SER
14	N	250	SER
15	O	18	MET
15	O	21	LYS
15	O	140	ARG
15	O	182	ARG

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Mol	Chain	Res	Type
15	O	196	SER
15	O	206	TYR
15	O	224	SER
15	O	226	TRP
15	O	250	ASP
16	P	73	TRP
16	P	263	TYR
16	P	264	ARG
18	R	4	THR
18	R	34	GLU
19	S	25	ARG
19	S	38	LYS
19	S	74	LYS
20	T	13	ASP
20	T	31	SER
20	T	37	MET
22	W	89	GLU
23	X	13	LYS
23	X	152	GLU
23	X	154	GLU
24	Y	5	LEU
24	Y	76	SER
24	Y	105	ARG
25	Z	106	VAL
25	Z	130	SER
26	a	70	ASP
27	b	33	THR
27	b	61	ASN
28	c	1	LYS
28	c	6	GLU
28	c	11	SER
28	c	33	LYS
29	d	95	LYS
30	e	15	ARG
30	e	18	THR
30	e	97	HIS
31	f	8	ARG
31	f	30	ASN
32	g	26	TRP
32	g	57	ASN
32	g	86	GLN
32	g	109	GLU

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Mol	Chain	Res	Type
32	g	112	CYS
32	g	116	SER
32	g	122	GLU
33	h	23	LYS
34	i	12	GLN
34	i	120	LYS
35	j	6	HIS
35	j	40	PHE
35	j	44	SER
35	j	70	ASP
36	k	12	LYS
37	l	4	ILE
37	l	25	LYS
38	m	26	SER
38	m	29	ARG
38	m	84	LYS
39	n	8	TYR
39	n	84	SER
40	o	21	MET
40	o	69	LYS
40	o	80	LYS
40	o	109	GLN
40	o	111	LYS
41	p	42	ARG
41	p	126	LYS
42	q	26	VAL
42	q	145	LYS
43	r	60	ARG
43	r	104	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
16	P	87	HIS
35	j	6	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
34	SAC	i	1	34	7,8,9	0.97	0	8,9,11	1.29	2 (25%)
1	FME	A	1	1	8,9,10	0.92	0	7,9,11	1.13	1 (14%)
10	FME	J	1	10	8,9,10	0.96	0	7,9,11	0.99	0
8	FME	H	1	8	8,9,10	0.96	0	7,9,11	0.78	0
14	FME	N	1	14	8,9,10	0.93	0	7,9,11	1.05	0
4	2MR	D	85	4	10,12,13	2.62	4 (40%)	5,13,15	1.15	1 (20%)
43	AYA	r	1	43	6,7,8	1.80	2 (33%)	5,8,10	1.28	1 (20%)
11	FME	K	1	11	8,9,10	0.93	0	7,9,11	0.86	0
12	FME	L	1	12	8,9,10	0.99	1 (12%)	7,9,11	0.75	0
13	FME	M	1	13	8,9,10	0.99	1 (12%)	7,9,11	1.01	1 (14%)
24	AYA	Y	1	24	6,7,8	1.79	2 (33%)	5,8,10	1.38	1 (20%)

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
34	SAC	i	1	34	-	2/7/8/10	-
1	FME	A	1	1	-	0/7/9/11	-
10	FME	J	1	10	-	3/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
43	AYA	r	1	43	-	0/4/6/8	-
11	FME	K	1	11	-	1/7/9/11	-
12	FME	L	1	12	-	2/7/9/11	-
13	FME	M	1	13	-	0/7/9/11	-
24	AYA	Y	1	24	-	0/4/6/8	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.86	1.44	1.33
4	D	85	2MR	CZ-NE	4.54	1.44	1.34
4	D	85	2MR	O-C	3.94	1.35	1.19
24	Y	1	AYA	CT-N	3.26	1.45	1.34
43	r	1	AYA	CT-N	3.13	1.45	1.34
4	D	85	2MR	CQ1-NH1	-2.17	1.42	1.46
43	r	1	AYA	OT-CT	-2.16	1.18	1.23
12	L	1	FME	CA-N	-2.06	1.43	1.46
13	M	1	FME	CA-N	-2.06	1.43	1.46
24	Y	1	AYA	OT-CT	-2.00	1.18	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	1	SAC	C-CA-N	2.55	114.33	109.73
1	A	1	FME	C-CA-N	2.47	114.18	109.73
24	Y	1	AYA	CM-CT-N	2.37	120.11	116.10
4	D	85	2MR	NE-CZ-NH2	-2.31	117.36	119.48
43	r	1	AYA	CM-CT-N	2.27	119.94	116.10
13	M	1	FME	C-CA-N	2.12	113.56	109.73
34	i	1	SAC	OG-CB-CA	-2.06	105.72	110.97

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1	FME	C-CA-CB-CG
8	H	1	FME	CA-CB-CG-SD
10	J	1	FME	O1-CN-N-CA
12	L	1	FME	O1-CN-N-CA
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	N-CA-CB-CG
12	L	1	FME	CA-CB-CG-SD
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
10	J	1	FME	CB-CG-SD-CE
11	K	1	FME	CB-CG-SD-CE
14	N	1	FME	C-CA-CB-CG
8	H	1	FME	CB-CG-SD-CE
10	J	1	FME	CA-CB-CG-SD
8	H	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 57 ligands modelled in this entry, 3 are monoatomic - leaving 54 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
52	CDL	K	401	-	70,70,99	1.03	8 (11%)	76,82,111	1.04	4 (5%)
45	LMT	M	602	-	36,36,36	1.13	2 (5%)	47,47,47	0.93	1 (2%)
51	3PE	N	1301	-	50,50,50	0.87	3 (6%)	53,55,55	1.07	2 (3%)
51	3PE	N	1303	-	40,40,50	0.96	4 (10%)	43,45,55	1.08	2 (4%)
51	3PE	Y	802	-	34,34,50	1.04	3 (8%)	37,39,55	1.20	2 (5%)
47	SF4	F	502	6	0,12,12	-	-	-		
58	EHZ	T	101	20	29,36,37	1.68	6 (20%)	35,44,47	1.88	6 (17%)
59	MYR	o	201	40	5,5,15	0.85	0	4,4,15	1.01	0
45	LMT	M	603	-	36,36,36	1.16	2 (5%)	47,47,47	0.89	1 (2%)
45	LMT	L	702	-	36,36,36	1.18	2 (5%)	47,47,47	0.94	1 (2%)
45	LMT	J	702	-	36,36,36	1.22	3 (8%)	47,47,47	1.12	2 (4%)
49	FMN	F	501	-	33,33,33	1.11	2 (6%)	48,50,50	1.24	6 (12%)
53	I49	N	1305	-	15,17,17	1.46	2 (13%)	21,22,22	2.11	4 (19%)
52	CDL	J	701	-	61,61,99	1.08	8 (13%)	67,73,111	1.28	4 (5%)
47	SF4	G	802	7	0,12,12	-	-	-		
51	3PE	L	701	-	48,48,50	0.90	4 (8%)	51,53,55	1.13	2 (3%)
51	3PE	M	601	-	45,45,50	0.91	3 (6%)	48,50,55	1.04	2 (4%)
51	3PE	M	605	-	50,50,50	0.85	3 (6%)	53,55,55	1.06	2 (3%)
51	3PE	L	705	-	44,44,50	0.91	3 (6%)	47,49,55	1.24	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	PC1	A	303	-	20,20,53	1.86	3 (15%)	24,27,61	1.14	1 (4%)
45	LMT	j	101	-	36,36,36	1.22	4 (11%)	47,47,47	0.88	1 (2%)
45	LMT	Y	803	-	36,36,36	1.19	3 (8%)	47,47,47	1.00	1 (2%)
56	NDP	P	501	-	45,52,52	2.15	4 (8%)	53,80,80	1.69	12 (22%)
47	SF4	I	203	9	0,12,12	-	-	-		
45	LMT	A	301	-	36,36,36	1.15	2 (5%)	47,47,47	1.01	2 (4%)
52	CDL	L	703	-	68,68,99	1.04	5 (7%)	74,80,111	1.09	4 (5%)
46	PC1	L	707	-	48,48,53	0.98	4 (8%)	54,56,61	1.07	2 (3%)
48	FES	G	803	7	0,4,4	-	-	-		
45	LMT	M	604	-	36,36,36	1.21	3 (8%)	47,47,47	0.90	0
51	3PE	N	1304	-	28,28,50	1.14	4 (14%)	31,33,55	1.13	2 (6%)
45	LMT	L	706	-	36,36,36	1.17	2 (5%)	47,47,47	1.04	2 (4%)
45	LMT	N	1302	-	36,36,36	1.18	3 (8%)	47,47,47	0.93	0
45	LMT	L	704	-	36,36,36	1.25	4 (11%)	47,47,47	1.01	2 (4%)
47	SF4	B	201	2	0,12,12	-	-	-		
46	PC1	B	203	-	34,34,53	1.16	4 (11%)	40,42,61	1.12	2 (5%)
51	3PE	X	401	-	50,50,50	0.86	4 (8%)	53,55,55	1.11	2 (3%)
54	GTP	O	401	55	26,34,34	2.90	11 (42%)	32,54,54	1.64	9 (28%)
51	3PE	I	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
45	LMT	Y	801	-	36,36,36	1.19	3 (8%)	47,47,47	0.99	0
58	EHZ	U	101	20	29,36,37	1.65	6 (20%)	35,44,47	1.42	3 (8%)
46	PC1	B	202	-	53,53,53	0.93	3 (5%)	59,61,61	1.01	2 (3%)
51	3PE	P	502	-	36,36,50	1.03	4 (11%)	39,41,55	1.10	2 (5%)
47	SF4	G	801	7	0,12,12	-	-	-		
51	3PE	d	301	-	50,50,50	0.83	3 (6%)	53,55,55	1.18	4 (7%)
45	LMT	h	1002	-	36,36,36	1.13	2 (5%)	47,47,47	1.04	1 (2%)
52	CDL	h	1001	-	66,66,99	1.05	7 (10%)	72,78,111	1.20	4 (5%)
45	LMT	l	201	-	36,36,36	1.20	3 (8%)	47,47,47	1.00	2 (4%)
48	FES	E	301	5	0,4,4	-	-	-		
51	3PE	H	402	-	33,33,50	1.35	3 (9%)	34,37,55	1.15	2 (5%)
47	SF4	I	202	9	0,12,12	-	-	-		
52	CDL	q	201	-	75,75,99	0.99	6 (8%)	81,87,111	1.11	4 (4%)
45	LMT	Y	804	-	36,36,36	1.20	3 (8%)	47,47,47	1.11	3 (6%)
51	3PE	H	401	-	43,43,50	0.93	3 (6%)	46,48,55	1.08	2 (4%)
45	LMT	A	302	-	36,36,36	1.14	2 (5%)	47,47,47	1.64	7 (14%)

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
52	CDL	K	401	-	-	29/81/81/110	-
45	LMT	M	602	-	-	8/21/61/61	0/2/2/2
51	3PE	N	1301	-	-	20/54/54/54	-
51	3PE	N	1303	-	-	22/44/44/54	-
51	3PE	Y	802	-	-	17/38/38/54	-
58	EHZ	T	101	20	-	11/42/44/45	-
47	SF4	F	502	6	-	-	0/6/5/5
59	MYR	o	201	40	-	2/2/3/13	-
45	LMT	M	603	-	-	13/21/61/61	0/2/2/2
45	LMT	L	702	-	-	10/21/61/61	0/2/2/2
45	LMT	J	702	-	-	10/21/61/61	0/2/2/2
49	FMN	F	501	-	-	1/18/18/18	0/3/3/3
53	I49	N	1305	-	-	5/10/10/10	0/1/1/1
52	CDL	J	701	-	-	37/71/71/110	-
51	3PE	L	701	-	-	28/52/52/54	-
47	SF4	G	802	7	-	-	0/6/5/5
51	3PE	M	601	-	-	19/49/49/54	-
51	3PE	M	605	-	-	24/54/54/54	-
51	3PE	L	705	-	-	20/48/48/54	-
46	PC1	A	303	-	-	4/22/22/57	-
45	LMT	j	101	-	-	4/21/61/61	0/2/2/2
45	LMT	Y	803	-	-	8/21/61/61	0/2/2/2
56	NDP	P	501	-	-	7/30/77/77	0/5/5/5
47	SF4	I	203	9	-	-	0/6/5/5
45	LMT	A	301	-	-	5/21/61/61	0/2/2/2
52	CDL	L	703	-	-	34/79/79/110	-
46	PC1	L	707	-	-	25/52/52/57	-
48	FES	G	803	7	-	-	0/1/1/1
45	LMT	M	604	-	-	8/21/61/61	0/2/2/2
51	3PE	N	1304	-	-	17/32/32/54	-
45	LMT	L	706	-	-	8/21/61/61	0/2/2/2
45	LMT	N	1302	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	L	704	-	-	10/21/61/61	0/2/2/2
51	3PE	X	401	-	-	25/54/54/54	-
46	PC1	B	203	-	-	17/38/38/57	-
47	SF4	B	201	2	-	-	0/6/5/5
54	GTP	O	401	55	-	4/18/38/38	0/3/3/3
51	3PE	I	201	-	-	16/54/54/54	-
45	LMT	Y	801	-	-	8/21/61/61	0/2/2/2
58	EHZ	U	101	20	-	7/42/44/45	-
46	PC1	B	202	-	-	20/57/57/57	-
51	3PE	P	502	-	-	21/40/40/54	-
47	SF4	G	801	7	-	-	0/6/5/5
51	3PE	d	301	-	-	23/54/54/54	-
45	LMT	h	1002	-	-	8/21/61/61	0/2/2/2
52	CDL	h	1001	-	-	39/77/77/110	-
45	LMT	l	201	-	-	9/21/61/61	0/2/2/2
51	3PE	H	402	-	-	19/36/36/54	-
48	FES	E	301	5	-	-	0/1/1/1
47	SF4	I	202	9	-	-	0/6/5/5
52	CDL	q	201	-	-	36/86/86/110	-
45	LMT	Y	804	-	-	6/21/61/61	0/2/2/2
51	3PE	H	401	-	-	18/47/47/54	-
45	LMT	A	302	-	-	11/21/61/61	0/2/2/2

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	11.88	1.81	1.59
54	O	401	GTP	O6-C6	8.07	1.39	1.23
46	A	303	PC1	O21-C2	-5.79	1.40	1.46
54	O	401	GTP	O4'-C1'	5.41	1.48	1.41
58	T	101	EHZ	C12-N1	5.12	1.45	1.33
58	U	101	EHZ	C15-N2	5.11	1.44	1.33
51	H	402	3PE	O21-C2	-5.09	1.40	1.46
58	T	101	EHZ	C15-N2	5.08	1.44	1.33
58	U	101	EHZ	C12-N1	5.00	1.44	1.33
54	O	401	GTP	C2-N3	4.62	1.44	1.33
54	O	401	GTP	C2-N1	4.61	1.49	1.37
54	O	401	GTP	C2-N2	4.47	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	N	1305	I49	C15-N02	-4.35	1.31	1.37
56	P	501	NDP	PN-O5D	3.65	1.74	1.59
45	J	702	LMT	O5B-C1B	3.65	1.51	1.41
45	L	704	LMT	O5B-C1B	3.64	1.51	1.41
45	N	1302	LMT	O5B-C1B	3.55	1.50	1.41
45	Y	803	LMT	O5B-C1B	3.55	1.50	1.41
49	F	501	FMN	C4A-N5	3.52	1.37	1.30
45	j	101	LMT	O5B-C1B	3.48	1.50	1.41
45	l	201	LMT	O5'-C1'	3.38	1.50	1.41
45	L	704	LMT	O5'-C1'	3.38	1.50	1.41
45	M	604	LMT	O5B-C1B	3.37	1.50	1.41
45	M	603	LMT	O5B-C1B	3.36	1.50	1.41
45	Y	801	LMT	O5B-C1B	3.36	1.50	1.41
45	j	101	LMT	O5'-C1'	3.34	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.32	1.50	1.41
56	P	501	NDP	O2B-C2B	-3.32	1.32	1.44
45	l	201	LMT	O5B-C1B	3.32	1.50	1.41
45	Y	804	LMT	O5B-C1B	3.32	1.50	1.41
54	O	401	GTP	C2'-C1'	-3.31	1.48	1.53
45	M	602	LMT	O5B-C1B	3.30	1.50	1.41
45	L	702	LMT	O5B-C1B	3.28	1.50	1.41
45	M	604	LMT	O5'-C1'	3.25	1.50	1.41
45	L	706	LMT	O5B-C1B	3.21	1.50	1.41
54	O	401	GTP	C5-C6	-3.15	1.41	1.47
45	A	301	LMT	O5'-C1'	3.15	1.49	1.41
45	A	302	LMT	O5B-C1B	3.14	1.49	1.41
45	A	301	LMT	O5B-C1B	3.14	1.49	1.41
45	J	702	LMT	O5'-C1'	3.10	1.49	1.41
45	Y	804	LMT	O5'-C1'	3.07	1.49	1.41
51	H	402	3PE	O21-C21	3.07	1.40	1.33
53	N	1305	I49	C14-N03	3.07	1.38	1.29
45	L	706	LMT	O5'-C1'	3.03	1.49	1.41
46	A	303	PC1	O21-C21	3.02	1.40	1.33
45	M	603	LMT	O5'-C1'	3.00	1.49	1.41
45	L	702	LMT	O5'-C1'	2.98	1.49	1.41
45	N	1302	LMT	O5'-C1'	2.98	1.49	1.41
45	A	302	LMT	O5'-C1'	2.95	1.49	1.41
45	Y	803	LMT	O5'-C1'	2.95	1.49	1.41
45	Y	801	LMT	O5'-C1'	2.93	1.49	1.41
51	H	401	3PE	O21-C2	-2.85	1.39	1.46
45	M	602	LMT	O5'-C1'	2.83	1.49	1.41
51	L	701	3PE	O21-C2	-2.83	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	q	201	CDL	OA6-CA4	-2.81	1.39	1.46
51	N	1301	3PE	O21-C2	-2.80	1.39	1.46
45	h	1002	LMT	O5'-C1'	2.79	1.49	1.41
52	h	1001	CDL	OB6-CB4	-2.75	1.39	1.46
51	L	701	3PE	O31-C3	-2.72	1.39	1.45
52	q	201	CDL	OB6-CB4	-2.72	1.39	1.46
52	K	401	CDL	OA6-CA4	-2.70	1.39	1.46
51	X	401	3PE	O21-C2	-2.69	1.39	1.46
52	L	703	CDL	OA6-CA4	-2.69	1.39	1.46
52	L	703	CDL	OB6-CB4	-2.68	1.39	1.46
46	B	202	PC1	O21-C2	-2.62	1.40	1.46
51	Y	802	3PE	O21-C2	-2.60	1.40	1.46
51	M	601	3PE	O21-C2	-2.59	1.40	1.46
51	L	705	3PE	O21-C2	-2.59	1.40	1.46
52	h	1001	CDL	OA6-CA4	-2.59	1.40	1.46
52	J	701	CDL	OB6-CB4	-2.57	1.40	1.46
58	U	101	EHZ	O4-C15	-2.53	1.18	1.23
51	I	201	3PE	O31-C3	-2.53	1.39	1.45
52	L	703	CDL	OB8-CB7	2.51	1.40	1.33
52	q	201	CDL	OA8-CA6	-2.51	1.39	1.45
51	N	1304	3PE	O21-C2	-2.51	1.40	1.46
51	N	1303	3PE	O21-C2	-2.50	1.40	1.46
58	T	101	EHZ	O3-C12	-2.49	1.18	1.23
54	O	401	GTP	C2'-C3'	-2.49	1.46	1.53
58	T	101	EHZ	O4-C15	-2.49	1.18	1.23
46	B	203	PC1	O21-C2	-2.49	1.40	1.46
51	H	402	3PE	O31-C31	2.48	1.40	1.33
51	M	605	3PE	O31-C31	2.47	1.40	1.33
52	K	401	CDL	OB8-CB7	2.47	1.40	1.33
51	L	705	3PE	O31-C3	-2.46	1.39	1.45
51	H	401	3PE	O31-C3	-2.46	1.39	1.45
51	P	502	3PE	O31-C31	2.46	1.40	1.33
52	K	401	CDL	OB6-CB4	-2.44	1.40	1.46
51	I	201	3PE	O21-C2	-2.44	1.40	1.46
52	J	701	CDL	OA6-CA5	2.43	1.40	1.35
51	Y	802	3PE	O31-C31	2.43	1.40	1.33
51	M	601	3PE	O31-C31	2.41	1.40	1.33
46	L	707	PC1	O31-C31	2.40	1.40	1.33
51	X	401	3PE	O31-C3	-2.39	1.39	1.45
52	J	701	CDL	OB8-CB6	-2.38	1.39	1.45
52	h	1001	CDL	OA8-CA7	2.38	1.40	1.33
46	B	202	PC1	O31-C3	-2.37	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	K	401	CDL	OA8-CA6	-2.37	1.39	1.45
46	L	707	PC1	O21-C2	-2.36	1.40	1.46
51	N	1303	3PE	O31-C31	2.35	1.40	1.33
45	Y	804	LMT	O5B-C5B	2.35	1.50	1.44
51	N	1304	3PE	O31-C31	2.34	1.40	1.33
52	L	703	CDL	OA8-CA7	2.34	1.40	1.33
52	K	401	CDL	OA8-CA7	2.33	1.40	1.33
52	J	701	CDL	OA8-CA7	2.33	1.40	1.33
54	O	401	GTP	PG-O2G	-2.33	1.45	1.54
51	N	1301	3PE	O31-C3	-2.31	1.39	1.45
58	U	101	EHZ	O3-C12	-2.30	1.18	1.23
51	P	502	3PE	O21-C21	2.30	1.40	1.34
52	h	1001	CDL	OB8-CB7	2.29	1.40	1.33
54	O	401	GTP	PG-O3G	-2.28	1.46	1.54
52	h	1001	CDL	OB8-CB6	-2.28	1.40	1.45
51	Y	802	3PE	O31-C3	-2.27	1.40	1.45
52	q	201	CDL	OB8-CB7	2.26	1.39	1.33
51	M	605	3PE	O21-C2	-2.26	1.41	1.46
51	P	502	3PE	O31-C3	-2.25	1.40	1.45
51	N	1301	3PE	O31-C31	2.24	1.39	1.33
46	B	203	PC1	O31-C31	2.24	1.39	1.33
58	T	101	EHZ	C9-S1	2.24	1.81	1.76
52	K	401	CDL	OB6-CB5	2.22	1.40	1.34
51	N	1304	3PE	O31-C3	-2.22	1.40	1.45
51	N	1303	3PE	O31-C3	-2.21	1.40	1.45
52	J	701	CDL	OB6-CB5	2.20	1.40	1.34
52	K	401	CDL	OB8-CB6	-2.20	1.40	1.45
52	L	703	CDL	OA8-CA6	-2.20	1.40	1.45
46	B	203	PC1	O31-C3	-2.20	1.40	1.45
52	h	1001	CDL	OA8-CA6	-2.19	1.40	1.45
58	T	101	EHZ	O6-C20	-2.19	1.39	1.44
52	J	701	CDL	OA8-CA6	-2.18	1.40	1.45
51	d	301	3PE	O31-C3	-2.18	1.40	1.45
45	Y	803	LMT	O5B-C5B	2.17	1.49	1.44
46	B	203	PC1	O21-C21	2.17	1.40	1.34
46	B	202	PC1	O31-C31	2.17	1.39	1.33
51	L	705	3PE	O31-C31	2.17	1.39	1.33
56	P	501	NDP	O5D-C5D	-2.16	1.36	1.44
51	I	201	3PE	O31-C31	2.16	1.39	1.33
51	I	201	3PE	O21-C21	2.16	1.40	1.34
45	M	604	LMT	O5B-C5B	2.15	1.49	1.44
51	d	301	3PE	O21-C2	-2.15	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	M	605	3PE	O21-C21	2.15	1.40	1.34
52	J	701	CDL	OA6-CA4	-2.14	1.41	1.46
52	q	201	CDL	OB8-CB6	-2.14	1.40	1.45
51	H	401	3PE	O31-C31	2.13	1.39	1.33
45	J	702	LMT	O5B-C5B	2.13	1.49	1.44
51	M	601	3PE	O31-C3	-2.12	1.40	1.45
49	F	501	FMN	C10-N1	2.11	1.37	1.33
45	L	704	LMT	O5'-C5'	2.10	1.49	1.44
51	N	1303	3PE	O21-C21	2.10	1.40	1.34
51	d	301	3PE	O31-C31	2.10	1.39	1.33
46	L	707	PC1	O31-C3	-2.09	1.40	1.45
45	Y	801	LMT	O5B-C5B	2.08	1.49	1.44
51	L	701	3PE	O31-C31	2.08	1.39	1.33
45	N	1302	LMT	O5B-C5B	2.07	1.49	1.44
51	P	502	3PE	O21-C2	-2.07	1.41	1.46
51	X	401	3PE	O21-C21	2.07	1.40	1.34
51	N	1304	3PE	O21-C21	2.07	1.40	1.34
52	q	201	CDL	OA6-CA5	2.06	1.40	1.34
51	X	401	3PE	O31-C31	2.06	1.39	1.33
45	L	704	LMT	O5B-C5B	2.05	1.49	1.44
46	A	303	PC1	O31-C3	-2.05	1.40	1.45
58	U	101	EHZ	C9-S1	2.05	1.81	1.76
51	L	701	3PE	O21-C21	2.05	1.40	1.34
52	J	701	CDL	OB8-CB7	2.04	1.39	1.33
58	U	101	EHZ	O6-C20	-2.04	1.39	1.44
45	j	101	LMT	O5B-C5B	2.03	1.49	1.44
54	O	401	GTP	PA-O2A	-2.02	1.45	1.55
52	K	401	CDL	OA6-CA5	2.02	1.40	1.34
46	L	707	PC1	O21-C21	2.02	1.40	1.34
45	l	201	LMT	O5B-C5B	2.01	1.49	1.44
45	j	101	LMT	O5'-C5'	2.00	1.49	1.44
52	h	1001	CDL	OA6-CA5	2.00	1.40	1.34

