Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:47 PM UTC

PDB ID	:	6TDV / pdb_00006tdv
EMDB ID	:	EMD-10468
Title	:	Cryo-EM structure of Euglena gracilis mitochondrial ATP synthase, membrane region
Authors	:	Muhleip, A.; Amunts, A.
Deposited on	:	2019-11-10
Resolution	:	2.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

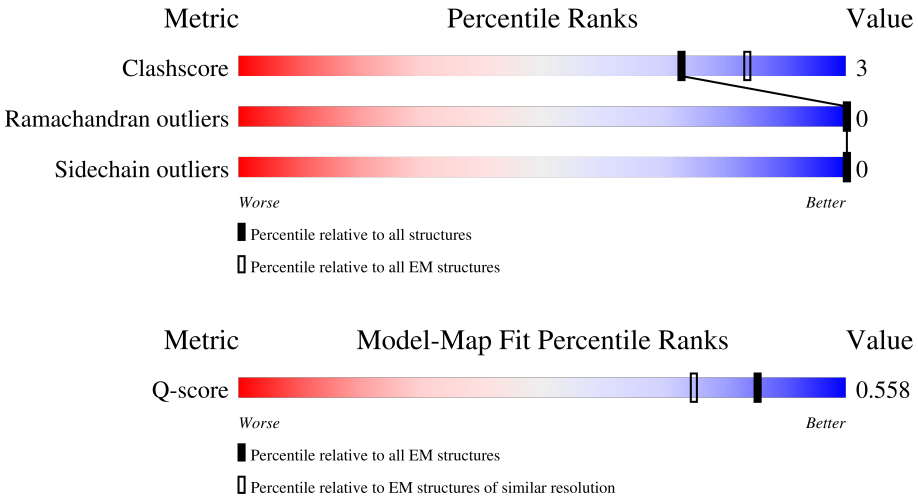
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.80 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	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	A	487	7% 93% 7%
1	a	487	7% 92% 7%
2	B	338	8% 9% 91%
2	b	338	8% 9% 91%

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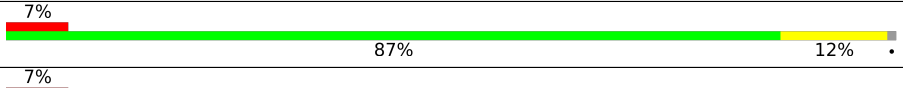
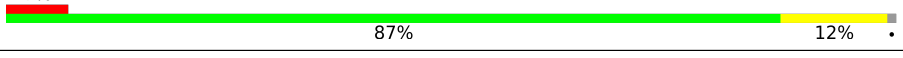
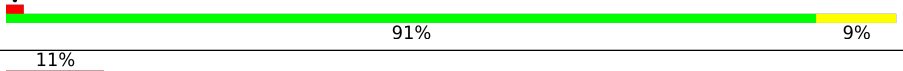
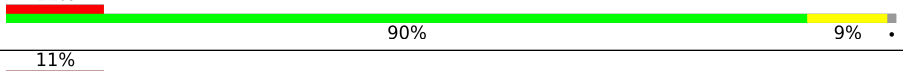
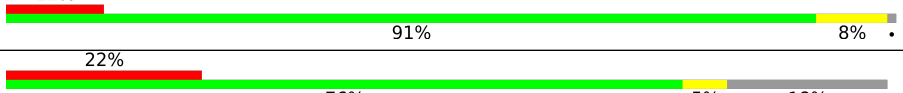
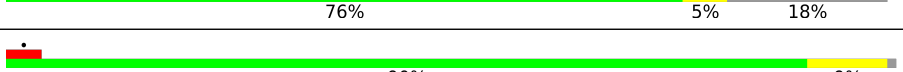
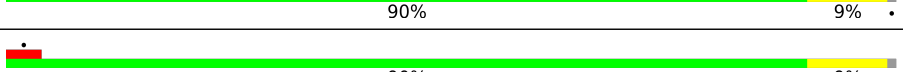
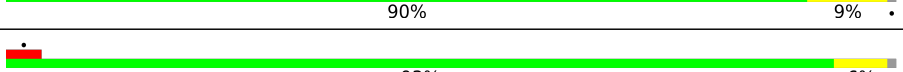
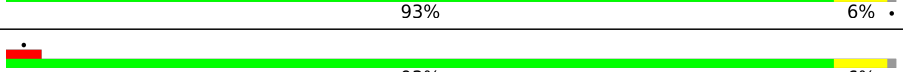
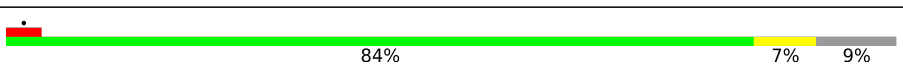
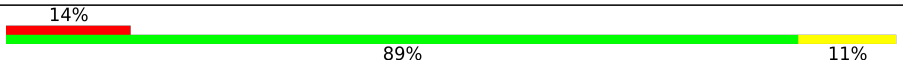
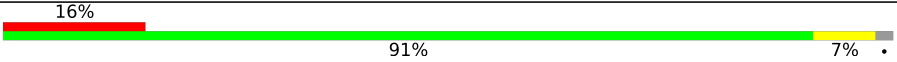
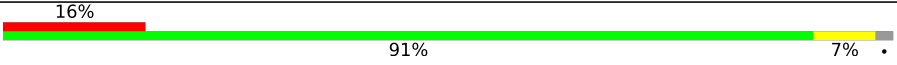
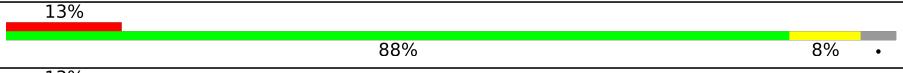
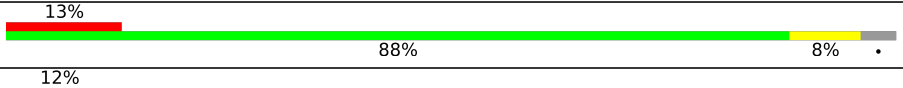
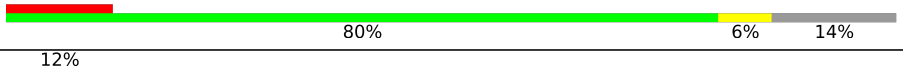
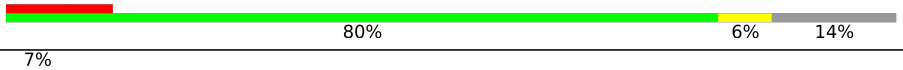
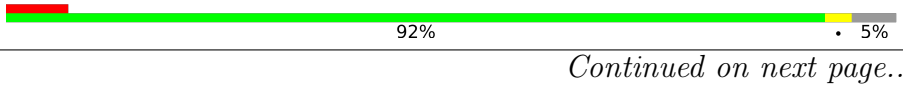
Mol	Chain	Length	Quality of chain
3	D	187	
3	d	187	
4	E	97	
4	e	97	
5	F	274	
5	f	274	
6	G	112	
6	g	112	
7	H	476	
7	h	476	
8	I	98	
8	i	98	
9	J	104	
9	j	104	
10	K	113	
10	k	113	
11	L	57	
11	l	57	
12	M	169	
12	m	169	
13	N	137	
13	n	137	
14	O	116	
14	o	116	
15	P	120	

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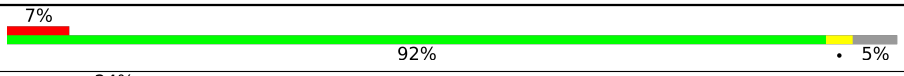
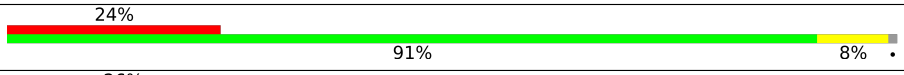
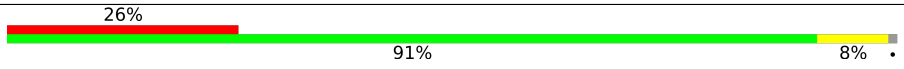
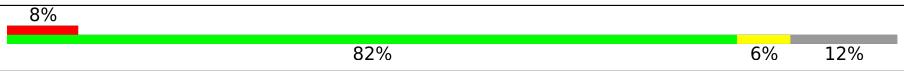
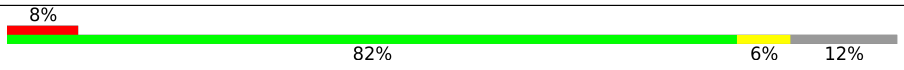
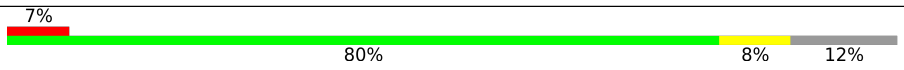
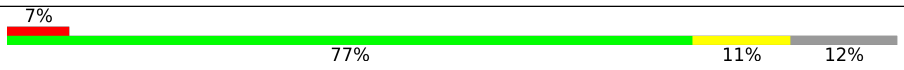
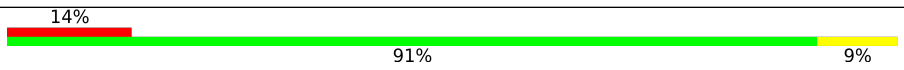
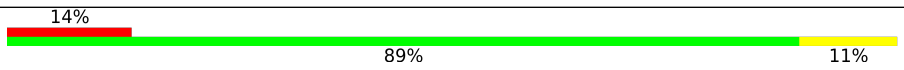
Mol	Chain	Length	Quality of chain
15	p	120	
16	Q	90	
16	q	90	
17	R	78	
17	r	78	
18	S	74	
18	s	74	
19	T	66	
19	t	66	

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 95420 atoms, of which 47674 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 ATPTB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	486	Total	C	H	N	O	S	0	0
			7864	2525	3919	677	733	10		
1	a	486	Total	C	H	N	O	S	0	0
			7864	2525	3919	677	733	10		

- Molecule 2 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	31	Total	C	H	N	O	0	0
			494	153	243	44	54		
2	b	31	Total	C	H	N	O	0	0
			494	153	243	44	54		

- Molecule 3 is a protein called ATPTB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	186	Total	C	H	N	O	S	0	0
			3040	977	1519	269	267	8		
3	d	186	Total	C	H	N	O	S	0	0
			3040	977	1519	269	267	8		

- Molecule 4 is a protein called ATPTB12.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	96	Total	C	H	N	O	S	0	0
			1574	509	777	144	141	3		
4	e	96	Total	C	H	N	O	S	0	0
			1577	510	779	144	141	3		

- Molecule 5 is a protein called subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	274	Total	C	H	N	O	S	0	0
			4639	1566	2327	341	391	14		
5	f	274	Total	C	H	N	O	S	0	0
			4642	1566	2329	342	391	14		

- Molecule 6 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	111	Total	C	H	N	O	S	0	0
			1803	566	924	160	146	7		
6	g	111	Total	C	H	N	O	S	0	0
			1803	566	924	160	146	7		

- Molecule 7 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	388	Total	C	H	N	O	S	0	0
			6165	1987	3059	512	598	9		
7	h	388	Total	C	H	N	O	S	0	0
			6165	1987	3059	512	598	9		

- Molecule 8 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	97	Total	C	H	N	O	S	0	0
			1553	504	771	140	135	3		
8	i	97	Total	C	H	N	O	S	0	0
			1553	504	771	140	135	3		

- Molecule 9 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	103	Total	C	H	N	O	S	0	0
			1734	581	853	151	146	3		
9	j	103	Total	C	H	N	O	S	0	0
			1734	581	853	151	146	3		

- Molecule 10 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	K	103	Total	C	H	N	O	S	0	0
			1637	530	821	136	144	6		

Continued on next page...

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	k	103	Total	C	H	N	O	S	0	0
			1637	530	821	136	144	6		

- Molecule 11 is a protein called subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	57	Total	C	H	N	O	0	0
			1008	350	507	69	82		
11	l	57	Total	C	H	N	O	0	0
			1008	350	507	69	82		

- Molecule 12 is a protein called ATPEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	M	166	Total	C	H	N	O	S	0	0
			2717	887	1354	228	240	8		
12	m	166	Total	C	H	N	O	S	0	0
			2717	887	1354	228	240	8		

- Molecule 13 is a protein called ATPEG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	N	131	Total	C	H	N	O	S	0	0
			2167	714	1070	198	182	3		
13	n	131	Total	C	H	N	O	S	0	0
			2167	714	1070	198	182	3		

- Molecule 14 is a protein called ATPEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	O	100	Total	C	H	N	O	S	0	0
			1652	556	803	146	145	2		
14	o	100	Total	C	H	N	O	S	0	0
			1652	556	803	146	145	2		

- Molecule 15 is a protein called ATPEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	114	Total	C	H	N	O	S	0	0
			1838	601	912	159	160	6		
15	p	114	Total	C	H	N	O	S	0	0
			1838	601	912	159	160	6		

- Molecule 16 is a protein called ATPEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	89	Total	C	H	N	O	S	0	0
			1476	475	723	137	137	4		
16	q	89	Total	C	H	N	O	S	0	0
			1476	475	723	137	137	4		

- Molecule 17 is a protein called ATPEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	69	Total	C	H	N	O	S	0	0
			1160	374	581	106	97	2		
17	r	69	Total	C	H	N	O	S	0	0
			1160	374	581	106	97	2		

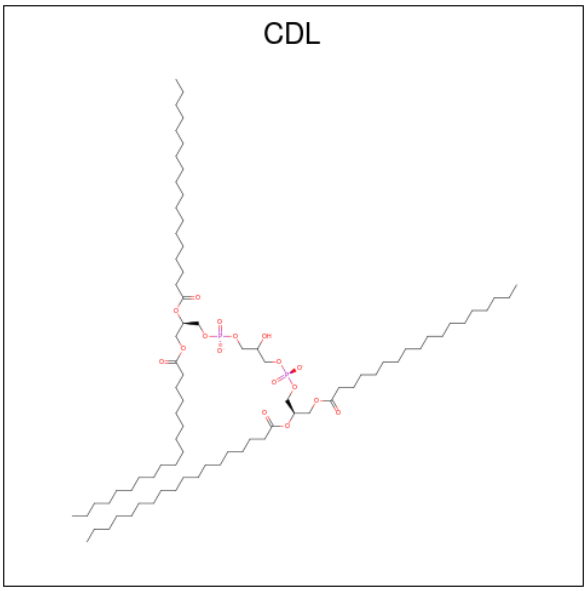
- Molecule 18 is a protein called ATPEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	S	65	Total	C	H	N	O	S	0	0
			1092	371	541	90	89	1		
18	s	65	Total	C	H	N	O	S	0	0
			1092	371	541	90	89	1		

- Molecule 19 is a protein called ATPEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	66	Total	C	H	N	O	S	0	0
			1080	349	552	95	83	1		
19	t	66	Total	C	H	N	O	S	0	0
			1080	349	552	95	83	1		

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	H	O	P	0
			183	62	102	17	2	
20	A	1	Total	C	H	O	P	0
			170	62	89	17	2	
20	A	1	Total	C	H	O	P	0
			184	63	102	17	2	
20	A	1	Total	C	H	O	P	0
			99	44	36	17	2	
20	D	1	Total	C	H	O	P	0
			228	72	137	17	2	
20	D	1	Total	C	H	O	P	0
			184	67	98	17	2	
20	E	1	Total	C	H	O	P	0
			95	44	32	17	2	
20	M	1	Total	C	H	O	P	0
			152	58	75	17	2	
20	M	1	Total	C	H	O	P	0
			80	34	27	17	2	
20	O	1	Total	C	H	O	P	0
			124	46	59	17	2	
20	P	1	Total	C	H	O	P	0
			75	29	27	17	2	
20	R	1	Total	C	H	O	P	0
			150	57	74	17	2	
20	a	1	Total	C	H	O	P	0
			183	62	102	17	2	
20	a	1	Total	C	H	O	P	0
			170	62	89	17	2	

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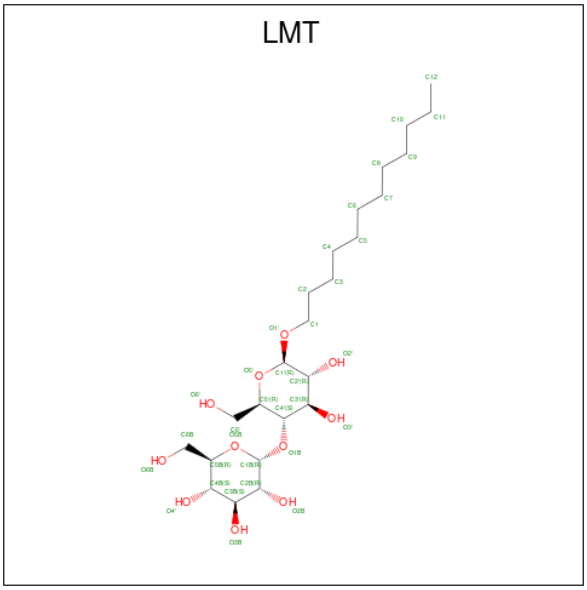
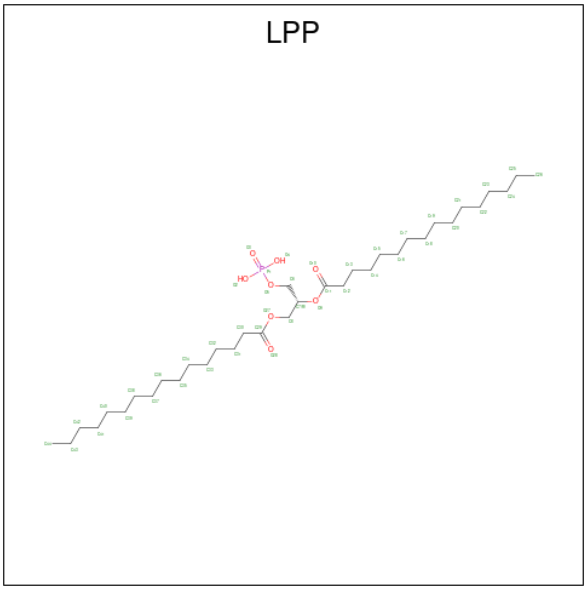
Mol	Chain	Residues	Atoms					AltConf
20	a	1	Total	C	H	O	P	0
			184	63	102	17	2	
20	a	1	Total	C	H	O	P	0
			99	44	36	17	2	
20	d	1	Total	C	H	O	P	0
			228	72	137	17	2	
20	d	1	Total	C	H	O	P	0
			184	67	98	17	2	
20	e	1	Total	C	H	O	P	0
			95	44	32	17	2	
20	m	1	Total	C	H	O	P	0
			152	58	75	17	2	
20	m	1	Total	C	H	O	P	0
			80	34	27	17	2	
20	o	1	Total	C	H	O	P	0
			124	46	59	17	2	
20	p	1	Total	C	H	O	P	0
			244	79	146	17	2	
20	p	1	Total	C	H	O	P	0
			75	29	27	17	2	
20	r	1	Total	C	H	O	P	0
			150	57	74	17	2	

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				AltConf
21	D	1	Total	C	H	O	0
			81	24	46	11	
21	F	1	Total	C	H	O	0
			81	24	46	11	
21	N	1	Total	C	H	O	0
			81	24	46	11	
21	Q	1	Total	C	H	O	0
			81	24	46	11	
21	d	1	Total	C	H	O	0
			81	24	46	11	
21	f	1	Total	C	H	O	0
			81	24	46	11	
21	n	1	Total	C	H	O	0
			81	24	46	11	
21	q	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 22 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	F	1	Total	C	H	O	P	0
			41	15	17	8	1	
22	I	1	Total	C	H	O	P	0
			111	35	67	8	1	
22	N	1	Total	C	H	O	P	0
			43	17	17	8	1	

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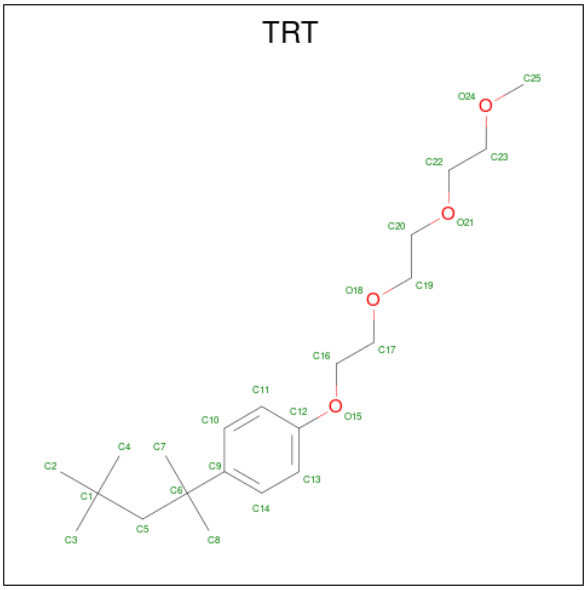
Mol	Chain	Residues	Atoms					AltConf
22	O	1	Total	C	H	O	P	0
			40	14	17	8	1	
22	O	1	Total	C	H	O	P	0
			73	23	41	8	1	
22	P	1	Total	C	H	O	P	0
			43	17	17	8	1	
22	R	1	Total	C	H	O	P	0
			48	22	17	8	1	
22	f	1	Total	C	H	O	P	0
			41	15	17	8	1	
22	i	1	Total	C	H	O	P	0
			111	35	67	8	1	
22	o	1	Total	C	H	O	P	0
			40	14	17	8	1	
22	o	1	Total	C	H	O	P	0
			73	23	41	8	1	
22	r	1	Total	C	H	O	P	0
			48	22	17	8	1	

- Molecule 23 is FRAGMENT OF TRITON X-100 (CCD ID: TRT) (formula: $C_{21}H_{36}O_4$).



Mol	Chain	Residues	Atoms				AltConf
23	G	1	Total	C	H	O	0
			61	21	36	4	
23	G	1	Total	C	H	O	0
			61	21	36	4	

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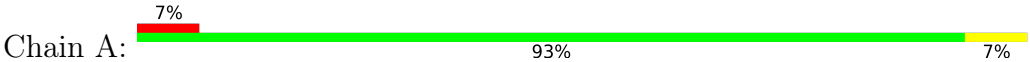
Mol	Chain	Residues	Atoms				AltConf
23	M	1	Total	C	H	O	0
			61	21	36	4	
23	M	1	Total	C	H	O	0
			61	21	36	4	
23	N	1	Total	C	H	O	0
			61	21	36	4	
23	N	1	Total	C	H	O	0
			61	21	36	4	
23	P	1	Total	C	H	O	0
			61	21	36	4	
23	R	1	Total	C	H	O	0
			61	21	36	4	
23	g	1	Total	C	H	O	0
			61	21	36	4	
23	g	1	Total	C	H	O	0
			61	21	36	4	
23	m	1	Total	C	H	O	0
			61	21	36	4	
23	m	1	Total	C	H	O	0
			61	21	36	4	
23	n	1	Total	C	H	O	0
			61	21	36	4	
23	n	1	Total	C	H	O	0
			61	21	36	4	
23	p	1	Total	C	H	O	0
			61	21	36	4	
23	r	1	Total	C	H	O	0
			61	21	36	4	

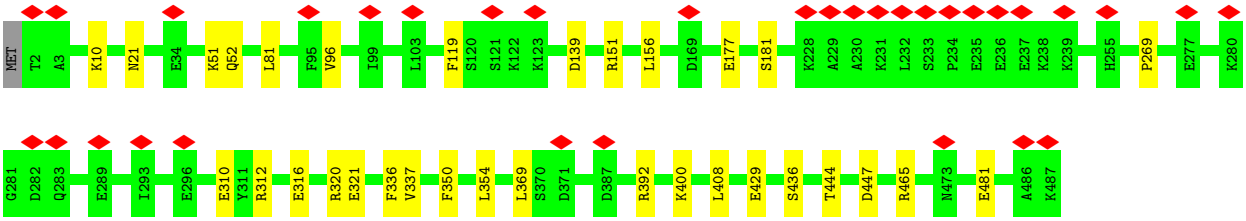
3 Residue-property plots (i)

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

• Molecule 1: ATPTB1

Chain A:

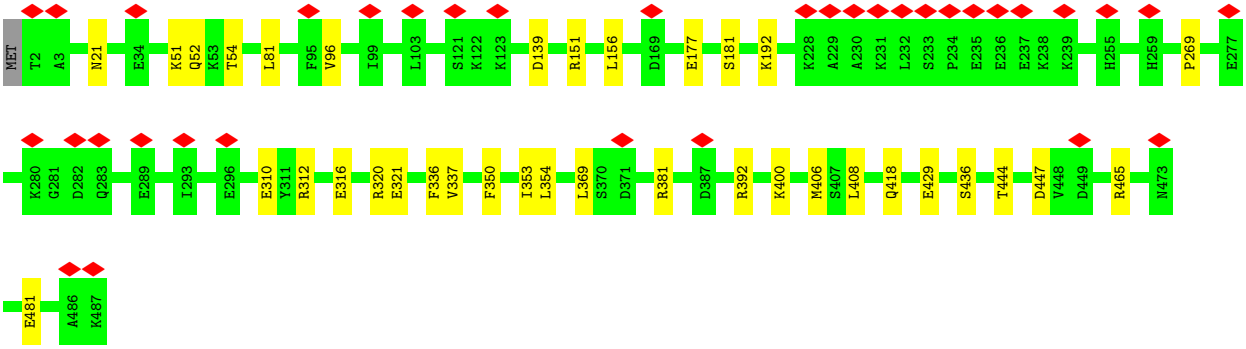




• Molecule 1: ATPTB1

Chain a:

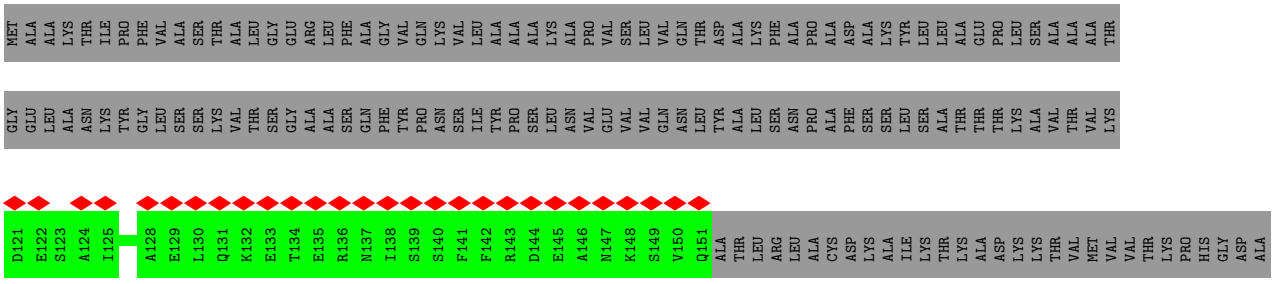


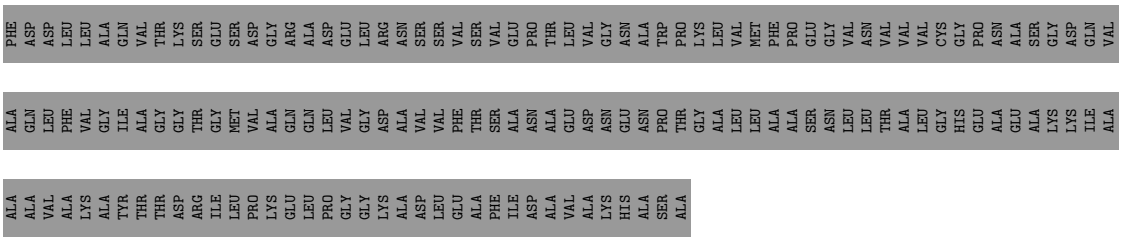


• Molecule 2: ATPTB3

Chain B:

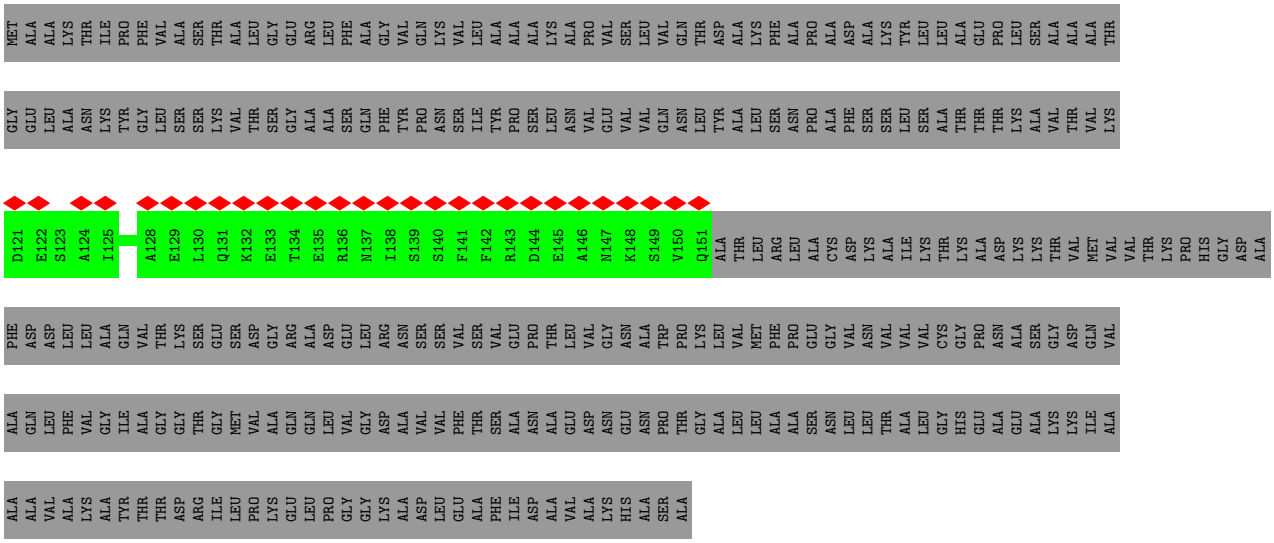




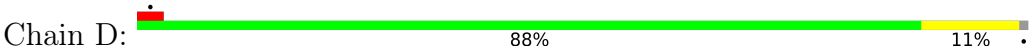


• Molecule 2: ATPTB3



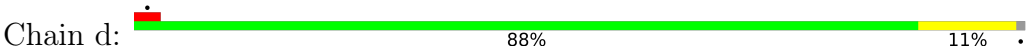


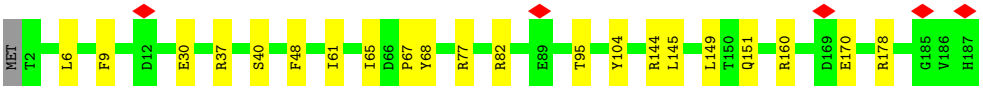
• Molecule 3: ATPTB6



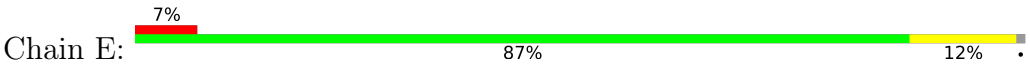


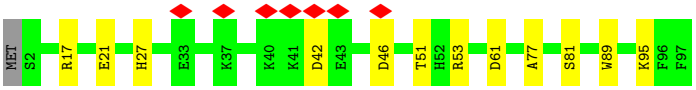
• Molecule 3: ATPTB6





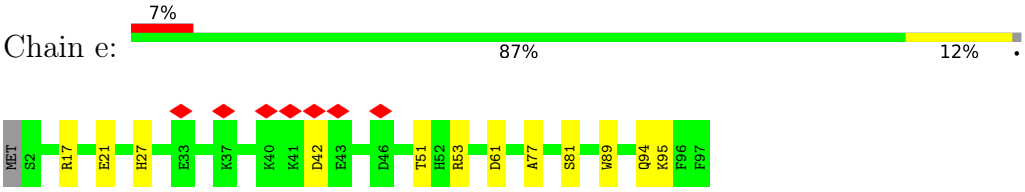
• Molecule 4: ATPTB12





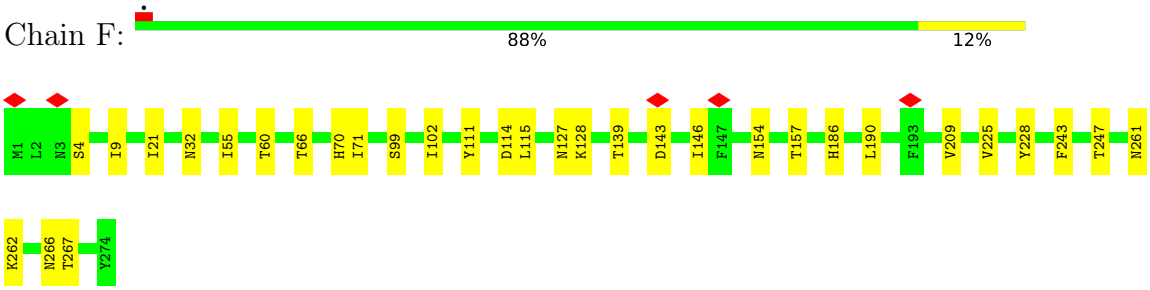
• Molecule 4: ATPTB12

Chain e:



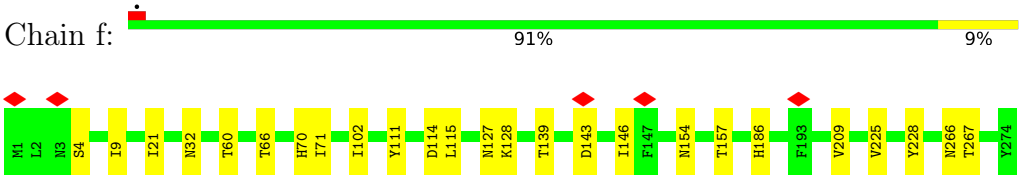
• Molecule 5: subunit a

Chain F:



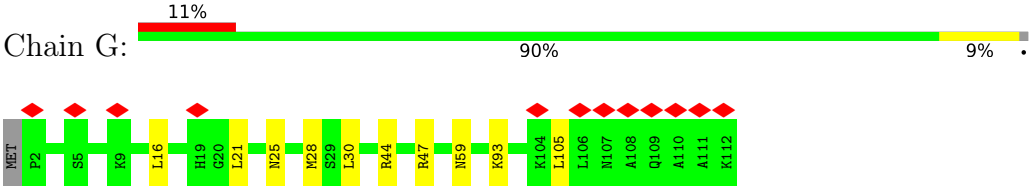
• Molecule 5: subunit a

Chain f:



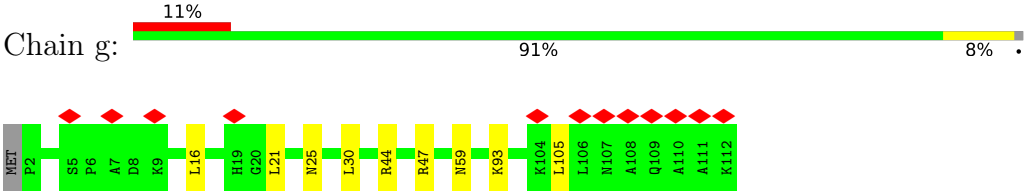
• Molecule 6: subunit b

Chain G:



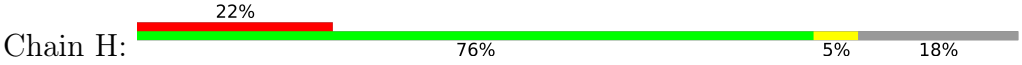
• Molecule 6: subunit b

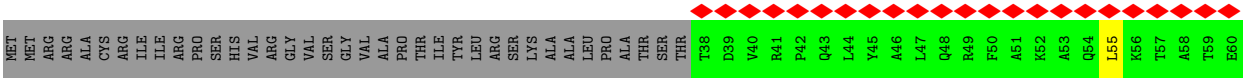
Chain g:

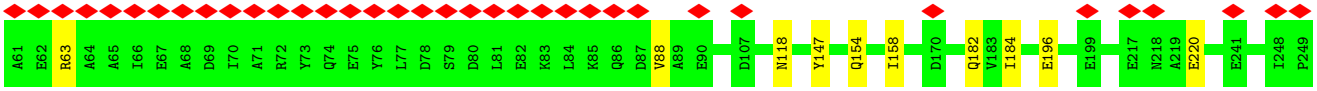


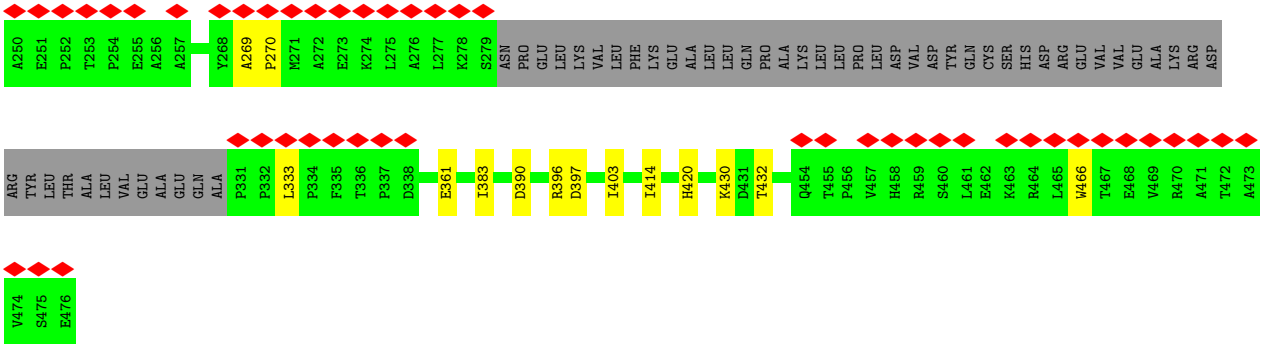
• Molecule 7: subunit d

Chain H:





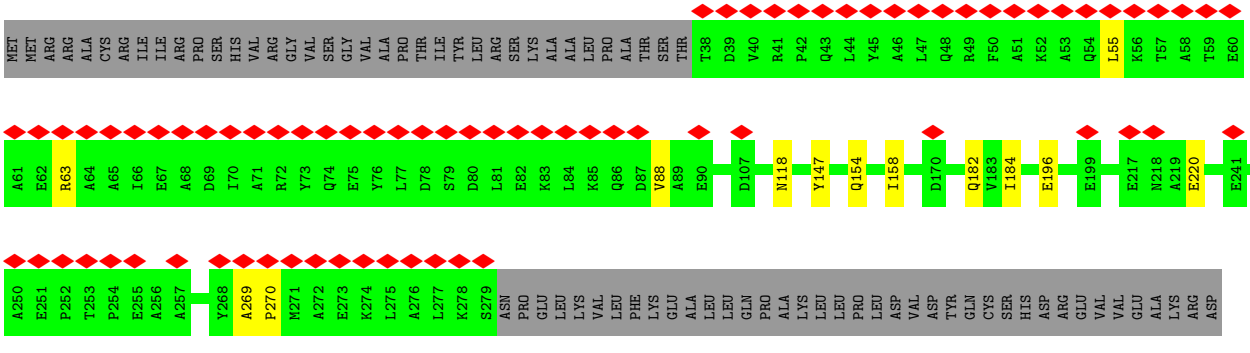




• Molecule 7: subunit d

Chain h:

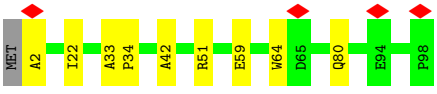




• Molecule 8: subunit f

Chain I:

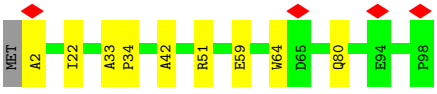




• Molecule 8: subunit f

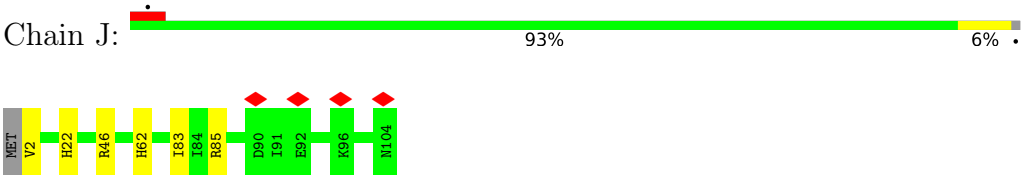
Chain i:





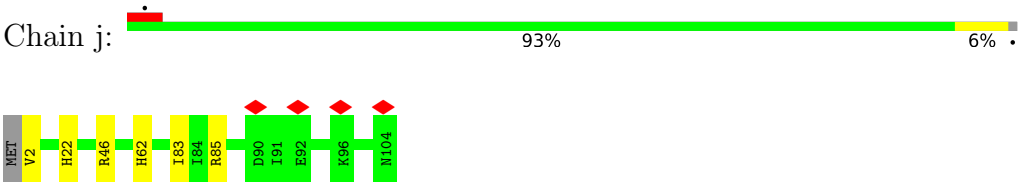
• Molecule 9: subunit i/j

Chain J:



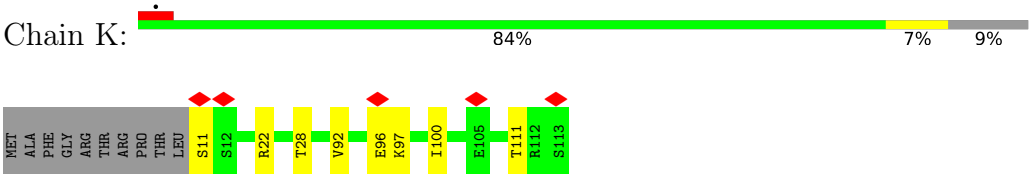
• Molecule 9: subunit i/j

Chain j:



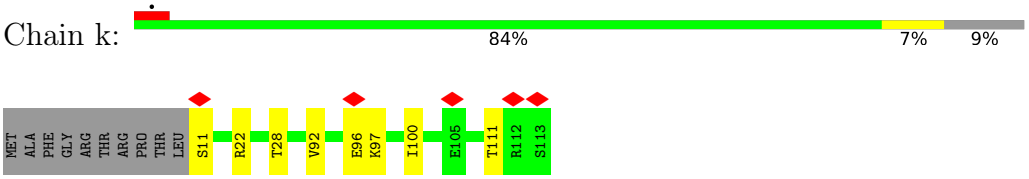
• Molecule 10: subunit k

Chain K:



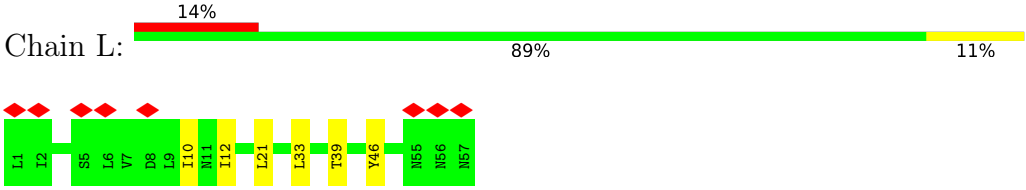
• Molecule 10: subunit k

Chain k:



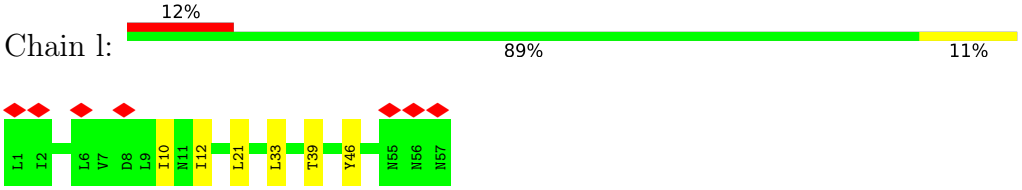
• Molecule 11: subunit 8

Chain L:



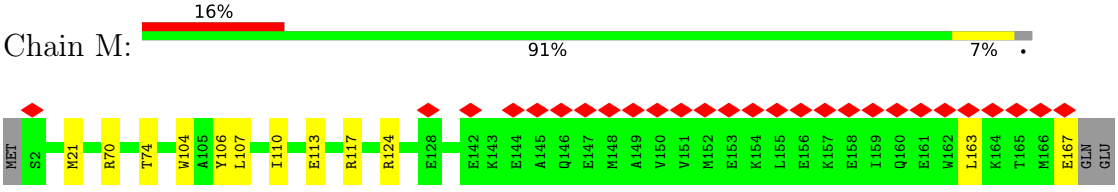
• Molecule 11: subunit 8

Chain l:



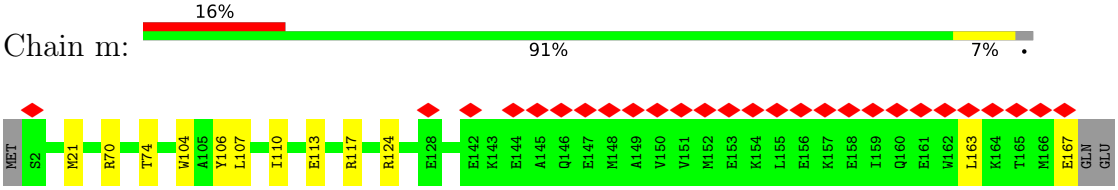
• Molecule 12: ATPEG1

Chain M:



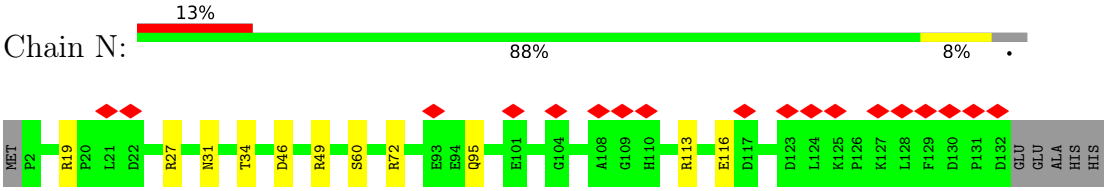
• Molecule 12: ATPEG1

Chain m:



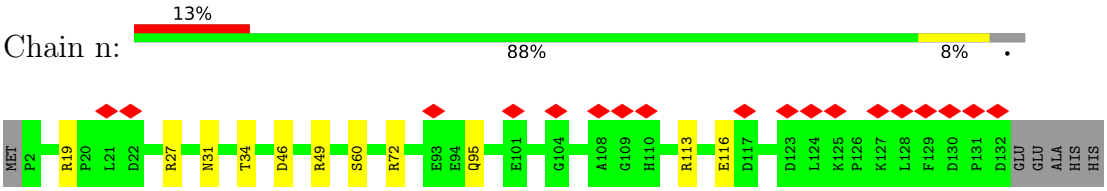
• Molecule 13: ATPEG2

Chain N:



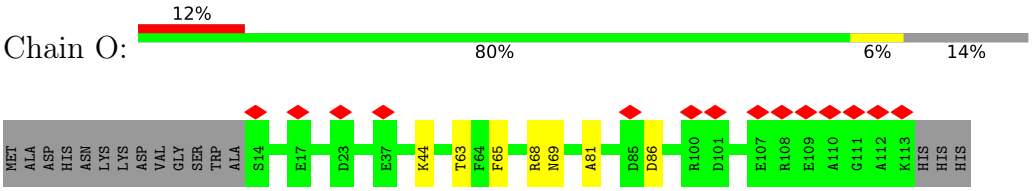
• Molecule 13: ATPEG2

Chain n:



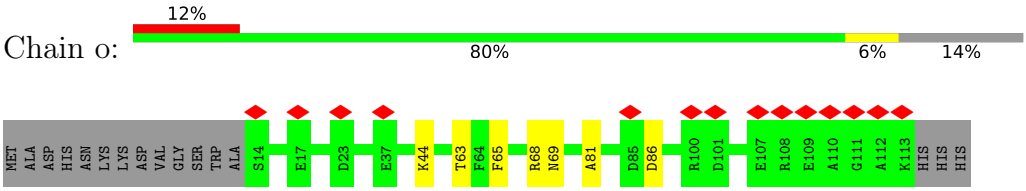
• Molecule 14: ATPEG3

Chain O:



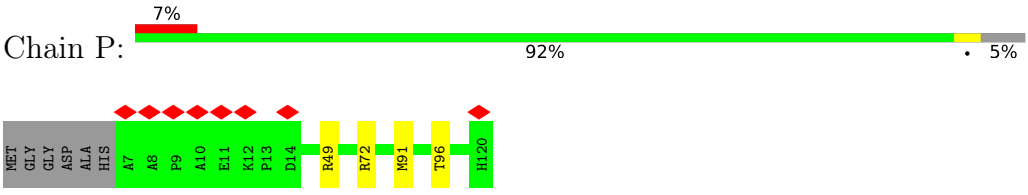
• Molecule 14: ATPEG3

Chain o:



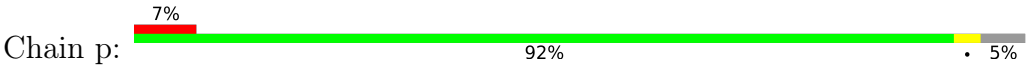
• Molecule 15: ATPEG4

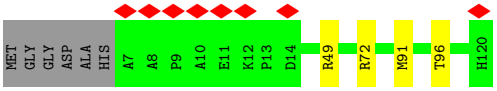
Chain P:



• Molecule 15: ATPEG4

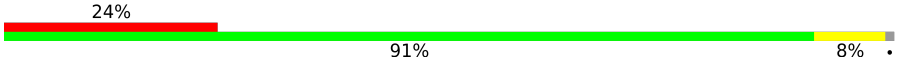
Chain p:

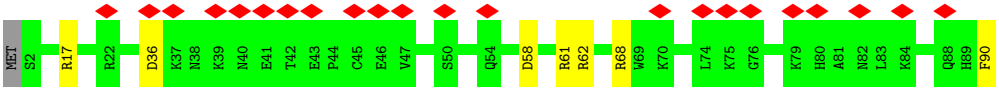




• Molecule 16: ATPEG5

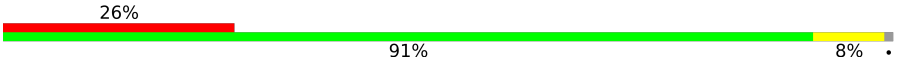
Chain Q:

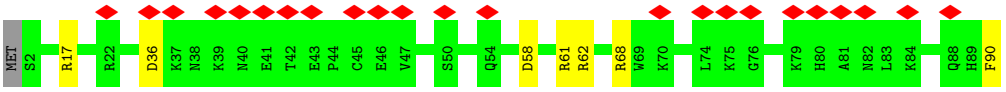




• Molecule 16: ATPEG5

Chain q:

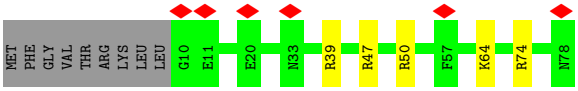




• Molecule 17: ATPEG6

Chain R:

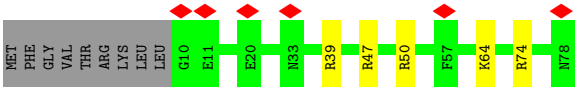




• Molecule 17: ATPEG6

Chain r:

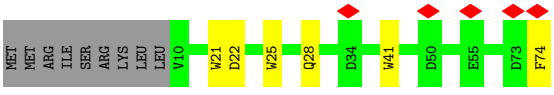




• Molecule 18: ATPEG7

Chain S:

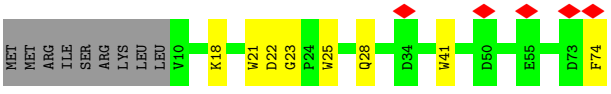




• Molecule 18: ATPEG7

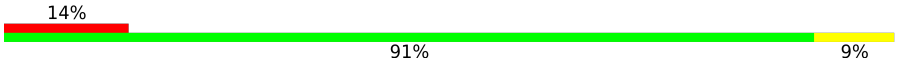
Chain s:

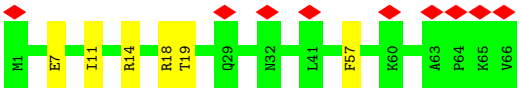




• Molecule 19: ATPEG8

Chain T:

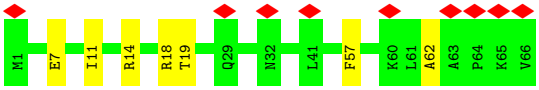




• Molecule 19: ATPEG8

Chain t:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	150242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	36.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, TRT, CDL, LPP

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	0.27	0/4047	0.38	0/5500
1	a	0.27	0/4047	0.38	0/5500
2	B	0.15	0/252	0.30	0/335
2	b	0.15	0/252	0.30	0/335
3	D	0.25	0/1559	0.37	0/2106
3	d	0.25	0/1559	0.37	0/2106
4	E	0.22	0/819	0.35	0/1096
4	e	0.22	0/821	0.35	0/1100
5	F	0.27	0/2377	0.38	0/3228
5	f	0.26	0/2379	0.38	0/3233
6	G	0.26	0/901	0.41	0/1218
6	g	0.26	0/901	0.41	0/1218
7	H	0.24	0/3185	0.34	0/4352
7	h	0.24	0/3185	0.34	0/4352
8	I	0.26	0/804	0.38	0/1084
8	i	0.26	0/804	0.38	0/1084
9	J	0.24	0/918	0.36	0/1255
9	j	0.25	0/918	0.36	0/1255
10	K	0.23	0/839	0.33	0/1135
10	k	0.23	0/839	0.33	0/1135
11	L	0.25	0/518	0.37	0/711
11	l	0.26	0/518	0.37	0/711
12	M	0.24	0/1399	0.35	0/1895
12	m	0.24	0/1399	0.35	0/1895
13	N	0.24	0/1137	0.31	0/1540
13	n	0.24	0/1137	0.31	0/1540
14	O	0.23	0/881	0.34	0/1193
14	o	0.23	0/881	0.34	0/1193
15	P	0.26	0/955	0.36	0/1292
15	p	0.27	0/955	0.36	0/1292
16	Q	0.20	0/774	0.40	0/1040
16	q	0.20	0/774	0.40	0/1040

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	R	0.21	0/594	0.38	0/798
17	r	0.21	0/594	0.38	0/798
18	S	0.24	0/575	0.37	0/785
18	s	0.24	0/575	0.37	0/785
19	T	0.23	0/543	0.35	0/730
19	t	0.23	0/543	0.35	0/730
All	All	0.25	0/46158	0.36	0/62595

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3945	3919	3919	22	0
1	a	3945	3919	3919	25	0
2	B	251	243	243	0	0
2	b	251	243	243	0	0
3	D	1521	1519	1519	15	0
3	d	1521	1519	1519	15	0
4	E	797	777	777	9	0
4	e	798	779	779	9	0
5	F	2312	2327	2327	23	0
5	f	2313	2329	2329	19	0
6	G	879	924	924	12	0
6	g	879	924	924	11	0
7	H	3106	3059	3059	19	0
7	h	3106	3059	3059	20	0
8	I	782	771	771	8	0
8	i	782	771	771	8	0
9	J	881	853	852	8	0
9	j	881	853	852	7	0
10	K	816	821	821	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	816	821	821	7	0
11	L	501	507	507	6	0
11	l	501	507	507	6	0
12	M	1363	1354	1354	7	0
12	m	1363	1354	1354	7	0
13	N	1097	1070	1070	8	0
13	n	1097	1070	1070	8	0
14	O	849	803	803	6	0
14	o	849	803	803	6	0
15	P	926	912	912	4	0
15	p	926	912	912	4	0
16	Q	753	723	723	5	0
16	q	753	723	723	5	0
17	R	579	581	581	7	0
17	r	579	581	581	7	0
18	S	551	541	541	6	0
18	s	551	541	541	7	0
19	T	528	552	552	6	0
19	t	528	552	552	7	0
20	A	307	329	395	8	0
20	D	177	235	255	6	0
20	E	63	32	73	6	0
20	M	130	102	151	4	0
20	O	65	59	77	4	0
20	P	48	27	40	1	0
20	R	76	74	99	2	0
20	a	307	329	395	7	0
20	d	177	235	255	6	0
20	e	63	32	73	7	0
20	m	130	102	151	1	0
20	o	65	59	77	3	0
20	p	146	173	189	1	0
20	r	76	74	99	2	0
21	D	35	46	44	0	0
21	F	35	46	44	2	0
21	N	35	46	44	0	0
21	Q	35	46	45	0	0
21	d	35	46	45	0	0
21	f	35	46	44	2	0
21	n	35	46	44	0	0
21	q	35	46	45	0	0
22	F	24	17	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	I	44	67	67	2	0
22	N	26	17	25	2	0
22	O	55	58	59	0	0
22	P	26	17	25	2	0
22	R	31	17	35	1	0
22	f	24	17	21	0	0
22	i	44	67	67	2	0
22	o	55	58	59	0	0
22	r	31	17	35	1	0
23	G	50	72	72	6	0
23	M	50	72	72	2	0
23	N	50	72	72	8	0
23	P	25	36	36	0	0
23	R	25	36	36	0	0
23	g	50	72	72	6	0
23	m	50	72	72	2	0
23	n	50	72	72	7	0
23	p	25	36	36	0	0
23	r	25	36	36	0	0
All	All	47746	47674	48188	317	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 (317) 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)
3:D:68:TYR:O	3:D:77:ARG:NH1	2.19	0.75
3:d:68:TYR:O	3:d:77:ARG:NH1	2.19	0.75
1:a:156:LEU:O	1:a:312:ARG:NH2	2.22	0.73
1:A:156:LEU:O	1:A:312:ARG:NH2	2.22	0.71
10:k:11:SER:OG	19:t:7:GLU:OE1	2.09	0.70
6:G:47:ARG:NH2	7:H:196:GLU:OE2	2.25	0.70
1:a:269:PRO:O	3:d:82:ARG:NH1	2.25	0.70
7:h:430:LYS:O	11:l:46:TYR:OH	2.10	0.70
1:A:177:GLU:O	1:A:181:SER:OG	2.10	0.69
6:g:47:ARG:NH2	7:h:196:GLU:OE2	2.25	0.69
4:e:17:ARG:NH1	4:e:21:GLU:OE2	2.25	0.69
4:E:61:ASP:OD1	9:J:46:ARG:NH1	2.25	0.69
1:a:177:GLU:O	1:a:181:SER:OG	2.10	0.69
1:a:369:LEU:O	1:a:392:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:61:ASP:OD1	9:j:46:ARG:NH1	2.25	0.69
1:A:369:LEU:O	1:A:392:ARG:NH1	2.26	0.69
4:E:17:ARG:NH1	4:E:21:GLU:OE2	2.25	0.68
1:A:269:PRO:O	3:D:82:ARG:NH1	2.26	0.68
15:p:49:ARG:NH1	20:p:202:CDL:OA3	2.26	0.68
7:H:430:LYS:O	11:L:46:TYR:OH	2.12	0.67
12:m:117:ARG:O	12:m:124:ARG:NH2	2.28	0.67
12:M:117:ARG:O	12:M:124:ARG:NH2	2.28	0.67
1:a:151:ARG:NH2	1:a:321:GLU:OE1	2.28	0.67
16:q:58:ASP:OD1	16:q:61:ARG:NH1	2.27	0.67
10:K:11:SER:OG	19:T:7:GLU:OE1	2.12	0.67
1:A:151:ARG:NH2	1:A:321:GLU:OE1	2.28	0.67
6:G:59:ASN:ND2	7:H:220:GLU:OE1	2.28	0.67
16:Q:58:ASP:OD1	16:Q:61:ARG:NH1	2.27	0.66
6:g:105:LEU:HD21	7:h:333:LEU:HD21	1.77	0.66
3:D:151:GLN:O	3:D:160:ARG:NH1	2.29	0.65
6:G:105:LEU:HD21	7:H:333:LEU:HD21	1.79	0.65
15:P:49:ARG:NH1	20:P:201:CDL:OA3	2.28	0.65
6:g:59:ASN:ND2	7:h:220:GLU:OE1	2.31	0.64
3:d:151:GLN:O	3:d:160:ARG:NH1	2.29	0.64
3:d:6:LEU:O	14:o:44:LYS:NZ	2.31	0.64
17:R:50:ARG:NH1	22:R:102:LPP:O3	2.31	0.64
17:r:50:ARG:NH1	22:r:102:LPP:O3	2.31	0.63
3:D:6:LEU:O	14:O:44:LYS:NZ	2.32	0.63
4:e:95:LYS:O	14:o:68:ARG:NH1	2.32	0.63
1:A:447:ASP:O	1:A:465:ARG:NH1	2.32	0.63
3:d:37:ARG:O	3:d:40:SER:OG	2.17	0.62
4:E:95:LYS:O	14:O:68:ARG:NH1	2.32	0.62
3:d:9:PHE:HZ	14:o:63:THR:HG22	1.64	0.62
5:F:143:ASP:HA	5:F:146:ILE:HD12	1.81	0.62
9:j:2:VAL:N	18:s:22:ASP:OD1	2.32	0.62
1:a:447:ASP:O	1:a:465:ARG:NH1	2.32	0.62
9:J:2:VAL:N	18:S:22:ASP:OD1	2.33	0.61
3:D:37:ARG:O	3:D:40:SER:OG	2.17	0.61
5:f:143:ASP:HA	5:f:146:ILE:HD12	1.81	0.61
5:F:114:ASP:OD2	19:T:14:ARG:NH2	2.33	0.61
1:a:139:ASP:OD1	18:s:21:TRP:NE1	2.34	0.60
5:f:114:ASP:OD2	19:t:14:ARG:NH2	2.33	0.60
12:M:70:ARG:O	12:M:74:THR:HG23	2.02	0.60
4:E:27:HIS:ND1	4:E:51:THR:OG1	2.26	0.60
1:A:139:ASP:OD1	18:S:21:TRP:NE1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLU:OE2	19:T:19:THR:HG21	2.02	0.59
12:m:70:ARG:O	12:m:74:THR:HG23	2.02	0.59
13:n:113:ARG:NH1	13:n:116:GLU:OE1	2.36	0.58
3:D:9:PHE:HZ	14:O:63:THR:HG22	1.69	0.58
14:o:81:ALA:HB3	14:o:86:ASP:HB2	1.85	0.58
6:G:47:ARG:NH1	7:H:147:TYR:O	2.36	0.58
14:O:69:ASN:ND2	20:O:201:CDL:OB2	2.36	0.58
13:N:113:ARG:NH1	13:N:116:GLU:OE1	2.36	0.58
16:Q:90:PHE:OXT	17:R:74:ARG:NH2	2.37	0.58
4:e:27:HIS:ND1	4:e:51:THR:OG1	2.26	0.58
4:e:89:TRP:CH2	20:e:101:CDL:H731	2.39	0.58
5:F:243:PHE:O	5:F:247:THR:OG1	2.11	0.57
14:o:69:ASN:ND2	20:o:201:CDL:OB2	2.37	0.57
16:q:90:PHE:OXT	17:r:74:ARG:NH2	2.37	0.57
6:g:47:ARG:NH1	7:h:147:TYR:O	2.36	0.57
6:G:44:ARG:NH1	23:G:202:TRT:H8C3	2.19	0.57
16:q:17:ARG:NH1	17:r:64:LYS:O	2.37	0.57
14:O:81:ALA:HB3	14:O:86:ASP:HB2	1.86	0.57
1:a:316:GLU:OE2	19:t:19:THR:HG21	2.04	0.56
4:E:89:TRP:CH2	20:E:101:CDL:H731	2.41	0.56
6:g:44:ARG:NH1	23:g:202:TRT:H8C3	2.21	0.56
3:D:170:GLU:OE1	3:D:170:GLU:N	2.40	0.55
6:G:44:ARG:HH12	23:G:202:TRT:H8C3	1.71	0.55
5:f:139:THR:OG1	5:f:143:ASP:OD2	2.13	0.55
7:h:420:HIS:NE2	7:h:432:THR:OG1	2.23	0.55
20:D:201:CDL:C67	20:E:101:CDL:H722	2.37	0.55
20:e:101:CDL:H661	20:e:101:CDL:H621	1.88	0.55
1:a:400:LYS:NZ	1:a:481:GLU:OE2	2.40	0.55
7:H:420:HIS:NE2	7:H:432:THR:OG1	2.23	0.55
12:m:163:LEU:O	12:m:167:GLU:N	2.40	0.55
1:A:10:LYS:NZ	1:A:119:PHE:O	2.30	0.55
3:d:170:GLU:OE1	3:d:170:GLU:N	2.40	0.55
20:d:201:CDL:C67	20:e:101:CDL:H722	2.37	0.55
5:F:139:THR:OG1	5:F:143:ASP:OD2	2.12	0.54
20:E:101:CDL:H661	20:E:101:CDL:H621	1.88	0.54
16:Q:17:ARG:NH1	17:R:64:LYS:O	2.39	0.54
13:n:72:ARG:NH1	15:p:96:THR:O	2.40	0.54
1:A:400:LYS:NZ	1:A:481:GLU:OE2	2.40	0.54
12:M:163:LEU:O	12:M:167:GLU:N	2.40	0.54
5:f:9:ILE:HG23	11:l:12:ILE:HG21	1.89	0.54
13:N:72:ARG:NH1	15:P:96:THR:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:53:ARG:NH1	5:F:4:SER:O	2.42	0.53
5:F:9:ILE:HG23	11:L:12:ILE:HG21	1.91	0.53
6:g:44:ARG:HH12	23:g:202:TRT:H8C3	1.73	0.53
21:F:302:LMT:O6B	21:F:302:LMT:O4'	2.21	0.53
1:a:336:PHE:HA	20:a:503:CDL:H722	1.91	0.52
4:e:53:ARG:NH1	5:f:4:SER:O	2.41	0.52
8:i:22:ILE:HD11	18:s:41:TRP:HE1	1.75	0.52
1:A:336:PHE:HA	20:A:503:CDL:H722	1.91	0.52
5:F:32:ASN:ND2	5:F:60:THR:OG1	2.43	0.52
13:n:46:ASP:OD1	13:n:49:ARG:NH1	2.42	0.52
17:r:50:ARG:NH2	20:r:101:CDL:OB4	2.43	0.51
8:I:33:ALA:HB3	8:I:34:PRO:HD3	1.93	0.51
7:h:158:ILE:HD12	7:h:184:ILE:CG2	2.41	0.51
13:N:27:ARG:NH1	23:N:201:TRT:H3C3	2.26	0.51
5:f:32:ASN:ND2	5:f:60:THR:OG1	2.43	0.51
8:I:22:ILE:HD11	18:S:41:TRP:NE1	2.26	0.51
13:n:95:GLN:OE1	13:n:95:GLN:N	2.44	0.51
8:I:22:ILE:HD11	18:S:41:TRP:HE1	1.75	0.51
3:d:145:LEU:HD23	19:t:57:PHE:CE1	2.45	0.51
4:e:77:ALA:O	4:e:81:SER:N	2.44	0.51
8:i:22:ILE:HD11	18:s:41:TRP:NE1	2.25	0.51
1:A:408:LEU:O	5:F:267:THR:HG21	2.11	0.50
7:H:158:ILE:HD12	7:H:184:ILE:CG2	2.41	0.50
1:a:408:LEU:O	5:f:267:THR:HG21	2.11	0.50
17:R:50:ARG:NH2	20:R:101:CDL:OB4	2.43	0.50
6:g:21:LEU:HD11	8:i:42:ALA:HA	1.94	0.50
14:O:65:PHE:CD1	20:O:201:CDL:HB62	2.47	0.50
20:d:201:CDL:H673	20:e:101:CDL:H722	1.93	0.50
7:H:154:GLN:O	7:H:182:GLN:NE2	2.45	0.50
8:i:33:ALA:HB3	8:i:34:PRO:HD3	1.93	0.50
13:n:27:ARG:NH1	23:n:202:TRT:H3C3	2.27	0.50
4:E:77:ALA:O	4:E:81:SER:N	2.44	0.50
7:h:154:GLN:O	7:h:182:GLN:NE2	2.45	0.50
20:m:201:CDL:H712	20:m:201:CDL:H371	1.94	0.50
14:o:65:PHE:CD1	20:o:201:CDL:HB62	2.47	0.50
22:N:203:LPP:O10	15:p:72:ARG:NH1	2.45	0.49
3:D:145:LEU:HD23	19:T:57:PHE:CE1	2.47	0.49
9:J:83:ILE:HD11	18:S:74:PHE:CE1	2.47	0.49
6:g:93:LYS:NZ	7:h:118:ASN:OD1	2.27	0.49
20:D:201:CDL:H673	20:E:101:CDL:H722	1.94	0.49
7:H:390:ASP:OD1	7:H:396:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:71:ILE:O	6:G:30:LEU:HD12	2.13	0.49
5:f:71:ILE:O	6:g:30:LEU:HD12	2.12	0.49
5:F:111:TYR:CE2	5:F:115:LEU:HD11	2.47	0.49
4:e:42:ASP:O	9:j:85:ARG:NH2	2.46	0.49
7:h:390:ASP:OD1	7:h:396:ARG:NH1	2.45	0.49
7:H:55:LEU:HD11	7:H:63:ARG:HG3	1.94	0.49
13:N:46:ASP:OD1	13:N:49:ARG:NH1	2.42	0.49
7:h:55:LEU:HD11	7:h:63:ARG:HG3	1.95	0.49
10:K:28:THR:HG21	17:R:39:ARG:HB3	1.94	0.48
8:I:59:GLU:OE1	8:I:64:TRP:N	2.44	0.48
13:N:95:GLN:OE1	13:N:95:GLN:N	2.44	0.48
23:G:201:TRT:H8C1	23:G:201:TRT:H3C2	1.95	0.48
20:a:502:CDL:H822	20:o:201:CDL:C75	2.43	0.48
5:f:102:ILE:HD13	9:j:22:HIS:HA	1.96	0.48
3:d:30:GLU:OE2	3:d:144:ARG:NH1	2.47	0.48
5:f:146:ILE:HD11	17:r:47:ARG:HB3	1.94	0.48
5:f:186:HIS:CE1	5:f:228:TYR:HH	2.26	0.48
23:g:201:TRT:H8C1	23:g:201:TRT:H3C2	1.95	0.48
20:A:502:CDL:H822	20:O:201:CDL:C75	2.43	0.48
5:F:102:ILE:HD13	9:J:22:HIS:HA	1.96	0.48
16:q:36:ASP:OD1	16:q:68:ARG:NH1	2.46	0.48
16:Q:36:ASP:OD1	16:Q:68:ARG:NH1	2.46	0.48
10:k:28:THR:HG21	17:r:39:ARG:HB3	1.94	0.48
5:F:146:ILE:HD11	17:R:47:ARG:HB3	1.95	0.47
20:M:203:CDL:H712	20:M:203:CDL:H371	1.96	0.47
9:j:83:ILE:HD11	18:s:74:PHE:CE1	2.49	0.47
3:d:61:ILE:HG23	3:d:104:TYR:HB3	1.97	0.47
4:E:42:ASP:O	9:J:85:ARG:NH2	2.46	0.47
7:H:414:ILE:HD11	11:L:39:THR:OG1	2.15	0.47
1:a:436:SER:OG	7:h:361:GLU:OE1	2.19	0.47
3:D:67:PRO:HD3	3:D:95:THR:HG22	1.96	0.47
1:a:96:VAL:CG1	20:d:202:CDL:H812	2.44	0.47
1:A:96:VAL:CG1	20:D:202:CDL:H812	2.45	0.46
3:D:61:ILE:HG23	3:D:104:TYR:HB3	1.96	0.46
20:a:503:CDL:H732	20:a:503:CDL:H771	1.97	0.46
5:f:111:TYR:CE2	5:f:115:LEU:HD11	2.51	0.46
3:d:67:PRO:HD3	3:d:95:THR:HG22	1.96	0.46
6:g:21:LEU:HD22	6:g:25:ASN:HB3	1.98	0.46
1:A:21:ASN:HB3	1:A:81:LEU:HD22	1.98	0.46
7:h:158:ILE:HD12	7:h:184:ILE:HG21	1.97	0.46
7:h:414:ILE:HD11	11:l:39:THR:OG1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:67:PRO:O	3:D:71:SER:OG	2.29	0.46
3:D:30:GLU:OE2	3:D:144:ARG:NH1	2.47	0.46
10:K:92:VAL:O	10:K:97:LYS:NZ	2.46	0.46
1:a:96:VAL:HG12	20:d:202:CDL:H812	1.97	0.46
1:a:177:GLU:OE1	1:a:192:LYS:NZ	2.30	0.46
20:a:502:CDL:H742	20:a:502:CDL:H772	1.28	0.46
20:d:202:CDL:H782	20:d:202:CDL:H751	1.55	0.46
6:G:93:LYS:NZ	7:H:118:ASN:OD1	2.27	0.46
10:K:100:ILE:O	17:R:74:ARG:NH1	2.48	0.46
12:M:113:GLU:N	13:N:60:SER:OG	2.49	0.45
20:E:101:CDL:H621	20:E:101:CDL:H591	1.82	0.45
6:G:21:LEU:HD22	6:G:25:ASN:HB3	1.98	0.45
8:I:51:ARG:NH2	22:I:101:LPP:O2	2.46	0.45
23:g:202:TRT:H8C1	23:g:202:TRT:C3	2.46	0.45
1:A:96:VAL:HG12	20:D:202:CDL:H812	1.97	0.45
12:M:21:MET:HE2	5:f:209:VAL:CG1	2.46	0.45
8:i:59:GLU:OE1	8:i:64:TRP:N	2.45	0.45
23:G:202:TRT:C3	23:G:202:TRT:H8C1	2.46	0.45
1:a:54:THR:OG1	20:a:502:CDL:OA3	2.32	0.45
4:e:89:TRP:N	4:e:94:GLN:OE1	2.49	0.45
12:m:113:GLU:N	13:n:60:SER:OG	2.50	0.45
23:n:202:TRT:H7C1	23:n:202:TRT:H2C3	1.99	0.45
1:a:21:ASN:HB3	1:a:81:LEU:HD22	1.98	0.45
8:i:51:ARG:NH2	22:i:101:LPP:O2	2.48	0.45
10:k:22:ARG:NH2	20:r:101:CDL:OB4	2.47	0.45
15:P:72:ARG:NH1	22:P:202:LPP:O10	2.48	0.45
6:G:21:LEU:HD11	8:I:42:ALA:HA	1.98	0.45
12:m:106:TYR:CZ	12:m:110:ILE:HD11	2.52	0.45
7:H:158:ILE:HD12	7:H:184:ILE:HG21	1.97	0.45
8:I:80:GLN:OE1	15:P:91:MET:HE2	2.16	0.45
12:M:106:TYR:CZ	12:M:110:ILE:HD11	2.52	0.45
5:F:186:HIS:CD2	5:F:228:TYR:HH	2.31	0.44
5:F:209:VAL:CG1	12:m:21:MET:HE2	2.47	0.44
7:H:397:ASP:CG	9:J:2:VAL:HG21	2.42	0.44
10:K:22:ARG:NH2	20:R:101:CDL:OB4	2.46	0.44
5:f:225:VAL:HG22	21:f:302:LMT:H32	1.99	0.44
20:A:503:CDL:H741	20:A:503:CDL:H712	1.52	0.44
5:f:66:THR:O	5:f:70:HIS:N	2.49	0.44
10:k:100:ILE:O	17:r:74:ARG:NH1	2.49	0.44
3:D:178:ARG:NH2	10:K:111:THR:O	2.48	0.44
7:H:403:ILE:HG23	11:L:33:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:96:GLU:OE1	16:Q:62:ARG:NH2	2.49	0.44
7:h:397:ASP:CG	9:j:2:VAL:HG21	2.43	0.44
20:A:501:CDL:H752	20:A:501:CDL:H722	1.77	0.44
23:N:202:TRT:H2C3	23:N:202:TRT:H7C1	1.99	0.44
21:f:302:LMT:O6B	21:f:302:LMT:O4'	2.21	0.44
12:m:104:TRP:CZ3	12:m:107:LEU:HD23	2.52	0.44
23:n:202:TRT:H3C2	23:n:202:TRT:C8	2.48	0.44
1:A:51:LYS:O	1:A:52:GLN:NE2	2.51	0.43
20:e:101:CDL:H621	20:e:101:CDL:H591	1.81	0.43
7:h:88:VAL:HG22	7:h:466:TRP:CE3	2.53	0.43
10:k:92:VAL:O	10:k:97:LYS:NZ	2.46	0.43
12:M:104:TRP:CZ3	12:M:107:LEU:HD23	2.52	0.43
5:f:21:ILE:HG21	11:l:21:LEU:HD11	1.99	0.43
5:F:127:ASN:OD1	5:F:128:LYS:N	2.52	0.43
23:N:201:TRT:H2C3	23:N:201:TRT:H7C1	1.99	0.43
23:n:203:TRT:H2C3	23:n:203:TRT:H7C1	1.99	0.43
7:H:88:VAL:HG22	7:H:466:TRP:CE3	2.53	0.43
7:H:269:ALA:HB3	7:H:270:PRO:HD3	2.01	0.43
13:N:19:ARG:NH2	7:h:383:ILE:O	2.51	0.43
5:f:127:ASN:OD1	5:f:128:LYS:N	2.52	0.43
20:D:202:CDL:H751	20:D:202:CDL:H782	1.55	0.43
5:F:21:ILE:HG21	11:L:21:LEU:HD11	2.00	0.43
8:i:80:GLN:OE1	15:p:91:MET:HE2	2.17	0.43
20:E:101:CDL:H661	20:E:101:CDL:H591	2.00	0.43
5:F:66:THR:O	5:F:70:HIS:N	2.49	0.43
23:M:202:TRT:H2C3	23:M:202:TRT:H7C1	2.01	0.43
1:a:51:LYS:O	1:a:52:GLN:NE2	2.51	0.43
1:a:350:PHE:CE2	1:a:354:LEU:HD11	2.54	0.43
7:h:269:ALA:HB3	7:h:270:PRO:HD3	2.01	0.43
1:A:444:THR:N	1:A:447:ASP:OD2	2.51	0.43
9:j:62:HIS:O	9:j:62:HIS:ND1	2.52	0.43
23:M:202:TRT:H3C2	23:M:202:TRT:C8	2.49	0.43
3:d:149:LEU:HD22	19:t:62:ALA:HB2	2.01	0.43
23:m:204:TRT:H2C3	23:m:204:TRT:H7C1	2.01	0.43
1:A:350:PHE:CE2	1:A:354:LEU:HD11	2.54	0.42
9:J:62:HIS:ND1	9:J:62:HIS:O	2.52	0.42
1:a:429:GLU:OE1	8:i:2:ALA:N	2.51	0.42
1:A:310:GLU:O	19:T:18:ARG:NH2	2.52	0.42
6:G:16:LEU:HD23	22:I:101:LPP:H441	2.00	0.42
23:N:201:TRT:C8	23:N:201:TRT:H3C2	2.48	0.42
7:h:403:ILE:HG23	11:l:33:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:10:ILE:HG22	11:l:10:ILE:O	2.19	0.42
1:a:320:ARG:NH2	1:a:337:VAL:O	2.52	0.42
23:g:201:TRT:H2C3	23:g:201:TRT:C7	2.50	0.42
11:L:10:ILE:HG22	11:L:10:ILE:O	2.19	0.42
5:f:154:ASN:O	5:f:157:THR:OG1	2.29	0.42
23:g:201:TRT:H2C3	23:g:201:TRT:H7C1	2.01	0.42
20:A:503:CDL:H732	20:A:503:CDL:H771	2.01	0.42
7:H:383:ILE:O	13:n:19:ARG:NH2	2.52	0.42
18:S:25:TRP:N	18:S:28:GLN:OE1	2.48	0.42
13:n:31:ASN:N	13:n:34:THR:OG1	2.48	0.42
20:D:202:CDL:H811	20:D:202:CDL:H781	1.77	0.42
20:e:101:CDL:H661	20:e:101:CDL:H591	2.01	0.42
20:a:503:CDL:H741	20:a:503:CDL:H712	1.69	0.42
3:d:178:ARG:NH2	10:k:111:THR:O	2.49	0.42
20:M:204:CDL:H742	20:M:204:CDL:H711	1.77	0.42
20:a:502:CDL:H711	3:d:48:PHE:CD2	2.55	0.42
18:s:25:TRP:N	18:s:28:GLN:OE1	2.47	0.42
20:A:502:CDL:H772	20:A:502:CDL:H742	1.28	0.41
5:F:154:ASN:O	5:F:157:THR:OG1	2.29	0.41
13:N:31:ASN:N	13:N:34:THR:OG1	2.48	0.41
23:N:201:TRT:H253	22:N:203:LPP:H321	2.00	0.41
22:P:202:LPP:H321	23:n:202:TRT:H253	2.01	0.41
6:g:16:LEU:HD23	22:i:101:LPP:H441	2.01	0.41
23:n:202:TRT:H3C2	23:n:202:TRT:H8C1	2.02	0.41
1:A:429:GLU:OE1	8:I:2:ALA:N	2.52	0.41
20:A:502:CDL:H711	3:D:48:PHE:CD2	2.55	0.41
23:G:201:TRT:H2C3	23:G:201:TRT:H7C1	2.01	0.41
5:F:266:ASN:N	5:F:266:ASN:OD1	2.53	0.41
20:M:203:CDL:H782	20:M:203:CDL:H752	1.92	0.41
23:N:201:TRT:H3C2	23:N:201:TRT:H8C1	2.02	0.41
5:F:190:LEU:HG	6:G:28:MET:HE2	2.02	0.41
23:G:201:TRT:H2C3	23:G:201:TRT:C7	2.50	0.41
7:h:55:LEU:O	7:h:63:ARG:NH2	2.51	0.41
23:m:204:TRT:H3C2	23:m:204:TRT:C8	2.49	0.41
4:E:46:ASP:OD2	9:J:85:ARG:NH2	2.48	0.41
1:a:353:ILE:HG21	1:a:406:MET:HE1	2.03	0.41
10:k:96:GLU:OE1	16:q:62:ARG:NH2	2.50	0.41
3:D:61:ILE:HG22	3:D:65:ILE:HD12	2.03	0.41
1:a:310:GLU:O	19:t:18:ARG:NH2	2.53	0.41
1:a:444:THR:N	1:a:447:ASP:OD2	2.51	0.41
23:n:203:TRT:H7C1	23:n:203:TRT:C2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:18:LYS:NZ	18:s:23:GLY:O	2.53	0.41
5:F:225:VAL:HG22	21:F:302:LMT:H32	2.03	0.41
19:t:11:ILE:O	19:t:11:ILE:HG22	2.21	0.41
1:a:381:ARG:O	1:a:418:GLN:NE2	2.54	0.40
3:d:61:ILE:HG22	3:d:65:ILE:HD12	2.03	0.40
1:A:320:ARG:NH2	1:A:337:VAL:O	2.52	0.40
23:N:201:TRT:H7C2	23:N:202:TRT:H14	2.04	0.40
23:N:202:TRT:H7C1	23:N:202:TRT:C2	2.51	0.40
5:f:266:ASN:OD1	5:f:266:ASN:N	2.53	0.40
1:A:436:SER:OG	7:H:361:GLU:OE1	2.20	0.40
5:F:55:ILE:HG21	5:F:99:SER:HB3	2.04	0.40
20:M:203:CDL:C85	20:M:203:CDL:H781	2.52	0.40
20:A:502:CDL:C83	20:O:201:CDL:H742	2.51	0.40
19:T:11:ILE:O	19:T:11:ILE:HG22	2.21	0.40
5:F:261:ASN:OD1	5:F:262:LYS:N	2.55	0.40
20:d:201:CDL:C67	20:e:101:CDL:H741	2.51	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	484/487 (99%)	467 (96%)	17 (4%)	0	100	100
1	a	484/487 (99%)	467 (96%)	17 (4%)	0	100	100
2	B	29/338 (9%)	29 (100%)	0	0	100	100
2	b	29/338 (9%)	29 (100%)	0	0	100	100
3	D	184/187 (98%)	180 (98%)	4 (2%)	0	100	100
3	d	184/187 (98%)	180 (98%)	4 (2%)	0	100	100
4	E	94/97 (97%)	91 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	e	94/97 (97%)	91 (97%)	3 (3%)	0	100	100
5	F	270/274 (98%)	262 (97%)	8 (3%)	0	100	100
5	f	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
6	G	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
6	g	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
7	H	384/476 (81%)	380 (99%)	4 (1%)	0	100	100
7	h	384/476 (81%)	380 (99%)	4 (1%)	0	100	100
8	I	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
8	i	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
9	J	101/104 (97%)	99 (98%)	2 (2%)	0	100	100
9	j	101/104 (97%)	99 (98%)	2 (2%)	0	100	100
10	K	101/113 (89%)	99 (98%)	2 (2%)	0	100	100
10	k	101/113 (89%)	99 (98%)	2 (2%)	0	100	100
11	L	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
11	l	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
12	M	164/169 (97%)	164 (100%)	0	0	100	100
12	m	164/169 (97%)	164 (100%)	0	0	100	100
13	N	129/137 (94%)	124 (96%)	5 (4%)	0	100	100
13	n	129/137 (94%)	124 (96%)	5 (4%)	0	100	100
14	O	98/116 (84%)	95 (97%)	3 (3%)	0	100	100
14	o	98/116 (84%)	95 (97%)	3 (3%)	0	100	100
15	P	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
15	p	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
16	Q	87/90 (97%)	80 (92%)	7 (8%)	0	100	100
16	q	87/90 (97%)	80 (92%)	7 (8%)	0	100	100
17	R	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
17	r	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
18	S	63/74 (85%)	61 (97%)	2 (3%)	0	100	100
18	s	63/74 (85%)	61 (97%)	2 (3%)	0	100	100
19	T	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
19	t	64/66 (97%)	63 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5382/6386 (84%)	5241 (97%)	141 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/427 (100%)	426 (100%)	0	100	100
1	a	426/427 (100%)	426 (100%)	0	100	100
2	B	28/259 (11%)	28 (100%)	0	100	100
2	b	28/259 (11%)	28 (100%)	0	100	100
3	D	159/160 (99%)	159 (100%)	0	100	100
3	d	159/160 (99%)	159 (100%)	0	100	100
4	E	80/82 (98%)	80 (100%)	0	100	100
4	e	81/82 (99%)	81 (100%)	0	100	100
5	F	258/259 (100%)	258 (100%)	0	100	100
5	f	259/259 (100%)	259 (100%)	0	100	100
6	G	98/99 (99%)	98 (100%)	0	100	100
6	g	98/99 (99%)	98 (100%)	0	100	100
7	H	339/414 (82%)	339 (100%)	0	100	100
7	h	339/414 (82%)	339 (100%)	0	100	100
8	I	82/83 (99%)	82 (100%)	0	100	100
8	i	82/83 (99%)	82 (100%)	0	100	100
9	J	94/95 (99%)	94 (100%)	0	100	100
9	j	94/95 (99%)	94 (100%)	0	100	100
10	K	89/97 (92%)	89 (100%)	0	100	100
10	k	89/97 (92%)	89 (100%)	0	100	100
11	L	56/56 (100%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	56/56 (100%)	56 (100%)	0	100	100
12	M	137/140 (98%)	137 (100%)	0	100	100
12	m	137/140 (98%)	137 (100%)	0	100	100
13	N	114/119 (96%)	114 (100%)	0	100	100
13	n	114/119 (96%)	114 (100%)	0	100	100
14	O	90/103 (87%)	90 (100%)	0	100	100
14	o	90/103 (87%)	90 (100%)	0	100	100
15	P	96/99 (97%)	96 (100%)	0	100	100
15	p	96/99 (97%)	96 (100%)	0	100	100
16	Q	82/83 (99%)	82 (100%)	0	100	100
16	q	82/83 (99%)	82 (100%)	0	100	100
17	R	59/67 (88%)	59 (100%)	0	100	100
17	r	59/67 (88%)	59 (100%)	0	100	100
18	S	59/68 (87%)	59 (100%)	0	100	100
18	s	59/68 (87%)	59 (100%)	0	100	100
19	T	54/54 (100%)	54 (100%)	0	100	100
19	t	54/54 (100%)	54 (100%)	0	100	100
All	All	4802/5528 (87%)	4802 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	3	HIS
4	E	52	HIS
5	F	3	ASN
5	F	125	ASN
5	F	163	ASN
7	H	370	GLN
9	J	44	ASN
11	L	55	ASN
11	L	57	ASN
12	M	130	HIS
13	N	62	HIS
13	N	65	ASN

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Mol	Chain	Res	Type
16	Q	40	ASN
16	Q	80	HIS
3	d	3	HIS
3	d	7	HIS
4	e	52	HIS
5	f	125	ASN
5	f	163	ASN
7	h	370	GLN
9	j	44	ASN
9	j	79	GLN
11	l	55	ASN
11	l	57	ASN
12	m	130	HIS
13	n	62	HIS
13	n	65	ASN
16	q	40	ASN
16	q	80	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

61 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	TRT	g	202	-	25,25,25	0.60	0	33,33,33	0.69	0
23	TRT	r	103	-	25,25,25	0.53	0	33,33,33	0.82	1 (3%)
20	CDL	A	504	-	62,62,99	1.11	8 (12%)	68,74,111	1.18	4 (5%)
20	CDL	a	503	-	80,80,99	0.98	8 (10%)	85,91,111	1.06	4 (4%)
21	LMT	n	201	-	36,36,36	1.17	6 (16%)	47,47,47	1.02	4 (8%)
23	TRT	G	202	-	25,25,25	0.60	0	33,33,33	0.69	0
23	TRT	p	203	-	25,25,25	1.25	3 (12%)	33,33,33	4.51	8 (24%)
22	LPP	o	203	-	31,31,43	1.28	4 (12%)	34,36,48	1.14	2 (5%)
22	LPP	o	202	-	22,22,43	1.41	3 (13%)	25,27,48	1.21	2 (8%)
23	TRT	N	201	-	25,25,25	0.51	0	33,33,33	0.85	1 (3%)
21	LMT	Q	101	-	36,36,36	1.14	6 (16%)	47,47,47	1.01	2 (4%)
20	CDL	R	101	-	75,75,99	1.01	8 (10%)	81,87,111	1.06	4 (4%)
20	CDL	M	203	-	76,76,99	1.00	8 (10%)	82,88,111	1.10	4 (4%)
20	CDL	A	503	-	80,80,99	0.98	8 (10%)	85,91,111	1.06	4 (4%)
23	TRT	m	204	-	25,25,25	0.55	0	33,33,33	0.78	1 (3%)
20	CDL	D	201	-	90,90,99	0.92	8 (8%)	96,102,111	1.04	4 (4%)
20	CDL	d	202	-	84,84,99	0.96	8 (9%)	90,96,111	1.02	4 (4%)
20	CDL	o	201	-	64,64,99	1.09	8 (12%)	70,76,111	1.08	4 (5%)
22	LPP	r	102	-	30,30,43	1.26	4 (13%)	33,35,48	1.26	2 (6%)
23	TRT	N	202	-	25,25,25	0.61	0	33,33,33	0.64	0
20	CDL	p	202	-	47,47,99	1.25	8 (17%)	53,59,111	1.31	5 (9%)
23	TRT	n	202	-	25,25,25	0.51	0	33,33,33	0.86	1 (3%)
20	CDL	A	502	-	80,80,99	0.99	8 (10%)	86,92,111	1.09	4 (4%)
20	CDL	a	502	-	80,80,99	0.98	8 (10%)	86,92,111	1.09	4 (4%)
21	LMT	q	101	-	36,36,36	1.15	6 (16%)	47,47,47	1.01	2 (4%)
22	LPP	F	301	-	23,23,43	1.39	3 (13%)	26,28,48	1.23	2 (7%)
20	CDL	m	202	-	52,52,99	1.20	8 (15%)	58,64,111	1.26	4 (6%)
23	TRT	G	201	-	25,25,25	0.54	0	33,33,33	0.79	0
23	TRT	g	201	-	25,25,25	0.53	0	33,33,33	0.79	0
23	TRT	P	203	-	25,25,25	1.25	3 (12%)	33,33,33	4.51	8 (24%)
20	CDL	a	501	-	80,80,99	0.98	7 (8%)	86,92,111	1.12	5 (5%)
20	CDL	e	101	-	62,62,99	1.09	8 (12%)	68,74,111	1.13	4 (5%)
22	LPP	I	101	-	43,43,43	1.13	3 (6%)	46,48,48	1.00	2 (4%)
23	TRT	M	201	-	25,25,25	0.55	0	33,33,33	0.68	1 (3%)
23	TRT	M	202	-	25,25,25	0.55	0	33,33,33	0.78	1 (3%)
23	TRT	n	203	-	25,25,25	0.61	0	33,33,33	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LPP	R	102	-	30,30,43	1.27	4 (13%)	33,35,48	1.25	2 (6%)
21	LMT	F	302	-	36,36,36	1.15	5 (13%)	47,47,47	0.96	2 (4%)
21	LMT	N	204	-	36,36,36	1.17	6 (16%)	47,47,47	1.03	4 (8%)
20	CDL	E	101	-	62,62,99	1.09	8 (12%)	68,74,111	1.12	4 (5%)
20	CDL	A	501	-	80,80,99	0.98	7 (8%)	86,92,111	1.12	5 (5%)
22	LPP	N	203	-	25,25,43	1.35	3 (12%)	28,30,48	1.28	2 (7%)
23	TRT	m	203	-	25,25,25	0.55	0	33,33,33	0.68	1 (3%)
20	CDL	d	201	-	90,90,99	0.92	8 (8%)	96,102,111	1.05	4 (4%)
22	LPP	i	101	-	43,43,43	1.13	3 (6%)	46,48,48	1.00	2 (4%)
20	CDL	D	202	-	84,84,99	0.96	8 (9%)	90,96,111	1.04	5 (5%)
21	LMT	d	203	-	36,36,36	1.17	6 (16%)	47,47,47	0.92	1 (2%)
20	CDL	r	101	-	75,75,99	1.01	8 (10%)	81,87,111	1.04	4 (4%)
22	LPP	O	203	-	31,31,43	1.28	4 (12%)	34,36,48	1.14	2 (5%)
22	LPP	P	202	-	25,25,43	1.35	3 (12%)	28,30,48	1.27	2 (7%)
22	LPP	f	301	-	23,23,43	1.39	3 (13%)	26,28,48	1.24	2 (7%)
23	TRT	R	103	-	25,25,25	0.53	0	33,33,33	0.82	1 (3%)
20	CDL	m	201	-	76,76,99	1.01	8 (10%)	82,88,111	1.10	4 (4%)
20	CDL	M	204	-	52,52,99	1.21	8 (15%)	58,64,111	1.27	4 (6%)
22	LPP	O	202	-	22,22,43	1.41	3 (13%)	25,27,48	1.21	2 (8%)
20	CDL	a	504	-	62,62,99	1.11	8 (12%)	68,74,111	1.18	4 (5%)
20	CDL	p	201	-	97,97,99	0.91	8 (8%)	103,109,111	1.00	4 (3%)
21	LMT	D	203	-	36,36,36	1.16	5 (13%)	47,47,47	0.92	1 (2%)
21	LMT	f	302	-	36,36,36	1.15	5 (13%)	47,47,47	0.96	2 (4%)
20	CDL	O	201	-	64,64,99	1.09	8 (12%)	70,76,111	1.07	4 (5%)
20	CDL	P	201	-	47,47,99	1.26	8 (17%)	53,59,111	1.32	5 (9%)

