Full wwPDB EM Validation Report

Aug 26, 2026 – 04:18 pm BST

PDB ID	:	8OLT / pdb_00008olt
EMDB ID	:	EMD-16962
Title	:	Mitochondrial complex I from Mus musculus in the active state bound with piericidin A
Authors	:	Grba, D.N.; Chung, I.; Bridges, H.R.; Agip, A.N.A.; Hirst, J.
Deposited on	:	2023-03-30
Resolution	:	2.84 Å(reported)
Based on initial model	:	6ZR2

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

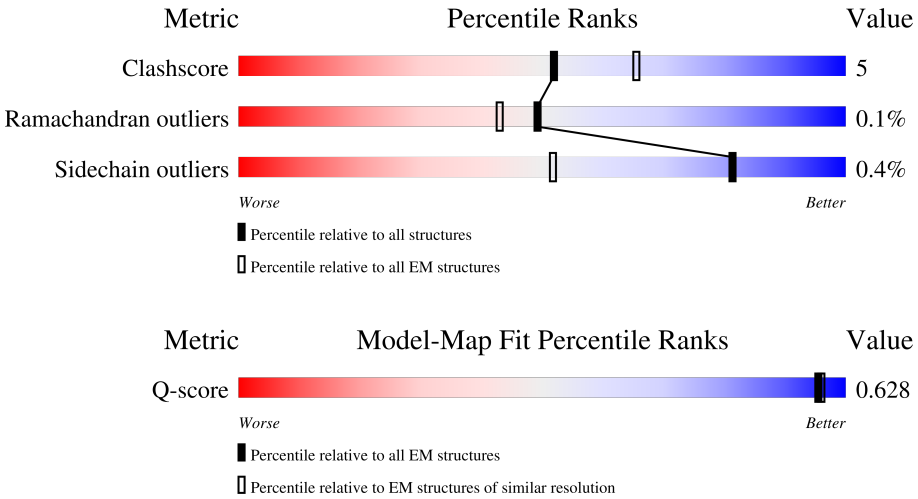
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.84 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.



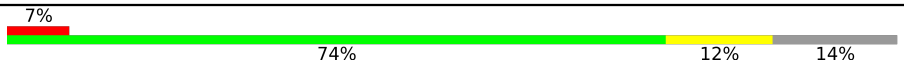
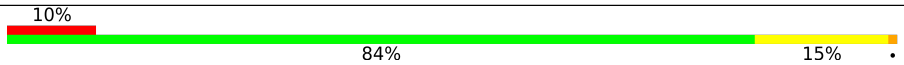
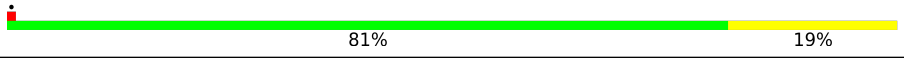
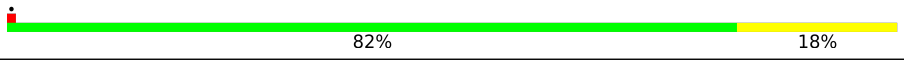
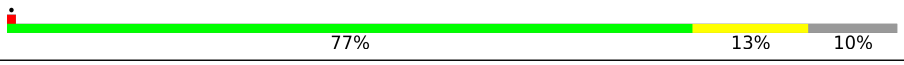
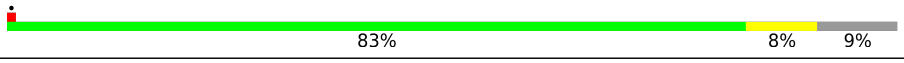
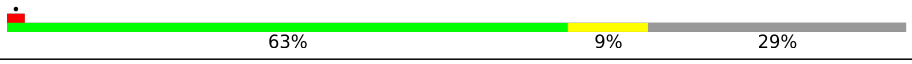
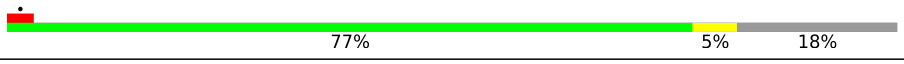
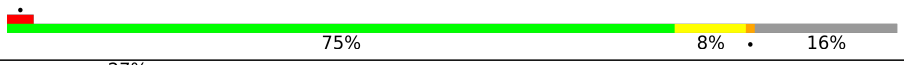
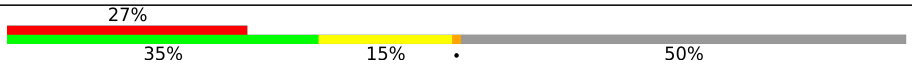
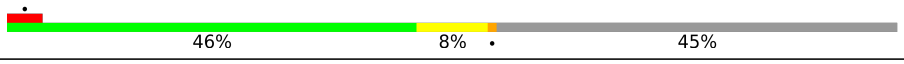
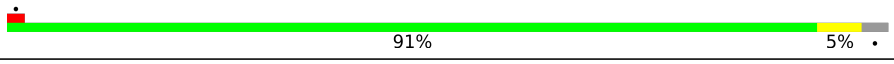
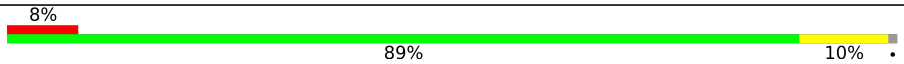
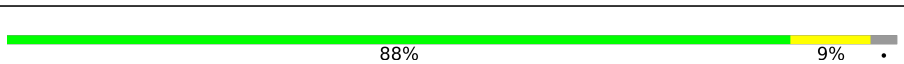
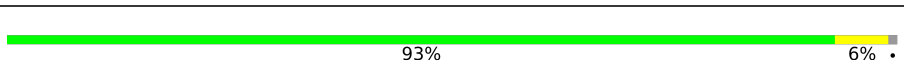
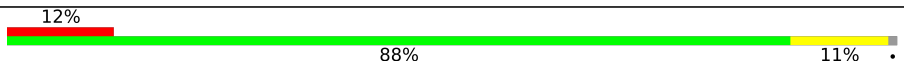
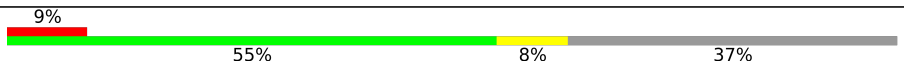
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	83% 17%
2	B	224	58% 10% 30%
3	C	263	70% 8% 21%
4	D	463	81% 11% 7%

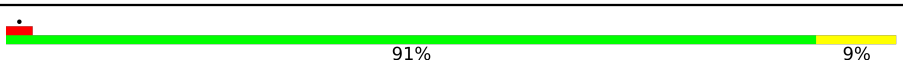
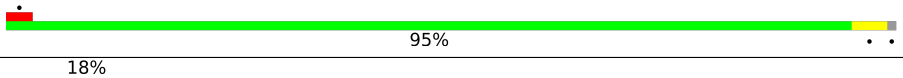
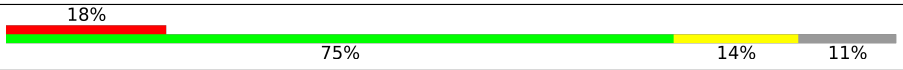
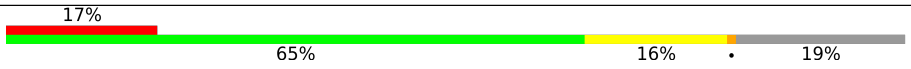
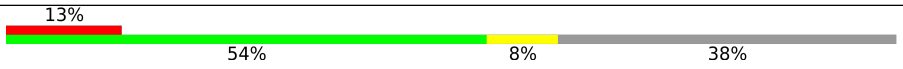
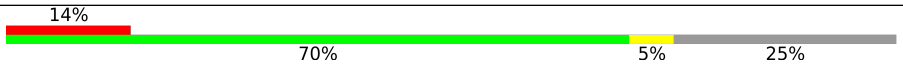
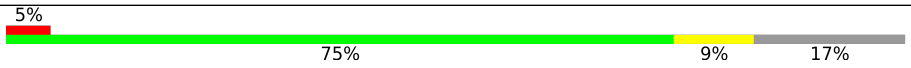
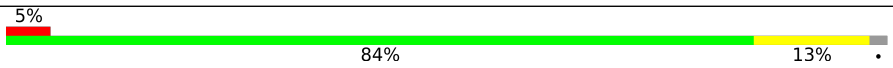
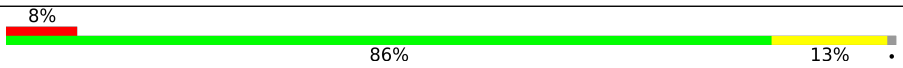
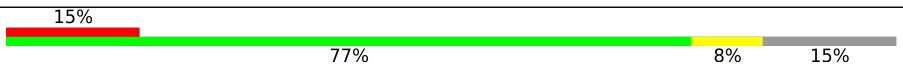
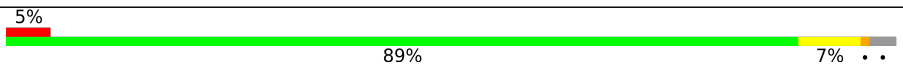
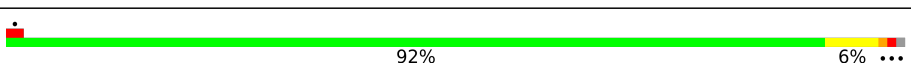
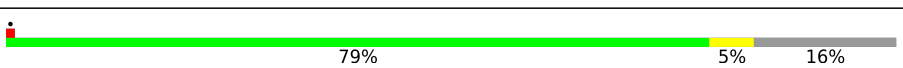
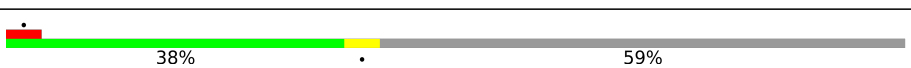
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Mol	Chain	Length	Quality of chain
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 68075 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	115	933	633	133	160	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	156	1247	796	223	214	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	208	1730	1116	297	314	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	430	3464	2215	595	630	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1660	1056	279	314	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	430	Total	C	N	O	S	0	0
			3321	2092	596	611	22		

- 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
			5296	3321	919	1015	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2540	1706	384	428	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	172	Total	C	N	O	S	0	0
			1308	878	186	229	15		

- 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
			737	477	112	137	11		

- 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
			4800	3182	746	827	45		

- 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
			3632	2408	567	617	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	345	Total	C	N	O	S	0	0
			2703	1795	417	454	37		

- 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
			2607	1674	431	492	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		

- 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
			1015	642	179	190	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	95	Total	C	N	O	S	0	0
			748	464	138	143	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	83	Total	C	N	O	S	0	0
			663	415	126	119	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	78	Total	C	N	O	S	0	0
			628	404	93	126	5		
20	U	86	Total	C	N	O	S	0	0
			692	446	102	139	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	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
			970	619	180	165	6		

- 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
			1396	889	250	247	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	142	Total	C	N	O	S	0	0
			1050	670	177	194	9		

- 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
			1161	747	206	200	8		

- 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
			564	366	100	94	4		

- 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
			648	425	105	114	4		

- 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	S	0	0
			398	261	69	67	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

- 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
			439	284	79	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	100	Total	C	N	O	S	0	0
			842	545	135	158	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
			1162	762	194	203	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	104	Total	C	N	O	S	0	0
			869	565	152	149	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	65	Total	C	N	O	S	0	0
			562	370	93	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	78	Total	C	N	O	S	0	0
			630	416	107	105	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
			1302	840	216	235	11		

- 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	676	189	185		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7, METHYLGLYOXAL BIS-(GUANYLHYDRAZONE), NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	117	Total	C	N	O	S	0	0
			1005	634	189	174	8		

- 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
			1439	904	258	269	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	144	Total	C	N	O	S	0	0
			1203	773	213	212	5		

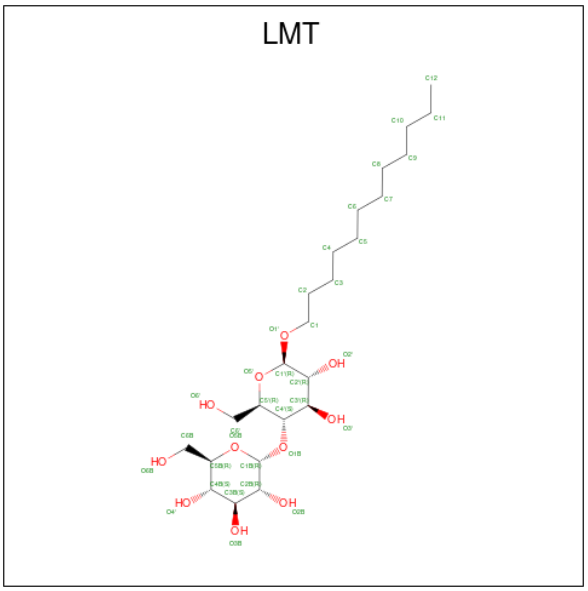
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	95	Total	C	N	O	S	0	0
			767	484	143	137	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	0	0
			361	225	65	71		

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



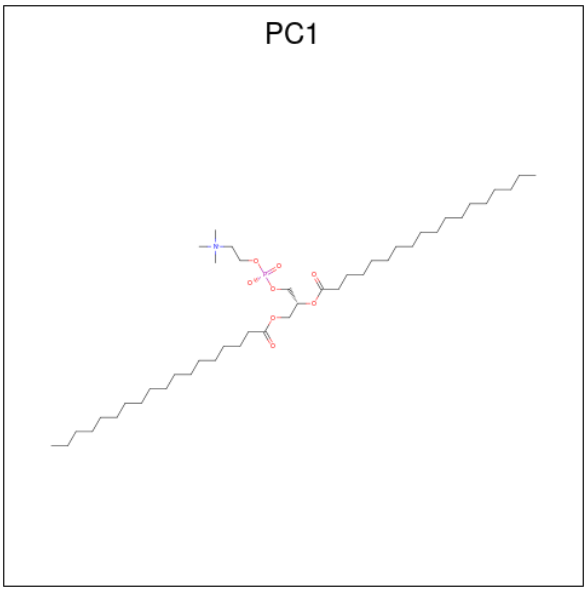
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	A	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	K	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	
45	O	1	Total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

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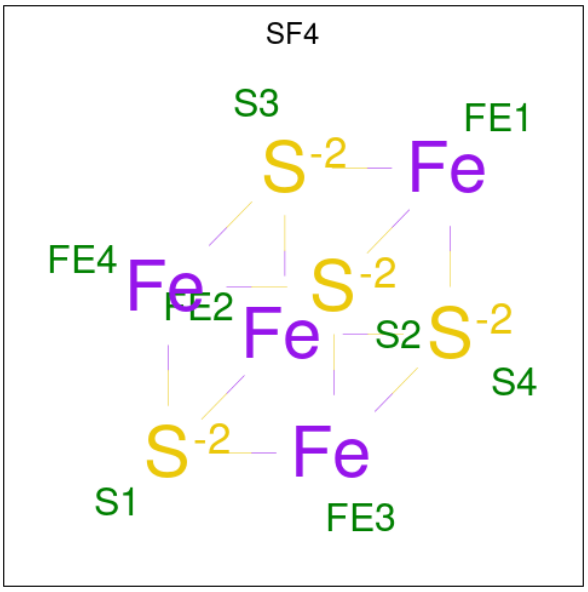
Mol	Chain	Residues	Atoms	AltConf
45	h	1	Total C O 35 24 11	0
45	j	1	Total C O 35 24 11	0

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



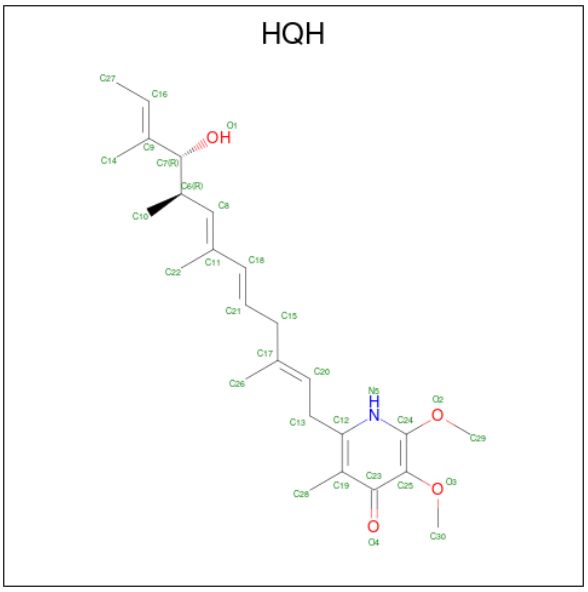
Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total C N O P 29 19 1 8 1	0
46	B	1	Total C N O P 38 28 1 8 1	0
46	B	1	Total C N O P 41 31 1 8 1	0

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



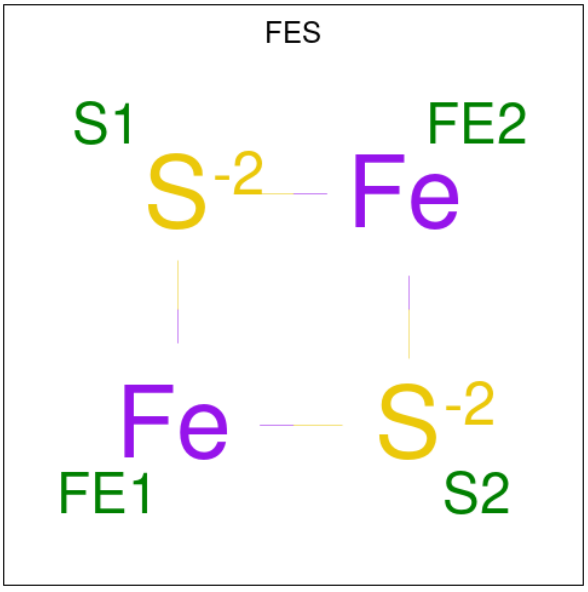
Mol	Chain	Residues	Atoms	AltConf
47	B	1	Total Fe S 8 4 4	0
47	F	1	Total Fe S 8 4 4	0
47	G	1	Total Fe S 8 4 4	0
47	G	1	Total Fe S 8 4 4	0
47	I	1	Total Fe S 8 4 4	0
47	I	1	Total Fe S 8 4 4	0

- Molecule 48 is Piericidin A (CCD ID: HQH) (formula: $C_{25}H_{37}NO_4$) (labeled as "Ligand of Interest" by depositor).



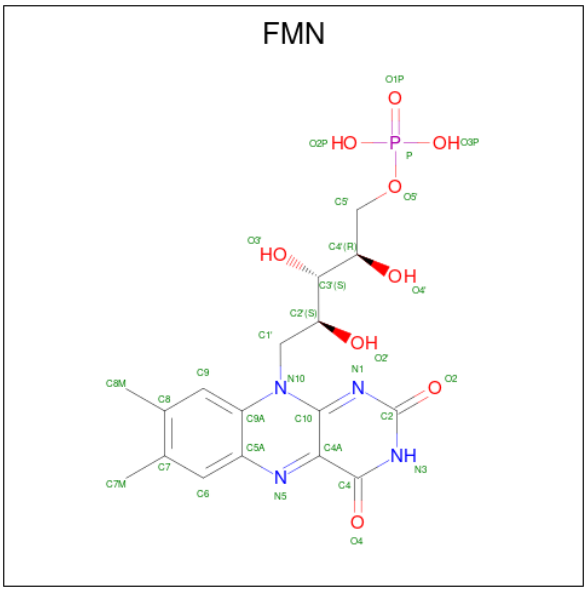
Mol	Chain	Residues	Atoms				AltConf
48	D	1	Total	C	N	O	0
			30	25	1	4	

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

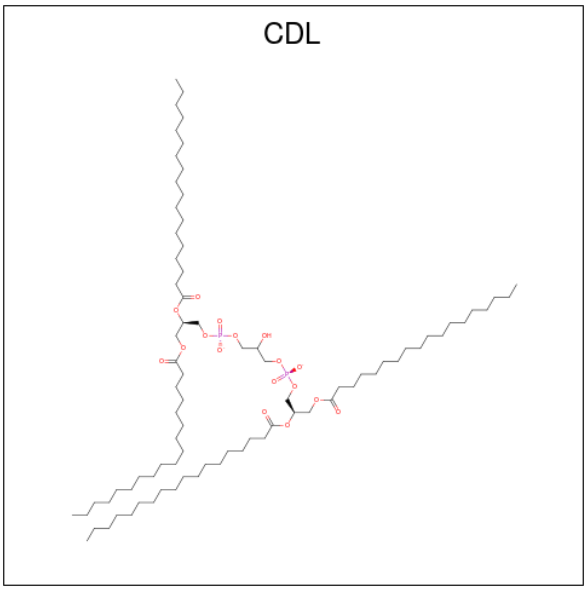


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is SODIUM ION (CCD ID: NA) (formula: Na).

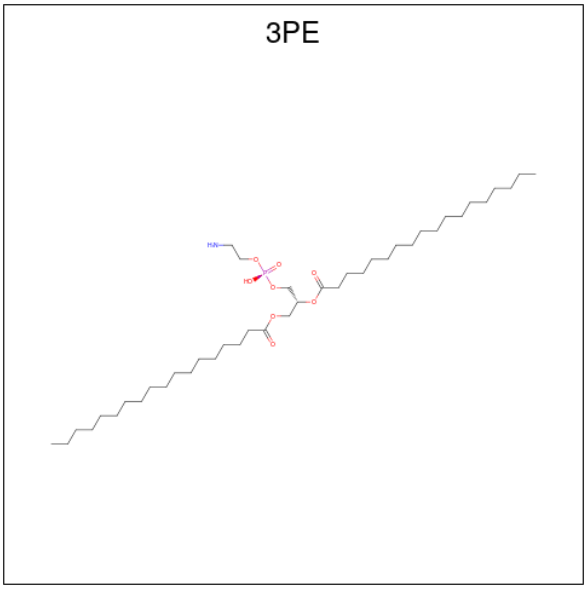
Mol	Chain	Residues	Atoms		AltConf
51	G	1	Total	Na	0
			1	1	

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



Mol	Chain	Residues	Atoms				AltConf
52	H	1	Total	C	O	P	0
			48	29	17	2	
52	L	1	Total	C	O	P	0
			64	45	17	2	
52	h	1	Total	C	O	P	0
			57	39	16	2	
52	h	1	Total	C	O	P	0
			48	29	17	2	
52	q	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 53 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
53	I	1	Total	C	N	O	P	0
			44	34	1	8	1	
53	L	1	Total	C	N	O	P	0
			41	31	1	8	1	
53	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
53	M	1	Total	C	N	O	P	0
			36	26	1	8	1	
53	M	1	Total	C	N	O	P	0
			36	26	1	8	1	
53	N	1	Total	C	N	O	P	0
			34	24	1	8	1	

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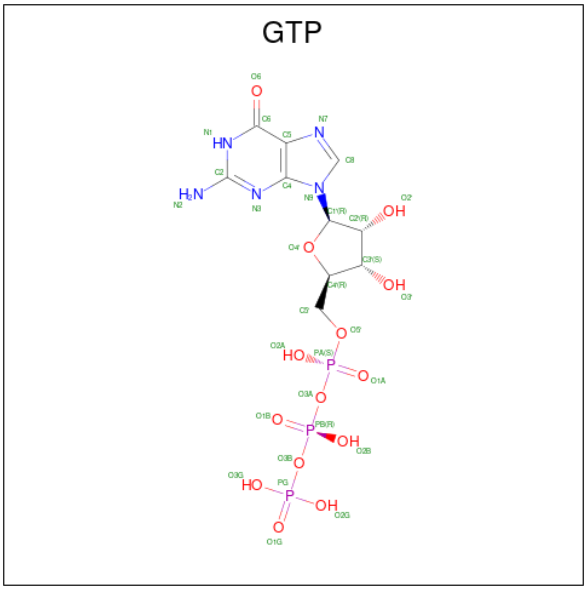
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Mol	Chain	Residues	Atoms					AltConf
53	N	1	Total	C	N	O	P	0
			33	23	1	8	1	
53	O	1	Total	C	N	O	P	0
			30	20	1	8	1	
53	X	1	Total	C	N	O	P	0
			36	26	1	8	1	
53	Z	1	Total	C	N	O	P	0
			31	21	1	8	1	
53	Z	1	Total	C	N	O	P	0
			41	31	1	8	1	
53	d	1	Total	C	N	O	P	0
			33	23	1	8	1	
53	i	1	Total	C	N	O	P	0
			30	20	1	8	1	
53	r	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

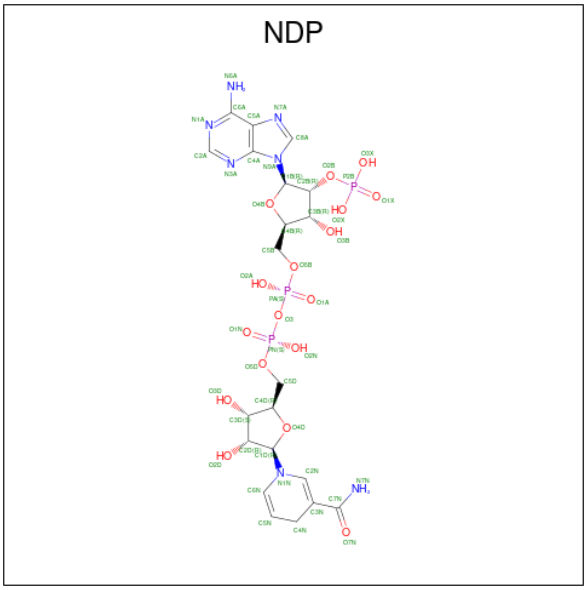
Mol	Chain	Residues	Atoms		AltConf
54	O	1	Total	Mg	0
			1	1	

- Molecule 55 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

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

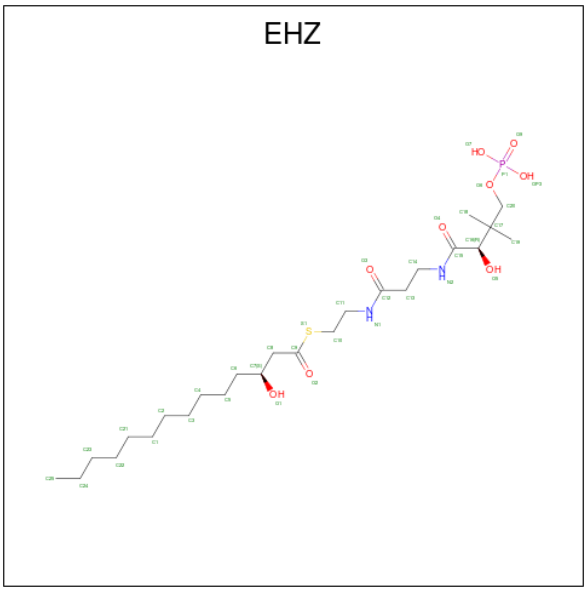


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

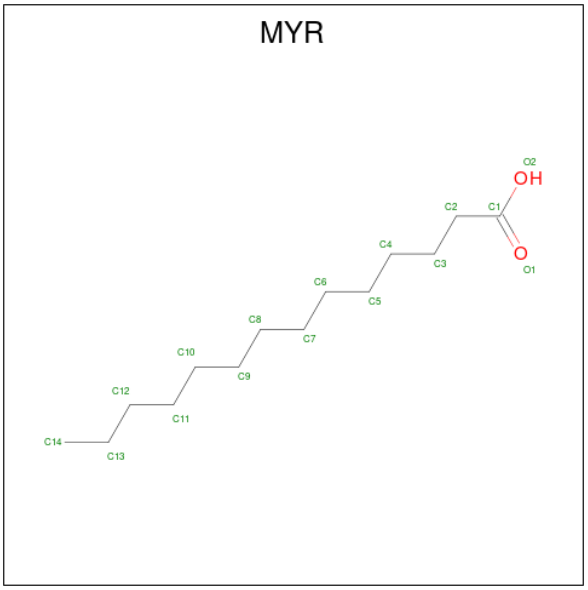
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- Molecule 58 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: 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 (CCD ID: 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	1	Total O 1 1	0
60	B	33	Total O 33 33	0
60	C	25	Total O 25 25	0
60	D	46	Total O 46 46	0
60	E	1	Total O 1 1	0
60	F	3	Total O 3 3	0
60	G	43	Total O 43 43	0
60	H	8	Total O 8 8	0
60	I	40	Total O 40 40	0
60	J	3	Total O 3 3	0
60	K	1	Total O 1 1	0
60	L	3	Total O 3 3	0
60	M	3	Total O 3 3	0
60	N	4	Total O 4 4	0
60	O	5	Total O 5 5	0
60	P	13	Total O 13 13	0
60	Q	9	Total O 9 9	0
60	R	5	Total O 5 5	0
60	W	1	Total O 1 1	0
60	X	4	Total O 4 4	0
60	Z	5	Total O 5 5	0
60	a	2	Total O 2 2	0

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Mol	Chain	Residues	Atoms	AltConf
60	d	1	Total O 1 1	0
60	e	2	Total O 2 2	0
60	g	1	Total O 1 1	0
60	h	3	Total O 3 3	0
60	i	1	Total O 1 1	0
60	l	3	Total O 3 3	0
60	m	1	Total O 1 1	0
60	n	1	Total O 1 1	0
60	p	1	Total O 1 1	0
60	q	5	Total O 5 5	0
60	r	3	Total O 3 3	0

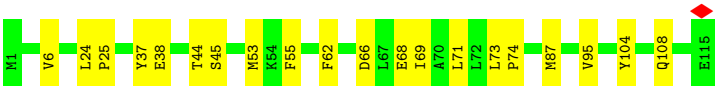
3 Residue-property plots (i)

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

• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:

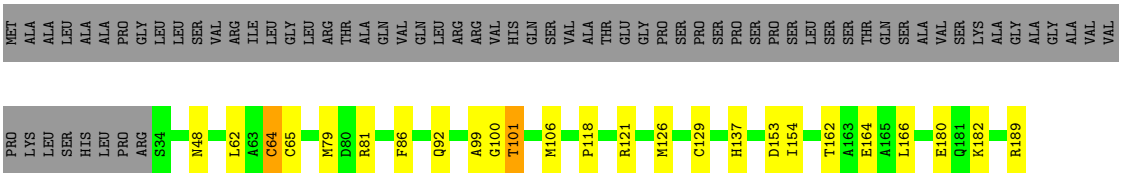




• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:

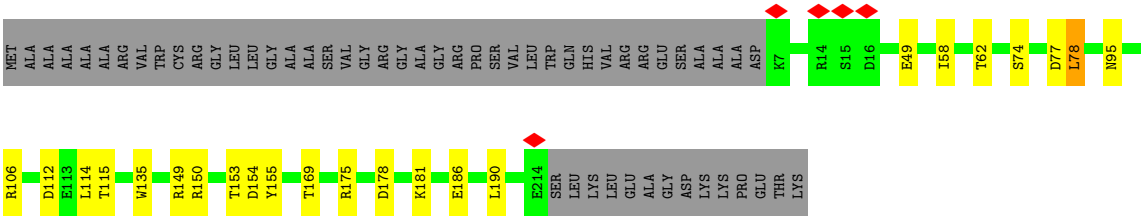




• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:

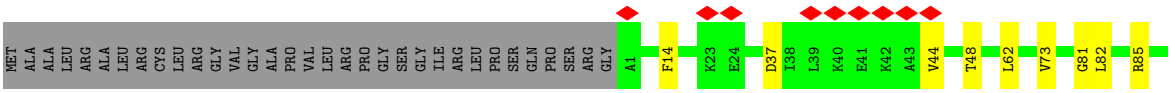


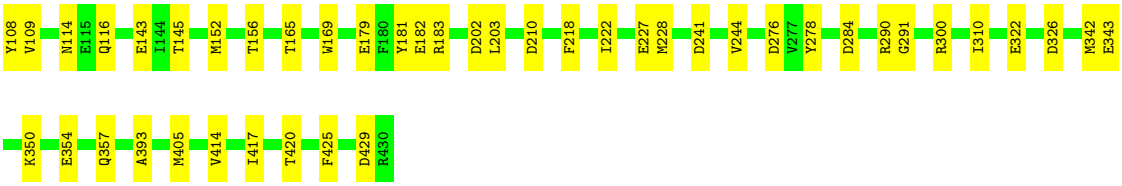


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:



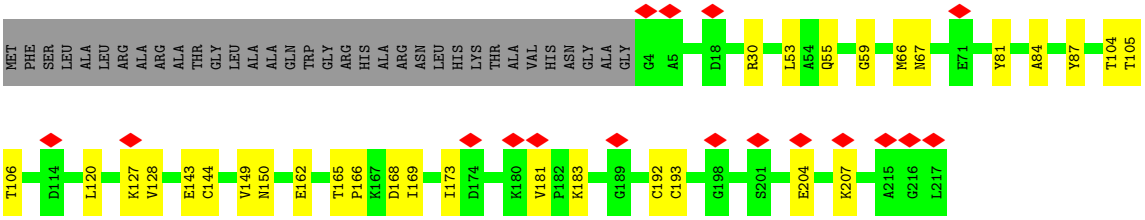




• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:

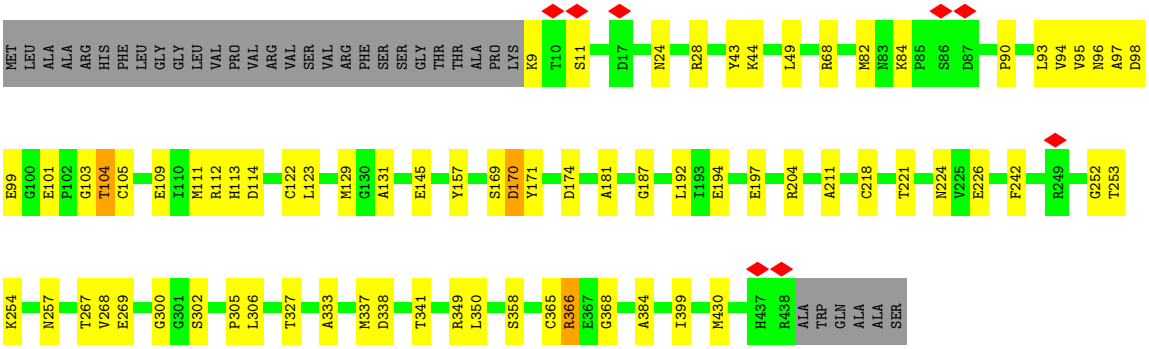




• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:

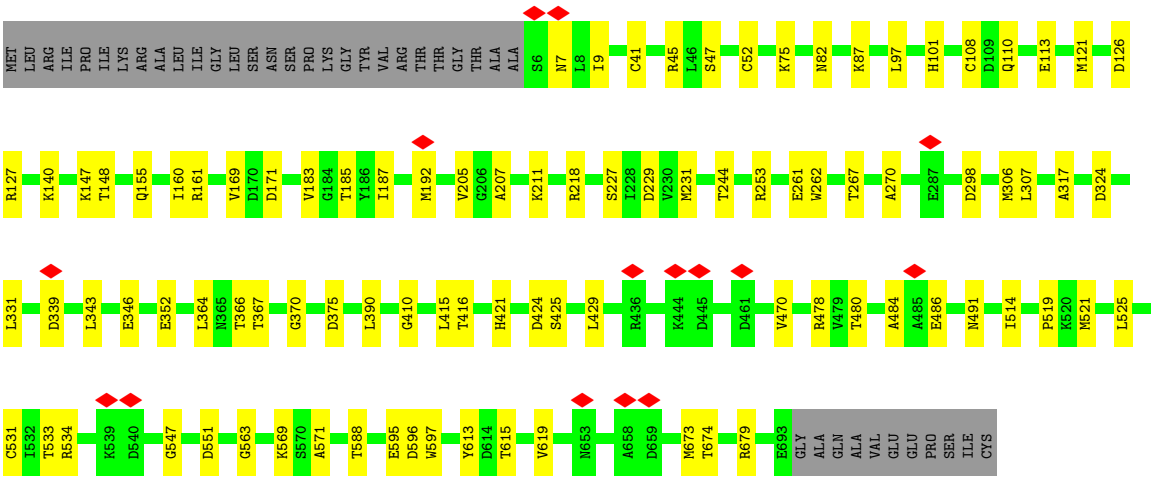




• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

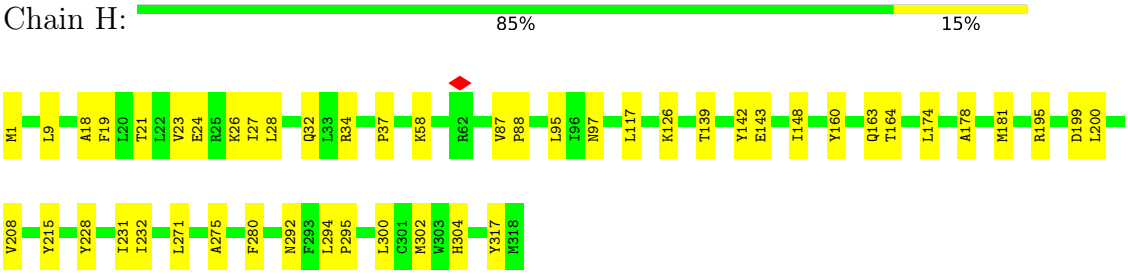
Chain G:





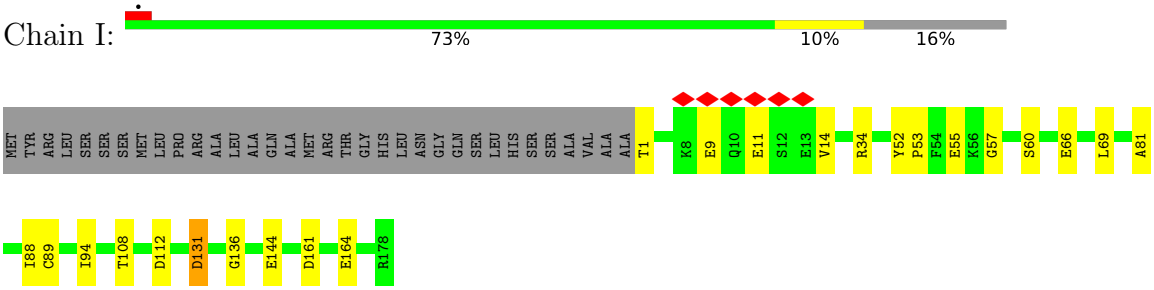
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



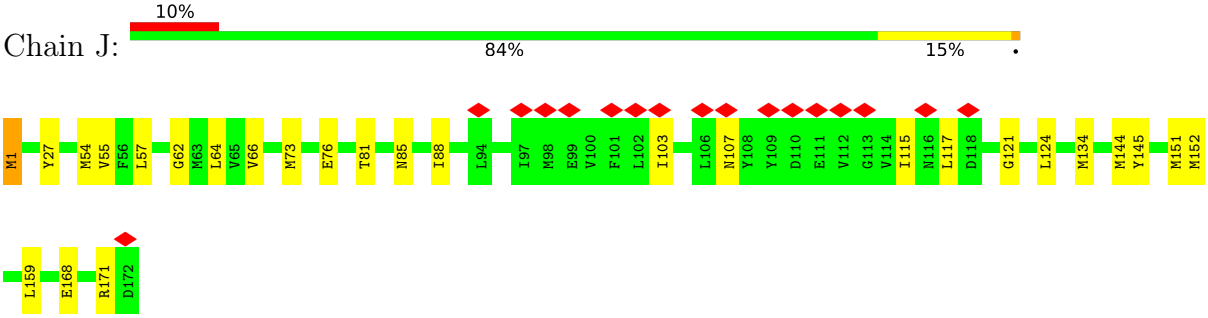
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



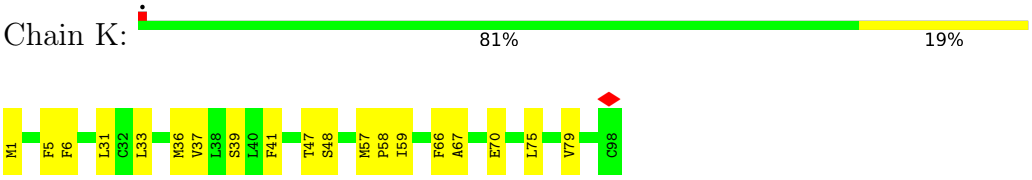
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



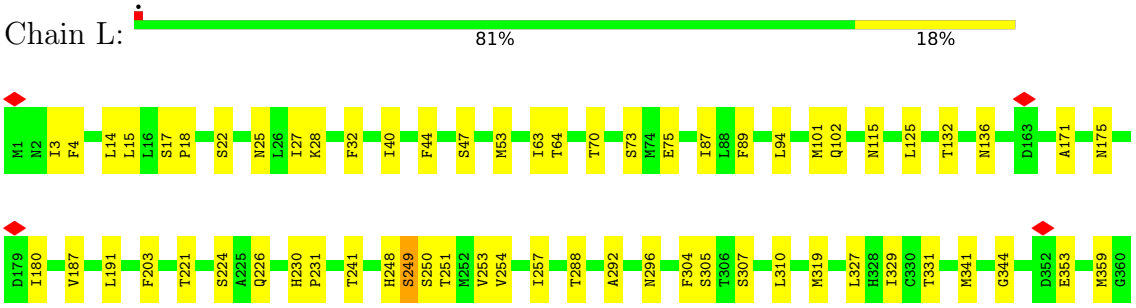
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

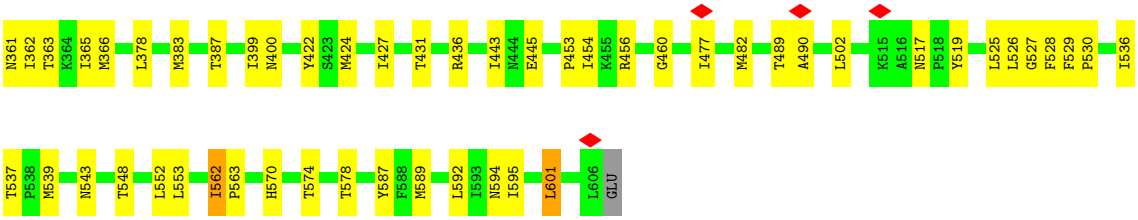
Chain K:



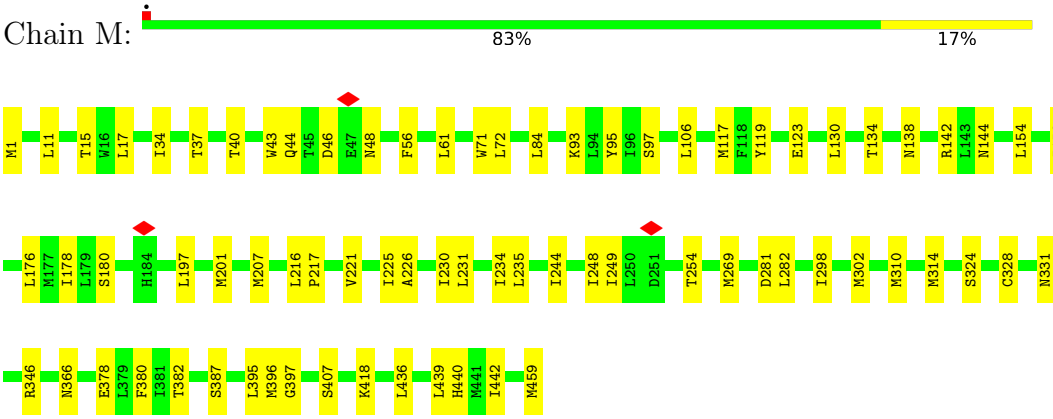
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:

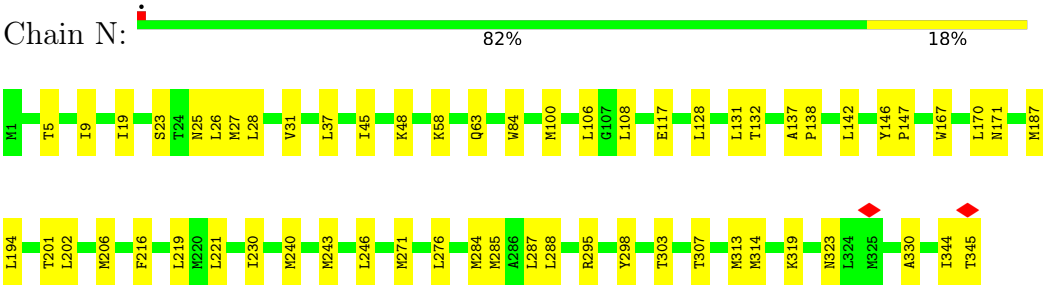




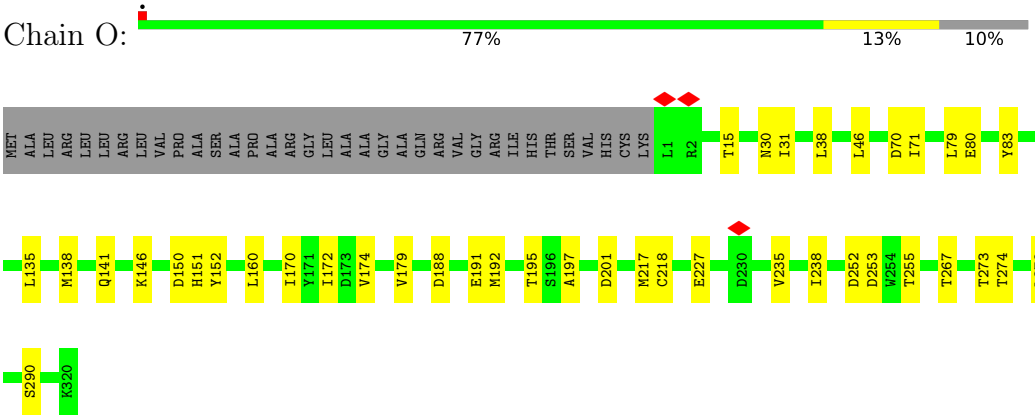
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