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	T	101	EHZ	C8-C9-S1	7.27	122.62	113.63
56	P	501	NDP	PN-O3-PA	-6.84	109.37	132.83
58	U	101	EHZ	C8-C9-S1	5.82	120.83	113.63
53	N	1305	I49	C14-N02-C15	-5.66	115.78	125.21
45	A	302	LMT	C1-O1'-C1'	5.27	122.58	113.84
53	N	1305	I49	N01-C14-N03	5.08	129.77	120.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	J	701	CDL	OA6-CA5-C11	4.98	120.25	111.09
52	J	701	CDL	OB6-CB5-C51	4.91	122.09	111.50
46	A	303	PC1	O21-C21-O22	-4.78	119.49	125.57
51	L	705	3PE	O21-C21-C22	4.75	121.74	111.50
51	I	201	3PE	O21-C21-C22	4.60	121.41	111.50
51	H	402	3PE	O21-C21-O22	-4.53	119.80	125.57
51	d	301	3PE	O21-C21-C22	4.51	121.23	111.50
46	B	203	PC1	O21-C21-C22	4.49	121.17	111.50
46	L	707	PC1	O21-C21-C22	4.48	121.15	111.50
45	A	302	LMT	O1'-C1'-C2'	4.46	115.26	108.30
51	N	1304	3PE	O21-C21-C22	4.38	120.94	111.50
52	h	1001	CDL	OB6-CB5-C51	4.27	120.70	111.50
51	Y	802	3PE	O21-C21-C22	4.25	120.66	111.50
51	L	701	3PE	O21-C21-C22	4.06	120.26	111.50
52	h	1001	CDL	OA6-CA5-C11	4.05	120.24	111.50
51	M	605	3PE	O21-C21-C22	4.05	120.22	111.50
46	B	202	PC1	O21-C21-C22	4.02	120.16	111.50
52	q	201	CDL	OA6-CA5-C11	3.99	120.11	111.50
51	X	401	3PE	O21-C21-C22	3.99	120.10	111.50
51	P	502	3PE	O21-C21-C22	3.97	120.05	111.50
45	Y	804	LMT	C3B-C4B-C5B	3.93	117.25	110.24
52	q	201	CDL	OB6-CB5-C51	3.92	119.96	111.50
51	N	1303	3PE	O21-C21-C22	3.84	119.78	111.50
52	L	703	CDL	OA6-CA5-C11	3.81	119.71	111.50
52	K	401	CDL	OB6-CB5-C51	3.75	119.59	111.50
45	A	302	LMT	C3B-C4B-C5B	3.63	116.71	110.24
56	P	501	NDP	O2B-P2B-O1X	-3.61	95.45	109.39
52	K	401	CDL	OA6-CA5-C11	3.56	119.18	111.50
51	H	401	3PE	O21-C21-C22	3.52	119.09	111.50
51	M	601	3PE	O21-C21-C22	3.51	119.08	111.50
52	L	703	CDL	OB6-CB5-C51	3.45	118.94	111.50
51	N	1301	3PE	O21-C21-C22	3.42	118.86	111.50
58	T	101	EHZ	C10-S1-C9	3.29	112.13	101.87
58	T	101	EHZ	C13-C14-N2	-3.28	105.27	111.90
54	O	401	GTP	C2-N1-C6	-3.26	119.09	125.10
54	O	401	GTP	C5-C6-N1	3.24	119.68	113.95
49	F	501	FMN	C4-N3-C2	-3.24	119.66	125.64
45	A	302	LMT	C4B-C3B-C2B	3.11	116.25	110.82
51	Y	802	3PE	O31-C31-C32	3.09	121.61	111.91
58	T	101	EHZ	C13-C12-N1	3.04	121.53	116.42
53	N	1305	I49	N05-C15-N04	-3.02	110.95	120.26
51	M	601	3PE	O31-C31-C32	3.01	121.36	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	h	1001	CDL	OA8-CA7-C31	2.99	121.28	111.91
51	N	1301	3PE	O31-C31-C32	2.97	121.22	111.91
45	Y	804	LMT	O5B-C5B-C4B	2.95	115.06	109.69
46	L	707	PC1	O31-C31-C32	2.92	121.06	111.91
54	O	401	GTP	PA-O3A-PB	-2.89	122.89	132.83
49	F	501	FMN	C4A-C10-N10	2.89	120.70	116.48
51	M	605	3PE	O31-C31-C32	2.87	120.92	111.91
51	P	502	3PE	O31-C31-C32	2.86	120.89	111.91
54	O	401	GTP	O2G-PG-O3B	2.86	114.23	104.64
58	T	101	EHZ	O2-C9-S1	-2.84	118.93	122.61
51	H	402	3PE	O31-C31-C32	2.80	120.70	111.91
46	B	203	PC1	O31-C31-C32	2.75	120.54	111.91
49	F	501	FMN	C4A-C4-N3	2.73	120.13	113.19
51	X	401	3PE	O31-C31-C32	2.73	120.47	111.91
56	P	501	NDP	PA-O5B-C5B	-2.72	105.72	121.68
52	J	701	CDL	OB8-CB7-C71	2.71	120.42	111.91
45	J	702	LMT	O5B-C1B-C2B	2.71	116.09	110.35
45	Y	803	LMT	C1-O1'-C1'	2.71	118.33	113.84
51	H	401	3PE	O31-C31-C32	2.71	120.40	111.91
51	N	1303	3PE	O31-C31-C32	2.69	120.35	111.91
52	h	1001	CDL	OB8-CB7-C71	2.66	120.27	111.91
51	L	701	3PE	O31-C31-C32	2.63	120.16	111.91
45	l	201	LMT	C1B-O1B-C4'	-2.63	111.46	117.96
51	d	301	3PE	O31-C31-C32	2.63	120.15	111.91
52	J	701	CDL	OA8-CA7-C31	2.60	120.05	111.91
52	L	703	CDL	OA8-CA7-C31	2.57	119.99	111.91
56	P	501	NDP	O3X-P2B-O2X	2.55	117.38	107.64
54	O	401	GTP	O3G-PG-O3B	2.53	113.11	104.64
56	P	501	NDP	O4B-C4B-C3B	2.53	110.11	105.11
52	q	201	CDL	OA8-CA7-C31	2.52	119.83	111.91
56	P	501	NDP	PN-O5D-C5D	-2.52	106.91	121.68
52	q	201	CDL	OB8-CB7-C71	2.51	119.77	111.91
45	L	706	LMT	C3B-C4B-C5B	2.48	114.67	110.24
45	J	702	LMT	C1B-O1B-C4'	-2.47	111.84	117.96
45	M	602	LMT	O1'-C1'-C2'	2.46	112.14	108.30
52	L	703	CDL	OB8-CB7-C71	2.45	119.60	111.91
45	L	704	LMT	C1B-C2B-C3B	2.45	115.09	110.00
51	L	705	3PE	O31-C31-C32	2.43	119.53	111.91
52	K	401	CDL	OB8-CB7-C71	2.42	119.50	111.91
54	O	401	GTP	PB-O3B-PG	-2.41	124.54	132.83
51	d	301	3PE	O21-C21-O22	-2.40	117.89	123.70
56	P	501	NDP	C2A-N1A-C6A	-2.39	114.66	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	F	501	FMN	O4-C4-C4A	-2.36	120.34	126.60
45	L	704	LMT	O5B-C1B-C2B	2.36	115.34	110.35
52	K	401	CDL	OA8-CA7-C31	2.34	119.26	111.91
49	F	501	FMN	C10-C4A-N5	-2.34	119.89	124.86
45	h	1002	LMT	C1B-O5B-C5B	-2.32	109.14	113.69
51	I	201	3PE	O31-C31-C32	2.31	119.16	111.91
56	P	501	NDP	O2N-PN-O1N	2.30	123.62	112.24
46	B	202	PC1	O31-C31-C32	2.29	119.10	111.91
58	U	101	EHZ	O2-C9-S1	-2.27	119.67	122.61
54	O	401	GTP	O2A-PA-O1A	-2.26	101.09	112.24
45	A	302	LMT	C1B-O5B-C5B	-2.25	109.27	113.69
45	Y	804	LMT	C1B-O1B-C4'	-2.22	112.47	117.96
51	N	1304	3PE	O31-C31-C32	2.22	118.87	111.91
58	T	101	EHZ	C14-N2-C15	-2.19	118.69	122.59
49	F	501	FMN	C4A-C10-N1	-2.19	119.66	124.73
56	P	501	NDP	O5D-PN-O1N	-2.18	100.54	109.07
45	A	301	LMT	C1B-O1B-C4'	-2.18	112.57	117.96
51	d	301	3PE	O21-C2-C3	2.18	116.28	108.40
45	A	302	LMT	C3'-C4'-C5'	2.18	115.92	110.93
51	L	705	3PE	C2-O21-C21	-2.17	112.44	117.79
53	N	1305	I49	N05-C15-N02	2.17	126.38	117.44
45	l	201	LMT	O5'-C1'-C2'	2.16	114.92	110.35
56	P	501	NDP	C5B-C4B-C3B	-2.14	107.18	115.18
54	O	401	GTP	O2B-PB-O1B	-2.13	101.72	112.24
56	P	501	NDP	O7N-C7N-C3N	2.12	124.90	120.90
54	O	401	GTP	C3'-C2'-C1'	2.12	104.17	100.98
45	M	603	LMT	C1B-O1B-C4'	-2.12	112.73	117.96
45	A	302	LMT	C2'-C3'-C4'	2.11	114.51	109.68
45	j	101	LMT	C1B-O1B-C4'	-2.09	112.78	117.96
45	A	301	LMT	C1B-O5B-C5B	-2.09	109.59	113.69
58	U	101	EHZ	C10-S1-C9	2.06	108.28	101.87
45	L	702	LMT	C1-O1'-C1'	2.04	117.22	113.84
56	P	501	NDP	O7N-C7N-N7N	-2.04	118.11	122.88
45	L	706	LMT	O5B-C5B-C4B	2.02	113.36	109.69

There are no chirality outliers.

All (702) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	302	LMT	C2'-C1'-O1'-C1
45	L	702	LMT	C2-C1-O1'-C1'
45	L	704	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
45	L	706	LMT	C2'-C1'-O1'-C1
45	L	706	LMT	O5'-C1'-O1'-C1
45	M	603	LMT	C2'-C1'-O1'-C1
45	M	603	LMT	O5'-C1'-O1'-C1
45	M	604	LMT	C2'-C1'-O1'-C1
45	M	604	LMT	O5'-C1'-O1'-C1
45	Y	803	LMT	O5'-C1'-O1'-C1
45	Y	804	LMT	C2-C1-O1'-C1'
45	h	1002	LMT	C2'-C1'-O1'-C1
45	h	1002	LMT	O5'-C1'-O1'-C1
45	l	201	LMT	C2'-C1'-O1'-C1
45	l	201	LMT	O5'-C1'-O1'-C1
46	A	303	PC1	C1-O11-P-O14
46	B	203	PC1	C11-O13-P-O14
51	H	402	3PE	C11-O13-P-O11
51	H	402	3PE	O13-C11-C12-N
51	H	402	3PE	C1-C2-O21-C21
51	H	402	3PE	O22-C21-O21-C2
51	L	701	3PE	C11-O13-P-O11
51	L	701	3PE	C11-O13-P-O12
51	L	701	3PE	C11-O13-P-O14
51	L	701	3PE	C22-C21-O21-C2
51	L	705	3PE	C11-O13-P-O14
51	L	705	3PE	O13-C11-C12-N
51	M	601	3PE	O13-C11-C12-N
51	M	605	3PE	C1-O11-P-O12
51	M	605	3PE	C1-O11-P-O14
51	M	605	3PE	O13-C11-C12-N
51	M	605	3PE	O32-C31-O31-C3
51	M	605	3PE	C32-C31-O31-C3
51	M	605	3PE	C22-C21-O21-C2
51	N	1301	3PE	C1-O11-P-O14
51	N	1301	3PE	C12-C11-O13-P
51	N	1301	3PE	O13-C11-C12-N
51	N	1303	3PE	O13-C11-C12-N
51	N	1304	3PE	C1-O11-P-O12
51	N	1304	3PE	O13-C11-C12-N
51	N	1304	3PE	O22-C21-O21-C2
51	P	502	3PE	C1-O11-P-O14
51	P	502	3PE	C11-O13-P-O11
51	P	502	3PE	C11-O13-P-O14
51	X	401	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
51	X	401	3PE	C1-O11-P-O13
51	X	401	3PE	C1-O11-P-O14
51	X	401	3PE	C22-C21-O21-C2
51	Y	802	3PE	O13-C11-C12-N
51	Y	802	3PE	O22-C21-O21-C2
51	d	301	3PE	C11-O13-P-O14
51	d	301	3PE	O22-C21-O21-C2
52	J	701	CDL	CB2-C1-CA2-OA2
52	J	701	CDL	OA7-CA5-OA6-CA4
52	J	701	CDL	C11-CA5-OA6-CA4
52	J	701	CDL	OB7-CB5-OB6-CB4
52	J	701	CDL	C51-CB5-OB6-CB4
52	K	401	CDL	CA2-OA2-PA1-OA3
52	K	401	CDL	CA2-OA2-PA1-OA4
52	L	703	CDL	C11-CA5-OA6-CA4
52	h	1001	CDL	CA2-OA2-PA1-OA5
52	h	1001	CDL	CA3-OA5-PA1-OA2
52	h	1001	CDL	CA3-OA5-PA1-OA3
52	h	1001	CDL	CA3-OA5-PA1-OA4
52	h	1001	CDL	CB2-OB2-PB2-OB3
52	h	1001	CDL	CB3-OB5-PB2-OB3
52	h	1001	CDL	OB7-CB5-OB6-CB4
52	h	1001	CDL	C51-CB5-OB6-CB4
52	q	201	CDL	CB2-OB2-PB2-OB3
52	q	201	CDL	CB2-OB2-PB2-OB4
52	q	201	CDL	CB2-OB2-PB2-OB5
53	N	1305	I49	C07-C06-C08-N01
53	N	1305	I49	N01-C14-N02-C15
53	N	1305	I49	N03-C14-N02-C15
54	O	401	GTP	C5'-O5'-PA-O3A
56	P	501	NDP	C2B-O2B-P2B-O1X
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	C16-C17-C20-O6
58	T	101	EHZ	O2-C9-S1-C10
58	T	101	EHZ	C8-C9-S1-C10
58	U	101	EHZ	C5-C6-C7-O1
58	U	101	EHZ	C5-C6-C7-C8
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
51	H	401	3PE	O32-C31-O31-C3
51	H	402	3PE	O32-C31-O31-C3
51	Y	802	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
51	L	701	3PE	O22-C21-O21-C2
51	P	502	3PE	O22-C21-O21-C2
51	X	401	3PE	O22-C21-O21-C2
52	L	703	CDL	OA7-CA5-OA6-CA4
51	H	401	3PE	C32-C31-O31-C3
51	P	502	3PE	C32-C31-O31-C3
51	Y	802	3PE	C32-C31-O31-C3
52	J	701	CDL	C31-CA7-OA8-CA6
45	L	702	LMT	O5B-C5B-C6B-O6B
51	N	1304	3PE	C22-C21-O21-C2
51	P	502	3PE	C22-C21-O21-C2
51	Y	802	3PE	C22-C21-O21-C2
51	d	301	3PE	C22-C21-O21-C2
45	J	702	LMT	C2B-C1B-O1B-C4'
45	A	301	LMT	O5'-C5'-C6'-O6'
51	H	402	3PE	C32-C31-O31-C3
51	L	701	3PE	C32-C31-O31-C3
51	N	1301	3PE	C32-C31-O31-C3
51	X	401	3PE	C32-C31-O31-C3
45	L	702	LMT	O5'-C5'-C6'-O6'
45	J	702	LMT	O5B-C1B-O1B-C4'
51	M	605	3PE	O22-C21-O21-C2
51	N	1301	3PE	O32-C31-O31-C3
51	P	502	3PE	O32-C31-O31-C3
51	X	401	3PE	O32-C31-O31-C3
52	J	701	CDL	OA9-CA7-OA8-CA6
45	A	302	LMT	O5B-C1B-O1B-C4'
52	J	701	CDL	O1-C1-CA2-OA2
52	q	201	CDL	O1-C1-CA2-OA2
46	L	707	PC1	C32-C31-O31-C3
51	N	1303	3PE	C32-C31-O31-C3
45	L	706	LMT	O5B-C5B-C6B-O6B
45	M	602	LMT	O5B-C5B-C6B-O6B
45	M	602	LMT	O5'-C5'-C6'-O6'
45	L	702	LMT	C4B-C5B-C6B-O6B
45	M	603	LMT	O5B-C1B-O1B-C4'
45	N	1302	LMT	O5B-C5B-C6B-O6B
45	Y	804	LMT	O5'-C5'-C6'-O6'
45	A	301	LMT	C4'-C5'-C6'-O6'
45	A	302	LMT	O5'-C5'-C6'-O6'
45	Y	801	LMT	C4B-C5B-C6B-O6B
45	L	704	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
45	L	706	LMT	O5'-C5'-C6'-O6'
45	h	1002	LMT	O5'-C5'-C6'-O6'
45	L	702	LMT	C4'-C5'-C6'-O6'
45	L	704	LMT	C4'-C5'-C6'-O6'
45	l	201	LMT	C4B-C5B-C6B-O6B
51	M	605	3PE	C2-C1-O11-P
51	L	701	3PE	O32-C31-O31-C3
51	N	1303	3PE	O32-C31-O31-C3
45	J	702	LMT	O5B-C5B-C6B-O6B
45	N	1302	LMT	O5'-C5'-C6'-O6'
45	Y	801	LMT	O5'-C5'-C6'-O6'
46	L	707	PC1	O32-C31-O31-C3
45	L	704	LMT	O5'-C1'-O1'-C1
52	q	201	CDL	C31-CA7-OA8-CA6
45	M	602	LMT	C4'-C5'-C6'-O6'
45	A	302	LMT	C2B-C1B-O1B-C4'
52	L	703	CDL	CB4-CB6-OB8-CB7
45	M	603	LMT	C4'-C5'-C6'-O6'
45	Y	801	LMT	O5B-C5B-C6B-O6B
52	q	201	CDL	CB2-C1-CA2-OA2
45	N	1302	LMT	C4'-C5'-C6'-O6'
52	q	201	CDL	OA9-CA7-OA8-CA6
45	L	706	LMT	C4B-C5B-C6B-O6B
45	L	706	LMT	C4'-C5'-C6'-O6'
45	M	604	LMT	C4B-C5B-C6B-O6B
52	K	401	CDL	CA5-C11-C12-C13
45	l	201	LMT	C4'-C5'-C6'-O6'
45	A	302	LMT	C4'-C5'-C6'-O6'
45	Y	801	LMT	C4'-C5'-C6'-O6'
45	J	702	LMT	O5'-C5'-C6'-O6'
45	l	201	LMT	O5B-C5B-C6B-O6B
51	L	705	3PE	C22-C21-O21-C2
45	N	1302	LMT	C4B-C5B-C6B-O6B
45	h	1002	LMT	C4'-C5'-C6'-O6'
45	M	602	LMT	C4B-C5B-C6B-O6B
46	B	203	PC1	C32-C31-O31-C3
52	h	1001	CDL	C31-CA7-OA8-CA6
45	N	1302	LMT	C5'-C4'-O1B-C1B
46	B	203	PC1	C21-C22-C23-C24
51	H	401	3PE	C31-C32-C33-C34
51	d	301	3PE	C21-C22-C23-C24
45	L	704	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
45	J	702	LMT	C4B-C5B-C6B-O6B
56	P	501	NDP	O4D-C4D-C5D-O5D
45	M	603	LMT	O5'-C5'-C6'-O6'
51	X	401	3PE	C21-C22-C23-C24
45	Y	803	LMT	C4'-C5'-C6'-O6'
52	q	201	CDL	C11-CA5-OA6-CA4
45	A	302	LMT	O5'-C1'-O1'-C1
45	L	702	LMT	O5'-C1'-O1'-C1
52	K	401	CDL	O1-C1-CB2-OB2
46	B	203	PC1	O32-C31-O31-C3
52	h	1001	CDL	OA9-CA7-OA8-CA6
45	h	1002	LMT	C2-C3-C4-C5
46	A	303	PC1	C1-O11-P-O13
46	B	202	PC1	C11-O13-P-O11
51	M	605	3PE	C1-O11-P-O13
51	N	1303	3PE	C11-O13-P-O11
51	N	1304	3PE	C1-O11-P-O13
51	P	502	3PE	C1-O11-P-O13
51	d	301	3PE	C11-O13-P-O11
52	J	701	CDL	CB3-OB5-PB2-OB2
52	K	401	CDL	CA2-OA2-PA1-OA5
52	K	401	CDL	CB3-OB5-PB2-OB2
52	L	703	CDL	CB3-OB5-PB2-OB2
52	h	1001	CDL	CB3-OB5-PB2-OB2
52	J	701	CDL	C71-CB7-OB8-CB6
45	M	603	LMT	O5B-C5B-C6B-O6B
52	K	401	CDL	CA2-C1-CB2-OB2
51	L	705	3PE	O22-C21-O21-C2
52	q	201	CDL	OA7-CA5-OA6-CA4
51	X	401	3PE	C3C-C3D-C3E-C3F
52	h	1001	CDL	C11-CA5-OA6-CA4
45	A	302	LMT	O1'-C1-C2-C3
45	J	702	LMT	C4-C5-C6-C7
46	B	202	PC1	C2C-C2D-C2E-C2F
46	L	707	PC1	C29-C2A-C2B-C2C
51	H	401	3PE	C3D-C3E-C3F-C3G
51	M	605	3PE	C2B-C2C-C2D-C2E
52	h	1001	CDL	C31-C32-C33-C34
58	T	101	EHZ	C18-C17-C20-O6
58	T	101	EHZ	C19-C17-C20-O6
51	H	402	3PE	C3D-C3E-C3F-C3G
51	X	401	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
52	K	401	CDL	C40-C41-C42-C43
58	U	101	EHZ	C21-C1-C2-C3
51	d	301	3PE	C3-C2-O21-C21
52	h	1001	CDL	OA7-CA5-OA6-CA4
46	B	202	PC1	C2A-C2B-C2C-C2D
51	I	201	3PE	C38-C39-C3A-C3B
51	M	605	3PE	C28-C29-C2A-C2B
52	h	1001	CDL	C14-C15-C16-C17
45	h	1002	LMT	C6-C7-C8-C9
52	h	1001	CDL	C72-C73-C74-C75
45	A	302	LMT	C11-C10-C9-C8
45	Y	803	LMT	C3-C4-C5-C6
52	L	703	CDL	C58-C59-C60-C61
52	L	703	CDL	CB5-C51-C52-C53
45	L	702	LMT	C2'-C1'-O1'-C1
45	J	702	LMT	C3-C4-C5-C6
46	L	707	PC1	C23-C24-C25-C26
51	L	701	3PE	C23-C24-C25-C26
51	X	401	3PE	C32-C33-C34-C35
45	M	604	LMT	O5B-C5B-C6B-O6B
45	M	604	LMT	C5'-C4'-O1B-C1B
45	N	1302	LMT	C3'-C4'-O1B-C1B
46	B	202	PC1	C3B-C3C-C3D-C3E
51	X	401	3PE	C23-C24-C25-C26
51	d	301	3PE	C39-C3A-C3B-C3C
52	L	703	CDL	CA7-C31-C32-C33
45	M	604	LMT	O1'-C1-C2-C3
51	N	1301	3PE	C23-C24-C25-C26
51	N	1301	3PE	C2D-C2E-C2F-C2G
52	q	201	CDL	C51-C52-C53-C54
45	l	201	LMT	O5'-C5'-C6'-O6'
45	j	101	LMT	C2B-C1B-O1B-C4'
45	Y	804	LMT	C4-C5-C6-C7
51	d	301	3PE	C26-C27-C28-C29
51	L	701	3PE	C29-C2A-C2B-C2C
51	M	601	3PE	C22-C23-C24-C25
51	M	605	3PE	C3E-C3F-C3G-C3H
51	M	605	3PE	C29-C2A-C2B-C2C
51	X	401	3PE	C28-C29-C2A-C2B
52	J	701	CDL	C75-C76-C77-C78
52	J	701	CDL	C78-C79-C80-C81
52	L	703	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
52	h	1001	CDL	C22-C23-C24-C25
51	d	301	3PE	C3E-C3F-C3G-C3H
52	J	701	CDL	C77-C78-C79-C80
46	L	707	PC1	C34-C35-C36-C37
51	N	1303	3PE	C29-C2A-C2B-C2C
52	h	1001	CDL	C13-C14-C15-C16
52	q	201	CDL	C38-C39-C40-C41
46	B	202	PC1	C31-C32-C33-C34
51	L	701	3PE	C21-C22-C23-C24
51	M	605	3PE	C31-C32-C33-C34
46	L	707	PC1	C24-C25-C26-C27
51	P	502	3PE	C33-C34-C35-C36
58	T	101	EHZ	C21-C22-C23-C24
51	M	601	3PE	C32-C31-O31-C3
52	J	701	CDL	C73-C74-C75-C76
45	Y	801	LMT	C2-C1-O1'-C1'
45	Y	803	LMT	C2-C1-O1'-C1'
45	j	101	LMT	C4-C5-C6-C7
51	I	201	3PE	C2B-C2C-C2D-C2E
51	L	705	3PE	C34-C35-C36-C37
52	q	201	CDL	C31-C32-C33-C34
52	J	701	CDL	OB9-CB7-OB8-CB6
45	Y	803	LMT	C2-C3-C4-C5
51	L	701	3PE	C28-C29-C2A-C2B
51	L	705	3PE	C33-C34-C35-C36
45	A	301	LMT	O5B-C5B-C6B-O6B
51	M	605	3PE	C2D-C2E-C2F-C2G
51	d	301	3PE	C24-C25-C26-C27
46	B	202	PC1	C28-C29-C2A-C2B
46	L	707	PC1	C36-C37-C38-C39
46	B	203	PC1	C22-C21-O21-C2
51	I	201	3PE	C22-C21-O21-C2
45	N	1302	LMT	O5B-C1B-O1B-C4'
45	M	604	LMT	C3'-C4'-O1B-C1B
52	q	201	CDL	C54-C55-C56-C57
46	B	203	PC1	C24-C25-C26-C27
45	Y	804	LMT	C4'-C5'-C6'-O6'
52	L	703	CDL	C34-C35-C36-C37
45	L	704	LMT	C4B-C5B-C6B-O6B
52	q	201	CDL	C11-C12-C13-C14
51	N	1304	3PE	C31-C32-C33-C34
45	j	101	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
45	M	604	LMT	C2-C3-C4-C5
46	B	203	PC1	O22-C21-O21-C2
51	N	1301	3PE	C3A-C3B-C3C-C3D
46	L	707	PC1	C2-C1-O11-P
45	Y	804	LMT	C4B-C5B-C6B-O6B
46	L	707	PC1	C37-C38-C39-C3A
51	Y	802	3PE	C36-C37-C38-C39
51	M	601	3PE	C38-C39-C3A-C3B
52	q	201	CDL	C57-C58-C59-C60
51	I	201	3PE	C32-C31-O31-C3
46	B	202	PC1	C33-C34-C35-C36
51	N	1301	3PE	C35-C36-C37-C38
46	L	707	PC1	C21-C22-C23-C24
51	M	601	3PE	O32-C31-O31-C3
46	L	707	PC1	C38-C39-C3A-C3B
51	I	201	3PE	O22-C21-O21-C2
52	K	401	CDL	OA7-CA5-OA6-CA4
45	L	704	LMT	O1'-C1-C2-C3
51	L	701	3PE	C2D-C2E-C2F-C2G
51	I	201	3PE	C33-C34-C35-C36
51	d	301	3PE	C32-C33-C34-C35
51	d	301	3PE	C23-C24-C25-C26
51	L	701	3PE	C2E-C2F-C2G-C2H
45	J	702	LMT	O5'-C1'-O1'-C1
46	L	707	PC1	C33-C34-C35-C36
51	N	1303	3PE	C23-C24-C25-C26
51	X	401	3PE	C36-C37-C38-C39
46	L	707	PC1	C22-C21-O21-C2
52	K	401	CDL	C11-CA5-OA6-CA4
52	K	401	CDL	C51-CB5-OB6-CB4
52	J	701	CDL	OB5-CB3-CB4-OB6
51	M	601	3PE	C34-C35-C36-C37
45	J	702	LMT	C2'-C1'-O1'-C1
45	M	602	LMT	C2'-C1'-O1'-C1
58	U	101	EHZ	C2-C3-C4-C5
51	M	601	3PE	C26-C27-C28-C29
51	I	201	3PE	O32-C31-O31-C3
46	B	202	PC1	C35-C36-C37-C38
46	L	707	PC1	C27-C28-C29-C2A
51	N	1301	3PE	C3D-C3E-C3F-C3G
51	L	705	3PE	C11-O13-P-O11
51	M	601	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
51	N	1301	3PE	C1-O11-P-O13
52	K	401	CDL	CA3-OA5-PA1-OA2
52	L	703	CDL	CA5-C11-C12-C13
46	L	707	PC1	C26-C27-C28-C29
52	K	401	CDL	C15-C16-C17-C18
52	K	401	CDL	C31-CA7-OA8-CA6
51	L	701	3PE	O11-C1-C2-C3
51	N	1301	3PE	O11-C1-C2-C3
51	N	1304	3PE	O11-C1-C2-C3
51	Y	802	3PE	O11-C1-C2-C3
52	h	1001	CDL	OB5-CB3-CB4-CB6
45	M	603	LMT	C2-C3-C4-C5
51	M	601	3PE	C37-C38-C39-C3A
52	K	401	CDL	C36-C37-C38-C39
52	L	703	CDL	C31-CA7-OA8-CA6
45	L	702	LMT	O1'-C1-C2-C3
46	B	203	PC1	C32-C33-C34-C35
52	q	201	CDL	C58-C59-C60-C61
52	q	201	CDL	O1-C1-CB2-OB2
46	B	203	PC1	C1-C2-C3-O31
46	L	707	PC1	C2C-C2D-C2E-C2F
51	L	705	3PE	C1-C2-C3-O31
51	M	605	3PE	C1-C2-C3-O31
52	J	701	CDL	CA3-CA4-CA6-OA8
52	L	703	CDL	CB3-CB4-CB6-OB8
51	P	502	3PE	C35-C36-C37-C38
51	d	301	3PE	C27-C28-C29-C2A
52	J	701	CDL	C72-C71-CB7-OB8
51	N	1304	3PE	C21-C22-C23-C24
45	Y	803	LMT	O5'-C5'-C6'-O6'
46	A	303	PC1	C32-C31-O31-C3
51	L	701	3PE	C33-C34-C35-C36
46	L	707	PC1	C2B-C2C-C2D-C2E
51	M	605	3PE	C32-C33-C34-C35
52	h	1001	CDL	C73-C74-C75-C76
46	L	707	PC1	C2F-C2G-C2H-C2I
51	P	502	3PE	C1-C2-O21-C21
52	h	1001	CDL	C71-CB7-OB8-CB6
46	B	202	PC1	C27-C28-C29-C2A
51	I	201	3PE	C29-C2A-C2B-C2C
52	J	701	CDL	CA4-CA6-OA8-CA7
51	H	402	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
46	L	707	PC1	O22-C21-O21-C2
52	K	401	CDL	OB7-CB5-OB6-CB4
52	K	401	CDL	OA9-CA7-OA8-CA6
46	B	203	PC1	C35-C36-C37-C38
51	H	402	3PE	C3C-C3D-C3E-C3F
52	q	201	CDL	C35-C36-C37-C38
52	q	201	CDL	C52-C53-C54-C55
51	L	701	3PE	C2F-C2G-C2H-C2I
52	q	201	CDL	CA2-C1-CB2-OB2
45	A	302	LMT	C7-C8-C9-C10
52	L	703	CDL	C55-C56-C57-C58
51	X	401	3PE	C2-C3-O31-C31
51	H	401	3PE	O11-C1-C2-C3
52	J	701	CDL	OB5-CB3-CB4-CB6
52	K	401	CDL	OB5-CB3-CB4-CB6
46	L	707	PC1	C2D-C2E-C2F-C2G
51	P	502	3PE	C24-C25-C26-C27
51	M	601	3PE	C31-C32-C33-C34
51	P	502	3PE	O13-C11-C12-N
52	L	703	CDL	O1-C1-CA2-OA2
52	L	703	CDL	OA9-CA7-OA8-CA6
51	Y	802	3PE	C2-C1-O11-P
52	J	701	CDL	C54-C55-C56-C57
52	q	201	CDL	C39-C40-C41-C42
45	A	302	LMT	C2-C1-O1'-C1'
45	L	704	LMT	C2-C1-O1'-C1'
45	L	706	LMT	C2-C1-O1'-C1'
45	M	603	LMT	C2-C1-O1'-C1'
45	j	101	LMT	C2-C1-O1'-C1'
45	l	201	LMT	C2-C1-O1'-C1'
51	H	401	3PE	C27-C28-C29-C2A
51	N	1301	3PE	C33-C34-C35-C36
51	N	1301	3PE	C3E-C3F-C3G-C3H
46	B	202	PC1	C2F-C2G-C2H-C2I
51	N	1301	3PE	C26-C27-C28-C29
52	K	401	CDL	C72-C73-C74-C75
46	B	203	PC1	C11-O13-P-O11
51	I	201	3PE	C1-O11-P-O13
45	L	702	LMT	C5-C6-C7-C8
51	I	201	3PE	O11-C1-C2-O21
51	L	701	3PE	O11-C1-C2-O21
51	N	1301	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
52	K	401	CDL	OB5-CB3-CB4-OB6
51	d	301	3PE	C2C-C2D-C2E-C2F
46	B	202	PC1	O21-C21-C22-C23
51	N	1301	3PE	C36-C37-C38-C39
52	h	1001	CDL	OB9-CB7-OB8-CB6
45	L	702	LMT	C6-C7-C8-C9
52	h	1001	CDL	C16-C17-C18-C19
51	H	401	3PE	O21-C2-C3-O31
51	L	705	3PE	O21-C2-C3-O31
51	M	605	3PE	O21-C2-C3-O31
52	h	1001	CDL	OB6-CB4-CB6-OB8
52	q	201	CDL	OB6-CB4-CB6-OB8
51	L	705	3PE	C32-C31-O31-C3
51	H	401	3PE	C36-C37-C38-C39
51	H	402	3PE	C3A-C3B-C3C-C3D
51	M	601	3PE	C35-C36-C37-C38
51	L	701	3PE	C34-C35-C36-C37
51	L	705	3PE	C37-C38-C39-C3A
52	L	703	CDL	C32-C33-C34-C35
52	h	1001	CDL	C11-C12-C13-C14
51	N	1303	3PE	C2-C1-O11-P
51	P	502	3PE	C2-C1-O11-P
51	L	701	3PE	C38-C39-C3A-C3B
52	L	703	CDL	C71-C72-C73-C74
52	K	401	CDL	C16-C17-C18-C19
45	l	201	LMT	O1'-C1-C2-C3
52	h	1001	CDL	OA5-CA3-CA4-CA6
45	M	602	LMT	C9-C10-C11-C12
51	L	705	3PE	C3A-C3B-C3C-C3D
45	Y	801	LMT	C3'-C4'-O1B-C1B
46	L	707	PC1	C25-C26-C27-C28
51	d	301	3PE	C2D-C2E-C2F-C2G
46	B	203	PC1	C31-C32-C33-C34
51	L	705	3PE	C31-C32-C33-C34
45	h	1002	LMT	C4B-C5B-C6B-O6B
45	L	706	LMT	C4-C5-C6-C7
46	B	202	PC1	C25-C26-C27-C28
45	L	704	LMT	C1-C2-C3-C4
45	Y	801	LMT	C5'-C4'-O1B-C1B
46	L	707	PC1	C3-C2-O21-C21
51	M	605	3PE	C1-C2-O21-C21
52	J	701	CDL	CA3-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
51	M	605	3PE	C33-C34-C35-C36
51	N	1303	3PE	C22-C23-C24-C25
51	H	402	3PE	C1-C2-C3-O31
51	d	301	3PE	C1-C2-C3-O31
52	q	201	CDL	CB3-CB4-CB6-OB8
46	L	707	PC1	O11-C1-C2-O21
51	H	401	3PE	O11-C1-C2-O21
54	O	401	GTP	PB-O3B-PG-O2G
58	T	101	EHZ	O1-C7-C8-C9
51	I	201	3PE	C26-C27-C28-C29
51	N	1304	3PE	C32-C33-C34-C35
46	B	203	PC1	O21-C2-C3-O31
51	L	705	3PE	O32-C31-O31-C3
46	B	202	PC1	C34-C35-C36-C37
56	P	501	NDP	C2B-O2B-P2B-O3X
45	M	603	LMT	C7-C8-C9-C10
52	q	201	CDL	C59-C60-C61-C62
45	N	1302	LMT	C11-C10-C9-C8
51	M	601	3PE	C36-C37-C38-C39
52	L	703	CDL	C38-C39-C40-C41
46	L	707	PC1	C35-C36-C37-C38
52	K	401	CDL	C11-C12-C13-C14
53	N	1305	I49	C08-C06-C07-C09
53	N	1305	I49	C08-C06-C07-C10
51	N	1304	3PE	C11-O13-P-O11
51	Y	802	3PE	C1-O11-P-O13
51	d	301	3PE	C1-O11-P-O13
52	J	701	CDL	C74-C75-C76-C77
51	d	301	3PE	C31-C32-C33-C34
51	H	402	3PE	C2-C1-O11-P
52	q	201	CDL	C1-CB2-OB2-PB2
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C1-O11-P-O14
51	H	402	3PE	C11-O13-P-O12
51	M	601	3PE	C11-O13-P-O14
51	N	1301	3PE	C1-O11-P-O12
51	N	1303	3PE	C1-O11-P-O12
51	N	1303	3PE	C11-O13-P-O12
51	N	1304	3PE	C1-O11-P-O14
51	P	502	3PE	C11-O13-P-O12
52	J	701	CDL	CB3-OB5-PB2-OB4
52	K	401	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
52	K	401	CDL	CB3-OB5-PB2-OB3
52	L	703	CDL	CB3-OB5-PB2-OB4
52	h	1001	CDL	CA2-OA2-PA1-OA4
52	h	1001	CDL	CB3-OB5-PB2-OB4
54	O	401	GTP	C5'-O5'-PA-O1A
58	T	101	EHZ	C6-C7-C8-C9
45	M	603	LMT	C3'-C4'-O1B-C1B
46	L	707	PC1	O11-C1-C2-C3
51	I	201	3PE	C36-C37-C38-C39
45	Y	803	LMT	C5'-C4'-O1B-C1B
51	H	401	3PE	C22-C23-C24-C25
51	M	601	3PE	C12-C11-O13-P
51	L	701	3PE	C35-C36-C37-C38
51	M	601	3PE	C2A-C2B-C2C-C2D
51	N	1304	3PE	O11-C1-C2-O21
51	X	401	3PE	O11-C1-C2-O21
51	Y	802	3PE	O11-C1-C2-O21
52	h	1001	CDL	OB5-CB3-CB4-OB6
45	M	603	LMT	C5'-C4'-O1B-C1B
51	M	605	3PE	C34-C35-C36-C37
45	J	702	LMT	C4'-C5'-C6'-O6'
51	H	401	3PE	C1-C2-C3-O31
59	o	201	MYR	C1-C2-C3-C4
51	H	402	3PE	O21-C2-C3-O31
51	d	301	3PE	O21-C2-C3-O31
52	J	701	CDL	OB6-CB4-CB6-OB8
52	L	703	CDL	OB6-CB4-CB6-OB8
51	Y	802	3PE	C39-C3A-C3B-C3C
52	L	703	CDL	C53-C54-C55-C56
45	M	602	LMT	C6-C7-C8-C9
52	L	703	CDL	C35-C36-C37-C38
51	L	701	3PE	C3D-C3E-C3F-C3G
51	X	401	3PE	C39-C3A-C3B-C3C
45	Y	803	LMT	C3'-C4'-O1B-C1B
51	X	401	3PE	C27-C28-C29-C2A
51	I	201	3PE	C3A-C3B-C3C-C3D
51	N	1303	3PE	O22-C21-O21-C2
46	B	203	PC1	C23-C24-C25-C26
51	N	1303	3PE	C33-C34-C35-C36
51	N	1303	3PE	C31-C32-C33-C34
45	M	603	LMT	C11-C10-C9-C8
51	X	401	3PE	C3F-C3G-C3H-C3I

