Full wwPDB EM Validation Report ⓘ

Feb 4, 2023 – 09:05 am GMT

PDB ID	:	7R47
EMDB ID	:	EMD-14282
Title	:	Bovine complex I in the presence of IM1761092, deactive class iii (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:

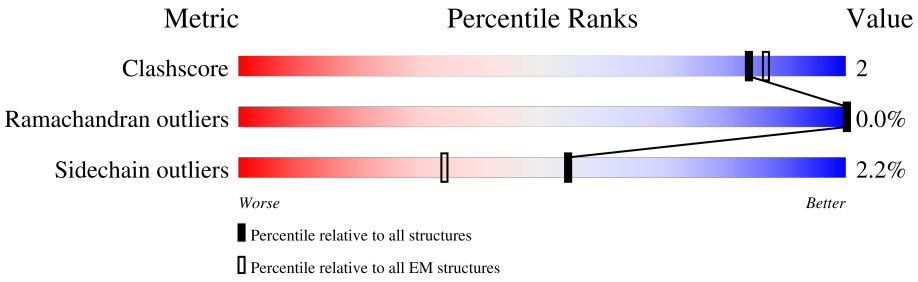
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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	7% 71% 14% 13%
2	B	216	65% 6% 29%
3	C	266	74% 23%
4	D	463	86% 10%
5	E	249	78% 8% 15%
6	F	464	87% 6% 8%
7	G	727	88% 6% 5%
8	H	318	86% 11%

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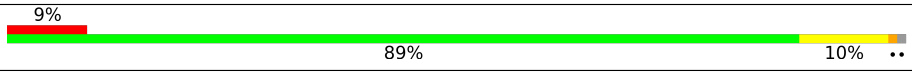
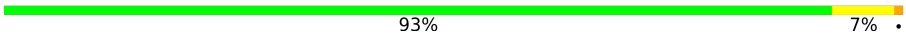
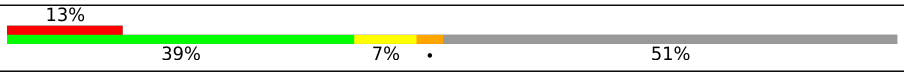
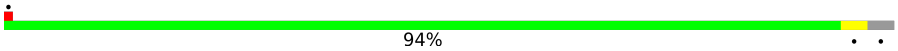
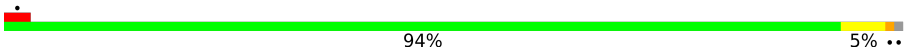
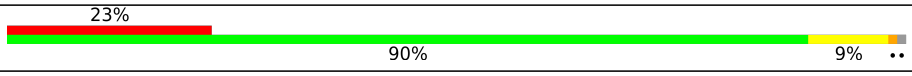
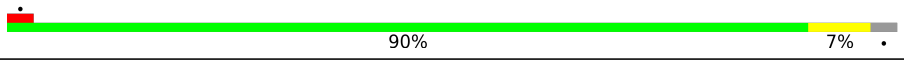
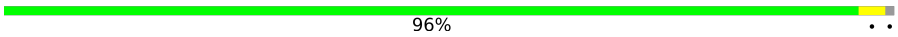
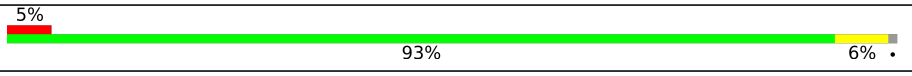
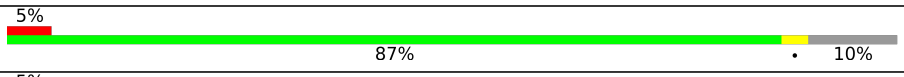
Mol	Chain	Length	Quality of chain
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	154	

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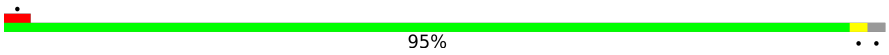
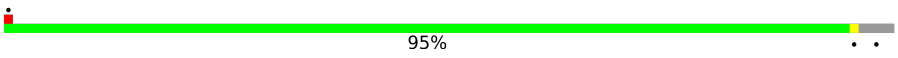
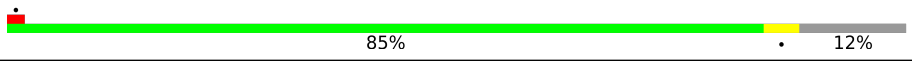
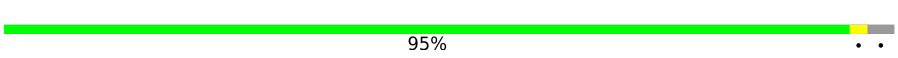
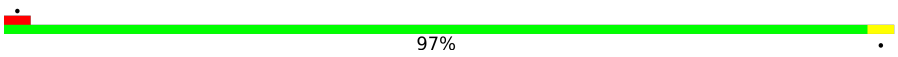
Mol	Chain	Length	Quality of chain
33	h	189	
34	i	127	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 68578 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	100	808	552	117	134	5	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	154	1230	786	220	210	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	206	1714	1107	295	309	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	415	3347	2138	575	609	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	212	Total	C	N	O	S	0	0
			1650	1054	276	310	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	429	Total	C	N	O	S	0	0
			3301	2080	589	612	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	307	Total	C	N	O	S	0	0
			2422	1625	370	404	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
			4784	3181	736	824	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	290	Total	C	N	O	S	0	0
			2309	1478	416	410	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	94	Total	C	N	O	S	0	0
			720	442	134	141	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	85	Total	C	N	O	S	0	0
			683	428	128	125	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	84	Total	C	N	O	S	0	0
			681	439	100	137	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	69	Total	C	N	O	S	0	0
			561	361	103	92	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	425	109	115	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	111	Total	C	N	O	S	0	0
			929	610	156	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	95	Total	C	N	O	S	0	0
			799	506	150	137	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total	C	N	O	S	0	0
			444	291	78	74	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	103	Total	C	N	O	S	0	0
			884	584	149	150	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	126	Total	C	N	O	0	0
			1050	672	186	192		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	0	0
			1487	952	272	256	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	121	Total	C	N	O	S	0	0
			1043	650	200	184	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	170	Total	C	N	O	S	0	0
			1435	900	265	262	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		

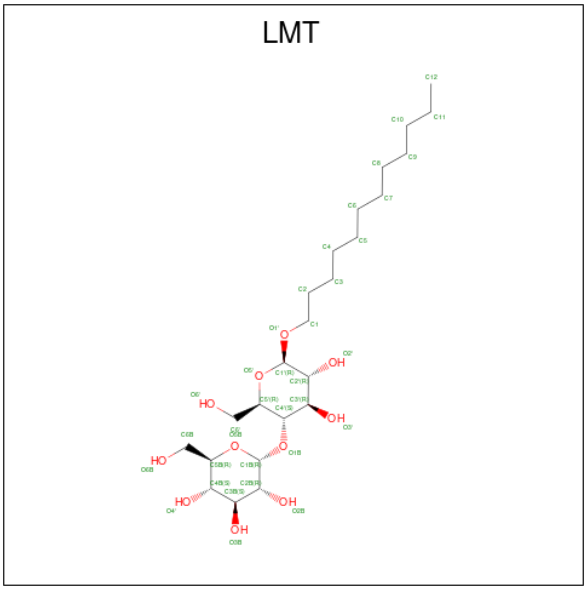
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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	43	Total	C	N	O	S	0	0
			364	228	65	70	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	B	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	N	1	Total	C	O	0
			35	24	11	
45	N	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	
45	d	1	Total	C	O	0
			35	24	11	

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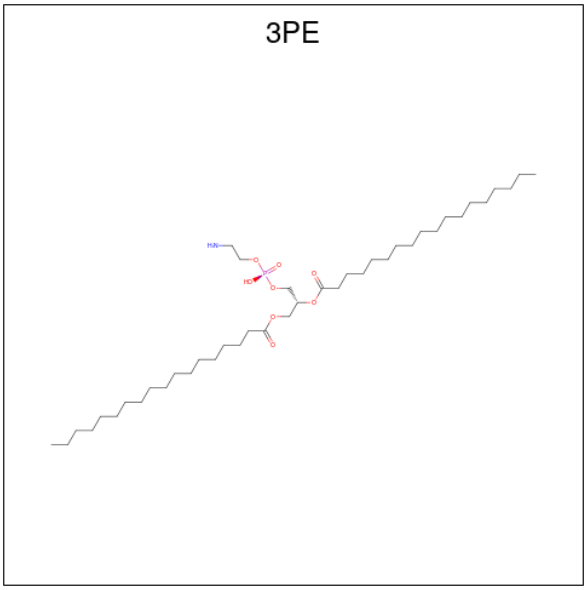
Mol	Chain	Residues	Atoms	AltConf
45	e	1	Total C O 35 24 11	0
45	f	1	Total C O 35 24 11	0
45	f	1	Total C O 35 24 11	0
45	h	1	Total C O 35 24 11	0
45	j	1	Total C O 35 24 11	0
45	l	1	Total C O 35 24 11	0

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total C N O P 38 28 1 8 1	0
46	H	1	Total C N O P 34 24 1 8 1	0
46	I	1	Total C N O P 51 41 1 8 1	0
46	L	1	Total C N O P 49 39 1 8 1	0
46	L	1	Total C N O P 45 35 1 8 1	0

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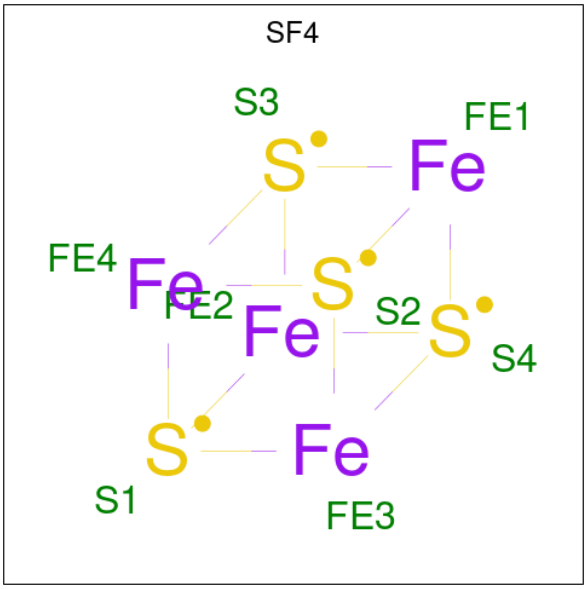
Mol	Chain	Residues	Atoms					AltConf
46	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	M	1	Total	C	N	O	P	0
			49	39	1	8	1	
46	N	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	b	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	d	1	Total	C	N	O	P	0
			47	37	1	8	1	

- 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	

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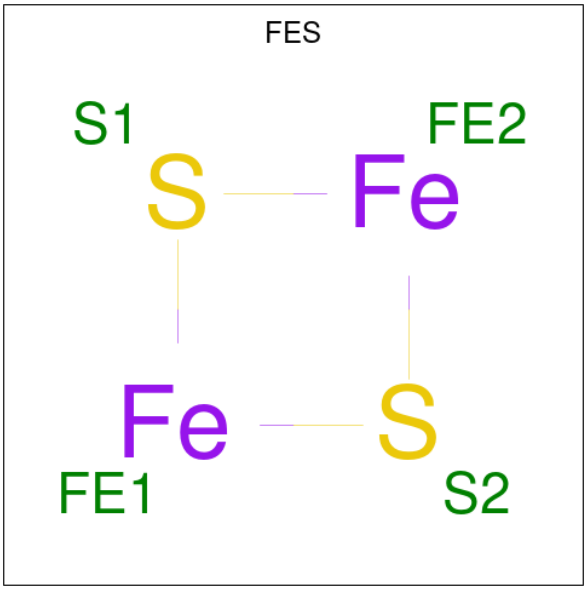
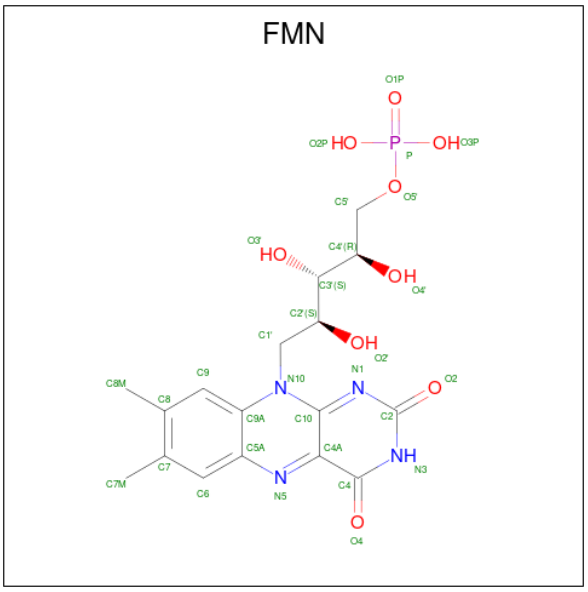
Mol	Chain	Residues	Atoms	AltConf
47	I	1	Total Fe S 8 4 4	0

- 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 4 2 2	0
48	G	1	Total Fe S 4 2 2	0

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

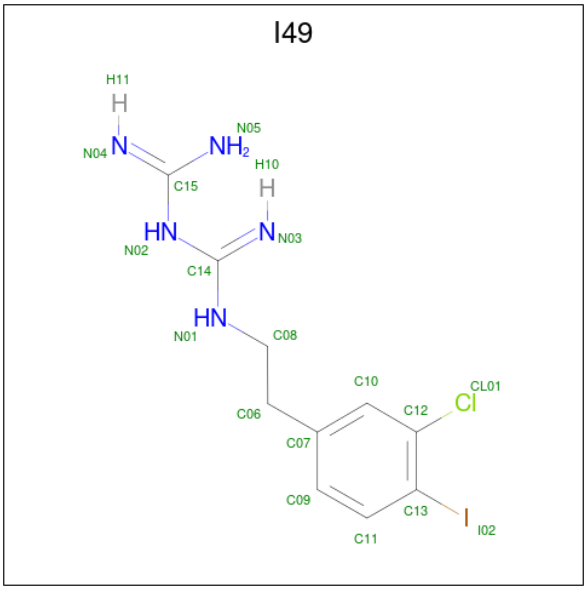


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

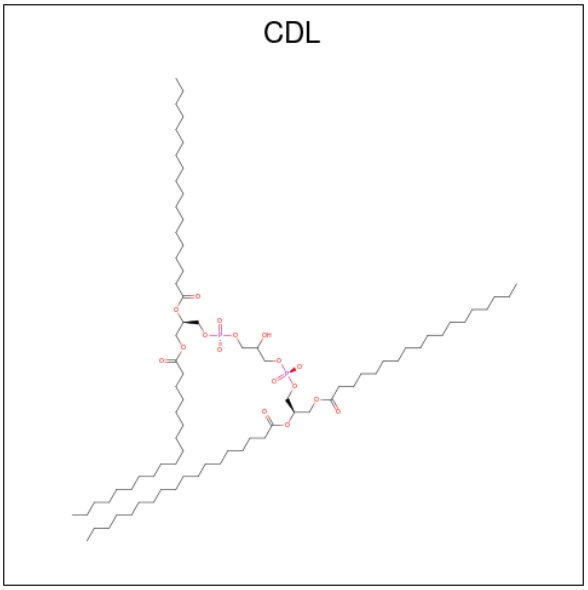
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 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).



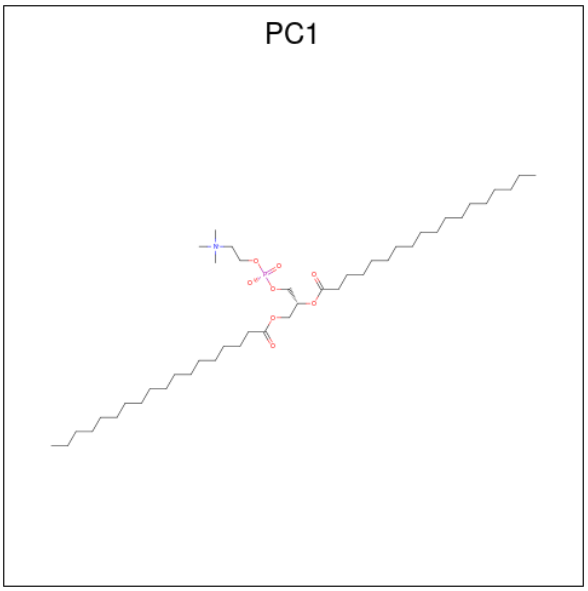
Mol	Chain	Residues	Atoms					AltConf
51	H	1	Total	C	Cl	I	N	0
			17	10	1	1	5	
51	N	1	Total	C	Cl	I	N	0
			17	10	1	1	5	

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



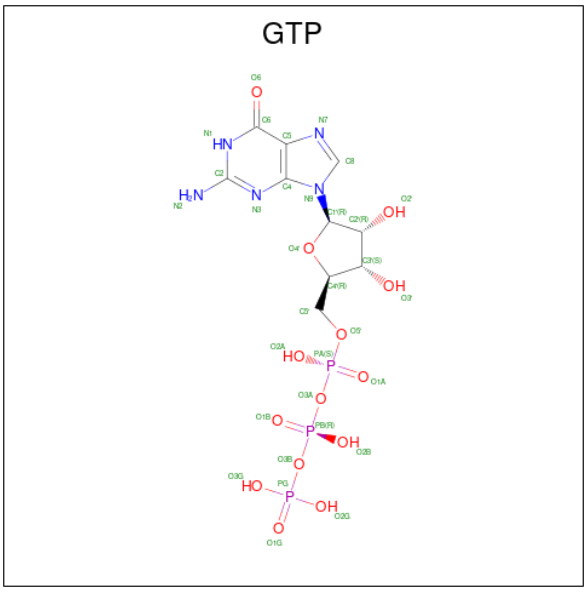
Mol	Chain	Residues	Atoms				AltConf
52	J	1	Total	C	O	P	0
			71	52	17	2	
52	L	1	Total	C	O	P	0
			69	50	17	2	
52	X	1	Total	C	O	P	0
			72	53	17	2	
52	d	1	Total	C	O	P	0
			65	46	17	2	
52	h	1	Total	C	O	P	0
			67	48	17	2	
52	q	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 53 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
53	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
53	q	1	Total	C	N	O	P	0
			35	25	1	8	1	

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

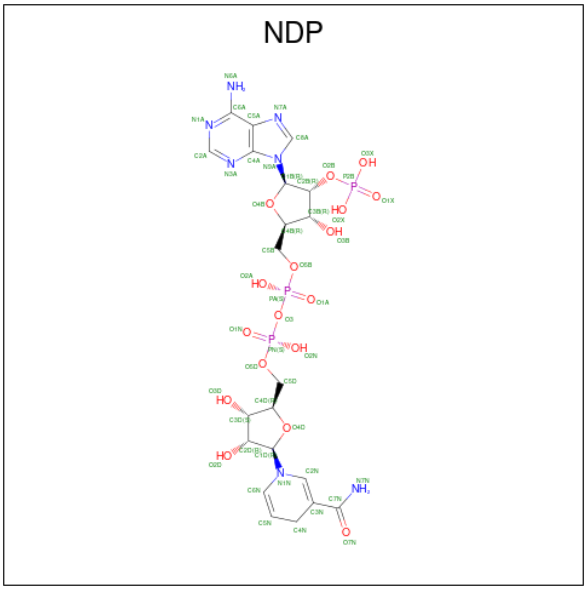


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- 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: $C_{21}H_{30}N_7O_{17}P_3$).

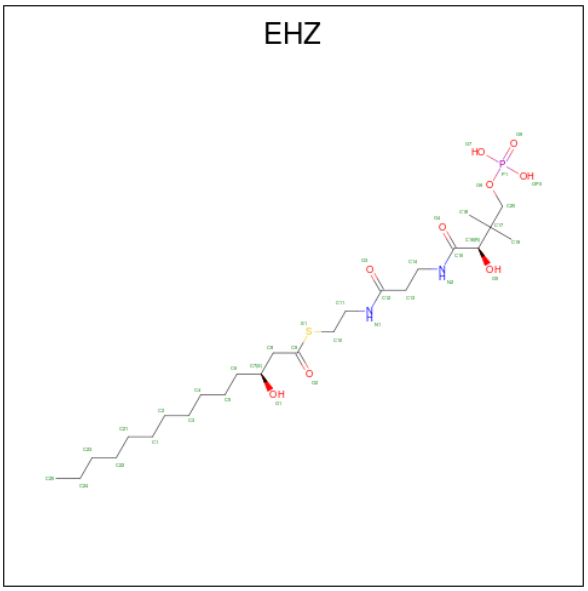


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

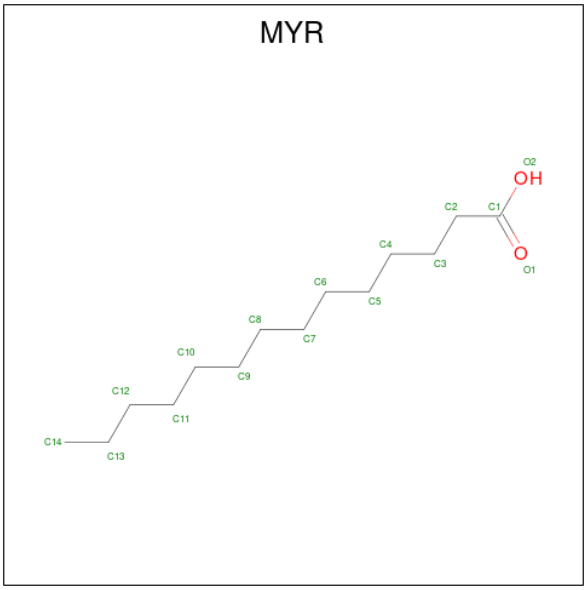
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- 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
			15	14	1	

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	A	11	Total O 11 11	0
60	B	60	Total O 60 60	0
60	C	109	Total O 109 109	0
60	D	177	Total O 177 177	0
60	E	27	Total O 27 27	0
60	F	78	Total O 78 78	0
60	G	228	Total O 228 228	0
60	H	56	Total O 56 56	0
60	I	107	Total O 107 107	0
60	J	15	Total O 15 15	0
60	K	12	Total O 12 12	0
60	L	71	Total O 71 71	0
60	M	83	Total O 83 83	0
60	N	56	Total O 56 56	0
60	O	30	Total O 30 30	0
60	P	47	Total O 47 47	0
60	Q	80	Total O 80 80	0
60	R	46	Total O 46 46	0
60	S	3	Total O 3 3	0
60	U	23	Total O 23 23	0
60	V	16	Total O 16 16	0
60	W	21	Total O 21 21	0

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Mol	Chain	Residues	Atoms	AltConf
60	X	34	Total O 34 34	0
60	Y	2	Total O 2 2	0
60	Z	32	Total O 32 32	0
60	a	23	Total O 23 23	0
60	b	10	Total O 10 10	0
60	c	1	Total O 1 1	0
60	d	16	Total O 16 16	0
60	e	30	Total O 30 30	0
60	f	10	Total O 10 10	0
60	g	16	Total O 16 16	0
60	h	33	Total O 33 33	0
60	i	12	Total O 12 12	0
60	j	4	Total O 4 4	0
60	k	10	Total O 10 10	0
60	l	38	Total O 38 38	0
60	m	20	Total O 20 20	0
60	n	40	Total O 40 40	0
60	o	24	Total O 24 24	0
60	p	39	Total O 39 39	0
60	q	42	Total O 42 42	0
60	r	33	Total O 33 33	0

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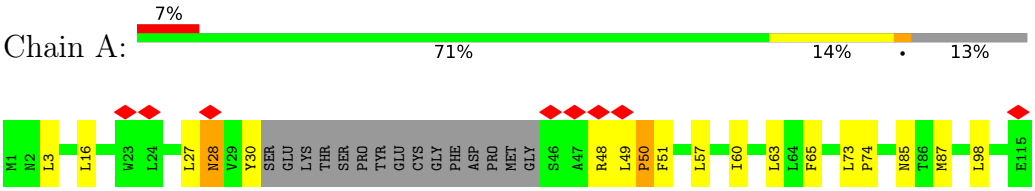
Mol	Chain	Residues	Atoms		AltConf
60	s	11	Total	O	0
			11	11	

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.

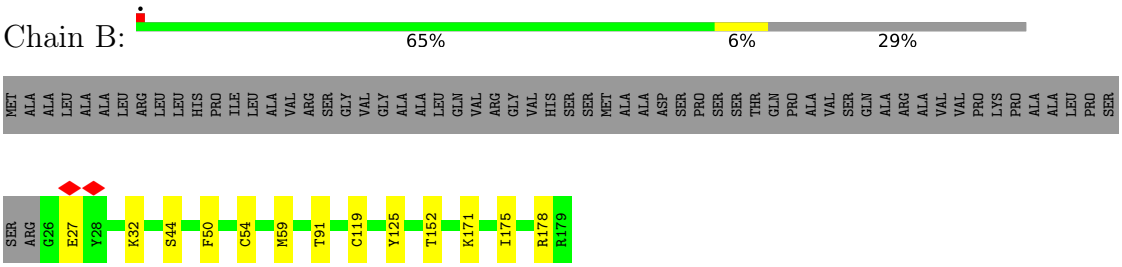
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



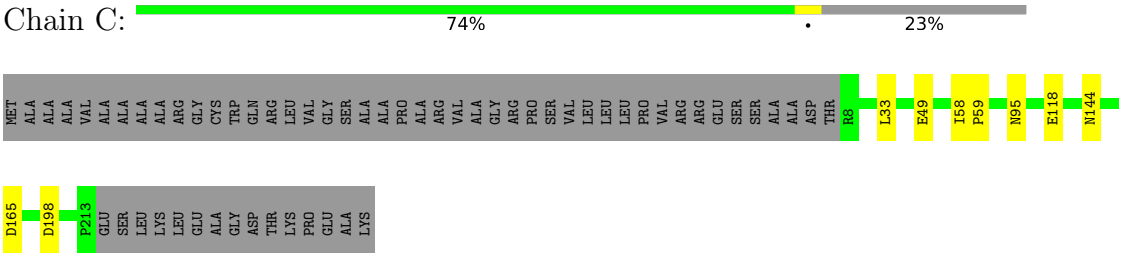
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:



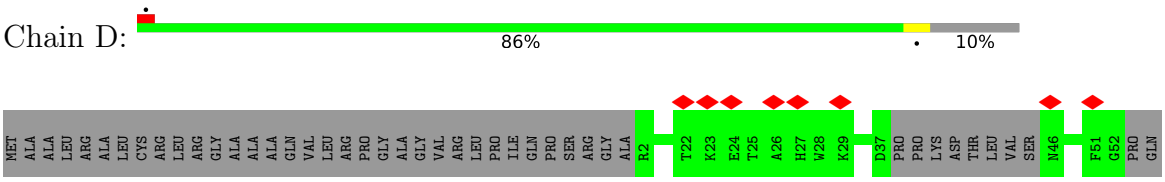
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:



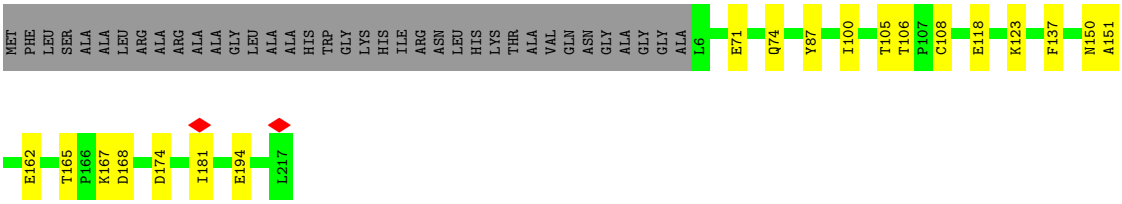
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:



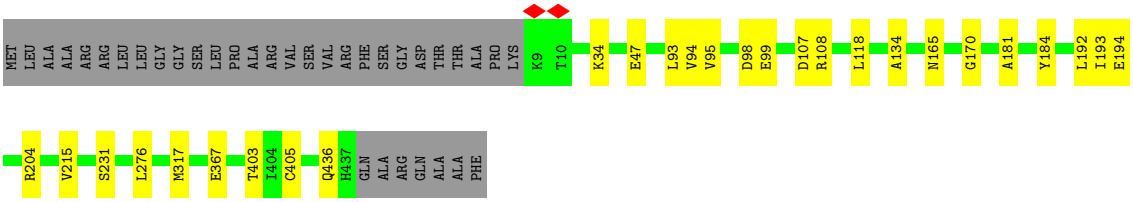
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



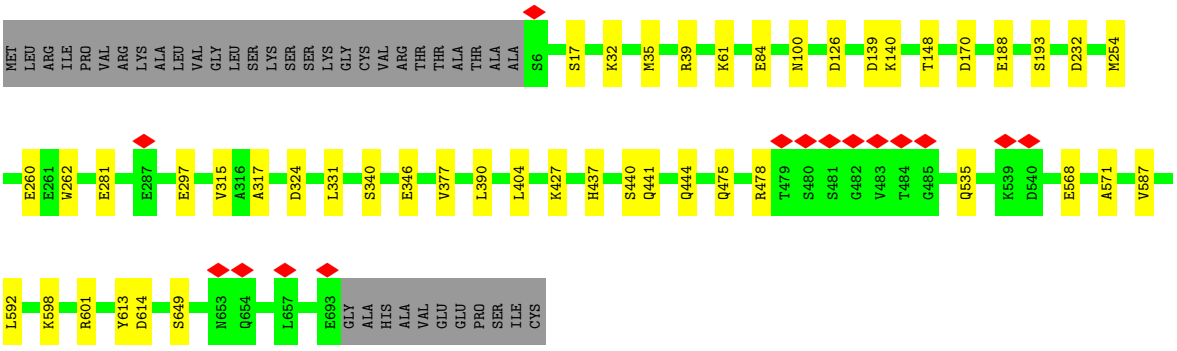
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:



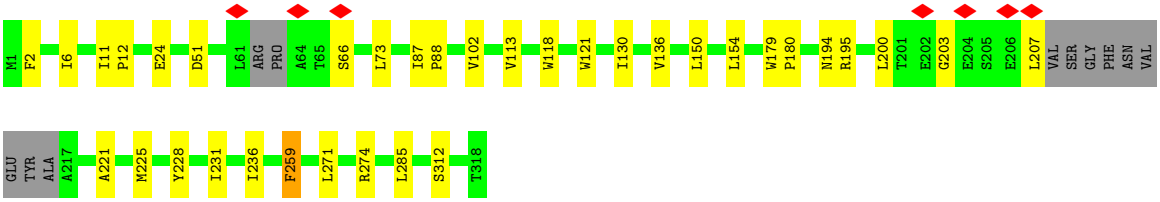
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:



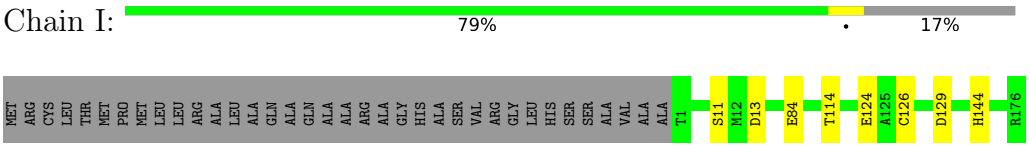
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



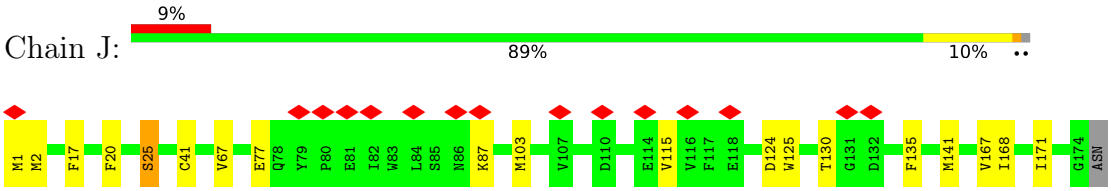
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



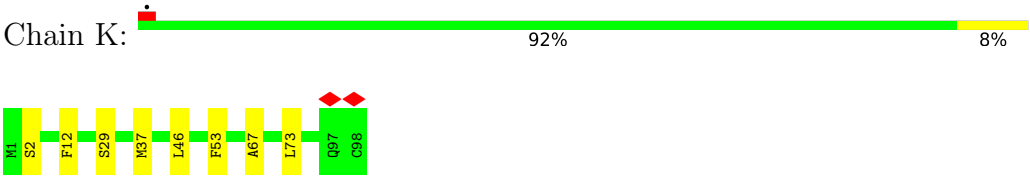
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



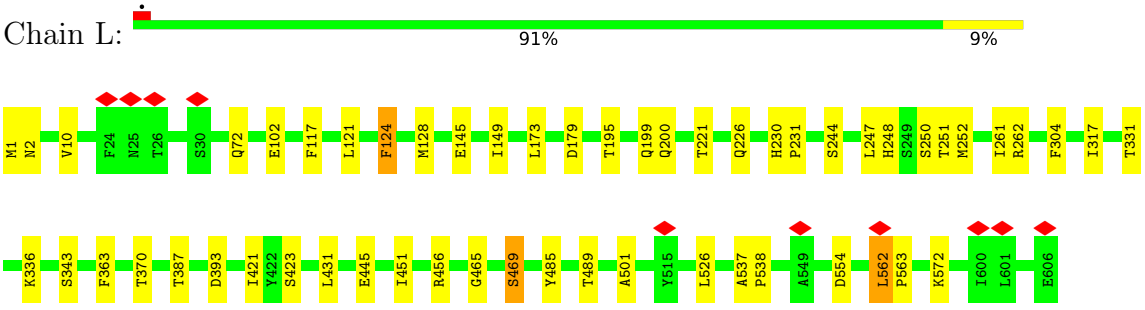
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:



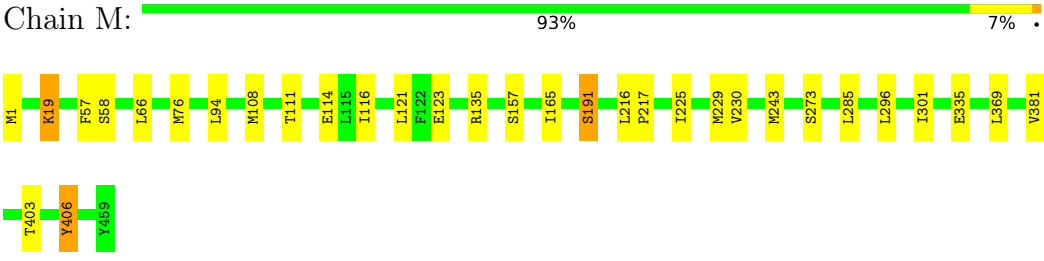
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:



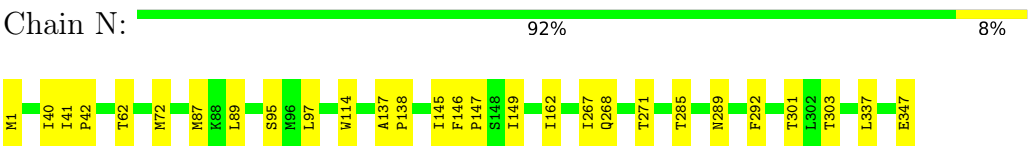
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



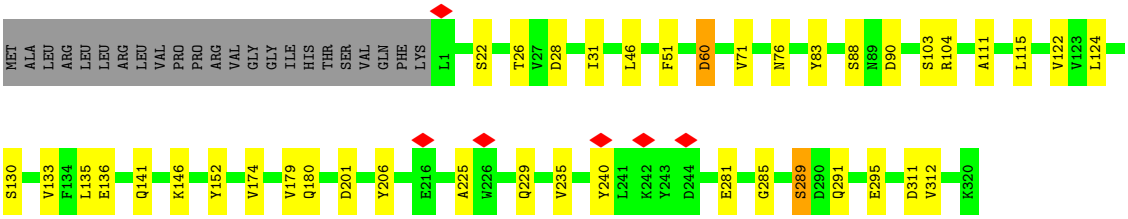
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



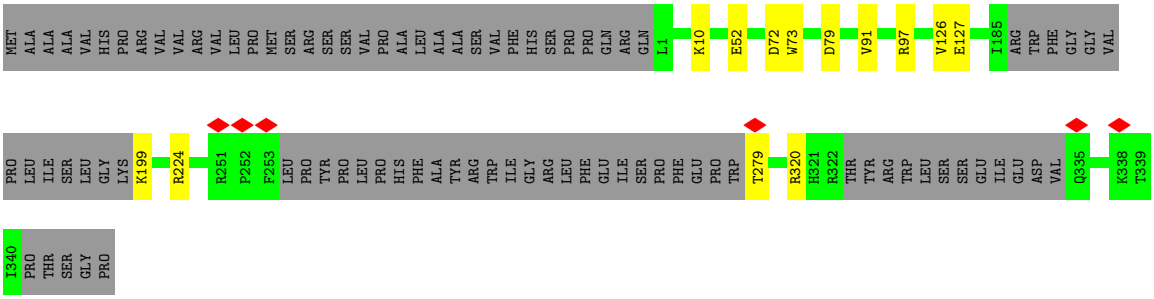
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



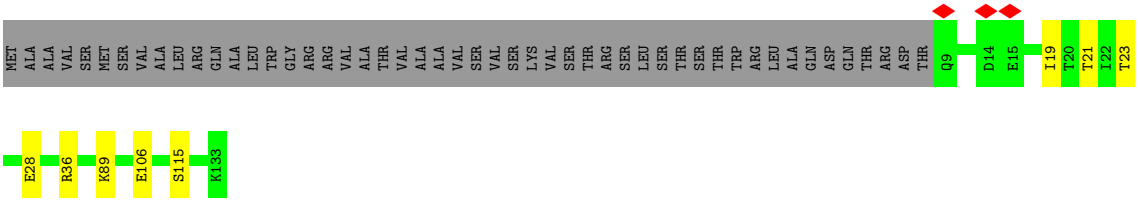
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



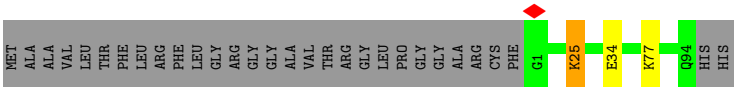
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



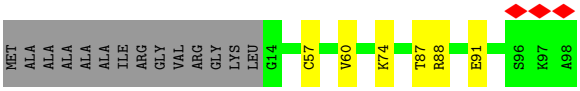
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



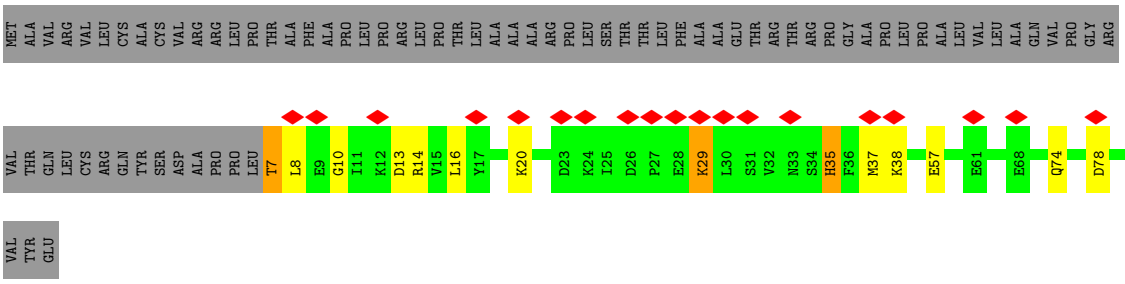
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



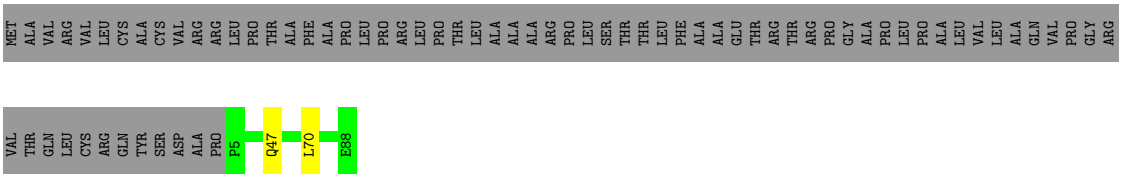
• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



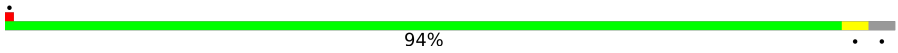
• Molecule 20: Acyl carrier protein, mitochondrial

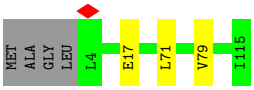
Chain U:



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

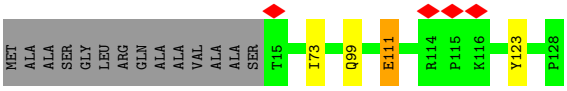
Chain V:





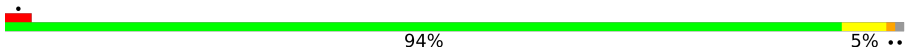
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



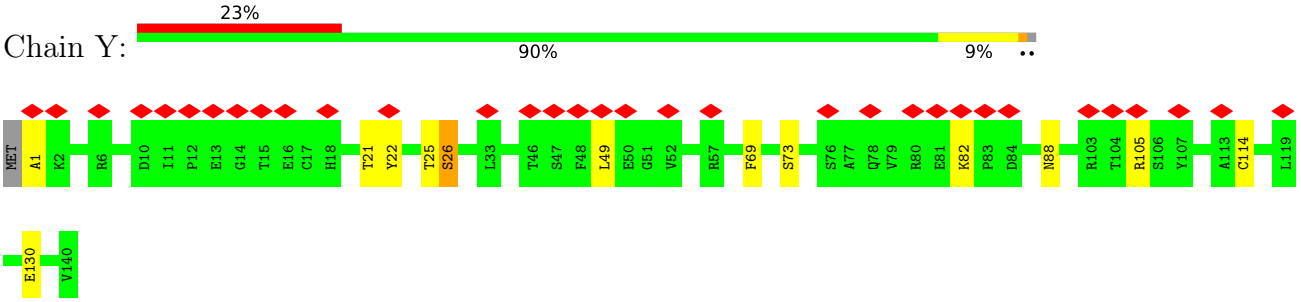
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



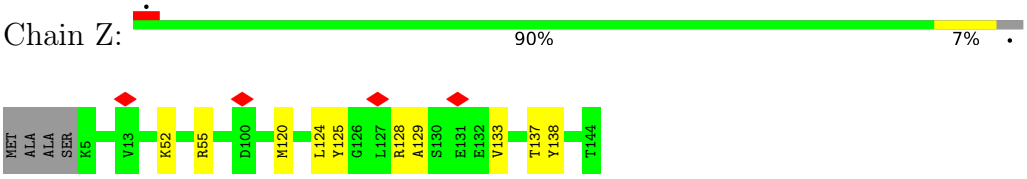
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:



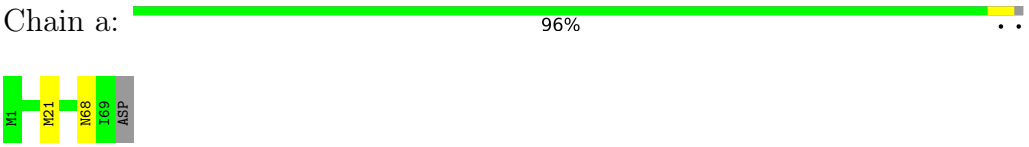
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



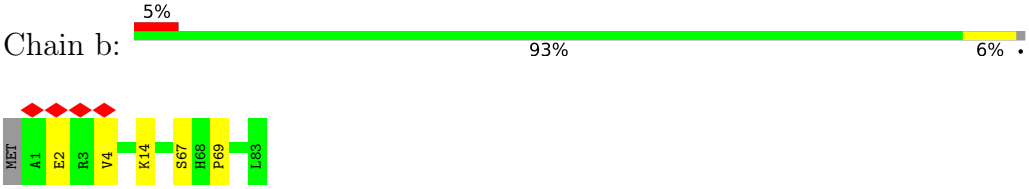
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:



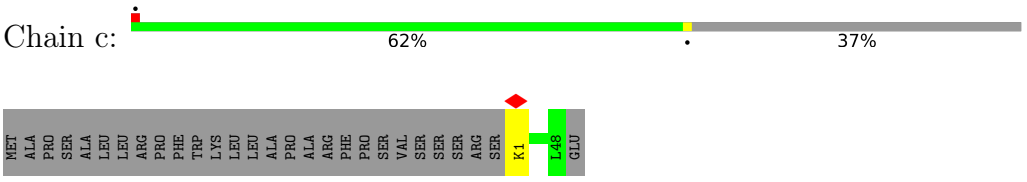
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:



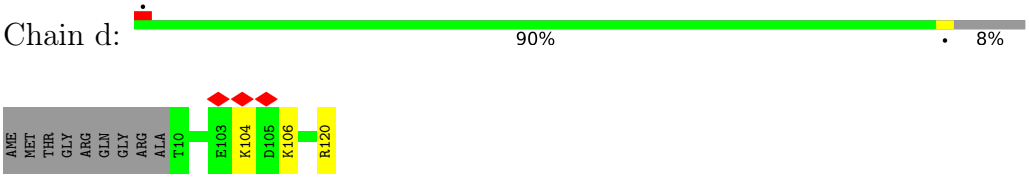
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:



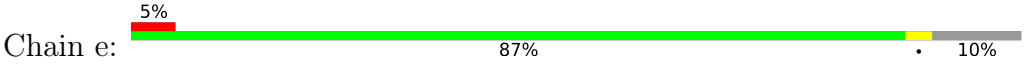
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

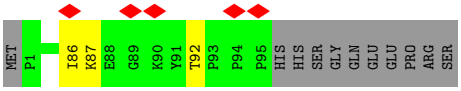
Chain d:



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

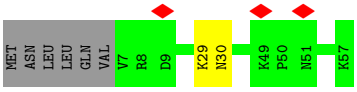
Chain e:





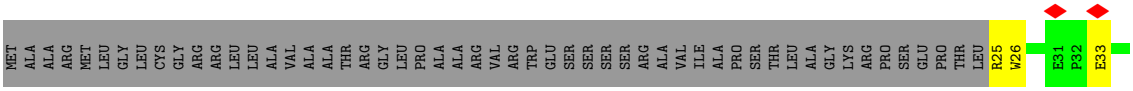
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

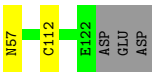
Chain f:



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

Chain g:



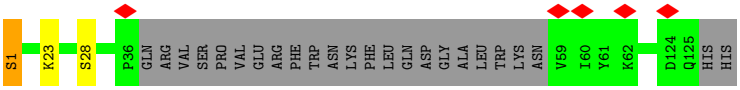


• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:

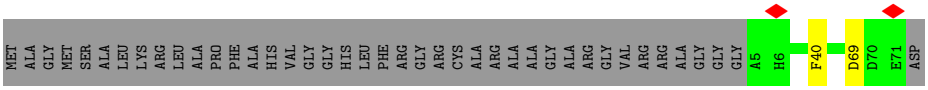
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



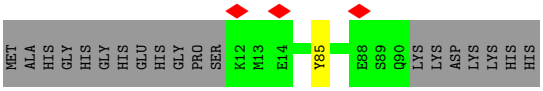
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



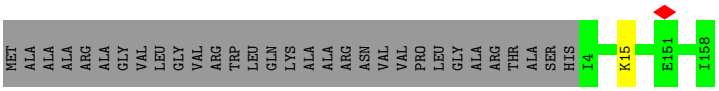
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



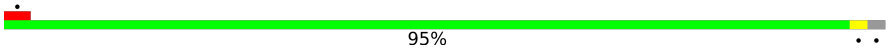
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

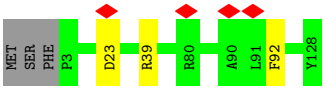
Chain l:



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

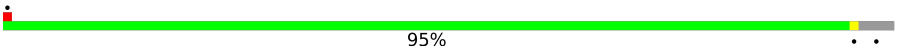
Chain m:

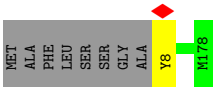




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

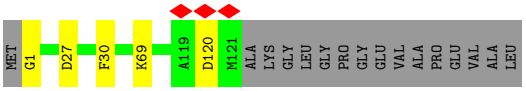
Chain n:





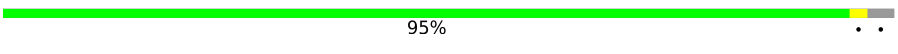
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



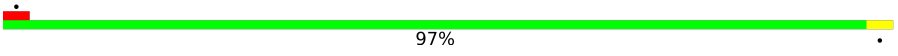
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

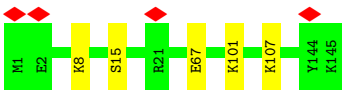
Chain p:



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

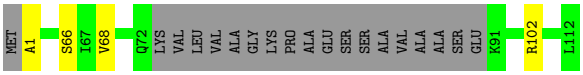
Chain q:





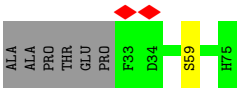
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

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	124012	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	44.627	Depositor
Minimum map value	-18.628	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.075	Depositor
Recommended contour level	6.0	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 (i)

5.1 Standard geometry (i)

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

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	0.29	0/818	0.42	0/1120
2	B	0.36	0/1261	0.46	0/1706
3	C	0.34	0/1765	0.45	0/2403
4	D	0.33	0/3417	0.45	0/4623
5	E	0.32	0/1690	0.45	0/2300
6	F	0.31	0/3375	0.45	0/4561
7	G	0.31	0/5367	0.47	0/7274
8	H	0.32	0/2479	0.44	0/3384
9	I	0.34	0/1445	0.47	0/1956
10	J	0.30	0/1362	0.41	0/1848
11	K	0.28	0/745	0.41	0/1008
12	L	0.32	0/4900	0.42	0/6667
13	M	0.32	0/3738	0.43	0/5097
14	N	0.30	0/2792	0.43	0/3800
15	O	0.34	0/2651	0.42	0/3587
16	P	0.30	0/2360	0.46	0/3188
17	Q	0.30	0/1039	0.46	0/1404
18	R	0.33	0/731	0.46	0/984
19	S	0.29	0/694	0.46	0/934
20	T	0.27	0/621	0.41	0/837
20	U	0.36	0/692	0.40	0/932
21	V	0.28	0/931	0.37	0/1261
22	W	0.30	0/995	0.42	0/1337
23	X	0.31	0/1439	0.42	0/1942
24	Y	0.26	0/1042	0.41	0/1414
25	Z	0.32	0/1175	0.43	0/1584
26	a	0.32	0/576	0.42	0/775
27	b	0.31	0/672	0.41	0/923
28	c	0.32	0/418	0.43	0/567
29	d	0.35	0/959	0.40	0/1298
30	e	0.29	0/818	0.42	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.31	0/457	0.40	0/616
32	g	0.35	0/850	0.41	0/1154
33	h	0.34	0/1188	0.43	0/1607
34	i	0.37	0/904	0.43	0/1230
35	j	0.37	0/607	0.39	0/833
36	k	0.33	0/657	0.41	0/887
37	l	0.39	0/1358	0.42	0/1858
38	m	0.34	0/1076	0.44	0/1455
39	n	0.36	0/1540	0.41	0/2085
40	o	0.38	1/1068 (0.1%)	0.43	0/1430
41	p	0.35	0/1468	0.42	0/1979
42	q	0.31	0/1250	0.47	0/1698
43	r	0.32	0/780	0.44	0/1056
44	s	0.30	0/375	0.43	0/507
All	All	0.32	1/66545 (0.0%)	0.44	0/90202

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
34	i	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	o	1	GLY	CA-C	5.17	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain
34	i	1	SAC	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	808	0	853	11	0
2	B	1230	0	1238	6	0
3	C	1714	0	1668	6	0
4	D	3347	0	3287	10	0
5	E	1650	0	1656	10	0
6	F	3301	0	3253	16	0
7	G	5279	0	5301	23	0
8	H	2422	0	2538	23	0
9	I	1414	0	1370	5	0
10	J	1337	0	1346	11	0
11	K	745	0	785	4	0
12	L	4784	0	4937	27	0
13	M	3654	0	3852	18	0
14	N	2733	0	2912	20	0
15	O	2589	0	2566	23	0
16	P	2309	0	2339	8	0
17	Q	1016	0	1014	4	0
18	R	720	0	700	2	0
19	S	683	0	695	2	0
20	T	612	0	604	7	0
20	U	681	0	677	1	0
21	V	911	0	950	2	0
22	W	971	0	989	4	0
23	X	1402	0	1381	2	0
24	Y	1030	0	1041	5	0
25	Z	1146	0	1146	7	0
26	a	561	0	564	0	0
27	b	651	0	662	0	0
28	c	405	0	409	0	0
29	d	929	0	914	0	0
30	e	799	0	807	0	0
31	f	444	0	444	0	0
32	g	824	0	772	0	0
33	h	1154	0	1168	0	0
34	i	884	0	905	0	0
35	j	580	0	519	0	0
36	k	638	0	621	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	l	1304	0	1203	0	0
38	m	1050	0	1051	0	0
39	n	1487	0	1433	0	0
40	o	1043	0	1011	0	0
41	p	1435	0	1411	0	0
42	q	1209	0	1182	0	0
43	r	767	0	776	0	0
44	s	364	0	336	0	0
45	A	35	0	46	0	0
45	B	35	0	46	2	0
45	L	35	0	46	0	0
45	N	70	0	92	2	0
45	Y	35	0	46	0	0
45	d	35	0	46	0	0
45	e	35	0	46	0	0
45	f	70	0	92	0	0
45	h	35	0	46	0	0
45	j	35	0	46	0	0
45	l	35	0	46	0	0
46	A	38	0	50	1	0
46	H	34	0	47	0	0
46	I	51	0	82	0	0
46	L	94	0	142	1	0
46	M	95	0	144	1	0
46	N	41	0	56	0	0
46	Y	35	0	44	0	0
46	b	48	0	73	0	0
46	d	47	0	71	0	0
47	B	8	0	0	0	0
47	F	8	0	0	1	0
47	G	16	0	0	0	0
47	I	16	0	0	1	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	17	0	0	3	0
51	N	17	0	0	1	0
52	J	71	0	86	0	0
52	L	69	0	82	0	0
52	X	72	0	88	1	0
52	d	65	0	77	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	h	67	0	81	0	0
52	q	76	0	96	0	0
53	M	40	0	57	1	0
53	q	35	0	44	0	0
54	O	32	0	12	2	0
55	O	1	0	0	0	0
56	P	48	0	26	2	0
57	R	1	0	0	0	0
58	T	37	0	0	1	0
58	U	37	0	0	0	0
59	o	15	0	27	0	0
60	A	11	0	0	0	0
60	B	60	0	0	0	0
60	C	109	0	0	4	0
60	D	177	0	0	2	0
60	E	27	0	0	0	0
60	F	78	0	0	1	0
60	G	228	0	0	5	0
60	H	56	0	0	0	0
60	I	107	0	0	2	0
60	J	15	0	0	0	0
60	K	12	0	0	0	0
60	L	71	0	0	2	0
60	M	83	0	0	1	0
60	N	56	0	0	2	0
60	O	30	0	0	2	0
60	P	47	0	0	1	0
60	Q	80	0	0	0	0
60	R	46	0	0	1	0
60	S	3	0	0	0	0
60	U	23	0	0	0	0
60	V	16	0	0	0	0
60	W	21	0	0	2	0
60	X	34	0	0	0	0
60	Y	2	0	0	0	0
60	Z	32	0	0	1	0
60	a	23	0	0	0	0
60	b	10	0	0	0	0
60	c	1	0	0	0	0
60	d	16	0	0	0	0
60	e	30	0	0	0	0
60	f	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	g	16	0	0	0	0
60	h	33	0	0	0	0
60	i	12	0	0	0	0
60	j	4	0	0	0	0
60	k	10	0	0	0	0
60	l	38	0	0	0	0
60	m	20	0	0	0	0
60	n	40	0	0	0	0
60	o	24	0	0	0	0
60	p	39	0	0	0	0
60	q	42	0	0	0	0
60	r	33	0	0	0	0
60	s	11	0	0	0	0
All	All	68578	0	67288	236	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 2.

All (236) 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)
9:I:11:SER:OG	9:I:13:ASP:OD1	1.92	0.86
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.12	0.83
4:D:279:ASP:OD2	60:D:501:HOH:O	1.98	0.82
22:W:111:GLU:OE1	60:W:201:HOH:O	1.97	0.81
7:G:232:ASP:OD2	60:G:901:HOH:O	1.98	0.80
7:G:346:GLU:OE2	60:G:902:HOH:O	2.00	0.80
8:H:225:MET:CE	51:H:602:I49:I02	3.00	0.80
12:L:465:GLY:O	12:L:469:SER:OG	2.00	0.79
14:N:347:GLU:OE2	60:N:1001:HOH:O	1.99	0.79
17:Q:36:ARG:NE	17:Q:106:GLU:OE1	2.16	0.77
7:G:260:GLU:OE1	60:G:903:HOH:O	2.02	0.76
5:E:165:THR:OG1	5:E:168:ASP:OD1	2.03	0.76
7:G:139:ASP:O	18:R:77:LYS:NZ	2.18	0.76
13:M:335:GLU:OE2	60:M:701:HOH:O	2.04	0.76
8:H:225:MET:HE3	51:H:602:I49:I02	2.56	0.76
9:I:124:GLU:OE2	60:I:301:HOH:O	2.06	0.74
8:H:225:MET:HE2	51:H:602:I49:I02	2.58	0.73
6:F:108:ARG:NH1	60:F:601:HOH:O	2.21	0.73
25:Z:138:TYR:OH	60:Z:201:HOH:O	2.02	0.72
7:G:598:LYS:NZ	60:G:905:HOH:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:83:TYR:OH	54:O:401:GTP:O3'	2.04	0.72
23:X:68:GLU:OE1	23:X:71:ARG:NH1	2.23	0.71
24:Y:69:PHE:O	24:Y:73:SER:OG	2.06	0.71
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.72	0.70
3:C:95:ASN:OD1	60:C:301:HOH:O	2.09	0.70
15:O:103:SER:OG	60:O:501:HOH:O	2.09	0.70
12:L:2:ASN:OD1	60:L:801:HOH:O	2.08	0.70
2:B:27:GLU:OE2	2:B:178:ARG:NH2	2.24	0.70
14:N:303:THR:O	60:N:1002:HOH:O	2.10	0.70
10:J:25:SER:OG	10:J:77:GLU:OE1	2.08	0.69
3:C:165:ASP:OD2	60:C:302:HOH:O	2.10	0.69
22:W:123:TYR:O	60:W:202:HOH:O	2.12	0.68
7:G:140:LYS:O	7:G:148:THR:OG1	2.08	0.68
8:H:24:GLU:OE2	8:H:228:TYR:OH	2.09	0.66
20:T:74:GLN:NE2	20:T:78:ASP:OD2	2.29	0.66
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.25	0.66
3:C:49:GLU:OE1	60:C:303:HOH:O	2.13	0.66
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.32	0.65
10:J:124:ASP:OD1	11:K:2:SER:OG	2.15	0.64
15:O:60:ASP:OD1	15:O:60:ASP:N	2.32	0.63
15:O:291:GLN:NE2	15:O:295:GLU:OE1	2.28	0.63
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.82	0.62
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.82	0.62
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.81	0.62
5:E:71:GLU:O	5:E:74:GLN:NE2	2.33	0.62
15:O:104:ARG:NH1	54:O:401:GTP:O6	2.32	0.62
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.80	0.62
24:Y:21:THR:O	24:Y:25:THR:OG1	2.11	0.61
16:P:72:ASP:O	60:P:601:HOH:O	2.16	0.59
18:R:25:LYS:O	60:R:301:HOH:O	2.17	0.59
5:E:181:ILE:HG23	5:E:181:ILE:O	2.03	0.58
3:C:118:GLU:OE2	3:C:144:ASN:ND2	2.36	0.58
1:A:49:LEU:O	1:A:50:PRO:C	2.42	0.57
1:A:49:LEU:O	1:A:51:PHE:N	2.38	0.57
15:O:26:THR:HG21	60:O:511:HOH:O	2.05	0.57
1:A:28:ASN:N	1:A:28:ASN:OD1	2.38	0.56
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.88	0.56
8:H:203:GLY:O	8:H:207:LEU:HD22	2.05	0.56
7:G:441:GLN:HA	7:G:441:GLN:OE1	2.06	0.56
9:I:84:GLU:OE2	60:I:302:HOH:O	2.18	0.56
12:L:128:MET:HB2	12:L:251:THR:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.87	0.55
12:L:173:LEU:HD13	46:L:701:3PE:H222	1.89	0.55
8:H:200:LEU:HD22	8:H:285:LEU:HD21	1.88	0.55
19:S:57:CYS:O	19:S:60:VAL:HG22	2.07	0.55
12:L:72:GLN:OE1	60:L:803:HOH:O	2.19	0.54
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.37	0.54
13:M:296:LEU:HD22	13:M:381:VAL:HG11	1.90	0.54
15:O:311:ASP:OD1	15:O:312:VAL:HG13	2.08	0.54
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.90	0.54
16:P:10:LYS:NZ	17:Q:28:GLU:OE2	2.41	0.54
45:B:202:LMT:O6'	45:B:202:LMT:O2B	2.26	0.53
5:E:105:THR:HG22	5:E:106:THR:H	1.73	0.53
13:M:135:ARG:NH1	14:N:301:THR:O	2.41	0.53
11:K:12:PHE:CD2	14:N:72:MET:HE2	2.43	0.53
4:D:415:VAL:HG21	8:H:207:LEU:HG	1.90	0.53
1:A:30:TYR:OH	56:P:501:NDP:O3X	2.22	0.53
12:L:195:THR:HG21	12:L:200:GLN:HB3	1.91	0.52
10:J:1:FME:SD	10:J:2:MET:N	2.83	0.52
45:N:902:LMT:O1B	45:N:902:LMT:O6'	2.26	0.52
7:G:170:ASP:OD2	60:G:904:HOH:O	2.18	0.52
7:G:315:VAL:O	7:G:340:SER:OG	2.23	0.52
2:B:44:SER:OG	8:H:51:ASP:OD1	2.19	0.52
14:N:267:ILE:O	14:N:271:THR:HG23	2.10	0.52
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.92	0.51
14:N:87:MET:O	14:N:145:ILE:HG22	2.10	0.51
15:O:281:GLU:N	15:O:281:GLU:OE1	2.43	0.51
5:E:123:LYS:NZ	5:E:174:ASP:OD1	2.23	0.51
14:N:97:LEU:HD21	45:N:902:LMT:H122	1.93	0.51
12:L:124:PHE:CD1	12:L:251:THR:HG21	2.45	0.51
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.46	0.51
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.46	0.51
6:F:47:GLU:OE2	6:F:47:GLU:HA	3.41	0.50
12:L:485:TYR:O	12:L:489:THR:OG1	2.29	0.50
5:E:194:GLU:OE1	5:E:194:GLU:N	2.43	0.50
7:G:377:VAL:HG23	7:G:404:LEU:HD11	1.94	0.50
15:O:285:GLY:O	15:O:289:SER:OG	2.29	0.50
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.94	0.50
1:A:27:LEU:HD11	45:B:202:LMT:H22	1.94	0.50
19:S:87:THR:O	19:S:91:GLU:HG3	2.12	0.49
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.95	0.49
13:M:296:LEU:HD21	13:M:396:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:174:VAL:HG22	15:O:225:ALA:HB2	1.95	0.49
20:T:29:LYS:HD2	20:T:29:LYS:O	2.13	0.49
6:F:99:GLU:OE1	6:F:107:ASP:N	2.46	0.48
16:P:97:ARG:NH2	56:P:501:NDP:O2X	2.44	0.48
8:H:11:ILE:HB	8:H:12:PRO:HD3	1.94	0.48
6:F:367:GLU:OE2	7:G:100:ASN:ND2	2.45	0.48
17:Q:21:THR:HG21	22:W:73:ILE:HD11	1.95	0.48
15:O:136:GLU:HA	15:O:136:GLU:OE2	2.14	0.48
14:N:337:LEU:HD23	52:X:1701:CDL:C60	2.44	0.48
2:B:91:THR:HA	2:B:119:CYS:HB3	1.96	0.48
12:L:251:THR:HG22	12:L:252:MET:N	2.29	0.48
7:G:297:GLU:HG3	22:W:123:TYR:CZ	2.49	0.48
16:P:224:ARG:HG2	16:P:224:ARG:HH11	1.78	0.48
16:P:279:THR:O	16:P:279:THR:HG23	2.14	0.47
25:Z:129:ALA:O	25:Z:133:VAL:HG23	2.14	0.47
10:J:103:MET:HG2	10:J:115:VAL:HG21	1.95	0.47
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.96	0.47
2:B:175:ILE:HD12	16:P:52:GLU:HG2	1.96	0.47
15:O:225:ALA:O	15:O:229:GLN:NE2	2.44	0.47
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.14	0.47
6:F:276:LEU:HD13	6:F:317:MET:SD	2.54	0.47
4:D:161:ILE:HD11	4:D:235:TRP:CZ3	2.50	0.47
12:L:124:PHE:CE1	12:L:251:THR:HG21	2.50	0.47
13:M:225:ILE:O	13:M:229:MET:HG3	2.15	0.47
20:U:47:GLN:NE2	20:U:70:LEU:O	2.47	0.47
12:L:562:LEU:HB2	12:L:563:PRO:CD	2.45	0.46
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.98	0.46
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.97	0.46
5:E:87:TYR:HB3	6:F:181:ALA:O	2.16	0.46
9:I:114:THR:HG21	9:I:144:HIS:CE1	2.50	0.46
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.50	0.46
20:T:7:THR:O	20:T:10:GLY:N	2.49	0.46
13:M:108:MET:HB3	13:M:121:LEU:HD13	1.98	0.46
20:T:82:ASP:OD2	20:T:82:ASP:N	2.48	0.46
25:Z:125:TYR:HB3	25:Z:133:VAL:HG22	1.97	0.46
12:L:445:GLU:O	12:L:451:ILE:HD11	2.16	0.46
12:L:149:ILE:HG13	13:M:369:LEU:HD13	1.97	0.46
14:N:347:GLU:HG3	51:N:904:I49:I02	2.86	0.46
12:L:331:THR:HB	12:L:387:THR:HG22	1.98	0.45
6:F:165:ASN:OD1	6:F:170:GLY:N	2.46	0.45
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.99	0.45
6:F:193:ILE:HG23	6:F:215:VAL:HA	1.98	0.45
3:C:58:ILE:HB	3:C:59:PRO:HD3	1.99	0.45
13:M:191:SER:OG	24:Y:130:GLU:OE1	2.35	0.45
24:Y:82:LYS:O	24:Y:88:ASN:ND2	2.48	0.45
6:F:184:TYR:CE2	49:F:501:FMN:HM73	2.52	0.45
13:M:19:LYS:CE	13:M:19:LYS:H	2.30	0.45
6:F:194:GLU:OE1	6:F:204:ARG:NE	2.42	0.44
8:H:102:VAL:HG11	8:H:154:LEU:HD11	1.99	0.44
58:T:101:EHZ:O2	58:T:101:EHZ:O1	2.34	0.44
12:L:230:HIS:N	12:L:231:PRO:CD	2.80	0.44
7:G:317:ALA:HB1	7:G:331:LEU:HD21	1.98	0.44
8:H:87:ILE:N	8:H:88:PRO:CD	2.81	0.44
6:F:93:LEU:O	6:F:134:ALA:HA	2.17	0.44
7:G:281:GLU:HG2	7:G:592:LEU:HD12	2.00	0.44
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.53	0.44
8:H:179:TRP:N	8:H:180:PRO:CD	2.81	0.44
13:M:123:GLU:OE2	13:M:157:SER:HB2	2.16	0.44
20:T:35:HIS:CE1	20:T:38:LYS:HE2	2.53	0.44
25:Z:124:LEU:O	25:Z:128:ARG:NH1	2.51	0.44
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.47	0.44
7:G:437:HIS:O	7:G:440:SER:OG	2.27	0.43
8:H:73:LEU:HD23	8:H:118:TRP:CZ3	2.53	0.43
14:N:146:PHE:HA	14:N:149:ILE:HD12	1.99	0.43
15:O:51:PHE:HB2	15:O:124:LEU:HD23	1.98	0.43
8:H:87:ILE:HG12	8:H:88:PRO:HD3	2.00	0.43
12:L:247:LEU:HD22	12:L:248:HIS:CD2	2.54	0.43
14:N:41:ILE:N	14:N:42:PRO:HD2	2.34	0.43
12:L:421:ILE:HA	12:L:501:ALA:HB2	1.99	0.43
53:M:603:PC1:O13	53:M:603:PC1:H132	2.18	0.43
4:D:157:HIS:ND1	60:D:502:HOH:O	2.27	0.43
4:D:417:ILE:O	4:D:420:THR:HG22	2.18	0.43
11:K:73:LEU:HD21	14:N:41:ILE:HG13	1.99	0.43
12:L:562:LEU:CB	12:L:563:PRO:CD	2.96	0.43
16:P:127:GLU:O	16:P:224:ARG:NH1	2.51	0.43
12:L:363:PHE:CD1	12:L:370:THR:HG21	2.54	0.43
23:X:154:GLU:OE1	23:X:154:GLU:N	2.51	0.43
1:A:63:LEU:HB2	10:J:67:VAL:HG21	2.01	0.43
11:K:37:MET:HG3	11:K:67:ALA:CB	2.48	0.43
4:D:328:ALA:HB3	7:G:126:ASP:HB2	2.01	0.42
5:E:108:CYS:HA	5:E:151:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:285:LEU:HD23	13:M:285:LEU:C	2.40	0.42
10:J:130:THR:HG21	25:Z:124:LEU:HD12	2.01	0.42
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.01	0.42
8:H:221:ALA:O	8:H:225:MET:HG3	2.18	0.42
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.55	0.42
15:O:31:ILE:O	15:O:179:VAL:HG13	2.19	0.42
15:O:88:SER:OG	15:O:90:ASP:OD1	2.17	0.42
21:V:17:GLU:OE1	21:V:17:GLU:HA	2.19	0.42
8:H:113:VAL:HG22	8:H:136:VAL:HG22	2.01	0.42
9:I:126:CYS:HA	47:I:203:SF4:S2	2.59	0.42
7:G:568:GLU:HA	7:G:587:VAL:O	2.20	0.42
8:H:102:VAL:HG13	8:H:150:LEU:HD21	2.00	0.42
10:J:17:PHE:HA	10:J:20:PHE:CE2	2.55	0.42
12:L:145:GLU:OE1	12:L:179:ASP:OD2	2.37	0.42
15:O:130:SER:O	15:O:133:VAL:HG22	2.19	0.42
4:D:117:ALA:HB2	4:D:367:ILE:HG12	2.01	0.42
6:F:184:TYR:CZ	49:F:501:FMN:HM73	2.54	0.42
1:A:65:PHE:CD2	1:A:98:LEU:HD11	2.55	0.42
1:A:3:LEU:HD22	46:A:302:3PE:H31	2.01	0.41
20:T:16:LEU:O	20:T:20:LYS:HG3	2.20	0.41
14:N:146:PHE:N	14:N:147:PRO:CD	2.83	0.41
16:P:91:VAL:HG23	16:P:126:VAL:HG11	2.02	0.41
7:G:535:GLN:OE1	7:G:535:GLN:HA	2.20	0.41
2:B:152:THR:HG22	4:D:188:ARG:HD3	2.01	0.41
4:D:322:GLU:OE1	4:D:322:GLU:N	2.43	0.41
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.56	0.41
14:N:89:LEU:HD12	14:N:95:SER:HA	2.03	0.41
6:F:403:THR:HB	47:F:502:SF4:S4	2.60	0.41
8:H:312:SER:HG	25:Z:55:ARG:HH21	1.67	0.41
15:O:46:LEU:HD21	15:O:235:VAL:HG13	2.03	0.41
21:V:71:LEU:HD13	21:V:79:VAL:HG11	2.02	0.41
1:A:73:LEU:N	1:A:74:PRO:CD	2.84	0.41
3:C:198:ASP:O	60:C:304:HOH:O	2.22	0.41
5:E:100:ILE:HD11	5:E:137:PHE:CD1	2.56	0.41
15:O:22:SER:HB3	15:O:115:LEU:HD11	2.02	0.41
1:A:49:LEU:HD21	8:H:130:ILE:HG13	2.03	0.41
5:E:150:ASN:HB3	5:E:162:GLU:HB3	2.03	0.41
10:J:125:TRP:HB2	25:Z:137:THR:HG21	2.03	0.41
13:M:403:THR:HA	13:M:406:TYR:CE2	2.55	0.41
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.56	0.40
14:N:162:ILE:HG22	14:N:285:THR:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:14:ARG:HD2	20:T:57:GLU:OE2	2.22	0.40
12:L:261:ILE:HG13	12:L:317:ILE:HD11	2.03	0.40
2:B:32:LYS:HA	2:B:32:LYS:HD3	1.92	0.40
13:M:94:LEU:HD21	46:M:602:3PE:O32	2.21	0.40
14:N:137:ALA:HB3	14:N:138:PRO:HD3	2.03	0.40
24:Y:22:TYR:O	24:Y:26:SER:OG	2.32	0.40
6:F:98:ASP:O	6:F:99:GLU:C	2.60	0.40
7:G:254:MET:HA	7:G:260:GLU:O	2.22	0.40
10:J:141:MET:CE	10:J:141:MET:HA	2.51	0.40
13:M:76:MET:SD	13:M:230:VAL:HB	2.62	0.40
15:O:240:TYR:N	15:O:240:TYR:CD2	2.89	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	96/115 (84%)	93 (97%)	2 (2%)	1 (1%)	15	17
2	B	152/216 (70%)	147 (97%)	5 (3%)	0	100	100
3	C	204/266 (77%)	199 (98%)	5 (2%)	0	100	100
4	D	408/463 (88%)	397 (97%)	11 (3%)	0	100	100
5	E	210/249 (84%)	207 (99%)	3 (1%)	0	100	100
6	F	427/464 (92%)	422 (99%)	5 (1%)	0	100	100
7	G	686/727 (94%)	670 (98%)	16 (2%)	0	100	100
8	H	301/318 (95%)	293 (97%)	8 (3%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	172/175 (98%)	164 (95%)	8 (5%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	604/606 (100%)	586 (97%)	17 (3%)	1 (0%)	47	58
13	M	457/459 (100%)	449 (98%)	8 (2%)	0	100	100
14	N	345/347 (99%)	338 (98%)	7 (2%)	0	100	100
15	O	318/343 (93%)	312 (98%)	6 (2%)	0	100	100
16	P	282/380 (74%)	276 (98%)	6 (2%)	0	100	100
17	Q	123/175 (70%)	122 (99%)	1 (1%)	0	100	100
18	R	92/124 (74%)	91 (99%)	1 (1%)	0	100	100
19	S	83/99 (84%)	81 (98%)	2 (2%)	0	100	100
20	T	74/156 (47%)	70 (95%)	4 (5%)	0	100	100
20	U	82/156 (53%)	82 (100%)	0	0	100	100
21	V	110/116 (95%)	110 (100%)	0	0	100	100
22	W	112/128 (88%)	110 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
25	Z	138/144 (96%)	136 (99%)	2 (1%)	0	100	100
26	a	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	109/120 (91%)	108 (99%)	1 (1%)	0	100	100
30	e	93/106 (88%)	92 (99%)	1 (1%)	0	100	100
31	f	49/57 (86%)	49 (100%)	0	0	100	100
32	g	96/154 (62%)	92 (96%)	4 (4%)	0	100	100
33	h	136/189 (72%)	136 (100%)	0	0	100	100
34	i	99/127 (78%)	95 (96%)	4 (4%)	0	100	100
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	77/98 (79%)	77 (100%)	0	0	100	100
37	l	153/186 (82%)	148 (97%)	5 (3%)	0	100	100
38	m	124/129 (96%)	120 (97%)	4 (3%)	0	100	100
39	n	169/179 (94%)	165 (98%)	4 (2%)	0	100	100
40	o	119/137 (87%)	114 (96%)	5 (4%)	0	100	100
41	p	168/176 (96%)	168 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	87 (97%)	3 (3%)	0	100	100
44	s	41/109 (38%)	40 (98%)	1 (2%)	0	100	100
All	All	7978/9212 (87%)	7809 (98%)	167 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	PRO
12	L	562	LEU

