Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:58 pm BST

PDB ID	:	6YNX / pdb_00006ynx
EMDB ID	:	EMD-10859
Title	:	Cryo-EM structure of Tetrahymena thermophila mitochondrial ATP synthase - Fo-subcomplex
Authors	:	Kock Flygaard, R.; Muhleip, A.; Amunts, A.
Deposited on	:	2020-04-14
Resolution	:	2.50 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:

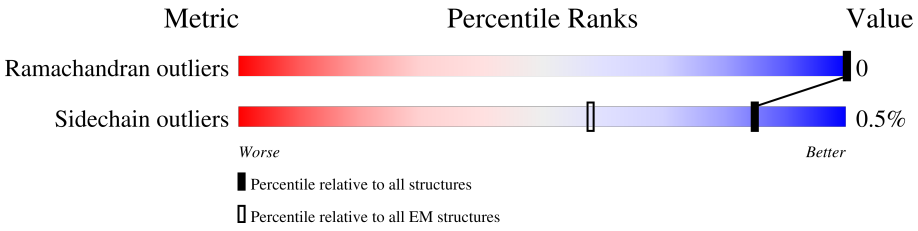
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	446	97%
1	a	446	96%
2	B	381	42% 58%
2	b	381	42% 58%
3	D	234	47% 53%
3	d	234	47% 53%
4	F	204	98%
4	f	204	98%
5	I	209	99%

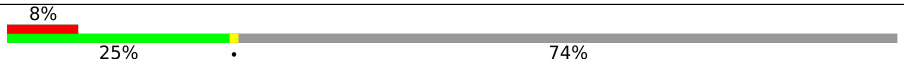
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	i	209	100%
6	K	179	99%
6	k	179	99%
7	C	100	95%
7	c	100	94%
8	G	286	89% 10%
8	g	286	89% 10%
9	H	268	86% 14%
9	h	268	86% 14%
10	J	273	99%
10	j	273	99%
11	L	247	99%
11	l	247	99%
12	M	221	100%
12	m	221	100%
13	N	179	66% 34%
13	n	179	66% 34%
14	O	154	64% 36%
14	o	154	64% 36%
15	P	152	99%
15	p	152	99%
16	Q	152	71% 29%
16	q	152	71% 29%
17	R	149	93% 6%
17	r	149	97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	S	145	
18	s	145	
19	E	480	
19	e	480	
20	i1	108	
20	i2	108	
21	t	460	

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 139915 atoms, of which 70075 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 subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	a	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		
1	A	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		

- Molecule 2 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	161	Total	C	H	N	O	S	0	0
			2678	903	1310	223	232	10		
2	B	161	Total	C	H	N	O	S	0	0
			2675	903	1307	223	232	10		

- Molecule 3 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	110	Total	C	H	N	O	S	0	0
			1764	591	846	147	176	4		
3	D	110	Total	C	H	N	O	S	0	0
			1764	591	846	147	176	4		

- Molecule 4 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	f	200	Total	C	H	N	O	S	0	0
			3373	1095	1691	299	278	10		
4	F	200	Total	C	H	N	O	S	0	0
			3374	1095	1692	299	278	10		

- Molecule 5 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	i	209	Total	C	H	N	O	S	0	0
			3461	1121	1741	304	285	10		
5	I	209	Total	C	H	N	O	S	0	0
			3461	1121	1741	304	285	10		

- Molecule 6 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k	179	Total	C	H	N	O	S	0	0
			2903	939	1430	257	266	11		
6	K	179	Total	C	H	N	O	S	0	0
			2903	939	1430	257	266	11		

- Molecule 7 is a protein called subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	c	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		
7	C	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		

- Molecule 8 is a protein called ATPTT3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	g	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		
8	G	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		

- Molecule 9 is a protein called ATPTT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	h	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		
9	H	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		

- Molecule 10 is a protein called ATPTT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	j	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	269	Total	C	H	N	O	S	0	0
			4344	1381	2145	406	404	8		

- Molecule 11 is a protein called ATPTT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	l	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	L	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		

- Molecule 12 is a protein called ATPTT7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	m	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	M	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		

- Molecule 13 is a protein called ATPTT8.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	n	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	N	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		

- Molecule 14 is a protein called ATPTT9.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	o	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		
14	O	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		

- Molecule 15 is a protein called ATPTT10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	P	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		

- Molecule 16 is a protein called ATPTT11.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	Q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		

- Molecule 17 is a protein called ATPTT12.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	r	145	Total	C	H	N	O	S	0	0
			2373	776	1180	201	212	4		
17	R	140	Total	C	H	N	O	S	0	0
			2288	750	1134	194	206	4		

- Molecule 18 is a protein called ATPTT13.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	s	105	Total	C	H	N	O	S	0	0
			1714	552	849	148	160	5		
18	S	106	Total	C	H	N	O	S	0	0
			1728	556	856	149	162	5		

- Molecule 19 is a protein called ATPTT1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	e	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	E	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		

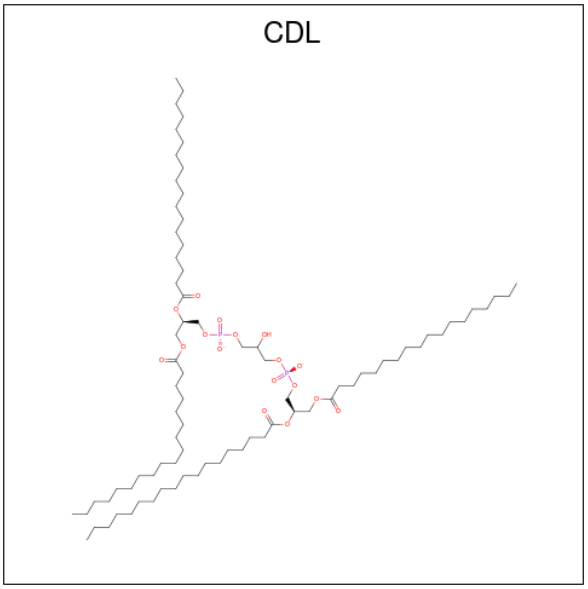
- Molecule 20 is a protein called Inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i1	28	Total	C	H	N	O	0	0
			474	154	236	39	45		
20	i2	32	Total	C	H	N	O	0	0
			529	171	262	45	51		

- Molecule 21 is a protein called ATPTT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	t	365	Total	C	H	N	O	S	0	0
			5889	1925	2876	533	544	11		

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



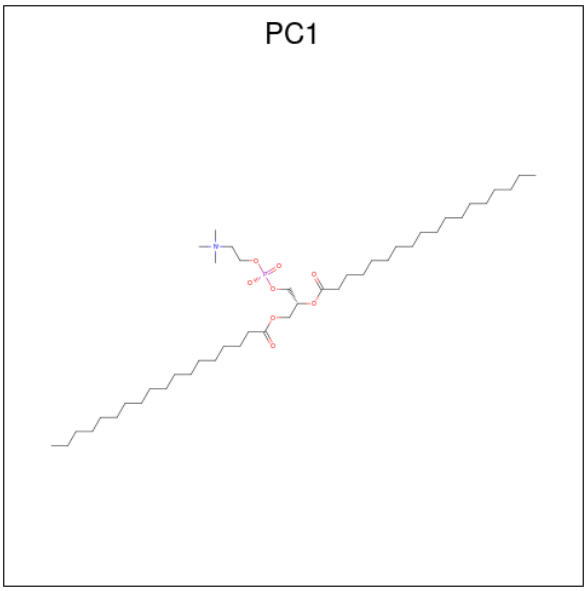
Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	i	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	j	1	Total	C	H	O	P	0
			256	81	156	17	2	

Continued on next page...

Continued from previous page...

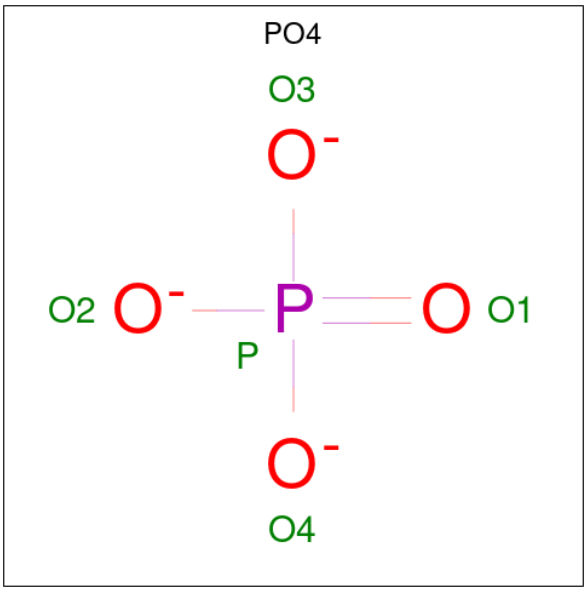
Mol	Chain	Residues	Atoms					AltConf
22	j	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	p	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	r	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	A	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	B	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	B	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	B	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	B	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	B	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	I	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	I	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	K	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	K	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	J	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	J	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	L	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	P	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 23 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



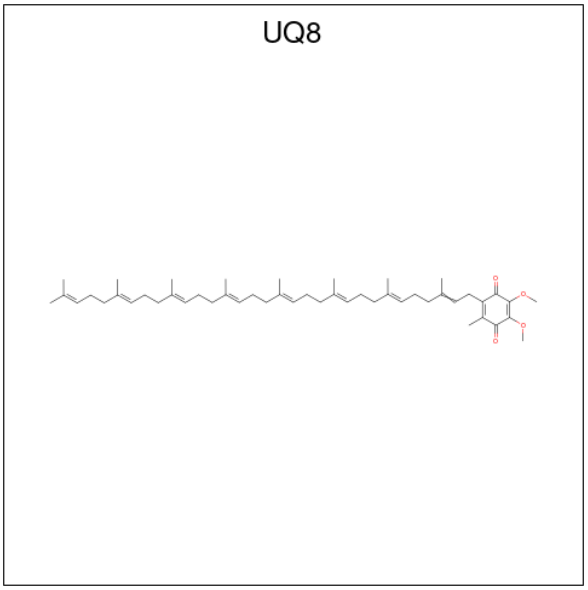
Mol	Chain	Residues	Atoms						AltConf
23	d	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	i	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	D	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 24 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



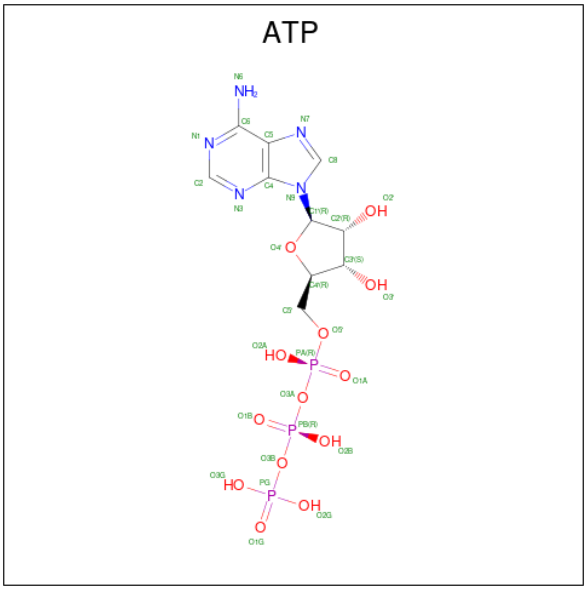
Mol	Chain	Residues	Atoms			AltConf
24	f	1	Total 5	O 4	P 1	0
24	F	1	Total 5	O 4	P 1	0