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Mol	Chain	Res	Type	Atoms
51	N	1301	3PE	C2-C1-O11-P
52	h	1001	CDL	OA5-CA3-CA4-OA6
51	H	402	3PE	C34-C35-C36-C37
51	M	605	3PE	C23-C24-C25-C26
52	L	703	CDL	C71-CB7-OB8-CB6
46	A	303	PC1	O32-C31-O31-C3
51	N	1303	3PE	C22-C21-O21-C2
52	L	703	CDL	OB9-CB7-OB8-CB6
52	q	201	CDL	CA3-OA5-PA1-OA2
51	L	705	3PE	C28-C29-C2A-C2B
51	M	601	3PE	C21-C22-C23-C24
52	h	1001	CDL	CB3-CB4-CB6-OB8
45	L	704	LMT	C4-C5-C6-C7
51	N	1304	3PE	C33-C34-C35-C36
51	Y	802	3PE	C3B-C3C-C3D-C3E
51	H	401	3PE	C26-C27-C28-C29
52	J	701	CDL	C1-CB2-OB2-PB2
51	L	701	3PE	C37-C38-C39-C3A
46	B	202	PC1	C24-C25-C26-C27
52	J	701	CDL	CA7-C31-C32-C33
51	X	401	3PE	O11-C1-C2-C3
56	P	501	NDP	O4D-C1D-N1N-C6N
51	X	401	3PE	C2A-C2B-C2C-C2D
52	J	701	CDL	C72-C73-C74-C75
51	L	701	3PE	C3C-C3D-C3E-C3F
51	M	605	3PE	C37-C38-C39-C3A
51	H	401	3PE	C3A-C3B-C3C-C3D
51	M	605	3PE	C2F-C2G-C2H-C2I
51	H	402	3PE	C31-C32-C33-C34
51	L	701	3PE	C25-C26-C27-C28
51	H	401	3PE	C28-C29-C2A-C2B
51	Y	802	3PE	C38-C39-C3A-C3B
58	T	101	EHZ	S1-C10-C11-N1
56	P	501	NDP	C2D-C1D-N1N-C6N
51	I	201	3PE	C34-C35-C36-C37
51	Y	802	3PE	C32-C33-C34-C35
51	N	1303	3PE	C21-C22-C23-C24
56	P	501	NDP	O4B-C4B-C5B-O5B
52	J	701	CDL	CB3-CB4-CB6-OB8
52	L	703	CDL	CB2-C1-CA2-OA2
52	K	401	CDL	C33-C34-C35-C36
52	q	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
58	U	101	EHZ	C21-C22-C23-C24
45	Y	804	LMT	O5B-C5B-C6B-O6B
52	h	1001	CDL	CA7-C31-C32-C33
51	P	502	3PE	C39-C3A-C3B-C3C
45	A	302	LMT	C2-C3-C4-C5
59	o	201	MYR	C2-C3-C4-C5
58	T	101	EHZ	C2-C3-C4-C5
56	P	501	NDP	C3D-C4D-C5D-O5D
52	q	201	CDL	OB9-CB7-OB8-CB6
51	P	502	3PE	C36-C37-C38-C39
52	J	701	CDL	C72-C71-CB7-OB9
45	M	603	LMT	C4B-C5B-C6B-O6B
51	N	1303	3PE	C32-C33-C34-C35
52	h	1001	CDL	C24-C25-C26-C27
51	d	301	3PE	C3F-C3G-C3H-C3I
54	O	401	GTP	PB-O3A-PA-O1A
45	Y	801	LMT	C1-C2-C3-C4
51	X	401	3PE	C2C-C2D-C2E-C2F
52	q	201	CDL	C73-C74-C75-C76
51	N	1304	3PE	C1-C2-C3-O31
52	K	401	CDL	C14-C15-C16-C17
51	L	705	3PE	C38-C39-C3A-C3B
51	I	201	3PE	O11-C1-C2-C3
51	L	705	3PE	C25-C26-C27-C28
52	J	701	CDL	OA6-CA4-CA6-OA8
45	N	1302	LMT	C2B-C1B-O1B-C4'
52	q	201	CDL	C13-C14-C15-C16
52	q	201	CDL	CA5-C11-C12-C13
52	J	701	CDL	CA3-OA5-PA1-OA2
52	h	1001	CDL	CB2-OB2-PB2-OB5
51	X	401	3PE	O21-C21-C22-C23
52	L	703	CDL	C13-C14-C15-C16
51	L	701	3PE	O21-C21-C22-C23
51	N	1304	3PE	O21-C21-C22-C23
52	q	201	CDL	C32-C31-CA7-OA8
52	J	701	CDL	C35-C36-C37-C38
52	L	703	CDL	C32-C31-CA7-OA8
51	Y	802	3PE	C1-C2-C3-O31
45	h	1002	LMT	C7-C8-C9-C10
45	M	602	LMT	O1'-C1-C2-C3
52	q	201	CDL	C15-C16-C17-C18
51	H	401	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
51	L	705	3PE	C39-C3A-C3B-C3C
51	Y	802	3PE	O21-C2-C3-O31
52	J	701	CDL	C79-C80-C81-C82
52	L	703	CDL	C56-C57-C58-C59
46	B	203	PC1	O21-C21-C22-C23
51	I	201	3PE	C25-C26-C27-C28
46	B	202	PC1	O22-C21-C22-C23
51	P	502	3PE	O21-C21-C22-C23
45	A	301	LMT	O5'-C1'-O1'-C1
52	L	703	CDL	C31-C32-C33-C34
45	l	201	LMT	C5-C6-C7-C8
52	J	701	CDL	C71-C72-C73-C74
51	Y	802	3PE	C22-C23-C24-C25
51	P	502	3PE	C23-C24-C25-C26
52	L	703	CDL	C32-C31-CA7-OA9
51	M	601	3PE	C28-C29-C2A-C2B
51	L	705	3PE	C3C-C3D-C3E-C3F
51	M	601	3PE	C11-O13-P-O11
51	N	1303	3PE	C1-O11-P-O13
52	h	1001	CDL	C15-C16-C17-C18
51	N	1304	3PE	O22-C21-C22-C23
51	X	401	3PE	O22-C21-C22-C23
52	q	201	CDL	C32-C31-CA7-OA9
51	H	402	3PE	C36-C37-C38-C39
46	B	202	PC1	C39-C3A-C3B-C3C
51	d	301	3PE	C3B-C3C-C3D-C3E
51	L	701	3PE	C39-C3A-C3B-C3C
46	B	202	PC1	C11-O13-P-O12
51	H	402	3PE	C1-O11-P-O14
51	L	701	3PE	C1-O11-P-O14
51	N	1301	3PE	C11-O13-P-O14
51	N	1303	3PE	C11-O13-P-O14
51	d	301	3PE	C1-O11-P-O14
52	J	701	CDL	CB2-OB2-PB2-OB3
52	J	701	CDL	CB3-OB5-PB2-OB3
52	K	401	CDL	CA3-OA5-PA1-OA4
52	L	703	CDL	CA3-OA5-PA1-OA3
52	L	703	CDL	CB3-OB5-PB2-OB3
52	q	201	CDL	CA3-OA5-PA1-OA3
51	L	705	3PE	C29-C2A-C2B-C2C
52	K	401	CDL	C12-C11-CA5-OA6
51	N	1303	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
52	q	201	CDL	C17-C18-C19-C20
51	H	401	3PE	O13-C11-C12-N
51	L	701	3PE	O22-C21-C22-C23
46	B	203	PC1	O22-C21-C22-C23
52	L	703	CDL	CB7-C71-C72-C73
52	L	703	CDL	C36-C37-C38-C39
51	H	401	3PE	C12-C11-O13-P
51	H	402	3PE	C12-C11-O13-P
51	P	502	3PE	C12-C11-O13-P
51	d	301	3PE	C12-C11-O13-P
52	h	1001	CDL	CA6-CA4-OA6-CA5
45	A	301	LMT	O1'-C1-C2-C3
51	M	601	3PE	C25-C26-C27-C28
51	X	401	3PE	C26-C27-C28-C29
51	N	1303	3PE	O31-C31-C32-C33
52	h	1001	CDL	C32-C31-CA7-OA8
46	B	203	PC1	C2-C1-O11-P
51	N	1304	3PE	C23-C24-C25-C26
49	F	501	FMN	N10-C1'-C2'-O2'
51	P	502	3PE	O22-C21-C22-C23
52	K	401	CDL	C52-C53-C54-C55
46	B	202	PC1	O31-C31-C32-C33
52	h	1001	CDL	CB7-C71-C72-C73
52	h	1001	CDL	C32-C31-CA7-OA9
51	H	401	3PE	O22-C21-C22-C23
51	N	1303	3PE	O32-C31-C32-C33
51	N	1303	3PE	O21-C21-C22-C23

There are no ring outliers.