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	87/100 (87%)	81 (93%)	6 (7%)	15	20
2	B	130/175 (74%)	125 (96%)	5 (4%)	33	47
3	C	187/228 (82%)	186 (100%)	1 (0%)	88	95
4	D	357/392 (91%)	354 (99%)	3 (1%)	81	91
5	E	183/205 (89%)	181 (99%)	2 (1%)	73	86
6	F	343/368 (93%)	339 (99%)	4 (1%)	71	84
7	G	578/608 (95%)	564 (98%)	14 (2%)	49	66
8	H	265/274 (97%)	260 (98%)	5 (2%)	57	73
9	I	151/175 (86%)	150 (99%)	1 (1%)	84	92
10	J	140/141 (99%)	135 (96%)	5 (4%)	35	49
11	K	85/85 (100%)	82 (96%)	3 (4%)	36	50
12	L	529/533 (99%)	516 (98%)	13 (2%)	47	65
13	M	412/412 (100%)	403 (98%)	9 (2%)	52	69
14	N	315/315 (100%)	314 (100%)	1 (0%)	92	97
15	O	283/303 (93%)	277 (98%)	6 (2%)	53	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	P	249/327 (76%)	245 (98%)	4 (2%)	62 78
17	Q	112/153 (73%)	110 (98%)	2 (2%)	59 75
18	R	77/97 (79%)	75 (97%)	2 (3%)	46 63
19	S	75/82 (92%)	73 (97%)	2 (3%)	44 61
20	T	70/135 (52%)	63 (90%)	7 (10%)	7 9
20	U	78/135 (58%)	78 (100%)	0	100 100
21	V	100/102 (98%)	100 (100%)	0	100 100
22	W	107/114 (94%)	105 (98%)	2 (2%)	57 73
23	X	154/155 (99%)	146 (95%)	8 (5%)	23 32
24	Y	101/102 (99%)	97 (96%)	4 (4%)	31 44
25	Z	119/121 (98%)	117 (98%)	2 (2%)	60 76
26	a	58/59 (98%)	56 (97%)	2 (3%)	37 51
27	b	71/72 (99%)	66 (93%)	5 (7%)	15 19
28	c	44/68 (65%)	43 (98%)	1 (2%)	50 67
29	d	100/105 (95%)	97 (97%)	3 (3%)	41 57
30	e	86/96 (90%)	83 (96%)	3 (4%)	36 50
31	f	48/54 (89%)	46 (96%)	2 (4%)	30 42
32	g	89/131 (68%)	84 (94%)	5 (6%)	21 29
33	h	121/158 (77%)	121 (100%)	0	100 100
34	i	98/120 (82%)	96 (98%)	2 (2%)	55 72
35	j	61/84 (73%)	59 (97%)	2 (3%)	38 53
36	k	61/76 (80%)	60 (98%)	1 (2%)	62 78
37	l	139/159 (87%)	138 (99%)	1 (1%)	84 92
38	m	112/115 (97%)	109 (97%)	3 (3%)	44 61
39	n	156/161 (97%)	155 (99%)	1 (1%)	86 94
40	o	110/120 (92%)	106 (96%)	4 (4%)	35 49
41	p	154/157 (98%)	151 (98%)	3 (2%)	57 73
42	q	131/131 (100%)	126 (96%)	5 (4%)	33 47
43	r	84/97 (87%)	81 (96%)	3 (4%)	35 49
44	s	42/92 (46%)	41 (98%)	1 (2%)	49 66
All	All	7052/7892 (89%)	6894 (98%)	158 (2%)	54 69

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	28	ASN
1	A	48	ARG
1	A	57	LEU
1	A	85	ASN
1	A	87	MET
2	B	50	PHE
2	B	54	CYS
2	B	59	MET
2	B	125	TYR
2	B	171	LYS
3	C	33	LEU
4	D	69	SER
4	D	341	SER
4	D	420	THR
5	E	118	GLU
5	E	167	LYS
6	F	34	LYS
6	F	231	SER
6	F	405	CYS
6	F	436	GLN
7	G	17	SER
7	G	32	LYS
7	G	35	MET
7	G	39	ARG
7	G	61	LYS
7	G	84	GLU
7	G	188	GLU
7	G	193	SER
7	G	427	LYS
7	G	444	GLN
7	G	475	GLN
7	G	478	ARG
7	G	613	TYR
7	G	649	SER
8	H	66	SER
8	H	121	TRP
8	H	194	ASN
8	H	259	PHE
8	H	274	ARG
9	I	129	ASP
10	J	25	SER

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Mol	Chain	Res	Type
10	J	41	CYS
10	J	87	LYS
10	J	135	PHE
10	J	171	ILE
11	K	29	SER
11	K	46	LEU
11	K	53	PHE
12	L	10	VAL
12	L	124	PHE
12	L	199	GLN
12	L	244	SER
12	L	250	SER
12	L	262	ARG
12	L	336	LYS
12	L	343	SER
12	L	393	ASP
12	L	423	SER
12	L	469	SER
12	L	554	ASP
12	L	572	LYS
13	M	19	LYS
13	M	57	PHE
13	M	58	SER
13	M	114	GLU
13	M	116	ILE
13	M	191	SER
13	M	273	SER
13	M	393	ILE
13	M	406	TYR
14	N	40	ILE
15	O	28	ASP
15	O	60	ASP
15	O	146	LYS
15	O	180	GLN
15	O	206	TYR
15	O	289	SER
16	P	73	TRP
16	P	79	ASP
16	P	199	LYS
16	P	320	ARG
17	Q	89	LYS
17	Q	115	SER

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Mol	Chain	Res	Type
18	R	25	LYS
18	R	34	GLU
19	S	74	LYS
19	S	88	ARG
20	T	7	THR
20	T	8	LEU
20	T	13	ASP
20	T	29	LYS
20	T	35	HIS
20	T	37	MET
20	T	82	ASP
22	W	99	GLN
22	W	111	GLU
23	X	15	GLN
23	X	17	VAL
23	X	22	SER
23	X	47	TRP
23	X	63	ASN
23	X	77	CYS
23	X	130	VAL
23	X	154	GLU
24	Y	26	SER
24	Y	49	LEU
24	Y	105	ARG
24	Y	114	CYS
25	Z	52	LYS
25	Z	120	MET
26	a	21	MET
26	a	68	ASN
27	b	2	GLU
27	b	4	VAL
27	b	14	LYS
27	b	67	SER
27	b	69	PRO
28	c	1	LYS
29	d	104	LYS
29	d	106	LYS
29	d	120	ARG
30	e	86	ILE
30	e	87	LYS
30	e	92	THR
31	f	29	LYS

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Mol	Chain	Res	Type
31	f	30	ASN
32	g	25	ARG
32	g	26	TRP
32	g	33	GLU
32	g	57	ASN
32	g	112	CYS
34	i	23	LYS
34	i	28	SER
35	j	40	PHE
35	j	69	ASP
36	k	85	TYR
37	l	15	LYS
38	m	23	ASP
38	m	39	ARG
38	m	92	PHE
39	n	8	TYR
40	o	27	ASP
40	o	30	PHE
40	o	69	LYS
40	o	120	ASP
41	p	3	SER
41	p	42	ARG
41	p	68	ARG
42	q	8	LYS
42	q	15	SER
42	q	67	GLU
42	q	101	LYS
42	q	107	LYS
43	r	66	SER
43	r	68	VAL
43	r	102	ARG
44	s	59	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
16	P	250	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	$\#\|Z\| > 2$
4	2MR	D	85	4	10,12,13	2.63	4 (40%)	5,13,15	1.14	1 (20%)
10	FME	J	1	10	8,9,10	0.99	0	7,9,11	0.75	0
34	SAC	i	1	34	7,8,9	1.85	1 (14%)	8,9,11	1.74	1 (12%)
43	AYA	r	1	43	6,7,8	1.78	2 (33%)	5,8,10	1.40	1 (20%)
8	FME	H	1	8	8,9,10	0.94	0	7,9,11	0.89	0
14	FME	N	1	14	8,9,10	0.98	0	7,9,11	1.02	1 (14%)
1	FME	A	1	1	8,9,10	0.95	0	7,9,11	0.96	0
13	FME	M	1	13	8,9,10	0.99	1 (12%)	7,9,11	1.03	1 (14%)
24	AYA	Y	1	24	6,7,8	1.80	2 (33%)	5,8,10	1.20	1 (20%)
12	FME	L	1	12	8,9,10	0.97	0	7,9,11	0.97	1 (14%)
11	FME	K	1	11	8,9,10	0.90	0	7,9,11	0.87	0

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

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.94	1.44	1.33
4	D	85	2MR	CZ-NE	4.59	1.44	1.34
34	i	1	SAC	O-C	4.15	1.36	1.19
4	D	85	2MR	O-C	3.86	1.35	1.19
24	Y	1	AYA	CT-N	3.27	1.45	1.34
43	r	1	AYA	CT-N	3.25	1.45	1.34
4	D	85	2MR	CQ1-NH1	-2.08	1.42	1.46
13	M	1	FME	CA-N	-2.06	1.43	1.46
43	r	1	AYA	OT-CT	-2.00	1.18	1.23
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	O-C-CA	-4.45	113.12	124.78
43	r	1	AYA	CM-CT-N	2.51	120.35	116.10
14	N	1	FME	C-CA-N	2.19	113.69	109.73
13	M	1	FME	C-CA-N	2.14	113.59	109.73
24	Y	1	AYA	CM-CT-N	2.13	119.71	116.10
4	D	85	2MR	NE-CZ-NH2	-2.10	117.56	119.48
12	L	1	FME	C-CA-N	2.01	113.36	109.73

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
34	i	1	SAC	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	J	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 51 ligands modelled in this entry, 3 are monoatomic - leaving 48 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	$\#\|Z\| > 2$
45	LMT	B	202	-	36,36,36	1.20	2 (5%)	47,47,47	0.93	0
53	PC1	M	603	-	39,39,53	1.10	3 (7%)	45,47,61	1.00	2 (4%)
45	LMT	d	1203	-	36,36,36	1.23	4 (11%)	47,47,47	1.01	3 (6%)
45	LMT	e	201	-	36,36,36	1.21	3 (8%)	47,47,47	1.18	5 (10%)
45	LMT	l	201	-	36,36,36	1.20	3 (8%)	47,47,47	0.97	3 (6%)
46	3PE	Y	401	-	34,34,50	1.04	4 (11%)	37,39,55	1.18	2 (5%)
46	3PE	A	302	-	37,37,50	0.97	4 (10%)	40,42,55	1.08	2 (5%)
54	GTP	O	401	55	26,34,34	2.91	10 (38%)	32,54,54	1.67	9 (28%)
52	CDL	q	202	-	75,75,99	0.99	8 (10%)	81,87,111	1.05	3 (3%)
45	LMT	A	301	-	36,36,36	1.21	3 (8%)	47,47,47	0.90	1 (2%)
45	LMT	L	704	-	36,36,36	1.19	3 (8%)	47,47,47	0.79	1 (2%)
48	FES	G	803	7	0,4,4	-	-	-		
47	SF4	I	202	9	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	LMT	N	901	-	36,36,36	1.19	3 (8%)	47,47,47	0.81	2 (4%)
46	3PE	L	701	-	48,48,50	0.87	2 (4%)	51,53,55	1.00	2 (3%)
46	3PE	d	1201	-	46,46,50	0.90	4 (8%)	49,51,55	1.11	2 (4%)
49	FMN	F	501	-	33,33,33	1.08	2 (6%)	48,50,50	1.26	6 (12%)
45	LMT	N	902	-	36,36,36	1.17	3 (8%)	47,47,47	0.89	1 (2%)
47	SF4	G	802	7	0,12,12	-	-	-		
45	LMT	f	1801	-	36,36,36	1.19	3 (8%)	47,47,47	1.19	4 (8%)
47	SF4	G	801	7	0,12,12	-	-	-		
53	PC1	q	201	-	34,34,53	1.15	4 (11%)	40,42,61	1.15	2 (5%)
46	3PE	M	601	-	45,45,50	0.89	4 (8%)	48,50,55	1.09	2 (4%)
56	NDP	P	501	-	45,52,52	2.13	5 (11%)	53,80,80	1.63	10 (18%)
59	MYR	o	201	40	14,14,15	0.90	0	13,13,15	0.70	0
51	I49	H	602	-	15,17,17	1.51	2 (13%)	21,22,22	1.87	5 (23%)
52	CDL	h	1001	-	66,66,99	1.06	7 (10%)	72,78,111	1.20	5 (6%)
46	3PE	M	602	-	48,48,50	0.87	3 (6%)	51,53,55	1.15	2 (3%)
46	3PE	N	903	-	40,40,50	0.96	4 (10%)	43,45,55	1.06	2 (4%)
52	CDL	J	401	-	70,70,99	1.03	6 (8%)	76,82,111	1.09	4 (5%)
45	LMT	h	1002	-	36,36,36	1.16	3 (8%)	47,47,47	1.07	2 (4%)
48	FES	E	301	5	0,4,4	-	-	-		
52	CDL	L	702	-	68,68,99	1.03	7 (10%)	74,80,111	1.09	4 (5%)
47	SF4	F	502	6	0,12,12	-	-	-		
47	SF4	B	201	2	0,12,12	-	-	-		
45	LMT	Y	402	-	36,36,36	1.19	3 (8%)	47,47,47	1.00	3 (6%)
58	EHZ	U	101	20	29,36,37	1.66	5 (17%)	35,44,47	1.41	2 (5%)
45	LMT	f	1802	-	36,36,36	1.21	3 (8%)	47,47,47	0.92	0
47	SF4	I	203	9	0,12,12	-	-	-		
46	3PE	H	601	-	33,33,50	1.42	3 (9%)	34,37,55	1.05	2 (5%)
51	I49	N	904	-	15,17,17	1.55	2 (13%)	21,22,22	1.69	5 (23%)
52	CDL	d	1202	-	64,64,99	1.08	8 (12%)	70,76,111	1.13	4 (5%)
46	3PE	b	901	-	47,47,50	0.87	4 (8%)	50,52,55	1.06	2 (4%)
52	CDL	X	1701	-	71,71,99	1.03	8 (11%)	77,83,111	1.17	4 (5%)
46	3PE	L	703	-	44,44,50	0.92	3 (6%)	47,49,55	1.07	2 (4%)
58	EHZ	T	101	20	29,36,37	1.66	5 (17%)	35,44,47	1.41	4 (11%)
46	3PE	I	201	-	50,50,50	0.87	4 (8%)	53,55,55	0.97	2 (3%)
45	LMT	j	101	-	36,36,36	1.16	2 (5%)	47,47,47	0.87	1 (2%)

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
45	LMT	B	202	-	-	8/21/61/61	0/2/2/2
53	PC1	M	603	-	-	13/43/43/57	-
45	LMT	d	1203	-	-	7/21/61/61	0/2/2/2
45	LMT	e	201	-	-	8/21/61/61	0/2/2/2
45	LMT	l	201	-	-	4/21/61/61	0/2/2/2
46	3PE	Y	401	-	-	20/38/38/54	-
46	3PE	A	302	-	-	12/41/41/54	-
54	GTP	O	401	55	-	4/18/38/38	0/3/3/3
52	CDL	q	202	-	-	41/86/86/110	-
45	LMT	A	301	-	-	9/21/61/61	0/2/2/2
45	LMT	L	704	-	-	9/21/61/61	0/2/2/2
48	FES	G	803	7	-	-	0/1/1/1
47	SF4	I	202	9	-	-	0/6/5/5
45	LMT	N	901	-	-	2/21/61/61	0/2/2/2
46	3PE	L	701	-	-	20/52/52/54	-
46	3PE	d	1201	-	-	22/50/50/54	-
49	FMN	F	501	-	-	2/18/18/18	0/3/3/3
45	LMT	N	902	-	-	7/21/61/61	0/2/2/2
47	SF4	G	802	7	-	-	0/6/5/5
45	LMT	f	1801	-	-	9/21/61/61	0/2/2/2
47	SF4	G	801	7	-	-	0/6/5/5
53	PC1	q	201	-	-	9/38/38/57	-
46	3PE	M	601	-	-	21/49/49/54	-
56	NDP	P	501	-	-	9/30/77/77	0/5/5/5
59	MYR	o	201	40	-	4/11/12/13	-
51	I49	H	602	-	-	6/10/10/10	0/1/1/1
52	CDL	h	1001	-	-	29/77/77/110	-
46	3PE	M	602	-	-	20/52/52/54	-
46	3PE	N	903	-	-	22/44/44/54	-
52	CDL	J	401	-	-	30/81/81/110	-
45	LMT	h	1002	-	-	7/21/61/61	0/2/2/2
48	FES	E	301	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	CDL	L	702	-	-	30/79/79/110	-
47	SF4	F	502	6	-	-	0/6/5/5
47	SF4	B	201	2	-	-	0/6/5/5
45	LMT	Y	402	-	-	9/21/61/61	0/2/2/2
58	EHZ	U	101	20	-	10/42/44/45	-
45	LMT	f	1802	-	-	6/21/61/61	0/2/2/2
52	CDL	d	1202	-	-	28/75/75/110	-
46	3PE	H	601	-	-	13/36/36/54	-
51	I49	N	904	-	-	5/10/10/10	0/1/1/1
47	SF4	I	203	9	-	-	0/6/5/5
46	3PE	b	901	-	-	27/51/51/54	-
52	CDL	X	1701	-	-	36/82/82/110	-
46	3PE	L	703	-	-	23/48/48/54	-
58	EHZ	T	101	20	-	9/42/44/45	-
46	3PE	I	201	-	-	19/54/54/54	-
45	LMT	j	101	-	-	7/21/61/61	0/2/2/2

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	11.62	1.81	1.59
54	O	401	GTP	O6-C6	8.16	1.39	1.23
46	H	601	3PE	O21-C2	-5.66	1.40	1.46
54	O	401	GTP	O4'-C1'	5.39	1.48	1.41
58	U	101	EHZ	C15-N2	5.38	1.45	1.33
58	T	101	EHZ	C12-N1	5.25	1.45	1.33
58	T	101	EHZ	C15-N2	5.10	1.44	1.33
58	U	101	EHZ	C12-N1	4.93	1.44	1.33
51	N	904	I49	C15-N02	-4.80	1.31	1.37
54	O	401	GTP	C2-N1	4.70	1.49	1.37
51	H	602	I49	C15-N02	-4.54	1.31	1.37
54	O	401	GTP	C2-N2	4.52	1.44	1.34
54	O	401	GTP	C2-N3	4.50	1.44	1.33
56	P	501	NDP	PN-O5D	3.67	1.74	1.59
45	N	901	LMT	O5B-C1B	3.61	1.51	1.41
45	l	201	LMT	O5B-C1B	3.60	1.51	1.41
49	F	501	FMN	C4A-N5	3.56	1.37	1.30
45	f	1802	LMT	O5B-C1B	3.55	1.50	1.41
45	e	201	LMT	O5B-C1B	3.53	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B	202	LMT	O5B-C1B	3.48	1.50	1.41
45	f	1801	LMT	O5B-C1B	3.48	1.50	1.41
45	A	301	LMT	O5B-C1B	3.38	1.50	1.41
45	N	902	LMT	O5B-C1B	3.38	1.50	1.41
45	L	704	LMT	O5B-C1B	3.36	1.50	1.41
45	d	1203	LMT	O5B-C1B	3.35	1.50	1.41
45	d	1203	LMT	O5'-C1'	3.34	1.50	1.41
45	Y	402	LMT	O5B-C1B	3.34	1.50	1.41
54	O	401	GTP	C2'-C1'	-3.31	1.48	1.53
45	j	101	LMT	O5B-C1B	3.29	1.50	1.41
45	Y	402	LMT	O5'-C1'	3.25	1.50	1.41
45	L	704	LMT	O5'-C1'	3.24	1.50	1.41
45	f	1802	LMT	O5'-C1'	3.21	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.19	1.50	1.41
46	H	601	3PE	O21-C21	3.19	1.40	1.33
45	j	101	LMT	O5'-C1'	3.18	1.49	1.41
45	A	301	LMT	O5'-C1'	3.18	1.49	1.41
56	P	501	NDP	O2B-C2B	-3.13	1.32	1.44
51	N	904	I49	C14-N03	3.12	1.38	1.29
51	H	602	I49	C14-N03	3.08	1.38	1.29
45	N	902	LMT	O5'-C1'	3.07	1.49	1.41
54	O	401	GTP	C5-C6	-3.04	1.41	1.47
45	l	201	LMT	O5'-C1'	3.03	1.49	1.41
45	B	202	LMT	O5'-C1'	2.97	1.49	1.41
45	f	1801	LMT	O5'-C1'	2.97	1.49	1.41
45	e	201	LMT	O5'-C1'	2.93	1.49	1.41
45	h	1002	LMT	O5'-C1'	2.93	1.49	1.41
45	N	901	LMT	O5'-C1'	2.92	1.49	1.41
52	h	1001	CDL	OA6-CA4	-2.88	1.39	1.46
46	L	703	3PE	O21-C2	-2.77	1.39	1.46
52	h	1001	CDL	OB6-CB4	-2.76	1.39	1.46
53	M	603	PC1	O21-C2	-2.75	1.39	1.46
46	M	602	3PE	O21-C2	-2.72	1.39	1.46
52	d	1202	CDL	OA6-CA4	-2.70	1.39	1.46
52	L	702	CDL	OB6-CB4	-2.67	1.39	1.46
52	q	202	CDL	OB6-CB4	-2.65	1.40	1.46
52	X	1701	CDL	OA6-CA4	-2.63	1.40	1.46
46	L	701	3PE	O21-C2	-2.62	1.40	1.46
52	L	702	CDL	OA6-CA4	-2.61	1.40	1.46
46	N	903	3PE	O21-C2	-2.60	1.40	1.46
52	q	202	CDL	OA6-CA4	-2.60	1.40	1.46
52	d	1202	CDL	OB6-CB4	-2.58	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	CDL	OA6-CA4	-2.56	1.40	1.46
46	d	1201	3PE	O21-C2	-2.56	1.40	1.46
46	H	601	3PE	O31-C31	2.55	1.40	1.33
58	U	101	EHZ	O4-C15	-2.55	1.18	1.23
46	I	201	3PE	O21-C2	-2.54	1.40	1.46
52	X	1701	CDL	OB6-CB4	-2.54	1.40	1.46
58	T	101	EHZ	O4-C15	-2.52	1.18	1.23
46	L	701	3PE	O31-C3	-2.51	1.39	1.45
46	I	201	3PE	O31-C3	-2.50	1.39	1.45
46	N	903	3PE	O31-C3	-2.50	1.39	1.45
52	q	202	CDL	OB8-CB7	2.49	1.40	1.33
52	J	401	CDL	OB8-CB7	2.49	1.40	1.33
52	d	1202	CDL	OB8-CB7	2.46	1.40	1.33
52	J	401	CDL	OB6-CB4	-2.43	1.40	1.46
46	A	302	3PE	O21-C2	-2.43	1.40	1.46
52	h	1001	CDL	OB8-CB6	-2.42	1.39	1.45
46	b	901	3PE	O31-C31	2.42	1.40	1.33
52	X	1701	CDL	OB8-CB7	2.42	1.40	1.33
54	O	401	GTP	C2'-C3'	-2.42	1.46	1.53
52	X	1701	CDL	OA8-CA7	2.40	1.40	1.33
53	q	201	PC1	O21-C2	-2.39	1.40	1.46
52	L	702	CDL	OA8-CA7	2.38	1.40	1.33
52	d	1202	CDL	OA8-CA6	-2.37	1.39	1.45
46	Y	401	3PE	O21-C2	-2.37	1.40	1.46
58	T	101	EHZ	O3-C12	-2.37	1.18	1.23
52	J	401	CDL	OA8-CA6	-2.36	1.39	1.45
52	L	702	CDL	OB8-CB7	2.36	1.40	1.33
46	d	1201	3PE	O31-C31	2.35	1.40	1.33
46	M	602	3PE	O31-C3	-2.35	1.39	1.45
58	U	101	EHZ	O3-C12	-2.35	1.18	1.23
52	X	1701	CDL	OB8-CB6	-2.34	1.39	1.45
46	Y	401	3PE	O31-C31	2.34	1.40	1.33
52	L	702	CDL	OB8-CB6	-2.33	1.39	1.45
52	q	202	CDL	OA8-CA6	-2.32	1.39	1.45
46	L	703	3PE	O31-C31	2.32	1.40	1.33
53	M	603	PC1	O31-C3	-2.32	1.39	1.45
52	J	401	CDL	OA8-CA7	2.32	1.40	1.33
45	f	1801	LMT	O5B-C5B	2.32	1.50	1.44
46	M	601	3PE	O21-C2	-2.31	1.40	1.46
54	O	401	GTP	PG-O2G	-2.31	1.45	1.54
52	d	1202	CDL	OB8-CB6	-2.30	1.39	1.45
46	L	703	3PE	O31-C3	-2.29	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	q	201	PC1	O21-C21	2.29	1.40	1.34
54	O	401	GTP	PG-O3G	-2.29	1.46	1.54
53	M	603	PC1	O31-C31	2.28	1.40	1.33
46	I	201	3PE	O31-C31	2.28	1.40	1.33
46	A	302	3PE	O31-C31	2.27	1.40	1.33
46	M	601	3PE	O31-C31	2.26	1.39	1.33
46	A	302	3PE	O31-C3	-2.26	1.40	1.45
46	M	602	3PE	O31-C31	2.23	1.39	1.33
53	q	201	PC1	O31-C31	2.22	1.39	1.33
45	e	201	LMT	O5B-C5B	2.21	1.49	1.44
46	Y	401	3PE	O31-C3	-2.21	1.40	1.45
46	d	1201	3PE	O21-C21	2.20	1.40	1.34
52	h	1001	CDL	OA8-CA7	2.19	1.39	1.33
52	X	1701	CDL	OA8-CA6	-2.19	1.40	1.45
52	q	202	CDL	OA8-CA7	2.19	1.39	1.33
46	b	901	3PE	O21-C2	-2.18	1.41	1.46
45	f	1802	LMT	O5B-C5B	2.18	1.49	1.44
46	d	1201	3PE	O31-C3	-2.18	1.40	1.45
52	J	401	CDL	OB6-CB5	2.18	1.40	1.34
46	b	901	3PE	O21-C21	2.16	1.40	1.34
46	Y	401	3PE	O21-C21	2.16	1.40	1.34
52	h	1001	CDL	OB8-CB7	2.15	1.39	1.33
46	M	601	3PE	O21-C21	2.14	1.40	1.34
46	A	302	3PE	O21-C21	2.14	1.40	1.34
52	h	1001	CDL	OA8-CA6	-2.14	1.40	1.45
53	q	201	PC1	O31-C3	-2.14	1.40	1.45
52	d	1202	CDL	OA8-CA7	2.13	1.39	1.33
45	l	201	LMT	O5B-C5B	2.13	1.49	1.44
52	L	702	CDL	OA8-CA6	-2.13	1.40	1.45
52	q	202	CDL	OB6-CB5	2.12	1.40	1.34
45	Y	402	LMT	O5B-C5B	2.12	1.49	1.44
46	N	903	3PE	O31-C31	2.11	1.39	1.33
45	N	901	LMT	O5B-C5B	2.11	1.49	1.44
52	d	1202	CDL	OB6-CB5	2.09	1.40	1.34
56	P	501	NDP	O5D-C5D	-2.09	1.36	1.44
46	M	601	3PE	O31-C3	-2.09	1.40	1.45
52	q	202	CDL	OB8-CB6	-2.09	1.40	1.45
45	N	902	LMT	O5B-C5B	2.08	1.49	1.44
49	F	501	FMN	C10-N1	2.08	1.37	1.33
52	L	702	CDL	OB6-CB5	2.07	1.40	1.34
46	I	201	3PE	O21-C21	2.06	1.40	1.34
45	d	1203	LMT	O5B-C5B	2.05	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	T	101	EHZ	C9-S1	2.05	1.81	1.76
52	X	1701	CDL	OA6-CA5	2.05	1.40	1.34
46	N	903	3PE	O21-C21	2.04	1.40	1.34
45	L	704	LMT	O5B-C5B	2.04	1.49	1.44
52	q	202	CDL	OA6-CA5	2.03	1.40	1.34
52	h	1001	CDL	OB6-CB5	2.03	1.40	1.34
52	d	1202	CDL	OA6-CA5	2.03	1.40	1.34
45	d	1203	LMT	O5'-C5'	2.03	1.49	1.44
52	X	1701	CDL	OB6-CB5	2.03	1.40	1.34
46	b	901	3PE	O31-C3	-2.02	1.40	1.45
58	U	101	EHZ	C9-S1	2.01	1.81	1.76
56	P	501	NDP	C2A-N1A	2.01	1.37	1.33
45	A	301	LMT	O1B-C4'	2.01	1.49	1.43
45	h	1002	LMT	O5'-C5'	2.00	1.49	1.44