- Molecule 25 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms				AltConf
25	i	1	Total 127	C 49	H 74	O 4	0
25	I	1	Total 127	C 49	H 74	O 4	0

- Molecule 26 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

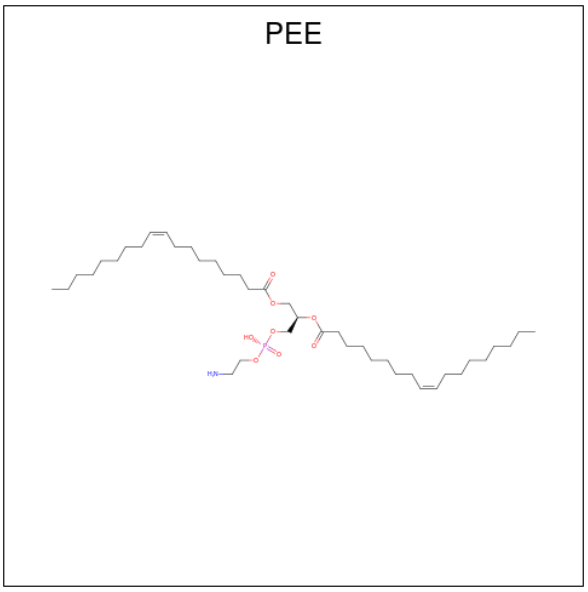


Mol	Chain	Residues	Atoms						AltConf
26	g	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
26	G	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

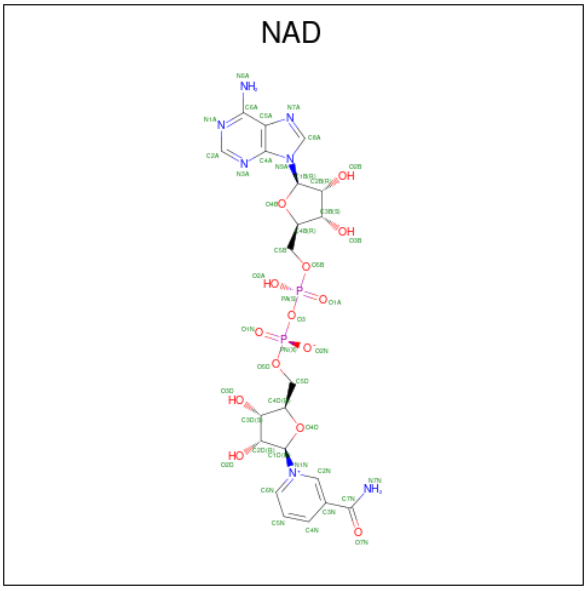
Mol	Chain	Residues	Atoms		AltConf
27	g	1	Total	Mg	0
			1	1	
27	G	1	Total	Mg	0
			1	1	

- Molecule 28 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
28	l	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
28	l	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	J	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
28	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 29 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



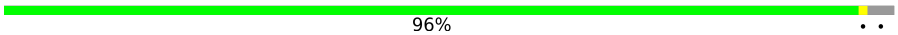
Mol	Chain	Residues	Atoms						AltConf
29	e	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
29	E	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

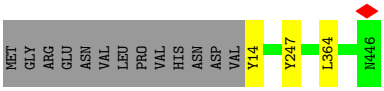
3 Residue-property plots (i)

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: subunit a

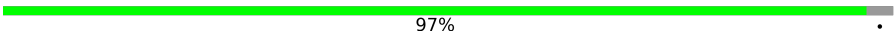
Chain a:





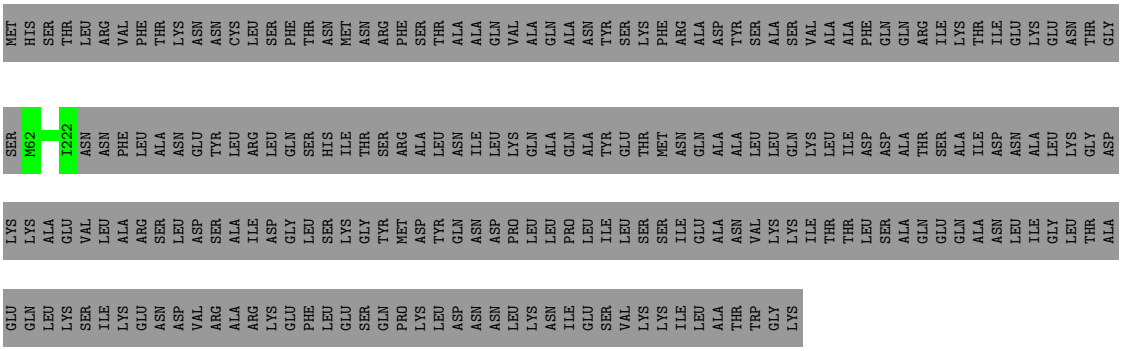
• Molecule 1: subunit a

Chain A:



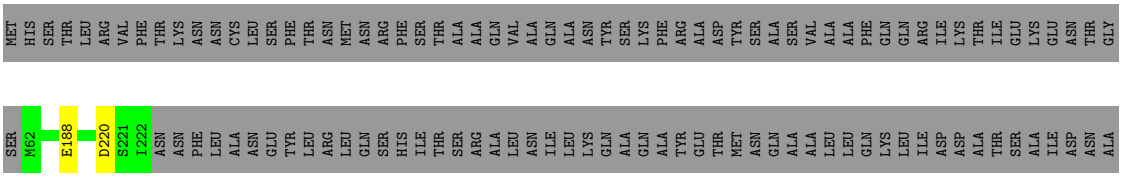
• Molecule 2: subunit b

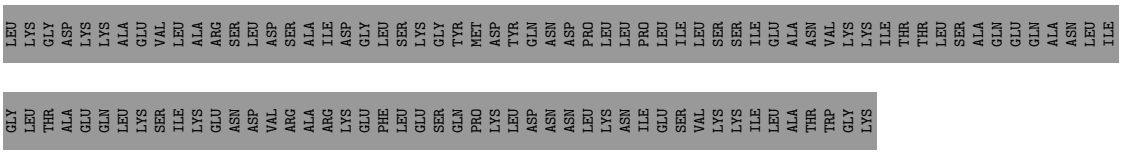
Chain b:



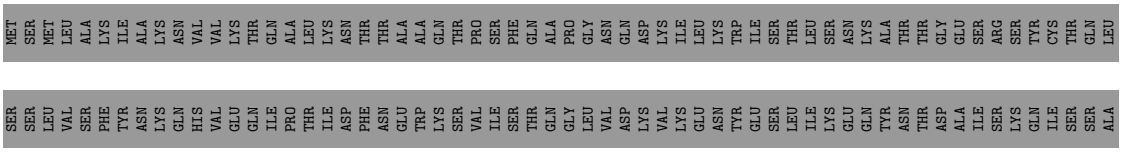
• Molecule 2: subunit b

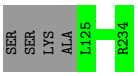
Chain B:



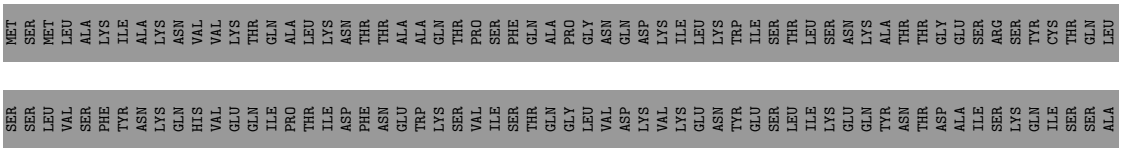


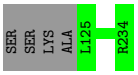
• Molecule 3: subunit d



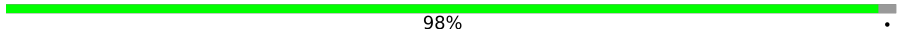


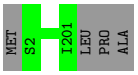
• Molecule 3: subunit d



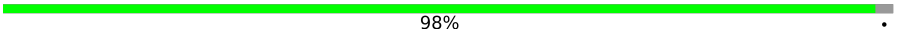


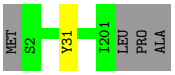
• Molecule 4: subunit f



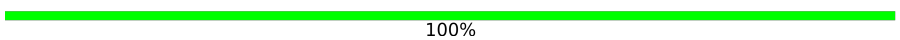


• Molecule 4: subunit f



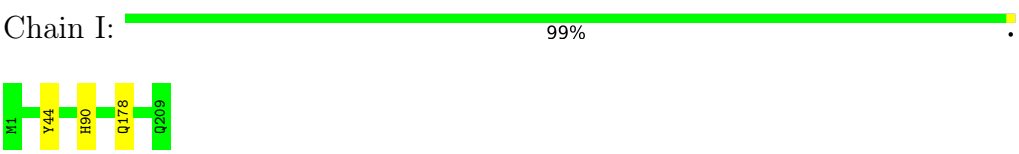


• Molecule 5: subunit i/j



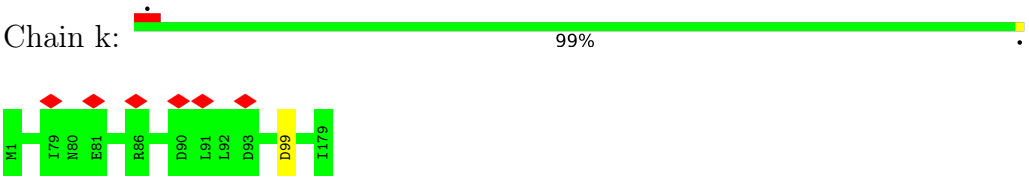
• Molecule 5: subunit i/j

Chain I:



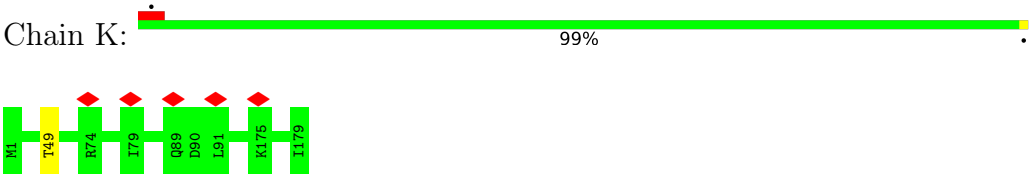
• Molecule 6: subunit k

Chain k:



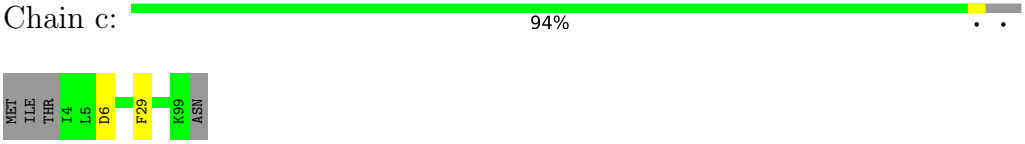
• Molecule 6: subunit k

Chain K:



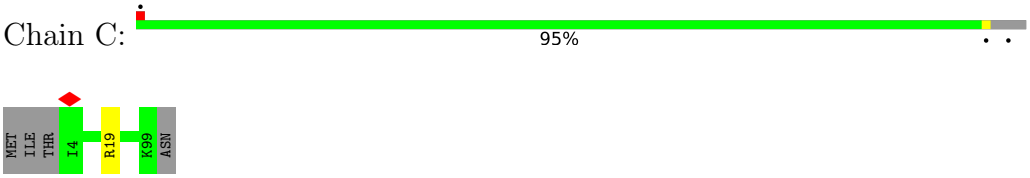
• Molecule 7: subunit 8

Chain c:



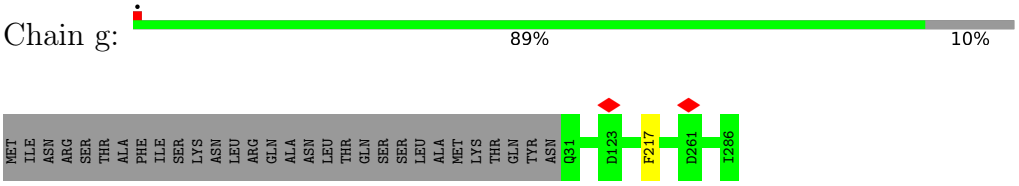
• Molecule 7: subunit 8

Chain C:



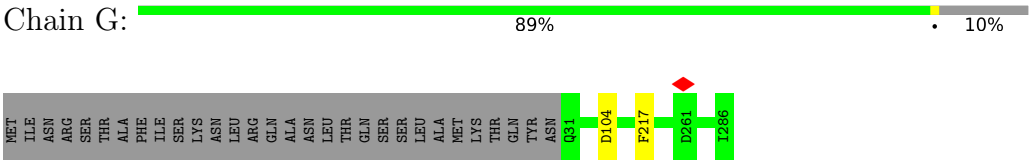
• Molecule 8: ATPTT3

Chain g:



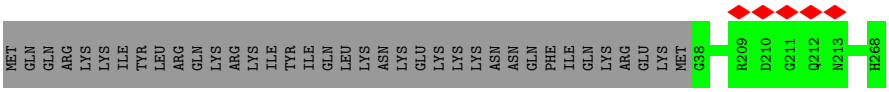
• Molecule 8: ATPTT3

Chain G:



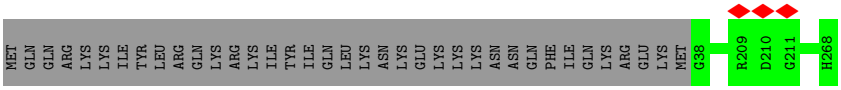
• Molecule 9: ATPTT4

Chain h:



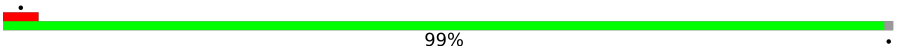
• Molecule 9: ATPTT4

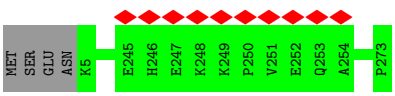
Chain H:



• Molecule 10: ATPTT5

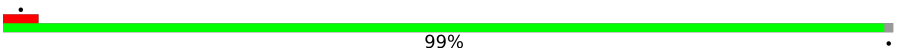
Chain j:

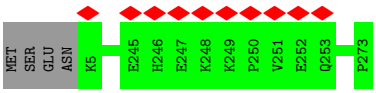




• Molecule 10: ATPTT5

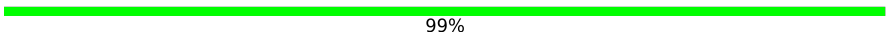
Chain J:





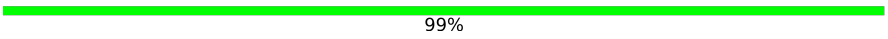
• Molecule 11: ATPTT6

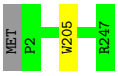
Chain l:



• Molecule 11: ATPTT6

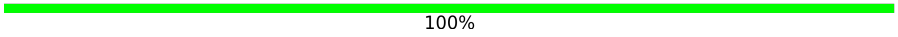
Chain L:





• Molecule 12: ATPTT7

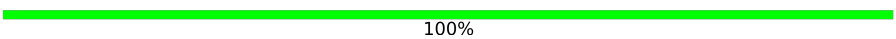
Chain m:



There are no outlier residues recorded for this chain.

• Molecule 12: ATPTT7

Chain M:



• Molecule 13: ATPTT8

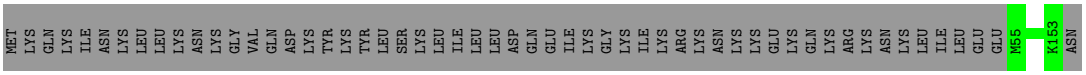
Chain n:

• Molecule 13: ATPTT8

Chain N:

• Molecule 14: ATPTT9

Chain o:

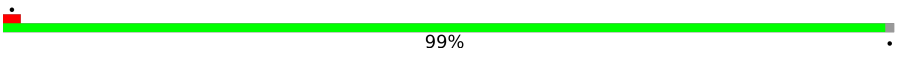


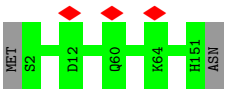
• Molecule 14: ATPTT9

Chain O:

• Molecule 15: ATPTT10

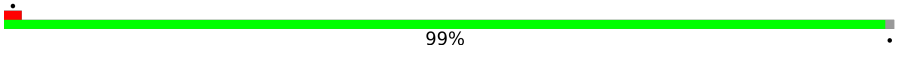
Chain p:

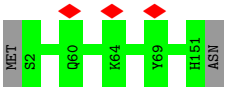




• Molecule 15: ATPTT10

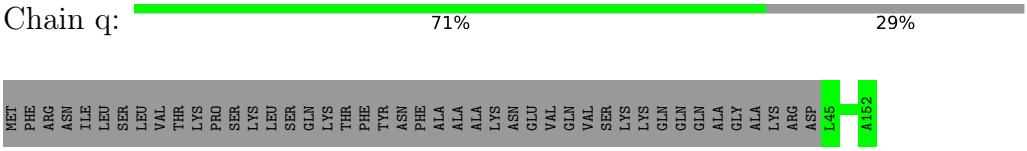
Chain P:





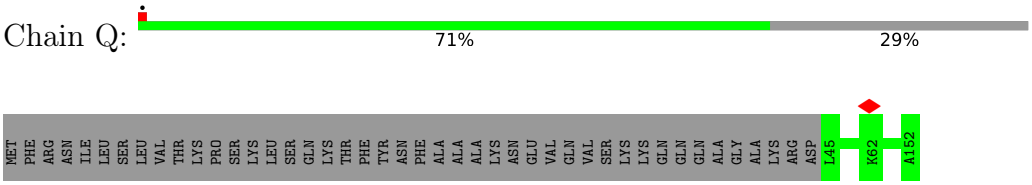
• Molecule 16: ATPTT11

Chain q:



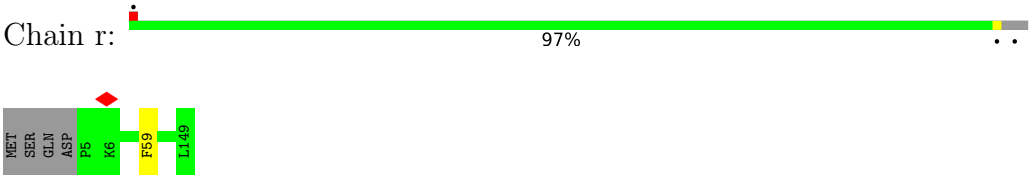
• Molecule 16: ATPTT11

Chain Q:



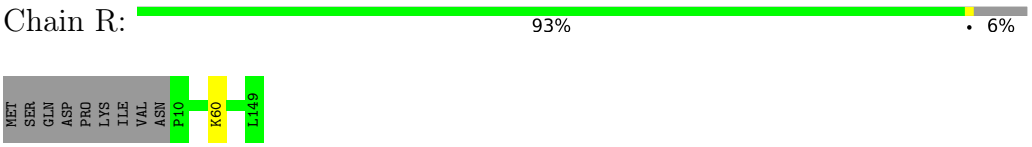
• Molecule 17: ATPTT12

Chain r:



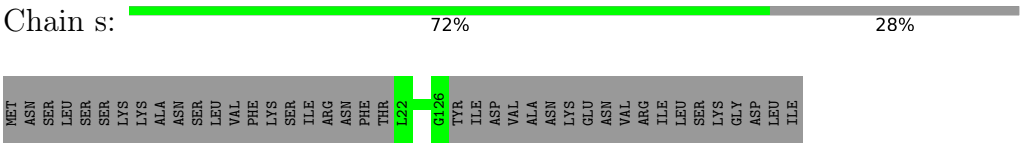
• Molecule 17: ATPTT12

Chain R:



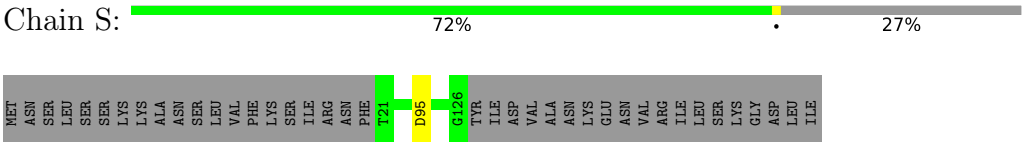
• Molecule 18: ATPTT13

Chain s:



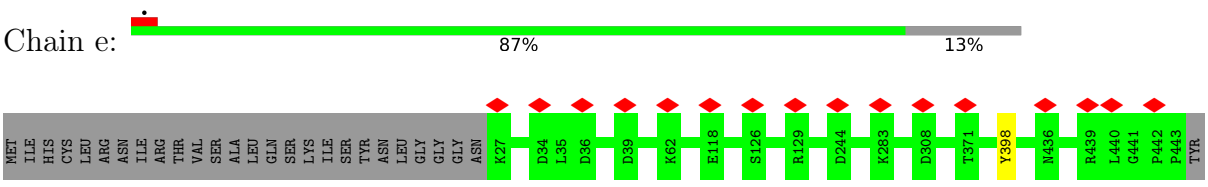
• Molecule 18: ATPTT13

Chain S:



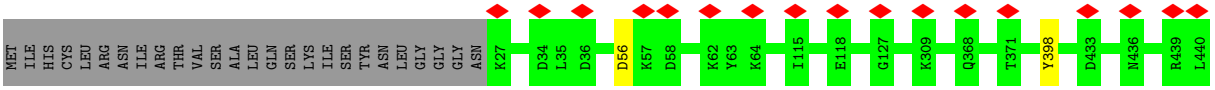
• Molecule 19: ATPTT1

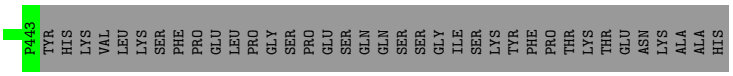
Chain e:



• Molecule 19: ATPTT1

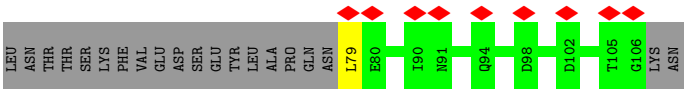
Chain E:





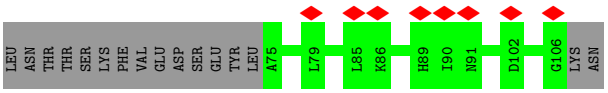
• Molecule 20: Inhibitor of F1 (IF1)

Chain i1:



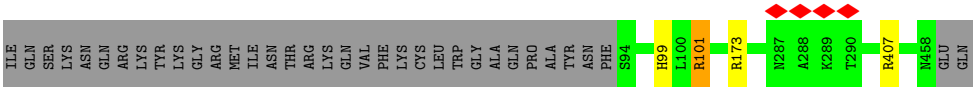
• Molecule 20: Inhibitor of F1 (IF1)

Chain i2:



• Molecule 21: ATPTT2

Chain t:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61157	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 ($e^-/Å^2$)	30.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: NAD, PO4, ATP, PEE, PC1, UQ8, CDL, MG

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	0.40	0/3752	0.41	0/5109
1	a	0.40	0/3752	0.41	0/5109
2	B	0.41	0/1417	0.42	0/1915
2	b	0.41	0/1417	0.40	0/1915
3	D	0.40	0/944	0.40	0/1278
3	d	0.39	0/944	0.41	0/1278
4	F	0.40	0/1733	0.44	0/2327
4	f	0.40	0/1733	0.43	0/2327
5	I	0.39	0/1771	0.43	0/2394
5	i	0.39	0/1771	0.44	0/2394
6	K	0.33	0/1508	0.42	0/2024
6	k	0.33	0/1508	0.41	0/2024
7	C	0.39	0/866	0.43	0/1176
7	c	0.40	0/866	0.43	0/1176
8	G	0.39	0/2302	0.44	0/3115
8	g	0.39	0/2302	0.43	0/3115
9	H	0.38	0/2006	0.43	0/2704
9	h	0.37	0/2006	0.42	0/2704
10	J	0.38	0/2256	0.43	0/3069
10	j	0.38	0/2256	0.44	0/3069
11	L	0.40	0/2140	0.42	0/2903
11	l	0.39	0/2140	0.42	0/2903
12	M	0.40	0/1912	0.40	0/2598
12	m	0.40	0/1912	0.40	0/2598
13	N	0.42	0/1030	0.44	0/1393
13	n	0.42	0/1030	0.45	0/1393
14	O	0.34	0/821	0.42	0/1104
14	o	0.33	0/821	0.43	0/1104
15	P	0.31	0/1249	0.39	0/1695
15	p	0.31	0/1249	0.40	0/1695
16	Q	0.35	0/888	0.41	0/1200
16	q	0.35	0/888	0.42	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	R	0.40	0/1185	0.41	0/1594
17	r	0.40	0/1225	0.41	0/1649
18	S	0.37	0/892	0.45	0/1209
18	s	0.38	0/885	0.45	0/1199
19	E	0.29	0/3492	0.42	0/4720
19	e	0.30	0/3492	0.42	0/4720
20	i1	0.45	0/242	0.50	0/328
20	i2	0.25	0/272	0.36	0/370
21	t	0.37	0/3103	0.44	1/4200 (0.0%)
All	All	0.38	0/67978	0.42	1/91997 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	t	101	ARG	NE-CZ-NH2	5.96	123.28	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	431/446 (97%)	425 (99%)	6 (1%)	0	100	100
1	a	431/446 (97%)	425 (99%)	6 (1%)	0	100	100
2	B	159/381 (42%)	153 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	159/381 (42%)	154 (97%)	5 (3%)	0	100	100
3	D	108/234 (46%)	106 (98%)	2 (2%)	0	100	100
3	d	108/234 (46%)	107 (99%)	1 (1%)	0	100	100
4	F	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
5	I	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
5	i	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
6	K	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
6	k	177/179 (99%)	168 (95%)	9 (5%)	0	100	100
7	C	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c	94/100 (94%)	91 (97%)	3 (3%)	0	100	100
8	G	254/286 (89%)	246 (97%)	8 (3%)	0	100	100
8	g	254/286 (89%)	243 (96%)	11 (4%)	0	100	100
9	H	229/268 (85%)	223 (97%)	6 (3%)	0	100	100
9	h	229/268 (85%)	227 (99%)	2 (1%)	0	100	100
10	J	267/273 (98%)	259 (97%)	8 (3%)	0	100	100
10	j	267/273 (98%)	259 (97%)	8 (3%)	0	100	100
11	L	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	l	244/247 (99%)	240 (98%)	4 (2%)	0	100	100
12	M	219/221 (99%)	217 (99%)	2 (1%)	0	100	100
12	m	219/221 (99%)	218 (100%)	1 (0%)	0	100	100
13	N	117/179 (65%)	113 (97%)	4 (3%)	0	100	100
13	n	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
14	O	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	o	97/154 (63%)	96 (99%)	1 (1%)	0	100	100
15	P	148/152 (97%)	142 (96%)	6 (4%)	0	100	100
15	p	148/152 (97%)	143 (97%)	5 (3%)	0	100	100
16	Q	106/152 (70%)	104 (98%)	2 (2%)	0	100	100
16	q	106/152 (70%)	103 (97%)	3 (3%)	0	100	100
17	R	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
17	r	143/149 (96%)	141 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	S	104/145 (72%)	101 (97%)	3 (3%)	0	100	100
18	s	103/145 (71%)	100 (97%)	3 (3%)	0	100	100
19	E	415/480 (86%)	408 (98%)	7 (2%)	0	100	100
19	e	415/480 (86%)	406 (98%)	9 (2%)	0	100	100
20	i1	26/108 (24%)	26 (100%)	0	0	100	100
20	i2	30/108 (28%)	30 (100%)	0	0	100	100
21	t	363/460 (79%)	356 (98%)	7 (2%)	0	100	100
All	All	7847/9594 (82%)	7667 (98%)	180 (2%)	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	397/409 (97%)	395 (100%)	2 (0%)	86	95
1	a	397/409 (97%)	394 (99%)	3 (1%)	79	91
2	B	143/331 (43%)	141 (99%)	2 (1%)	62	83
2	b	143/331 (43%)	143 (100%)	0	100	100
3	D	95/206 (46%)	95 (100%)	0	100	100
3	d	95/206 (46%)	95 (100%)	0	100	100
4	F	175/178 (98%)	174 (99%)	1 (1%)	84	94
4	f	175/178 (98%)	175 (100%)	0	100	100
5	I	182/182 (100%)	179 (98%)	3 (2%)	58	80
5	i	182/182 (100%)	181 (100%)	1 (0%)	86	95
6	K	152/152 (100%)	151 (99%)	1 (1%)	81	93
6	k	152/152 (100%)	151 (99%)	1 (1%)	81	93
7	C	93/97 (96%)	92 (99%)	1 (1%)	70	87
7	c	93/97 (96%)	91 (98%)	2 (2%)	47	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	G	235/262 (90%)	233 (99%)	2 (1%)	75 90
8	g	235/262 (90%)	234 (100%)	1 (0%)	89 96
9	H	208/245 (85%)	208 (100%)	0	100 100
9	h	208/245 (85%)	208 (100%)	0	100 100
10	J	235/239 (98%)	235 (100%)	0	100 100
10	j	235/239 (98%)	235 (100%)	0	100 100
11	L	219/220 (100%)	218 (100%)	1 (0%)	86 95
11	l	219/220 (100%)	218 (100%)	1 (0%)	86 95
12	M	202/202 (100%)	201 (100%)	1 (0%)	86 95
12	m	202/202 (100%)	202 (100%)	0	100 100
13	N	104/162 (64%)	104 (100%)	0	100 100
13	n	104/162 (64%)	104 (100%)	0	100 100
14	O	89/142 (63%)	89 (100%)	0	100 100
14	o	89/142 (63%)	89 (100%)	0	100 100
15	P	131/133 (98%)	131 (100%)	0	100 100
15	p	131/133 (98%)	131 (100%)	0	100 100
16	Q	97/135 (72%)	97 (100%)	0	100 100
16	q	97/135 (72%)	97 (100%)	0	100 100
17	R	120/129 (93%)	119 (99%)	1 (1%)	79 91
17	r	125/129 (97%)	124 (99%)	1 (1%)	79 91
18	S	95/131 (72%)	94 (99%)	1 (1%)	70 87
18	s	94/131 (72%)	94 (100%)	0	100 100
19	E	359/414 (87%)	357 (99%)	2 (1%)	84 94
19	e	359/414 (87%)	358 (100%)	1 (0%)	91 97
20	i1	26/101 (26%)	25 (96%)	1 (4%)	28 53
20	i2	29/101 (29%)	29 (100%)	0	100 100
21	t	325/414 (78%)	321 (99%)	4 (1%)	67 86
All	All	7046/8554 (82%)	7012 (100%)	34 (0%)	85 95