21 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	M	602	LMT	4	0
51	N	1301	3PE	2	0
47	F	502	SF4	1	0
45	J	702	LMT	1	0
49	F	501	FMN	2	0
53	N	1305	I49	1	0
52	J	701	CDL	1	0
51	M	601	3PE	3	0
51	M	605	3PE	1	0
46	A	303	PC1	1	0

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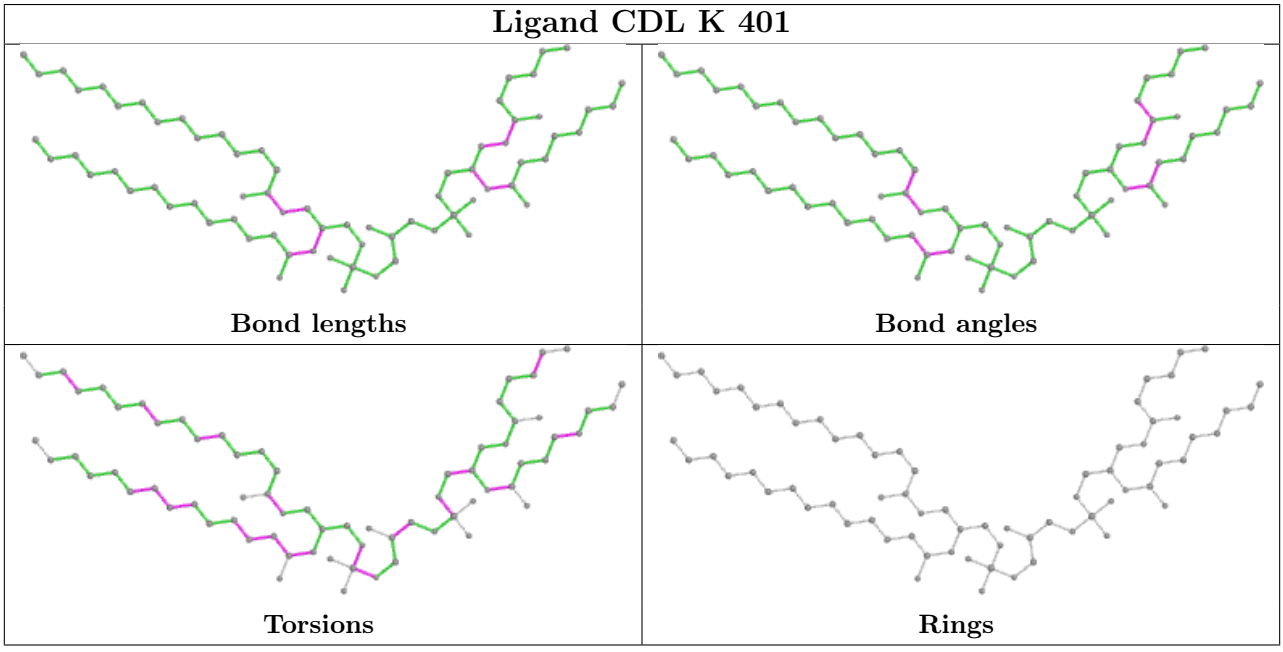
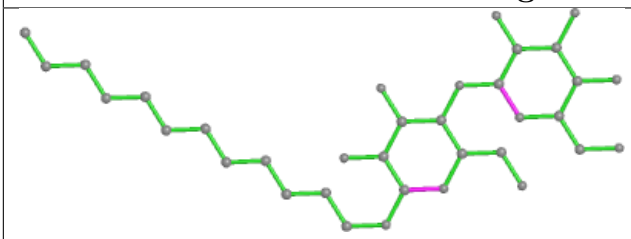
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	P	501	NDP	1	0
45	L	706	LMT	1	0
47	B	201	SF4	1	0
46	B	203	PC1	1	0
51	X	401	3PE	4	0
54	O	401	GTP	3	0
45	Y	801	LMT	2	0
46	B	202	PC1	1	0
45	Y	804	LMT	2	0
51	H	401	3PE	1	0
45	A	302	LMT	1	0

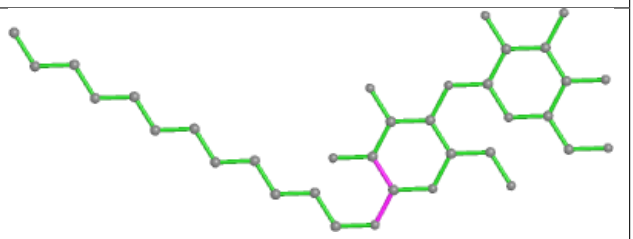
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



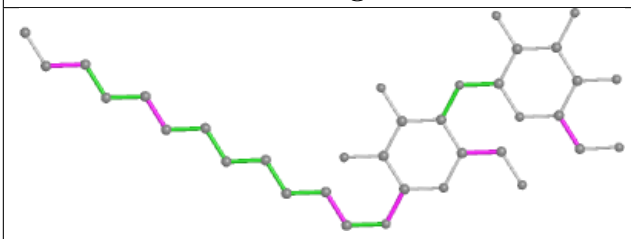
Ligand LMT M 602



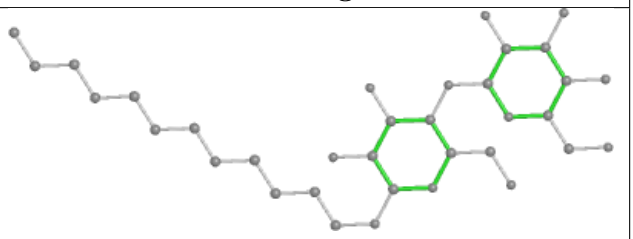
Bond lengths



Bond angles

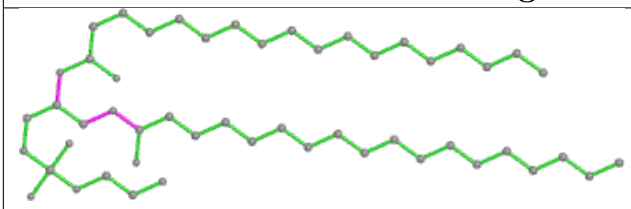


Torsions

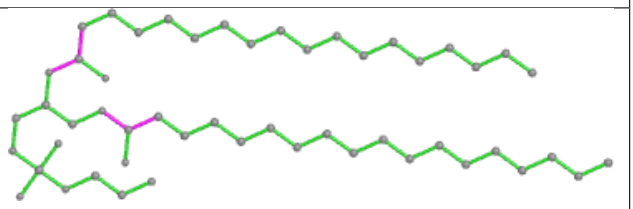


Rings

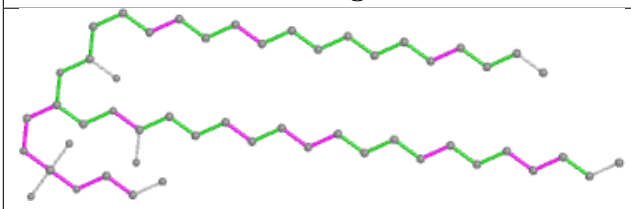
Ligand 3PE N 1301



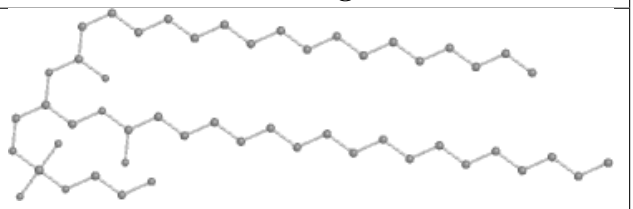
Bond lengths



Bond angles

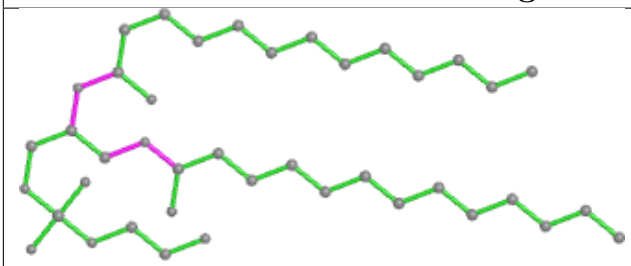


Torsions

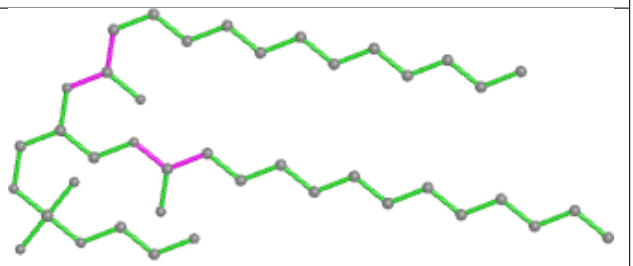


Rings

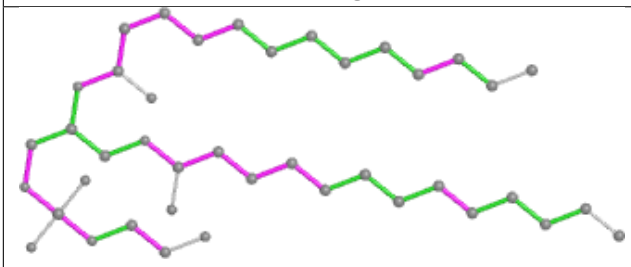
Ligand 3PE N 1303



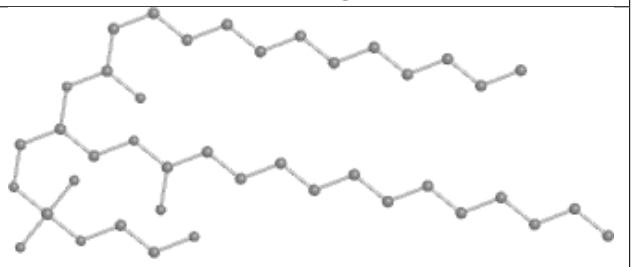
Bond lengths



Bond angles

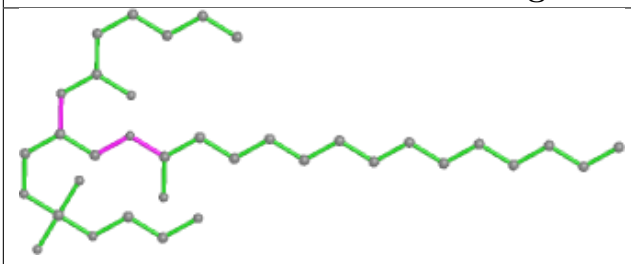


Torsions

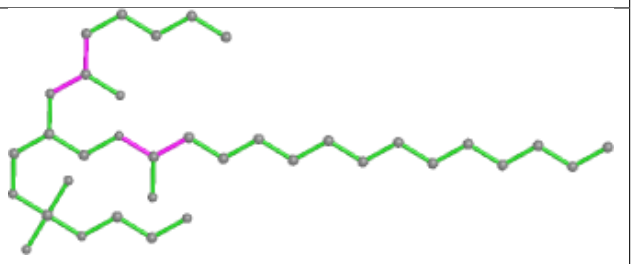


Rings

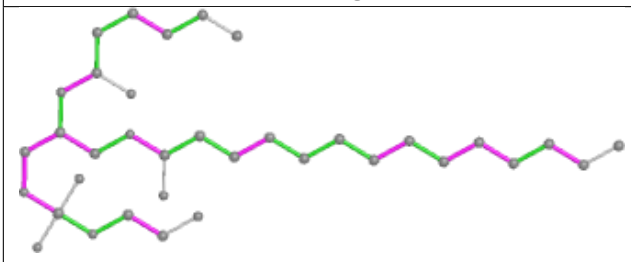
Ligand 3PE Y 802



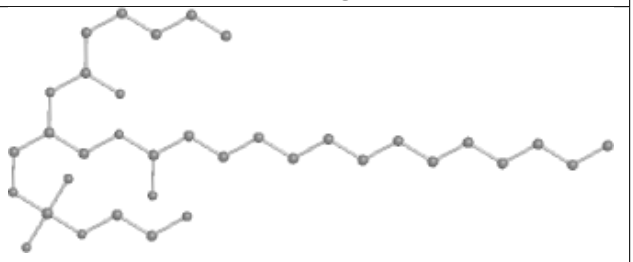
Bond lengths



Bond angles

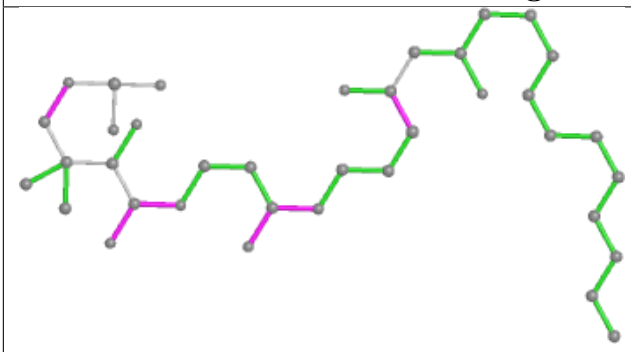


Torsions

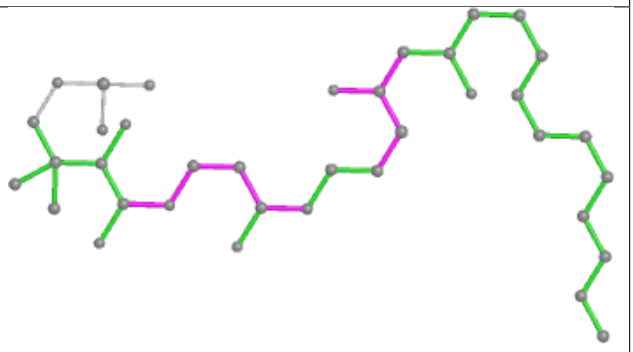


Rings

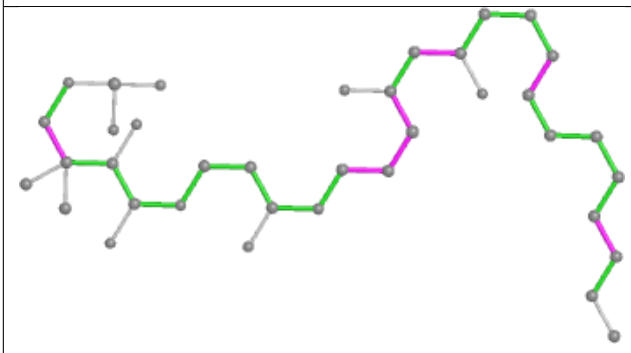
Ligand EHZ T 101



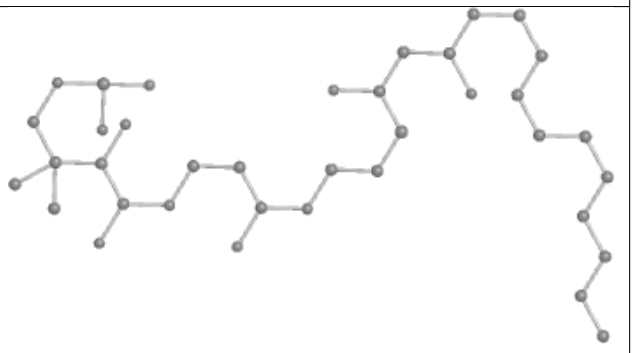
Bond lengths



Bond angles

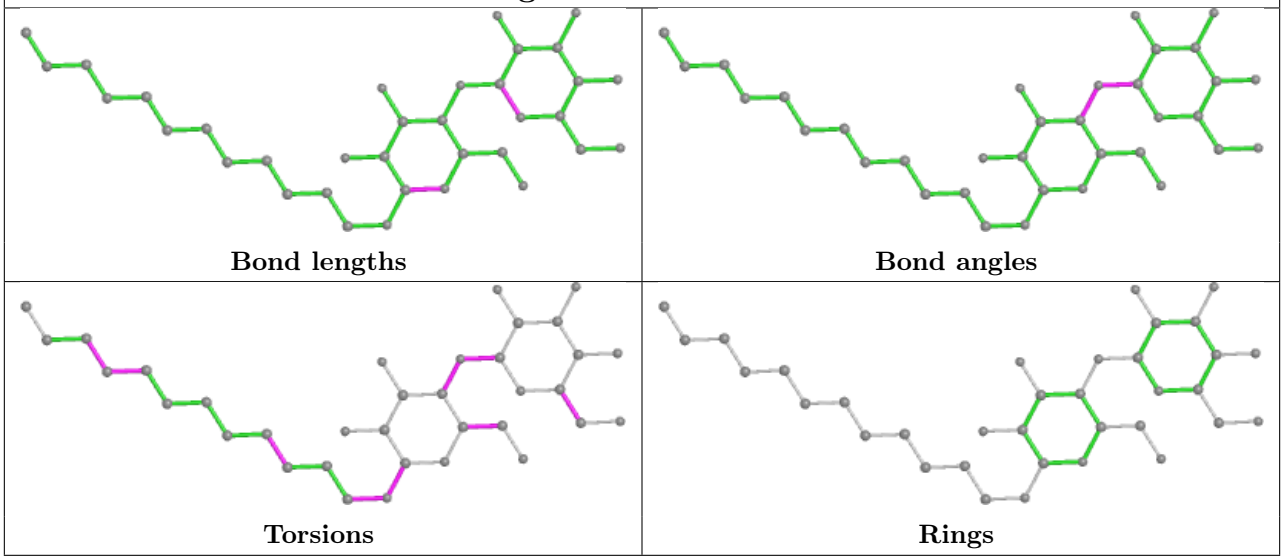


Torsions

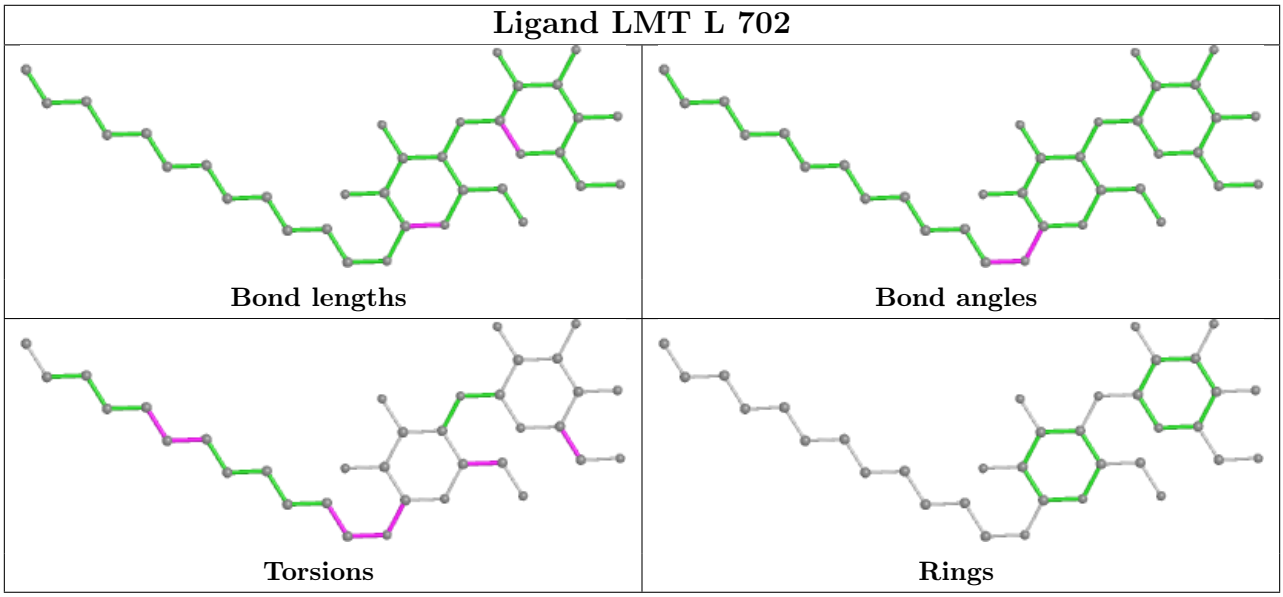


Rings

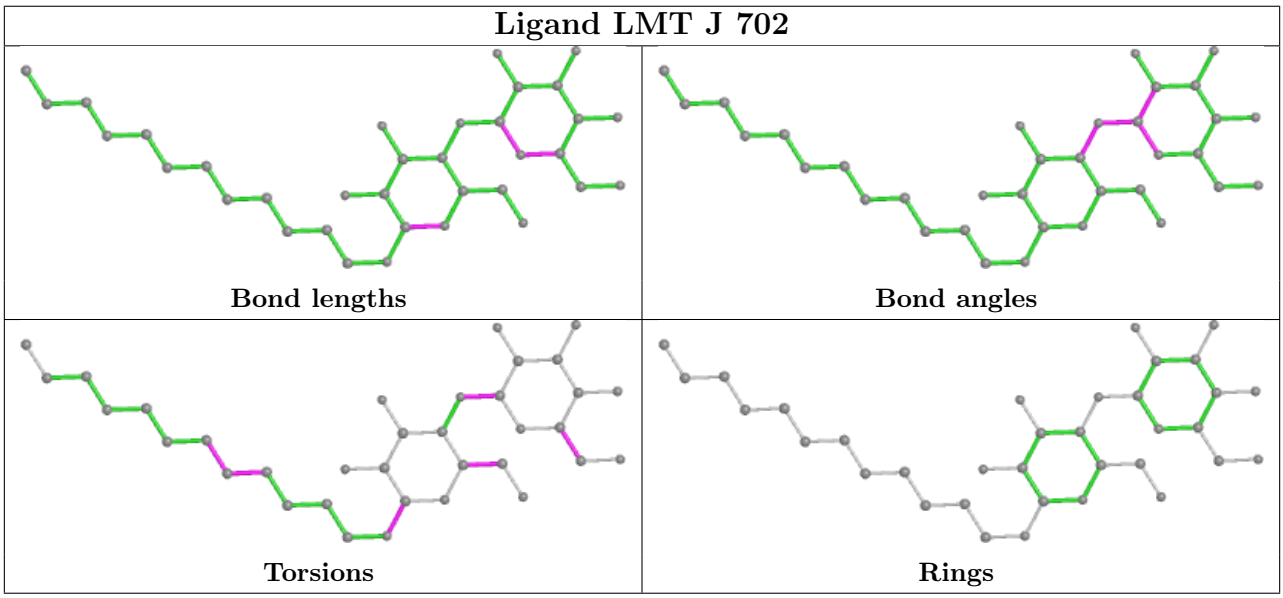
Ligand LMT M 603



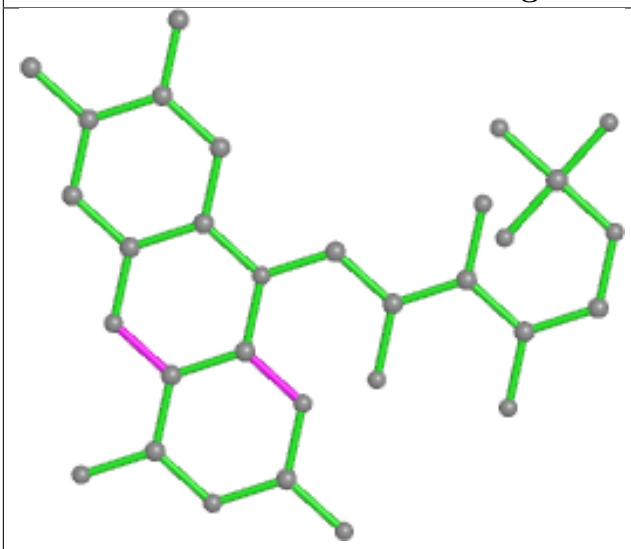
Ligand LMT L 702



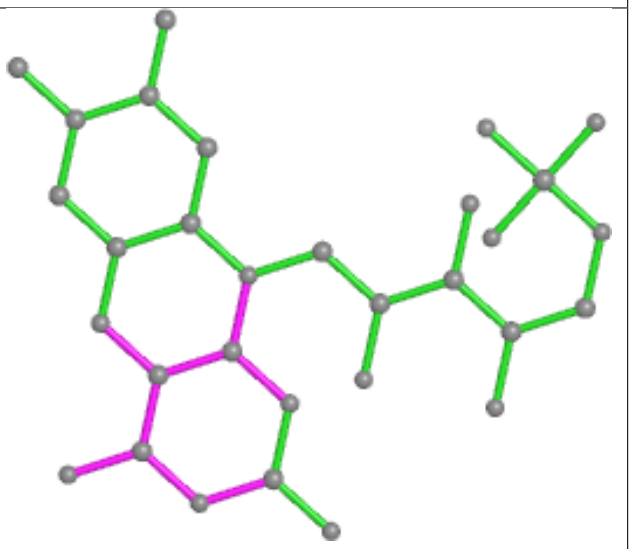
Ligand LMT J 702



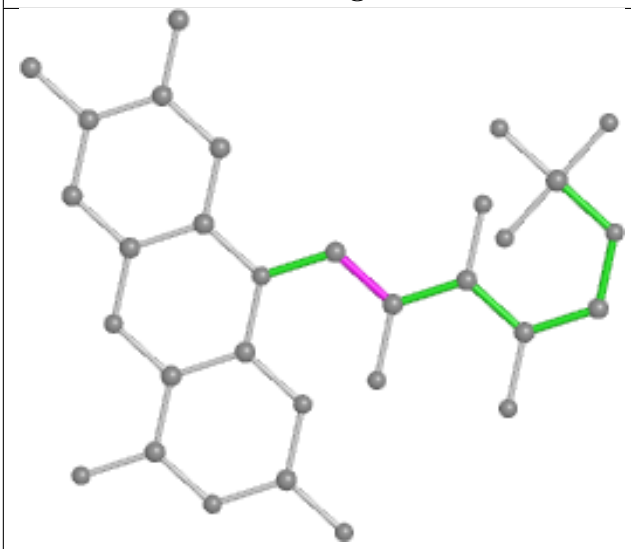
Ligand FMN F 501



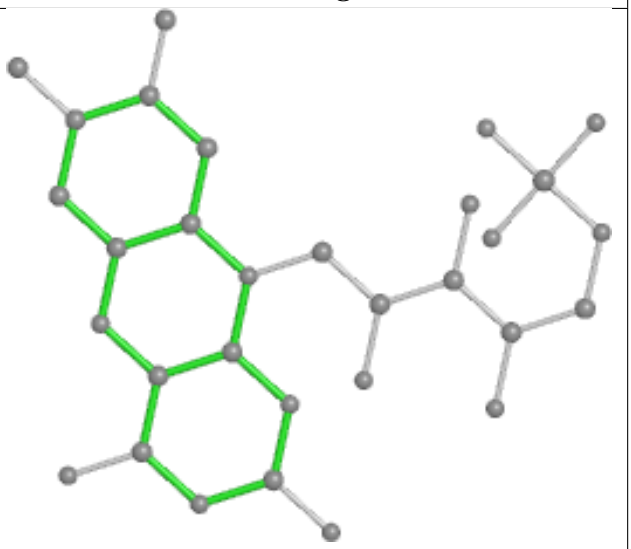
Bond lengths



Bond angles

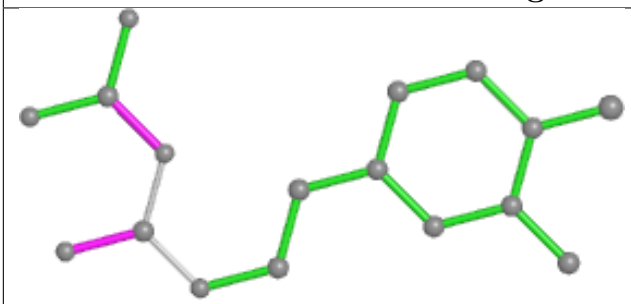


Torsions

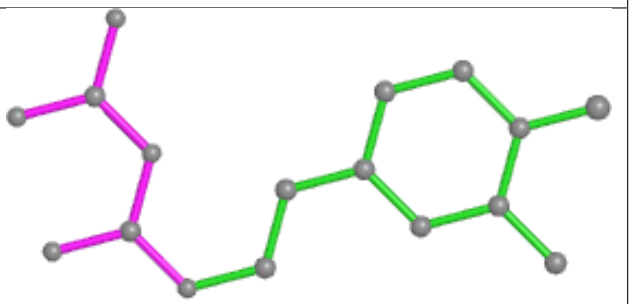


Rings

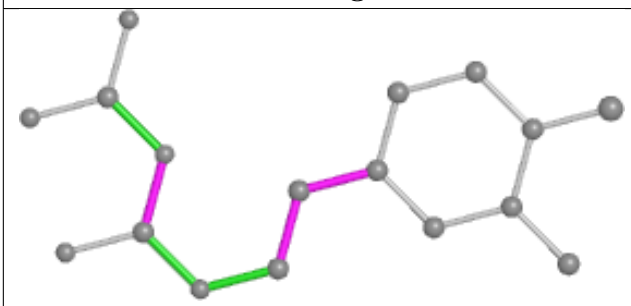
Ligand I49 N 1305



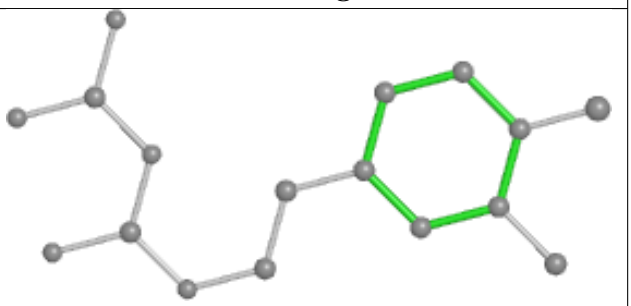
Bond lengths



Bond angles

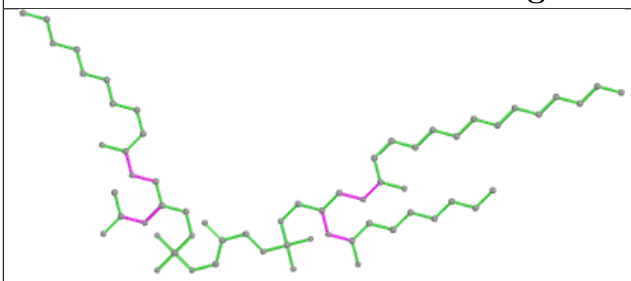


Torsions



Rings

Ligand CDL J 701



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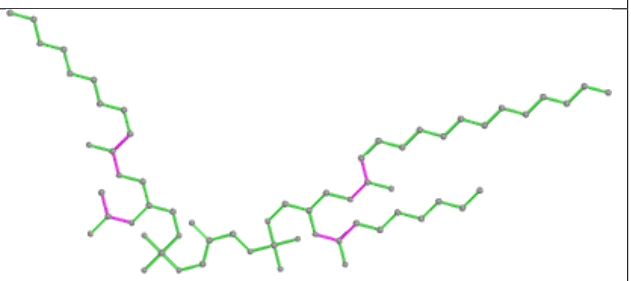
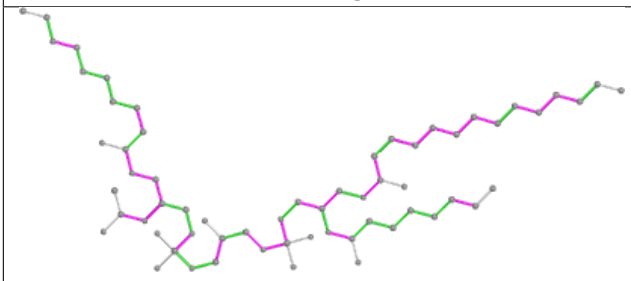
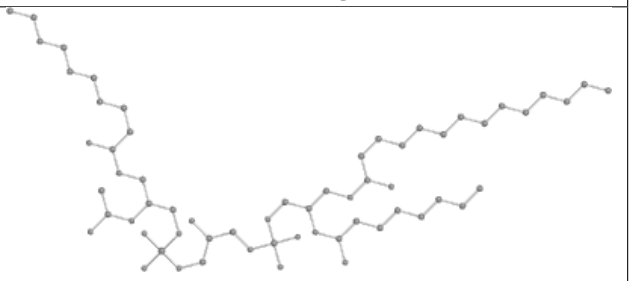


