



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 07:16 PM UTC

PDB ID : 8OM1 / pdb_00008om1
EMDB ID : EMD-16965
Title : Mitochondrial complex I from Mus musculus in the active state
Authors : Grba, D.N.; Chung, I.; Bridges, H.R.; Agip, A.N.A.; Hirst, J.
Deposited on : 2023-03-31
Resolution : 2.39 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

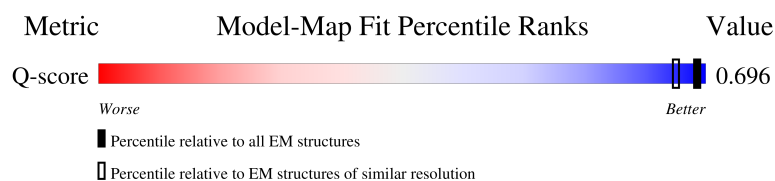
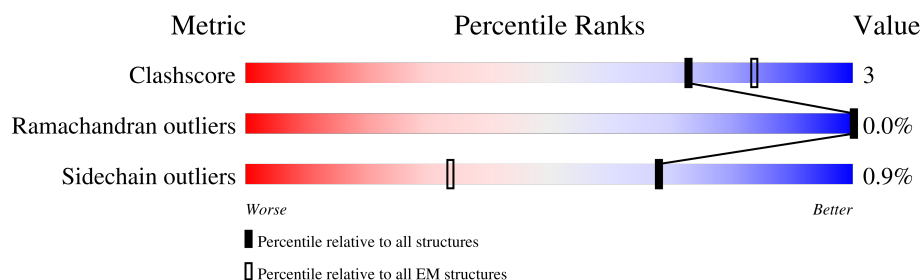
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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) : 2.49

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 2.39 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	4884 (1.90 - 2.89)

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 $\leq 5\%$. 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	 92% 8%
2	B	224	 60% 10% 30%
3	C	263	 71% 7% 21%
4	D	463	 86% 7% 7%

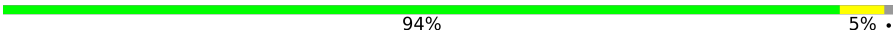
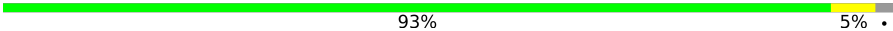
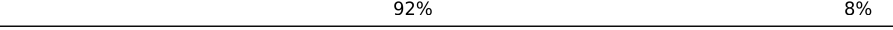
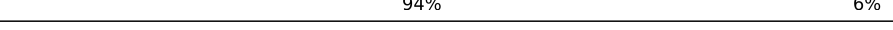
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Mol	Chain	Length	Quality of chain
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	142	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	 91% 9%
30	e	106	 94% 5%
31	f	57	 93% 5%
32	g	151	 60% 7% 33%
33	h	189	 72% 26%
34	i	127	 72% 9% 18%
35	j	105	 58% 5% 37%
36	k	104	 69% 6% 25%
37	l	186	 79% 5% 16%
38	m	129	 90% 8%
39	n	179	 92% 8%
40	o	136	 82% 5% 12%
41	p	176	 91% 5%
42	q	145	 94% 6%
43	r	112	 85% 5% 10%
44	s	104	 37% 6% 58%

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 71256 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
1	A	115	Total	C	N	O	S	0	0
			933	633	133	160	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1259	802	227	216	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	208	Total	C	N	O	S	0	0
			1730	1116	297	314	3		

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

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

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

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

- 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	689	Total	C	N	O	S	0	0
			5301	3324	920	1016	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	607	Total	C	N	O	S	0	0
			4809	3187	747	830	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	126	Total	C	N	O	S	0	0
			1021	646	179	192	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	86	Total	C	N	O	S	0	0
			685	430	130	122	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	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	114	Total	C	N	O	S	0	0
			927	604	154	166	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	49	Total	C	N	O	S	0	0
			407	266	70	70	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	56	Total	C	N	O	S	0	0
			482	314	85	81	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	139	Total	C	N	O	S	0	0
			1166	764	195	204	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	66	Total	C	N	O	S	0	0
			566	372	94	99	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	157	Total	C	N	O	S	0	0
			1323	855	220	237	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	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	119	Total	C	N	O	S	0	0
			1019	642	191	178	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	145	Total	C	N	O	S	0	0
			1212	779	215	213	5		

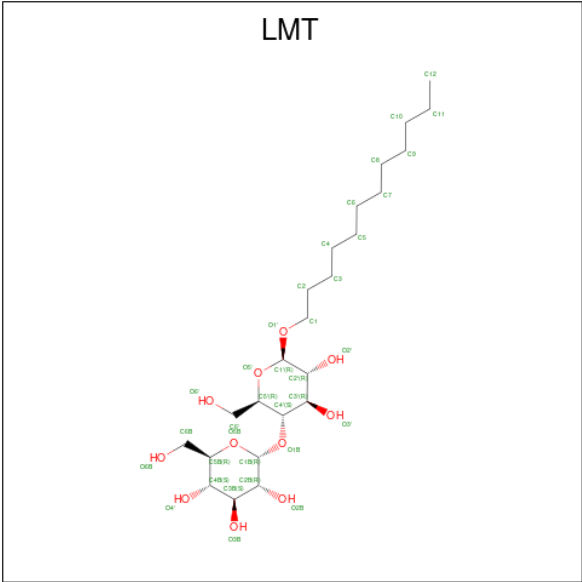
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	101	Total	C	N	O	S	0	0
			809	511	150	145	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	44	Total	C	N	O	0	0
			368	230	66	72		

- Molecule 45 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



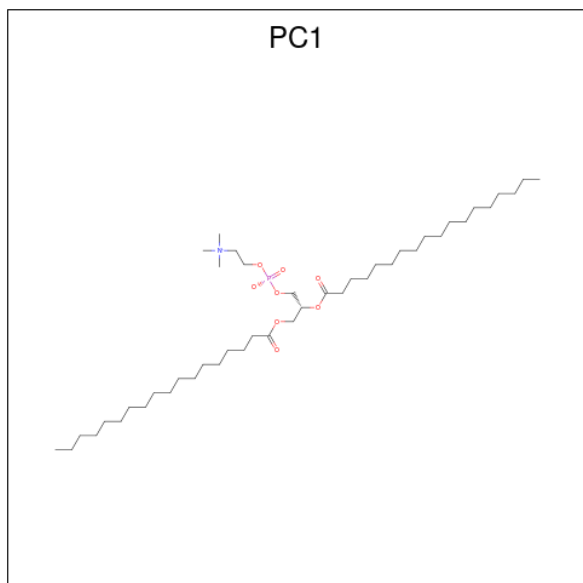
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	A	1	Total	C	O	0
			35	24	11	
45	H	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	M	1	Total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

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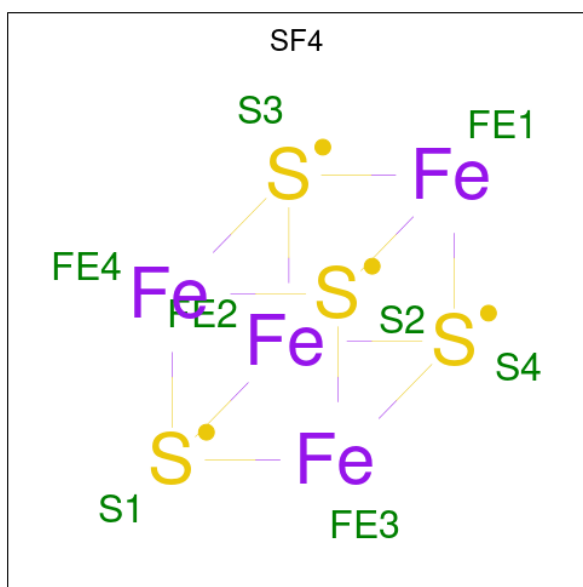
Mol	Chain	Residues	Atoms			AltConf
45	h	1	Total	C	O	0
			35	24	11	
45	j	1	Total	C	O	0
			35	24	11	

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



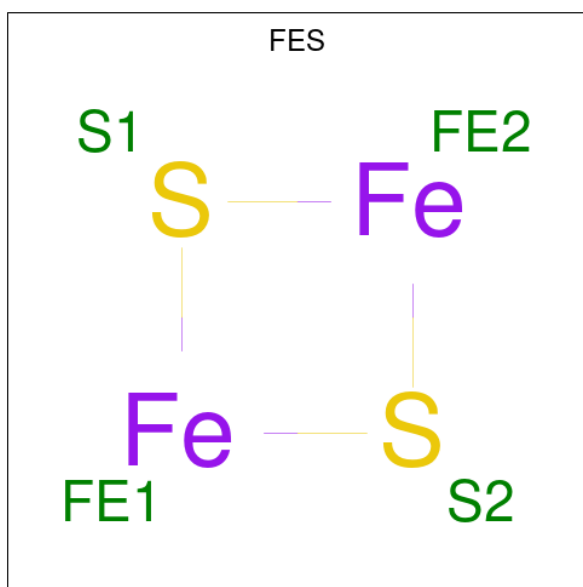
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
46	L	1	Total	C	N	O	P	0
			27	17	1	8	1	
46	p	1	Total	C	N	O	P	0
			36	26	1	8	1	

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



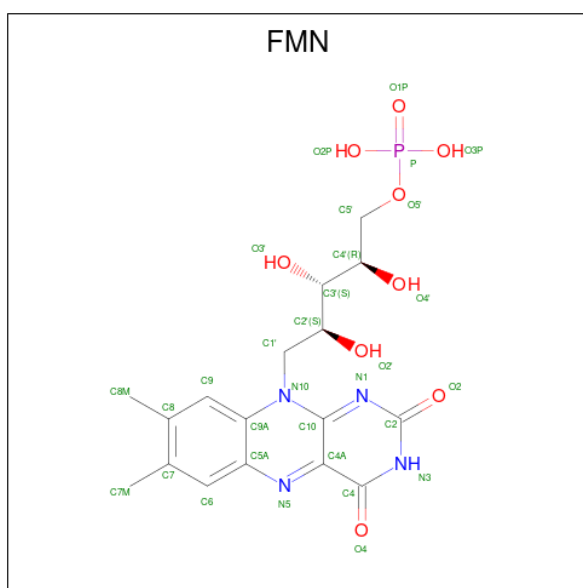
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

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

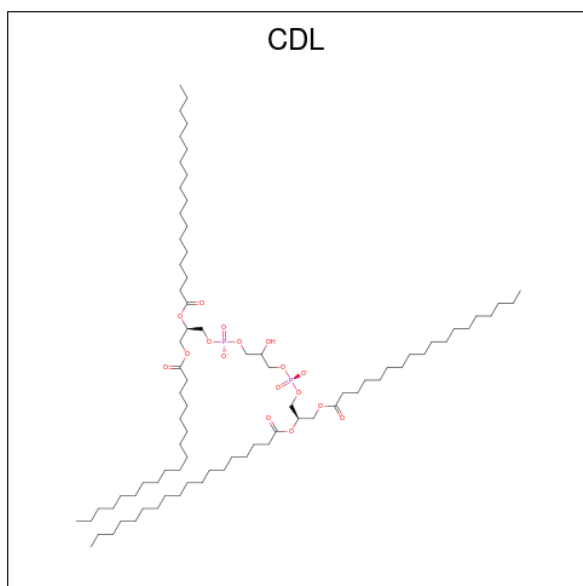


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is SODIUM ION (CCD ID: NA) (formula: Na).

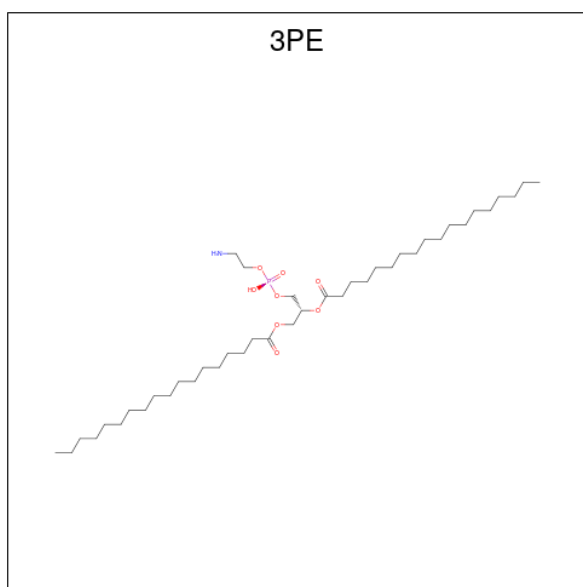
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	Na	0
			1	1	

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
51	H	1	Total	C	O	P	0
			51	33	16	2	
51	K	1	Total	C	O	P	0
			71	52	17	2	
51	L	1	Total	C	O	P	0
			68	49	17	2	
51	h	1	Total	C	O	P	0
			58	39	17	2	
51	h	1	Total	C	O	P	0
			78	60	16	2	
51	q	1	Total	C	O	P	0
			62	43	17	2	

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
52	I	1	Total	C	N	O	P	0
			36	26	1	8	1	
52	I	1	Total	C	N	O	P	0
			44	34	1	8	1	
52	L	1	Total	C	N	O	P	0
			43	33	1	8	1	
52	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
52	M	1	Total	C	N	O	P	0
			41	31	1	8	1	
52	N	1	Total	C	N	O	P	0
			34	24	1	8	1	
52	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
52	O	1	Total	C	N	O	P	0
			30	20	1	8	1	
52	X	1	Total	C	N	O	P	0
			37	27	1	8	1	
52	Y	1	Total	C	N	O	P	0
			38	28	1	8	1	
52	Z	1	Total	C	N	O	P	0
			43	33	1	8	1	
52	d	1	Total	C	N	O	P	0
			43	33	1	8	1	
52	d	1	Total	C	N	O	P	0
			32	22	1	8	1	
52	f	1	Total	C	N	O	P	0
			42	32	1	8	1	

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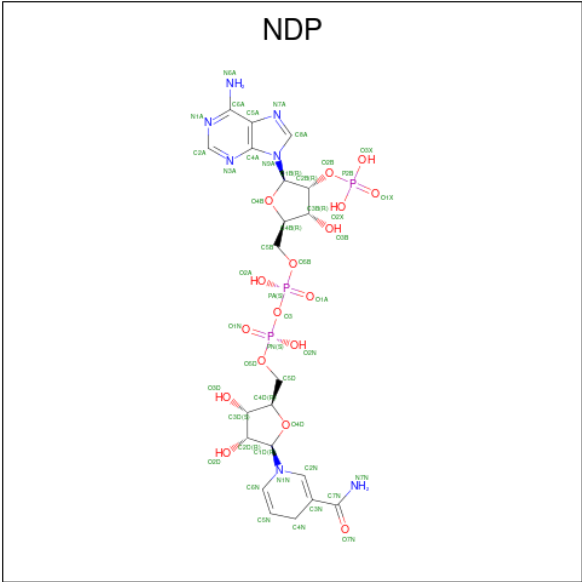
Mol	Chain	Residues	Atoms					AltConf
52	i	1	Total 30	C 20	N 1	O 8	P 1	0
52	r	1	Total 46	C 36	N 1	O 8	P 1	0

- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 53 | O | 1 | Total Mg
1 1 | 0 |

- # DGT

Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total 31	C 10	N 5	O 13	P 3	0

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

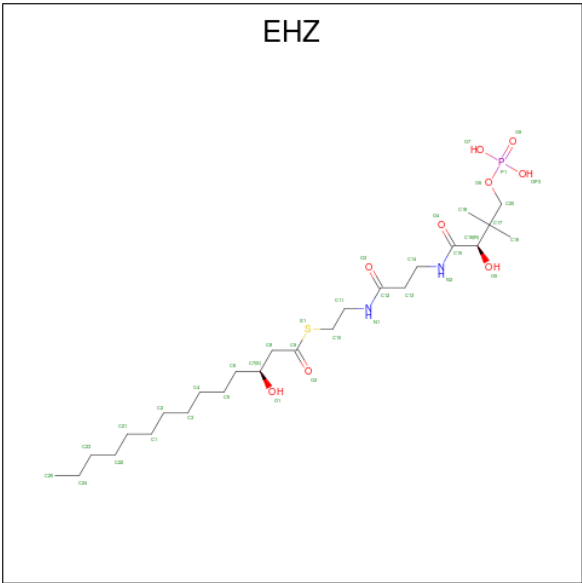


Mol	Chain	Residues	Atoms					AltConf
55	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

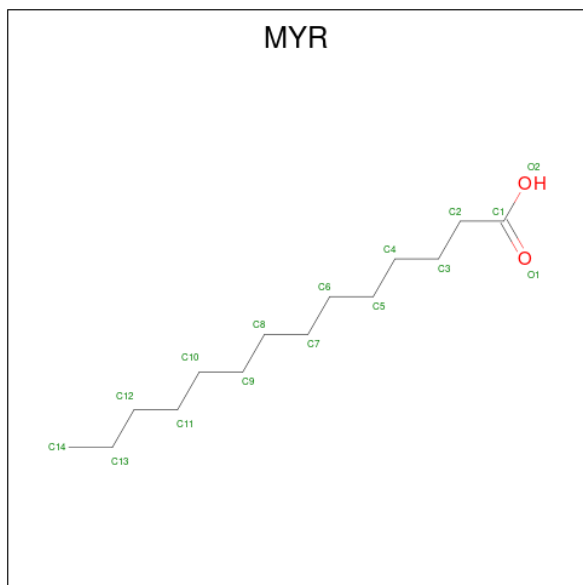
Mol	Chain	Residues	Atoms		AltConf
56	R	1	Total	Zn	0
			1	1	

- Molecule 57 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: C₂₅H₄₉N₂O₉PS).



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

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
58	o	1	Total	C	O	
			15	14	1	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		AltConf
59	A	59	Total	O	
			59	59	0
59	B	96	Total	O	
			96	96	0
59	C	160	Total	O	
			160	160	0
59	D	257	Total	O	
			257	257	0
59	E	43	Total	O	
			43	43	0
59	F	85	Total	O	
			85	85	0
59	G	300	Total	O	
			300	300	0

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Mol	Chain	Residues	Atoms		AltConf
59	H	120	Total 120	O 120	0
59	I	124	Total 124	O 124	0
59	J	60	Total 60	O 60	0
59	K	41	Total 41	O 41	0
59	L	105	Total 105	O 105	0
59	M	190	Total 190	O 190	0
59	N	123	Total 123	O 123	0
59	O	108	Total 108	O 108	0
59	P	149	Total 149	O 149	0
59	Q	120	Total 120	O 120	0
59	R	52	Total 52	O 52	0
59	S	2	Total 2	O 2	0
59	T	1	Total 1	O 1	0
59	U	3	Total 3	O 3	0
59	V	35	Total 35	O 35	0
59	W	58	Total 58	O 58	0
59	X	64	Total 64	O 64	0
59	Y	2	Total 2	O 2	0
59	Z	73	Total 73	O 73	0
59	a	37	Total 37	O 37	0
59	b	15	Total 15	O 15	0

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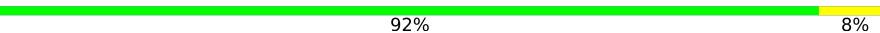
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
59	c	4	Total 4	O 4	0
59	d	31	Total 31	O 31	0
59	e	44	Total 44	O 44	0
59	f	11	Total 11	O 11	0
59	g	27	Total 27	O 27	0
59	h	45	Total 45	O 45	0
59	i	6	Total 6	O 6	0
59	j	2	Total 2	O 2	0
59	k	3	Total 3	O 3	0
59	l	37	Total 37	O 37	0
59	m	34	Total 34	O 34	0
59	n	31	Total 31	O 31	0
59	p	45	Total 45	O 45	0
59	q	84	Total 84	O 84	0
59	r	51	Total 51	O 51	0
59	s	8	Total 8	O 8	0

3 Residue-property plots

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.

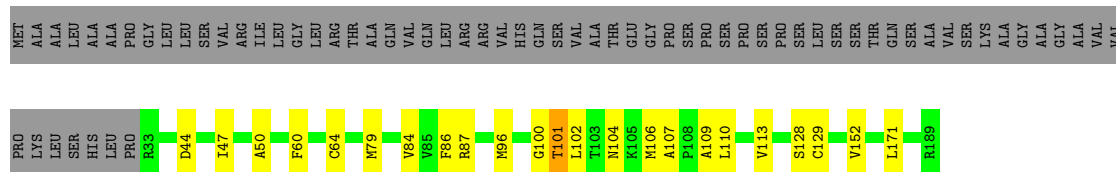
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



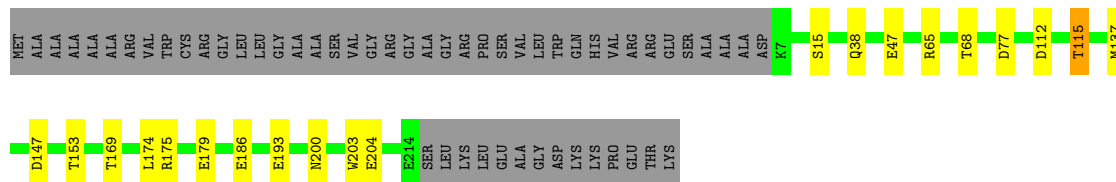
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



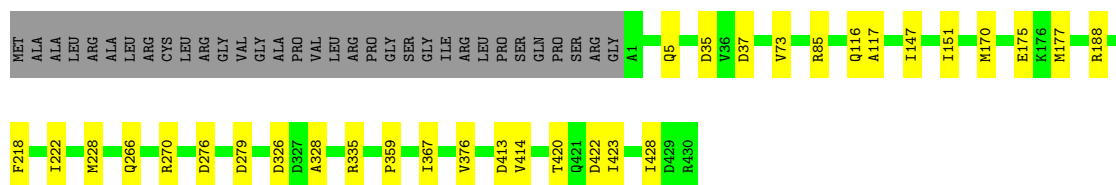
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

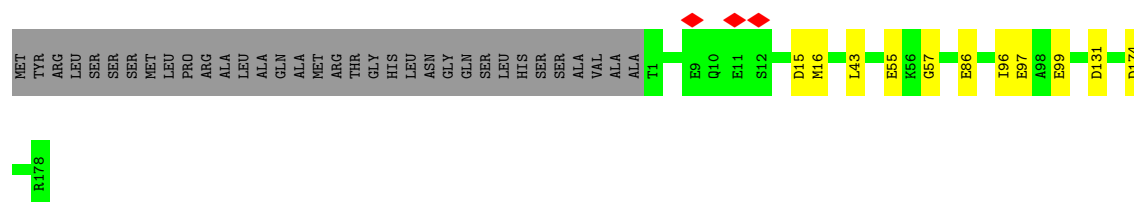
Chain C: 



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

Chain D: 





- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 90% 10%



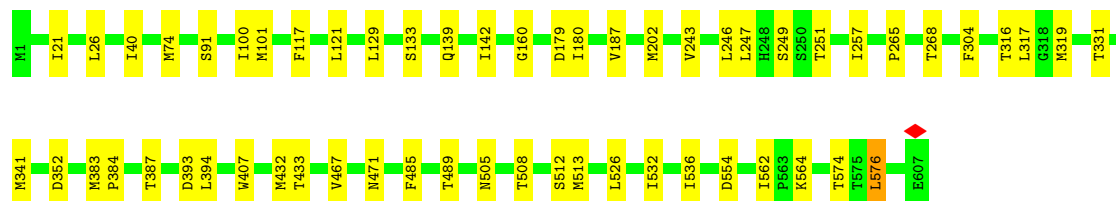
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K: 92% 8%



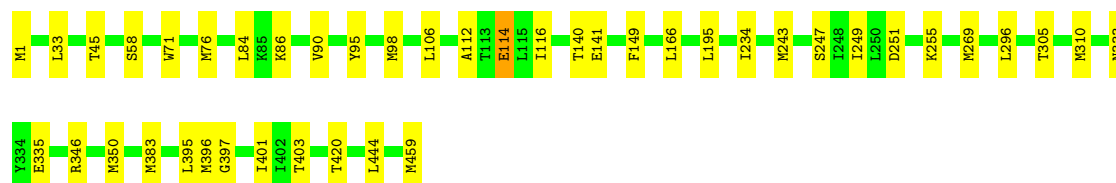
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 91% 9%



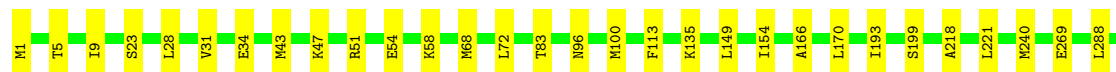
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 91% 9%



- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

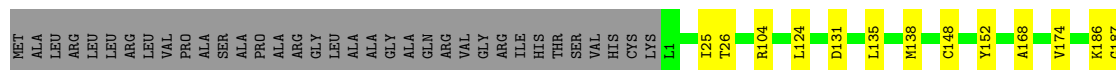
Chain N: 90% 10%





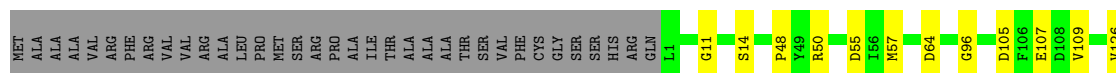
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 84% 6% 10%



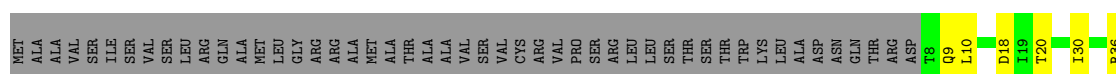
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 84% 7% 9%



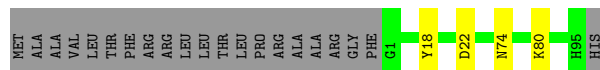
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 63% 9% 28%



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

Chain R: 78% 18%

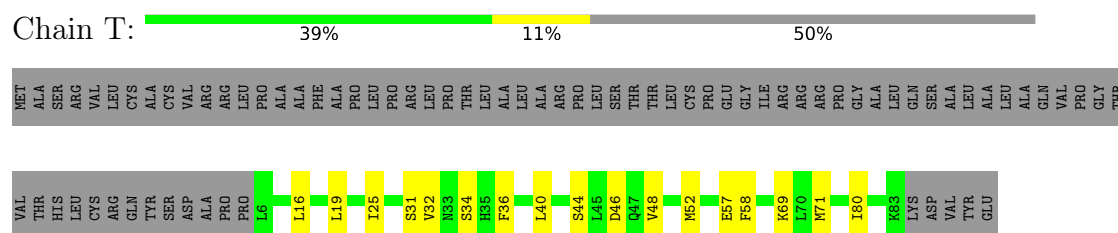


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

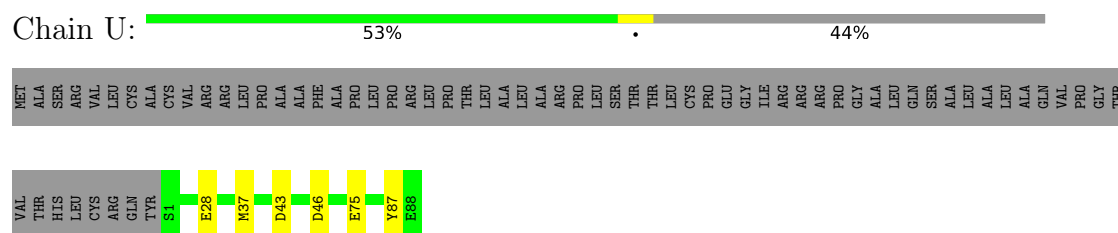
Chain S: 79% 8% 13%



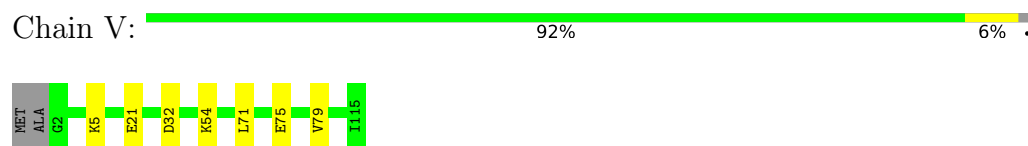
- Molecule 20: Acyl carrier protein, mitochondrial



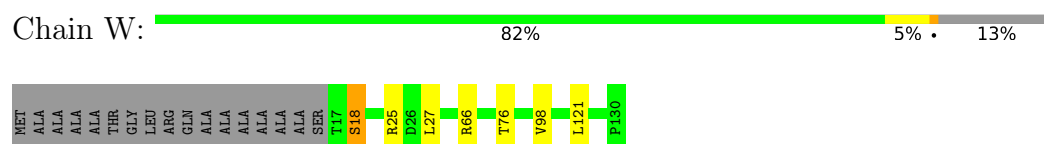
- Molecule 20: Acyl carrier protein, mitochondrial



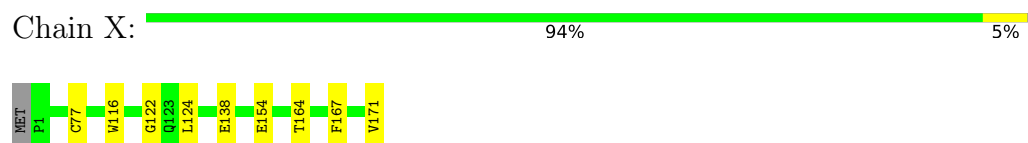
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



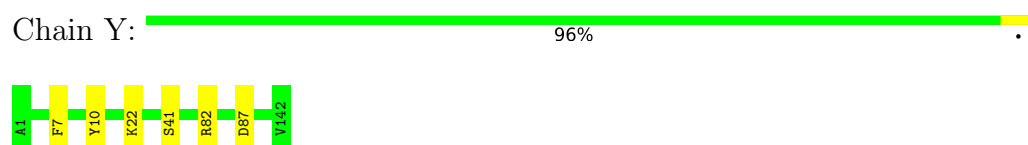
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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



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



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

Chain Z:  88% 9% .

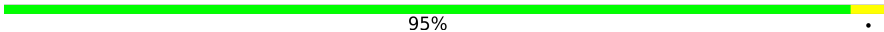


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  94% . .



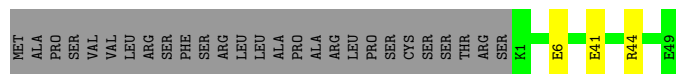
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  95% . .



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

Chain c:  61% . 36%



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

Chain d:  91% 9%



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

Chain e:  94% 5% .



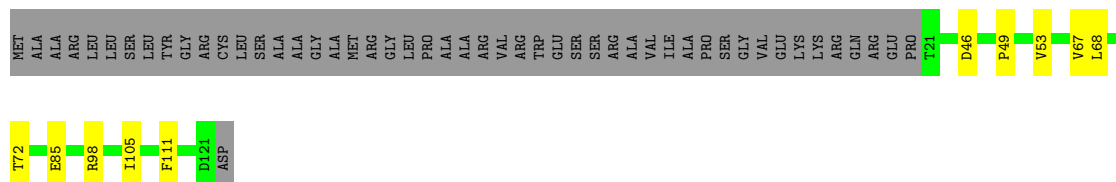
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:  93% 5% .



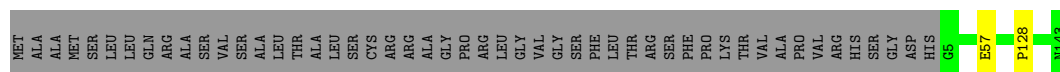
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g: 



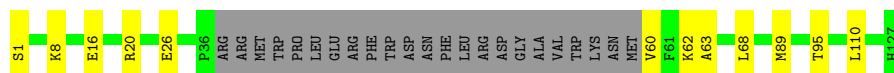
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h: 



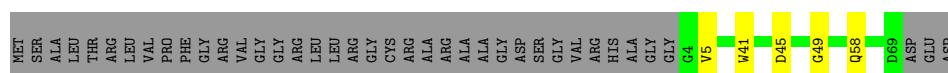
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i: 



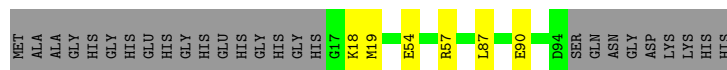
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j: 



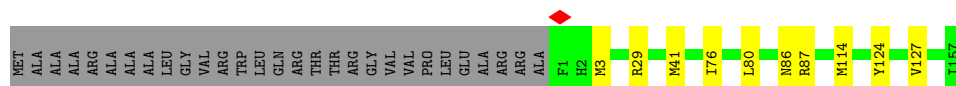
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k: 

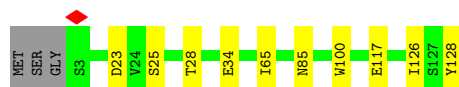
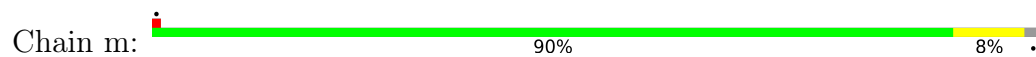


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l: 



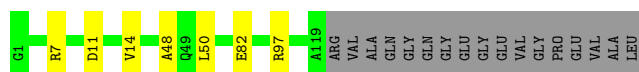
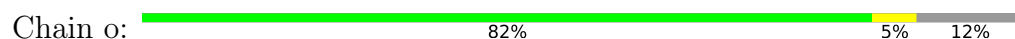
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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



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



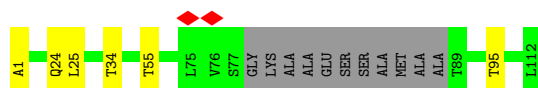
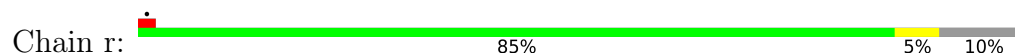
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



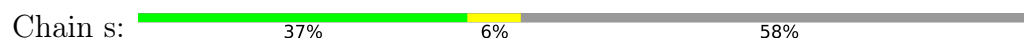
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



P26	T27	D28	T29	T30	L46	D47	L52	S53	H59
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	109866	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 ($e^-/\text{\AA}^2$)	39.94	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	44.320	Depositor
Minimum map value	-20.720	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.927	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	480.62003, 480.62003, 480.62003	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6866, 0.6866, 0.6866	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/949	0.40	0/1297
2	B	0.32	0/1277	0.46	0/1727
3	C	0.29	0/1780	0.45	0/2424
4	D	0.29	0/3540	0.41	0/4795
5	E	0.25	0/1700	0.41	0/2316
6	F	0.29	0/3396	0.37	0/4586
7	G	0.29	0/5388	0.39	0/7300
8	H	0.31	0/2607	0.49	1/3564 (0.0%)
9	I	0.30	0/1461	0.43	0/1974
10	J	0.25	0/1330	0.35	0/1810
11	K	0.25	0/738	0.34	0/1002
12	L	0.29	0/4922	0.36	0/6698
13	M	0.28	0/3709	0.38	0/5052
14	N	0.29	0/2755	0.41	0/3751
15	O	0.28	0/2674	0.36	0/3626
16	P	0.28	0/2823	0.39	0/3828
17	Q	0.28	0/1044	0.37	0/1409
18	R	0.28	0/762	0.36	0/1026
19	S	0.29	0/696	0.39	0/938
20	T	0.21	0/637	0.40	0/858
20	U	0.30	0/718	0.34	0/970
21	V	0.25	0/949	0.31	0/1286
22	W	0.27	0/993	0.40	0/1335
23	X	0.26	0/1434	0.38	0/1937
24	Y	0.27	0/1074	0.30	0/1456
25	Z	0.28	0/1192	0.38	0/1608
26	a	0.28	0/577	0.40	0/777
27	b	0.26	0/671	0.34	0/921
28	c	0.28	0/418	0.43	0/567
29	d	0.28	0/1028	0.40	0/1387
30	e	0.27	0/900	0.41	0/1199

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.26	0/495	0.33	0/667
32	g	0.27	0/878	0.41	0/1196
33	h	0.30	0/1201	0.40	0/1626
34	i	0.29	0/889	0.42	0/1210
35	j	0.28	0/591	0.33	0/809
36	k	0.28	0/650	0.32	0/878
37	l	0.29	0/1379	0.38	0/1882
38	m	0.31	0/1079	0.42	0/1463
39	n	0.31	0/1596	0.36	0/2162
40	o	0.29	0/1044	0.40	0/1401
41	p	0.29	0/1472	0.40	0/1989
42	q	0.28	0/1243	0.39	0/1692
43	r	0.29	0/819	0.42	0/1108
44	s	0.26	0/379	0.48	0/515
All	All	0.28	0/67857	0.39	1/92022 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	202	GLU	N-CA-C	-5.01	106.01	112.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	8	0
2	B	1259	0	1255	14	0
3	C	1730	0	1686	17	0
4	D	3464	0	3416	22	0
5	E	1660	0	1653	17	0
6	F	3321	0	3278	22	0
7	G	5301	0	5327	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	2540	0	2626	23	0
9	I	1431	0	1383	8	0
10	J	1308	0	1319	17	0
11	K	737	0	768	6	0
12	L	4809	0	4991	38	0
13	M	3632	0	3853	35	0
14	N	2703	0	2902	27	0
15	O	2607	0	2566	17	0
16	P	2748	0	2768	19	0
17	Q	1021	0	1022	13	0
18	R	748	0	724	4	0
19	S	685	0	706	4	0
20	T	628	0	626	9	0
20	U	706	0	698	5	0
21	V	927	0	968	5	0
22	W	970	0	991	7	0
23	X	1396	0	1385	8	0
24	Y	1050	0	1039	4	0
25	Z	1161	0	1161	9	0
26	a	564	0	579	3	0
27	b	648	0	652	3	0
28	c	407	0	407	2	0
29	d	996	0	1001	10	0
30	e	877	0	871	3	0
31	f	482	0	482	3	0
32	g	850	0	783	6	0
33	h	1166	0	1166	2	0
34	i	869	0	863	8	0
35	j	566	0	518	3	0
36	k	630	0	623	4	0
37	l	1323	0	1216	9	0
38	m	1050	0	1061	9	0
39	n	1541	0	1473	9	0
40	o	1019	0	1008	6	0
41	p	1439	0	1408	8	0
42	q	1212	0	1171	9	0
43	r	809	0	843	5	0
44	s	368	0	346	5	0
45	A	70	0	88	1	0
45	H	35	0	45	2	0
45	J	70	0	89	2	0
45	L	105	0	131	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	M	35	0	40	0	0
45	N	70	0	89	0	0
45	Y	105	0	133	1	0
45	h	35	0	46	0	0
45	j	35	0	45	0	0
46	A	34	0	42	0	0
46	B	95	0	141	1	0
46	L	27	0	28	0	0
46	p	36	0	46	0	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	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	2	0
50	G	1	0	0	0	0
51	H	51	0	52	0	0
51	K	71	0	86	0	0
51	L	68	0	80	0	0
51	h	136	0	174	0	0
51	q	62	0	68	0	0
52	I	80	0	108	1	0
52	L	88	0	127	2	0
52	M	41	0	59	0	0
52	N	72	0	97	1	0
52	O	30	0	34	0	0
52	X	37	0	48	1	0
52	Y	38	0	50	1	0
52	Z	43	0	60	0	0
52	d	75	0	98	2	0
52	f	42	0	58	0	0
52	i	30	0	34	1	0
52	r	46	0	66	1	0
53	O	1	0	0	0	0
54	O	31	0	12	2	0
55	P	48	0	26	2	0
56	R	1	0	0	0	0
57	T	37	0	0	0	0
57	U	37	0	0	1	0
58	o	15	0	27	0	0
59	A	59	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	B	96	0	0	2	0
59	C	160	0	0	11	0
59	D	257	0	0	10	0
59	E	43	0	0	3	0
59	F	85	0	0	6	0
59	G	300	0	0	21	0
59	H	120	0	0	6	0
59	I	124	0	0	3	0
59	J	60	0	0	4	0
59	K	41	0	0	2	0
59	L	105	0	0	6	0
59	M	190	0	0	14	0
59	N	123	0	0	7	0
59	O	108	0	0	6	0
59	P	149	0	0	13	0
59	Q	120	0	0	6	0
59	R	52	0	0	3	0
59	S	2	0	0	0	0
59	T	1	0	0	0	0
59	U	3	0	0	0	0
59	V	35	0	0	2	0
59	W	58	0	0	0	0
59	X	64	0	0	3	0
59	Y	2	0	0	0	0
59	Z	73	0	0	4	0
59	a	37	0	0	0	0
59	b	15	0	0	1	0
59	c	4	0	0	0	0
59	d	31	0	0	2	0
59	e	44	0	0	2	0
59	f	11	0	0	1	0
59	g	27	0	0	1	0
59	h	45	0	0	1	0
59	i	6	0	0	0	0
59	j	2	0	0	0	0
59	k	3	0	0	0	0
59	l	37	0	0	2	0
59	m	34	0	0	2	0
59	n	31	0	0	1	0
59	p	45	0	0	1	0
59	q	84	0	0	2	0
59	r	51	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	s	8	0	0	0	0
All	All	71256	0	68897	449	0