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	14	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	247	TYR
1	a	364	LEU
5	i	44	TYR
6	k	99	ASP
7	c	6	ASP
7	c	29	PHE
8	g	217	PHE
11	l	205	TRP
17	r	59	PHE
19	e	398	TYR
1	A	14	TYR
1	A	247	TYR
2	B	188	GLU
2	B	220	ASP
4	F	31	TYR
5	I	44	TYR
5	I	90	HIS
5	I	178	GLN
6	K	49	THR
7	C	19	ARG
8	G	104	ASP
8	G	217	PHE
11	L	205	TRP
12	M	37	ASP
17	R	60	LYS
18	S	95	ASP
19	E	56	ASP
19	E	398	TYR
20	i1	79	LEU
21	t	99	HIS
21	t	101	ARG
21	t	173	ARG
21	t	407	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
12	m	74	HIS
19	e	165	ASN
5	I	83	HIS
9	H	136	HIS
10	J	130	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	M	74	HIS
19	E	361	ASN
21	t	170	ASN
21	t	234	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 50 ligands modelled in this entry, 2 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CDL	B	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.06	4 (3%)
22	CDL	B	404	-	99,99,99	0.89	8 (8%)	105,111,111	0.95	4 (3%)
22	CDL	i	302	-	99,99,99	0.89	8 (8%)	105,111,111	0.94	4 (3%)
28	PEE	J	303	10	47,47,50	1.18	6 (12%)	50,52,55	1.13	4 (8%)
22	CDL	I	301	5	99,99,99	0.88	6 (6%)	105,111,111	0.95	3 (2%)
22	CDL	K	202	-	99,99,99	0.88	7 (7%)	105,111,111	1.07	5 (4%)
22	CDL	f	303	-	99,99,99	0.89	8 (8%)	105,111,111	1.12	5 (4%)
22	CDL	l	304	-	99,99,99	0.89	7 (7%)	105,111,111	1.04	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PEE	J	304	-	50,50,50	1.16	6 (12%)	53,55,55	1.12	3 (5%)
22	CDL	a	501	-	99,99,99	0.89	7 (7%)	105,111,111	1.02	3 (2%)
29	NAD	E	900	-	42,48,48	3.83	19 (45%)	50,73,73	2.10	6 (12%)
25	UQ8	i	303	-	53,53,53	1.80	7 (13%)	64,67,67	1.60	15 (23%)
22	CDL	L	301	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	4 (3%)
23	PC1	g	303	8	53,53,53	0.97	3 (5%)	59,61,61	1.04	2 (3%)
22	CDL	J	302	-	99,99,99	0.87	7 (7%)	105,111,111	0.99	4 (3%)
22	CDL	l	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.02	4 (3%)
22	CDL	J	301	-	99,99,99	0.89	6 (6%)	105,111,111	1.07	4 (3%)
22	CDL	B	401	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	5 (4%)
23	PC1	d	301	3	53,53,53	0.93	4 (7%)	59,61,61	1.08	3 (5%)
23	PC1	G	303	-	53,53,53	0.97	4 (7%)	59,61,61	0.94	2 (3%)
23	PC1	G	304	8	53,53,53	0.97	3 (5%)	59,61,61	1.04	2 (3%)
24	PO4	f	301	-	4,4,4	1.06	0	6,6,6	0.42	0
22	CDL	k	202	-	99,99,99	0.89	7 (7%)	105,111,111	1.04	5 (4%)
22	CDL	A	501	-	99,99,99	0.88	7 (7%)	105,111,111	1.01	5 (4%)
22	CDL	k	203	-	99,99,99	0.89	7 (7%)	105,111,111	0.99	4 (3%)
22	CDL	r	201	-	99,99,99	0.87	5 (5%)	105,111,111	0.97	4 (3%)
22	CDL	b	402	-	99,99,99	0.89	7 (7%)	105,111,111	0.93	4 (3%)
22	CDL	B	405	2	99,99,99	0.88	8 (8%)	105,111,111	1.10	5 (4%)
28	PEE	l	302	-	47,47,50	1.18	6 (12%)	50,52,55	1.09	3 (6%)
22	CDL	k	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	5 (4%)
22	CDL	f	304	4	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
22	CDL	I	302	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	4 (3%)
26	ATP	G	301	27	26,33,33	4.75	7 (26%)	31,52,52	2.46	7 (22%)
22	CDL	K	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.01	4 (3%)
23	PC1	D	301	3	53,53,53	0.95	4 (7%)	59,61,61	1.10	2 (3%)
22	CDL	j	301	-	99,99,99	0.89	7 (7%)	105,111,111	1.07	4 (3%)
22	CDL	B	403	2	99,99,99	0.87	7 (7%)	105,111,111	1.09	4 (3%)
25	UQ8	I	303	-	53,53,53	1.81	7 (13%)	64,67,67	1.57	13 (20%)
24	PO4	F	900	-	4,4,4	1.06	0	6,6,6	0.46	0
22	CDL	p	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.00	4 (3%)
28	PEE	l	303	-	50,50,50	1.15	6 (12%)	53,55,55	1.13	3 (5%)
23	PC1	i	301	-	53,53,53	0.96	4 (7%)	59,61,61	0.96	2 (3%)
29	NAD	e	900	-	42,48,48	3.83	19 (45%)	50,73,73	2.17	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CDL	f	302	4	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
22	CDL	b	401	-	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
22	CDL	j	302	-	99,99,99	0.87	7 (7%)	105,111,111	1.02	4 (3%)
22	CDL	P	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	5 (4%)
26	ATP	g	301	27	26,33,33	4.76	7 (26%)	31,52,52	2.45	7 (22%)

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
22	CDL	B	402	-	-	53/110/110/110	-
22	CDL	B	404	-	-	40/110/110/110	-
22	CDL	i	302	-	-	41/110/110/110	-
28	PEE	J	303	10	-	23/51/51/54	-
22	CDL	I	301	5	-	50/110/110/110	-
22	CDL	K	202	-	-	39/110/110/110	-
22	CDL	f	303	-	-	42/110/110/110	-
22	CDL	l	304	-	-	41/110/110/110	-
28	PEE	J	304	-	-	24/54/54/54	-
22	CDL	a	501	-	-	47/110/110/110	-
29	NAD	E	900	-	-	7/26/62/62	0/5/5/5
25	UQ8	i	303	-	-	8/51/75/75	0/1/1/1
22	CDL	L	301	-	-	44/110/110/110	-
23	PC1	g	303	8	-	17/57/57/57	-
22	CDL	J	302	-	-	36/110/110/110	-
22	CDL	l	301	-	-	37/110/110/110	-
22	CDL	J	301	-	-	35/110/110/110	-
22	CDL	B	401	-	-	52/110/110/110	-
23	PC1	d	301	3	-	17/57/57/57	-
23	PC1	G	303	-	-	16/57/57/57	-
23	PC1	G	304	8	-	19/57/57/57	-
22	CDL	k	202	-	-	44/110/110/110	-
22	CDL	A	501	-	-	51/110/110/110	-
22	CDL	k	203	-	-	45/110/110/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CDL	r	201	-	-	47/110/110/110	-
22	CDL	b	402	-	-	43/110/110/110	-
22	CDL	B	405	2	-	40/110/110/110	-
28	PEE	l	302	-	-	26/51/51/54	-
22	CDL	k	201	-	-	35/110/110/110	-
22	CDL	f	304	4	-	59/110/110/110	-
22	CDL	I	302	-	-	41/110/110/110	-
26	ATP	G	301	27	-	0/18/38/38	0/3/3/3
22	CDL	K	201	-	-	33/110/110/110	-
23	PC1	D	301	3	-	14/57/57/57	-
22	CDL	j	301	-	-	41/110/110/110	-
22	CDL	B	403	2	-	43/110/110/110	-
25	UQ8	I	303	-	-	11/51/75/75	0/1/1/1
22	CDL	p	201	-	-	34/110/110/110	-
28	PEE	l	303	-	-	24/54/54/54	-
23	PC1	i	301	-	-	16/57/57/57	-
29	NAD	e	900	-	-	8/26/62/62	0/5/5/5
22	CDL	f	302	4	-	43/110/110/110	-
22	CDL	b	401	-	-	55/110/110/110	-
22	CDL	j	302	-	-	37/110/110/110	-
22	CDL	P	201	-	-	39/110/110/110	-
26	ATP	g	301	27	-	0/18/38/38	0/3/3/3