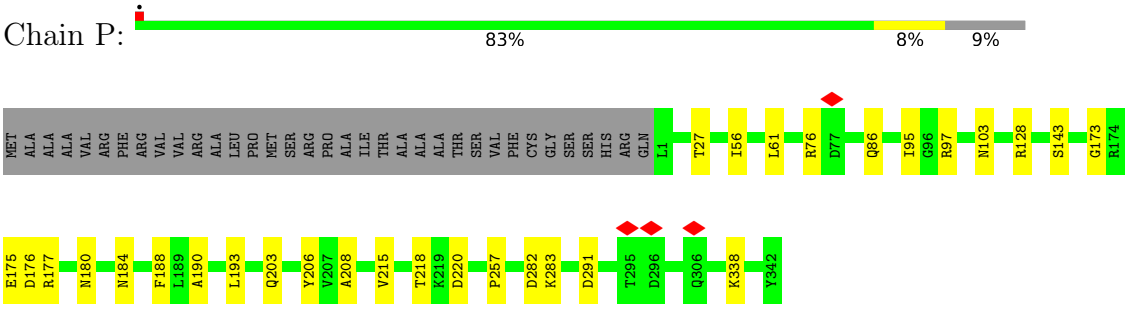


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



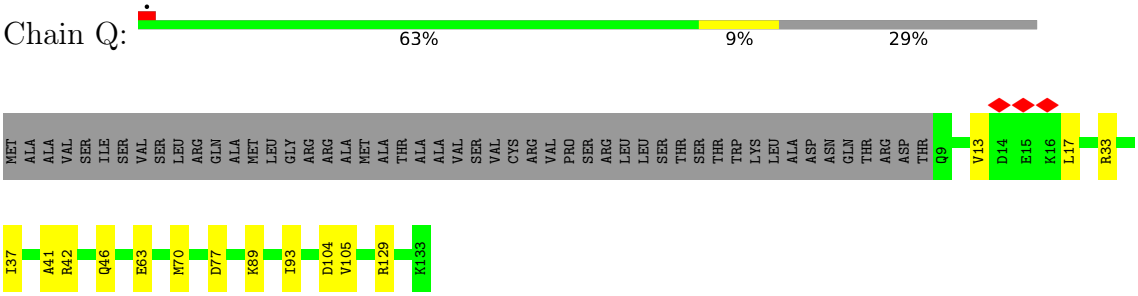
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



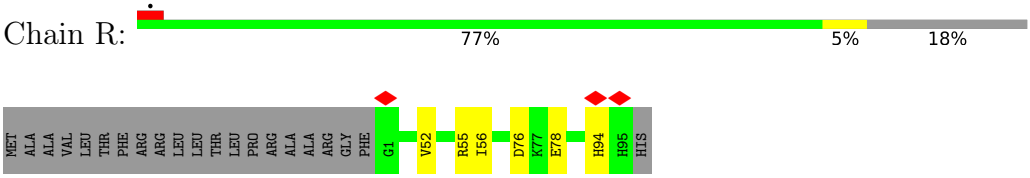
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



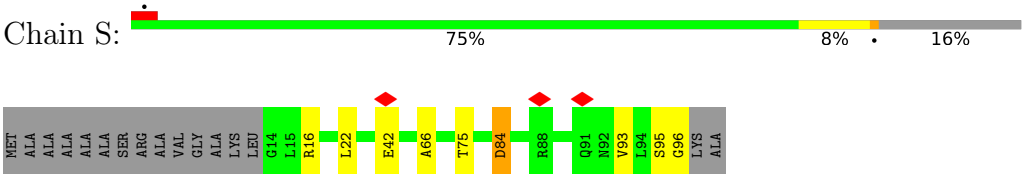
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



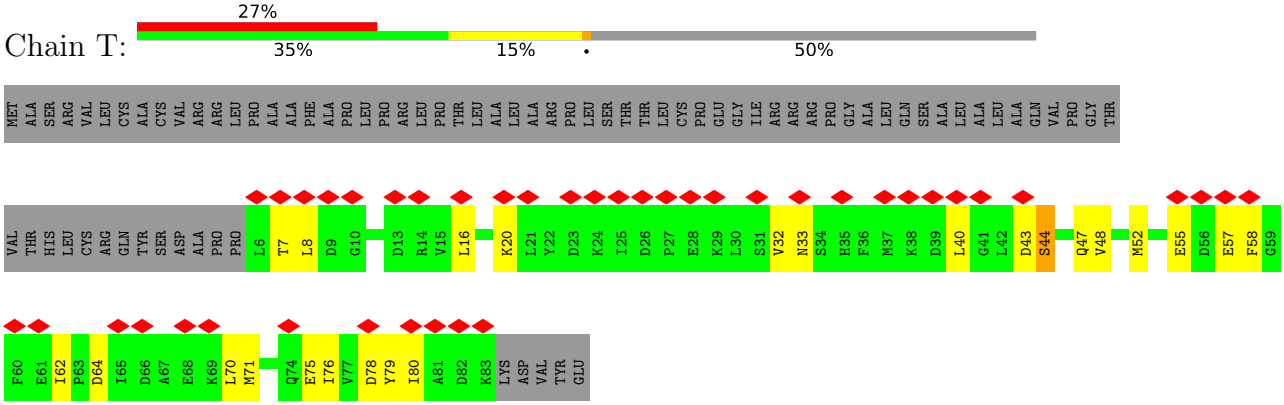
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



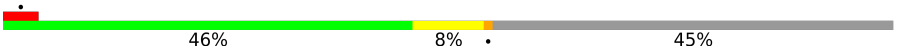
• Molecule 20: Acyl carrier protein, mitochondrial

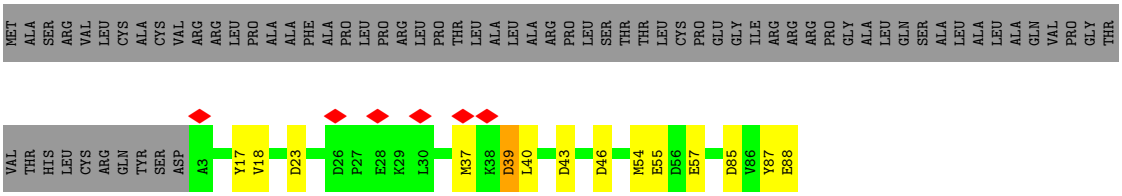
Chain T:



• Molecule 20: Acyl carrier protein, mitochondrial

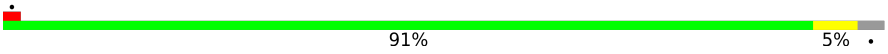
Chain U:

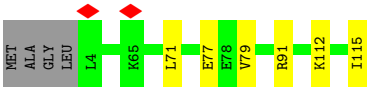




• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:

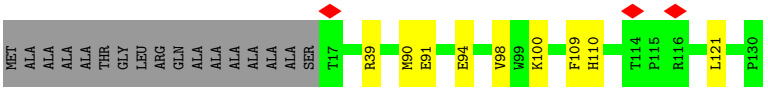




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:





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

Chain X:

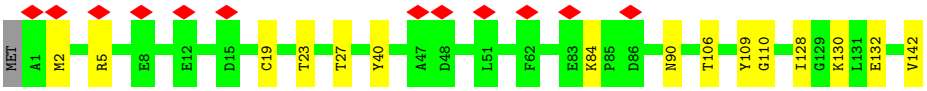




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:





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

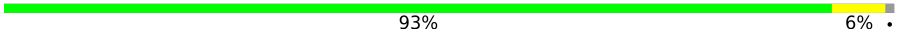
Chain Z:

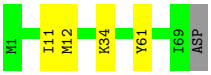




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:





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

Chain b:





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

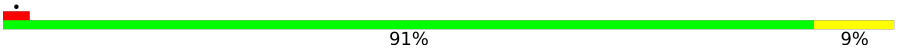
Chain c:

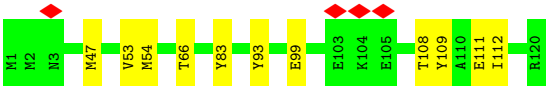




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

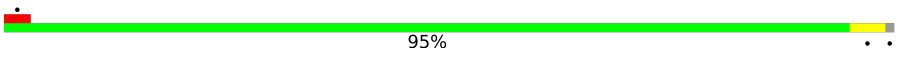
Chain d:





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

Chain e:

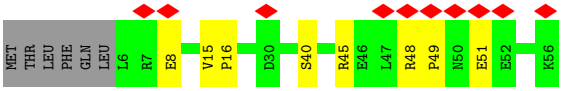




• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:

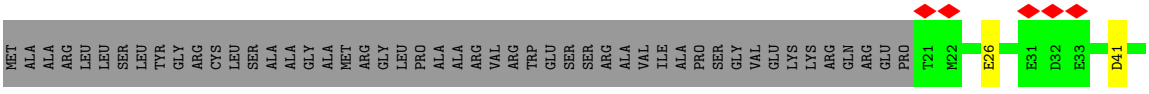


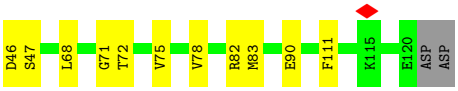


• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:





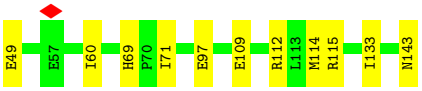


• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



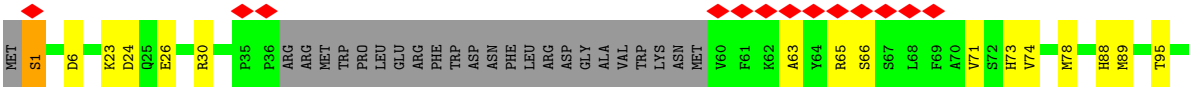


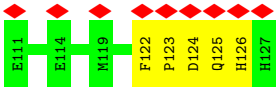


• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



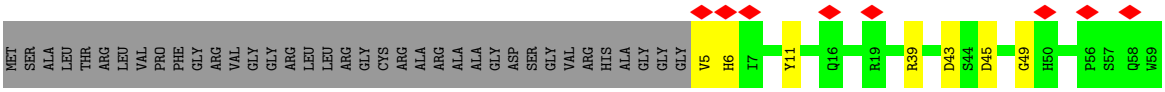


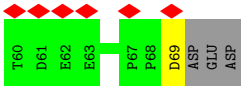


• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



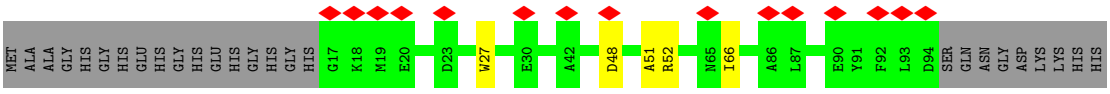




• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:

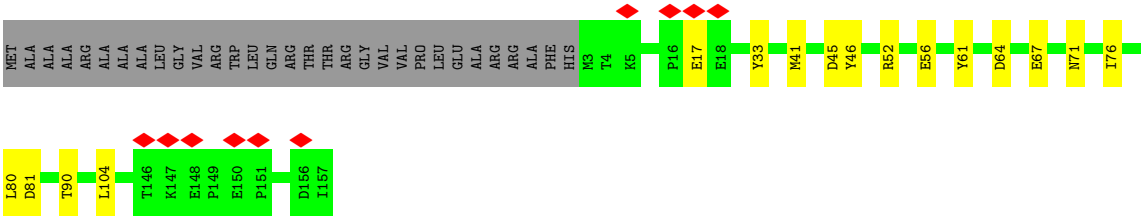




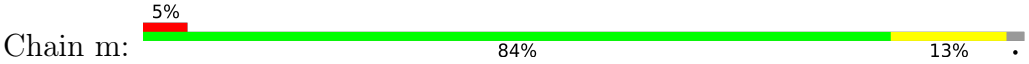
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

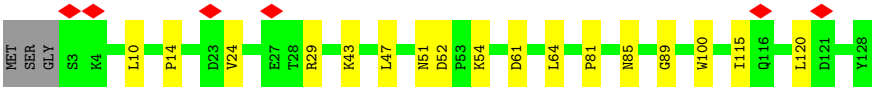
Chain l:



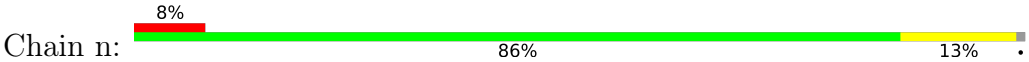


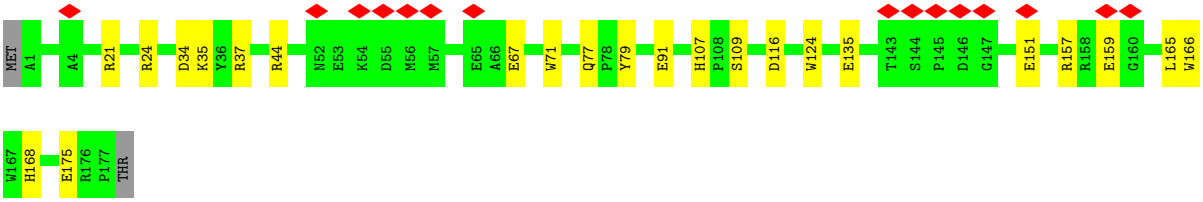
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



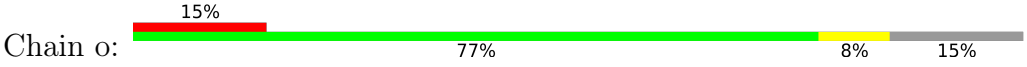


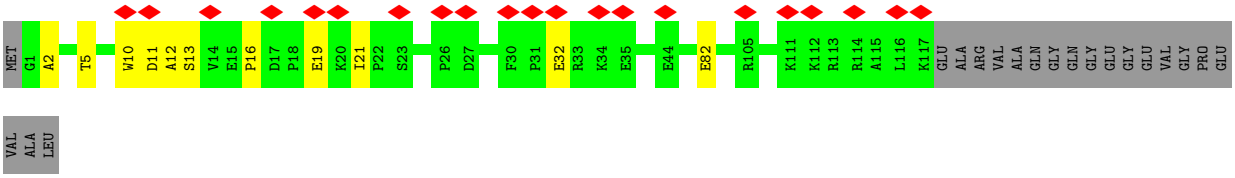
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



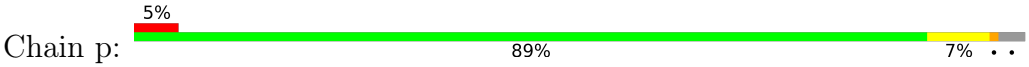


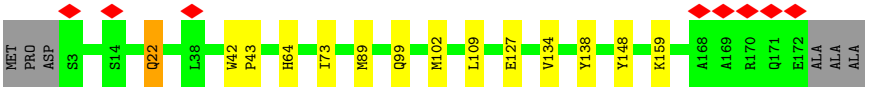
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7, METHYLGLYOXAL BIS-(GUANYLHYDRAZONE), NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



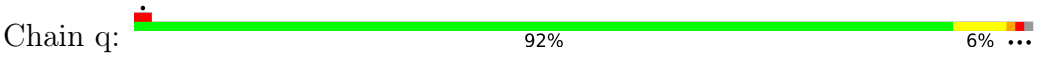


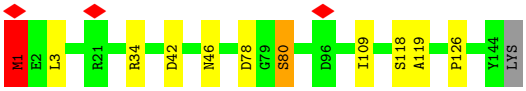
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10





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

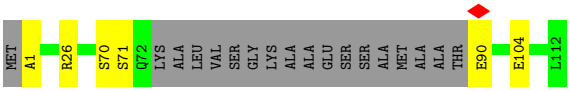




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



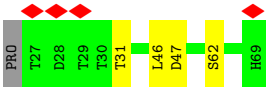


• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50, 46	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	47600	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.386	Depositor
Minimum map value	-0.195	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	535.5, 535.5, 535.5	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0625, 1.0625, 1.0625	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: CDL, 3PE, ZN, MG, EHZ, MYR, AME, NA, SF4, LMT, SAC, PC1, FMN, NDP, AYA, GTP, HQH, FME, FES, 2MR

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	0.35	0/949	0.35	0/1297
2	B	0.44	0/1278	0.40	0/1730
3	C	0.39	0/1780	0.40	0/2424
4	D	0.39	0/3540	0.38	0/4795
5	E	0.34	0/1700	0.39	0/2316
6	F	0.36	0/3396	0.38	0/4586
7	G	0.37	0/5383	0.38	0/7293
8	H	0.38	0/2607	0.37	0/3564
9	I	0.43	0/1461	0.40	0/1974
10	J	0.35	0/1330	0.33	0/1810
11	K	0.37	0/738	0.33	0/1002
12	L	0.36	0/4913	0.36	0/6686
13	M	0.38	0/3709	0.35	0/5052
14	N	0.37	0/2755	0.35	0/3751
15	O	0.38	0/2674	0.35	0/3626
16	P	0.36	0/2823	0.35	0/3828
17	Q	0.37	0/1038	0.34	0/1401
18	R	0.38	0/762	0.32	0/1026
19	S	0.32	0/674	0.38	0/909
20	T	0.30	0/637	0.36	0/858
20	U	0.34	0/704	0.32	0/951
21	V	0.36	0/937	0.30	0/1270
22	W	0.39	0/993	0.38	0/1335
23	X	0.36	0/1434	0.36	0/1937
24	Y	0.35	0/1074	0.33	0/1456
25	Z	0.37	0/1192	0.36	0/1608
26	a	0.39	0/577	0.35	0/777
27	b	0.34	0/671	0.36	0/921
28	c	0.36	0/409	0.32	0/555
29	d	0.37	0/1028	0.35	0/1387
30	e	0.37	0/900	0.37	0/1199

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
31	f	0.32	0/451	0.37	0/607
32	g	0.37	0/870	0.37	0/1185
33	h	0.39	0/1197	0.34	0/1621
34	i	0.36	0/889	0.40	0/1210
35	j	0.36	0/587	0.37	0/804
36	k	0.33	0/650	0.36	0/878
37	l	0.37	0/1356	0.36	0/1851
38	m	0.37	0/1079	0.40	0/1463
39	n	0.37	0/1589	0.37	0/2152
40	o	0.35	0/1030	0.40	0/1382
41	p	0.36	0/1472	0.36	0/1989
42	q	0.37	0/1234	0.35	0/1681
43	r	0.37	0/777	0.38	0/1051
44	s	0.31	0/371	0.37	0/504
All	All	0.37	0/67618	0.37	0/91702