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

All (449) 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)
37:l:41:MET:SD	38:m:85:ASN:ND2	2.42	0.93
14:N:47:LYS:NZ	59:N:504:HOH:O	2.07	0.85
14:N:34:GLU:OE1	59:N:501:HOH:O	1.94	0.84
45:L:701:LMT:O2B	45:L:701:LMT:O3'	1.95	0.83
3:C:112:ASP:OD2	3:C:115:THR:OG1	1.98	0.82
12:L:179:ASP:OD2	59:L:801:HOH:O	1.97	0.82
15:O:227:GLU:OE2	59:O:601:HOH:O	1.97	0.82
3:C:147:ASP:OD2	59:C:301:HOH:O	1.99	0.81
52:X:201:3PE:O12	52:d:201:3PE:N	2.14	0.81
3:C:15:SER:O	59:C:302:HOH:O	2.00	0.80
23:X:124:LEU:O	59:X:301:HOH:O	2.00	0.79
13:M:251:ASP:OD1	59:M:601:HOH:O	2.00	0.79
7:G:396:ARG:NH1	59:G:916:HOH:O	2.16	0.79
14:N:113:PHE:O	59:N:502:HOH:O	1.99	0.79
29:d:18:ALA:O	59:d:301:HOH:O	2.00	0.79
7:G:225:THR:OG1	59:G:901:HOH:O	1.97	0.78
4:D:35:ASP:OD2	59:D:501:HOH:O	2.01	0.78
27:b:81:LYS:NZ	59:b:101:HOH:O	2.17	0.78
12:L:179:ASP:OD1	59:L:802:HOH:O	2.01	0.78
13:M:335:GLU:OE2	59:M:602:HOH:O	2.00	0.78
7:G:91:GLU:OE2	59:G:902:HOH:O	2.02	0.78
10:J:78:TYR:O	59:J:301:HOH:O	2.02	0.78
21:V:21:GLU:OE2	59:V:201:HOH:O	2.02	0.77
7:G:14:ASP:OD1	59:G:903:HOH:O	2.02	0.77
16:P:55:ASP:OD2	59:P:601:HOH:O	2.01	0.77
9:I:97:GLU:OE2	59:I:301:HOH:O	2.01	0.77
24:Y:41:SER:OG	52:Y:203:3PE:O12	2.03	0.77
42:q:136:GLU:OE2	59:q:301:HOH:O	2.03	0.77
15:O:237:ASP:OD1	59:O:602:HOH:O	2.04	0.76
1:A:73:LEU:HD12	10:J:54:MET:HE1	1.66	0.76
46:B:204:PC1:O12	59:B:301:HOH:O	2.03	0.76
4:D:413:ASP:OD2	59:D:502:HOH:O	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:66:GLU:OE1	59:Q:201:HOH:O	2.03	0.76
7:G:232:ASP:O	59:G:904:HOH:O	2.04	0.76
4:D:279:ASP:OD2	59:D:503:HOH:O	2.04	0.76
10:J:48:GLY:O	59:J:302:HOH:O	2.03	0.75
10:J:124:LEU:O	59:J:303:HOH:O	2.03	0.75
16:P:286:ARG:NH1	59:P:609:HOH:O	2.20	0.75
9:I:57:GLY:O	59:I:302:HOH:O	2.05	0.75
3:C:47:GLU:O	59:C:303:HOH:O	2.04	0.74
3:C:200:ASN:OD1	59:C:305:HOH:O	2.05	0.74
4:D:359:PRO:O	59:D:504:HOH:O	2.05	0.74
54:O:502:DGT:O2G	59:O:603:HOH:O	2.05	0.74
14:N:96:ASN:OD1	59:N:503:HOH:O	2.04	0.74
45:L:701:LMT:O4'	52:L:706:3PE:O12	2.06	0.74
17:Q:39:VAL:O	59:Q:202:HOH:O	2.05	0.74
4:D:266:GLN:O	59:D:505:HOH:O	2.06	0.74
8:H:61:MET:O	59:H:502:HOH:O	2.06	0.74
18:R:22:ASP:OD2	59:R:301:HOH:O	2.04	0.74
13:M:114:GLU:OE2	13:M:116:ILE:HG22	1.88	0.74
39:n:75:HIS:O	59:n:201:HOH:O	2.06	0.73
13:M:251:ASP:OD2	59:M:603:HOH:O	2.06	0.73
20:U:87:TYR:OH	34:i:26:GLU:OE1	2.05	0.73
3:C:204:GLU:OE2	59:C:304:HOH:O	2.05	0.73
7:G:617:ASP:OD2	59:G:905:HOH:O	2.05	0.73
6:F:380:VAL:O	6:F:429:ARG:NH2	2.22	0.73
12:L:352:ASP:OD2	59:L:803:HOH:O	2.06	0.73
13:M:243:MET:O	13:M:247:SER:OG	2.05	0.73
13:M:251:ASP:OD2	59:M:604:HOH:O	2.06	0.73
43:r:95:THR:O	59:r:301:HOH:O	2.07	0.73
6:F:304:THR:O	59:F:601:HOH:O	2.07	0.72
16:P:127:GLU:O	59:P:603:HOH:O	2.06	0.72
4:D:270:ARG:NH2	59:D:509:HOH:O	2.21	0.72
7:G:31:GLU:OE1	59:G:906:HOH:O	2.06	0.72
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.71	0.72
7:G:58:GLU:OE2	7:G:80:LEU:HD12	1.89	0.72
7:G:246:GLU:OE2	59:G:908:HOH:O	2.07	0.72
7:G:635:ASP:O	59:G:907:HOH:O	2.06	0.72
3:C:203:TRP:O	59:C:306:HOH:O	2.08	0.72
7:G:588:THR:O	59:G:912:HOH:O	2.08	0.72
12:L:21:ILE:HD12	12:L:26:LEU:HD23	1.71	0.72
7:G:154:ILE:O	59:G:913:HOH:O	2.08	0.71
24:Y:7:PHE:O	45:Y:201:LMT:O6'	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:109:ASP:OD2	59:G:910:HOH:O	2.07	0.71
9:I:174:ASP:OD1	59:I:303:HOH:O	2.09	0.71
14:N:135:LYS:NZ	59:N:507:HOH:O	2.23	0.71
39:n:34:ASP:OD2	39:n:35:LYS:N	2.24	0.71
4:D:335:ARG:NH2	9:I:131:ASP:OD2	2.23	0.71
7:G:595:GLU:OE2	59:G:911:HOH:O	2.08	0.71
4:D:422:ASP:OD2	59:D:506:HOH:O	2.08	0.70
4:D:5:GLN:O	59:D:507:HOH:O	2.09	0.70
7:G:232:ASP:OD2	59:G:909:HOH:O	2.07	0.70
7:G:595:GLU:OE2	59:G:914:HOH:O	2.09	0.70
23:X:171:VAL:O	59:X:302:HOH:O	2.10	0.70
33:h:128:PRO:O	59:h:301:HOH:O	2.08	0.70
3:C:77:ASP:OD2	59:C:307:HOH:O	2.08	0.70
5:E:45:ALA:O	59:E:403:HOH:O	2.10	0.70
3:C:38:GLN:O	59:C:309:HOH:O	2.09	0.70
16:P:170:ASP:OD2	59:P:605:HOH:O	2.10	0.70
3:C:179:GLU:OE1	59:C:308:HOH:O	2.09	0.69
5:E:90:TYR:O	59:E:402:HOH:O	2.09	0.69
38:m:128:TYR:O	59:m:203:HOH:O	2.10	0.69
8:H:199:ASP:OD2	59:H:504:HOH:O	2.10	0.69
6:F:175:VAL:O	59:F:602:HOH:O	2.10	0.69
24:Y:82:ARG:NH2	24:Y:87:ASP:OD2	2.25	0.69
25:Z:116:VAL:O	59:Z:301:HOH:O	2.10	0.69
8:H:143:GLU:OE2	59:H:503:HOH:O	2.10	0.69
21:V:32:ASP:OD1	59:V:202:HOH:O	2.11	0.68
16:P:177:ARG:NH2	59:P:613:HOH:O	2.26	0.68
34:i:110:LEU:HD21	41:p:18:ALA:O	1.93	0.68
16:P:64:ASP:OD1	59:P:606:HOH:O	2.11	0.68
38:m:117:GLU:OE1	59:m:202:HOH:O	2.09	0.68
17:Q:61:THR:O	59:Q:203:HOH:O	2.11	0.68
43:r:55:THR:OG1	59:r:302:HOH:O	2.11	0.68
3:C:179:GLU:OE2	59:C:310:HOH:O	2.11	0.68
30:e:16:HIS:O	59:e:201:HOH:O	2.11	0.68
5:E:30:ARG:NH2	44:s:47:ASP:OD2	2.26	0.67
7:G:95:GLU:OE1	59:G:915:HOH:O	2.13	0.67
32:g:46:ASP:OD1	59:g:201:HOH:O	2.11	0.67
8:H:206:GLU:OE2	59:H:505:HOH:O	2.12	0.67
1:A:68:GLU:HG2	10:J:159:LEU:HD13	1.77	0.67
13:M:114:GLU:OE1	59:M:606:HOH:O	2.11	0.67
42:q:78:ASP:OD1	59:q:302:HOH:O	2.12	0.67
21:V:5:LYS:NZ	21:V:75:GLU:OE1	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:77:GLU:OE2	59:Z:302:HOH:O	2.12	0.66
15:O:304:TYR:O	59:O:605:HOH:O	2.14	0.66
4:D:328:ALA:HB3	7:G:126:ASP:HB2	1.78	0.66
6:F:208:PRO:O	59:F:603:HOH:O	2.14	0.66
17:Q:130:VAL:O	59:Q:204:HOH:O	2.14	0.66
18:R:18:TYR:O	59:R:302:HOH:O	2.13	0.66
30:e:79:LYS:O	59:e:202:HOH:O	2.13	0.66
1:A:73:LEU:CD1	10:J:54:MET:HE1	2.25	0.65
14:N:23:SER:O	59:N:505:HOH:O	2.15	0.65
37:l:86:ASN:OD1	59:l:201:HOH:O	2.14	0.65
7:G:331:LEU:HD22	7:G:525:LEU:HD22	1.79	0.64
3:C:65:ARG:NH2	59:C:316:HOH:O	2.30	0.64
1:A:38:GLU:OE2	59:A:302:HOH:O	2.15	0.64
2:B:44:ASP:OD2	59:B:302:HOH:O	2.15	0.64
23:X:116:TRP:O	59:X:303:HOH:O	2.15	0.64
49:F:502:FMN:O1P	59:F:604:HOH:O	2.15	0.64
57:U:201:EHZ:O2	57:U:201:EHZ:O1	2.07	0.64
15:O:174:VAL:O	59:O:606:HOH:O	2.15	0.64
12:L:393:ASP:OD1	12:L:394:LEU:N	2.31	0.63
43:r:24:GLN:NE2	59:r:305:HOH:O	2.29	0.63
13:M:140:THR:HG23	13:M:141:GLU:OE1	1.99	0.63
34:i:89:MET:O	34:i:95:THR:OG1	2.13	0.63
32:g:98:ARG:NH1	32:g:105:ILE:O	2.32	0.63
14:N:345:THR:O	29:d:79:GLN:NE2	2.33	0.62
7:G:143:GLY:HA2	7:G:190:MET:HE2	1.82	0.62
7:G:237:ASN:ND2	59:G:928:HOH:O	2.33	0.61
9:I:55:GLU:OE1	42:q:34:ARG:NH1	2.33	0.61
20:U:75:GLU:OE2	34:i:8:LYS:NZ	2.34	0.61
32:g:68:LEU:O	32:g:72:THR:OG1	2.10	0.61
41:p:67:TYR:OH	59:p:401:HOH:O	2.13	0.61
55:P:501:NDP:O1X	59:P:607:HOH:O	2.15	0.61
10:J:2:ASN:OD1	45:J:202:LMT:O6'	2.18	0.61
2:B:50:ALA:HB2	8:H:53:MET:HE2	1.83	0.61
3:C:137:MET:HE1	3:C:153:THR:HG23	1.82	0.61
45:J:202:LMT:O3'	45:J:202:LMT:O5B	2.19	0.61
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.31	0.60
4:D:326:ASP:OD1	59:D:508:HOH:O	2.17	0.60
5:E:214:GLN:NE2	6:F:235:CYS:O	2.35	0.60
20:T:46:ASP:OD1	22:W:66:ARG:NH2	2.35	0.60
25:Z:122:GLU:OE1	59:Z:303:HOH:O	2.17	0.59
13:M:112:ALA:O	59:M:608:HOH:O	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.84	0.59
39:n:126:LYS:NZ	39:n:130:GLU:OE2	2.31	0.59
14:N:221:LEU:HD22	14:N:240:MET:HE2	1.85	0.59
35:j:58:GLN:N	35:j:58:GLN:OE1	2.35	0.59
12:L:485:PHE:O	12:L:489:THR:OG1	2.20	0.58
14:N:83:THR:OG1	59:N:506:HOH:O	2.16	0.58
14:N:193:ILE:HD11	14:N:269:GLU:HB3	1.85	0.58
20:T:31:SER:O	20:T:34:SER:OG	2.15	0.58
34:i:16:GLU:OE2	34:i:20:ARG:NH1	2.36	0.58
15:O:26:THR:HG22	15:O:124:LEU:HB2	1.84	0.58
6:F:342:ASP:OD1	6:F:429:ARG:NH1	2.36	0.58
10:J:66:VAL:HG11	11:K:31:LEU:HD21	1.85	0.58
20:T:25:ILE:HG12	20:T:40:LEU:HD13	1.86	0.58
7:G:283:MET:HE3	7:G:293:TYR:CD2	2.39	0.57
12:L:407:TRP:CZ3	37:l:114:MET:HE2	2.39	0.57
15:O:25:ILE:HD12	15:O:168:ALA:HB3	1.86	0.57
16:P:179:LEU:HD11	16:P:310:LEU:HD11	1.86	0.57
22:W:27:LEU:HD13	22:W:76:THR:O	2.04	0.57
13:M:296:LEU:CD2	13:M:396:MET:HE1	2.35	0.57
13:M:116:ILE:HG21	23:X:167:PHE:CD1	2.40	0.56
13:M:149:PHE:O	59:M:609:HOH:O	2.18	0.56
12:L:257:ILE:HG23	12:L:317:LEU:HD11	1.88	0.56
2:B:106:MET:HE3	2:B:109:ALA:HB3	1.87	0.56
6:F:99:GLU:OE1	6:F:108:ARG:N	2.38	0.56
42:q:78:ASP:OD2	42:q:80:SER:OG	2.25	0.55
7:G:272:ASP:OD1	7:G:681:SER:OG	2.25	0.55
20:U:46:ASP:OD1	39:n:44:ARG:NH2	2.40	0.55
12:L:467:VAL:O	12:L:471:ASN:ND2	2.39	0.55
13:M:166:LEU:HD23	13:M:195:LEU:HD13	1.89	0.55
25:Z:142:TYR:CZ	26:a:48:MET:HE1	2.42	0.54
5:E:53:LEU:HD13	44:s:46:LEU:HD12	1.90	0.54
11:K:12:PHE:CE1	14:N:72:LEU:HD22	2.42	0.54
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.42	0.54
42:q:95:ASP:HB2	43:r:34:THR:HG22	1.89	0.54
1:A:79:ILE:HD12	8:H:314:VAL:HG13	1.90	0.54
3:C:175:ARG:NH2	3:C:186:GLU:OE1	2.40	0.54
5:E:192:CYS:SG	5:E:193:CYS:N	2.79	0.54
31:f:41:MET:HE2	31:f:41:MET:HA	1.89	0.54
5:E:27:ASN:OD1	5:E:53:LEU:HD11	2.08	0.53
25:Z:65:GLU:OE1	59:Z:304:HOH:O	2.18	0.53
7:G:613:TYR:CD1	7:G:619:VAL:HG22	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:10:TYR:O	24:Y:22:LYS:NZ	2.40	0.53
31:f:43:PHE:O	59:f:202:HOH:O	2.18	0.53
15:O:297:ARG:NH2	59:O:610:HOH:O	2.31	0.53
15:O:320:LYS:O	29:d:60:ARG:NH2	2.39	0.53
5:E:105:THR:HG22	5:E:106:THR:H	1.73	0.53
17:Q:18:ASP:OD2	17:Q:20:THR:OG1	2.22	0.53
29:d:108:THR:OG1	29:d:111:GLU:OE2	2.27	0.53
7:G:366:THR:O	7:G:367:THR:OG1	2.20	0.53
14:N:221:LEU:HD22	14:N:240:MET:CE	2.39	0.52
25:Z:121:GLY:HA2	25:Z:132:MET:HE1	1.92	0.52
2:B:60:PHE:HZ	2:B:110:LEU:HD12	1.74	0.52
13:M:249:ILE:O	59:M:611:HOH:O	2.18	0.52
45:L:705:LMT:O3'	45:L:705:LMT:O2B	2.20	0.52
23:X:138:GLU:OE1	23:X:138:GLU:N	2.36	0.52
1:A:44:THR:HG22	22:W:98:VAL:HB	1.91	0.52
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.42	0.52
12:L:505:ASN:O	12:L:508:THR:OG1	2.23	0.52
13:M:296:LEU:HD22	13:M:396:MET:HE1	1.91	0.52
16:P:126:VAL:O	59:P:608:HOH:O	2.19	0.52
34:i:68:LEU:HD13	34:i:68:LEU:O	2.09	0.52
5:E:136:LEU:HD23	5:E:137:PHE:CE2	2.44	0.52
12:L:331:THR:HB	12:L:387:THR:HG22	1.91	0.52
12:L:532:ILE:O	12:L:536:ILE:HG22	2.10	0.52
10:J:69:TYR:HB3	11:K:27:MET:HE1	1.92	0.51
6:F:300:GLY:HA3	6:F:304:THR:HG21	1.92	0.51
12:L:180:ILE:HD12	13:M:397:GLY:HA2	1.92	0.51
17:Q:10:LEU:HD13	22:W:18:SER:HB3	1.92	0.51
13:M:98:MET:HE2	13:M:98:MET:HA	1.91	0.51
5:E:164:LEU:HD13	5:E:169:ILE:HD13	1.93	0.51
20:T:36:PHE:HD1	20:T:40:LEU:HD12	1.76	0.51
37:l:76:ILE:HG23	37:l:80:LEU:HD22	1.92	0.51
40:o:82:GLU:N	40:o:82:GLU:OE1	2.41	0.51
17:Q:46:GLN:OE1	59:Q:205:HOH:O	2.19	0.51
6:F:197:GLU:OE1	6:F:216:PHE:N	2.42	0.51
8:H:250:ASN:O	8:H:251:LEU:HD22	2.10	0.51
6:F:154:ARG:HA	44:s:52:LEU:HD21	1.92	0.51
25:Z:68:ILE:HD11	27:b:49:PRO:HB2	1.92	0.51
42:q:55:PHE:CD2	43:r:25:LEU:HD13	2.46	0.50
5:E:79:ARG:NH2	5:E:82:GLU:OE2	2.45	0.50
35:j:45:ASP:O	35:j:49:GLY:N	2.45	0.50
9:I:99:GLU:OE1	42:q:131:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:40:ILE:CD1	12:L:101:MET:HE3	2.41	0.50
13:M:350:MET:HE3	59:M:761:HOH:O	2.11	0.50
15:O:186:LYS:NZ	15:O:191:GLU:OE1	2.39	0.50
40:o:11:ASP:OD1	40:o:14:VAL:HG22	2.11	0.50
12:L:74:MET:HE1	59:L:885:HOH:O	2.10	0.50
16:P:50:ARG:NH2	59:P:624:HOH:O	2.45	0.50
18:R:80:LYS:NZ	59:R:303:HOH:O	2.20	0.50
12:L:100:ILE:HD13	12:L:341:MET:CE	2.42	0.50
12:L:383:MET:HE3	12:L:384:PRO:HD2	1.94	0.50
7:G:391:PHE:CE2	7:G:395:ILE:HD11	2.47	0.49
11:K:92:ASN:O	59:K:201:HOH:O	2.19	0.49
7:G:375:ASP:OD2	7:G:375:ASP:N	2.45	0.49
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.95	0.49
6:F:224:ASN:ND2	49:F:502:FMN:O2	2.36	0.49
38:m:23:ASP:OD2	38:m:28:THR:OG1	2.26	0.49
1:A:53:MET:HE2	1:A:55:PHE:CE2	2.47	0.49
4:D:423:ILE:HG23	4:D:428:ILE:CD1	2.42	0.49
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.47	0.49
16:P:105:ASP:OD1	16:P:107:GLU:N	2.43	0.49
16:P:244:TYR:OH	59:P:602:HOH:O	2.03	0.49
37:l:127:VAL:HG22	40:o:97:ARG:HB3	1.95	0.49
10:J:114:VAL:C	10:J:115:ILE:HD13	2.37	0.49
36:k:18:LYS:NZ	36:k:19:MET:O	2.45	0.49
8:H:264:LEU:HD21	26:a:12:MET:HB3	1.95	0.49
5:E:53:LEU:HD13	44:s:46:LEU:CD1	2.42	0.48
12:L:513:MET:HE3	12:L:513:MET:HA	1.94	0.48
7:G:324:ASP:HB3	7:G:571:ALA:HB1	1.94	0.48
7:G:615:THR:O	7:G:619:VAL:HG23	2.13	0.48
12:L:513:MET:HE1	39:n:30:CYS:SG	2.53	0.48
29:d:112:ILE:O	41:p:159:LYS:NZ	2.46	0.48
9:I:43:LEU:HD11	52:r:201:3PE:H3F1	1.96	0.48
12:L:564:LYS:NZ	45:L:705:LMT:O6B	2.30	0.48
15:O:25:ILE:CD1	15:O:168:ALA:HB3	2.43	0.48
29:d:22:PRO:O	59:d:302:HOH:O	2.20	0.48
8:H:139:THR:OG1	59:H:506:HOH:O	2.20	0.47
12:L:129:LEU:O	12:L:133:SER:OG	2.23	0.47
6:F:111:MET:SD	6:F:138:ILE:HD12	2.54	0.47
13:M:71:TRP:HZ3	32:g:67:VAL:HG11	1.78	0.47
15:O:174:VAL:HG22	15:O:225:SER:OG	2.15	0.47
29:d:25:LYS:NZ	52:d:201:3PE:O14	2.47	0.47
35:j:41:TRP:NE1	36:k:87:LEU:HD11	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:231:MET:HE2	7:G:231:MET:HA	1.96	0.47
45:L:701:LMT:O1B	45:L:701:LMT:O6'	2.30	0.47
8:H:209:SER:OG	8:H:212:ASN:OD1	2.31	0.47
45:H:402:LMT:O1B	45:H:402:LMT:O6'	2.32	0.47
13:M:106:LEU:HD13	13:M:234:ILE:HG21	1.96	0.47
16:P:14:SER:OG	59:P:604:HOH:O	2.10	0.47
5:E:101:GLN:HG2	5:E:140:ILE:HD11	1.97	0.47
8:H:23:VAL:HG12	8:H:27:ILE:HD12	1.97	0.47
20:U:37:MET:HE1	20:U:43:ASP:O	2.14	0.47
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.50	0.47
16:P:96:GLY:O	55:P:501:NDP:H8A	2.15	0.47
2:B:101:THR:HA	2:B:129:CYS:HB3	1.96	0.46
5:E:99:HIS:ND1	59:E:407:HOH:O	2.35	0.46
7:G:20:VAL:HG21	7:G:73:VAL:HG21	1.97	0.46
12:L:187:VAL:HG12	13:M:383:MET:HG3	1.96	0.46
36:k:54:GLU:OE1	36:k:57:ARG:NH1	2.48	0.46
39:n:146:ASP:OD1	39:n:146:ASP:N	2.46	0.46
13:M:444:LEU:HD22	59:M:745:HOH:O	2.15	0.46
15:O:187:GLY:HA2	15:O:192:MET:HE2	1.98	0.46
16:P:293:MET:HE3	16:P:294:PRO:HD2	1.97	0.46
2:B:79:MET:HE1	2:B:86:PHE:CE2	2.50	0.46
7:G:339:ASP:OD1	19:S:16:ARG:NH2	2.49	0.46
2:B:102:LEU:HD11	2:B:107:ALA:HA	1.98	0.46
7:G:606:ILE:CD1	22:W:121:LEU:HD11	2.46	0.46
15:O:138:MET:HE3	54:O:502:DGT:HN2	1.80	0.46
9:I:86:GLU:HB2	9:I:96:ILE:HD12	1.97	0.45
38:m:23:ASP:OD1	38:m:25:SER:OG	2.26	0.45
1:A:98:LEU:HD22	8:H:298:LEU:HD22	1.99	0.45
10:J:168:GLU:CG	14:N:5:THR:HG21	2.46	0.45
6:F:200:GLN:NE2	59:F:610:HOH:O	2.48	0.45
8:H:187:ILE:HD12	52:I:204:3PE:H271	1.98	0.45
13:M:346:ARG:HB2	13:M:420:THR:HG23	1.98	0.45
16:P:294:PRO:O	16:P:295:THR:HG23	2.16	0.45
37:l:3:MET:HG3	38:m:65:ILE:HG21	1.98	0.45
4:D:151:ILE:HG23	4:D:170:MET:HB3	1.98	0.45
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.98	0.45
13:M:333:ASN:ND2	59:M:616:HOH:O	2.34	0.45
39:n:140:GLN:O	39:n:143:THR:HG22	2.16	0.45
4:D:37:ASP:OD2	14:N:51:ARG:NE	2.46	0.45
4:D:228:MET:HE2	59:D:749:HOH:O	2.16	0.45
12:L:554:ASP:OD2	59:L:804:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:MET:CE	2:B:113:VAL:HG23	2.47	0.45
52:L:702:3PE:H2D2	13:M:401:ILE:HG21	1.99	0.45
13:M:45:THR:OG1	59:M:610:HOH:O	2.18	0.45
2:B:47:ILE:HG22	8:H:57:MET:SD	2.57	0.45
4:D:73:VAL:HG21	4:D:414:VAL:HG21	1.97	0.45
6:F:370:ASP:OD2	6:F:374:LYS:NZ	2.43	0.45
10:J:76:GLU:OE2	59:J:301:HOH:O	2.21	0.45
38:m:126:ILE:HD13	41:p:102:MET:HE2	1.98	0.45
13:M:296:LEU:HD21	13:M:396:MET:HE1	1.99	0.44
2:B:60:PHE:CZ	2:B:110:LEU:HD12	2.50	0.44
3:C:68:THR:HG21	21:V:54:LYS:HE3	1.99	0.44
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.99	0.44
10:J:114:VAL:HG23	10:J:115:ILE:HG12	2.00	0.44
13:M:403:THR:OG1	59:M:605:HOH:O	2.08	0.44
33:h:57:GLU:OE2	33:h:57:GLU:HA	2.18	0.44
17:Q:69:LEU:HD11	42:q:126:PRO:HG2	1.99	0.44
25:Z:93:GLU:HG2	25:Z:105:VAL:HG13	1.99	0.44
5:E:145:LEU:HD12	5:E:153:MET:HE1	2.00	0.44
5:E:204:GLU:OE2	5:E:204:GLU:N	2.51	0.44
10:J:151:MET:SD	14:N:28:LEU:HD21	2.58	0.44
12:L:100:ILE:HD13	12:L:341:MET:HE1	2.00	0.44
20:T:48:VAL:HG12	20:T:52:MET:HE2	2.00	0.44
2:B:152:VAL:O	16:P:57:MET:HE1	2.18	0.44
12:L:246:LEU:O	12:L:251:THR:OG1	2.36	0.44
26:a:53:ARG:NE	30:e:104:ARG:O	2.49	0.44
7:G:481:THR:OG1	7:G:483:VAL:HG13	2.18	0.43
28:c:6:GLU:HA	28:c:6:GLU:OE1	2.18	0.43
7:G:53:ARG:NH2	59:G:941:HOH:O	2.42	0.43
7:G:232:ASP:OD1	59:G:918:HOH:O	2.21	0.43
8:H:31:MET:HE1	8:H:272:TRP:CD1	2.52	0.43
12:L:432:MET:O	12:L:433:THR:OG1	2.25	0.43
45:A:201:LMT:H5B	45:A:201:LMT:H4'	1.99	0.43
59:K:205:HOH:O	14:N:68:MET:HE3	2.18	0.43
4:D:147:ILE:HG22	4:D:177:MET:HE1	1.99	0.43
12:L:574:THR:OG1	14:N:170:LEU:HD23	2.18	0.43
13:M:395:LEU:HD21	38:m:100:TRP:CZ2	2.53	0.43
16:P:11:GLY:O	59:P:611:HOH:O	2.21	0.43
17:Q:36:ARG:NH2	17:Q:106:GLU:OE2	2.46	0.43
23:X:122:GLY:CA	27:b:77:LEU:HD12	2.49	0.43
31:f:44:GLN:O	41:p:68:ARG:NH2	2.49	0.43
52:i:201:3PE:P	52:i:201:3PE:HN2	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:174:ARG:NH1	39:n:177:PRO:O	2.52	0.43
2:B:104:ASN:HB3	3:C:174:LEU:HD22	2.00	0.43
11:K:12:PHE:CD1	14:N:72:LEU:HD22	2.54	0.43
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.53	0.43
14:N:304:MET:HE3	15:O:286:ALA:HB1	1.99	0.43
19:S:33:ARG:O	19:S:37:VAL:HG23	2.18	0.43
14:N:343:LEU:HD22	52:N:402:3PE:H262	2.01	0.43
16:P:330:GLU:OE2	16:P:330:GLU:N	2.50	0.43
21:V:71:LEU:HD13	21:V:79:VAL:HG11	2.00	0.43
41:p:18:ALA:HB3	41:p:19:PRO:C	2.44	0.43
42:q:1:AME:HA	42:q:1:AME:HT23	1.78	0.43
44:s:28:ASP:OD1	44:s:30:THR:HG22	2.18	0.43
16:P:48:PRO:O	59:P:610:HOH:O	2.21	0.43
7:G:136:ALA:O	18:R:74:ASN:ND2	2.48	0.43
12:L:187:VAL:HG12	13:M:383:MET:CG	2.48	0.42
13:M:76:MET:HE1	59:M:708:HOH:O	2.19	0.42
17:Q:41:ALA:O	59:Q:206:HOH:O	2.21	0.42
14:N:54:GLU:OE2	14:N:58:LYS:NZ	2.46	0.42
37:l:124:TYR:OH	40:o:7:ARG:NH2	2.52	0.42
6:F:182:GLY:N	59:F:608:HOH:O	2.46	0.42
7:G:39:ARG:NH1	59:G:906:HOH:O	2.48	0.42
7:G:140:LYS:O	7:G:148:THR:OG1	2.34	0.42
8:H:202:GLU:O	8:H:203:GLY:C	2.62	0.42
10:J:89:LEU:O	10:J:93:VAL:HG23	2.19	0.42
17:Q:9:GLN:O	22:W:25:ARG:NH1	2.52	0.42
28:c:41:GLU:OE1	28:c:44:ARG:NH1	2.52	0.42
34:i:60:VAL:O	34:i:60:VAL:HG12	2.20	0.42
7:G:315:VAL:O	7:G:340:SER:OG	2.34	0.42
12:L:202:MET:HA	12:L:202:MET:HE2	2.02	0.42
12:L:243:VAL:HG13	12:L:247:LEU:HD13	2.01	0.42
14:N:149:LEU:HB3	14:N:154:ILE:HD11	2.02	0.42
14:N:240:MET:SD	29:d:48:LEU:HD22	2.59	0.42
10:J:121:GLY:O	25:Z:136:ASN:ND2	2.51	0.42
15:O:104:ARG:NE	15:O:131:ASP:OD1	2.46	0.42
17:Q:20:THR:HG22	17:Q:30:ILE:HD13	2.01	0.42
20:T:25:ILE:HG23	20:T:40:LEU:HD22	2.02	0.42
20:T:58:PHE:CE2	20:T:80:ILE:HD13	2.54	0.42
2:B:79:MET:HE3	2:B:84:VAL:HG12	2.02	0.42
6:F:93:LEU:HD13	6:F:129:MET:HE1	2.01	0.42
6:F:193:ILE:HG23	6:F:215:VAL:HA	2.01	0.42
7:G:431:ASP:N	7:G:431:ASP:OD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:576:LEU:HD12	12:L:576:LEU:C	2.45	0.42
14:N:166:ALA:HB1	14:N:288:LEU:HD23	2.01	0.42
40:o:48:ALA:HB3	40:o:50:LEU:HD13	2.01	0.42
6:F:192:LEU:HD23	6:F:192:LEU:O	2.20	0.42
6:F:367:GLU:OE2	7:G:100:ASN:ND2	2.51	0.42
7:G:434:SER:OG	7:G:436:ARG:NH1	2.53	0.42
8:H:250:ASN:ND2	45:H:402:LMT:O6'	2.42	0.42
4:D:218:PHE:CE2	4:D:222:ILE:HD11	2.54	0.41
4:D:117:ALA:HB2	4:D:367:ILE:HG12	2.02	0.41
7:G:606:ILE:HD13	22:W:121:LEU:HD11	2.01	0.41
12:L:160:GLY:O	59:L:805:HOH:O	2.22	0.41
13:M:269:MET:HE1	13:M:396:MET:SD	2.60	0.41
7:G:638:GLU:O	19:S:24:GLN:NE2	2.42	0.41
8:H:198:PHE:CD1	8:H:285:LEU:HD13	2.55	0.41
11:K:66:PHE:CZ	14:N:31:VAL:HG13	2.56	0.41
23:X:164:THR:HG22	29:d:83:TYR:CE2	2.55	0.41
4:D:175:GLU:OE1	4:D:188:ARG:NH2	2.51	0.41
7:G:610:THR:OG1	59:G:917:HOH:O	2.21	0.41
8:H:204:GLU:HG3	59:H:562:HOH:O	2.21	0.41
23:X:154:GLU:OE1	23:X:154:GLU:N	2.46	0.41
32:g:49:PRO:O	32:g:53:VAL:HG13	2.20	0.41
12:L:40:ILE:HD11	12:L:101:MET:HE3	2.01	0.41
29:d:120:ARG:NH2	41:p:144:ASP:OD2	2.54	0.41
4:D:423:ILE:HG23	4:D:428:ILE:HD12	2.01	0.41
13:M:98:MET:HE2	13:M:98:MET:CA	2.50	0.41
13:M:84:LEU:HD11	13:M:95:TYR:CD2	2.56	0.41
13:M:310:MET:HE3	13:M:310:MET:HB3	1.99	0.41
20:T:69:LYS:O	20:T:71:MET:N	2.54	0.41
20:U:28:GLU:OE2	20:U:28:GLU:HA	2.20	0.41
34:i:62:LYS:O	34:i:63:ALA:HB3	2.20	0.41
37:l:29:ARG:NH2	38:m:34:GLU:OE2	2.49	0.41
37:l:87:ARG:O	59:l:202:HOH:O	2.21	0.41
3:C:193:GLU:OE1	17:Q:80:SER:OG	2.33	0.41
10:J:69:TYR:CD2	10:J:73:MET:HE1	2.56	0.41
14:N:218:ALA:HA	14:N:240:MET:HE3	2.03	0.41
15:O:148:CYS:HA	15:O:279:LEU:HD11	2.02	0.41
6:F:194:GLU:OE2	6:F:204:ARG:NE	2.52	0.40
8:H:18:ALA:O	8:H:21:THR:OG1	2.26	0.40
12:L:265:PRO:O	12:L:268:THR:HG22	2.21	0.40
14:N:9:ILE:CG2	14:N:43:MET:HE2	2.51	0.40
36:k:54:GLU:OE2	39:n:33:ARG:NH2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:11:ASP:OD1	40:o:11:ASP:C	2.65	0.40
12:L:139:GLN:HA	12:L:142:ILE:HD12	2.04	0.40
19:S:43:LEU:HD21	19:S:90:MET:HE3	2.04	0.40
20:T:16:LEU:HD21	20:T:32:VAL:HG22	2.03	0.40
2:B:100:GLY:HA2	47:B:201:SF4:S4	2.61	0.40
12:L:316:THR:HA	12:L:319:MET:HE2	2.04	0.40
32:g:111:PHE:CE1	41:p:73:ILE:HG22	2.56	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%)	201 (98%)	5 (2%)	0	100	100
4	D	427/463 (92%)	413 (97%)	14 (3%)	0	100	100
5	E	212/248 (86%)	205 (97%)	6 (3%)	1 (0%)	24	37
6	F	428/464 (92%)	417 (97%)	11 (3%)	0	100	100
7	G	687/727 (94%)	667 (97%)	20 (3%)	0	100	100
8	H	316/318 (99%)	305 (96%)	9 (3%)	2 (1%)	21	32
9	I	176/212 (83%)	171 (97%)	5 (3%)	0	100	100
10	J	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	605/607 (100%)	583 (96%)	21 (4%)	1 (0%)	43	58
13	M	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
14	N	343/345 (99%)	340 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	318/355 (90%)	313 (98%)	5 (2%)	0	100	100
16	P	340/377 (90%)	332 (98%)	8 (2%)	0	100	100
17	Q	124/175 (71%)	123 (99%)	1 (1%)	0	100	100
18	R	93/116 (80%)	90 (97%)	3 (3%)	0	100	100
19	S	84/99 (85%)	82 (98%)	2 (2%)	0	100	100
20	T	76/156 (49%)	71 (93%)	5 (7%)	0	100	100
20	U	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
21	V	112/116 (97%)	112 (100%)	0	0	100	100
22	W	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
24	Y	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
25	Z	138/144 (96%)	136 (99%)	2 (1%)	0	100	100
26	a	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	118 (100%)	0	0	100	100
30	e	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
31	f	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
32	g	99/151 (66%)	98 (99%)	1 (1%)	0	100	100
33	h	137/189 (72%)	134 (98%)	3 (2%)	0	100	100
34	i	100/127 (79%)	94 (94%)	6 (6%)	0	100	100
35	j	64/105 (61%)	62 (97%)	2 (3%)	0	100	100
36	k	76/104 (73%)	73 (96%)	3 (4%)	0	100	100
37	l	155/186 (83%)	151 (97%)	4 (3%)	0	100	100
38	m	124/129 (96%)	121 (98%)	3 (2%)	0	100	100
39	n	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
40	o	117/136 (86%)	112 (96%)	5 (4%)	0	100	100
41	p	168/176 (96%)	165 (98%)	3 (2%)	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	97/112 (87%)	90 (93%)	7 (7%)	0	100	100
44	s	42/104 (40%)	39 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8150/9210 (88%)	7934 (97%)	212 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	183	LYS
8	H	203	GLY
8	H	244	GLY
12	L	562	ILE

5.3.2 Protein sidechains ⓘ

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%)	103 (100%)	0	100	100
2	B	132/184 (72%)	128 (97%)	4 (3%)	36	58
3	C	190/227 (84%)	188 (99%)	2 (1%)	65	82
4	D	370/394 (94%)	368 (100%)	2 (0%)	81	91
5	E	184/206 (89%)	181 (98%)	3 (2%)	55	76
6	F	345/370 (93%)	342 (99%)	3 (1%)	70	85
7	G	580/610 (95%)	575 (99%)	5 (1%)	70	85
8	H	279/279 (100%)	273 (98%)	6 (2%)	45	67
9	I	152/178 (85%)	150 (99%)	2 (1%)	61	80
10	J	137/137 (100%)	137 (100%)	0	100	100
11	K	87/87 (100%)	85 (98%)	2 (2%)	44	66
12	L	549/549 (100%)	545 (99%)	4 (1%)	76	88
13	M	414/414 (100%)	406 (98%)	8 (2%)	50	71
14	N	307/307 (100%)	305 (99%)	2 (1%)	76	88
15	O	284/309 (92%)	284 (100%)	0	100	100
16	P	299/325 (92%)	296 (99%)	3 (1%)	68	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	80/96 (83%)	80 (100%)	0	100	100
19	S	75/80 (94%)	73 (97%)	2 (3%)	39	62
20	T	72/135 (53%)	69 (96%)	3 (4%)	26	45
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	107 (99%)	1 (1%)	70	85
23	X	153/154 (99%)	152 (99%)	1 (1%)	76	88
24	Y	106/106 (100%)	106 (100%)	0	100	100
25	Z	121/123 (98%)	119 (98%)	2 (2%)	53	74
26	a	59/60 (98%)	59 (100%)	0	100	100
27	b	72/73 (99%)	72 (100%)	0	100	100
28	c	43/67 (64%)	43 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	93/94 (99%)	91 (98%)	2 (2%)	45	67
31	f	52/53 (98%)	52 (100%)	0	100	100
32	g	92/129 (71%)	91 (99%)	1 (1%)	65	82
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	95/118 (80%)	95 (100%)	0	100	100
35	j	61/87 (70%)	60 (98%)	1 (2%)	55	76
36	k	60/78 (77%)	59 (98%)	1 (2%)	53	74
37	l	142/161 (88%)	142 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	163/164 (99%)	162 (99%)	1 (1%)	78	89
40	o	109/120 (91%)	109 (100%)	0	100	100
41	p	155/158 (98%)	154 (99%)	1 (1%)	78	89
42	q	130/130 (100%)	130 (100%)	0	100	100
43	r	90/95 (95%)	90 (100%)	0	100	100
44	s	43/95 (45%)	42 (98%)	1 (2%)	44	66
All	All	7222/7942 (91%)	7159 (99%)	63 (1%)	68	85

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	64	CYS
2	B	101	THR
2	B	128	SER
2	B	171	LEU
3	C	115	THR
3	C	169	THR
4	D	376	VAL
4	D	420	THR
5	E	29	LYS
5	E	48	LEU
5	E	64	SER
6	F	104	THR
6	F	105	CYS
6	F	262	VAL
7	G	18	VAL
7	G	31	GLU
7	G	58	GLU
7	G	329	VAL
7	G	341	ASP
8	H	54	LYS
8	H	76	THR
8	H	176	LEU
8	H	202	GLU
8	H	204	GLU
8	H	296	LEU
9	I	15	ASP
9	I	16	MET
11	K	17	LEU
11	K	82	SER
12	L	91	SER
12	L	249	SER
12	L	512	SER
12	L	576	LEU
13	M	33	LEU
13	M	58	SER
13	M	86	LYS
13	M	90	VAL
13	M	114	GLU
13	M	255	LYS
13	M	305	THR
13	M	459	MET
14	N	100	MET
14	N	199	SER

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Mol	Chain	Res	Type
16	P	109	VAL
16	P	142	SER
16	P	148	SER
19	S	58	SER
19	S	97	LYS
20	T	19	LEU
20	T	44	SER
20	T	57	GLU
22	W	18	SER
23	X	77	CYS
25	Z	29	LEU
25	Z	113	THR
30	e	37	LYS
30	e	72	MET
32	g	85	GLU
35	j	5	VAL
36	k	90	GLU
39	n	175	GLU
41	p	129	GLU
44	s	53	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
3	C	39	GLN
3	C	88	ASN
4	D	54	GLN
4	D	135	GLN
4	D	217	ASN
5	E	91	ASN
6	F	200	GLN
6	F	264	HIS
7	G	100	ASN
7	G	401	HIS
7	G	402	ASN
7	G	535	GLN
8	H	47	GLN
8	H	93	HIS
10	J	3	ASN
12	L	113	ASN
12	L	170	GLN