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
23	TRT	g	202	-	-	15/23/23/23	0/1/1/1
23	TRT	r	103	-	-	9/23/23/23	0/1/1/1
20	CDL	A	504	-	-	33/73/73/110	-
20	CDL	a	503	-	-	31/89/89/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMT	n	201	-	-	9/21/61/61	0/2/2/2
23	TRT	G	202	-	-	15/23/23/23	0/1/1/1
23	TRT	p	203	-	-	15/23/23/23	0/1/1/1
22	LPP	o	203	-	-	15/33/33/45	-
22	LPP	o	202	-	-	10/24/24/45	-
23	TRT	N	201	-	-	7/23/23/23	0/1/1/1
21	LMT	Q	101	-	-	6/21/61/61	0/2/2/2
20	CDL	R	101	-	-	33/86/86/110	-
20	CDL	M	203	-	-	39/87/87/110	-
20	CDL	A	503	-	-	33/89/89/110	-
23	TRT	m	204	-	-	8/23/23/23	0/1/1/1
20	CDL	D	201	-	-	35/101/101/110	-
20	CDL	d	202	-	-	44/95/95/110	-
20	CDL	o	201	-	-	38/75/75/110	-
22	LPP	r	102	-	-	13/32/32/45	-
23	TRT	N	202	-	-	14/23/23/23	0/1/1/1
20	CDL	p	202	-	-	23/57/57/110	-
23	TRT	n	202	-	-	7/23/23/23	0/1/1/1
20	CDL	A	502	-	-	30/91/91/110	-
20	CDL	a	502	-	-	33/91/91/110	-
21	LMT	q	101	-	-	6/21/61/61	0/2/2/2
22	LPP	F	301	-	-	5/25/25/45	-
20	CDL	m	202	-	-	30/63/63/110	-
23	TRT	G	201	-	-	8/23/23/23	0/1/1/1
23	TRT	g	201	-	-	8/23/23/23	0/1/1/1
23	TRT	P	203	-	-	15/23/23/23	0/1/1/1
20	CDL	a	501	-	-	28/91/91/110	-
20	CDL	e	101	-	-	40/73/73/110	-
22	LPP	I	101	-	-	13/45/45/45	-
23	TRT	M	201	-	-	10/23/23/23	0/1/1/1
23	TRT	M	202	-	-	8/23/23/23	0/1/1/1
23	TRT	n	203	-	-	14/23/23/23	0/1/1/1
22	LPP	R	102	-	-	13/32/32/45	-
21	LMT	F	302	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMT	N	204	-	-	9/21/61/61	0/2/2/2
20	CDL	E	101	-	-	40/73/73/110	-
20	CDL	A	501	-	-	27/91/91/110	-
22	LPP	N	203	-	-	12/27/27/45	-
23	TRT	m	203	-	-	10/23/23/23	0/1/1/1
20	CDL	d	201	-	-	33/101/101/110	-
22	LPP	i	101	-	-	13/45/45/45	-
20	CDL	D	202	-	-	43/95/95/110	-
21	LMT	d	203	-	-	7/21/61/61	0/2/2/2
20	CDL	r	101	-	-	36/86/86/110	-
22	LPP	O	203	-	-	15/33/33/45	-
22	LPP	P	202	-	-	12/27/27/45	-
22	LPP	f	301	-	-	5/25/25/45	-
23	TRT	R	103	-	-	9/23/23/23	0/1/1/1
20	CDL	m	201	-	-	39/87/87/110	-
20	CDL	M	204	-	-	29/63/63/110	-
22	LPP	O	202	-	-	10/24/24/45	-
20	CDL	a	504	-	-	33/73/73/110	-
20	CDL	p	201	-	-	45/108/108/110	-
21	LMT	D	203	-	-	7/21/61/61	0/2/2/2
21	LMT	f	302	-	-	8/21/61/61	0/2/2/2
20	CDL	O	201	-	-	34/75/75/110	-
20	CDL	P	201	-	-	24/57/57/110	-

All (289) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	203	TRT	C6-C9	4.13	1.60	1.53
23	p	203	TRT	C6-C9	4.13	1.60	1.53
22	P	202	LPP	O9-C11	3.36	1.43	1.34
22	N	203	LPP	O9-C11	3.34	1.43	1.34
22	I	101	LPP	O9-C11	3.25	1.43	1.34
22	i	101	LPP	O9-C11	3.25	1.43	1.34
22	r	102	LPP	O9-C11	3.21	1.43	1.34
22	R	102	LPP	O9-C11	3.20	1.43	1.34
22	o	202	LPP	O9-C11	3.19	1.43	1.34
22	O	202	LPP	O9-C11	3.19	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	203	LPP	O9-C11	3.18	1.43	1.34
22	o	203	LPP	O9-C11	3.18	1.43	1.34
22	F	301	LPP	O9-C11	3.15	1.43	1.34
22	f	301	LPP	O9-C11	3.15	1.43	1.34
22	i	101	LPP	O27-C29	2.97	1.42	1.33
20	D	202	CDL	OB6-CB4	-2.97	1.39	1.46
22	I	101	LPP	O27-C29	2.96	1.42	1.33
20	d	202	CDL	OB6-CB4	-2.96	1.39	1.46
20	A	501	CDL	OB6-CB4	-2.95	1.39	1.46
20	a	501	CDL	OB6-CB4	-2.95	1.39	1.46
22	o	203	LPP	O27-C29	2.93	1.41	1.33
22	o	202	LPP	O27-C29	2.92	1.41	1.33
22	O	203	LPP	O27-C29	2.91	1.41	1.33
20	d	201	CDL	OB6-CB4	-2.91	1.39	1.46
22	O	202	LPP	O27-C29	2.89	1.41	1.33
20	D	201	CDL	OB6-CB4	-2.89	1.39	1.46
21	n	201	LMT	O3'-C3'	-2.83	1.35	1.43
20	m	201	CDL	OA6-CA4	-2.81	1.40	1.46
21	N	204	LMT	O3'-C3'	-2.81	1.36	1.43
20	M	203	CDL	OA6-CA4	-2.80	1.40	1.46
20	m	202	CDL	OA6-CA4	-2.79	1.40	1.46
20	M	204	CDL	OA6-CA4	-2.79	1.40	1.46
22	F	301	LPP	O27-C29	2.79	1.41	1.33
22	f	301	LPP	O27-C29	2.78	1.41	1.33
20	m	201	CDL	OB6-CB4	-2.77	1.40	1.46
22	R	102	LPP	O27-C29	2.76	1.41	1.33
22	N	203	LPP	O27-C29	2.76	1.41	1.33
22	P	202	LPP	O27-C29	2.76	1.41	1.33
20	P	201	CDL	OB6-CB4	-2.75	1.40	1.46
22	r	102	LPP	O27-C29	2.75	1.41	1.33
20	p	201	CDL	OB6-CB4	-2.73	1.40	1.46
20	a	501	CDL	OA6-CA4	-2.73	1.40	1.46
20	p	202	CDL	OB6-CB4	-2.73	1.40	1.46
20	A	501	CDL	OA6-CA4	-2.73	1.40	1.46
21	D	203	LMT	O3'-C3'	-2.72	1.36	1.43
20	M	204	CDL	OB6-CB4	-2.71	1.40	1.46
20	m	202	CDL	OB6-CB4	-2.71	1.40	1.46
20	M	203	CDL	OB6-CB4	-2.71	1.40	1.46
20	a	504	CDL	OB6-CB4	-2.70	1.40	1.46
21	d	203	LMT	O3'-C3'	-2.69	1.36	1.43
20	o	201	CDL	OB6-CB4	-2.68	1.40	1.46
20	A	504	CDL	OB6-CB4	-2.67	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	201	CDL	OA6-CA4	-2.66	1.40	1.46
20	r	101	CDL	OB6-CB4	-2.65	1.40	1.46
20	R	101	CDL	OB6-CB4	-2.65	1.40	1.46
20	A	503	CDL	OB6-CB4	-2.65	1.40	1.46
20	a	504	CDL	OA6-CA4	-2.65	1.40	1.46
20	d	201	CDL	OA6-CA4	-2.65	1.40	1.46
20	O	201	CDL	OB6-CB4	-2.65	1.40	1.46
21	F	302	LMT	O3'-C3'	-2.61	1.36	1.43
20	a	503	CDL	OB6-CB4	-2.61	1.40	1.46
20	A	504	CDL	OA6-CA4	-2.60	1.40	1.46
20	p	201	CDL	OA6-CA4	-2.60	1.40	1.46
20	a	502	CDL	OB6-CB4	-2.60	1.40	1.46
21	f	302	LMT	O3'-C3'	-2.59	1.36	1.43
20	E	101	CDL	OB6-CB4	-2.59	1.40	1.46
20	A	502	CDL	OB6-CB4	-2.58	1.40	1.46
21	q	101	LMT	O3'-C3'	-2.57	1.36	1.43
20	r	101	CDL	OA6-CA4	-2.56	1.40	1.46
21	Q	101	LMT	O3'-C3'	-2.56	1.36	1.43
20	e	101	CDL	OB6-CB4	-2.55	1.40	1.46
20	R	101	CDL	OA6-CA4	-2.55	1.40	1.46
20	o	201	CDL	OA6-CA4	-2.53	1.40	1.46
20	O	201	CDL	OA6-CA4	-2.51	1.40	1.46
20	a	502	CDL	OA6-CA4	-2.50	1.40	1.46
20	A	504	CDL	OA8-CA7	2.49	1.40	1.33
20	a	504	CDL	OA8-CA7	2.49	1.40	1.33
21	D	203	LMT	O2'-C2'	-2.48	1.36	1.43
21	d	203	LMT	O2'-C2'	-2.47	1.36	1.43
20	A	502	CDL	OB8-CB7	2.47	1.40	1.33
20	a	502	CDL	OB8-CB7	2.47	1.40	1.33
21	f	302	LMT	O2B-C2B	-2.46	1.36	1.43
21	F	302	LMT	O2B-C2B	-2.45	1.36	1.43
21	d	203	LMT	O2B-C2B	-2.45	1.36	1.43
21	D	203	LMT	O2B-C2B	-2.44	1.36	1.43
20	D	202	CDL	OA6-CA4	-2.44	1.40	1.46
20	e	101	CDL	OA6-CA4	-2.43	1.40	1.46
20	r	101	CDL	OB8-CB7	2.43	1.40	1.33
20	m	201	CDL	OA8-CA7	2.43	1.40	1.33
20	r	101	CDL	OA8-CA6	-2.42	1.39	1.45
20	a	504	CDL	OB8-CB7	2.41	1.40	1.33
20	O	201	CDL	OA8-CA7	2.41	1.40	1.33
20	R	101	CDL	OB8-CB7	2.41	1.40	1.33
20	A	502	CDL	OA8-CA6	-2.41	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	E	101	CDL	OA6-CA4	-2.40	1.40	1.46
20	M	204	CDL	OB8-CB7	2.40	1.40	1.33
20	O	201	CDL	OB8-CB7	2.40	1.40	1.33
20	A	503	CDL	OA6-CA4	-2.40	1.41	1.46
20	D	201	CDL	OA8-CA7	2.40	1.40	1.33
20	P	201	CDL	OA6-CA5	2.40	1.41	1.34
20	d	202	CDL	OA6-CA4	-2.40	1.41	1.46
20	A	502	CDL	OA6-CA4	-2.40	1.41	1.46
20	d	202	CDL	OA8-CA7	2.39	1.40	1.33
20	A	504	CDL	OB8-CB7	2.39	1.40	1.33
20	M	203	CDL	OA8-CA7	2.39	1.40	1.33
20	D	201	CDL	OB8-CB7	2.39	1.40	1.33
20	D	202	CDL	OB8-CB7	2.39	1.40	1.33
20	E	101	CDL	OB8-CB7	2.39	1.40	1.33
20	a	502	CDL	OA8-CA6	-2.39	1.39	1.45
20	d	201	CDL	OA8-CA7	2.38	1.40	1.33
20	m	202	CDL	OB8-CB7	2.38	1.40	1.33
20	A	501	CDL	OA8-CA6	-2.38	1.39	1.45
20	o	201	CDL	OB8-CB7	2.38	1.40	1.33
20	P	201	CDL	OA8-CA7	2.38	1.40	1.33
20	R	101	CDL	OA8-CA6	-2.38	1.39	1.45
20	d	202	CDL	OB8-CB7	2.37	1.40	1.33
20	e	101	CDL	OB8-CB7	2.37	1.40	1.33
20	P	201	CDL	OB8-CB7	2.37	1.40	1.33
20	a	503	CDL	OA6-CA4	-2.37	1.41	1.46
20	d	201	CDL	OB8-CB7	2.37	1.40	1.33
20	p	202	CDL	OA8-CA7	2.37	1.40	1.33
20	a	503	CDL	OA8-CA6	-2.37	1.39	1.45
20	D	202	CDL	OA8-CA6	-2.37	1.39	1.45
20	A	503	CDL	OA8-CA6	-2.36	1.39	1.45
20	P	201	CDL	OB6-CB5	2.36	1.40	1.35
20	a	502	CDL	OB6-CB5	2.36	1.40	1.34
20	o	201	CDL	OA8-CA7	2.35	1.40	1.33
20	p	202	CDL	OB8-CB7	2.35	1.40	1.33
20	A	502	CDL	OB6-CB5	2.35	1.40	1.34
20	D	202	CDL	OA8-CA7	2.35	1.40	1.33
20	a	501	CDL	OA8-CA6	-2.35	1.39	1.45
20	e	101	CDL	OA8-CA7	2.35	1.40	1.33
20	M	203	CDL	OB8-CB7	2.35	1.40	1.33
20	p	202	CDL	OA6-CA4	-2.35	1.41	1.46
20	E	101	CDL	OA8-CA7	2.34	1.40	1.33
20	a	503	CDL	OA8-CA7	2.34	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	m	201	CDL	OB8-CB7	2.34	1.40	1.33
20	p	201	CDL	OA8-CA6	-2.33	1.40	1.45
20	M	204	CDL	OA8-CA7	2.33	1.40	1.33
20	a	501	CDL	OB8-CB7	2.33	1.40	1.33
20	A	501	CDL	OA8-CA7	2.33	1.40	1.33
20	p	202	CDL	OA6-CA5	2.33	1.40	1.34
20	p	201	CDL	OA8-CA7	2.33	1.40	1.33
20	M	204	CDL	OA8-CA6	-2.33	1.40	1.45
20	A	503	CDL	OA8-CA7	2.32	1.40	1.33
21	F	302	LMT	O3B-C3B	-2.32	1.37	1.43
20	p	202	CDL	OB6-CB5	2.32	1.40	1.35
21	N	204	LMT	O2B-C2B	-2.32	1.37	1.43
20	p	201	CDL	OB8-CB7	2.32	1.40	1.33
21	n	201	LMT	O2B-C2B	-2.32	1.37	1.43
20	a	501	CDL	OA8-CA7	2.31	1.40	1.33
20	A	501	CDL	OB8-CB7	2.31	1.40	1.33
20	a	503	CDL	OB8-CB7	2.31	1.40	1.33
20	A	503	CDL	OB8-CB7	2.30	1.40	1.33
20	A	502	CDL	OA8-CA7	2.30	1.40	1.33
20	m	202	CDL	OA8-CA6	-2.30	1.40	1.45
20	d	202	CDL	OA8-CA6	-2.30	1.40	1.45
20	P	201	CDL	OA6-CA4	-2.30	1.41	1.46
20	m	202	CDL	OA8-CA7	2.30	1.40	1.33
20	e	101	CDL	OB6-CB5	2.29	1.40	1.34
20	R	101	CDL	OA6-CA5	2.29	1.40	1.34
21	N	204	LMT	O2'-C2'	-2.29	1.37	1.43
21	f	302	LMT	O3B-C3B	-2.29	1.37	1.43
20	a	503	CDL	OB8-CB6	-2.28	1.40	1.45
20	r	101	CDL	OA8-CA7	2.28	1.40	1.33
20	a	504	CDL	OB6-CB5	2.28	1.40	1.34
21	n	201	LMT	O2'-C2'	-2.27	1.37	1.43
20	E	101	CDL	OB6-CB5	2.27	1.40	1.34
20	r	101	CDL	OA6-CA5	2.27	1.40	1.34
21	q	101	LMT	O3B-C3B	-2.27	1.37	1.43
21	Q	101	LMT	O3B-C3B	-2.27	1.37	1.43
23	p	203	TRT	C8-C6	2.27	1.60	1.53
20	R	101	CDL	OA8-CA7	2.27	1.40	1.33
20	A	504	CDL	OB6-CB5	2.26	1.40	1.34
23	P	203	TRT	C8-C6	2.26	1.59	1.53
20	A	501	CDL	OB8-CB6	-2.26	1.40	1.45
20	A	503	CDL	OB8-CB6	-2.25	1.40	1.45
20	a	501	CDL	OB8-CB6	-2.25	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	502	CDL	OA8-CA7	2.25	1.39	1.33
20	P	201	CDL	OB8-CB6	-2.25	1.40	1.45
20	p	202	CDL	OB8-CB6	-2.25	1.40	1.45
23	p	203	TRT	C7-C6	2.25	1.59	1.53
20	E	101	CDL	OA6-CA5	2.24	1.40	1.34
20	e	101	CDL	OA8-CA6	-2.24	1.40	1.45
20	d	202	CDL	OB8-CB6	-2.24	1.40	1.45
21	N	204	LMT	O3B-C3B	-2.24	1.37	1.43
20	D	202	CDL	OB8-CB6	-2.24	1.40	1.45
20	o	201	CDL	OB6-CB5	2.24	1.40	1.34
20	p	201	CDL	OA6-CA5	2.24	1.40	1.34
20	p	201	CDL	OB8-CB6	-2.23	1.40	1.45
20	A	502	CDL	OA6-CA5	2.23	1.40	1.34
23	P	203	TRT	C7-C6	2.23	1.59	1.53
20	O	201	CDL	OB6-CB5	2.23	1.40	1.34
20	a	504	CDL	OA8-CA6	-2.23	1.40	1.45
21	n	201	LMT	O3B-C3B	-2.23	1.37	1.43
21	F	302	LMT	O2'-C2'	-2.23	1.37	1.43
20	D	202	CDL	OA6-CA5	2.23	1.40	1.34
20	e	101	CDL	OA6-CA5	2.22	1.40	1.34
20	A	504	CDL	OA8-CA6	-2.22	1.40	1.45
20	a	501	CDL	OA6-CA5	2.22	1.40	1.34
20	o	201	CDL	OA6-CA5	2.21	1.40	1.34
20	A	502	CDL	OB8-CB6	-2.21	1.40	1.45
20	m	201	CDL	OB6-CB5	2.21	1.40	1.34
21	D	203	LMT	O3B-C3B	-2.21	1.37	1.43
21	d	203	LMT	O3B-C3B	-2.21	1.37	1.43
21	f	302	LMT	O2'-C2'	-2.21	1.37	1.43
20	d	202	CDL	OA6-CA5	2.21	1.40	1.34
20	a	504	CDL	OB8-CB6	-2.21	1.40	1.45
20	a	502	CDL	OA6-CA5	2.21	1.40	1.34
20	o	201	CDL	OA8-CA6	-2.21	1.40	1.45
22	o	203	LPP	O9-C7	-2.21	1.41	1.46
21	Q	101	LMT	O4'-C4B	-2.21	1.37	1.43
22	O	203	LPP	O9-C7	-2.21	1.41	1.46
20	a	504	CDL	OA6-CA5	2.20	1.40	1.34
20	M	204	CDL	OA6-CA5	2.20	1.40	1.34
20	A	503	CDL	OA6-CA5	2.20	1.40	1.34
20	m	202	CDL	OA6-CA5	2.20	1.40	1.34
20	m	202	CDL	OB8-CB6	-2.19	1.40	1.45
22	R	102	LPP	O9-C7	-2.19	1.41	1.46
20	A	501	CDL	OA6-CA5	2.19	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	E	101	CDL	OA8-CA6	-2.19	1.40	1.45
20	a	502	CDL	OB8-CB6	-2.19	1.40	1.45
20	D	201	CDL	OA6-CA5	2.18	1.40	1.34
20	A	504	CDL	OB8-CB6	-2.18	1.40	1.45
20	a	503	CDL	OA6-CA5	2.18	1.40	1.34
20	M	204	CDL	OB6-CB5	2.18	1.40	1.34
20	r	101	CDL	OB6-CB5	2.18	1.40	1.34
20	d	201	CDL	OA6-CA5	2.18	1.40	1.34
21	f	302	LMT	O4'-C4B	-2.18	1.37	1.43
20	A	504	CDL	OA6-CA5	2.18	1.40	1.34
20	M	203	CDL	OB6-CB5	2.18	1.40	1.34
21	q	101	LMT	O1'-C1'	-2.18	1.36	1.40
20	m	202	CDL	OB6-CB5	2.18	1.40	1.34
20	M	204	CDL	OB8-CB6	-2.17	1.40	1.45
21	q	101	LMT	O4'-C4B	-2.17	1.37	1.43
21	Q	101	LMT	O1'-C1'	-2.17	1.36	1.40
20	D	201	CDL	OA8-CA6	-2.17	1.40	1.45
20	R	101	CDL	OB6-CB5	2.17	1.40	1.34
22	F	301	LPP	O9-C7	-2.17	1.41	1.46
21	F	302	LMT	O4'-C4B	-2.17	1.37	1.43
21	Q	101	LMT	O2B-C2B	-2.16	1.37	1.43
20	O	201	CDL	OA8-CA6	-2.16	1.40	1.45
20	O	201	CDL	OA6-CA5	2.16	1.40	1.34
22	f	301	LPP	O9-C7	-2.16	1.41	1.46
21	q	101	LMT	O2B-C2B	-2.16	1.37	1.43
20	d	201	CDL	OA8-CA6	-2.16	1.40	1.45
20	P	201	CDL	OA8-CA6	-2.16	1.40	1.45
21	D	203	LMT	O4'-C4B	-2.16	1.37	1.43
20	a	503	CDL	OB6-CB5	2.15	1.40	1.34
20	E	101	CDL	OB8-CB6	-2.15	1.40	1.45
20	M	203	CDL	OA8-CA6	-2.15	1.40	1.45
20	m	201	CDL	OB8-CB6	-2.15	1.40	1.45
21	d	203	LMT	O4'-C4B	-2.15	1.37	1.43
21	q	101	LMT	O2'-C2'	-2.15	1.37	1.43
22	i	101	LPP	O9-C7	-2.14	1.41	1.46
20	m	201	CDL	OA8-CA6	-2.14	1.40	1.45
20	M	203	CDL	OB8-CB6	-2.14	1.40	1.45
22	r	102	LPP	O9-C7	-2.14	1.41	1.46
20	p	201	CDL	OB6-CB5	2.14	1.40	1.34
22	O	202	LPP	O9-C7	-2.14	1.41	1.46
20	A	503	CDL	OB6-CB5	2.13	1.40	1.34
20	o	201	CDL	OB8-CB6	-2.13	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Q	101	LMT	O2'-C2'	-2.13	1.37	1.43
20	e	101	CDL	OB8-CB6	-2.13	1.40	1.45
20	r	101	CDL	OB8-CB6	-2.12	1.40	1.45
20	R	101	CDL	OB8-CB6	-2.12	1.40	1.45
20	O	201	CDL	OB8-CB6	-2.12	1.40	1.45
22	o	202	LPP	O9-C7	-2.12	1.41	1.46
22	I	101	LPP	O9-C7	-2.11	1.41	1.46
20	m	201	CDL	OA6-CA5	2.11	1.40	1.34
20	p	202	CDL	OA8-CA6	-2.10	1.40	1.45
20	M	203	CDL	OA6-CA5	2.10	1.40	1.34
21	N	204	LMT	O1'-C1'	-2.09	1.36	1.40
21	n	201	LMT	O1'-C1'	-2.09	1.36	1.40
20	D	201	CDL	OB8-CB6	-2.09	1.40	1.45
21	N	204	LMT	O4'-C4B	-2.08	1.37	1.43
20	d	201	CDL	OB8-CB6	-2.06	1.40	1.45
21	d	203	LMT	O1'-C1'	-2.04	1.36	1.40
22	R	102	LPP	C12-C11	2.04	1.56	1.50
20	d	201	CDL	OB6-CB5	2.04	1.40	1.34
22	N	203	LPP	P1-O5	2.03	1.66	1.60
21	n	201	LMT	O4'-C4B	-2.03	1.37	1.43
22	r	102	LPP	C12-C11	2.03	1.56	1.50
22	o	203	LPP	P1-O5	2.02	1.66	1.60
20	D	201	CDL	OB6-CB5	2.02	1.40	1.34
20	D	202	CDL	OB6-CB5	2.02	1.40	1.34
22	P	202	LPP	P1-O5	2.01	1.66	1.60
22	O	203	LPP	P1-O5	2.01	1.66	1.60
20	d	202	CDL	OB6-CB5	2.00	1.39	1.34

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	203	TRT	C7-C6-C8	14.88	152.16	107.26
23	p	203	TRT	C7-C6-C8	14.88	152.14	107.26
23	P	203	TRT	C5-C6-C9	11.75	139.47	112.00
23	p	203	TRT	C5-C6-C9	11.75	139.46	112.00
23	p	203	TRT	C8-C6-C9	-11.22	81.81	110.18
23	P	203	TRT	C8-C6-C9	-11.21	81.85	110.18
23	P	203	TRT	C7-C6-C9	-10.90	82.62	110.18
23	p	203	TRT	C7-C6-C9	-10.89	82.65	110.18
20	P	201	CDL	OB6-CB5-C51	4.99	119.99	111.09
20	p	202	CDL	OB6-CB5-C51	4.99	119.98	111.09
20	M	204	CDL	OA6-CA5-C11	4.66	121.55	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	m	202	CDL	OA6-CA5-C11	4.55	121.31	111.48
23	p	203	TRT	C8-C6-C5	-4.34	88.00	109.11
23	P	203	TRT	C8-C6-C5	-4.34	88.01	109.11
20	a	504	CDL	OA6-CA5-C11	4.23	120.63	111.48
20	A	504	CDL	OA6-CA5-C11	4.21	120.59	111.48
22	P	202	LPP	O9-C11-C12	4.19	120.54	111.48
22	N	203	LPP	O9-C11-C12	4.18	120.53	111.48
23	P	203	TRT	C7-C6-C5	-4.15	88.94	109.11
23	p	203	TRT	C7-C6-C5	-4.15	88.94	109.11
22	r	102	LPP	O9-C11-C12	4.13	120.42	111.48
22	R	102	LPP	O9-C11-C12	4.13	120.41	111.48
20	O	201	CDL	OB6-CB5-C51	4.05	120.24	111.48
20	o	201	CDL	OB6-CB5-C51	4.04	120.22	111.48
20	R	101	CDL	OA6-CA5-C11	4.03	120.20	111.48
20	e	101	CDL	OA6-CA5-C11	4.03	120.20	111.48
20	a	502	CDL	OB6-CB5-C51	4.01	120.16	111.48
20	A	502	CDL	OB6-CB5-C51	3.98	120.09	111.48
20	E	101	CDL	OA6-CA5-C11	3.97	120.08	111.48
20	A	501	CDL	OA6-CA5-C11	3.96	120.05	111.48
20	a	501	CDL	OA6-CA5-C11	3.93	119.99	111.48
20	m	202	CDL	OB6-CB5-C51	3.89	119.89	111.48
20	p	201	CDL	OB6-CB5-C51	3.88	119.89	111.48
22	O	203	LPP	O9-C11-C12	3.88	119.87	111.48
20	M	204	CDL	OB6-CB5-C51	3.87	119.85	111.48
22	o	203	LPP	O9-C11-C12	3.86	119.84	111.48
20	r	101	CDL	OA6-CA5-C11	3.85	119.82	111.48
20	a	504	CDL	OB6-CB5-C51	3.80	119.71	111.48
20	A	504	CDL	OB6-CB5-C51	3.79	119.69	111.48
20	m	201	CDL	OB6-CB5-C51	3.77	119.64	111.48
20	M	203	CDL	OB6-CB5-C51	3.76	119.62	111.48
20	a	503	CDL	OA6-CA5-C11	3.75	119.58	111.48
20	A	503	CDL	OA6-CA5-C11	3.75	119.58	111.48
20	d	201	CDL	OB6-CB5-C51	3.75	119.58	111.48
20	D	201	CDL	OB6-CB5-C51	3.72	119.53	111.48
20	d	201	CDL	OA6-CA5-C11	3.69	119.47	111.48
20	D	201	CDL	OA6-CA5-C11	3.69	119.47	111.48
20	P	201	CDL	OA6-CA5-C11	3.69	119.46	111.48
22	f	301	LPP	O9-C11-C12	3.69	119.46	111.48
22	O	202	LPP	O9-C11-C12	3.68	119.44	111.48
22	o	202	LPP	O9-C11-C12	3.68	119.43	111.48
20	m	201	CDL	OA6-CA5-C11	3.67	119.42	111.48
20	M	203	CDL	OA6-CA5-C11	3.66	119.40	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	301	LPP	O9-C11-C12	3.66	119.40	111.48
20	R	101	CDL	OB6-CB5-C51	3.65	119.37	111.48
20	r	101	CDL	OB6-CB5-C51	3.64	119.36	111.48
20	a	501	CDL	OB6-CB5-C51	3.64	119.35	111.48
20	A	503	CDL	OB6-CB5-C51	3.63	119.34	111.48
20	a	503	CDL	OB6-CB5-C51	3.63	119.33	111.48
20	A	501	CDL	OB6-CB5-C51	3.63	119.33	111.48
20	a	502	CDL	OA6-CA5-C11	3.60	119.27	111.48
20	e	101	CDL	OB6-CB5-C51	3.60	119.26	111.48
20	p	202	CDL	OA6-CA5-C11	3.59	119.25	111.48
20	E	101	CDL	OB6-CB5-C51	3.56	119.18	111.48
20	A	502	CDL	OA6-CA5-C11	3.49	119.03	111.48
20	p	201	CDL	OA6-CA5-C11	3.45	118.94	111.48
22	i	101	LPP	O9-C11-C12	3.37	118.77	111.48
22	I	101	LPP	O9-C11-C12	3.36	118.75	111.48
20	a	504	CDL	OA8-CA7-C31	3.32	121.95	111.83
20	A	504	CDL	OA8-CA7-C31	3.28	121.83	111.83
20	D	202	CDL	OB6-CB5-C51	3.26	118.53	111.48
20	d	202	CDL	OB6-CB5-C51	3.26	118.53	111.48
20	O	201	CDL	OA6-CA5-C11	3.22	118.44	111.48
20	o	201	CDL	OA6-CA5-C11	3.22	118.44	111.48
23	p	203	TRT	C1-C5-C6	-3.14	111.62	123.78
23	P	203	TRT	C1-C5-C6	-3.13	111.65	123.78
20	D	202	CDL	OA6-CA5-C11	3.11	118.21	111.48
20	d	201	CDL	OA8-CA7-C31	2.98	120.93	111.83
20	d	202	CDL	OA6-CA5-C11	2.98	117.92	111.48
20	D	201	CDL	OA8-CA7-C31	2.97	120.90	111.83
20	M	203	CDL	OA8-CA7-C31	2.97	120.90	111.83
20	m	201	CDL	OA8-CA7-C31	2.96	120.87	111.83
20	A	503	CDL	OB8-CB7-C71	2.96	120.86	111.83
20	a	503	CDL	OB8-CB7-C71	2.94	120.81	111.83
20	M	204	CDL	OA8-CA7-C31	2.93	120.76	111.83
20	o	201	CDL	OA8-CA7-C31	2.90	119.94	111.15
20	m	202	CDL	OA8-CA7-C31	2.88	120.60	111.83
20	D	202	CDL	OB8-CB7-C71	2.85	120.53	111.83
20	p	201	CDL	OB8-CB7-C71	2.84	120.48	111.83
20	a	501	CDL	OA8-CA7-C31	2.83	120.47	111.83
20	A	501	CDL	OA8-CA7-C31	2.81	120.41	111.83
22	f	301	LPP	O27-C29-C30	2.79	120.35	111.83
20	A	502	CDL	OB8-CB7-C71	2.78	120.31	111.83
20	a	502	CDL	OB8-CB7-C71	2.78	120.31	111.83
22	F	301	LPP	O27-C29-C30	2.77	120.29	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	M	203	CDL	OB8-CB7-C71	2.75	120.23	111.83
20	m	201	CDL	OB8-CB7-C71	2.74	120.20	111.83
20	O	201	CDL	OA8-CA7-C31	2.74	119.47	111.15
20	d	202	CDL	OB8-CB7-C71	2.71	120.11	111.83
20	P	201	CDL	OA8-CA7-C31	2.71	120.09	111.83
20	e	101	CDL	OB8-CB7-C71	2.70	120.07	111.83
20	p	202	CDL	OA8-CA7-C31	2.70	120.07	111.83
20	p	202	CDL	OB8-CB7-C71	2.69	120.02	111.83
20	E	101	CDL	OB8-CB7-C71	2.68	120.02	111.83
20	M	204	CDL	OB8-CB7-C71	2.67	119.97	111.83
20	m	202	CDL	OB8-CB7-C71	2.66	119.96	111.83
20	A	501	CDL	OB8-CB7-C71	2.66	119.94	111.83
20	P	201	CDL	OB8-CB7-C71	2.65	119.93	111.83
20	a	504	CDL	OB8-CB7-C71	2.65	119.92	111.83
20	A	502	CDL	OA8-CA7-C31	2.65	119.92	111.83
20	p	201	CDL	OA8-CA7-C31	2.65	119.90	111.83
20	a	501	CDL	OB8-CB7-C71	2.64	119.89	111.83
23	P	203	TRT	C14-C9-C6	2.63	126.28	121.52
22	N	203	LPP	O27-C29-C30	2.63	119.86	111.83
20	A	504	CDL	OB8-CB7-C71	2.63	119.86	111.83
22	P	202	LPP	O27-C29-C30	2.63	119.85	111.83
23	p	203	TRT	C14-C9-C6	2.62	126.25	121.52
20	o	201	CDL	OB8-CB7-C71	2.61	119.79	111.83
20	P	201	CDL	CB4-OB6-CB5	-2.60	113.25	117.85
20	O	201	CDL	OB8-CB7-C71	2.60	119.76	111.83
22	o	203	LPP	O27-C29-C30	2.59	119.72	111.83
20	p	202	CDL	CB4-OB6-CB5	-2.59	113.28	117.85
22	r	102	LPP	O27-C29-C30	2.58	119.70	111.83
22	O	203	LPP	O27-C29-C30	2.58	119.69	111.83
20	a	502	CDL	OA8-CA7-C31	2.57	119.67	111.83
22	R	102	LPP	O27-C29-C30	2.57	119.66	111.83
21	n	201	LMT	C3B-C4B-C5B	-2.55	105.61	110.23
20	d	202	CDL	OA8-CA7-C31	2.55	119.60	111.83
21	N	204	LMT	C3B-C4B-C5B	-2.55	105.62	110.23
20	D	202	CDL	OA8-CA7-C31	2.54	119.58	111.83
20	R	101	CDL	OB8-CB7-C71	2.52	119.53	111.83
20	r	101	CDL	OB8-CB7-C71	2.52	119.52	111.83
20	a	503	CDL	OA8-CA7-C31	2.52	119.51	111.83
20	A	503	CDL	OA8-CA7-C31	2.51	119.49	111.83
20	A	501	CDL	CB4-OB6-CB5	-2.48	111.85	117.80
22	o	202	LPP	O27-C29-C30	2.47	119.36	111.83
20	e	101	CDL	OA8-CA7-C31	2.47	119.36	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	E	101	CDL	OA8-CA7-C31	2.46	119.34	111.83
22	O	202	LPP	O27-C29-C30	2.45	119.29	111.83
20	a	501	CDL	CB4-OB6-CB5	-2.44	111.97	117.80
20	R	101	CDL	OA8-CA7-C31	2.43	119.23	111.83
20	r	101	CDL	OA8-CA7-C31	2.42	119.20	111.83
22	i	101	LPP	O27-C29-C30	2.41	119.19	111.83
21	N	204	LMT	C3'-C4'-C5'	-2.41	105.59	110.93
22	I	101	LPP	O27-C29-C30	2.41	119.18	111.83
23	n	202	TRT	C5-C6-C9	-2.41	106.37	112.00
21	n	201	LMT	C3'-C4'-C5'	-2.40	105.61	110.93
23	N	201	TRT	C5-C6-C9	-2.39	106.42	112.00
20	d	201	CDL	OB8-CB7-C71	2.37	119.07	111.83
21	Q	101	LMT	C3B-C4B-C5B	-2.35	105.97	110.23
21	q	101	LMT	C3B-C4B-C5B	-2.34	106.00	110.23
20	D	201	CDL	OB8-CB7-C71	2.31	118.87	111.83
21	q	101	LMT	C3'-C4'-C5'	-2.25	105.95	110.93
21	Q	101	LMT	C3'-C4'-C5'	-2.24	105.96	110.93
23	m	203	TRT	C5-C6-C9	2.21	117.15	112.00
23	R	103	TRT	C5-C6-C9	-2.19	106.87	112.00
23	r	103	TRT	C5-C6-C9	-2.19	106.88	112.00
23	M	201	TRT	C5-C6-C9	2.19	117.11	112.00
21	f	302	LMT	C3'-C4'-C5'	-2.17	106.12	110.93
21	F	302	LMT	C3'-C4'-C5'	-2.16	106.14	110.93
21	d	203	LMT	C3'-C4'-C5'	-2.12	106.23	110.93
21	D	203	LMT	C3'-C4'-C5'	-2.12	106.23	110.93
21	f	302	LMT	C3B-C4B-C5B	-2.10	106.43	110.23
21	F	302	LMT	C3B-C4B-C5B	-2.09	106.44	110.23
21	n	201	LMT	O5B-C5B-C6B	2.06	111.55	106.44
21	N	204	LMT	O5B-C1B-C2B	2.06	114.60	110.37
21	N	204	LMT	O5B-C5B-C6B	2.05	111.52	106.44
21	n	201	LMT	O5B-C1B-C2B	2.05	114.58	110.37
23	m	204	TRT	C5-C6-C9	-2.03	107.25	112.00
20	D	202	CDL	CB4-OB6-CB5	-2.03	112.94	117.80
23	M	202	TRT	C5-C6-C9	-2.02	107.27	112.00

There are no chirality outliers.