Bond angles

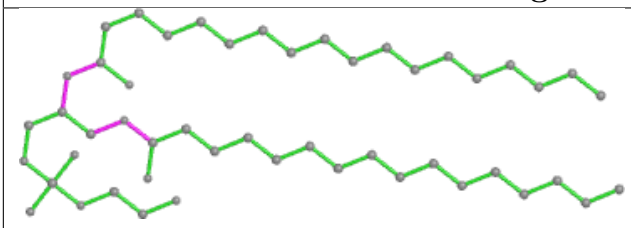


Torsions

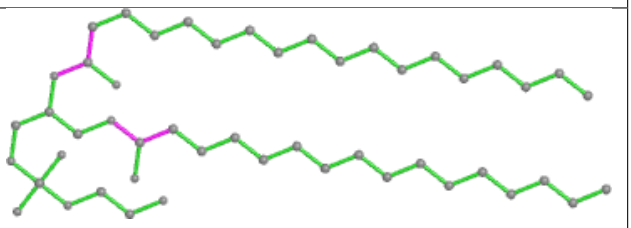


Rings

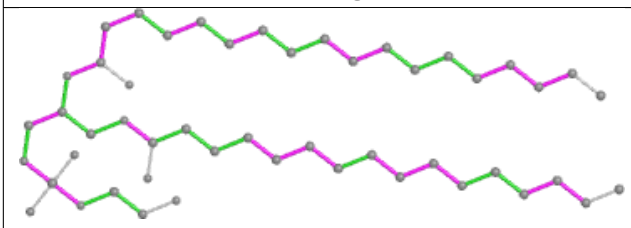
Ligand 3PE L 701



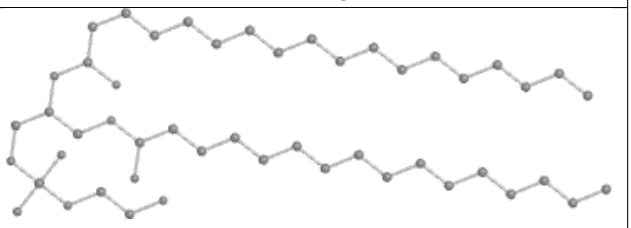
Bond lengths



Bond angles

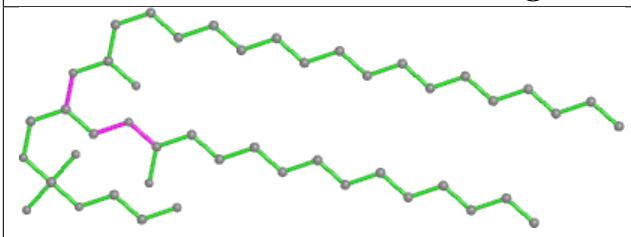


Torsions

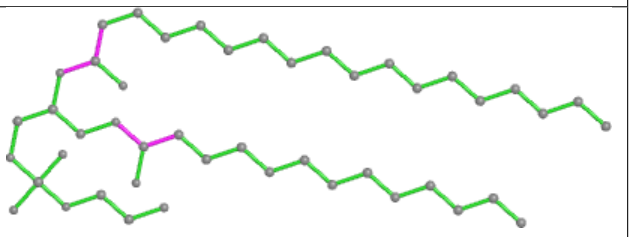


Rings

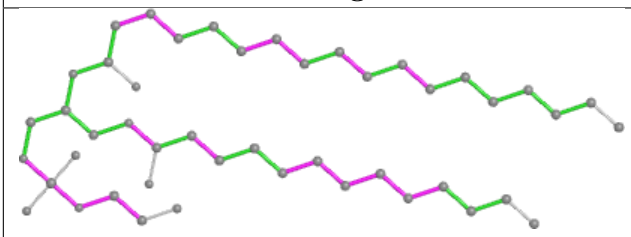
Ligand 3PE M 601



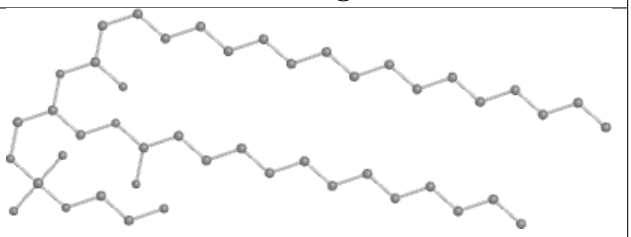
Bond lengths



Bond angles

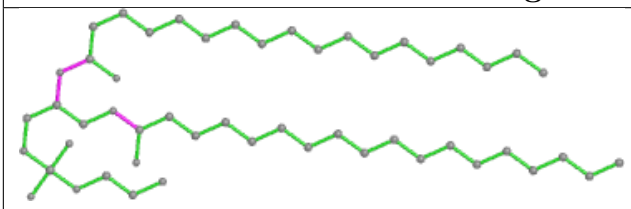


Torsions

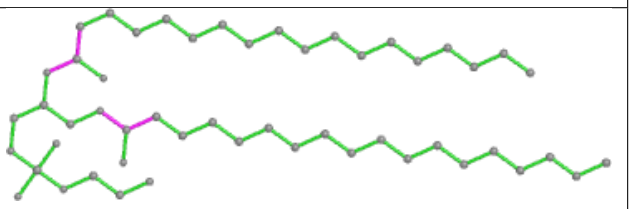


Rings

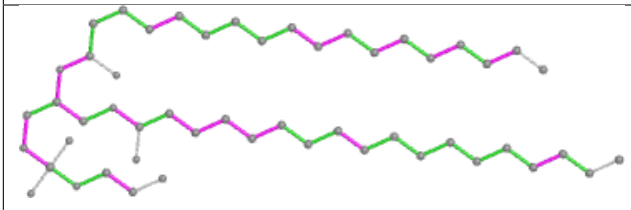
Ligand 3PE M 605



Bond lengths



Bond angles



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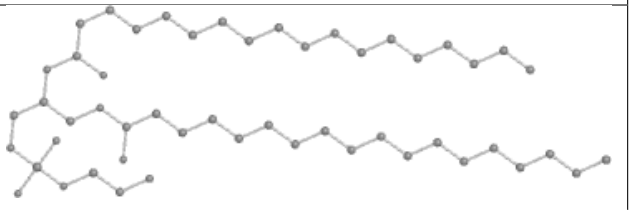
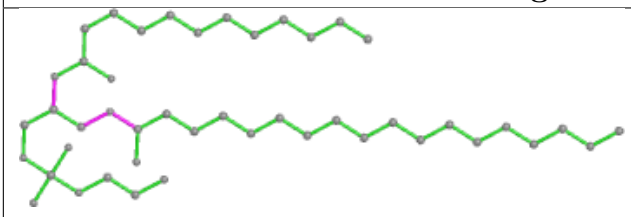
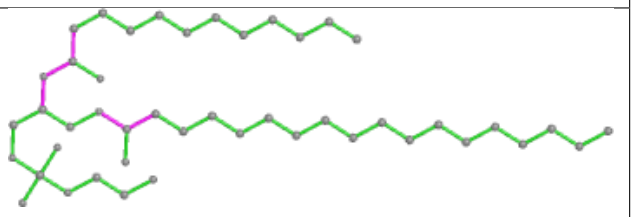


Rings

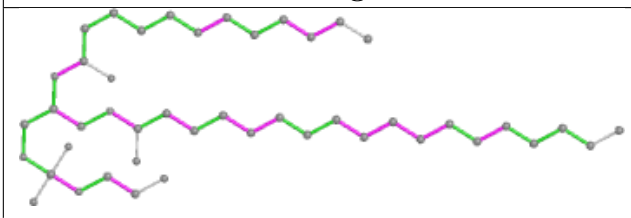
Ligand 3PE L 705



Bond lengths



Bond angles



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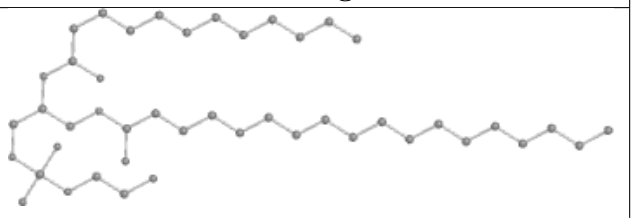
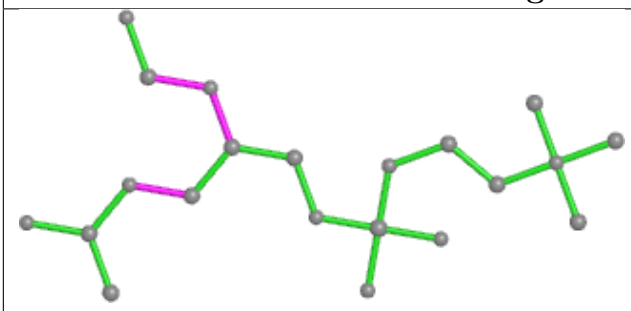
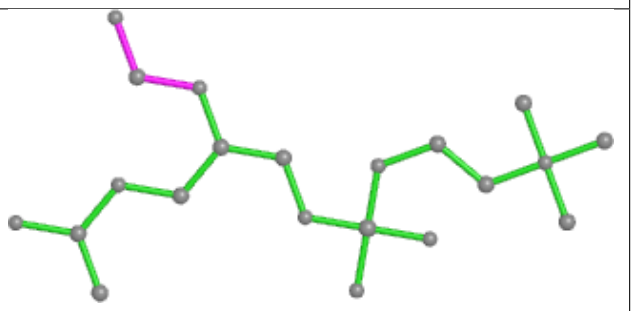


Rings

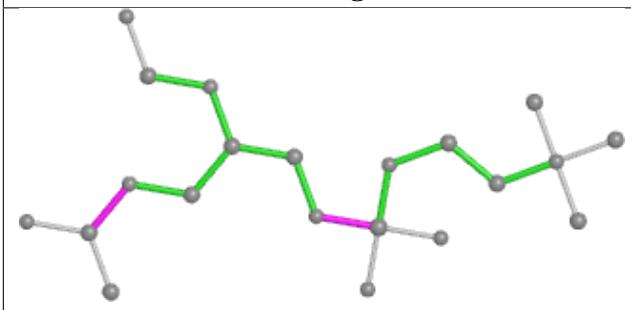
Ligand PC1 A 303



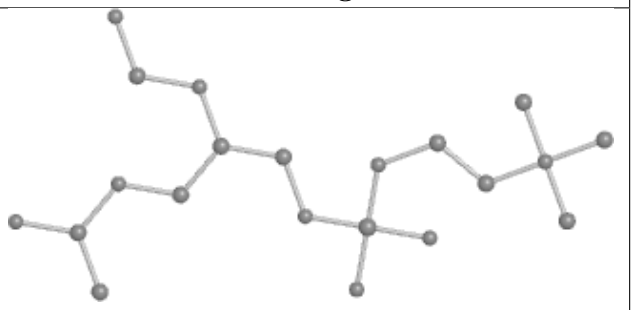
Bond lengths



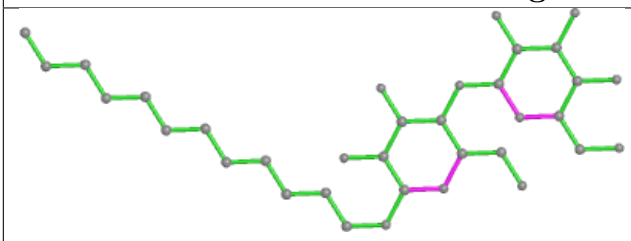
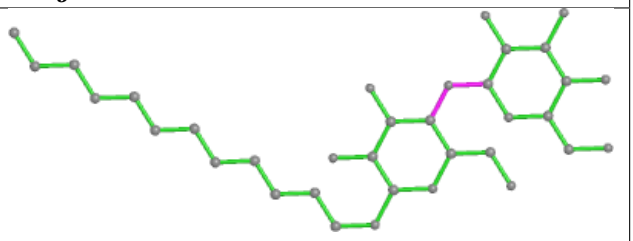
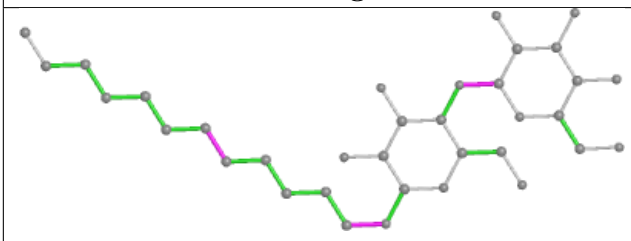
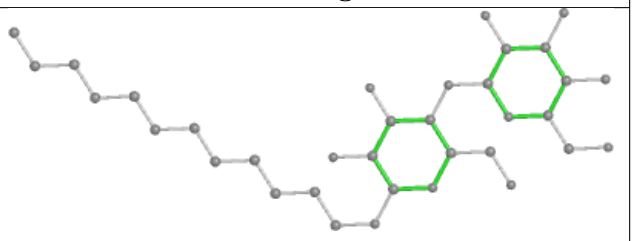
Bond angles

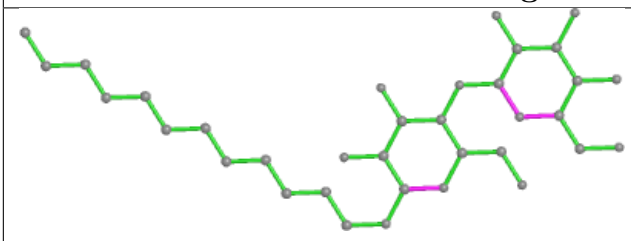
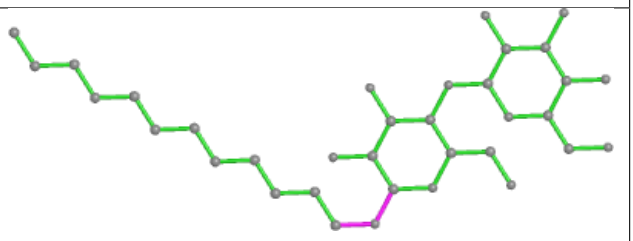
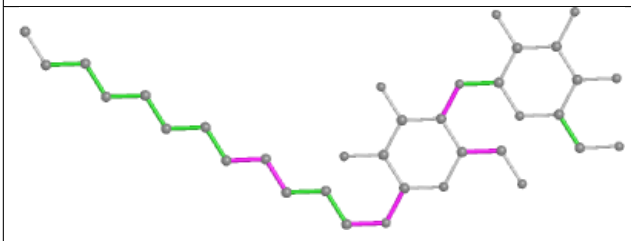
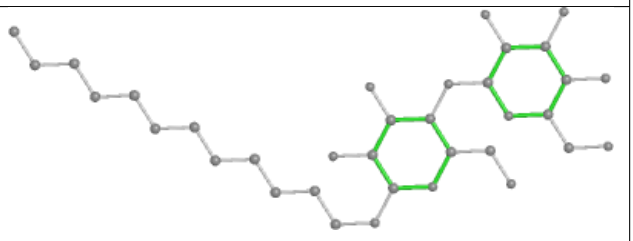


Torsions

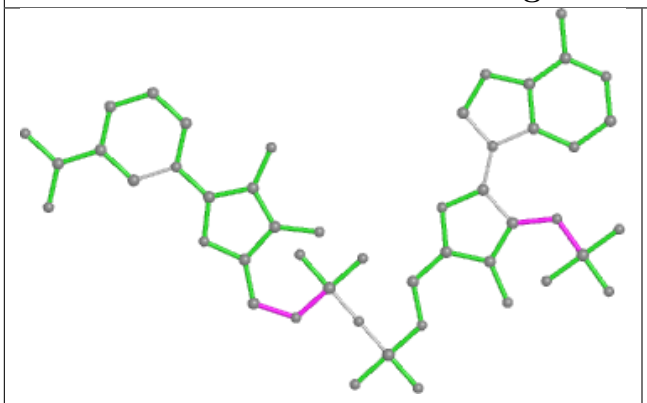


Rings

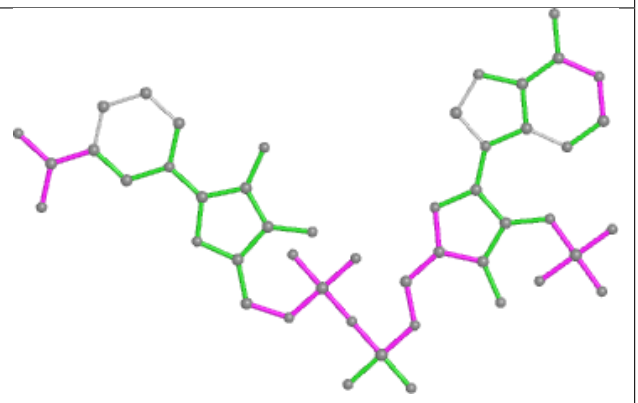
Ligand LMT j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT Y 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

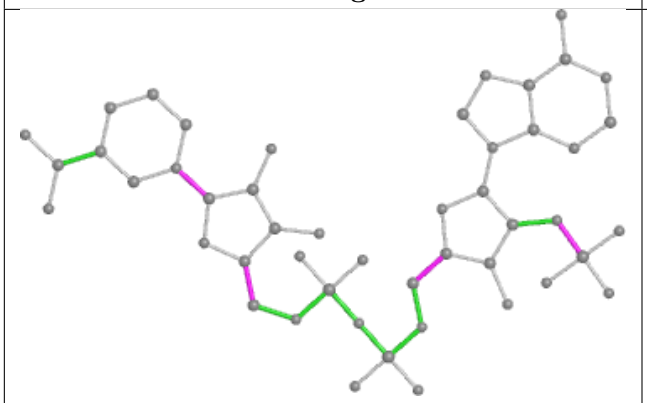
Ligand NDP P 501



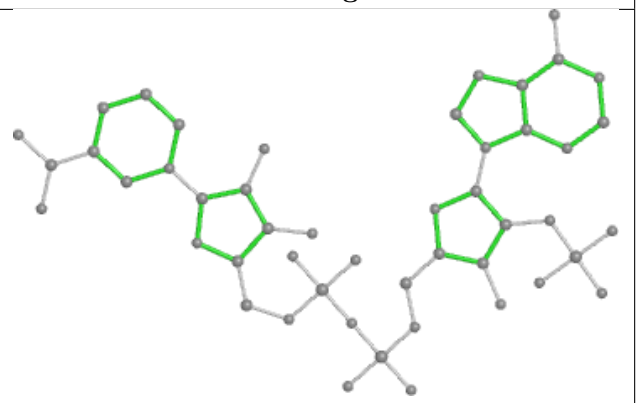
Bond lengths



Bond angles

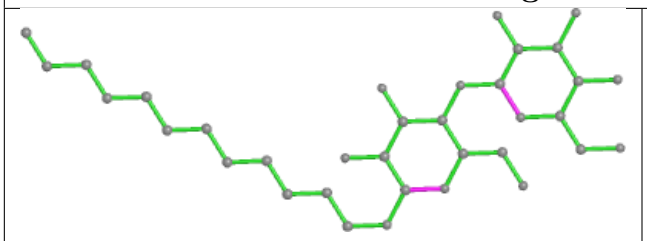


Torsions

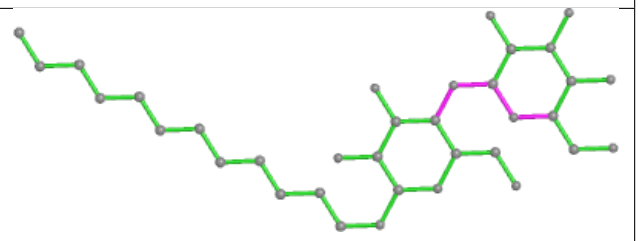


Rings

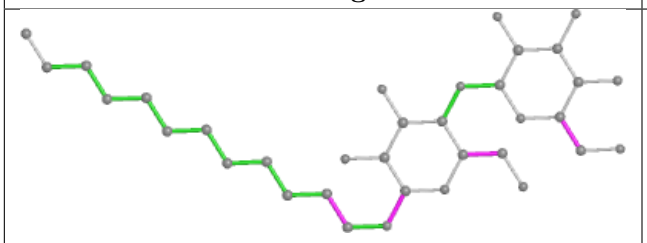
Ligand LMT A 301



Bond lengths



Bond angles



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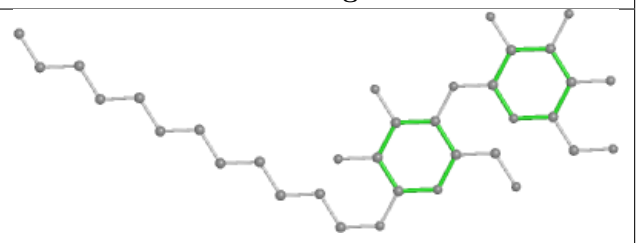
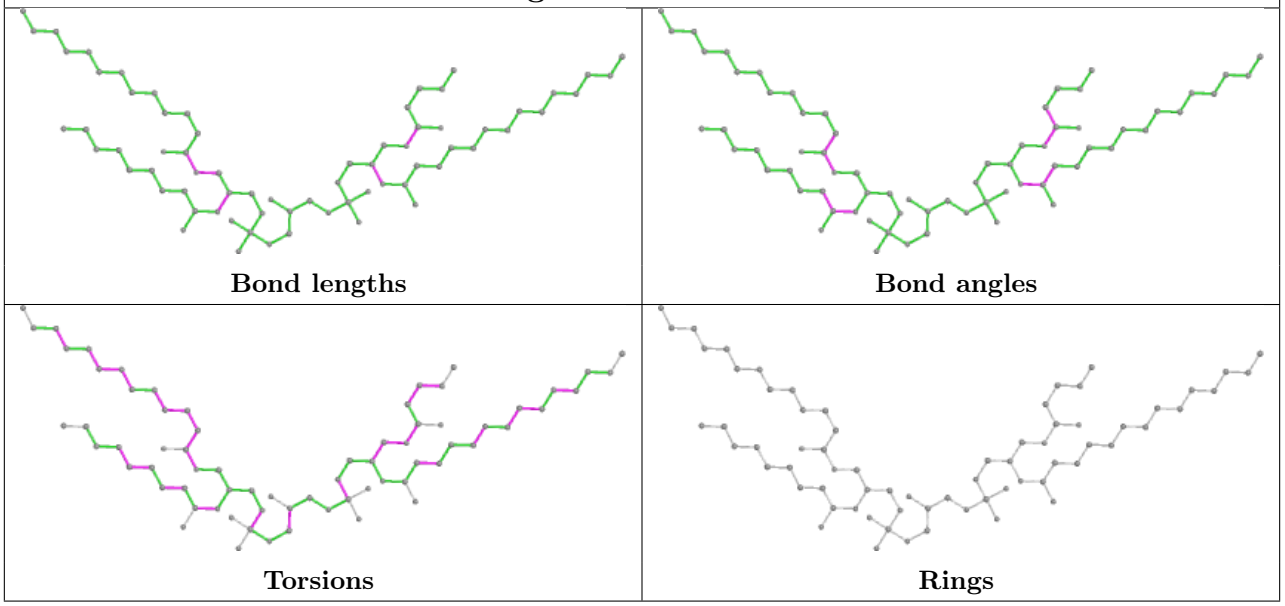
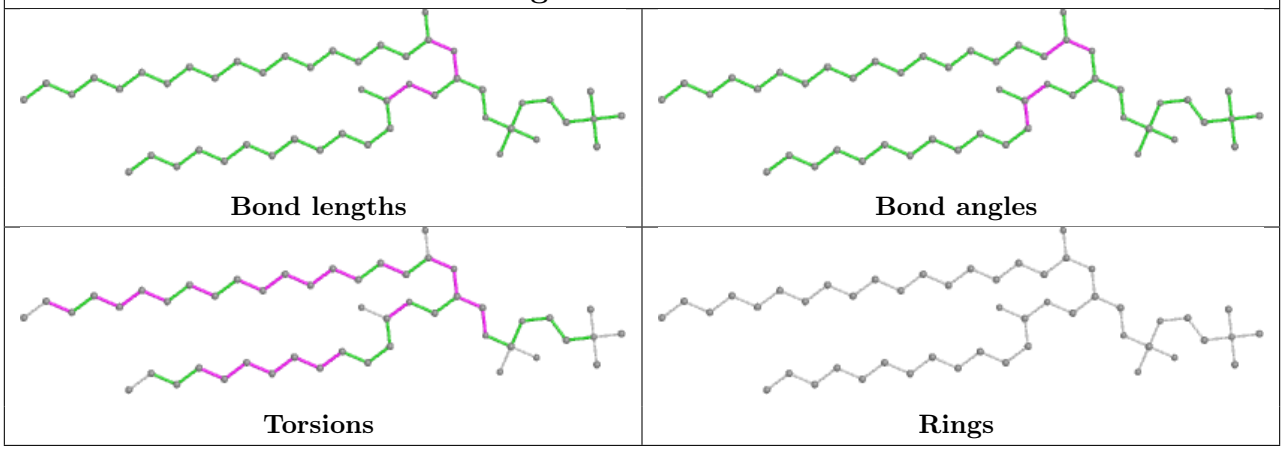