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	P	501	NDP	PN-O3-PA	-6.22	111.49	132.83
58	U	101	EHZ	C8-C9-S1	5.96	121.00	113.63
58	T	101	EHZ	C8-C9-S1	5.68	120.65	113.63
51	N	904	I49	N01-C14-N03	5.12	129.85	120.26
52	h	1001	CDL	OB6-CB5-C51	4.41	121.00	111.50
53	q	201	PC1	O21-C21-C22	4.38	120.93	111.50
52	X	1701	CDL	OB6-CB5-C51	4.28	120.73	111.50
46	d	1201	3PE	O21-C21-C22	4.27	120.71	111.50
46	Y	401	3PE	O21-C21-C22	4.21	120.58	111.50
46	M	602	3PE	O21-C21-C22	4.10	120.33	111.50
52	q	202	CDL	OA6-CA5-C11	4.07	120.28	111.50
52	d	1202	CDL	OA6-CA5-C11	4.03	120.19	111.50
51	H	602	I49	N01-C14-N03	4.00	127.76	120.26
46	H	601	3PE	O21-C21-O22	-3.97	120.52	125.57
46	N	903	3PE	O21-C21-C22	3.94	119.99	111.50
46	b	901	3PE	O21-C21-C22	3.91	119.94	111.50
46	M	601	3PE	O21-C21-C22	3.91	119.92	111.50
52	h	1001	CDL	OA6-CA5-C11	3.90	119.90	111.50
52	X	1701	CDL	OA6-CA5-C11	3.89	119.88	111.50
46	L	701	3PE	O21-C21-C22	3.87	119.84	111.50
52	L	702	CDL	OA6-CA5-C11	3.82	119.73	111.50
46	A	302	3PE	O21-C21-C22	3.79	119.67	111.50
52	J	401	CDL	OA6-CA5-C11	3.77	119.63	111.50
52	J	401	CDL	OB6-CB5-C51	3.68	119.44	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	I	201	3PE	O21-C21-C22	3.58	119.22	111.50
51	H	602	I49	C14-N02-C15	-3.54	119.31	125.21
52	L	702	CDL	OB6-CB5-C51	3.52	119.08	111.50
46	L	703	3PE	O21-C21-C22	3.51	119.08	111.50
53	M	603	PC1	O21-C21-C22	3.51	119.06	111.50
52	q	202	CDL	OB6-CB5-C51	3.50	119.05	111.50
56	P	501	NDP	O2B-P2B-O1X	-3.47	96.01	109.39
52	d	1202	CDL	OB6-CB5-C51	3.44	120.38	110.80
45	h	1002	LMT	O5'-C5'-C4'	3.21	116.51	109.75
54	O	401	GTP	C2-N1-C6	-3.14	119.31	125.10
54	O	401	GTP	C5-C6-N1	3.14	119.49	113.95
49	F	501	FMN	C4-N3-C2	-3.13	119.86	125.64
45	e	201	LMT	O5'-C5'-C4'	3.07	116.23	109.75
49	F	501	FMN	C4A-C10-N10	3.07	120.97	116.48
52	X	1701	CDL	OB8-CB7-C71	3.06	121.51	111.91
45	f	1801	LMT	C1'-C2'-C3'	3.03	116.30	110.00
46	M	601	3PE	O31-C31-C32	2.99	121.28	111.91
51	H	602	I49	C08-N01-C14	-2.89	118.23	123.50
46	Y	401	3PE	O31-C31-C32	2.87	120.93	111.91
54	O	401	GTP	PB-O3B-PG	-2.86	123.01	132.83
54	O	401	GTP	O2G-PG-O3B	2.84	114.17	104.64
52	h	1001	CDL	OA8-CA7-C31	2.83	120.80	111.91
54	O	401	GTP	O3G-PG-O3B	2.83	114.14	104.64
53	q	201	PC1	O31-C31-C32	2.83	120.79	111.91
56	P	501	NDP	PA-O5B-C5B	-2.83	105.11	121.68
46	A	302	3PE	O31-C31-C32	2.76	120.56	111.91
46	d	1201	3PE	O31-C31-C32	2.75	120.53	111.91
58	T	101	EHZ	O2-C9-S1	-2.75	119.05	122.61
54	O	401	GTP	PA-O3A-PB	-2.75	123.41	132.83
45	h	1002	LMT	C1B-O1B-C4'	-2.73	111.20	117.96
52	J	401	CDL	OB8-CB7-C71	2.72	120.44	111.91
46	L	703	3PE	O31-C31-C32	2.69	120.36	111.91
53	M	603	PC1	O31-C31-C32	2.67	120.30	111.91
52	q	202	CDL	OB8-CB7-C71	2.67	120.28	111.91
52	d	1202	CDL	OB8-CB7-C71	2.67	120.28	111.91
45	f	1801	LMT	C1'-O5'-C5'	-2.67	108.45	113.69
46	M	602	3PE	O31-C31-C32	2.67	120.27	111.91
49	F	501	FMN	C4A-C4-N3	2.65	119.93	113.19
52	h	1001	CDL	OB8-CB7-C71	2.64	120.18	111.91
56	P	501	NDP	PN-O5D-C5D	-2.61	106.38	121.68
51	N	904	I49	N05-C15-N04	-2.59	112.30	120.26
52	X	1701	CDL	OA8-CA7-C31	2.58	120.00	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	H	602	I49	N05-C15-N04	-2.57	112.36	120.26
45	f	1801	LMT	C2'-C3'-C4'	2.55	115.50	109.68
56	P	501	NDP	O3X-P2B-O2X	2.54	117.34	107.64
46	b	901	3PE	O31-C31-C32	2.52	119.81	111.91
52	J	401	CDL	OA8-CA7-C31	2.50	119.77	111.91
52	L	702	CDL	OB8-CB7-C71	2.49	119.73	111.91
46	H	601	3PE	O31-C31-C32	2.49	119.72	111.91
56	P	501	NDP	O5D-PN-O1N	-2.48	99.39	109.07
45	e	201	LMT	O5B-C5B-C4B	2.47	114.18	109.69
45	e	201	LMT	C3B-C4B-C5B	2.47	114.64	110.24
58	T	101	EHZ	C13-C12-N1	2.47	120.57	116.42
56	P	501	NDP	O4B-C4B-C3B	2.47	109.99	105.11
51	N	904	I49	N05-C15-N02	2.44	127.50	117.44
49	F	501	FMN	O4-C4-C4A	-2.44	120.12	126.60
45	f	1801	LMT	O5B-C5B-C4B	2.43	114.11	109.69
52	d	1202	CDL	OA8-CA7-C31	2.43	119.52	111.91
45	d	1203	LMT	C3B-C4B-C5B	2.42	114.56	110.24
45	j	101	LMT	C1B-O1B-C4'	-2.41	112.01	117.96
52	L	702	CDL	OA8-CA7-C31	2.40	119.45	111.91
49	F	501	FMN	C10-C4A-N5	-2.39	119.78	124.86
45	l	201	LMT	C1B-O1B-C4'	-2.36	112.13	117.96
45	N	901	LMT	C1B-O1B-C4'	-2.35	112.14	117.96
54	O	401	GTP	O2B-PB-O1B	-2.35	100.64	112.24
56	P	501	NDP	C2A-N1A-C6A	-2.32	114.78	118.75
46	I	201	3PE	O31-C31-C32	2.32	119.19	111.91
51	H	602	I49	C12-C13-I02	-2.32	119.28	121.72
45	d	1203	LMT	O5B-C5B-C4B	2.30	113.86	109.69
45	Y	402	LMT	C3B-C4B-C5B	2.29	114.32	110.24
54	O	401	GTP	O2A-PA-O1A	-2.27	101.04	112.24
45	e	201	LMT	C4B-C3B-C2B	2.26	114.78	110.82
56	P	501	NDP	O2N-PN-O1N	2.25	123.34	112.24
45	l	201	LMT	C6B-C5B-C4B	-2.21	107.83	113.00
54	O	401	GTP	C3'-C2'-C1'	2.21	104.30	100.98
49	F	501	FMN	C4A-C10-N1	-2.20	119.63	124.73
52	h	1001	CDL	CA4-OA6-CA5	-2.19	112.41	117.79
45	L	704	LMT	C1B-O5B-C5B	-2.18	109.42	113.69
58	T	101	EHZ	C13-C14-N2	-2.17	107.51	111.90
46	L	701	3PE	O31-C31-C32	2.17	118.71	111.91
46	N	903	3PE	O31-C31-C32	2.15	118.66	111.91
51	N	904	I49	N02-C14-N01	-2.15	112.54	118.08
58	U	101	EHZ	C13-C12-N1	2.14	120.02	116.42
51	N	904	I49	C09-C07-C10	2.12	121.51	118.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	e	201	LMT	C3'-C4'-C5'	2.12	115.79	110.93
45	l	201	LMT	O5B-C5B-C4B	2.11	113.53	109.69
45	Y	402	LMT	C1B-O1B-C4'	-2.10	112.76	117.96
45	A	301	LMT	O1B-C4'-C3'	2.07	112.80	107.28
45	d	1203	LMT	O5'-C5'-C4'	2.07	114.11	109.75
56	P	501	NDP	O7N-C7N-N7N	-2.05	118.08	122.88
45	N	902	LMT	O1B-C4'-C3'	2.04	112.72	107.28
45	Y	402	LMT	C6B-C5B-C4B	-2.03	108.24	113.00
45	N	901	LMT	O1'-C1'-C2'	2.00	111.43	108.30

There are no chirality outliers.

All (576) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	B	202	LMT	O5'-C1'-O1'-C1
45	Y	402	LMT	C2-C1-O1'-C1'
45	e	201	LMT	C2-C1-O1'-C1'
45	f	1801	LMT	O5'-C1'-O1'-C1
45	f	1802	LMT	O5'-C1'-O1'-C1
45	j	101	LMT	O5'-C1'-O1'-C1
46	H	601	3PE	O13-C11-C12-N
46	H	601	3PE	O22-C21-O21-C2
46	L	703	3PE	C1-O11-P-O12
46	L	703	3PE	C1-O11-P-O13
46	L	703	3PE	C1-O11-P-O14
46	L	703	3PE	C11-O13-P-O11
46	L	703	3PE	C11-O13-P-O12
46	L	703	3PE	C11-O13-P-O14
46	M	601	3PE	O13-C11-C12-N
46	M	602	3PE	O13-C11-C12-N
46	N	903	3PE	C11-O13-P-O11
46	N	903	3PE	C11-O13-P-O12
46	N	903	3PE	C11-O13-P-O14
46	N	903	3PE	O13-C11-C12-N
46	Y	401	3PE	C11-O13-P-O14
46	Y	401	3PE	O13-C11-C12-N
46	Y	401	3PE	C22-C21-O21-C2
46	b	901	3PE	C1-O11-P-O12
46	b	901	3PE	C1-O11-P-O14
46	b	901	3PE	O13-C11-C12-N
46	b	901	3PE	O21-C2-C3-O31
46	b	901	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
46	d	1201	3PE	C1-O11-P-O12
46	d	1201	3PE	C1-O11-P-O13
46	d	1201	3PE	C1-O11-P-O14
46	d	1201	3PE	O13-C11-C12-N
46	d	1201	3PE	C22-C21-O21-C2
51	H	602	I49	C07-C06-C08-N01
51	N	904	I49	C07-C06-C08-N01
51	N	904	I49	N05-C15-N02-C14
52	J	401	CDL	CB2-OB2-PB2-OB3
52	J	401	CDL	CB2-OB2-PB2-OB4
52	J	401	CDL	CB3-OB5-PB2-OB3
52	J	401	CDL	CB3-OB5-PB2-OB4
52	X	1701	CDL	CA2-C1-CB2-OB2
52	X	1701	CDL	C11-CA5-OA6-CA4
52	d	1202	CDL	CA3-OA5-PA1-OA4
52	d	1202	CDL	C11-CA5-OA6-CA4
52	d	1202	CDL	CB2-OB2-PB2-OB3
52	d	1202	CDL	C51-CB5-OB6-CB4
52	h	1001	CDL	CA2-OA2-PA1-OA5
52	h	1001	CDL	CB3-OB5-PB2-OB2
52	h	1001	CDL	CB3-OB5-PB2-OB3
52	h	1001	CDL	OB7-CB5-OB6-CB4
52	q	202	CDL	O1-C1-CB2-OB2
52	q	202	CDL	CA2-OA2-PA1-OA3
52	q	202	CDL	CA2-OA2-PA1-OA4
52	q	202	CDL	C11-CA5-OA6-CA4
52	q	202	CDL	CB3-OB5-PB2-OB3
54	O	401	GTP	C5'-O5'-PA-O3A
56	P	501	NDP	C2B-O2B-P2B-O1X
58	U	101	EHZ	C5-C6-C7-C8
58	U	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
45	d	1203	LMT	O5B-C1B-O1B-C4'
46	M	602	3PE	O32-C31-O31-C3
45	d	1203	LMT	C2B-C1B-O1B-C4'
45	A	301	LMT	C3'-C4'-O1B-C1B
46	M	602	3PE	C32-C31-O31-C3
46	A	302	3PE	O32-C31-O31-C3
46	L	703	3PE	O32-C31-O31-C3
46	d	1201	3PE	O32-C31-O31-C3
52	X	1701	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
52	X	1701	CDL	OB9-CB7-OB8-CB6
52	d	1202	CDL	OB9-CB7-OB8-CB6
52	J	401	CDL	OA7-CA5-OA6-CA4
52	X	1701	CDL	OA7-CA5-OA6-CA4
52	d	1202	CDL	OA7-CA5-OA6-CA4
52	d	1202	CDL	OB7-CB5-OB6-CB4
52	q	202	CDL	OA7-CA5-OA6-CA4
46	A	302	3PE	C32-C31-O31-C3
46	L	703	3PE	C32-C31-O31-C3
52	X	1701	CDL	C31-CA7-OA8-CA6
52	X	1701	CDL	C71-CB7-OB8-CB6
46	b	901	3PE	C22-C21-O21-C2
52	J	401	CDL	C11-CA5-OA6-CA4
52	h	1001	CDL	C51-CB5-OB6-CB4
46	d	1201	3PE	C32-C31-O31-C3
52	d	1202	CDL	C71-CB7-OB8-CB6
45	N	902	LMT	C3'-C4'-O1B-C1B
46	Y	401	3PE	O22-C21-O21-C2
46	d	1201	3PE	O22-C21-O21-C2
45	N	901	LMT	C4B-C5B-C6B-O6B
45	N	902	LMT	C4'-C5'-C6'-O6'
45	Y	402	LMT	C4'-C5'-C6'-O6'
46	Y	401	3PE	C32-C31-O31-C3
46	Y	401	3PE	O32-C31-O31-C3
45	e	201	LMT	C4B-C5B-C6B-O6B
45	f	1801	LMT	O5'-C5'-C6'-O6'
45	A	301	LMT	C4B-C5B-C6B-O6B
45	L	704	LMT	O5'-C5'-C6'-O6'
52	J	401	CDL	CB4-CB3-OB5-PB2
45	N	901	LMT	O5B-C5B-C6B-O6B
45	N	902	LMT	O5'-C5'-C6'-O6'
45	Y	402	LMT	O5'-C5'-C6'-O6'
45	e	201	LMT	O5'-C1'-O1'-C1
45	A	301	LMT	O5B-C5B-C6B-O6B
52	q	202	CDL	CA2-C1-CB2-OB2
46	N	903	3PE	C32-C31-O31-C3
52	L	702	CDL	C31-CA7-OA8-CA6
52	h	1001	CDL	C71-CB7-OB8-CB6
53	M	603	PC1	C32-C31-O31-C3
53	q	201	PC1	C32-C31-O31-C3
45	A	301	LMT	C2-C3-C4-C5
46	N	903	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	f	1801	LMT	C4'-C5'-C6'-O6'
52	X	1701	CDL	O1-C1-CB2-OB2
45	A	301	LMT	C2'-C1'-O1'-C1
45	L	704	LMT	C2'-C1'-O1'-C1
46	N	903	3PE	O21-C2-C3-O31
45	e	201	LMT	O5B-C5B-C6B-O6B
45	j	101	LMT	O5B-C1B-O1B-C4'
45	L	704	LMT	C4'-C5'-C6'-O6'
52	J	401	CDL	CA5-C11-C12-C13
52	h	1001	CDL	CB5-C51-C52-C53
52	h	1001	CDL	OB9-CB7-OB8-CB6
53	M	603	PC1	O32-C31-O31-C3
45	j	101	LMT	C2B-C1B-O1B-C4'
45	f	1801	LMT	C5'-C4'-O1B-C1B
52	X	1701	CDL	CB7-C71-C72-C73
45	f	1802	LMT	C4B-C5B-C6B-O6B
45	B	202	LMT	C3'-C4'-O1B-C1B
45	j	101	LMT	O5'-C5'-C6'-O6'
52	L	702	CDL	OA9-CA7-OA8-CA6
53	q	201	PC1	O32-C31-O31-C3
46	A	302	3PE	C31-C32-C33-C34
46	I	201	3PE	C21-C22-C23-C24
46	L	701	3PE	C31-C32-C33-C34
46	M	602	3PE	C31-C32-C33-C34
46	M	601	3PE	C21-C22-C23-C24
53	q	201	PC1	C31-C32-C33-C34
45	d	1203	LMT	C3'-C4'-O1B-C1B
52	J	401	CDL	CB7-C71-C72-C73
52	J	401	CDL	C31-CA7-OA8-CA6
45	h	1002	LMT	C4'-C5'-C6'-O6'
46	I	201	3PE	C11-O13-P-O11
46	Y	401	3PE	C1-O11-P-O13
46	b	901	3PE	C1-O11-P-O13
52	J	401	CDL	CA3-OA5-PA1-OA2
52	J	401	CDL	CB2-OB2-PB2-OB5
52	J	401	CDL	CB3-OB5-PB2-OB2
52	d	1202	CDL	CA3-OA5-PA1-OA2
52	q	202	CDL	CA2-OA2-PA1-OA5
45	e	201	LMT	O5'-C5'-C6'-O6'
52	L	702	CDL	C71-CB7-OB8-CB6
45	A	301	LMT	O5'-C5'-C6'-O6'
52	q	202	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
45	Y	402	LMT	C3-C4-C5-C6
52	L	702	CDL	C11-CA5-OA6-CA4
52	L	702	CDL	C51-CB5-OB6-CB4
46	L	701	3PE	C29-C2A-C2B-C2C
46	Y	401	3PE	C37-C38-C39-C3A
46	b	901	3PE	C28-C29-C2A-C2B
46	b	901	3PE	C2A-C2B-C2C-C2D
52	X	1701	CDL	C54-C55-C56-C57
52	h	1001	CDL	C72-C73-C74-C75
52	X	1701	CDL	C15-C16-C17-C18
46	b	901	3PE	C1-C2-O21-C21
52	L	702	CDL	OA7-CA5-OA6-CA4
52	L	702	CDL	OB7-CB5-OB6-CB4
46	L	701	3PE	C37-C38-C39-C3A
52	q	202	CDL	C57-C58-C59-C60
45	f	1802	LMT	C5'-C4'-O1B-C1B
46	M	602	3PE	C2B-C2C-C2D-C2E
46	N	903	3PE	C29-C2A-C2B-C2C
45	d	1203	LMT	C5'-C4'-O1B-C1B
46	I	201	3PE	C33-C34-C35-C36
45	f	1801	LMT	C3'-C4'-O1B-C1B
52	L	702	CDL	C55-C56-C57-C58
46	d	1201	3PE	C21-C22-C23-C24
46	I	201	3PE	C2C-C2D-C2E-C2F
46	L	703	3PE	C38-C39-C3A-C3B
59	o	201	MYR	C2-C3-C4-C5
52	L	702	CDL	OB9-CB7-OB8-CB6
52	h	1001	CDL	C22-C23-C24-C25
46	L	701	3PE	C22-C21-O21-C2
46	M	602	3PE	C26-C27-C28-C29
52	X	1701	CDL	C20-C21-C22-C23
46	L	703	3PE	C32-C33-C34-C35
46	N	903	3PE	C32-C33-C34-C35
46	d	1201	3PE	C33-C34-C35-C36
46	d	1201	3PE	C37-C38-C39-C3A
52	d	1202	CDL	C33-C34-C35-C36
45	L	704	LMT	O1'-C1-C2-C3
52	X	1701	CDL	C11-C12-C13-C14
52	q	202	CDL	C31-C32-C33-C34
52	q	202	CDL	C72-C73-C74-C75
53	M	603	PC1	C29-C2A-C2B-C2C
45	e	201	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
46	L	701	3PE	C34-C35-C36-C37
52	J	401	CDL	C16-C17-C18-C19
45	L	704	LMT	C5-C6-C7-C8
46	I	201	3PE	C23-C24-C25-C26
45	L	704	LMT	C2-C1-O1'-C1'
45	d	1203	LMT	C2-C1-O1'-C1'
45	h	1002	LMT	C2-C1-O1'-C1'
52	X	1701	CDL	CB5-C51-C52-C53
52	J	401	CDL	OA9-CA7-OA8-CA6
46	b	901	3PE	C26-C27-C28-C29
46	L	701	3PE	O22-C21-O21-C2
46	b	901	3PE	C37-C38-C39-C3A
45	N	902	LMT	C1-C2-C3-C4
52	h	1001	CDL	C11-CA5-OA6-CA4
46	M	602	3PE	C3D-C3E-C3F-C3G
52	q	202	CDL	C39-C40-C41-C42
45	f	1802	LMT	C3'-C4'-O1B-C1B
46	L	701	3PE	C22-C23-C24-C25
46	L	701	3PE	C2E-C2F-C2G-C2H
46	b	901	3PE	C3E-C3F-C3G-C3H
45	l	201	LMT	C4-C5-C6-C7
52	h	1001	CDL	C12-C13-C14-C15
52	h	1001	CDL	O1-C1-CB2-OB2
52	h	1001	CDL	C71-C72-C73-C74
52	q	202	CDL	C51-C52-C53-C54
52	q	202	CDL	OB9-CB7-OB8-CB6
52	J	401	CDL	C36-C37-C38-C39
52	h	1001	CDL	OA7-CA5-OA6-CA4
46	H	601	3PE	C3C-C3D-C3E-C3F
46	N	903	3PE	C23-C24-C25-C26
52	L	702	CDL	C34-C35-C36-C37
52	q	202	CDL	C11-C12-C13-C14
46	N	903	3PE	C21-C22-C23-C24
46	M	602	3PE	C3C-C3D-C3E-C3F
52	h	1001	CDL	C31-CA7-OA8-CA6
46	M	602	3PE	C23-C24-C25-C26
46	N	903	3PE	C33-C34-C35-C36
46	I	201	3PE	C3B-C3C-C3D-C3E
45	l	201	LMT	O1'-C1-C2-C3
59	o	201	MYR	C9-C10-C11-C12
51	N	904	I49	N04-C15-N02-C14
46	M	601	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
52	d	1202	CDL	CB7-C71-C72-C73
52	h	1001	CDL	C31-C32-C33-C34
46	M	602	3PE	C22-C21-O21-C2
45	e	201	LMT	C2B-C1B-O1B-C4'
58	T	101	EHZ	C1-C2-C3-C4
52	q	202	CDL	O1-C1-CA2-OA2
46	M	602	3PE	O22-C21-O21-C2
46	b	901	3PE	C2C-C2D-C2E-C2F
52	J	401	CDL	C12-C13-C14-C15
52	q	202	CDL	C59-C60-C61-C62
45	f	1801	LMT	O5B-C5B-C6B-O6B
46	A	302	3PE	C32-C33-C34-C35
52	X	1701	CDL	C74-C75-C76-C77
53	M	603	PC1	C2C-C2D-C2E-C2F
52	h	1001	CDL	OA9-CA7-OA8-CA6
46	N	903	3PE	C22-C21-O21-C2
46	M	601	3PE	C37-C38-C39-C3A
52	X	1701	CDL	CA2-OA2-PA1-OA5
52	d	1202	CDL	CB2-OB2-PB2-OB5
52	q	202	CDL	CB3-OB5-PB2-OB2
58	T	101	EHZ	C3-C4-C5-C6
52	q	202	CDL	C1-CA2-OA2-PA1
58	U	101	EHZ	C1-C21-C22-C23
46	L	703	3PE	O11-C1-C2-C3
52	X	1701	CDL	OA5-CA3-CA4-CA6
52	d	1202	CDL	OA5-CA3-CA4-CA6
52	q	202	CDL	OA5-CA3-CA4-CA6
51	H	602	I49	N05-C15-N02-C14
45	Y	402	LMT	C2-C3-C4-C5
46	M	602	3PE	C3A-C3B-C3C-C3D
45	e	201	LMT	O5B-C1B-O1B-C4'
52	h	1001	CDL	CA2-C1-CB2-OB2
46	M	601	3PE	C36-C37-C38-C39
45	L	704	LMT	C6-C7-C8-C9
46	A	302	3PE	C1-C2-C3-O31
46	L	701	3PE	C1-C2-C3-O31
46	Y	401	3PE	C1-C2-C3-O31
46	b	901	3PE	C35-C36-C37-C38
46	d	1201	3PE	C1-C2-C3-O31
52	J	401	CDL	CA3-CA4-CA6-OA8
52	L	702	CDL	CA3-CA4-CA6-OA8
53	M	603	PC1	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
53	q	201	PC1	C1-C2-C3-O31
45	L	704	LMT	O5'-C1'-O1'-C1
52	q	202	CDL	C35-C36-C37-C38
46	M	601	3PE	C22-C21-O21-C2
58	U	101	EHZ	C1-C2-C3-C4
45	B	202	LMT	O5'-C5'-C6'-O6'
46	Y	401	3PE	C31-C32-C33-C34
45	N	902	LMT	O5B-C5B-C6B-O6B
45	B	202	LMT	C5'-C4'-O1B-C1B
46	d	1201	3PE	C35-C36-C37-C38
45	h	1002	LMT	C4B-C5B-C6B-O6B
46	I	201	3PE	C37-C38-C39-C3A
46	L	703	3PE	C25-C26-C27-C28
53	M	603	PC1	C2E-C2F-C2G-C2H
46	M	601	3PE	C28-C29-C2A-C2B
52	X	1701	CDL	C57-C58-C59-C60
46	L	703	3PE	O11-C1-C2-O21
46	M	602	3PE	O11-C1-C2-O21
46	M	601	3PE	C2A-C2B-C2C-C2D
46	H	601	3PE	C3E-C3F-C3G-C3H
58	T	101	EHZ	C1-C21-C22-C23
52	L	702	CDL	OB6-CB4-CB6-OB8
53	M	603	PC1	O21-C2-C3-O31
46	I	201	3PE	C32-C31-O31-C3
45	f	1802	LMT	O5B-C5B-C6B-O6B
46	I	201	3PE	C27-C28-C29-C2A
46	b	901	3PE	C39-C3A-C3B-C3C
52	J	401	CDL	C39-C40-C41-C42
46	H	601	3PE	C35-C36-C37-C38
46	L	701	3PE	C2A-C2B-C2C-C2D
52	J	401	CDL	C19-C20-C21-C22
46	A	302	3PE	C24-C25-C26-C27
46	H	601	3PE	C37-C38-C39-C3A
52	X	1701	CDL	C75-C76-C77-C78
54	O	401	GTP	PG-O3B-PB-O1B
46	L	701	3PE	C38-C39-C3A-C3B
58	T	101	EHZ	C5-C6-C7-C8
52	X	1701	CDL	CB2-C1-CA2-OA2
46	M	601	3PE	O11-C1-C2-C3
46	Y	401	3PE	O11-C1-C2-C3
52	q	202	CDL	C37-C38-C39-C40
52	X	1701	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
46	N	903	3PE	O22-C21-O21-C2
45	f	1802	LMT	C1-C2-C3-C4
53	M	603	PC1	C23-C24-C25-C26
46	L	701	3PE	C36-C37-C38-C39
46	b	901	3PE	C27-C28-C29-C2A
53	M	603	PC1	C2-C1-O11-P
45	j	101	LMT	O5B-C5B-C6B-O6B
52	q	202	CDL	C15-C16-C17-C18
46	N	903	3PE	C1-C2-C3-O31
46	b	901	3PE	C1-C2-C3-O31
52	h	1001	CDL	CB3-CB4-CB6-OB8
52	q	202	CDL	CA3-CA4-CA6-OA8
45	A	301	LMT	O1'-C1-C2-C3
52	h	1001	CDL	C15-C16-C17-C18
46	Y	401	3PE	C11-O13-P-O11
52	L	702	CDL	CB3-OB5-PB2-OB2
52	X	1701	CDL	OB5-CB3-CB4-OB6
52	d	1202	CDL	OA5-CA3-CA4-OA6
52	q	202	CDL	OA5-CA3-CA4-OA6
46	A	302	3PE	C39-C3A-C3B-C3C
52	L	702	CDL	CB5-C51-C52-C53
56	P	501	NDP	O4D-C4D-C5D-O5D
46	I	201	3PE	O32-C31-O31-C3
52	X	1701	CDL	C60-C61-C62-C63
45	f	1801	LMT	O5B-C1B-O1B-C4'
46	A	302	3PE	O21-C2-C3-O31
46	L	703	3PE	O21-C2-C3-O31
46	M	601	3PE	O21-C2-C3-O31
46	Y	401	3PE	O21-C2-C3-O31
46	d	1201	3PE	O21-C2-C3-O31
52	q	202	CDL	OB6-CB4-CB6-OB8
53	q	201	PC1	O21-C2-C3-O31
46	I	201	3PE	C2B-C2C-C2D-C2E
46	M	601	3PE	O22-C21-O21-C2
46	d	1201	3PE	C38-C39-C3A-C3B
46	H	601	3PE	C2-C1-O11-P
52	L	702	CDL	CA4-CA3-OA5-PA1
52	d	1202	CDL	CA5-C11-C12-C13
52	J	401	CDL	C54-C55-C56-C57
46	L	701	3PE	C21-C22-C23-C24
46	M	602	3PE	O11-C1-C2-C3
52	X	1701	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
46	L	701	3PE	C24-C25-C26-C27
59	o	201	MYR	C11-C12-C13-C14
52	X	1701	CDL	C53-C54-C55-C56
52	X	1701	CDL	C52-C53-C54-C55
52	d	1202	CDL	C31-C32-C33-C34
46	M	601	3PE	C3-C2-O21-C21
46	d	1201	3PE	C3A-C3B-C3C-C3D
52	h	1001	CDL	C73-C74-C75-C76
52	q	202	CDL	C56-C57-C58-C59
46	I	201	3PE	C32-C33-C34-C35
52	q	202	CDL	C38-C39-C40-C41
53	q	201	PC1	C22-C23-C24-C25
46	M	601	3PE	C1-C2-C3-O31
51	N	904	I49	N01-C14-N02-C15
52	L	702	CDL	CB3-CB4-CB6-OB8
52	q	202	CDL	CB3-CB4-CB6-OB8
46	M	601	3PE	O11-C1-C2-O21
46	L	703	3PE	C3C-C3D-C3E-C3F
58	T	101	EHZ	O1-C7-C8-C9
46	I	201	3PE	C26-C27-C28-C29
46	L	701	3PE	O21-C2-C3-O31
52	J	401	CDL	OA6-CA4-CA6-OA8
52	h	1001	CDL	OB6-CB4-CB6-OB8
52	h	1001	CDL	C17-C18-C19-C20
56	P	501	NDP	C2B-O2B-P2B-O3X
53	M	603	PC1	C31-C32-C33-C34
54	O	401	GTP	PB-O3A-PA-O1A
56	P	501	NDP	PN-O3-PA-O1A
52	X	1701	CDL	C52-C51-CB5-OB6
45	N	902	LMT	C5'-C4'-O1B-C1B
52	J	401	CDL	C71-CB7-OB8-CB6
52	L	702	CDL	CA2-OA2-PA1-OA5
46	A	302	3PE	C35-C36-C37-C38
52	X	1701	CDL	CB4-CB3-OB5-PB2
52	q	202	CDL	CA4-CA3-OA5-PA1
46	H	601	3PE	C11-O13-P-O14
46	I	201	3PE	C11-O13-P-O12
46	I	201	3PE	C11-O13-P-O14
46	M	601	3PE	C1-O11-P-O12
46	Y	401	3PE	C1-O11-P-O12
46	Y	401	3PE	C11-O13-P-O12
52	J	401	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
52	X	1701	CDL	CA2-OA2-PA1-OA4
52	X	1701	CDL	CA3-OA5-PA1-OA3
52	d	1202	CDL	CA3-OA5-PA1-OA3
52	d	1202	CDL	CB2-OB2-PB2-OB4
52	q	202	CDL	CA3-OA5-PA1-OA3
52	q	202	CDL	CB2-OB2-PB2-OB3
54	O	401	GTP	C5'-O5'-PA-O1A
58	T	101	EHZ	C6-C7-C8-C9
45	B	202	LMT	C7-C8-C9-C10
52	L	702	CDL	OB5-CB3-CB4-CB6
59	o	201	MYR	C7-C8-C9-C10
45	B	202	LMT	C3-C4-C5-C6
52	L	702	CDL	C38-C39-C40-C41
46	A	302	3PE	C12-C11-O13-P
46	M	602	3PE	C12-C11-O13-P
52	d	1202	CDL	CA2-C1-CB2-OB2
46	Y	401	3PE	O11-C1-C2-O21
52	d	1202	CDL	C52-C51-CB5-OB6
52	d	1202	CDL	O1-C1-CB2-OB2
46	b	901	3PE	C34-C35-C36-C37
52	L	702	CDL	C33-C34-C35-C36
52	q	202	CDL	C54-C55-C56-C57
53	M	603	PC1	C1-C2-C3-O31
52	L	702	CDL	OA6-CA4-CA6-OA8
52	q	202	CDL	OA6-CA4-CA6-OA8
45	B	202	LMT	C5-C6-C7-C8
46	L	703	3PE	C2-C1-O11-P
52	L	702	CDL	C54-C55-C56-C57
46	N	903	3PE	O31-C31-C32-C33
52	J	401	CDL	OB9-CB7-OB8-CB6
46	L	703	3PE	O21-C21-C22-C23
45	d	1203	LMT	C9-C10-C11-C12
58	T	101	EHZ	C5-C6-C7-O1
52	q	202	CDL	C17-C18-C19-C20
45	h	1002	LMT	O5'-C5'-C6'-O6'
46	b	901	3PE	C21-C22-C23-C24
46	I	201	3PE	C25-C26-C27-C28
52	L	702	CDL	C14-C15-C16-C17
46	Y	401	3PE	C32-C33-C34-C35
46	L	701	3PE	C2C-C2D-C2E-C2F
52	X	1701	CDL	OA5-CA3-CA4-OA6
45	d	1203	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
52	X	1701	CDL	CA3-OA5-PA1-OA2
46	L	703	3PE	C1-C2-C3-O31
58	U	101	EHZ	C2-C3-C4-C5
52	d	1202	CDL	C38-C39-C40-C41
56	P	501	NDP	PN-O3-PA-O2A
45	f	1801	LMT	C2B-C1B-O1B-C4'
46	d	1201	3PE	C2-C1-O11-P
49	F	501	FMN	C4'-C5'-O5'-P
45	j	101	LMT	C4'-C5'-C6'-O6'
46	M	601	3PE	C3A-C3B-C3C-C3D
45	L	704	LMT	C9-C10-C11-C12
46	M	601	3PE	C23-C24-C25-C26
46	M	602	3PE	C35-C36-C37-C38
52	L	702	CDL	C56-C57-C58-C59
56	P	501	NDP	O4D-C1D-N1N-C6N
52	q	202	CDL	OB5-CB3-CB4-OB6
52	J	401	CDL	O1-C1-CB2-OB2
46	H	601	3PE	C3D-C3E-C3F-C3G
52	d	1202	CDL	C52-C51-CB5-OB7
53	q	201	PC1	C2-C1-O11-P
52	L	702	CDL	C31-C32-C33-C34
46	I	201	3PE	O22-C21-O21-C2
56	P	501	NDP	C2D-C1D-N1N-C6N
46	M	602	3PE	C33-C34-C35-C36
46	b	901	3PE	C22-C23-C24-C25
56	P	501	NDP	O4B-C4B-C5B-O5B
46	L	703	3PE	C36-C37-C38-C39
46	Y	401	3PE	C39-C3A-C3B-C3C
52	d	1202	CDL	C77-C78-C79-C80
45	Y	402	LMT	C3'-C4'-O1B-C1B
46	H	601	3PE	C3A-C3B-C3C-C3D
52	h	1001	CDL	C16-C17-C18-C19
58	U	101	EHZ	C21-C1-C2-C3
46	M	601	3PE	C1-O11-P-O13
52	h	1001	CDL	C52-C53-C54-C55
46	M	601	3PE	C25-C26-C27-C28
46	L	701	3PE	C32-C31-O31-C3
45	Y	402	LMT	C11-C10-C9-C8
46	L	703	3PE	C3E-C3F-C3G-C3H
46	L	703	3PE	C22-C23-C24-C25
46	Y	401	3PE	C3B-C3C-C3D-C3E
52	h	1001	CDL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
53	q	201	PC1	C24-C25-C26-C27
45	h	1002	LMT	C11-C10-C9-C8
45	j	101	LMT	C2'-C1'-O1'-C1
58	T	101	EHZ	C11-C10-S1-C9
58	U	101	EHZ	C5-C6-C7-O1
46	N	903	3PE	C26-C27-C28-C29
45	N	902	LMT	O5'-C1'-O1'-C1
51	H	602	I49	C08-C06-C07-C09
46	b	901	3PE	C23-C24-C25-C26
46	L	701	3PE	O32-C31-O31-C3
52	h	1001	CDL	C32-C33-C34-C35
46	d	1201	3PE	C31-C32-C33-C34
46	L	703	3PE	C35-C36-C37-C38
51	H	602	I49	C08-C06-C07-C10
46	b	901	3PE	C32-C33-C34-C35
45	Y	402	LMT	C5'-C4'-O1B-C1B
46	M	601	3PE	C26-C27-C28-C29
52	J	401	CDL	C52-C53-C54-C55
45	Y	402	LMT	C1-C2-C3-C4
46	I	201	3PE	C22-C21-O21-C2
46	N	903	3PE	C22-C23-C24-C25
52	L	702	CDL	C35-C36-C37-C38
52	J	401	CDL	C53-C54-C55-C56
52	L	702	CDL	C53-C54-C55-C56
46	H	601	3PE	C36-C37-C38-C39
46	d	1201	3PE	C39-C3A-C3B-C3C
52	J	401	CDL	C33-C34-C35-C36
45	A	301	LMT	C4'-C5'-C6'-O6'
46	Y	401	3PE	C23-C24-C25-C26
46	b	901	3PE	C2B-C2C-C2D-C2E
46	d	1201	3PE	C32-C33-C34-C35
52	q	202	CDL	C52-C53-C54-C55
46	L	701	3PE	O21-C21-C22-C23
45	l	201	LMT	C5-C6-C7-C8
45	A	301	LMT	O5'-C1'-O1'-C1
46	N	903	3PE	O21-C21-C22-C23
46	L	703	3PE	C28-C29-C2A-C2B
51	H	602	I49	N01-C14-N02-C15
45	h	1002	LMT	O5B-C5B-C6B-O6B
52	d	1202	CDL	C72-C71-CB7-OB8
52	q	202	CDL	C52-C51-CB5-OB6
46	H	601	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
52	L	702	CDL	C71-C72-C73-C74
46	N	903	3PE	O11-C1-C2-C3
46	b	901	3PE	O21-C21-C22-C23
46	d	1201	3PE	O21-C21-C22-C23
45	l	201	LMT	C1-C2-C3-C4
53	M	603	PC1	O31-C31-C32-C33
46	I	201	3PE	C3A-C3B-C3C-C3D
45	h	1002	LMT	O5'-C1'-O1'-C1
52	X	1701	CDL	C32-C31-CA7-OA8
52	X	1701	CDL	CA5-C11-C12-C13
45	f	1801	LMT	C5-C6-C7-C8
46	M	602	3PE	C36-C37-C38-C39
46	M	602	3PE	C27-C28-C29-C2A
52	h	1001	CDL	C51-C52-C53-C54
51	H	602	I49	N03-C14-N02-C15
51	N	904	I49	N03-C14-N02-C15
52	d	1202	CDL	C72-C71-CB7-OB9
52	d	1202	CDL	C32-C33-C34-C35
58	T	101	EHZ	C22-C23-C24-C25
52	q	202	CDL	CB2-OB2-PB2-OB5
52	X	1701	CDL	C32-C31-CA7-OA9
46	L	701	3PE	O22-C21-C22-C23
46	M	602	3PE	C1-O11-P-O14
52	J	401	CDL	CA3-OA5-PA1-OA4
52	L	702	CDL	CA2-OA2-PA1-OA3
52	L	702	CDL	CB3-OB5-PB2-OB4
52	X	1701	CDL	CA2-OA2-PA1-OA3
56	P	501	NDP	C3D-C4D-C5D-O5D
46	N	903	3PE	O22-C21-C22-C23
46	b	901	3PE	O22-C21-C22-C23
58	U	101	EHZ	C3-C4-C5-C6
46	M	601	3PE	C12-C11-O13-P
52	q	202	CDL	C52-C51-CB5-OB7
46	b	901	3PE	O31-C31-C32-C33
53	q	201	PC1	O21-C21-C22-C23
46	d	1201	3PE	O22-C21-C22-C23
46	H	601	3PE	O11-C1-C2-O21
49	F	501	FMN	N10-C1'-C2'-O2'
46	A	302	3PE	O31-C31-C32-C33
46	A	302	3PE	O21-C21-C22-C23
53	M	603	PC1	O32-C31-C32-C33
45	B	202	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
52	d	1202	CDL	C71-C72-C73-C74
46	N	903	3PE	C28-C29-C2A-C2B