All (1221) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	501	CDL	CB2-OB2-PB2-OB3
20	A	501	CDL	CB3-OB5-PB2-OB3
20	A	501	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
20	A	502	CDL	O1-C1-CB2-OB2
20	A	502	CDL	CA3-OA5-PA1-OA3
20	A	502	CDL	OA7-CA5-OA6-CA4
20	A	502	CDL	C11-CA5-OA6-CA4
20	A	502	CDL	CB2-OB2-PB2-OB3
20	A	502	CDL	OB7-CB5-OB6-CB4
20	A	503	CDL	CA2-OA2-PA1-OA3
20	A	503	CDL	CB3-OB5-PB2-OB2
20	A	503	CDL	CB3-OB5-PB2-OB3
20	A	504	CDL	O1-C1-CB2-OB2
20	A	504	CDL	CA2-C1-CB2-OB2
20	A	504	CDL	OA7-CA5-OA6-CA4
20	A	504	CDL	CB3-OB5-PB2-OB2
20	A	504	CDL	CB3-OB5-PB2-OB4
20	D	201	CDL	CA2-OA2-PA1-OA3
20	D	201	CDL	CA2-OA2-PA1-OA4
20	D	201	CDL	CB2-OB2-PB2-OB3
20	D	201	CDL	CB2-OB2-PB2-OB5
20	D	202	CDL	O1-C1-CA2-OA2
20	D	202	CDL	CA2-OA2-PA1-OA3
20	D	202	CDL	CA2-OA2-PA1-OA5
20	D	202	CDL	CA3-OA5-PA1-OA2
20	D	202	CDL	CA3-OA5-PA1-OA4
20	D	202	CDL	CB2-OB2-PB2-OB5
20	D	202	CDL	CB3-OB5-PB2-OB2
20	D	202	CDL	CB3-OB5-PB2-OB4
20	D	202	CDL	C51-CB5-OB6-CB4
20	E	101	CDL	O1-C1-CB2-OB2
20	E	101	CDL	CA3-OA5-PA1-OA3
20	E	101	CDL	CB2-OB2-PB2-OB3
20	E	101	CDL	CB2-OB2-PB2-OB5
20	E	101	CDL	CB3-OB5-PB2-OB2
20	E	101	CDL	CB3-OB5-PB2-OB3
20	E	101	CDL	CB3-OB5-PB2-OB4
20	E	101	CDL	OB5-CB3-CB4-OB6
20	M	203	CDL	CA2-OA2-PA1-OA4
20	M	203	CDL	CA2-OA2-PA1-OA5
20	M	203	CDL	CB3-OB5-PB2-OB4
20	M	203	CDL	OB5-CB3-CB4-OB6
20	M	204	CDL	CA2-OA2-PA1-OA5
20	M	204	CDL	CA3-OA5-PA1-OA2
20	M	204	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
20	M	204	CDL	CB2-OB2-PB2-OB3
20	M	204	CDL	CB3-OB5-PB2-OB2
20	M	204	CDL	CB3-OB5-PB2-OB3
20	M	204	CDL	CB3-OB5-PB2-OB4
20	O	201	CDL	CA2-OA2-PA1-OA4
20	O	201	CDL	CA2-OA2-PA1-OA5
20	O	201	CDL	CA3-OA5-PA1-OA2
20	O	201	CDL	CA3-OA5-PA1-OA3
20	O	201	CDL	CA3-OA5-PA1-OA4
20	O	201	CDL	CB2-OB2-PB2-OB3
20	O	201	CDL	CB2-OB2-PB2-OB4
20	O	201	CDL	CB2-OB2-PB2-OB5
20	O	201	CDL	CB3-OB5-PB2-OB2
20	O	201	CDL	CB3-OB5-PB2-OB3
20	O	201	CDL	CB3-OB5-PB2-OB4
20	P	201	CDL	CA2-OA2-PA1-OA3
20	P	201	CDL	CA2-OA2-PA1-OA5
20	P	201	CDL	CA3-OA5-PA1-OA2
20	P	201	CDL	CA3-OA5-PA1-OA3
20	P	201	CDL	OA9-CA7-OA8-CA6
20	P	201	CDL	CB2-OB2-PB2-OB3
20	P	201	CDL	CB2-OB2-PB2-OB4
20	P	201	CDL	CB2-OB2-PB2-OB5
20	P	201	CDL	C51-CB5-OB6-CB4
20	R	101	CDL	CB2-OB2-PB2-OB5
20	a	501	CDL	CB2-OB2-PB2-OB3
20	a	501	CDL	CB3-OB5-PB2-OB3
20	a	501	CDL	C51-CB5-OB6-CB4
20	a	502	CDL	C11-CA5-OA6-CA4
20	a	502	CDL	CB2-OB2-PB2-OB3
20	a	502	CDL	OB7-CB5-OB6-CB4
20	a	503	CDL	CA2-OA2-PA1-OA3
20	a	503	CDL	CB3-OB5-PB2-OB2
20	a	503	CDL	CB3-OB5-PB2-OB3
20	a	504	CDL	O1-C1-CB2-OB2
20	a	504	CDL	CA2-C1-CB2-OB2
20	a	504	CDL	OA7-CA5-OA6-CA4
20	a	504	CDL	CB3-OB5-PB2-OB2
20	a	504	CDL	CB3-OB5-PB2-OB4
20	d	201	CDL	CA2-OA2-PA1-OA3
20	d	201	CDL	CA2-OA2-PA1-OA4
20	d	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
20	d	201	CDL	CB2-OB2-PB2-OB5
20	d	202	CDL	CA2-OA2-PA1-OA3
20	d	202	CDL	CA2-OA2-PA1-OA5
20	d	202	CDL	CA3-OA5-PA1-OA2
20	d	202	CDL	CA3-OA5-PA1-OA4
20	d	202	CDL	CB2-OB2-PB2-OB5
20	d	202	CDL	CB3-OB5-PB2-OB2
20	d	202	CDL	CB3-OB5-PB2-OB4
20	d	202	CDL	C51-CB5-OB6-CB4
20	e	101	CDL	O1-C1-CB2-OB2
20	e	101	CDL	CA3-OA5-PA1-OA3
20	e	101	CDL	CB2-OB2-PB2-OB3
20	e	101	CDL	CB2-OB2-PB2-OB5
20	e	101	CDL	CB3-OB5-PB2-OB2
20	e	101	CDL	CB3-OB5-PB2-OB3
20	e	101	CDL	CB3-OB5-PB2-OB4
20	e	101	CDL	OB5-CB3-CB4-OB6
20	m	201	CDL	CA2-OA2-PA1-OA4
20	m	201	CDL	CA2-OA2-PA1-OA5
20	m	201	CDL	CB3-OB5-PB2-OB4
20	m	201	CDL	OB5-CB3-CB4-OB6
20	m	202	CDL	CA2-OA2-PA1-OA5
20	m	202	CDL	CA3-OA5-PA1-OA2
20	m	202	CDL	CA3-OA5-PA1-OA3
20	m	202	CDL	CB2-OB2-PB2-OB3
20	m	202	CDL	CB3-OB5-PB2-OB2
20	m	202	CDL	CB3-OB5-PB2-OB3
20	m	202	CDL	CB3-OB5-PB2-OB4
20	o	201	CDL	O1-C1-CA2-OA2
20	o	201	CDL	CA2-OA2-PA1-OA4
20	o	201	CDL	CA2-OA2-PA1-OA5
20	o	201	CDL	CA3-OA5-PA1-OA2
20	o	201	CDL	CA3-OA5-PA1-OA3
20	o	201	CDL	CA3-OA5-PA1-OA4
20	o	201	CDL	CB2-OB2-PB2-OB3
20	o	201	CDL	CB2-OB2-PB2-OB4
20	o	201	CDL	CB2-OB2-PB2-OB5
20	o	201	CDL	CB3-OB5-PB2-OB2
20	o	201	CDL	CB3-OB5-PB2-OB3
20	o	201	CDL	CB3-OB5-PB2-OB4
20	p	201	CDL	CA3-OA5-PA1-OA2
20	p	201	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
20	p	201	CDL	OA5-CA3-CA4-OA6
20	p	201	CDL	CB2-OB2-PB2-OB4
20	p	201	CDL	CB2-OB2-PB2-OB5
20	p	201	CDL	CB3-OB5-PB2-OB2
20	p	201	CDL	CB3-OB5-PB2-OB3
20	p	201	CDL	CB3-OB5-PB2-OB4
20	p	202	CDL	CA2-OA2-PA1-OA3
20	p	202	CDL	CA2-OA2-PA1-OA5
20	p	202	CDL	CA3-OA5-PA1-OA2
20	p	202	CDL	CA3-OA5-PA1-OA3
20	p	202	CDL	CB2-OB2-PB2-OB3
20	p	202	CDL	CB2-OB2-PB2-OB4
20	p	202	CDL	CB2-OB2-PB2-OB5
20	p	202	CDL	C51-CB5-OB6-CB4
20	r	101	CDL	CB2-OB2-PB2-OB5
21	N	204	LMT	C2'-C1'-O1'-C1
21	N	204	LMT	O5'-C1'-O1'-C1
21	n	201	LMT	C2'-C1'-O1'-C1
21	n	201	LMT	O5'-C1'-O1'-C1
22	I	101	LPP	C6-O5-P1-O2
22	O	203	LPP	C6-O5-P1-O2
22	O	203	LPP	C6-O5-P1-O4
22	O	203	LPP	O5-C6-C7-O9
22	R	102	LPP	O10-C11-O9-C7
22	i	101	LPP	C6-O5-P1-O2
22	o	203	LPP	C6-O5-P1-O2
22	o	203	LPP	C6-O5-P1-O4
22	o	203	LPP	O5-C6-C7-O9
22	r	102	LPP	O10-C11-O9-C7
20	P	201	CDL	OB7-CB5-OB6-CB4
20	p	202	CDL	OB7-CB5-OB6-CB4
20	M	204	CDL	OA9-CA7-OA8-CA6
20	m	202	CDL	OA9-CA7-OA8-CA6
22	R	102	LPP	O28-C29-O27-C8
22	r	102	LPP	O28-C29-O27-C8
20	p	202	CDL	C31-CA7-OA8-CA6
20	A	501	CDL	OA9-CA7-OA8-CA6
20	D	201	CDL	OA9-CA7-OA8-CA6
20	M	203	CDL	OA9-CA7-OA8-CA6
20	a	501	CDL	OA9-CA7-OA8-CA6
20	d	201	CDL	OA9-CA7-OA8-CA6
20	m	201	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
20	p	201	CDL	OA9-CA7-OA8-CA6
20	p	201	CDL	OB9-CB7-OB8-CB6
20	p	202	CDL	OA9-CA7-OA8-CA6
21	Q	101	LMT	C4B-C5B-C6B-O6B
21	q	101	LMT	C4B-C5B-C6B-O6B
20	A	501	CDL	OB7-CB5-OB6-CB4
20	D	202	CDL	OB7-CB5-OB6-CB4
20	a	501	CDL	OB7-CB5-OB6-CB4
20	a	502	CDL	OA7-CA5-OA6-CA4
20	d	202	CDL	OB7-CB5-OB6-CB4
20	A	501	CDL	C31-CA7-OA8-CA6
20	D	201	CDL	C31-CA7-OA8-CA6
20	M	203	CDL	C31-CA7-OA8-CA6
20	M	204	CDL	C31-CA7-OA8-CA6
20	P	201	CDL	C31-CA7-OA8-CA6
20	a	501	CDL	C31-CA7-OA8-CA6
20	d	201	CDL	C31-CA7-OA8-CA6
20	m	201	CDL	C31-CA7-OA8-CA6
20	m	202	CDL	C31-CA7-OA8-CA6
20	p	201	CDL	C71-CB7-OB8-CB6
22	R	102	LPP	C30-C29-O27-C8
22	r	102	LPP	C30-C29-O27-C8
20	A	502	CDL	C51-CB5-OB6-CB4
20	A	504	CDL	C11-CA5-OA6-CA4
20	a	502	CDL	C51-CB5-OB6-CB4
20	a	504	CDL	C11-CA5-OA6-CA4
22	R	102	LPP	C12-C11-O9-C7
22	r	102	LPP	C12-C11-O9-C7
21	Q	101	LMT	O5B-C5B-C6B-O6B
21	q	101	LMT	O5B-C5B-C6B-O6B
20	P	201	CDL	C71-CB7-OB8-CB6
20	p	201	CDL	C31-CA7-OA8-CA6
20	p	202	CDL	C71-CB7-OB8-CB6
22	N	203	LPP	O28-C29-O27-C8
22	P	202	LPP	O28-C29-O27-C8
21	N	204	LMT	O5'-C5'-C6'-O6'
21	n	201	LMT	O5'-C5'-C6'-O6'
20	A	503	CDL	O1-C1-CA2-OA2
20	O	201	CDL	O1-C1-CA2-OA2
20	a	502	CDL	O1-C1-CB2-OB2
20	a	503	CDL	O1-C1-CA2-OA2
20	d	202	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
20	D	202	CDL	C71-CB7-OB8-CB6
20	R	101	CDL	C31-CA7-OA8-CA6
20	d	202	CDL	C71-CB7-OB8-CB6
20	r	101	CDL	C31-CA7-OA8-CA6
22	N	203	LPP	C30-C29-O27-C8
22	P	202	LPP	C30-C29-O27-C8
21	D	203	LMT	O5B-C5B-C6B-O6B
21	d	203	LMT	O5B-C5B-C6B-O6B
23	P	203	TRT	C2-C1-C5-C6
23	P	203	TRT	C4-C1-C5-C6
23	p	203	TRT	C2-C1-C5-C6
23	p	203	TRT	C4-C1-C5-C6
20	d	202	CDL	OB9-CB7-OB8-CB6
20	p	202	CDL	OB9-CB7-OB8-CB6
20	D	202	CDL	OB9-CB7-OB8-CB6
20	P	201	CDL	OB9-CB7-OB8-CB6
23	R	103	TRT	C13-C12-O15-C16
23	r	103	TRT	C13-C12-O15-C16
23	P	203	TRT	O15-C16-C17-O18
23	p	203	TRT	O15-C16-C17-O18
20	R	101	CDL	OA9-CA7-OA8-CA6
20	r	101	CDL	OA9-CA7-OA8-CA6
21	F	302	LMT	O5B-C5B-C6B-O6B
21	f	302	LMT	O5B-C5B-C6B-O6B
23	R	103	TRT	C11-C12-O15-C16
20	A	502	CDL	C74-C75-C76-C77
20	a	502	CDL	C74-C75-C76-C77
23	r	103	TRT	C11-C12-O15-C16
23	P	203	TRT	C3-C1-C5-C6
23	p	203	TRT	C3-C1-C5-C6
23	G	202	TRT	O21-C22-C23-O24
23	P	203	TRT	O21-C22-C23-O24
23	g	202	TRT	O21-C22-C23-O24
23	p	203	TRT	O21-C22-C23-O24
20	M	203	CDL	C11-CA5-OA6-CA4
20	m	201	CDL	C11-CA5-OA6-CA4
21	N	204	LMT	C4'-C5'-C6'-O6'
21	n	201	LMT	C4'-C5'-C6'-O6'
23	N	201	TRT	C13-C12-O15-C16
23	n	202	TRT	C13-C12-O15-C16
20	A	502	CDL	CA2-C1-CB2-OB2
20	A	503	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
20	a	503	CDL	CB2-C1-CA2-OA2
20	A	502	CDL	C31-CA7-OA8-CA6
20	A	503	CDL	C31-CA7-OA8-CA6
20	A	503	CDL	C71-CB7-OB8-CB6
20	E	101	CDL	C71-CB7-OB8-CB6
20	a	502	CDL	C31-CA7-OA8-CA6
20	a	503	CDL	C31-CA7-OA8-CA6
20	a	503	CDL	C71-CB7-OB8-CB6
20	e	101	CDL	C71-CB7-OB8-CB6
21	D	203	LMT	C4B-C5B-C6B-O6B
20	M	204	CDL	C71-C72-C73-C74
20	m	202	CDL	C71-C72-C73-C74
22	R	102	LPP	C37-C38-C39-C40
22	r	102	LPP	C37-C38-C39-C40
23	G	201	TRT	O18-C19-C20-O21
23	g	201	TRT	O18-C19-C20-O21
21	d	203	LMT	C4B-C5B-C6B-O6B
23	N	201	TRT	C11-C12-O15-C16
23	n	202	TRT	C11-C12-O15-C16
20	M	203	CDL	O1-C1-CB2-OB2
20	m	201	CDL	O1-C1-CB2-OB2
23	P	203	TRT	C13-C12-O15-C16
23	P	203	TRT	C11-C12-O15-C16
23	p	203	TRT	C13-C12-O15-C16
23	p	203	TRT	C11-C12-O15-C16
20	a	503	CDL	OB9-CB7-OB8-CB6
23	R	103	TRT	O21-C22-C23-O24
23	r	103	TRT	O21-C22-C23-O24
23	G	201	TRT	C11-C12-O15-C16
23	g	201	TRT	C11-C12-O15-C16
23	G	201	TRT	C13-C12-O15-C16
23	g	201	TRT	C13-C12-O15-C16
20	A	503	CDL	OB9-CB7-OB8-CB6
20	M	203	CDL	OA5-CA3-CA4-OA6
20	m	201	CDL	OA5-CA3-CA4-OA6
20	d	202	CDL	C75-C76-C77-C78
20	D	202	CDL	C75-C76-C77-C78
20	a	504	CDL	CB5-C51-C52-C53
20	a	504	CDL	CA5-C11-C12-C13
23	G	202	TRT	C11-C12-O15-C16
23	g	202	TRT	C11-C12-O15-C16
20	M	203	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
20	m	201	CDL	OA7-CA5-OA6-CA4
20	a	501	CDL	C72-C73-C74-C75
23	R	103	TRT	O18-C19-C20-O21
23	r	103	TRT	O18-C19-C20-O21
23	G	202	TRT	C13-C12-O15-C16
23	g	202	TRT	C13-C12-O15-C16
20	p	201	CDL	C57-C58-C59-C60
20	A	501	CDL	C72-C73-C74-C75
20	A	503	CDL	CB5-C51-C52-C53
20	A	504	CDL	CB5-C51-C52-C53
20	a	503	CDL	CB5-C51-C52-C53
20	a	504	CDL	CA7-C31-C32-C33
20	p	201	CDL	CB5-C51-C52-C53
22	N	203	LPP	C29-C30-C31-C32
22	P	202	LPP	C29-C30-C31-C32
23	M	201	TRT	O15-C16-C17-O18
23	m	203	TRT	O15-C16-C17-O18
23	N	202	TRT	O18-C19-C20-O21
20	A	504	CDL	CA7-C31-C32-C33
20	A	503	CDL	OA9-CA7-OA8-CA6
20	a	503	CDL	OA9-CA7-OA8-CA6
20	e	101	CDL	OB9-CB7-OB8-CB6
23	n	203	TRT	O18-C19-C20-O21
20	d	201	CDL	CB5-C51-C52-C53
20	A	502	CDL	OA9-CA7-OA8-CA6
20	E	101	CDL	OB9-CB7-OB8-CB6
20	a	502	CDL	OA9-CA7-OA8-CA6
20	D	201	CDL	CB5-C51-C52-C53
23	P	203	TRT	C1-C5-C6-C8
23	P	203	TRT	C1-C5-C6-C7
23	p	203	TRT	C1-C5-C6-C8
23	p	203	TRT	C1-C5-C6-C7
20	D	202	CDL	CB2-C1-CA2-OA2
20	E	101	CDL	CA2-C1-CB2-OB2
20	d	202	CDL	CB2-C1-CA2-OA2
20	e	101	CDL	CA2-C1-CB2-OB2
20	o	201	CDL	CB2-C1-CA2-OA2
20	R	101	CDL	C51-CB5-OB6-CB4
20	r	101	CDL	C51-CB5-OB6-CB4
23	P	203	TRT	C5-C6-C9-C14
23	p	203	TRT	C5-C6-C9-C14
20	R	101	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
20	r	101	CDL	OB7-CB5-OB6-CB4
23	M	202	TRT	C13-C12-O15-C16
23	m	204	TRT	C13-C12-O15-C16
20	D	201	CDL	O1-C1-CB2-OB2
20	d	201	CDL	O1-C1-CB2-OB2
20	d	202	CDL	C78-C79-C80-C81
21	F	302	LMT	O1'-C1-C2-C3
21	f	302	LMT	O1'-C1-C2-C3
23	N	202	TRT	C13-C12-O15-C16
23	n	203	TRT	C13-C12-O15-C16
20	D	202	CDL	C78-C79-C80-C81
23	P	203	TRT	C5-C6-C9-C10
23	p	203	TRT	C5-C6-C9-C10
20	E	101	CDL	C11-CA5-OA6-CA4
20	P	201	CDL	C11-CA5-OA6-CA4
20	e	101	CDL	C11-CA5-OA6-CA4
20	R	101	CDL	CA5-C11-C12-C13
21	F	302	LMT	C4B-C5B-C6B-O6B
21	f	302	LMT	C4B-C5B-C6B-O6B
20	E	101	CDL	C72-C73-C74-C75
20	A	503	CDL	C74-C75-C76-C77
20	M	203	CDL	C13-C14-C15-C16
20	a	503	CDL	C74-C75-C76-C77
20	m	201	CDL	C13-C14-C15-C16
22	O	203	LPP	C18-C19-C20-C21
22	o	203	LPP	C18-C19-C20-C21
20	M	203	CDL	C73-C74-C75-C76
20	M	203	CDL	C79-C80-C81-C82
22	O	203	LPP	C17-C18-C19-C20
22	o	203	LPP	C17-C18-C19-C20
20	A	502	CDL	C72-C73-C74-C75
20	A	503	CDL	C72-C73-C74-C75
20	M	203	CDL	C32-C33-C34-C35
20	a	503	CDL	C72-C73-C74-C75
20	e	101	CDL	C72-C73-C74-C75
20	m	201	CDL	C32-C33-C34-C35
20	m	201	CDL	C73-C74-C75-C76
20	m	201	CDL	C79-C80-C81-C82
20	P	201	CDL	OA7-CA5-OA6-CA4
20	p	201	CDL	C15-C16-C17-C18
22	I	101	LPP	C35-C36-C37-C38
22	i	101	LPP	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
20	D	202	CDL	CA5-C11-C12-C13
20	D	201	CDL	C17-C18-C19-C20
20	a	502	CDL	C72-C73-C74-C75
20	d	201	CDL	C17-C18-C19-C20
20	m	201	CDL	C71-C72-C73-C74
22	I	101	LPP	C21-C22-C23-C24
22	i	101	LPP	C21-C22-C23-C24
20	D	202	CDL	C11-CA5-OA6-CA4
20	M	204	CDL	C51-CB5-OB6-CB4
20	O	201	CDL	C51-CB5-OB6-CB4
20	p	202	CDL	C11-CA5-OA6-CA4
20	r	101	CDL	C55-C56-C57-C58
21	N	204	LMT	C11-C10-C9-C8
21	n	201	LMT	C11-C10-C9-C8
23	M	202	TRT	C11-C12-O15-C16
23	m	204	TRT	C11-C12-O15-C16
20	d	202	CDL	C81-C82-C83-C84
20	A	502	CDL	C60-C61-C62-C63
20	D	202	CDL	C72-C73-C74-C75
20	D	202	CDL	C81-C82-C83-C84
20	E	101	CDL	C56-C57-C58-C59
20	M	203	CDL	C71-C72-C73-C74
20	M	204	CDL	C53-C54-C55-C56
20	a	502	CDL	C60-C61-C62-C63
20	d	202	CDL	C72-C73-C74-C75
20	p	201	CDL	C18-C19-C20-C21
20	A	502	CDL	C13-C14-C15-C16
20	R	101	CDL	C55-C56-C57-C58
20	r	101	CDL	CA5-C11-C12-C13
23	N	202	TRT	C11-C12-O15-C16
23	n	203	TRT	C11-C12-O15-C16
20	A	503	CDL	C21-C22-C23-C24
20	D	201	CDL	C42-C43-C44-C45
20	E	101	CDL	OA7-CA5-OA6-CA4
20	e	101	CDL	OA7-CA5-OA6-CA4
20	a	503	CDL	C21-C22-C23-C24
20	d	201	CDL	C42-C43-C44-C45
20	d	202	CDL	C37-C38-C39-C40
22	R	102	LPP	C30-C31-C32-C33
22	r	102	LPP	C30-C31-C32-C33
20	d	202	CDL	CA5-C11-C12-C13
20	A	503	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
20	D	202	CDL	C34-C35-C36-C37
20	D	202	CDL	C37-C38-C39-C40
20	D	202	CDL	C77-C78-C79-C80
20	R	101	CDL	C57-C58-C59-C60
20	a	502	CDL	C13-C14-C15-C16
20	a	503	CDL	C33-C34-C35-C36
20	p	201	CDL	C55-C56-C57-C58
21	q	101	LMT	O5'-C5'-C6'-O6'
20	e	101	CDL	C56-C57-C58-C59
20	r	101	CDL	C57-C58-C59-C60
23	M	201	TRT	C5-C6-C9-C10
23	m	203	TRT	C5-C6-C9-C10
20	A	501	CDL	C17-C18-C19-C20
20	A	503	CDL	C31-C32-C33-C34
21	Q	101	LMT	O5'-C5'-C6'-O6'
21	Q	101	LMT	C1-C2-C3-C4
21	q	101	LMT	C1-C2-C3-C4
20	d	202	CDL	C77-C78-C79-C80
20	e	101	CDL	C71-C72-C73-C74
20	p	201	CDL	C31-C32-C33-C34
20	r	101	CDL	C36-C37-C38-C39
20	p	201	CDL	CA5-C11-C12-C13
22	R	102	LPP	C11-C12-C13-C14
22	r	102	LPP	C11-C12-C13-C14
20	a	502	CDL	C11-C12-C13-C14
20	a	503	CDL	C31-C32-C33-C34
20	a	503	CDL	C52-C53-C54-C55
20	o	201	CDL	C51-CB5-OB6-CB4
20	D	201	CDL	C71-CB7-OB8-CB6
22	O	202	LPP	C30-C29-O27-C8
22	o	202	LPP	C30-C29-O27-C8
20	M	204	CDL	C1-CA2-OA2-PA1
20	m	202	CDL	C1-CA2-OA2-PA1
20	A	503	CDL	C52-C53-C54-C55
20	a	501	CDL	C17-C18-C19-C20
20	d	202	CDL	C34-C35-C36-C37
20	M	204	CDL	CA5-C11-C12-C13
20	m	202	CDL	CA5-C11-C12-C13
20	O	201	CDL	C71-C72-C73-C74
20	R	101	CDL	C36-C37-C38-C39
23	G	201	TRT	O21-C22-C23-O24
20	A	502	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	o	201	CDL	C71-C72-C73-C74
20	O	201	CDL	OB7-CB5-OB6-CB4
20	p	202	CDL	OA7-CA5-OA6-CA4
23	g	201	TRT	O21-C22-C23-O24
20	P	201	CDL	C72-C73-C74-C75
21	N	204	LMT	C3-C4-C5-C6
21	n	201	LMT	C3-C4-C5-C6
20	d	201	CDL	C71-CB7-OB8-CB6
22	R	102	LPP	C32-C33-C34-C35
22	r	102	LPP	C32-C33-C34-C35
20	E	101	CDL	C71-C72-C73-C74
20	M	203	CDL	C77-C78-C79-C80
22	O	203	LPP	C19-C20-C21-C22
22	o	203	LPP	C19-C20-C21-C22
20	D	202	CDL	C74-C75-C76-C77
20	d	202	CDL	C74-C75-C76-C77
20	p	202	CDL	C72-C73-C74-C75
20	A	503	CDL	C11-CA5-OA6-CA4
20	A	503	CDL	C51-CB5-OB6-CB4
20	D	201	CDL	C11-CA5-OA6-CA4
20	D	201	CDL	C51-CB5-OB6-CB4
20	M	203	CDL	C51-CB5-OB6-CB4
20	M	204	CDL	C11-CA5-OA6-CA4
20	O	201	CDL	C11-CA5-OA6-CA4
20	a	503	CDL	C11-CA5-OA6-CA4
20	a	503	CDL	C51-CB5-OB6-CB4
20	d	201	CDL	C11-CA5-OA6-CA4
20	d	201	CDL	C51-CB5-OB6-CB4
20	d	202	CDL	C11-CA5-OA6-CA4
20	m	201	CDL	C51-CB5-OB6-CB4
20	m	202	CDL	C11-CA5-OA6-CA4
20	m	202	CDL	C51-CB5-OB6-CB4
20	o	201	CDL	C11-CA5-OA6-CA4
20	p	201	CDL	C51-CB5-OB6-CB4
22	N	203	LPP	C12-C11-O9-C7
22	P	202	LPP	C12-C11-O9-C7
20	m	201	CDL	C77-C78-C79-C80
20	A	503	CDL	OA7-CA5-OA6-CA4
20	A	503	CDL	OB7-CB5-OB6-CB4
20	D	202	CDL	OA7-CA5-OA6-CA4
20	M	204	CDL	OA7-CA5-OA6-CA4
20	a	503	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
20	a	503	CDL	OB7-CB5-OB6-CB4
20	d	201	CDL	OA7-CA5-OA6-CA4
20	d	201	CDL	OB7-CB5-OB6-CB4
20	d	202	CDL	OA7-CA5-OA6-CA4
20	m	202	CDL	OA7-CA5-OA6-CA4
20	m	202	CDL	OB7-CB5-OB6-CB4
20	o	201	CDL	OB7-CB5-OB6-CB4
20	R	101	CDL	C62-C63-C64-C65
20	r	101	CDL	C62-C63-C64-C65
20	M	203	CDL	C82-C83-C84-C85
20	m	201	CDL	C82-C83-C84-C85
20	a	501	CDL	C34-C35-C36-C37
23	M	201	TRT	C5-C6-C9-C14
23	m	203	TRT	C5-C6-C9-C14
20	M	203	CDL	C74-C75-C76-C77
20	m	201	CDL	C74-C75-C76-C77
21	D	203	LMT	C3-C4-C5-C6
21	d	203	LMT	C3-C4-C5-C6
20	D	201	CDL	OB9-CB7-OB8-CB6
20	a	501	CDL	CB7-C71-C72-C73
20	D	201	CDL	OA7-CA5-OA6-CA4
20	M	203	CDL	OB7-CB5-OB6-CB4
20	M	204	CDL	OB7-CB5-OB6-CB4
20	m	201	CDL	OB7-CB5-OB6-CB4
22	N	203	LPP	O10-C11-O9-C7
22	P	202	LPP	O10-C11-O9-C7
20	A	502	CDL	OB5-CB3-CB4-OB6
20	a	502	CDL	OB5-CB3-CB4-OB6
20	A	501	CDL	C34-C35-C36-C37
20	p	201	CDL	C37-C38-C39-C40
20	A	502	CDL	C23-C24-C25-C26
22	O	202	LPP	O28-C29-O27-C8
22	o	202	LPP	O28-C29-O27-C8
20	a	502	CDL	C23-C24-C25-C26
20	A	501	CDL	CB7-C71-C72-C73
20	A	504	CDL	OA6-CA4-CA6-OA8
20	E	101	CDL	OB6-CB4-CB6-OB8
20	a	504	CDL	OA6-CA4-CA6-OA8
20	e	101	CDL	OB6-CB4-CB6-OB8
20	r	101	CDL	C74-C75-C76-C77
20	R	101	CDL	C74-C75-C76-C77
23	G	202	TRT	C5-C6-C9-C10

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Mol	Chain	Res	Type	Atoms
23	N	202	TRT	C5-C6-C9-C10
23	g	202	TRT	C5-C6-C9-C10
23	n	203	TRT	C5-C6-C9-C10
20	O	201	CDL	C1-CB2-OB2-PB2
21	n	201	LMT	O5B-C5B-C6B-O6B
22	R	102	LPP	C34-C35-C36-C37
20	D	201	CDL	OB7-CB5-OB6-CB4
20	p	201	CDL	OB7-CB5-OB6-CB4
20	O	201	CDL	CB2-C1-CA2-OA2
20	a	502	CDL	CA2-C1-CB2-OB2
20	O	201	CDL	C55-C56-C57-C58
20	o	201	CDL	C55-C56-C57-C58
22	r	102	LPP	C34-C35-C36-C37
21	N	204	LMT	O5B-C5B-C6B-O6B
22	N	203	LPP	C13-C14-C15-C16
22	P	202	LPP	C13-C14-C15-C16
20	A	503	CDL	C71-C72-C73-C74
20	d	201	CDL	OB9-CB7-OB8-CB6
20	A	502	CDL	C73-C74-C75-C76
20	A	503	CDL	OB5-CB3-CB4-CB6
20	D	201	CDL	OB5-CB3-CB4-CB6
20	M	203	CDL	OA5-CA3-CA4-CA6
20	M	203	CDL	OB5-CB3-CB4-CB6
20	a	503	CDL	OB5-CB3-CB4-CB6
20	d	201	CDL	OB5-CB3-CB4-CB6
20	e	101	CDL	OA5-CA3-CA4-CA6
20	m	201	CDL	OA5-CA3-CA4-CA6
20	m	201	CDL	OB5-CB3-CB4-CB6
22	O	203	LPP	O5-C6-C7-C8
22	o	203	LPP	O5-C6-C7-C8
20	O	201	CDL	OA7-CA5-OA6-CA4
20	o	201	CDL	OA7-CA5-OA6-CA4
20	D	202	CDL	C31-C32-C33-C34
20	a	504	CDL	C74-C75-C76-C77
20	a	502	CDL	C73-C74-C75-C76
21	d	203	LMT	O1'-C1-C2-C3
21	D	203	LMT	O1'-C1-C2-C3
20	A	501	CDL	CA7-C31-C32-C33
20	a	501	CDL	CA7-C31-C32-C33
20	A	504	CDL	C74-C75-C76-C77
22	R	102	LPP	C36-C37-C38-C39
22	r	102	LPP	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
20	O	201	CDL	C20-C21-C22-C23
20	A	504	CDL	CA5-C11-C12-C13
20	o	201	CDL	C20-C21-C22-C23
23	G	202	TRT	C5-C6-C9-C14
23	N	202	TRT	C5-C6-C9-C14
23	g	202	TRT	C5-C6-C9-C14
23	n	203	TRT	C5-C6-C9-C14
23	G	201	TRT	O15-C16-C17-O18
20	D	202	CDL	CB3-CB4-CB6-OB8
20	M	204	CDL	CB3-CB4-CB6-OB8
20	m	202	CDL	CB3-CB4-CB6-OB8
20	r	101	CDL	CB3-CB4-CB6-OB8
20	M	204	CDL	C73-C74-C75-C76
20	p	201	CDL	C81-C82-C83-C84
23	g	201	TRT	O15-C16-C17-O18
20	p	201	CDL	C79-C80-C81-C82
21	F	302	LMT	C5-C6-C7-C8
21	f	302	LMT	C5-C6-C7-C8
20	m	202	CDL	C73-C74-C75-C76
20	M	203	CDL	C71-CB7-OB8-CB6
20	a	502	CDL	C75-C76-C77-C78
20	A	502	CDL	C75-C76-C77-C78
20	A	502	CDL	C20-C21-C22-C23
20	a	502	CDL	C20-C21-C22-C23
20	o	201	CDL	C1-CB2-OB2-PB2
20	M	204	CDL	C51-C52-C53-C54
22	O	203	LPP	C6-O5-P1-O3
22	o	203	LPP	C6-O5-P1-O3
20	m	201	CDL	C71-CB7-OB8-CB6
20	A	503	CDL	C18-C19-C20-C21
22	I	101	LPP	C30-C29-O27-C8
22	i	101	LPP	C30-C29-O27-C8
20	p	201	CDL	C41-C42-C43-C44
20	D	202	CDL	C43-C44-C45-C46
20	E	101	CDL	C53-C54-C55-C56
20	d	202	CDL	C43-C44-C45-C46
20	M	203	CDL	C81-C82-C83-C84
20	a	503	CDL	C18-C19-C20-C21
20	R	101	CDL	OA6-CA4-CA6-OA8
20	R	101	CDL	OB6-CB4-CB6-OB8
20	o	201	CDL	OA6-CA4-CA6-OA8
20	r	101	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
20	E	101	CDL	C62-C63-C64-C65
20	r	101	CDL	C75-C76-C77-C78
20	e	101	CDL	C53-C54-C55-C56
20	R	101	CDL	C75-C76-C77-C78
20	d	202	CDL	C31-C32-C33-C34
22	N	203	LPP	C32-C33-C34-C35
22	P	202	LPP	C32-C33-C34-C35
20	A	502	CDL	C31-C32-C33-C34
20	m	201	CDL	C81-C82-C83-C84
20	A	501	CDL	C55-C56-C57-C58
20	e	101	CDL	C62-C63-C64-C65
22	f	301	LPP	C12-C13-C14-C15
22	F	301	LPP	C12-C13-C14-C15
20	a	504	CDL	C71-C72-C73-C74
22	I	101	LPP	C31-C32-C33-C34
20	A	504	CDL	C71-C72-C73-C74
20	a	501	CDL	C55-C56-C57-C58
22	i	101	LPP	C31-C32-C33-C34
20	D	201	CDL	C12-C13-C14-C15
20	M	203	CDL	C72-C73-C74-C75
20	a	504	CDL	C57-C58-C59-C60
20	m	201	CDL	C72-C73-C74-C75
20	p	201	CDL	CA7-C31-C32-C33
20	D	202	CDL	C53-C54-C55-C56
20	r	101	CDL	C59-C60-C61-C62
20	A	504	CDL	C57-C58-C59-C60
20	d	202	CDL	C53-C54-C55-C56
20	A	502	CDL	OB5-CB3-CB4-CB6
20	E	101	CDL	OA5-CA3-CA4-CA6
20	E	101	CDL	OB5-CB3-CB4-CB6
20	a	502	CDL	OB5-CB3-CB4-CB6
20	e	101	CDL	OB5-CB3-CB4-CB6
20	R	101	CDL	C59-C60-C61-C62
20	d	201	CDL	C12-C13-C14-C15
22	R	102	LPP	C38-C39-C40-C41
20	E	101	CDL	C12-C11-CA5-OA6
22	r	102	LPP	C38-C39-C40-C41
20	O	201	CDL	C15-C16-C17-C18
23	M	201	TRT	O18-C19-C20-O21
22	I	101	LPP	O28-C29-O27-C8
22	i	101	LPP	O28-C29-O27-C8
23	m	203	TRT	O18-C19-C20-O21

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Mol	Chain	Res	Type	Atoms
20	m	202	CDL	C51-C52-C53-C54
20	o	201	CDL	C15-C16-C17-C18
20	A	504	CDL	CA3-CA4-CA6-OA8
20	E	101	CDL	CB3-CB4-CB6-OB8
20	R	101	CDL	CB3-CB4-CB6-OB8
20	a	504	CDL	CA3-CA4-CA6-OA8
20	e	101	CDL	CB3-CB4-CB6-OB8
23	P	203	TRT	C17-C16-O15-C12
23	p	203	TRT	C17-C16-O15-C12
20	M	203	CDL	OB9-CB7-OB8-CB6
20	a	502	CDL	C31-C32-C33-C34
20	d	201	CDL	C34-C35-C36-C37
23	p	203	TRT	C22-C23-O24-C25
20	D	201	CDL	C11-C12-C13-C14
20	p	201	CDL	C20-C21-C22-C23
20	D	201	CDL	OB5-CB3-CB4-OB6
20	d	201	CDL	OB5-CB3-CB4-OB6
20	R	101	CDL	C31-C32-C33-C34
23	R	103	TRT	C17-C16-O15-C12
23	r	103	TRT	C17-C16-O15-C12
20	p	201	CDL	C1-CA2-OA2-PA1
23	P	203	TRT	C22-C23-O24-C25
20	a	502	CDL	C32-C33-C34-C35
20	D	201	CDL	C34-C35-C36-C37
20	r	101	CDL	C31-C32-C33-C34
20	e	101	CDL	C12-C11-CA5-OA6
20	m	202	CDL	OB6-CB4-CB6-OB8
20	p	201	CDL	OB6-CB4-CB6-OB8
20	r	101	CDL	OB6-CB4-CB6-OB8
20	m	201	CDL	OB9-CB7-OB8-CB6
20	A	502	CDL	C77-C78-C79-C80
20	d	201	CDL	C11-C12-C13-C14
20	m	202	CDL	C53-C54-C55-C56
20	p	201	CDL	C59-C60-C61-C62
20	A	501	CDL	C15-C16-C17-C18
20	A	504	CDL	C52-C53-C54-C55
23	R	103	TRT	C22-C23-O24-C25
23	r	103	TRT	C22-C23-O24-C25
20	D	202	CDL	C13-C14-C15-C16
22	f	301	LPP	C30-C29-O27-C8
22	N	203	LPP	O9-C11-C12-C13
22	P	202	LPP	O9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	A	501	CDL	C11-CA5-OA6-CA4
20	a	501	CDL	C11-CA5-OA6-CA4
20	p	201	CDL	C11-CA5-OA6-CA4
23	R	103	TRT	C1-C5-C6-C8
23	r	103	TRT	C1-C5-C6-C8
23	G	202	TRT	C20-C19-O18-C17
23	g	202	TRT	C20-C19-O18-C17
22	F	301	LPP	C30-C29-O27-C8
20	e	101	CDL	C63-C64-C65-C66
20	p	201	CDL	OA5-CA3-CA4-CA6
20	a	501	CDL	C15-C16-C17-C18
23	N	201	TRT	O21-C22-C23-O24
23	n	202	TRT	O21-C22-C23-O24
22	I	101	LPP	C6-O5-P1-O4
22	i	101	LPP	C6-O5-P1-O4
20	E	101	CDL	C63-C64-C65-C66
20	e	101	CDL	C51-C52-C53-C54
20	o	201	CDL	C31-CA7-OA8-CA6
23	G	202	TRT	C17-C16-O15-C12
23	g	202	TRT	C17-C16-O15-C12
20	A	502	CDL	CA6-CA4-OA6-CA5
20	A	503	CDL	CA6-CA4-OA6-CA5
20	E	101	CDL	CA6-CA4-OA6-CA5
20	P	201	CDL	CA6-CA4-OA6-CA5
20	a	502	CDL	CA6-CA4-OA6-CA5
20	a	503	CDL	CA6-CA4-OA6-CA5
20	e	101	CDL	CA6-CA4-OA6-CA5
20	p	202	CDL	CA6-CA4-OA6-CA5
23	M	202	TRT	C16-C17-O18-C19
23	m	204	TRT	C16-C17-O18-C19
23	m	203	TRT	C13-C12-O15-C16
20	A	502	CDL	C76-C77-C78-C79
20	d	202	CDL	C13-C14-C15-C16
21	F	302	LMT	C11-C10-C9-C8
20	A	501	CDL	OA7-CA5-OA6-CA4
20	A	503	CDL	OA5-CA3-CA4-OA6
20	E	101	CDL	OA5-CA3-CA4-OA6
20	O	201	CDL	OB5-CB3-CB4-OB6
20	a	503	CDL	OA5-CA3-CA4-OA6
20	e	101	CDL	OA5-CA3-CA4-OA6
20	o	201	CDL	OB5-CB3-CB4-OB6
23	N	202	TRT	C16-C17-O18-C19

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Mol	Chain	Res	Type	Atoms
23	n	203	TRT	C16-C17-O18-C19
20	p	201	CDL	C74-C75-C76-C77
21	f	302	LMT	C11-C10-C9-C8
20	a	501	CDL	C20-C21-C22-C23
23	M	201	TRT	C13-C12-O15-C16
20	d	202	CDL	CB3-CB4-CB6-OB8
20	p	201	CDL	CB3-CB4-CB6-OB8
20	a	504	CDL	C52-C53-C54-C55
20	m	201	CDL	C21-C22-C23-C24
22	R	102	LPP	C35-C36-C37-C38
22	r	102	LPP	C35-C36-C37-C38
20	R	101	CDL	CA7-C31-C32-C33
20	D	202	CDL	OB6-CB4-CB6-OB8
20	d	202	CDL	OB6-CB4-CB6-OB8
20	a	501	CDL	OA7-CA5-OA6-CA4
20	p	201	CDL	OA7-CA5-OA6-CA4
20	a	501	CDL	C40-C41-C42-C43
22	F	301	LPP	O28-C29-O27-C8
22	f	301	LPP	O28-C29-O27-C8
22	i	101	LPP	C23-C24-C25-C26
20	p	201	CDL	C38-C39-C40-C41
22	i	101	LPP	C12-C13-C14-C15
20	A	501	CDL	C40-C41-C42-C43
22	I	101	LPP	C12-C13-C14-C15
22	I	101	LPP	C23-C24-C25-C26
20	r	101	CDL	CA7-C31-C32-C33
23	M	202	TRT	O18-C19-C20-O21
23	m	204	TRT	O18-C19-C20-O21
20	M	203	CDL	C17-C18-C19-C20
20	a	502	CDL	C77-C78-C79-C80
20	d	202	CDL	C39-C40-C41-C42
20	m	201	CDL	C17-C18-C19-C20
23	m	203	TRT	C11-C12-O15-C16
20	M	203	CDL	CA2-C1-CB2-OB2
20	m	201	CDL	CA2-C1-CB2-OB2
23	M	201	TRT	C11-C12-O15-C16
20	o	201	CDL	OA9-CA7-OA8-CA6
20	D	202	CDL	C39-C40-C41-C42
20	M	203	CDL	C21-C22-C23-C24
22	I	101	LPP	C18-C19-C20-C21
22	i	101	LPP	C18-C19-C20-C21
20	a	502	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
20	r	101	CDL	C72-C73-C74-C75
23	N	202	TRT	C22-C23-O24-C25
23	n	203	TRT	C22-C23-O24-C25
23	R	103	TRT	O15-C16-C17-O18
23	r	103	TRT	O15-C16-C17-O18
23	R	103	TRT	C1-C5-C6-C9
23	r	103	TRT	C1-C5-C6-C9
20	R	101	CDL	C72-C73-C74-C75
20	M	204	CDL	OA5-CA3-CA4-CA6
20	O	201	CDL	OB5-CB3-CB4-CB6
20	o	201	CDL	OB5-CB3-CB4-CB6
21	D	203	LMT	C6-C7-C8-C9
21	d	203	LMT	C6-C7-C8-C9
20	m	201	CDL	C75-C76-C77-C78
21	q	101	LMT	C3-C4-C5-C6
21	Q	101	LMT	C3-C4-C5-C6
22	O	203	LPP	C12-C13-C14-C15
22	o	203	LPP	C12-C13-C14-C15
20	a	501	CDL	C51-C52-C53-C54
20	p	201	CDL	C53-C54-C55-C56
20	o	201	CDL	C1-CA2-OA2-PA1
20	A	502	CDL	C32-C33-C34-C35
22	I	101	LPP	C39-C40-C41-C42
20	e	101	CDL	CA7-C31-C32-C33
20	m	201	CDL	C16-C17-C18-C19
22	i	101	LPP	C39-C40-C41-C42
20	A	504	CDL	C53-C54-C55-C56
23	M	202	TRT	O21-C22-C23-O24
23	m	204	TRT	O21-C22-C23-O24
20	A	501	CDL	C51-C52-C53-C54
20	D	201	CDL	C55-C56-C57-C58
20	d	201	CDL	C40-C41-C42-C43
20	M	204	CDL	OB6-CB4-CB6-OB8
20	d	202	CDL	OA6-CA4-CA6-OA8
20	o	201	CDL	C17-C18-C19-C20
20	M	203	CDL	C16-C17-C18-C19
20	R	101	CDL	CA3-CA4-CA6-OA8
20	o	201	CDL	CA3-CA4-CA6-OA8
20	r	101	CDL	CA3-CA4-CA6-OA8
22	O	202	LPP	C6-C7-C8-O27
22	o	202	LPP	C6-C7-C8-O27
20	M	204	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
20	A	501	CDL	C58-C59-C60-C61
20	d	201	CDL	C55-C56-C57-C58
20	p	202	CDL	C32-C33-C34-C35
20	M	203	CDL	C75-C76-C77-C78
20	a	501	CDL	C58-C59-C60-C61
20	m	201	CDL	CB7-C71-C72-C73
20	O	201	CDL	C17-C18-C19-C20
20	d	202	CDL	C73-C74-C75-C76
22	O	202	LPP	C13-C14-C15-C16
22	o	202	LPP	C13-C14-C15-C16
20	A	502	CDL	CA2-OA2-PA1-OA3
20	A	502	CDL	CA3-OA5-PA1-OA2
20	A	503	CDL	CA3-OA5-PA1-OA2
20	A	503	CDL	CA3-OA5-PA1-OA4
20	A	503	CDL	CB2-OB2-PB2-OB3
20	A	504	CDL	CA2-OA2-PA1-OA3
20	A	504	CDL	CB2-OB2-PB2-OB3
20	D	201	CDL	CA2-OA2-PA1-OA5
20	D	201	CDL	CB2-OB2-PB2-OB4
20	D	202	CDL	CA3-OA5-PA1-OA3
20	D	202	CDL	CB2-OB2-PB2-OB3
20	E	101	CDL	CA2-OA2-PA1-OA3
20	E	101	CDL	CA2-OA2-PA1-OA5
20	E	101	CDL	CB2-OB2-PB2-OB4
20	M	203	CDL	CA2-OA2-PA1-OA3
20	M	203	CDL	CB2-OB2-PB2-OB3
20	M	203	CDL	CB3-OB5-PB2-OB2
20	M	203	CDL	CB3-OB5-PB2-OB3
20	M	204	CDL	CA2-OA2-PA1-OA3
20	P	201	CDL	CA2-OA2-PA1-OA4
20	R	101	CDL	CA2-OA2-PA1-OA5
20	R	101	CDL	CA3-OA5-PA1-OA3
20	a	502	CDL	CA2-OA2-PA1-OA3
20	a	502	CDL	CA3-OA5-PA1-OA2
20	a	502	CDL	CA3-OA5-PA1-OA3
20	a	502	CDL	CA3-OA5-PA1-OA4
20	a	502	CDL	CB2-OB2-PB2-OB5
20	a	503	CDL	CA3-OA5-PA1-OA2
20	a	503	CDL	CA3-OA5-PA1-OA4
20	a	504	CDL	CA2-OA2-PA1-OA3
20	a	504	CDL	CB2-OB2-PB2-OB3
20	d	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
20	d	201	CDL	CB2-OB2-PB2-OB4
20	d	202	CDL	CA3-OA5-PA1-OA3
20	d	202	CDL	CB2-OB2-PB2-OB3
20	e	101	CDL	CA2-OA2-PA1-OA3
20	e	101	CDL	CA2-OA2-PA1-OA5
20	e	101	CDL	CB2-OB2-PB2-OB4
20	m	201	CDL	CA2-OA2-PA1-OA3
20	m	201	CDL	CB2-OB2-PB2-OB3
20	m	201	CDL	CB3-OB5-PB2-OB2
20	m	201	CDL	CB3-OB5-PB2-OB3
20	m	202	CDL	CA2-OA2-PA1-OA3
20	p	201	CDL	CA3-OA5-PA1-OA3
20	p	202	CDL	CA2-OA2-PA1-OA4
20	r	101	CDL	CA2-OA2-PA1-OA4
20	r	101	CDL	CA2-OA2-PA1-OA5
20	r	101	CDL	CA3-OA5-PA1-OA3
22	O	203	LPP	C23-C24-C25-C26
22	o	203	LPP	C23-C24-C25-C26
20	a	504	CDL	C53-C54-C55-C56
20	p	201	CDL	C76-C77-C78-C79
20	A	504	CDL	CA4-CA3-OA5-PA1
20	E	101	CDL	C1-CB2-OB2-PB2
20	O	201	CDL	C1-CA2-OA2-PA1
20	a	504	CDL	CA4-CA3-OA5-PA1
20	a	503	CDL	C55-C56-C57-C58
20	E	101	CDL	CA7-C31-C32-C33
20	A	501	CDL	C12-C11-CA5-OA6
20	A	503	CDL	C55-C56-C57-C58
23	G	201	TRT	C23-C22-O21-C20
23	G	201	TRT	C16-C17-O18-C19
23	g	201	TRT	C23-C22-O21-C20
20	M	203	CDL	CB7-C71-C72-C73
21	Q	101	LMT	C7-C8-C9-C10
21	q	101	LMT	C7-C8-C9-C10
23	g	201	TRT	C16-C17-O18-C19
22	R	102	LPP	C39-C40-C41-C42
20	D	202	CDL	CA6-CA4-OA6-CA5
20	O	201	CDL	CA3-CA4-OA6-CA5
20	d	202	CDL	CA6-CA4-OA6-CA5
20	o	201	CDL	CA3-CA4-OA6-CA5
22	N	203	LPP	C8-C7-O9-C11
22	P	202	LPP	C8-C7-O9-C11