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Mol	Chain	Res	Type
12	L	296	ASN
12	L	320	ASN
13	M	88	ASN
13	M	139	GLN
13	M	331	ASN
13	M	366	ASN
13	M	374	ASN
13	M	399	ASN
13	M	415	GLN
14	N	2	ASN
14	N	87	GLN
14	N	222	ASN
14	N	228	ASN
14	N	308	ASN
15	O	44	GLN
15	O	140	ASN
15	O	288	GLN
16	P	93	ASN
18	R	50	ASN
19	S	47	HIS
21	V	36	HIS
22	W	110	HIS
23	X	142	HIS
25	Z	89	ASN
27	b	68	HIS
28	c	35	HIS
29	d	117	HIS
30	e	96	HIS
32	g	25	GLN
32	g	84	GLN
33	h	135	HIS
37	l	27	ASN
37	l	103	HIS
37	l	125	GLN
38	m	51	ASN
38	m	125	ASN
39	n	25	HIS
39	n	72	GLN
39	n	77	GLN
40	o	83	GLN
41	p	27	ASN
42	q	54	GLN

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Mol	Chain	Res	Type
42	q	112	ASN
43	r	24	GLN
43	r	35	GLN
43	r	51	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	2MR	D	85	4	10,12,13	2.44	3 (30%)	5,13,15	1.15	0
8	FME	H	1	8	8,9,10	1.01	1 (12%)	8,9,11	1.04	0
34	SAC	i	1	34	7,8,9	0.53	0	7,9,11	0.87	1 (14%)
12	FME	L	1	12	8,9,10	0.97	0	8,9,11	1.11	0
10	FME	J	1	10	8,9,10	0.97	0	8,9,11	0.94	0
14	FME	N	1	14	8,9,10	1.05	1 (12%)	8,9,11	0.83	0
13	FME	M	1	13	8,9,10	0.94	0	8,9,11	1.32	1 (12%)
11	FME	K	1	11	8,9,10	1.02	1 (12%)	8,9,11	1.15	1 (12%)
1	FME	A	1	1	8,9,10	1.00	1 (12%)	8,9,11	0.81	0
42	AME	q	1	42	9,10,11	1.53	1 (11%)	9,11,13	1.77	3 (33%)
43	AYA	r	1	43	6,7,8	1.16	1 (16%)	6,8,10	1.07	0
2	WYK	B	87	2	9,11,12	2.58	3 (33%)	8,13,15	1.63	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
4	2MR	D	85	4	-	0/10/13/15	-
8	FME	H	1	8	-	4/7/9/11	-
34	SAC	i	1	34	-	5/7/8/10	-
12	FME	L	1	12	-	1/7/9/11	-
10	FME	J	1	10	-	4/7/9/11	-
14	FME	N	1	14	-	0/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
11	FME	K	1	11	-	4/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
42	AME	q	1	42	-	3/9/10/12	-
43	AYA	r	1	43	-	1/5/6/8	-
2	WYK	B	87	2	-	0/10/11/13	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	87	WYK	CZ-NE	6.53	1.45	1.33
4	D	85	2MR	CZ-NH2	5.10	1.44	1.33
4	D	85	2MR	CZ-NE	4.78	1.44	1.34
42	q	1	AME	CT1-N	3.59	1.45	1.34
2	B	87	WYK	CZ-NH2	-2.62	1.24	1.34
4	D	85	2MR	CQ1-NH1	-2.38	1.41	1.46
43	r	1	AYA	CA-N	-2.28	1.44	1.46
8	H	1	FME	CA-N	-2.24	1.43	1.46
2	B	87	WYK	CZ-NH1	-2.21	1.24	1.32
14	N	1	FME	CA-N	-2.19	1.43	1.46
11	K	1	FME	CA-N	-2.15	1.43	1.46
1	A	1	FME	CA-N	-2.13	1.43	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1	FME	C-CA-N	3.08	115.45	109.50
2	B	87	WYK	CB-CA-N	2.91	116.84	110.48
2	B	87	WYK	CB-CA-C	2.90	115.46	110.99
42	q	1	AME	CT2-CT1-N	2.62	120.47	116.12
42	q	1	AME	O-C-CA	-2.51	118.31	124.77
34	i	1	SAC	O-C-CA	-2.15	119.25	124.77
11	K	1	FME	C-CA-N	2.09	113.53	109.50
42	q	1	AME	CE-SD-CG	2.06	110.99	100.32

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	1	FME	C-CA-CB-CG
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
13	M	1	FME	CB-CA-N-CN
43	r	1	AYA	O-C-CA-CB
11	K	1	FME	CA-CB-CG-SD
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
10	J	1	FME	CA-CB-CG-SD
42	q	1	AME	CT2-CT1-N-CA
42	q	1	AME	OT-CT1-N-CA
8	H	1	FME	CA-CB-CG-SD
42	q	1	AME	CA-CB-CG-SD
8	H	1	FME	C-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
11	K	1	FME	CB-CG-SD-CE
34	i	1	SAC	C-CA-N-C1A
12	L	1	FME	CB-CA-N-CN
10	J	1	FME	N-CA-CB-CG
8	H	1	FME	CB-CG-SD-CE
34	i	1	SAC	CB-CA-N-C1A
34	i	1	SAC	N-CA-CB-OG
1	A	1	FME	N-CA-CB-CG
8	H	1	FME	CB-CA-N-CN
10	J	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 3 are monoatomic - leaving 57 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	$\# Z > 2$
47	SF4	I	202	9	0,12,12	-	-	-		
45	LMT	H	402	-	36,36,36	1.20	6 (16%)	47,47,47	1.08	5 (10%)
51	CDL	h	201	-	57,57,99	1.31	8 (14%)	61,68,111	1.21	4 (6%)
52	3PE	r	201	-	45,45,50	0.94	4 (8%)	48,50,55	1.10	2 (4%)
52	3PE	Z	201	-	42,42,50	0.97	3 (7%)	45,47,55	1.01	2 (4%)
52	3PE	d	202	-	31,31,50	1.12	4 (12%)	34,36,55	1.10	2 (5%)
57	EHZ	T	201	20	31,36,37	1.62	5 (16%)	36,44,47	1.64	7 (19%)
45	LMT	A	201	-	36,36,36	1.08	5 (13%)	47,47,47	1.30	4 (8%)
47	SF4	I	201	9	0,12,12	-	-	-		
45	LMT	Y	202	-	36,36,36	1.16	6 (16%)	47,47,47	0.94	0
47	SF4	B	201	2	0,12,12	-	-	-		
47	SF4	G	802	7	0,12,12	-	-	-		
58	MYR	o	201	40	13,14,15	0.81	0	12,13,15	0.52	0
46	PC1	B	203	-	42,42,53	1.08	4 (9%)	48,50,61	1.16	3 (6%)
52	3PE	f	101	-	41,41,50	0.97	4 (9%)	44,46,55	1.12	2 (4%)
45	LMT	L	701	-	36,36,36	1.25	6 (16%)	47,47,47	0.98	1 (2%)
52	3PE	N	402	-	33,33,50	0.95	2 (6%)	34,37,55	0.99	1 (2%)
45	LMT	h	203	-	36,36,36	1.14	4 (11%)	47,47,47	0.97	1 (2%)
45	LMT	j	101	-	36,36,36	1.17	6 (16%)	47,47,47	0.92	0
51	CDL	h	202	-	77,77,99	0.92	6 (7%)	82,88,111	1.08	3 (3%)
45	LMT	Y	204	-	36,36,36	1.19	6 (16%)	47,47,47	0.97	1 (2%)
54	DGT	O	502	53	32,33,33	3.22	15 (46%)	48,52,52	1.95	14 (29%)
45	LMT	J	202	-	36,36,36	1.09	5 (13%)	47,47,47	1.17	5 (10%)
46	PC1	A	203	-	33,33,53	1.22	5 (15%)	39,41,61	0.93	2 (5%)
45	LMT	L	704	-	36,36,36	1.12	5 (13%)	47,47,47	1.00	2 (4%)
48	FES	E	301	5	0,4,4	-	-	-		
51	CDL	H	401	-	50,50,99	1.11	6 (12%)	55,61,111	1.06	3 (5%)
52	3PE	X	201	-	36,36,50	1.04	4 (11%)	39,41,55	1.10	2 (5%)
46	PC1	L	707	-	26,26,53	1.30	4 (15%)	32,34,61	0.98	2 (6%)
47	SF4	F	501	6	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	LMT	L	705	-	36,36,36	1.17	5 (13%)	47,47,47	0.98	3 (6%)
51	CDL	L	703	-	67,67,99	1.09	7 (10%)	73,79,111	1.13	5 (6%)
45	LMT	J	201	-	36,36,36	1.17	5 (13%)	47,47,47	0.94	1 (2%)
52	3PE	Y	203	-	37,37,50	1.00	4 (10%)	40,42,55	1.15	2 (5%)
52	3PE	L	706	-	44,44,50	0.90	4 (9%)	47,49,55	1.03	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
52	3PE	i	201	-	29,29,50	1.17	4 (13%)	32,34,55	1.25	3 (9%)
46	PC1	p	302	-	35,35,53	1.16	4 (11%)	41,43,61	1.12	2 (4%)
52	3PE	I	204	-	43,43,50	0.93	4 (9%)	46,48,55	1.05	2 (4%)
46	PC1	B	204	-	51,51,53	0.97	4 (7%)	57,59,61	0.92	2 (3%)
45	LMT	N	401	-	36,36,36	1.16	5 (13%)	47,47,47	1.21	4 (8%)
55	NDP	P	501	-	51,52,52	2.26	8 (15%)	71,80,80	1.48	17 (23%)
52	3PE	O	503	-	29,29,50	1.12	4 (13%)	32,34,55	1.10	2 (6%)
51	CDL	K	101	-	70,70,99	1.07	7 (10%)	76,82,111	1.10	4 (5%)
52	3PE	d	201	-	42,42,50	0.97	3 (7%)	45,47,55	1.10	3 (6%)
45	LMT	N	404	-	36,36,36	1.14	5 (13%)	47,47,47	0.90	0
48	FES	G	803	7	0,4,4	-	-	-	-	-
49	FMN	F	502	-	33,33,33	2.40	6 (18%)	48,50,50	1.69	13 (27%)
52	3PE	I	203	-	35,35,50	1.05	4 (11%)	38,40,55	1.03	2 (5%)
45	LMT	M	502	-	36,36,36	1.30	6 (16%)	47,47,47	1.03	1 (2%)
51	CDL	q	201	-	61,61,99	1.12	6 (9%)	67,73,111	1.14	4 (5%)
45	LMT	Y	201	-	36,36,36	1.15	6 (16%)	47,47,47	1.12	3 (6%)
52	3PE	N	403	-	37,37,50	1.01	4 (10%)	40,42,55	1.10	2 (5%)
57	EHZ	U	201	20	31,36,37	1.54	4 (12%)	36,44,47	1.74	8 (22%)
52	3PE	L	702	-	42,42,50	1.00	4 (9%)	45,47,55	0.94	2 (4%)
52	3PE	M	501	-	40,40,50	0.99	3 (7%)	43,45,55	0.98	2 (4%)
45	LMT	A	202	-	36,36,36	1.19	6 (16%)	47,47,47	0.91	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SF4	I	202	9	-	-	0/6/5/5
45	LMT	H	402	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	CDL	h	201	-	-	27/67/67/110	-
52	3PE	r	201	-	-	21/49/49/54	-
52	3PE	Z	201	-	-	17/46/46/54	-
52	3PE	d	202	-	-	17/35/35/54	-
57	EHZ	T	201	20	-	21/42/44/45	-
45	LMT	A	201	-	-	8/21/61/61	0/2/2/2
47	SF4	I	201	9	-	-	0/6/5/5
45	LMT	Y	202	-	-	7/21/61/61	0/2/2/2
47	SF4	B	201	2	-	-	0/6/5/5
58	MYR	o	201	40	-	6/12/12/13	-
47	SF4	G	802	7	-	-	0/6/5/5
46	PC1	B	203	-	-	20/46/46/57	-
52	3PE	f	101	-	-	13/45/45/54	-
45	LMT	L	701	-	-	12/21/61/61	0/2/2/2
52	3PE	N	402	-	-	11/36/36/54	-
45	LMT	h	203	-	-	8/21/61/61	0/2/2/2
45	LMT	j	101	-	-	9/21/61/61	0/2/2/2
51	CDL	h	202	-	-	42/87/87/110	-
45	LMT	Y	204	-	-	11/21/61/61	0/2/2/2
54	DGT	O	502	53	-	10/22/34/34	0/3/3/3
45	LMT	J	202	-	-	7/21/61/61	0/2/2/2
46	PC1	A	203	-	-	10/37/37/57	-
45	LMT	L	704	-	-	7/21/61/61	0/2/2/2
48	FES	E	301	5	-	-	0/1/1/1
51	CDL	H	401	-	-	31/59/59/110	-
52	3PE	X	201	-	-	21/40/40/54	-
46	PC1	L	707	-	-	15/30/30/57	-
51	CDL	L	703	-	-	26/78/78/110	-
45	LMT	L	705	-	-	7/21/61/61	0/2/2/2
47	SF4	F	501	6	-	-	0/6/5/5
45	LMT	J	201	-	-	5/21/61/61	0/2/2/2
52	3PE	Y	203	-	-	24/41/41/54	-
52	3PE	L	706	-	-	17/48/48/54	-
47	SF4	G	801	7	-	-	0/6/5/5
52	3PE	i	201	-	-	14/33/33/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	p	302	-	-	11/39/39/57	-
52	3PE	I	204	-	-	14/47/47/54	-
46	PC1	B	204	-	-	28/55/55/57	-
45	LMT	N	401	-	-	8/21/61/61	0/2/2/2
55	NDP	P	501	-	-	4/34/77/77	0/5/5/5
52	3PE	O	503	-	-	14/33/33/54	-
51	CDL	K	101	-	-	32/81/81/110	-
52	3PE	d	201	-	-	21/46/46/54	-
45	LMT	N	404	-	-	12/21/61/61	0/2/2/2
48	FES	G	803	7	-	-	0/1/1/1
49	FMN	F	502	-	-	8/18/18/18	0/3/3/3
52	3PE	I	203	-	-	18/39/39/54	-
45	LMT	M	502	-	-	11/21/61/61	0/2/2/2
51	CDL	q	201	-	-	34/72/72/110	-
45	LMT	Y	201	-	-	12/21/61/61	0/2/2/2
52	3PE	N	403	-	-	11/41/41/54	-
57	EHZ	U	201	20	-	15/42/44/45	-
52	3PE	L	702	-	-	22/46/46/54	-
52	3PE	M	501	-	-	24/44/44/54	-
45	LMT	A	202	-	-	8/21/61/61	0/2/2/2

All (245) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	P	501	NDP	P2B-O2B	12.38	1.81	1.59
54	O	502	DGT	O6-C6	8.54	1.39	1.23
49	F	502	FMN	O4-C4	8.39	1.39	1.23
49	F	502	FMN	O2-C2	7.24	1.38	1.24
54	O	502	DGT	C5-N7	6.66	1.52	1.39
55	P	501	NDP	PA-O3	5.55	1.65	1.59
57	T	201	EHZ	C15-N2	5.20	1.45	1.33
51	h	201	CDL	OA6-CA4	-5.03	1.40	1.46
57	U	201	EHZ	C12-N1	4.81	1.44	1.33
57	U	201	EHZ	C15-N2	4.80	1.44	1.33
57	T	201	EHZ	C12-N1	4.71	1.44	1.33
54	O	502	DGT	PA-O3A	4.69	1.64	1.59
54	O	502	DGT	PB-O3B	4.63	1.64	1.59
54	O	502	DGT	C2-N2	4.60	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	O	502	DGT	C2-N1	4.52	1.48	1.37
54	O	502	DGT	PB-O3A	4.49	1.64	1.59
54	O	502	DGT	C8-N9	-4.40	1.27	1.37
54	O	502	DGT	C2-N3	4.16	1.43	1.33
54	O	502	DGT	C4-N9	-4.15	1.27	1.38
55	P	501	NDP	PN-O5D	3.90	1.74	1.59
49	F	502	FMN	C2-N1	3.58	1.44	1.36
55	P	501	NDP	O2B-C2B	-3.53	1.32	1.44
51	h	201	CDL	OA6-CA5	3.22	1.40	1.33
45	M	502	LMT	O3'-C3'	-3.15	1.35	1.43
45	L	701	LMT	O2B-C2B	-3.14	1.35	1.43
45	M	502	LMT	O2'-C2'	-3.09	1.35	1.43
51	q	201	CDL	OB6-CB4	-3.08	1.39	1.46
52	Z	201	3PE	O21-C2	-3.07	1.39	1.46
51	K	101	CDL	OB6-CB4	-2.99	1.39	1.46
45	L	701	LMT	O3'-C3'	-2.97	1.35	1.43
51	h	202	CDL	OA6-CA4	-2.97	1.39	1.46
45	L	701	LMT	O2'-C2'	-2.96	1.35	1.43
52	d	201	3PE	O21-C2	-2.93	1.39	1.46
51	K	101	CDL	OA6-CA4	-2.86	1.39	1.46
45	N	401	LMT	O3'-C3'	-2.86	1.35	1.43
46	B	204	PC1	O21-C2	-2.83	1.39	1.46
52	r	201	3PE	O21-C2	-2.82	1.40	1.46
52	N	403	3PE	O21-C2	-2.79	1.40	1.46
51	H	401	CDL	OA6-CA4	-2.78	1.40	1.46
51	h	202	CDL	OB6-CB4	-2.77	1.40	1.46
45	L	704	LMT	O3'-C3'	-2.75	1.36	1.43
51	L	703	CDL	OA6-CA4	-2.74	1.40	1.46
52	I	204	3PE	O21-C2	-2.74	1.40	1.46
57	T	201	EHZ	O3-C12	-2.74	1.17	1.23
52	I	203	3PE	O21-C2	-2.73	1.40	1.46
52	d	202	3PE	O21-C2	-2.73	1.40	1.46
57	T	201	EHZ	O4-C15	-2.71	1.18	1.23
54	O	502	DGT	C1'-N9	-2.70	1.41	1.48
51	K	101	CDL	OB8-CB6	-2.70	1.39	1.45
45	A	202	LMT	O3'-C3'	-2.70	1.36	1.43
52	i	201	3PE	O21-C2	-2.69	1.40	1.46
51	L	703	CDL	OB6-CB4	-2.69	1.40	1.46
51	L	703	CDL	OA8-CA7	2.69	1.41	1.33
45	J	201	LMT	O3'-C3'	-2.68	1.36	1.43
51	h	201	CDL	OB6-CB4	-2.68	1.40	1.46
45	M	502	LMT	O3B-C3B	-2.66	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	M	501	3PE	O21-C2	-2.66	1.40	1.46
45	H	402	LMT	O3'-C3'	-2.66	1.36	1.43
45	Y	202	LMT	O3'-C3'	-2.66	1.36	1.43
52	O	503	3PE	O21-C2	-2.65	1.40	1.46
52	X	201	3PE	O21-C2	-2.65	1.40	1.46
46	L	707	PC1	O21-C2	-2.64	1.40	1.46
45	j	101	LMT	O3'-C3'	-2.64	1.36	1.43
52	d	202	3PE	O31-C31	2.63	1.41	1.33
46	p	302	PC1	O21-C2	-2.63	1.40	1.46
45	J	201	LMT	O2'-C2'	-2.62	1.36	1.43
51	q	201	CDL	OA6-CA4	-2.61	1.40	1.46
49	F	502	FMN	P-O3P	-2.61	1.45	1.54
45	A	201	LMT	O3'-C3'	-2.60	1.36	1.43
46	B	203	PC1	O31-C3	-2.60	1.39	1.45
57	U	201	EHZ	O4-C15	-2.59	1.18	1.23
52	f	101	3PE	O31-C31	2.59	1.40	1.33
46	p	302	PC1	O31-C31	2.58	1.40	1.33
52	L	702	3PE	O31-C3	-2.58	1.39	1.45
45	N	404	LMT	O3'-C3'	-2.58	1.36	1.43
51	K	101	CDL	OA8-CA7	2.57	1.40	1.33
46	B	203	PC1	O21-C2	-2.57	1.40	1.46
52	f	101	3PE	O21-C2	-2.57	1.40	1.46
45	L	705	LMT	O3'-C3'	-2.57	1.36	1.43
49	F	502	FMN	P-O2P	-2.57	1.45	1.54
46	A	203	PC1	O31-C31	2.54	1.40	1.33
52	L	702	3PE	O21-C2	-2.53	1.40	1.46
52	M	501	3PE	O31-C31	2.53	1.40	1.33
45	J	202	LMT	O3'-C3'	-2.53	1.36	1.43
45	M	502	LMT	O2B-C2B	-2.52	1.36	1.43
52	X	201	3PE	O31-C31	2.52	1.40	1.33
45	Y	204	LMT	O3'-C3'	-2.52	1.36	1.43
52	L	702	3PE	O21-C21	2.51	1.41	1.34
52	L	706	3PE	O21-C2	-2.51	1.40	1.46
51	q	201	CDL	OB8-CB7	2.51	1.40	1.33
52	Y	203	3PE	O21-C2	-2.50	1.40	1.46
52	d	201	3PE	O31-C3	-2.50	1.39	1.45
46	A	203	PC1	O21-C2	-2.49	1.40	1.46
45	Y	201	LMT	O3'-C3'	-2.48	1.36	1.43
51	q	201	CDL	OA8-CA7	2.47	1.40	1.33
52	i	201	3PE	O31-C31	2.46	1.40	1.33
52	Z	201	3PE	O31-C3	-2.45	1.39	1.45
57	T	201	EHZ	C9-S1	2.45	1.82	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	h	201	CDL	OB8-CB6	-2.43	1.39	1.45
54	O	502	DGT	PG-O1G	-2.43	1.45	1.54
45	H	402	LMT	O1'-C1'	-2.42	1.36	1.40
45	L	705	LMT	O2B-C2B	-2.42	1.37	1.43
52	r	201	3PE	O31-C31	2.42	1.40	1.33
52	N	402	3PE	O21-C21	2.42	1.41	1.34
51	H	401	CDL	OB8-CB6	-2.42	1.39	1.45
52	Y	203	3PE	O31-C3	-2.42	1.39	1.45
52	X	201	3PE	O31-C3	-2.41	1.39	1.45
45	L	704	LMT	O2B-C2B	-2.41	1.37	1.43
45	Y	202	LMT	O2'-C2'	-2.39	1.37	1.43
51	H	401	CDL	OB8-CB7	2.39	1.40	1.33
45	M	502	LMT	O1'-C1'	-2.38	1.36	1.40
45	N	404	LMT	O2B-C2B	-2.38	1.37	1.43
45	h	203	LMT	O3'-C3'	-2.38	1.37	1.43
52	N	402	3PE	O21-C2	-2.37	1.41	1.46
52	I	203	3PE	O31-C31	2.37	1.40	1.33
46	L	707	PC1	O31-C31	2.37	1.40	1.33
57	U	201	EHZ	O3-C12	-2.37	1.18	1.23
51	h	202	CDL	OB8-CB6	-2.37	1.39	1.45
45	L	705	LMT	O2'-C2'	-2.36	1.37	1.43
46	B	203	PC1	O21-C21	2.36	1.40	1.34
52	N	403	3PE	O31-C31	2.36	1.40	1.33
45	H	402	LMT	O2B-C2B	-2.35	1.37	1.43
45	J	201	LMT	O1'-C1'	-2.35	1.36	1.40
45	A	201	LMT	O3B-C3B	-2.35	1.37	1.43
52	O	503	3PE	O31-C31	2.35	1.40	1.33
51	q	201	CDL	OB8-CB6	-2.35	1.39	1.45
45	h	203	LMT	O2'-C2'	-2.34	1.37	1.43
45	M	502	LMT	O4'-C4B	-2.34	1.37	1.43
45	j	101	LMT	O2'-C2'	-2.34	1.37	1.43
45	Y	202	LMT	O2B-C2B	-2.34	1.37	1.43
51	H	401	CDL	OA8-CA6	-2.34	1.39	1.45
45	Y	201	LMT	O2B-C2B	-2.33	1.37	1.43
45	j	101	LMT	O3B-C3B	-2.32	1.37	1.43
52	L	706	3PE	O21-C21	2.32	1.40	1.34
49	F	502	FMN	C6-C5A	-2.32	1.36	1.40
45	L	704	LMT	O2'-C2'	-2.32	1.37	1.43
45	N	401	LMT	O2B-C2B	-2.32	1.37	1.43
45	A	202	LMT	O1'-C1'	-2.32	1.36	1.40
45	Y	204	LMT	O2'-C2'	-2.30	1.37	1.43
45	h	203	LMT	O3B-C3B	-2.30	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	Y	203	3PE	O21-C21	2.30	1.40	1.34
54	O	502	DGT	PG-O2G	-2.30	1.46	1.54
45	J	201	LMT	O2B-C2B	-2.30	1.37	1.43
51	L	703	CDL	OB8-CB7	2.29	1.40	1.33
52	O	503	3PE	O31-C3	-2.29	1.40	1.45
51	h	201	CDL	OA8-CA7	2.29	1.40	1.33
52	O	503	3PE	O21-C21	2.28	1.40	1.34
51	L	703	CDL	OB6-CB5	2.28	1.40	1.34
51	q	201	CDL	OA8-CA6	-2.28	1.40	1.45
45	H	402	LMT	O2'-C2'	-2.27	1.37	1.43
55	P	501	NDP	O2D-C2D	-2.27	1.37	1.43
45	L	704	LMT	O3B-C3B	-2.27	1.37	1.43
45	A	202	LMT	O2'-C2'	-2.26	1.37	1.43
45	Y	201	LMT	O2'-C2'	-2.26	1.37	1.43
45	Y	202	LMT	O3B-C3B	-2.26	1.37	1.43
51	L	703	CDL	OA6-CA5	2.25	1.40	1.34
51	h	201	CDL	OB8-CB7	2.25	1.39	1.33
45	Y	204	LMT	O3B-C3B	-2.25	1.37	1.43
51	L	703	CDL	OB8-CB6	-2.25	1.40	1.45
45	h	203	LMT	O2B-C2B	-2.24	1.37	1.43
52	I	204	3PE	O31-C3	-2.22	1.40	1.45
52	r	201	3PE	O21-C21	2.22	1.40	1.34
51	h	201	CDL	OB6-CB5	2.22	1.40	1.34
45	L	705	LMT	O1'-C1'	-2.21	1.36	1.40
55	P	501	NDP	O5D-C5D	-2.21	1.36	1.44
45	A	201	LMT	O2B-C2B	-2.21	1.37	1.43
45	L	705	LMT	O3B-C3B	-2.21	1.37	1.43
45	Y	204	LMT	O2B-C2B	-2.20	1.37	1.43
46	B	204	PC1	O31-C31	2.20	1.39	1.33
52	N	403	3PE	O31-C3	-2.20	1.40	1.45
45	L	701	LMT	O3B-C3B	-2.20	1.37	1.43
45	J	202	LMT	O2'-C2'	-2.20	1.37	1.43
51	H	401	CDL	OA8-CA7	2.18	1.39	1.33
51	h	202	CDL	OB8-CB7	2.18	1.39	1.33
45	Y	201	LMT	O3B-C3B	-2.18	1.37	1.43
52	i	201	3PE	O21-C21	2.17	1.40	1.34
45	N	404	LMT	O3B-C3B	-2.17	1.37	1.43
46	B	204	PC1	O31-C3	-2.17	1.40	1.45
45	Y	202	LMT	O4'-C4B	-2.16	1.37	1.43
45	N	401	LMT	O2'-C2'	-2.16	1.37	1.43
52	I	203	3PE	O31-C3	-2.16	1.40	1.45
46	B	203	PC1	O31-C31	2.16	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Y	202	LMT	O1'-C1'	-2.15	1.36	1.40
52	f	101	3PE	O21-C21	2.15	1.40	1.34
52	f	101	3PE	O31-C3	-2.15	1.40	1.45
45	j	101	LMT	O2B-C2B	-2.15	1.37	1.43
52	M	501	3PE	O21-C21	2.15	1.40	1.34
52	N	403	3PE	O21-C21	2.14	1.40	1.34
45	J	202	LMT	O2B-C2B	-2.14	1.37	1.43
51	H	401	CDL	OA6-CA5	2.14	1.40	1.34
45	J	202	LMT	O3B-C3B	-2.14	1.37	1.43
51	K	101	CDL	OA6-CA5	2.14	1.40	1.34
45	N	401	LMT	O3B-C3B	-2.14	1.37	1.43
45	N	404	LMT	O1'-C1'	-2.14	1.36	1.40
45	Y	204	LMT	O4'-C4B	-2.14	1.37	1.43
52	L	706	3PE	O31-C3	-2.13	1.40	1.45
45	Y	204	LMT	O1'-C1'	-2.13	1.36	1.40
46	L	707	PC1	O21-C21	2.13	1.40	1.34
46	p	302	PC1	O21-C21	2.13	1.40	1.34
45	J	202	LMT	O4'-C4B	-2.13	1.37	1.43
45	H	402	LMT	O3B-C3B	-2.13	1.37	1.43
52	i	201	3PE	O31-C3	-2.12	1.40	1.45
51	h	201	CDL	OA8-CA6	-2.12	1.40	1.45
45	Y	201	LMT	O4'-C4B	-2.12	1.37	1.43
46	L	707	PC1	O31-C3	-2.11	1.40	1.45
52	d	202	3PE	O21-C21	2.11	1.40	1.34
52	I	203	3PE	O21-C21	2.11	1.40	1.34
45	A	201	LMT	O2'-C2'	-2.11	1.37	1.43
52	X	201	3PE	O21-C21	2.11	1.40	1.34
45	A	202	LMT	O4'-C4B	-2.10	1.37	1.43
45	A	202	LMT	O3B-C3B	-2.10	1.37	1.43
54	O	502	DGT	PB-O1B	-2.10	1.45	1.55
52	d	201	3PE	O31-C31	2.10	1.39	1.33
52	r	201	3PE	O31-C3	-2.10	1.40	1.45
51	K	101	CDL	OB8-CB7	2.09	1.39	1.33
45	H	402	LMT	O4'-C4B	-2.09	1.37	1.43
54	O	502	DGT	PA-O1A	-2.09	1.45	1.55
52	Y	203	3PE	O31-C31	2.09	1.39	1.33
45	L	704	LMT	O4'-C4B	-2.08	1.37	1.43
51	h	202	CDL	OB6-CB5	2.08	1.40	1.34
45	j	101	LMT	O1'-C1'	-2.08	1.36	1.40
45	L	701	LMT	O4'-C4B	-2.08	1.37	1.43
45	N	404	LMT	O2'-C2'	-2.08	1.37	1.43
46	A	203	PC1	O31-C3	-2.08	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Y	201	LMT	O1'-C1'	-2.08	1.36	1.40
51	h	202	CDL	OA6-CA5	2.07	1.40	1.34
45	A	202	LMT	O2B-C2B	-2.06	1.37	1.43
52	Z	201	3PE	O31-C31	2.06	1.39	1.33
46	A	203	PC1	O21-C21	2.06	1.40	1.34
52	d	202	3PE	O31-C3	-2.05	1.40	1.45
45	L	701	LMT	O1'-C1'	-2.05	1.36	1.40
45	A	201	LMT	O4'-C4B	-2.04	1.37	1.43
45	N	401	LMT	O5'-C5'	-2.04	1.39	1.44
52	I	204	3PE	O21-C21	2.03	1.40	1.34
52	L	706	3PE	O31-C31	2.03	1.39	1.33
45	j	101	LMT	O4'-C4B	-2.02	1.37	1.43
46	p	302	PC1	O31-C3	-2.02	1.40	1.45
55	P	501	NDP	O3D-C3D	-2.02	1.38	1.43
45	J	201	LMT	O3B-C3B	-2.02	1.38	1.43
46	A	203	PC1	C12-N	-2.02	1.45	1.51
52	I	204	3PE	O31-C31	2.01	1.39	1.33
46	B	204	PC1	O21-C21	2.01	1.40	1.34
51	K	101	CDL	OA8-CA6	-2.01	1.40	1.45
52	L	702	3PE	O31-C31	2.01	1.39	1.33
55	P	501	NDP	O4B-C4B	-2.00	1.40	1.45

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	502	DGT	C8-N9-C4	7.46	120.01	106.03
57	U	201	EHZ	C8-C9-S1	5.70	120.75	113.56
46	B	203	PC1	O21-C21-C22	5.28	122.90	111.48
57	T	201	EHZ	C8-C9-S1	5.19	120.11	113.56
52	i	201	3PE	O21-C21-C22	4.71	121.67	111.48
52	Y	203	3PE	O21-C21-C22	4.44	121.09	111.48
52	r	201	3PE	O21-C21-C22	4.37	120.93	111.48
51	h	202	CDL	OB6-CB5-C51	4.34	120.87	111.48
46	p	302	PC1	O21-C21-C22	4.31	120.81	111.48
45	A	201	LMT	O5B-C5B-C4B	4.26	117.37	109.70
52	d	201	3PE	O21-C21-C22	4.21	120.59	111.48
51	q	201	CDL	OA6-CA5-C11	4.18	120.52	111.48
51	L	703	CDL	OA6-CA5-C11	4.14	120.45	111.48
52	X	201	3PE	O21-C21-C22	4.08	120.31	111.48
52	L	702	3PE	O21-C21-C22	4.08	120.30	111.48
51	K	101	CDL	OA6-CA5-C11	4.04	120.22	111.48
52	f	101	3PE	O21-C21-C22	4.03	120.21	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	h	201	CDL	OB6-CB5-C51	3.98	120.10	111.48
49	F	502	FMN	O5'-P-O1P	3.93	117.05	106.44
51	h	201	CDL	OA6-CA5-OA7	-3.92	120.67	125.70
52	I	204	3PE	O21-C21-C22	3.87	119.85	111.48
52	N	402	3PE	O21-C21-C22	3.85	119.81	111.48
52	Z	201	3PE	O21-C21-C22	3.85	119.81	111.48
52	M	501	3PE	O21-C21-C22	3.82	119.75	111.48
51	L	703	CDL	OB6-CB5-C51	3.81	119.72	111.48
52	d	202	3PE	O21-C21-C22	3.73	119.56	111.48
51	h	202	CDL	OA6-CA5-C11	3.73	119.54	111.48
45	A	201	LMT	C1B-O5B-C5B	3.67	120.88	113.72
52	N	403	3PE	O21-C21-C22	3.65	119.38	111.48
52	O	503	3PE	O21-C21-C22	3.57	119.21	111.48
49	F	502	FMN	C9-C9A-N10	3.57	126.66	121.85
52	I	203	3PE	O21-C21-C22	3.49	119.04	111.48
49	F	502	FMN	C4-N3-C2	-3.48	119.46	125.64
51	L	703	CDL	OA8-CA7-C31	3.47	122.40	111.83
51	q	201	CDL	OB6-CB5-C51	3.44	118.93	111.48
55	P	501	NDP	O2B-P2B-O1X	-3.38	97.29	109.33
45	N	401	LMT	C3'-C4'-C5'	-3.38	103.44	110.93
57	T	201	EHZ	C10-S1-C9	3.36	111.77	101.84
49	F	502	FMN	O2P-P-O5'	3.32	115.33	106.67
49	F	502	FMN	C6-C5A-N5	-3.31	112.94	118.44
51	K	101	CDL	OB6-CB5-C51	3.31	118.63	111.48
54	O	502	DGT	C1'-N9-C8	-3.23	120.66	127.91
51	H	401	CDL	OA6-CA5-C11	3.20	118.41	111.48
55	P	501	NDP	P2B-O2B-C2B	-3.19	114.92	123.43
55	P	501	NDP	O3-PA-O1A	-3.16	101.19	110.70
54	O	502	DGT	C2-N1-C6	-3.13	119.44	125.11
46	B	204	PC1	O31-C31-C32	3.11	121.32	111.83
52	I	204	3PE	O31-C31-C32	3.09	121.25	111.83
46	p	302	PC1	O31-C31-C32	3.05	121.14	111.83
54	O	502	DGT	O2G-PG-O3B	3.00	114.69	104.64
54	O	502	DGT	C2'-C3'-C4'	2.97	108.83	102.80
57	T	201	EHZ	O2-C9-S1	-2.96	118.92	122.68
51	K	101	CDL	OA8-CA7-C31	2.94	120.81	111.83
55	P	501	NDP	C2B-C1B-N9A	-2.93	108.94	113.75
45	L	701	LMT	C3'-C4'-C5'	-2.92	104.45	110.93
51	q	201	CDL	OB8-CB7-C71	2.92	120.73	111.83
51	h	201	CDL	OA8-CA7-C31	2.91	120.69	111.83
55	P	501	NDP	O2N-PN-O3	2.89	115.08	107.27
52	f	101	3PE	O31-C31-C32	2.87	120.58	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	L	707	PC1	O31-C31-C32	2.86	120.56	111.83
52	d	201	3PE	O31-C31-C32	2.86	120.55	111.83
52	L	706	3PE	O21-C21-C22	2.83	117.61	111.48
51	H	401	CDL	OB8-CB7-C71	2.82	120.43	111.83
52	I	203	3PE	O31-C31-C32	2.81	120.40	111.83
46	A	203	PC1	O21-C21-C22	2.80	121.23	110.93
57	T	201	EHZ	C5-C6-C7	-2.80	106.97	114.68
46	B	204	PC1	O21-C21-C22	2.79	117.52	111.48
51	H	401	CDL	OA8-CA7-C31	2.79	120.33	111.83
52	N	403	3PE	O31-C31-C32	2.79	120.33	111.83
45	N	401	LMT	O5B-C5B-C4B	2.78	114.71	109.70
57	U	201	EHZ	C7-C8-C9	-2.78	107.65	113.86
52	Y	203	3PE	O31-C31-C32	2.78	120.31	111.83
52	d	202	3PE	O31-C31-C32	2.77	120.27	111.83
52	X	201	3PE	O31-C31-C32	2.73	120.17	111.83
57	T	201	EHZ	C19-C17-C16	2.73	113.42	108.77
57	U	201	EHZ	C14-C13-C12	-2.73	107.85	112.39
52	i	201	3PE	O31-C31-C32	2.71	120.09	111.83
52	M	501	3PE	O31-C31-C32	2.69	120.05	111.83
51	h	202	CDL	OB8-CB7-C71	2.67	119.97	111.83
49	F	502	FMN	C9A-C5A-N5	2.67	125.28	122.45
52	r	201	3PE	O31-C31-C32	2.66	119.94	111.83
46	B	203	PC1	O31-C31-C32	2.66	119.93	111.83
57	T	201	EHZ	C7-C8-C9	-2.65	107.95	113.86
52	O	503	3PE	O31-C31-C32	2.65	119.90	111.83
45	J	202	LMT	C3'-C4'-C5'	-2.64	105.08	110.93
45	J	202	LMT	C1-O1'-C1'	2.63	118.17	113.68
51	h	201	CDL	OB8-CB7-C71	2.62	119.83	111.83
55	P	501	NDP	N3A-C4A-N9A	2.61	131.60	127.17
49	F	502	FMN	O4-C4-C4A	-2.60	119.67	126.53
57	U	201	EHZ	O2-C9-C8	-2.60	119.65	123.74
49	F	502	FMN	C4A-C4-N3	2.59	119.85	113.25
45	H	402	LMT	C3B-C4B-C5B	-2.59	105.54	110.23
57	T	201	EHZ	C13-C12-N1	2.59	121.06	116.34
52	L	706	3PE	O31-C31-C32	2.58	119.69	111.83
54	O	502	DGT	O1G-PG-O3B	2.54	113.16	104.64
55	P	501	NDP	PA-O5B-C5B	-2.53	106.84	121.35
54	O	502	DGT	O1A-PA-O2A	-2.53	100.68	112.44
46	L	707	PC1	O21-C21-C22	2.52	120.18	110.93
45	Y	201	LMT	O5'-C5'-C6'	2.52	112.68	106.44
54	O	502	DGT	C5-C6-N1	2.49	119.58	113.25
54	O	502	DGT	O1B-PB-O2B	-2.48	100.92	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	P	501	NDP	O3X-P2B-O2X	2.44	116.94	107.80
55	P	501	NDP	O7N-C7N-C3N	2.43	125.48	120.90
57	U	201	EHZ	O2-C9-S1	-2.43	119.59	122.68
55	P	501	NDP	O7N-C7N-N7N	-2.42	117.46	122.89
46	A	203	PC1	O31-C31-C32	2.42	119.20	111.83
55	P	501	NDP	PN-O5D-C5D	-2.40	107.58	121.35
45	A	202	LMT	C3B-C4B-C5B	-2.40	105.88	110.23
54	O	502	DGT	O6-C6-C5	-2.39	120.22	126.53
51	K	101	CDL	OB8-CB7-C71	2.39	119.11	111.83
55	P	501	NDP	C2A-N1A-C6A	-2.38	114.83	118.73
45	Y	204	LMT	C1'-O5'-C5'	-2.37	109.08	113.72
51	L	703	CDL	OB8-CB7-C71	2.35	119.00	111.83
57	U	201	EHZ	C19-C17-C16	2.35	112.78	108.77
49	F	502	FMN	O4'-C4'-C5'	-2.35	104.81	109.99
57	U	201	EHZ	C13-C12-N1	2.34	120.61	116.34
55	P	501	NDP	C5A-C4A-N3A	-2.33	123.51	126.72
45	H	402	LMT	O5B-C1B-C2B	2.32	115.13	110.37
45	Y	201	LMT	C2'-C3'-C4'	2.31	114.93	109.68
45	N	401	LMT	O5'-C1'-O1'	-2.31	104.58	110.04
52	Z	201	3PE	O31-C31-C32	2.31	118.88	111.83
55	P	501	NDP	O4B-C4B-C3B	2.30	109.72	105.15
45	H	402	LMT	C1B-C2B-C3B	2.30	114.85	110.01
45	M	502	LMT	C3B-C4B-C5B	-2.29	106.08	110.23
54	O	502	DGT	C1'-N9-C4	-2.29	119.33	125.50
45	H	402	LMT	C3'-C4'-C5'	-2.27	105.89	110.93
45	L	705	LMT	O1'-C1'-C2'	2.26	111.71	108.27
54	O	502	DGT	C6-C5-N7	2.25	134.39	130.29
45	J	202	LMT	O5B-C5B-C4B	2.25	113.75	109.70
45	J	201	LMT	C3B-C4B-C5B	-2.24	106.17	110.23
45	J	202	LMT	O1'-C1'-C2'	2.23	111.66	108.27
51	q	201	CDL	OA8-CA7-C31	2.21	118.58	111.83
45	J	202	LMT	C1'-O5'-C5'	-2.18	109.46	113.72
45	A	201	LMT	C1'-O5'-C5'	-2.17	109.48	113.72
49	F	502	FMN	C4A-C10-N10	2.16	119.57	116.48
55	P	501	NDP	O5D-PN-O1N	-2.15	100.40	108.94
54	O	502	DGT	N9-C8-N7	-2.13	109.44	113.40
55	P	501	NDP	O2N-PN-O1N	2.13	122.36	112.44
49	F	502	FMN	O3P-P-O5'	2.12	112.20	106.67
45	Y	201	LMT	O5'-C1'-O1'	-2.11	105.05	110.04
45	N	401	LMT	O1B-C4'-C3'	2.11	112.59	107.23
52	i	201	3PE	C2-O21-C21	-2.07	112.84	117.80
45	h	203	LMT	C1'-O5'-C5'	-2.07	109.68	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	L	705	LMT	C3B-C4B-C5B	-2.06	106.49	110.23
55	P	501	NDP	C5B-C4B-C3B	-2.06	107.80	115.21
46	B	203	PC1	O21-C21-O22	-2.05	118.91	123.70
49	F	502	FMN	O3P-P-O1P	-2.04	102.89	110.83
57	U	201	EHZ	C11-N1-C12	-2.03	119.03	122.82
45	H	402	LMT	O5B-C5B-C6B	2.02	111.45	106.44
45	L	704	LMT	O5B-C5B-C4B	2.02	113.34	109.70
54	O	502	DGT	C5-C4-N9	-2.01	102.05	105.66
52	L	702	3PE	O31-C31-C32	2.01	117.96	111.83
51	L	703	CDL	OA8-CA6-CA4	2.01	114.19	108.40
45	L	705	LMT	O5'-C5'-C4'	2.01	113.87	109.72
49	F	502	FMN	O2-C2-N1	-2.00	118.47	121.80
52	d	201	3PE	O21-C21-O22	-2.00	119.02	123.70
45	A	201	LMT	C1B-O1B-C4'	2.00	122.72	117.98
45	L	704	LMT	O1'-C1'-C2'	2.00	111.31	108.27

There are no chirality outliers.