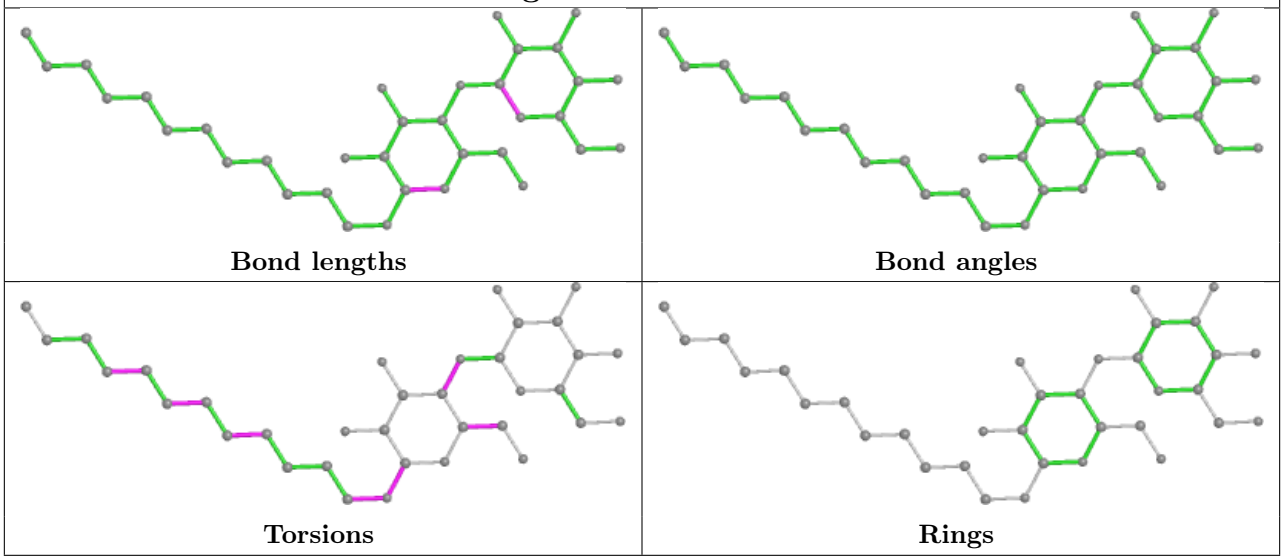
There are no ring outliers.

15 monomers are involved in 22 short contacts:

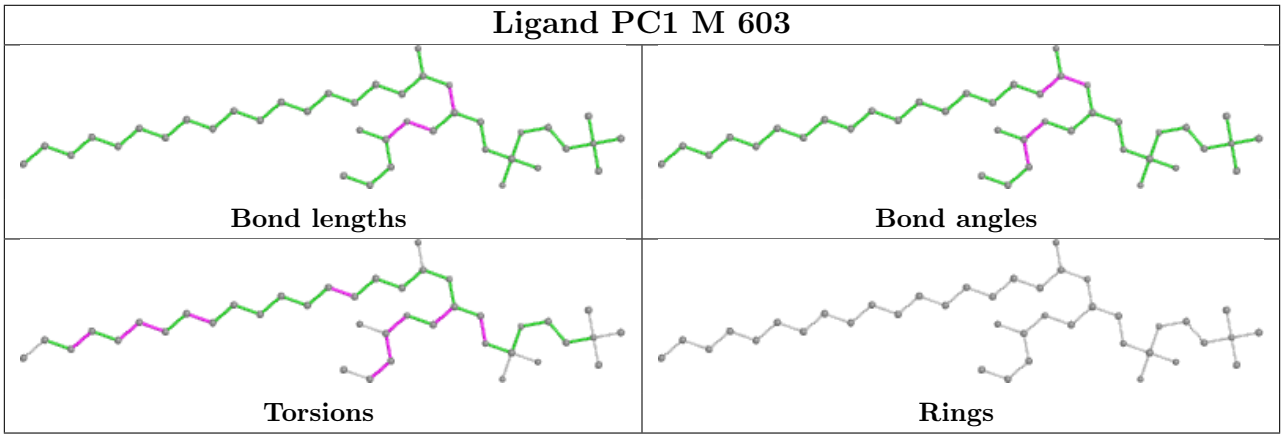
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	B	202	LMT	2	0
53	M	603	PC1	1	0
46	A	302	3PE	1	0
54	O	401	GTP	2	0
46	L	701	3PE	1	0
49	F	501	FMN	2	0
45	N	902	LMT	2	0
56	P	501	NDP	2	0
51	H	602	I49	3	0
46	M	602	3PE	1	0
47	F	502	SF4	1	0
47	I	203	SF4	1	0
51	N	904	I49	1	0
52	X	1701	CDL	1	0
58	T	101	EHZ	1	0

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.

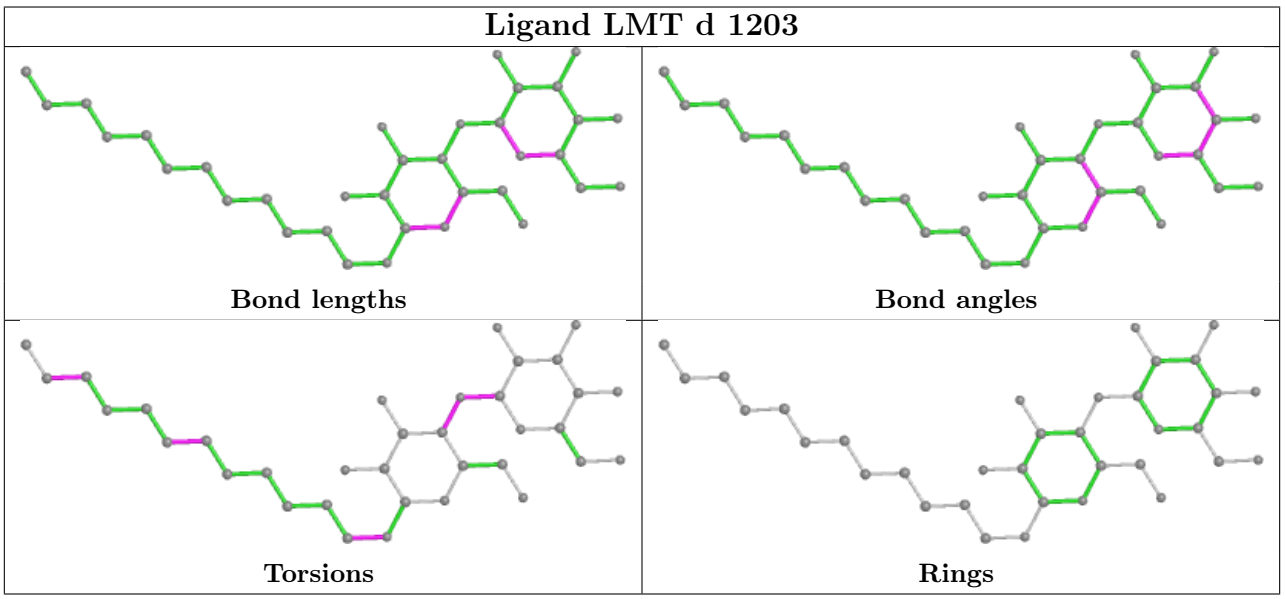
Ligand LMT B 202

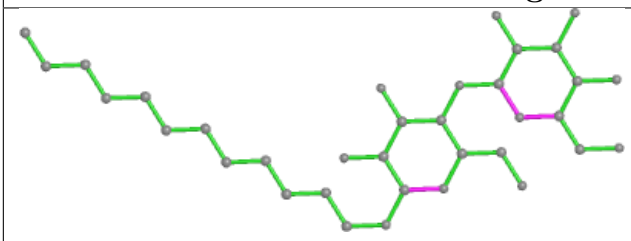
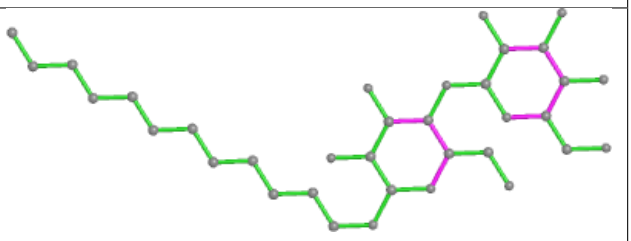
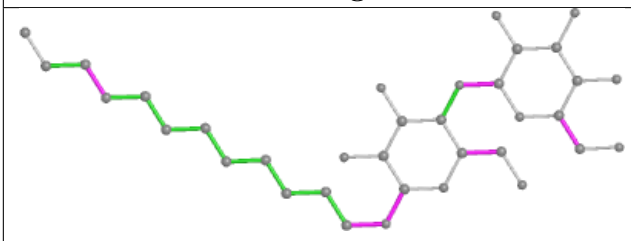
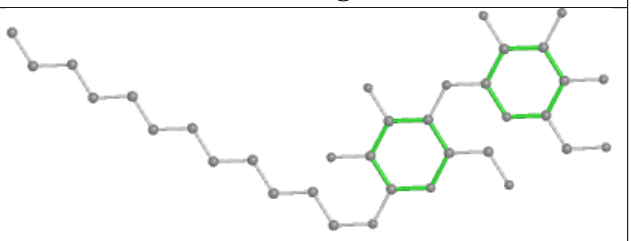


Ligand PC1 M 603



Ligand LMT d 1203



Ligand LMT e 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

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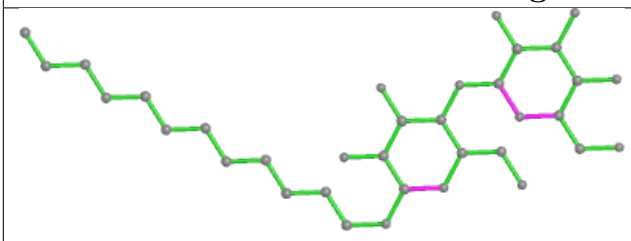
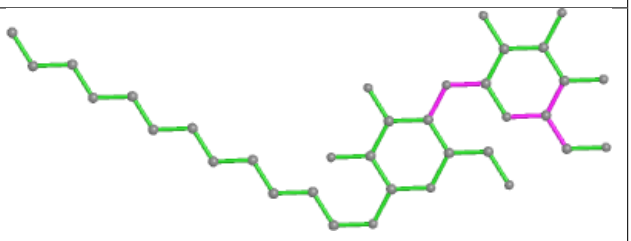
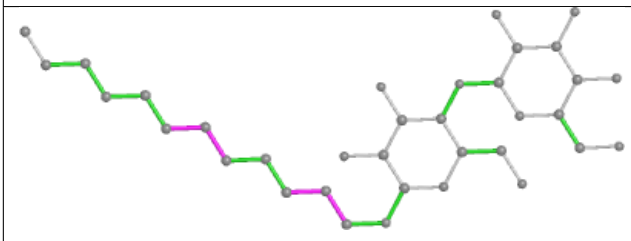
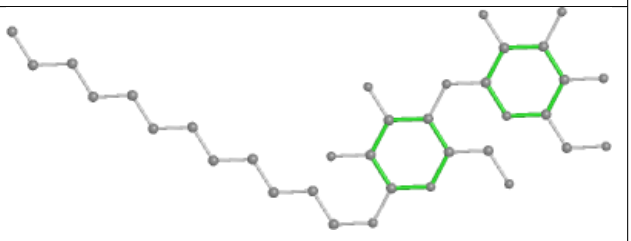
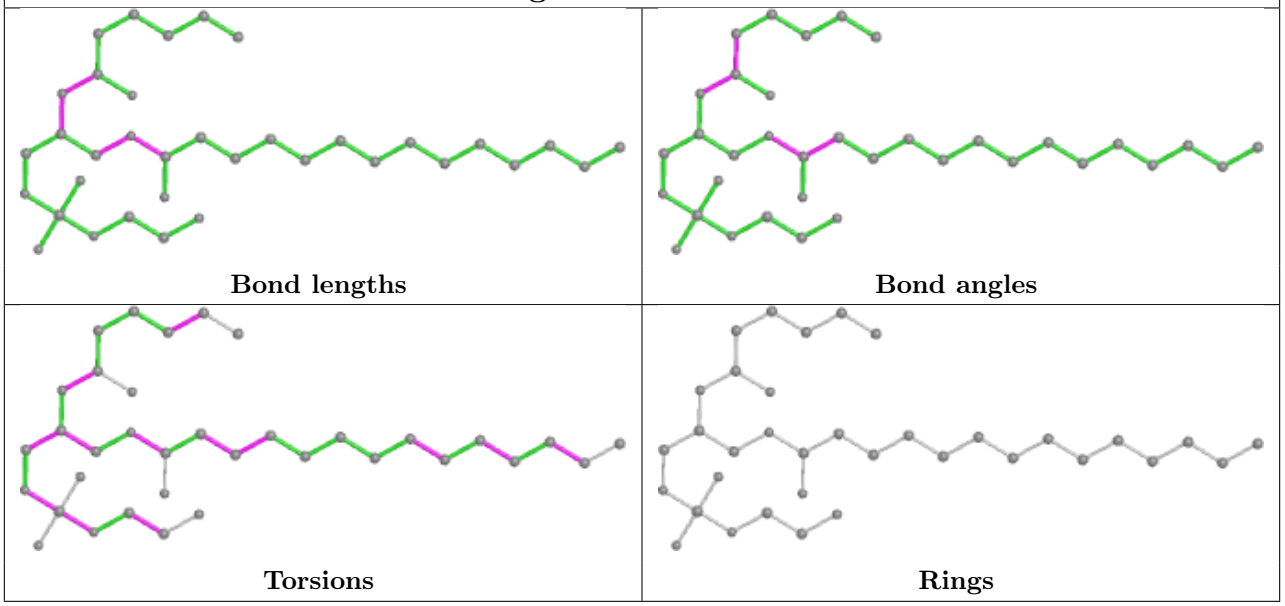
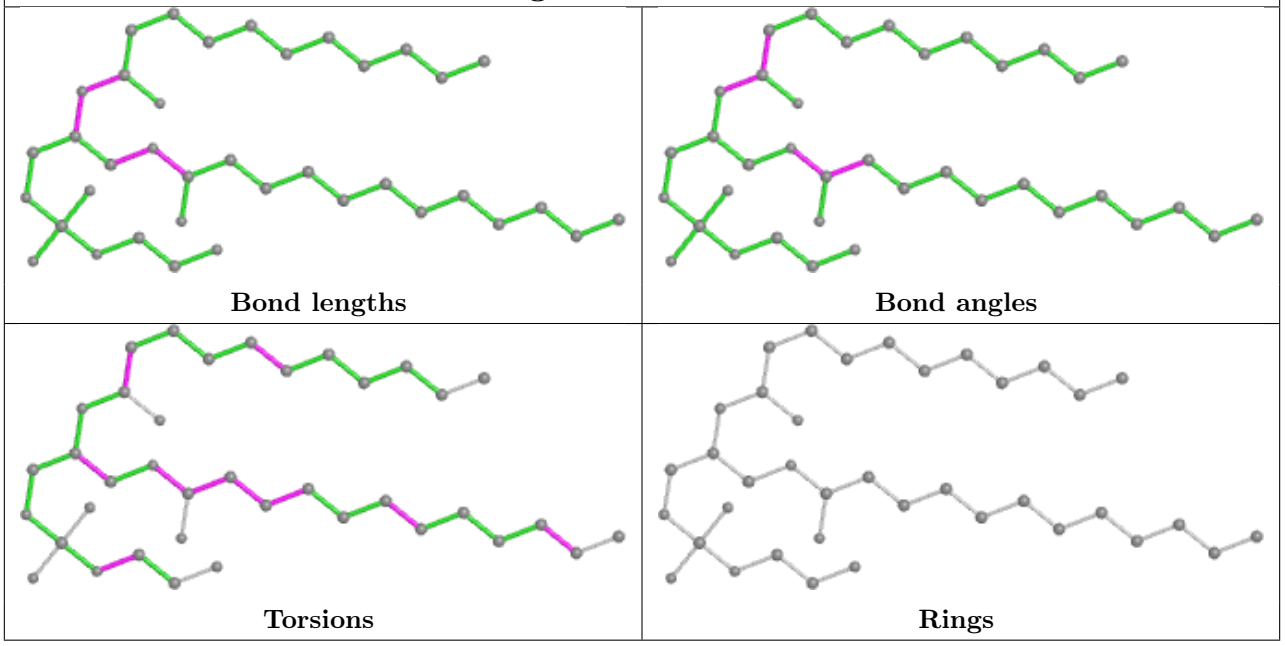
 Bond lengths	 Bond angles
 Torsions	 Rings

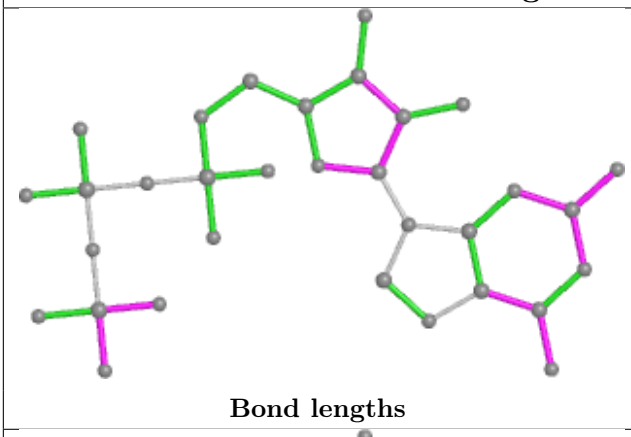
Ligand 3PE Y 401



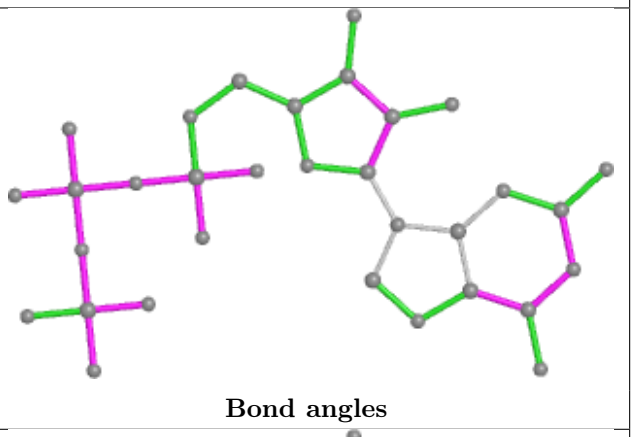
Ligand 3PE A 302



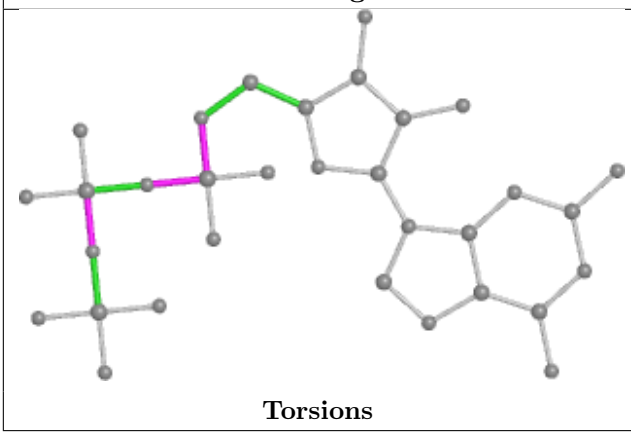
Ligand GTP O 401



Bond lengths



Bond angles



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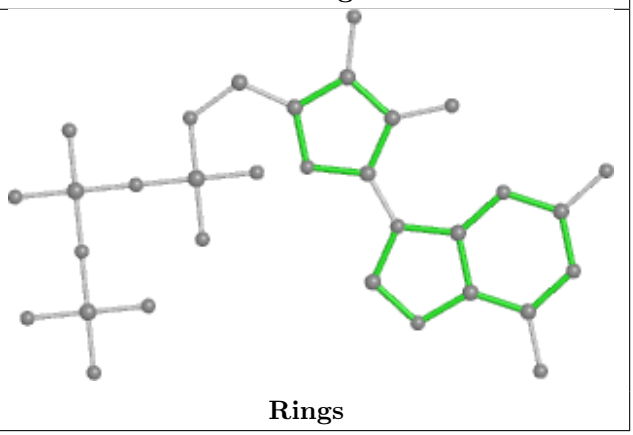
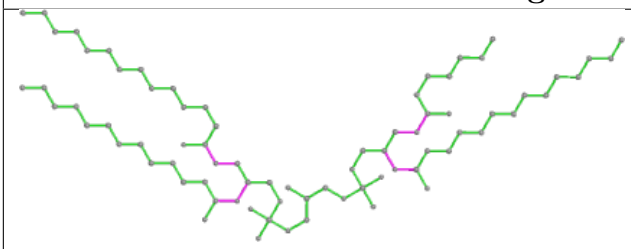