Rings

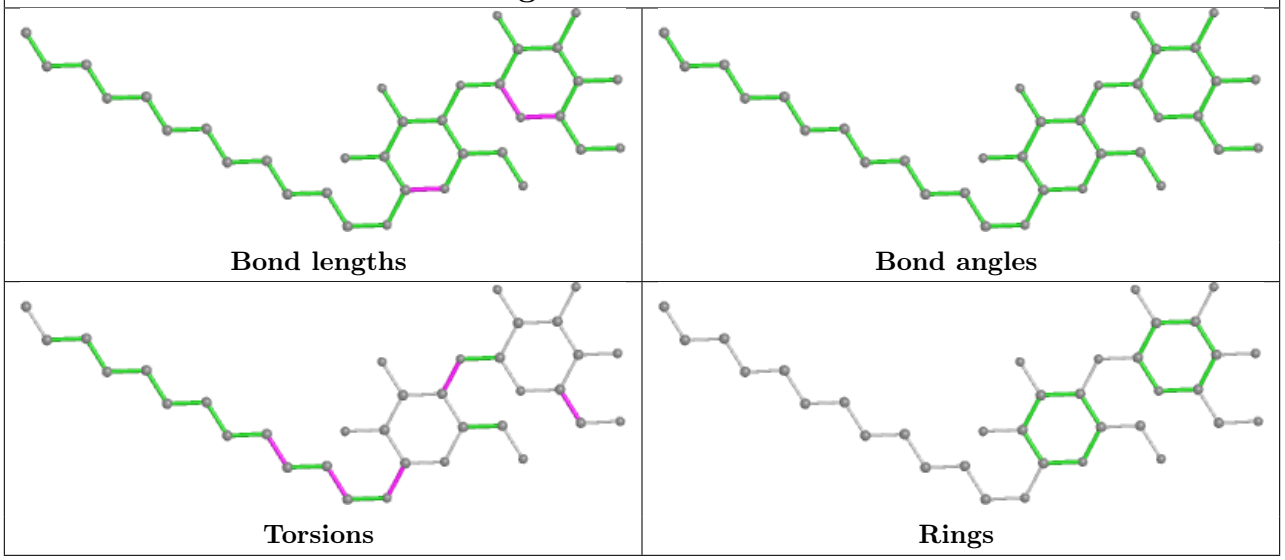
Ligand CDL L 703



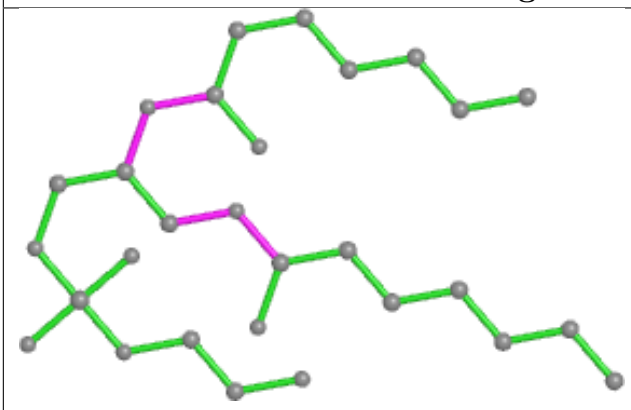
Ligand PC1 L 707



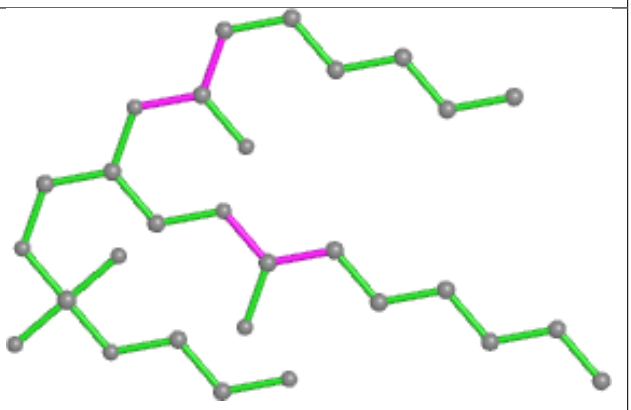
Ligand LMT M 604



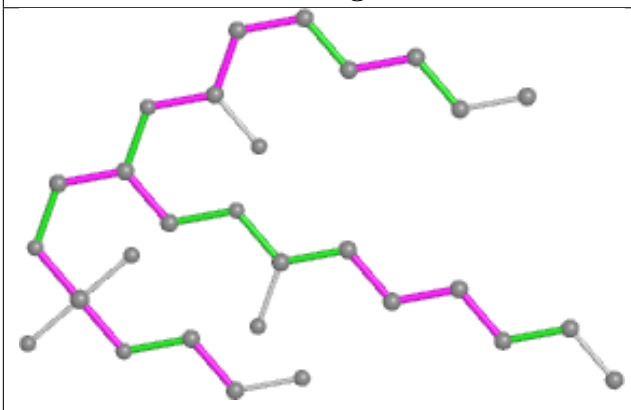
Ligand 3PE N 1304



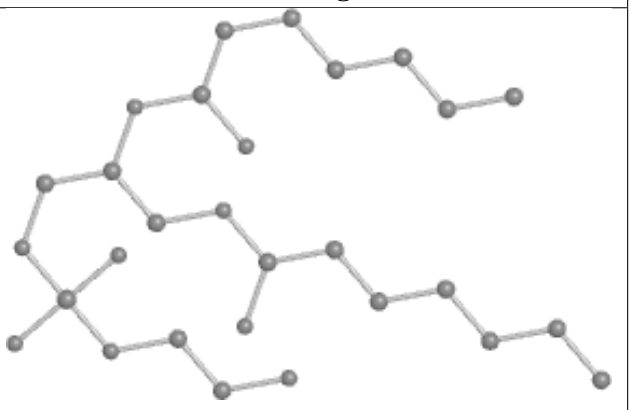
Bond lengths



Bond angles

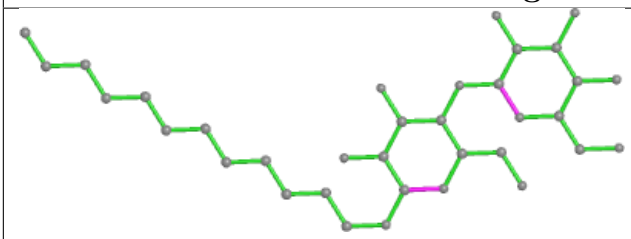


Torsions

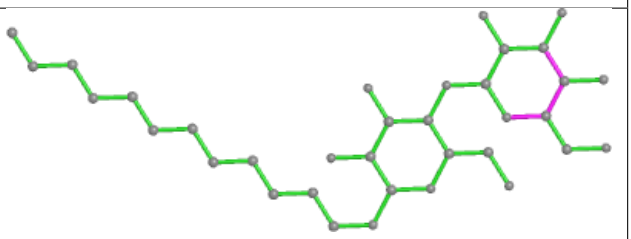


Rings

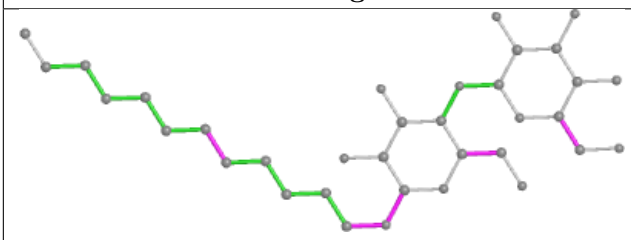
Ligand LMT L 706



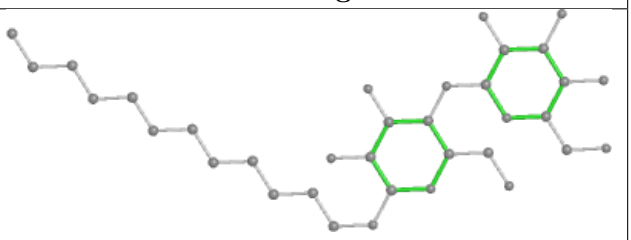
Bond lengths



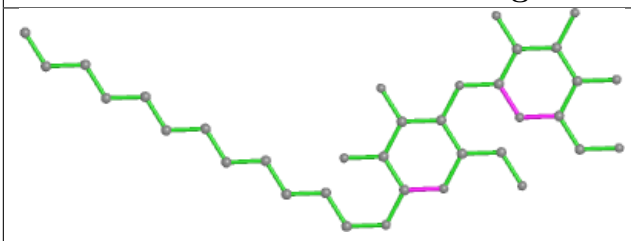
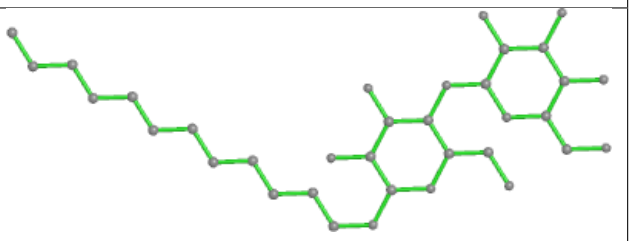
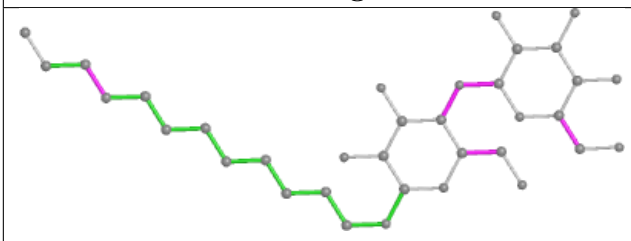
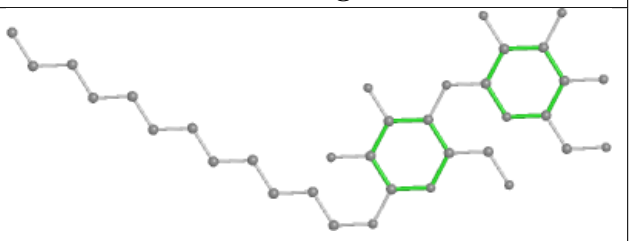
Bond angles

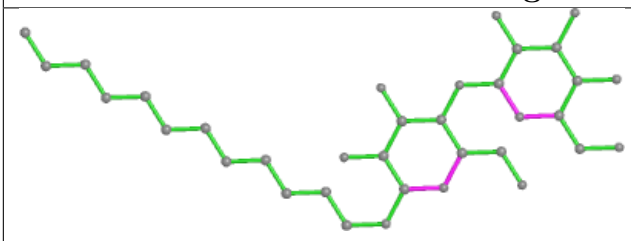
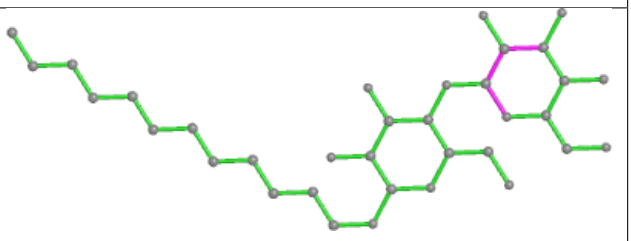
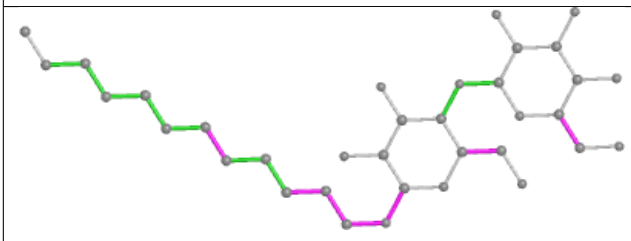
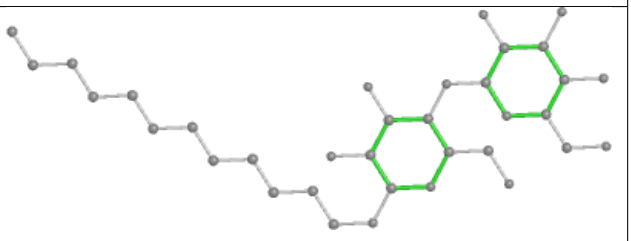


Torsions

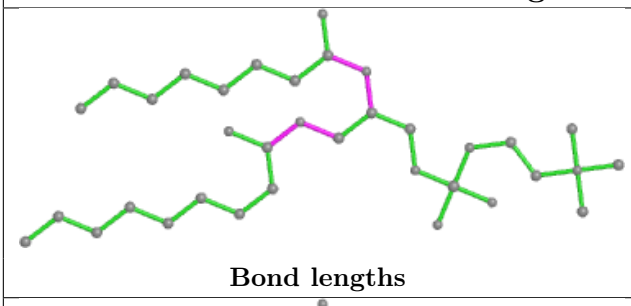


Rings

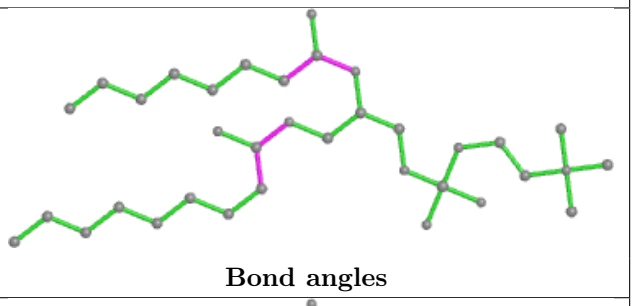
Ligand LMT N 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT L 704	
 Bond lengths	 Bond angles
 Torsions	 Rings

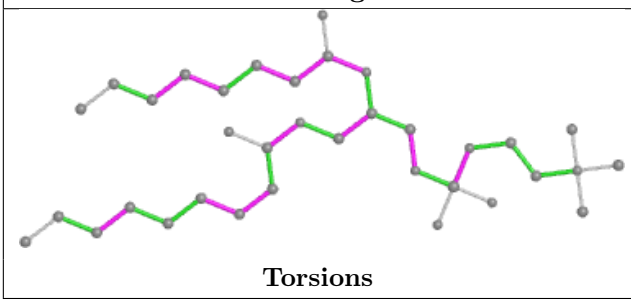
Ligand PC1 B 203



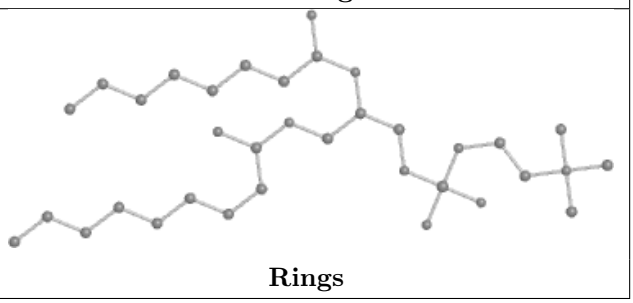
Bond lengths



Bond angles

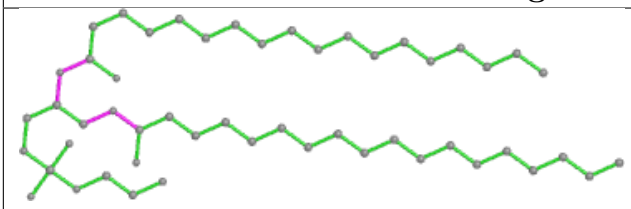


Torsions

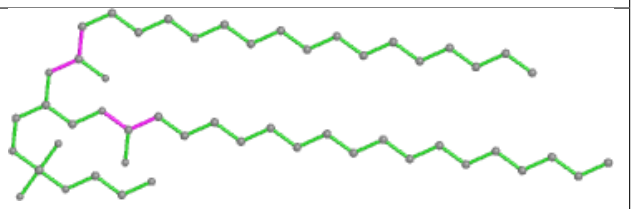


Rings

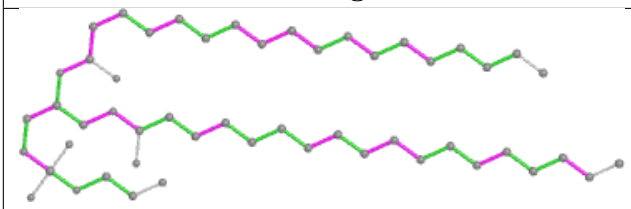
Ligand 3PE X 401



Bond lengths



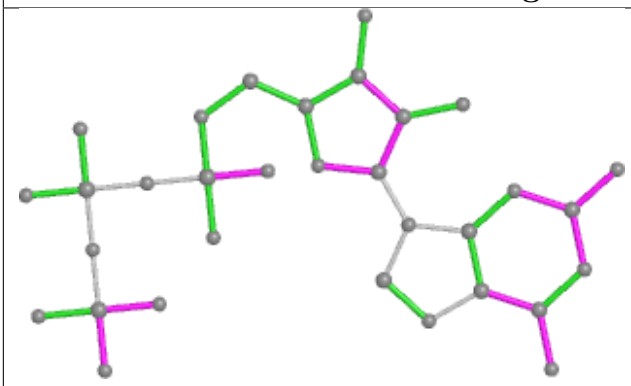
Bond angles



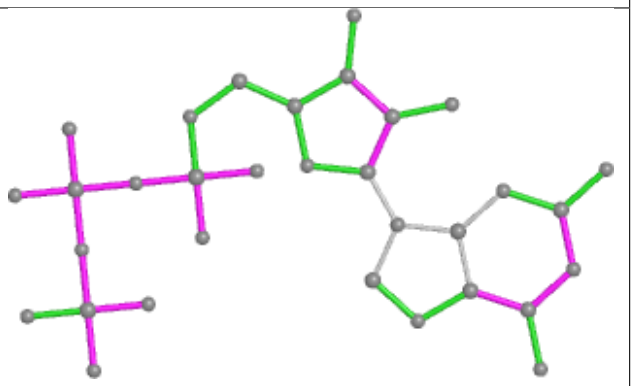
Torsions

Rings

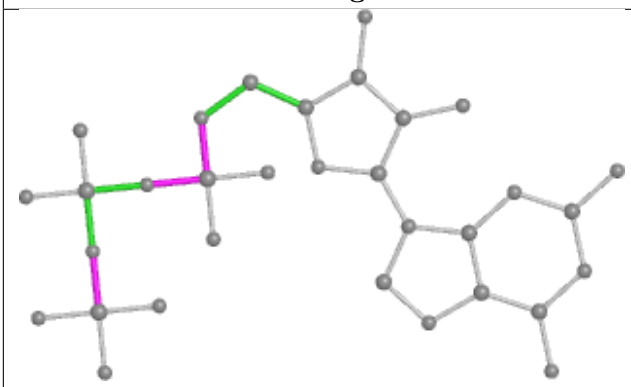
Ligand GTP O 401



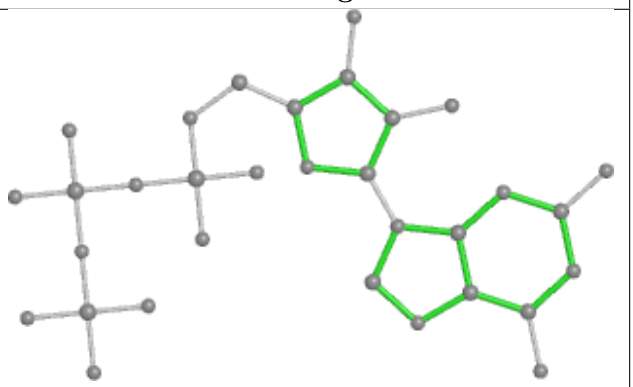
Bond lengths



Bond angles

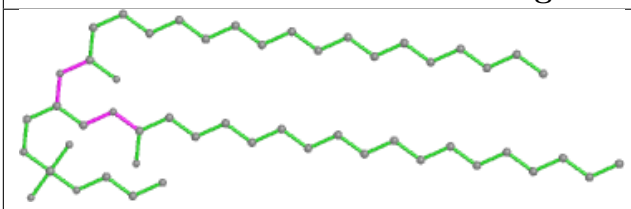


Torsions

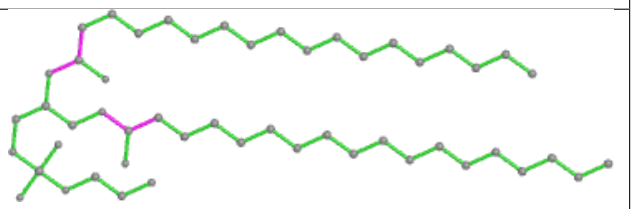


Rings

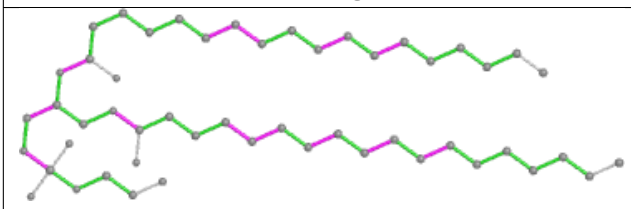
Ligand 3PE I 201



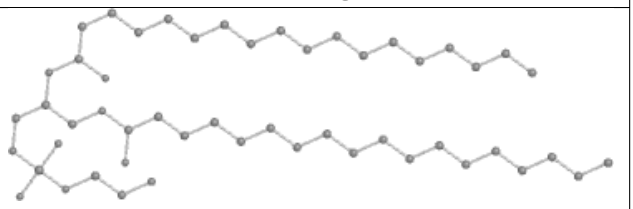
Bond lengths



Bond angles

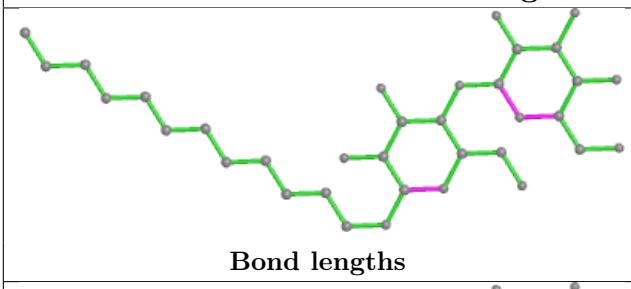


Torsions

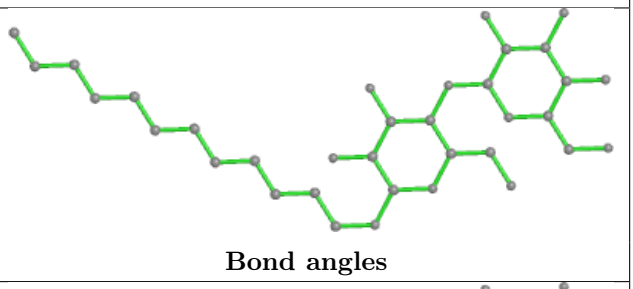


Rings

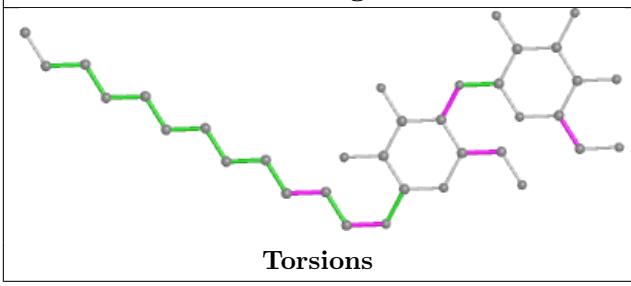
Ligand LMT Y 801



Bond lengths



Bond angles



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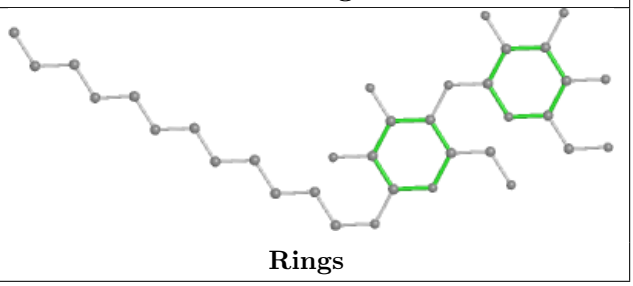
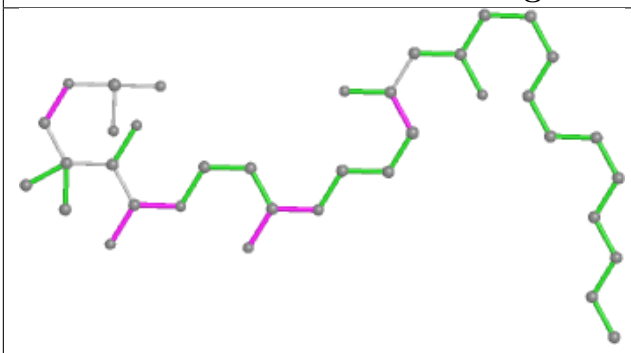
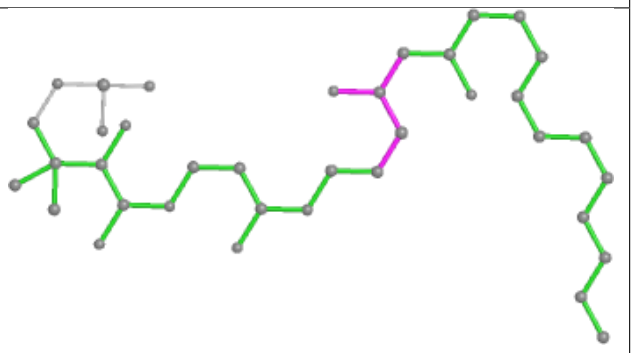