All (333) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	301	ATP	C2'-C1'	-17.21	1.27	1.53
26	G	301	ATP	C2'-C1'	-17.05	1.27	1.53
26	G	301	ATP	O4'-C1'	11.06	1.56	1.41
26	g	301	ATP	O4'-C1'	10.92	1.56	1.41
29	e	900	NAD	O4D-C1D	-9.81	1.27	1.41
25	i	303	UQ8	C6-C1	9.81	1.53	1.35
25	I	303	UQ8	C6-C1	9.75	1.53	1.35
29	E	900	NAD	O4D-C1D	-9.74	1.27	1.41
26	G	301	ATP	C3'-C4'	-9.54	1.28	1.53
26	g	301	ATP	C3'-C4'	-9.51	1.28	1.53
29	E	900	NAD	C3B-C4B	-9.28	1.29	1.53
29	e	900	NAD	C3B-C4B	-9.25	1.29	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	E	900	NAD	C3D-C4D	-8.50	1.31	1.53
29	e	900	NAD	C3D-C4D	-8.48	1.31	1.53
29	E	900	NAD	C7N-N7N	8.42	1.49	1.33
29	e	900	NAD	C7N-N7N	8.40	1.49	1.33
29	e	900	NAD	O4D-C4D	7.54	1.61	1.45
29	E	900	NAD	O4D-C4D	7.52	1.61	1.45
29	e	900	NAD	O4B-C4B	7.51	1.61	1.45
29	E	900	NAD	O4B-C4B	7.50	1.61	1.45
29	e	900	NAD	O4B-C1B	-6.62	1.31	1.41
29	E	900	NAD	O4B-C1B	-6.28	1.32	1.41
29	E	900	NAD	C3N-C7N	4.72	1.57	1.50
26	G	301	ATP	C2'-C3'	4.69	1.66	1.53
26	g	301	ATP	C2'-C3'	4.61	1.66	1.53
29	e	900	NAD	C3N-C7N	4.60	1.57	1.50
29	E	900	NAD	O3D-C3D	4.54	1.53	1.43
29	e	900	NAD	O3D-C3D	4.53	1.53	1.43
26	g	301	ATP	O4'-C4'	4.43	1.54	1.45
26	G	301	ATP	O4'-C4'	4.42	1.54	1.45
29	e	900	NAD	C6A-N6A	4.22	1.49	1.34
29	E	900	NAD	C6A-N6A	4.21	1.49	1.34
25	I	303	UQ8	C4-C3	4.10	1.53	1.36
25	i	303	UQ8	C4-C3	4.06	1.52	1.36
28	J	303	PEE	C39-C38	3.77	1.53	1.31
28	l	303	PEE	C18-C19	3.76	1.53	1.31
28	J	304	PEE	C39-C38	3.74	1.53	1.31
28	l	303	PEE	C39-C38	3.73	1.53	1.31
28	J	304	PEE	C18-C19	3.71	1.53	1.31
28	l	302	PEE	C39-C38	3.67	1.53	1.31
28	l	302	PEE	C18-C19	3.61	1.52	1.31
28	J	303	PEE	C18-C19	3.59	1.52	1.31
29	e	900	NAD	O3B-C3B	3.15	1.50	1.43
26	G	301	ATP	C6-N6	3.13	1.45	1.34
29	E	900	NAD	O3B-C3B	3.13	1.50	1.43
26	g	301	ATP	C6-N6	3.05	1.45	1.34
22	A	501	CDL	OA6-CA4	-2.95	1.39	1.46
22	l	301	CDL	OA6-CA4	-2.93	1.39	1.46
22	K	202	CDL	OA6-CA4	-2.91	1.39	1.46
22	k	202	CDL	OA6-CA4	-2.88	1.39	1.46
22	a	501	CDL	OA6-CA4	-2.84	1.39	1.46
22	L	301	CDL	OA6-CA4	-2.83	1.39	1.46
22	B	403	CDL	OA6-CA4	-2.83	1.39	1.46
29	E	900	NAD	O2B-C2B	-2.79	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	301	ATP	C5-C4	-2.78	1.33	1.40
22	B	404	CDL	OB6-CB4	-2.77	1.39	1.46
22	f	302	CDL	OB6-CB4	-2.77	1.39	1.46
22	J	301	CDL	OA6-CA4	-2.74	1.39	1.46
22	f	302	CDL	OA6-CA4	-2.74	1.39	1.46
22	b	402	CDL	OB6-CB4	-2.74	1.39	1.46
26	G	301	ATP	C5-C4	-2.74	1.33	1.40
22	I	301	CDL	OB6-CB4	-2.73	1.39	1.46
29	e	900	NAD	O2B-C2B	-2.72	1.36	1.43
22	a	501	CDL	OB6-CB4	-2.72	1.39	1.46
22	L	301	CDL	OB6-CB4	-2.71	1.39	1.46
22	r	201	CDL	OB6-CB4	-2.71	1.39	1.46
23	G	303	PC1	O21-C2	-2.70	1.39	1.46
22	l	304	CDL	OA8-CA7	2.69	1.41	1.33
23	i	301	PC1	O21-C2	-2.67	1.39	1.46
29	E	900	NAD	C2N-N1N	2.67	1.38	1.35
22	j	301	CDL	OA6-CA4	-2.66	1.39	1.46
22	B	401	CDL	OB6-CB4	-2.66	1.39	1.46
22	b	402	CDL	OA8-CA7	2.65	1.41	1.33
22	K	202	CDL	OB6-CB4	-2.63	1.40	1.46
22	A	501	CDL	OB6-CB4	-2.63	1.40	1.46
22	I	302	CDL	OA6-CA4	-2.62	1.40	1.46
22	p	201	CDL	OA6-CA4	-2.61	1.40	1.46
28	J	303	PEE	O2-C2	-2.61	1.40	1.46
22	p	201	CDL	OB6-CB4	-2.61	1.40	1.46
22	B	401	CDL	OA6-CA4	-2.60	1.40	1.46
22	P	201	CDL	OA6-CA4	-2.59	1.40	1.46
22	J	302	CDL	OB6-CB4	-2.59	1.40	1.46
22	b	401	CDL	OB6-CB4	-2.59	1.40	1.46
22	J	301	CDL	OA8-CA7	2.59	1.40	1.33
22	j	301	CDL	OB6-CB4	-2.59	1.40	1.46
29	e	900	NAD	C2N-N1N	2.59	1.38	1.35
22	i	302	CDL	OA6-CA4	-2.57	1.40	1.46
22	f	302	CDL	OA8-CA7	2.57	1.40	1.33
22	l	304	CDL	OB6-CB4	-2.57	1.40	1.46
22	k	203	CDL	OA8-CA7	2.57	1.40	1.33
22	j	302	CDL	OB6-CB4	-2.56	1.40	1.46
22	f	303	CDL	OA8-CA7	2.55	1.40	1.33
22	k	202	CDL	OA8-CA7	2.55	1.40	1.33
22	B	402	CDL	OB6-CB4	-2.55	1.40	1.46
22	I	301	CDL	OA8-CA7	2.55	1.40	1.33
22	K	202	CDL	OA8-CA7	2.54	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	j	301	CDL	OA8-CA7	2.54	1.40	1.33
22	K	201	CDL	OB8-CB7	2.53	1.40	1.33
28	l	302	PEE	O2-C2	-2.53	1.40	1.46
23	g	303	PC1	O31-C31	2.53	1.40	1.33
22	r	201	CDL	OA8-CA7	2.53	1.40	1.33
22	J	301	CDL	OB6-CB4	-2.53	1.40	1.46
23	G	304	PC1	O21-C2	-2.53	1.40	1.46
22	f	304	CDL	OA6-CA4	-2.53	1.40	1.46
22	J	302	CDL	OB8-CB7	2.53	1.40	1.33
22	I	301	CDL	OA6-CA4	-2.53	1.40	1.46
22	j	302	CDL	OB8-CB7	2.52	1.40	1.33
22	B	404	CDL	OA8-CA7	2.52	1.40	1.33
22	l	301	CDL	OB6-CB4	-2.52	1.40	1.46
23	G	304	PC1	O31-C31	2.52	1.40	1.33
29	E	900	NAD	C5A-C4A	-2.52	1.34	1.40
28	J	304	PEE	O2-C2	-2.52	1.40	1.46
28	l	303	PEE	O2-C2	-2.52	1.40	1.46
22	k	201	CDL	OB8-CB7	2.51	1.40	1.33
22	B	405	CDL	OA8-CA7	2.51	1.40	1.33
22	j	302	CDL	OA8-CA7	2.51	1.40	1.33
29	e	900	NAD	C5A-C4A	-2.51	1.34	1.40
22	B	405	CDL	OB6-CB4	-2.51	1.40	1.46
22	K	201	CDL	OB6-CB4	-2.50	1.40	1.46
22	k	202	CDL	OB6-CB4	-2.50	1.40	1.46
22	B	405	CDL	OB8-CB7	2.50	1.40	1.33
22	b	401	CDL	OB8-CB6	-2.50	1.39	1.45
22	k	203	CDL	OB6-CB4	-2.50	1.40	1.46
22	P	201	CDL	OB8-CB7	2.49	1.40	1.33
22	P	201	CDL	OB6-CB4	-2.49	1.40	1.46
22	p	201	CDL	OB8-CB7	2.49	1.40	1.33
22	f	303	CDL	OB6-CB4	-2.49	1.40	1.46
22	J	302	CDL	OA6-CA4	-2.48	1.40	1.46
22	l	301	CDL	OB8-CB6	-2.48	1.39	1.45
23	i	301	PC1	O31-C31	2.48	1.40	1.33
22	a	501	CDL	OA8-CA7	2.47	1.40	1.33
22	r	201	CDL	OA6-CA4	-2.47	1.40	1.46
22	k	201	CDL	OA6-CA5	2.47	1.41	1.34
22	j	301	CDL	OB8-CB7	2.47	1.40	1.33
29	e	900	NAD	C2A-N1A	2.47	1.38	1.33
22	f	303	CDL	OB8-CB7	2.46	1.40	1.33
22	B	403	CDL	OB6-CB4	-2.46	1.40	1.46
22	b	401	CDL	OA6-CA4	-2.46	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	301	CDL	OB8-CB7	2.46	1.40	1.33
29	E	900	NAD	C2A-N1A	2.46	1.38	1.33
22	f	303	CDL	OA6-CA5	2.46	1.41	1.34
22	k	201	CDL	OA8-CA7	2.46	1.40	1.33
22	a	501	CDL	OB8-CB7	2.46	1.40	1.33
22	P	201	CDL	OA8-CA7	2.45	1.40	1.33
23	g	303	PC1	O21-C2	-2.45	1.40	1.46
22	I	302	CDL	OB6-CB4	-2.45	1.40	1.46
22	f	304	CDL	OB6-CB4	-2.44	1.40	1.46
22	L	301	CDL	OA8-CA7	2.44	1.40	1.33
22	b	401	CDL	OA8-CA7	2.44	1.40	1.33
22	l	304	CDL	OB8-CB7	2.44	1.40	1.33
22	B	404	CDL	OA6-CA4	-2.44	1.40	1.46
22	B	403	CDL	OA8-CA7	2.43	1.40	1.33
25	i	303	UQ8	O4-C4M	-2.43	1.39	1.45
22	k	203	CDL	OB8-CB7	2.43	1.40	1.33
22	r	201	CDL	OB8-CB6	-2.43	1.39	1.45
22	i	302	CDL	OA8-CA7	2.43	1.40	1.33
22	i	302	CDL	OB6-CB4	-2.43	1.40	1.46
22	B	401	CDL	OB8-CB7	2.43	1.40	1.33
22	k	201	CDL	OB6-CB4	-2.42	1.40	1.46
22	I	302	CDL	OA8-CA7	2.42	1.40	1.33
22	J	301	CDL	OB8-CB7	2.42	1.40	1.33
22	A	501	CDL	OB8-CB7	2.42	1.40	1.33
22	B	402	CDL	OB8-CB6	-2.41	1.39	1.45
22	f	304	CDL	OA8-CA7	2.41	1.40	1.33
22	K	201	CDL	OA8-CA7	2.41	1.40	1.33