Rings

Ligand CDL q 202



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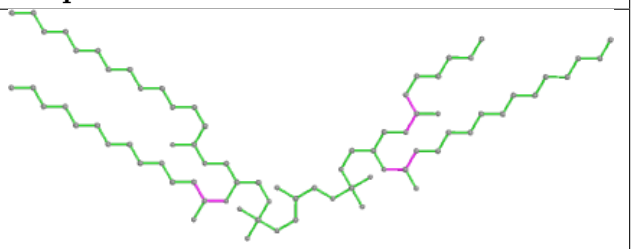
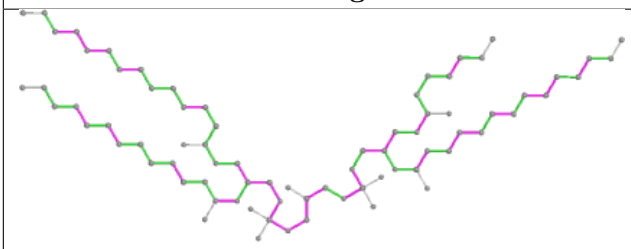


Bond angles



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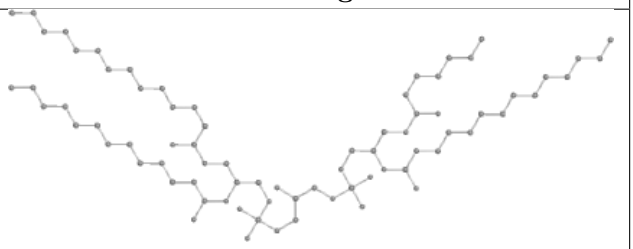
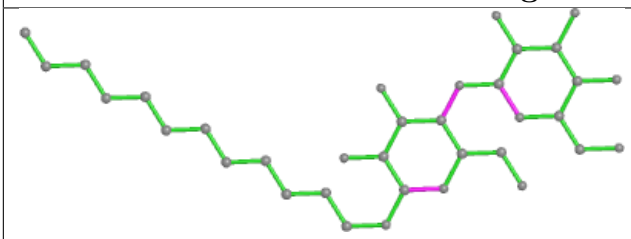


Rings

Ligand LMT A 301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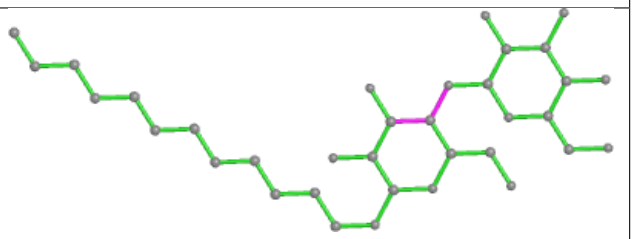
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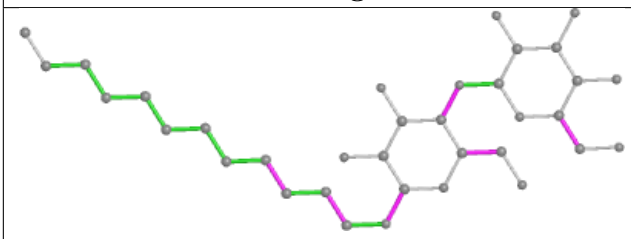
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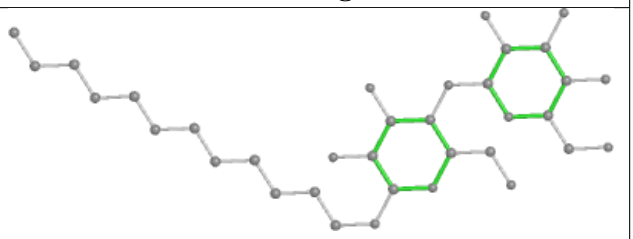
Rings

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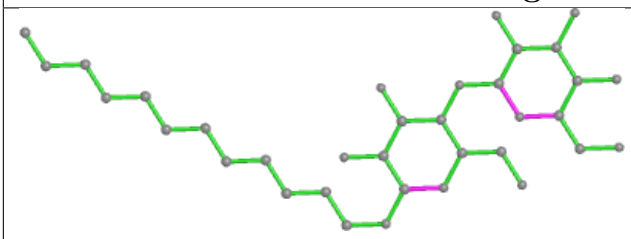
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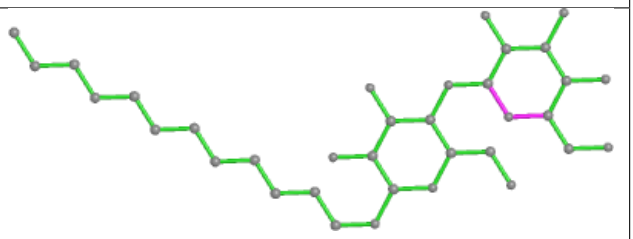
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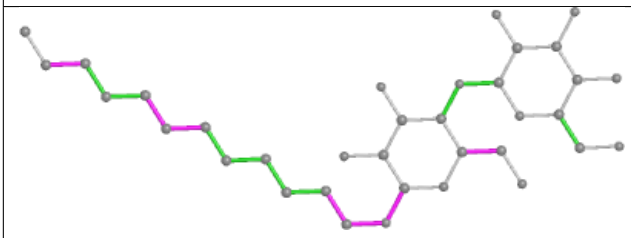
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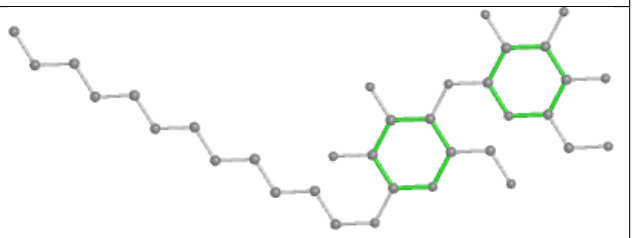
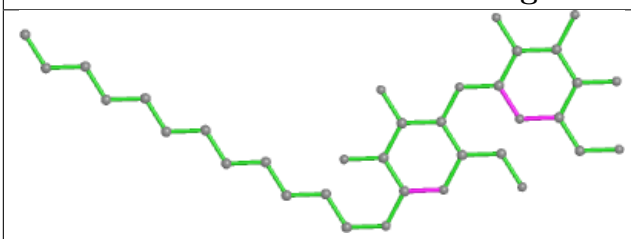

Rings

Ligand LMT N 901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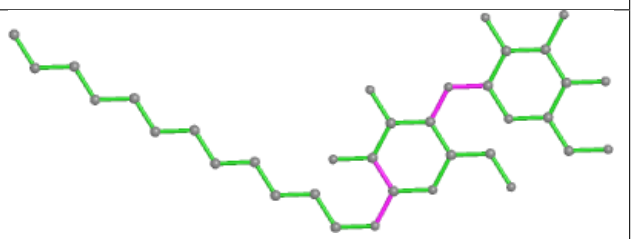
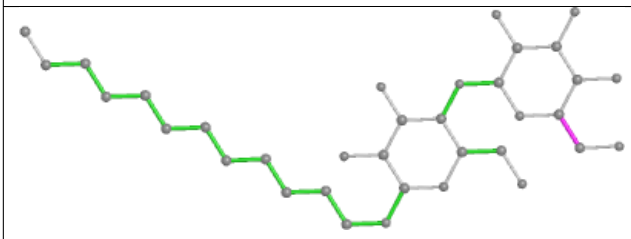

Bond angles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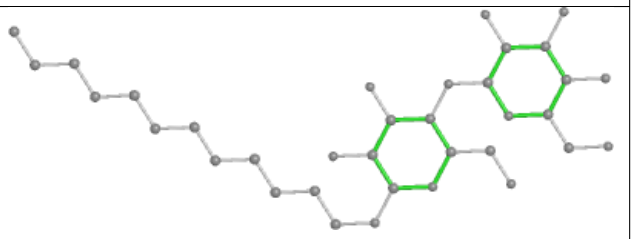
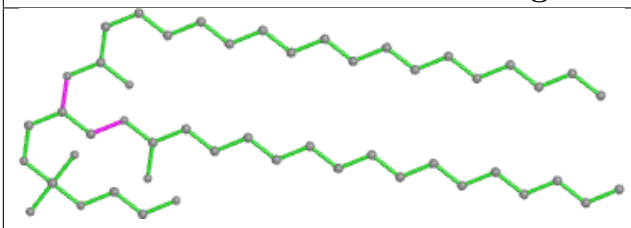

Rings

Ligand 3PE L 701



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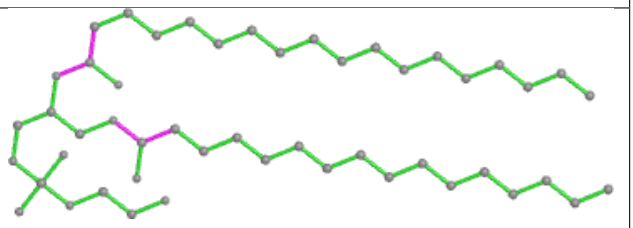
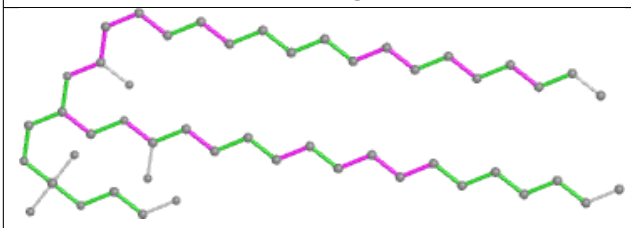


Bond angles



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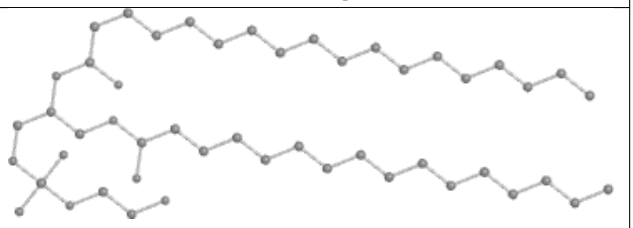
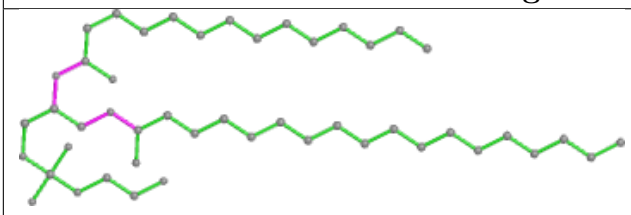


Rings

Ligand 3PE d 1201



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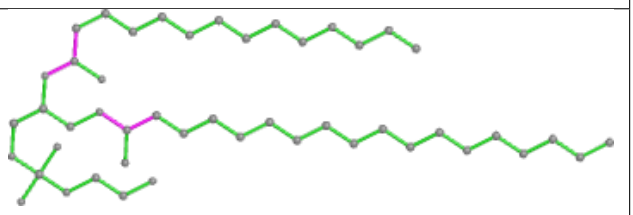
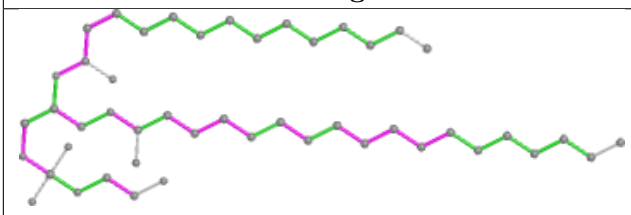


Bond angles



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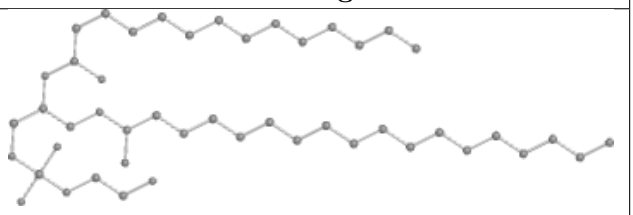
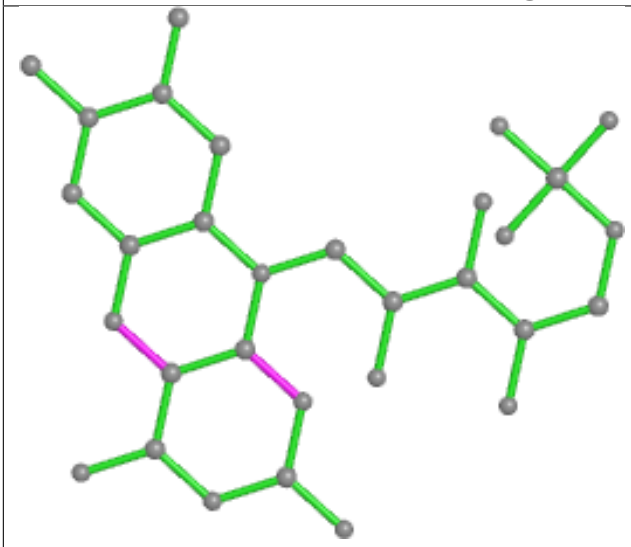
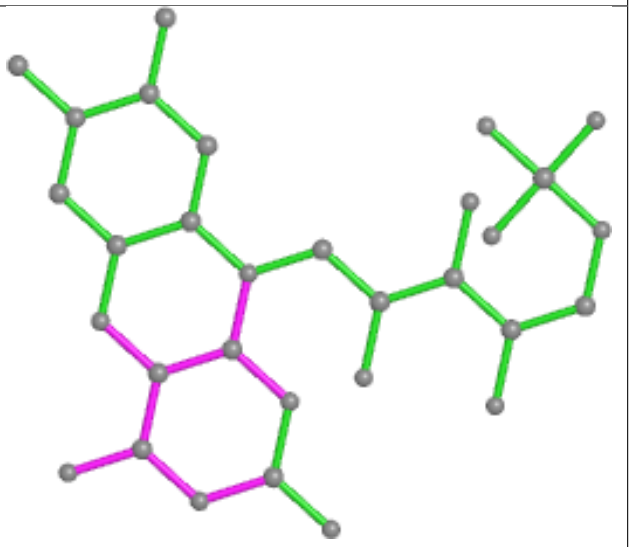


Rings

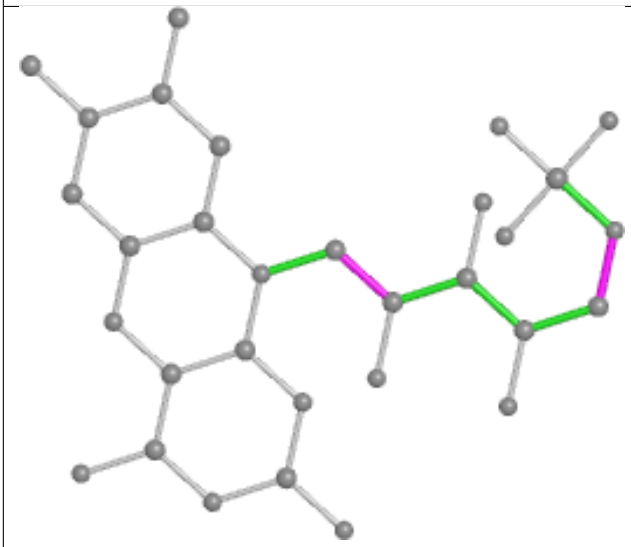
Ligand FMN F 501



Bond lengths



Bond angles



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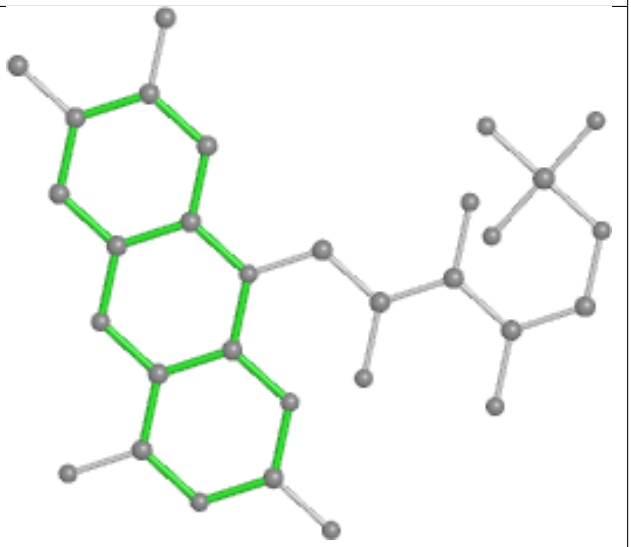
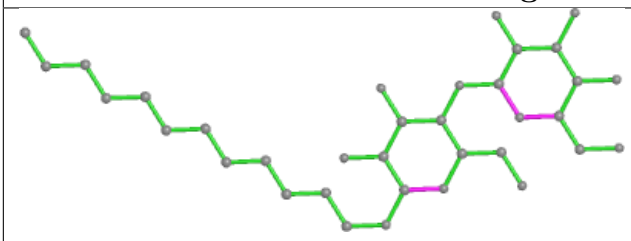
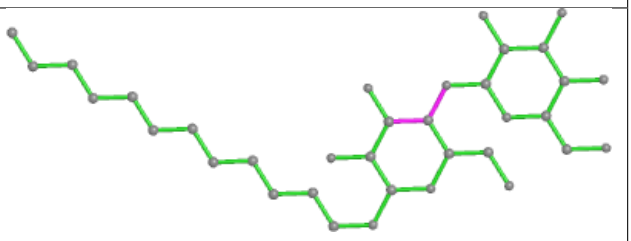
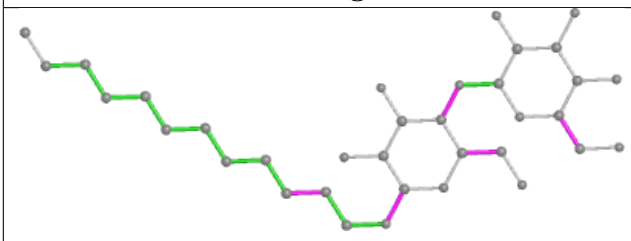
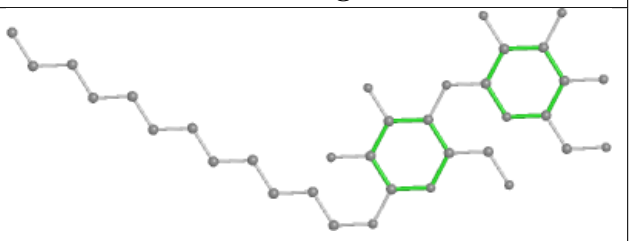
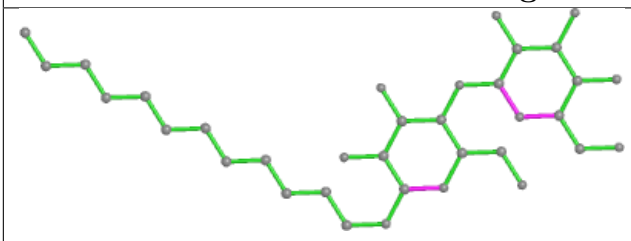
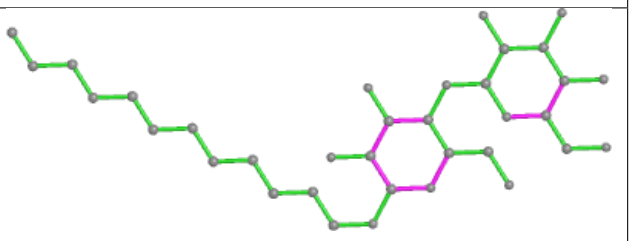
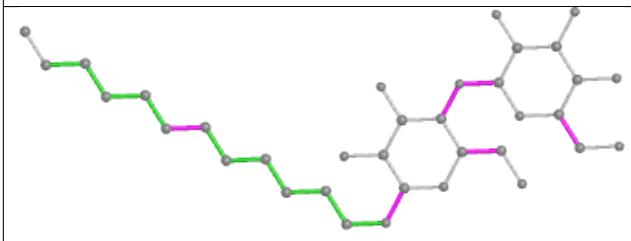
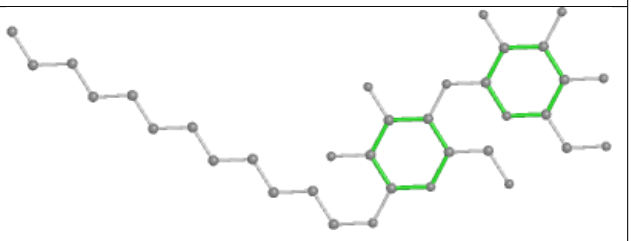
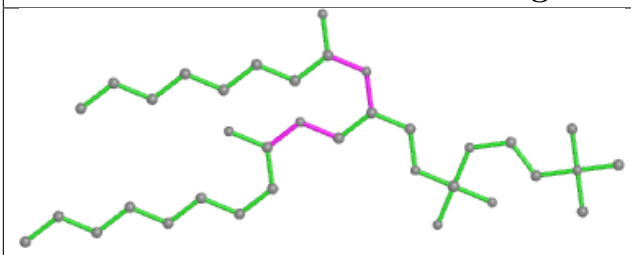


Rings

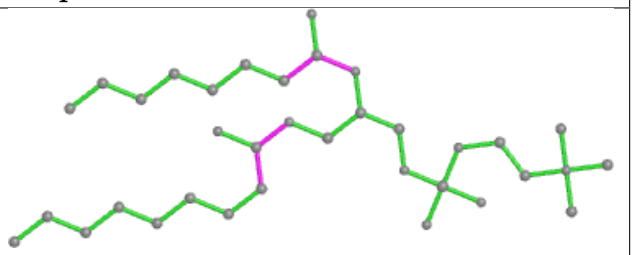
Ligand LMT N 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT f 1801	
 Bond lengths	 Bond angles
 Torsions	 Rings