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Mol	Chain	Res	Type	Atoms
22	r	102	LPP	C39-C40-C41-C42
20	a	501	CDL	C12-C11-CA5-OA6
21	N	204	LMT	C2-C3-C4-C5
21	n	201	LMT	C2-C3-C4-C5
20	A	503	CDL	OA5-CA3-CA4-CA6
20	a	503	CDL	OA5-CA3-CA4-CA6
20	m	202	CDL	OA5-CA3-CA4-CA6
20	A	504	CDL	C75-C76-C77-C78
20	A	503	CDL	OB5-CB3-CB4-OB6
20	M	204	CDL	OA5-CA3-CA4-OA6
20	a	503	CDL	OB5-CB3-CB4-OB6
20	m	202	CDL	C12-C11-CA5-OA6
20	D	201	CDL	CB7-C71-C72-C73
20	p	201	CDL	C61-C62-C63-C64
20	a	504	CDL	C75-C76-C77-C78
20	P	201	CDL	C32-C33-C34-C35
20	r	101	CDL	C63-C64-C65-C66
20	A	501	CDL	CB4-CB3-OB5-PB2
20	a	501	CDL	CB4-CB3-OB5-PB2
20	e	101	CDL	C1-CB2-OB2-PB2
20	A	504	CDL	C32-C31-CA7-OA8
20	A	502	CDL	CB5-C51-C52-C53
20	R	101	CDL	C63-C64-C65-C66
20	o	201	CDL	C72-C71-CB7-OB8
20	a	504	CDL	C59-C60-C61-C62
20	a	502	CDL	CB5-C51-C52-C53
20	A	501	CDL	C13-C14-C15-C16
20	O	201	CDL	C72-C71-CB7-OB8
20	a	504	CDL	C32-C31-CA7-OA8
22	O	202	LPP	C14-C15-C16-C17
22	o	202	LPP	C14-C15-C16-C17
20	D	201	CDL	C33-C34-C35-C36
20	D	202	CDL	C73-C74-C75-C76
20	a	501	CDL	C13-C14-C15-C16
20	A	504	CDL	C59-C60-C61-C62
21	F	302	LMT	C2-C1-O1'-C1'
21	f	302	LMT	C2-C1-O1'-C1'
20	d	201	CDL	C33-C34-C35-C36
20	M	204	CDL	CB4-CB3-OB5-PB2
20	d	202	CDL	C15-C16-C17-C18
22	F	301	LPP	C14-C15-C16-C17
22	f	301	LPP	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	A	501	CDL	C71-CB7-OB8-CB6
23	P	203	TRT	C1-C5-C6-C9
23	p	203	TRT	C1-C5-C6-C9
20	P	201	CDL	C71-C72-C73-C74
20	D	201	CDL	C40-C41-C42-C43
20	R	101	CDL	C77-C78-C79-C80
20	p	201	CDL	C42-C43-C44-C45
20	r	101	CDL	C77-C78-C79-C80
20	A	504	CDL	C31-CA7-OA8-CA6
20	A	501	CDL	OB9-CB7-OB8-CB6
23	N	201	TRT	O15-C16-C17-O18
20	d	201	CDL	C53-C54-C55-C56
20	p	201	CDL	C73-C74-C75-C76
20	d	201	CDL	CB7-C71-C72-C73
23	g	202	TRT	O15-C16-C17-O18
23	n	202	TRT	O15-C16-C17-O18
23	G	202	TRT	O15-C16-C17-O18
20	d	202	CDL	C71-C72-C73-C74
20	A	504	CDL	C1-CA2-OA2-PA1
20	P	201	CDL	CA4-CA3-OA5-PA1
20	a	504	CDL	C1-CA2-OA2-PA1
20	m	202	CDL	CB4-CB3-OB5-PB2
20	p	202	CDL	CA4-CA3-OA5-PA1
20	E	101	CDL	C51-C52-C53-C54
20	D	202	CDL	C15-C16-C17-C18
20	r	101	CDL	C13-C14-C15-C16
23	M	202	TRT	C1-C5-C6-C9
23	N	201	TRT	C1-C5-C6-C9
23	m	204	TRT	C1-C5-C6-C9
23	n	202	TRT	C1-C5-C6-C9
20	R	101	CDL	C13-C14-C15-C16
20	D	201	CDL	C53-C54-C55-C56
20	E	101	CDL	C59-C60-C61-C62
20	p	201	CDL	C83-C84-C85-C86
20	D	202	CDL	C40-C41-C42-C43
20	a	501	CDL	C71-CB7-OB8-CB6
20	A	504	CDL	OA9-CA7-OA8-CA6
20	D	202	CDL	C1-CA2-OA2-PA1
20	d	202	CDL	CB4-CB3-OB5-PB2
20	A	501	CDL	OB5-CB3-CB4-CB6
20	a	501	CDL	OB5-CB3-CB4-CB6
20	p	202	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
20	d	202	CDL	C40-C41-C42-C43
20	d	201	CDL	CB2-C1-CA2-OA2
20	D	202	CDL	C32-C31-CA7-OA8
20	O	201	CDL	C52-C51-CB5-OB6
20	A	504	CDL	C56-C57-C58-C59
20	a	501	CDL	OB9-CB7-OB8-CB6
20	o	201	CDL	C72-C73-C74-C75
20	a	504	CDL	C56-C57-C58-C59
22	N	203	LPP	C31-C32-C33-C34
22	P	202	LPP	C31-C32-C33-C34
20	O	201	CDL	C72-C73-C74-C75
20	D	202	CDL	CB4-CB3-OB5-PB2
20	d	202	CDL	C1-CA2-OA2-PA1
20	o	201	CDL	C52-C51-CB5-OB6
20	e	101	CDL	C59-C60-C61-C62
20	A	502	CDL	C24-C25-C26-C27
20	a	502	CDL	C24-C25-C26-C27
22	I	101	LPP	C37-C38-C39-C40
22	i	101	LPP	C37-C38-C39-C40
20	A	504	CDL	C73-C74-C75-C76
22	o	202	LPP	O10-C11-O9-C7
20	d	201	CDL	C59-C60-C61-C62
20	D	201	CDL	C22-C23-C24-C25
20	d	201	CDL	C22-C23-C24-C25
20	E	101	CDL	C12-C11-CA5-OA7
20	a	504	CDL	C73-C74-C75-C76
20	d	202	CDL	C32-C31-CA7-OA8
20	R	101	CDL	C60-C61-C62-C63
23	G	201	TRT	C1-C5-C6-C9
23	g	201	TRT	C1-C5-C6-C9
22	O	202	LPP	O10-C11-O9-C7
21	D	203	LMT	C1-C2-C3-C4
20	D	201	CDL	CB2-C1-CA2-OA2
20	D	201	CDL	C59-C60-C61-C62
21	d	203	LMT	C1-C2-C3-C4
20	P	201	CDL	OA5-CA3-CA4-CA6
20	O	201	CDL	OA6-CA4-CA6-OA8
22	F	301	LPP	O9-C7-C8-O27
22	f	301	LPP	O9-C7-C8-O27
20	r	101	CDL	C60-C61-C62-C63
20	M	203	CDL	C80-C81-C82-C83
20	E	101	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
20	p	201	CDL	C52-C53-C54-C55
20	E	101	CDL	C32-C33-C34-C35
20	e	101	CDL	C32-C33-C34-C35
20	e	101	CDL	C12-C11-CA5-OA7
20	R	101	CDL	C37-C38-C39-C40
20	O	201	CDL	C18-C19-C20-C21
20	R	101	CDL	C76-C77-C78-C79
20	p	202	CDL	C71-C72-C73-C74
20	e	101	CDL	C72-C71-CB7-OB8
23	G	202	TRT	C7-C6-C9-C10
23	g	202	TRT	C7-C6-C9-C10
20	a	503	CDL	C71-C72-C73-C74
20	o	201	CDL	C18-C19-C20-C21
20	r	101	CDL	C76-C77-C78-C79
21	F	302	LMT	C7-C8-C9-C10
21	f	302	LMT	C7-C8-C9-C10
20	a	504	CDL	C31-CA7-OA8-CA6
23	G	202	TRT	C1-C5-C6-C9
23	N	202	TRT	C1-C5-C6-C9
23	g	202	TRT	C1-C5-C6-C9
23	n	203	TRT	C1-C5-C6-C9
20	e	101	CDL	C60-C61-C62-C63
20	E	101	CDL	C60-C61-C62-C63
20	P	201	CDL	C31-C32-C33-C34
23	N	202	TRT	C8-C6-C9-C10
23	n	203	TRT	C8-C6-C9-C10
20	D	202	CDL	C71-C72-C73-C74
20	A	501	CDL	CB3-CB4-CB6-OB8
20	a	504	CDL	OA9-CA7-OA8-CA6
23	N	202	TRT	C7-C6-C9-C14
23	n	203	TRT	C7-C6-C9-C14
21	N	204	LMT	C5'-C4'-O1B-C1B
22	O	203	LPP	C14-C15-C16-C17
21	n	201	LMT	C5'-C4'-O1B-C1B
23	M	201	TRT	C7-C6-C9-C10
23	N	202	TRT	C7-C6-C9-C10
23	m	203	TRT	C7-C6-C9-C10
23	n	203	TRT	C7-C6-C9-C10
20	a	502	CDL	CA5-C11-C12-C13
22	o	203	LPP	C14-C15-C16-C17
20	D	202	CDL	C12-C13-C14-C15
21	F	302	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
21	f	302	LMT	C1-C2-C3-C4
20	m	201	CDL	C80-C81-C82-C83
23	N	201	TRT	C17-C16-O15-C12
23	M	202	TRT	C1-C5-C6-C8
20	r	101	CDL	C32-C33-C34-C35
23	n	202	TRT	C17-C16-O15-C12
20	E	101	CDL	C73-C74-C75-C76
20	D	202	CDL	C32-C33-C34-C35
22	O	202	LPP	O9-C7-C8-O27
20	d	201	CDL	C13-C14-C15-C16
20	R	101	CDL	C32-C31-CA7-OA8
20	r	101	CDL	C32-C31-CA7-OA8
22	O	202	LPP	O5-C6-C7-C8
22	o	202	LPP	O5-C6-C7-C8
20	A	501	CDL	C19-C20-C21-C22
22	N	203	LPP	O10-C11-C12-C13
22	P	202	LPP	O10-C11-C12-C13
22	O	203	LPP	C21-C22-C23-C24
22	o	203	LPP	C21-C22-C23-C24
20	O	201	CDL	C13-C14-C15-C16
23	G	202	TRT	C7-C6-C9-C14
23	g	202	TRT	C7-C6-C9-C14
22	O	202	LPP	C12-C11-O9-C7
23	N	201	TRT	O18-C19-C20-O21
23	n	202	TRT	O18-C19-C20-O21
20	A	504	CDL	OB7-CB5-OB6-CB4
22	O	203	LPP	O10-C11-O9-C7
22	o	203	LPP	O10-C11-O9-C7
20	d	201	CDL	C56-C57-C58-C59
20	D	201	CDL	C13-C14-C15-C16
20	O	201	CDL	C12-C13-C14-C15
23	m	204	TRT	C1-C5-C6-C8
20	M	203	CDL	C72-C71-CB7-OB8
20	o	201	CDL	C13-C14-C15-C16
20	D	201	CDL	C56-C57-C58-C59
20	a	504	CDL	OB7-CB5-OB6-CB4
22	o	202	LPP	C12-C11-O9-C7
20	m	201	CDL	C72-C71-CB7-OB8
20	d	202	CDL	C12-C13-C14-C15
23	M	201	TRT	C8-C6-C9-C14
23	N	202	TRT	C8-C6-C9-C14
23	n	203	TRT	C8-C6-C9-C14

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Mol	Chain	Res	Type	Atoms
20	e	101	CDL	C73-C74-C75-C76
20	a	504	CDL	CB7-C71-C72-C73
23	P	203	TRT	O18-C19-C20-O21
23	p	203	TRT	O18-C19-C20-O21
20	m	202	CDL	C52-C51-CB5-OB6
20	A	503	CDL	C23-C24-C25-C26
20	o	201	CDL	C12-C13-C14-C15
23	m	203	TRT	C8-C6-C9-C14
20	A	504	CDL	CB7-C71-C72-C73
20	R	101	CDL	C51-C52-C53-C54
20	a	504	CDL	C72-C73-C74-C75
20	d	202	CDL	C32-C33-C34-C35
20	R	101	CDL	C53-C54-C55-C56
23	M	201	TRT	C8-C6-C9-C10
23	g	202	TRT	C8-C6-C9-C14
23	m	203	TRT	C8-C6-C9-C10
20	A	501	CDL	C54-C55-C56-C57
20	A	504	CDL	C72-C73-C74-C75
20	a	501	CDL	C54-C55-C56-C57
20	r	101	CDL	C53-C54-C55-C56
20	A	504	CDL	C52-C51-CB5-OB6
20	a	501	CDL	CB3-CB4-CB6-OB8
20	a	501	CDL	C19-C20-C21-C22
21	D	203	LMT	O5'-C1'-O1'-C1
21	d	203	LMT	O5'-C1'-O1'-C1
20	a	504	CDL	C52-C51-CB5-OB6
22	N	203	LPP	O9-C7-C8-O27
22	P	202	LPP	O9-C7-C8-O27
22	o	202	LPP	O9-C7-C8-O27
23	G	202	TRT	C8-C6-C9-C14
23	M	201	TRT	C7-C6-C9-C14
23	m	203	TRT	C7-C6-C9-C14
20	a	503	CDL	C23-C24-C25-C26
20	r	101	CDL	C51-C52-C53-C54
20	A	504	CDL	C55-C56-C57-C58
20	M	204	CDL	C52-C51-CB5-OB6
20	r	101	CDL	C52-C51-CB5-OB6
20	m	201	CDL	C72-C71-CB7-OB9
20	E	101	CDL	OB7-CB5-OB6-CB4
23	M	202	TRT	O15-C16-C17-O18
23	m	204	TRT	O15-C16-C17-O18
20	o	201	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
23	g	202	TRT	C2-C1-C5-C6
20	M	203	CDL	C72-C71-CB7-OB9
22	o	203	LPP	C15-C16-C17-C18
22	O	203	LPP	C15-C16-C17-C18
22	O	202	LPP	O5-C6-C7-O9
22	o	202	LPP	O5-C6-C7-O9
20	E	101	CDL	C54-C55-C56-C57
20	R	101	CDL	C52-C51-CB5-OB6
23	g	202	TRT	C8-C6-C9-C10
20	m	202	CDL	C52-C51-CB5-OB7
23	G	202	TRT	C2-C1-C5-C6
23	N	202	TRT	O15-C16-C17-O18
23	n	203	TRT	O15-C16-C17-O18
20	a	504	CDL	C52-C51-CB5-OB7
23	G	202	TRT	C8-C6-C9-C10
20	A	504	CDL	C52-C51-CB5-OB7
20	R	101	CDL	C32-C31-CA7-OA9
23	G	202	TRT	C23-C22-O21-C20
23	g	202	TRT	C23-C22-O21-C20
20	D	201	CDL	C72-C71-CB7-OB8
20	e	101	CDL	C31-CA7-OA8-CA6
20	e	101	CDL	C54-C55-C56-C57
20	r	101	CDL	C32-C31-CA7-OA9
20	m	202	CDL	OB9-CB7-OB8-CB6
20	p	201	CDL	C32-C33-C34-C35
23	N	202	TRT	O21-C22-C23-O24
23	n	203	TRT	O21-C22-C23-O24
20	r	101	CDL	C33-C34-C35-C36
20	M	204	CDL	C52-C51-CB5-OB7
20	M	204	CDL	C1-CB2-OB2-PB2
20	A	503	CDL	C12-C11-CA5-OA6
22	i	101	LPP	C19-C20-C21-C22
22	I	101	LPP	C19-C20-C21-C22
22	o	203	LPP	C12-C11-O9-C7
20	m	202	CDL	OB5-CB3-CB4-CB6
20	r	101	CDL	OB5-CB3-CB4-CB6
20	m	202	CDL	C71-CB7-OB8-CB6
20	D	201	CDL	C23-C24-C25-C26
20	P	201	CDL	C72-C71-CB7-OB8
22	O	203	LPP	C12-C11-O9-C7
20	a	504	CDL	C55-C56-C57-C58
20	p	202	CDL	C72-C71-CB7-OB8

There are no ring outliers.

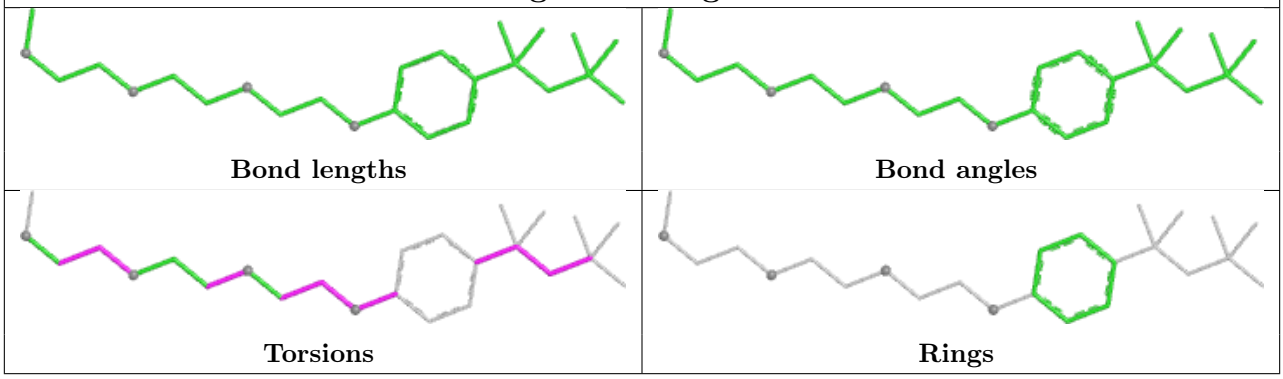
38 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	g	202	TRT	3	0
20	a	503	CDL	3	0
23	G	202	TRT	3	0
23	N	201	TRT	6	0
20	R	101	CDL	2	0
20	M	203	CDL	3	0
20	A	503	CDL	3	0
23	m	204	TRT	2	0
20	D	201	CDL	2	0
20	d	202	CDL	3	0
20	o	201	CDL	3	0
22	r	102	LPP	1	0
23	N	202	TRT	3	0
20	p	202	CDL	1	0
23	n	202	TRT	5	0
20	A	502	CDL	4	0
20	a	502	CDL	4	0
23	G	201	TRT	3	0
23	g	201	TRT	3	0
20	e	101	CDL	7	0
22	I	101	LPP	2	0
23	M	202	TRT	2	0
23	n	203	TRT	2	0
22	R	102	LPP	1	0
21	F	302	LMT	2	0
20	E	101	CDL	6	0
20	A	501	CDL	1	0
22	N	203	LPP	2	0
20	d	201	CDL	3	0
22	i	101	LPP	2	0
20	D	202	CDL	4	0
20	r	101	CDL	2	0
22	P	202	LPP	2	0
20	m	201	CDL	1	0
20	M	204	CDL	1	0
21	f	302	LMT	2	0
20	O	201	CDL	4	0
20	P	201	CDL	1	0

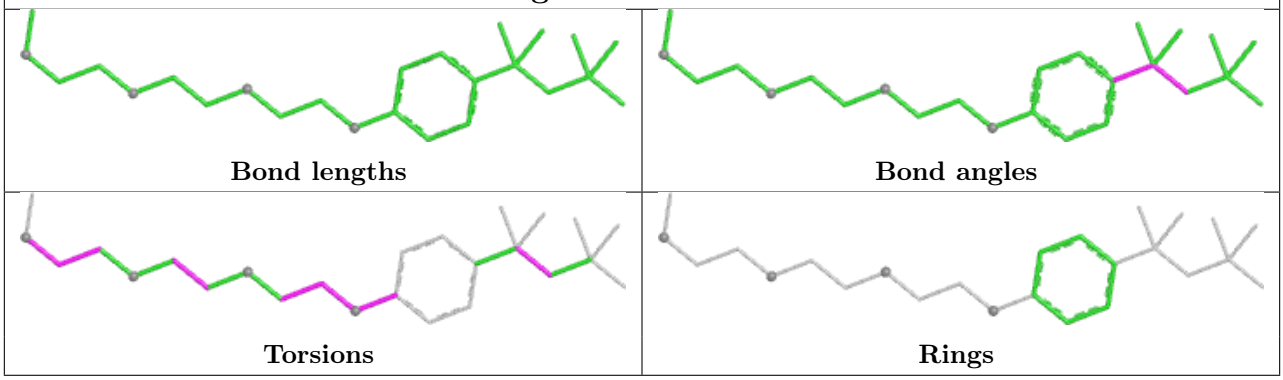
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

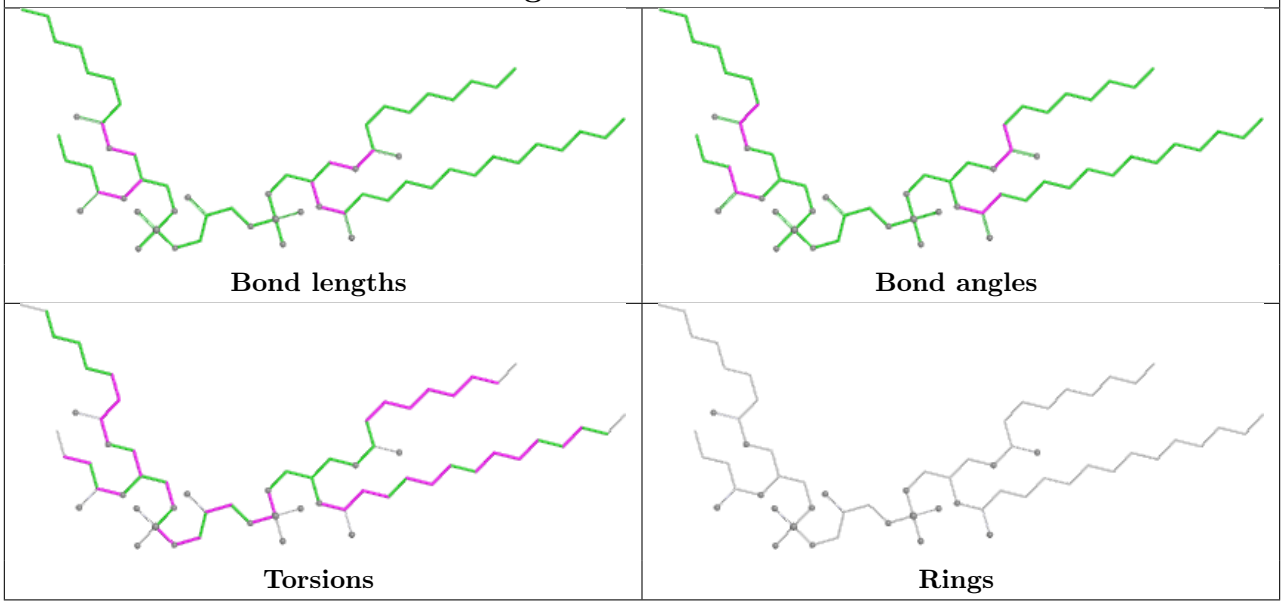
Ligand TRT g 202



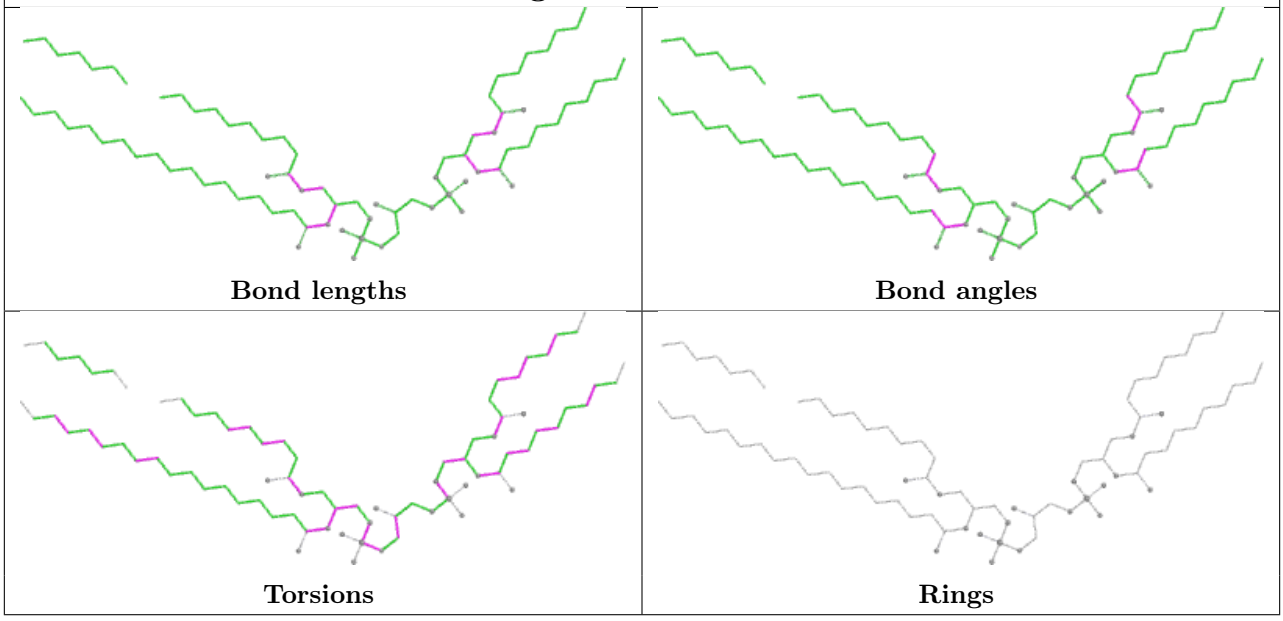
Ligand TRT r 103



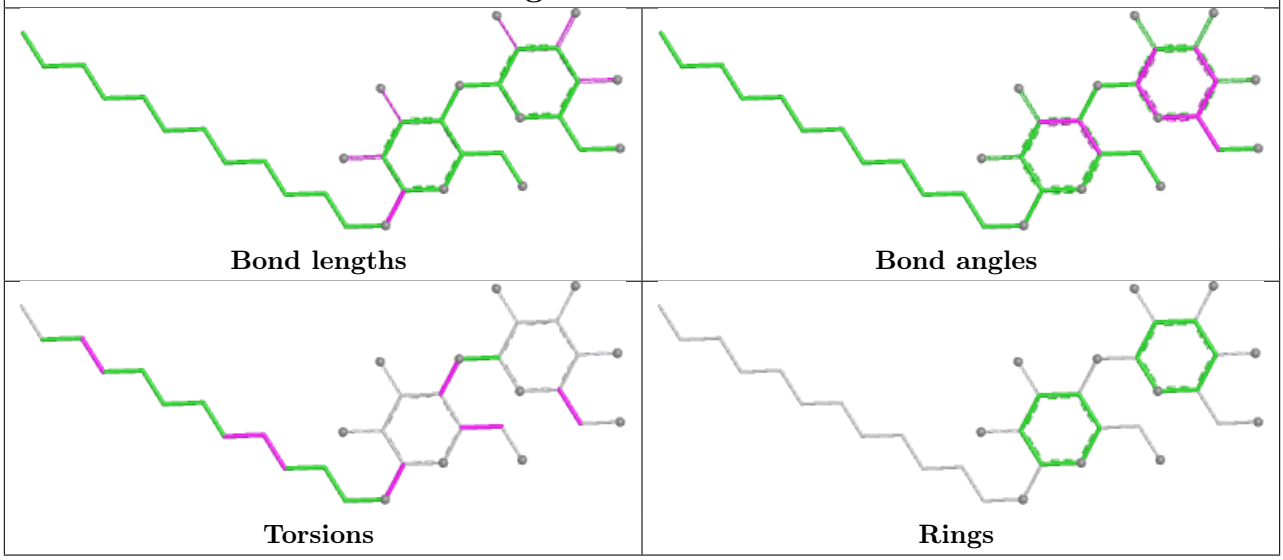
Ligand CDL A 504



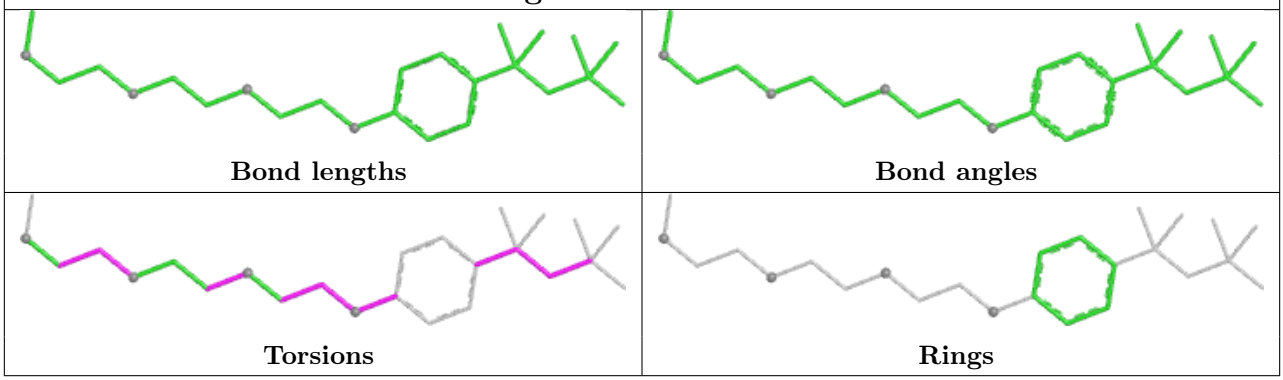
Ligand CDL a 503



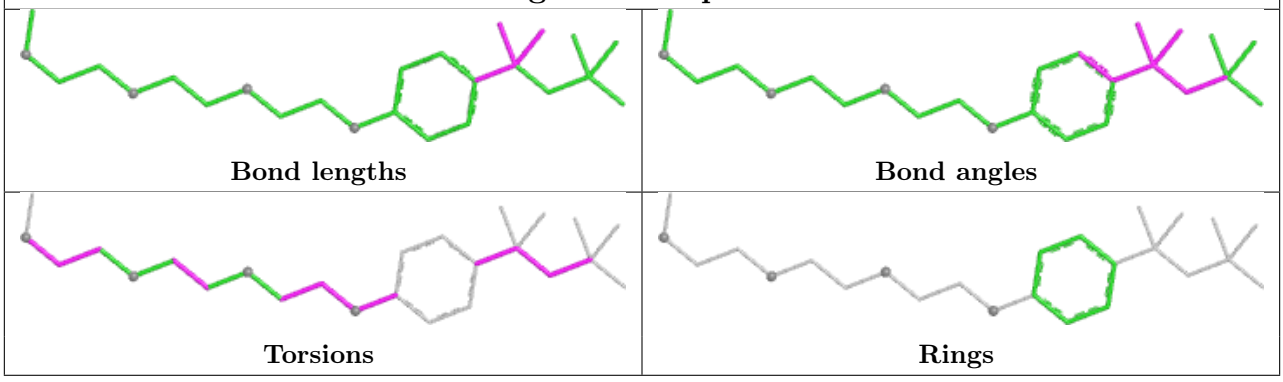
Ligand LMT n 201



Ligand TRT G 202



Ligand TRT p 203



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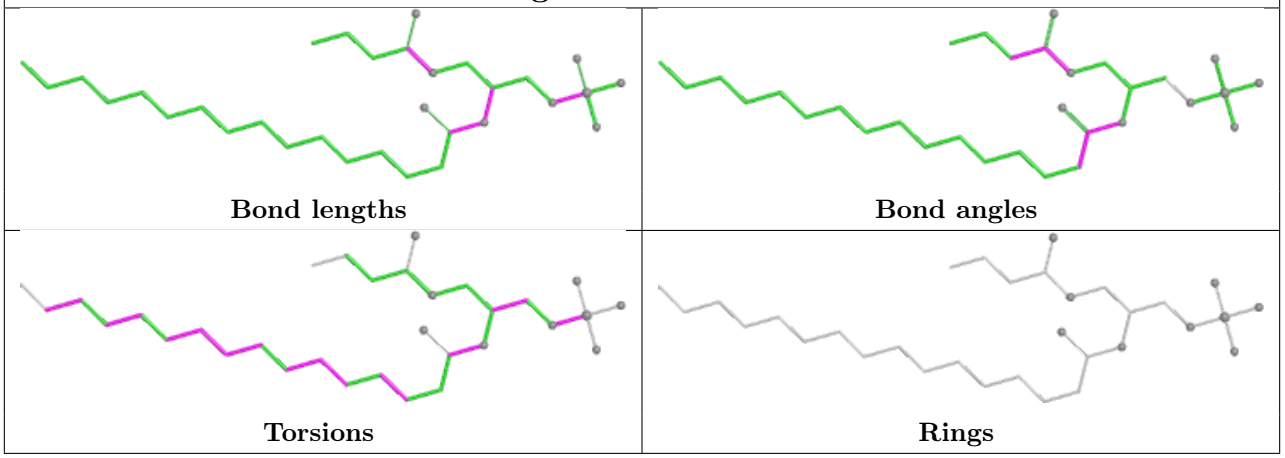

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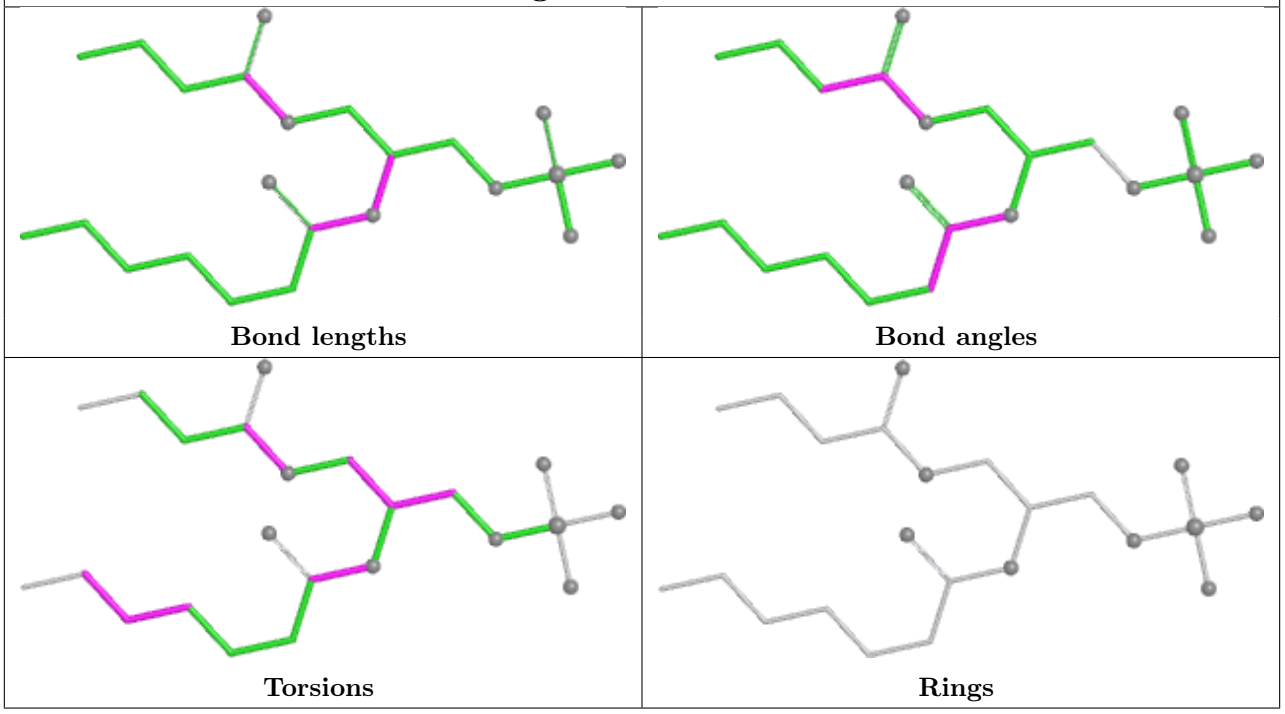

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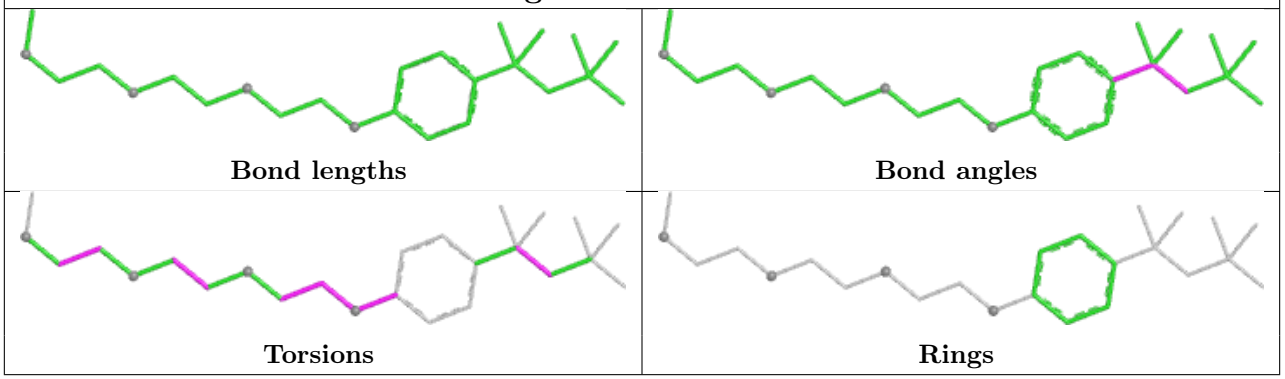
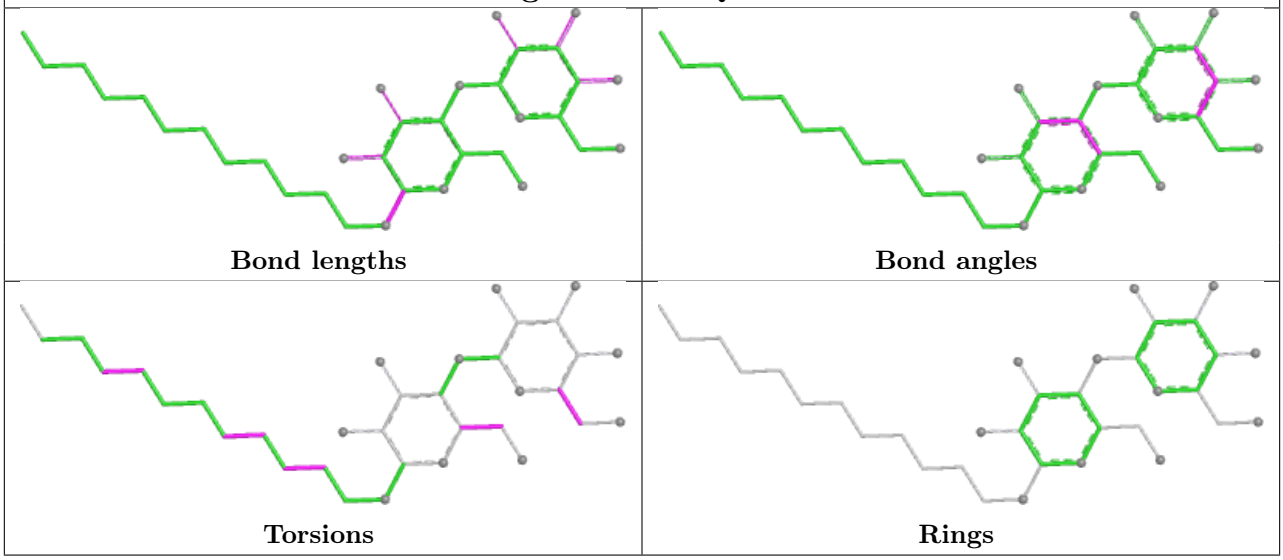


Ligand LMT Q 101



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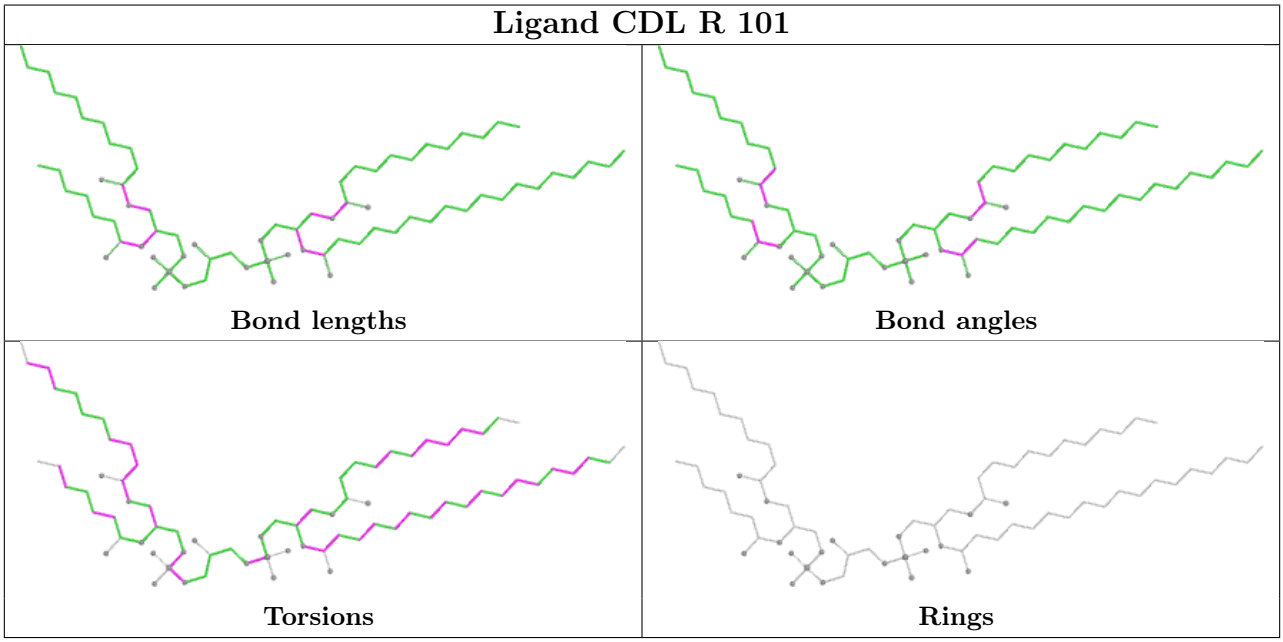

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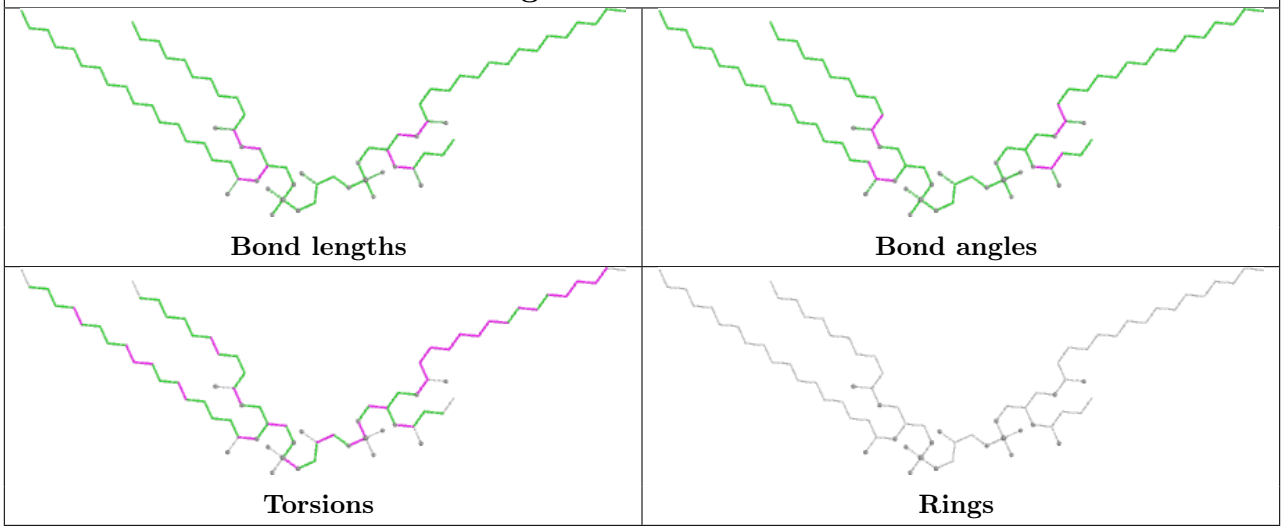

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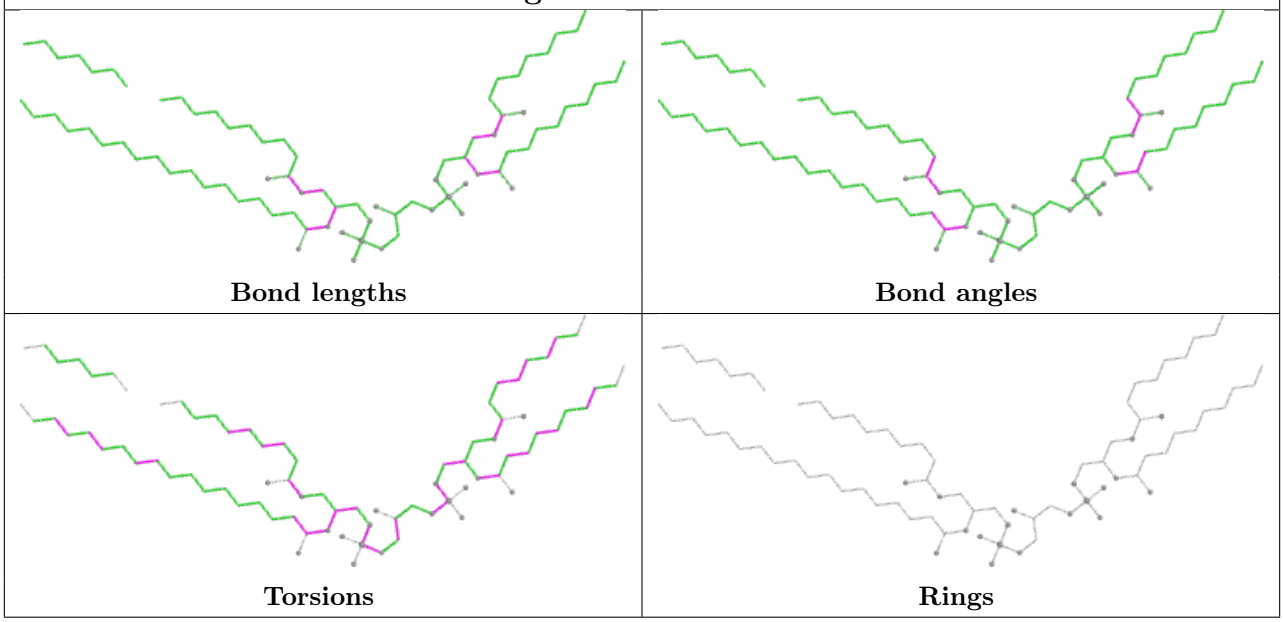

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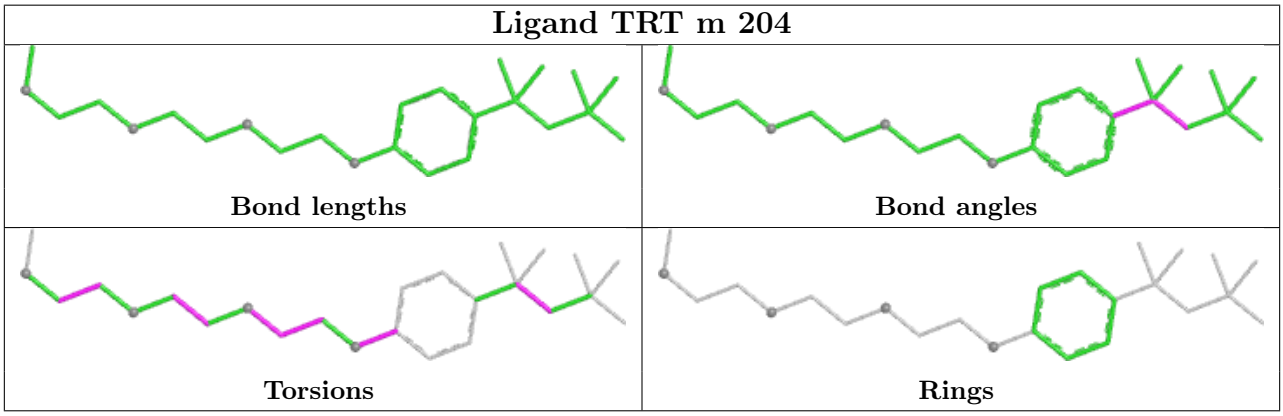