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
34	i	0	1
42	q	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	i	1	SAC	Mainchain
42	q	1	AME	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	933	0	969	18	0
2	B	1247	0	1255	23	0
3	C	1730	0	1686	16	0
4	D	3464	0	3416	38	0
5	E	1660	0	1653	22	0
6	F	3321	0	3278	44	0
7	G	5296	0	5322	64	0
8	H	2540	0	2626	39	0
9	I	1431	0	1383	21	0
10	J	1308	0	1319	31	0
11	K	737	0	768	16	0
12	L	4800	0	4985	85	0
13	M	3632	0	3853	59	0
14	N	2703	0	2902	55	0
15	O	2607	0	2566	34	0
16	P	2748	0	2768	18	0
17	Q	1015	0	1016	12	0
18	R	748	0	724	3	0
19	S	663	0	677	7	0
20	T	628	0	626	19	0
20	U	692	0	686	14	0
21	V	915	0	954	4	0
22	W	970	0	991	7	0
23	X	1396	0	1383	17	0
24	Y	1050	0	1039	12	0
25	Z	1161	0	1161	10	0
26	a	564	0	579	3	0
27	b	648	0	652	6	0
28	c	398	0	401	4	0
29	d	996	0	1001	9	0
30	e	877	0	871	4	0
31	f	439	0	433	5	0
32	g	842	0	779	11	0
33	h	1162	0	1163	11	0
34	i	869	0	863	18	0
35	j	562	0	515	5	0
36	k	630	0	623	7	0
37	l	1302	0	1197	13	0
38	m	1050	0	1061	15	0
39	n	1534	0	1466	21	0
40	o	1005	0	996	7	0
41	p	1439	0	1408	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	q	1203	0	1158	9	0
43	r	767	0	793	4	0
44	s	361	0	338	4	0
45	A	70	0	87	0	0
45	J	70	0	88	0	0
45	K	35	0	43	0	0
45	L	70	0	87	2	0
45	M	35	0	41	1	0
45	O	35	0	45	1	0
45	P	35	0	45	0	0
45	Y	140	0	175	10	0
45	h	35	0	43	0	0
45	j	35	0	45	1	0
46	A	29	0	32	0	0
46	B	79	0	106	1	0
47	B	8	0	0	1	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	D	30	0	0	0	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	2	0
51	G	1	0	0	0	0
52	H	48	0	42	0	0
52	L	64	0	72	1	0
52	h	105	0	104	2	0
52	q	64	0	72	1	0
53	I	44	0	62	0	0
53	L	85	0	118	2	0
53	M	72	0	95	0	0
53	N	67	0	82	1	0
53	O	30	0	34	1	0
53	X	36	0	46	1	0
53	Z	72	0	92	0	0
53	d	33	0	40	1	0
53	i	30	0	34	0	0
53	r	45	0	64	0	0
54	O	1	0	0	0	0
55	O	32	0	12	5	0
56	P	48	0	26	1	0
57	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	T	37	0	0	0	0
58	U	37	0	0	1	0
59	o	15	0	27	0	0
60	A	1	0	0	0	0
60	B	33	0	0	5	0
60	C	25	0	0	2	0
60	D	46	0	0	5	0
60	E	1	0	0	0	0
60	F	3	0	0	0	0
60	G	43	0	0	6	0
60	H	8	0	0	1	0
60	I	40	0	0	3	0
60	J	3	0	0	0	0
60	K	1	0	0	0	0
60	L	3	0	0	0	0
60	M	3	0	0	0	0
60	N	4	0	0	0	0
60	O	5	0	0	1	0
60	P	13	0	0	3	0
60	Q	9	0	0	1	0
60	R	5	0	0	0	0
60	W	1	0	0	0	0
60	X	4	0	0	1	0
60	Z	5	0	0	1	0
60	a	2	0	0	0	0
60	d	1	0	0	0	0
60	e	2	0	0	0	0
60	g	1	0	0	0	0
60	h	3	0	0	0	0
60	i	1	0	0	0	0
60	l	3	0	0	1	0
60	m	1	0	0	0	0
60	n	1	0	0	0	0
60	p	1	0	0	0	0
60	q	5	0	0	0	0
60	r	3	0	0	0	0
All	All	68075	0	68181	730	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (730) 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)
13:M:231:LEU:HD23	13:M:235:LEU:HD12	1.37	1.05
2:B:121:ARG:O	60:B:301:HOH:O	1.87	0.93
4:D:114:ASN:ND2	60:D:703:HOH:O	2.01	0.93
7:G:161:ARG:NH1	60:G:906:HOH:O	2.06	0.89
10:J:168:GLU:OE1	10:J:171:ARG:NH2	2.07	0.86
53:X:201:3PE:O12	53:d:201:3PE:N	2.06	0.86
7:G:110:GLN:OE1	60:G:901:HOH:O	1.93	0.86
42:q:78:ASP:OD1	42:q:80:SER:OG	1.92	0.86
7:G:113:GLU:OE2	60:G:902:HOH:O	1.93	0.86
2:B:79:MET:HE1	2:B:86:PHE:CD2	2.10	0.86
16:P:86:GLN:OE1	60:P:601:HOH:O	1.92	0.86
12:L:427:ILE:O	12:L:431:THR:OG1	1.94	0.85
7:G:366:THR:O	7:G:367:THR:OG1	1.93	0.84
12:L:587:TYR:OH	14:N:117:GLU:OE1	1.93	0.84
15:O:83:TYR:OH	55:O:502:GTP:O2'	1.96	0.84
15:O:273:THR:O	60:O:601:HOH:O	1.95	0.83
4:D:393:ALA:O	60:D:701:HOH:O	1.95	0.83
16:P:338:LYS:O	60:P:602:HOH:O	1.94	0.83
1:A:71:LEU:O	10:J:145:TYR:OH	1.97	0.83
34:i:63:ALA:O	34:i:66:SER:N	2.12	0.82
7:G:244:THR:O	60:G:903:HOH:O	1.96	0.82
6:F:366:ARG:NH1	7:G:155:GLN:OE1	2.12	0.82
15:O:80:GLU:N	15:O:80:GLU:OE1	2.12	0.81
21:V:112:LYS:NZ	21:V:115:ILE:O	2.12	0.81
20:T:57:GLU:N	20:T:57:GLU:OE2	2.13	0.81
6:F:9:LYS:NZ	6:F:11:SER:O	2.14	0.81
21:V:77:GLU:OE2	21:V:77:GLU:N	2.14	0.81
37:l:41:MET:SD	38:m:85:ASN:ND2	2.54	0.81
25:Z:51:ARG:O	60:Z:301:HOH:O	1.98	0.81
8:H:24:GLU:OE1	8:H:228:TYR:OH	2.00	0.79
20:U:87:TYR:OH	34:i:26:GLU:OE2	1.99	0.79
24:Y:130:LYS:NZ	45:Y:203:LMT:O3'	2.13	0.79
17:Q:41:ALA:O	60:Q:201:HOH:O	1.99	0.79
4:D:14:PHE:O	60:D:702:HOH:O	2.00	0.78
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.15	0.78
23:X:49:GLU:OE2	23:X:134:ARG:NH1	2.17	0.77
4:D:143:GLU:OE2	4:D:278:TYR:OH	2.02	0.77
9:I:9:GLU:N	9:I:9:GLU:OE1	2.17	0.77
11:K:70:GLU:OE1	11:K:70:GLU:N	2.18	0.77
14:N:221:LEU:HD22	14:N:240:MET:HE2	1.66	0.77
20:U:55:GLU:OE1	39:n:24:ARG:NH2	2.18	0.77
3:C:49:GLU:OE2	3:C:106:ARG:NH1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:8:GLU:N	31:f:8:GLU:OE1	2.18	0.77
12:L:539:MET:SD	38:m:10:LEU:HD21	2.26	0.76
2:B:48:ASN:OD1	60:B:302:HOH:O	2.03	0.76
5:E:30:ARG:NH2	44:s:47:ASP:OD1	2.18	0.76
7:G:47:SER:OG	60:G:905:HOH:O	1.99	0.76
4:D:284:ASP:OD1	9:I:1:THR:OG1	2.03	0.76
14:N:298:TYR:O	14:N:303:THR:OG1	2.04	0.76
20:U:57:GLU:OE1	35:j:11:TYR:OH	2.04	0.76
13:M:244:ILE:O	41:p:148:TYR:OH	2.04	0.75
45:Y:201:LMT:O6'	45:Y:201:LMT:O5B	2.05	0.75
7:G:415:LEU:O	7:G:416:THR:OG1	2.01	0.74
20:T:75:GLU:OE1	20:T:75:GLU:N	2.18	0.74
15:O:38:LEU:HD23	15:O:172:ILE:HD11	1.68	0.74
6:F:82:MET:SD	6:F:221:THR:OG1	2.44	0.74
6:F:84:LYS:NZ	6:F:211:ALA:O	2.20	0.74
6:F:338:ASP:O	6:F:341:THR:HG22	1.88	0.74
34:i:125:GLN:O	34:i:126:HIS:ND1	2.21	0.73
33:h:39:GLY:O	33:h:43:VAL:HG23	1.88	0.73
40:o:2:ALA:O	40:o:5:THR:OG1	2.05	0.73
8:H:181:MET:SD	8:H:300:LEU:HD13	2.27	0.73
53:L:703:3PE:O11	45:Y:201:LMT:O4'	2.06	0.73
20:T:64:ASP:OD2	22:W:39:ARG:NH1	2.21	0.73
7:G:569:LYS:NZ	7:G:596:ASP:OD2	2.19	0.73
16:P:180:ASN:O	16:P:184:ASN:ND2	2.21	0.73
43:r:90:GLU:N	43:r:90:GLU:OE1	2.21	0.73
2:B:126:MET:SD	2:B:166:LEU:HD13	2.29	0.72
9:I:164:GLU:OE1	60:I:301:HOH:O	2.05	0.72
16:P:76:ARG:NH2	16:P:103:ASN:O	2.22	0.72
23:X:102:GLN:N	23:X:102:GLN:OE1	2.22	0.72
40:o:32:GLU:N	40:o:32:GLU:OE1	2.22	0.72
12:L:25:ASN:OD1	12:L:28:LYS:NZ	2.14	0.72
4:D:145:THR:HG1	4:D:181:TYR:HH	1.36	0.72
20:T:76:ILE:O	20:T:80:ILE:HD12	1.88	0.72
7:G:97:LEU:O	60:G:907:HOH:O	2.06	0.71
7:G:352:GLU:N	7:G:352:GLU:OE2	2.23	0.71
25:Z:130:GLU:N	25:Z:130:GLU:OE1	2.23	0.71
29:d:109:TYR:O	41:p:159:LYS:NZ	2.24	0.71
30:e:21:SER:OG	33:h:133:ILE:HG23	1.90	0.70
6:F:358:SER:OG	6:F:365:CYS:SG	2.45	0.70
8:H:95:LEU:O	60:H:501:HOH:O	2.07	0.70
12:L:102:GLN:OE1	12:L:456:ARG:NH2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:88:GLU:OE1	34:i:23:LYS:NZ	2.24	0.70
14:N:58:LYS:NZ	14:N:117:GLU:OE2	2.22	0.70
12:L:89:PHE:CE2	12:L:132:THR:HG21	2.27	0.70
40:o:11:ASP:OD1	40:o:12:ALA:N	2.25	0.70
9:I:55:GLU:OE2	42:q:34:ARG:NH1	2.25	0.69
6:F:224:ASN:ND2	50:F:502:FMN:O2	2.24	0.69
20:U:23:ASP:OD1	36:k:52:ARG:NH2	2.25	0.69
24:Y:109:TYR:N	45:Y:201:LMT:O6B	2.24	0.69
39:n:107:HIS:ND1	39:n:109:SER:OG	2.25	0.69
4:D:342:MET:HE2	7:G:101:HIS:HD2	1.57	0.69
12:L:359:MET:O	12:L:436:ARG:NH1	2.26	0.68
42:q:3:LEU:HD11	52:q:501:CDL:C31	2.23	0.68
10:J:76:GLU:N	10:J:76:GLU:OE1	2.27	0.68
53:N:402:3PE:N	53:O:504:3PE:O12	2.24	0.68
12:L:594:ASN:OD1	24:Y:40:TYR:OH	2.04	0.68
45:L:701:LMT:O3'	13:M:144:ASN:ND2	2.27	0.67
4:D:203:LEU:O	60:D:704:HOH:O	2.11	0.67
58:U:201:EHZ:O3	58:U:201:EHZ:N2	2.21	0.67
14:N:108:LEU:HD13	14:N:191:LEU:HD22	1.77	0.67
28:c:41:GLU:OE2	28:c:45:ARG:NE	2.28	0.67
39:n:34:ASP:OD1	39:n:35:LYS:N	2.27	0.67
7:G:486:GLU:OE1	7:G:486:GLU:N	2.27	0.66
32:g:46:ASP:OD1	32:g:47:SER:N	2.28	0.66
40:o:11:ASP:OD1	40:o:13:SER:N	2.26	0.66
5:E:53:LEU:HD13	44:s:46:LEU:HD13	1.76	0.66
15:O:170:ILE:HD11	15:O:238:ILE:HD11	1.77	0.66
2:B:153:ASP:OD2	60:B:303:HOH:O	2.14	0.66
13:M:324:SER:OG	13:M:440:HIS:NE2	2.24	0.66
37:l:71:ASN:O	60:l:201:HOH:O	2.14	0.65
7:G:324:ASP:HB3	7:G:571:ALA:HB1	1.79	0.65
20:U:46:ASP:OD1	39:n:44:ARG:NH2	2.30	0.65
9:I:14:VAL:HG23	9:I:14:VAL:O	1.96	0.65
12:L:365:ILE:HD12	12:L:443:ILE:HD13	1.80	0.64
2:B:79:MET:HE1	2:B:86:PHE:CE2	2.32	0.64
8:H:32:GLN:OE1	8:H:34:ARG:NH2	2.28	0.64
12:L:248:HIS:O	12:L:249:SER:OG	2.12	0.64
6:F:194:GLU:OE2	6:F:204:ARG:NE	2.29	0.64
12:L:362:ILE:HD13	12:L:365:ILE:HD11	1.80	0.64
20:U:85:ASP:OD2	39:n:175:GLU:N	2.26	0.64
23:X:48:GLU:OE1	23:X:134:ARG:NH2	2.31	0.64
25:Z:49:MET:HE2	25:Z:49:MET:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:179:GLU:OE1	43:r:26:ARG:NH1	2.29	0.63
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.79	0.63
27:b:59:ASP:OD1	27:b:60:GLY:N	2.31	0.63
20:T:55:GLU:OE2	20:T:62:ILE:N	2.31	0.63
24:Y:2:MET:O	24:Y:5:ARG:N	2.32	0.63
6:F:257:ASN:ND2	6:F:267:THR:OG1	2.32	0.63
8:H:24:GLU:HG3	8:H:271:LEU:HD22	1.79	0.63
5:E:204:GLU:OE2	5:E:207:LYS:NZ	2.31	0.63
7:G:160:ILE:HD11	7:G:183:VAL:HG13	1.80	0.63
12:L:3:ILE:HG23	12:L:53:MET:HE1	1.79	0.63
40:o:16:PRO:HB2	40:o:21:ILE:HD11	1.81	0.63
41:p:22:GLN:O	41:p:22:GLN:NE2	2.32	0.63
1:A:73:LEU:O	8:H:160:TYR:OH	2.14	0.63
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.79	0.63
13:M:48:ASN:ND2	41:p:89:MET:SD	2.72	0.62
6:F:197:GLU:OE2	17:Q:129:ARG:NH1	2.32	0.62
8:H:117:LEU:HD11	10:J:64:LEU:HD12	1.81	0.62
3:C:95:ASN:ND2	60:C:301:HOH:O	2.32	0.62
7:G:317:ALA:HB1	7:G:331:LEU:HD21	1.81	0.62
37:l:17:GLU:OE1	37:l:17:GLU:N	2.32	0.62
14:N:128:LEU:O	14:N:132:THR:OG1	2.11	0.62
6:F:109:GLU:OE1	6:F:112:ARG:NH1	2.32	0.61
13:M:418:LYS:NZ	39:n:91:GLU:OE2	2.31	0.61
23:X:108:GLN:NE2	23:X:112:ASP:OD1	2.33	0.61
12:L:365:ILE:HD12	12:L:443:ILE:CD1	2.29	0.61
7:G:227:SER:O	7:G:253:ARG:NH1	2.32	0.61
12:L:589:MET:HE3	12:L:592:LEU:HD23	1.82	0.61
13:M:395:LEU:HD21	38:m:100:TRP:CZ2	2.35	0.61
12:L:40:ILE:CD1	12:L:101:MET:HE3	2.30	0.61
7:G:45:ARG:HE	7:G:261:GLU:CD	2.09	0.61
5:E:104:THR:OG1	6:F:349:ARG:NH2	2.33	0.61
23:X:129:LYS:NZ	27:b:62:MET:O	2.32	0.61
4:D:218:PHE:CE2	4:D:222:ILE:HD11	2.36	0.60
38:m:47:LEU:HB3	39:n:165:LEU:HD13	1.82	0.60
5:E:165:THR:HG22	5:E:166:PRO:HD2	1.82	0.60
12:L:341:MET:HE1	12:L:453:PRO:HB2	1.83	0.60
14:N:142:LEU:HB3	14:N:194:LEU:HD21	1.82	0.60
38:m:61:ASP:OD2	38:m:64:LEU:N	2.31	0.60
13:M:302:MET:HA	13:M:302:MET:HE2	1.82	0.60
4:D:343:GLU:N	4:D:343:GLU:OE1	2.35	0.60
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:589:MET:CE	12:L:592:LEU:HD23	2.32	0.59
36:k:48:ASP:OD1	39:n:37:ARG:NE	2.27	0.59
1:A:68:GLU:CG	10:J:159:LEU:HD13	2.31	0.59
16:P:143:SER:OG	16:P:282:ASP:OD1	2.20	0.59
1:A:68:GLU:HG2	10:J:159:LEU:HD13	1.83	0.59
4:D:81:GLY:N	4:D:429:ASP:OD1	2.26	0.59
20:T:16:LEU:HD23	20:T:16:LEU:O	2.02	0.59
23:X:43:MET:HE3	23:X:47:TRP:HZ3	1.67	0.59
6:F:49:LEU:HD11	6:F:123:LEU:HD21	1.85	0.59
10:J:66:VAL:HG11	11:K:31:LEU:HD21	1.84	0.59
26:a:34:LYS:NZ	26:a:61:TYR:O	2.34	0.59
43:r:70:SER:OG	43:r:71:SER:N	2.35	0.59
12:L:22:SER:HA	12:L:27:ILE:HD12	1.84	0.58
12:L:574:THR:OG1	14:N:167:TRP:O	2.13	0.58
15:O:286:ALA:O	15:O:290:SER:OG	2.12	0.58
40:o:82:GLU:N	40:o:82:GLU:OE1	2.36	0.58
15:O:128:ILE:HD12	15:O:160:LEU:HD12	1.85	0.58
12:L:44:PHE:O	12:L:47:SER:OG	2.18	0.58
7:G:429:LEU:HD22	7:G:470:VAL:HG22	1.86	0.58
11:K:37:VAL:HG11	11:K:67:ALA:CB	2.34	0.57
7:G:140:LYS:O	7:G:148:THR:OG1	2.21	0.57
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.34	0.57
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.39	0.57
20:T:43:ASP:OD1	20:T:44:SER:N	2.37	0.57
22:W:91:GLU:OE1	22:W:100:LYS:NZ	2.23	0.57
37:l:52:ARG:NH1	37:l:56:GLU:OE1	2.34	0.57
20:T:16:LEU:HD21	20:T:20:LYS:HE3	1.86	0.57
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.86	0.57
15:O:146:LYS:NZ	15:O:150:ASP:OD1	2.37	0.57
4:D:322:GLU:OE2	4:D:322:GLU:N	2.37	0.57
38:m:52:ASP:OD1	38:m:54:LYS:N	2.34	0.57
4:D:165:THR:OG1	8:H:275:ALA:O	2.20	0.57
17:Q:13:VAL:HG23	17:Q:13:VAL:O	2.05	0.57
30:e:3:LEU:O	30:e:5:ILE:N	2.35	0.57
20:T:48:VAL:HG12	20:T:52:MET:HE2	1.86	0.56
6:F:157:TYR:OH	6:F:174:ASP:OD1	2.22	0.56
7:G:82:ASN:O	7:G:87:LYS:NZ	2.37	0.56
7:G:514:ILE:HG23	7:G:519:PRO:HD3	1.87	0.56
10:J:27:TYR:CE2	10:J:81:THR:HG22	2.40	0.56
13:M:106:LEU:HD13	13:M:234:ILE:HG21	1.86	0.56
13:M:328:CYS:SG	13:M:436:LEU:HD21	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:195:THR:HG22	15:O:197:ALA:H	1.71	0.56
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.39	0.56
23:X:43:MET:HE3	23:X:47:TRP:CZ3	2.40	0.56
34:i:30:ARG:NH2	39:n:116:ASP:OD2	2.36	0.56
8:H:28:LEU:HD23	8:H:275:ALA:HB2	1.88	0.56
16:P:215:VAL:O	16:P:218:THR:OG1	2.23	0.56
6:F:169:SER:O	6:F:170:ASP:CB	2.54	0.56
40:o:19:GLU:N	40:o:19:GLU:OE2	2.35	0.56
23:X:8:THR:OG1	23:X:10:GLU:OE2	2.23	0.56
37:l:33:TYR:OH	37:l:45:ASP:O	2.17	0.56
12:L:378:LEU:HD23	12:L:383:MET:SD	2.46	0.55
13:M:37:THR:O	13:M:40:THR:HG22	2.06	0.55
5:E:66:MET:HE3	5:E:84:ALA:CB	2.37	0.55
12:L:4:PHE:HZ	12:L:87:ILE:HD11	1.71	0.55
6:F:68:ARG:NH2	6:F:253:THR:O	2.39	0.55
16:P:27:THR:HG22	16:P:56:ILE:HG22	1.88	0.55
37:l:76:ILE:HG23	37:l:80:LEU:HD22	1.89	0.55
10:J:54:MET:HE1	10:J:57:LEU:HD12	1.89	0.55
11:K:33:LEU:HD23	11:K:36:MET:CE	2.37	0.55
14:N:285:MET:CE	14:N:288:LEU:HD12	2.37	0.54
13:M:138:ASN:ND2	13:M:334:TYR:OH	2.39	0.54
25:Z:86:LEU:HD11	25:Z:118:PRO:HG3	1.88	0.54
32:g:68:LEU:O	32:g:72:THR:OG1	2.11	0.54
42:q:118:SER:O	42:q:119:ALA:HB3	2.05	0.54
6:F:302:SER:CB	6:F:350:LEU:HD22	2.36	0.54
10:J:151:MET:CE	14:N:28:LEU:HD21	2.38	0.54
19:S:84:ASP:OD1	19:S:84:ASP:N	2.39	0.54
4:D:326:ASP:OD1	7:G:127:ARG:NH2	2.39	0.54
4:D:342:MET:HE2	7:G:101:HIS:CD2	2.42	0.54
13:M:324:SER:HG	13:M:440:HIS:CD2	2.24	0.54
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.38	0.54
25:Z:93:GLU:OE2	30:e:74:ARG:NH2	2.40	0.54
27:b:64:ASP:N	27:b:64:ASP:OD1	2.40	0.54
52:h:202:CDL:OB3	34:i:88:HIS:NE2	2.41	0.54
34:i:71:VAL:HG12	34:i:71:VAL:O	2.07	0.54
8:H:18:ALA:O	8:H:21:THR:OG1	2.17	0.54
12:L:570:HIS:ND1	14:N:288:LEU:HD11	2.23	0.54
10:J:54:MET:CE	10:J:57:LEU:HD12	2.37	0.54
6:F:145:GLU:OE2	6:F:145:GLU:N	2.40	0.54
10:J:85:ASN:HB3	10:J:88:ILE:HG22	1.90	0.54
14:N:313:MET:HG3	15:O:99:TRP:CH2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:341:MET:HE2	12:L:454:ILE:CG1	2.38	0.53
16:P:95:ILE:O	60:P:604:HOH:O	2.19	0.53
2:B:164:GLU:OE2	9:I:57:GLY:N	2.32	0.53
7:G:429:LEU:CD2	7:G:470:VAL:HG22	2.38	0.53
2:B:162:THR:HG23	60:B:331:HOH:O	2.09	0.53
7:G:229:ASP:OD2	7:G:267:THR:OG1	2.27	0.53
29:d:112:ILE:O	41:p:159:LYS:NZ	2.39	0.53
33:h:109:GLU:OE2	33:h:112:ARG:NH1	2.39	0.53
6:F:306:LEU:C	6:F:306:LEU:HD12	2.33	0.53
12:L:73:SER:O	12:L:73:SER:OG	2.23	0.53
6:F:226:GLU:OE2	6:F:254:LYS:NZ	2.41	0.53
12:L:40:ILE:HD11	12:L:101:MET:HE3	1.91	0.53
12:L:319:MET:HE2	12:L:399:ILE:HD13	1.91	0.53
32:g:111:PHE:CE1	41:p:73:ILE:HG22	2.43	0.53
2:B:92:GLN:NE2	8:H:215:TYR:O	2.35	0.53
4:D:350:LYS:NZ	60:D:708:HOH:O	2.29	0.53
8:H:26:LYS:NZ	8:H:37:PRO:O	2.25	0.53
14:N:146:TYR:N	14:N:147:PRO:HD2	2.24	0.53
15:O:15:THR:OG1	15:O:253:ASP:OD1	2.15	0.53
24:Y:84:LYS:O	24:Y:90:ASN:ND2	2.40	0.53
13:M:310:MET:HE1	13:M:380:PHE:CE1	2.44	0.52
14:N:25:ASN:HB3	14:N:28:LEU:HD23	1.91	0.52
3:C:77:ASP:OD1	3:C:77:ASP:N	2.42	0.52
38:m:24:VAL:HG22	38:m:24:VAL:O	2.09	0.52
2:B:65:CYS:HB3	2:B:126:MET:HE3	1.92	0.52
37:l:46:TYR:OH	37:l:76:ILE:O	2.21	0.52
7:G:674:THR:O	7:G:679:ARG:NH1	2.43	0.52
8:H:97:ASN:ND2	8:H:163:GLN:OE1	2.40	0.52
19:S:66:ALA:HB2	19:S:93:VAL:HG11	1.92	0.52
7:G:108:CYS:O	7:G:218:ARG:NH2	2.39	0.52
7:G:185:THR:O	7:G:187:ILE:N	2.42	0.52
18:R:76:ASP:O	18:R:78:GLU:N	2.43	0.52
17:Q:33:ARG:NH1	17:Q:77:ASP:OD1	2.38	0.52
24:Y:106:THR:HG22	24:Y:106:THR:O	2.10	0.52
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.91	0.51
7:G:366:THR:HG22	7:G:370:GLY:HA3	1.91	0.51
14:N:19:ILE:O	14:N:23:SER:OG	2.25	0.51
38:m:51:ASN:OD1	39:n:168:HIS:ND1	2.43	0.51
4:D:152:MET:O	4:D:156:THR:OG1	2.13	0.51
13:M:225:ILE:HD13	13:M:331:ASN:HB2	1.91	0.51
4:D:44:VAL:O	4:D:44:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:190:MET:HB3	14:N:201:THR:HG23	1.92	0.51
7:G:9:ILE:HG22	7:G:75:LYS:HE3	1.93	0.51
12:L:424:MET:HE2	12:L:502:LEU:CD2	2.41	0.51
11:K:66:PHE:CZ	14:N:31:VAL:HG13	2.45	0.51
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.45	0.51
12:L:363:THR:HG22	36:k:66:ILE:HD13	1.91	0.51
11:K:75:LEU:O	11:K:79:VAL:HG23	2.10	0.51
12:L:361:ASN:OD1	36:k:66:ILE:HD11	2.10	0.51
13:M:44:GLN:NE2	13:M:48:ASN:O	2.42	0.51
13:M:176:LEU:O	13:M:180:SER:OG	2.24	0.51
7:G:613:TYR:CD2	7:G:619:VAL:HG22	2.45	0.51
14:N:25:ASN:OD1	14:N:27:MET:N	2.41	0.51
15:O:135:LEU:HD22	15:O:152:TYR:CG	2.46	0.51
12:L:601:LEU:C	12:L:601:LEU:HD23	2.36	0.50
2:B:101:THR:HA	2:B:129:CYS:HB3	1.92	0.50
12:L:363:THR:CG2	36:k:66:ILE:HD13	2.41	0.50
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.93	0.50
35:j:39:ARG:NH1	35:j:43:ASP:OD1	2.39	0.50
31:f:45:ARG:NH1	33:h:60:ILE:HG21	2.26	0.50
12:L:424:MET:HE2	12:L:502:LEU:HD22	1.93	0.50
15:O:70:ASP:OD1	15:O:71:ILE:N	2.45	0.50
32:g:90:GLU:OE1	41:p:64:HIS:NE2	2.33	0.50
8:H:200:LEU:HD21	8:H:280:PHE:O	2.12	0.50
12:L:341:MET:HE2	12:L:454:ILE:HG13	1.93	0.50
13:M:56:PHE:CE1	13:M:117:MET:HE1	2.47	0.50
14:N:131:LEU:HD12	14:N:216:PHE:CZ	2.47	0.50
19:S:22:LEU:HD23	19:S:22:LEU:N	2.26	0.50
7:G:339:ASP:OD1	19:S:16:ARG:NH2	2.40	0.50
10:J:62:GLY:O	10:J:66:VAL:HG23	2.12	0.50
4:D:183:ARG:NH1	4:D:210:ASP:OD2	2.45	0.50
12:L:64:THR:O	34:i:95:THR:HG23	2.11	0.50
12:L:230:HIS:N	12:L:231:PRO:CD	2.75	0.50
13:M:159:PRO:HD3	14:N:284:MET:HE2	1.94	0.50
15:O:188:ASP:OD2	15:O:191:GLU:N	2.39	0.50
16:P:188:PHE:O	16:P:190:ALA:N	2.40	0.50
4:D:202:ASP:OD1	4:D:203:LEU:N	2.45	0.49
12:L:327:LEU:O	12:L:331:THR:HG23	2.12	0.49
13:M:310:MET:SD	13:M:314:MET:HE2	2.52	0.49
20:T:40:LEU:HD12	20:T:40:LEU:H	1.77	0.49
7:G:424:ASP:OD1	7:G:425:SER:N	2.45	0.49
19:S:95:SER:OG	19:S:96:GLY:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:7:ASN:OD1	7:G:7:ASN:N	2.44	0.49
39:n:21:ARG:NH2	39:n:67:GLU:OE2	2.45	0.49
41:p:102:MET:SD	41:p:134:VAL:HG12	2.52	0.49
5:E:66:MET:HE3	5:E:84:ALA:HB3	1.94	0.49
24:Y:110:GLY:N	45:Y:201:LMT:O6B	2.39	0.49
2:B:64:CYS:HB3	4:D:108:TYR:HB2	1.93	0.49
7:G:231:MET:HE3	7:G:270:ALA:HB3	1.93	0.49
12:L:15:LEU:HD22	12:L:125:LEU:HD23	1.95	0.49
23:X:141:TYR:OH	33:h:143:ASN:O	2.19	0.49
37:l:56:GLU:OE2	37:l:90:THR:OG1	2.30	0.49
7:G:615:THR:O	7:G:619:VAL:HG23	2.12	0.49
12:L:89:PHE:CD2	12:L:132:THR:HG21	2.47	0.49
3:C:175:ARG:HE	3:C:186:GLU:CD	2.21	0.49
20:T:58:PHE:CD2	20:T:80:ILE:HG12	2.48	0.49
7:G:298:ASP:C	7:G:298:ASP:OD1	2.55	0.49
4:D:405:MET:HE2	4:D:417:ILE:HG23	1.93	0.48
9:I:161:ASP:OD1	60:I:302:HOH:O	2.19	0.48
10:J:168:GLU:HG3	14:N:5:THR:HG21	1.94	0.48
12:L:3:ILE:CG2	12:L:53:MET:HE1	2.43	0.48
15:O:151:HIS:CB	15:O:279:LEU:HD11	2.43	0.48
3:C:58:ILE:O	3:C:62:THR:OG1	2.20	0.48
7:G:205:VAL:HG23	7:G:207:ALA:H	1.79	0.48
13:M:46:ASP:HA	32:g:83:MET:HG3	1.94	0.48
13:M:130:LEU:O	13:M:134:THR:OG1	2.26	0.48
12:L:257:ILE:CG2	12:L:329:ILE:HD11	2.43	0.48
13:M:216:LEU:HB3	13:M:217:PRO:HD3	1.94	0.48
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.96	0.48
12:L:180:ILE:HD12	13:M:397:GLY:HA2	1.94	0.48
15:O:138:MET:HE3	55:O:502:GTP:HN21	1.78	0.48
34:i:24:ASP:OD2	39:n:124:TRP:NE1	2.40	0.48
5:E:192:CYS:SG	5:E:193:CYS:N	2.87	0.48
23:X:122:GLY:N	25:Z:65:GLU:OE2	2.43	0.48
19:S:42:GLU:N	19:S:42:GLU:OE1	2.46	0.48
5:E:149:VAL:HG23	5:E:150:ASN:OD1	2.12	0.48
12:L:17:SER:OG	12:L:18:PRO:HD3	2.14	0.48
20:U:39:ASP:OD1	20:U:39:ASP:N	2.46	0.48
6:F:131:ALA:O	6:F:171:TYR:OH	2.21	0.48
45:L:704:LMT:O5B	45:L:704:LMT:O6'	2.32	0.48
15:O:227:GLU:OE2	21:V:91:ARG:NH1	2.40	0.48
1:A:104:TYR:O	1:A:108:GLN:HG2	2.13	0.48
14:N:344:ILE:O	14:N:345:THR:OG1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:32:VAL:O	20:T:32:VAL:HG12	2.13	0.48
3:C:150:ARG:NH1	3:C:153:THR:OG1	2.46	0.48
3:C:178:ASP:O	3:C:181:LYS:NZ	2.43	0.48
12:L:552:LEU:HD21	38:m:89:GLY:HA2	1.95	0.48
5:E:53:LEU:CD1	44:s:46:LEU:HD13	2.44	0.47
6:F:384:ALA:HB3	6:F:430:MET:HE2	1.96	0.47
4:D:227:GLU:OE2	9:I:34:ARG:NE	2.47	0.47
7:G:595:GLU:OE2	7:G:597:TRP:NE1	2.47	0.47
11:K:33:LEU:HD23	11:K:36:MET:HE3	1.96	0.47
12:L:253:VAL:HB	12:L:310:LEU:HD11	1.95	0.47
32:g:41:ASP:OD1	32:g:41:ASP:N	2.47	0.47
2:B:81:ARG:HA	8:H:37:PRO:HA	1.95	0.47
9:I:131:ASP:N	9:I:131:ASP:OD1	2.47	0.47
12:L:14:LEU:HD21	34:i:73:HIS:O	2.13	0.47
13:M:378:GLU:O	13:M:382:THR:OG1	2.27	0.47
15:O:174:VAL:HG12	15:O:179:VAL:HG23	1.96	0.47
18:R:52:VAL:O	18:R:94:HIS:N	2.47	0.47
11:K:33:LEU:O	11:K:37:VAL:HG23	2.14	0.47
6:F:368:GLY:HA3	6:F:399:ILE:HD11	1.96	0.47
13:M:343:ILE:O	13:M:346:ARG:NH1	2.39	0.47
14:N:170:LEU:O	14:N:295:ARG:NH1	2.48	0.47
14:N:276:LEU:HD22	45:Y:202:LMT:H12	1.96	0.47
25:Z:93:GLU:OE2	25:Z:103:TRP:NE1	2.42	0.47
29:d:47:MET:HG3	29:d:53:VAL:HG22	1.97	0.47
30:e:21:SER:OG	30:e:21:SER:O	2.31	0.47
8:H:181:MET:HE1	8:H:304:HIS:NE2	2.30	0.47
10:J:73:MET:HE1	11:K:79:VAL:HG22	1.96	0.47
20:U:37:MET:HE1	20:U:43:ASP:O	2.15	0.47
2:B:189:ARG:NE	46:B:203:PC1:O12	2.48	0.47
4:D:241:ASP:OD1	4:D:290:ARG:NH2	2.40	0.47
12:L:288:THR:HG21	12:L:307:SER:HB3	1.96	0.47
53:L:703:3PE:O31	45:Y:201:LMT:O2B	2.33	0.47
14:N:25:ASN:OD1	14:N:26:LEU:N	2.48	0.47
15:O:252:ASP:OD1	15:O:252:ASP:N	2.46	0.47
13:M:11:LEU:HD11	13:M:34:ILE:CD1	2.45	0.47
23:X:164:THR:HG22	29:d:83:TYR:CE2	2.50	0.47
2:B:62:LEU:HB2	2:B:100:GLY:HA3	1.98	0.46
7:G:533:THR:HG22	7:G:534:ARG:N	2.30	0.46
15:O:138:MET:CE	55:O:502:GTP:HN21	2.28	0.46
15:O:252:ASP:OD1	15:O:255:THR:HG23	2.14	0.46
24:Y:110:GLY:H	45:Y:201:LMT:H6B	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:GLU:OE2	6:F:105:CYS:HA	2.15	0.46
15:O:170:ILE:CD1	15:O:238:ILE:HD11	2.43	0.46
4:D:300:ARG:NH2	4:D:420:THR:O	2.45	0.46
15:O:217:MET:HG3	15:O:218:CYS:SG	2.55	0.46
20:T:75:GLU:O	20:T:79:TYR:N	2.41	0.46
1:A:37:TYR:HE2	8:H:208:VAL:HG21	1.80	0.46
10:J:168:GLU:CG	14:N:5:THR:HG21	2.46	0.46
2:B:81:ARG:NH2	9:I:52:TYR:O	2.48	0.46
13:M:158:ILE:HB	13:M:159:PRO:HD3	1.98	0.46
37:l:61:TYR:OH	39:n:151:GLU:OE1	2.20	0.46
2:B:180:GLU:OE2	2:B:182:LYS:NZ	2.46	0.46
10:J:115:ILE:HD11	11:K:6:PHE:CD2	2.51	0.46
5:E:143:GLU:O	5:E:144:CYS:C	2.58	0.46
10:J:151:MET:HE1	14:N:28:LEU:HD21	1.97	0.46
12:L:288:THR:HG21	12:L:307:SER:CB	2.46	0.46
13:M:310:MET:HE1	13:M:380:PHE:CD1	2.49	0.46
4:D:62:LEU:HB2	4:D:425:PHE:CZ	2.51	0.46
13:M:269:MET:HE1	13:M:396:MET:HG2	1.98	0.46
20:T:7:THR:C	20:T:8:LEU:HD12	2.41	0.46
28:c:27:MET:HE3	29:d:66:THR:HG22	1.98	0.46
39:n:135:GLU:OE2	39:n:166:TRP:NE1	2.49	0.46
8:H:164:THR:HG22	8:H:164:THR:O	2.15	0.45
13:M:248:ILE:HG23	13:M:249:ILE:HG23	1.98	0.45
35:j:45:ASP:O	35:j:49:GLY:N	2.46	0.45
5:E:105:THR:HG22	5:E:106:THR:H	1.81	0.45
11:K:57:MET:N	11:K:58:PRO:CD	2.78	0.45
13:M:166:LEU:HD21	14:N:271:MET:SD	2.56	0.45
28:c:19:LEU:C	28:c:19:LEU:HD23	2.41	0.45
1:A:68:GLU:HG3	10:J:159:LEU:HD13	1.98	0.45
5:E:165:THR:O	5:E:168:ASP:N	2.46	0.45
6:F:97:ALA:HB1	6:F:111:MET:SD	2.56	0.45
11:K:5:PHE:HZ	11:K:47:THR:OG1	1.99	0.45
12:L:32:PHE:CD2	12:L:115:ASN:HB2	2.51	0.45
13:M:459:MET:O	32:g:82:ARG:NH1	2.46	0.45
17:Q:93:ILE:HD11	17:Q:105:VAL:HG21	1.97	0.45
3:C:112:ASP:OD2	3:C:115:THR:N	2.49	0.45
3:C:169:THR:HG21	3:C:190:LEU:HD11	1.98	0.45
9:I:88:ILE:O	9:I:89:CYS:C	2.60	0.45
12:L:539:MET:O	12:L:543:ASN:HB2	2.16	0.45
14:N:243:MET:HE2	14:N:330:ALA:HB1	1.98	0.45
23:X:152:VAL:HG12	23:X:153:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:562:ILE:HG22	12:L:563:PRO:N	2.31	0.45
12:L:578:THR:HG21	14:N:171:ASN:HD22	1.82	0.45
13:M:442:ILE:HG21	32:g:68:LEU:HD13	1.99	0.45
32:g:26:GLU:OE1	32:g:26:GLU:HA	2.16	0.45
12:L:187:VAL:O	12:L:191:LEU:HD13	2.17	0.45
20:U:17:TYR:HH	36:k:27:TRP:HE1	1.60	0.45
34:i:6:ASP:OD2	39:n:157:ARG:NH1	2.48	0.45
6:F:305:PRO:HD2	6:F:327:THR:HA	1.99	0.45
8:H:199:ASP:OD1	8:H:199:ASP:N	2.48	0.45
10:J:55:VAL:HB	11:K:41:PHE:CE2	2.52	0.45
12:L:171:ALA:O	12:L:175:ASN:ND2	2.45	0.45
12:L:254:VAL:HG11	12:L:329:ILE:HG23	1.98	0.45
52:L:705:CDL:CB5	52:L:705:CDL:OB8	2.65	0.45
14:N:131:LEU:HD12	14:N:216:PHE:HZ	1.81	0.45
21:V:71:LEU:HD13	21:V:79:VAL:HG11	1.98	0.45
23:X:14:VAL:HG22	23:X:15:GLU:H	1.81	0.45
12:L:241:THR:HG21	12:L:344:GLY:HA3	1.98	0.45
13:M:225:ILE:HG23	13:M:226:ALA:N	2.31	0.45
23:X:10:GLU:H	23:X:10:GLU:CD	2.25	0.45
2:B:137:HIS:NE2	60:B:305:HOH:O	2.23	0.45
7:G:147:LYS:HB2	7:G:211:LYS:HG3	1.98	0.45
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.99	0.45
13:M:11:LEU:HD11	13:M:34:ILE:HD12	1.99	0.45
31:f:45:ARG:NH2	31:f:51:GLU:OE1	2.49	0.45
1:A:69:ILE:HD11	8:H:148:ILE:HD11	1.98	0.44
17:Q:37:ILE:HB	17:Q:105:VAL:HG22	1.99	0.44
20:U:18:VAL:HB	20:U:54:MET:HE1	1.99	0.44
12:L:529:PHE:HB3	12:L:530:PRO:HD3	1.98	0.44
4:D:182:GLU:OE2	9:I:60:SER:OG	2.25	0.44
5:E:87:TYR:CG	6:F:181:ALA:HB3	2.52	0.44
14:N:45:ILE:O	14:N:48:LYS:HG2	2.17	0.44
16:P:128:ARG:NH2	16:P:220:ASP:O	2.48	0.44
42:q:42:ASP:OD1	42:q:46:ASN:N	2.51	0.44
6:F:242:PHE:CE2	6:F:252:GLY:HA3	2.52	0.44
7:G:307:LEU:N	7:G:521:MET:HE1	2.32	0.44
12:L:191:LEU:HD21	13:M:387:SER:HB3	1.98	0.44
14:N:5:THR:HG22	14:N:9:ILE:HD12	2.00	0.44
37:l:64:ASP:OD1	38:m:43:LYS:NZ	2.42	0.44
1:A:6:VAL:HG21	8:H:87:VAL:HG11	1.99	0.44
6:F:93:LEU:HD13	6:F:129:MET:HE1	1.98	0.44
12:L:250:SER:O	12:L:251:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:61:LEU:HD22	13:M:244:ILE:HG21	1.99	0.44
14:N:219:LEU:CD2	14:N:230:ILE:HD13	2.47	0.44
14:N:344:ILE:HG13	14:N:345:THR:N	2.32	0.44
13:M:207:MET:CB	13:M:298:ILE:HD11	2.47	0.44
14:N:285:MET:HE1	14:N:288:LEU:HD12	2.00	0.44
16:P:177:ARG:O	16:P:283:LYS:NZ	2.45	0.44
45:Y:201:LMT:H4'	38:m:81:PRO:HG2	2.00	0.44
27:b:27:LEU:O	27:b:31:MET:HG2	2.18	0.44
6:F:90:PRO:O	6:F:218:CYS:HB3	2.18	0.44
6:F:337:MET:HB3	6:F:341:THR:HG21	2.00	0.44
8:H:139:THR:HB	10:J:64:LEU:HD21	1.99	0.44
10:J:107:ASN:ND2	10:J:117:LEU:HD12	2.33	0.44
12:L:70:THR:HG23	12:L:75:GLU:HG2	2.00	0.44
14:N:307:THR:O	15:O:284:ILE:N	2.43	0.44
14:N:319:LYS:HG2	15:O:267:THR:HG21	1.99	0.44
1:A:73:LEU:N	1:A:74:PRO:CD	2.81	0.44
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.49	0.44
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.99	0.44
12:L:362:ILE:CD1	12:L:365:ILE:HD11	2.48	0.44
15:O:170:ILE:O	15:O:170:ILE:HG22	2.18	0.44
34:i:89:MET:O	34:i:95:THR:HB	2.18	0.44
9:I:66:GLU:O	9:I:136:GLY:N	2.45	0.44
11:K:59:ILE:HD13	14:N:84:TRP:CE2	2.53	0.44
14:N:323:ASN:OD1	14:N:323:ASN:N	2.44	0.44
23:X:14:VAL:HG22	23:X:15:GLU:N	2.32	0.44
36:k:48:ASP:OD2	36:k:51:ALA:N	2.51	0.44
5:E:165:THR:O	5:E:166:PRO:C	2.61	0.43
4:D:73:VAL:HG21	4:D:414:VAL:HG21	2.00	0.43
6:F:24:ASN:ND2	6:F:113:HIS:O	2.50	0.43
8:H:174:LEU:O	8:H:178:ALA:HB3	2.18	0.43
9:I:9:GLU:O	9:I:11:GLU:N	2.52	0.43
12:L:525:LEU:HD12	12:L:528:PHE:HE1	1.84	0.43
13:M:154:LEU:HB3	14:N:287:LEU:CD2	2.48	0.43
14:N:314:MET:HE2	15:O:274:THR:HG21	1.98	0.43
22:W:98:VAL:HG12	22:W:98:VAL:O	2.17	0.43
7:G:169:VAL:O	7:G:171:ASP:N	2.48	0.43
8:H:139:THR:HG22	8:H:143:GLU:HG3	2.00	0.43
10:J:1:FME:HE2	25:Z:141:TRP:CH2	2.53	0.43
13:M:366:ASN:ND2	13:M:407:SER:OG	2.49	0.43
16:P:203:GLN:N	16:P:291:ASP:OD2	2.37	0.43
11:K:66:PHE:O	11:K:70:GLU:OE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:366:MET:HA	12:L:445:GLU:OE1	2.19	0.43
12:L:517:ASN:OD1	12:L:519:TYR:N	2.51	0.43
14:N:106:LEU:HD21	14:N:138:PRO:HB2	2.00	0.43
20:T:47:GLN:OE1	20:T:71:MET:HE1	2.17	0.43
43:r:104:GLU:OE1	43:r:104:GLU:N	2.44	0.43
1:A:44:THR:HG21	4:D:48:THR:HB	1.99	0.43
2:B:99:ALA:CB	2:B:126:MET:HE2	2.48	0.43
6:F:96:ASN:ND2	6:F:187:GLY:O	2.41	0.43
7:G:41:CYS:HB3	7:G:52:CYS:HB3	2.00	0.43
25:Z:134:ASN:O	25:Z:138:GLY:N	2.48	0.43
41:p:127:GLU:OE1	41:p:127:GLU:N	2.51	0.43
7:G:317:ALA:CB	7:G:331:LEU:HD21	2.49	0.43
7:G:673:MET:HE3	7:G:679:ARG:HA	2.00	0.43
9:I:69:LEU:HD13	60:I:340:HOH:O	2.17	0.43
39:n:159:GLU:OE1	39:n:159:GLU:HA	2.19	0.43
2:B:100:GLY:HA2	47:B:201:SF4:S4	2.59	0.43
5:E:55:GLN:O	5:E:59:GLY:N	2.39	0.43
8:H:292:ASN:HA	27:b:17:VAL:HG11	2.00	0.43
13:M:197:LEU:O	13:M:201:MET:HG2	2.19	0.43
34:i:123:PRO:O	34:i:124:ASP:HB3	2.18	0.43
12:L:203:PHE:CZ	41:p:109:LEU:HD11	2.53	0.43
12:L:536:ILE:HG23	12:L:537:THR:N	2.34	0.43
29:d:108:THR:OG1	29:d:111:GLU:OE1	2.30	0.43
35:j:69:ASP:OD1	35:j:69:ASP:N	2.47	0.43
37:l:81:ASP:OD1	37:l:81:ASP:N	2.51	0.43
1:A:24:LEU:HB3	1:A:25:PRO:HD3	2.00	0.43
3:C:78:LEU:HD23	3:C:78:LEU:C	2.43	0.43
15:O:124:LEU:HD12	15:O:124:LEU:N	2.33	0.43
34:i:74:VAL:O	34:i:78:MET:HB2	2.18	0.43
39:n:107:HIS:CE1	39:n:109:SER:HG	2.30	0.43
3:C:114:LEU:HD12	17:Q:17:LEU:HD11	2.01	0.43
3:C:149:ARG:NH1	60:C:306:HOH:O	2.49	0.43
9:I:14:VAL:O	9:I:14:VAL:CG2	2.64	0.43
10:J:145:TYR:CG	10:J:152:MET:HE1	2.54	0.43
10:J:151:MET:CE	14:N:28:LEU:HD11	2.49	0.43
12:L:296:ASN:OD1	39:n:77:GLN:NE2	2.48	0.43
19:S:75:THR:HG23	19:S:75:THR:O	2.18	0.43
1:A:45:SER:O	8:H:126:LYS:NZ	2.52	0.42
13:M:72:LEU:HD23	13:M:230:ILE:HD12	2.01	0.42
13:M:221:VAL:O	13:M:221:VAL:HG12	2.18	0.42
13:M:282:LEU:HD12	13:M:282:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:344:ILE:HD13	23:X:166:PHE:CE1	2.54	0.42
41:p:42:TRP:HB3	41:p:43:PRO:HD3	2.01	0.42
6:F:95:VAL:HG21	6:F:122:CYS:SG	2.60	0.42
15:O:79:LEU:HD11	55:O:502:GTP:H1'	2.01	0.42
24:Y:23:THR:O	24:Y:27:THR:OG1	2.23	0.42
27:b:4:ILE:HG13	27:b:5:SER:N	2.34	0.42
4:D:143:GLU:HG3	4:D:310:ILE:HG21	2.01	0.42
5:E:120:LEU:HD21	5:E:169:ILE:CG1	2.50	0.42
6:F:94:VAL:HG11	6:F:192:LEU:HD22	2.01	0.42
7:G:192:MET:HE2	7:G:192:MET:HA	2.01	0.42
10:J:145:TYR:CD1	10:J:152:MET:HE1	2.54	0.42
12:L:595:ILE:HG12	14:N:100:MET:SD	2.58	0.42
22:W:109:PHE:O	22:W:110:HIS:C	2.62	0.42
24:Y:142:VAL:O	33:h:115:ARG:NH2	2.41	0.42
33:h:49:GLU:OE2	33:h:49:GLU:N	2.52	0.42
41:p:99:GLN:NE2	41:p:138:TYR:OH	2.52	0.42
12:L:341:MET:HE2	12:L:454:ILE:HG12	2.00	0.42
1:A:53:MET:HE2	1:A:55:PHE:CE1	2.55	0.42
3:C:175:ARG:NE	3:C:186:GLU:OE1	2.51	0.42
10:J:151:MET:HE3	14:N:28:LEU:HD21	2.00	0.42
12:L:400:ASN:OD1	12:L:489:THR:HG21	2.19	0.42
13:M:43:TRP:CE3	32:g:78:VAL:HG22	2.55	0.42
15:O:30:ASN:OD1	15:O:31:ILE:N	2.44	0.42
55:O:502:GTP:H5'	55:O:502:GTP:H8	1.84	0.42
42:q:118:SER:O	42:q:119:ALA:CB	2.67	0.42
2:B:118:PRO:O	8:H:58:LYS:NZ	2.51	0.42
6:F:98:ASP:O	6:F:99:GLU:C	2.63	0.42
6:F:169:SER:O	6:F:170:ASP:HB2	2.19	0.42
7:G:126:ASP:OD2	7:G:127:ARG:NH1	2.53	0.42
14:N:106:LEU:HD22	14:N:187:MET:HE2	2.00	0.42
20:U:46:ASP:OD1	39:n:44:ARG:CZ	2.68	0.42
24:Y:128:ILE:O	24:Y:132:GLU:HG2	2.20	0.42
32:g:71:GLY:O	32:g:75:VAL:HG23	2.19	0.42
33:h:36:VAL:HG12	33:h:40:ILE:HD12	2.01	0.42
33:h:69:HIS:CE1	33:h:71:ILE:HD12	2.54	0.42
1:A:62:PHE:O	1:A:66:ASP:HB2	2.20	0.42
4:D:350:LYS:HG3	7:G:121:MET:HG3	2.02	0.42
5:E:67:ASN:OD1	5:E:81:TYR:OH	2.20	0.42
7:G:480:THR:O	7:G:480:THR:HG22	2.19	0.42
9:I:164:GLU:HB3	42:q:109:ILE:HG12	2.02	0.42
12:L:63:ILE:CG2	34:i:89:MET:HE1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:28:LEU:N	14:N:28:LEU:HD22	2.34	0.42
35:j:5:VAL:HG23	35:j:6:HIS:N	2.35	0.42
4:D:109:VAL:O	4:D:109:VAL:HG12	2.19	0.42
7:G:306:MET:C	7:G:521:MET:HE1	2.45	0.42
7:G:410:GLY:O	7:G:421:HIS:NE2	2.53	0.42
45:M:501:LMT:H71	14:N:246:LEU:HD21	2.00	0.42
22:W:121:LEU:HD23	22:W:121:LEU:HA	1.94	0.42
7:G:346:GLU:OE1	7:G:531:CYS:SG	2.77	0.42
12:L:422:TYR:C	12:L:422:TYR:CD2	2.98	0.42
20:U:39:ASP:O	20:U:40:LEU:HD23	2.20	0.42
29:d:93:TYR:CG	33:h:114:MET:HE2	2.55	0.42
34:i:71:VAL:O	34:i:71:VAL:CG1	2.67	0.42
8:H:9:LEU:HD22	8:H:95:LEU:HD22	2.00	0.41
8:H:232:ILE:HD11	26:a:12:MET:HE3	2.02	0.41
20:U:88:GLU:HG3	20:U:88:GLU:O	2.20	0.41
2:B:106:MET:SD	4:D:82:LEU:HD23	2.60	0.41
50:F:502:FMN:HM73	50:F:502:FMN:HM81	1.82	0.41
7:G:547:GLY:O	7:G:563:GLY:N	2.37	0.41
13:M:119:TYR:O	13:M:123:GLU:HG2	2.20	0.41
17:Q:89:LYS:HD2	17:Q:105:VAL:HG11	2.01	0.41
4:D:244:VAL:HA	4:D:291:GLY:O	2.20	0.41
10:J:103:ILE:HG23	10:J:115:ILE:HG21	2.01	0.41
11:K:37:VAL:HG11	11:K:67:ALA:HB1	2.03	0.41
12:L:387:THR:OG1	12:L:460:GLY:O	2.37	0.41
13:M:15:THR:O	13:M:93:LYS:NZ	2.54	0.41
13:M:281:ASP:OD1	13:M:281:ASP:C	2.62	0.41
16:P:177:ARG:NH2	56:P:501:NDP:O2N	2.43	0.41
24:Y:110:GLY:N	45:Y:201:LMT:H6B	2.16	0.41
10:J:121:GLY:HA2	10:J:124:LEU:HD13	2.03	0.41
12:L:136:ASN:OD1	12:L:136:ASN:N	2.53	0.41
12:L:251:THR:O	12:L:254:VAL:HG22	2.20	0.41
12:L:353:GLU:OE2	39:n:79:TYR:HE1	2.04	0.41
12:L:548:THR:O	12:L:553:LEU:HD23	2.20	0.41
13:M:310:MET:SD	13:M:314:MET:CE	3.09	0.41
20:T:32:VAL:O	20:T:32:VAL:CG1	2.68	0.41
3:C:154:ASP:OD1	3:C:155:TYR:N	2.53	0.41
6:F:197:GLU:OE2	17:Q:129:ARG:NH2	2.53	0.41
6:F:268:VAL:HG22	6:F:269:GLU:N	2.36	0.41
13:M:93:LYS:O	13:M:97:SER:OG	2.33	0.41
13:M:134:THR:O	13:M:142:ARG:NE	2.54	0.41
16:P:193:LEU:O	16:P:257:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:33:ASN:OD1	20:T:33:ASN:N	2.51	0.41
28:c:4:VAL:HG23	28:c:5:ARG:N	2.36	0.41
45:j:101:LMT:O6'	45:j:101:LMT:O2B	2.32	0.41
5:E:181:VAL:O	5:E:181:VAL:HG13	2.20	0.41
7:G:478:ARG:NH2	7:G:484:ALA:O	2.53	0.41
13:M:254:THR:O	13:M:254:THR:HG22	2.21	0.41
13:M:346:ARG:HE	37:l:67:GLU:CD	2.29	0.41
3:C:135:TRP:CE2	22:W:90:MET:HE1	2.56	0.41
6:F:103:GLY:O	6:F:333:ALA:HB1	2.20	0.41
7:G:588:THR:HG21	17:Q:63:GLU:HA	2.03	0.41
7:G:613:TYR:CD2	7:G:613:TYR:O	2.73	0.41
12:L:94:LEU:HD23	12:L:125:LEU:HD21	2.01	0.41
13:M:382:THR:OG1	13:M:396:MET:HE1	2.21	0.41
14:N:108:LEU:CD1	14:N:191:LEU:HD22	2.47	0.41
15:O:188:ASP:O	15:O:192:MET:HG3	2.21	0.41
18:R:55:ARG:NH1	18:R:56:ILE:HD11	2.36	0.41
38:m:52:ASP:OD1	38:m:52:ASP:C	2.63	0.41
6:F:43:TYR:OH	6:F:44:LYS:NZ	2.49	0.41
12:L:292:ALA:HB2	12:L:304:PHE:HB3	2.03	0.41
13:M:178:ILE:HD12	33:h:97:GLU:HB3	2.03	0.41
31:f:48:ARG:O	31:f:49:PRO:C	2.64	0.41
1:A:71:LEU:HD22	10:J:144:MET:HE1	2.02	0.41
5:E:173:ILE:O	5:E:173:ILE:HG22	2.20	0.41
6:F:28:ARG:HD3	44:s:31:THR:O	2.20	0.41
7:G:551:ASP:OD2	7:G:679:ARG:NH2	2.47	0.41
8:H:19:PHE:CE2	26:a:11:ILE:HG21	2.55	0.41
12:L:527:GLY:O	37:l:104:LEU:HD13	2.21	0.41
13:M:71:TRP:CH2	13:M:439:LEU:HD22	2.56	0.41
14:N:37:LEU:HD13	14:N:63:GLN:HB2	2.03	0.41
45:O:503:LMT:O2'	45:O:503:LMT:H12	2.21	0.41
16:P:61:LEU:H	16:P:61:LEU:HD23	1.86	0.41
16:P:206:TYR:CE2	16:P:208:ALA:HB3	2.56	0.41
20:T:70:LEU:N	20:T:70:LEU:HD12	2.36	0.41
34:i:122:PHE:N	34:i:122:PHE:CD1	2.89	0.41
6:F:101:GLU:O	6:F:104:THR:HG22	2.21	0.41
12:L:224:SER:O	12:L:310:LEU:HD13	2.21	0.41
13:M:17:LEU:HD21	29:d:54:MET:SD	2.62	0.41
20:T:40:LEU:HD12	20:T:40:LEU:N	2.36	0.41
34:i:63:ALA:O	34:i:65:ARG:N	2.54	0.41
38:m:115:ILE:CG1	38:m:120:LEU:HD12	2.51	0.41
42:q:1:AME:HA	42:q:1:AME:HT23	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:MET:SD	1:A:87:MET:C	3.05	0.40
3:C:150:ARG:NE	22:W:94:GLU:OE2	2.43	0.40
7:G:317:ALA:HB3	7:G:343:LEU:HD13	2.03	0.40
9:I:81:ALA:HB2	9:I:108:THR:HG22	2.02	0.40
12:L:477:ILE:HD12	12:L:477:ILE:H	1.87	0.40
12:L:489:THR:HG23	12:L:490:ALA:N	2.36	0.40
16:P:175:GLU:N	16:P:175:GLU:OE2	2.54	0.40
29:d:99:GLU:OE1	29:d:99:GLU:N	2.41	0.40
38:m:14:PRO:HG3	39:n:71:TRP:CZ2	2.57	0.40
8:H:23:VAL:HG12	8:H:27:ILE:HD12	2.03	0.40
8:H:87:VAL:CG2	8:H:88:PRO:HD3	2.51	0.40
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.04	0.40
9:I:94:ILE:HA	9:I:112:ASP:O	2.21	0.40
13:M:84:LEU:HD11	13:M:95:TYR:CD2	2.55	0.40
14:N:45:ILE:O	14:N:45:ILE:HG23	2.20	0.40
14:N:202:LEU:O	14:N:206:MET:HG2	2.21	0.40
16:P:173:GLY:O	16:P:176:ASP:OD2	2.39	0.40
38:m:24:VAL:HG23	38:m:29:ARG:CZ	2.52	0.40
4:D:169:TRP:CH2	4:D:228:MET:SD	3.14	0.40
5:E:127:LYS:O	5:E:128:VAL:C	2.65	0.40
8:H:142:TYR:CD2	8:H:142:TYR:C	2.98	0.40
8:H:317:TYR:CG	10:J:134:MET:HE1	2.55	0.40
9:I:52:TYR:CG	9:I:53:PRO:HA	2.57	0.40
15:O:46:LEU:HD21	15:O:235:VAL:HG13	2.03	0.40
25:Z:44:PHE:CZ	25:Z:48:ARG:HD2	2.56	0.40
31:f:15:VAL:HB	31:f:16:PRO:HD3	2.03	0.40
52:h:201:CDL:OA2	52:h:201:CDL:OB2	2.39	0.40
17:Q:70:MET:SD	42:q:126:PRO:HB2	2.62	0.40
2:B:154:ILE:HD13	9:I:144:GLU:HG2	2.02	0.40
7:G:331:LEU:HD22	7:G:525:LEU:HD22	2.03	0.40
8:H:87:VAL:N	8:H:88:PRO:CD	2.85	0.40
23:X:118:ARG:NE	60:X:301:HOH:O	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
2	B	154/224 (69%)	147 (96%)	7 (4%)	0	100	100
3	C	206/263 (78%)	196 (95%)	10 (5%)	0	100	100
4	D	427/463 (92%)	410 (96%)	17 (4%)	0	100	100
5	E	212/248 (86%)	192 (91%)	19 (9%)	1 (0%)	24	43
6	F	428/464 (92%)	410 (96%)	16 (4%)	2 (0%)	24	43
7	G	686/727 (94%)	652 (95%)	34 (5%)	0	100	100
8	H	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
9	I	176/212 (83%)	169 (96%)	7 (4%)	0	100	100
10	J	170/172 (99%)	153 (90%)	17 (10%)	0	100	100
11	K	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
12	L	604/607 (100%)	568 (94%)	34 (6%)	2 (0%)	36	55
13	M	457/459 (100%)	444 (97%)	13 (3%)	0	100	100
14	N	343/345 (99%)	332 (97%)	11 (3%)	0	100	100
15	O	318/355 (90%)	310 (98%)	8 (2%)	0	100	100
16	P	340/377 (90%)	328 (96%)	12 (4%)	0	100	100
17	Q	123/175 (70%)	117 (95%)	6 (5%)	0	100	100
18	R	93/116 (80%)	84 (90%)	9 (10%)	0	100	100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
20	T	76/156 (49%)	64 (84%)	12 (16%)	0	100	100
20	U	84/156 (54%)	83 (99%)	1 (1%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
22	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
23	X	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
24	Y	140/143 (98%)	138 (99%)	2 (1%)	0	100	100
25	Z	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
26	a	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	72 (89%)	9 (11%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	d	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
30	e	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
31	f	49/57 (86%)	45 (92%)	4 (8%)	0	100	100
32	g	98/151 (65%)	98 (100%)	0	0	100	100
33	h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
34	i	100/128 (78%)	90 (90%)	10 (10%)	0	100	100
35	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
36	k	76/104 (73%)	74 (97%)	2 (3%)	0	100	100
37	l	153/186 (82%)	145 (95%)	8 (5%)	0	100	100
38	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
39	n	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
40	o	115/137 (84%)	105 (91%)	9 (8%)	1 (1%)	14	27
41	p	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
42	q	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
43	r	91/113 (80%)	84 (92%)	7 (8%)	0	100	100
44	s	41/104 (39%)	38 (93%)	3 (7%)	0	100	100
All	All	8118/9214 (88%)	7731 (95%)	381 (5%)	6 (0%)	49	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	170	ASP
12	L	562	ILE
40	o	10	TRP
12	L	249	SER
5	E	183	LYS
6	F	300	GLY

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	103/103 (100%)	102 (99%)	1 (1%)	68 83
2	B	132/185 (71%)	130 (98%)	2 (2%)	57 77
3	C	190/227 (84%)	188 (99%)	2 (1%)	65 81
4	D	370/394 (94%)	369 (100%)	1 (0%)	86 94
5	E	184/206 (89%)	184 (100%)	0	100 100
6	F	345/370 (93%)	342 (99%)	3 (1%)	70 84
7	G	580/610 (95%)	579 (100%)	1 (0%)	87 95
8	H	279/279 (100%)	279 (100%)	0	100 100
9	I	152/178 (85%)	151 (99%)	1 (1%)	76 88
10	J	137/137 (100%)	137 (100%)	0	100 100
11	K	87/87 (100%)	85 (98%)	2 (2%)	44 68
12	L	548/549 (100%)	545 (100%)	3 (0%)	81 90
13	M	414/414 (100%)	414 (100%)	0	100 100
14	N	307/307 (100%)	307 (100%)	0	100 100
15	O	284/309 (92%)	284 (100%)	0	100 100
16	P	299/325 (92%)	298 (100%)	1 (0%)	86 94
17	Q	112/153 (73%)	111 (99%)	1 (1%)	70 84
18	R	80/96 (83%)	80 (100%)	0	100 100
19	S	73/80 (91%)	72 (99%)	1 (1%)	59 78
20	T	72/135 (53%)	70 (97%)	2 (3%)	38 62
20	U	79/135 (58%)	78 (99%)	1 (1%)	61 79
21	V	100/102 (98%)	100 (100%)	0	100 100
22	W	108/114 (95%)	108 (100%)	0	100 100
23	X	153/154 (99%)	153 (100%)	0	100 100
24	Y	106/107 (99%)	105 (99%)	1 (1%)	70 84
25	Z	121/123 (98%)	121 (100%)	0	100 100
26	a	59/60 (98%)	59 (100%)	0	100 100
27	b	72/73 (99%)	72 (100%)	0	100 100
28	c	42/67 (63%)	42 (100%)	0	100 100
29	d	107/107 (100%)	107 (100%)	0	100 100
30	e	93/94 (99%)	93 (100%)	0	100 100
31	f	47/53 (89%)	46 (98%)	1 (2%)	47 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	g	91/129 (70%)	91 (100%)	0	100 100
33	h	123/162 (76%)	123 (100%)	0	100 100
34	i	95/119 (80%)	95 (100%)	0	100 100
35	j	61/87 (70%)	61 (100%)	0	100 100
36	k	60/78 (77%)	60 (100%)	0	100 100
37	l	140/161 (87%)	140 (100%)	0	100 100
38	m	112/114 (98%)	112 (100%)	0	100 100
39	n	162/164 (99%)	162 (100%)	0	100 100
40	o	108/121 (89%)	108 (100%)	0	100 100
41	p	155/158 (98%)	154 (99%)	1 (1%)	78 89
42	q	129/130 (99%)	128 (99%)	1 (1%)	73 86
43	r	85/96 (88%)	85 (100%)	0	100 100
44	s	42/95 (44%)	41 (98%)	1 (2%)	43 67
All	All	7198/7947 (91%)	7171 (100%)	27 (0%)	81 92

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
2	B	64	CYS
2	B	101	THR
3	C	74	SER
3	C	78	LEU
4	D	37	ASP
6	F	104	THR
6	F	114	ASP
6	F	366	ARG
7	G	375	ASP
9	I	131	ASP
11	K	39	SER
11	K	48	SER
12	L	305	SER
12	L	482	MET
12	L	601	LEU
16	P	97	ARG
17	Q	104	ASP
19	S	84	ASP

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Mol	Chain	Res	Type
20	T	44	SER
20	T	78	ASP
20	U	39	ASP
24	Y	19	CYS
31	f	40	SER
41	p	22	GLN
42	q	80	SER
44	s	62	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	19	HIS
4	D	135	GLN
5	E	155	GLN
6	F	24	ASN
6	F	402	HIS
6	F	436	GLN
7	G	401	HIS
7	G	402	ASN
7	G	629	ASN
7	G	643	GLN
8	H	5	ASN
8	H	47	GLN
8	H	97	ASN
8	H	163	GLN
10	J	107	ASN
12	L	109	HIS
12	L	200	GLN
12	L	209	ASN
12	L	248	HIS
12	L	269	ASN
12	L	295	GLN
12	L	354	GLN
13	M	51	ASN
13	M	81	GLN
13	M	82	ASN
13	M	139	GLN
13	M	184	HIS
13	M	331	ASN
13	M	366	ASN
13	M	374	ASN

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Mol	Chain	Res	Type
13	M	422	HIS
14	N	174	GLN
14	N	228	ASN
14	N	289	ASN
15	O	45	GLN
16	P	67	GLN
16	P	93	ASN
16	P	250	HIS
18	R	95	HIS
22	W	93	GLN
23	X	123	GLN
25	Z	102	ASN
27	b	51	ASN
28	c	9	ASN
29	d	8	HIS
30	e	44	HIS
30	e	76	HIS
30	e	97	HIS
37	l	54	GLN
37	l	65	HIS
37	l	125	GLN
38	m	85	ASN
38	m	125	ASN
40	o	42	GLN
40	o	49	GLN
40	o	81	HIS
41	p	22	GLN
41	p	122	GLN
42	q	123	GLN
42	q	135	HIS

5.3.3 RNA (i)

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	$\#\|Z\| > 2$
11	FME	K	1	11	8,9,10	1.02	1 (12%)	7,9,11	1.21	1 (14%)
8	FME	H	1	8	8,9,10	1.02	1 (12%)	7,9,11	1.08	0
13	FME	M	1	13	8,9,10	1.10	1 (12%)	7,9,11	0.71	0
14	FME	N	1	14	8,9,10	0.88	0	7,9,11	0.83	0
10	FME	J	1	10	8,9,10	0.97	1 (12%)	7,9,11	0.91	0
43	AYA	r	1	43	6,7,8	1.41	1 (16%)	5,8,10	1.17	1 (20%)
1	FME	A	1	1	8,9,10	0.92	0	7,9,11	0.86	0
12	FME	L	1	12	8,9,10	0.97	0	7,9,11	0.65	0
42	AME	q	1	42	9,10,11	1.50	1 (11%)	9,11,13	1.88	2 (22%)
4	2MR	D	85	4	10,12,13	2.25	2 (20%)	5,13,15	1.23	1 (20%)
34	SAC	i	1	34	7,8,9	1.83	1 (14%)	8,9,11	1.88	2 (25%)

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
11	FME	K	1	11	-	2/7/9/11	-
8	FME	H	1	8	-	3/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
14	FME	N	1	14	-	4/7/9/11	-
10	FME	J	1	10	-	3/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
1	FME	A	1	1	-	1/7/9/11	-
12	FME	L	1	12	-	2/7/9/11	-
42	AME	q	1	42	-	5/9/10/12	-
4	2MR	D	85	4	-	0/10/13/15	-
34	SAC	i	1	34	-	2/7/8/10	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.62	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	4.48	1.43	1.34
34	i	1	SAC	O-C	4.21	1.36	1.19
42	q	1	AME	CT1-N	3.41	1.46	1.34
43	r	1	AYA	CA-N	-3.03	1.43	1.46
13	M	1	FME	CA-N	-2.49	1.42	1.46
8	H	1	FME	CA-N	-2.14	1.43	1.46
11	K	1	FME	CA-N	-2.13	1.43	1.46
10	J	1	FME	CA-N	-2.04	1.43	1.46

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	-4.52	112.94	124.78
42	q	1	AME	CT2-CT1-N	3.67	122.31	116.10
42	q	1	AME	CE-SD-CG	2.74	109.81	100.40
34	i	1	SAC	OG-CB-CA	-2.57	104.41	110.97
11	K	1	FME	C-CA-N	2.34	113.95	109.73
4	D	85	2MR	NE-CZ-NH2	-2.28	117.39	119.48
43	r	1	AYA	CB-CA-N	2.26	112.12	109.61