All (761) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	L	701	LMT	O5'-C1'-O1'-C1
45	Y	204	LMT	C2-C1-O1'-C1'
46	A	203	PC1	C11-O13-P-O14
46	A	203	PC1	C11-O13-P-O11
46	A	203	PC1	C1-O11-P-O13
46	A	203	PC1	O13-C11-C12-N
46	A	203	PC1	O22-C21-O21-C2
46	B	203	PC1	C1-O11-P-O12
46	B	203	PC1	C1-O11-P-O14
46	B	203	PC1	C1-O11-P-O13
46	B	203	PC1	O22-C21-O21-C2
46	B	204	PC1	C11-O13-P-O12
46	B	204	PC1	C11-O13-P-O14
46	B	204	PC1	C11-O13-P-O11
46	B	204	PC1	C1-O11-P-O12
46	B	204	PC1	C1-O11-P-O13
46	B	204	PC1	O13-C11-C12-N
46	L	707	PC1	C11-O13-P-O11
46	L	707	PC1	C1-O11-P-O12
46	L	707	PC1	C22-C21-O21-C2
46	p	302	PC1	C11-O13-P-O14
46	p	302	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
46	p	302	PC1	C22-C21-O21-C2
49	F	502	FMN	C3'-C4'-C5'-O5'
51	H	401	CDL	CA2-OA2-PA1-OA3
51	H	401	CDL	CA2-OA2-PA1-OA5
51	H	401	CDL	CB3-OB5-PB2-OB2
51	H	401	CDL	CB3-OB5-PB2-OB4
51	K	101	CDL	CA3-OA5-PA1-OA2
51	K	101	CDL	C11-CA5-OA6-CA4
51	K	101	CDL	CB3-OB5-PB2-OB3
51	L	703	CDL	OA7-CA5-OA6-CA4
51	h	201	CDL	CA2-OA2-PA1-OA5
51	h	201	CDL	OA7-CA5-OA6-CA4
51	h	201	CDL	CB2-OB2-PB2-OB4
51	h	202	CDL	CA2-OA2-PA1-OA3
51	h	202	CDL	CA2-OA2-PA1-OA5
51	h	202	CDL	CA3-CA4-CA6-OA8
51	h	202	CDL	OA6-CA4-CA6-OA8
51	q	201	CDL	CA2-OA2-PA1-OA5
51	q	201	CDL	CA3-OA5-PA1-OA4
51	q	201	CDL	CA4-CA3-OA5-PA1
51	q	201	CDL	C51-CB5-OB6-CB4
52	I	203	3PE	C1-O11-P-O12
52	I	203	3PE	C1-O11-P-O13
52	L	702	3PE	O13-C11-C12-N
52	L	702	3PE	C22-C21-O21-C2
52	L	706	3PE	C1-O11-P-O14
52	N	402	3PE	C11-O13-P-O11
52	N	402	3PE	O13-C11-C12-N
52	N	403	3PE	C1-O11-P-O14
52	O	503	3PE	C1-O11-P-O14
52	O	503	3PE	C11-O13-P-O11
52	O	503	3PE	C11-O13-P-O14
52	O	503	3PE	O21-C2-C3-O31
52	X	201	3PE	C1-O11-P-O13
52	X	201	3PE	C1-O11-P-O14
52	X	201	3PE	O13-C11-C12-N
52	X	201	3PE	O22-C21-O21-C2
52	X	201	3PE	C22-C21-O21-C2
52	Y	203	3PE	C1-O11-P-O12
52	Y	203	3PE	C1-O11-P-O13
52	Y	203	3PE	C11-O13-P-O11
52	Y	203	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
52	Y	203	3PE	C22-C21-O21-C2
52	d	201	3PE	C1-O11-P-O13
52	d	201	3PE	C1-O11-P-O14
52	d	201	3PE	C22-C21-O21-C2
52	d	202	3PE	C1-O11-P-O14
52	d	202	3PE	O13-C11-C12-N
52	f	101	3PE	C22-C21-O21-C2
52	i	201	3PE	C11-O13-P-O12
52	i	201	3PE	O13-C11-C12-N
52	i	201	3PE	O22-C21-O21-C2
52	i	201	3PE	C22-C21-O21-C2
52	r	201	3PE	C1-O11-P-O12
52	r	201	3PE	C1-O11-P-O13
52	r	201	3PE	C11-O13-P-O11
52	r	201	3PE	C11-O13-P-O14
52	r	201	3PE	C12-C11-O13-P
52	r	201	3PE	O13-C11-C12-N
52	r	201	3PE	C22-C21-O21-C2
54	O	502	DGT	PB-O3B-PG-O2G
57	T	201	EHZ	C7-C8-C9-S1
57	T	201	EHZ	S1-C10-C11-N1
57	T	201	EHZ	C15-C16-C17-C18
57	T	201	EHZ	C15-C16-C17-C19
57	T	201	EHZ	C15-C16-C17-C20
57	T	201	EHZ	O5-C16-C17-C18
57	T	201	EHZ	O5-C16-C17-C19
57	T	201	EHZ	O5-C16-C17-C20
57	T	201	EHZ	O2-C9-S1-C10
57	T	201	EHZ	C8-C9-S1-C10
57	U	201	EHZ	O1-C7-C8-C9
57	U	201	EHZ	C15-C16-C17-C18
57	U	201	EHZ	C15-C16-C17-C19
57	U	201	EHZ	C15-C16-C17-C20
57	U	201	EHZ	O5-C16-C17-C18
57	U	201	EHZ	O2-C9-S1-C10
57	U	201	EHZ	C8-C9-S1-C10
58	o	201	MYR	C1-C2-C3-C4
45	J	202	LMT	C3'-C4'-O1B-C1B
45	A	201	LMT	O5B-C1B-O1B-C4'
45	Y	201	LMT	O5B-C1B-O1B-C4'
46	p	302	PC1	O32-C31-O31-C3
51	H	401	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
52	L	706	3PE	O32-C31-O31-C3
46	p	302	PC1	C32-C31-O31-C3
52	d	202	3PE	C32-C31-O31-C3
46	B	203	PC1	O32-C31-O31-C3
51	L	703	CDL	OA9-CA7-OA8-CA6
51	h	202	CDL	OB9-CB7-OB8-CB6
52	Y	203	3PE	O32-C31-O31-C3
52	d	201	3PE	O32-C31-O31-C3
52	d	202	3PE	O32-C31-O31-C3
52	i	201	3PE	O32-C31-O31-C3
45	N	401	LMT	C3'-C4'-O1B-C1B
46	L	707	PC1	O22-C21-O21-C2
46	p	302	PC1	O22-C21-O21-C2
51	K	101	CDL	OA7-CA5-OA6-CA4
51	q	201	CDL	OB7-CB5-OB6-CB4
52	L	702	3PE	O22-C21-O21-C2
52	Y	203	3PE	O22-C21-O21-C2
52	d	201	3PE	O22-C21-O21-C2
52	f	101	3PE	O22-C21-O21-C2
52	r	201	3PE	O22-C21-O21-C2
51	H	401	CDL	C71-CB7-OB8-CB6
51	L	703	CDL	C31-CA7-OA8-CA6
51	h	202	CDL	C71-CB7-OB8-CB6
52	L	706	3PE	C32-C31-O31-C3
52	Y	203	3PE	C32-C31-O31-C3
52	d	201	3PE	C32-C31-O31-C3
52	i	201	3PE	C32-C31-O31-C3
45	A	201	LMT	O5'-C5'-C6'-O6'
46	A	203	PC1	C22-C21-O21-C2
46	B	203	PC1	C22-C21-O21-C2
51	L	703	CDL	C11-CA5-OA6-CA4
46	B	203	PC1	C32-C31-O31-C3
51	K	101	CDL	OA9-CA7-OA8-CA6
52	O	503	3PE	O32-C31-O31-C3
45	Y	202	LMT	O5B-C1B-O1B-C4'
45	j	101	LMT	O5'-C5'-C6'-O6'
51	H	401	CDL	O1-C1-CA2-OA2
51	L	703	CDL	O1-C1-CA2-OA2
51	q	201	CDL	O1-C1-CB2-OB2
51	K	101	CDL	C31-CA7-OA8-CA6
45	N	401	LMT	O5'-C5'-C6'-O6'
45	h	203	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
45	J	202	LMT	O5B-C1B-O1B-C4'
51	H	401	CDL	OB6-CB4-CB6-OB8
45	A	201	LMT	C4'-C5'-C6'-O6'
57	T	201	EHZ	C13-C14-N2-C15
52	O	503	3PE	C32-C31-O31-C3
46	L	707	PC1	C2-C1-O11-P
45	Y	201	LMT	O5'-C5'-C6'-O6'
45	Y	204	LMT	O5'-C5'-C6'-O6'
45	j	101	LMT	C4B-C5B-C6B-O6B
45	H	402	LMT	O5'-C1'-O1'-C1
45	j	101	LMT	O5'-C1'-O1'-C1
45	j	101	LMT	C4'-C5'-C6'-O6'
52	X	201	3PE	C32-C31-O31-C3
45	L	705	LMT	O5'-C5'-C6'-O6'
45	N	404	LMT	O5'-C5'-C6'-O6'
52	X	201	3PE	O32-C31-O31-C3
51	h	202	CDL	C11-CA5-OA6-CA4
45	M	502	LMT	O5B-C1B-O1B-C4'
45	N	401	LMT	C4'-C5'-C6'-O6'
51	H	401	CDL	CB2-C1-CA2-OA2
51	H	401	CDL	C31-CA7-OA8-CA6
51	h	201	CDL	C71-CB7-OB8-CB6
52	I	203	3PE	C32-C31-O31-C3
52	I	204	3PE	C32-C31-O31-C3
52	f	101	3PE	C32-C31-O31-C3
52	r	201	3PE	C32-C31-O31-C3
45	Y	201	LMT	C4'-C5'-C6'-O6'
51	h	201	CDL	OB9-CB7-OB8-CB6
45	N	404	LMT	C4'-C5'-C6'-O6'
51	L	703	CDL	CA4-CA6-OA8-CA7
45	H	402	LMT	C2'-C1'-O1'-C1
45	L	701	LMT	C2'-C1'-O1'-C1
45	j	101	LMT	C2'-C1'-O1'-C1
51	h	202	CDL	O1-C1-CB2-OB2
45	Y	201	LMT	C4B-C5B-C6B-O6B
45	h	203	LMT	C4'-C5'-C6'-O6'
52	I	204	3PE	O32-C31-O31-C3
52	f	101	3PE	O32-C31-O31-C3
52	r	201	3PE	O32-C31-O31-C3
45	j	101	LMT	O5B-C5B-C6B-O6B
45	Y	204	LMT	O5B-C1B-O1B-C4'
45	Y	204	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
52	M	501	3PE	C31-C32-C33-C34
51	h	201	CDL	C31-CA7-OA8-CA6
52	Y	203	3PE	C21-C22-C23-C24
49	F	502	FMN	O3'-C3'-C4'-C5'
45	M	502	LMT	O1'-C1-C2-C3
49	F	502	FMN	C2'-C3'-C4'-C5'
46	B	203	PC1	C21-C22-C23-C24
52	I	203	3PE	O32-C31-O31-C3
51	K	101	CDL	C51-CB5-OB6-CB4
45	L	701	LMT	O5'-C5'-C6'-O6'
52	I	203	3PE	C31-C32-C33-C34
52	d	202	3PE	C21-C22-C23-C24
51	H	401	CDL	OA9-CA7-OA8-CA6
45	A	202	LMT	O5'-C1'-O1'-C1
45	L	701	LMT	O5B-C1B-O1B-C4'
51	H	401	CDL	OB5-CB3-CB4-OB6
46	L	707	PC1	C32-C31-O31-C3
51	h	202	CDL	OA7-CA5-OA6-CA4
45	L	705	LMT	C4'-C5'-C6'-O6'
45	N	404	LMT	O1'-C1-C2-C3
45	Y	202	LMT	O1'-C1-C2-C3
45	M	502	LMT	C5'-C4'-O1B-C1B
52	Z	201	3PE	C32-C31-O31-C3
52	d	202	3PE	C31-C32-C33-C34
51	K	101	CDL	OB7-CB5-OB6-CB4
51	H	401	CDL	OB5-CB3-CB4-CB6
51	L	703	CDL	CB2-C1-CA2-OA2
51	h	202	CDL	CA2-C1-CB2-OB2
51	q	201	CDL	CA2-C1-CB2-OB2
51	q	201	CDL	C71-CB7-OB8-CB6
45	Y	201	LMT	C5'-C4'-O1B-C1B
45	L	701	LMT	C2B-C1B-O1B-C4'
51	h	201	CDL	OA9-CA7-OA8-CA6
51	q	201	CDL	C11-CA5-OA6-CA4
45	L	701	LMT	C4B-C5B-C6B-O6B
51	q	201	CDL	OA7-CA5-OA6-CA4
45	A	202	LMT	C2'-C1'-O1'-C1
51	H	401	CDL	CB4-CB3-OB5-PB2
52	Z	201	3PE	O32-C31-O31-C3
46	L	707	PC1	O32-C31-O31-C3
51	h	201	CDL	C51-CB5-OB6-CB4
45	Y	202	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
52	L	702	3PE	C33-C34-C35-C36
57	U	201	EHZ	C1-C21-C22-C23
45	H	402	LMT	O5'-C5'-C6'-O6'
46	p	302	PC1	C34-C35-C36-C37
52	M	501	3PE	C26-C27-C28-C29
51	K	101	CDL	C71-CB7-OB8-CB6
52	N	403	3PE	C32-C31-O31-C3
45	H	402	LMT	C6-C7-C8-C9
52	I	203	3PE	C28-C29-C2A-C2B
51	h	201	CDL	OB7-CB5-OB6-CB4
52	M	501	3PE	C2A-C2B-C2C-C2D
46	B	204	PC1	C33-C34-C35-C36
46	B	204	PC1	C22-C21-O21-C2
52	M	501	3PE	C22-C21-O21-C2
51	L	703	CDL	C51-C52-C53-C54
52	I	204	3PE	C31-C32-C33-C34
52	L	702	3PE	C2E-C2F-C2G-C2H
52	L	706	3PE	C24-C25-C26-C27
52	Z	201	3PE	C23-C24-C25-C26
45	N	401	LMT	C3-C4-C5-C6
52	L	702	3PE	C2C-C2D-C2E-C2F
46	L	707	PC1	C31-C32-C33-C34
45	Y	201	LMT	O5B-C5B-C6B-O6B
45	J	202	LMT	C1-C2-C3-C4
51	q	201	CDL	OB9-CB7-OB8-CB6
45	Y	204	LMT	C5-C6-C7-C8
52	I	203	3PE	C32-C33-C34-C35
45	Y	201	LMT	C7-C8-C9-C10
46	B	204	PC1	C37-C38-C39-C3A
52	L	702	3PE	C27-C28-C29-C2A
52	L	706	3PE	C3C-C3D-C3E-C3F
52	d	201	3PE	C23-C24-C25-C26
52	L	702	3PE	C21-C22-C23-C24
52	N	402	3PE	C2A-C2B-C2C-C2D
52	d	201	3PE	C34-C35-C36-C37
58	o	201	MYR	C9-C10-C11-C12
45	L	704	LMT	O1'-C1-C2-C3
45	J	201	LMT	C11-C10-C9-C8
52	N	403	3PE	C36-C37-C38-C39
52	Z	201	3PE	C22-C23-C24-C25
51	H	401	CDL	C13-C14-C15-C16
51	q	201	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
46	A	203	PC1	C36-C37-C38-C39
51	K	101	CDL	C54-C55-C56-C57
51	q	201	CDL	C14-C15-C16-C17
52	Z	201	3PE	C33-C34-C35-C36
52	N	403	3PE	O32-C31-O31-C3
52	M	501	3PE	C24-C25-C26-C27
52	i	201	3PE	C22-C23-C24-C25
57	T	201	EHZ	C1-C21-C22-C23
51	K	101	CDL	C52-C53-C54-C55
51	h	202	CDL	CA5-C11-C12-C13
52	L	702	3PE	C32-C33-C34-C35
45	N	404	LMT	O5B-C5B-C6B-O6B
45	L	705	LMT	C2'-C1'-O1'-C1
51	K	101	CDL	C56-C57-C58-C59
52	L	702	3PE	C2B-C2C-C2D-C2E
45	H	402	LMT	C4-C5-C6-C7
52	L	702	3PE	C29-C2A-C2B-C2C
52	Y	203	3PE	C34-C35-C36-C37
45	N	401	LMT	O5B-C5B-C6B-O6B
51	h	202	CDL	C51-CB5-OB6-CB4
52	N	403	3PE	C22-C21-O21-C2
52	d	202	3PE	C22-C21-O21-C2
52	X	201	3PE	C21-C22-C23-C24
45	L	701	LMT	C3-C4-C5-C6
52	X	201	3PE	C22-C23-C24-C25
46	B	204	PC1	O22-C21-O21-C2
52	M	501	3PE	O22-C21-O21-C2
52	d	202	3PE	O22-C21-O21-C2
45	A	202	LMT	C11-C10-C9-C8
46	B	204	PC1	C26-C27-C28-C29
46	B	204	PC1	C29-C2A-C2B-C2C
51	K	101	CDL	OB9-CB7-OB8-CB6
45	A	202	LMT	C4-C5-C6-C7
45	Y	201	LMT	C3'-C4'-O1B-C1B
45	Y	201	LMT	C4-C5-C6-C7
52	M	501	3PE	C22-C23-C24-C25
45	h	203	LMT	O5B-C5B-C6B-O6B
52	M	501	3PE	C28-C29-C2A-C2B
58	o	201	MYR	C7-C8-C9-C10
51	h	201	CDL	C52-C53-C54-C55
52	N	403	3PE	C34-C35-C36-C37
45	Y	201	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
52	L	702	3PE	C35-C36-C37-C38
45	J	202	LMT	C4'-C5'-C6'-O6'
51	h	201	CDL	C78-C79-C80-C81
45	A	202	LMT	O5'-C5'-C6'-O6'
52	N	403	3PE	O22-C21-O21-C2
52	I	203	3PE	C29-C2A-C2B-C2C
51	K	101	CDL	C72-C73-C74-C75
51	L	703	CDL	C14-C15-C16-C17
46	L	707	PC1	C32-C33-C34-C35
52	f	101	3PE	C29-C2A-C2B-C2C
45	J	201	LMT	O5B-C5B-C6B-O6B
52	d	202	3PE	C33-C34-C35-C36
52	X	201	3PE	C36-C37-C38-C39
45	L	704	LMT	C4-C5-C6-C7
51	h	201	CDL	C31-C32-C33-C34
52	I	204	3PE	C28-C29-C2A-C2B
45	M	502	LMT	C3'-C4'-O1B-C1B
51	h	202	CDL	C72-C73-C74-C75
52	L	706	3PE	C28-C29-C2A-C2B
46	B	204	PC1	C24-C25-C26-C27
51	h	202	CDL	C79-C80-C81-C82
45	N	404	LMT	C1-C2-C3-C4
52	O	503	3PE	C24-C25-C26-C27
52	I	203	3PE	C26-C27-C28-C29
52	X	201	3PE	C3C-C3D-C3E-C3F
52	i	201	3PE	C32-C33-C34-C35
49	F	502	FMN	C2'-C3'-C4'-O4'
46	B	204	PC1	C3A-C3B-C3C-C3D
45	Y	204	LMT	C4'-C5'-C6'-O6'
58	o	201	MYR	C2-C3-C4-C5
51	K	101	CDL	CB7-C71-C72-C73
52	O	503	3PE	C1-C2-C3-O31
52	Z	201	3PE	C1-C2-C3-O31
57	T	201	EHZ	C21-C22-C23-C24
52	d	201	3PE	C28-C29-C2A-C2B
51	q	201	CDL	C19-C20-C21-C22
46	B	203	PC1	C26-C27-C28-C29
52	d	201	3PE	C37-C38-C39-C3A
51	q	201	CDL	C72-C73-C74-C75
52	Y	203	3PE	C31-C32-C33-C34
45	A	201	LMT	O5B-C5B-C6B-O6B
52	L	706	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
45	M	502	LMT	C6-C7-C8-C9
46	B	203	PC1	C2B-C2C-C2D-C2E
45	Y	202	LMT	C3-C4-C5-C6
51	h	201	CDL	OB5-CB3-CB4-OB6
52	I	203	3PE	O11-C1-C2-O21
51	L	703	CDL	C71-CB7-OB8-CB6
45	M	502	LMT	C1-C2-C3-C4
45	N	404	LMT	C5-C6-C7-C8
52	I	204	3PE	C37-C38-C39-C3A
52	N	402	3PE	C26-C27-C28-C29
51	q	201	CDL	C74-C75-C76-C77
52	I	204	3PE	C22-C23-C24-C25
51	H	401	CDL	OA6-CA4-CA6-OA8
51	h	202	CDL	C81-C82-C83-C84
52	r	201	3PE	C3E-C3F-C3G-C3H
52	Z	201	3PE	O21-C21-C22-C23
51	L	703	CDL	C17-C18-C19-C20
57	T	201	EHZ	C1-C2-C3-C4
52	M	501	3PE	C35-C36-C37-C38
45	J	202	LMT	C3-C4-C5-C6
51	h	202	CDL	C59-C60-C61-C62
52	M	501	3PE	C2B-C2C-C2D-C2E
51	h	201	CDL	C34-C35-C36-C37
57	U	201	EHZ	O5-C16-C17-C19
52	N	402	3PE	C2F-C2G-C2H-C2I
54	O	502	DGT	PB-O3A-PA-O2A
55	P	501	NDP	PN-O3-PA-O1A
46	B	204	PC1	C32-C31-O31-C3
45	Y	201	LMT	C1-C2-C3-C4
52	L	702	3PE	C37-C38-C39-C3A
45	L	704	LMT	C7-C8-C9-C10
45	Y	202	LMT	C7-C8-C9-C10
57	U	201	EHZ	C3-C4-C5-C6
51	h	202	CDL	OB7-CB5-OB6-CB4
45	Y	201	LMT	C2-C1-O1'-C1'
49	F	502	FMN	C4'-C5'-O5'-P
51	h	202	CDL	C1-CA2-OA2-PA1
46	L	707	PC1	C33-C34-C35-C36
49	F	502	FMN	O4'-C4'-C5'-O5'
45	J	202	LMT	C2'-C1'-O1'-C1
46	B	203	PC1	C36-C37-C38-C39
51	q	201	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
57	U	201	EHZ	C22-C23-C24-C25
52	d	202	3PE	O11-C1-C2-C3
51	H	401	CDL	C19-C20-C21-C22
52	L	706	3PE	C3A-C3B-C3C-C3D
52	r	201	3PE	C28-C29-C2A-C2B
52	f	101	3PE	C34-C35-C36-C37
51	h	201	CDL	C72-C73-C74-C75
52	L	706	3PE	C36-C37-C38-C39
46	B	204	PC1	C1-C2-C3-O31
52	I	204	3PE	C1-C2-C3-O31
52	i	201	3PE	C1-C2-C3-O31
52	L	702	3PE	C25-C26-C27-C28
57	U	201	EHZ	C5-C6-C7-O1
52	r	201	3PE	C24-C25-C26-C27
51	q	201	CDL	OA5-CA3-CA4-OA6
52	L	702	3PE	O11-C1-C2-O21
46	B	203	PC1	C2-C1-O11-P
45	N	404	LMT	O5B-C1B-O1B-C4'
52	N	403	3PE	C39-C3A-C3B-C3C
52	I	204	3PE	C25-C26-C27-C28
51	h	201	CDL	OA6-CA4-CA6-OA8
52	I	204	3PE	O21-C2-C3-O31
52	M	501	3PE	O21-C2-C3-O31
52	d	201	3PE	O21-C2-C3-O31
51	h	202	CDL	C75-C76-C77-C78
45	N	401	LMT	C5'-C4'-O1B-C1B
45	J	201	LMT	C9-C10-C11-C12
51	L	703	CDL	C18-C19-C20-C21
52	f	101	3PE	C25-C26-C27-C28
45	L	705	LMT	O5'-C1'-O1'-C1
45	h	203	LMT	C3-C4-C5-C6
57	U	201	EHZ	C6-C7-C8-C9
51	L	703	CDL	C20-C21-C22-C23
52	Z	201	3PE	C24-C25-C26-C27
45	H	402	LMT	C5'-C4'-O1B-C1B
51	L	703	CDL	OB9-CB7-OB8-CB6
46	B	203	PC1	C31-C32-C33-C34
52	I	204	3PE	C32-C33-C34-C35
51	h	202	CDL	C24-C25-C26-C27
51	L	703	CDL	OA5-CA3-CA4-CA6
52	I	203	3PE	O11-C1-C2-C3
52	L	702	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
52	M	501	3PE	O11-C1-C2-C3
52	I	203	3PE	C22-C23-C24-C25
52	f	101	3PE	C21-C22-C23-C24
52	I	204	3PE	C34-C35-C36-C37
58	o	201	MYR	C10-C11-C12-C13
52	Y	203	3PE	C24-C25-C26-C27
51	H	401	CDL	CA5-C11-C12-C13
52	O	503	3PE	C23-C24-C25-C26
51	L	703	CDL	C72-C73-C74-C75
51	h	201	CDL	C80-C81-C82-C83
51	q	201	CDL	CA6-CA4-OA6-CA5
57	T	201	EHZ	C5-C6-C7-O1
45	L	701	LMT	O5B-C5B-C6B-O6B
45	Y	204	LMT	C4B-C5B-C6B-O6B
52	d	201	3PE	C3A-C3B-C3C-C3D
45	H	402	LMT	C5-C6-C7-C8
46	B	204	PC1	O11-C1-C2-O21
52	Y	203	3PE	O11-C1-C2-O21
52	d	202	3PE	O11-C1-C2-O21
45	A	201	LMT	O5'-C1'-O1'-C1
52	d	201	3PE	C1-C2-C3-O31
57	T	201	EHZ	N1-C12-C13-C14
45	N	404	LMT	C2B-C1B-O1B-C4'
46	B	204	PC1	O32-C31-O31-C3
51	q	201	CDL	C51-C52-C53-C54
52	Y	203	3PE	C22-C23-C24-C25
52	r	201	3PE	C37-C38-C39-C3A
46	L	707	PC1	C12-C11-O13-P
52	Y	203	3PE	C12-C11-O13-P
52	i	201	3PE	C12-C11-O13-P
45	L	701	LMT	O1'-C1-C2-C3
52	d	202	3PE	C23-C24-C25-C26
46	B	204	PC1	O21-C2-C3-O31
51	K	101	CDL	OB6-CB4-CB6-OB8
51	q	201	CDL	OB6-CB4-CB6-OB8
52	N	403	3PE	O21-C2-C3-O31
52	i	201	3PE	O21-C2-C3-O31
51	H	401	CDL	CB3-CB4-CB6-OB8
52	r	201	3PE	C33-C34-C35-C36
45	L	701	LMT	C9-C10-C11-C12
51	K	101	CDL	C1-CB2-OB2-PB2
46	L	707	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
52	Y	203	3PE	C26-C27-C28-C29
51	h	202	CDL	C55-C56-C57-C58
51	h	202	CDL	C20-C21-C22-C23
52	I	204	3PE	C3B-C3C-C3D-C3E
45	A	201	LMT	C2-C1-O1'-C1'
45	j	101	LMT	C2-C1-O1'-C1'
45	M	502	LMT	C7-C8-C9-C10
57	T	201	EHZ	O3-C12-C13-C14
52	I	204	3PE	C3C-C3D-C3E-C3F
51	h	201	CDL	OB5-CB3-CB4-CB6
52	X	201	3PE	O11-C1-C2-C3
52	Y	203	3PE	O11-C1-C2-C3
45	N	404	LMT	C6-C7-C8-C9
52	M	501	3PE	C29-C2A-C2B-C2C
52	Y	203	3PE	C33-C34-C35-C36
45	Y	204	LMT	C5'-C4'-O1B-C1B
45	N	404	LMT	C7-C8-C9-C10
57	T	201	EHZ	C2-C1-C21-C22
51	h	202	CDL	C1-CB2-OB2-PB2
46	B	203	PC1	C34-C35-C36-C37
57	T	201	EHZ	C11-C10-S1-C9
45	L	704	LMT	C6-C7-C8-C9
46	B	204	PC1	C32-C33-C34-C35
51	L	703	CDL	OA5-CA3-CA4-OA6
52	M	501	3PE	O11-C1-C2-O21
52	X	201	3PE	O11-C1-C2-O21
52	r	201	3PE	C26-C27-C28-C29
52	X	201	3PE	C3B-C3C-C3D-C3E
52	X	201	3PE	O21-C2-C3-O31
52	Z	201	3PE	O21-C2-C3-O31
51	h	201	CDL	C74-C75-C76-C77
51	K	101	CDL	CB3-CB4-CB6-OB8
51	h	201	CDL	CA3-CA4-CA6-OA8
51	q	201	CDL	CB3-CB4-CB6-OB8
52	M	501	3PE	C1-C2-C3-O31
52	L	702	3PE	C22-C23-C24-C25
52	M	501	3PE	O32-C31-O31-C3
52	N	402	3PE	C27-C28-C29-C2A
52	Z	201	3PE	C26-C27-C28-C29
51	h	202	CDL	CB5-C51-C52-C53
45	J	201	LMT	C4-C5-C6-C7
46	A	203	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	B	203	PC1	C11-O13-P-O12
46	B	203	PC1	C11-O13-P-O11
46	L	707	PC1	C1-O11-P-O13
51	H	401	CDL	CA2-OA2-PA1-OA4
51	H	401	CDL	CB2-OB2-PB2-OB3
51	H	401	CDL	CB3-OB5-PB2-OB3
51	K	101	CDL	CB2-OB2-PB2-OB3
51	K	101	CDL	CB2-OB2-PB2-OB4
51	K	101	CDL	CB2-OB2-PB2-OB5
51	K	101	CDL	CB3-OB5-PB2-OB2
51	K	101	CDL	CB3-OB5-PB2-OB4
51	L	703	CDL	CA2-OA2-PA1-OA3
51	L	703	CDL	CB2-OB2-PB2-OB3
51	h	201	CDL	CA2-OA2-PA1-OA3
51	h	201	CDL	CB2-OB2-PB2-OB3
51	h	201	CDL	CB2-OB2-PB2-OB5
51	h	201	CDL	CB3-OB5-PB2-OB3
51	h	202	CDL	CA3-OA5-PA1-OA3
51	q	201	CDL	CA2-OA2-PA1-OA3
51	q	201	CDL	CA3-OA5-PA1-OA2
51	q	201	CDL	CA3-OA5-PA1-OA3
52	M	501	3PE	C1-O11-P-O14
52	M	501	3PE	C11-O13-P-O14
52	N	402	3PE	C1-O11-P-O14
52	O	503	3PE	C1-O11-P-O12
52	O	503	3PE	C1-O11-P-O13
52	O	503	3PE	C11-O13-P-O12
52	Y	203	3PE	C11-O13-P-O12
52	Y	203	3PE	O13-C11-C12-N
52	d	201	3PE	C11-O13-P-O11
52	d	201	3PE	C11-O13-P-O12
52	d	201	3PE	C11-O13-P-O14
52	d	202	3PE	C1-O11-P-O12
52	d	202	3PE	C1-O11-P-O13
52	f	101	3PE	C11-O13-P-O14
52	i	201	3PE	C11-O13-P-O11
52	i	201	3PE	C11-O13-P-O14
52	r	201	3PE	C11-O13-P-O12
54	O	502	DGT	C5'-O5'-PA-O3A
54	O	502	DGT	C5'-O5'-PA-O1A
54	O	502	DGT	C5'-O5'-PA-O2A
57	U	201	EHZ	O5-C16-C17-C20

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Mol	Chain	Res	Type	Atoms
52	d	201	3PE	C35-C36-C37-C38
51	h	202	CDL	C56-C57-C58-C59
52	L	702	3PE	C24-C25-C26-C27
51	K	101	CDL	C1-CA2-OA2-PA1
52	L	706	3PE	C1-C2-O21-C21
51	q	201	CDL	CB5-C51-C52-C53
52	d	201	3PE	C21-C22-C23-C24
51	K	101	CDL	C76-C77-C78-C79
45	A	201	LMT	C4-C5-C6-C7
52	M	501	3PE	C32-C31-O31-C3
52	d	202	3PE	C2-C1-O11-P
46	p	302	PC1	C21-C22-C23-C24
51	h	202	CDL	C19-C20-C21-C22
52	I	203	3PE	C34-C35-C36-C37
51	L	703	CDL	C13-C14-C15-C16
45	Y	202	LMT	C6-C7-C8-C9
45	N	404	LMT	C3'-C4'-O1B-C1B
51	H	401	CDL	CA3-CA4-CA6-OA8
52	X	201	3PE	C1-C2-C3-O31
45	L	701	LMT	C5-C6-C7-C8
51	h	202	CDL	C61-C62-C63-C64
45	Y	204	LMT	C7-C8-C9-C10
57	T	201	EHZ	C7-C8-C9-O2
51	h	202	CDL	C51-C52-C53-C54
52	N	402	3PE	C24-C25-C26-C27
45	H	402	LMT	C11-C10-C9-C8
45	L	701	LMT	C4'-C5'-C6'-O6'
45	M	502	LMT	C2-C1-O1'-C1'
51	H	401	CDL	C1-CA2-OA2-PA1
45	M	502	LMT	C9-C10-C11-C12
45	L	704	LMT	C3-C4-C5-C6
51	H	401	CDL	C72-C73-C74-C75
45	M	502	LMT	C2-C3-C4-C5
51	h	202	CDL	OB5-CB3-CB4-OB6
45	Y	204	LMT	O1'-C1-C2-C3
51	H	401	CDL	C18-C19-C20-C21
45	L	705	LMT	C11-C10-C9-C8
51	L	703	CDL	O1-C1-CB2-OB2
51	H	401	CDL	C31-C32-C33-C34
49	F	502	FMN	O3'-C3'-C4'-O4'
51	q	201	CDL	C20-C21-C22-C23
46	B	204	PC1	C3F-C3G-C3H-C3I

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Mol	Chain	Res	Type	Atoms
45	J	201	LMT	C7-C8-C9-C10
52	r	201	3PE	C25-C26-C27-C28
45	Y	202	LMT	O5'-C1'-O1'-C1
52	Z	201	3PE	O22-C21-C22-C23
51	L	703	CDL	C16-C17-C18-C19
52	Z	201	3PE	C27-C28-C29-C2A
51	q	201	CDL	C1-CA2-OA2-PA1
52	Z	201	3PE	C38-C39-C3A-C3B
52	d	201	3PE	C32-C33-C34-C35
45	A	202	LMT	C7-C8-C9-C10
52	Z	201	3PE	C22-C21-O21-C2
52	N	403	3PE	C1-C2-C3-O31
46	B	204	PC1	C35-C36-C37-C38
52	L	706	3PE	C3E-C3F-C3G-C3H
51	h	202	CDL	CB7-C71-C72-C73
51	h	202	CDL	OA5-CA3-CA4-OA6
52	X	201	3PE	C31-C32-C33-C34
52	f	101	3PE	C32-C33-C34-C35
46	B	203	PC1	C24-C25-C26-C27
46	B	204	PC1	O11-C1-C2-C3
45	j	101	LMT	C7-C8-C9-C10
52	L	706	3PE	C34-C35-C36-C37
45	H	402	LMT	C3'-C4'-O1B-C1B
45	A	202	LMT	C1-C2-C3-C4
54	O	502	DGT	O4'-C4'-C5'-O5'
55	P	501	NDP	O4D-C1D-N1N-C6N
52	M	501	3PE	C25-C26-C27-C28
52	N	402	3PE	C25-C26-C27-C28
45	h	203	LMT	O1'-C1-C2-C3
52	N	402	3PE	C29-C2A-C2B-C2C
45	L	705	LMT	C1-C2-C3-C4
45	N	401	LMT	C6-C7-C8-C9
51	h	202	CDL	C57-C58-C59-C60
52	i	201	3PE	C23-C24-C25-C26
52	N	402	3PE	C2D-C2E-C2F-C2G
52	L	706	3PE	C2A-C2B-C2C-C2D
51	h	201	CDL	CA4-CA3-OA5-PA1
52	I	203	3PE	C33-C34-C35-C36
52	Z	201	3PE	O22-C21-O21-C2
52	L	702	3PE	C1-C2-C3-O31
51	h	202	CDL	C23-C24-C25-C26
52	L	706	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
52	d	202	3PE	C35-C36-C37-C38
52	f	101	3PE	C28-C29-C2A-C2B
57	T	201	EHZ	C3-C4-C5-C6
51	q	201	CDL	OA5-CA3-CA4-CA6
58	o	201	MYR	C5-C6-C7-C8
51	h	202	CDL	C16-C17-C18-C19
55	P	501	NDP	C2D-C1D-N1N-C6N
45	L	705	LMT	C7-C8-C9-C10
54	O	502	DGT	PB-O3B-PG-O1G
45	h	203	LMT	O5B-C1B-O1B-C4'
52	r	201	3PE	C3C-C3D-C3E-C3F
51	h	201	CDL	C51-C52-C53-C54
51	h	202	CDL	CB4-CB3-OB5-PB2
45	H	402	LMT	C2-C3-C4-C5
52	d	202	3PE	C38-C39-C3A-C3B
52	f	101	3PE	C37-C38-C39-C3A
46	B	204	PC1	C3C-C3D-C3E-C3F
52	L	702	3PE	C32-C31-O31-C3
45	Y	204	LMT	C3'-C4'-O1B-C1B
51	K	101	CDL	C77-C78-C79-C80
52	L	702	3PE	C34-C35-C36-C37
52	r	201	3PE	C34-C35-C36-C37
52	Y	203	3PE	O21-C2-C3-O31
52	I	204	3PE	C24-C25-C26-C27
51	K	101	CDL	C12-C11-CA5-OA6
51	L	703	CDL	C32-C31-CA7-OA8
46	p	302	PC1	O11-C1-C2-C3
51	h	202	CDL	OB5-CB3-CB4-CB6
51	K	101	CDL	C57-C58-C59-C60
46	B	204	PC1	C11-C12-N-C13
46	B	204	PC1	C11-C12-N-C15
51	q	201	CDL	C32-C31-CA7-OA8
52	L	702	3PE	O32-C31-O31-C3
45	J	202	LMT	C4-C5-C6-C7
51	H	401	CDL	C12-C13-C14-C15
52	N	403	3PE	C32-C33-C34-C35
54	O	502	DGT	PG-O3B-PB-O1B
55	P	501	NDP	PN-O3-PA-O2A
45	L	704	LMT	C11-C10-C9-C8
52	d	201	3PE	C2A-C2B-C2C-C2D
52	Z	201	3PE	C39-C3A-C3B-C3C
51	h	202	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
51	L	703	CDL	C34-C35-C36-C37
52	M	501	3PE	O21-C21-C22-C23
51	K	101	CDL	OB5-CB3-CB4-OB6
51	h	202	CDL	C58-C59-C60-C61
46	L	707	PC1	O31-C31-C32-C33
52	I	203	3PE	O21-C21-C22-C23
51	L	703	CDL	C53-C54-C55-C56
46	p	302	PC1	O31-C31-C32-C33
51	h	202	CDL	C76-C77-C78-C79
52	I	203	3PE	C25-C26-C27-C28
51	h	201	CDL	CB4-CB3-OB5-PB2
52	L	706	3PE	C2-C1-O11-P
46	B	203	PC1	C1-C2-C3-O31
46	B	204	PC1	C11-C12-N-C14
46	A	203	PC1	O31-C31-C32-C33
51	H	401	CDL	C72-C71-CB7-OB8
52	Y	203	3PE	O31-C31-C32-C33
51	q	201	CDL	C72-C71-CB7-OB8
52	O	503	3PE	O31-C31-C32-C33
54	O	502	DGT	PB-O3B-PG-O3G
52	M	501	3PE	O31-C31-C32-C33
51	K	101	CDL	C32-C33-C34-C35
49	F	502	FMN	N10-C1'-C2'-O2'
52	X	201	3PE	C35-C36-C37-C38
46	B	204	PC1	C34-C35-C36-C37
52	X	201	3PE	C33-C34-C35-C36
57	U	201	EHZ	C21-C22-C23-C24
45	j	101	LMT	C1-C2-C3-C4
51	h	202	CDL	C11-C12-C13-C14
52	X	201	3PE	C2-C1-O11-P
52	f	101	3PE	C35-C36-C37-C38
51	q	201	CDL	C32-C31-CA7-OA9
52	X	201	3PE	C38-C39-C3A-C3B
51	K	101	CDL	C12-C11-CA5-OA7
52	M	501	3PE	O22-C21-C22-C23
46	p	302	PC1	O32-C31-C32-C33
51	q	201	CDL	C11-C12-C13-C14
52	I	203	3PE	C21-C22-C23-C24
51	K	101	CDL	C74-C75-C76-C77
45	A	202	LMT	C4B-C5B-C6B-O6B
45	M	502	LMT	C5-C6-C7-C8
46	A	203	PC1	O32-C31-C32-C33

Continued on next page...