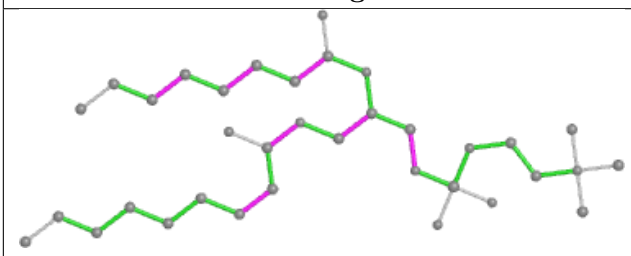
Ligand PC1 q 201



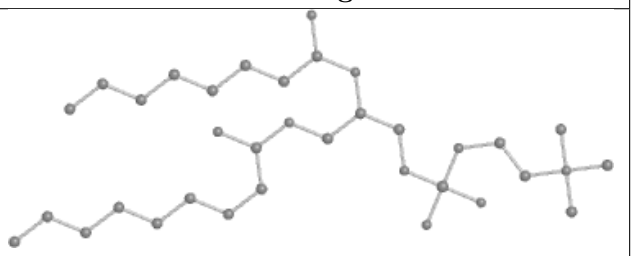
Bond lengths



Bond angles

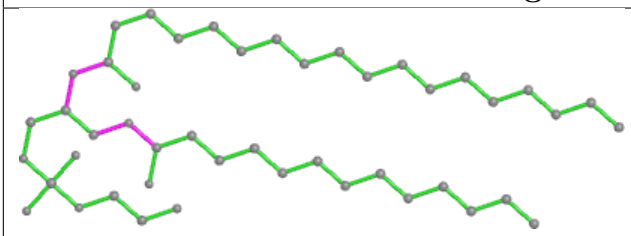


Torsions

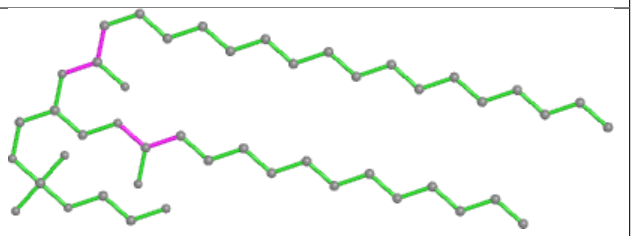


Rings

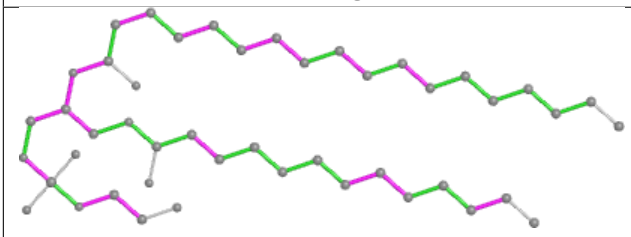
Ligand 3PE M 601



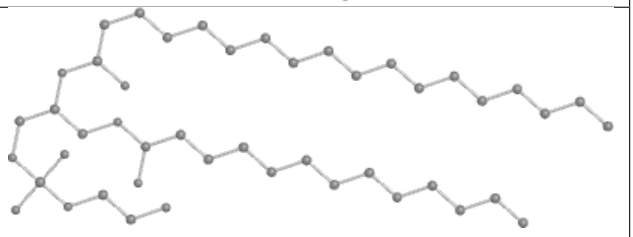
Bond lengths



Bond angles

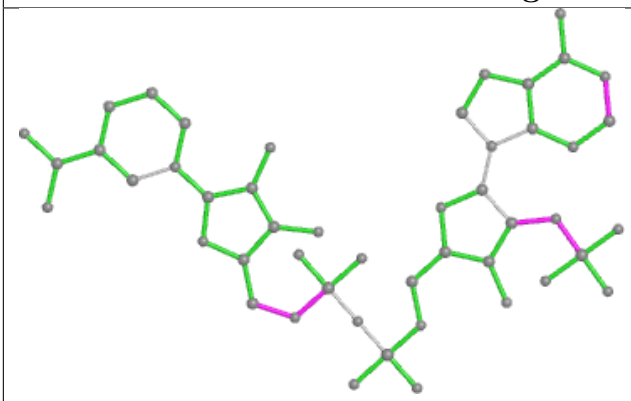


Torsions

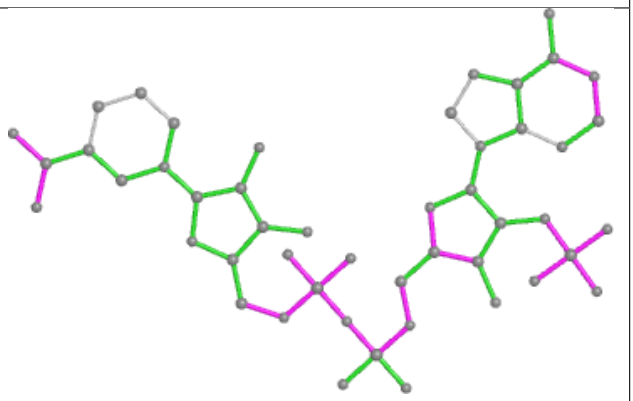


Rings

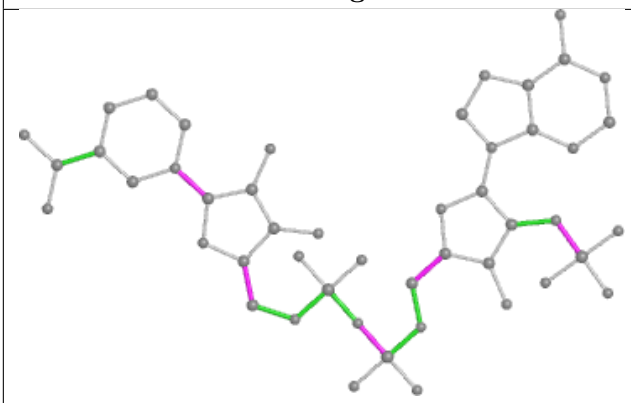
Ligand NDP P 501



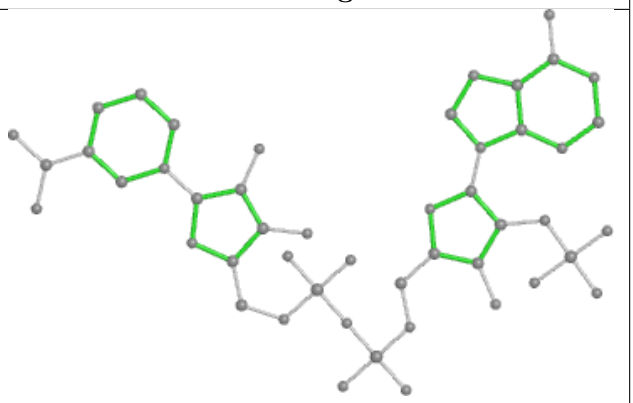
Bond lengths



Bond angles

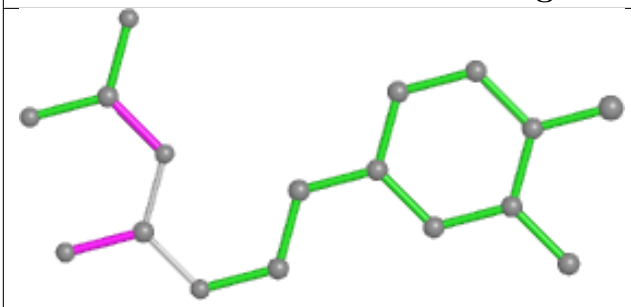


Torsions

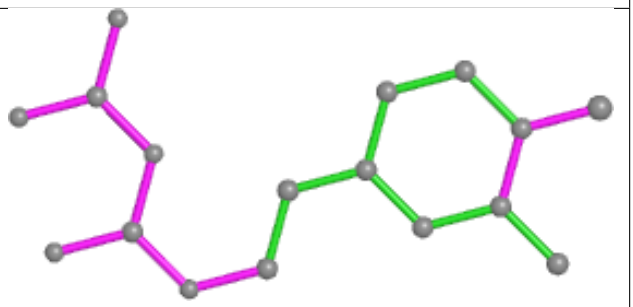


Rings

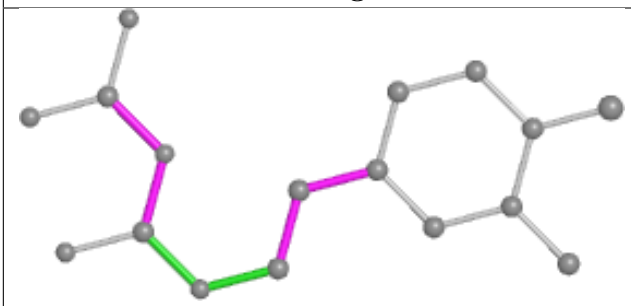
Ligand I49 H 602



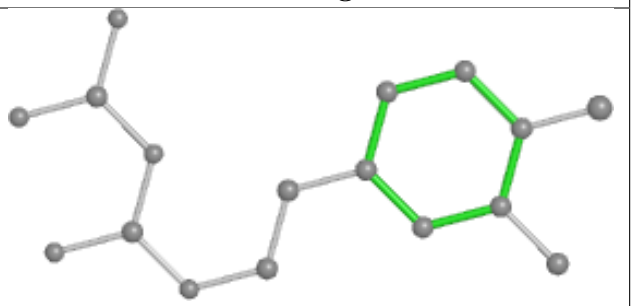
Bond lengths



Bond angles

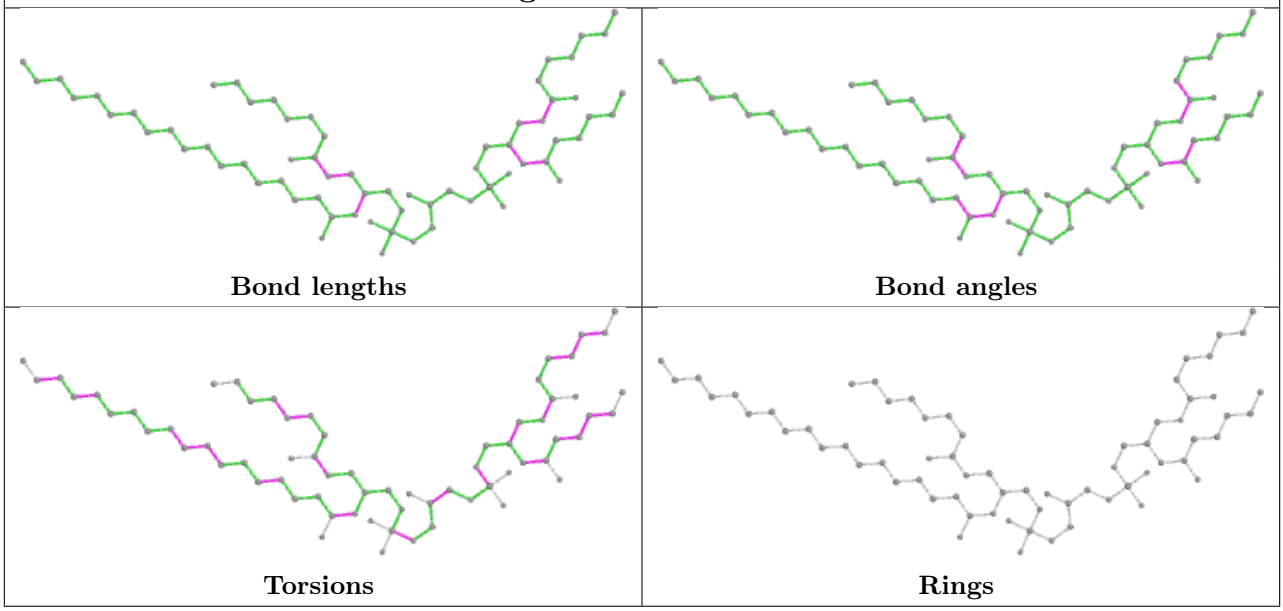


Torsions

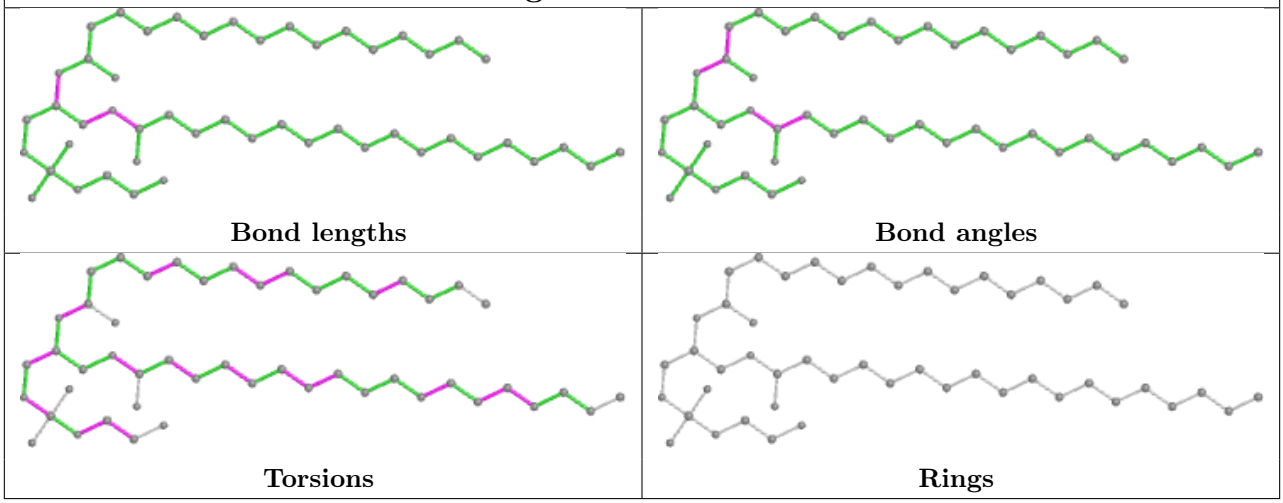


Rings

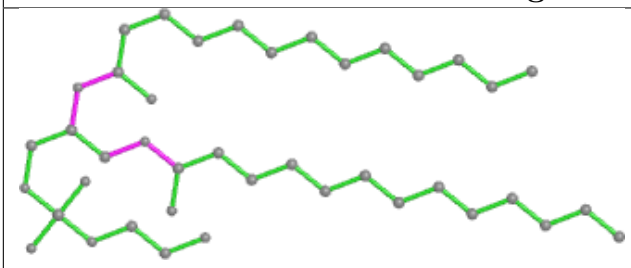
Ligand CDL h 1001



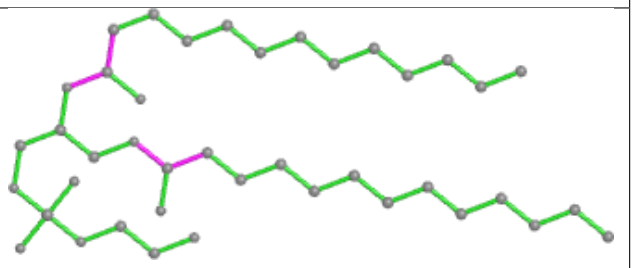
Ligand 3PE M 602



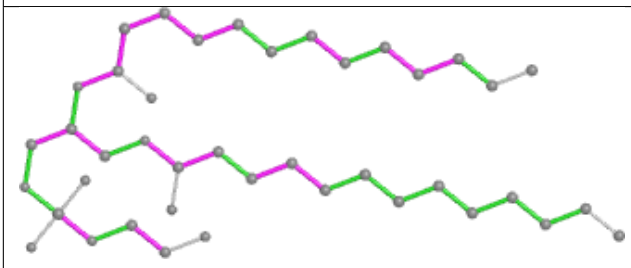
Ligand 3PE N 903



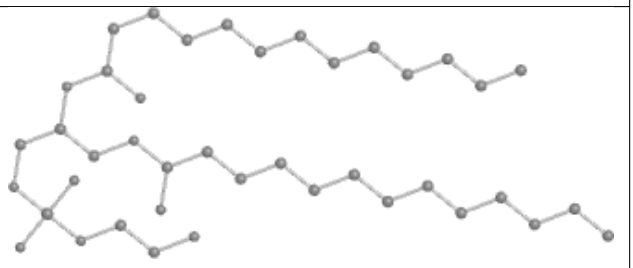
Bond lengths



Bond angles

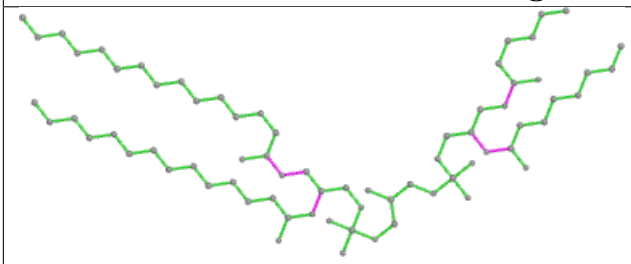


Torsions

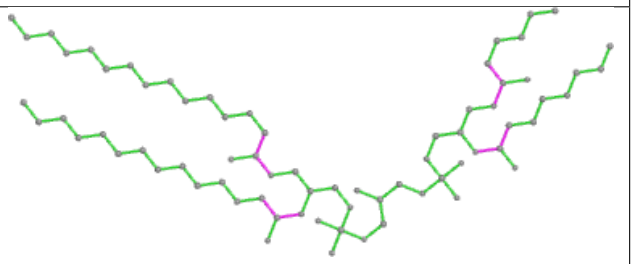


Rings

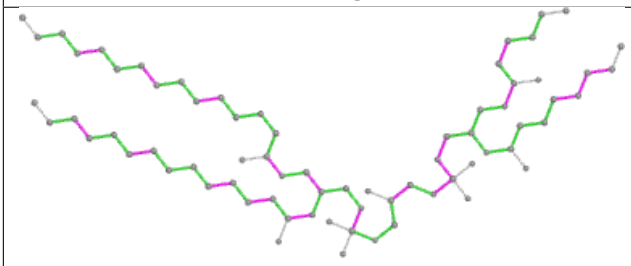
Ligand CDL J 401



Bond lengths



Bond angles



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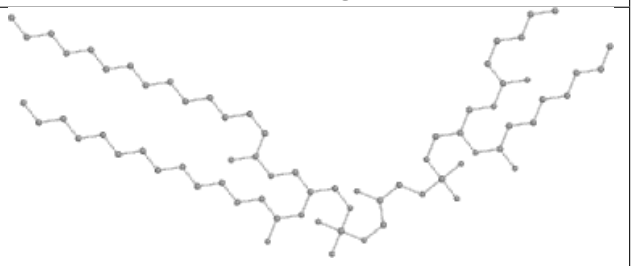
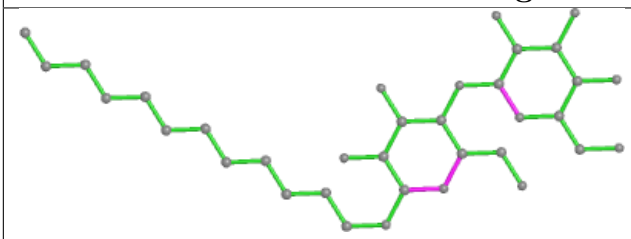
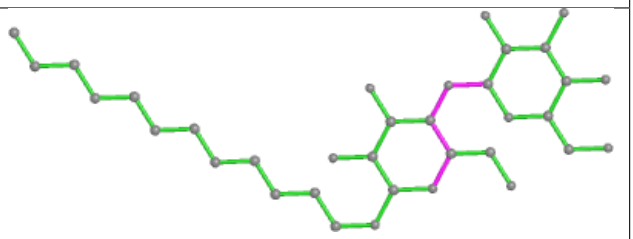


Rings

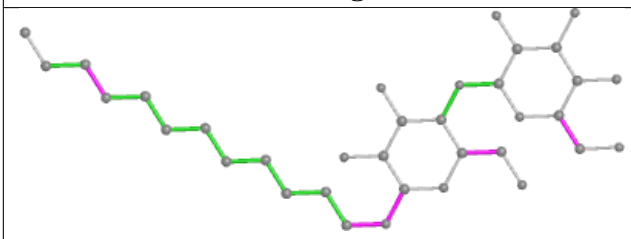
Ligand LMT h 1002



Bond lengths



Bond angles



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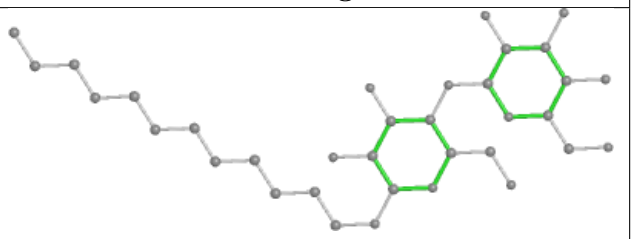
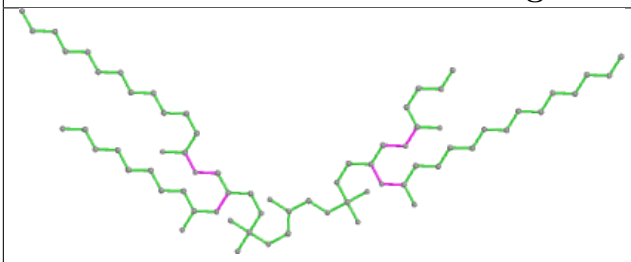


Rings

Ligand CDL L 702



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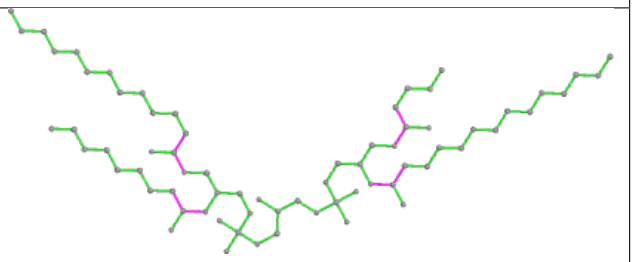
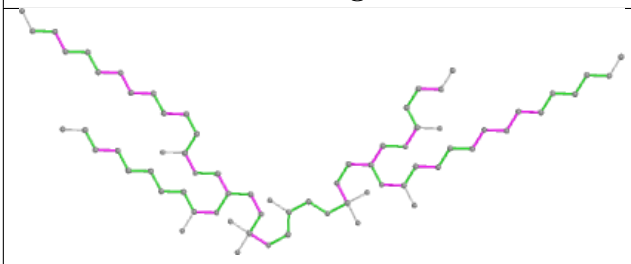
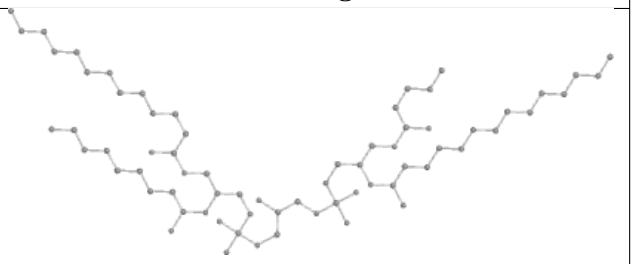


Bond angles

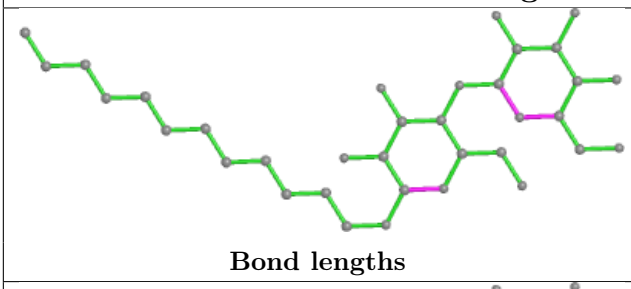


Torsions



Rings

Ligand LMT Y 402



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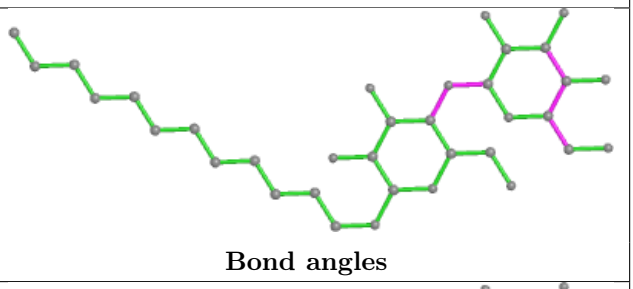
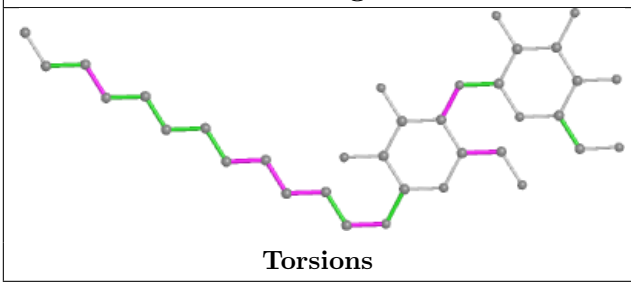


Bond angles



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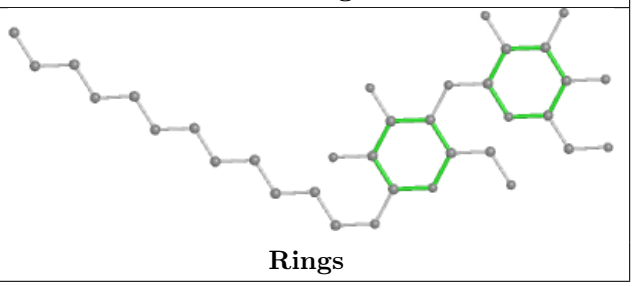
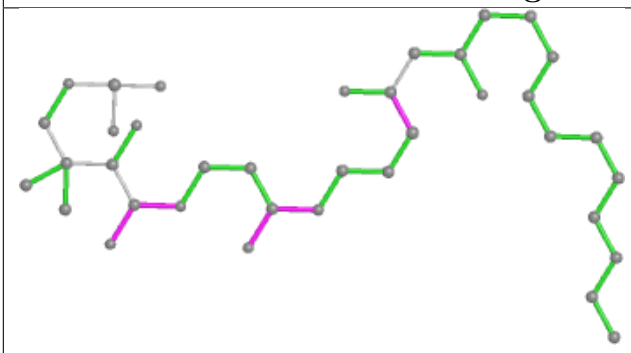


Rings

Ligand EHZ U 101



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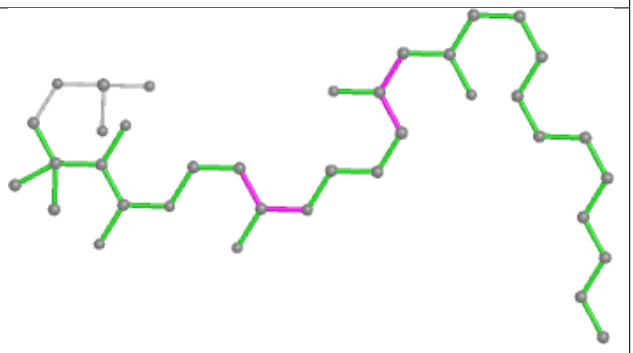
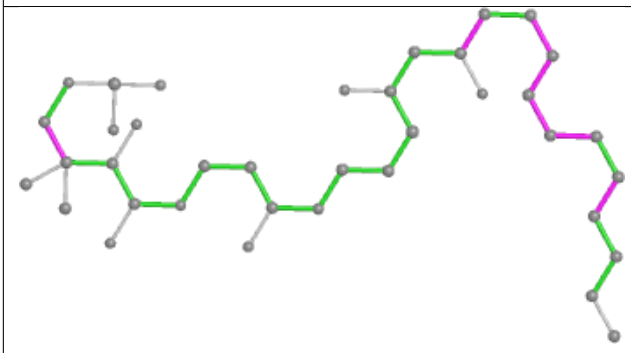
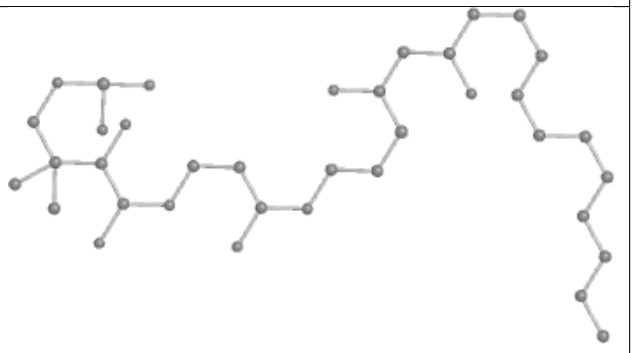


Bond angles

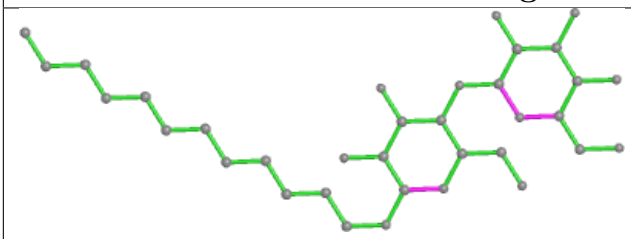


Torsions

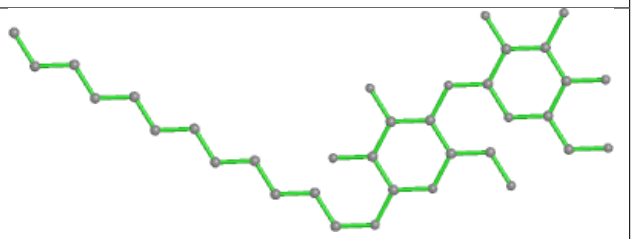


Rings

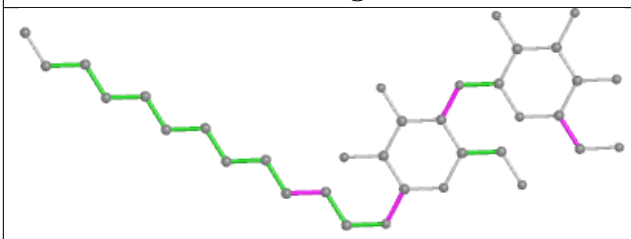
Ligand LMT f 1802



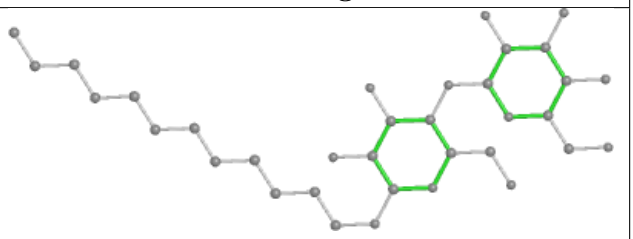
Bond lengths



Bond angles

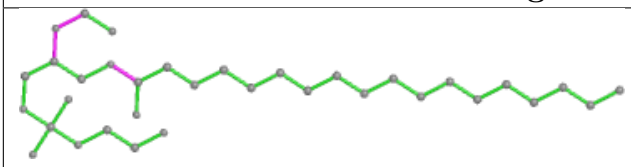


Torsions

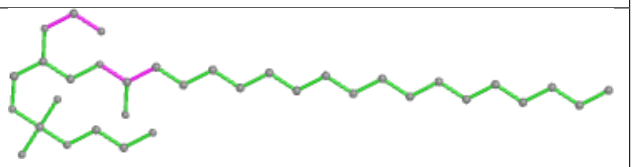


Rings

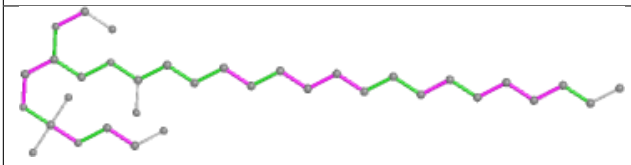
Ligand 3PE H 601



Bond lengths



Bond angles



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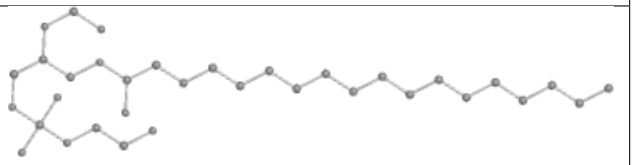
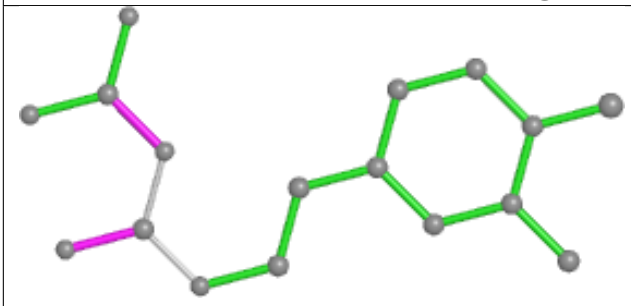
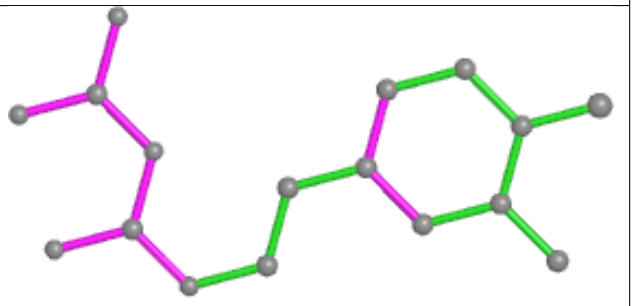