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	C-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
12	L	1	FME	CB-CA-N-CN
14	N	1	FME	N-CA-CB-CG
14	N	1	FME	C-CA-CB-CG
34	i	1	SAC	N-CA-CB-OG
34	i	1	SAC	C-CA-CB-OG
42	q	1	AME	C-CA-CB-CG
8	H	1	FME	CA-CB-CG-SD
10	J	1	FME	CA-CB-CG-SD
42	q	1	AME	CT2-CT1-N-CA
42	q	1	AME	OT-CT1-N-CA
1	A	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CG-SD-CE
14	N	1	FME	CB-CG-SD-CE
10	J	1	FME	N-CA-CB-CG
11	K	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
13	M	1	FME	CB-CA-N-CN
12	L	1	FME	CA-CB-CG-SD
42	q	1	AME	CB-CG-SD-CE
14	N	1	FME	CB-CA-N-CN
42	q	1	AME	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 3 are monoatomic - leaving 53 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	L	701	-	36,36,36	1.25	6 (16%)	47,47,47	0.94	1 (2%)
48	HQH	D	601	-	29,30,30	0.83	2 (6%)	28,40,40	1.40	4 (14%)
47	SF4	G	801	7	0,12,12	-	-	-		
58	EHZ	T	201	20	29,36,37	1.67	5 (17%)	35,44,47	1.63	9 (25%)
45	LMT	Y	204	-	36,36,36	1.22	6 (16%)	47,47,47	1.05	3 (6%)
45	LMT	j	101	-	36,36,36	1.15	4 (11%)	47,47,47	0.95	1 (2%)
53	3PE	i	201	34	29,29,50	1.14	3 (10%)	32,34,55	1.25	2 (6%)
55	GTP	O	502	-	30,34,34	3.04	13 (43%)	46,54,54	2.06	16 (34%)
45	LMT	Y	201	-	36,36,36	1.29	6 (16%)	47,47,47	1.02	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
46	PC1	B	203	-	40,40,53	1.09	2 (5%)	46,48,61	1.14	2 (4%)
45	LMT	K	201	-	36,36,36	1.33	7 (19%)	47,47,47	1.07	2 (4%)
50	FMN	F	502	-	33,33,33	2.51	6 (18%)	48,50,50	1.51	10 (20%)
45	LMT	L	704	-	36,36,36	1.23	7 (19%)	47,47,47	1.12	4 (8%)
53	3PE	N	402	-	32,32,50	1.06	4 (12%)	35,37,55	1.11	2 (5%)
53	3PE	Z	201	-	30,30,50	1.09	3 (10%)	33,35,55	1.10	2 (6%)
53	3PE	Z	202	-	40,40,50	0.97	4 (10%)	43,45,55	1.05	2 (4%)
45	LMT	A	403	-	36,36,36	1.18	4 (11%)	47,47,47	1.06	2 (4%)
53	3PE	I	203	-	43,43,50	0.92	3 (6%)	46,48,55	1.08	2 (4%)
53	3PE	N	401	-	33,33,50	1.07	4 (12%)	36,38,55	1.05	2 (5%)
45	LMT	J	202	-	36,36,36	1.19	6 (16%)	47,47,47	1.00	0
46	PC1	A	402	-	28,28,53	1.29	3 (10%)	34,36,61	0.98	2 (5%)
49	FES	G	803	7	0,4,4	-	-	-		
45	LMT	P	502	-	36,36,36	1.18	5 (13%)	47,47,47	1.19	4 (8%)
47	SF4	I	202	9	0,12,12	-	-	-		
45	LMT	J	201	-	36,36,36	1.22	5 (13%)	47,47,47	1.15	2 (4%)
52	CDL	L	705	-	63,63,99	1.08	7 (11%)	69,75,111	1.20	4 (5%)
59	MYR	o	201	40	14,14,15	0.75	0	13,13,15	0.63	0
52	CDL	q	501	-	63,63,99	1.06	5 (7%)	69,75,111	1.03	4 (5%)
53	3PE	d	201	-	32,32,50	1.06	3 (9%)	35,37,55	1.11	2 (5%)
47	SF4	I	201	9	0,12,12	-	-	-		
45	LMT	Y	202	-	36,36,36	1.22	6 (16%)	47,47,47	0.96	2 (4%)
53	3PE	r	201	-	44,44,50	0.93	4 (9%)	47,49,55	1.08	2 (4%)
47	SF4	G	802	7	0,12,12	-	-	-		
56	NDP	P	501	-	49,52,52	2.00	8 (16%)	66,80,80	1.62	13 (19%)
53	3PE	M	502	-	35,35,50	1.00	3 (8%)	38,40,55	1.13	2 (5%)
52	CDL	h	201	-	56,56,99	1.05	5 (8%)	61,67,111	1.18	4 (6%)
52	CDL	h	202	-	46,46,99	1.53	8 (17%)	50,57,111	1.36	4 (8%)
45	LMT	M	501	-	36,36,36	1.27	7 (19%)	47,47,47	1.19	3 (6%)
53	3PE	L	702	-	40,40,50	0.96	3 (7%)	43,45,55	1.12	2 (4%)
53	3PE	L	703	-	43,43,50	0.91	4 (9%)	46,48,55	1.07	3 (6%)
58	EHZ	U	201	20	29,36,37	1.62	5 (17%)	35,44,47	1.72	8 (22%)
45	LMT	A	401	-	36,36,36	1.23	6 (16%)	47,47,47	1.01	2 (4%)
45	LMT	Y	203	-	36,36,36	1.15	5 (13%)	47,47,47	1.07	2 (4%)
52	CDL	H	401	-	47,47,99	1.16	6 (12%)	51,58,111	1.26	3 (5%)
53	3PE	O	504	-	29,29,50	1.10	4 (13%)	32,34,55	1.04	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	FES	E	301	5	0,4,4	-	-	-		
53	3PE	M	503	-	35,35,50	1.01	4 (11%)	38,40,55	1.11	2 (5%)
47	SF4	F	501	6	0,12,12	-	-	-		
47	SF4	B	201	2	0,12,12	-	-	-		
53	3PE	X	201	-	35,35,50	1.00	4 (11%)	38,40,55	1.22	2 (5%)
45	LMT	h	203	-	36,36,36	1.22	5 (13%)	47,47,47	1.02	2 (4%)
45	LMT	O	503	-	36,36,36	1.15	5 (13%)	47,47,47	1.48	4 (8%)
46	PC1	B	202	-	37,37,53	1.12	4 (10%)	43,45,61	1.15	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	L	701	-	-	7/21/61/61	0/2/2/2
48	HQH	D	601	-	-	10/27/29/29	0/1/1/1
58	EHZ	T	201	20	-	17/42/44/45	-
47	SF4	G	801	7	-	-	0/6/5/5
45	LMT	Y	204	-	-	11/21/61/61	0/2/2/2
45	LMT	j	101	-	-	11/21/61/61	0/2/2/2
53	3PE	i	201	34	-	19/33/33/54	-
55	GTP	O	502	-	-	7/22/38/38	0/3/3/3
45	LMT	Y	201	-	-	12/21/61/61	0/2/2/2
46	PC1	B	203	-	-	20/44/44/57	-
45	LMT	K	201	-	-	6/21/61/61	0/2/2/2
50	FMN	F	502	-	-	9/18/18/18	0/3/3/3
45	LMT	L	704	-	-	11/21/61/61	0/2/2/2
53	3PE	N	402	-	-	16/36/36/54	-
53	3PE	Z	201	-	-	21/34/34/54	-
53	3PE	Z	202	-	-	20/44/44/54	-
45	LMT	A	403	-	-	10/21/61/61	0/2/2/2
53	3PE	I	203	-	-	16/47/47/54	-
53	3PE	N	401	-	-	19/37/37/54	-
45	LMT	J	202	-	-	8/21/61/61	0/2/2/2
46	PC1	A	402	-	-	15/32/32/57	-
49	FES	G	803	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	P	502	-	-	13/21/61/61	0/2/2/2
47	SF4	I	202	9	-	-	0/6/5/5
45	LMT	J	201	-	-	10/21/61/61	0/2/2/2
52	CDL	L	705	-	-	36/74/74/110	-
59	MYR	o	201	40	-	6/11/12/13	-
52	CDL	q	501	-	-	36/73/73/110	-
53	3PE	d	201	-	-	18/36/36/54	-
47	SF4	I	201	9	-	-	0/6/5/5
45	LMT	Y	202	-	-	9/21/61/61	0/2/2/2
53	3PE	r	201	-	-	16/48/48/54	-
47	SF4	G	802	7	-	-	0/6/5/5
56	NDP	P	501	-	-	3/34/77/77	0/5/5/5
53	3PE	M	502	-	-	19/39/39/54	-
52	CDL	h	201	-	-	31/65/65/110	-
52	CDL	h	202	-	-	32/56/56/110	-
45	LMT	M	501	-	-	14/21/61/61	0/2/2/2
53	3PE	L	702	-	-	20/44/44/54	-
53	3PE	L	703	-	-	24/47/47/54	-
58	EHZ	U	201	20	-	16/42/44/45	-
45	LMT	A	401	-	-	10/21/61/61	0/2/2/2
45	LMT	Y	203	-	-	15/21/61/61	0/2/2/2
52	CDL	H	401	-	-	24/57/57/110	-
53	3PE	O	504	-	-	14/33/33/54	-
53	3PE	M	503	-	-	17/39/39/54	-
49	FES	E	301	5	-	-	0/1/1/1
47	SF4	F	501	6	-	-	0/6/5/5
47	SF4	B	201	2	-	-	0/6/5/5
53	3PE	X	201	-	-	16/39/39/54	-
45	LMT	h	203	-	-	7/21/61/61	0/2/2/2
45	LMT	O	503	-	-	9/21/61/61	0/2/2/2
46	PC1	B	202	-	-	19/41/41/57	-

All (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	10.62	1.79	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	O	502	GTP	O6-C6	8.59	1.39	1.23
50	F	502	FMN	O4-C4	8.42	1.39	1.23
50	F	502	FMN	O2-C2	8.16	1.39	1.24
55	O	502	GTP	C5-N7	6.57	1.51	1.39
52	h	202	CDL	OA6-CA4	-6.08	1.39	1.46
58	T	201	EHZ	C15-N2	5.62	1.45	1.33
58	U	201	EHZ	C15-N2	4.92	1.44	1.33
58	U	201	EHZ	C12-N1	4.77	1.44	1.33
58	T	201	EHZ	C12-N1	4.77	1.44	1.33
55	O	502	GTP	C8-N9	-4.60	1.27	1.37
55	O	502	GTP	C2-N1	4.58	1.49	1.37
55	O	502	GTP	C2-N3	4.51	1.44	1.33
55	O	502	GTP	C2-N2	4.42	1.44	1.34
50	F	502	FMN	C2-N1	3.89	1.46	1.36
55	O	502	GTP	C4-N9	-3.75	1.28	1.38
56	P	501	NDP	O2B-C2B	-3.33	1.32	1.44
56	P	501	NDP	PN-O5D	3.26	1.72	1.59
45	M	501	LMT	O3'-C3'	-3.14	1.35	1.43
45	K	201	LMT	O2B-C2B	-3.07	1.35	1.43
52	h	202	CDL	OA6-CA5	3.03	1.40	1.33
45	A	401	LMT	O3'-C3'	-3.00	1.35	1.43
45	J	201	LMT	O3'-C3'	-2.97	1.36	1.43
45	M	501	LMT	O2'-C2'	-2.96	1.36	1.43
45	Y	203	LMT	O3'-C3'	-2.94	1.36	1.43
45	L	704	LMT	O3'-C3'	-2.90	1.36	1.43
45	Y	202	LMT	O3'-C3'	-2.90	1.36	1.43
52	h	201	CDL	OB6-CB4	-2.89	1.39	1.46
53	I	203	3PE	O21-C2	-2.89	1.39	1.46
45	Y	201	LMT	O3'-C3'	-2.87	1.36	1.43
45	Y	202	LMT	O2'-C2'	-2.87	1.36	1.43
52	q	501	CDL	OA6-CA4	-2.87	1.39	1.46
53	Z	202	3PE	O21-C2	-2.87	1.39	1.46
46	B	203	PC1	O21-C2	-2.85	1.39	1.46
45	J	202	LMT	O3'-C3'	-2.84	1.36	1.43
45	Y	204	LMT	O3'-C3'	-2.82	1.36	1.43
53	L	702	3PE	O21-C2	-2.82	1.39	1.46
45	j	101	LMT	O3'-C3'	-2.81	1.36	1.43
55	O	502	GTP	O4'-C1'	2.80	1.48	1.42
45	K	201	LMT	O3'-C3'	-2.77	1.36	1.43
45	Y	201	LMT	O2'-C2'	-2.77	1.36	1.43
52	h	202	CDL	OB6-CB4	-2.77	1.39	1.46
52	L	705	CDL	OB6-CB4	-2.76	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	q	501	CDL	OB6-CB4	-2.75	1.39	1.46
53	i	201	3PE	O31-C31	2.74	1.41	1.33
46	A	402	PC1	O21-C2	-2.74	1.39	1.46
45	L	701	LMT	O3'-C3'	-2.73	1.36	1.43
45	Y	204	LMT	O2'-C2'	-2.73	1.36	1.43
45	K	201	LMT	O2'-C2'	-2.72	1.36	1.43
52	h	201	CDL	OA6-CA4	-2.72	1.39	1.46
53	X	201	3PE	O21-C2	-2.69	1.39	1.46
53	i	201	3PE	O21-C2	-2.68	1.39	1.46
45	L	701	LMT	O2B-C2B	-2.67	1.36	1.43
45	Y	201	LMT	O2B-C2B	-2.66	1.36	1.43
45	A	403	LMT	O2'-C2'	-2.66	1.36	1.43
53	Z	201	3PE	O21-C2	-2.65	1.40	1.46
45	O	503	LMT	O3'-C3'	-2.65	1.36	1.43
53	N	401	3PE	O31-C31	2.65	1.41	1.33
53	r	201	3PE	O21-C2	-2.64	1.40	1.46
53	N	401	3PE	O21-C2	-2.64	1.40	1.46
45	A	403	LMT	O3'-C3'	-2.63	1.36	1.43
58	U	201	EHZ	O3-C12	-2.63	1.17	1.23
52	L	705	CDL	OA6-CA4	-2.63	1.40	1.46
45	J	201	LMT	O2B-C2B	-2.63	1.36	1.43
45	h	203	LMT	O3'-C3'	-2.61	1.36	1.43
45	M	501	LMT	O2B-C2B	-2.61	1.36	1.43
56	P	501	NDP	O4B-C4B	-2.61	1.39	1.45
45	P	502	LMT	O3'-C3'	-2.60	1.36	1.43
45	P	502	LMT	O2'-C2'	-2.60	1.36	1.43
53	d	201	3PE	O21-C2	-2.59	1.40	1.46
50	F	502	FMN	P-O2P	-2.58	1.44	1.54
46	B	202	PC1	O21-C2	-2.57	1.40	1.46
45	M	501	LMT	O4'-C4B	-2.57	1.36	1.43
45	O	503	LMT	O2'-C2'	-2.56	1.36	1.43
53	N	402	3PE	O21-C2	-2.56	1.40	1.46
45	L	701	LMT	O2'-C2'	-2.55	1.37	1.43
55	O	502	GTP	C2'-C3'	-2.54	1.46	1.53
46	B	203	PC1	O31-C3	-2.53	1.39	1.45
45	h	203	LMT	O3B-C3B	-2.52	1.37	1.43
53	r	201	3PE	O31-C31	2.52	1.40	1.33
53	O	504	3PE	O31-C31	2.51	1.40	1.33
45	K	201	LMT	O1'-C1'	-2.50	1.35	1.40
45	J	202	LMT	O3B-C3B	-2.49	1.37	1.43
58	T	201	EHZ	O3-C12	-2.48	1.18	1.23
45	O	503	LMT	O2B-C2B	-2.48	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	J	202	LMT	O2B-C2B	-2.47	1.37	1.43
58	U	201	EHZ	O4-C15	-2.47	1.18	1.23
45	Y	201	LMT	O4'-C4B	-2.47	1.37	1.43
52	h	201	CDL	OB8-CB7	2.47	1.40	1.33
53	M	502	3PE	O31-C31	2.46	1.40	1.33
50	F	502	FMN	P-O3P	-2.46	1.45	1.54
52	L	705	CDL	OA8-CA7	2.45	1.40	1.33
53	M	503	3PE	O21-C2	-2.44	1.40	1.46
52	q	501	CDL	OB8-CB7	2.43	1.40	1.33
48	D	601	HQH	C12-C19	2.43	1.40	1.37
45	P	502	LMT	O2B-C2B	-2.42	1.37	1.43
52	H	401	CDL	OB6-CB4	-2.42	1.40	1.46
53	X	201	3PE	O31-C3	-2.42	1.39	1.45
58	T	201	EHZ	O4-C15	-2.42	1.18	1.23
55	O	502	GTP	PG-O2G	-2.42	1.45	1.54
55	O	502	GTP	PG-O3G	-2.41	1.45	1.54
45	P	502	LMT	O3B-C3B	-2.41	1.37	1.43
53	Z	201	3PE	O31-C31	2.41	1.40	1.33
46	B	202	PC1	O31-C31	2.41	1.40	1.33
52	h	202	CDL	OB8-CB7	2.41	1.40	1.33
53	M	502	3PE	O21-C2	-2.40	1.40	1.46
45	L	701	LMT	O4'-C4B	-2.39	1.37	1.43
50	F	502	FMN	C4A-N5	2.39	1.35	1.30
45	J	202	LMT	O2'-C2'	-2.39	1.37	1.43
45	A	401	LMT	O3B-C3B	-2.39	1.37	1.43
45	K	201	LMT	O3B-C3B	-2.39	1.37	1.43
46	A	402	PC1	O31-C3	-2.39	1.39	1.45
45	j	101	LMT	O3B-C3B	-2.38	1.37	1.43
45	L	704	LMT	O2B-C2B	-2.38	1.37	1.43
53	L	702	3PE	O31-C31	2.38	1.40	1.33
53	O	504	3PE	O21-C2	-2.37	1.40	1.46
53	M	503	3PE	O31-C3	-2.36	1.39	1.45
45	O	503	LMT	O3B-C3B	-2.36	1.37	1.43
45	Y	204	LMT	O3B-C3B	-2.35	1.37	1.43
45	Y	203	LMT	O3B-C3B	-2.35	1.37	1.43
45	A	403	LMT	O2B-C2B	-2.35	1.37	1.43
45	Y	202	LMT	O2B-C2B	-2.34	1.37	1.43
53	d	201	3PE	O31-C3	-2.33	1.39	1.45
45	J	201	LMT	O3B-C3B	-2.33	1.37	1.43
45	A	403	LMT	O3B-C3B	-2.33	1.37	1.43
45	A	401	LMT	O2'-C2'	-2.32	1.37	1.43
53	N	402	3PE	O31-C31	2.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Y	204	LMT	O2B-C2B	-2.31	1.37	1.43
45	h	203	LMT	O2'-C2'	-2.31	1.37	1.43
52	h	202	CDL	OA8-CA7	2.30	1.40	1.33
45	L	701	LMT	O3B-C3B	-2.29	1.37	1.43
52	H	401	CDL	OB8-CB7	2.28	1.40	1.33
45	h	203	LMT	O2B-C2B	-2.28	1.37	1.43
45	K	201	LMT	O5'-C5'	-2.28	1.38	1.44
45	Y	201	LMT	O1'-C1'	-2.28	1.36	1.40
53	Z	202	3PE	O31-C31	2.28	1.40	1.33
45	A	401	LMT	O4'-C4B	-2.27	1.37	1.43
45	j	101	LMT	O2'-C2'	-2.27	1.37	1.43
52	h	202	CDL	OB8-CB6	-2.27	1.40	1.45
56	P	501	NDP	C7N-C3N	-2.26	1.43	1.48
46	B	202	PC1	O31-C3	-2.26	1.40	1.45
56	P	501	NDP	O3B-C3B	-2.26	1.37	1.43
45	j	101	LMT	O2B-C2B	-2.25	1.37	1.43
53	O	504	3PE	O21-C21	2.25	1.40	1.34
53	I	203	3PE	O31-C3	-2.24	1.40	1.45
45	Y	203	LMT	O2B-C2B	-2.24	1.37	1.43
52	h	202	CDL	OA8-CA6	-2.24	1.40	1.45
45	L	704	LMT	O2'-C2'	-2.24	1.37	1.43
53	d	201	3PE	O31-C31	2.23	1.39	1.33
45	P	502	LMT	O1'-C1'	-2.23	1.36	1.40
45	Y	204	LMT	O1'-C1'	-2.23	1.36	1.40
45	J	202	LMT	O1'-C1'	-2.22	1.36	1.40
45	L	701	LMT	O1'-C1'	-2.22	1.36	1.40
45	Y	201	LMT	O3B-C3B	-2.22	1.37	1.43
45	A	401	LMT	O2B-C2B	-2.21	1.37	1.43
53	L	703	3PE	O31-C31	2.21	1.39	1.33
45	Y	203	LMT	O2'-C2'	-2.21	1.37	1.43
56	P	501	NDP	O2D-C2D	-2.21	1.37	1.43
52	L	705	CDL	OB8-CB7	2.20	1.39	1.33
45	M	501	LMT	O3B-C3B	-2.20	1.37	1.43
52	H	401	CDL	OA6-CA4	-2.20	1.41	1.46
45	h	203	LMT	O4'-C4B	-2.20	1.37	1.43
53	I	203	3PE	O31-C31	2.20	1.39	1.33
53	Z	202	3PE	O31-C3	-2.19	1.40	1.45
52	L	705	CDL	OB8-CB6	-2.19	1.40	1.45
45	Y	203	LMT	O4'-C4B	-2.19	1.37	1.43
45	J	201	LMT	O4'-C4B	-2.19	1.37	1.43
53	L	703	3PE	O21-C2	-2.18	1.41	1.46
45	Y	202	LMT	O3B-C3B	-2.18	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Y	204	LMT	O4'-C4B	-2.18	1.37	1.43
46	A	402	PC1	O31-C31	2.17	1.39	1.33
53	N	402	3PE	O21-C21	2.17	1.40	1.34
45	M	501	LMT	O5'-C5'	-2.17	1.39	1.44
52	H	401	CDL	OA6-CA5	2.17	1.40	1.34
45	L	704	LMT	O4'-C4B	-2.17	1.37	1.43
53	L	702	3PE	O31-C3	-2.16	1.40	1.45
53	L	703	3PE	O21-C21	2.16	1.40	1.34
45	J	201	LMT	O2'-C2'	-2.16	1.37	1.43
45	L	704	LMT	O3B-C3B	-2.16	1.37	1.43
58	U	201	EHZ	C9-S1	2.15	1.81	1.76
56	P	501	NDP	O5D-C5D	-2.15	1.36	1.44
52	H	401	CDL	OB8-CB6	-2.15	1.40	1.45
45	L	704	LMT	O1'-C1'	-2.13	1.36	1.40
45	A	401	LMT	O1'-C1'	-2.13	1.36	1.40
45	L	704	LMT	O5'-C5'	-2.12	1.39	1.44
52	q	501	CDL	OB6-CB5	2.12	1.40	1.34
46	B	202	PC1	O21-C21	2.11	1.40	1.34
45	O	503	LMT	O4'-C4B	-2.11	1.38	1.43
52	H	401	CDL	OB6-CB5	2.11	1.40	1.34
53	Z	201	3PE	O31-C3	-2.10	1.40	1.45
53	L	703	3PE	O31-C3	-2.10	1.40	1.45
53	X	201	3PE	O31-C31	2.10	1.39	1.33
45	M	501	LMT	O1'-C1'	-2.09	1.36	1.40
53	M	503	3PE	O21-C21	2.09	1.40	1.34
45	K	201	LMT	O4'-C4B	-2.09	1.38	1.43
52	h	201	CDL	OA6-CA5	2.09	1.39	1.35
53	N	402	3PE	O31-C3	-2.09	1.40	1.45
53	r	201	3PE	O31-C3	-2.09	1.40	1.45
52	h	201	CDL	OB8-CB6	-2.08	1.40	1.45
58	T	201	EHZ	O6-C20	-2.08	1.39	1.44
53	N	401	3PE	O21-C21	2.07	1.40	1.34
53	M	503	3PE	O31-C31	2.06	1.39	1.33
48	D	601	HQH	C22-C11	-2.06	1.46	1.50
53	r	201	3PE	O21-C21	2.06	1.40	1.34
53	i	201	3PE	O21-C21	2.04	1.40	1.34
52	L	705	CDL	OA6-CA5	2.04	1.40	1.34
53	M	502	3PE	O21-C21	2.04	1.40	1.34
53	Z	202	3PE	O21-C21	2.04	1.40	1.34
55	O	502	GTP	C1'-N9	-2.04	1.41	1.47
45	Y	202	LMT	O4'-C4B	-2.03	1.38	1.43
52	q	501	CDL	OB8-CB6	-2.03	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	L	705	CDL	OA8-CA6	-2.03	1.40	1.45
55	O	502	GTP	PB-O2B	-2.03	1.45	1.55
45	Y	202	LMT	O1'-C1'	-2.02	1.36	1.40
53	O	504	3PE	O31-C3	-2.02	1.40	1.45
45	J	202	LMT	O4'-C4B	-2.01	1.38	1.43
53	X	201	3PE	O21-C21	2.00	1.40	1.34
53	N	401	3PE	O31-C3	-2.00	1.40	1.45
52	h	202	CDL	OB6-CB5	2.00	1.40	1.34

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	O	502	GTP	C8-N9-C4	7.41	120.16	106.05
56	P	501	NDP	PN-O3-PA	-6.41	110.84	132.83
45	O	503	LMT	C1-O1'-C1'	5.12	122.33	113.84
45	O	503	LMT	O1'-C1'-C2'	4.97	116.06	108.30
52	H	401	CDL	OB6-CB5-C51	4.79	121.83	111.50
52	L	705	CDL	OA6-CA5-C11	4.57	121.35	111.50
52	h	201	CDL	OA6-CA5-C11	4.51	119.39	111.09
52	h	202	CDL	OB6-CB5-C51	4.51	121.22	111.50
45	M	501	LMT	O5B-C5B-C4B	4.42	117.72	109.69
58	U	201	EHZ	C8-C9-S1	4.36	119.03	113.63
52	h	202	CDL	OA6-CA5-OA7	-4.25	120.17	125.57
55	O	502	GTP	PB-O3B-PG	-4.24	118.27	132.83
46	B	202	PC1	O21-C21-C22	4.21	120.57	111.50
46	B	203	PC1	O21-C21-C22	4.18	120.52	111.50
53	X	201	3PE	O21-C21-C22	4.17	120.48	111.50
58	T	201	EHZ	C8-C9-S1	4.17	118.78	113.63
53	M	502	3PE	O21-C21-C22	4.13	120.41	111.50
52	H	401	CDL	OA6-CA5-C11	4.10	120.33	111.50
58	U	201	EHZ	C14-C13-C12	-4.08	105.56	112.36
53	L	702	3PE	O21-C21-C22	4.07	120.28	111.50
52	L	705	CDL	OB6-CB5-C51	3.98	120.08	111.50
53	M	503	3PE	O21-C21-C22	3.96	120.04	111.50
53	N	401	3PE	O21-C21-C22	3.92	119.95	111.50
53	r	201	3PE	O21-C21-C22	3.91	119.93	111.50
52	h	201	CDL	OB6-CB5-C51	3.86	119.83	111.50
53	i	201	3PE	O21-C21-C22	3.86	119.83	111.50
53	Z	201	3PE	O21-C21-C22	3.85	119.80	111.50
53	N	402	3PE	O21-C21-C22	3.78	119.66	111.50
55	O	502	GTP	PA-O3A-PB	-3.75	119.96	132.83
52	q	501	CDL	OB6-CB5-C51	3.74	119.56	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	d	201	3PE	O21-C21-C22	3.69	119.46	111.50
52	q	501	CDL	OA6-CA5-C11	3.68	119.42	111.50
53	Z	202	3PE	O21-C21-C22	3.67	119.41	111.50
53	i	201	3PE	O31-C31-C32	3.65	123.37	111.91
53	I	203	3PE	O21-C21-C22	3.65	119.37	111.50
53	O	504	3PE	O21-C21-C22	3.58	119.22	111.50
53	L	703	3PE	O21-C21-C22	3.55	119.16	111.50
50	F	502	FMN	C4-N3-C2	-3.54	119.10	125.64
50	F	502	FMN	C9-C9A-N10	3.49	126.56	121.84
56	P	501	NDP	O2B-P2B-O1X	-3.34	96.49	109.39
58	U	201	EHZ	C13-C12-N1	3.34	122.04	116.42
58	T	201	EHZ	C11-N1-C12	-3.29	116.73	122.84
52	H	401	CDL	OB8-CB7-C71	3.28	119.98	111.38
55	O	502	GTP	C2-N1-C6	-3.27	119.13	125.10
45	J	201	LMT	C3'-C4'-C5'	-3.22	103.54	110.93
46	A	402	PC1	O21-C21-C22	3.21	119.76	110.80
58	T	201	EHZ	C13-C12-N1	3.19	121.80	116.42
48	D	601	HQH	O2-C24-N5	3.18	123.05	113.49
53	M	502	3PE	O31-C31-C32	3.17	119.70	111.38
50	F	502	FMN	O5'-P-O1P	3.13	115.24	106.47
52	h	202	CDL	OB8-CB7-C71	3.11	121.68	111.91
45	K	201	LMT	C2'-C3'-C4'	3.11	116.79	109.68
55	O	502	GTP	C3'-C2'-C1'	3.10	107.32	101.43
45	A	403	LMT	C3B-C4B-C5B	-3.08	104.74	110.24
46	B	202	PC1	O31-C31-C32	3.06	121.50	111.91
45	Y	203	LMT	C3'-C4'-C5'	-2.98	104.08	110.93
45	L	704	LMT	C3'-C4'-C5'	-2.97	104.12	110.93
55	O	502	GTP	O3G-PG-O3B	2.96	114.56	104.64
48	D	601	HQH	O3-C25-C23	2.95	126.53	116.56
45	Y	204	LMT	C1'-O5'-C5'	-2.94	107.92	113.69
56	P	501	NDP	PA-O5B-C5B	-2.93	104.50	121.68
45	K	201	LMT	C1'-O5'-C5'	-2.86	108.07	113.69
53	Z	202	3PE	O31-C31-C32	2.86	120.88	111.91
45	P	502	LMT	C1'-O5'-C5'	-2.84	108.11	113.69
45	Y	202	LMT	C1'-O5'-C5'	-2.81	108.18	113.69
53	L	703	3PE	O31-C31-C32	2.81	120.71	111.91
53	d	201	3PE	O31-C31-C32	2.79	120.67	111.91
50	F	502	FMN	C4A-C4-N3	2.78	120.26	113.19
52	L	705	CDL	OA8-CA7-C31	2.77	120.60	111.91
50	F	502	FMN	C6-C5A-N5	-2.75	113.71	118.51
53	r	201	3PE	O31-C31-C32	2.74	120.52	111.91
50	F	502	FMN	O2P-P-O5'	2.69	113.90	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	h	203	LMT	C1'-O5'-C5'	-2.69	108.40	113.69
46	B	203	PC1	O31-C31-C32	2.68	120.31	111.91
55	O	502	GTP	C2'-C3'-C4'	2.65	107.79	102.64
56	P	501	NDP	PN-O5D-C5D	-2.64	106.19	121.68
52	L	705	CDL	OB8-CB7-C71	2.64	120.19	111.91
52	q	501	CDL	OB8-CB7-C71	2.62	120.12	111.91
53	X	201	3PE	O31-C31-C32	2.61	120.10	111.91
58	T	201	EHZ	C7-C8-C9	-2.60	107.95	113.89
52	h	201	CDL	OB8-CB7-C71	2.60	120.08	111.91
45	L	704	LMT	C1'-O5'-C5'	-2.59	108.60	113.69
53	Z	201	3PE	O31-C31-C32	2.59	120.03	111.91
48	D	601	HQH	C15-C21-C18	2.58	128.19	124.18
56	P	501	NDP	N3A-C4A-N9A	2.58	131.33	127.08
56	P	501	NDP	C4B-O4B-C1B	-2.57	103.79	109.47
50	F	502	FMN	O3P-P-O5'	2.54	113.49	106.73
53	N	402	3PE	O31-C31-C32	2.54	119.88	111.91
48	D	601	HQH	C10-C6-C8	-2.54	105.83	110.05
56	P	501	NDP	O3X-P2B-O2X	2.53	117.32	107.64
45	J	201	LMT	C1'-O5'-C5'	-2.52	108.75	113.69
52	h	202	CDL	OA8-CA7-C31	2.50	119.75	111.91
56	P	501	NDP	O5D-PN-O1N	-2.49	99.33	109.07
56	P	501	NDP	C5A-C4A-N3A	-2.49	123.50	126.75
55	O	502	GTP	C5-C6-N1	2.49	119.51	113.19
53	I	203	3PE	O31-C31-C32	2.49	119.72	111.91
52	h	201	CDL	CA4-OA6-CA5	-2.47	113.29	117.90
55	O	502	GTP	C1'-N9-C8	-2.47	119.67	126.70
45	A	401	LMT	C3'-C4'-C5'	-2.47	105.27	110.93
53	L	702	3PE	O31-C31-C32	2.46	119.64	111.91
53	O	504	3PE	O31-C31-C32	2.45	119.60	111.91
50	F	502	FMN	O4-C4-C4A	-2.45	120.10	126.60
55	O	502	GTP	O6-C6-C5	-2.44	120.11	126.60
45	P	502	LMT	O1'-C1'-C2'	2.44	112.12	108.30
56	P	501	NDP	C2A-N1A-C6A	-2.43	114.60	118.77
45	A	403	LMT	C1'-O5'-C5'	-2.41	108.95	113.69
55	O	502	GTP	C5-C4-N9	-2.41	101.25	105.63
45	P	502	LMT	O5B-C5B-C4B	2.40	114.06	109.69
53	N	401	3PE	O31-C31-C32	2.39	119.42	111.91
53	M	503	3PE	O31-C31-C32	2.39	119.40	111.91
58	U	201	EHZ	C11-N1-C12	-2.38	118.42	122.84
45	j	101	LMT	C3'-C4'-C5'	-2.36	105.51	110.93
45	O	503	LMT	O5'-C1'-C2'	-2.35	105.37	110.35
58	U	201	EHZ	C10-S1-C9	2.35	109.18	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	h	203	LMT	O1'-C1'-C2'	2.30	111.90	108.30
58	T	201	EHZ	C19-C17-C16	2.30	112.81	108.82
58	U	201	EHZ	C7-C8-C9	-2.29	108.66	113.89
45	O	503	LMT	C1'-O5'-C5'	-2.29	109.20	113.69
58	T	201	EHZ	O2-C9-S1	-2.27	119.67	122.61
45	M	501	LMT	C1'-O5'-C5'	-2.26	109.25	113.69
45	Y	204	LMT	C3'-C4'-C5'	-2.25	105.77	110.93
45	L	701	LMT	O5B-C5B-C4B	2.23	113.74	109.69
45	Y	204	LMT	C3B-C4B-C5B	-2.23	106.27	110.24
50	F	502	FMN	C5'-C4'-C3'	-2.22	107.92	112.20
45	P	502	LMT	O5B-C5B-C6B	2.21	111.93	106.44
45	Y	201	LMT	C1-O1'-C1'	2.20	117.48	113.84
53	L	703	3PE	O31-C31-O32	-2.17	118.11	123.59
56	P	501	NDP	O2N-PN-O1N	2.14	122.82	112.24
55	O	502	GTP	C1'-N9-C4	-2.14	120.15	126.50
56	P	501	NDP	O3X-P2B-O2B	-2.14	96.41	105.99
45	A	401	LMT	O5'-C1'-O1'	-2.11	104.97	109.97
58	U	201	EHZ	C10-C11-N1	-2.10	108.00	112.42
45	Y	202	LMT	O5B-C5B-C4B	2.10	113.50	109.69
55	O	502	GTP	N9-C8-N7	-2.10	109.44	113.39
50	F	502	FMN	C9A-C5A-N5	2.10	124.71	122.43
46	A	402	PC1	O31-C31-C32	2.09	118.48	111.91
58	T	201	EHZ	C14-C13-C12	-2.09	108.87	112.36
58	U	201	EHZ	C13-C14-N2	-2.09	107.68	111.90
45	M	501	LMT	C3'-C4'-C5'	-2.07	106.19	110.93
45	Y	203	LMT	C3B-C4B-C5B	-2.06	106.57	110.24
55	O	502	GTP	O2A-PA-O1A	-2.05	102.11	112.24
55	O	502	GTP	O2B-PB-O1B	-2.04	102.15	112.24
56	P	501	NDP	C5A-C6A-N1A	2.03	121.75	117.39
55	O	502	GTP	N9-C4-N3	2.02	130.00	125.94
45	L	704	LMT	O5B-C5B-C4B	2.02	113.36	109.69
45	L	704	LMT	O5'-C1'-O1'	-2.02	105.20	109.97
52	q	501	CDL	OA8-CA7-C31	2.01	121.16	112.38
58	T	201	EHZ	C13-C14-N2	2.01	115.95	111.90
58	T	201	EHZ	C10-S1-C9	2.00	108.10	101.87

There are no chirality outliers.