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Mol	Chain	Res	Type	Atoms
51	H	401	CDL	C72-C71-CB7-OB9
51	L	703	CDL	C32-C31-CA7-OA9
52	I	203	3PE	O22-C21-C22-C23
52	d	201	3PE	C24-C25-C26-C27
45	L	704	LMT	C9-C10-C11-C12
52	L	706	3PE	C25-C26-C27-C28
45	A	201	LMT	C9-C10-C11-C12
52	L	706	3PE	O22-C21-O21-C2
46	B	203	PC1	O21-C2-C3-O31
52	Y	203	3PE	C32-C33-C34-C35
45	h	203	LMT	C2B-C1B-O1B-C4'
46	B	203	PC1	C37-C38-C39-C3A
52	r	201	3PE	C3D-C3E-C3F-C3G
45	N	404	LMT	C5'-C4'-O1B-C1B
45	h	203	LMT	C4-C5-C6-C7
52	O	503	3PE	O32-C31-C32-C33
51	H	401	CDL	C32-C31-CA7-OA8
46	L	707	PC1	O32-C31-C32-C33
54	O	502	DGT	PA-O3A-PB-O1B
52	M	501	3PE	O32-C31-C32-C33
52	Z	201	3PE	C36-C37-C38-C39
51	q	201	CDL	C72-C71-CB7-OB9
52	Y	203	3PE	O32-C31-C32-C33
45	N	401	LMT	C11-C10-C9-C8
51	h	202	CDL	C52-C53-C54-C55

There are no ring outliers.

21 monomers are involved in 28 short contacts:

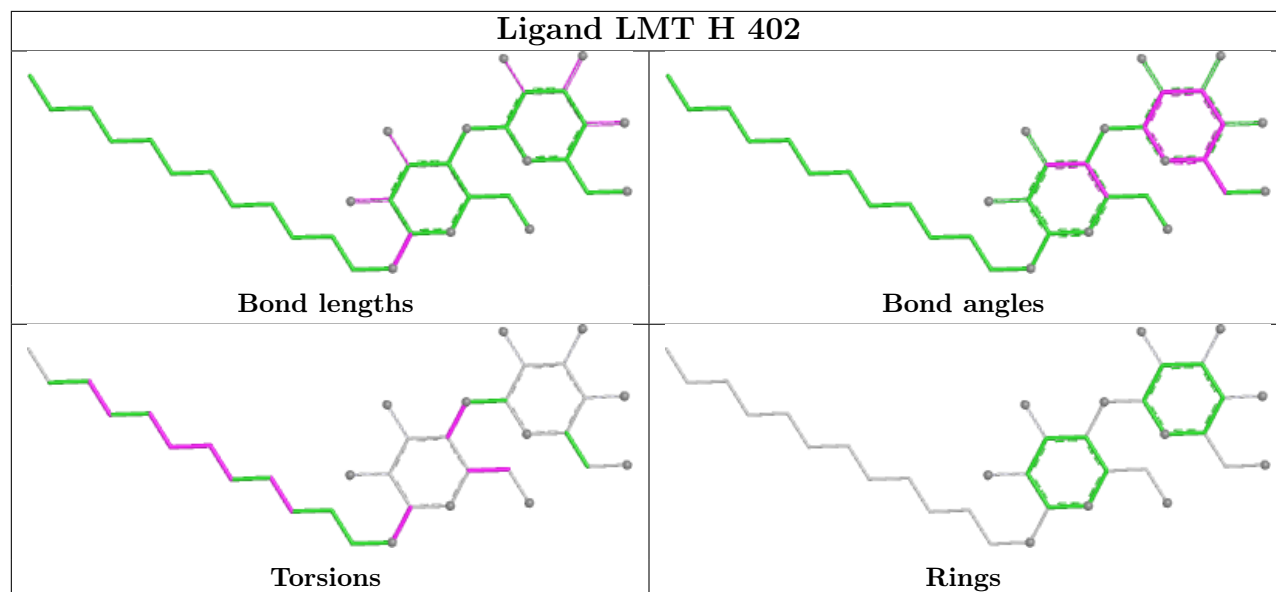
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	H	402	LMT	2	0
52	r	201	3PE	1	0
45	A	201	LMT	1	0
47	B	201	SF4	1	0
45	L	701	LMT	3	0
52	N	402	3PE	1	0
54	O	502	DGT	2	0
45	J	202	LMT	2	0
52	X	201	3PE	1	0
45	L	705	LMT	2	0
52	Y	203	3PE	1	0
52	L	706	3PE	1	0

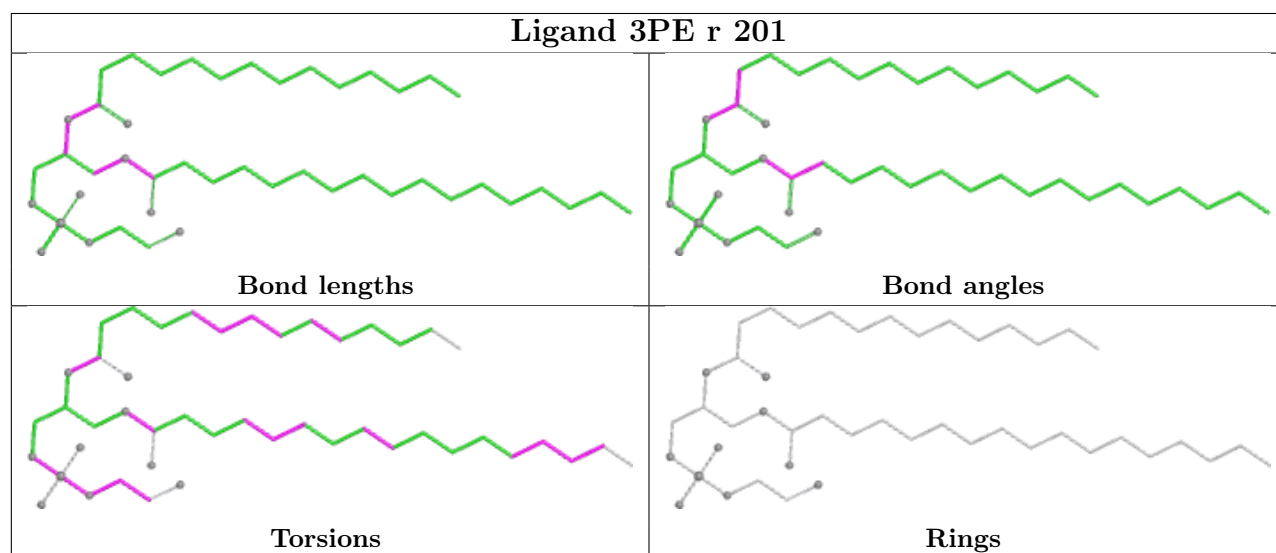
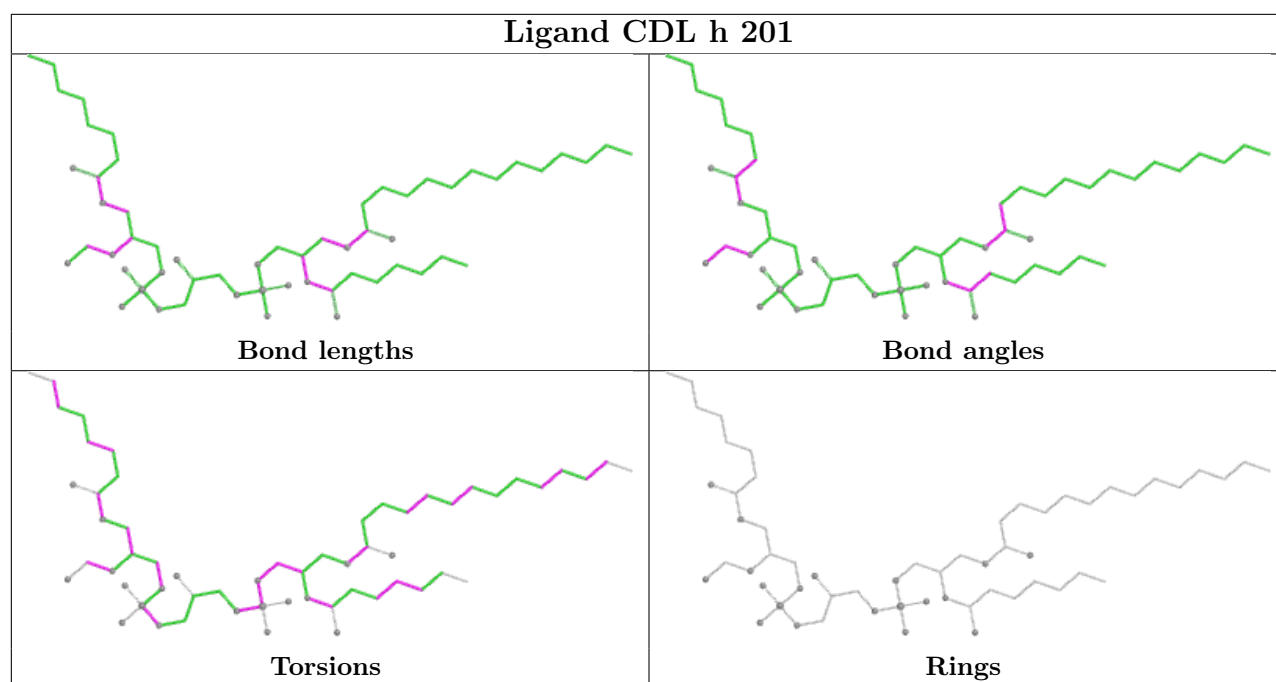
Continued on next page...

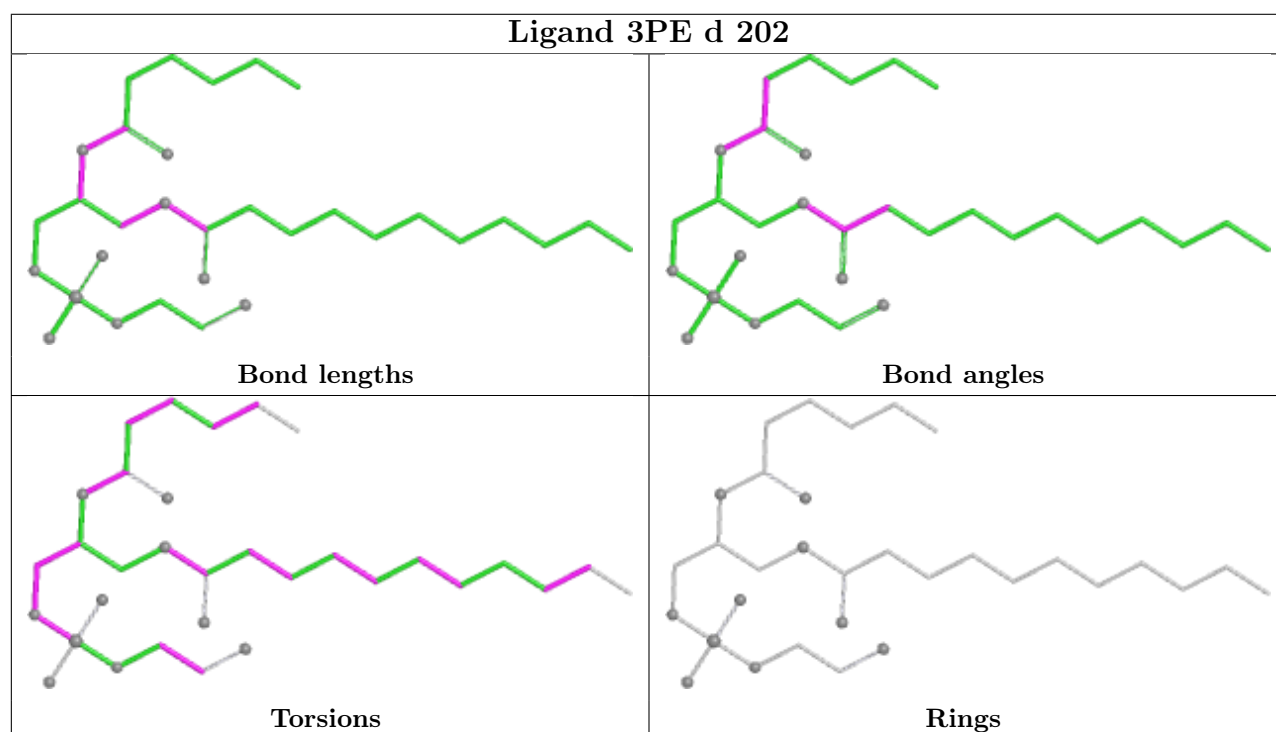
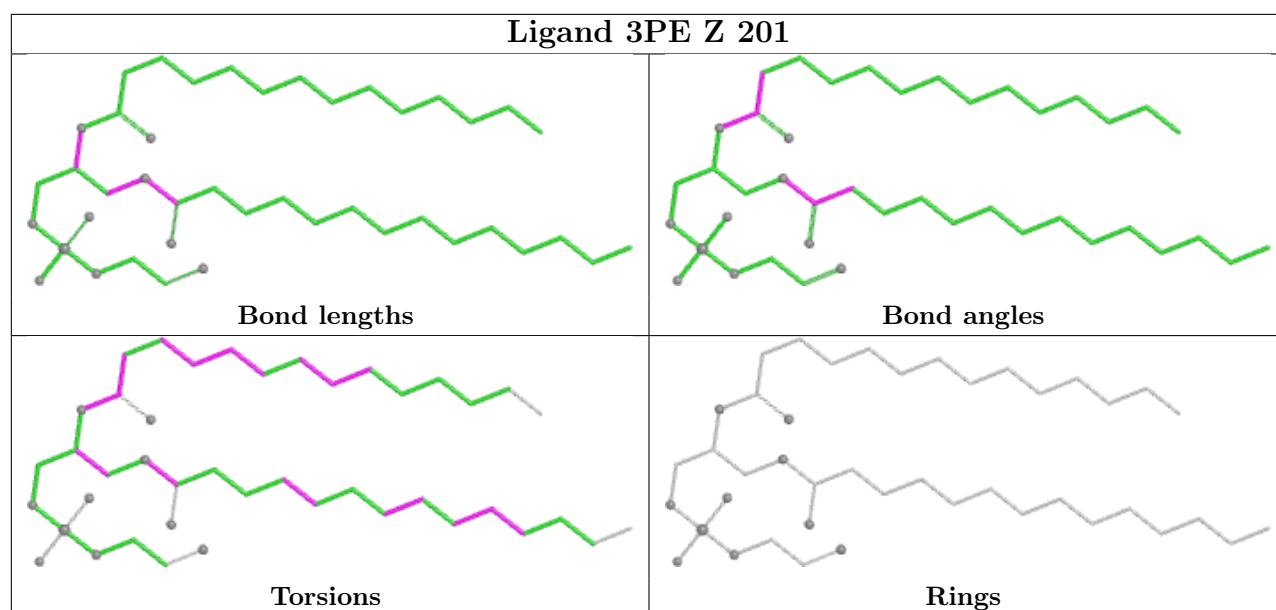
Continued from previous page...

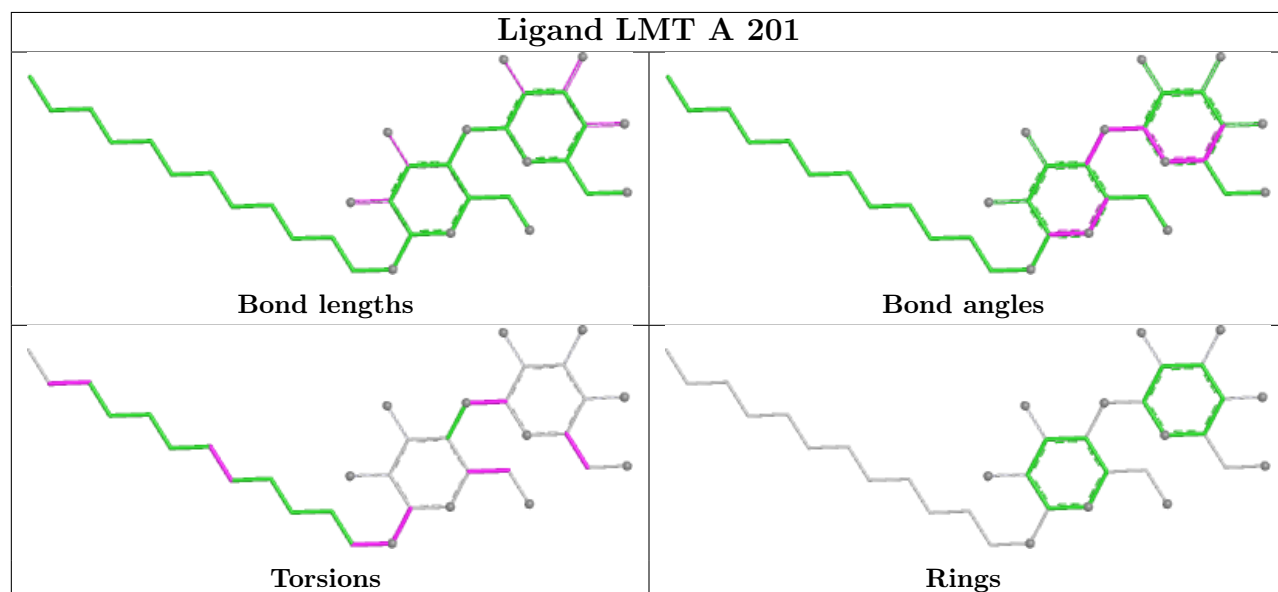
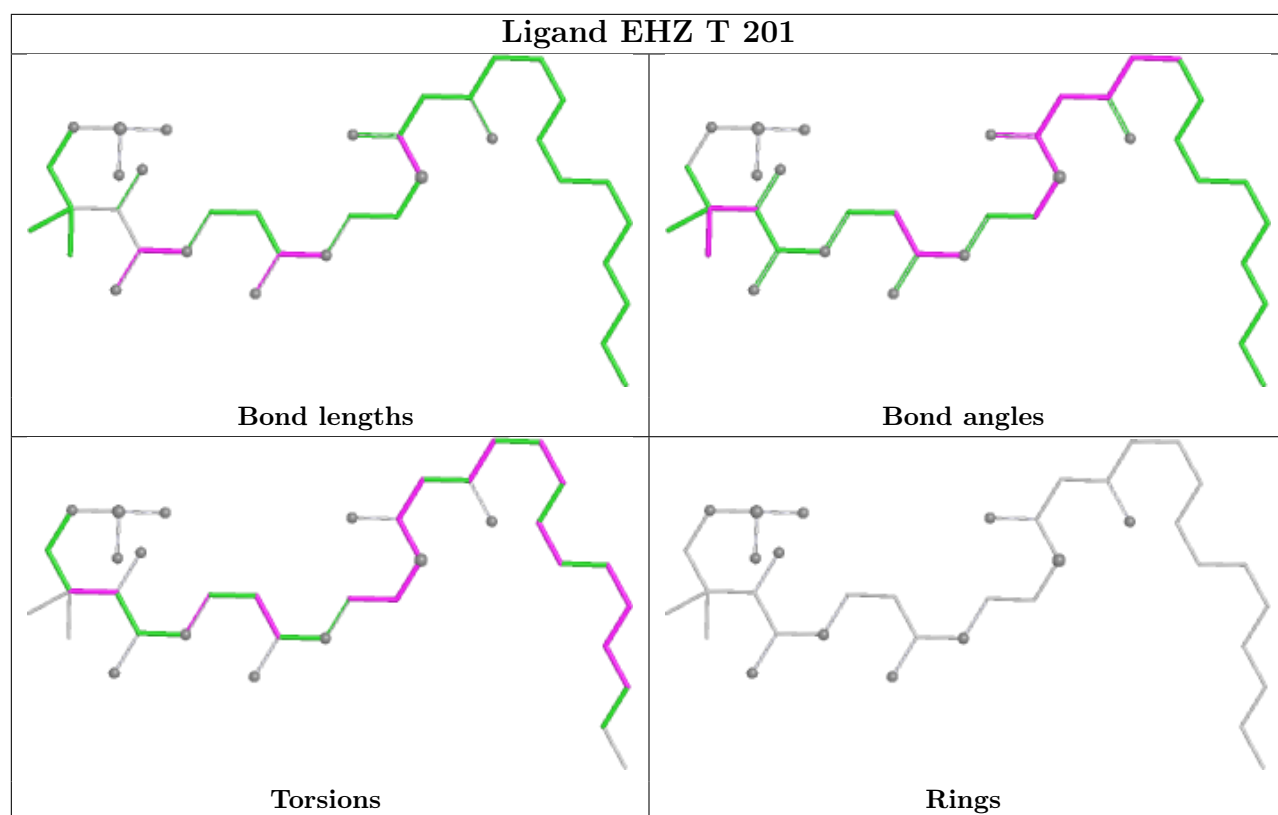
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	i	201	3PE	1	0
52	I	204	3PE	1	0
46	B	204	PC1	1	0
55	P	501	NDP	2	0
52	d	201	3PE	2	0
49	F	502	FMN	2	0
45	Y	201	LMT	1	0
57	U	201	EHZ	1	0
52	L	702	3PE	1	0

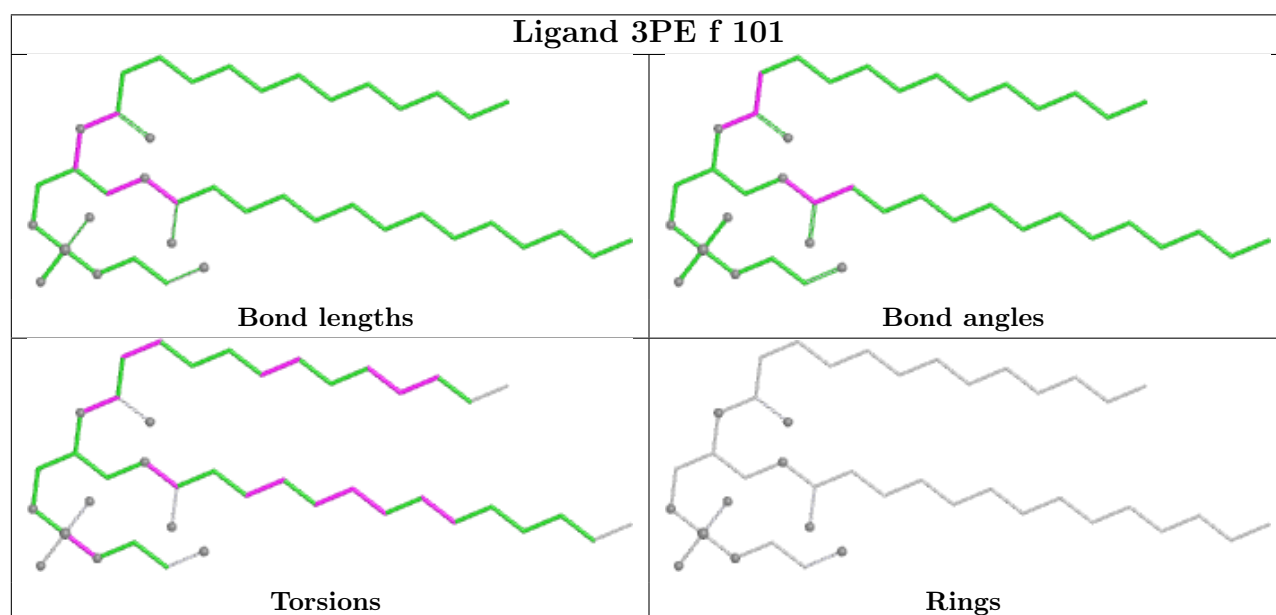
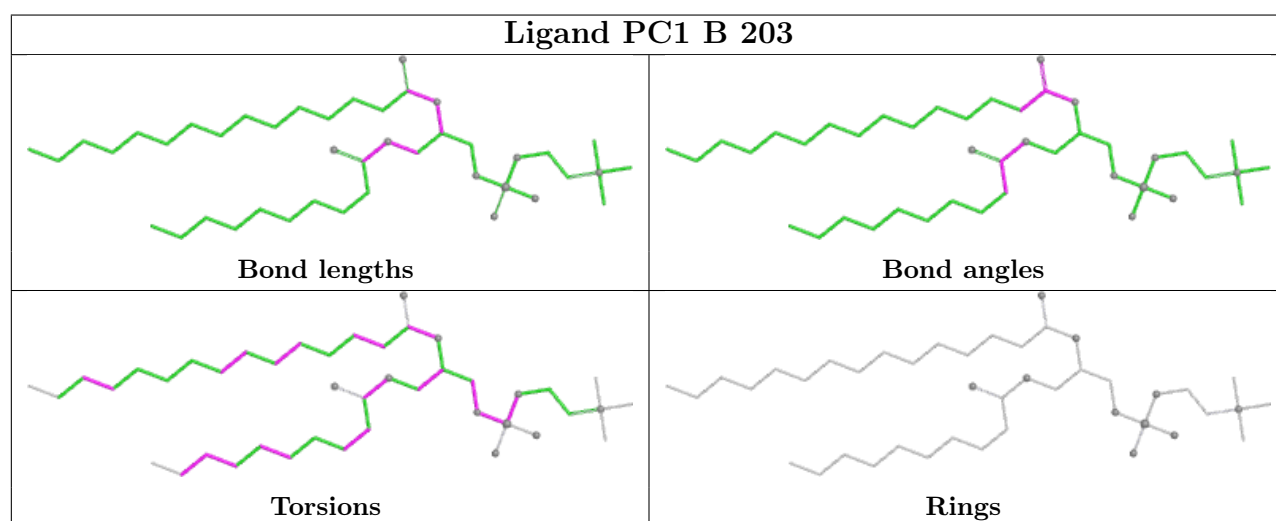
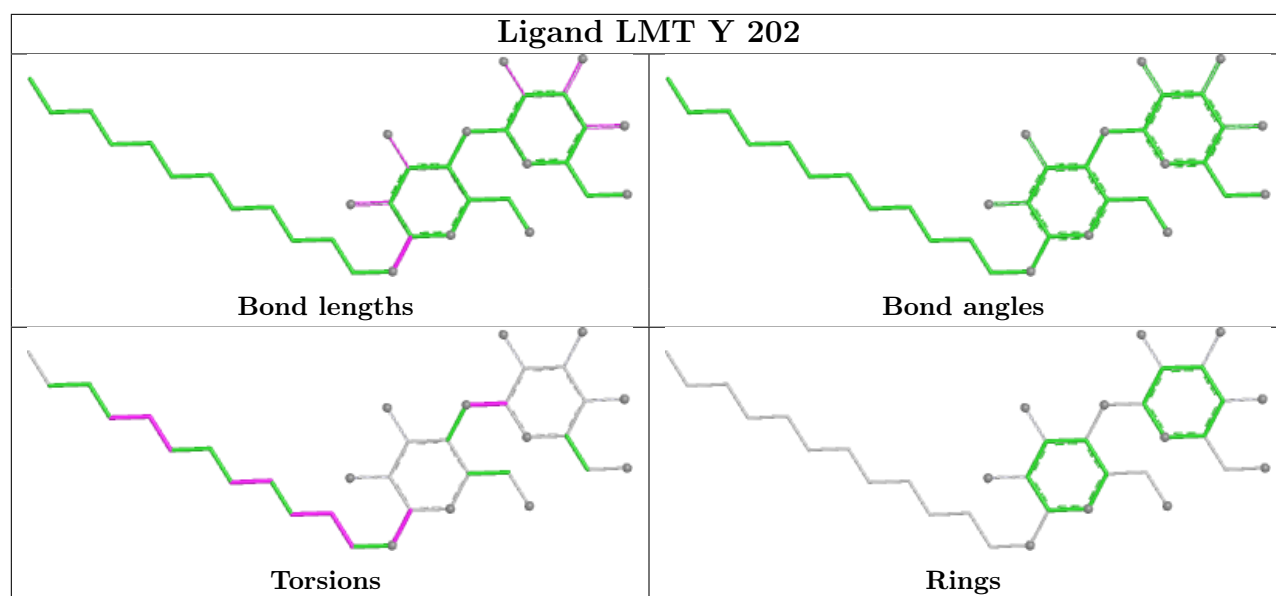
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

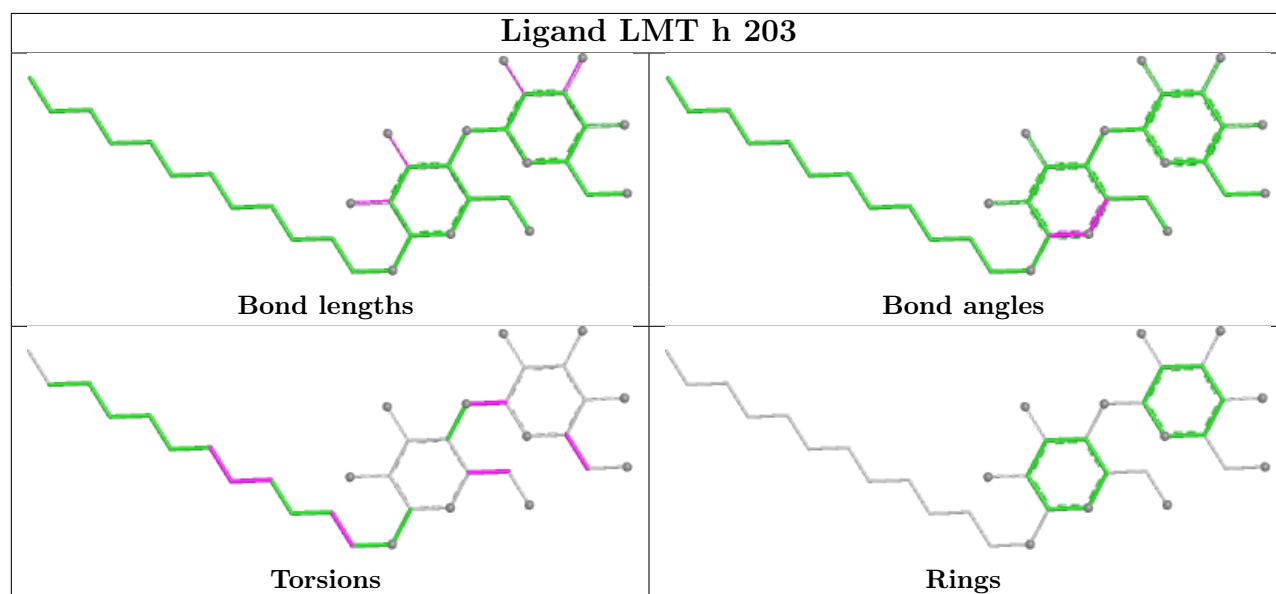
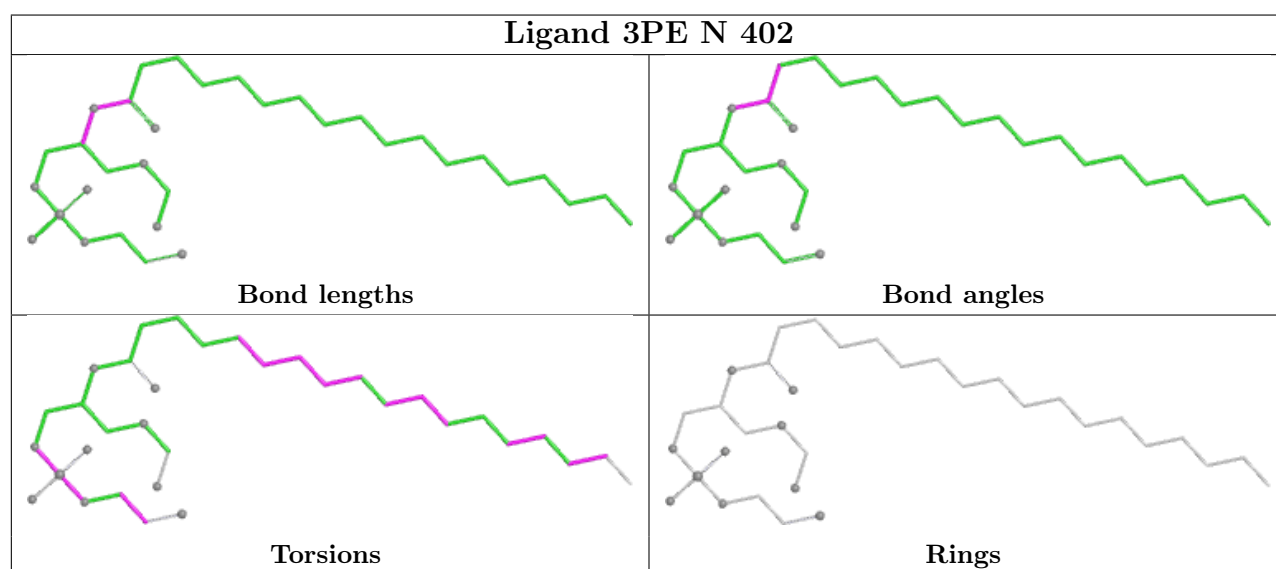
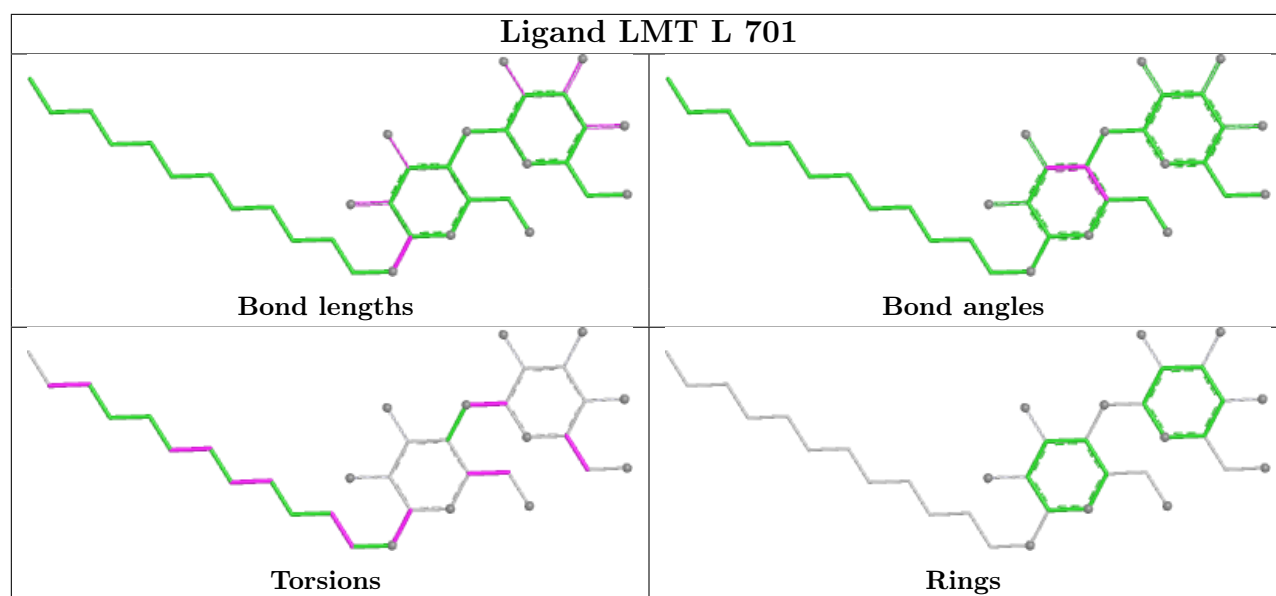


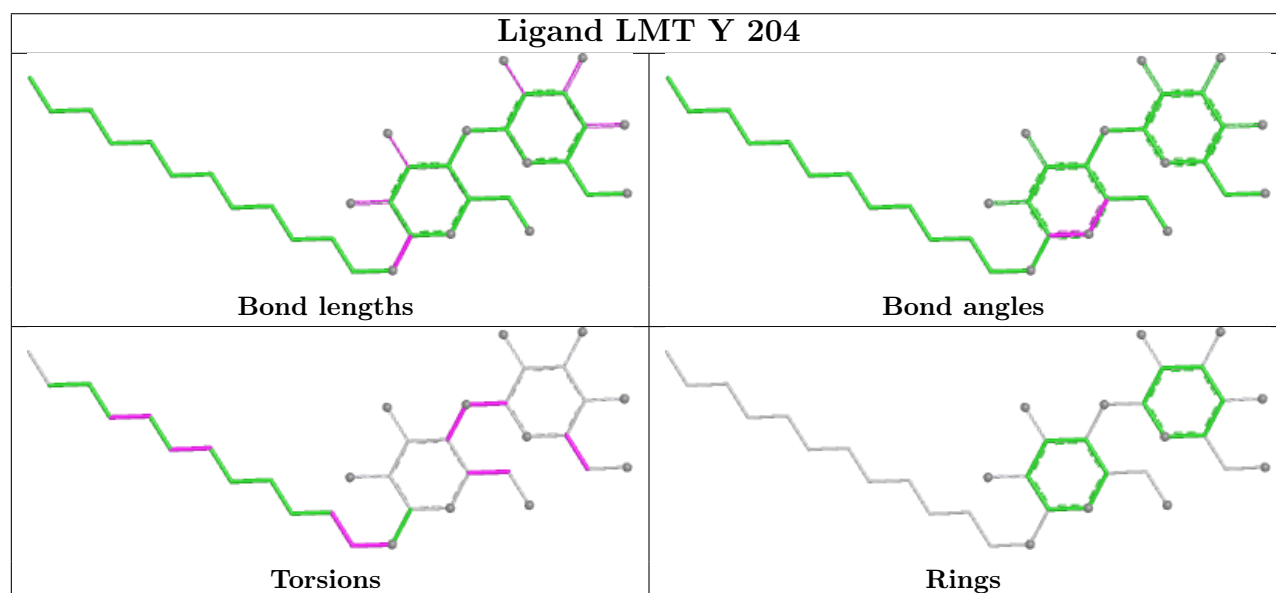
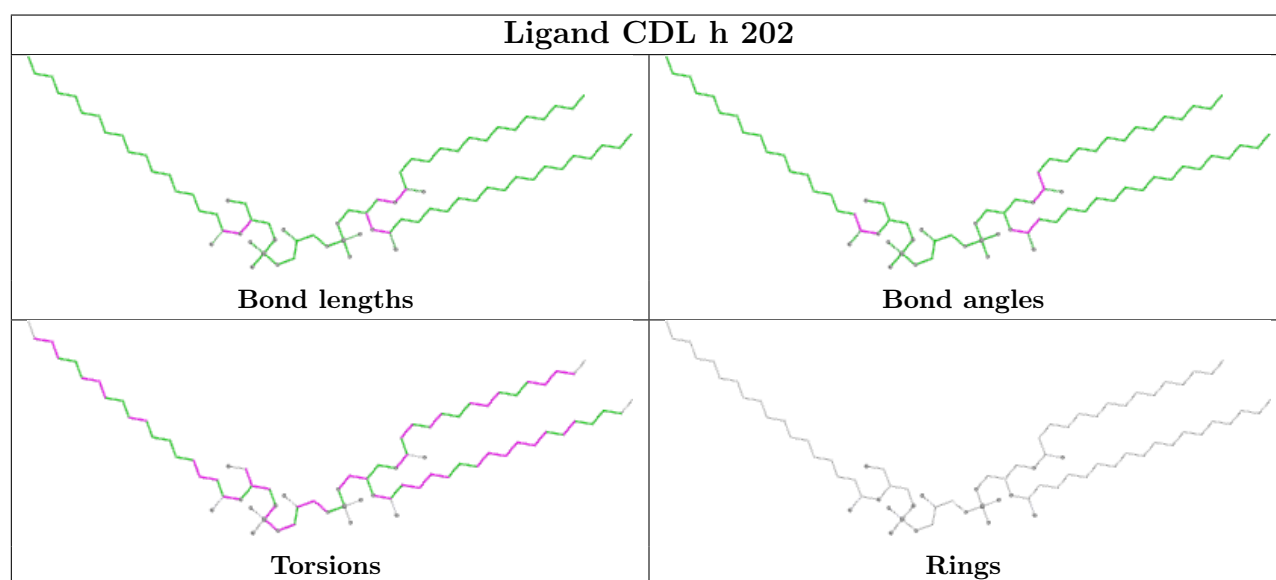
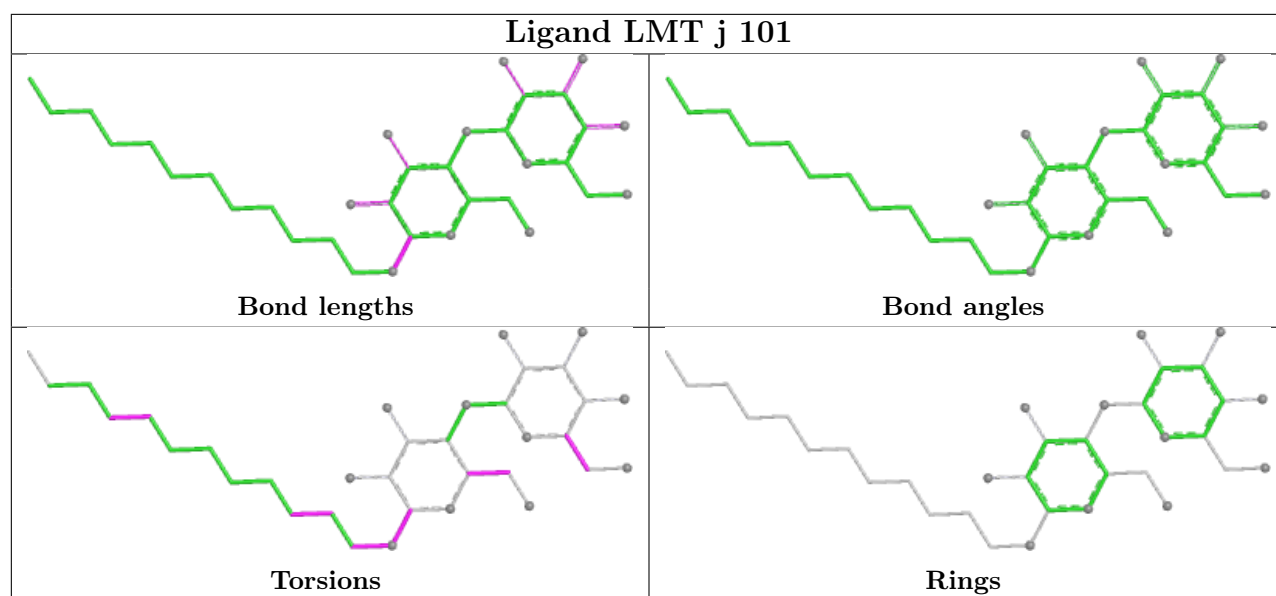