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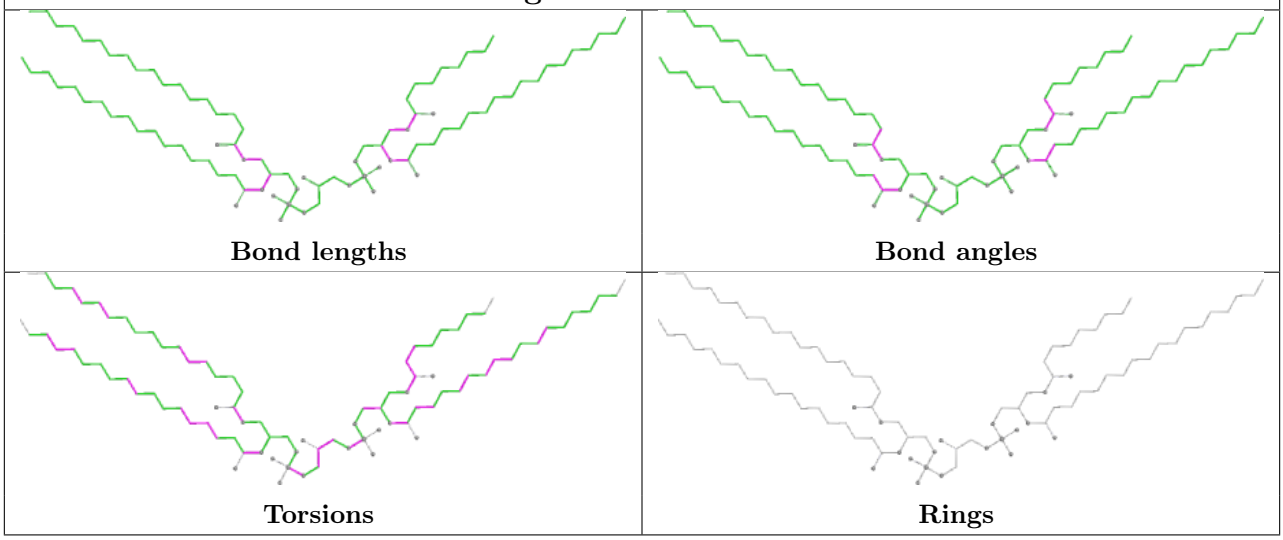

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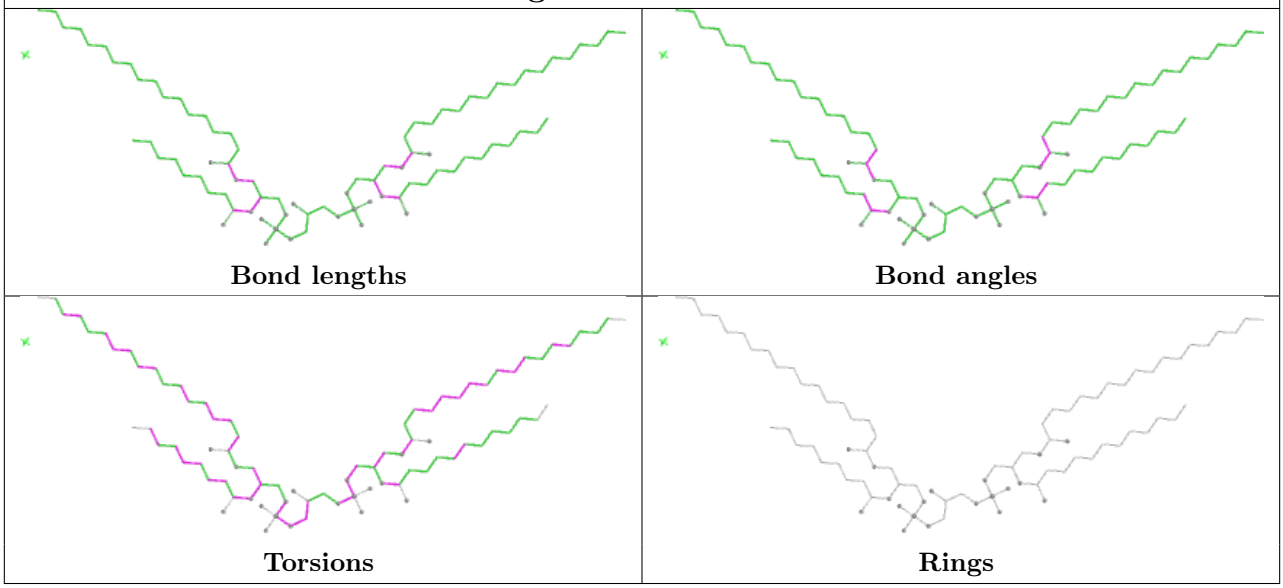

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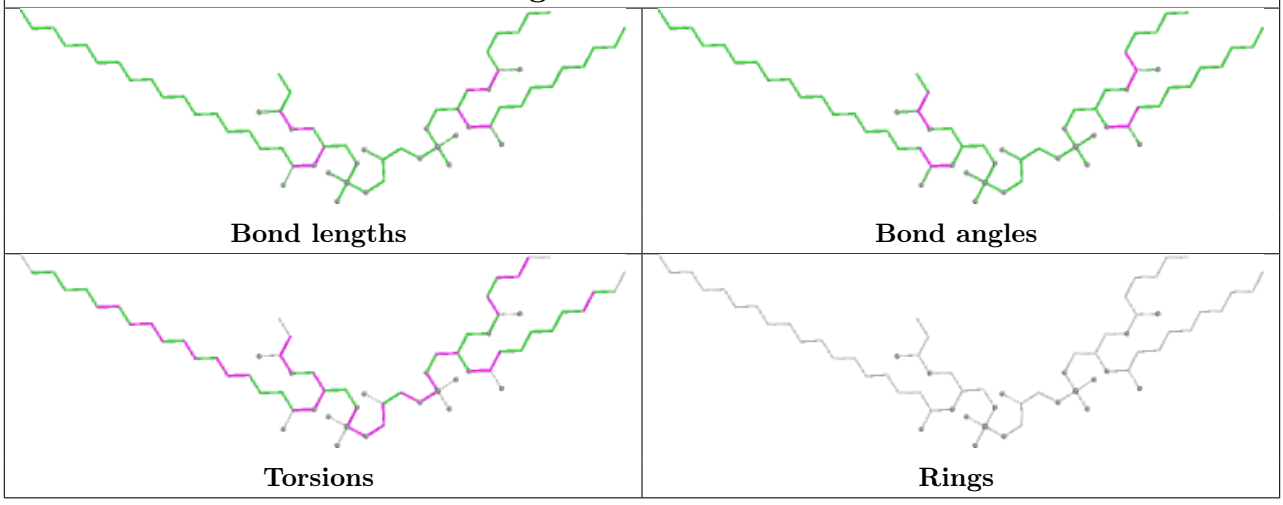

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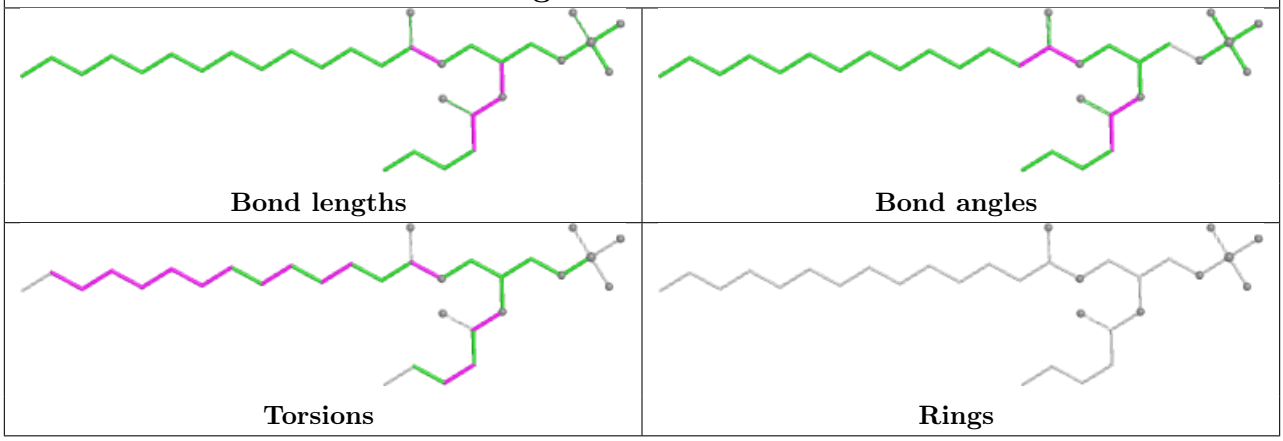

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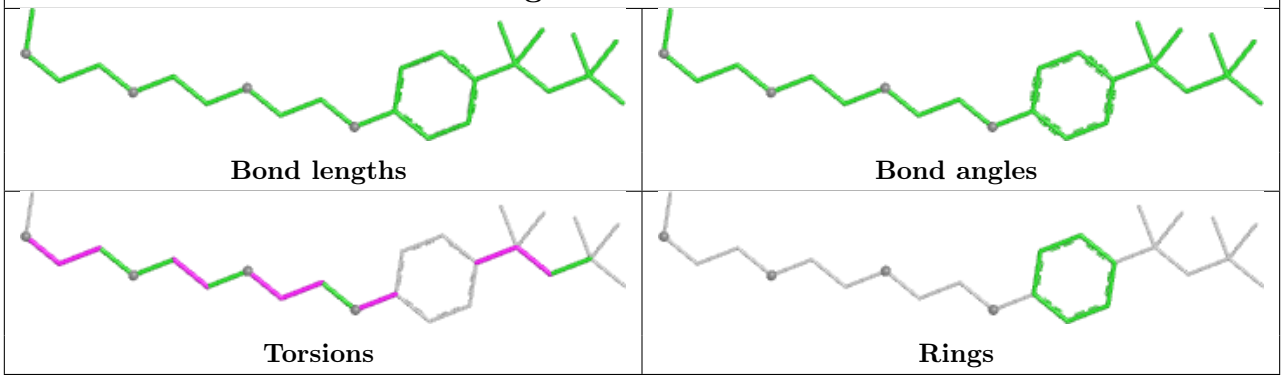
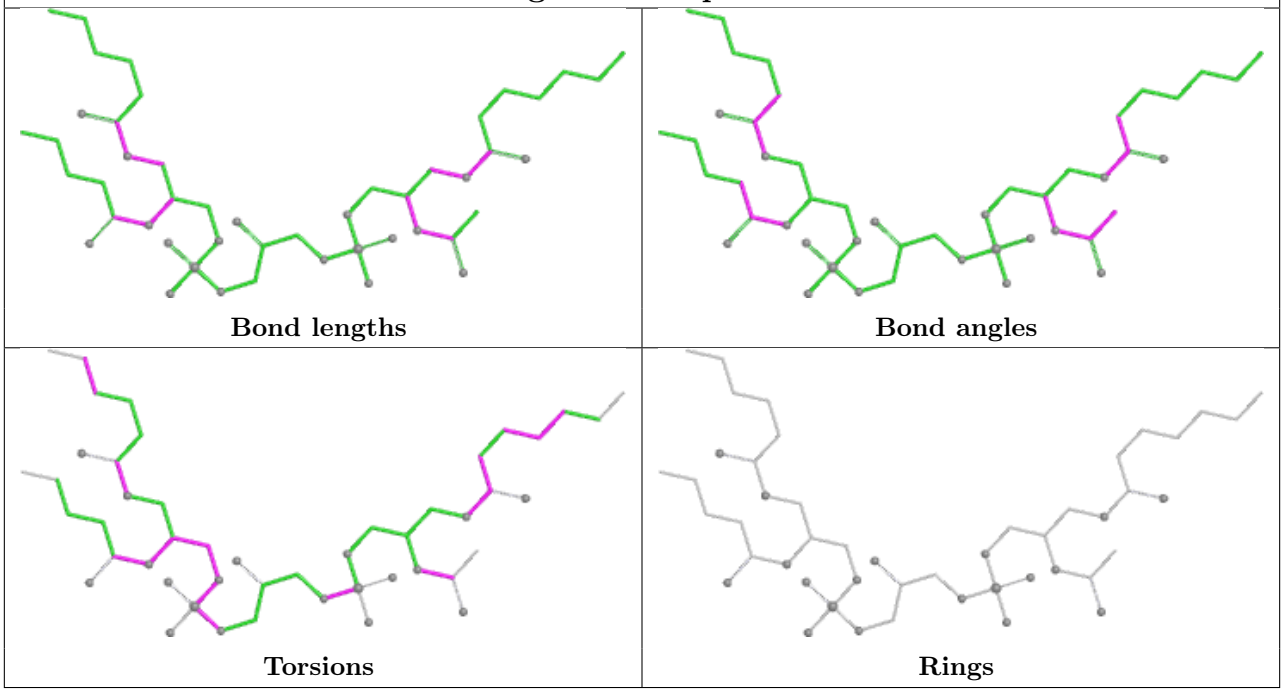


Ligand CDL p 202



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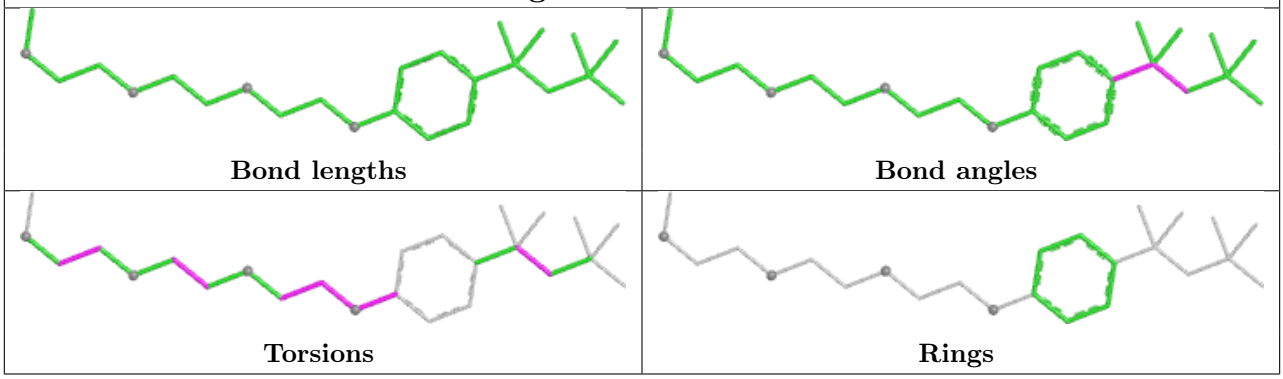

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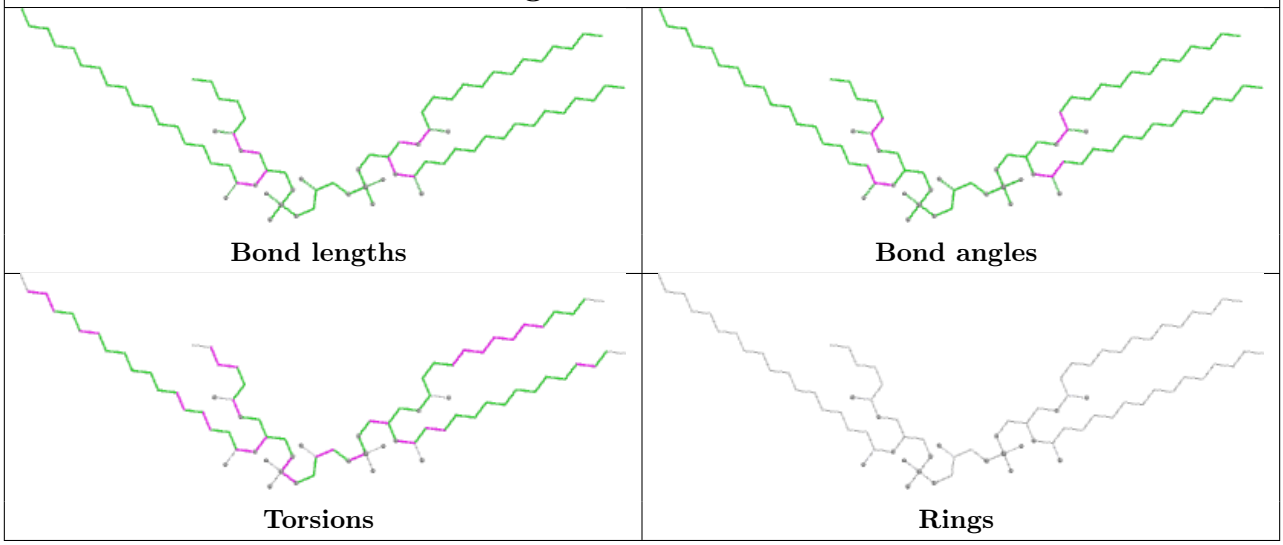

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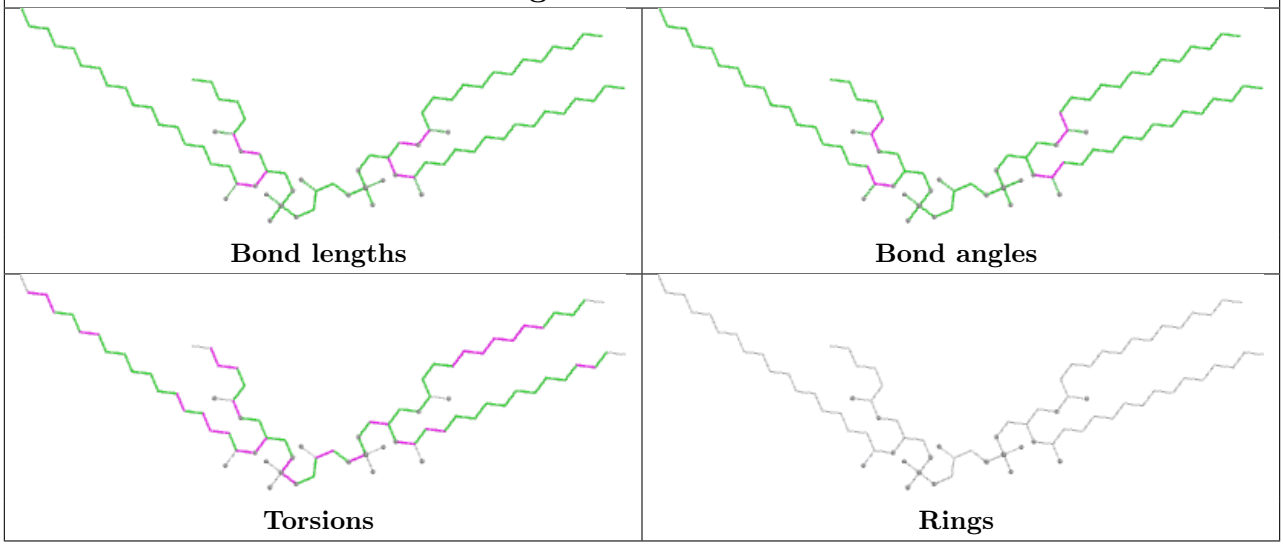

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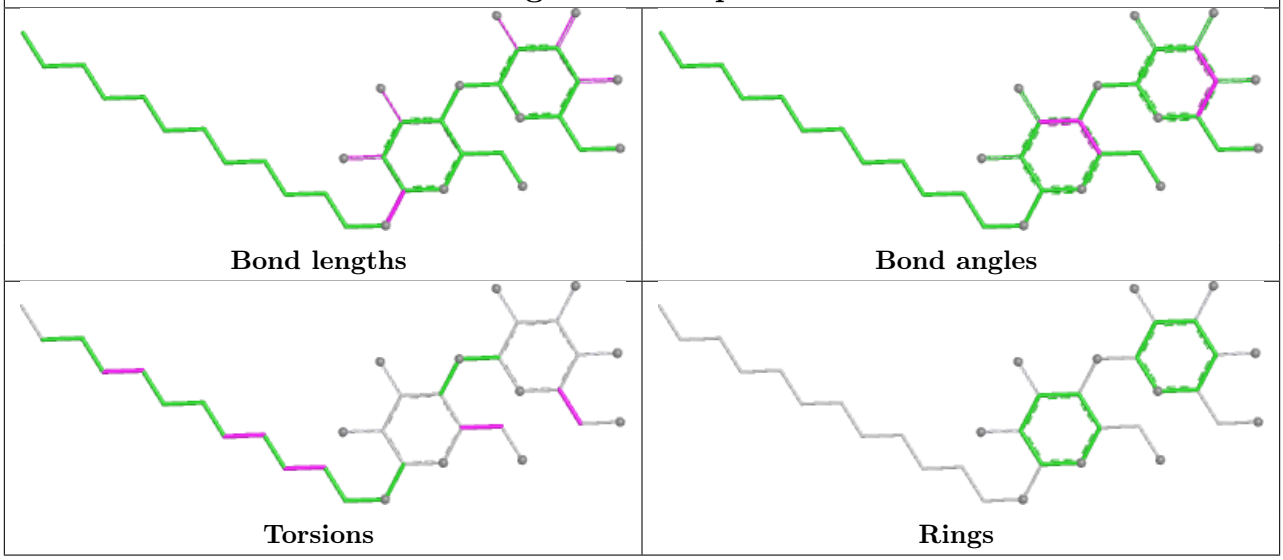

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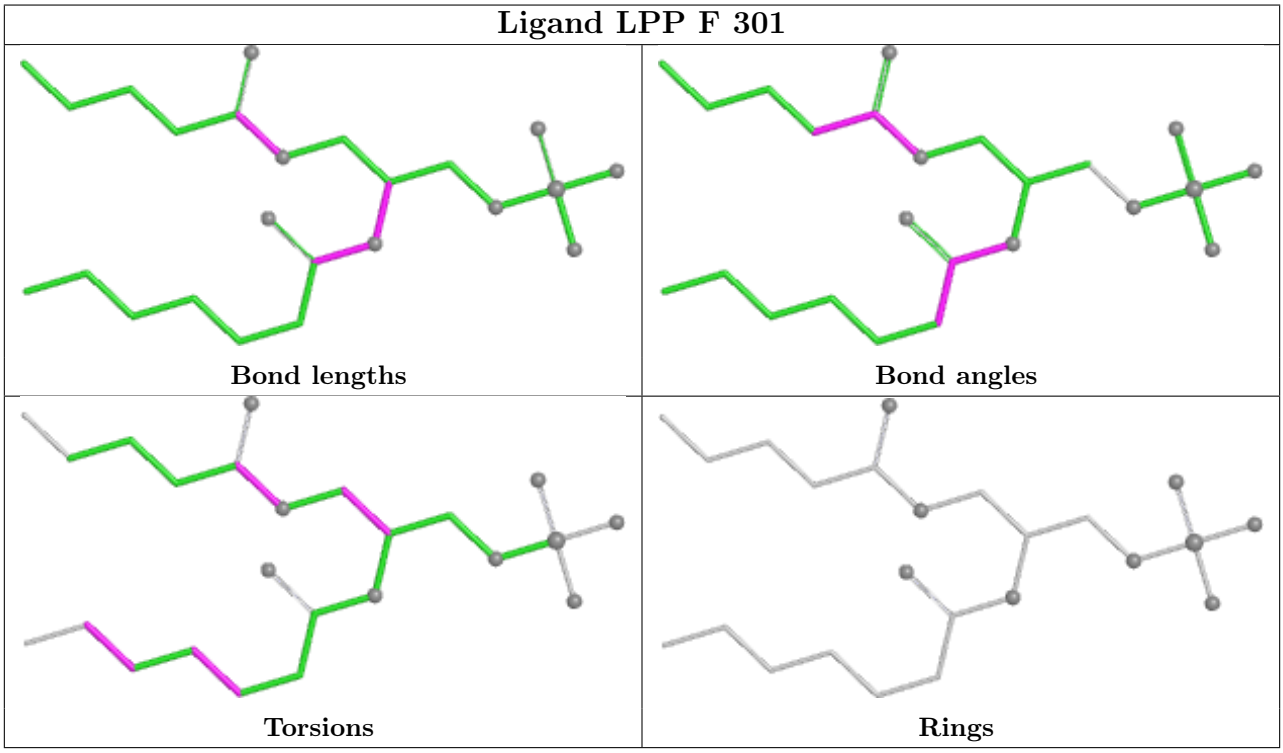

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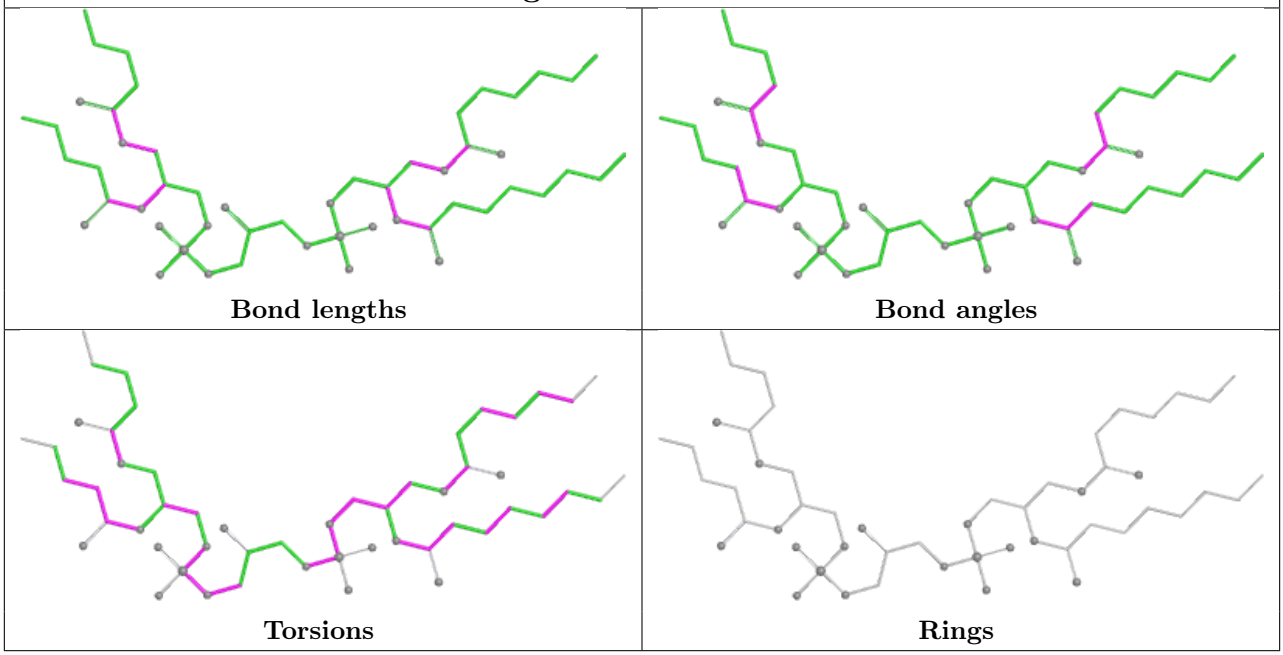

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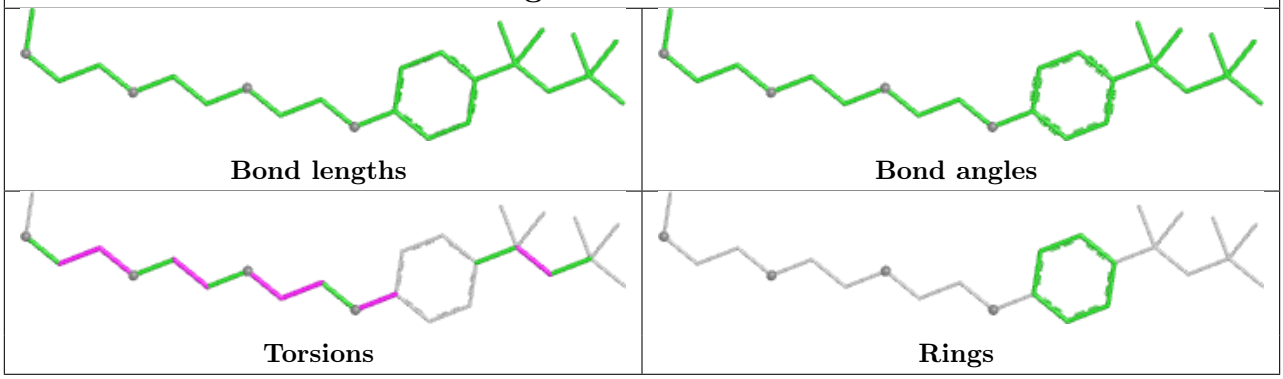

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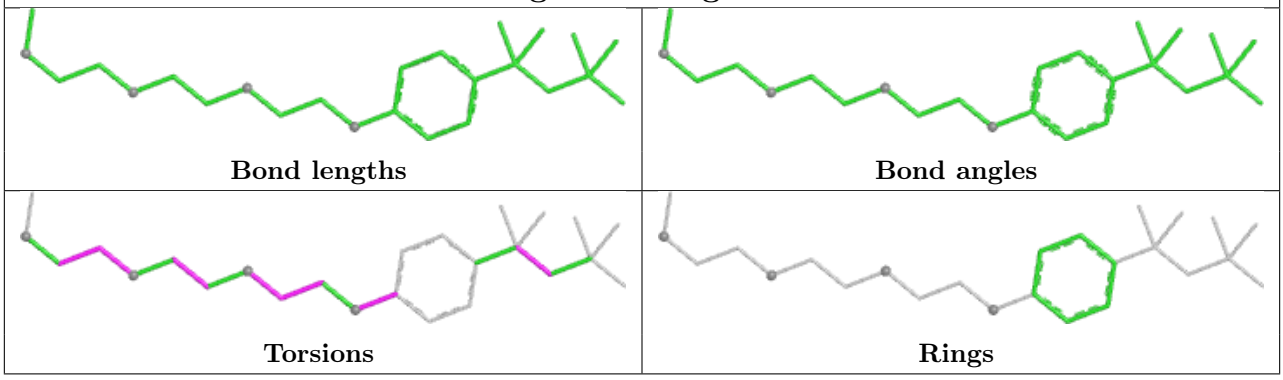

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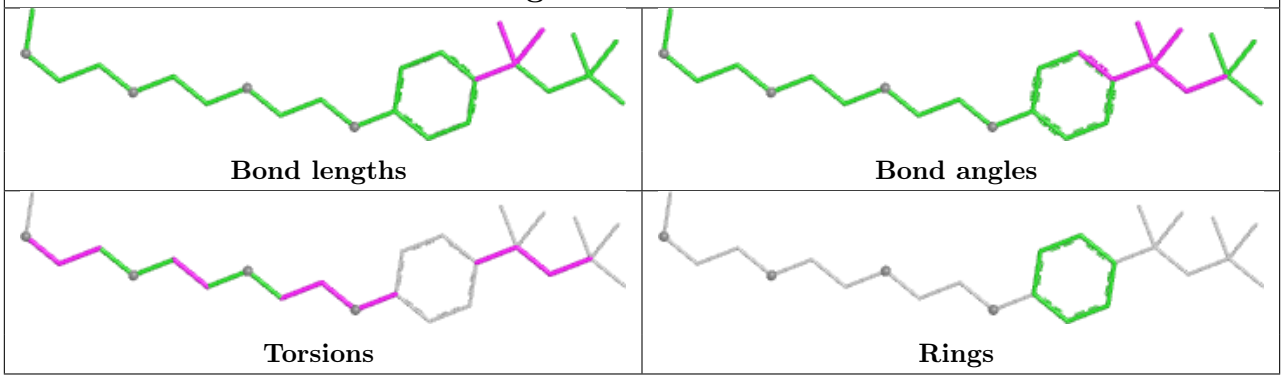

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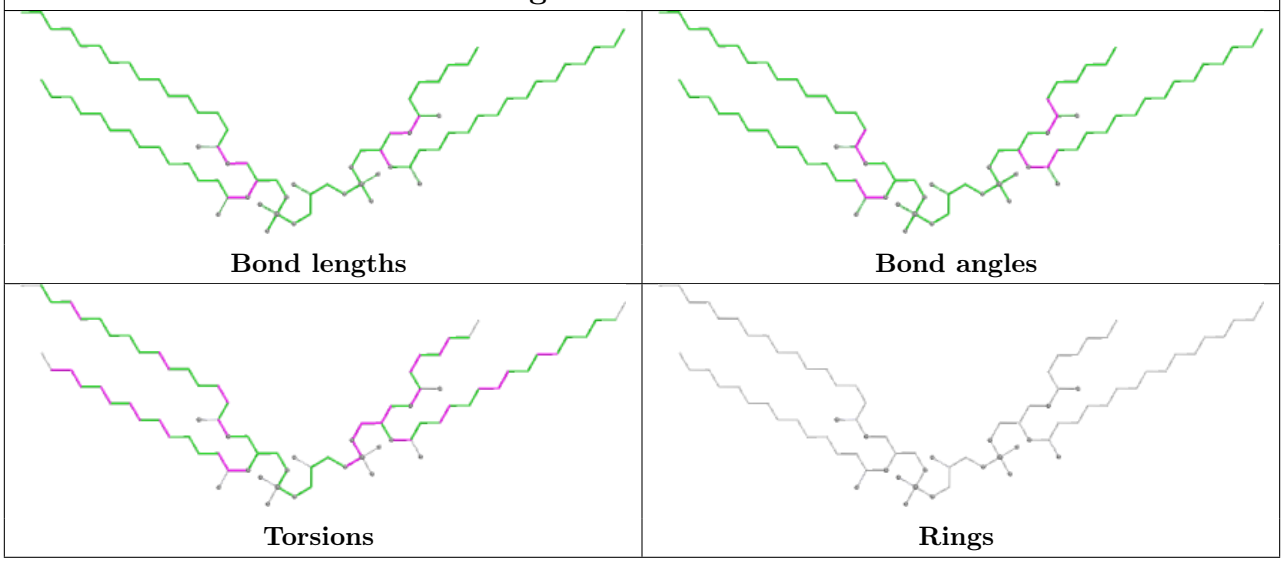

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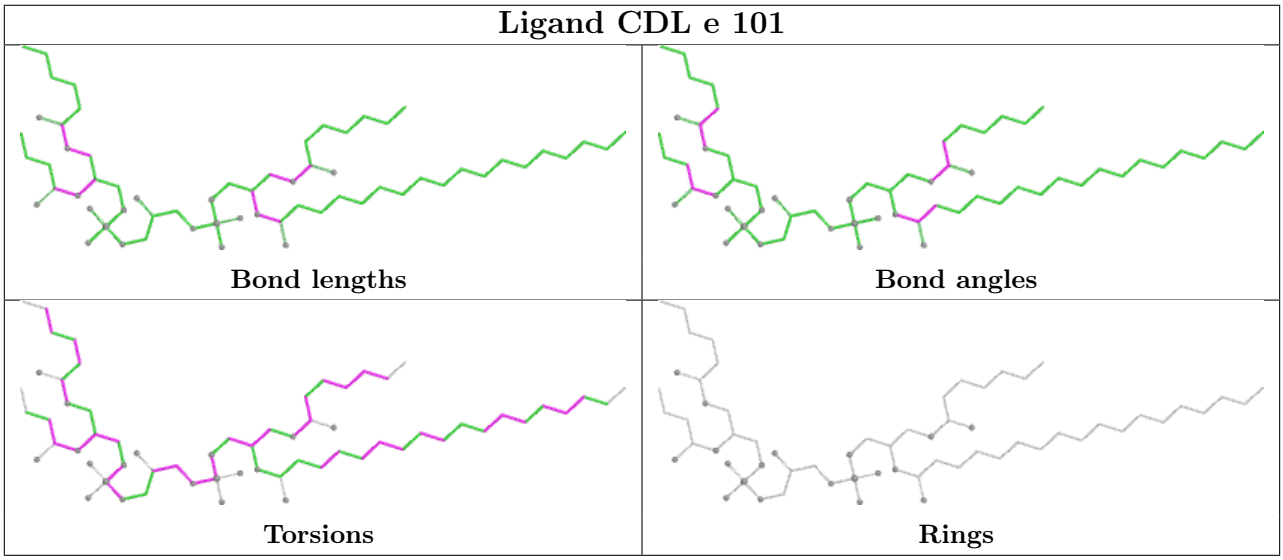

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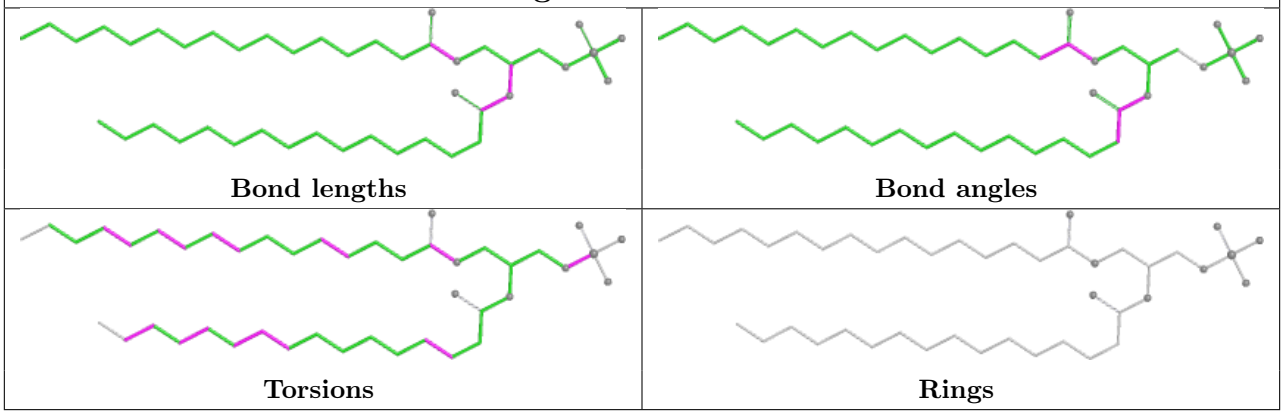

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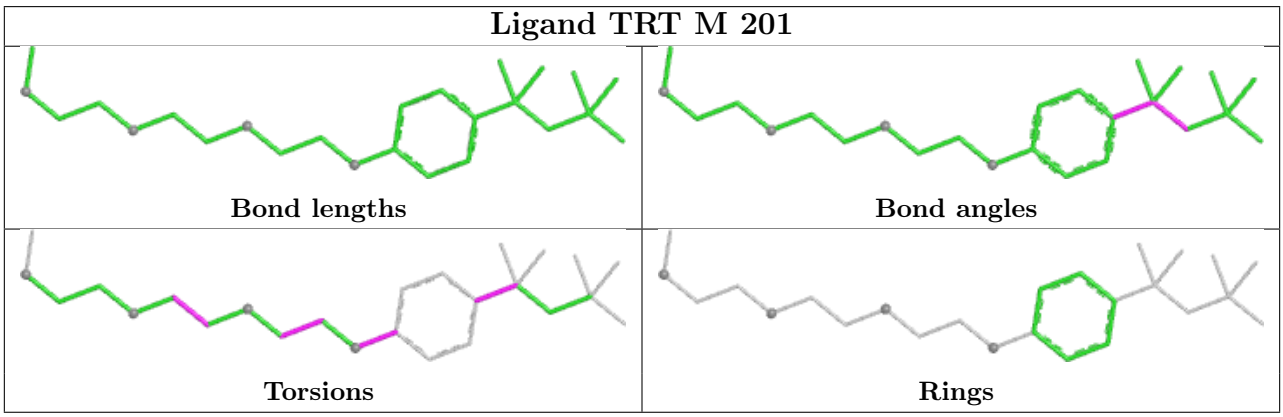

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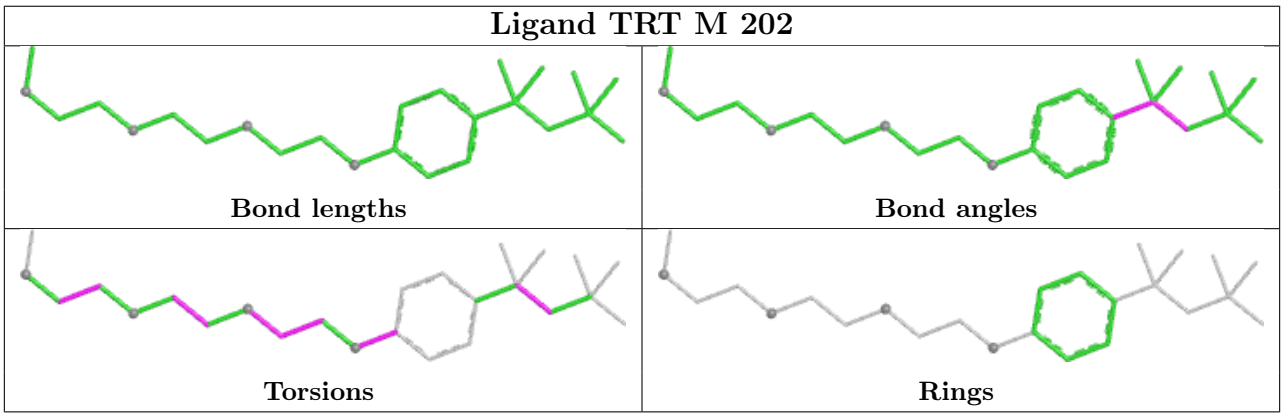

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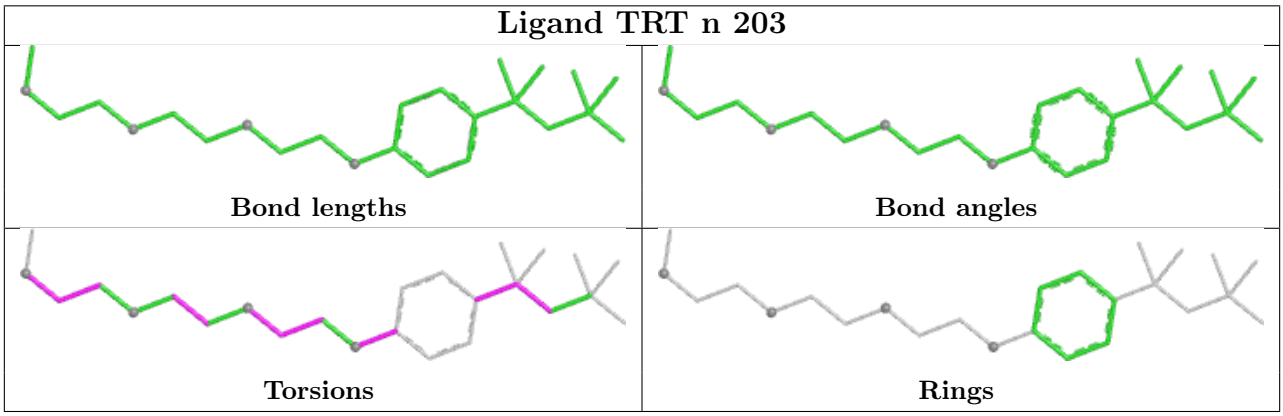

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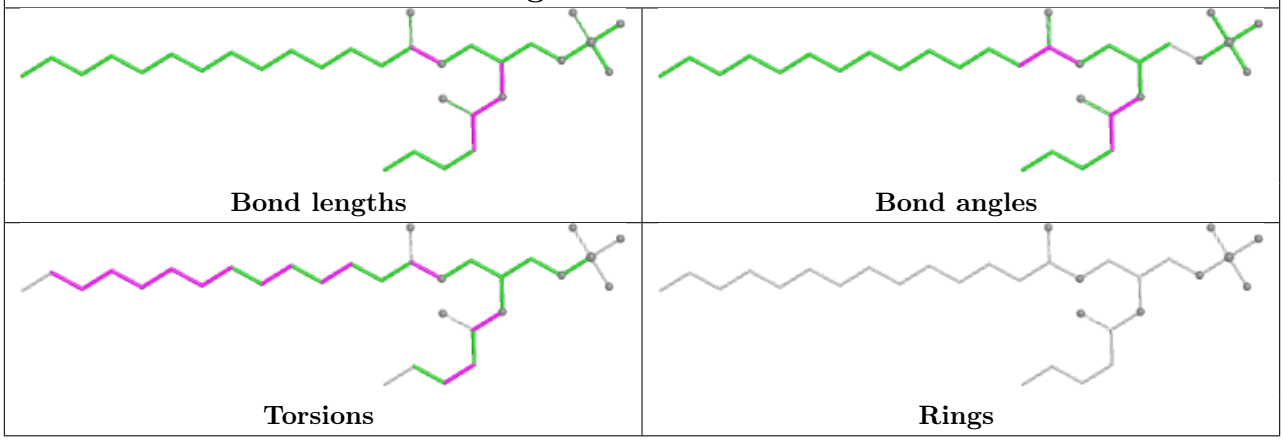

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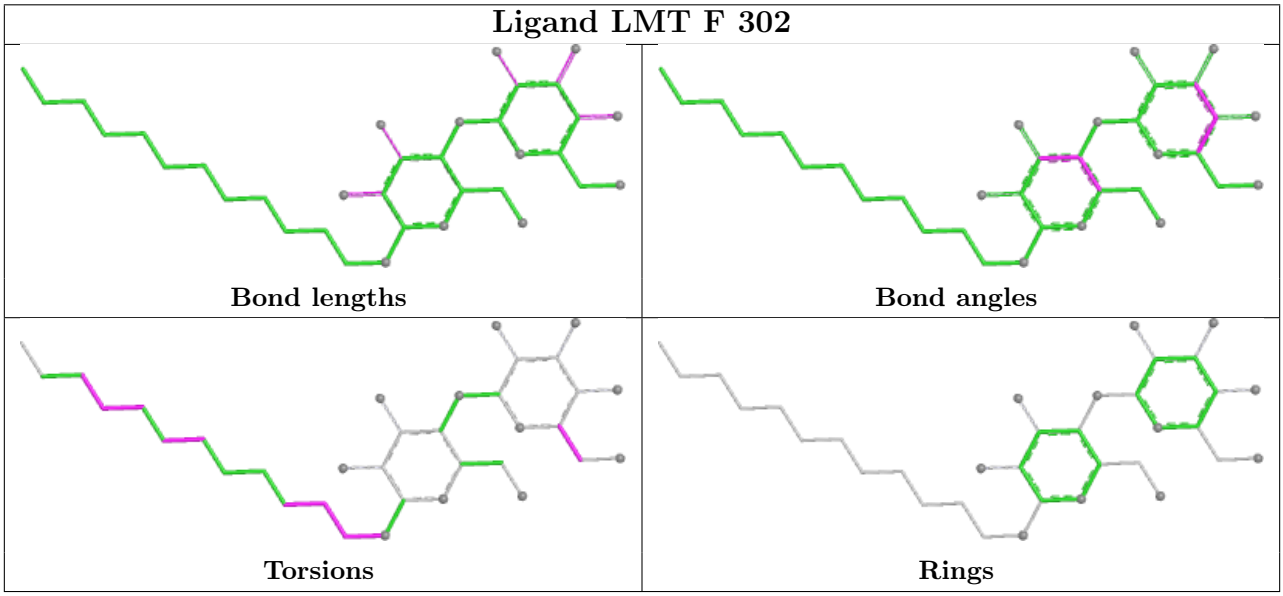