All (699) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	401	LMT	O5'-C1'-O1'-C1
45	A	401	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
45	K	201	LMT	O5'-C1'-O1'-C1
45	L	701	LMT	C2'-C1'-O1'-C1
45	L	701	LMT	O5'-C1'-O1'-C1
45	M	501	LMT	C2-C1-O1'-C1'
45	O	503	LMT	C2'-C1'-O1'-C1
45	O	503	LMT	C2-C1-O1'-C1'
45	Y	201	LMT	C2'-C1'-O1'-C1
45	Y	201	LMT	O5'-C1'-O1'-C1
45	Y	202	LMT	C2'-C1'-O1'-C1
45	Y	202	LMT	O5'-C1'-O1'-C1
45	Y	203	LMT	C2'-C1'-O1'-C1
45	Y	203	LMT	O5'-C1'-O1'-C1
45	Y	203	LMT	C2-C1-O1'-C1'
45	j	101	LMT	O5'-C1'-O1'-C1
46	A	402	PC1	C11-O13-P-O14
46	A	402	PC1	C11-O13-P-O11
46	A	402	PC1	C1-O11-P-O12
46	A	402	PC1	C1-O11-P-O13
46	A	402	PC1	O13-C11-C12-N
46	A	402	PC1	O22-C21-O21-C2
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	O22-C21-O21-C2
46	B	202	PC1	C22-C21-O21-C2
46	B	203	PC1	C11-O13-P-O11
46	B	203	PC1	O11-C1-C2-O21
46	B	203	PC1	C22-C21-O21-C2
48	D	601	HQH	C22-C11-C8-C6
48	D	601	HQH	C18-C11-C8-C6
48	D	601	HQH	C19-C12-C13-C20
48	D	601	HQH	N5-C12-C13-C20
50	F	502	FMN	C1'-C2'-C3'-O3'
50	F	502	FMN	C1'-C2'-C3'-C4'
50	F	502	FMN	C5'-O5'-P-O2P
50	F	502	FMN	C5'-O5'-P-O3P
52	H	401	CDL	CA4-CA3-OA5-PA1
52	H	401	CDL	OA9-CA7-OA8-CA6
52	H	401	CDL	CB3-OB5-PB2-OB2
52	H	401	CDL	CB3-OB5-PB2-OB4
52	L	705	CDL	C11-CA5-OA6-CA4
52	L	705	CDL	CB2-OB2-PB2-OB3
52	L	705	CDL	CB2-OB2-PB2-OB4
52	L	705	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
52	h	201	CDL	CA3-OA5-PA1-OA3
52	h	201	CDL	CA3-OA5-PA1-OA4
52	h	201	CDL	OA7-CA5-OA6-CA4
52	h	201	CDL	C11-CA5-OA6-CA4
52	h	201	CDL	CB3-OB5-PB2-OB3
52	h	201	CDL	OB6-CB4-CB6-OB8
52	h	202	CDL	CA2-C1-CB2-OB2
52	h	202	CDL	CA3-CA4-OA6-CA5
52	h	202	CDL	CA6-CA4-OA6-CA5
52	h	202	CDL	OA7-CA5-OA6-CA4
52	h	202	CDL	CB2-OB2-PB2-OB4
52	h	202	CDL	CB3-OB5-PB2-OB3
52	h	202	CDL	CB3-OB5-PB2-OB4
52	h	202	CDL	C51-CB5-OB6-CB4
52	q	501	CDL	CA2-OA2-PA1-OA4
52	q	501	CDL	CA3-OA5-PA1-OA3
52	q	501	CDL	CB3-OB5-PB2-OB2
52	q	501	CDL	CB3-OB5-PB2-OB3
53	I	203	3PE	O13-C11-C12-N
53	I	203	3PE	O11-C1-C2-O21
53	L	702	3PE	C1-O11-P-O14
53	L	702	3PE	O21-C2-C3-O31
53	L	703	3PE	C11-O13-P-O11
53	L	703	3PE	C11-O13-P-O14
53	L	703	3PE	O13-C11-C12-N
53	M	502	3PE	C1-O11-P-O12
53	M	503	3PE	C1-O11-P-O12
53	M	503	3PE	C1-O11-P-O14
53	N	401	3PE	C12-C11-O13-P
53	N	401	3PE	O13-C11-C12-N
53	N	401	3PE	O22-C21-O21-C2
53	N	402	3PE	C11-O13-P-O14
53	N	402	3PE	C12-C11-O13-P
53	N	402	3PE	O13-C11-C12-N
53	N	402	3PE	C22-C21-O21-C2
53	O	504	3PE	O21-C2-C3-O31
53	X	201	3PE	C12-C11-O13-P
53	X	201	3PE	O13-C11-C12-N
53	X	201	3PE	O22-C21-O21-C2
53	X	201	3PE	C22-C21-O21-C2
53	Z	201	3PE	C1-O11-P-O12
53	Z	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
53	Z	201	3PE	C11-O13-P-O12
53	Z	201	3PE	C11-O13-P-O14
53	Z	201	3PE	O13-C11-C12-N
53	Z	202	3PE	C12-C11-O13-P
53	Z	202	3PE	O13-C11-C12-N
53	d	201	3PE	C11-O13-P-O14
53	d	201	3PE	C22-C21-O21-C2
53	i	201	3PE	C11-O13-P-O12
53	i	201	3PE	C11-O13-P-O14
53	i	201	3PE	C12-C11-O13-P
53	i	201	3PE	O32-C31-O31-C3
53	i	201	3PE	C32-C31-O31-C3
53	i	201	3PE	C22-C21-O21-C2
55	O	502	GTP	PB-O3B-PG-O2G
55	O	502	GTP	C5'-O5'-PA-O3A
55	O	502	GTP	C5'-O5'-PA-O1A
58	T	201	EHZ	S1-C10-C11-N1
58	T	201	EHZ	C11-C10-S1-C9
58	T	201	EHZ	C15-C16-C17-C20
58	T	201	EHZ	O5-C16-C17-C19
58	T	201	EHZ	O5-C16-C17-C20
58	U	201	EHZ	C15-C16-C17-C19
58	U	201	EHZ	C15-C16-C17-C20
59	o	201	MYR	C1-C2-C3-C4
46	B	202	PC1	O32-C31-O31-C3
45	P	502	LMT	O5B-C1B-O1B-C4'
58	T	201	EHZ	C13-C14-N2-C15
46	B	202	PC1	C32-C31-O31-C3
52	H	401	CDL	C71-CB7-OB8-CB6
52	H	401	CDL	OB9-CB7-OB8-CB6
52	L	705	CDL	OA9-CA7-OA8-CA6
52	h	202	CDL	OA9-CA7-OA8-CA6
52	h	202	CDL	OB9-CB7-OB8-CB6
53	Z	201	3PE	O32-C31-O31-C3
45	O	503	LMT	O5B-C5B-C6B-O6B
46	B	203	PC1	O22-C21-O21-C2
52	L	705	CDL	OA7-CA5-OA6-CA4
52	h	202	CDL	OB7-CB5-OB6-CB4
53	N	402	3PE	O22-C21-O21-C2
53	d	201	3PE	O22-C21-O21-C2
53	i	201	3PE	O22-C21-O21-C2
52	L	705	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
52	h	202	CDL	C31-CA7-OA8-CA6
52	h	202	CDL	C71-CB7-OB8-CB6
53	Z	201	3PE	C32-C31-O31-C3
45	A	403	LMT	O5'-C5'-C6'-O6'
46	A	402	PC1	C22-C21-O21-C2
53	N	401	3PE	C22-C21-O21-C2
46	B	203	PC1	C32-C31-O31-C3
45	Y	203	LMT	O5B-C5B-C6B-O6B
45	J	202	LMT	O5'-C5'-C6'-O6'
45	Y	201	LMT	O5'-C5'-C6'-O6'
52	h	202	CDL	O1-C1-CB2-OB2
45	J	201	LMT	O5'-C5'-C6'-O6'
45	L	701	LMT	O5B-C5B-C6B-O6B
45	L	701	LMT	C4B-C5B-C6B-O6B
45	O	503	LMT	C4B-C5B-C6B-O6B
45	Y	202	LMT	O5B-C1B-O1B-C4'
45	M	501	LMT	O5'-C5'-C6'-O6'
45	J	202	LMT	O5B-C5B-C6B-O6B
45	A	403	LMT	C4'-C5'-C6'-O6'
45	J	201	LMT	C3'-C4'-O1B-C1B
45	h	203	LMT	O5B-C5B-C6B-O6B
45	j	101	LMT	O5B-C5B-C6B-O6B
46	B	203	PC1	O32-C31-O31-C3
45	Y	204	LMT	O5'-C5'-C6'-O6'
45	P	502	LMT	C4'-C5'-C6'-O6'
52	q	501	CDL	OA9-CA7-OA8-CA6
45	j	101	LMT	O5'-C5'-C6'-O6'
45	Y	203	LMT	C4B-C5B-C6B-O6B
45	M	501	LMT	O5B-C5B-C6B-O6B
45	J	201	LMT	C4'-C5'-C6'-O6'
45	Y	201	LMT	C4B-C5B-C6B-O6B
52	q	501	CDL	C31-CA7-OA8-CA6
45	O	503	LMT	O5B-C1B-O1B-C4'
52	L	705	CDL	CB2-C1-CA2-OA2
52	L	705	CDL	CA2-C1-CB2-OB2
52	q	501	CDL	C71-CB7-OB8-CB6
53	Z	202	3PE	C32-C31-O31-C3
53	r	201	3PE	C32-C31-O31-C3
45	j	101	LMT	C4'-C5'-C6'-O6'
45	L	701	LMT	O5'-C5'-C6'-O6'
45	O	503	LMT	C2B-C1B-O1B-C4'
53	N	401	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
45	L	704	LMT	C4B-C5B-C6B-O6B
53	Z	202	3PE	C31-C32-C33-C34
45	J	201	LMT	C2'-C1'-O1'-C1
45	K	201	LMT	C2'-C1'-O1'-C1
45	j	101	LMT	C2'-C1'-O1'-C1
53	Z	202	3PE	O21-C2-C3-O31
53	Z	202	3PE	O32-C31-O31-C3
45	J	202	LMT	C4'-C5'-C6'-O6'
45	M	501	LMT	O5B-C1B-O1B-C4'
48	D	601	HQH	C22-C11-C18-C21
48	D	601	HQH	C8-C11-C18-C21
45	Y	202	LMT	O5'-C5'-C6'-O6'
45	M	501	LMT	C4'-C5'-C6'-O6'
53	L	702	3PE	C21-C22-C23-C24
53	d	201	3PE	C21-C22-C23-C24
53	r	201	3PE	O32-C31-O31-C3
45	L	704	LMT	O5B-C5B-C6B-O6B
45	P	502	LMT	O5'-C5'-C6'-O6'
45	Y	204	LMT	C4'-C5'-C6'-O6'
52	L	705	CDL	CA7-C31-C32-C33
45	A	403	LMT	O5B-C5B-C6B-O6B
52	h	202	CDL	CB5-C51-C52-C53
52	H	401	CDL	CB5-C51-C52-C53
52	L	705	CDL	CB5-C51-C52-C53
52	q	501	CDL	CB7-C71-C72-C73
53	N	401	3PE	C21-C22-C23-C24
56	P	501	NDP	O4D-C4D-C5D-O5D
58	T	201	EHZ	C5-C6-C7-O1
53	M	503	3PE	C32-C31-O31-C3
45	j	101	LMT	C5'-C4'-O1B-C1B
45	j	101	LMT	C4B-C5B-C6B-O6B
46	A	402	PC1	C31-C32-C33-C34
53	X	201	3PE	C31-C32-C33-C34
52	q	501	CDL	OB9-CB7-OB8-CB6
52	L	705	CDL	O1-C1-CA2-OA2
52	L	705	CDL	O1-C1-CB2-OB2
45	Y	201	LMT	C4'-C5'-C6'-O6'
53	L	703	3PE	C22-C21-O21-C2
46	B	202	PC1	C11-O13-P-O11
46	B	203	PC1	C1-O11-P-O13
52	H	401	CDL	CA2-OA2-PA1-OA5
52	h	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
52	h	202	CDL	CB2-OB2-PB2-OB5
52	h	202	CDL	CB3-OB5-PB2-OB2
52	q	501	CDL	CA2-OA2-PA1-OA5
52	q	501	CDL	CA3-OA5-PA1-OA2
53	L	702	3PE	C1-O11-P-O13
53	M	502	3PE	C1-O11-P-O13
53	M	503	3PE	C1-O11-P-O13
53	M	503	3PE	C11-O13-P-O11
53	N	401	3PE	C11-O13-P-O11
53	N	402	3PE	C11-O13-P-O11
53	O	504	3PE	C11-O13-P-O11
53	Z	201	3PE	C1-O11-P-O13
53	Z	201	3PE	C11-O13-P-O11
53	i	201	3PE	C1-O11-P-O13
53	X	201	3PE	C32-C31-O31-C3
53	L	703	3PE	O22-C21-O21-C2
45	j	101	LMT	C3'-C4'-O1B-C1B
50	F	502	FMN	O2'-C2'-C3'-O3'
53	M	503	3PE	C22-C21-O21-C2
52	h	201	CDL	C57-C58-C59-C60
53	N	402	3PE	C34-C35-C36-C37
45	Y	204	LMT	C4B-C5B-C6B-O6B
53	L	702	3PE	C37-C38-C39-C3A
58	U	201	EHZ	C3-C4-C5-C6
59	o	201	MYR	C9-C10-C11-C12
45	M	501	LMT	O1'-C1-C2-C3
58	U	201	EHZ	C2-C1-C21-C22
45	P	502	LMT	C6-C7-C8-C9
45	h	203	LMT	C2-C3-C4-C5
46	B	203	PC1	C3A-C3B-C3C-C3D
53	I	203	3PE	C29-C2A-C2B-C2C
53	r	201	3PE	C26-C27-C28-C29
45	L	704	LMT	O1'-C1-C2-C3
46	B	203	PC1	C33-C34-C35-C36
45	A	401	LMT	C2'-C1'-O1'-C1
53	L	703	3PE	C32-C31-O31-C3
45	Y	202	LMT	C4-C5-C6-C7
45	Y	204	LMT	C6-C7-C8-C9
46	B	203	PC1	C37-C38-C39-C3A
52	L	705	CDL	C52-C53-C54-C55
53	O	504	3PE	C24-C25-C26-C27
53	d	201	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
53	r	201	3PE	C25-C26-C27-C28
53	X	201	3PE	O32-C31-O31-C3
45	A	403	LMT	C11-C10-C9-C8
46	B	202	PC1	C34-C35-C36-C37
46	B	202	PC1	C36-C37-C38-C39
52	H	401	CDL	C11-C12-C13-C14
53	M	502	3PE	C29-C2A-C2B-C2C
45	Y	201	LMT	O5B-C5B-C6B-O6B
53	M	503	3PE	O32-C31-O31-C3
45	P	502	LMT	C5'-C4'-O1B-C1B
52	q	501	CDL	C79-C80-C81-C82
53	i	201	3PE	C24-C25-C26-C27
53	M	503	3PE	O22-C21-O21-C2
52	H	401	CDL	C11-CA5-OA6-CA4
53	L	702	3PE	C22-C21-O21-C2
53	r	201	3PE	C22-C21-O21-C2
46	B	202	PC1	C24-C25-C26-C27
53	Z	201	3PE	C24-C25-C26-C27
45	J	201	LMT	C5'-C4'-O1B-C1B
45	Y	201	LMT	C5-C6-C7-C8
52	L	705	CDL	C71-C72-C73-C74
59	o	201	MYR	C3-C4-C5-C6
45	A	403	LMT	C1-C2-C3-C4
45	O	503	LMT	O5'-C1'-O1'-C1
52	H	401	CDL	C52-C53-C54-C55
53	M	502	3PE	O13-C11-C12-N
53	M	503	3PE	O13-C11-C12-N
52	h	202	CDL	C31-C32-C33-C34
58	U	201	EHZ	C1-C2-C3-C4
45	h	203	LMT	C4B-C5B-C6B-O6B
45	J	201	LMT	C3-C4-C5-C6
53	Z	202	3PE	C34-C35-C36-C37
45	K	201	LMT	C2-C1-O1'-C1'
45	P	502	LMT	C2-C1-O1'-C1'
45	Y	204	LMT	C2-C1-O1'-C1'
46	B	203	PC1	C24-C25-C26-C27
45	Y	203	LMT	C4-C5-C6-C7
53	M	503	3PE	C24-C25-C26-C27
52	H	401	CDL	OA7-CA5-OA6-CA4
53	r	201	3PE	O22-C21-O21-C2
45	O	503	LMT	O1'-C1-C2-C3
45	J	202	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
52	h	201	CDL	C51-CB5-OB6-CB4
53	L	703	3PE	C3C-C3D-C3E-C3F
52	q	501	CDL	CA5-C11-C12-C13
45	P	502	LMT	O5B-C5B-C6B-O6B
53	L	702	3PE	C26-C27-C28-C29
53	X	201	3PE	C33-C34-C35-C36
52	h	201	CDL	OB7-CB5-OB6-CB4
53	L	702	3PE	O22-C21-O21-C2
45	J	201	LMT	C1-C2-C3-C4
50	F	502	FMN	O2'-C2'-C3'-C4'
53	I	203	3PE	C26-C27-C28-C29
53	N	401	3PE	C35-C36-C37-C38
45	Y	204	LMT	O1'-C1-C2-C3
53	I	203	3PE	C32-C31-O31-C3
46	B	202	PC1	C33-C34-C35-C36
53	L	703	3PE	O32-C31-O31-C3
52	q	501	CDL	OA7-CA5-OA6-CA4
52	q	501	CDL	C75-C76-C77-C78
53	M	502	3PE	C2D-C2E-C2F-C2G
45	L	704	LMT	C6-C7-C8-C9
52	L	705	CDL	C18-C19-C20-C21
52	h	201	CDL	C59-C60-C61-C62
53	r	201	3PE	C28-C29-C2A-C2B
52	L	705	CDL	CA4-CA6-OA8-CA7
53	Z	202	3PE	C26-C27-C28-C29
52	q	501	CDL	C11-CA5-OA6-CA4
53	N	402	3PE	O11-C1-C2-O21
53	i	201	3PE	O11-C1-C2-O21
46	B	203	PC1	C23-C24-C25-C26
52	q	501	CDL	OB6-CB4-CB6-OB8
53	Z	201	3PE	O21-C2-C3-O31
53	d	201	3PE	C32-C31-O31-C3
45	J	201	LMT	C11-C10-C9-C8
53	Z	201	3PE	C23-C24-C25-C26
53	d	201	3PE	C36-C37-C38-C39
45	Y	203	LMT	O5'-C5'-C6'-O6'
52	L	705	CDL	C12-C13-C14-C15
53	I	203	3PE	O32-C31-O31-C3
53	N	401	3PE	C34-C35-C36-C37
52	h	201	CDL	CB3-OB5-PB2-OB2
53	L	702	3PE	C11-O13-P-O11
53	X	201	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
53	i	201	3PE	C11-O13-P-O11
45	Y	203	LMT	C3-C4-C5-C6
52	h	201	CDL	OA5-CA3-CA4-CA6
53	I	203	3PE	O11-C1-C2-C3
53	N	401	3PE	O11-C1-C2-C3
53	N	402	3PE	O11-C1-C2-C3
45	A	401	LMT	C5-C6-C7-C8
45	A	403	LMT	O1'-C1-C2-C3
45	M	501	LMT	C5'-C4'-O1B-C1B
45	A	401	LMT	O5B-C5B-C6B-O6B
53	M	502	3PE	C24-C25-C26-C27
45	M	501	LMT	C6-C7-C8-C9
45	L	704	LMT	C4-C5-C6-C7
52	q	501	CDL	C78-C79-C80-C81
53	d	201	3PE	C31-C32-C33-C34
45	Y	202	LMT	C11-C10-C9-C8
52	q	501	CDL	CA3-CA4-CA6-OA8
52	q	501	CDL	CB3-CB4-CB6-OB8
53	O	504	3PE	C23-C24-C25-C26
48	D	601	HQH	C24-C25-O3-C30
53	d	201	3PE	C39-C3A-C3B-C3C
45	L	704	LMT	O5'-C5'-C6'-O6'
53	M	503	3PE	C34-C35-C36-C37
45	Y	204	LMT	O5'-C1'-O1'-C1
45	L	701	LMT	C9-C10-C11-C12
45	Y	203	LMT	C2-C3-C4-C5
52	L	705	CDL	C22-C23-C24-C25
53	N	401	3PE	C36-C37-C38-C39
53	L	703	3PE	C25-C26-C27-C28
58	T	201	EHZ	C18-C17-C20-O6
58	T	201	EHZ	C19-C17-C20-O6
45	K	201	LMT	C9-C10-C11-C12
52	L	705	CDL	C55-C56-C57-C58
45	P	502	LMT	C11-C10-C9-C8
53	O	504	3PE	C27-C28-C29-C2A
50	F	502	FMN	C5'-O5'-P-O1P
53	L	703	3PE	C34-C35-C36-C37
53	d	201	3PE	C33-C34-C35-C36
52	h	202	CDL	OB5-CB3-CB4-OB6
52	q	501	CDL	OA5-CA3-CA4-OA6
53	d	201	3PE	O11-C1-C2-O21
53	r	201	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
45	J	202	LMT	C4B-C5B-C6B-O6B
53	d	201	3PE	O32-C31-O31-C3
45	L	704	LMT	C7-C8-C9-C10
45	P	502	LMT	C3'-C4'-O1B-C1B
46	A	402	PC1	C35-C36-C37-C38
52	q	501	CDL	OA6-CA4-CA6-OA8
53	M	502	3PE	O21-C2-C3-O31
58	T	201	EHZ	O5-C16-C17-C18
58	U	201	EHZ	O5-C16-C17-C18
58	U	201	EHZ	O5-C16-C17-C19
45	A	401	LMT	O1'-C1-C2-C3
46	B	202	PC1	C31-C32-C33-C34
45	O	503	LMT	C4-C5-C6-C7
58	T	201	EHZ	C5-C6-C7-C8
53	M	502	3PE	C22-C23-C24-C25
53	N	402	3PE	C36-C37-C38-C39
53	Z	201	3PE	C35-C36-C37-C38
45	M	501	LMT	C4B-C5B-C6B-O6B
45	h	203	LMT	C9-C10-C11-C12
45	j	101	LMT	C9-C10-C11-C12
45	P	502	LMT	C1-C2-C3-C4
52	L	705	CDL	OA5-CA3-CA4-CA6
53	Z	202	3PE	O11-C1-C2-C3
53	i	201	3PE	O11-C1-C2-C3
45	L	701	LMT	C2-C3-C4-C5
52	q	501	CDL	C71-C72-C73-C74
59	o	201	MYR	C7-C8-C9-C10
53	L	702	3PE	O13-C11-C12-N
52	h	202	CDL	CB7-C71-C72-C73
52	h	201	CDL	CA4-CA3-OA5-PA1
52	L	705	CDL	C72-C73-C74-C75
53	M	502	3PE	C2C-C2D-C2E-C2F
53	N	402	3PE	C31-C32-C33-C34
46	B	203	PC1	C1-C2-C3-O31
52	h	202	CDL	CA3-CA4-CA6-OA8
53	L	702	3PE	C1-C2-C3-O31
53	L	703	3PE	C1-C2-C3-O31
53	N	402	3PE	C1-C2-C3-O31
53	X	201	3PE	C1-C2-C3-O31
53	Z	201	3PE	C1-C2-C3-O31
53	Z	202	3PE	C1-C2-C3-O31
53	d	201	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
53	i	201	3PE	C1-C2-C3-O31
53	I	203	3PE	C32-C33-C34-C35
53	r	201	3PE	C33-C34-C35-C36
45	h	203	LMT	C4'-C5'-C6'-O6'
53	Z	201	3PE	C25-C26-C27-C28
45	P	502	LMT	C5-C6-C7-C8
52	h	201	CDL	C61-C62-C63-C64
45	P	502	LMT	C4-C5-C6-C7
52	q	501	CDL	OB5-CB3-CB4-OB6
53	Z	201	3PE	O11-C1-C2-O21
53	Z	202	3PE	O11-C1-C2-O21
52	H	401	CDL	C54-C55-C56-C57
52	h	201	CDL	C74-C75-C76-C77
48	D	601	HQH	C23-C25-O3-C30
52	h	201	CDL	C77-C78-C79-C80
52	h	202	CDL	OA6-CA4-CA6-OA8
45	h	203	LMT	O5'-C1'-O1'-C1
46	B	202	PC1	C22-C23-C24-C25
53	Z	202	3PE	C2A-C2B-C2C-C2D
53	Z	202	3PE	C24-C25-C26-C27
52	H	401	CDL	C1-CA2-OA2-PA1
52	H	401	CDL	CB4-CB3-OB5-PB2
52	L	705	CDL	C1-CB2-OB2-PB2
52	L	705	CDL	CB4-CB3-OB5-PB2
45	J	202	LMT	C4-C5-C6-C7
53	Z	202	3PE	C27-C28-C29-C2A
58	T	201	EHZ	C21-C22-C23-C24
58	U	201	EHZ	O2-C9-S1-C10
45	K	201	LMT	O1'-C1-C2-C3
53	O	504	3PE	C32-C33-C34-C35
45	Y	202	LMT	C5-C6-C7-C8
46	B	203	PC1	O11-C1-C2-C3
53	M	503	3PE	O11-C1-C2-C3
45	L	704	LMT	C3-C4-C5-C6
53	L	702	3PE	C23-C24-C25-C26
45	Y	202	LMT	C4'-C5'-C6'-O6'
53	I	203	3PE	C24-C25-C26-C27
53	N	401	3PE	C33-C34-C35-C36
52	H	401	CDL	CA6-CA4-OA6-CA5
58	U	201	EHZ	C8-C9-S1-C10
46	B	202	PC1	C25-C26-C27-C28
46	A	402	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
52	h	201	CDL	CB3-CB4-CB6-OB8
53	O	504	3PE	C1-C2-C3-O31
53	X	201	3PE	C2-C1-O11-P
45	A	403	LMT	C4B-C5B-C6B-O6B
45	M	501	LMT	C3'-C4'-O1B-C1B
46	B	202	PC1	O11-C1-C2-O21
45	M	501	LMT	C1-C2-C3-C4
58	T	201	EHZ	C15-C16-C17-C19
45	Y	201	LMT	C3'-C4'-O1B-C1B
52	q	501	CDL	C55-C56-C57-C58
53	L	703	3PE	C3B-C3C-C3D-C3E
46	B	203	PC1	O21-C2-C3-O31
53	L	703	3PE	O21-C2-C3-O31
53	i	201	3PE	O21-C2-C3-O31
53	L	703	3PE	C3A-C3B-C3C-C3D
53	Z	202	3PE	C2B-C2C-C2D-C2E
45	A	401	LMT	C11-C10-C9-C8
52	h	201	CDL	C76-C77-C78-C79
45	M	501	LMT	C2-C3-C4-C5
45	M	501	LMT	C9-C10-C11-C12
53	M	502	3PE	C25-C26-C27-C28
53	M	502	3PE	C11-O13-P-O11
53	N	401	3PE	C1-O11-P-O13
56	P	501	NDP	O4D-C1D-N1N-C6N
52	h	202	CDL	CA4-CA3-OA5-PA1
46	A	402	PC1	C1-O11-P-O14
46	B	203	PC1	C1-O11-P-O12
46	B	203	PC1	C1-O11-P-O14
52	H	401	CDL	CA2-OA2-PA1-OA4
52	H	401	CDL	CB3-OB5-PB2-OB3
52	h	201	CDL	CB2-OB2-PB2-OB4
52	h	202	CDL	CB2-OB2-PB2-OB3
52	q	501	CDL	CA2-OA2-PA1-OA3
53	L	702	3PE	C1-O11-P-O12
53	M	502	3PE	C1-O11-P-O14
53	M	503	3PE	C11-O13-P-O14
53	N	401	3PE	C1-O11-P-O12
53	N	401	3PE	C11-O13-P-O12
53	O	504	3PE	C11-O13-P-O12
53	O	504	3PE	C11-O13-P-O14
53	i	201	3PE	C1-O11-P-O14
53	I	203	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
45	A	403	LMT	O5'-C1'-O1'-C1
45	L	704	LMT	O5'-C1'-O1'-C1
46	B	202	PC1	O11-C1-C2-C3
52	q	501	CDL	OB5-CB3-CB4-CB6
53	Z	201	3PE	O11-C1-C2-C3
53	d	201	3PE	O11-C1-C2-C3
46	B	202	PC1	C27-C28-C29-C2A
53	i	201	3PE	C33-C34-C35-C36
52	q	501	CDL	C54-C55-C56-C57
45	Y	203	LMT	C11-C10-C9-C8
53	r	201	3PE	C22-C23-C24-C25
53	I	203	3PE	C12-C11-O13-P
53	L	703	3PE	C12-C11-O13-P
53	L	703	3PE	C3D-C3E-C3F-C3G
52	L	705	CDL	C53-C54-C55-C56
53	i	201	3PE	C31-C32-C33-C34
52	L	705	CDL	OA5-CA3-CA4-OA6
53	M	503	3PE	O11-C1-C2-O21
53	M	502	3PE	O31-C31-C32-C33
45	A	401	LMT	C2-C3-C4-C5
58	U	201	EHZ	C10-C11-N1-C12
53	M	502	3PE	C1-C2-C3-O31
58	T	201	EHZ	C16-C17-C20-O6
58	U	201	EHZ	O5-C16-C17-C20
46	A	402	PC1	O21-C2-C3-O31
46	B	202	PC1	O21-C2-C3-O31
53	N	402	3PE	O21-C2-C3-O31
53	X	201	3PE	O21-C2-C3-O31
53	d	201	3PE	O21-C2-C3-O31
53	X	201	3PE	C3C-C3D-C3E-C3F
53	r	201	3PE	C36-C37-C38-C39
45	j	101	LMT	C1-C2-C3-C4
45	Y	204	LMT	C7-C8-C9-C10
53	N	401	3PE	C32-C31-O31-C3
53	L	703	3PE	C37-C38-C39-C3A
45	P	502	LMT	C7-C8-C9-C10
45	Y	203	LMT	C6-C7-C8-C9
59	o	201	MYR	C5-C6-C7-C8
53	N	401	3PE	O32-C31-O31-C3
45	Y	203	LMT	O1'-C1-C2-C3
45	Y	204	LMT	O5B-C5B-C6B-O6B
53	L	702	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
45	L	704	LMT	C9-C10-C11-C12
53	L	703	3PE	C33-C34-C35-C36
53	L	703	3PE	C1-C2-O21-C21
53	X	201	3PE	C3-C2-O21-C21
52	h	202	CDL	OB5-CB3-CB4-CB6
45	Y	202	LMT	C2-C3-C4-C5
52	H	401	CDL	C51-C52-C53-C54
52	q	501	CDL	C1-CB2-OB2-PB2
52	H	401	CDL	OB5-CB3-CB4-OB6
52	h	201	CDL	OA5-CA3-CA4-OA6
53	M	502	3PE	C2B-C2C-C2D-C2E
45	A	401	LMT	C7-C8-C9-C10
45	M	501	LMT	O5'-C1'-O1'-C1
45	L	704	LMT	C2'-C1'-O1'-C1
45	h	203	LMT	C2'-C1'-O1'-C1
45	J	202	LMT	C2-C3-C4-C5
52	L	705	CDL	CA2-OA2-PA1-OA5
52	h	201	CDL	CA2-OA2-PA1-OA5
52	h	202	CDL	CA2-OA2-PA1-OA5
53	Z	202	3PE	C1-O11-P-O13
53	d	201	3PE	C1-O11-P-O13
53	d	201	3PE	C11-O13-P-O11
53	L	703	3PE	C39-C3A-C3B-C3C
58	U	201	EHZ	C21-C22-C23-C24
53	M	502	3PE	C2A-C2B-C2C-C2D
45	Y	201	LMT	C2-C3-C4-C5
59	o	201	MYR	C2-C3-C4-C5
55	O	502	GTP	PA-O3A-PB-O2B
53	X	201	3PE	C22-C23-C24-C25
53	Z	202	3PE	C32-C33-C34-C35
53	r	201	3PE	C3C-C3D-C3E-C3F
50	F	502	FMN	C4'-C5'-O5'-P
53	M	503	3PE	C2-C1-O11-P
52	H	401	CDL	OB7-CB5-OB6-CB4
46	B	203	PC1	C31-C32-C33-C34
53	i	201	3PE	O13-C11-C12-N
46	B	203	PC1	C35-C36-C37-C38
52	q	501	CDL	C76-C77-C78-C79
53	M	502	3PE	O32-C31-C32-C33
53	Z	201	3PE	C2-C1-O11-P
53	O	504	3PE	C25-C26-C27-C28
45	Y	203	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
53	M	503	3PE	C37-C38-C39-C3A
45	J	201	LMT	O5'-C1'-O1'-C1
52	q	501	CDL	C56-C57-C58-C59
52	h	201	CDL	CB2-OB2-PB2-OB5
52	h	201	CDL	C79-C80-C81-C82
53	N	401	3PE	C27-C28-C29-C2A
52	q	501	CDL	CB4-CB3-OB5-PB2
53	N	402	3PE	C2-C1-O11-P
53	I	203	3PE	C28-C29-C2A-C2B
58	U	201	EHZ	C1-C21-C22-C23
52	q	501	CDL	OA5-CA3-CA4-CA6
45	Y	201	LMT	C5'-C4'-O1B-C1B
58	U	201	EHZ	C11-C10-S1-C9
52	H	401	CDL	C51-CB5-OB6-CB4
52	h	201	CDL	C52-C53-C54-C55
53	r	201	3PE	C3A-C3B-C3C-C3D
58	U	201	EHZ	C22-C23-C24-C25
53	L	702	3PE	C24-C25-C26-C27
45	K	201	LMT	C6-C7-C8-C9
45	Y	201	LMT	C7-C8-C9-C10
52	L	705	CDL	C31-C32-C33-C34
45	Y	203	LMT	C7-C8-C9-C10
53	Z	202	3PE	C35-C36-C37-C38
53	r	201	3PE	O11-C1-C2-O21
45	A	401	LMT	O5'-C5'-C6'-O6'
45	Y	204	LMT	O5B-C1B-O1B-C4'
52	L	705	CDL	C17-C18-C19-C20
52	h	201	CDL	C51-C52-C53-C54
52	h	201	CDL	C60-C61-C62-C63
52	h	201	CDL	OA6-CA4-CA6-OA8
53	Z	202	3PE	O21-C21-C22-C23
45	A	403	LMT	C2'-C1'-O1'-C1
58	T	201	EHZ	C2-C1-C21-C22
53	N	401	3PE	O21-C2-C3-O31
52	h	201	CDL	C58-C59-C60-C61
52	h	202	CDL	C72-C73-C74-C75
58	T	201	EHZ	C1-C21-C22-C23
52	L	705	CDL	C52-C51-CB5-OB6
56	P	501	NDP	C3D-C4D-C5D-O5D
52	h	202	CDL	C52-C51-CB5-OB6
53	L	703	3PE	O21-C21-C22-C23
53	L	702	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
52	L	705	CDL	CB3-OB5-PB2-OB2
53	Z	202	3PE	C11-O13-P-O11
53	I	203	3PE	C37-C38-C39-C3A
52	L	705	CDL	C32-C31-CA7-OA8
48	D	601	HQH	C21-C15-C17-C26
52	h	201	CDL	C75-C76-C77-C78
45	J	202	LMT	C3-C4-C5-C6
52	h	202	CDL	C72-C71-CB7-OB8
53	L	702	3PE	O21-C21-C22-C23
53	Z	201	3PE	C34-C35-C36-C37
46	B	202	PC1	C1-C2-C3-O31
48	D	601	HQH	C17-C15-C21-C18
45	Y	203	LMT	C5'-C4'-O1B-C1B
45	A	403	LMT	C9-C10-C11-C12
53	L	703	3PE	C35-C36-C37-C38
55	O	502	GTP	PB-O3B-PG-O3G
58	U	201	EHZ	C15-C16-C17-C18
52	q	501	CDL	C59-C60-C61-C62
52	H	401	CDL	OB5-CB3-CB4-CB6
53	r	201	3PE	O11-C1-C2-C3
53	r	201	3PE	O21-C2-C3-O31
46	B	203	PC1	C21-C22-C23-C24
53	I	203	3PE	C33-C34-C35-C36
53	L	703	3PE	C38-C39-C3A-C3B
45	J	201	LMT	C6-C7-C8-C9
45	j	101	LMT	C4-C5-C6-C7
53	L	702	3PE	C32-C33-C34-C35
46	A	402	PC1	O21-C21-C22-C23
55	O	502	GTP	O4'-C4'-C5'-O5'
53	O	504	3PE	C22-C23-C24-C25
52	L	705	CDL	C51-CB5-OB6-CB4
53	L	702	3PE	C34-C35-C36-C37
52	h	202	CDL	C52-C51-CB5-OB7
52	H	401	CDL	CB2-C1-CA2-OA2
52	h	202	CDL	C72-C71-CB7-OB9
53	N	402	3PE	O31-C31-C32-C33
53	L	703	3PE	O22-C21-C22-C23
52	L	705	CDL	C52-C51-CB5-OB7
45	Y	204	LMT	C2B-C1B-O1B-C4'
55	O	502	GTP	C4'-C5'-O5'-PA
52	h	202	CDL	CA2-OA2-PA1-OA3
53	I	203	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
53	I	203	3PE	C11-O13-P-O14
53	X	201	3PE	C11-O13-P-O12
53	i	201	3PE	C1-O11-P-O12
53	M	503	3PE	O31-C31-C32-C33
53	M	502	3PE	O11-C1-C2-C3
46	B	202	PC1	C26-C27-C28-C29
52	q	501	CDL	C58-C59-C60-C61
53	L	702	3PE	O22-C21-C22-C23
46	A	402	PC1	O31-C31-C32-C33
53	M	502	3PE	O22-C21-O21-C2
52	L	705	CDL	C32-C31-CA7-OA9
53	N	402	3PE	C32-C33-C34-C35
53	Z	201	3PE	C12-C11-O13-P
52	q	501	CDL	C52-C53-C54-C55
53	d	201	3PE	C35-C36-C37-C38
53	Z	201	3PE	O21-C21-C22-C23
46	A	402	PC1	O32-C31-C32-C33
58	T	201	EHZ	O3-C12-C13-C14
50	F	502	FMN	N10-C1'-C2'-O2'
52	h	201	CDL	C52-C51-CB5-OB6
53	O	504	3PE	O31-C31-C32-C33
45	Y	201	LMT	C2-C1-O1'-C1'
53	O	504	3PE	O21-C21-C22-C23
52	L	705	CDL	OB7-CB5-OB6-CB4
53	O	504	3PE	O32-C31-C32-C33

There are no ring outliers.

23 monomers are involved in 32 short contacts:

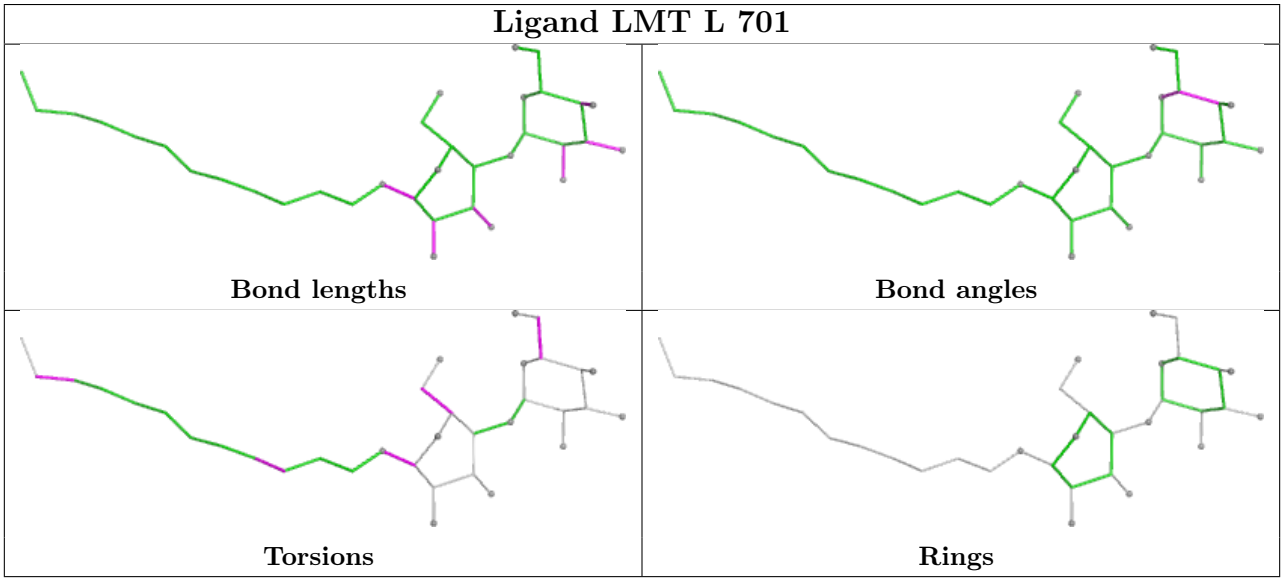
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	L	701	LMT	1	0
45	j	101	LMT	1	0
55	O	502	GTP	5	0
45	Y	201	LMT	8	0
46	B	203	PC1	1	0
50	F	502	FMN	2	0
45	L	704	LMT	1	0
53	N	402	3PE	1	0
52	L	705	CDL	1	0
52	q	501	CDL	1	0
53	d	201	3PE	1	0
45	Y	202	LMT	1	0

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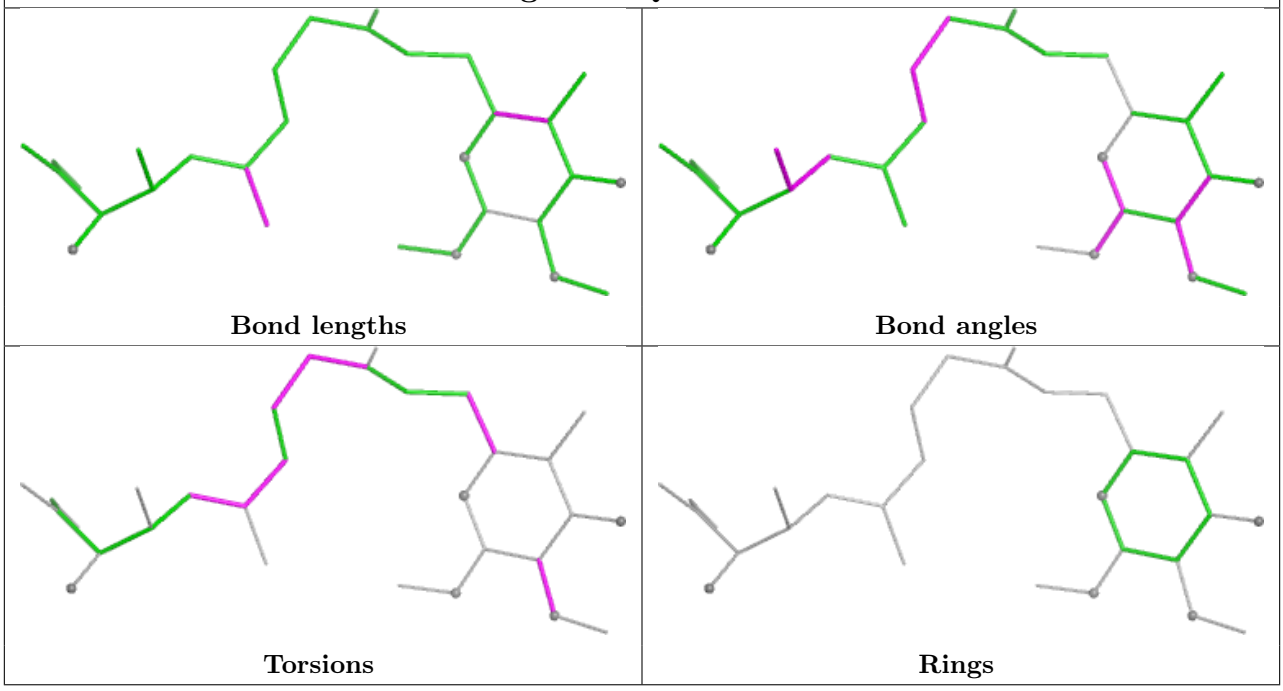
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	P	501	NDP	1	0
52	h	201	CDL	1	0
52	h	202	CDL	1	0
45	M	501	LMT	1	0
53	L	703	3PE	2	0
58	U	201	EHZ	1	0
45	Y	203	LMT	1	0
53	O	504	3PE	1	0
47	B	201	SF4	1	0
53	X	201	3PE	1	0
45	O	503	LMT	1	0

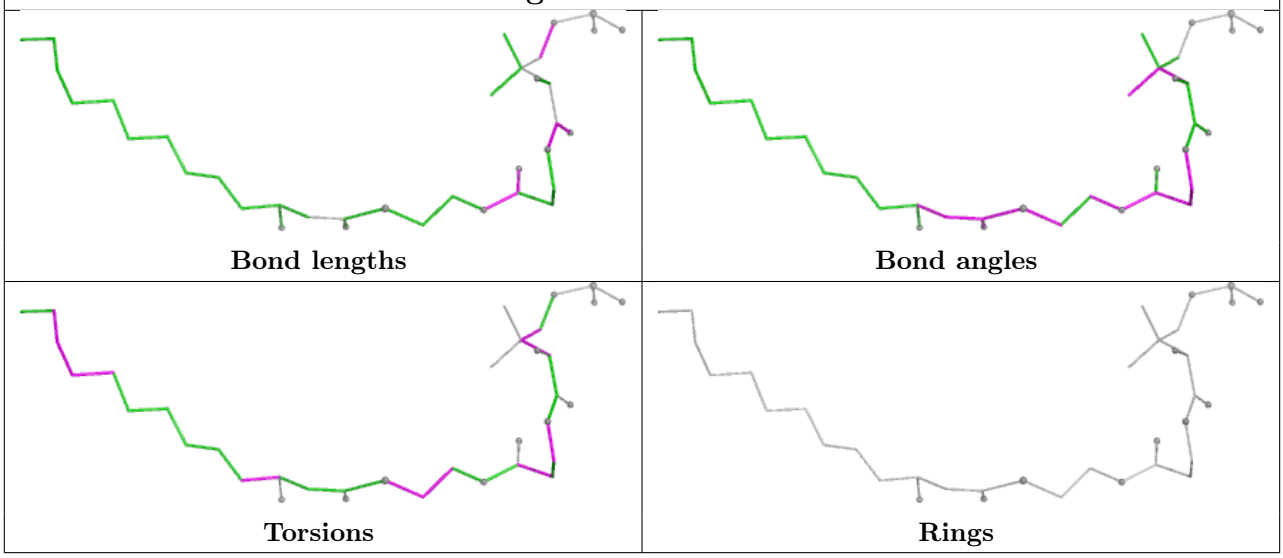
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



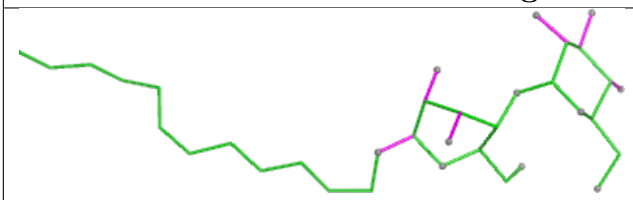
Ligand HQH D 601



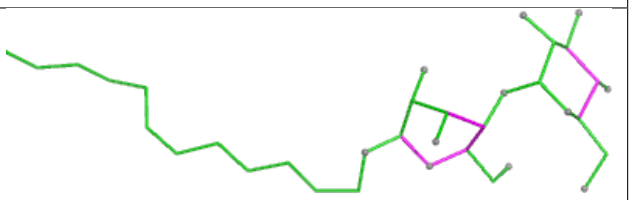
Ligand EHZ T 201



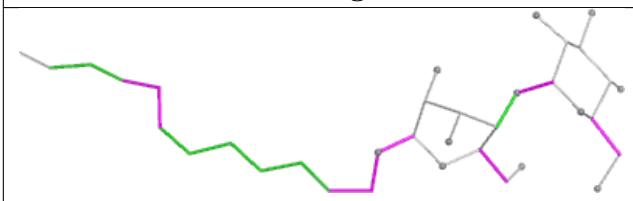
Ligand LMT Y 204



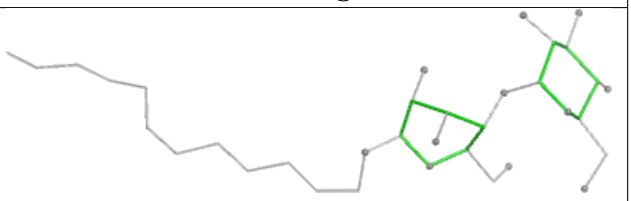
Bond lengths



Bond angles

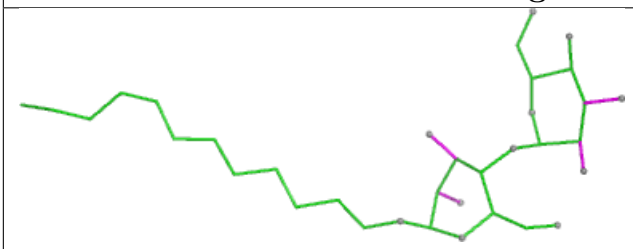


Torsions

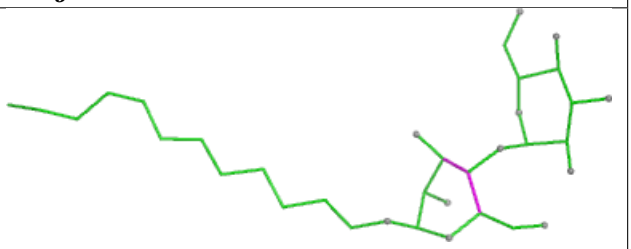


Rings

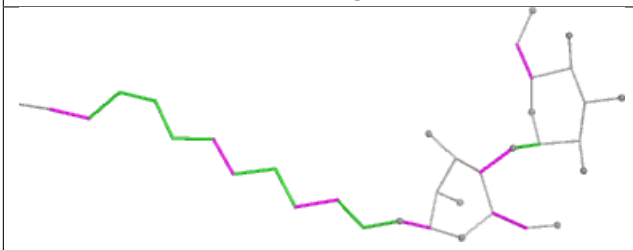
Ligand LMT j 101



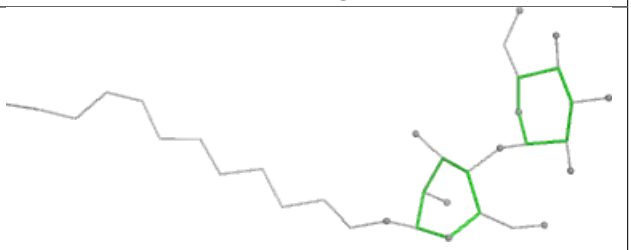
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Bond angles

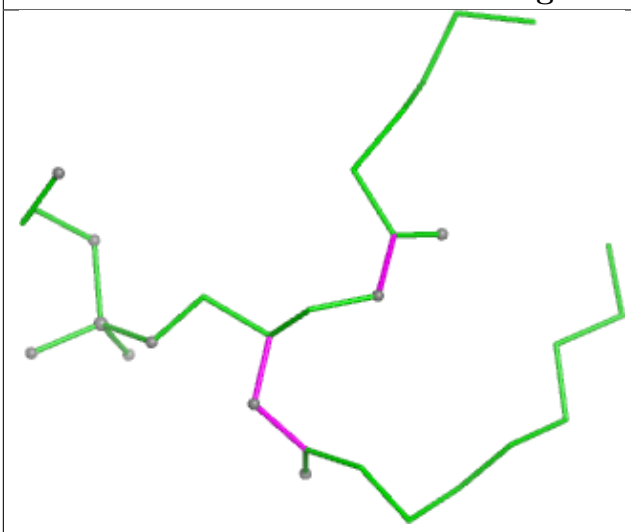


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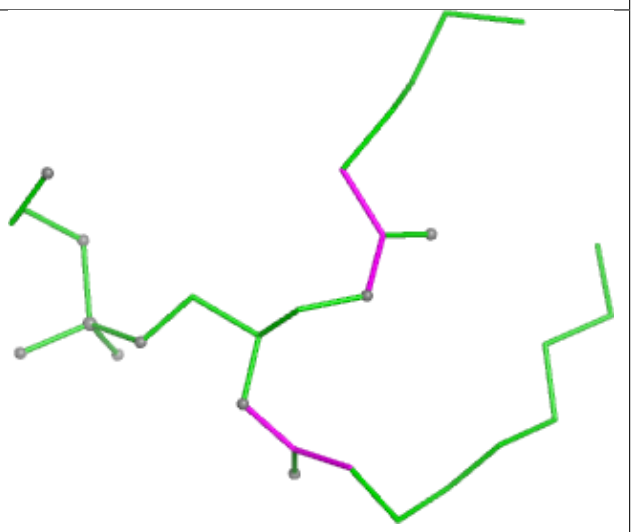


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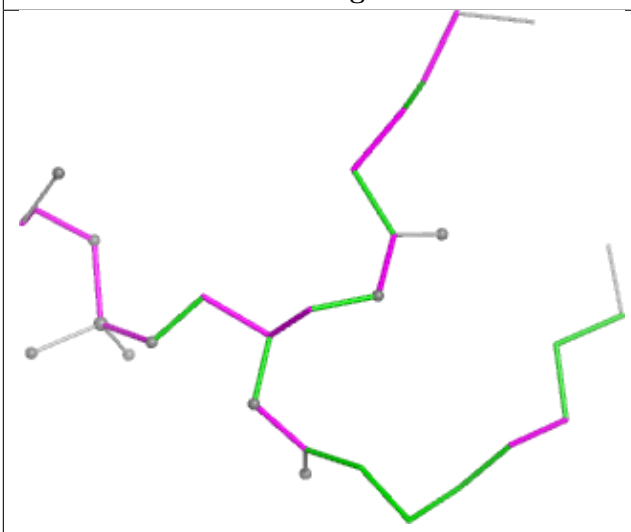
Ligand 3PE i 201



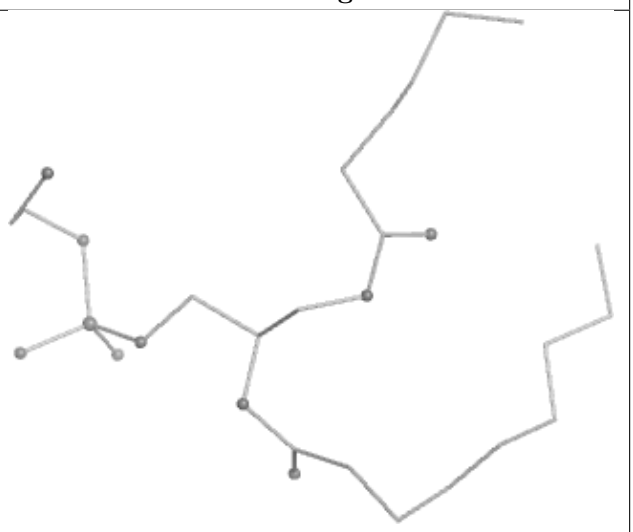
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Bond angles