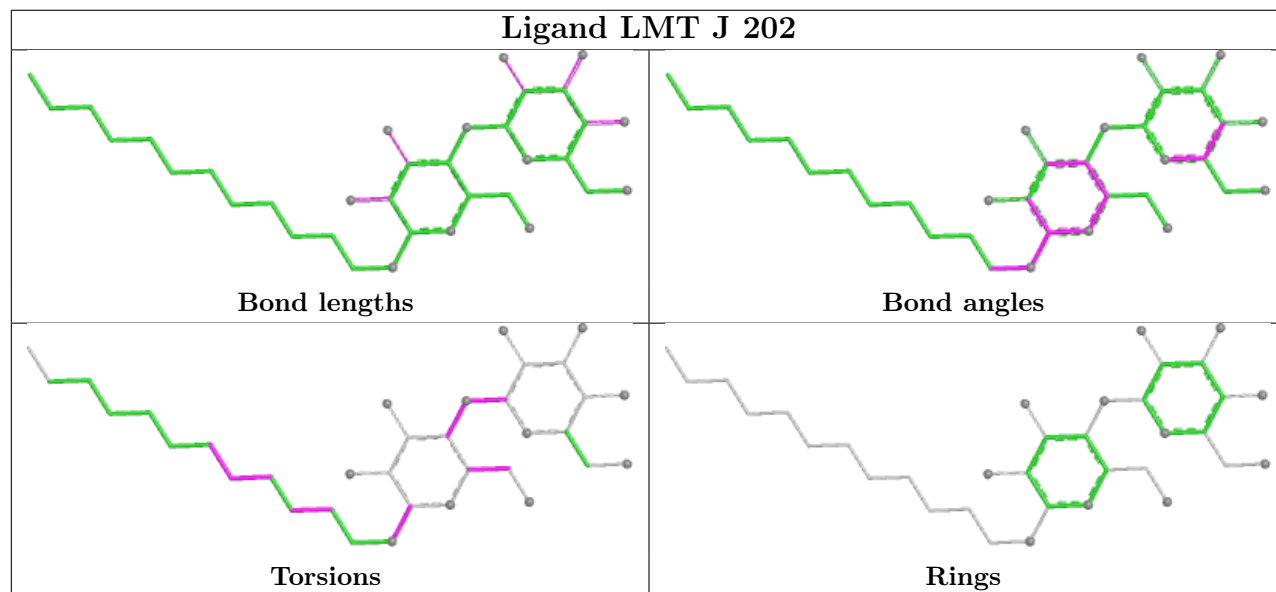
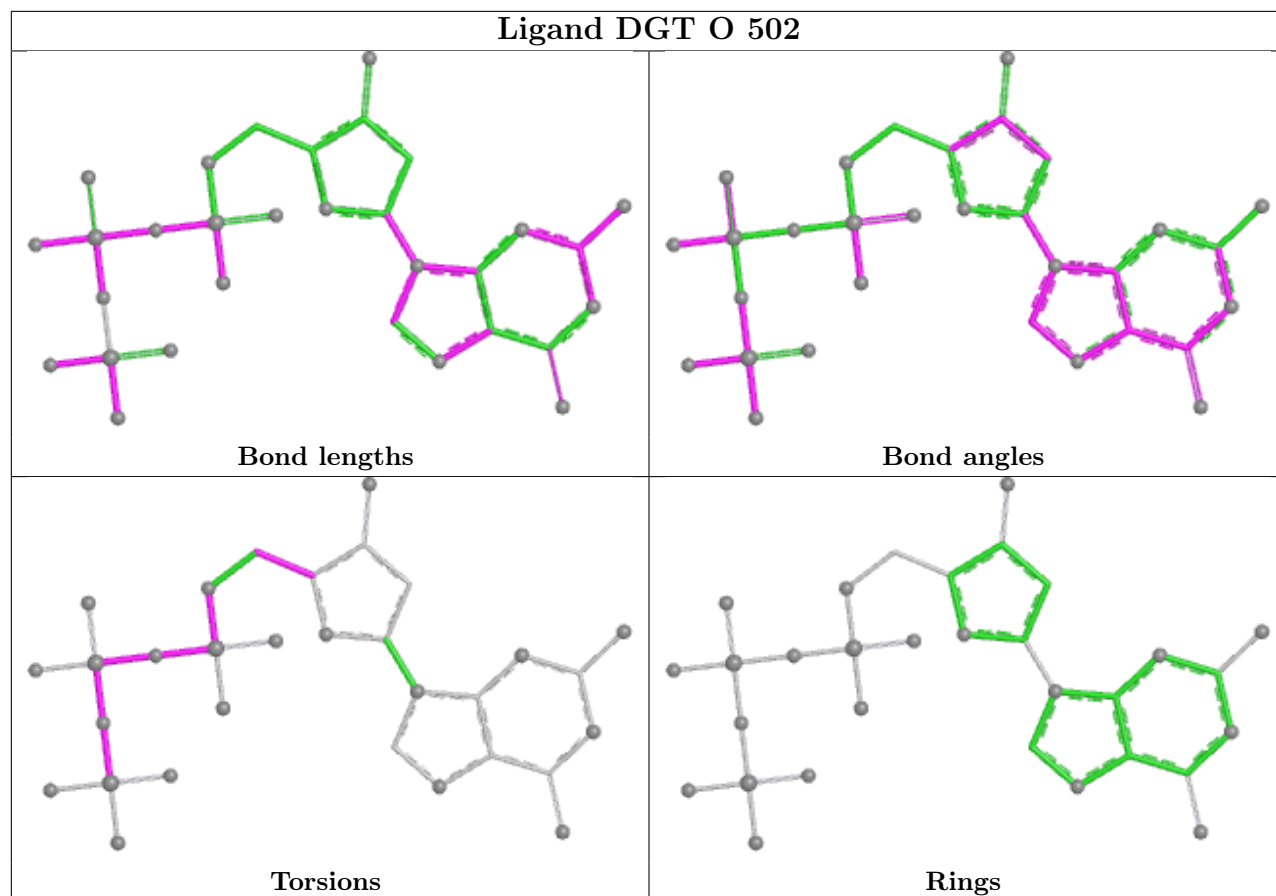


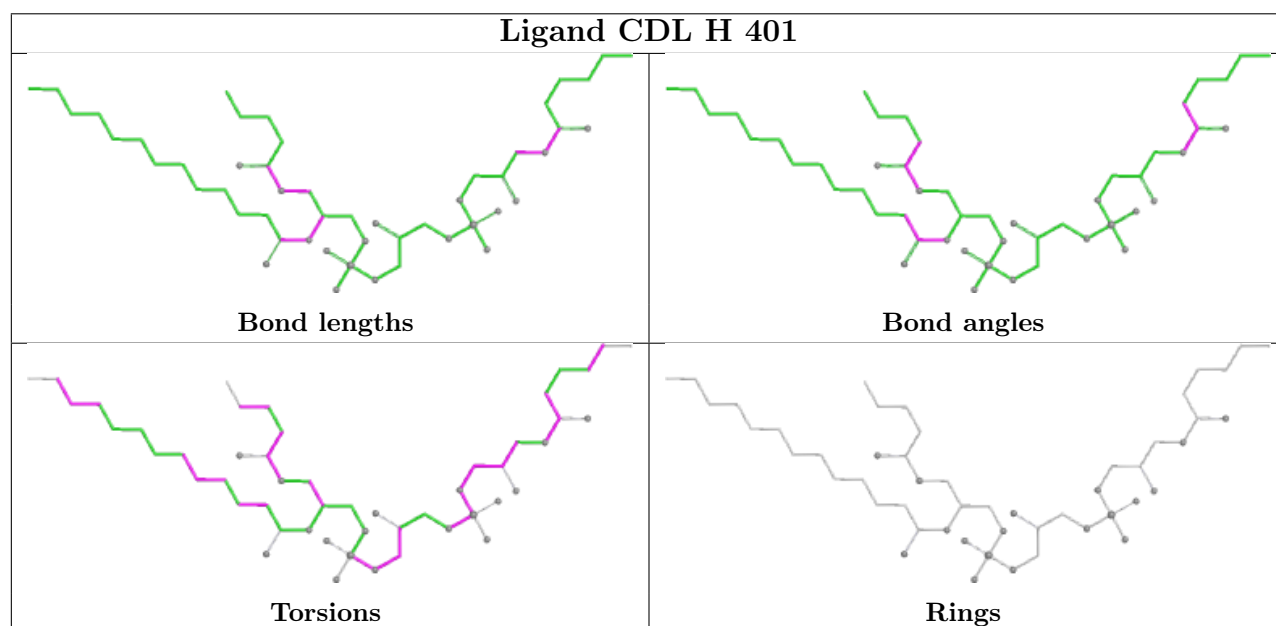
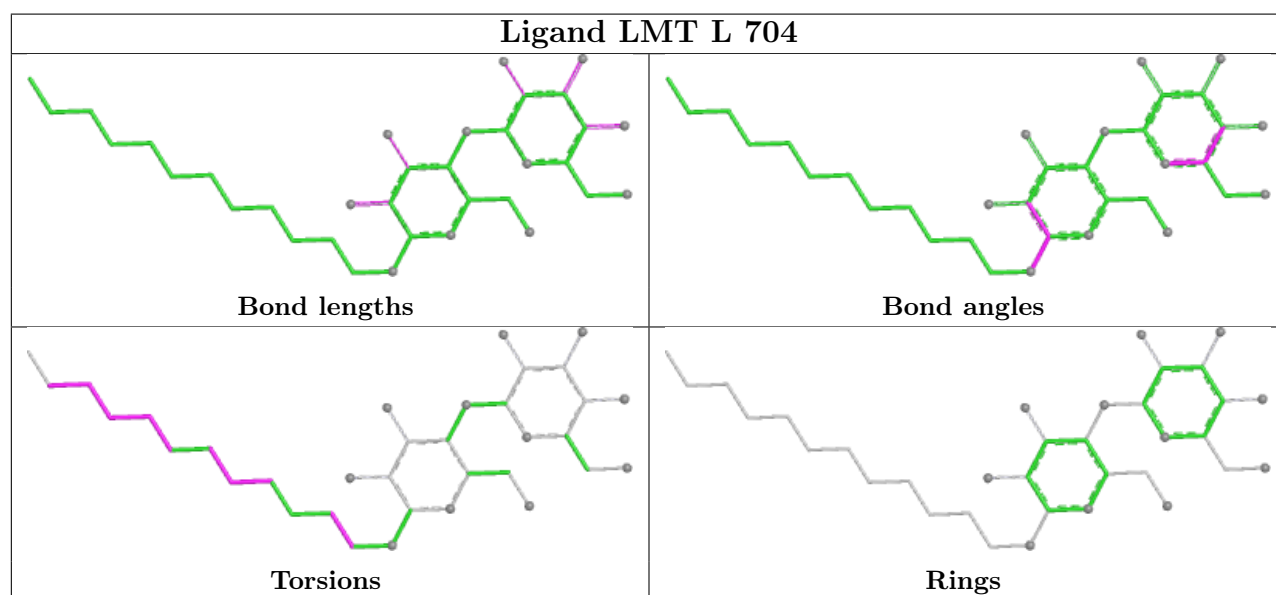
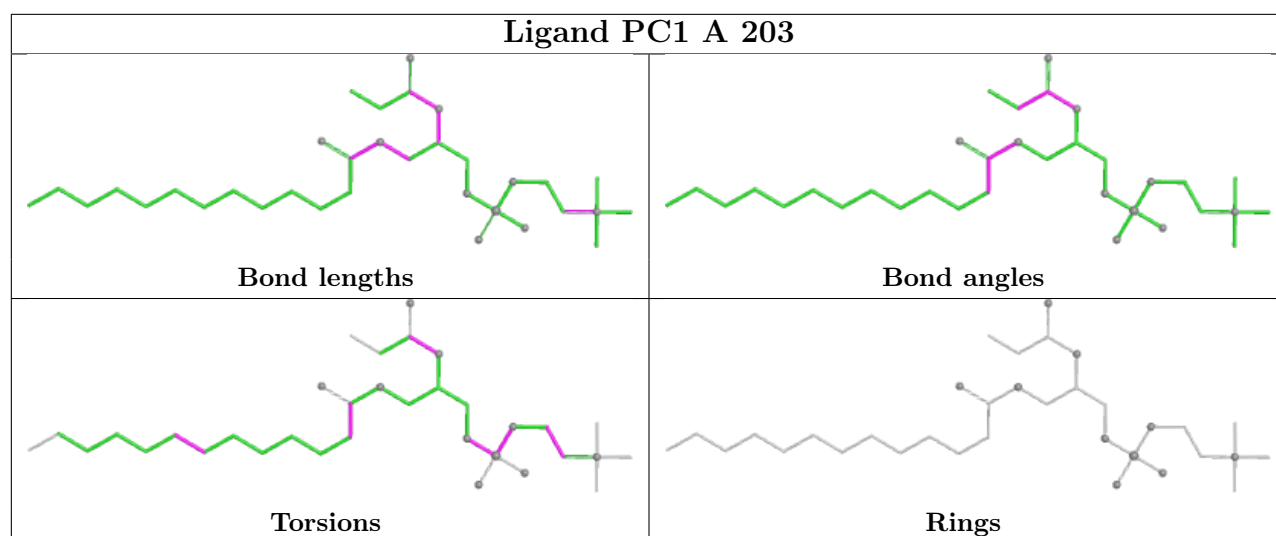


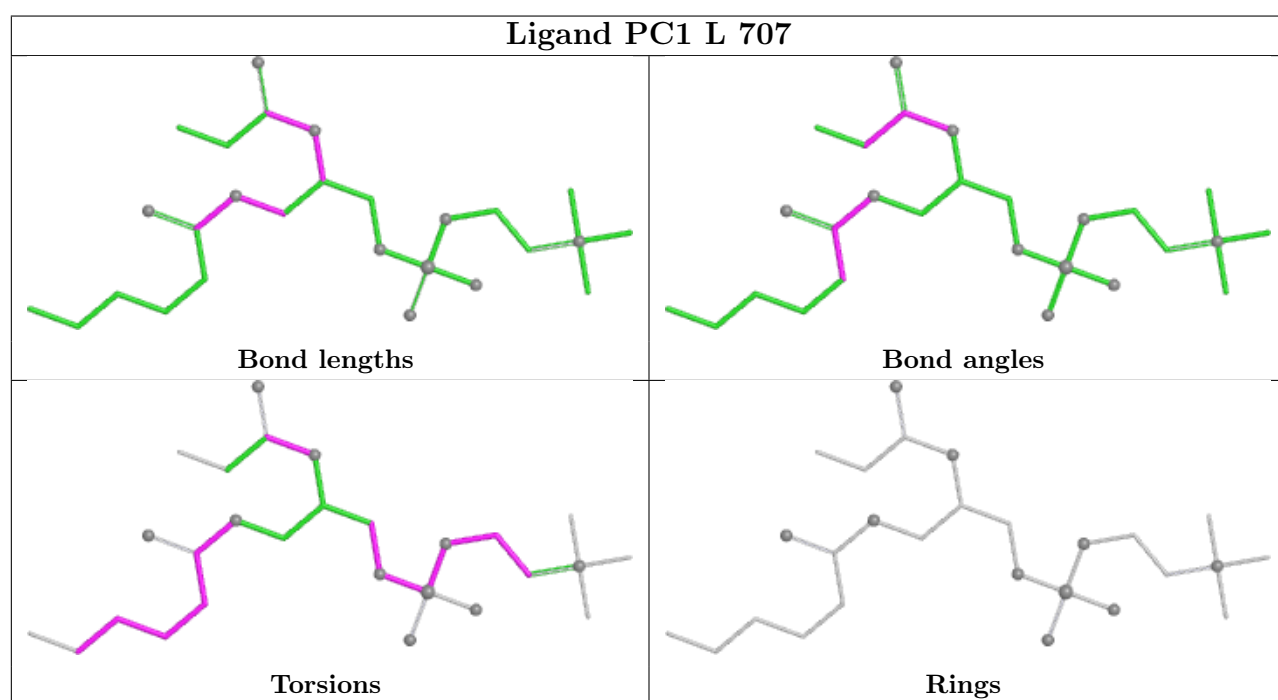
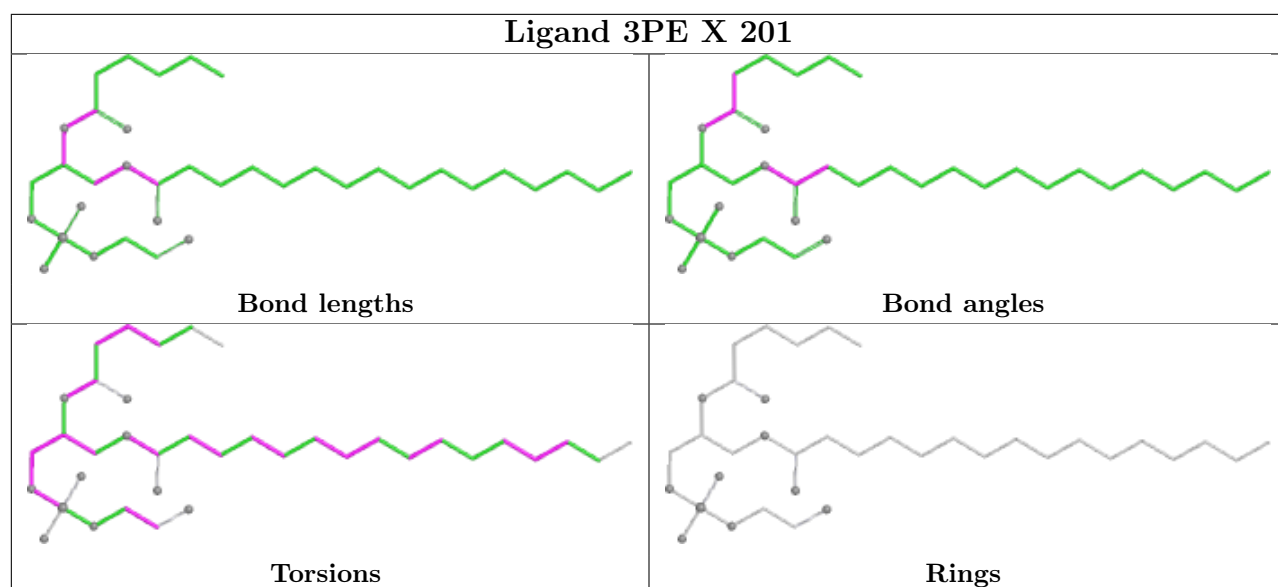


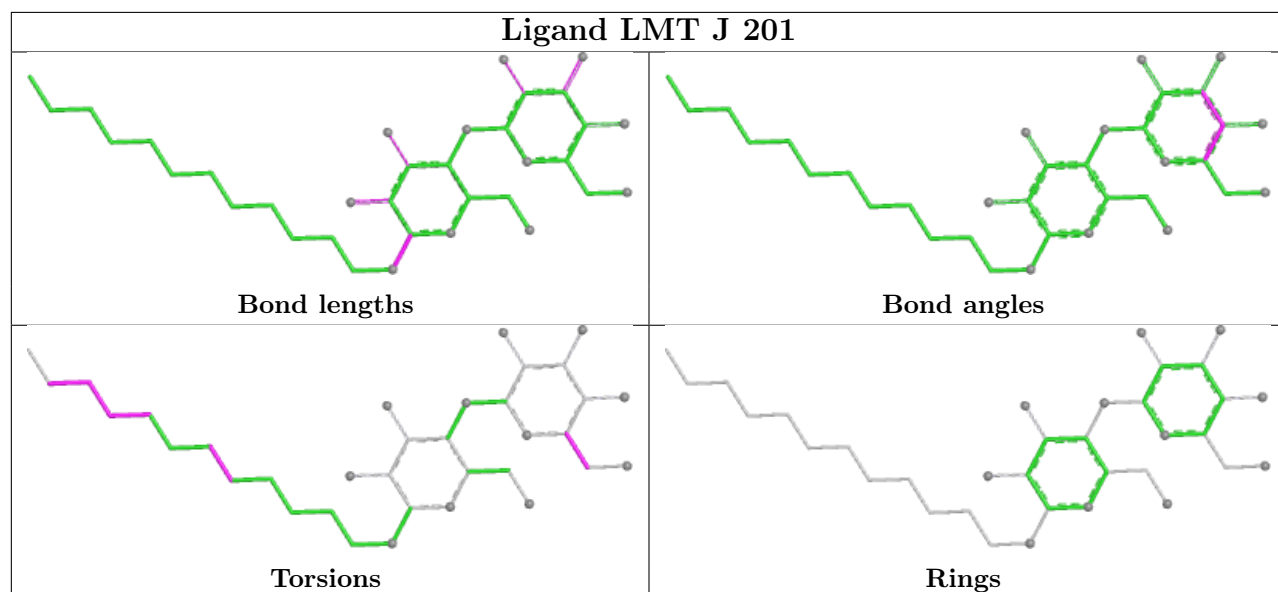
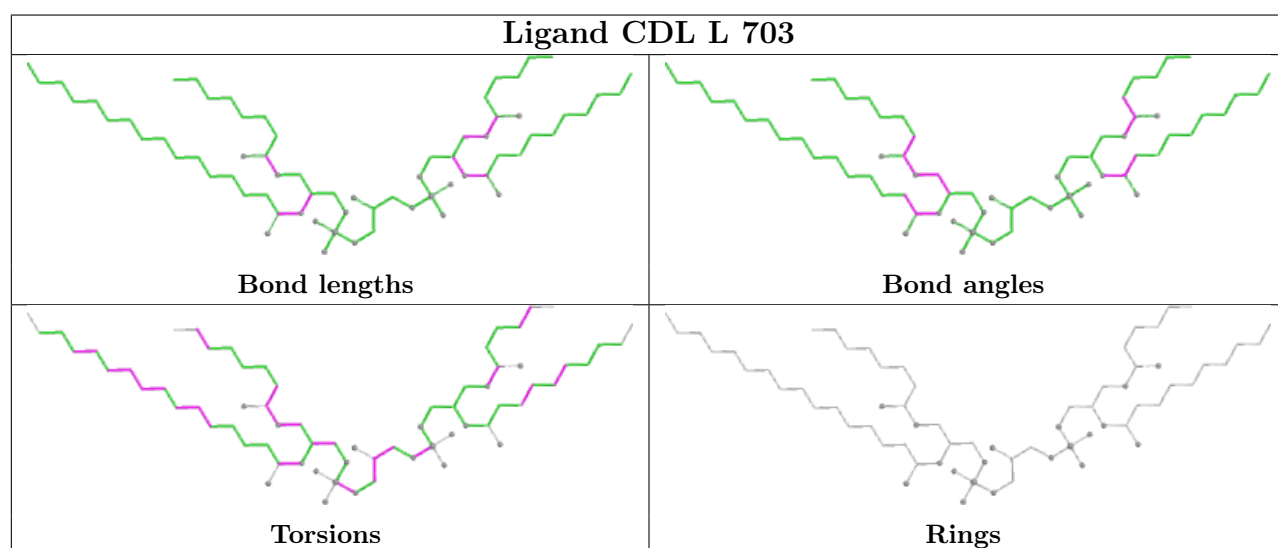
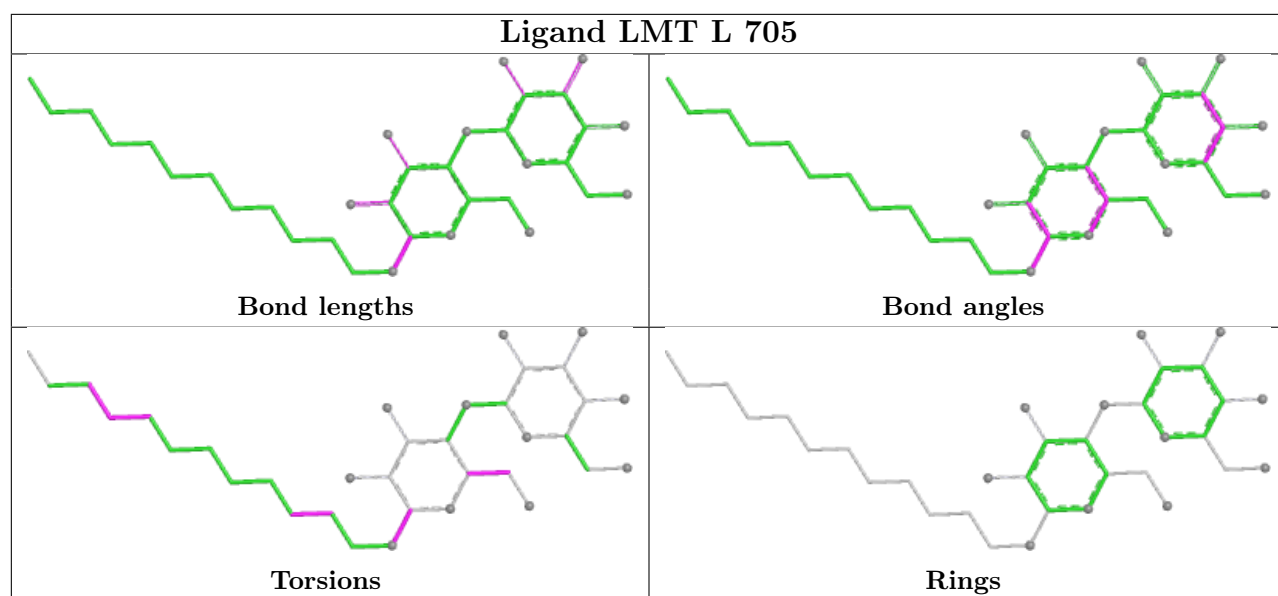


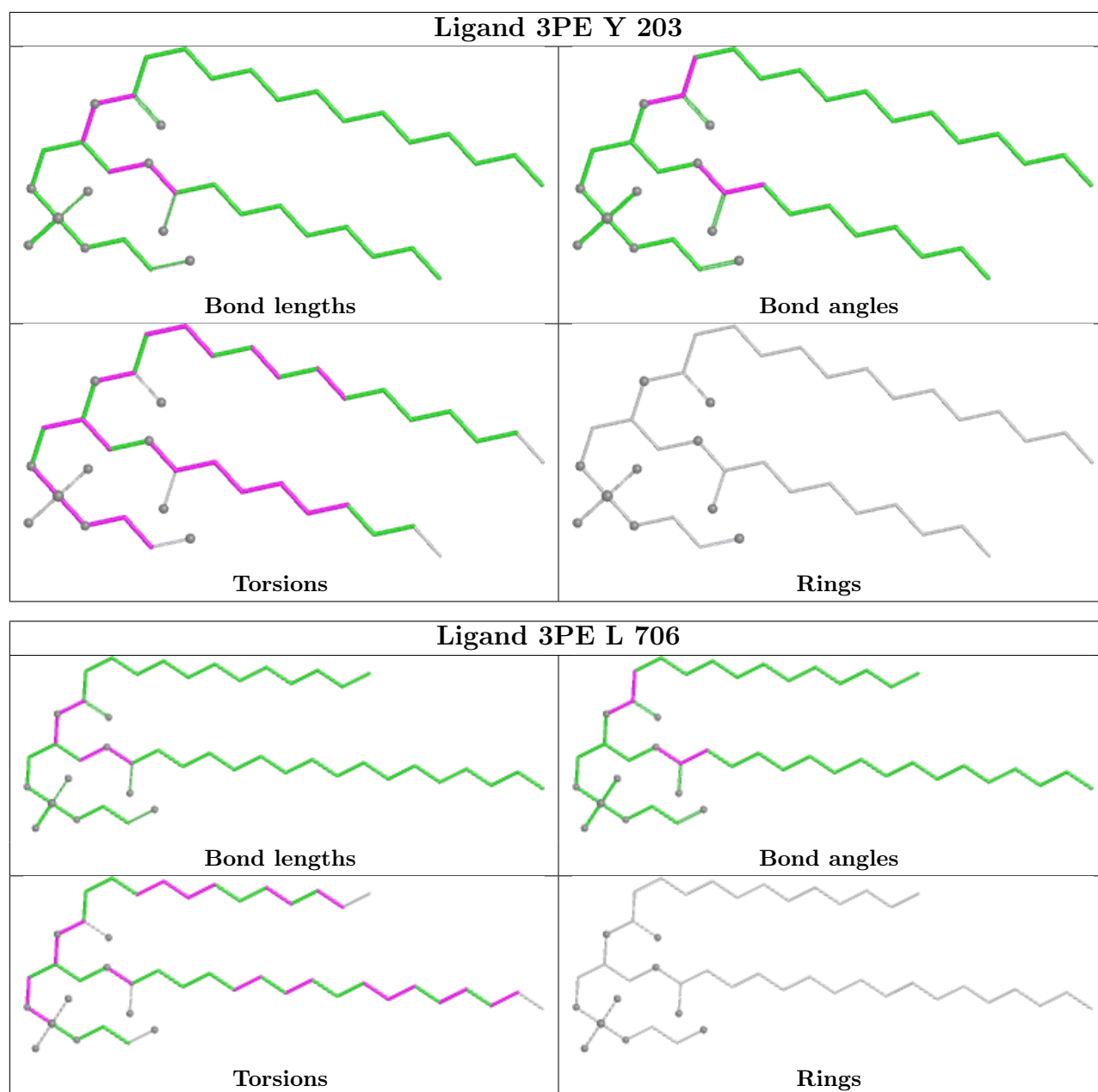


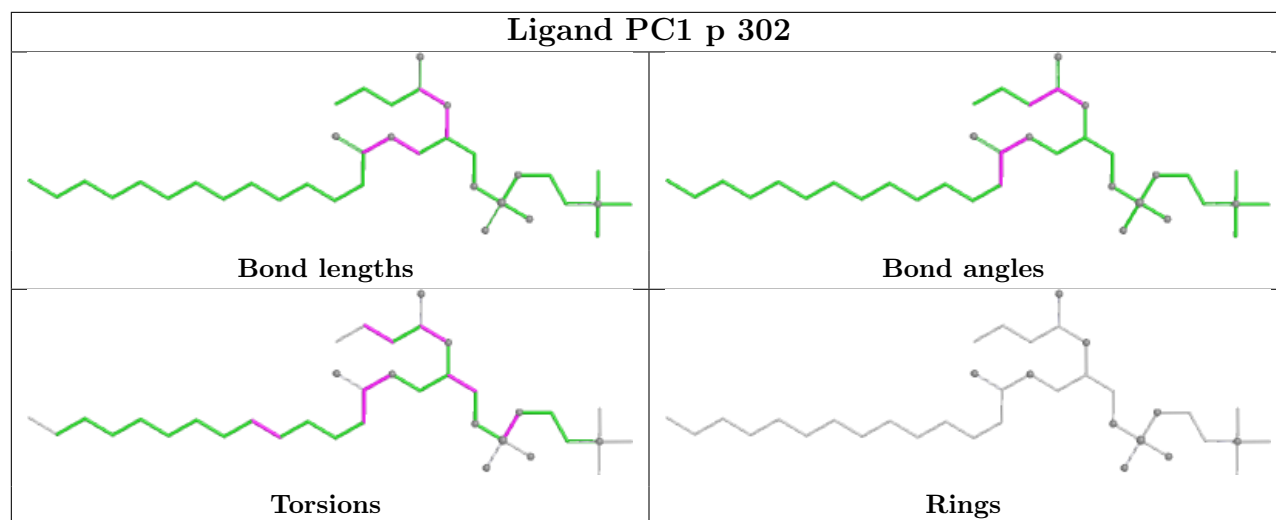
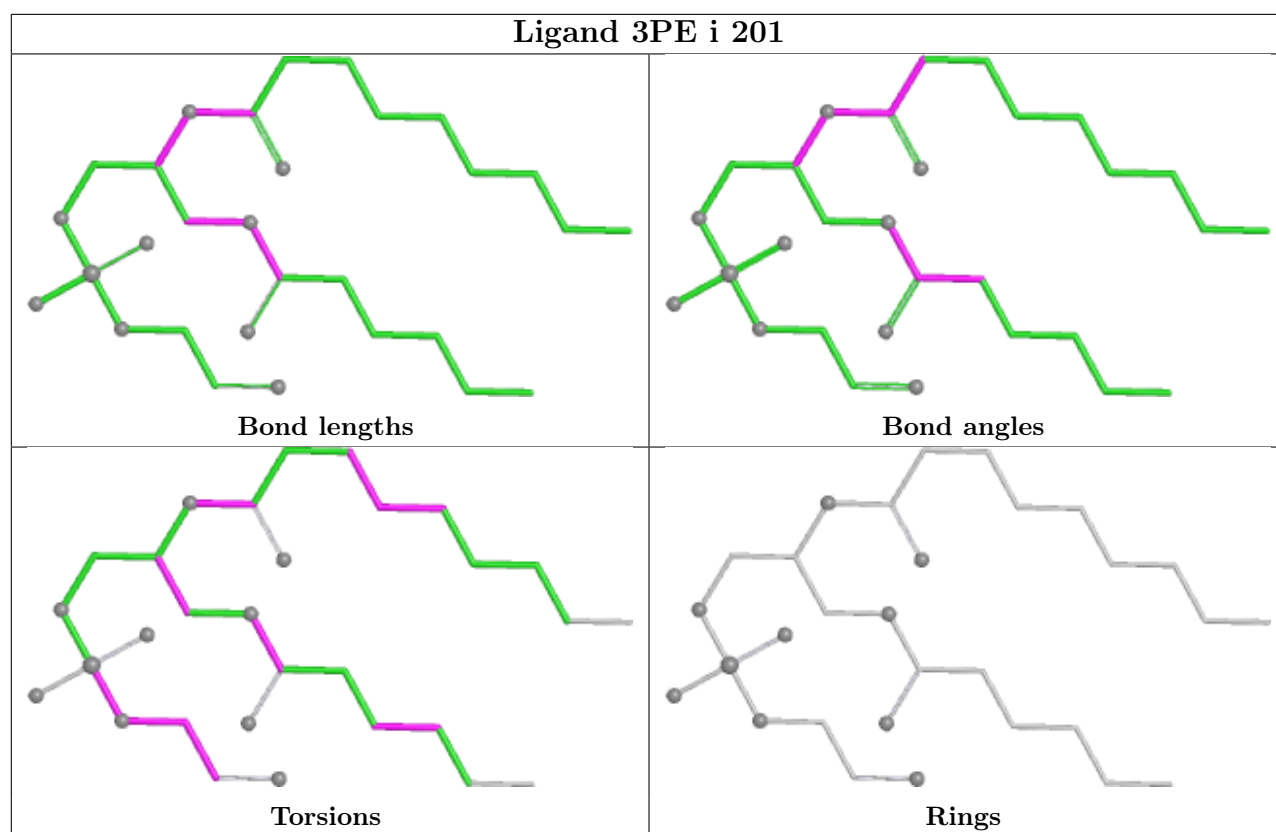


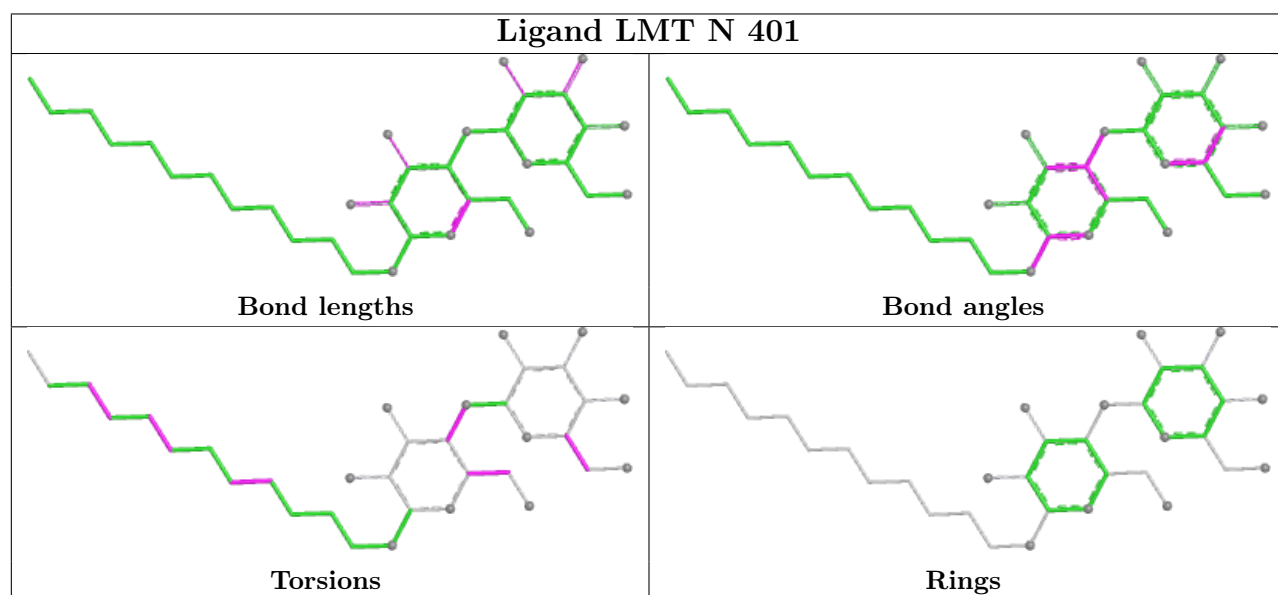
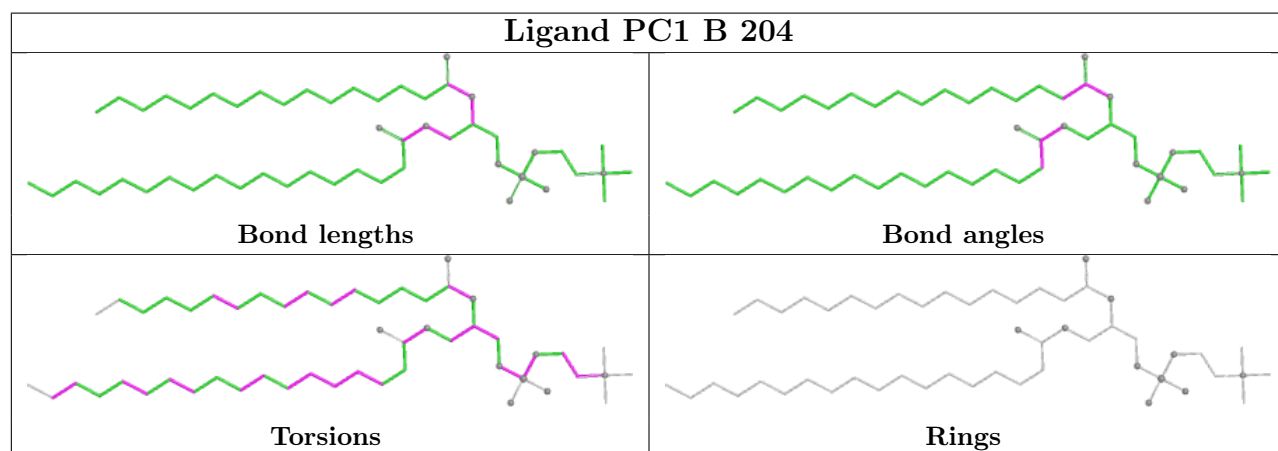
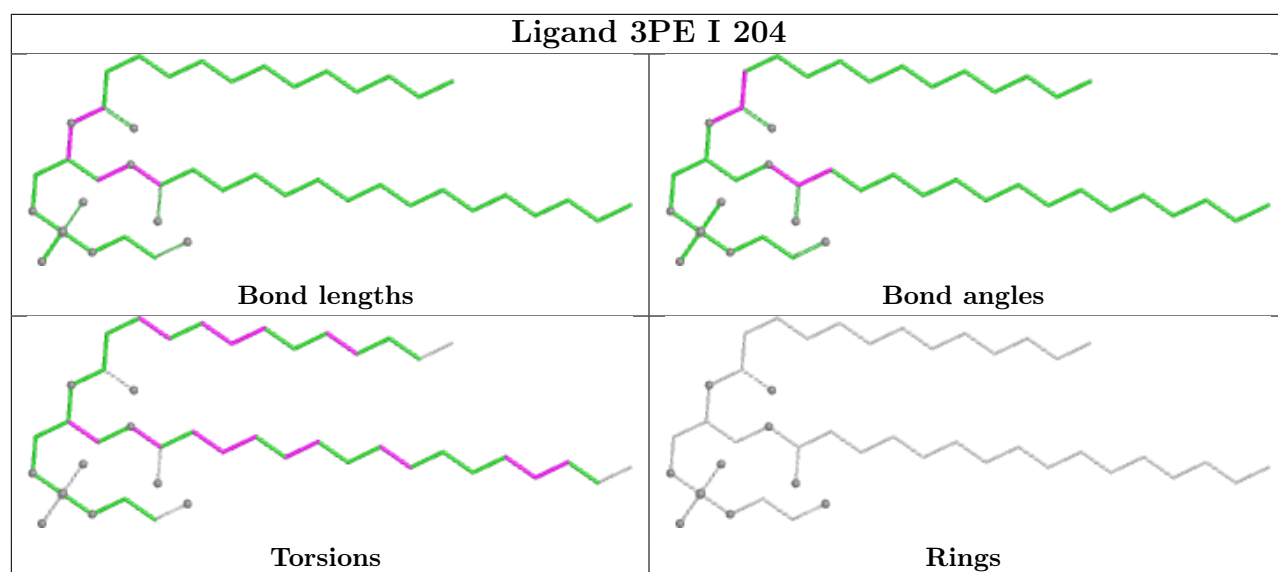