22	f	303	CDL	OA6-CA4	-2.41	1.40	1.46
22	B	402	CDL	OA8-CA6	-2.41	1.39	1.45
22	K	202	CDL	OB8-CB7	2.41	1.40	1.33
23	D	301	PC1	O21-C2	-2.41	1.40	1.46
29	E	900	NAD	O7N-C7N	-2.41	1.19	1.24
22	k	203	CDL	OA6-CA4	-2.40	1.40	1.46
22	j	302	CDL	OA6-CA4	-2.40	1.40	1.46
22	b	402	CDL	OA6-CA4	-2.40	1.40	1.46
22	J	302	CDL	OA8-CA7	2.39	1.40	1.33
22	p	201	CDL	OA8-CA7	2.38	1.40	1.33
22	B	402	CDL	OB8-CB7	2.38	1.40	1.33
22	l	304	CDL	OA6-CA4	-2.38	1.40	1.46
22	I	301	CDL	OB8-CB7	2.38	1.40	1.33
28	l	302	PEE	O3-C3	-2.37	1.39	1.45
25	i	303	UQ8	O3-C3M	-2.37	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	304	PEE	O3-C30	2.37	1.40	1.33
22	l	301	CDL	OA8-CA7	2.37	1.40	1.33
22	K	201	CDL	OA6-CA4	-2.37	1.40	1.46
22	i	302	CDL	OB8-CB7	2.37	1.40	1.33
22	B	405	CDL	OA6-CA4	-2.37	1.40	1.46
23	G	303	PC1	O31-C31	2.37	1.40	1.33
23	D	301	PC1	O31-C3	-2.36	1.39	1.45
22	k	202	CDL	OB8-CB7	2.36	1.40	1.33
28	l	303	PEE	O3-C30	2.35	1.40	1.33
22	b	402	CDL	OB8-CB7	2.35	1.40	1.33
29	E	900	NAD	C2D-C1D	2.35	1.57	1.53
28	J	303	PEE	O3-C3	-2.34	1.39	1.45
22	f	304	CDL	OB8-CB7	2.34	1.40	1.33
22	I	301	CDL	OB8-CB6	-2.34	1.39	1.45
25	I	303	UQ8	O3-C3M	-2.34	1.39	1.45
23	g	303	PC1	O21-C21	2.34	1.40	1.34
22	f	302	CDL	OB8-CB6	-2.34	1.39	1.45
22	B	402	CDL	OA6-CA4	-2.34	1.40	1.46
29	e	900	NAD	O7N-C7N	-2.34	1.19	1.24
22	B	401	CDL	OA8-CA7	2.33	1.40	1.33
22	b	401	CDL	OB8-CB7	2.33	1.40	1.33
23	d	301	PC1	O21-C21	2.33	1.40	1.34
23	D	301	PC1	O21-C21	2.33	1.40	1.34
22	B	404	CDL	OB8-CB7	2.33	1.40	1.33
25	I	303	UQ8	O4-C4M	-2.32	1.39	1.45
22	I	302	CDL	OB8-CB6	-2.32	1.39	1.45
22	f	302	CDL	OB8-CB7	2.32	1.40	1.33
22	I	302	CDL	OB8-CB7	2.31	1.40	1.33
22	B	403	CDL	OB8-CB6	-2.31	1.39	1.45
23	d	301	PC1	O31-C31	2.31	1.40	1.33
22	K	201	CDL	OA6-CA5	2.30	1.40	1.34
22	f	303	CDL	OB6-CB5	2.29	1.40	1.34
22	A	501	CDL	OA8-CA7	2.29	1.40	1.33
22	B	402	CDL	OA8-CA7	2.29	1.40	1.33
22	i	302	CDL	OB6-CB5	2.29	1.40	1.34
23	G	303	PC1	O31-C3	-2.29	1.39	1.45
22	A	501	CDL	OA8-CA6	-2.28	1.40	1.45
28	l	302	PEE	O3-C30	2.28	1.40	1.33
22	B	403	CDL	OB8-CB7	2.28	1.40	1.33
22	f	304	CDL	OB8-CB6	-2.28	1.40	1.45
22	l	301	CDL	OB8-CB7	2.27	1.40	1.33
28	J	304	PEE	O3-C3	-2.27	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	k	201	CDL	OA6-CA4	-2.27	1.40	1.46
22	i	302	CDL	OB8-CB6	-2.27	1.40	1.45
28	J	303	PEE	O3-C30	2.26	1.39	1.33
22	B	404	CDL	OB8-CB6	-2.26	1.40	1.45
22	B	405	CDL	OA6-CA5	2.26	1.40	1.34
22	k	201	CDL	OB6-CB5	2.25	1.40	1.34
22	r	201	CDL	OB8-CB7	2.25	1.39	1.33
22	I	302	CDL	OB6-CB5	2.25	1.40	1.34
22	B	402	CDL	OB6-CB5	2.25	1.40	1.34
22	A	501	CDL	OB8-CB6	-2.24	1.40	1.45
22	a	501	CDL	OA8-CA6	-2.24	1.40	1.45
23	d	301	PC1	O21-C2	-2.24	1.41	1.46
22	B	401	CDL	OA6-CA5	2.24	1.40	1.34
22	l	304	CDL	OB6-CB5	2.24	1.40	1.34
22	k	203	CDL	OB6-CB5	2.24	1.40	1.34
23	d	301	PC1	O31-C3	-2.23	1.40	1.45
22	k	202	CDL	OB8-CB6	-2.23	1.40	1.45
23	G	304	PC1	O21-C21	2.23	1.40	1.34
28	l	302	PEE	O2-C10	2.23	1.40	1.34
22	b	402	CDL	OB8-CB6	-2.23	1.40	1.45
22	K	201	CDL	OB6-CB5	2.22	1.40	1.34
22	k	202	CDL	OB6-CB5	2.22	1.40	1.34
25	i	303	UQ8	O2-C2	-2.22	1.18	1.23
22	f	304	CDL	OB6-CB5	2.21	1.40	1.34
25	I	303	UQ8	O5-C5	-2.21	1.18	1.23
22	L	301	CDL	OB8-CB6	-2.21	1.40	1.45
23	D	301	PC1	O31-C31	2.21	1.39	1.33
22	a	501	CDL	OB8-CB6	-2.21	1.40	1.45
22	k	203	CDL	OB8-CB6	-2.21	1.40	1.45
25	i	303	UQ8	O5-C5	-2.20	1.18	1.23
28	J	304	PEE	O2-C10	2.20	1.40	1.34
22	l	301	CDL	OA8-CA6	-2.20	1.40	1.45
22	B	405	CDL	OB6-CB5	2.20	1.40	1.34
22	B	401	CDL	OA8-CA6	-2.20	1.40	1.45
22	k	203	CDL	OA6-CA5	2.19	1.40	1.34
22	i	302	CDL	OA6-CA5	2.19	1.40	1.34
25	I	303	UQ8	C6-C5	2.19	1.52	1.46
22	J	302	CDL	OA8-CA6	-2.18	1.40	1.45
22	J	301	CDL	OB6-CB5	2.18	1.40	1.34
22	P	201	CDL	OB6-CB5	2.18	1.40	1.34
22	j	301	CDL	OB6-CB5	2.18	1.40	1.34
28	l	303	PEE	O2-C10	2.17	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	l	304	CDL	OB8-CB6	-2.17	1.40	1.45
22	B	404	CDL	OA6-CA5	2.16	1.40	1.34
25	I	303	UQ8	O2-C2	-2.16	1.18	1.23
22	K	202	CDL	OB6-CB5	2.16	1.40	1.34
22	j	302	CDL	OA8-CA6	-2.16	1.40	1.45
22	L	301	CDL	OA8-CA6	-2.16	1.40	1.45
22	B	402	CDL	OA6-CA5	2.15	1.40	1.34
22	b	401	CDL	OA6-CA5	2.15	1.40	1.34
22	b	402	CDL	OA6-CA5	2.15	1.40	1.34
22	I	302	CDL	OA6-CA5	2.15	1.40	1.34
28	J	303	PEE	O2-C10	2.14	1.40	1.34
22	f	304	CDL	OA8-CA6	-2.14	1.40	1.45
22	f	304	CDL	OA6-CA5	2.13	1.40	1.34
22	J	302	CDL	OB6-CB5	2.13	1.40	1.34
22	f	303	CDL	OB8-CB6	-2.12	1.40	1.45
22	j	302	CDL	OB6-CB5	2.12	1.40	1.34
22	p	201	CDL	OA6-CA5	2.12	1.40	1.34
22	K	201	CDL	OA8-CA6	-2.12	1.40	1.45
29	e	900	NAD	C2D-C1D	2.12	1.57	1.53
22	p	201	CDL	OB6-CB5	2.11	1.40	1.34
22	i	302	CDL	OA8-CA6	-2.11	1.40	1.45
28	l	303	PEE	O3-C3	-2.11	1.40	1.45
22	j	301	CDL	OB8-CB6	-2.11	1.40	1.45
22	B	401	CDL	OB8-CB6	-2.11	1.40	1.45
22	J	301	CDL	OB8-CB6	-2.11	1.40	1.45
25	i	303	UQ8	C6-C5	2.11	1.52	1.46
22	K	202	CDL	OA8-CA6	-2.10	1.40	1.45
22	K	202	CDL	OB8-CB6	-2.10	1.40	1.45
22	L	301	CDL	OB6-CB5	2.10	1.40	1.34
22	J	302	CDL	OB8-CB6	-2.10	1.40	1.45
22	b	401	CDL	OA8-CA6	-2.09	1.40	1.45
22	A	501	CDL	OB6-CB5	2.09	1.40	1.34
22	b	402	CDL	OB6-CB5	2.09	1.40	1.34
22	l	304	CDL	OA6-CA5	2.09	1.40	1.34
22	k	202	CDL	OA8-CA6	-2.08	1.40	1.45
23	G	303	PC1	O21-C21	2.08	1.40	1.34
22	B	403	CDL	OA8-CA6	-2.08	1.40	1.45
22	P	201	CDL	OA8-CA6	-2.08	1.40	1.45
22	B	404	CDL	OA8-CA6	-2.08	1.40	1.45
22	f	302	CDL	OB6-CB5	2.07	1.40	1.34
22	I	302	CDL	OA8-CA6	-2.07	1.40	1.45
23	i	301	PC1	O31-C3	-2.07	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	E	900	NAD	C2A-N3A	2.07	1.35	1.32
22	P	201	CDL	OA6-CA5	2.06	1.40	1.34
22	j	301	CDL	OA6-CA5	2.06	1.40	1.34
22	f	302	CDL	OA6-CA5	2.06	1.40	1.34
22	k	201	CDL	OB8-CB6	-2.05	1.40	1.45
22	p	201	CDL	OA8-CA6	-2.05	1.40	1.45
22	B	403	CDL	OB6-CB5	2.05	1.40	1.34
22	a	501	CDL	OA6-CA5	2.04	1.40	1.34
22	K	201	CDL	OB8-CB6	-2.04	1.40	1.45
29	e	900	NAD	PA-O5B	2.04	1.67	1.59
22	B	401	CDL	OB6-CB5	2.04	1.40	1.34
23	i	301	PC1	O21-C21	2.04	1.40	1.34
22	k	201	CDL	OA8-CA6	-2.03	1.40	1.45
29	e	900	NAD	C2A-N3A	2.03	1.35	1.32
22	f	302	CDL	OA8-CA6	-2.03	1.40	1.45
22	j	302	CDL	OB8-CB6	-2.02	1.40	1.45
22	b	401	CDL	OB6-CB5	2.02	1.40	1.34
22	B	404	CDL	OB6-CB5	2.02	1.40	1.34
22	P	201	CDL	OB8-CB6	-2.02	1.40	1.45
22	B	405	CDL	OA8-CA6	-2.02	1.40	1.45
29	E	900	NAD	PA-O5B	2.01	1.67	1.59
22	B	405	CDL	OB8-CB6	-2.01	1.40	1.45
22	f	303	CDL	OA8-CA6	-2.01	1.40	1.45
22	l	301	CDL	OB6-CB5	2.01	1.40	1.34
22	L	301	CDL	OA6-CA5	2.01	1.40	1.34
22	I	301	CDL	OA8-CA6	-2.00	1.40	1.45
22	p	201	CDL	OB8-CB6	-2.00	1.40	1.45