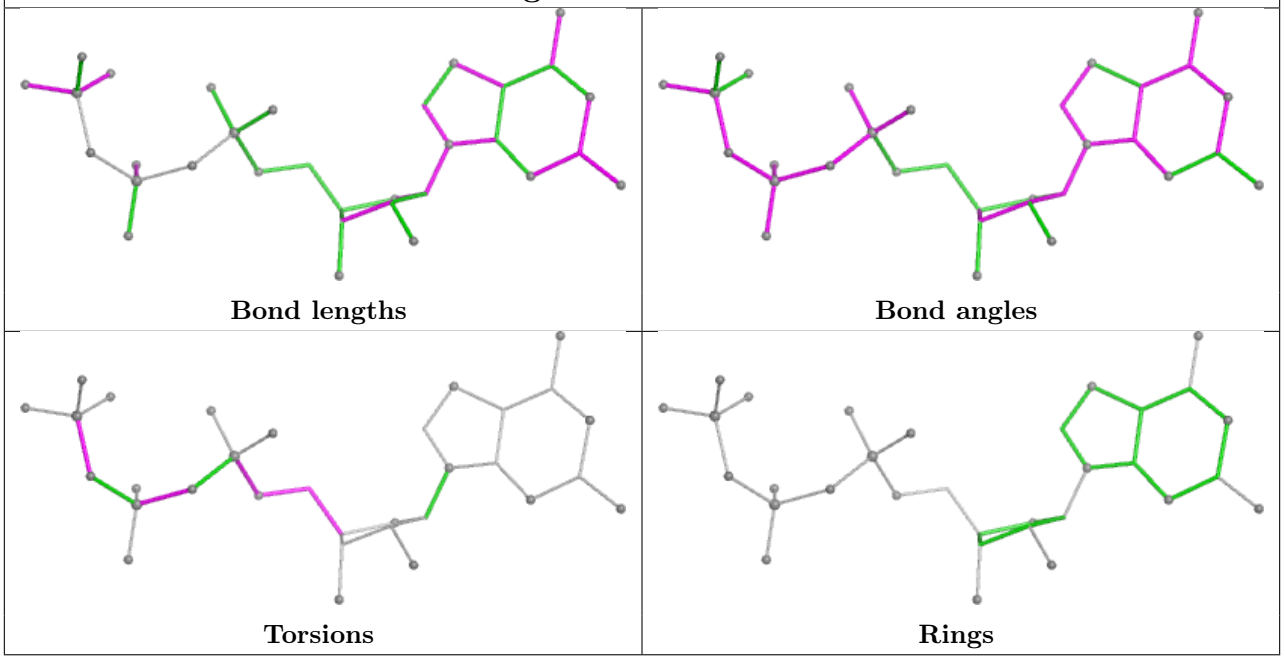


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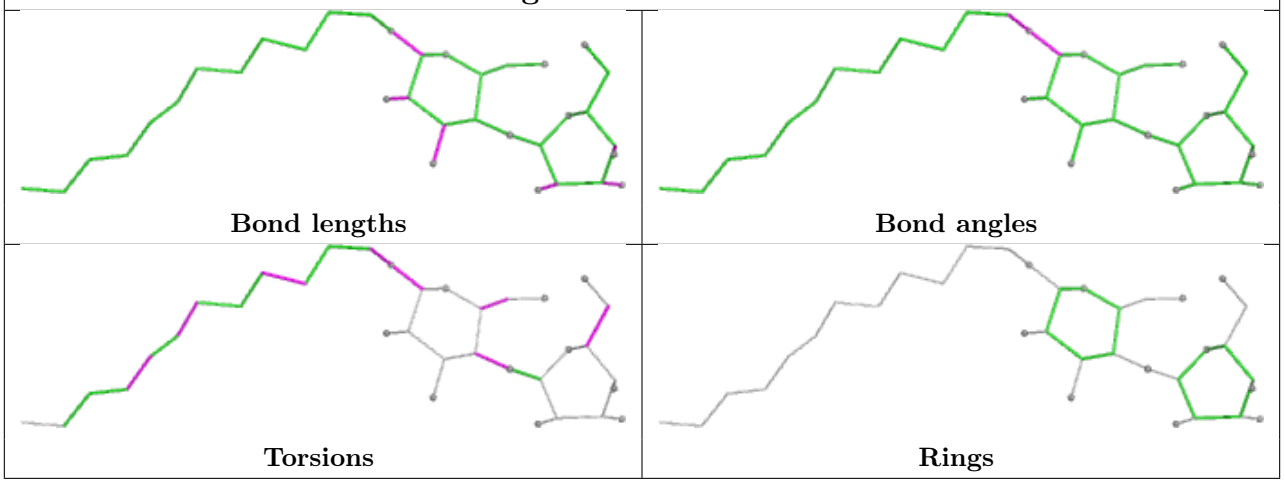


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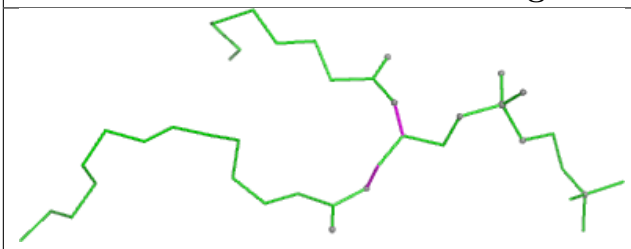
Ligand GTP O 502



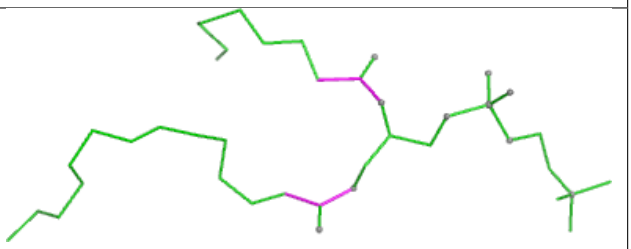
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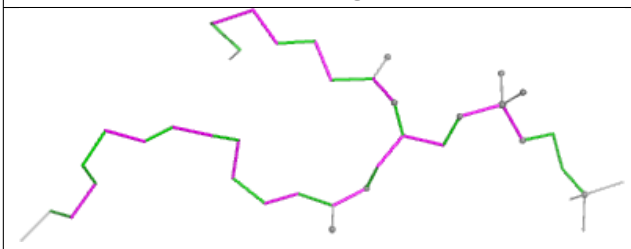
Ligand PC1 B 203



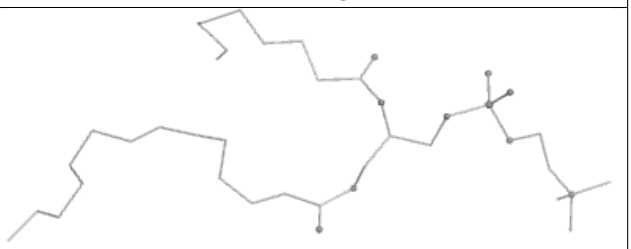
Bond lengths



Bond angles

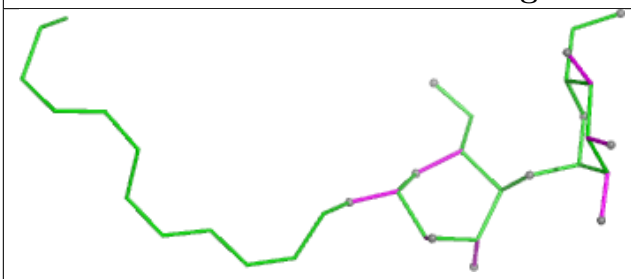


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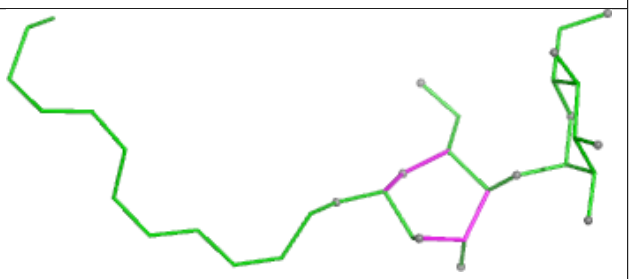


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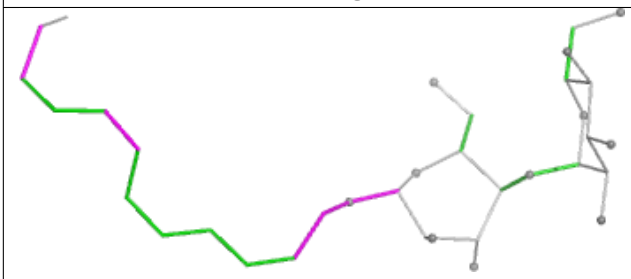
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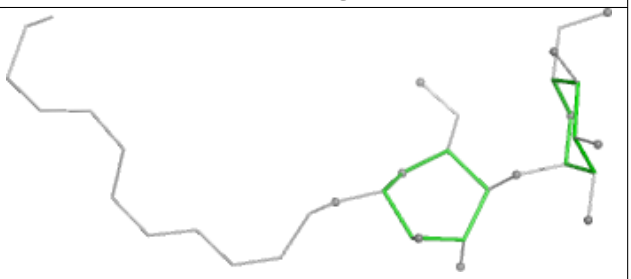
Bond lengths



Bond angles

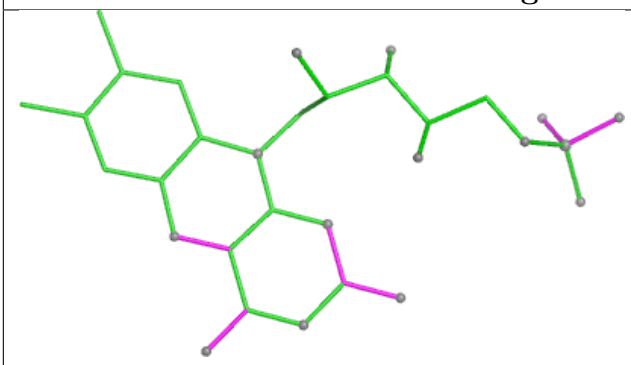


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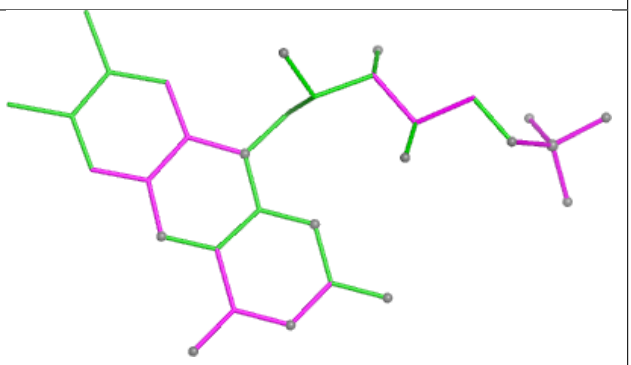


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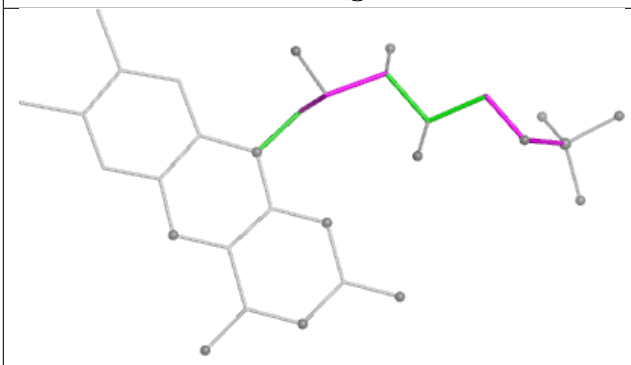
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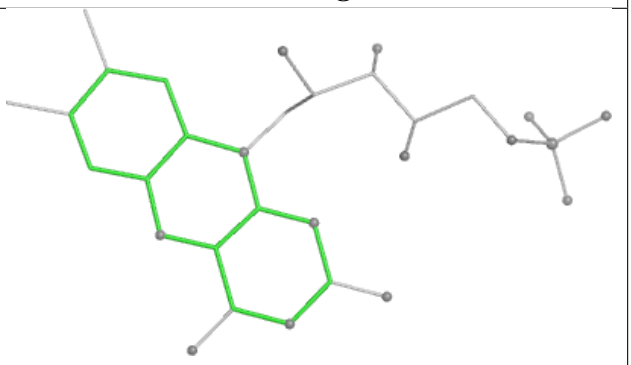
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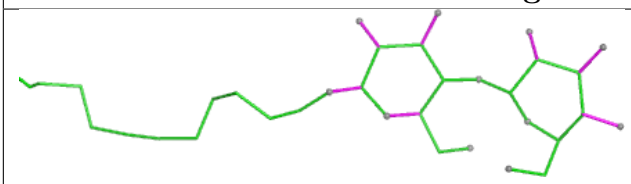


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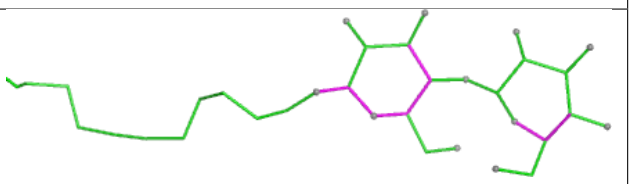


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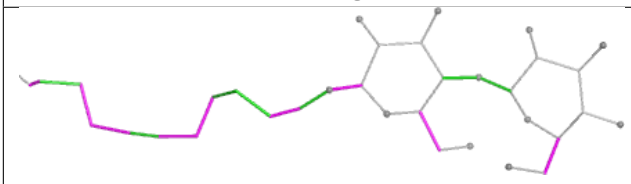
Ligand LMT L 704



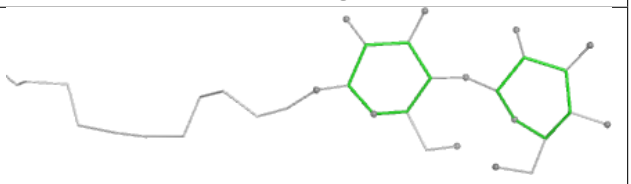
Bond lengths



Bond angles

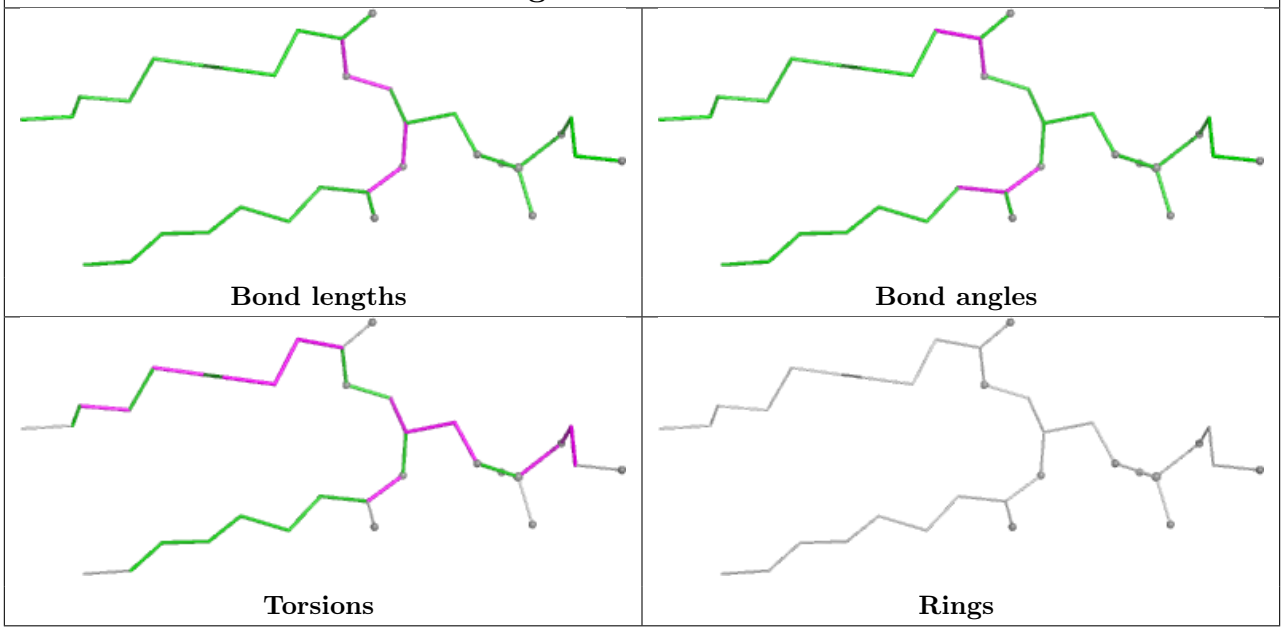


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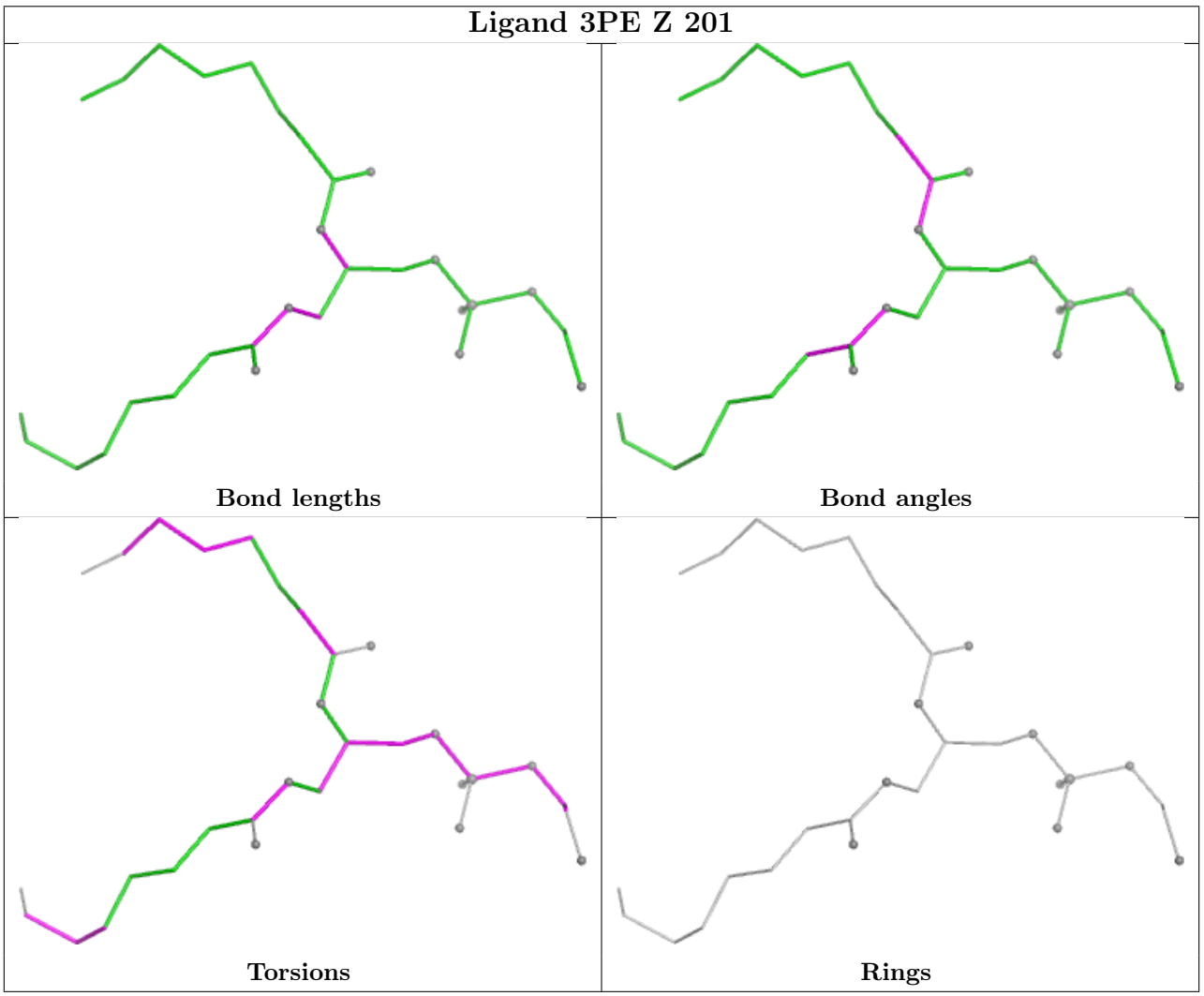


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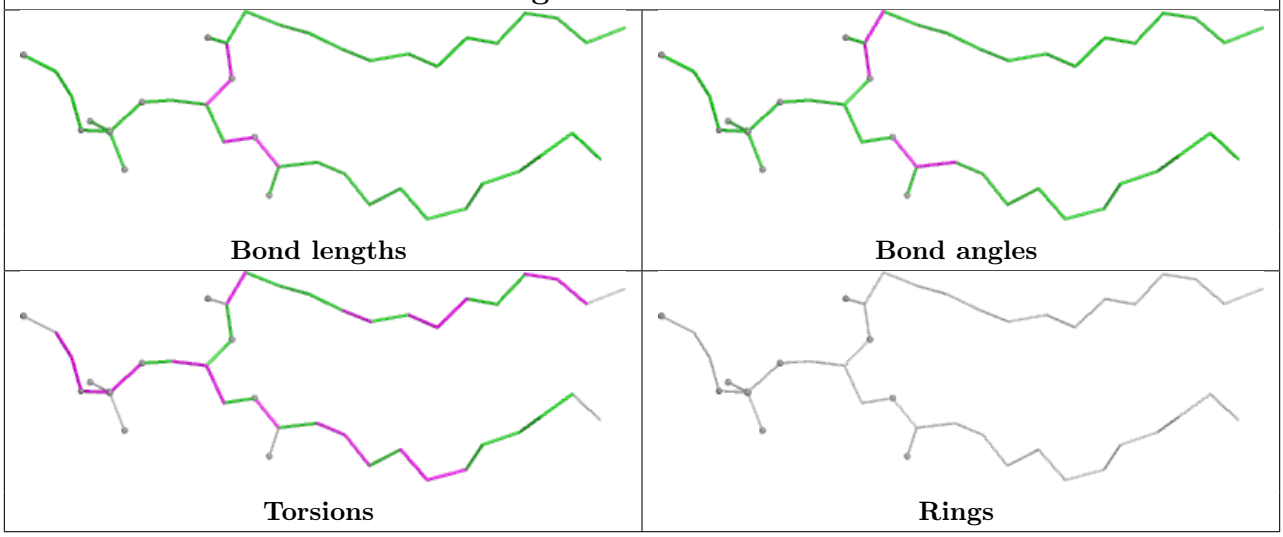
Ligand 3PE N 402



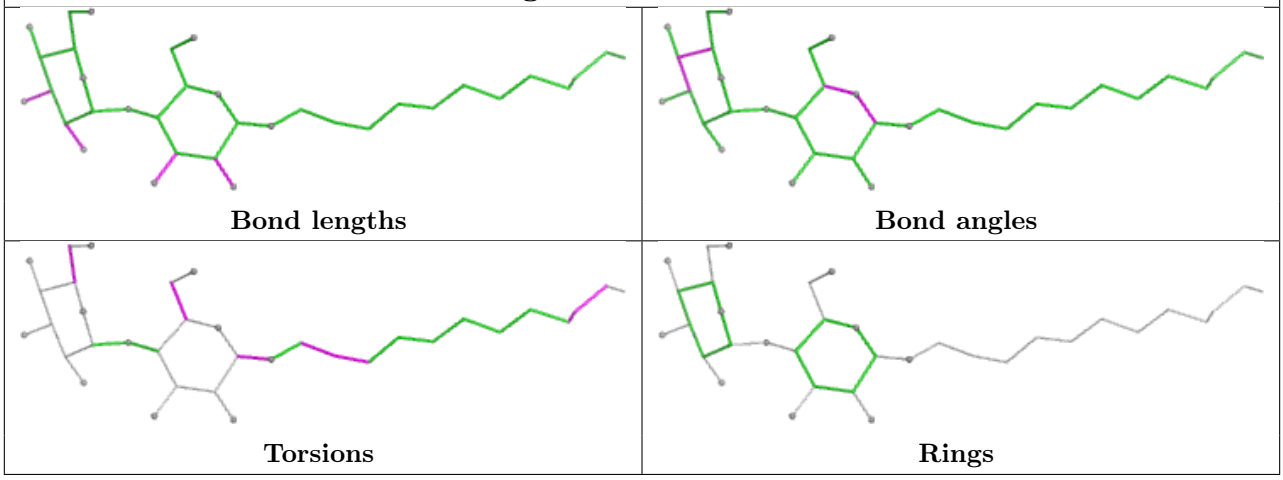
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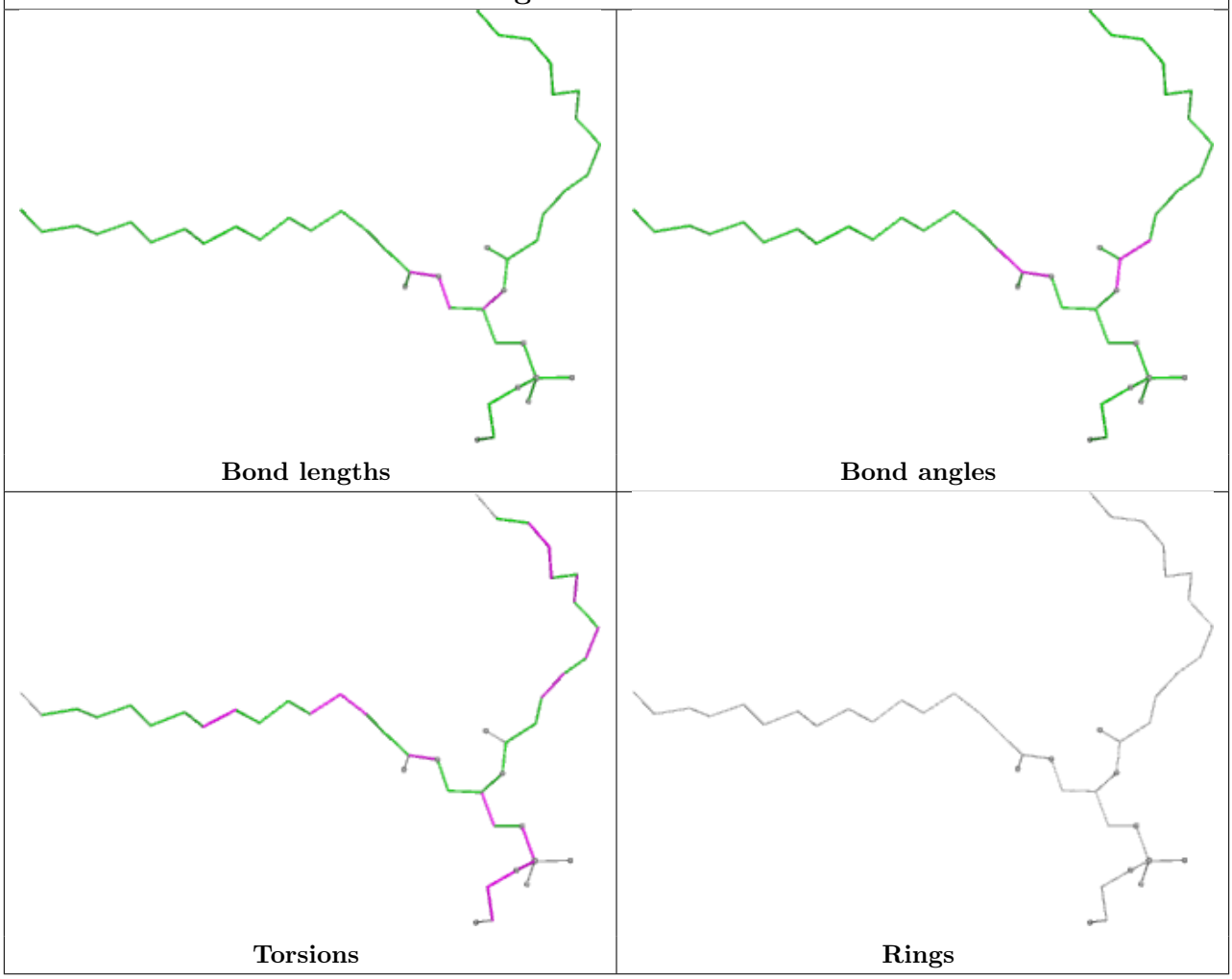
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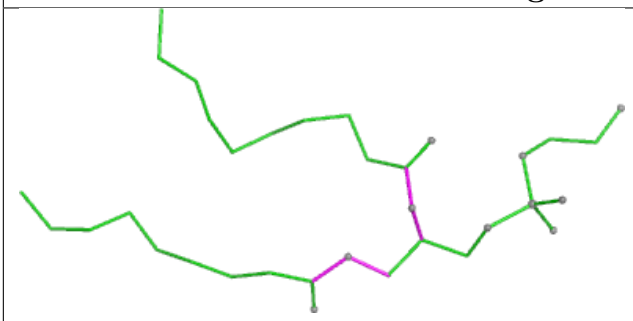
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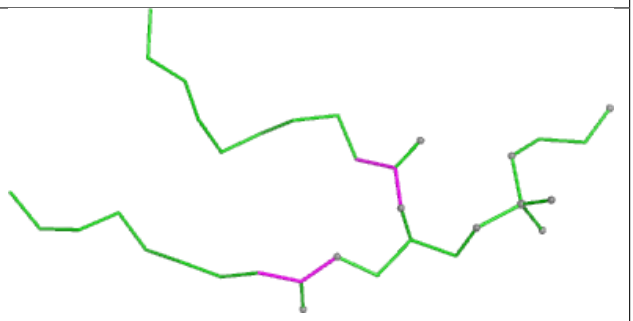
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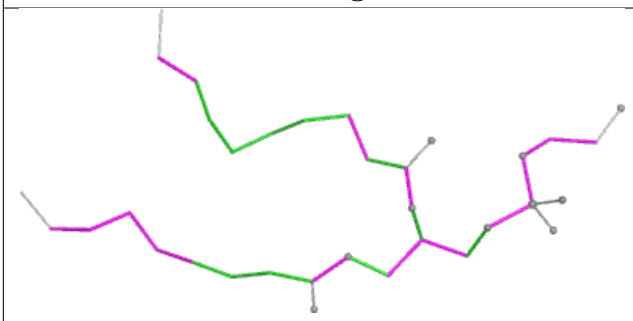
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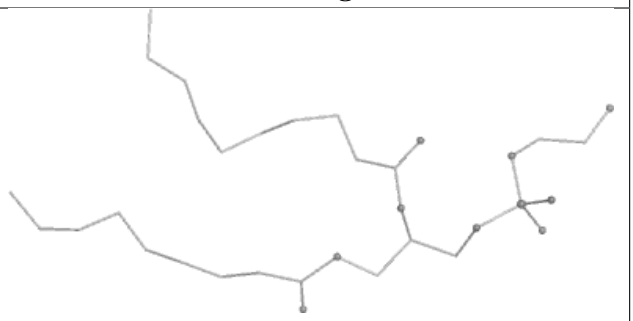
Bond lengths



Bond angles

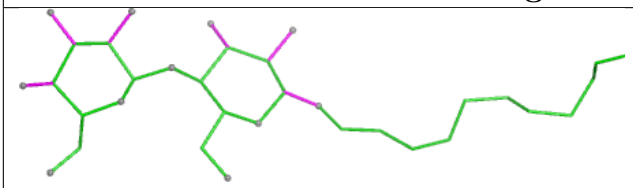


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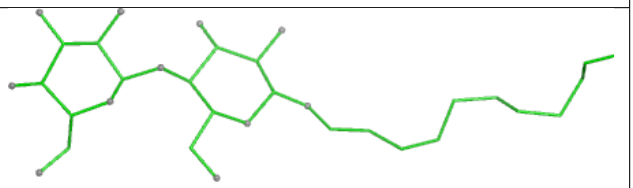


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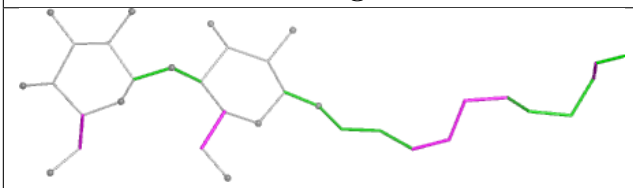
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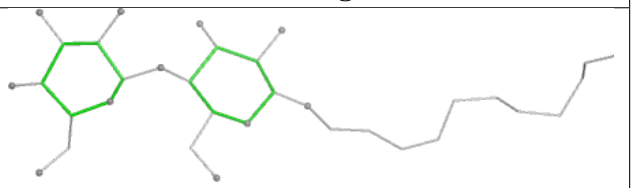
Bond lengths



Bond angles

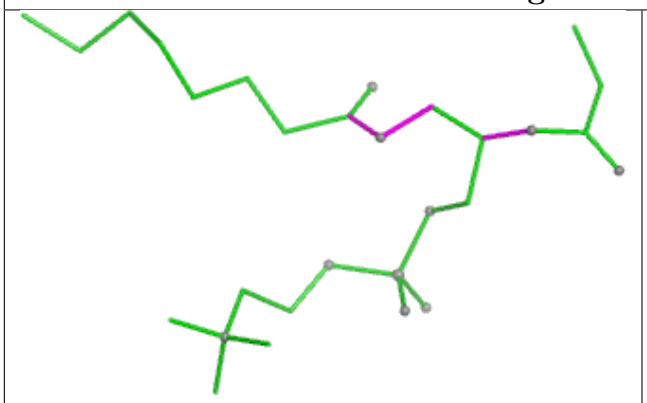


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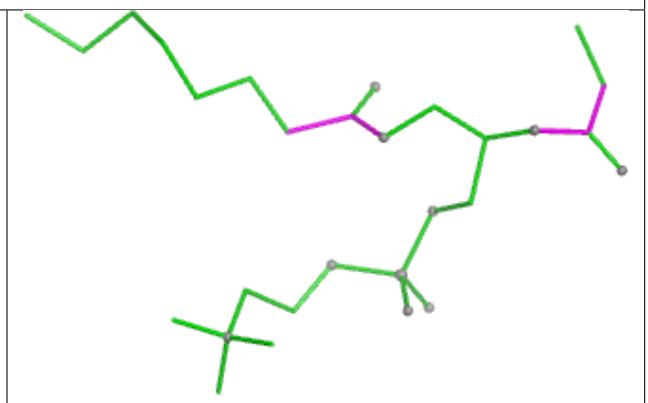


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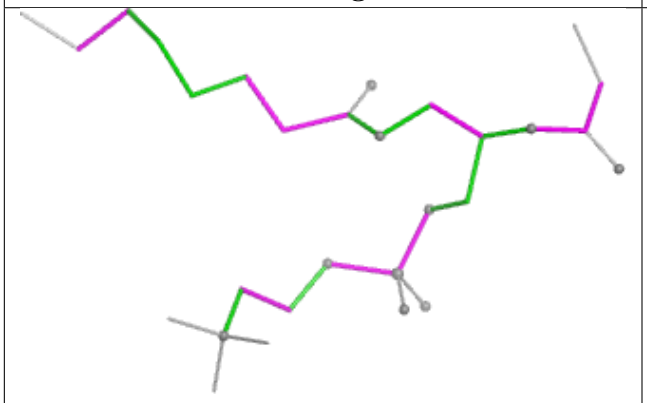
Ligand PC1 A 402



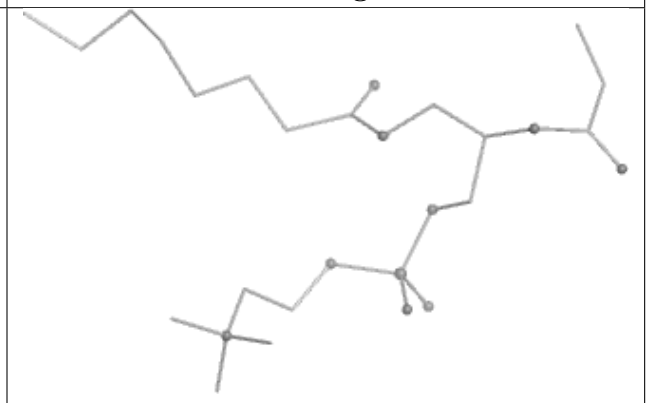
Bond lengths



Bond angles

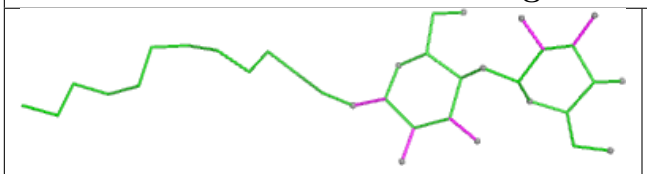


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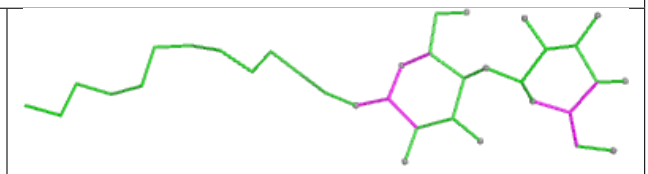


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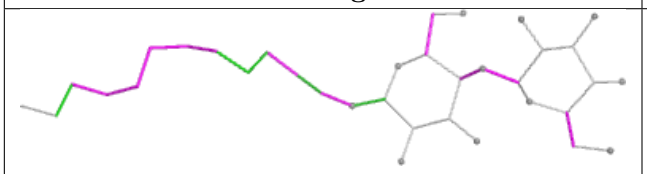
Ligand LMT P 502



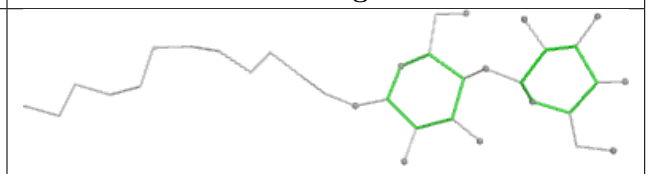
Bond lengths



Bond angles

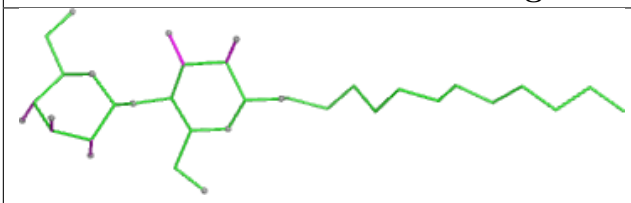


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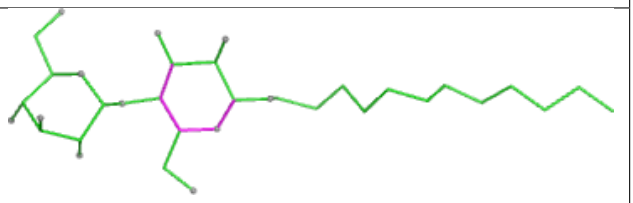


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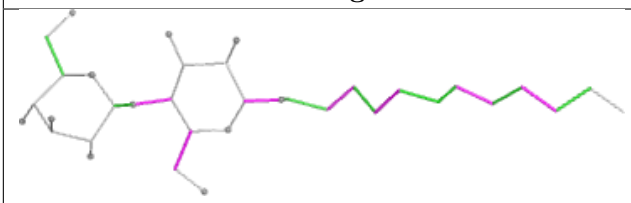
Ligand LMT J 201



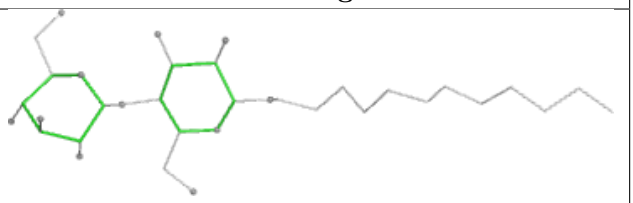
Bond lengths



Bond angles

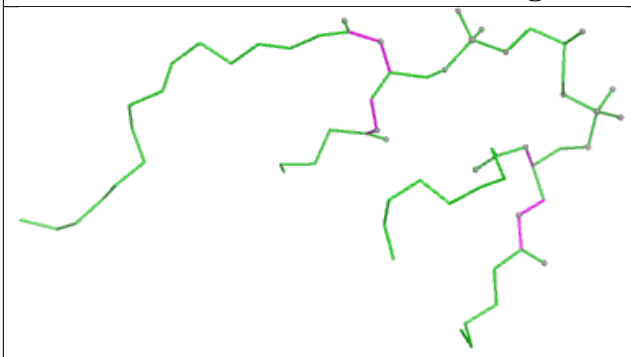


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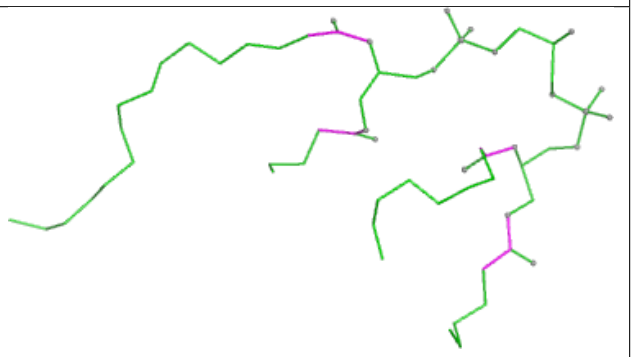


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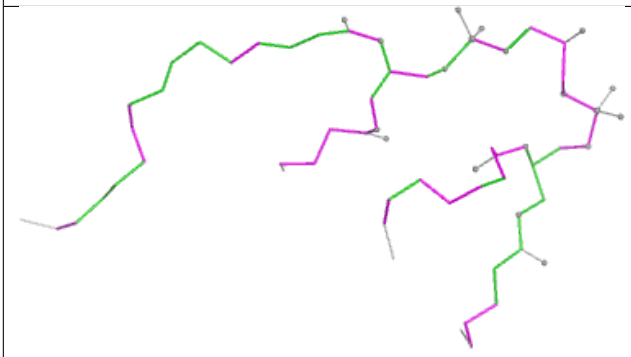
Ligand CDL L 705



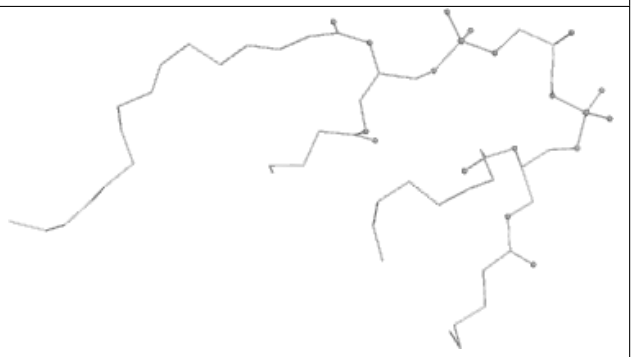
Bond lengths



Bond angles

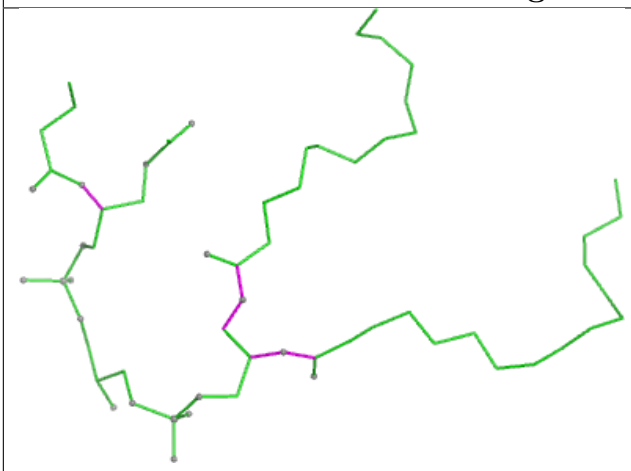


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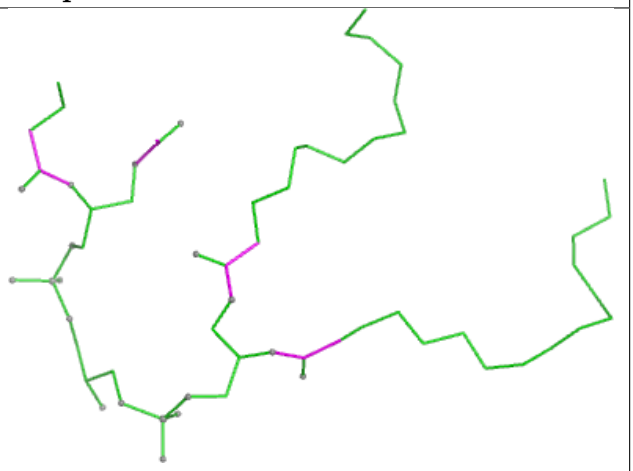


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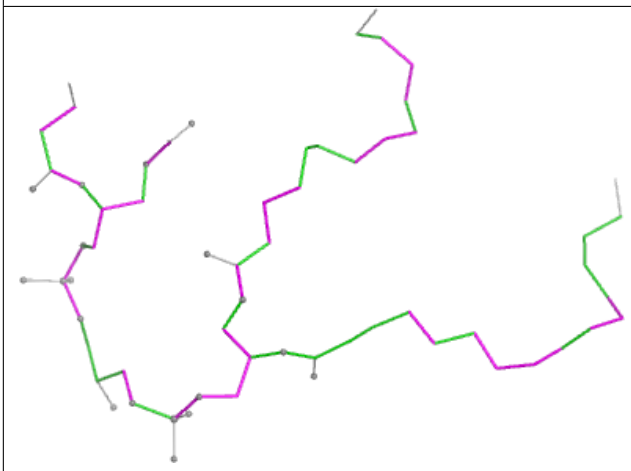
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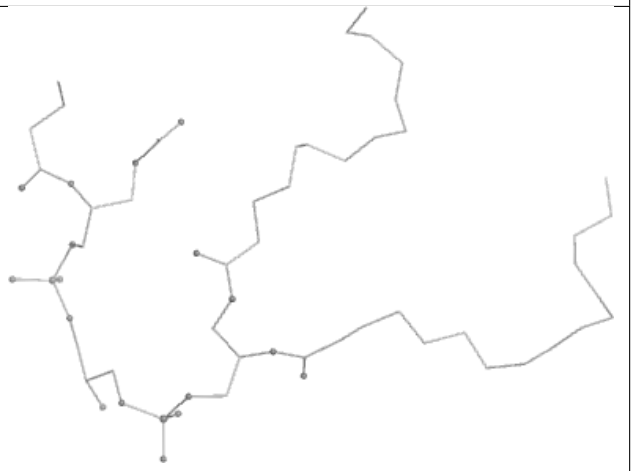
Bond lengths