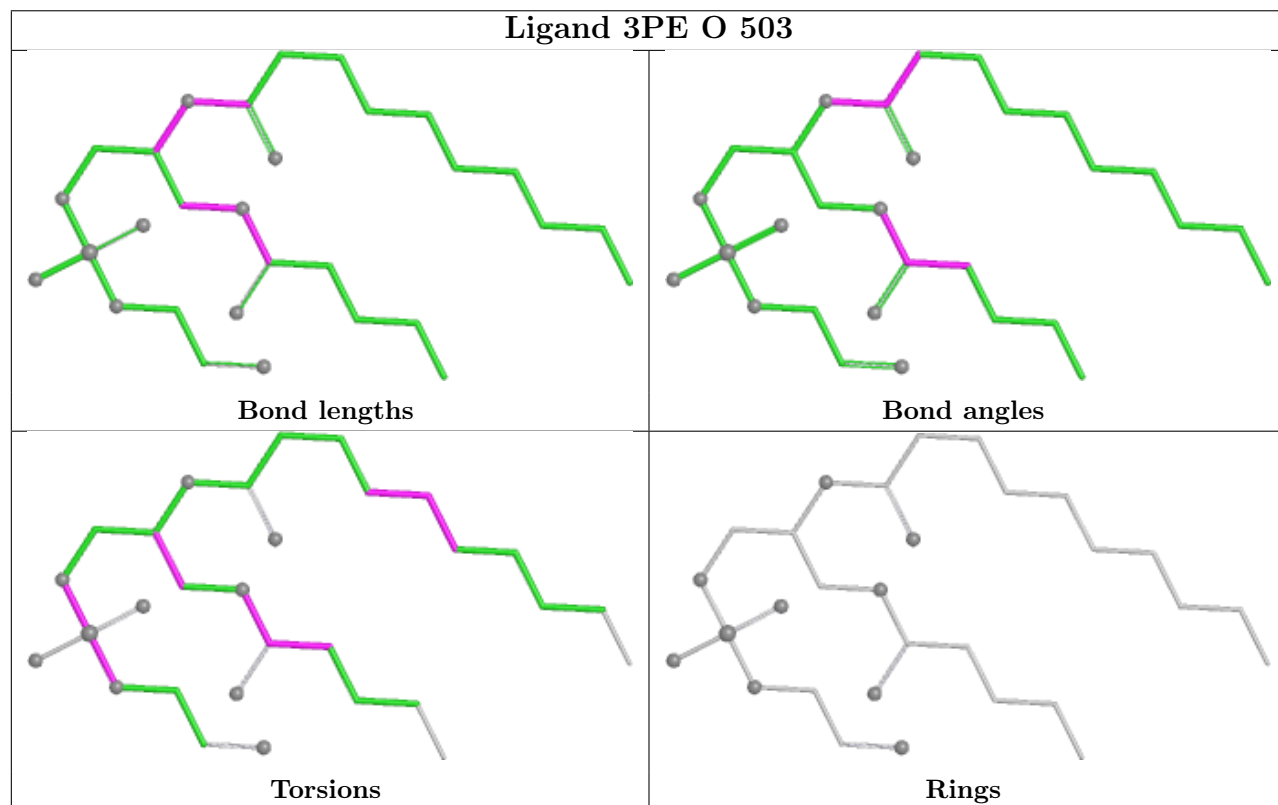
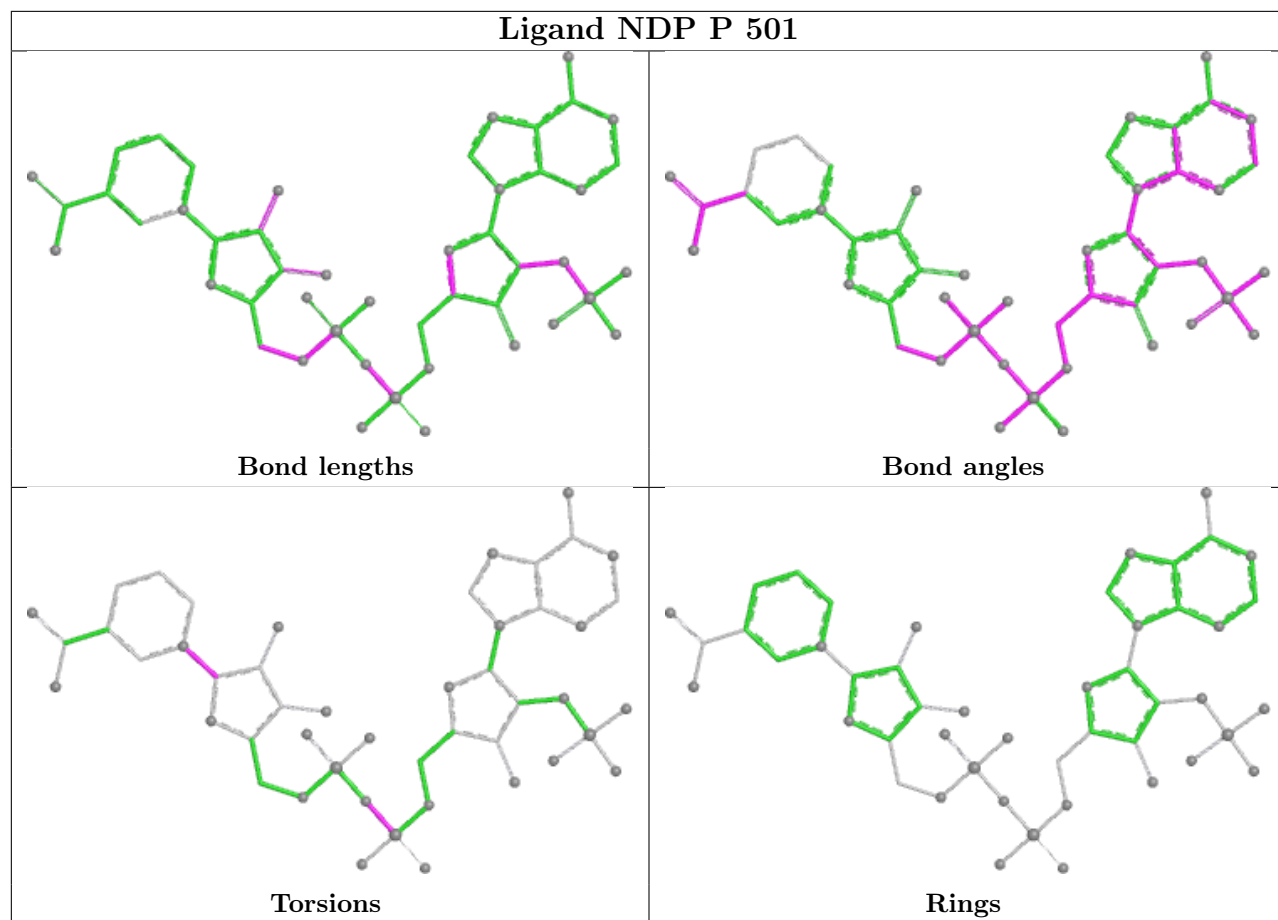


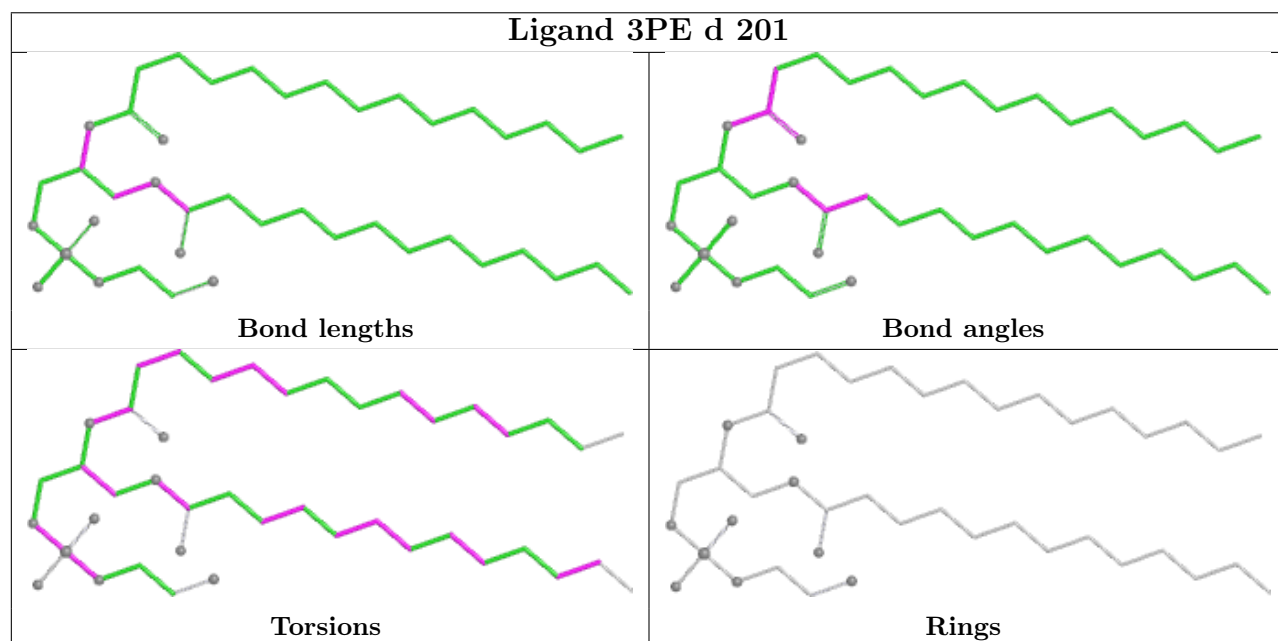
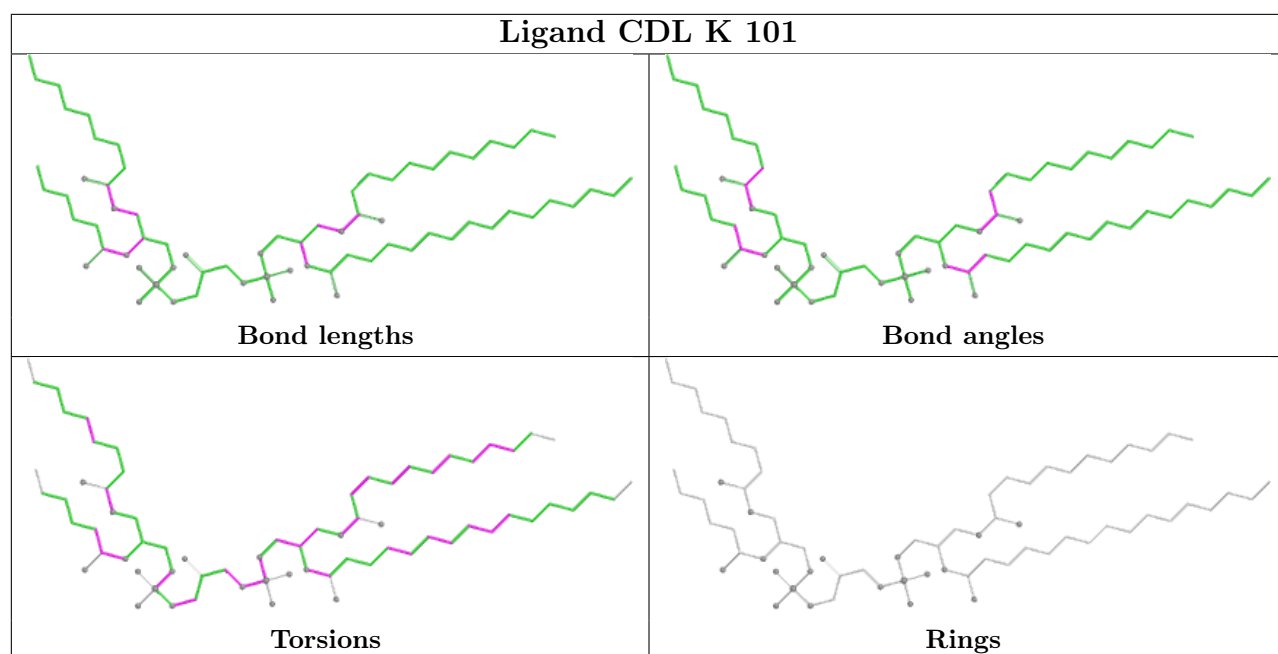


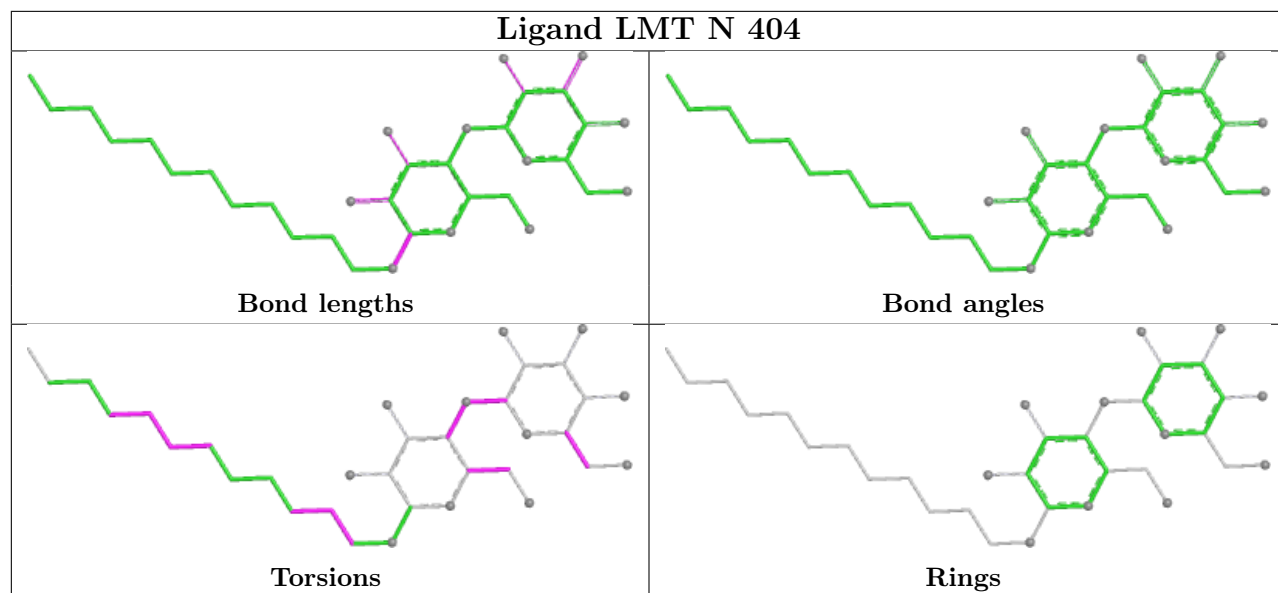


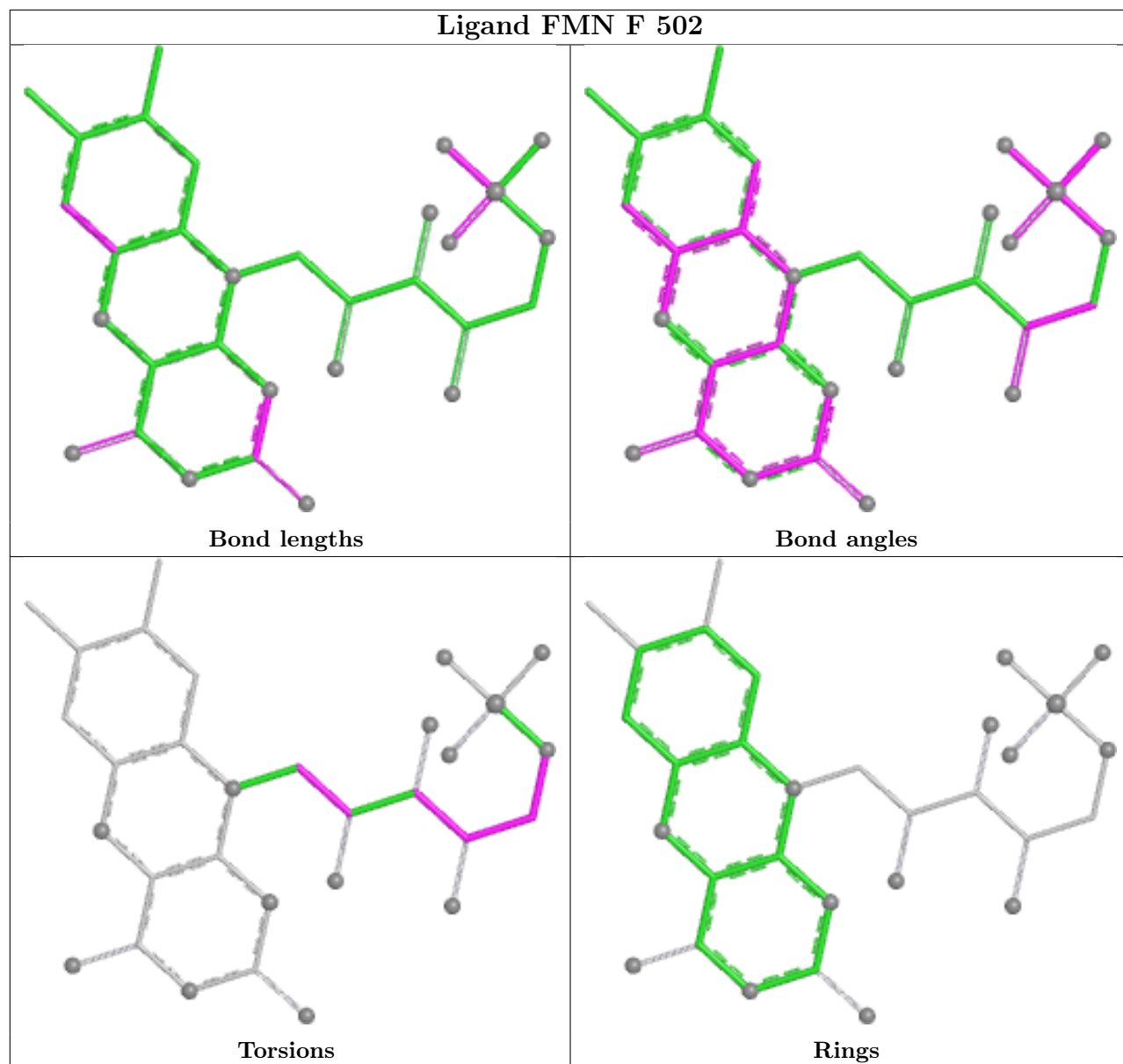


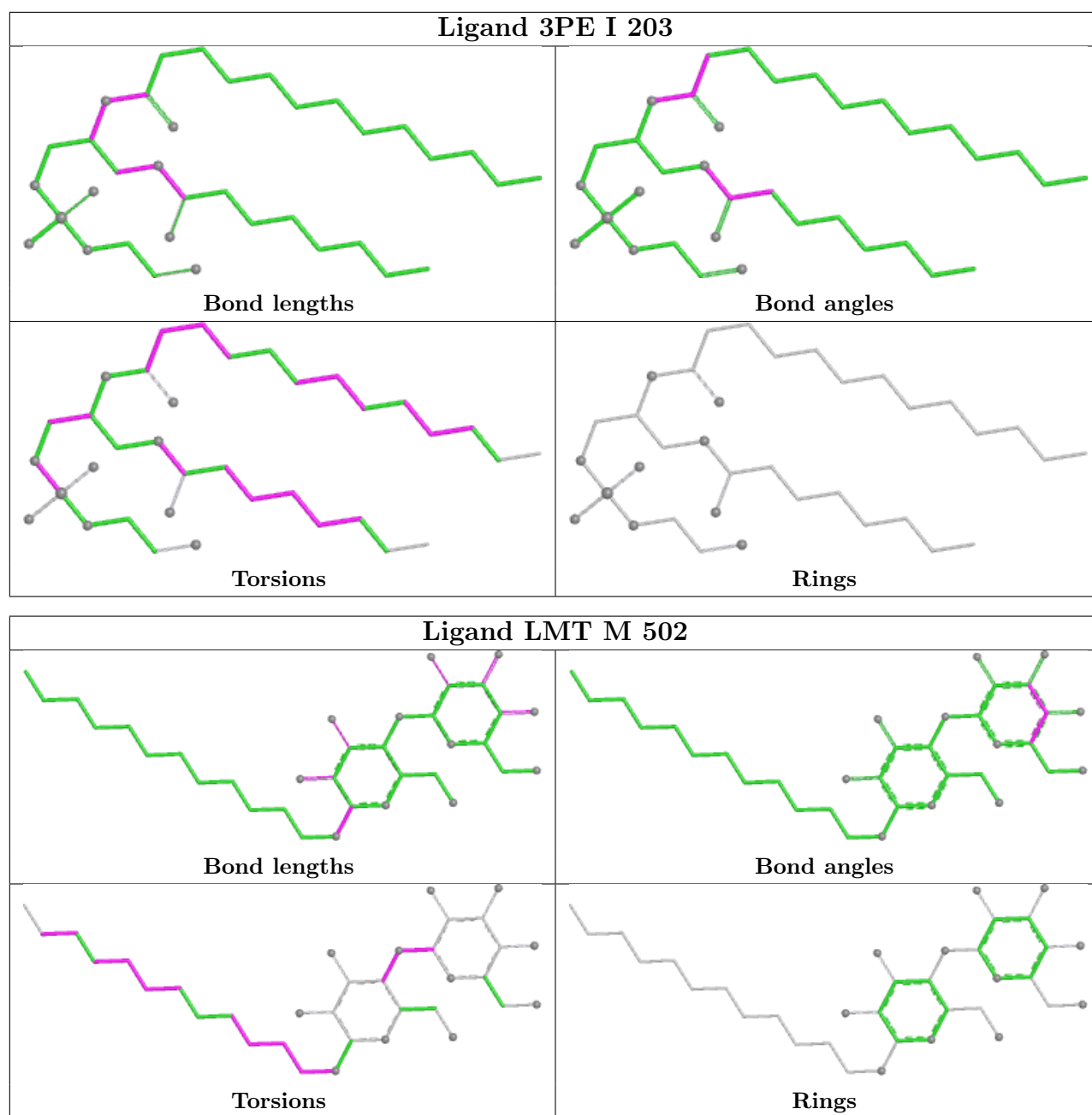


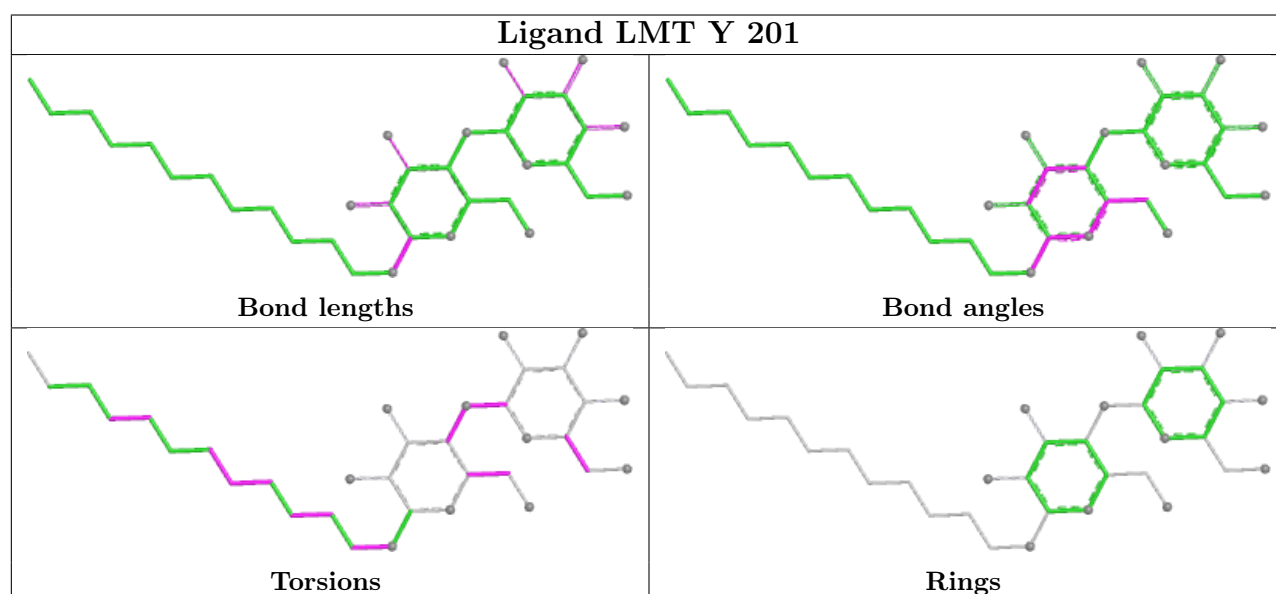
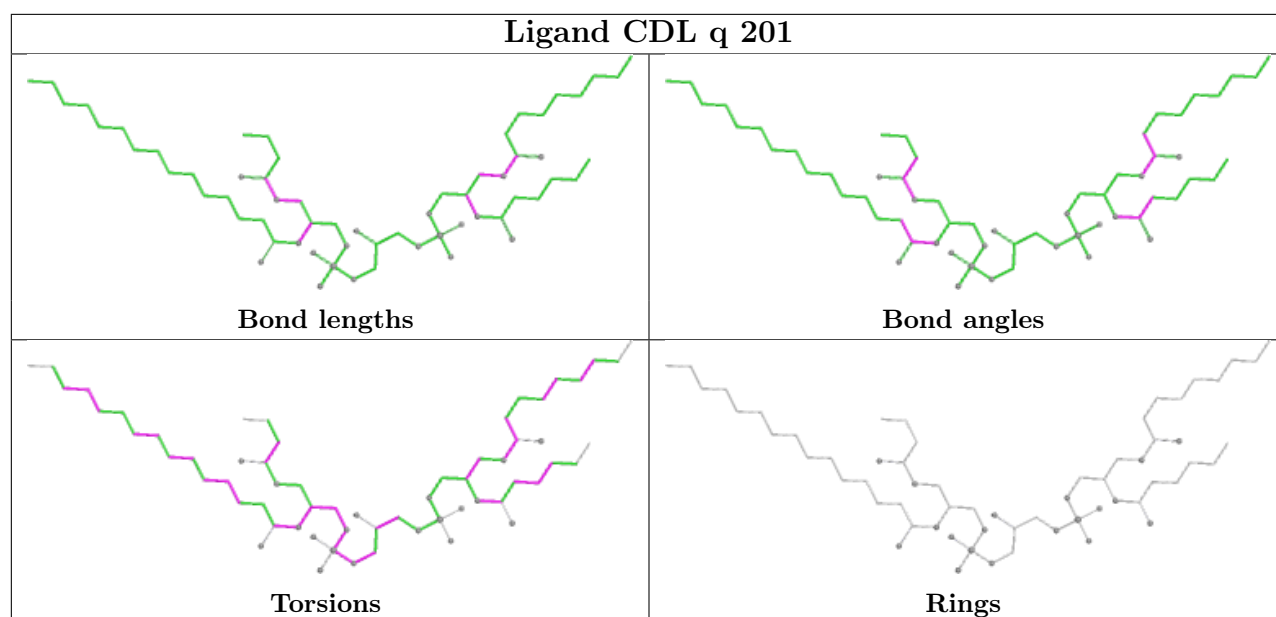




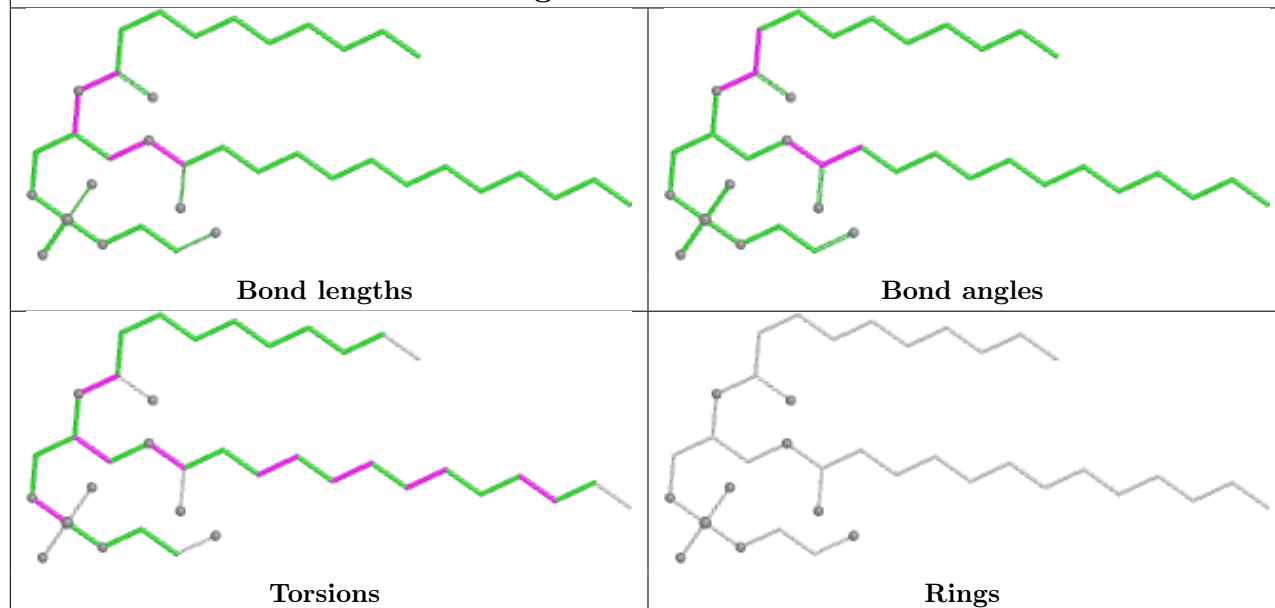




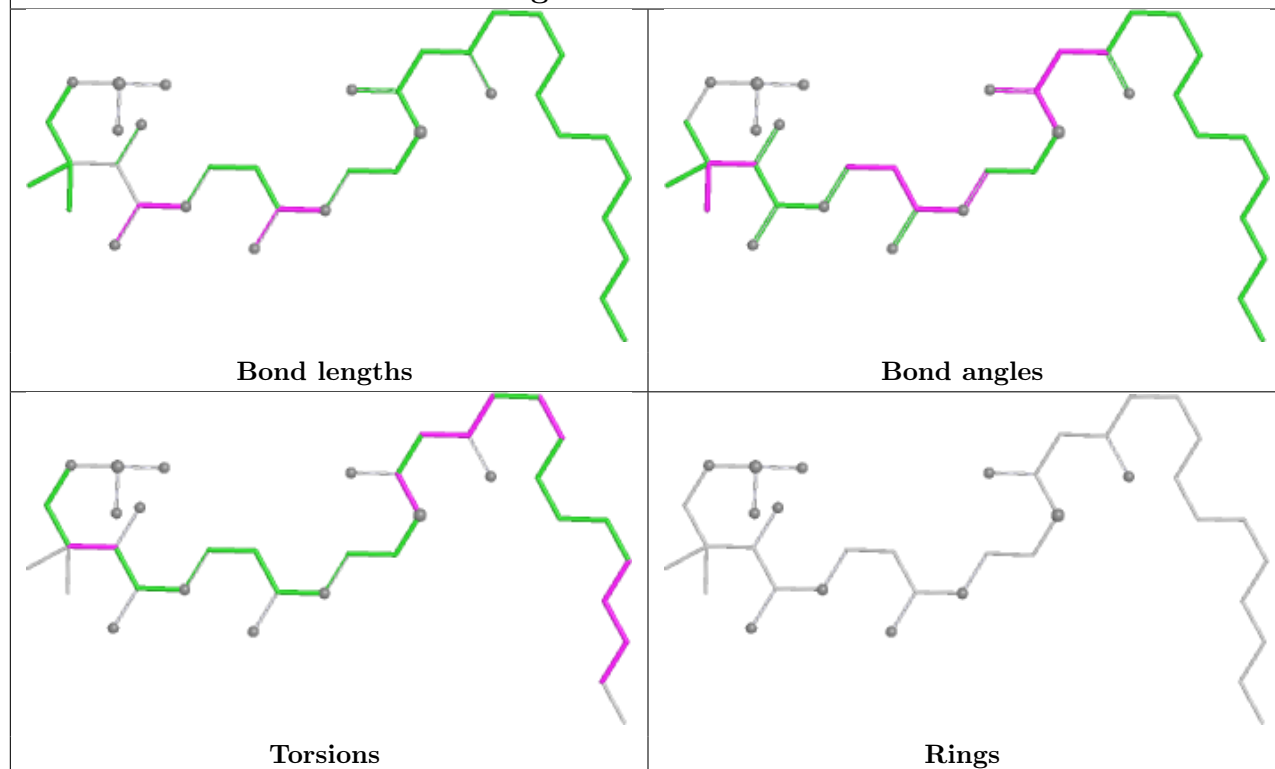


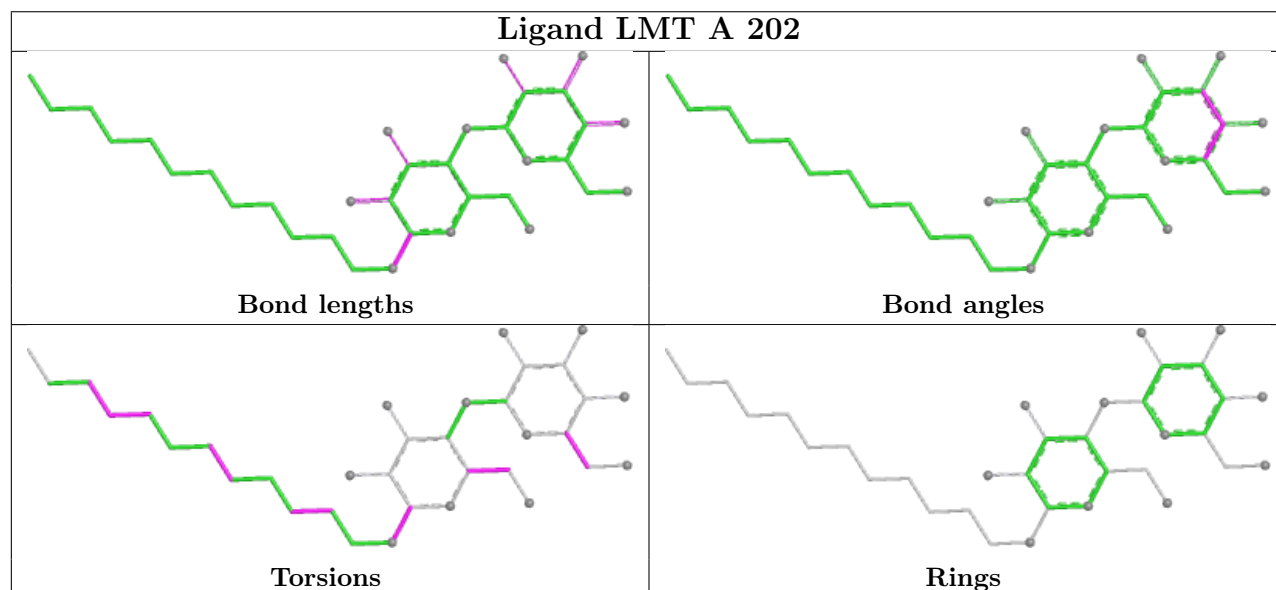
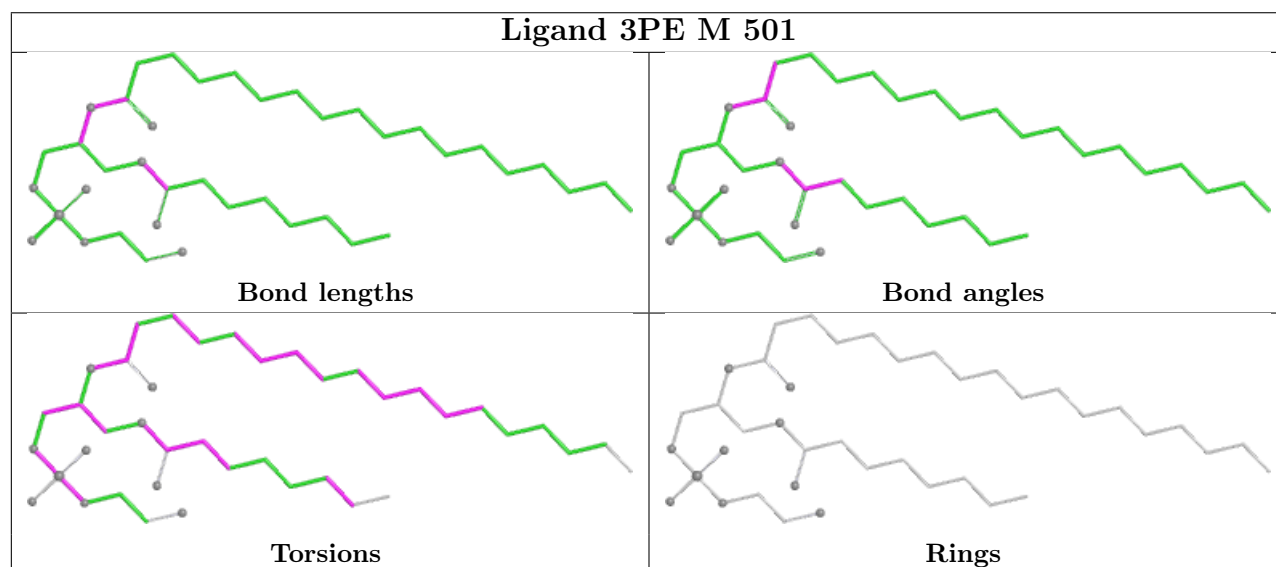
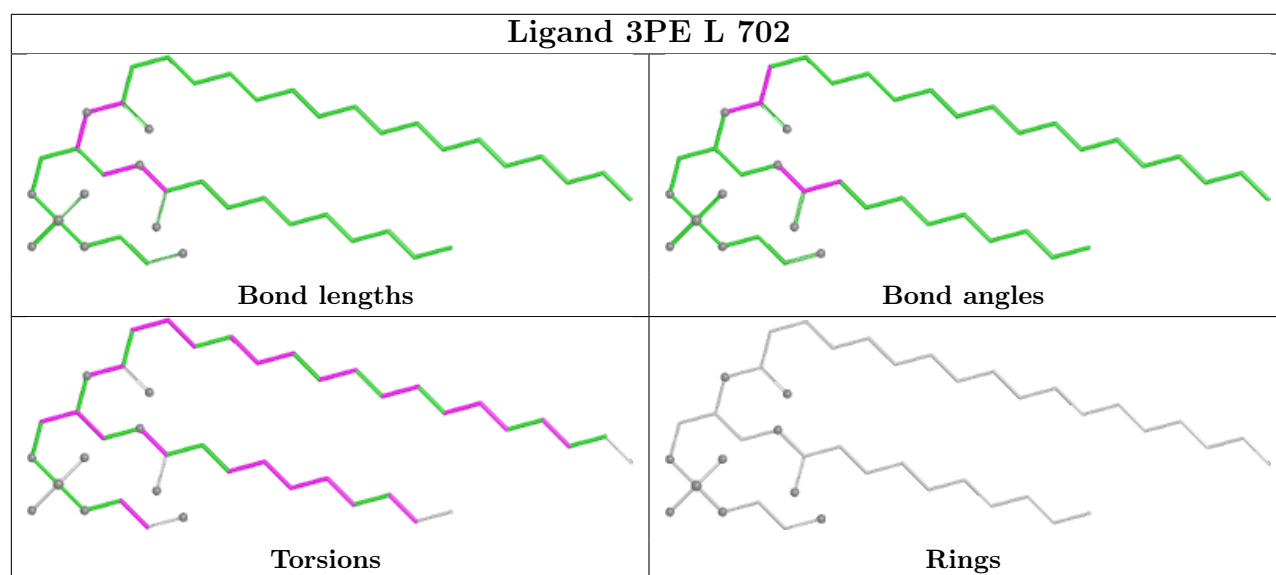


Ligand 3PE N 403



Ligand EHZ U 201





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.

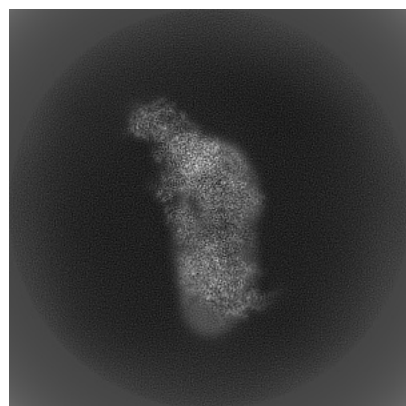
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16965. These allow visual inspection of the internal detail of the map and identification of artifacts.