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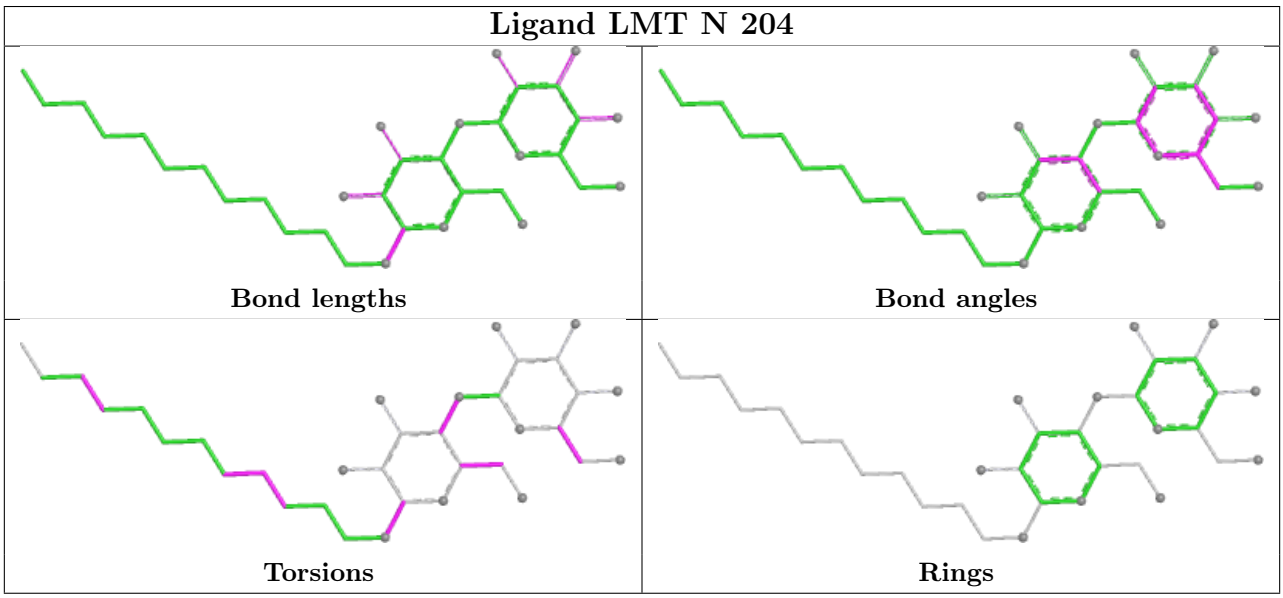

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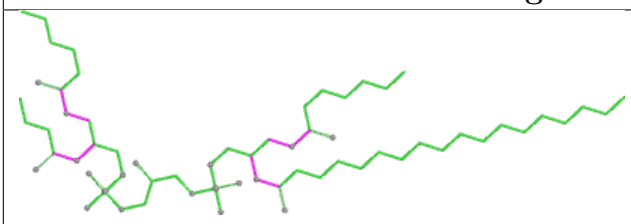

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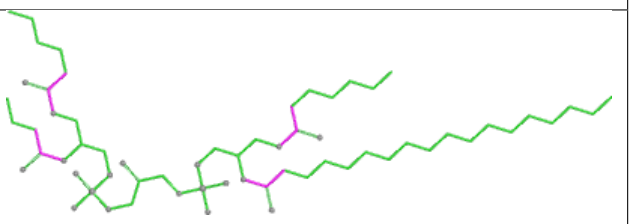
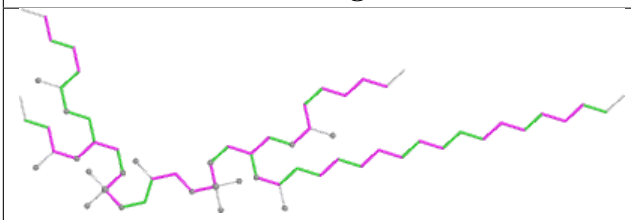
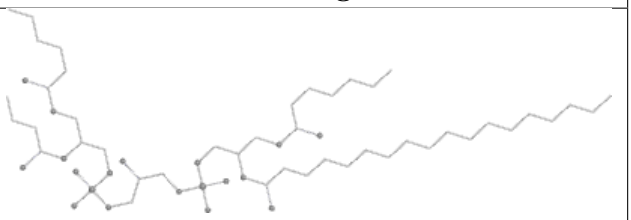


Bond angles

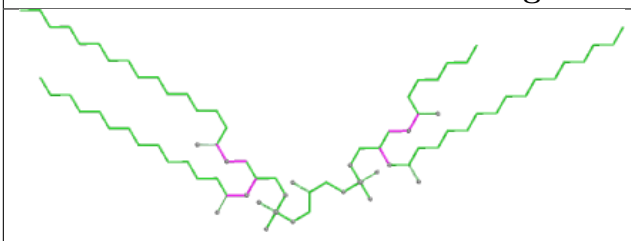


Torsions



Rings

Ligand CDL A 501



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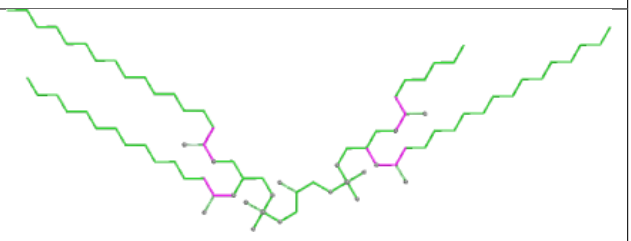

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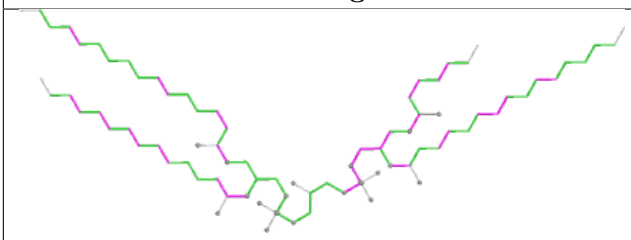

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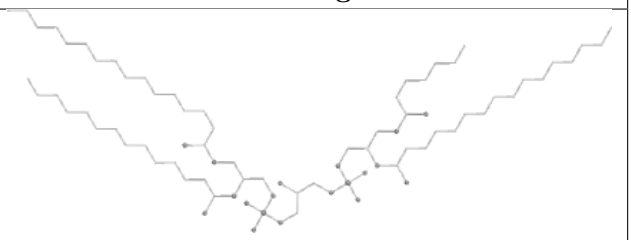

Rings

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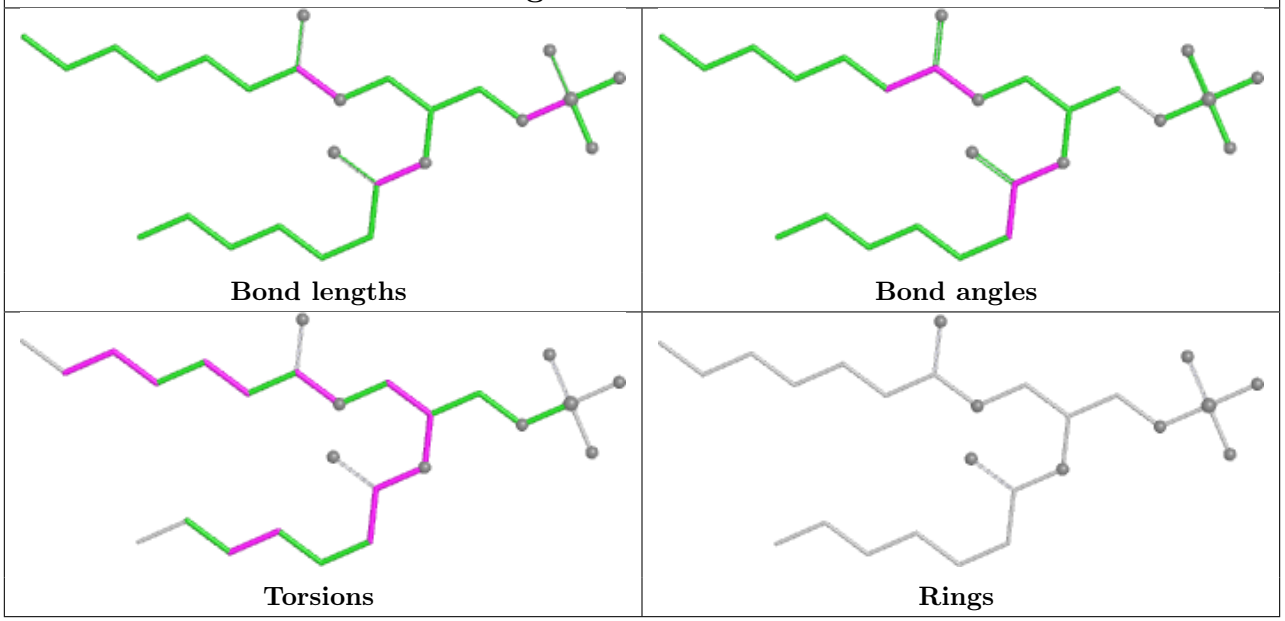
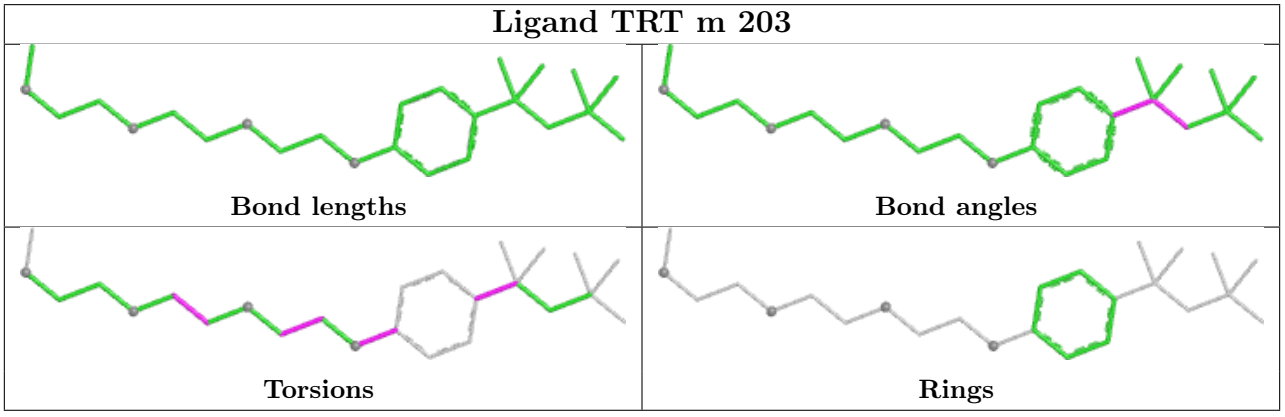


Ligand TRT m 203



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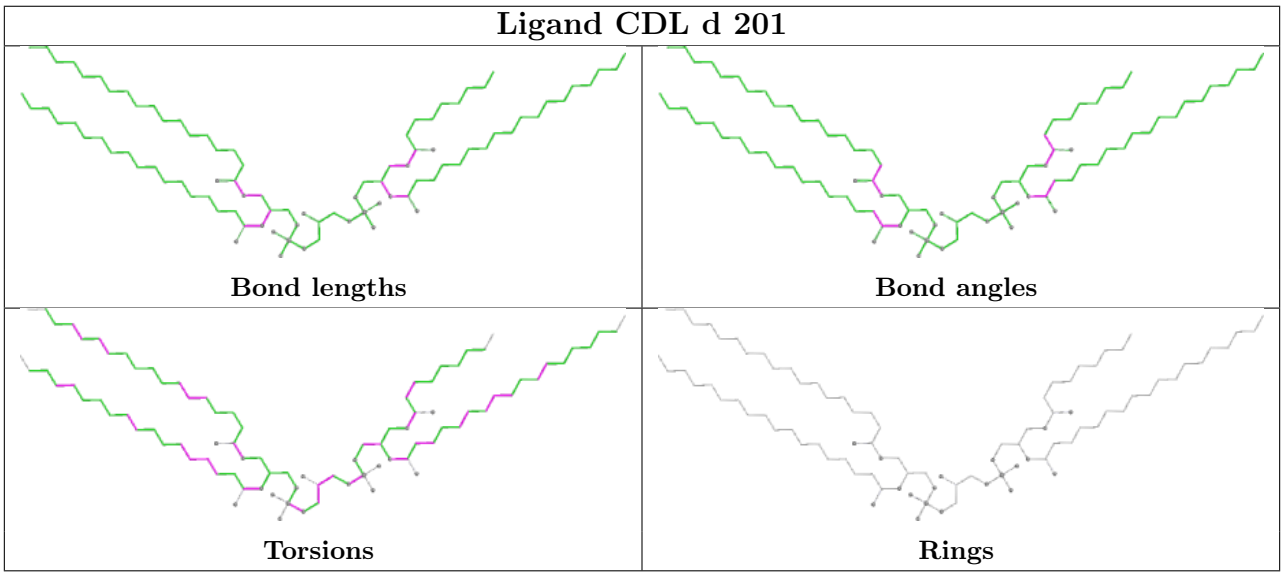
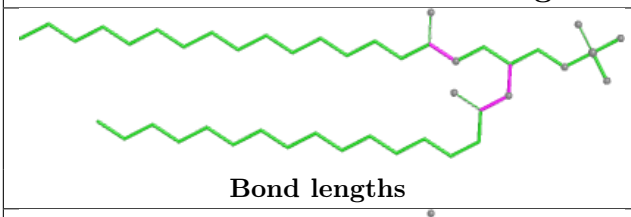
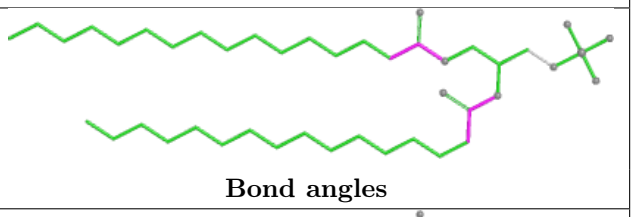


Ligand LPP i 101


Bond lengths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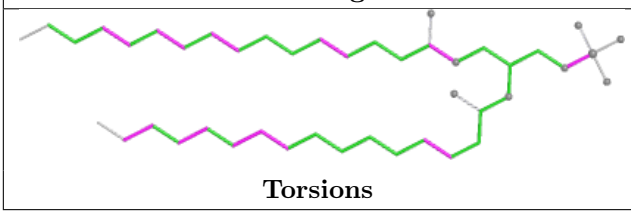
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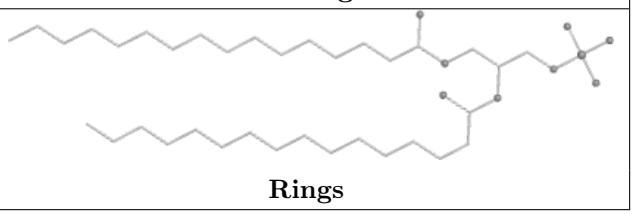
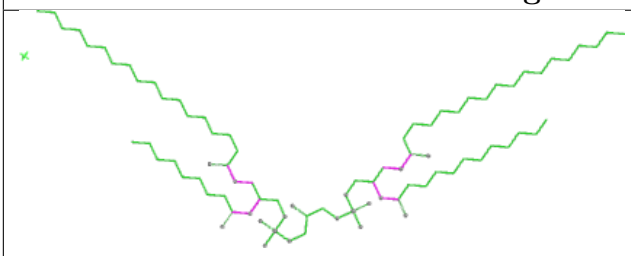

Rings

Ligand CDL D 202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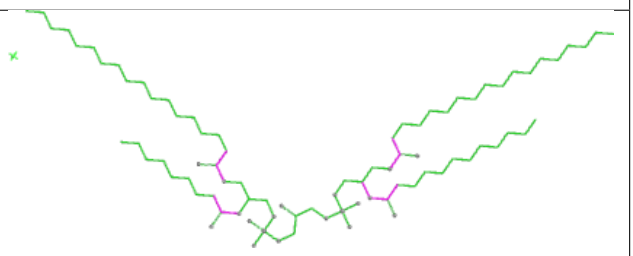
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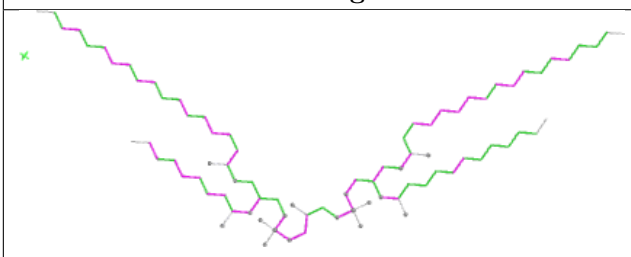
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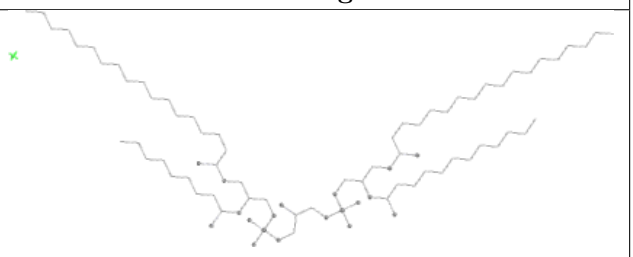
Rings

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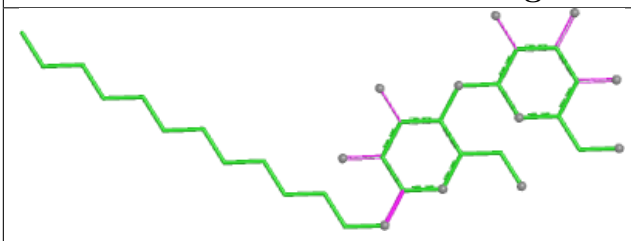
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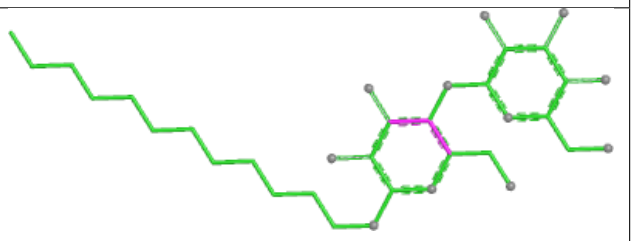
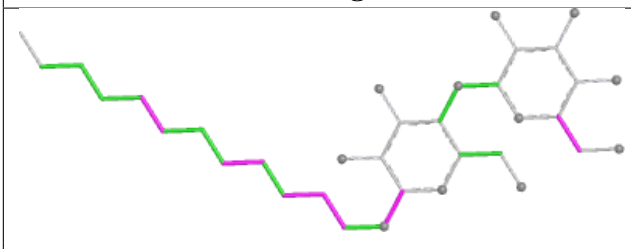

Bond angles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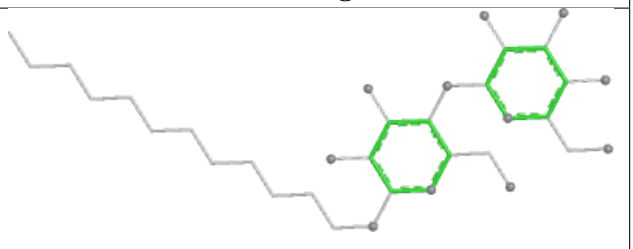
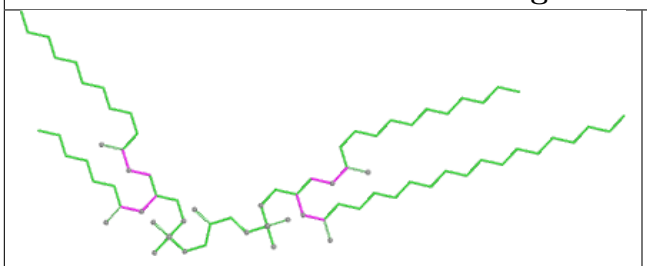

Rings

Ligand CDL r 101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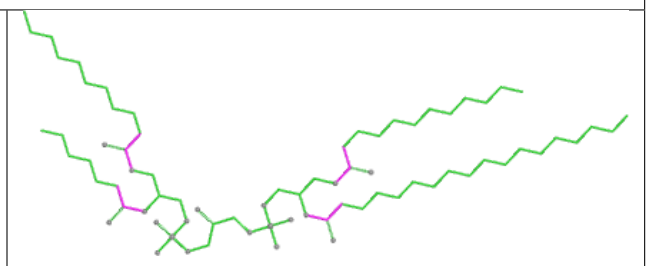
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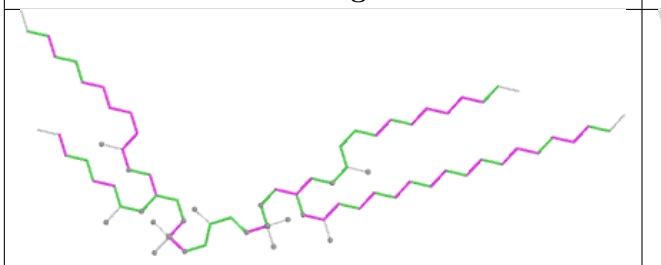
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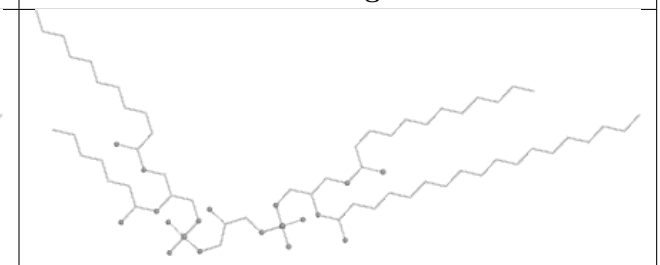
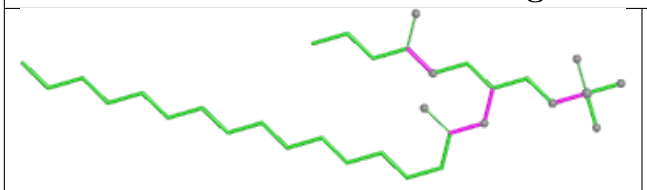

Rings

Ligand LPP O 203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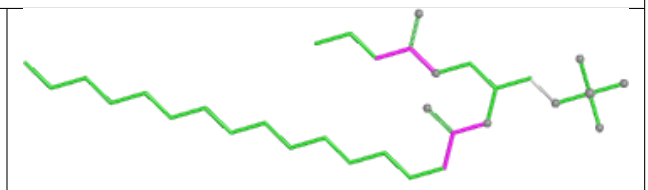
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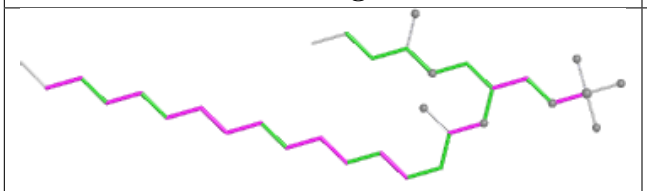
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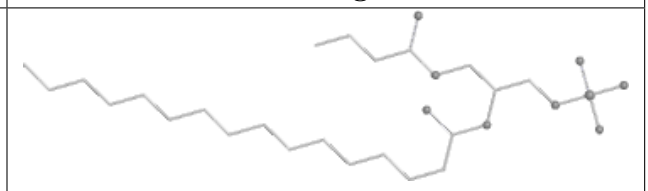
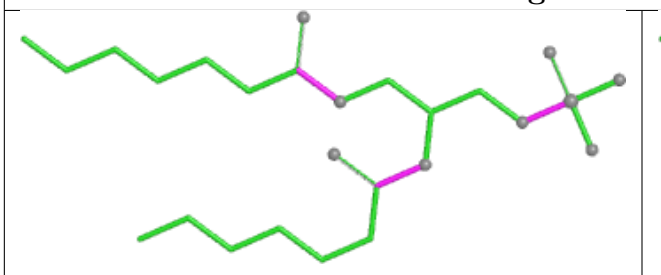

Rings

Ligand LPP P 202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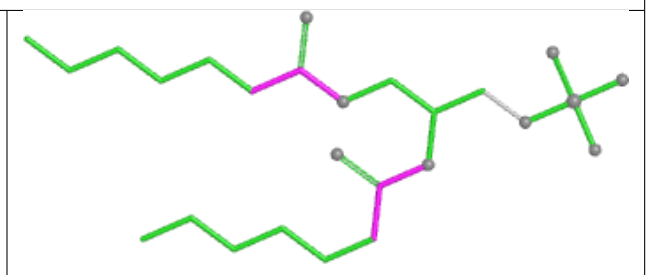
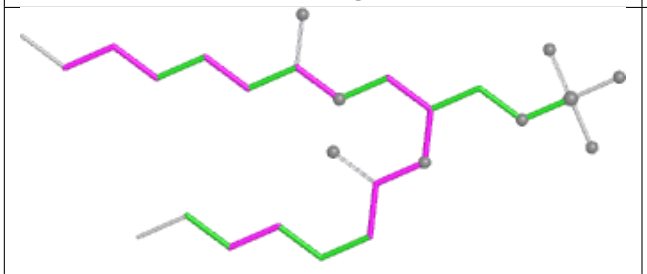

Bond angles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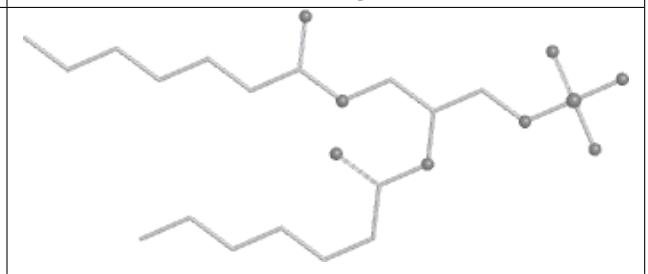
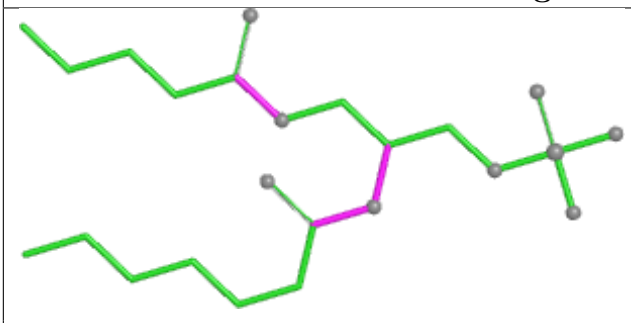

Rings

Ligand LPP f 301



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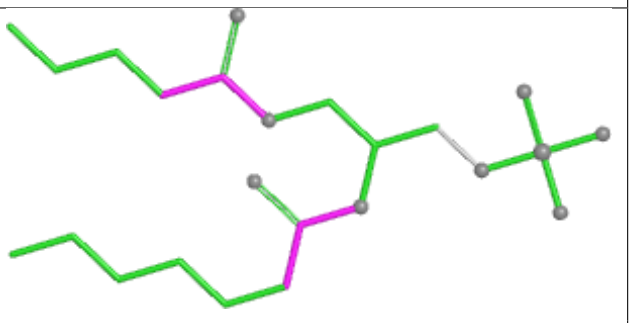
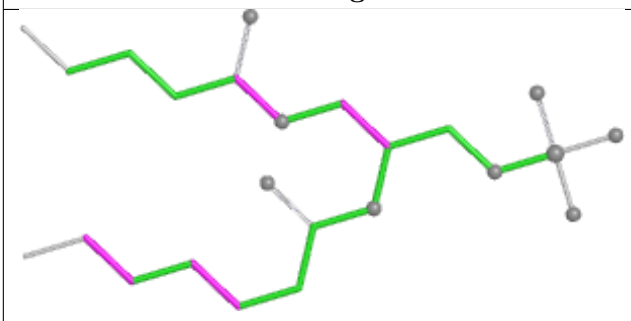


Bond angles



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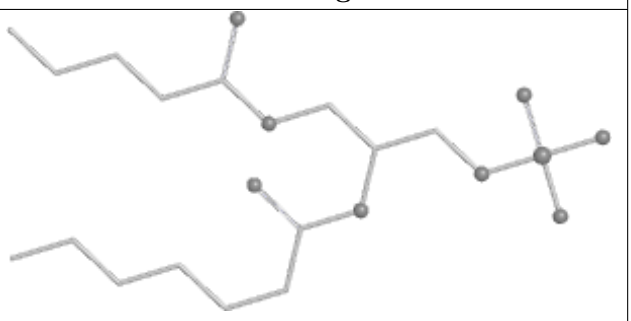
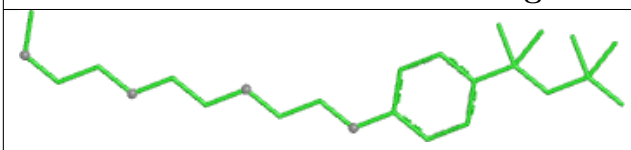


Rings

Ligand TRT R 103



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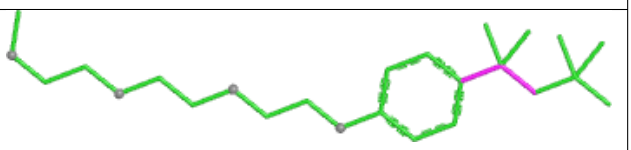
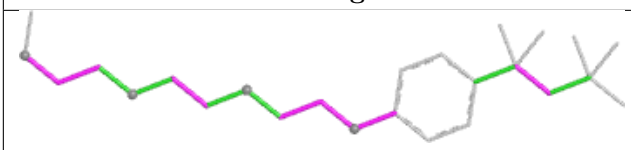


Bond angles



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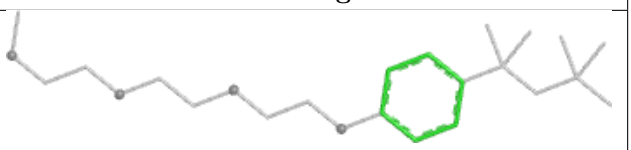
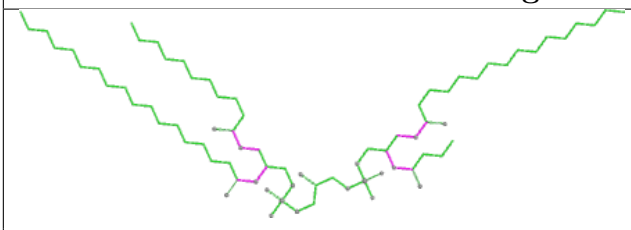
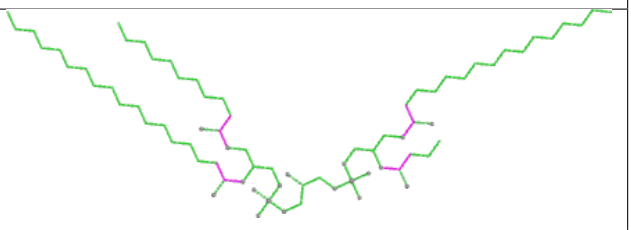


Rings

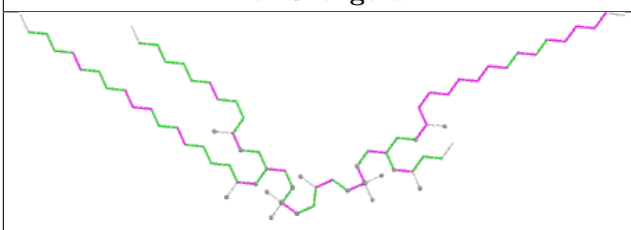
Ligand CDL m 201



Bond lengths



Bond angles



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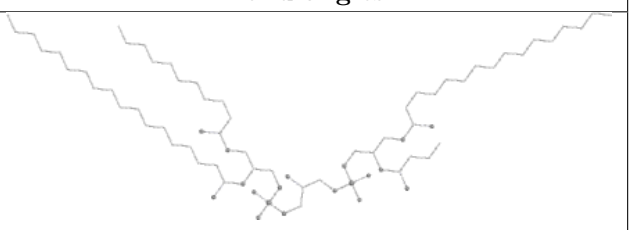
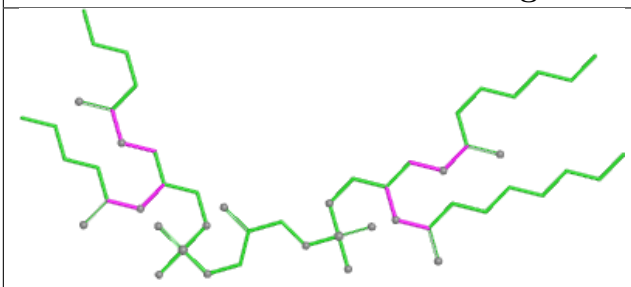


Rings

Ligand CDL M 204



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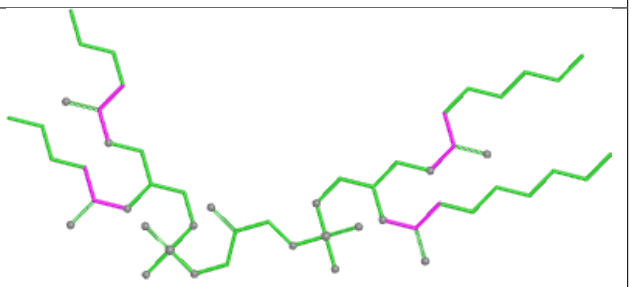

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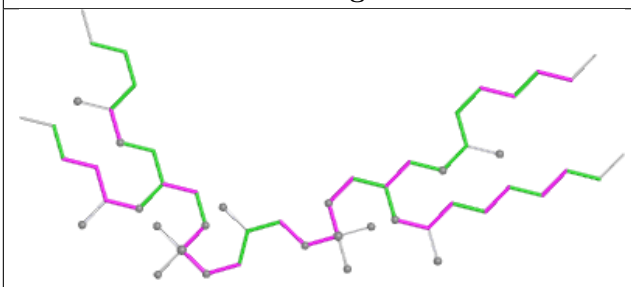

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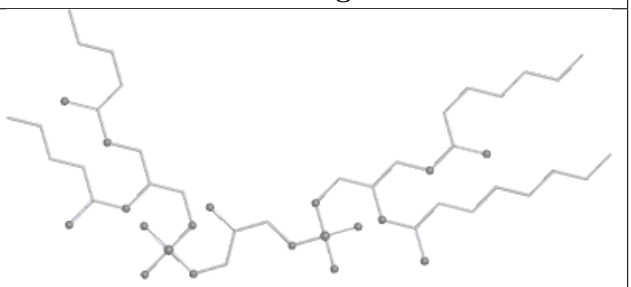
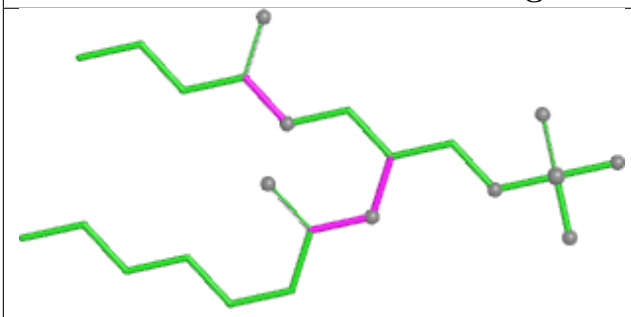


Rings

Ligand LPP O 202



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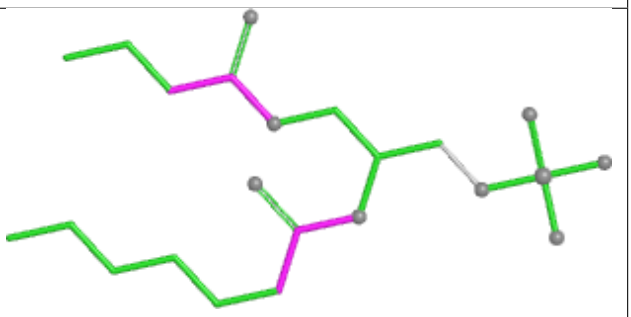
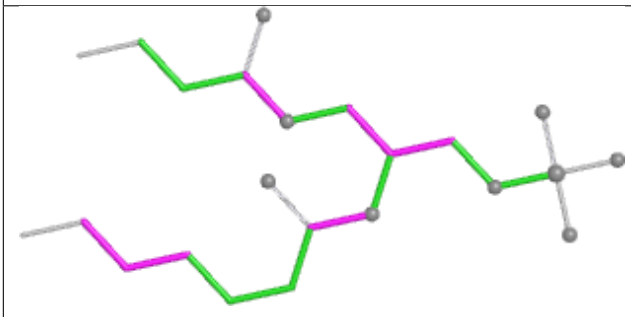


Bond angles



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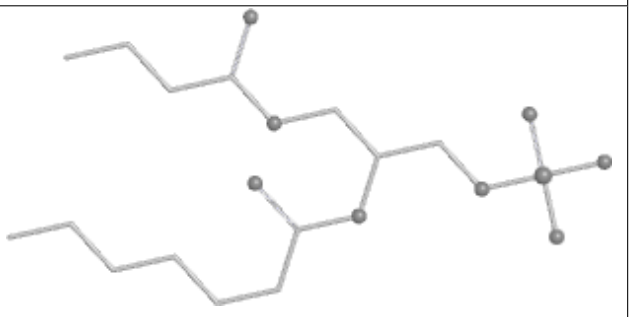
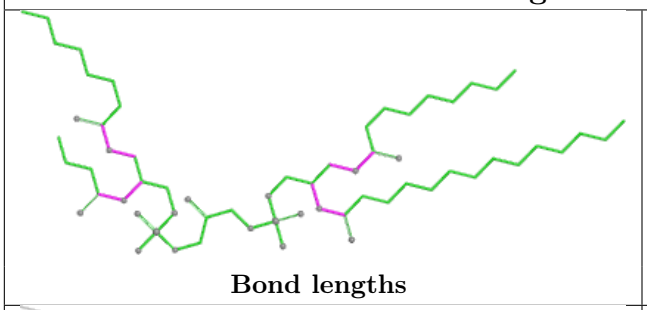
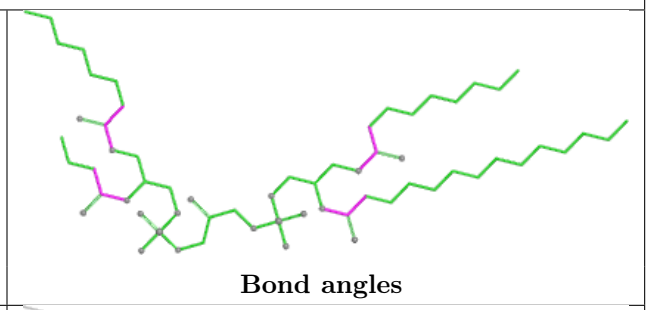


Rings

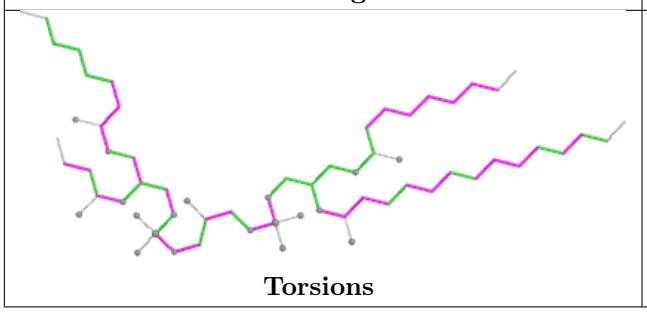
Ligand CDL a 504



Bond lengths



Bond angles



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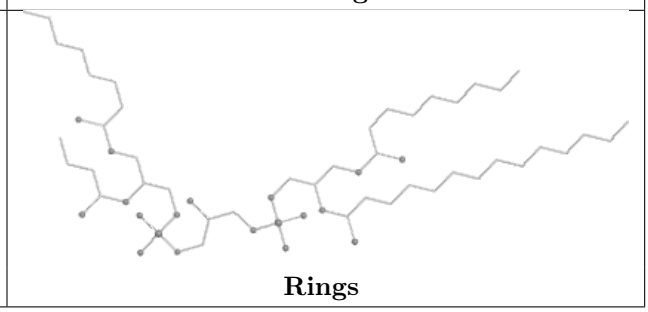
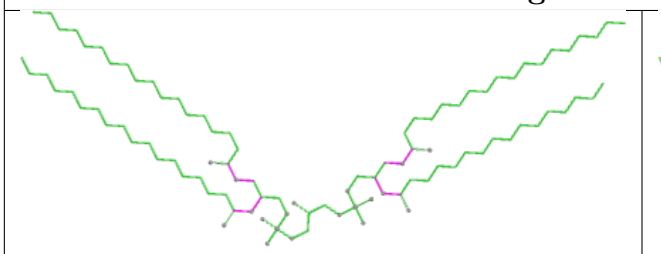


Rings

Ligand CDL p 201



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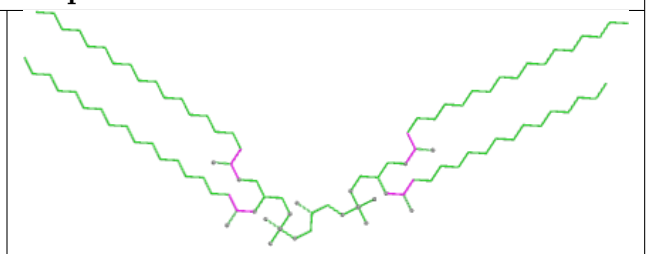
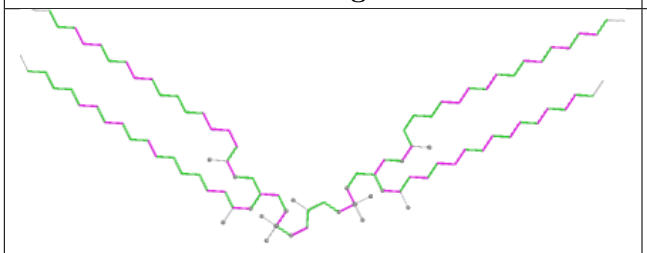


Bond angles



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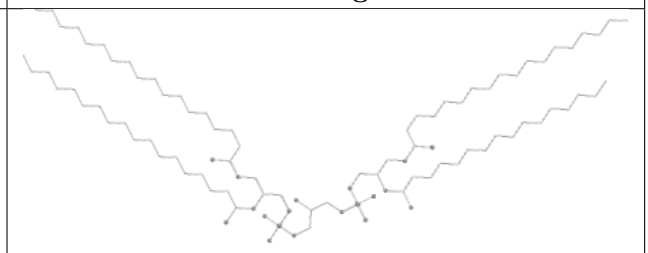
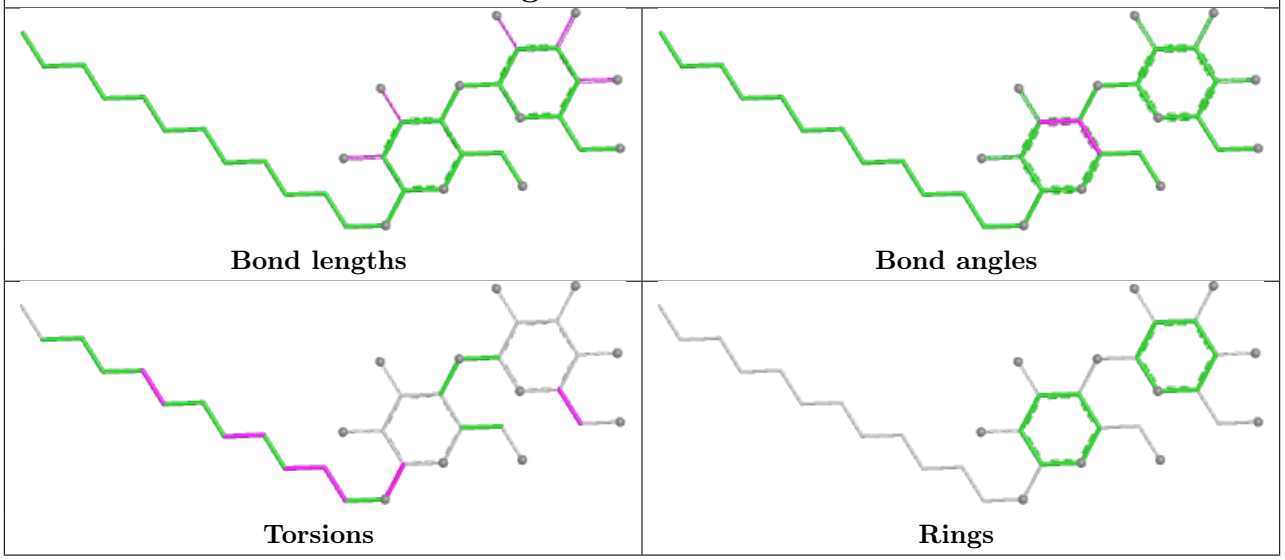
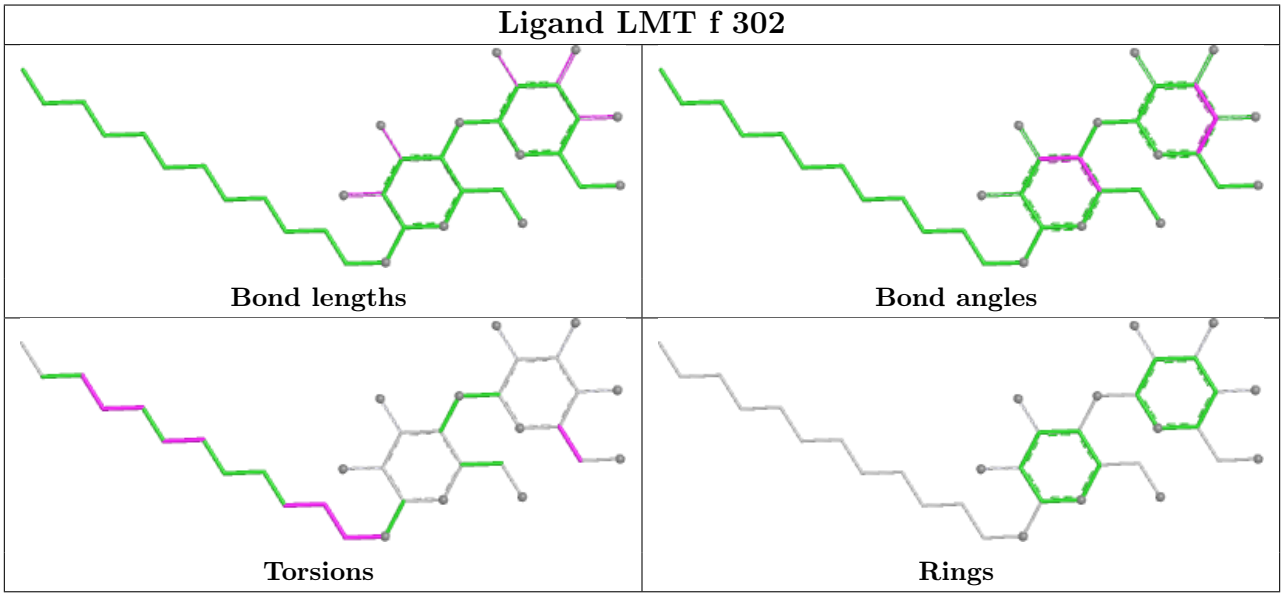


Rings

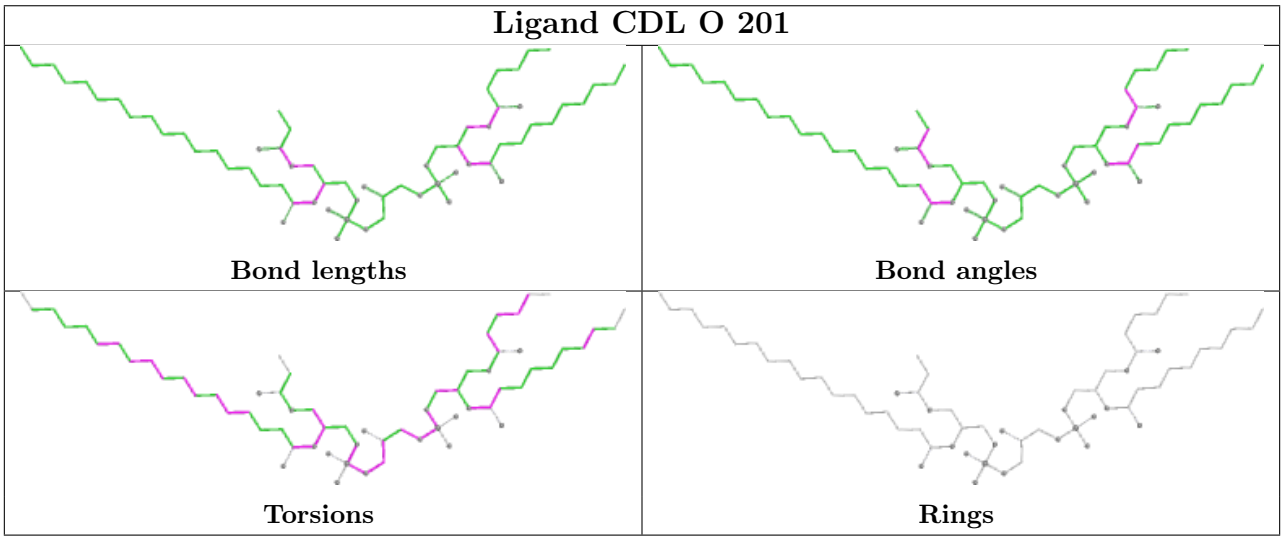
Ligand LMT D 203



Ligand LMT f 302



Ligand CDL O 201



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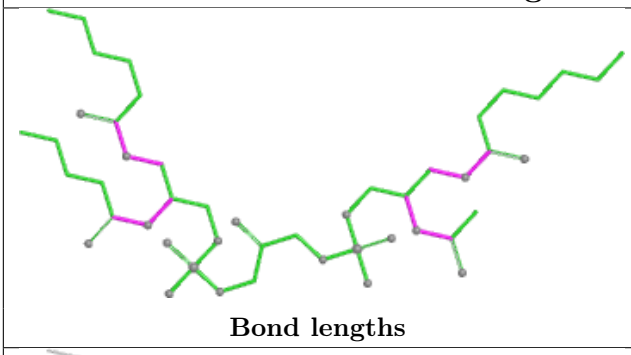
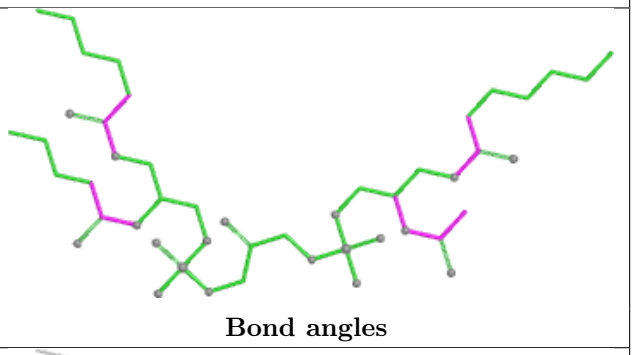
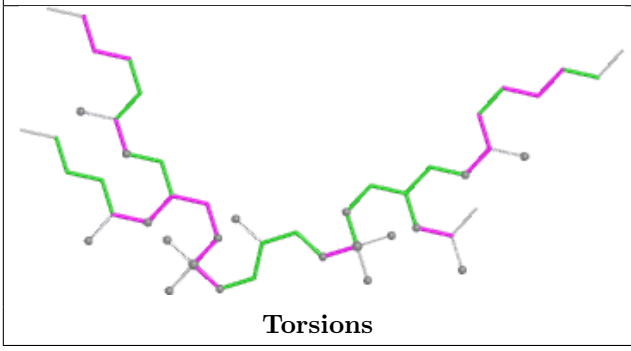


Bond lengths



Bond angles



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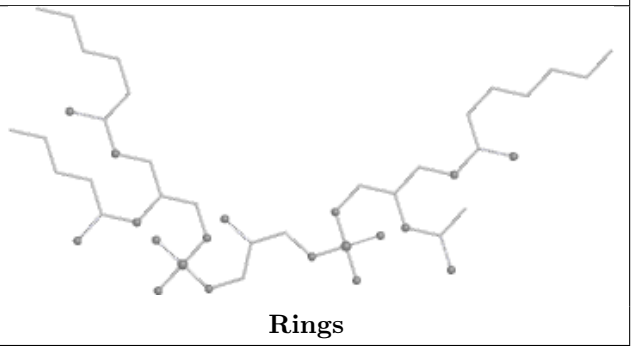


Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

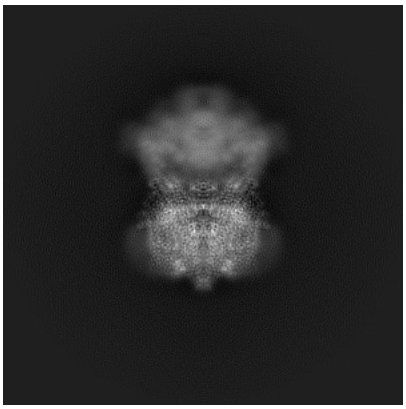
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10468. These allow visual inspection of the internal detail of the map and identification of artifacts.