Bond angles

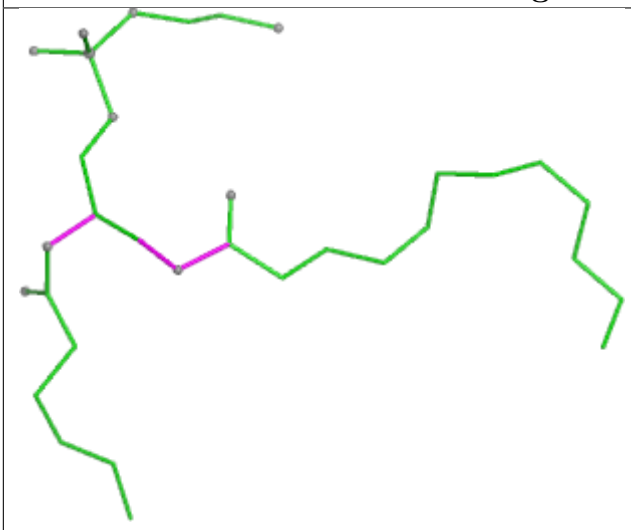


Torsions

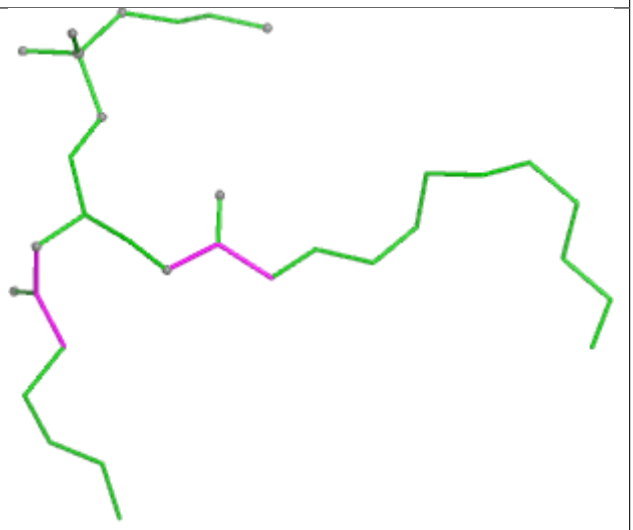


Rings

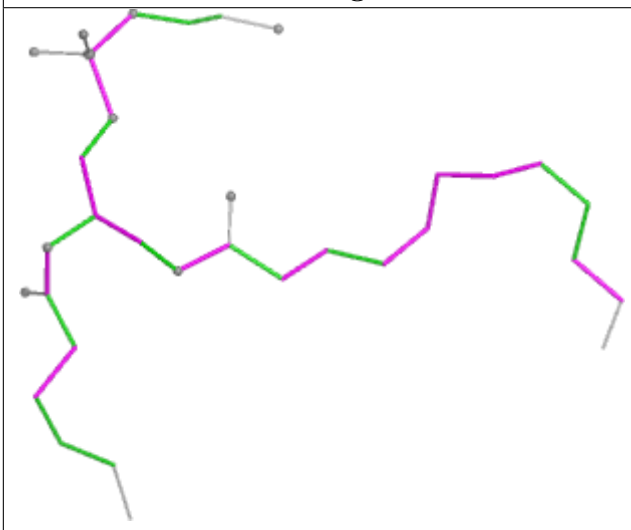
Ligand 3PE d 201



Bond lengths



Bond angles

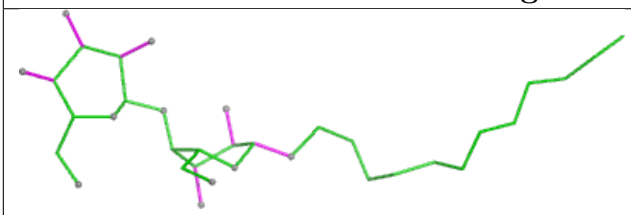


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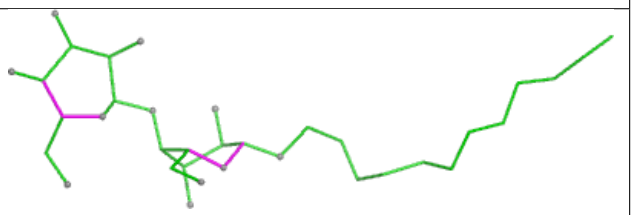


Rings

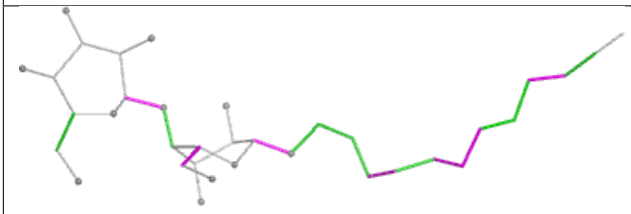
Ligand LMT Y 202



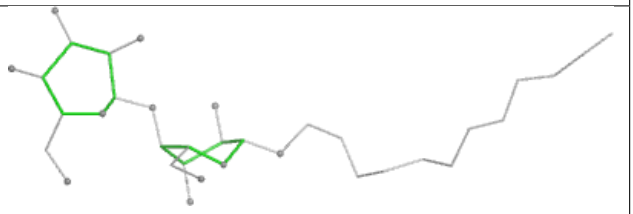
Bond lengths



Bond angles

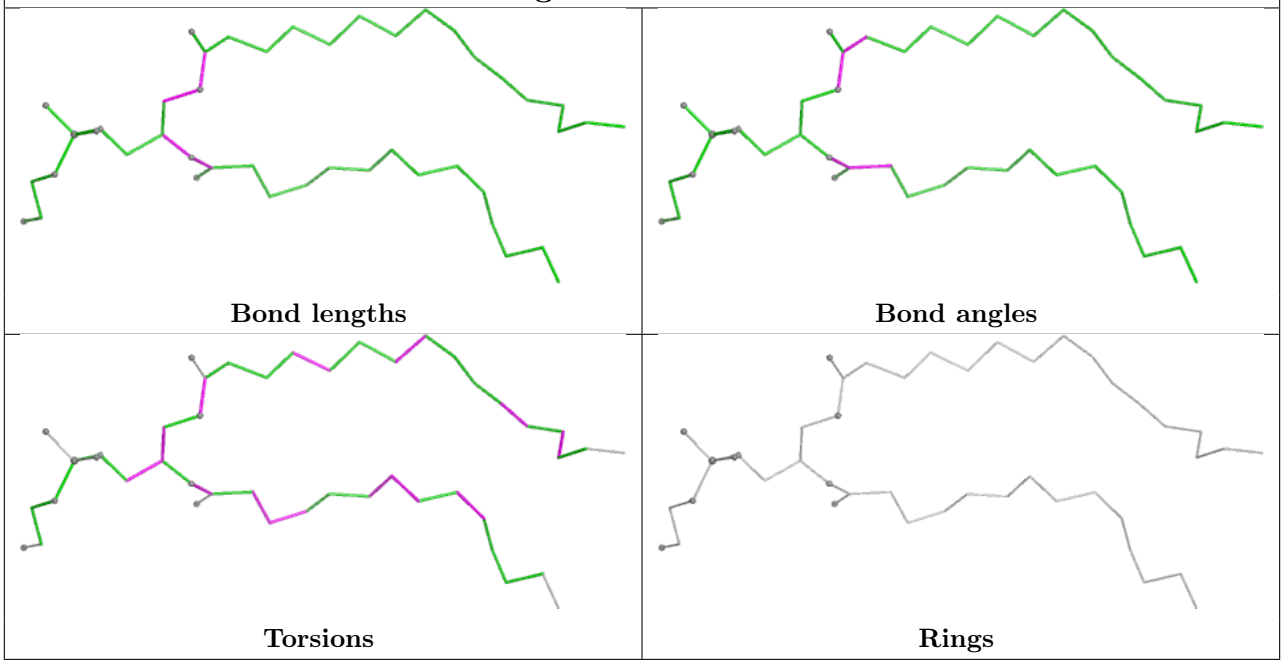


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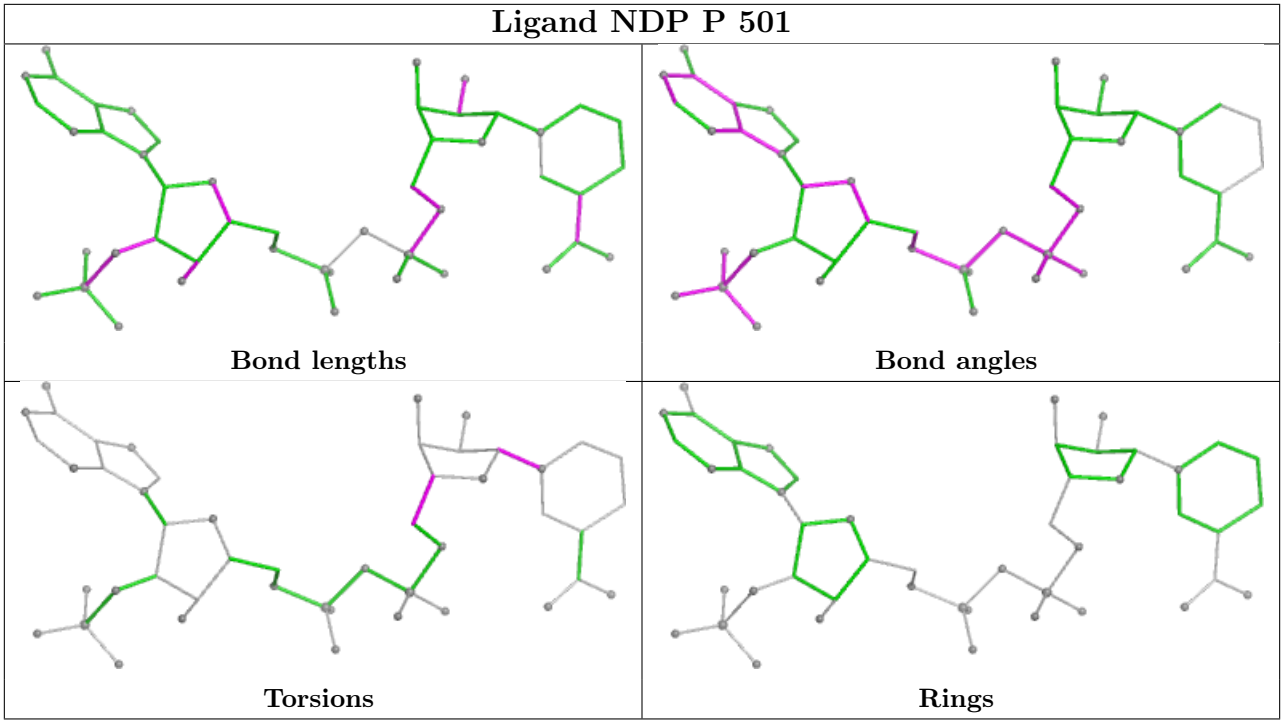


Rings

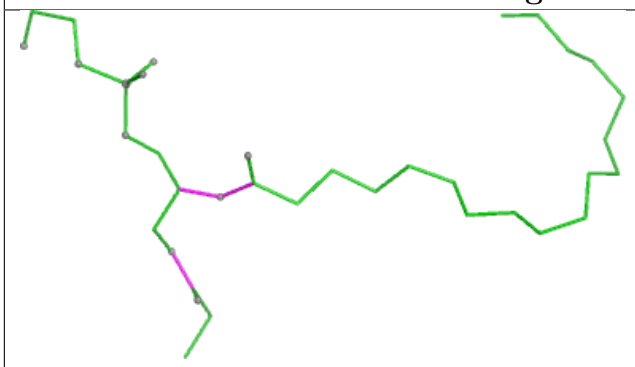
Ligand 3PE r 201



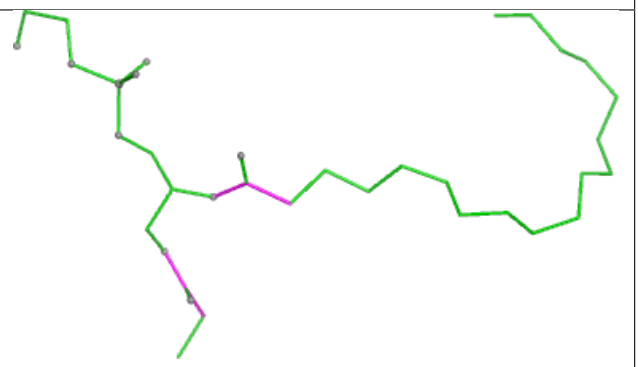
Ligand NDP P 501



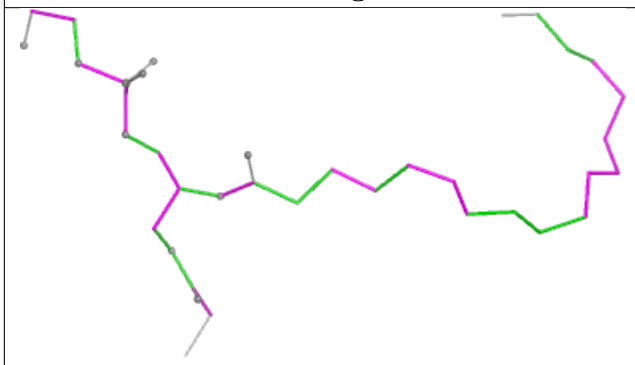
Ligand 3PE M 502



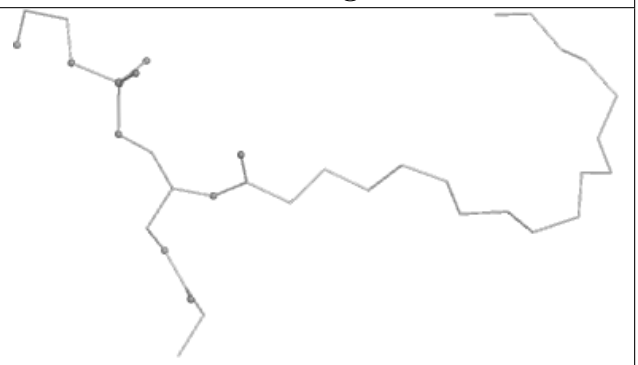
Bond lengths



Bond angles

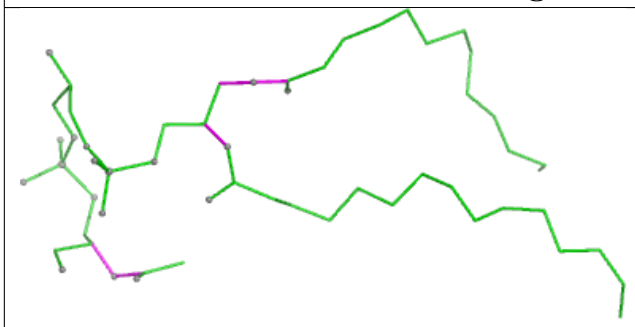


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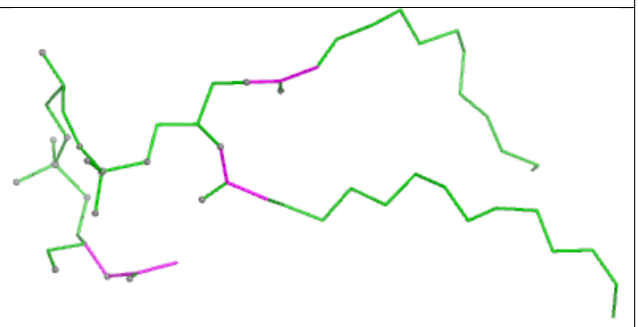


Rings

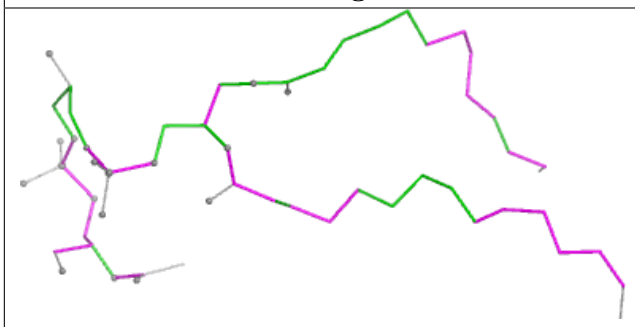
Ligand CDL h 201



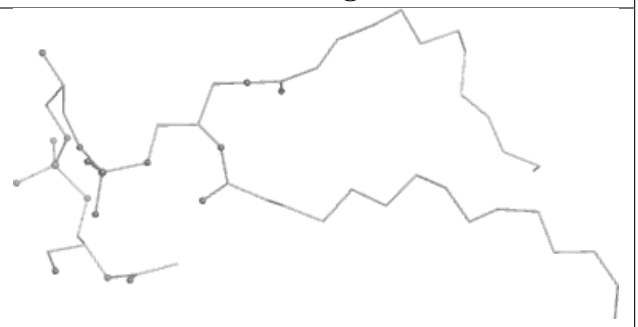
Bond lengths



Bond angles

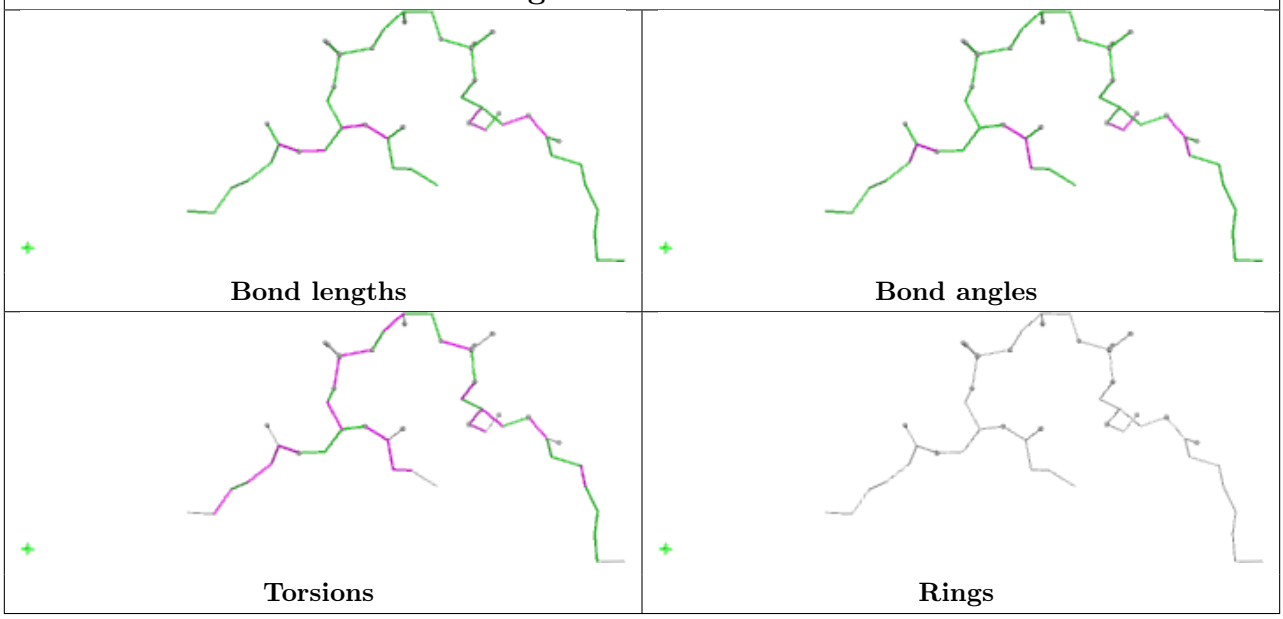


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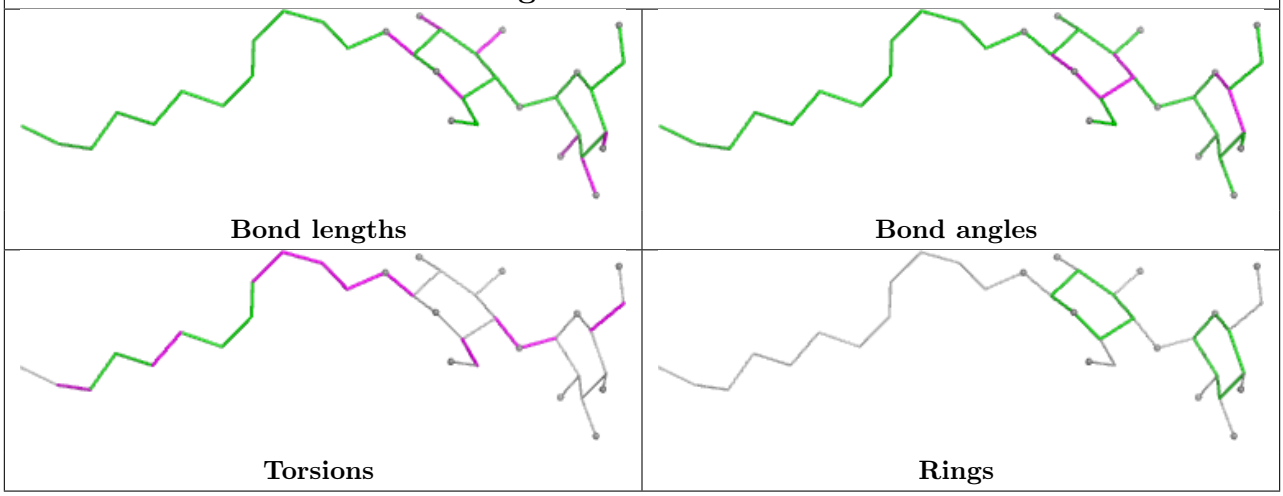


Rings

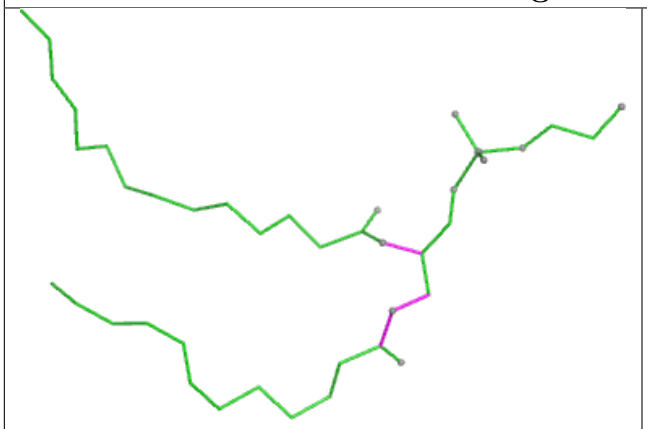
Ligand CDL h 202



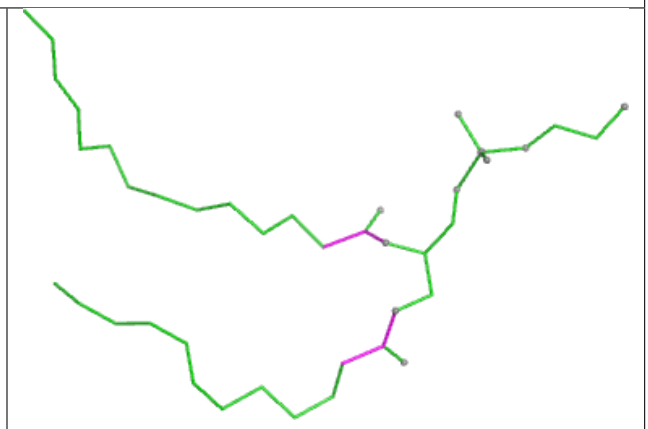
Ligand LMT M 501



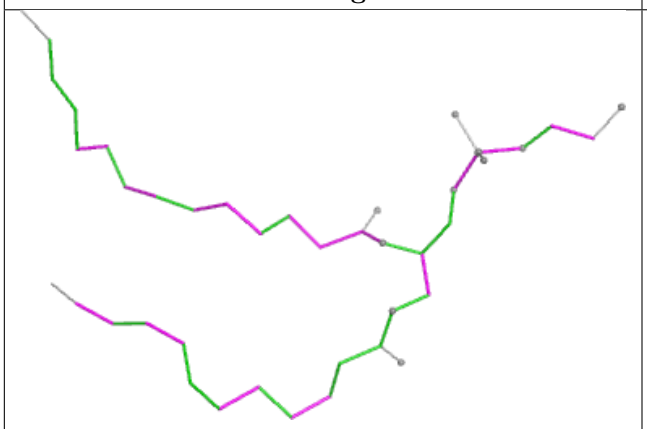
Ligand 3PE L 702



Bond lengths



Bond angles

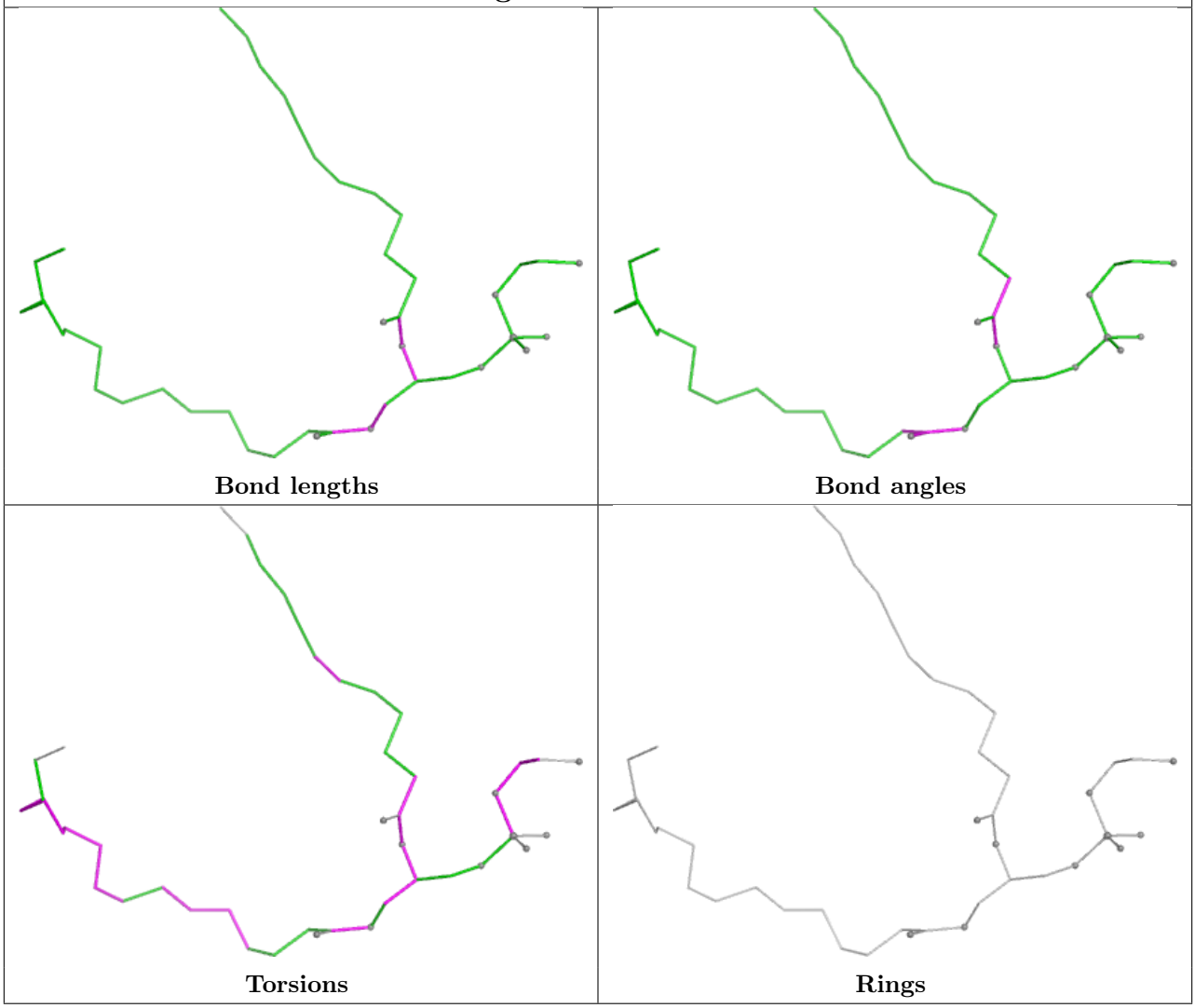


Torsions

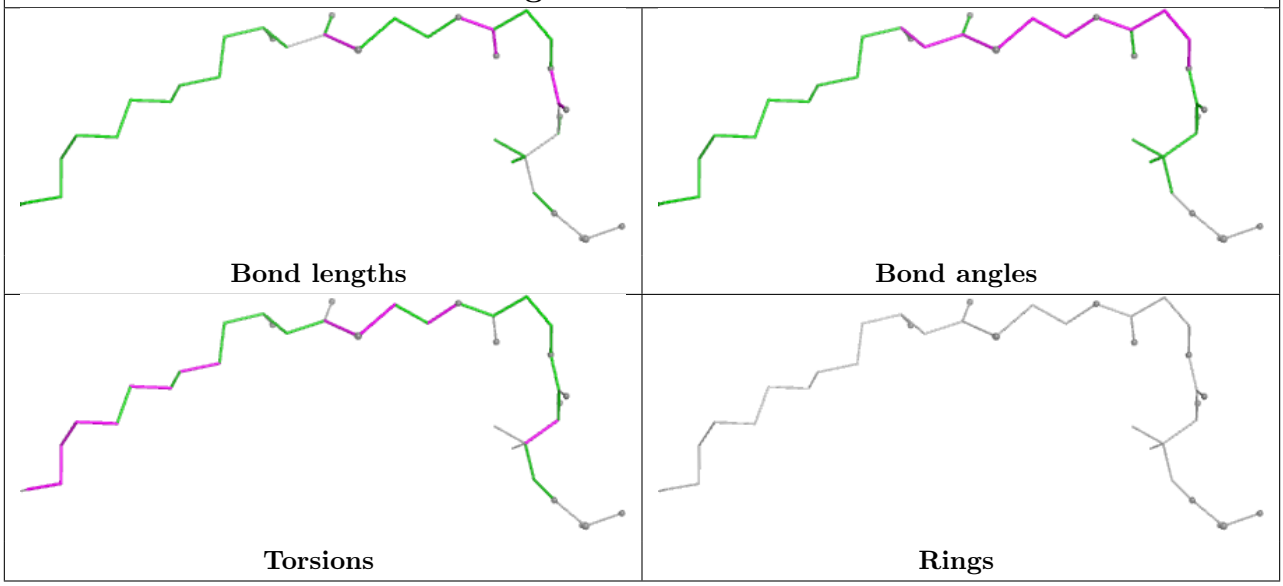


Rings

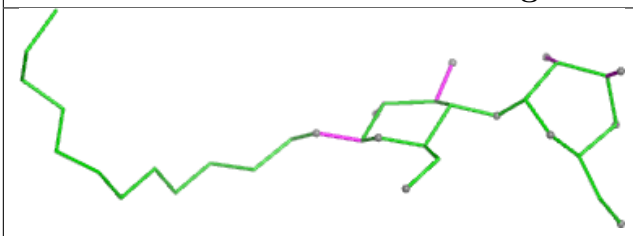
Ligand 3PE L 703



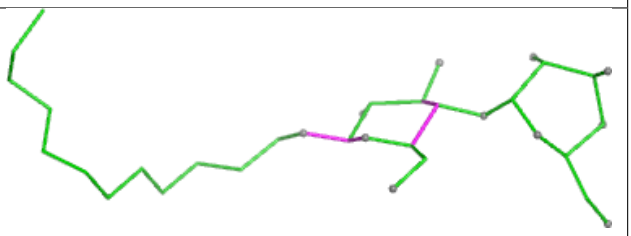
Ligand EHZ U 201



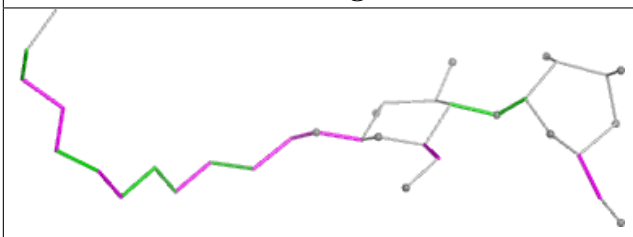
Ligand LMT A 401



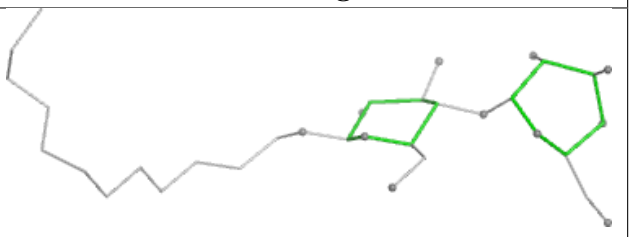
Bond lengths



Bond angles

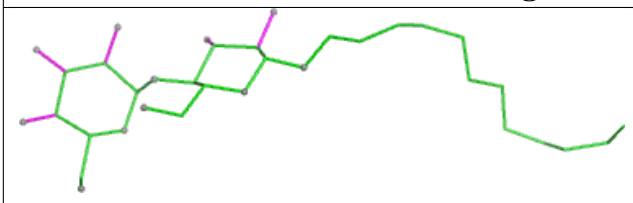


Torsions

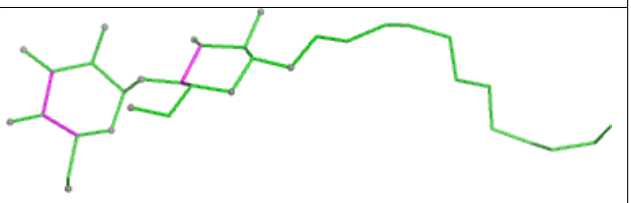


Rings

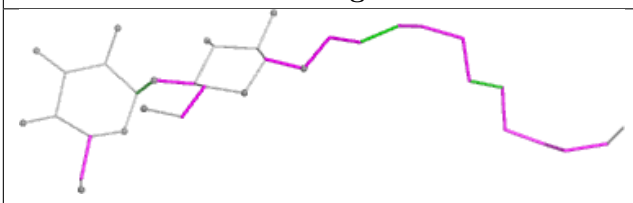
Ligand LMT Y 203



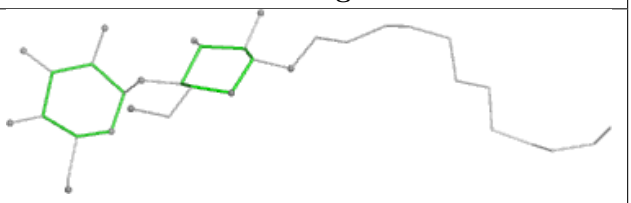
Bond lengths



Bond angles

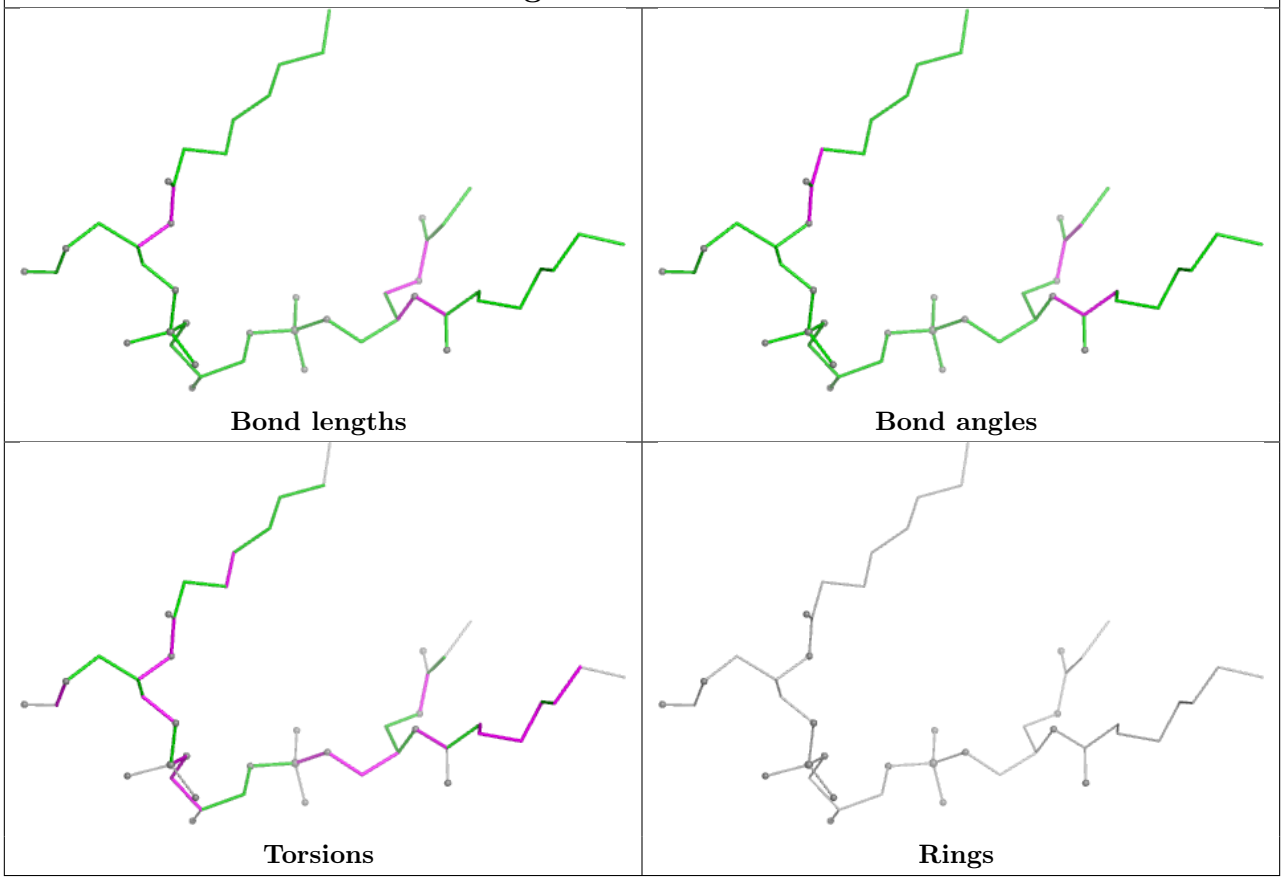


Torsions

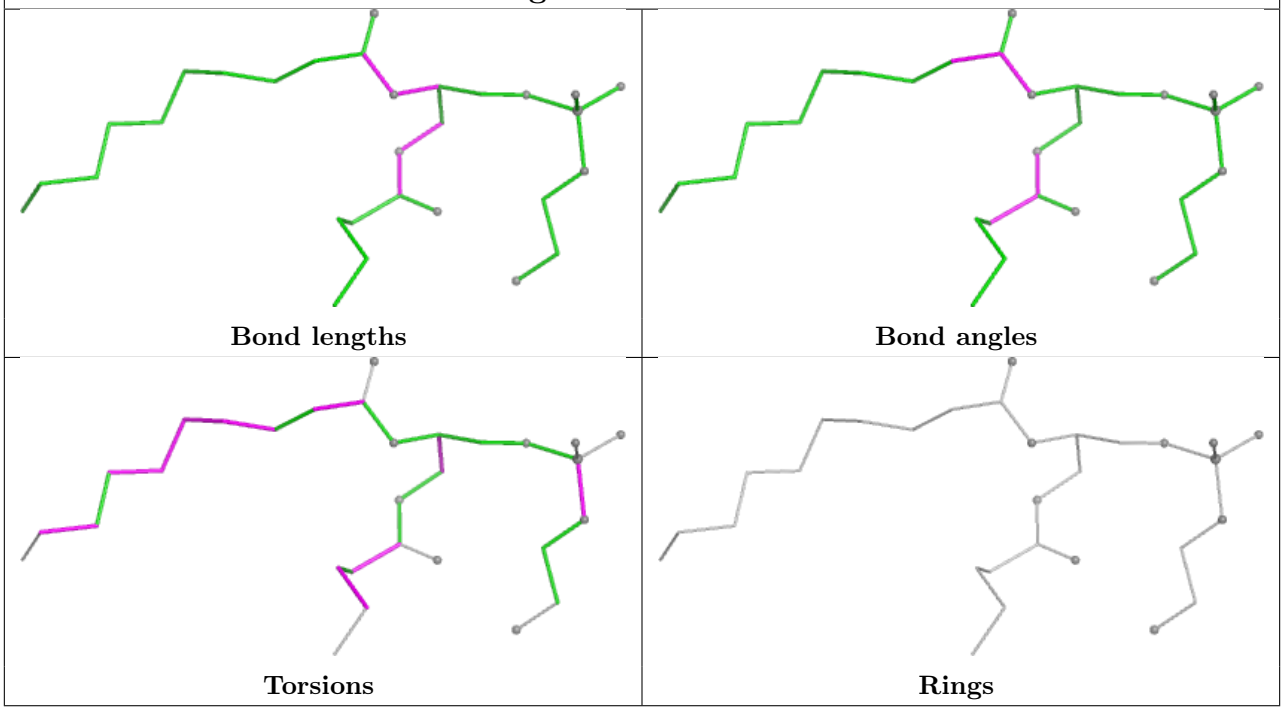


Rings

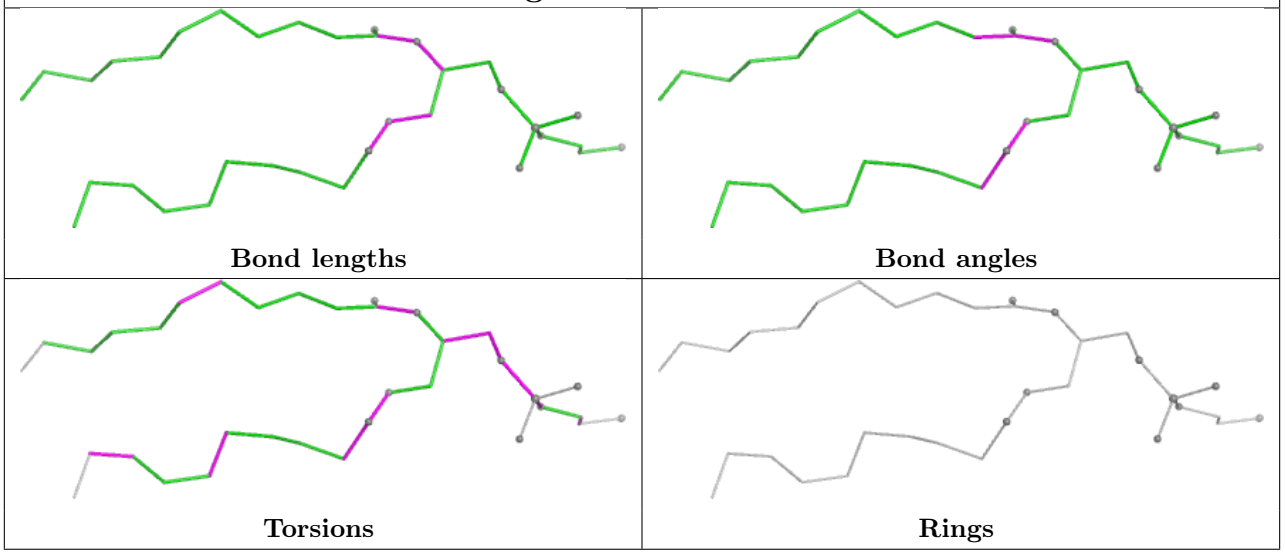
Ligand CDL H 401



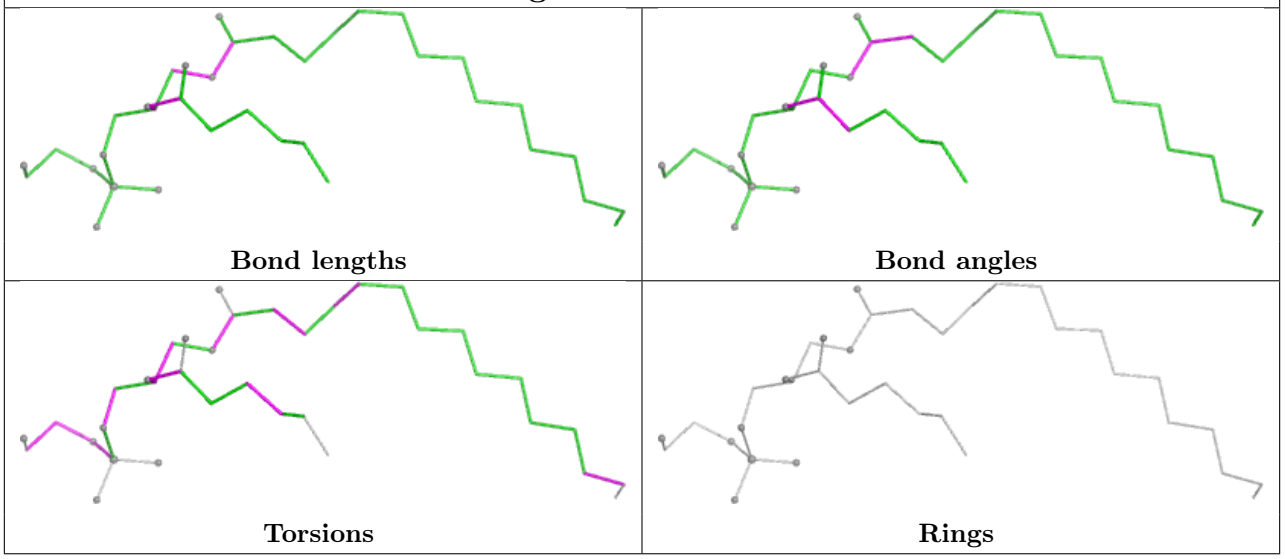
Ligand 3PE O 504



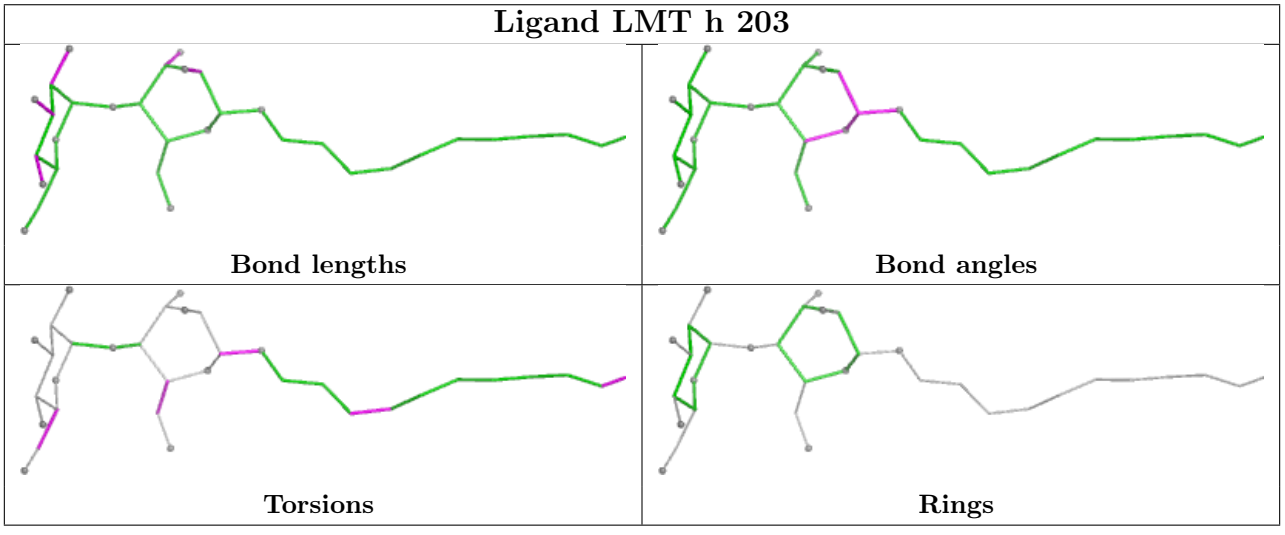
Ligand 3PE M 503



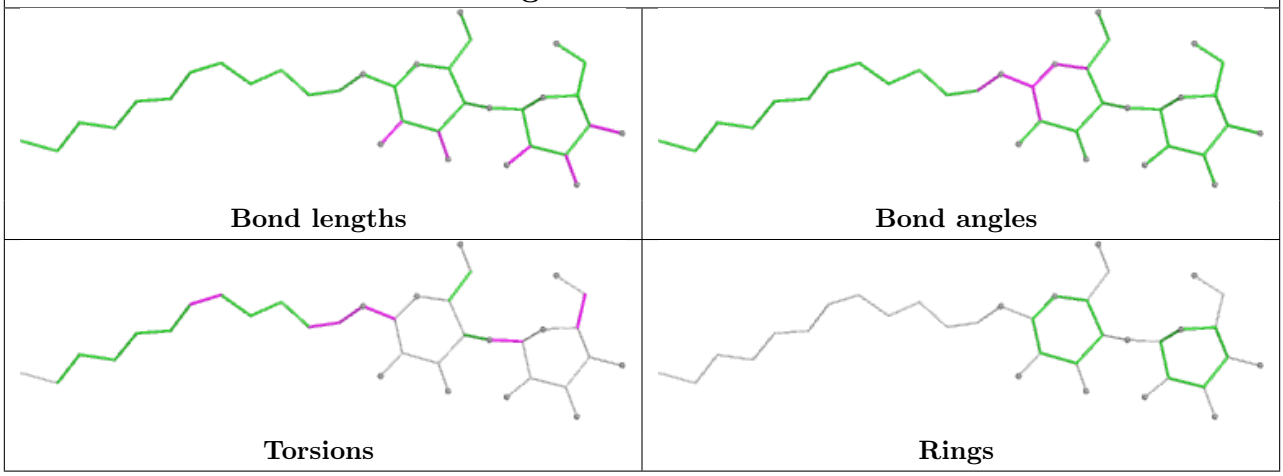
Ligand 3PE X 201



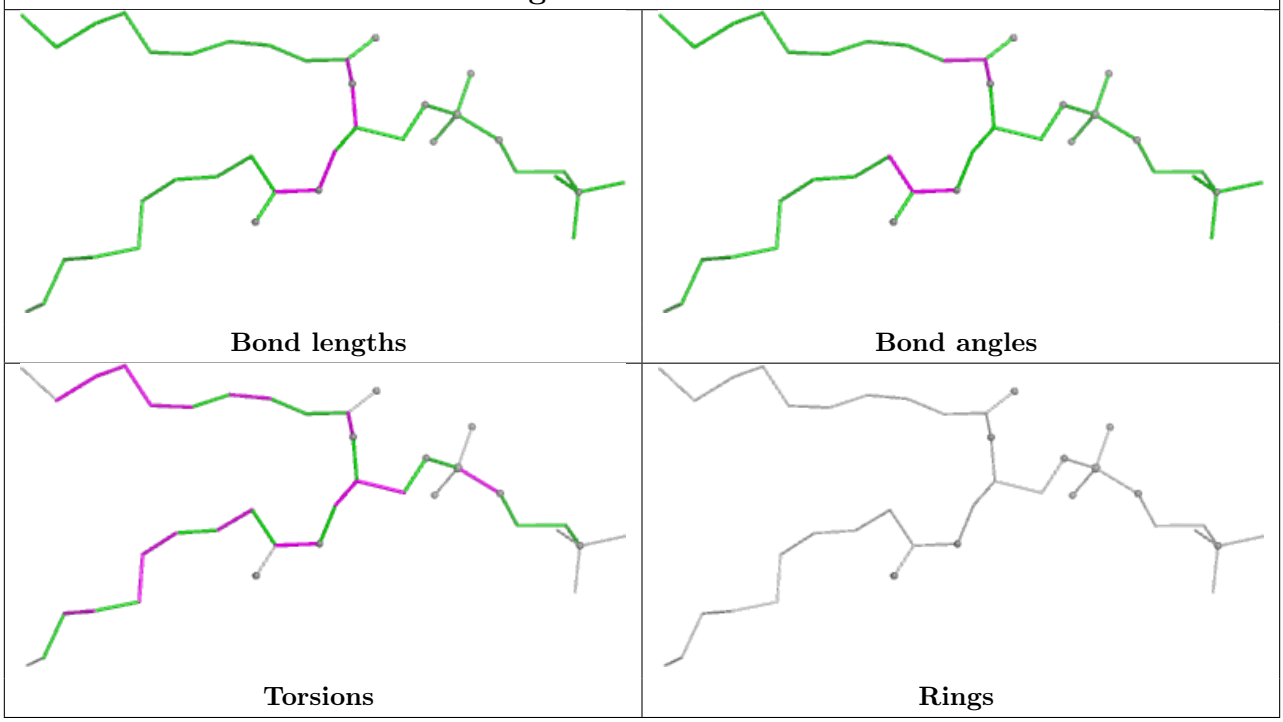
Ligand LMT h 203



Ligand LMT O 503



Ligand PC1 B 202



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.