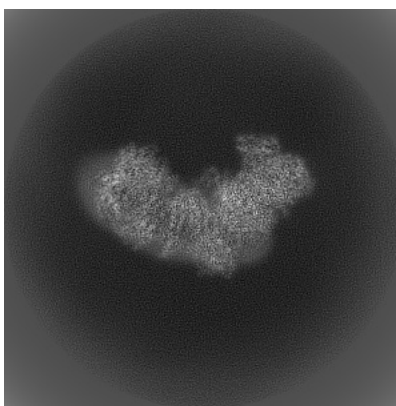
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

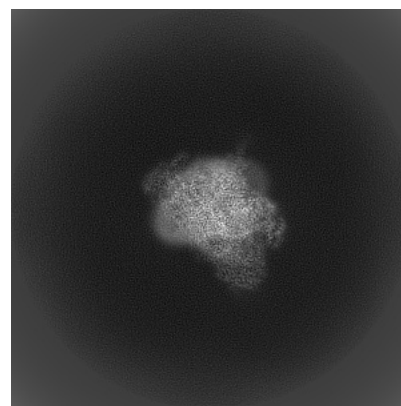
6.1.1 Primary map



X

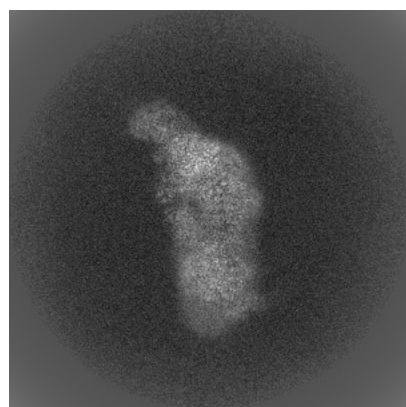


Y

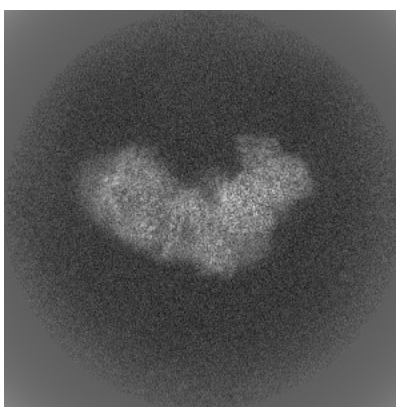


Z

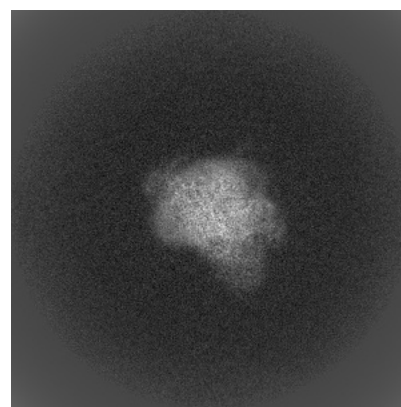
6.1.2 Raw map



X



Y

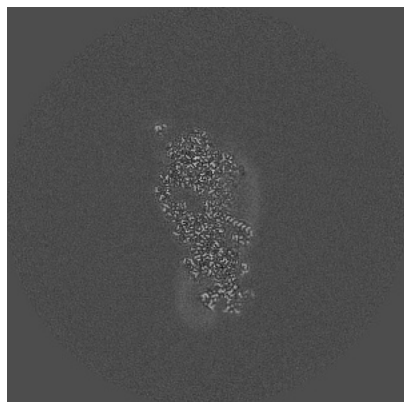


Z

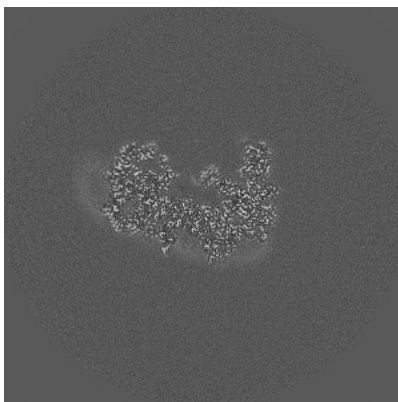
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

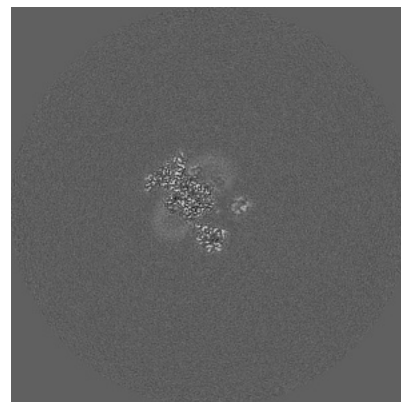
6.2.1 Primary map



X Index: 350

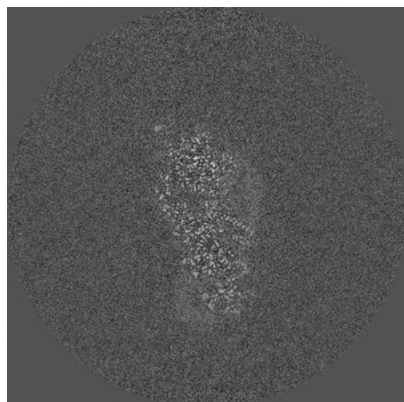


Y Index: 350

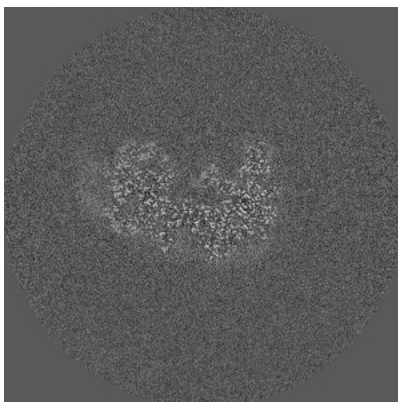


Z Index: 350

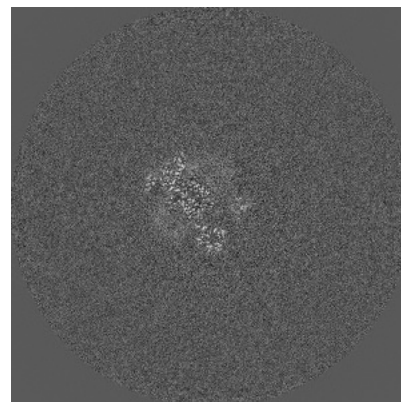
6.2.2 Raw map



X Index: 350



Y Index: 350



Z Index: 350

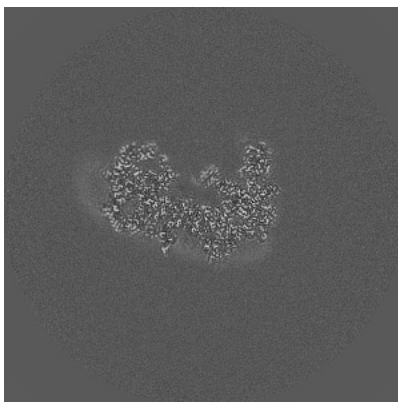
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

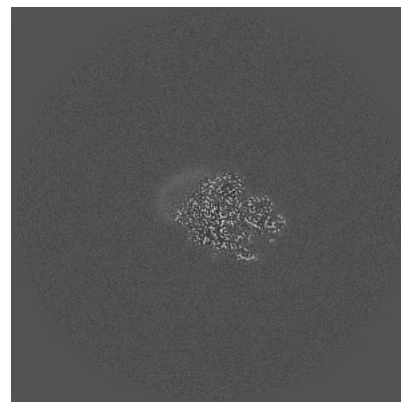
6.3.1 Primary map



X Index: 370

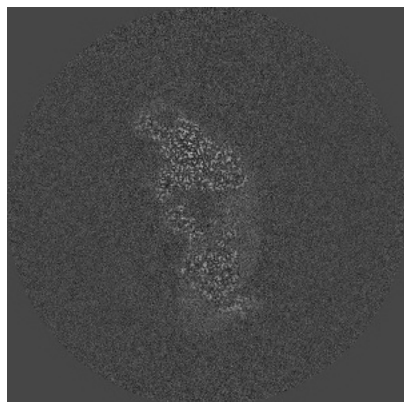


Y Index: 350

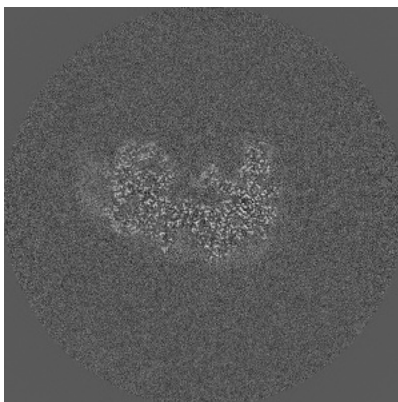


Z Index: 438

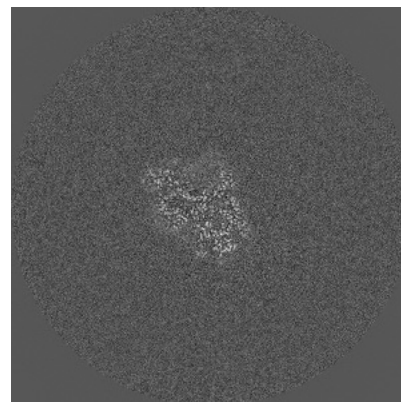
6.3.2 Raw map



X Index: 370



Y Index: 350

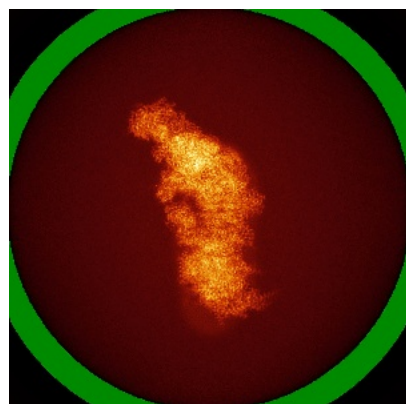


Z Index: 386

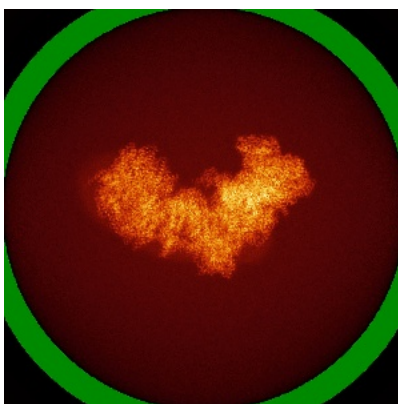
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

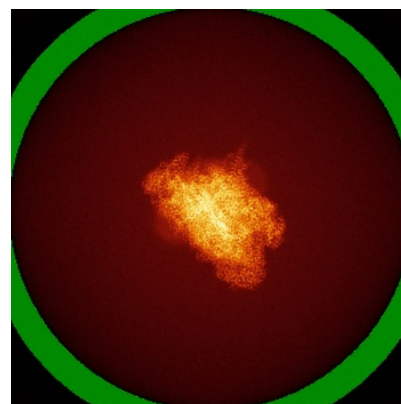
6.4.1 Primary map



X

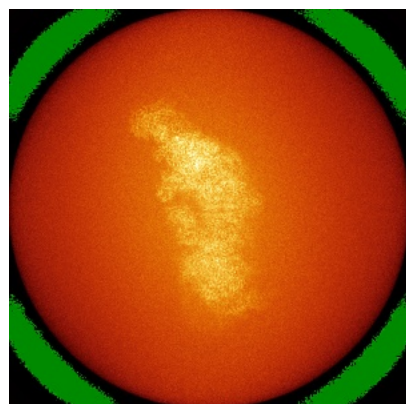


Y

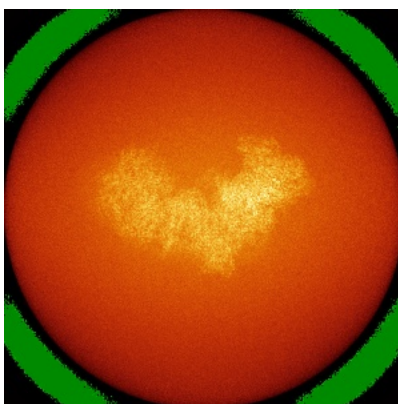


Z

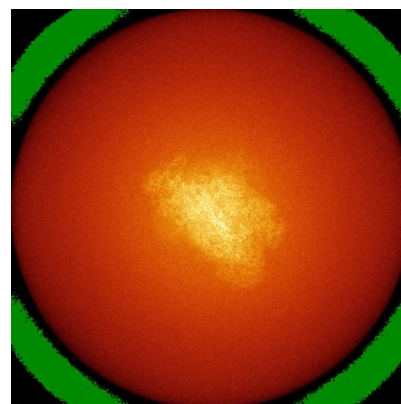
6.4.2 Raw map



X



Y

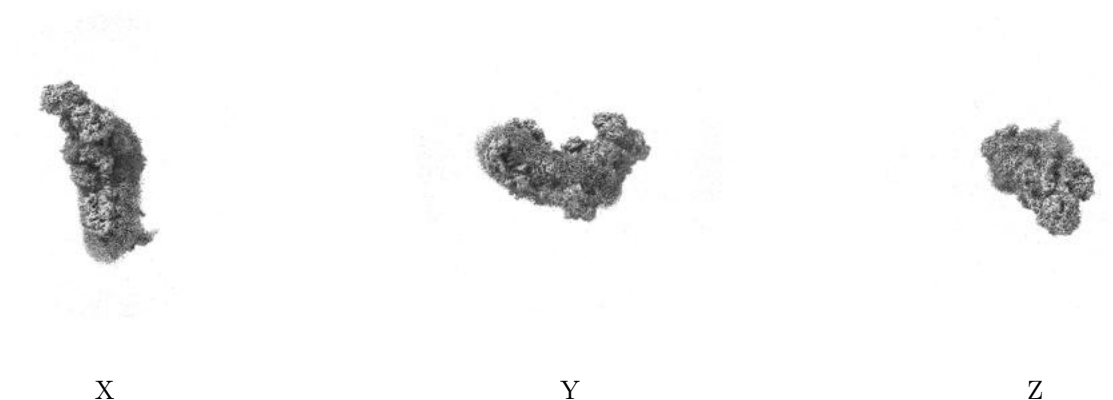


Z

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.

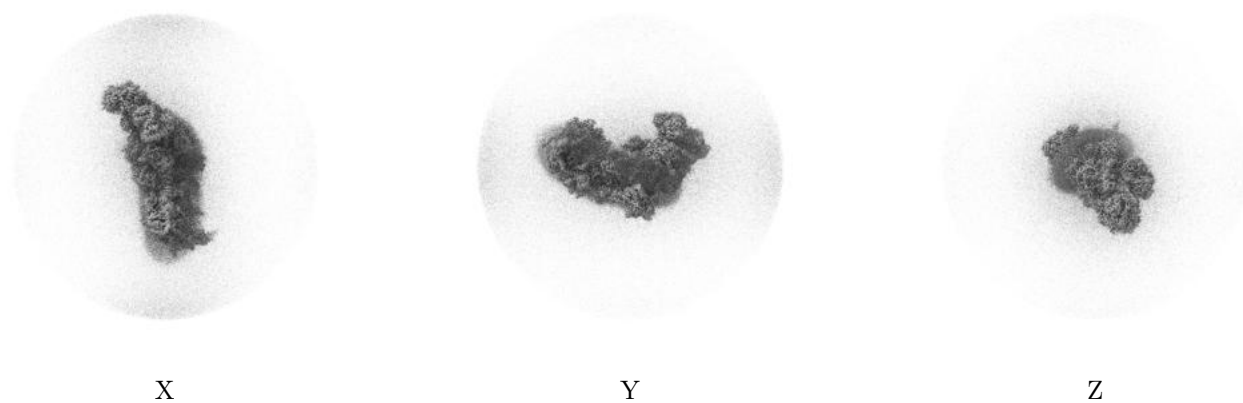
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. 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



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.

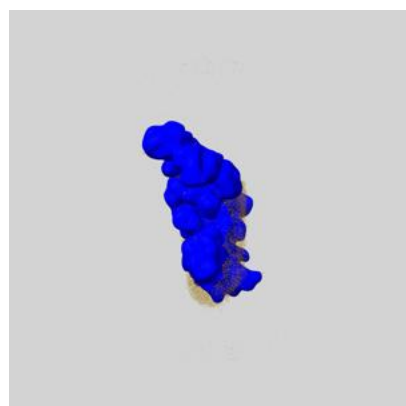
6.6 Mask visualisation [i](#)

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

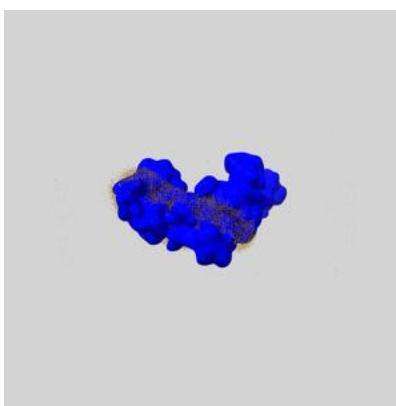
A mask typically either:

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

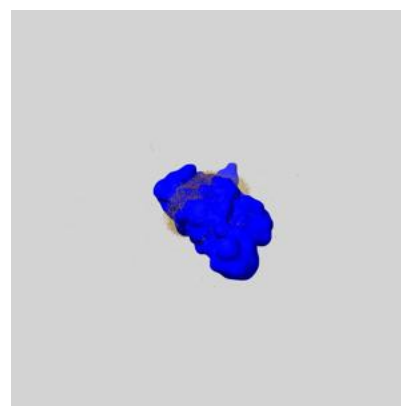
6.6.1 emd_16965_msk_1.map [i](#)



X



Y

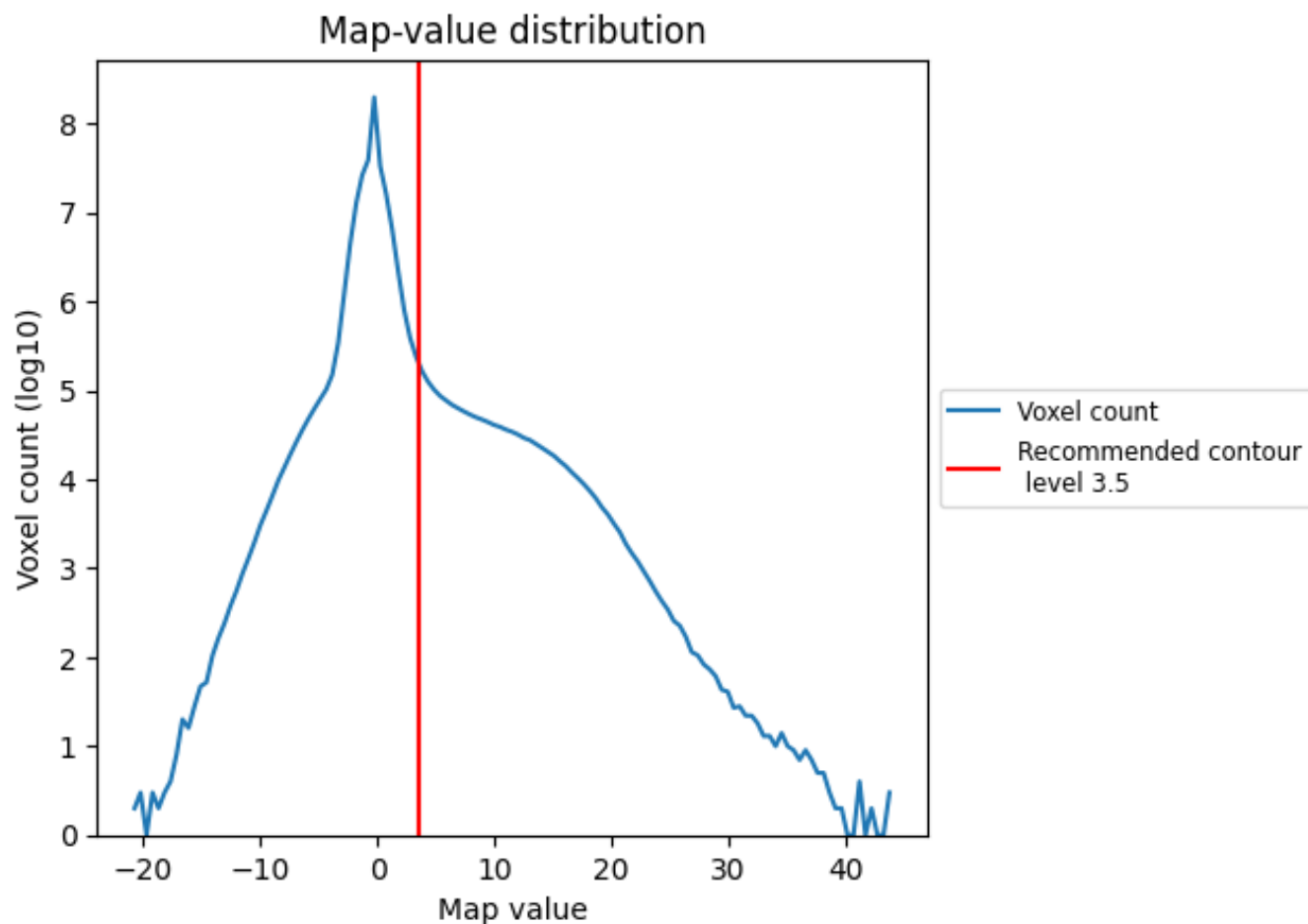


Z

7 Map analysis [i](#)

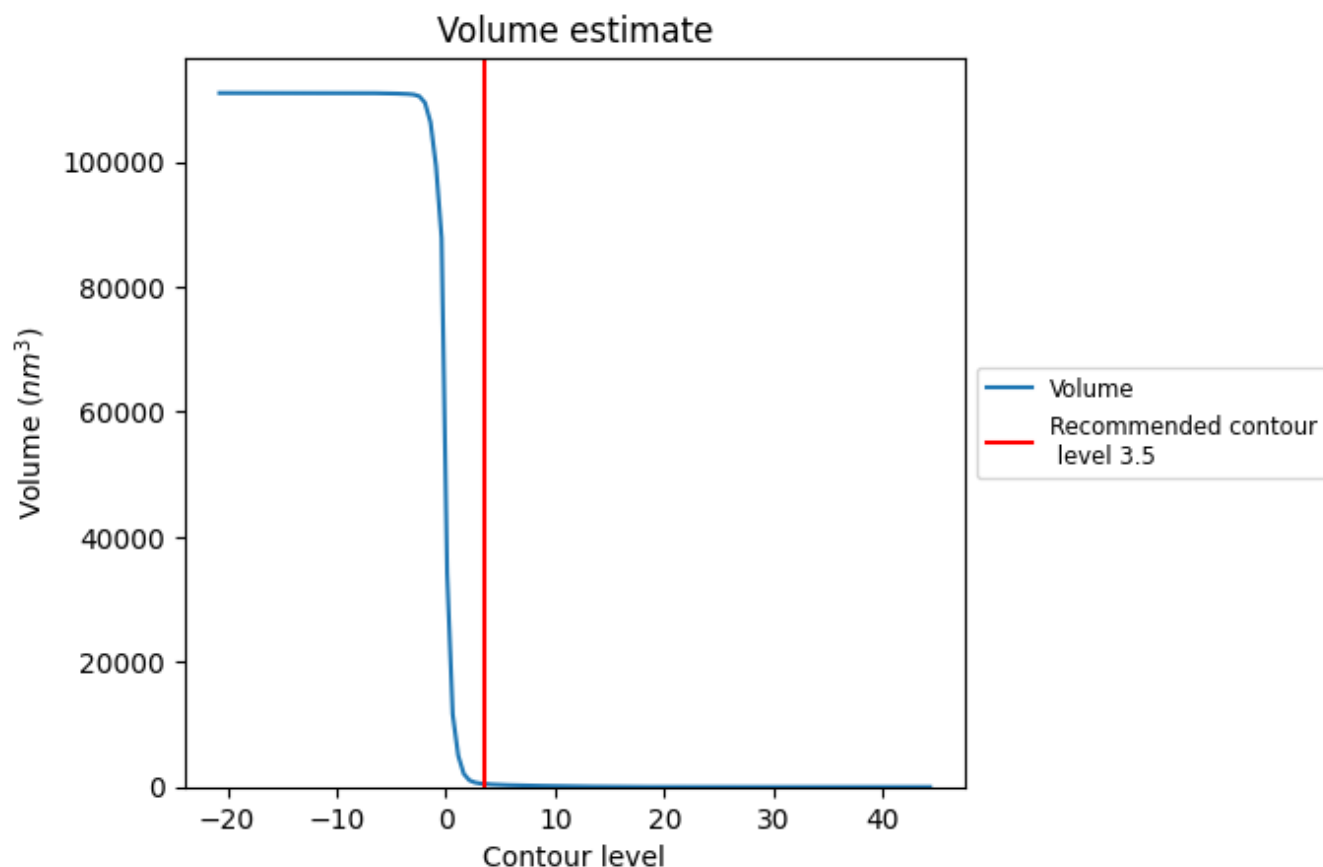
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

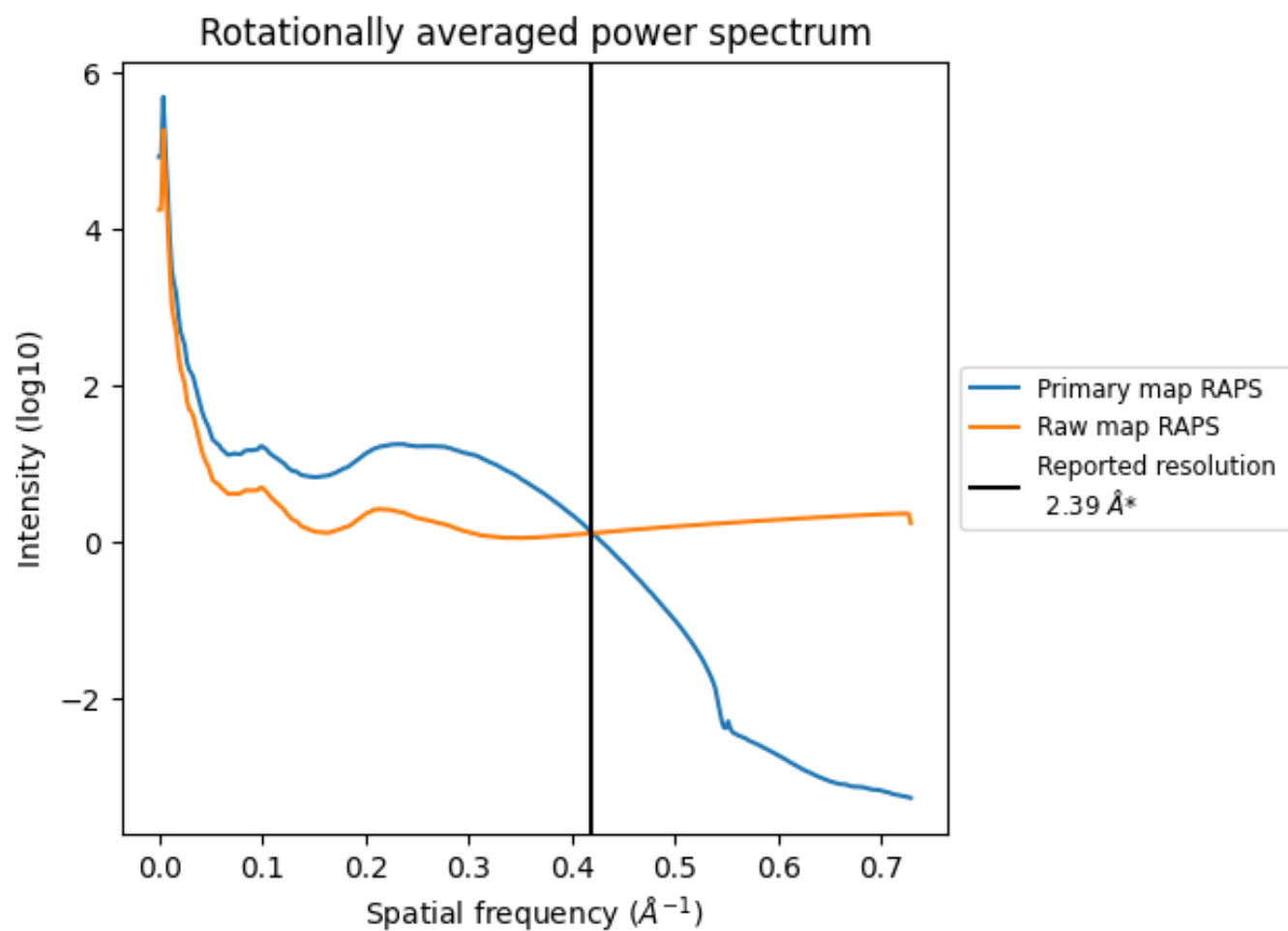
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 496 nm³; this corresponds to an approximate mass of 448 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](#)

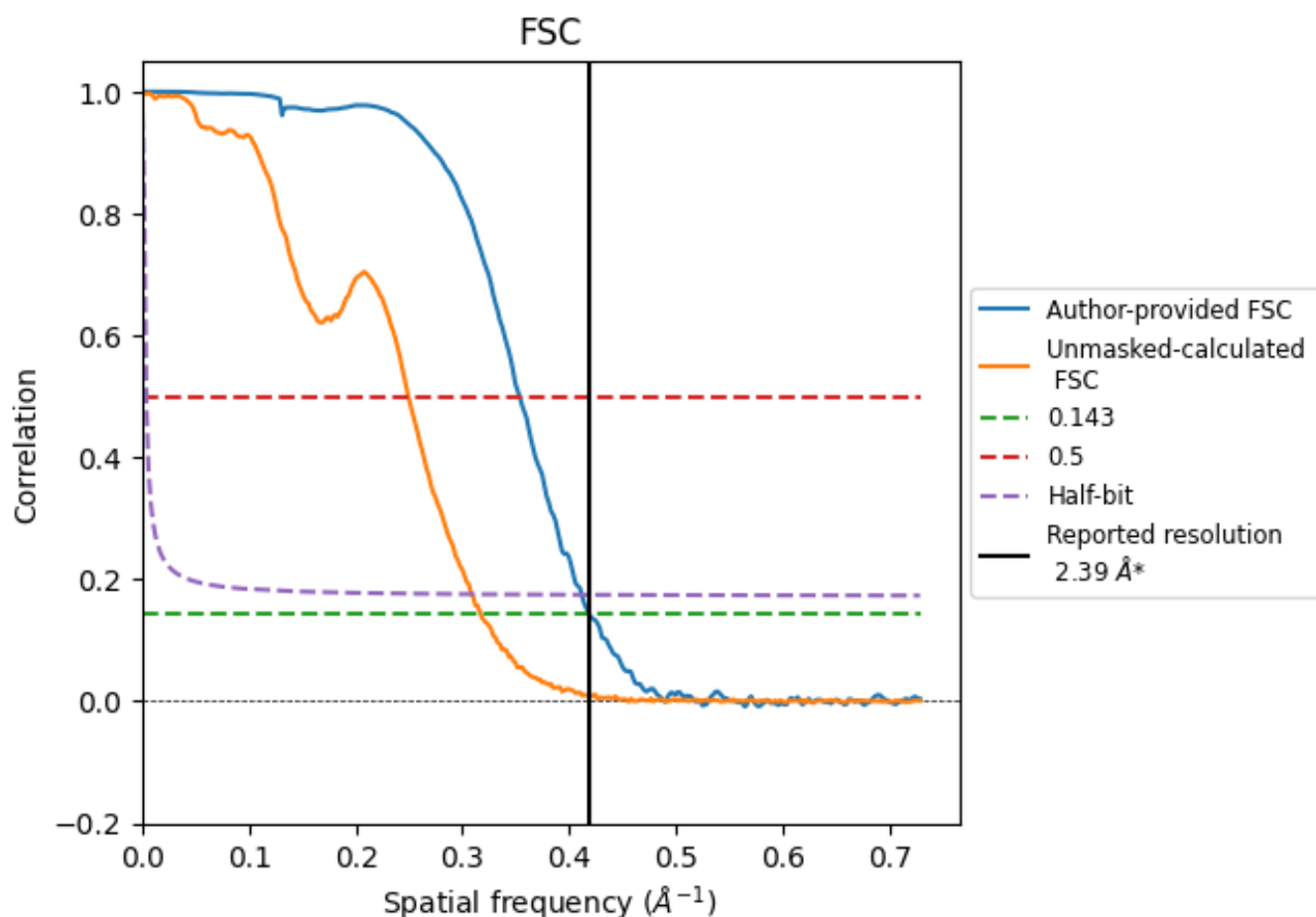


*Reported resolution corresponds to spatial frequency of 0.418 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.418 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

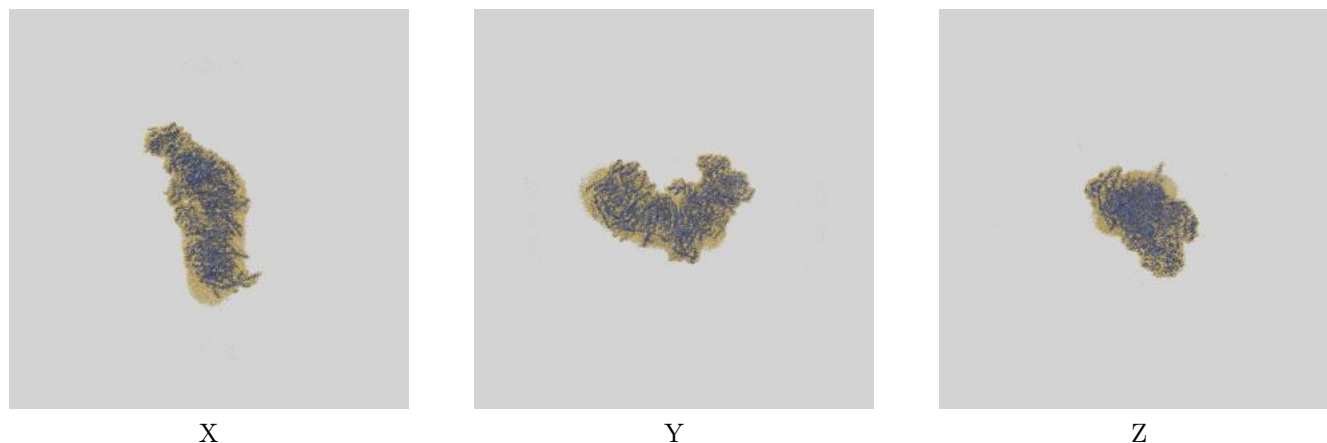
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.39	2.83	2.43
Unmasked-calculated*	3.15	4.01	3.24

*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 3.15 differs from the reported value 2.39 by more than 10 %

9 Map-model fit [i](#)

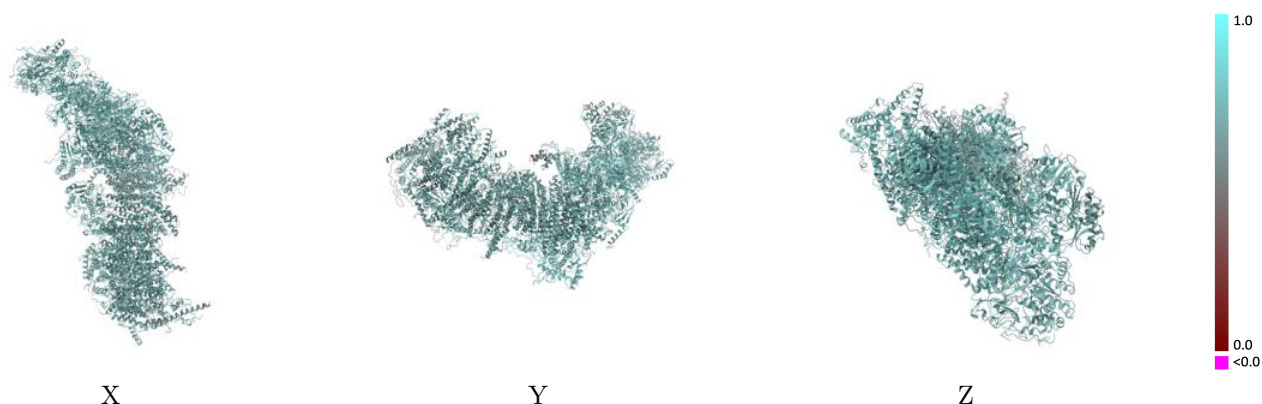
This section contains information regarding the fit between EMDB map EMD-16965 and PDB model 8OM1. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



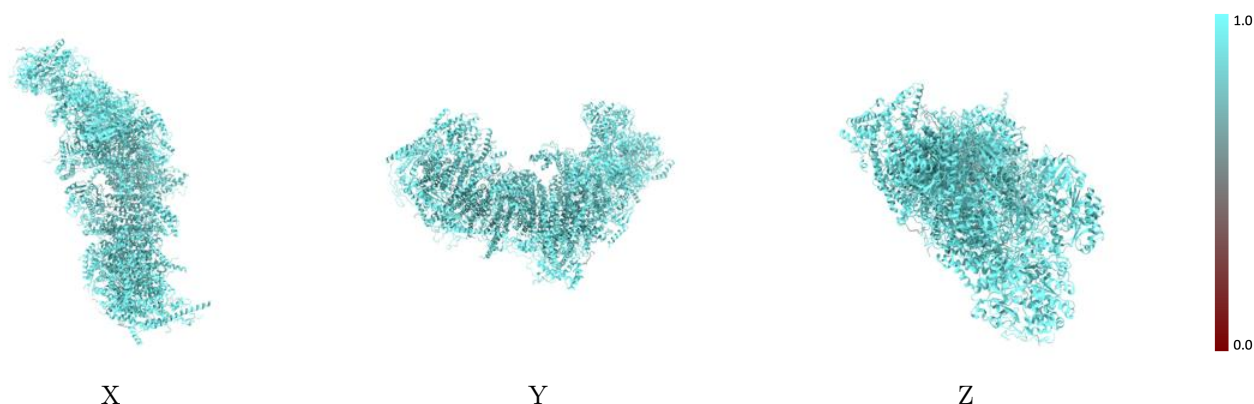
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



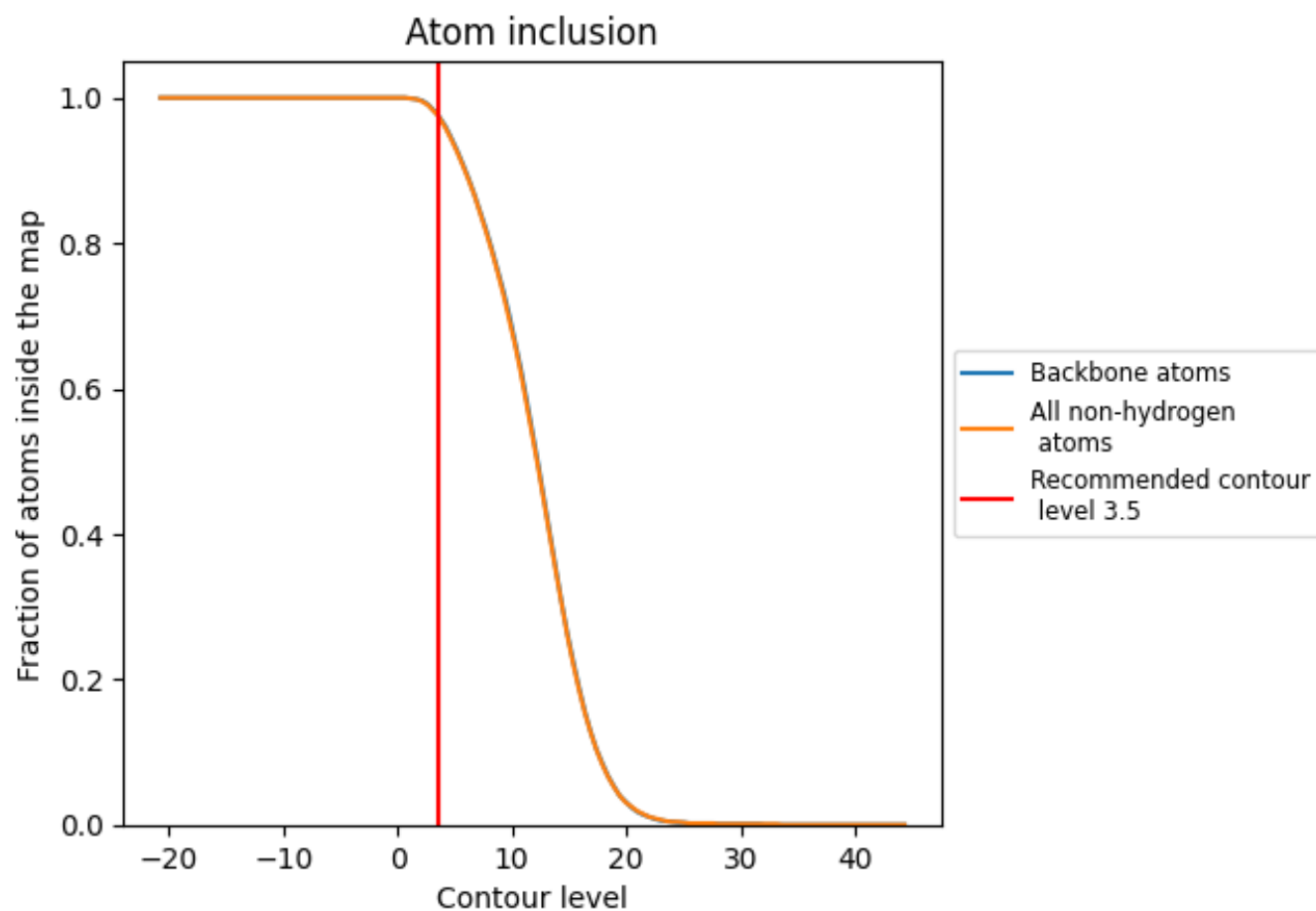
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9760	 0.6960
A	 0.9820	 0.7130
B	 0.9890	 0.7390
C	 0.9870	 0.7410
D	 0.9870	 0.7410
E	 0.9710	 0.6690
F	 0.9860	 0.6800
G	 0.9820	 0.7010
H	 0.9920	 0.7310
I	 0.9750	 0.7350
J	 0.9670	 0.6970
K	 0.9860	 0.7290
L	 0.9800	 0.6810
M	 0.9950	 0.7290
N	 0.9910	 0.7270
O	 0.9820	 0.7090
P	 0.9850	 0.7150
Q	 0.9750	 0.7180
R	 0.9840	 0.7070
S	 0.9700	 0.6370
T	 0.8920	 0.5780
U	 0.9610	 0.6330
V	 0.9710	 0.7130
W	 0.9790	 0.7120
X	 0.9740	 0.6960
Y	 0.9580	 0.6530
Z	 0.9850	 0.7070
a	 0.9960	 0.7230
b	 0.9770	 0.6820
c	 0.9370	 0.6540
d	 0.9720	 0.6940
e	 0.9720	 0.6980
f	 0.9350	 0.6500
g	 0.9770	 0.6930
h	 0.9640	 0.6890



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Chain	Atom inclusion	Q-score
i	 0.9520	 0.6290
j	 0.9420	 0.6120
k	 0.9580	 0.6190
l	 0.9620	 0.6640
m	 0.9640	 0.6750
n	 0.9600	 0.6550
o	 0.9410	 0.6080
p	 0.9700	 0.6640
q	 0.9790	 0.7060
r	 0.9600	 0.6970
s	 0.9440	 0.6380