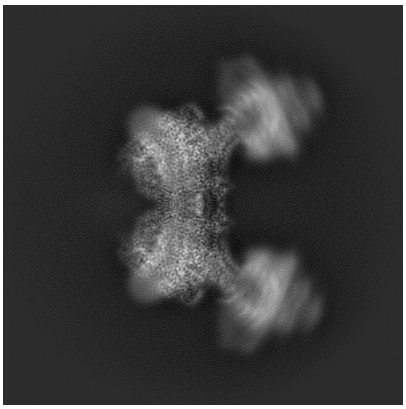
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

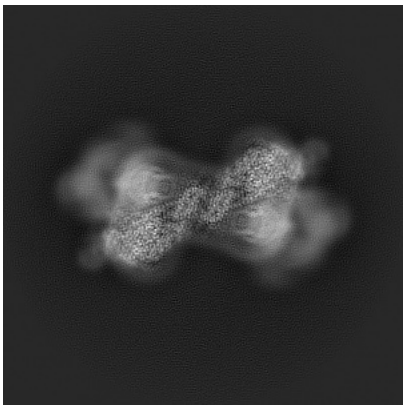
6.1.1 Primary map



X

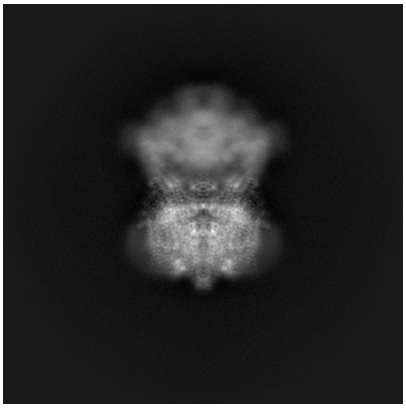


Y

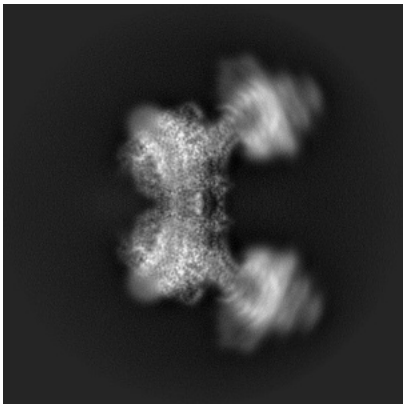


Z

6.1.2 Raw map



X



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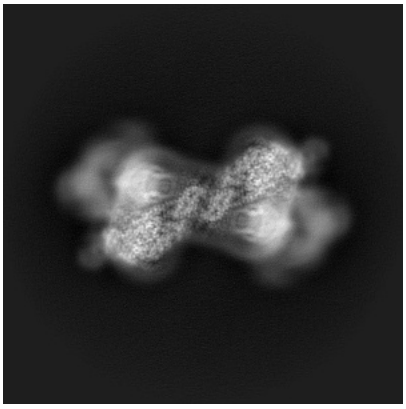
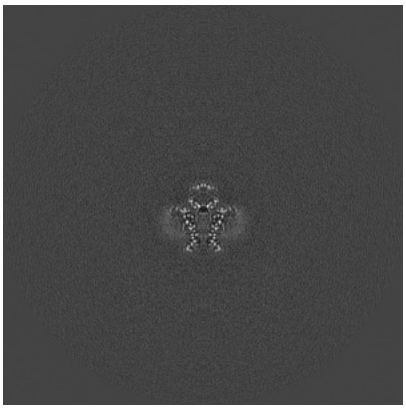


Z

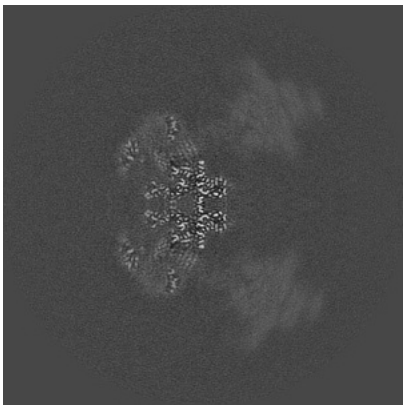
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

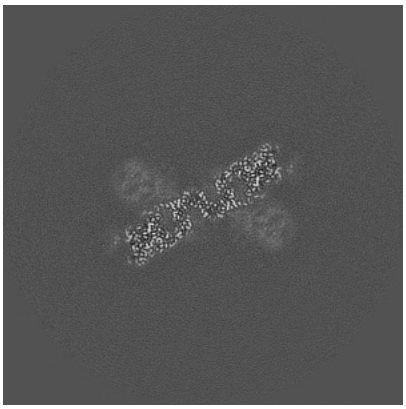
6.2.1 Primary map



X Index: 220

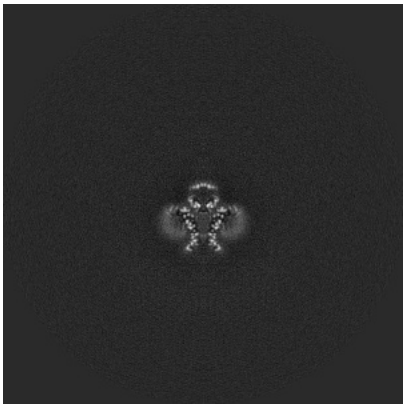


Y Index: 220

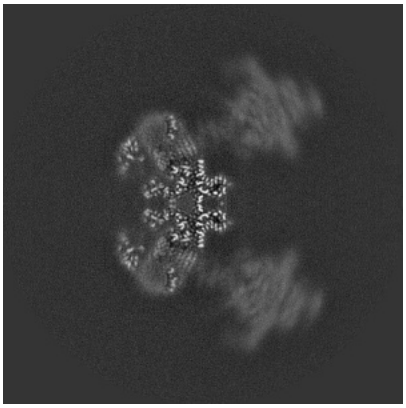


Z Index: 220

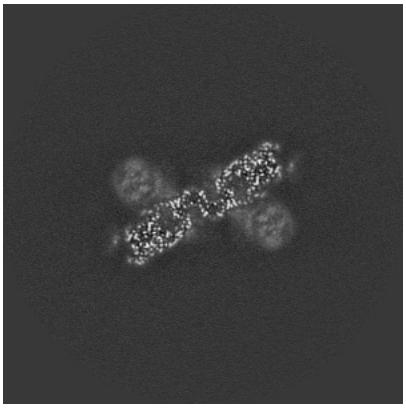
6.2.2 Raw map



X Index: 220



Y Index: 220

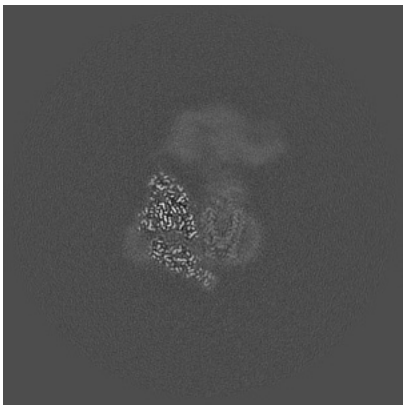


Z Index: 220

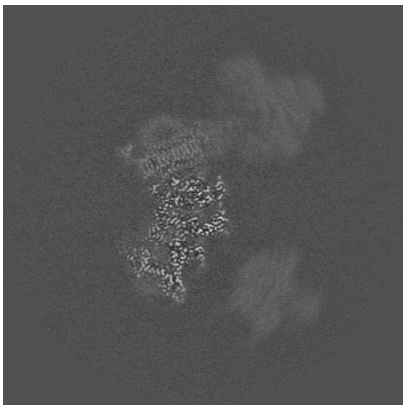
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

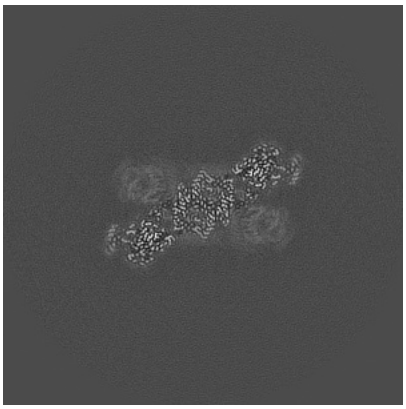
6.3.1 Primary map



X Index: 158

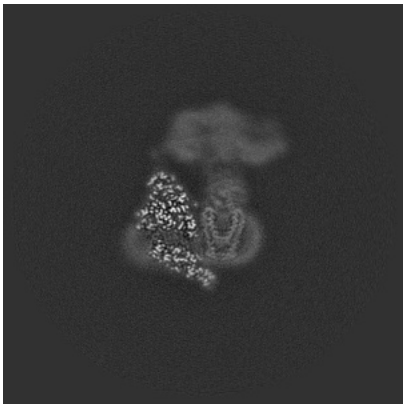


Y Index: 210

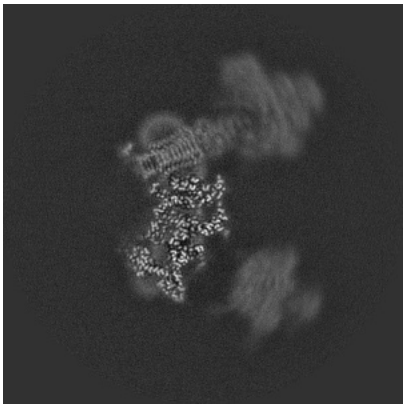


Z Index: 214

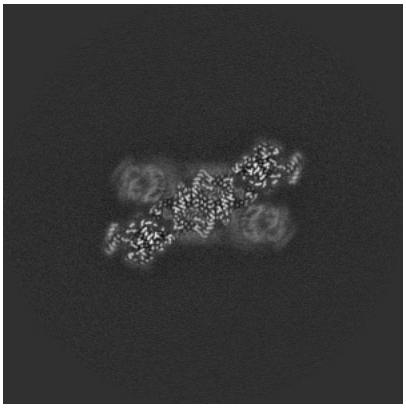
6.3.2 Raw map



X Index: 157



Y Index: 209

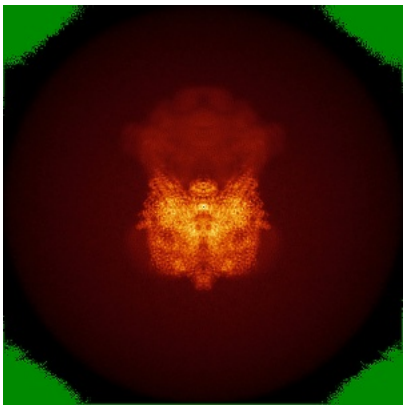


Z Index: 214

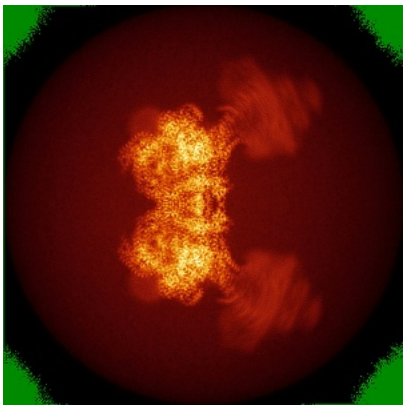
The images above show the largest variance slices of the map in three orthogonal directions.

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

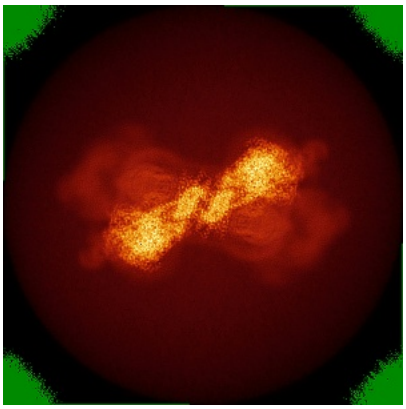
6.4.1 Primary map



X

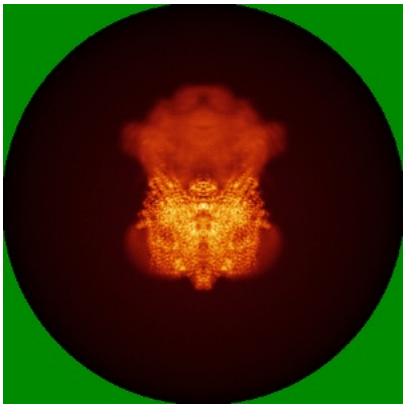


Y

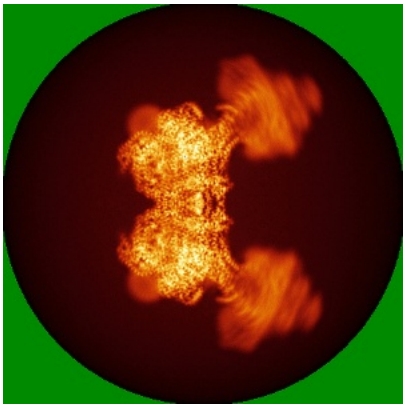


Z

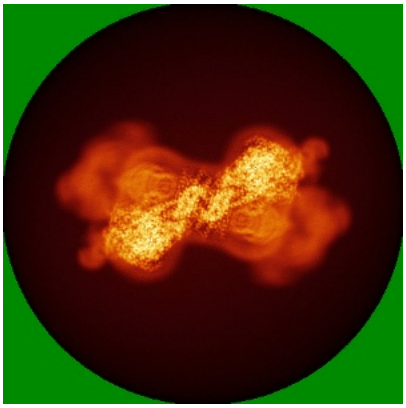
6.4.2 Raw map



X



Y

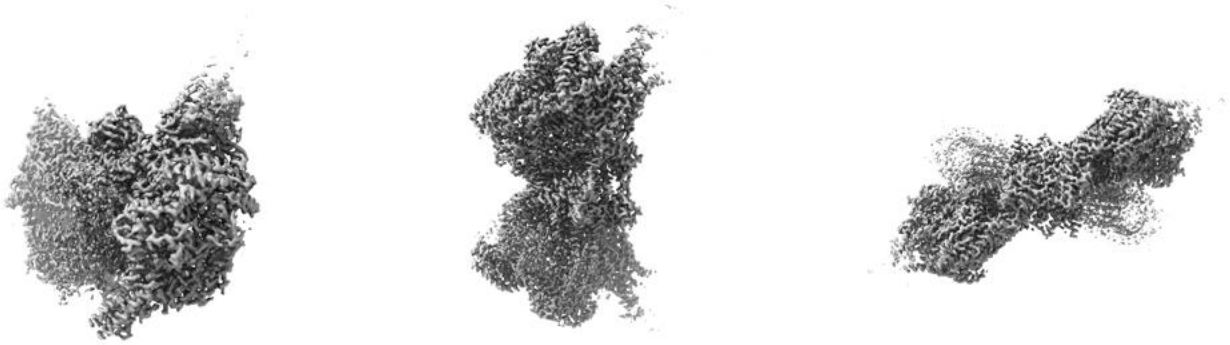


Z

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

6.5 Orthogonal surface views (i)

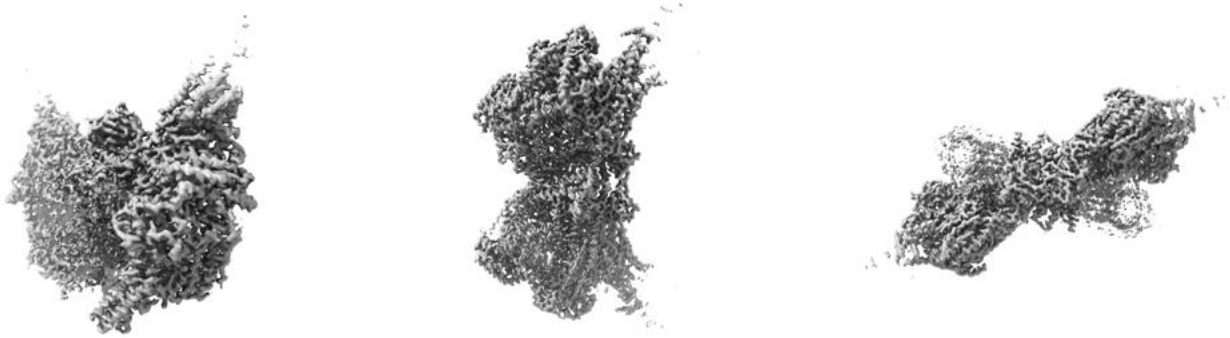
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

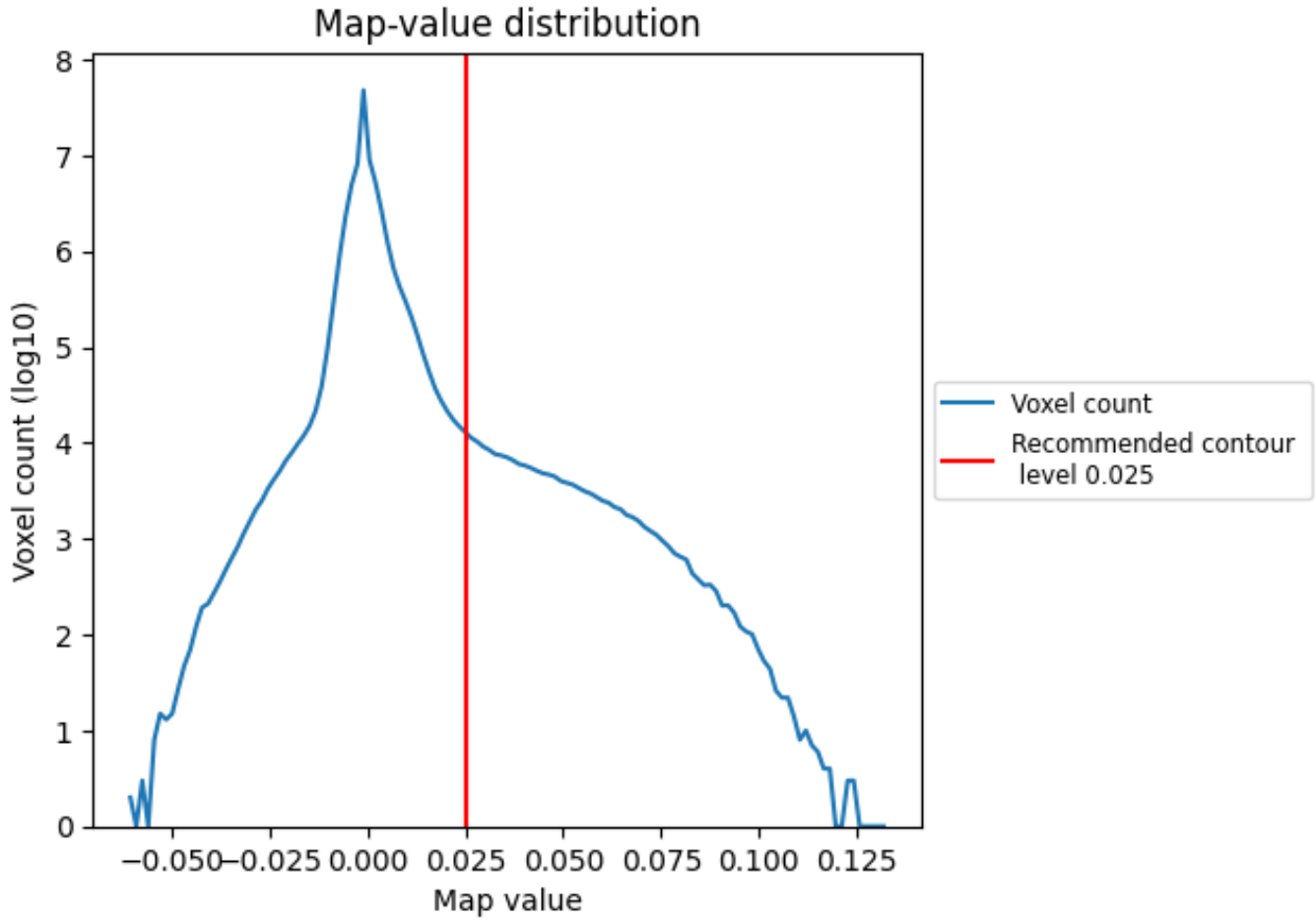
6.6 Mask visualisation (i)

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

7 Map analysis

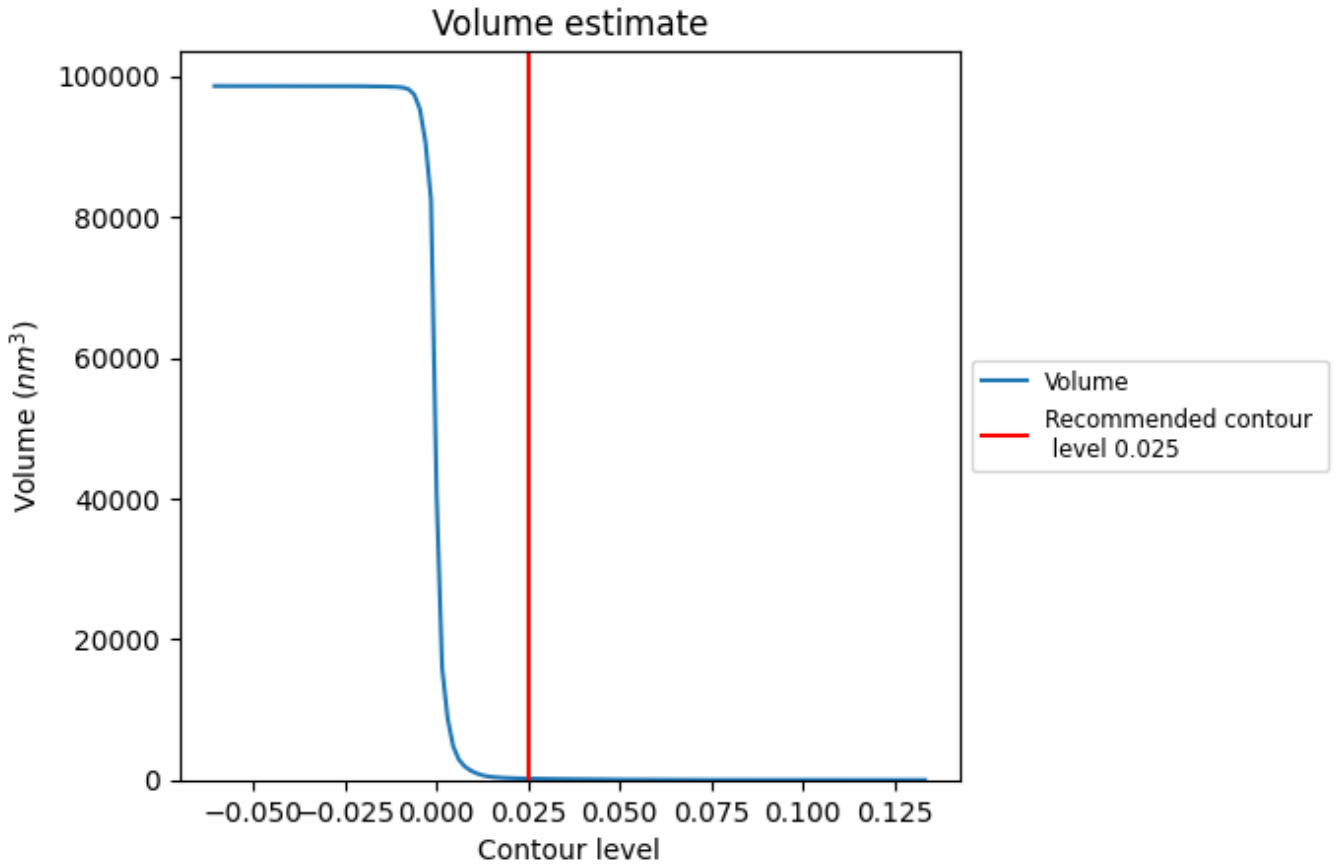
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

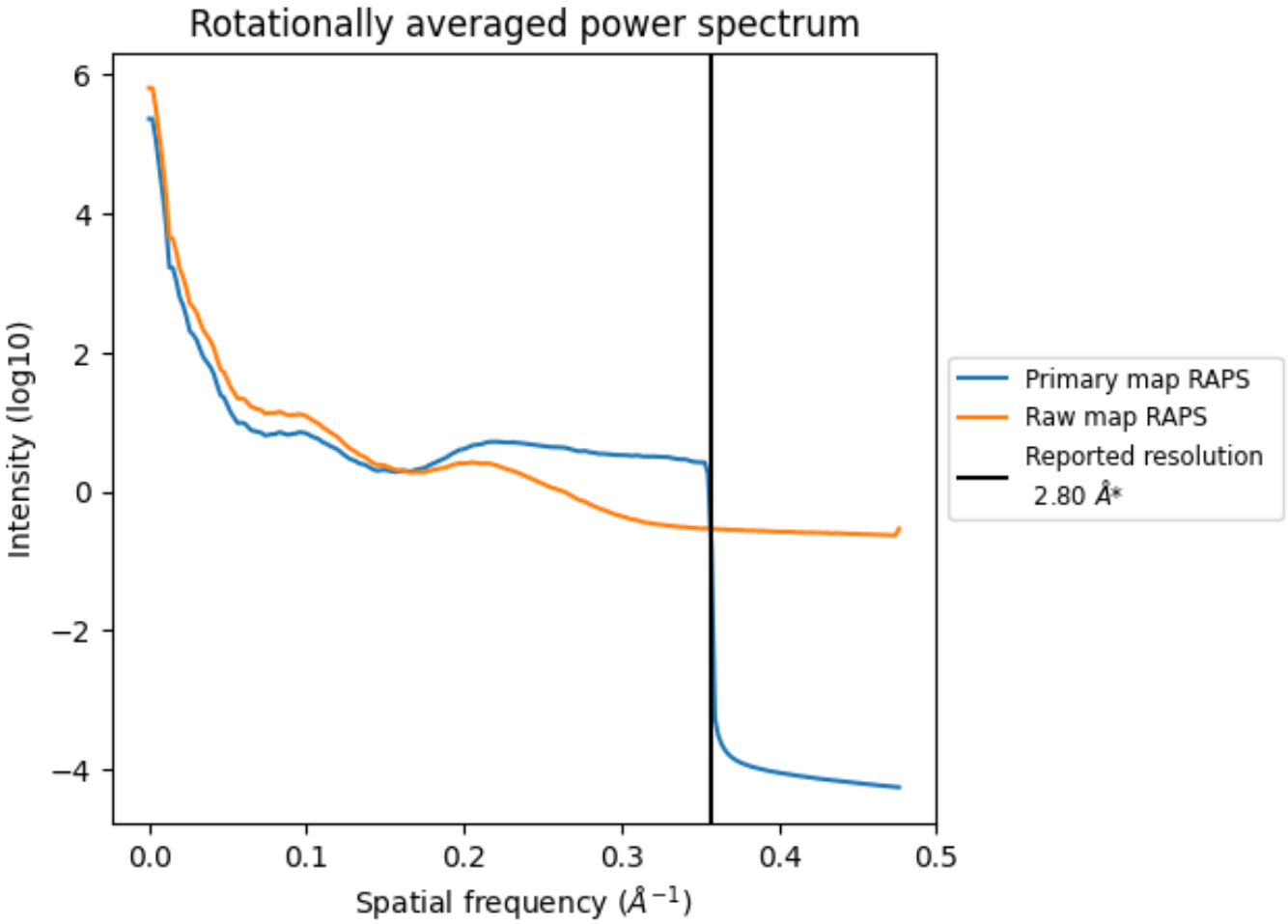
7.2 Volume estimate



The volume at the recommended contour level is 192 nm^3; this corresponds to an approximate mass of 173 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)

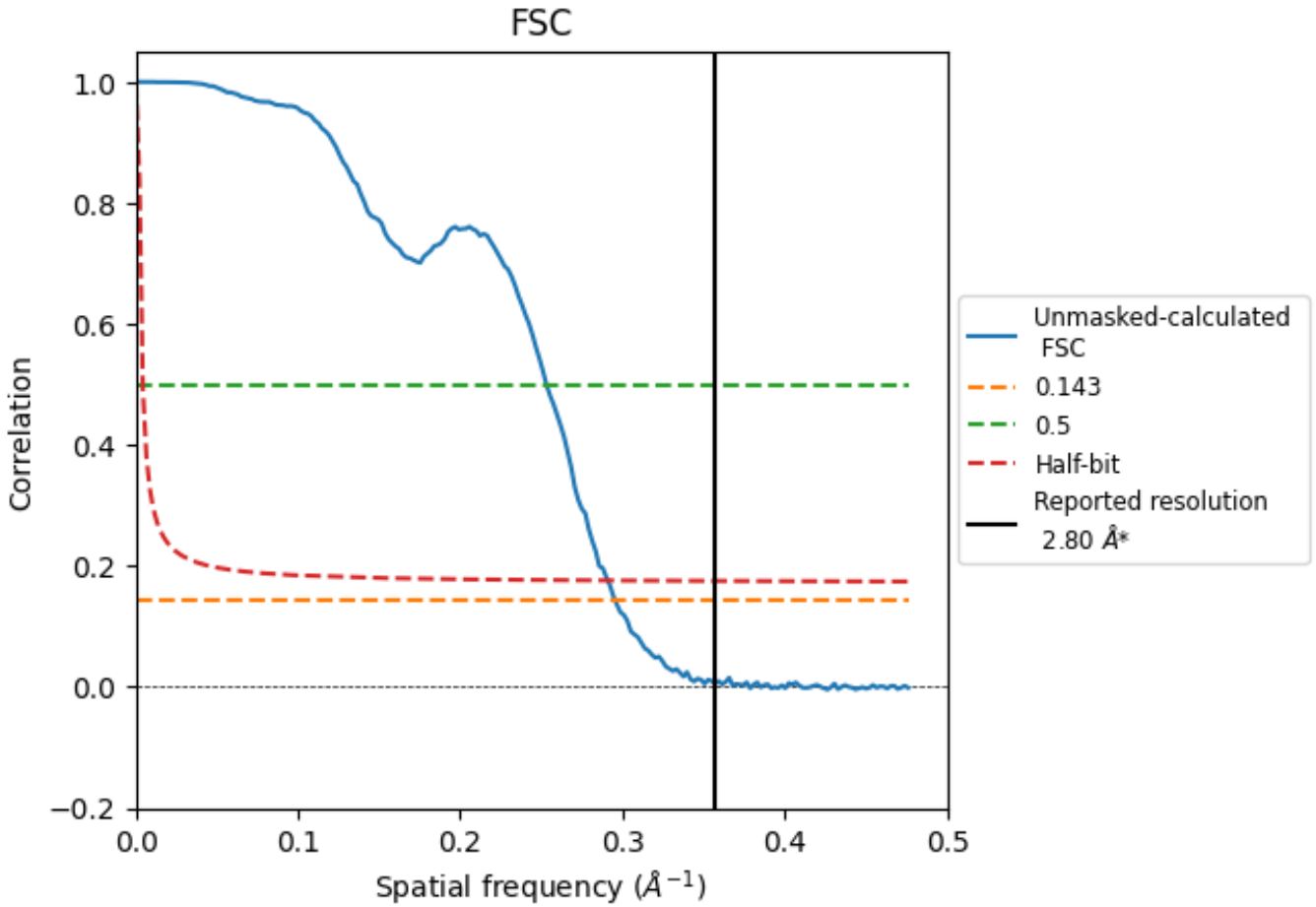


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

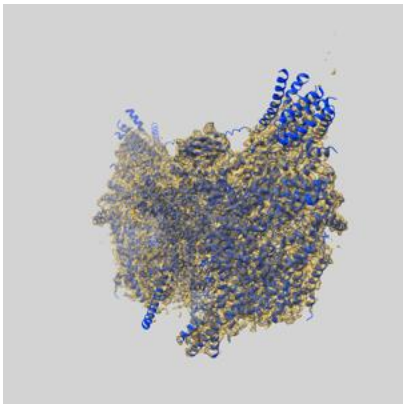
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	3.95	3.44

*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 3.38 differs from the reported value 2.8 by more than 10 %

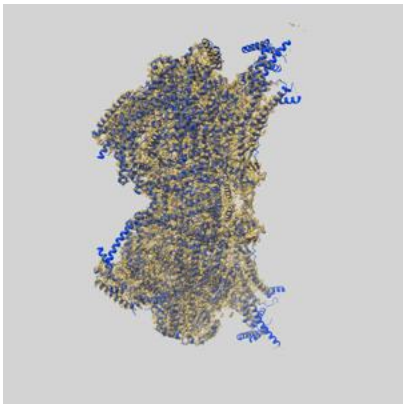
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10468 and PDB model 6TDV. Per-residue inclusion information can be found in section 3 on page 14.

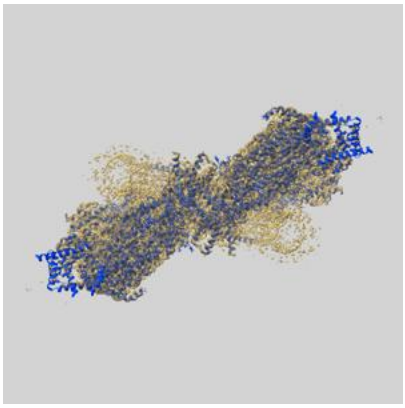
9.1 Map-model overlay



X



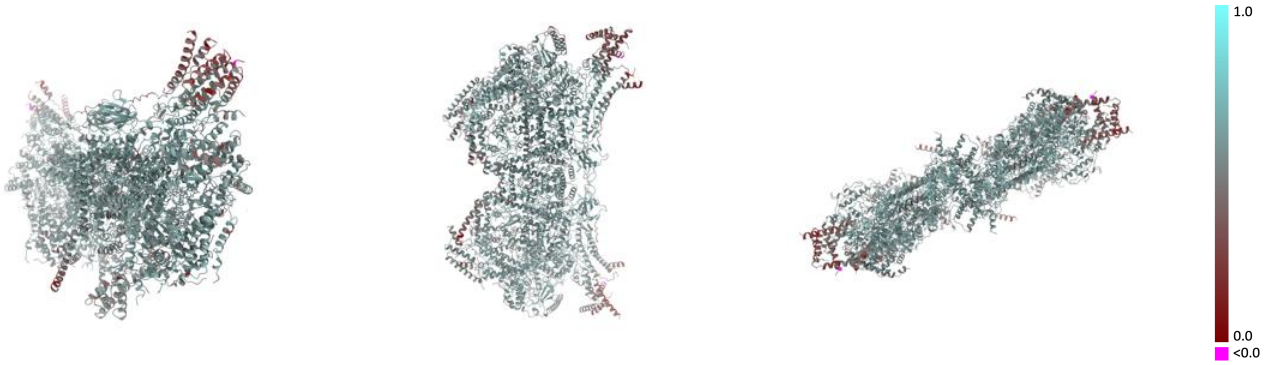
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

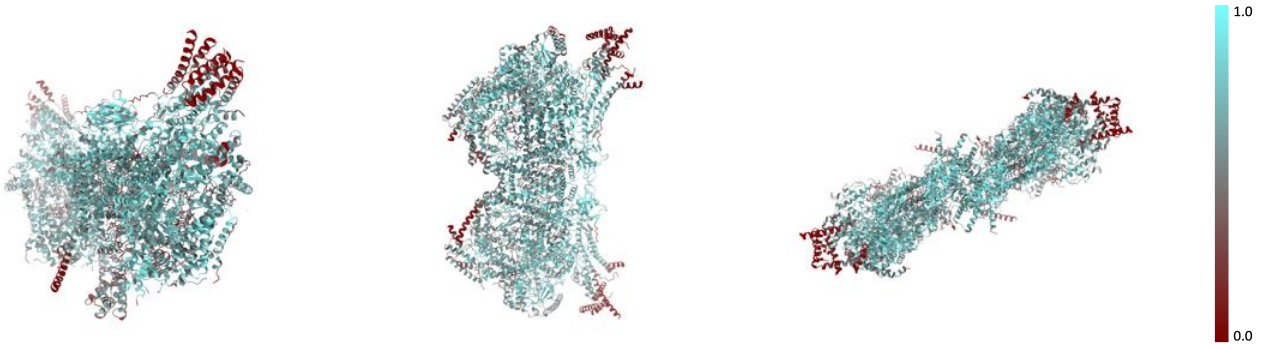
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

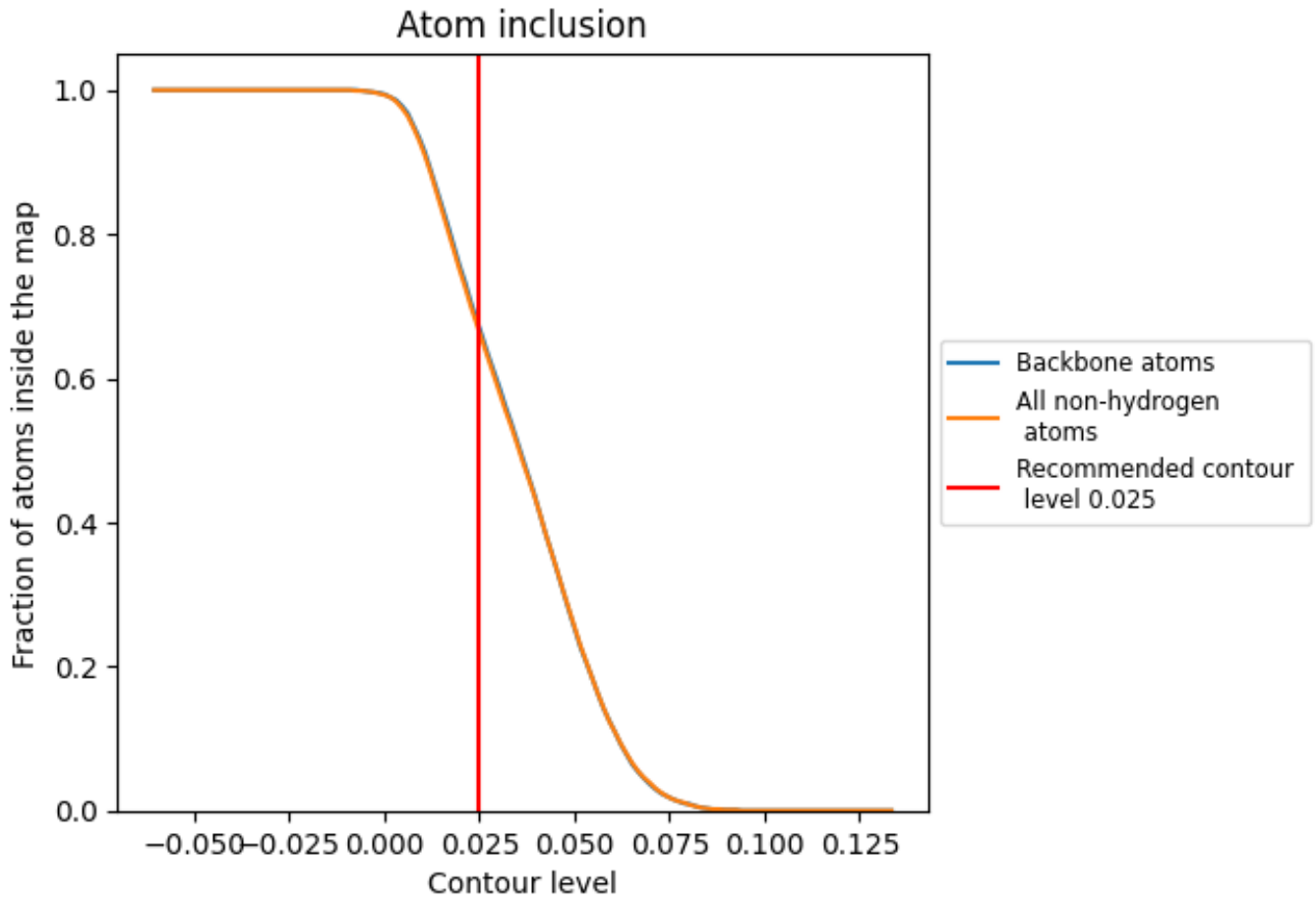
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6640	0.5580
A	0.6970	0.5680
B	0.1210	0.3190
D	0.7070	0.5750
E	0.6790	0.5630
F	0.7500	0.5880
G	0.6710	0.5580
H	0.5710	0.5090
I	0.7140	0.5740
J	0.7450	0.5960
K	0.7150	0.5700
L	0.7070	0.5760
M	0.6170	0.5500
N	0.6530	0.5720
O	0.6210	0.5540
P	0.7080	0.5750
Q	0.5480	0.4960
R	0.6090	0.5520
S	0.7360	0.5960
T	0.7060	0.5710
a	0.6970	0.5700
b	0.1210	0.3130
d	0.7080	0.5750
e	0.6780	0.5630
f	0.7500	0.5880
g	0.6710	0.5580
h	0.5730	0.5080
i	0.7140	0.5770
j	0.7450	0.5930
k	0.7140	0.5740
l	0.7070	0.5750
m	0.6220	0.5480
n	0.6570	0.5760
o	0.6210	0.5540
p	0.6640	0.5740



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
q	0.5480	0.4990
r	0.6090	0.5530
s	0.7340	0.5990
t	0.7120	0.5730