Rings

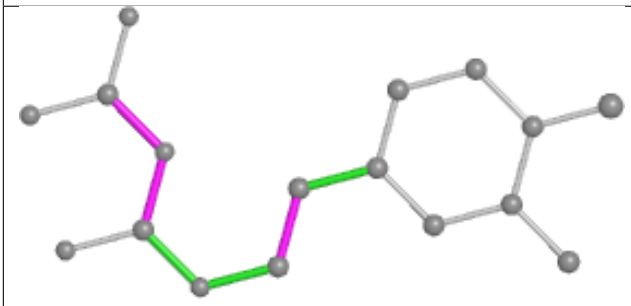
Ligand I49 N 904



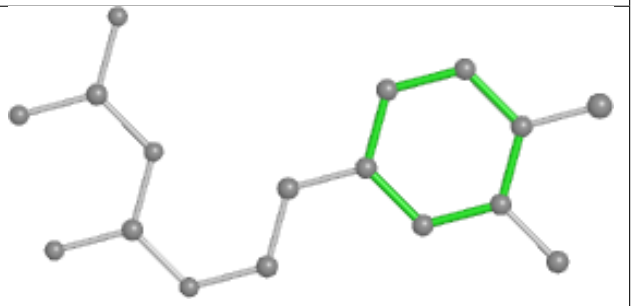
Bond lengths



Bond angles

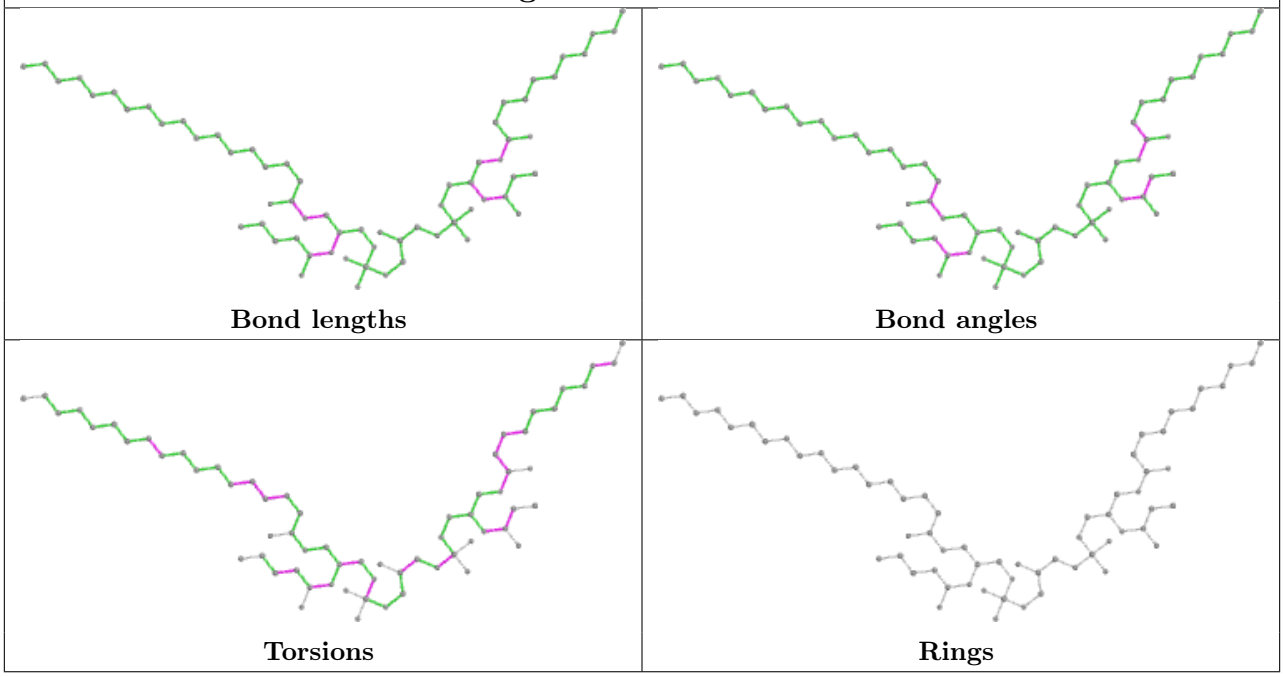


Torsions

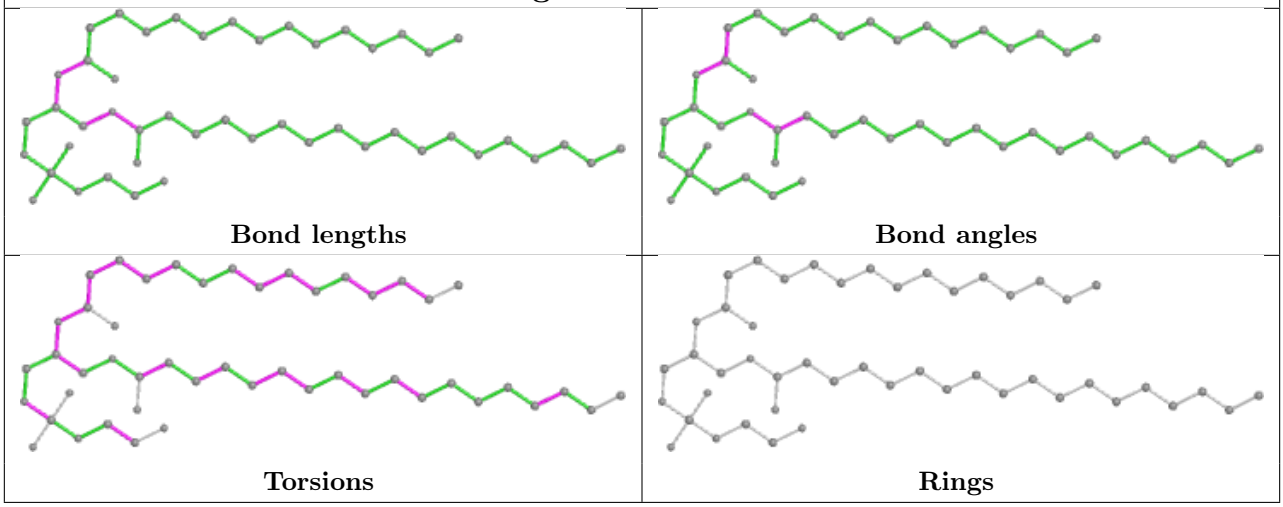


Rings

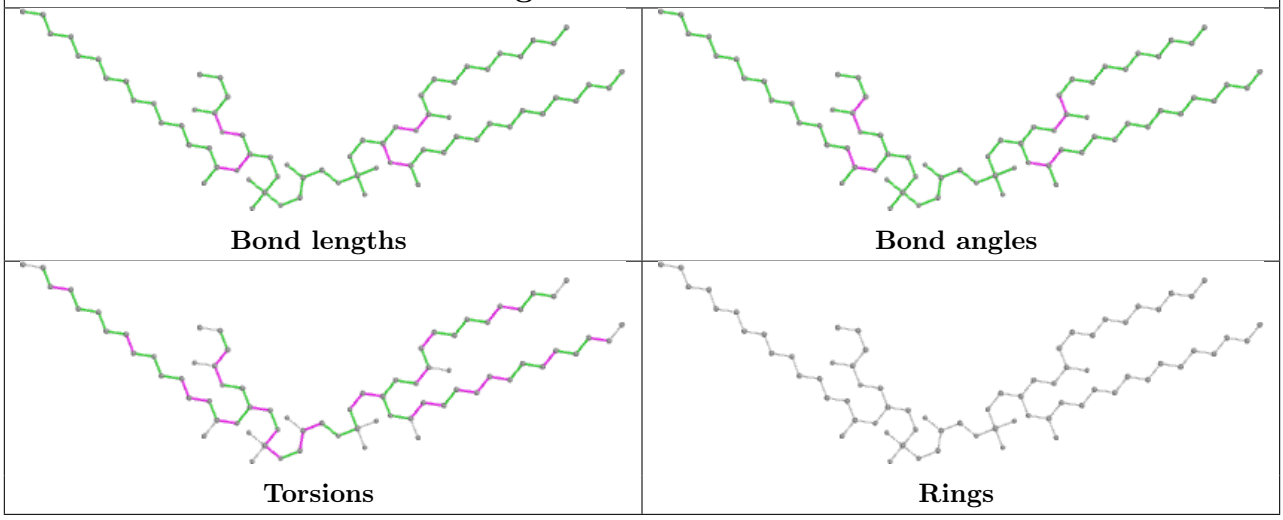
Ligand CDL d 1202



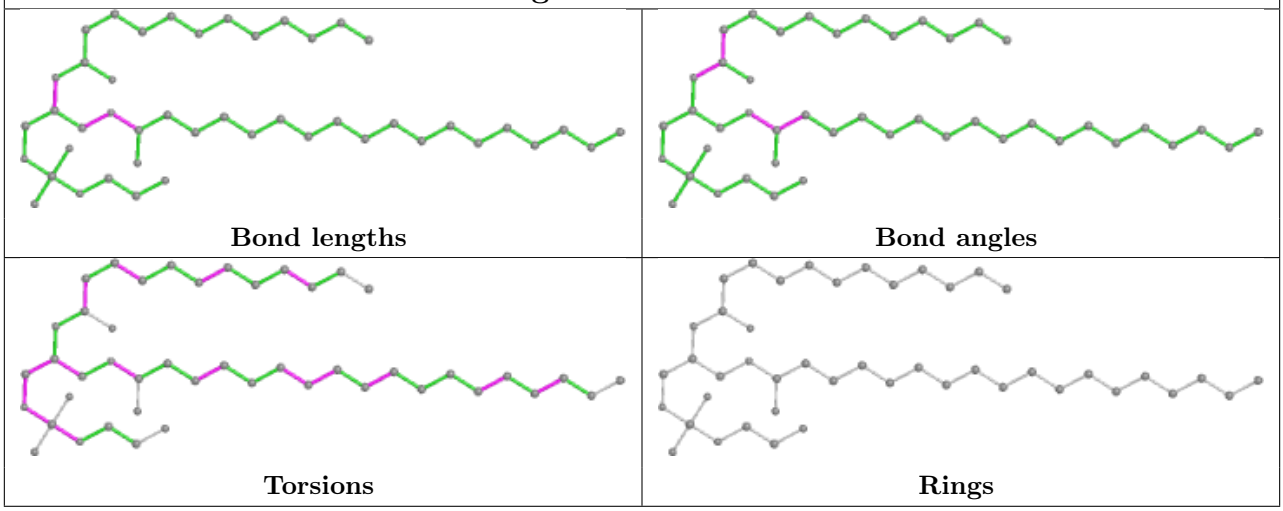
Ligand 3PE b 901



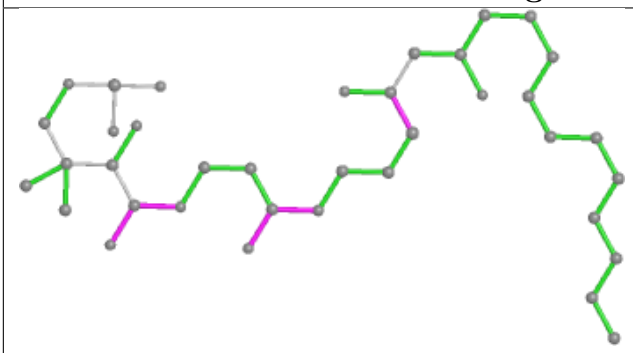
Ligand CDL X 1701



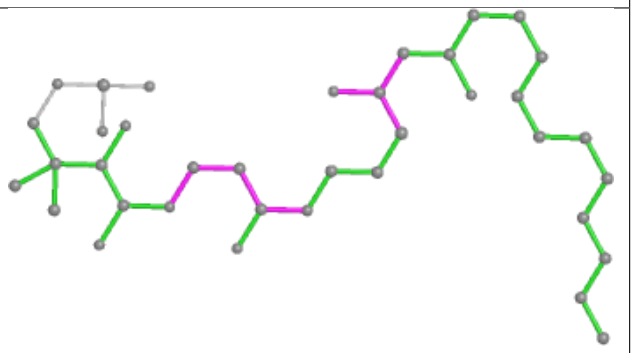
Ligand 3PE L 703



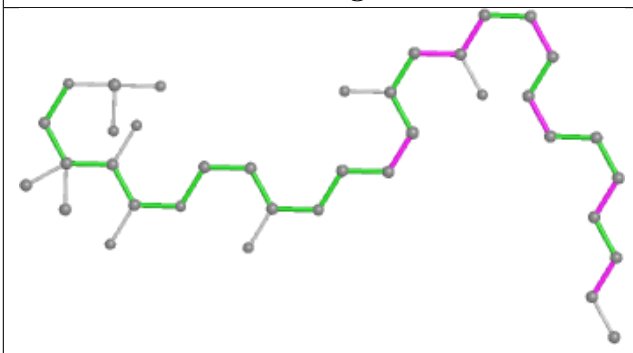
Ligand EHZ T 101



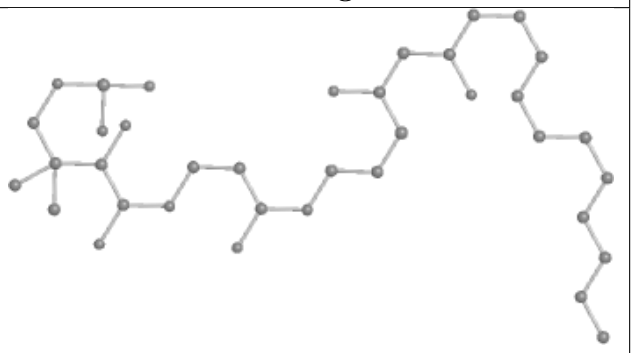
Bond lengths



Bond angles

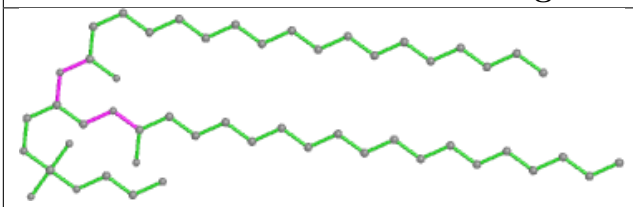


Torsions

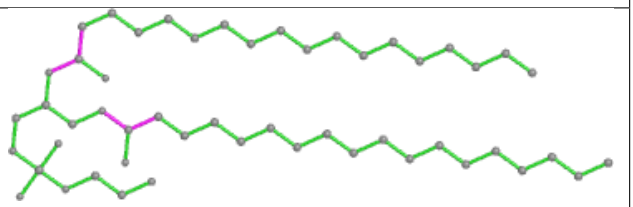


Rings

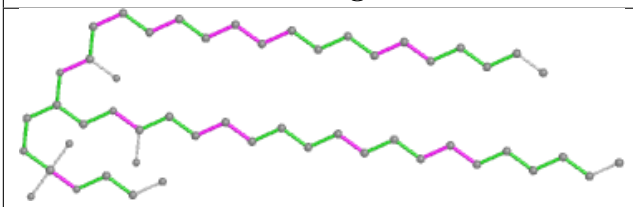
Ligand 3PE I 201



Bond lengths



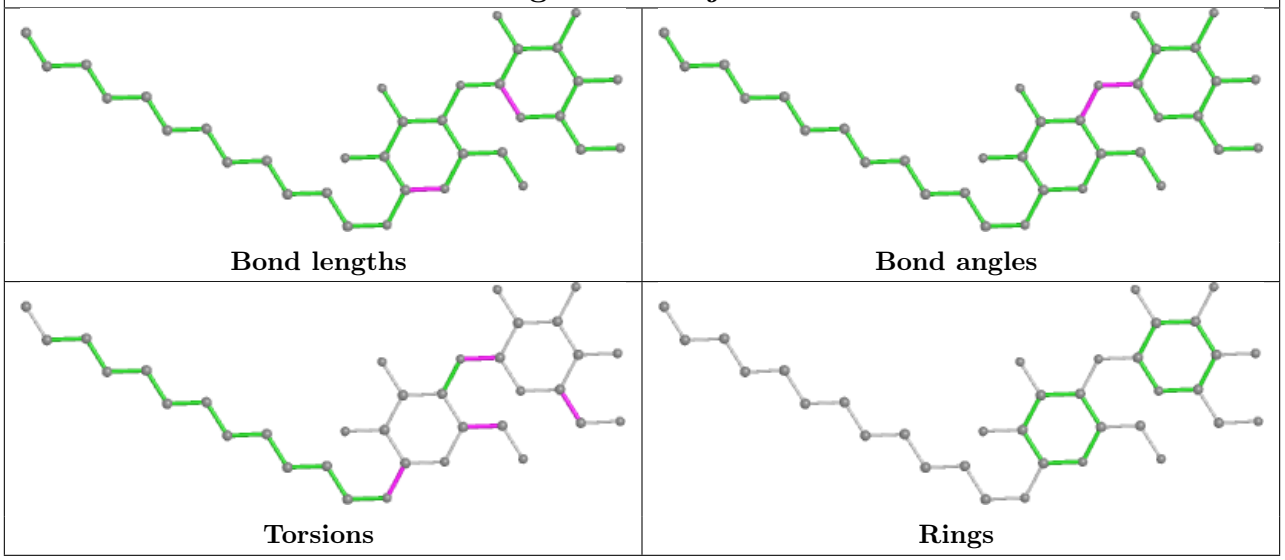
Bond angles



Torsions

Rings

Ligand LMT j 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

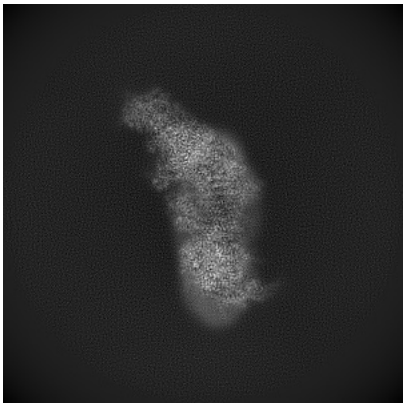
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14282. These allow visual inspection of the internal detail of the map and identification of artifacts.

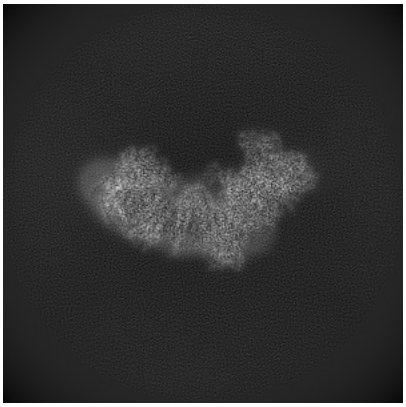
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

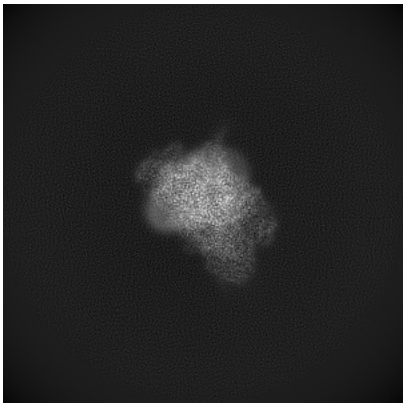
6.1.1 Primary map



X



Y

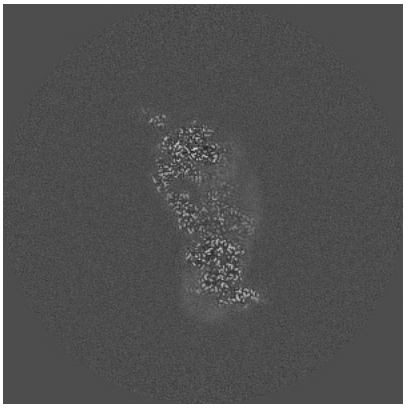


Z

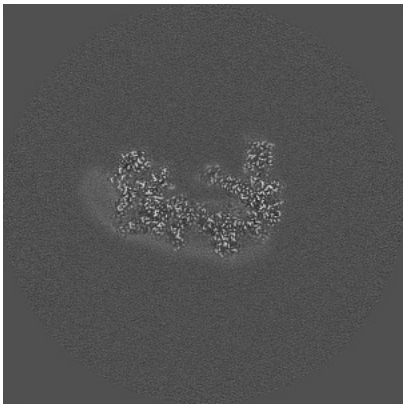
The images above show the map projected in three orthogonal directions.

6.2 Central slices

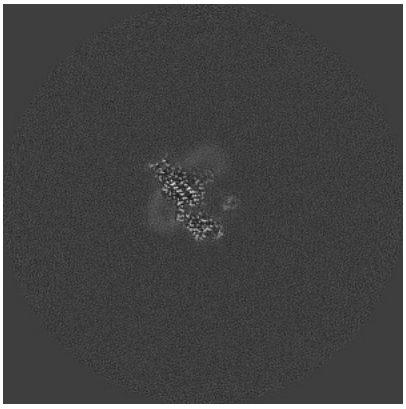
6.2.1 Primary map



X Index: 330



Y Index: 330

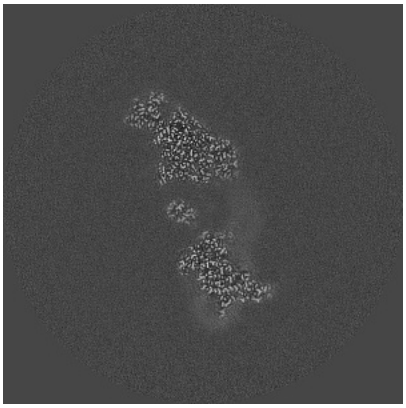


Z Index: 330

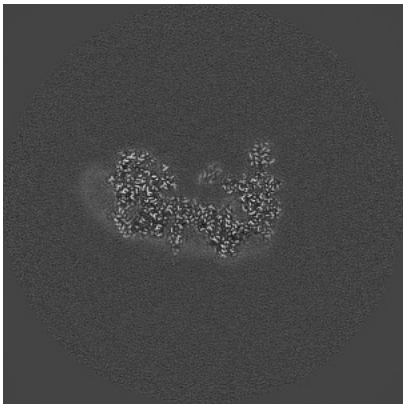
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

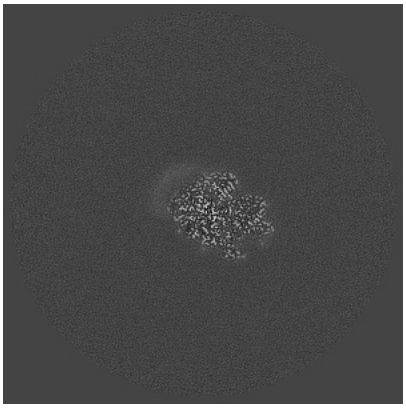
6.3.1 Primary map



X Index: 356



Y Index: 336



Z Index: 422

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

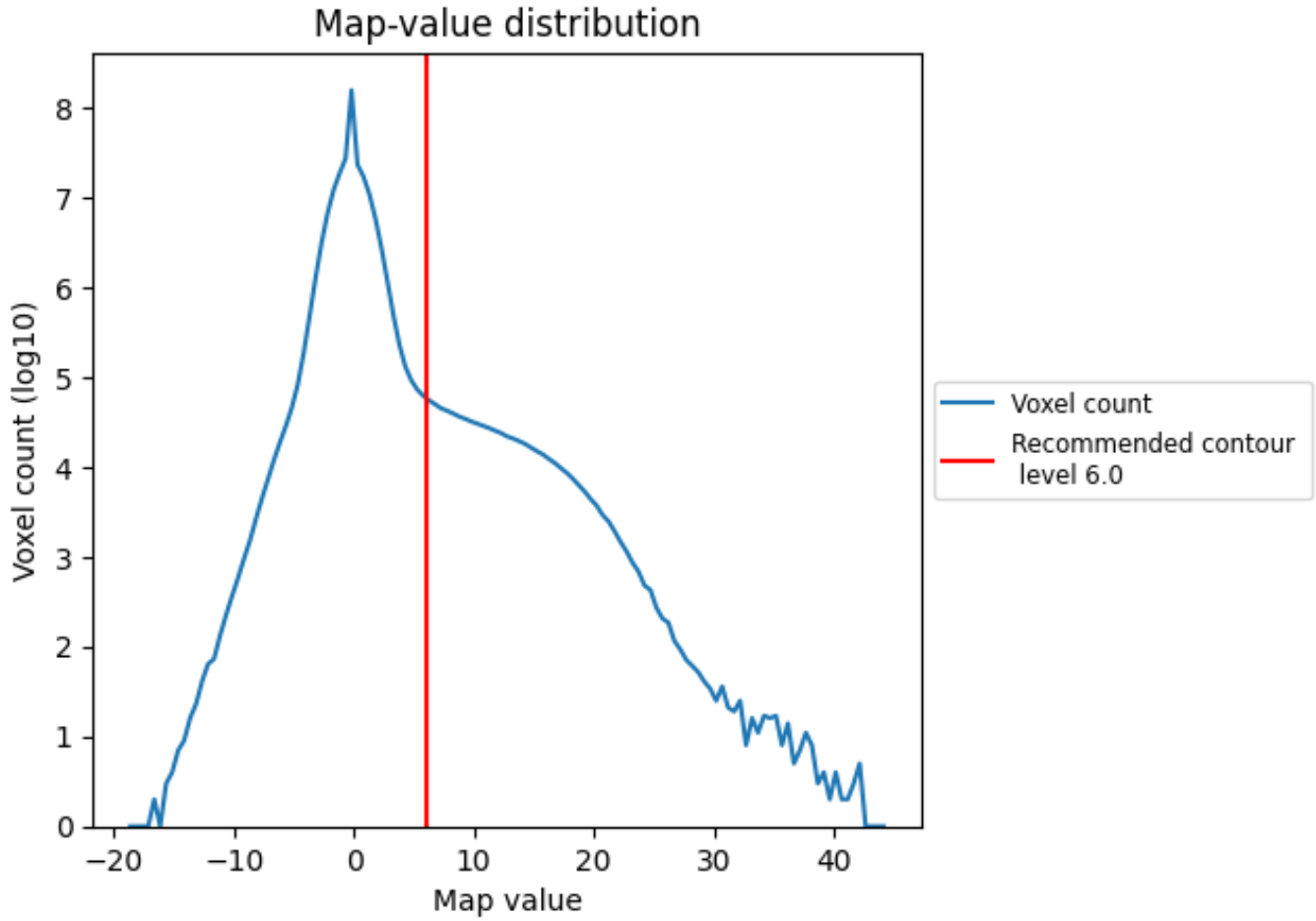
6.5 Mask visualisation (i)

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

7 Map analysis

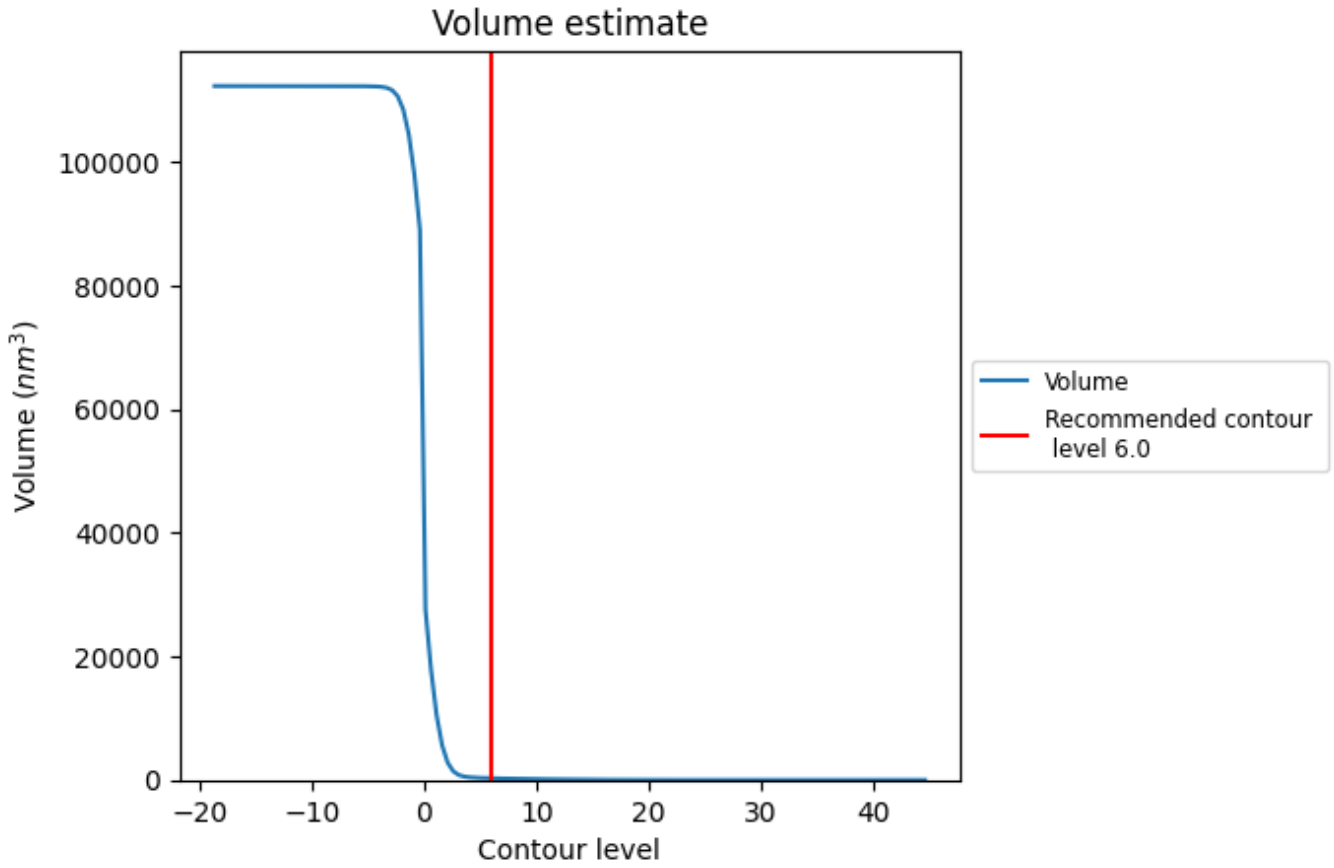
This section contains the results of statistical analysis of the map.

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.

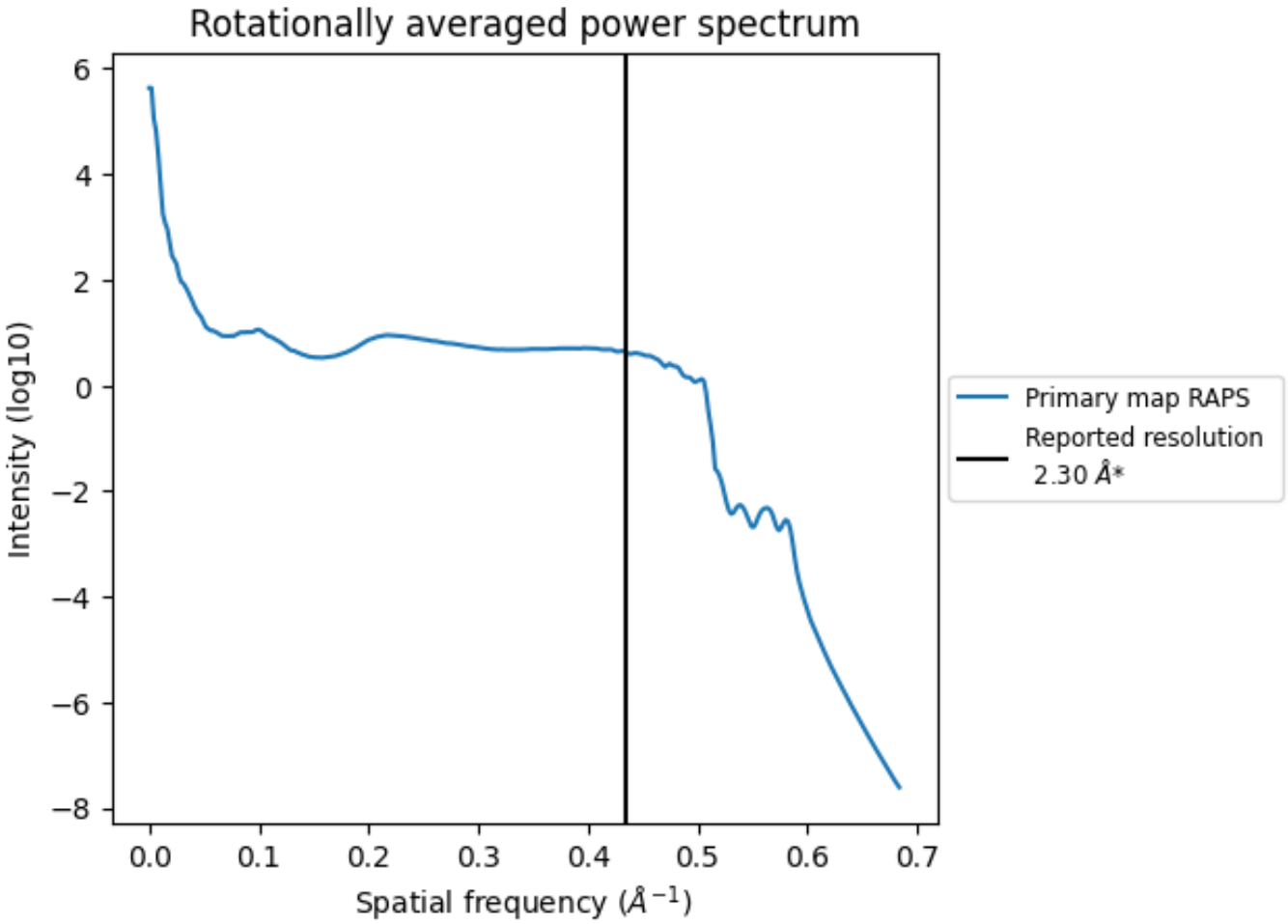
7.2 Volume estimate



The volume at the recommended contour level is 277 nm^3; this corresponds to an approximate mass of 251 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 $Å^{-1}$

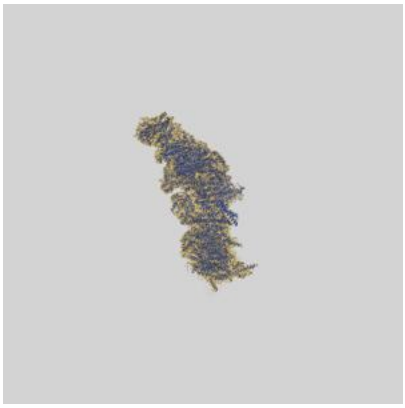
8 Fourier-Shell correlation (i)

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

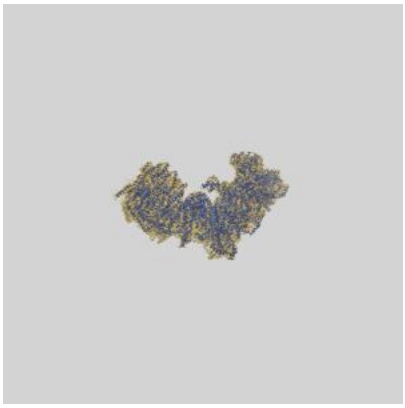
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14282 and PDB model 7R47. Per-residue inclusion information can be found in section 3 on page 24.

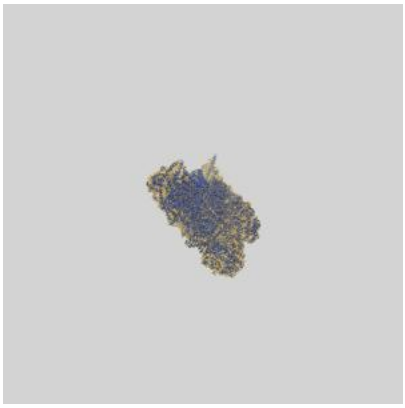
9.1 Map-model overlay



X



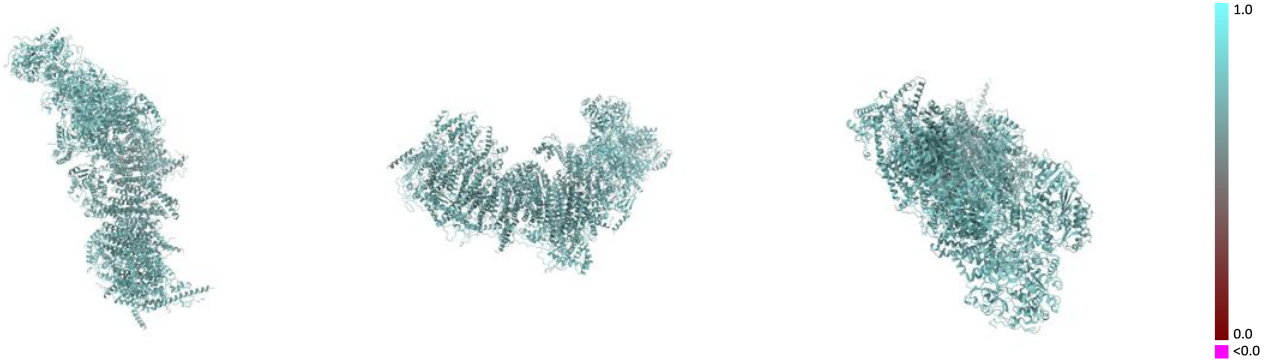
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 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.

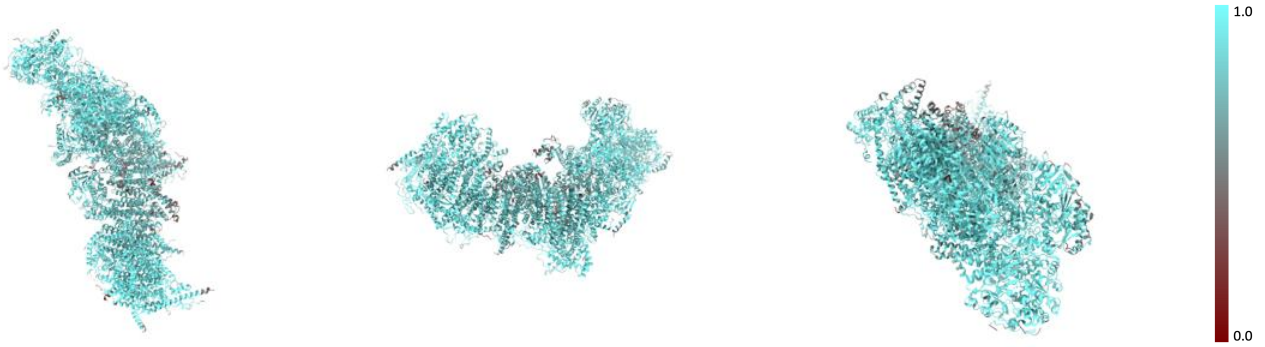
9.2 Q-score mapped to coordinate model (i)



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.

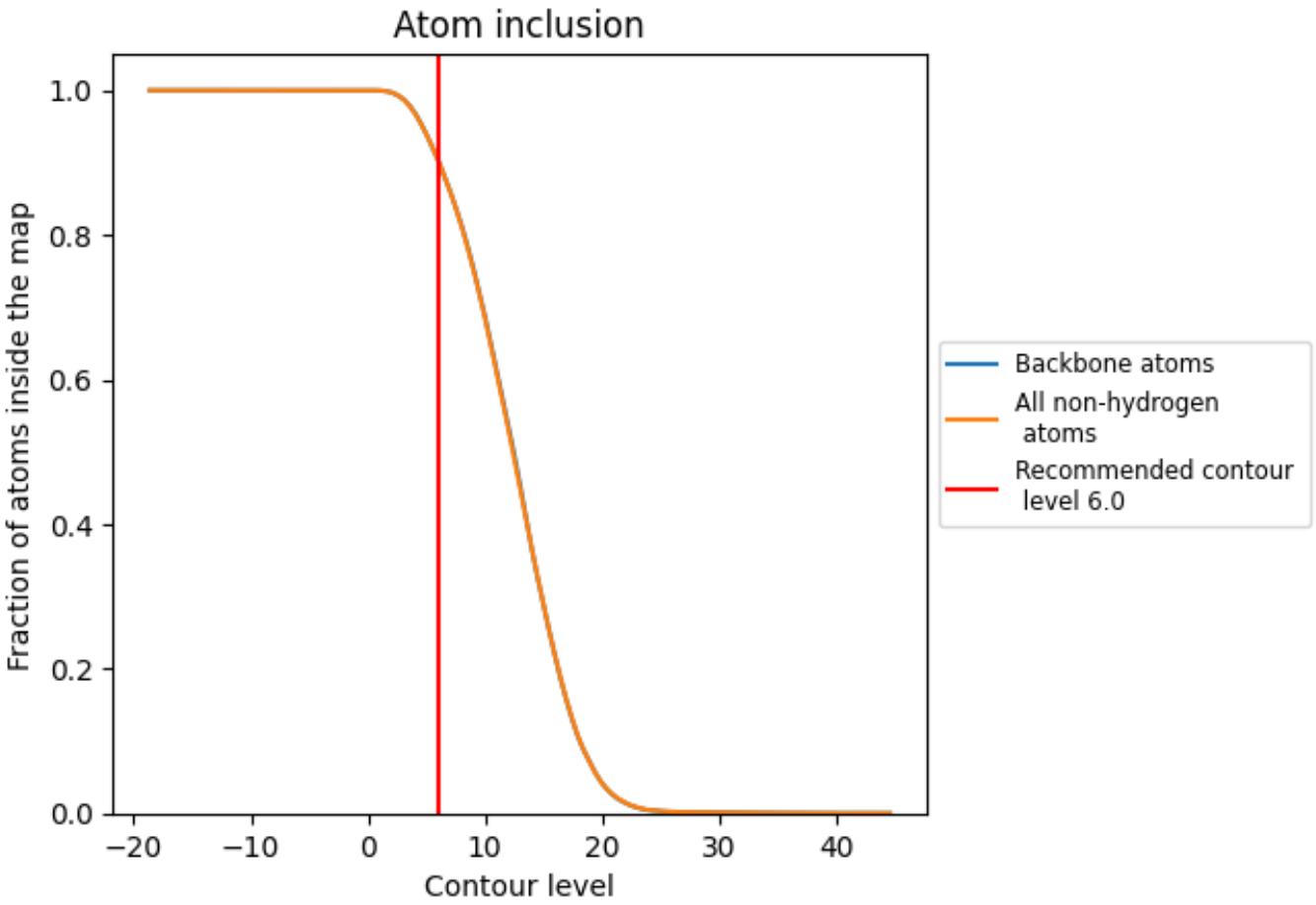
9.3 Atom inclusion mapped to coordinate model (i)



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 (6.0).

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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9041	0.7150
A	0.8270	0.6910
B	0.9333	0.7420
C	0.9718	0.7530
D	0.9473	0.7490
E	0.9048	0.7110
F	0.9458	0.7250
G	0.9285	0.7310
H	0.9430	0.7240
I	0.9736	0.7570
J	0.8039	0.7000
K	0.9499	0.7330
L	0.9363	0.7100
M	0.9740	0.7320
N	0.9549	0.7300
O	0.8801	0.6950
P	0.8877	0.7150
Q	0.9215	0.7410
R	0.9175	0.7370
S	0.8464	0.6980
T	0.6289	0.6360
U	0.9480	0.7010
V	0.8772	0.7210
W	0.8811	0.7190
X	0.8748	0.7000
Y	0.5915	0.6590
Z	0.8818	0.7070
a	0.9575	0.7170
b	0.8509	0.6830
c	0.8384	0.6710
d	0.8360	0.6990
e	0.8274	0.6890
f	0.7824	0.6640
g	0.9002	0.7040
h	0.9135	0.7070

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.8801	0.6800
j	0.8633	0.6720
k	0.8923	0.6710
l	0.9248	0.6990
m	0.8663	0.6960
n	0.9316	0.7060
o	0.8997	0.6790
p	0.9273	0.7040
q	0.8593	0.7210
r	0.9191	0.7340
s	0.8873	0.7110