Rings

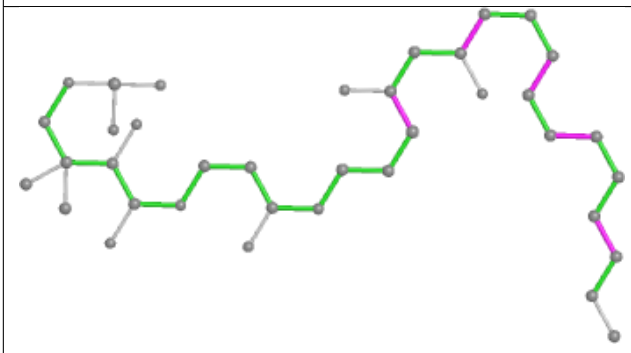
Ligand EHZ U 101



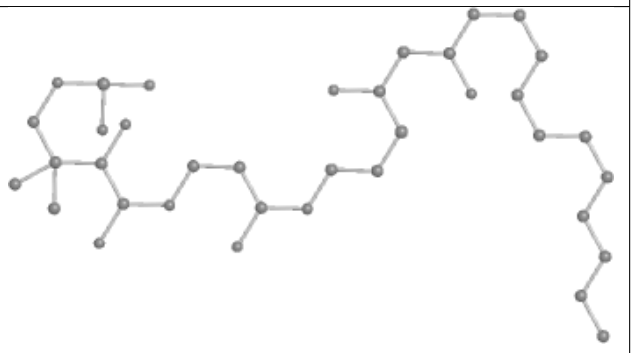
Bond lengths



Bond angles

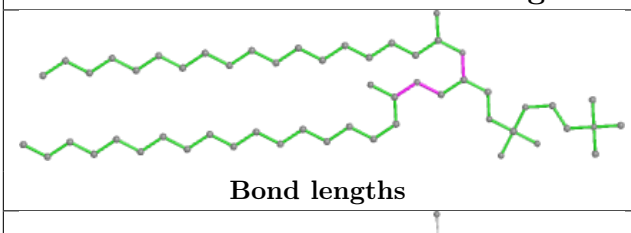


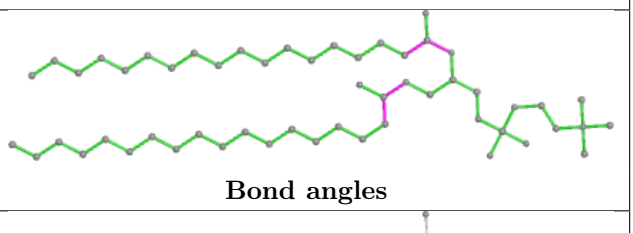
Torsions

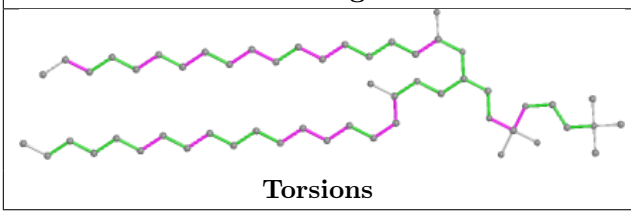


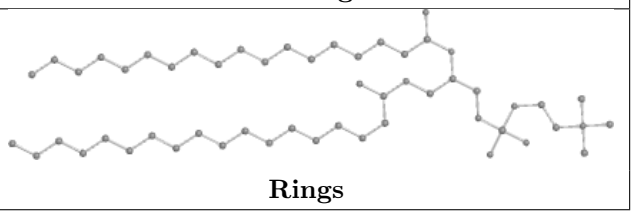
Rings

Ligand PC1 B 202

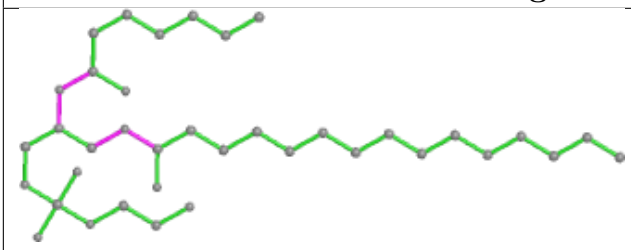

Bond lengths

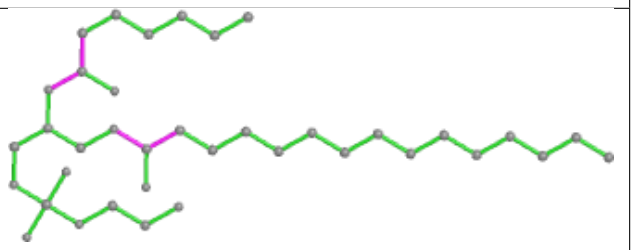

Bond angles

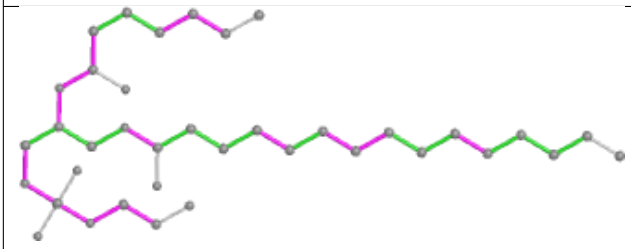

Torsions


Rings

Ligand 3PE P 502

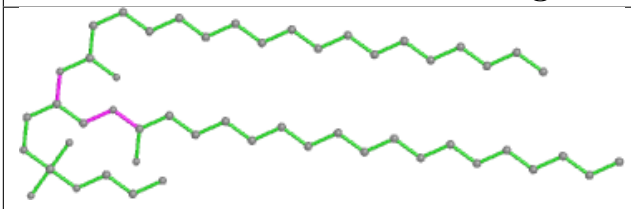

Bond lengths

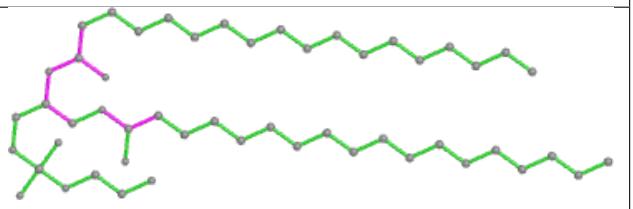

Bond angles

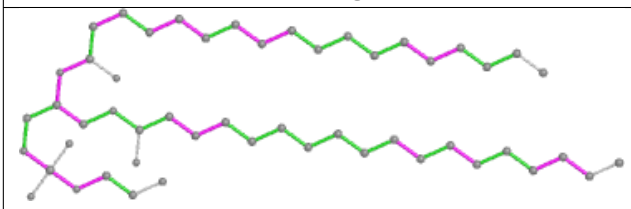

Torsions

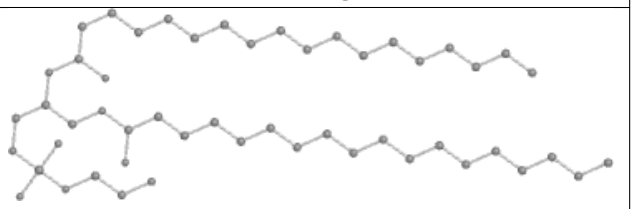

Rings

Ligand 3PE d 301

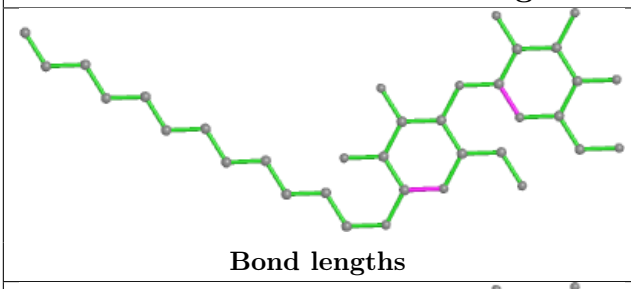

Bond lengths


Bond angles

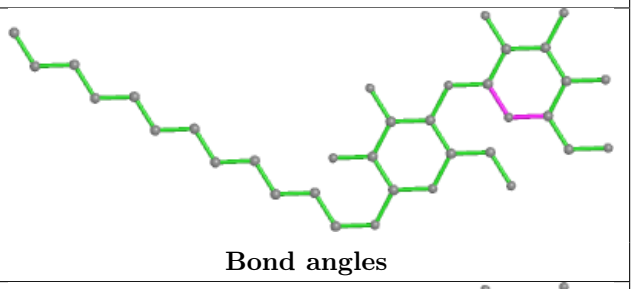

Torsions


Rings

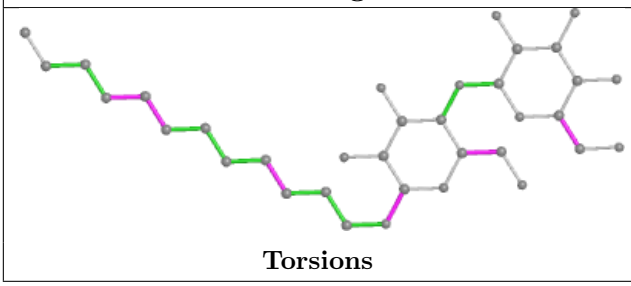
Ligand LMT h 1002



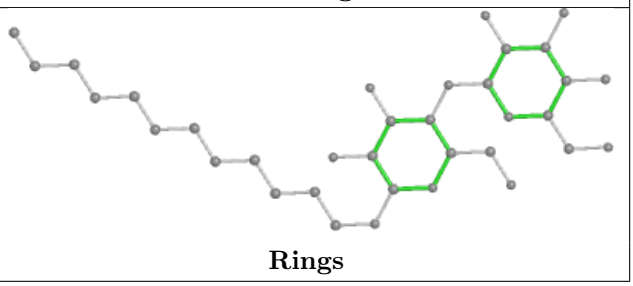
Bond lengths



Bond angles

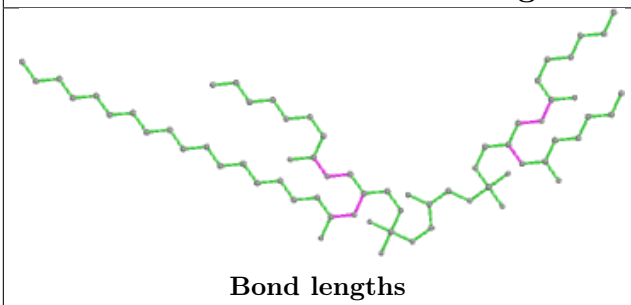


Torsions

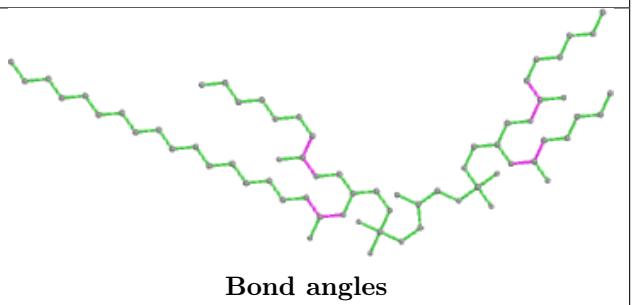


Rings

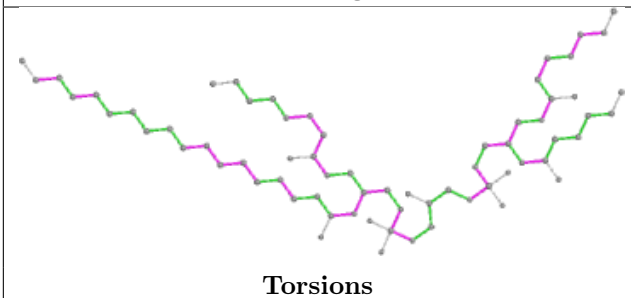
Ligand CDL h 1001



Bond lengths



Bond angles



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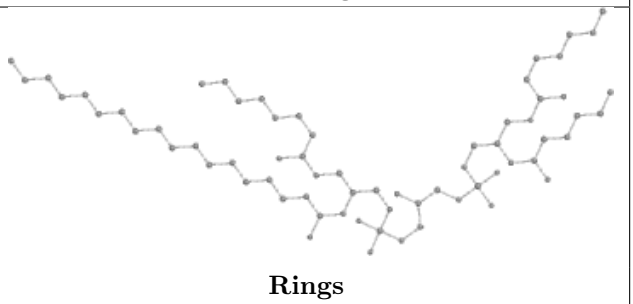
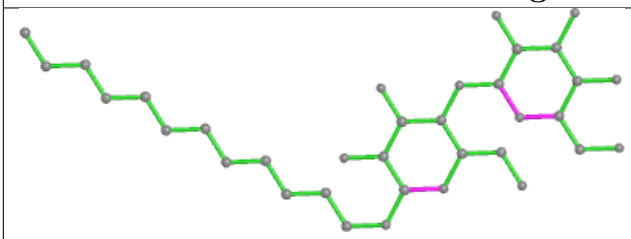
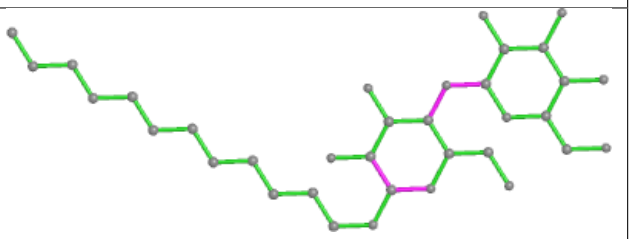


Rings

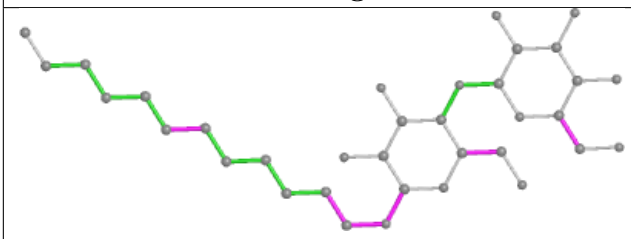
Ligand LMT l 201



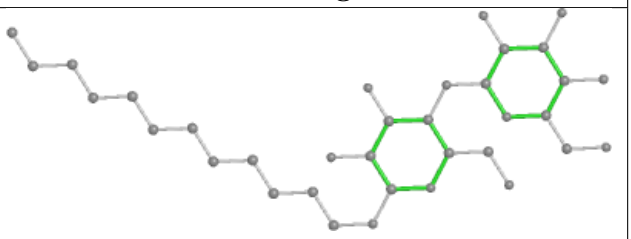
Bond lengths



Bond angles

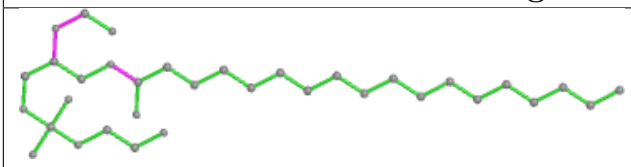


Torsions

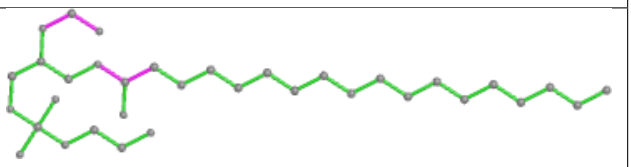


Rings

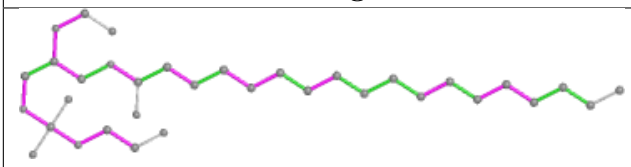
Ligand 3PE H 402



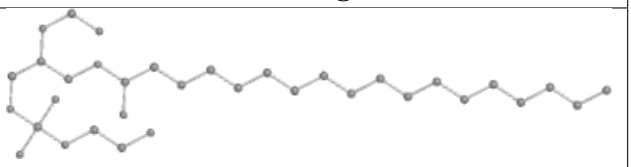
Bond lengths



Bond angles

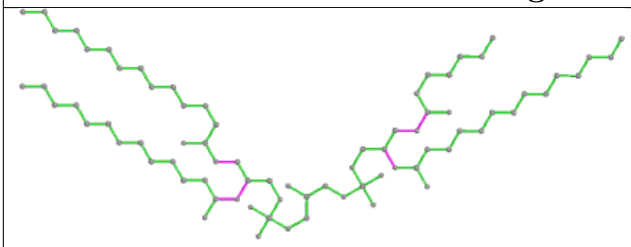


Torsions

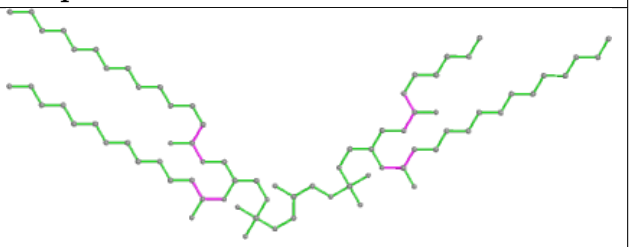


Rings

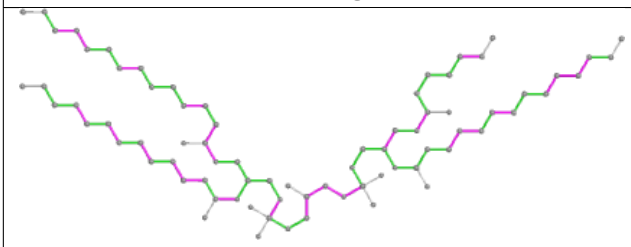
Ligand CDL q 201



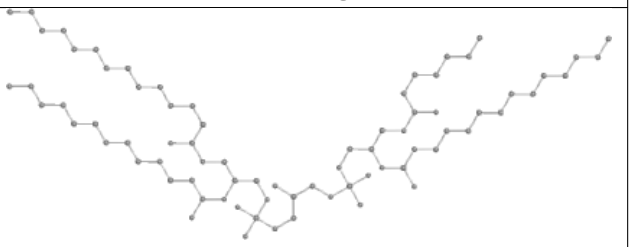
Bond lengths



Bond angles

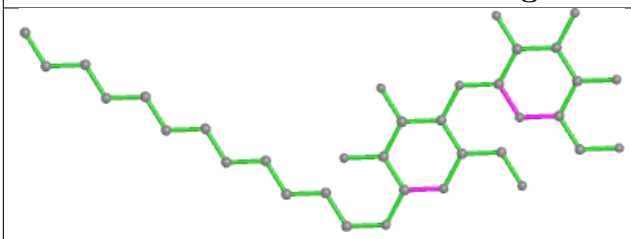


Torsions

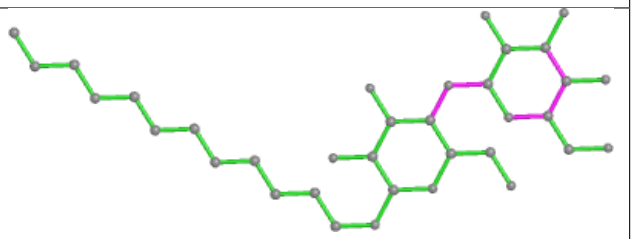


Rings

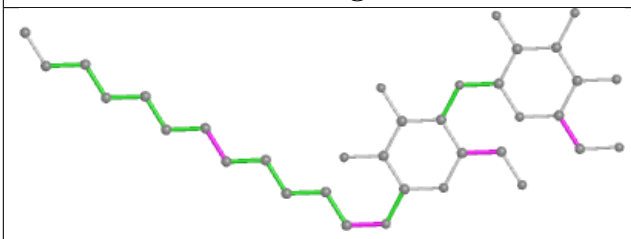
Ligand LMT Y 804



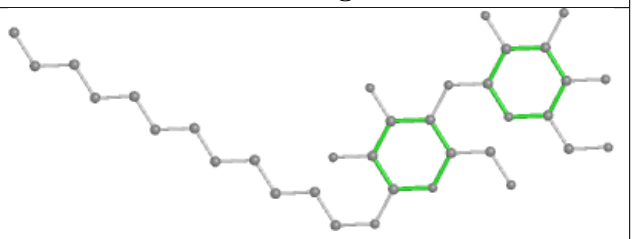
Bond lengths



Bond angles

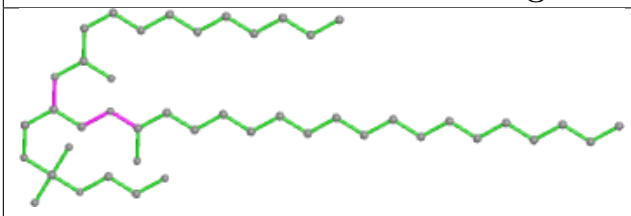


Torsions

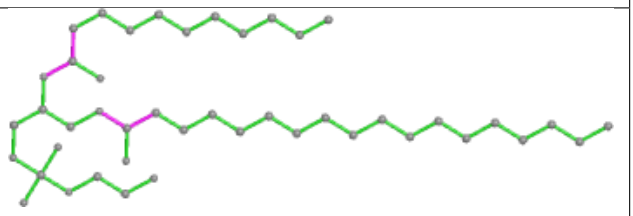


Rings

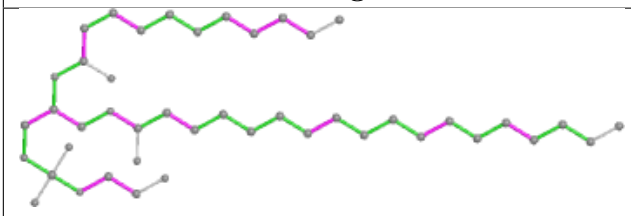
Ligand 3PE H 401



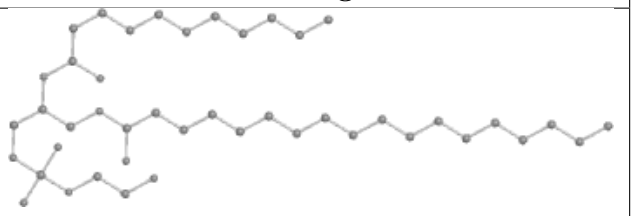
Bond lengths



Bond angles

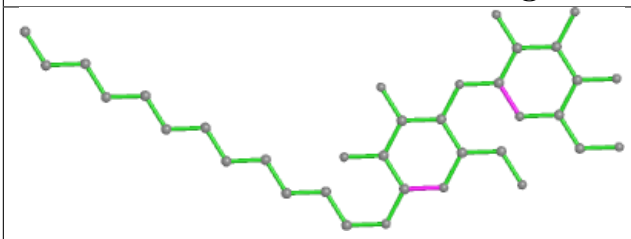


Torsions

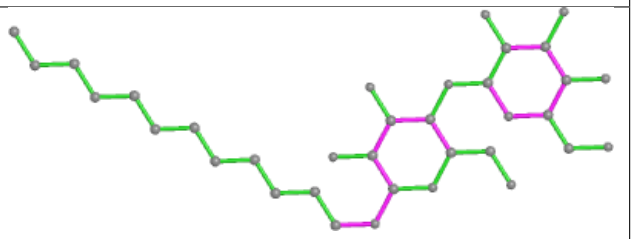


Rings

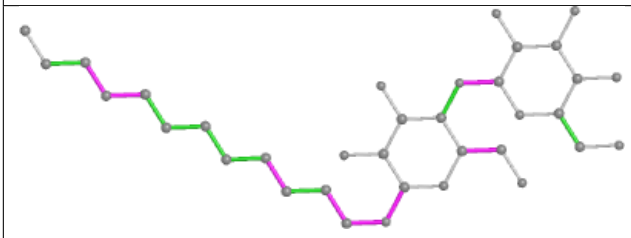
Ligand LMT A 302



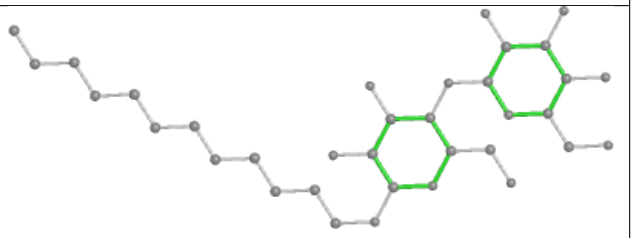
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

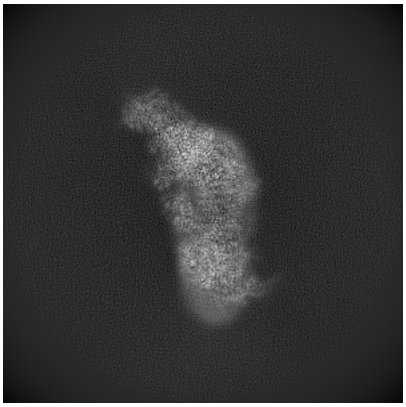
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14251. These allow visual inspection of the internal detail of the map and identification of artifacts.

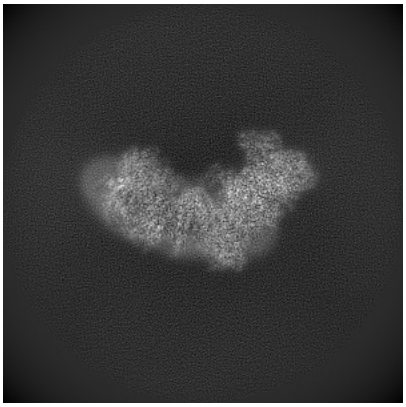
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

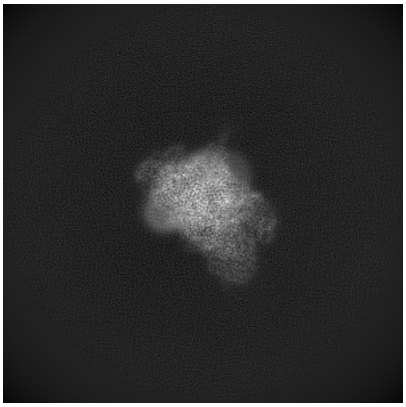
6.1.1 Primary map



X



Y

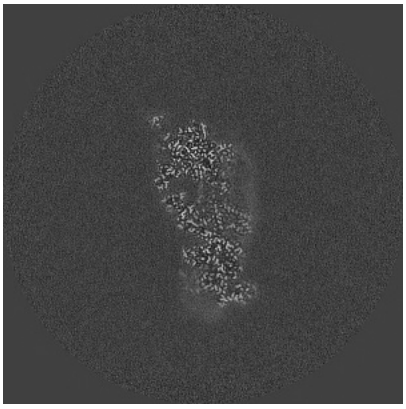


Z

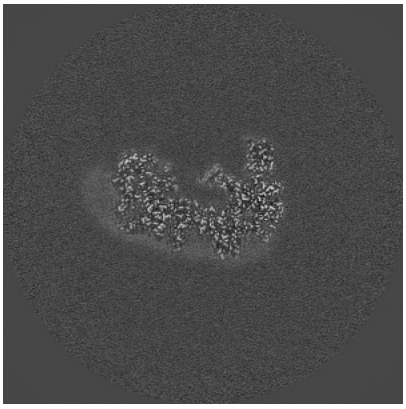
The images above show the map projected in three orthogonal directions.