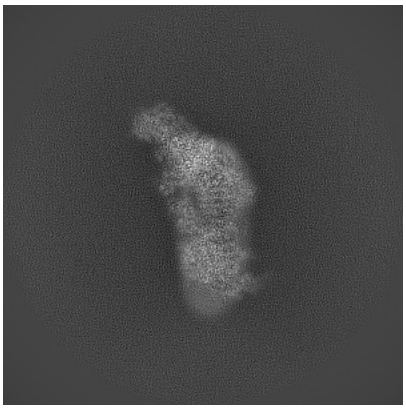
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16962. These allow visual inspection of the internal detail of the map and identification of artifacts.

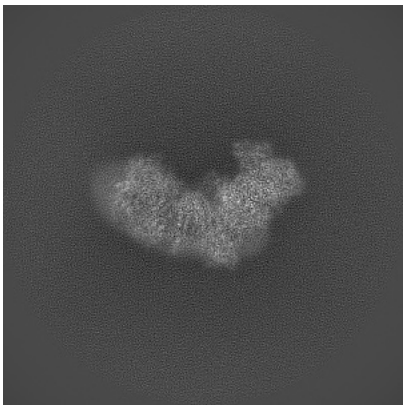
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

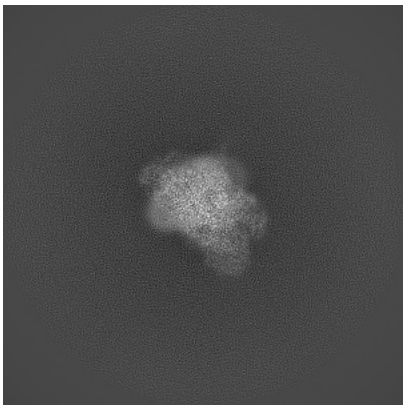
6.1.1 Primary map



X

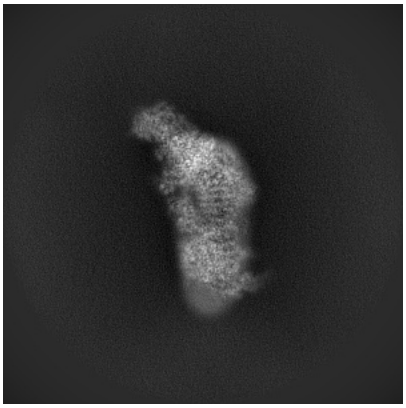


Y

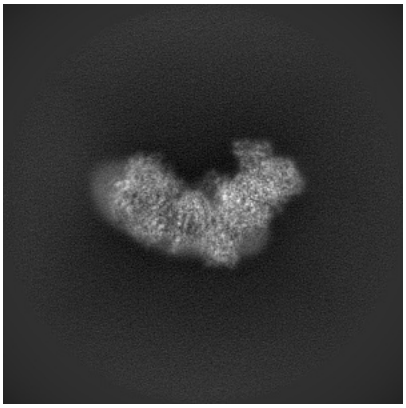


Z

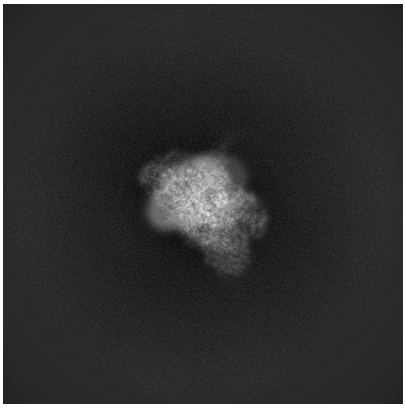
6.1.2 Raw map



X



Y

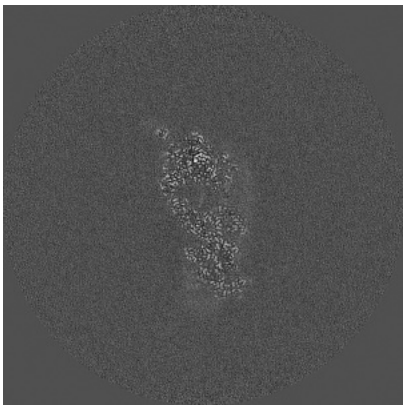


Z

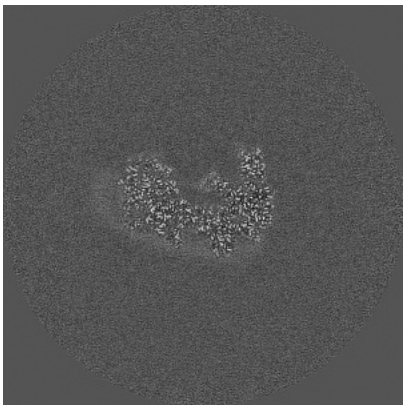
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

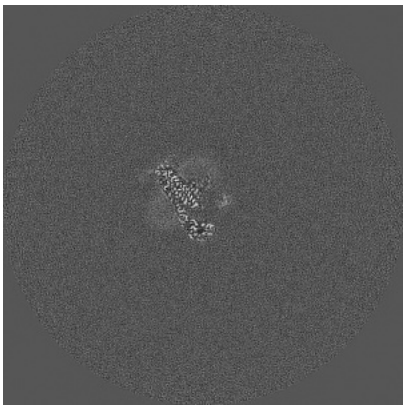
6.2.1 Primary map



X Index: 252

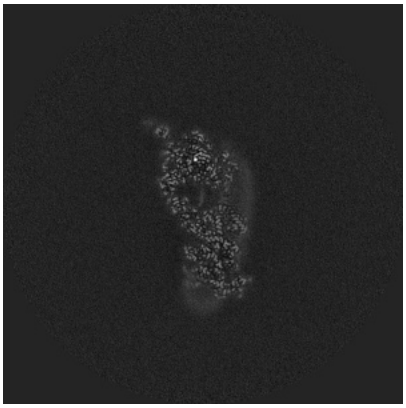


Y Index: 252

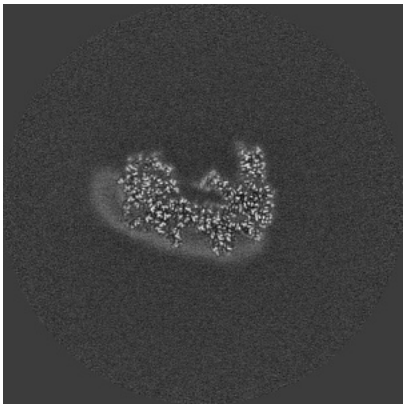


Z Index: 252

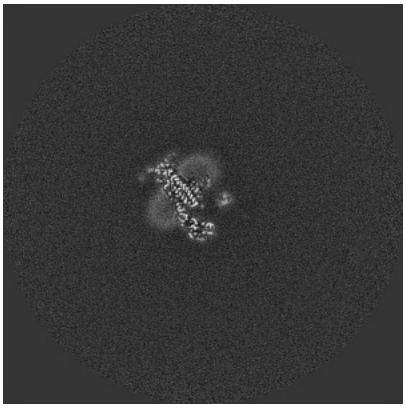
6.2.2 Raw map



X Index: 252



Y Index: 252

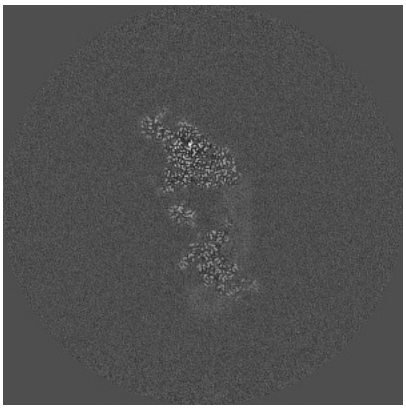


Z Index: 252

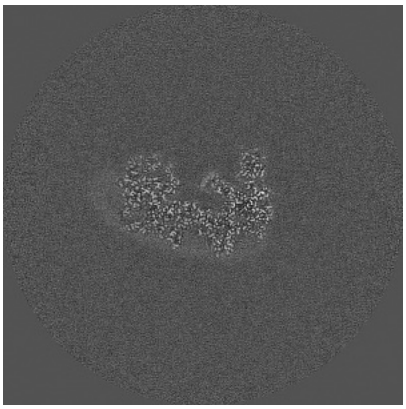
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

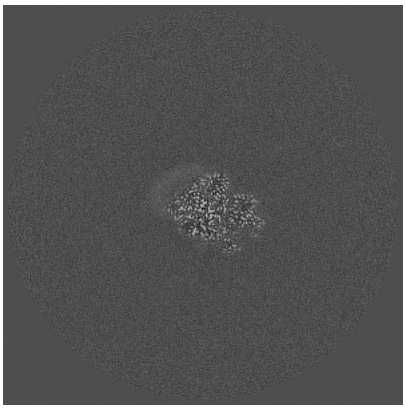
6.3.1 Primary map



X Index: 264

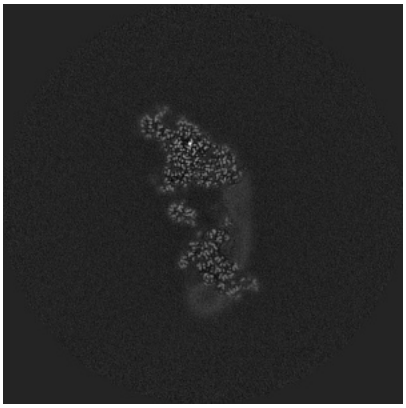


Y Index: 254

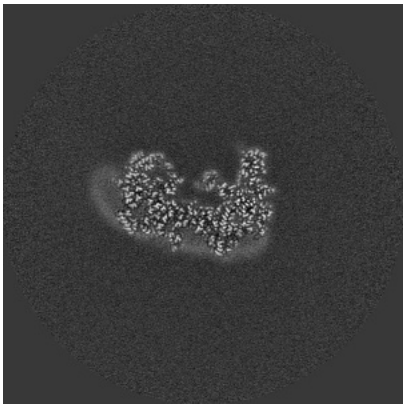


Z Index: 313

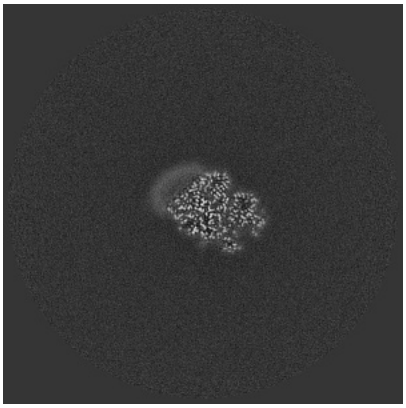
6.3.2 Raw map



X Index: 264



Y Index: 257

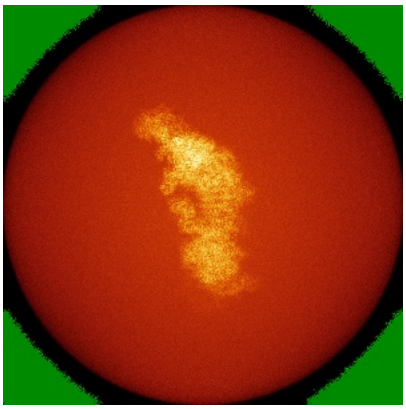


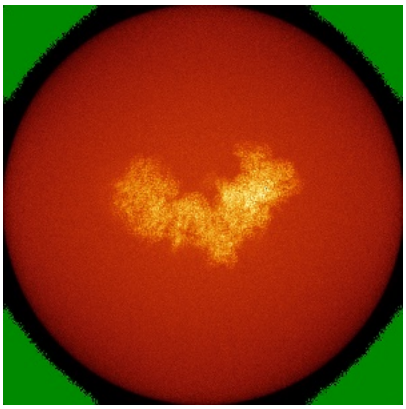
Z Index: 313

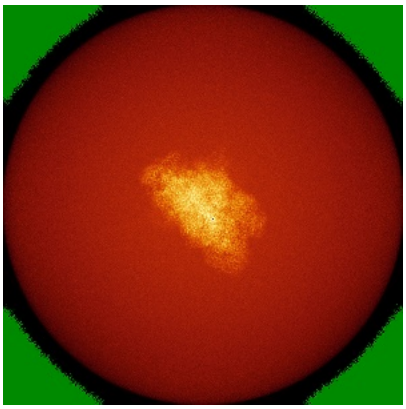
The images above show the largest variance slices of the map in three orthogonal directions.

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

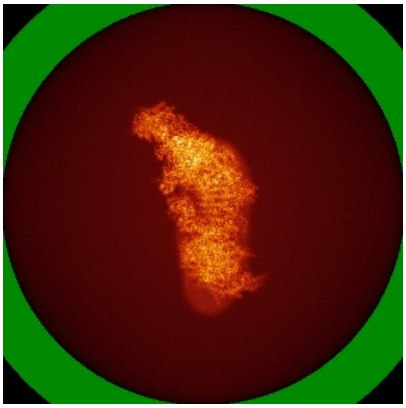
6.4.1 Primary map

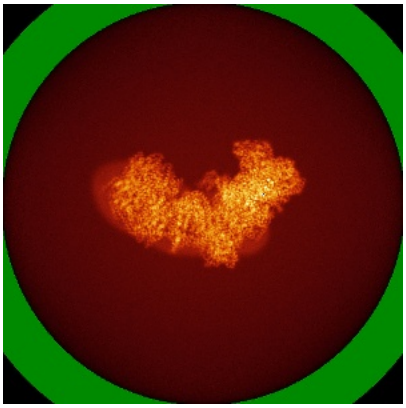

X

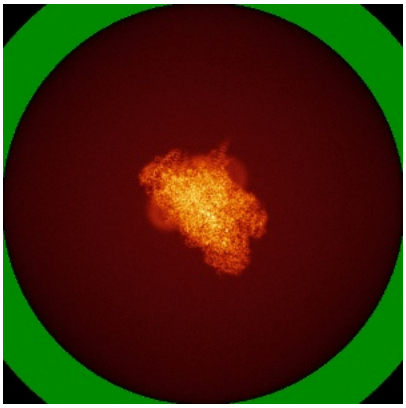

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

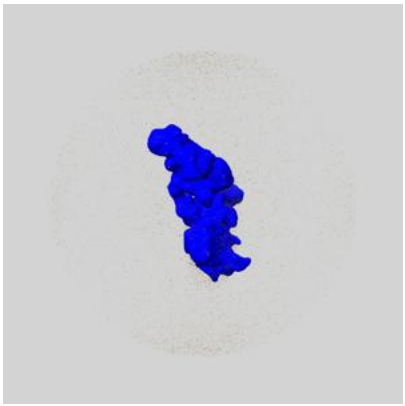
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

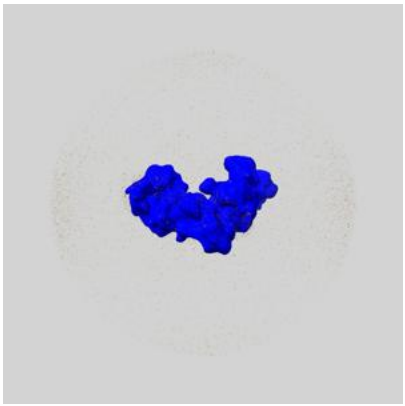
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

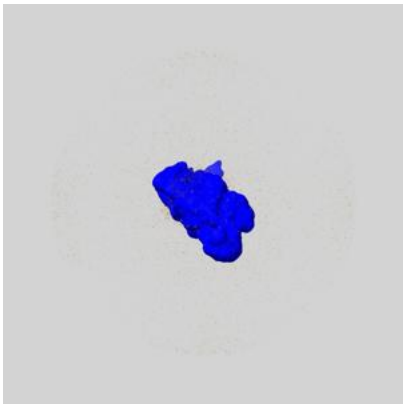
6.6.1 emd_16962_msk_1.map



X



Y

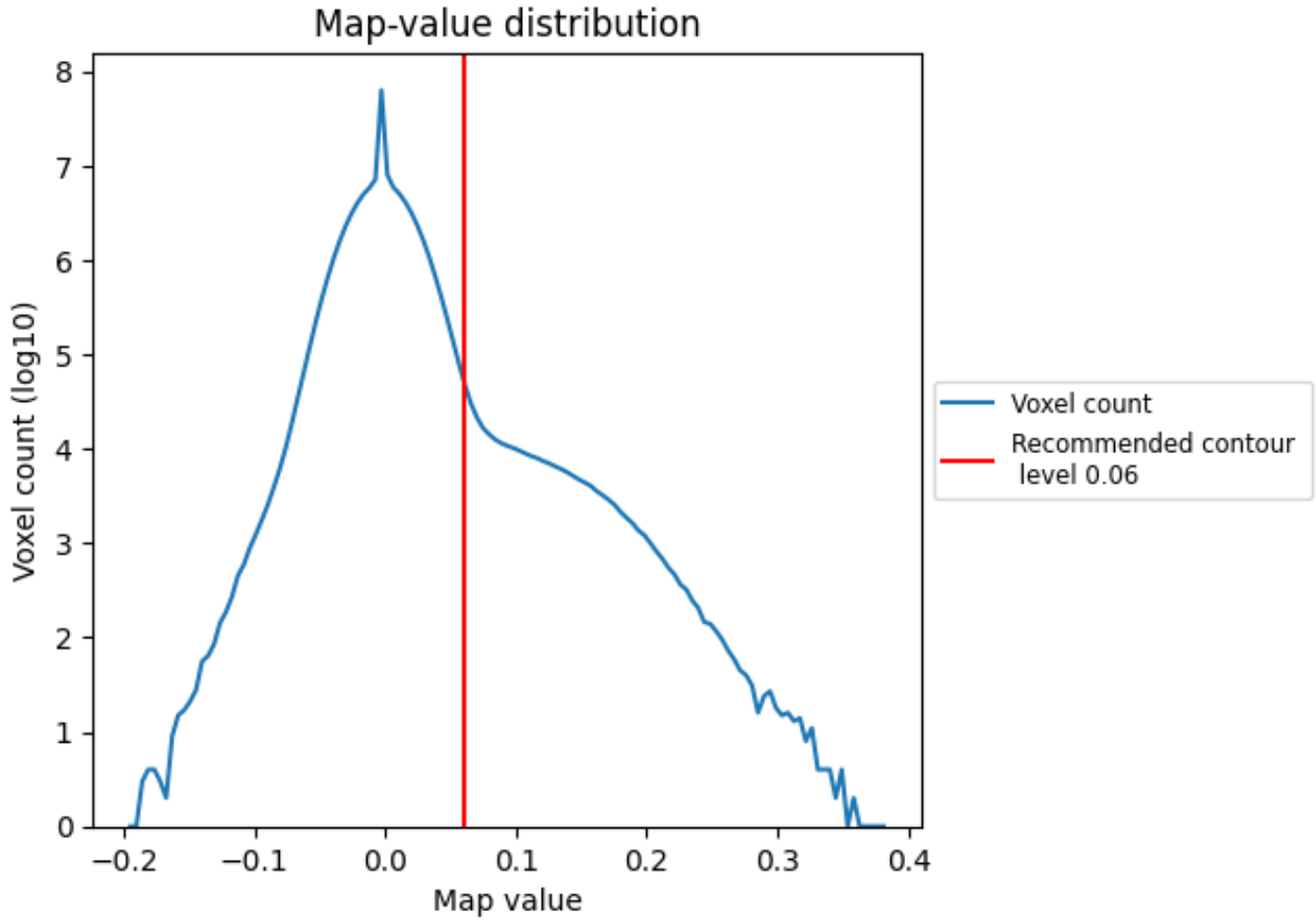


Z

7 Map analysis

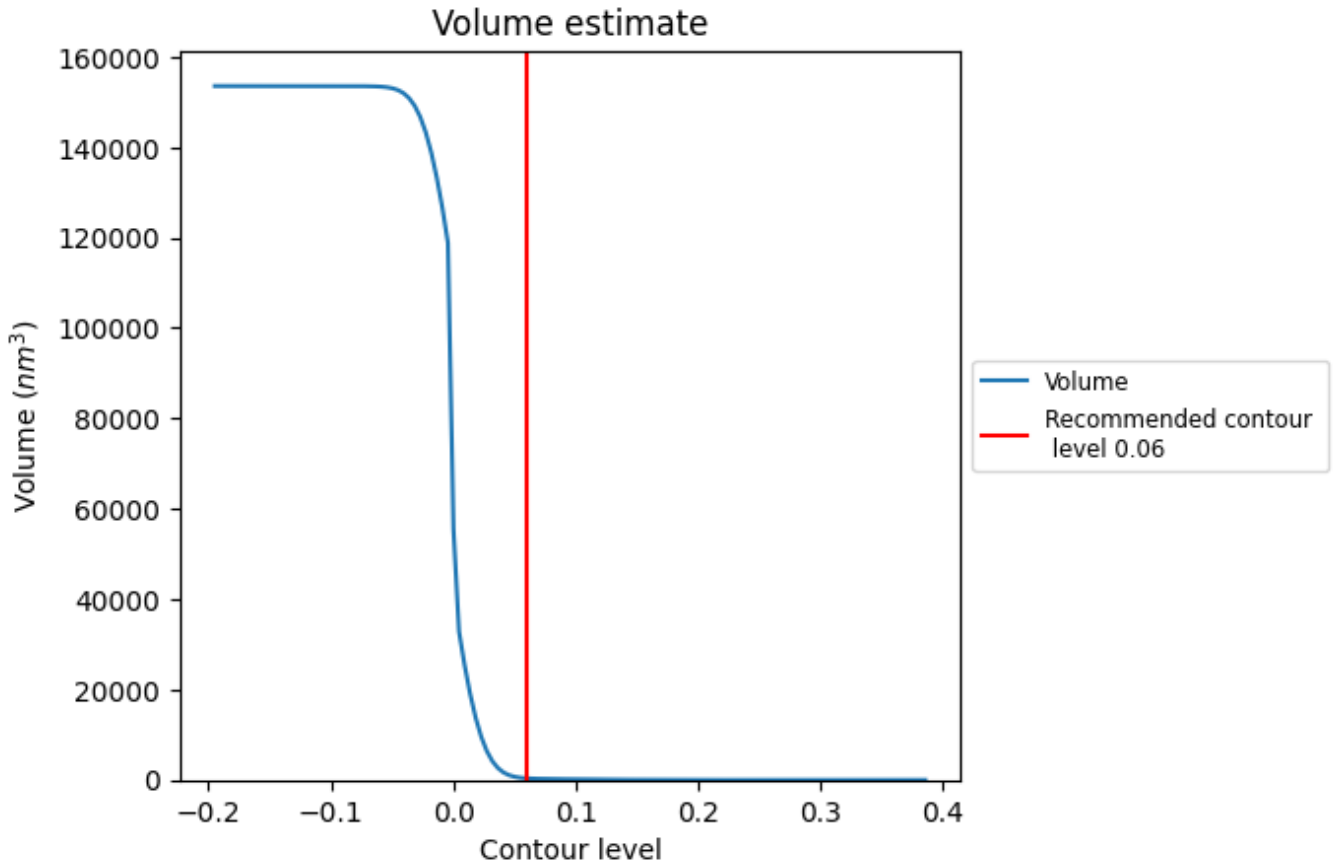
This section contains the results of statistical analysis of the map.

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.

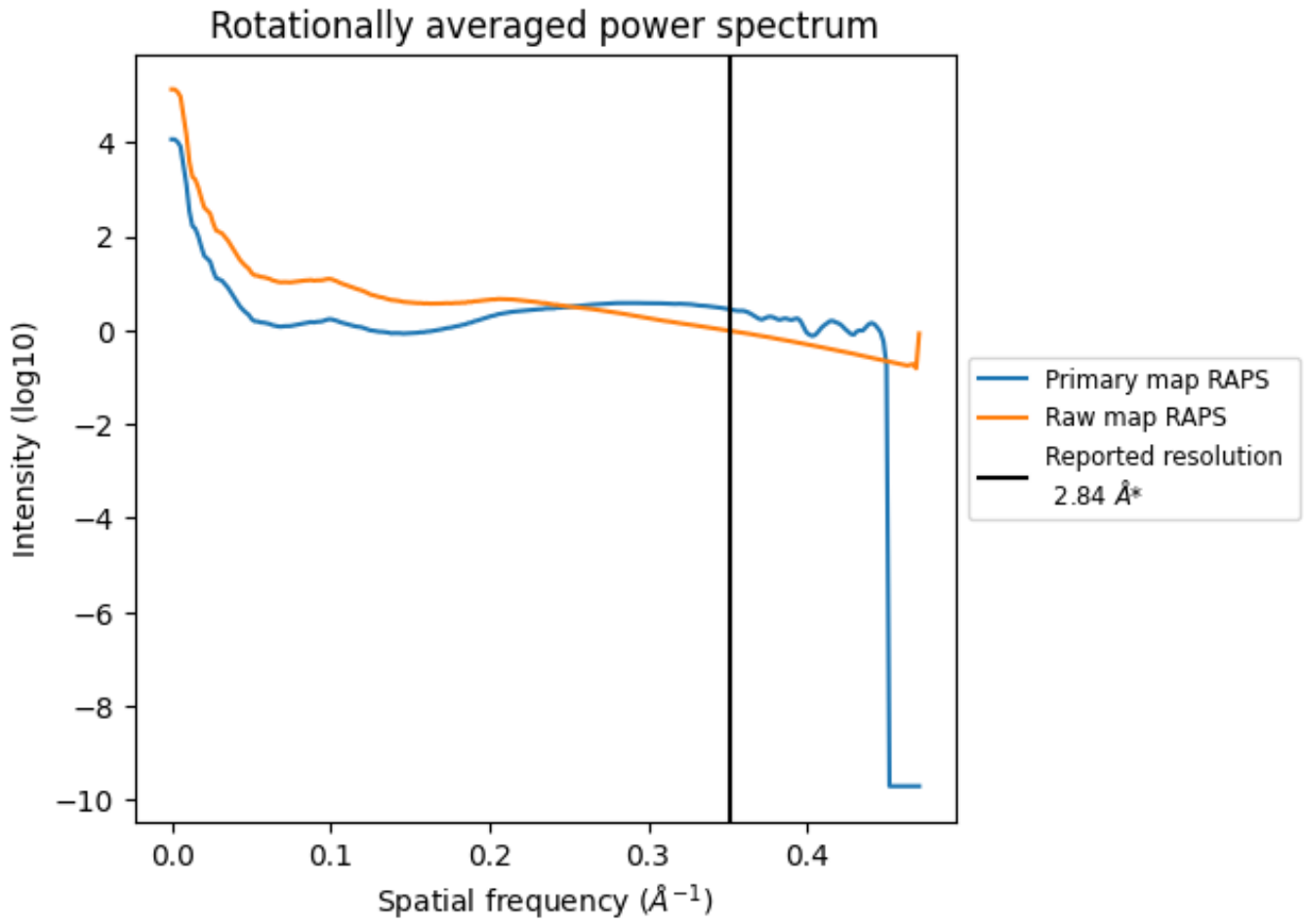
7.2 Volume estimate



The volume at the recommended contour level is 366 nm^3; this corresponds to an approximate mass of 331 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)

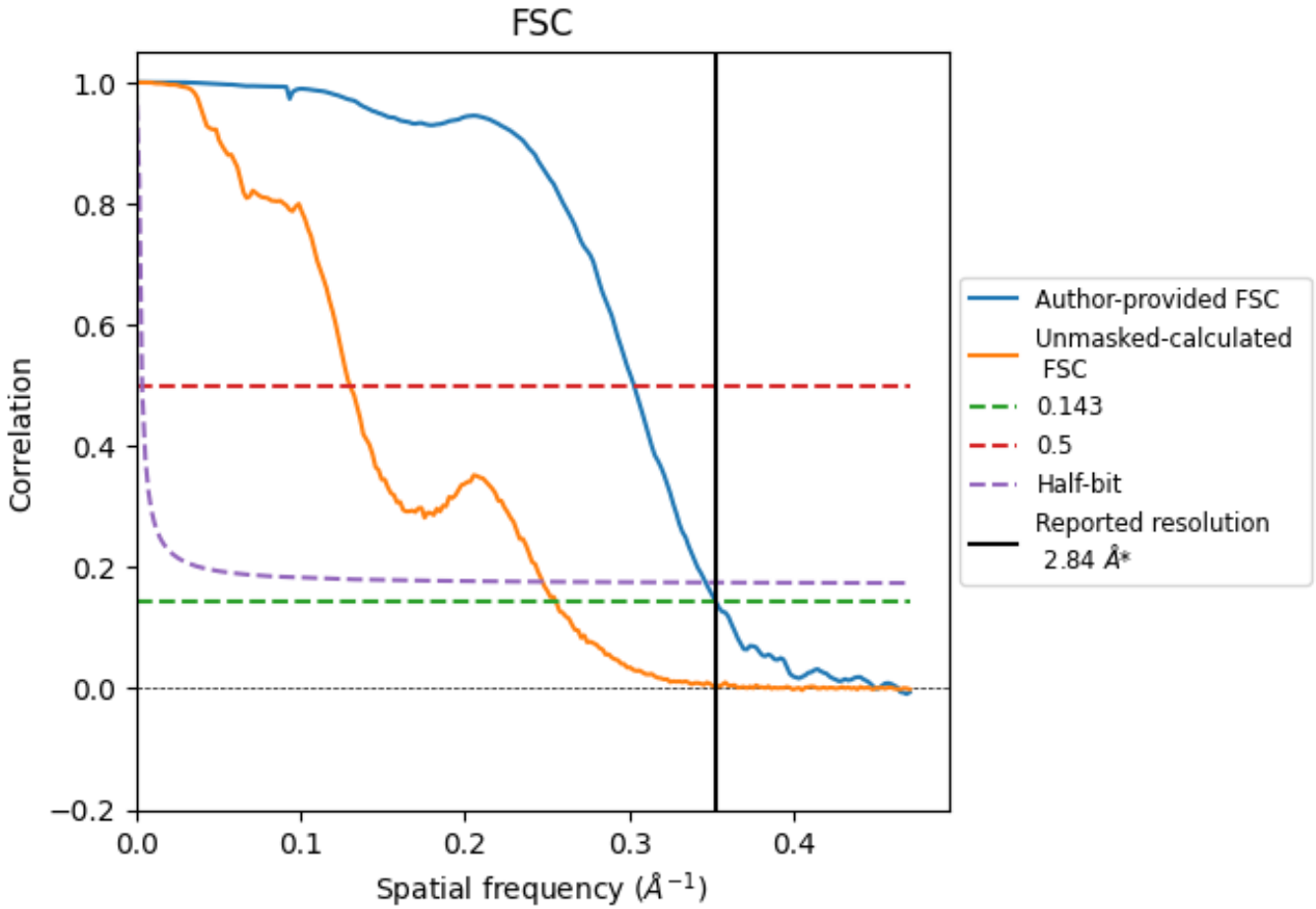


*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

8.2 Resolution estimates (i)

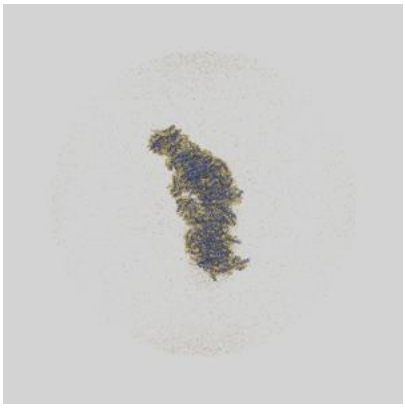
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.30	2.89
Unmasked-calculated*	3.91	7.69	4.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 2.84 by more than 10 %

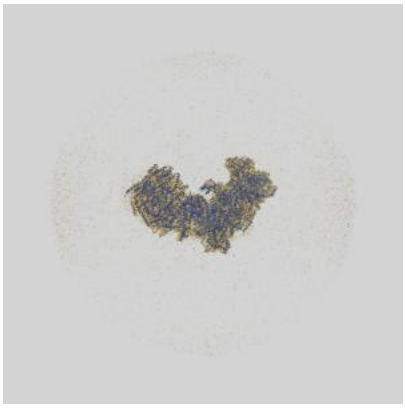
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16962 and PDB model 8OLT. Per-residue inclusion information can be found in section 3 on page 23.

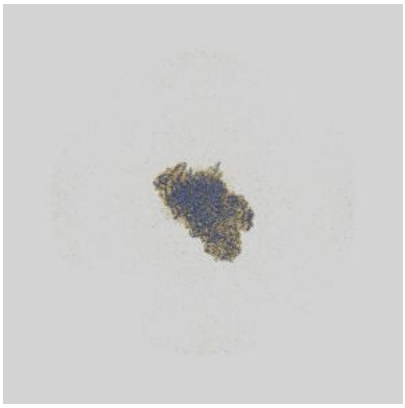
9.1 Map-model overlay



X



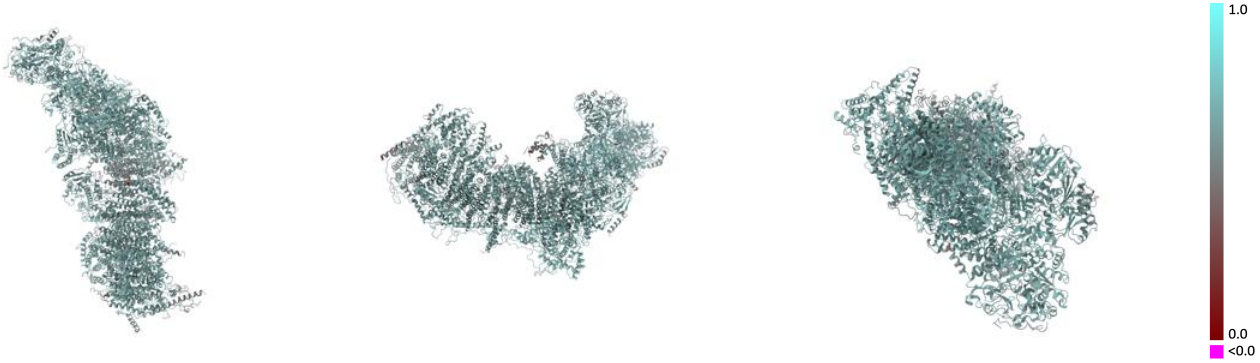
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

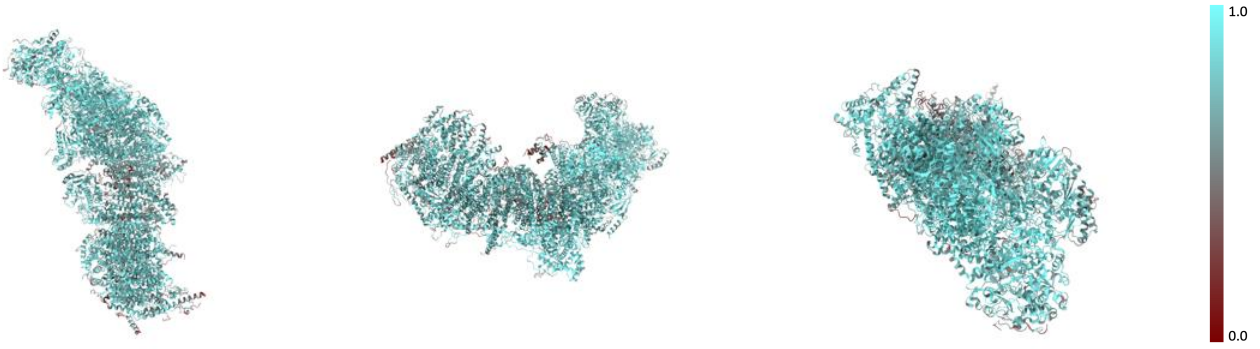
9.2 Q-score mapped to coordinate model



X Y Z

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

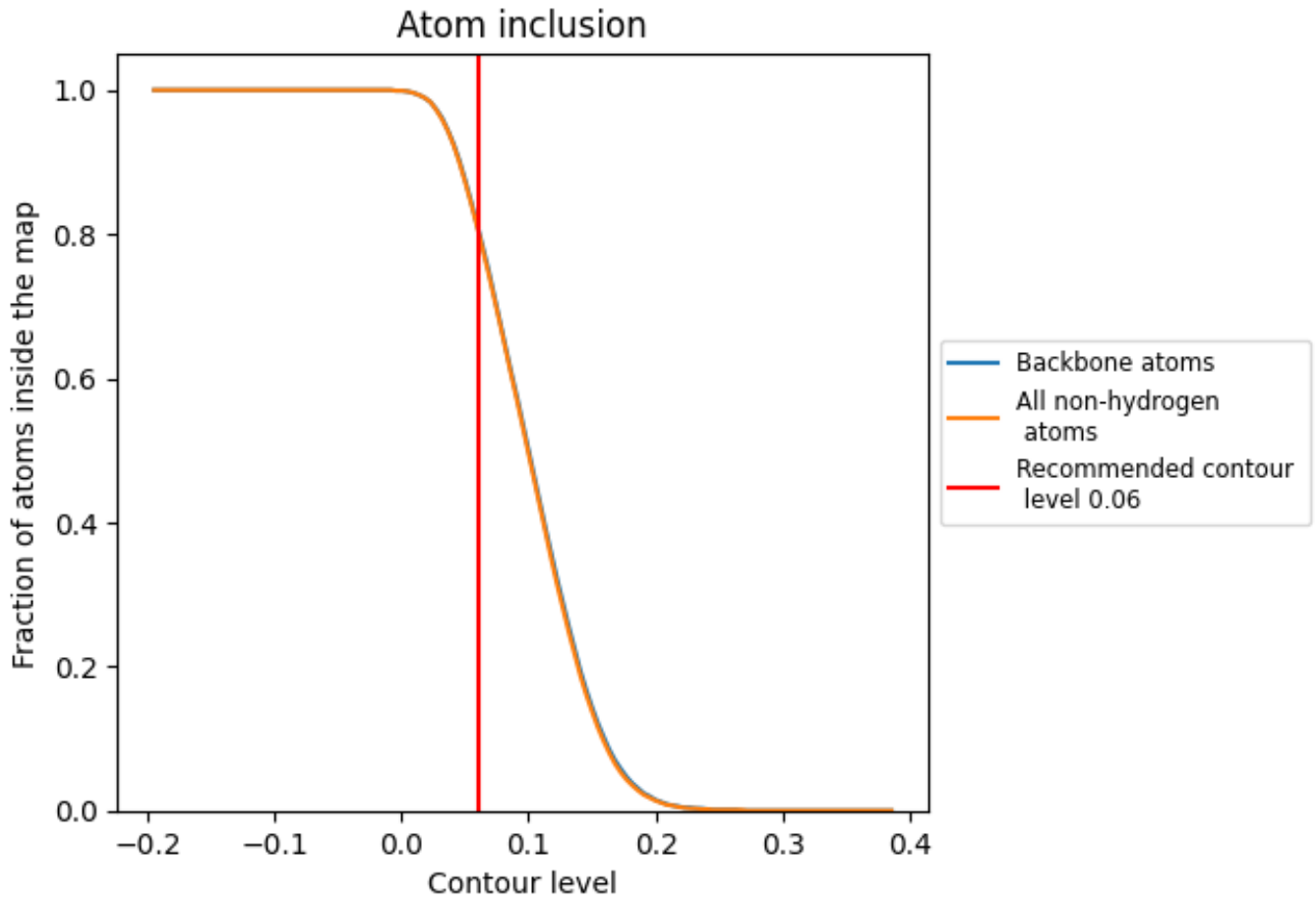
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.6280
A	0.7870	0.6350
B	0.9050	0.6610
C	0.9000	0.6610
D	0.8880	0.6560
E	0.7650	0.6010
F	0.8080	0.6180
G	0.8310	0.6320
H	0.8680	0.6510
I	0.8960	0.6550
J	0.7490	0.6110
K	0.8410	0.6450
L	0.8020	0.6270
M	0.8610	0.6470
N	0.8660	0.6520
O	0.8270	0.6390
P	0.8480	0.6380
Q	0.8560	0.6450
R	0.8460	0.6370
S	0.7190	0.5940
T	0.4240	0.4780
U	0.7080	0.6040
V	0.8160	0.6390
W	0.8190	0.6290
X	0.8150	0.6280
Y	0.6600	0.5890
Z	0.8270	0.6370
a	0.8790	0.6460
b	0.7520	0.6120
c	0.6980	0.5950
d	0.8170	0.6300
e	0.8260	0.6310
f	0.7140	0.5950
g	0.8060	0.6230
h	0.7960	0.6290



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Chain	Atom inclusion	Q-score
i	0.6630	0.5830
j	0.6320	0.5570
k	0.6220	0.5620
l	0.7790	0.6140
m	0.7690	0.6120
n	0.7680	0.6090
o	0.6330	0.5550
p	0.7710	0.6090
q	0.8410	0.6370
r	0.8130	0.6310
s	0.7440	0.5980