6.2 Central slices

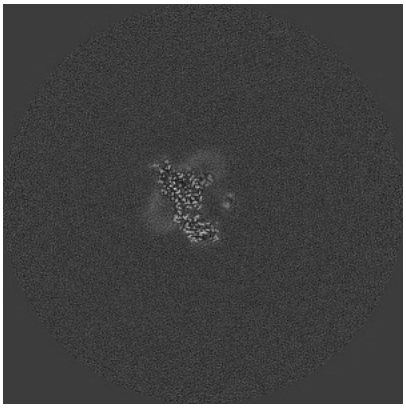
6.2.1 Primary map



X Index: 330



Y Index: 330

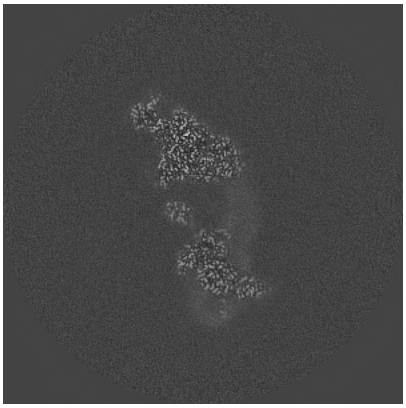


Z Index: 330

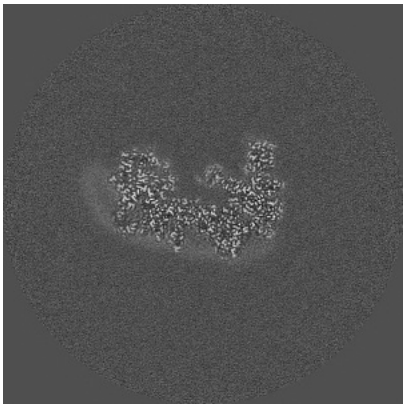
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

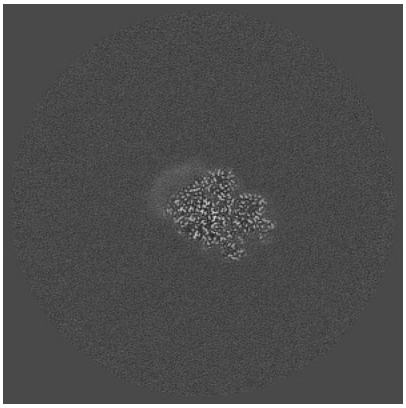
6.3.1 Primary map



X Index: 353



Y Index: 333

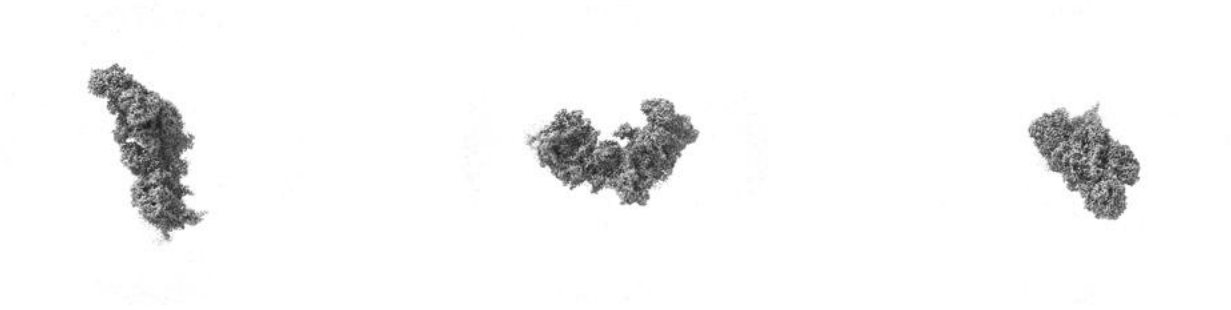


Z Index: 423

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

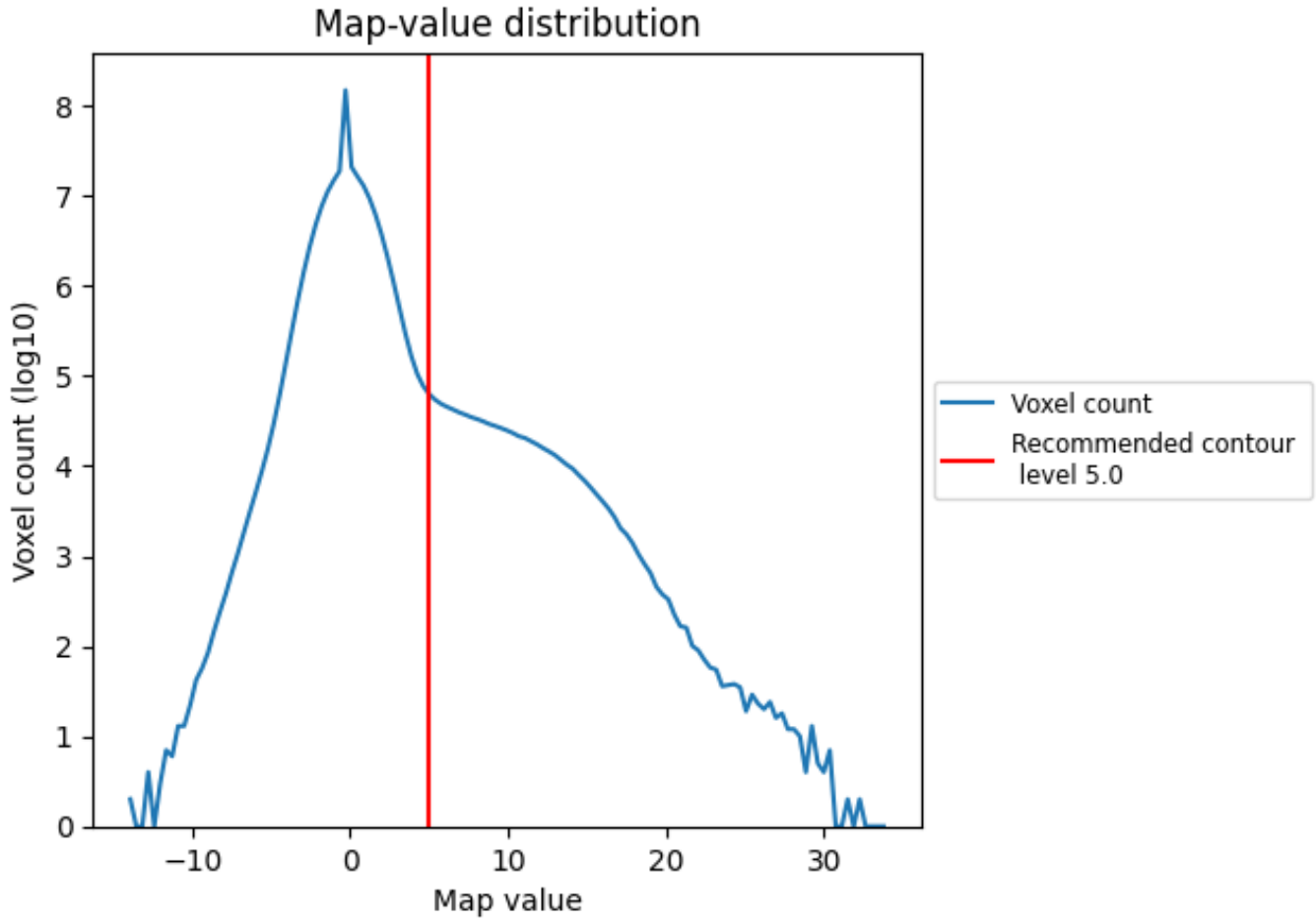
6.5 Mask visualisation (i)

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

7 Map analysis

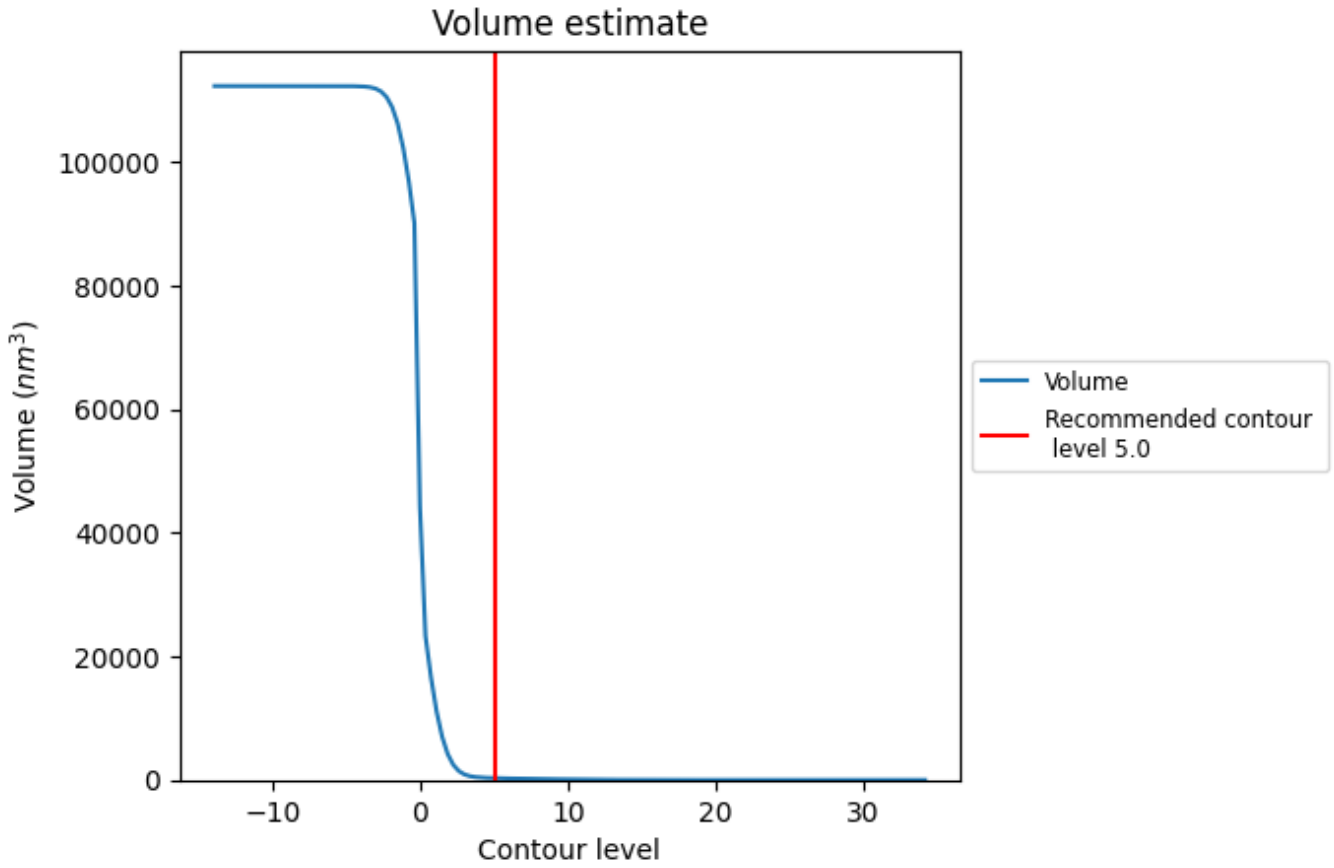
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

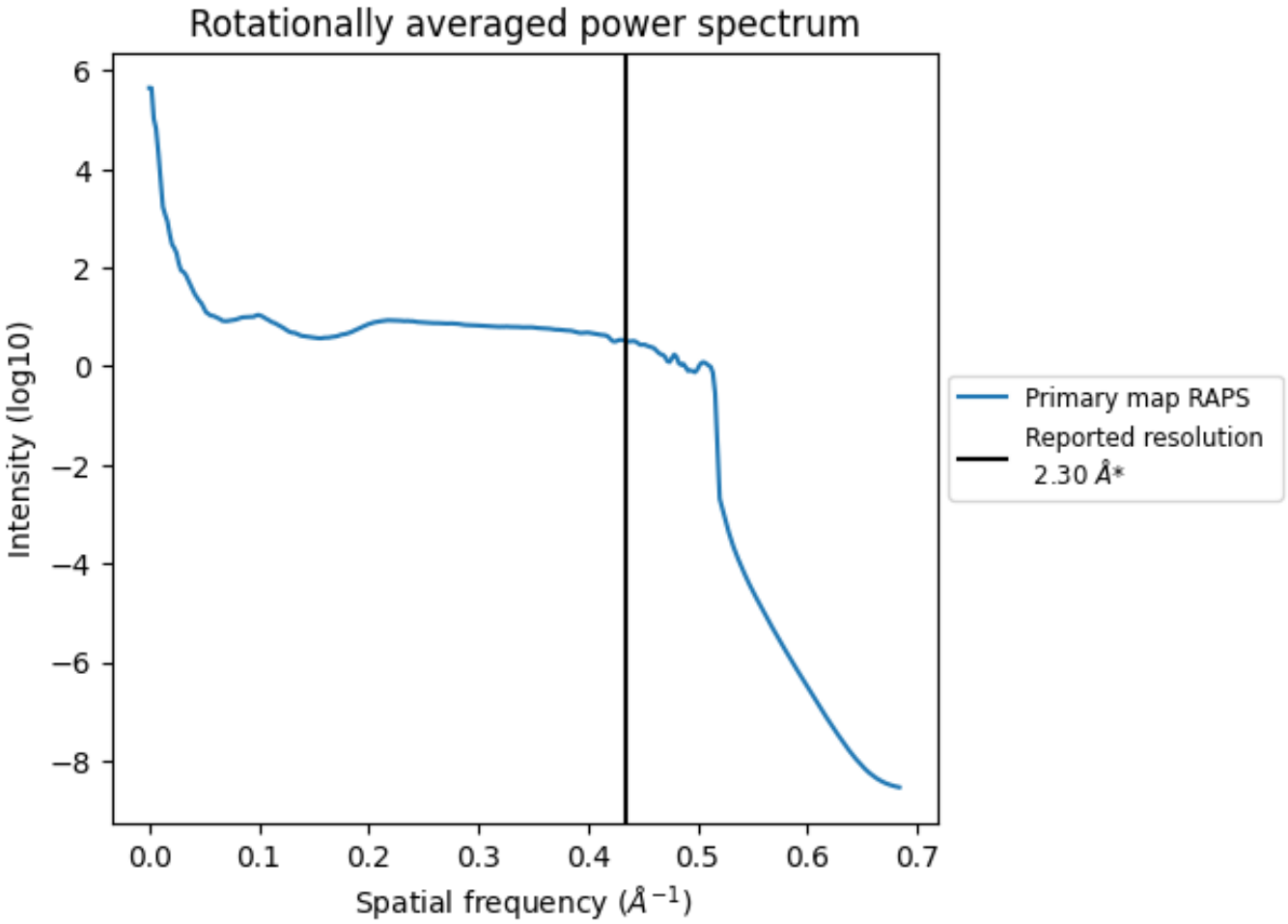
7.2 Volume estimate



The volume at the recommended contour level is 299 nm^3; this corresponds to an approximate mass of 270 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

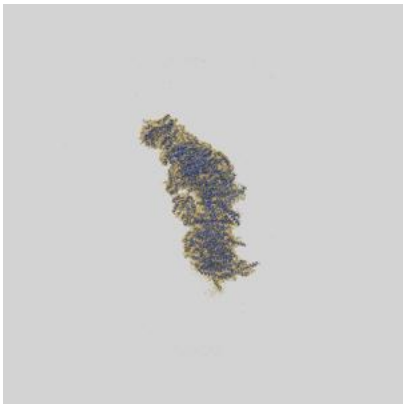
8 Fourier-Shell correlation (i)

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

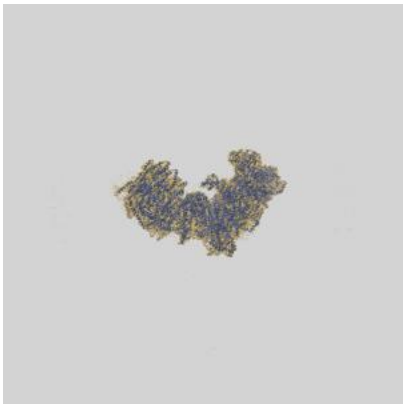
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14251 and PDB model 7R41. Per-residue inclusion information can be found in section 3 on page 23.

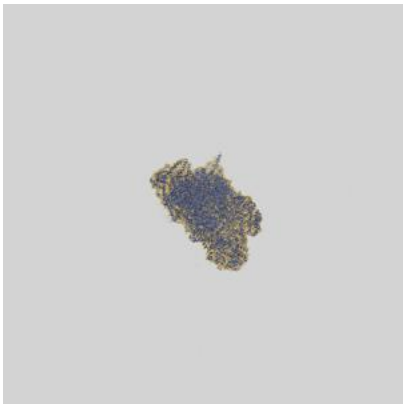
9.1 Map-model overlay



X



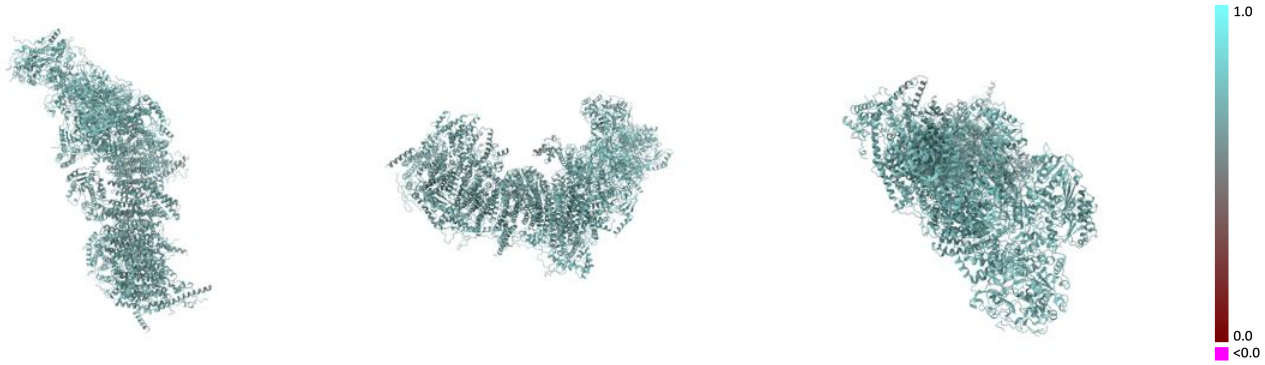
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 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.

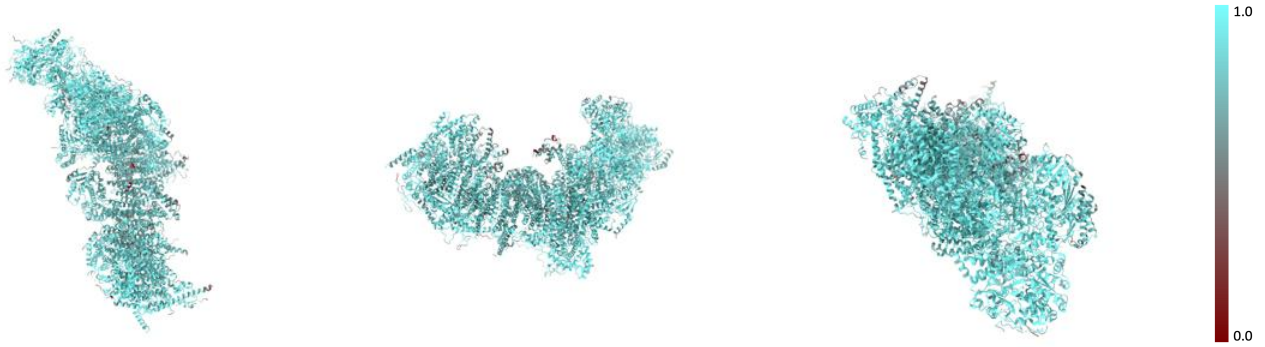
9.2 Q-score mapped to coordinate model (i)



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.

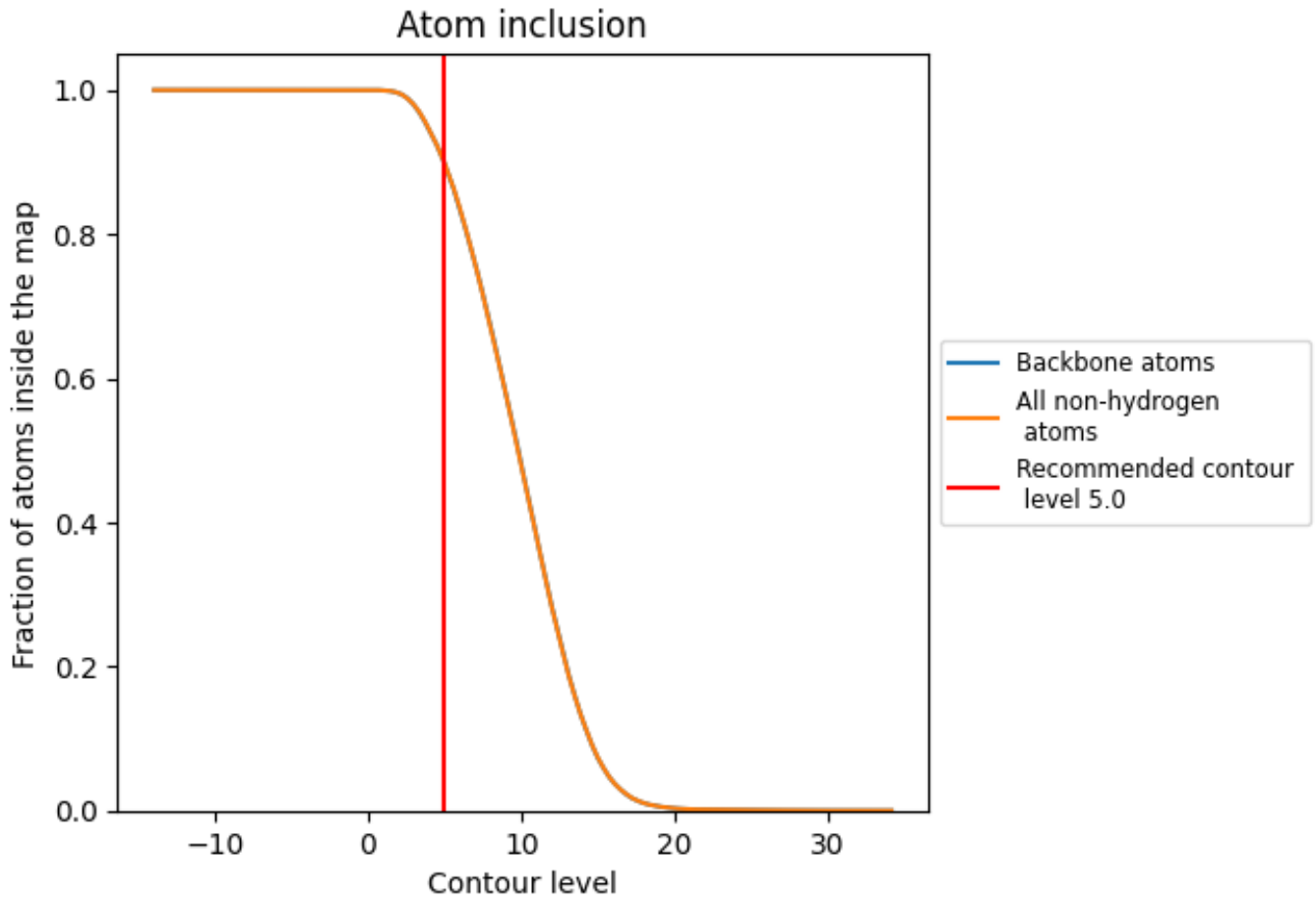
9.3 Atom inclusion mapped to coordinate model (i)



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 (5.0).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8992	0.6860
A	0.8863	0.6930
B	0.9519	0.7230
C	0.9636	0.7270
D	0.9526	0.7240
E	0.8923	0.6780
F	0.9478	0.6960
G	0.9283	0.7030
H	0.9635	0.7150
I	0.9708	0.7290
J	0.8836	0.6840
K	0.9198	0.7050
L	0.8983	0.6670
M	0.9519	0.6950
N	0.9472	0.7040
O	0.8972	0.6720
P	0.8970	0.6960
Q	0.9315	0.7130
R	0.9046	0.7040
S	0.8647	0.6730
T	0.6273	0.5950
U	0.9116	0.6660
V	0.8884	0.6930
W	0.8917	0.6960
X	0.8834	0.6700
Y	0.6975	0.6350
Z	0.8827	0.6780
a	0.9435	0.6960
b	0.8623	0.6590
c	0.7551	0.6470
d	0.8810	0.6790
e	0.8379	0.6660
f	0.8014	0.6470
g	0.8940	0.6700
h	0.9053	0.6820

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.8232	0.6480
j	0.8083	0.6350
k	0.8682	0.6390
l	0.8058	0.6420
m	0.7777	0.6540
n	0.8839	0.6670
o	0.8730	0.6420
p	0.8890	0.6650
q	0.8873	0.6950
r	0.9245	0.7040
s	0.8702	0.6780