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	e	900	NAD	C1B-N9A-C4A	-8.37	111.94	126.64
29	E	900	NAD	C1B-N9A-C4A	-8.11	112.38	126.64
29	e	900	NAD	C5A-C6A-N6A	8.10	132.67	120.35
29	E	900	NAD	C5A-C6A-N6A	7.92	132.39	120.35
26	G	301	ATP	C5-C6-N6	7.45	131.68	120.35
26	g	301	ATP	C5-C6-N6	7.44	131.66	120.35
26	G	301	ATP	C1'-N9-C4	5.59	136.46	126.64
26	g	301	ATP	C1'-N9-C4	5.46	136.23	126.64
29	e	900	NAD	N3A-C2A-N1A	-5.44	120.17	128.68
29	e	900	NAD	N6A-C6A-N1A	-5.41	107.34	118.57
26	G	301	ATP	N3-C2-N1	-5.39	120.26	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	E	900	NAD	N3A-C2A-N1A	-5.38	120.27	128.68
29	E	900	NAD	N6A-C6A-N1A	-5.33	107.51	118.57
26	g	301	ATP	N3-C2-N1	-5.31	120.37	128.68
26	g	301	ATP	N6-C6-N1	-5.04	108.10	118.57
22	k	201	CDL	OA6-CA5-C11	5.00	122.28	111.50
26	G	301	ATP	N6-C6-N1	-4.95	108.30	118.57
23	D	301	PC1	O21-C21-C22	4.94	122.14	111.50
23	d	301	PC1	O21-C21-C22	4.91	122.08	111.50
22	f	304	CDL	OB6-CB5-C51	4.82	121.90	111.50
23	g	303	PC1	O21-C21-C22	4.82	121.89	111.50
22	f	302	CDL	OB6-CB5-C51	4.74	121.71	111.50
22	f	303	CDL	OA6-CA5-C11	4.73	121.70	111.50
22	B	403	CDL	OB6-CB5-C51	4.69	121.62	111.50
23	G	304	PC1	O21-C21-C22	4.65	121.52	111.50
22	l	301	CDL	OB6-CB5-C51	4.45	121.10	111.50
22	B	405	CDL	OA6-CA5-C11	4.42	121.03	111.50
22	K	201	CDL	OA6-CA5-C11	4.37	120.91	111.50
22	B	402	CDL	OA6-CA5-C11	4.33	120.83	111.50
25	I	303	UQ8	C40-C39-C41	4.31	122.53	115.27
26	G	301	ATP	C3'-C2'-C1'	4.24	107.36	100.98
26	g	301	ATP	C3'-C2'-C1'	4.23	107.35	100.98
22	P	201	CDL	OB6-CB5-C51	4.18	120.51	111.50
22	j	301	CDL	OA6-CA5-C11	4.18	120.50	111.50
22	J	301	CDL	OA6-CA5-C11	4.13	120.39	111.50
28	l	303	PEE	O2-C10-C11	4.12	120.39	111.50
22	J	301	CDL	OB6-CB5-C51	4.12	120.38	111.50
22	j	301	CDL	OB6-CB5-C51	4.12	120.37	111.50
22	k	203	CDL	OB6-CB5-C51	4.06	120.24	111.50
22	j	302	CDL	OB6-CB5-C51	4.04	120.21	111.50
22	k	202	CDL	OB6-CB5-C51	4.00	120.11	111.50
22	I	302	CDL	OB6-CB5-C51	3.98	120.08	111.50
22	J	302	CDL	OB6-CB5-C51	3.97	120.06	111.50
22	k	201	CDL	OB6-CB5-C51	3.97	120.06	111.50
22	K	202	CDL	OB6-CB5-C51	3.95	120.01	111.50
22	b	401	CDL	OB6-CB5-C51	3.94	120.00	111.50
22	i	302	CDL	OB6-CB5-C51	3.91	119.93	111.50
22	B	401	CDL	OA6-CA5-C11	3.90	119.90	111.50
22	f	303	CDL	OB6-CB5-C51	3.89	119.88	111.50
22	l	304	CDL	OB6-CB5-C51	3.85	119.80	111.50
22	p	201	CDL	OA6-CA5-C11	3.84	119.79	111.50
22	a	501	CDL	OB6-CB5-C51	3.81	119.72	111.50
22	B	404	CDL	OA6-CA5-C11	3.81	119.72	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	401	CDL	OA6-CA5-C11	3.81	119.71	111.50
22	I	302	CDL	OA6-CA5-C11	3.80	119.69	111.50
23	i	301	PC1	O21-C21-C22	3.78	119.66	111.50
22	p	201	CDL	OB6-CB5-C51	3.78	119.64	111.50
22	B	405	CDL	OB6-CB5-C51	3.78	119.64	111.50
22	f	304	CDL	OA6-CA5-C11	3.76	119.61	111.50
22	A	501	CDL	OB6-CB5-C51	3.71	119.49	111.50
22	P	201	CDL	OA6-CA5-C11	3.70	119.48	111.50
22	L	301	CDL	OA6-CA5-C11	3.68	119.42	111.50
23	G	303	PC1	O21-C21-C22	3.66	119.38	111.50
22	B	401	CDL	OB6-CB5-C51	3.65	119.36	111.50
28	J	304	PEE	O2-C10-C11	3.62	119.30	111.50
22	A	501	CDL	OA6-CA5-C11	3.61	119.28	111.50
22	f	302	CDL	OA6-CA5-C11	3.60	119.25	111.50
22	l	304	CDL	OA6-CA5-C11	3.59	119.23	111.50
22	a	501	CDL	OA6-CA5-C11	3.58	119.21	111.50
28	l	302	PEE	O2-C10-C11	3.57	119.20	111.50
22	B	402	CDL	OB6-CB5-C51	3.56	119.18	111.50
25	i	303	UQ8	C25-C24-C26	3.56	121.26	115.27
22	L	301	CDL	OB6-CB5-C51	3.49	119.03	111.50
22	b	402	CDL	OA6-CA5-C11	3.48	119.00	111.50
22	k	202	CDL	OA6-CA5-C11	3.47	118.97	111.50
22	K	201	CDL	OB6-CB5-C51	3.45	118.93	111.50
28	J	303	PEE	O2-C10-C11	3.40	118.84	111.50
25	I	303	UQ8	C27-C28-C29	-3.40	119.48	127.66
22	f	303	CDL	OA8-CA7-C31	3.35	122.44	111.91
22	l	301	CDL	OA6-CA5-C11	3.35	118.72	111.50
25	i	303	UQ8	C7-C8-C9	-3.34	121.23	126.79
22	k	203	CDL	OA6-CA5-C11	3.33	118.68	111.50
22	B	403	CDL	OA6-CA5-C11	3.31	118.63	111.50
25	I	303	UQ8	C20-C19-C21	3.28	120.79	115.27
22	K	202	CDL	OA6-CA5-C11	3.26	118.52	111.50
25	I	303	UQ8	C17-C18-C19	-3.26	119.82	127.66
22	I	301	CDL	OA6-CA5-C11	3.25	118.51	111.50
25	i	303	UQ8	C35-C34-C36	3.25	120.74	115.27
25	I	303	UQ8	C7-C8-C9	-3.24	121.41	126.79
26	G	301	ATP	PB-O3B-PG	-3.21	121.81	132.83
22	r	201	CDL	OA6-CA5-C11	3.21	118.42	111.50
22	i	302	CDL	OA6-CA5-C11	3.20	118.41	111.50
29	e	900	NAD	PN-O3-PA	-3.15	122.01	132.83
26	g	301	ATP	PB-O3B-PG	-3.14	122.04	132.83
22	r	201	CDL	OB6-CB5-C51	3.14	118.26	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	i	303	UQ8	C30-C29-C31	3.13	120.54	115.27
25	i	303	UQ8	C17-C18-C19	-3.12	120.15	127.66
25	I	303	UQ8	C25-C24-C26	3.08	120.45	115.27
22	I	301	CDL	OB6-CB5-C51	3.07	118.13	111.50
22	l	304	CDL	OA8-CA7-C31	3.04	121.46	111.91
22	b	402	CDL	OB6-CB5-C51	3.02	118.01	111.50
29	E	900	NAD	PN-O3-PA	-2.97	122.62	132.83
22	j	302	CDL	OA8-CA7-C31	2.93	121.10	111.91
22	K	201	CDL	OB8-CB7-C71	2.91	121.04	111.91
22	f	302	CDL	OA8-CA7-C31	2.90	120.99	111.91
22	B	404	CDL	OB6-CB5-C51	2.89	117.73	111.50
25	i	303	UQ8	C40-C39-C41	2.89	120.13	115.27
23	G	304	PC1	O31-C31-C32	2.89	120.96	111.91
22	J	302	CDL	OA6-CA5-C11	2.83	117.61	111.50
22	J	301	CDL	OB8-CB7-C71	2.83	120.80	111.91
22	B	403	CDL	OA8-CA7-C31	2.83	120.78	111.91
25	i	303	UQ8	C27-C28-C29	-2.82	120.87	127.66
22	K	202	CDL	OA8-CA7-C31	2.82	120.76	111.91
22	I	301	CDL	OA8-CA7-C31	2.79	120.67	111.91
28	J	304	PEE	O3-C30-C31	2.78	120.63	111.91
22	B	405	CDL	OA8-CA7-C31	2.78	120.63	111.91
22	p	201	CDL	OB8-CB7-C71	2.77	120.61	111.91
22	k	201	CDL	OB8-CB7-C71	2.75	120.55	111.91
22	j	302	CDL	OA6-CA5-C11	2.75	117.42	111.50
28	l	303	PEE	O3-C30-C31	2.74	120.49	111.91
22	p	201	CDL	OA8-CA7-C31	2.72	120.46	111.91
22	J	301	CDL	OA8-CA7-C31	2.72	120.45	111.91
22	P	201	CDL	OA8-CA7-C31	2.72	120.44	111.91
22	B	405	CDL	OB8-CB7-C71	2.71	120.41	111.91
22	j	301	CDL	OA8-CA7-C31	2.71	120.41	111.91
25	i	303	UQ8	C22-C23-C24	-2.70	121.16	127.66
22	k	202	CDL	OA8-CA7-C31	2.69	120.33	111.91
22	f	303	CDL	OB8-CB7-C71	2.68	120.33	111.91
28	J	303	PEE	O3-C30-C31	2.67	120.27	111.91
25	I	303	UQ8	C22-C23-C24	-2.64	121.31	127.66
22	r	201	CDL	OA8-CA7-C31	2.62	120.12	111.91
23	G	303	PC1	O31-C31-C32	2.61	120.10	111.91
25	i	303	UQ8	C20-C19-C21	2.60	119.65	115.27
22	j	302	CDL	OB8-CB7-C71	2.60	120.07	111.91
22	K	202	CDL	CA4-OA6-CA5	-2.60	111.39	117.79
22	B	401	CDL	OA8-CA7-C31	2.58	120.01	111.91
22	k	201	CDL	OA8-CA7-C31	2.57	119.97	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	i	301	PC1	O31-C31-C32	2.55	119.92	111.91
22	b	401	CDL	OA8-CA7-C31	2.53	119.86	111.91
22	P	201	CDL	OB8-CB7-C71	2.53	119.86	111.91
22	k	202	CDL	CA4-OA6-CA5	-2.53	111.56	117.79
22	K	202	CDL	OB8-CB7-C71	2.53	119.83	111.91
25	i	303	UQ8	C12-C13-C14	-2.52	121.59	127.66
22	i	302	CDL	OB8-CB7-C71	2.51	119.79	111.91
22	a	501	CDL	OB8-CB7-C71	2.51	119.77	111.91
26	G	301	ATP	PA-O3A-PB	-2.51	124.23	132.83
22	K	201	CDL	OA8-CA7-C31	2.50	119.75	111.91
22	j	301	CDL	OB8-CB7-C71	2.50	119.74	111.91
22	b	402	CDL	OB8-CB7-C71	2.47	119.65	111.91
22	L	301	CDL	OA8-CA7-C31	2.47	119.65	111.91
22	f	304	CDL	OA8-CA7-C31	2.46	119.62	111.91
22	J	302	CDL	OB8-CB7-C71	2.43	119.55	111.91
22	l	301	CDL	OA8-CA7-C31	2.42	119.52	111.91
22	B	404	CDL	OA8-CA7-C31	2.41	119.47	111.91
22	r	201	CDL	OB8-CB7-C71	2.40	119.43	111.91
22	A	501	CDL	OA8-CA7-C31	2.40	119.42	111.91
22	I	302	CDL	OA8-CA7-C31	2.39	119.40	111.91
23	g	303	PC1	O31-C31-C32	2.39	119.39	111.91
22	k	203	CDL	OA8-CA7-C31	2.38	119.38	111.91
23	D	301	PC1	O31-C31-C32	2.38	119.37	111.91
25	I	303	UQ8	C1M-C1-C6	-2.38	120.52	124.40
22	I	302	CDL	OB8-CB7-C71	2.37	119.36	111.91
22	B	403	CDL	OB8-CB7-C71	2.37	119.35	111.91
28	l	302	PEE	O3-C30-C31	2.37	119.33	111.91
22	f	304	CDL	OB8-CB7-C71	2.35	119.28	111.91
22	i	302	CDL	OA8-CA7-C31	2.34	119.26	111.91
22	b	402	CDL	OA8-CA7-C31	2.34	119.25	111.91
22	L	301	CDL	OB8-CB7-C71	2.34	119.25	111.91
26	g	301	ATP	PA-O3A-PB	-2.34	124.80	132.83
22	A	501	CDL	CB4-OB6-CB5	-2.33	112.05	117.79
22	B	401	CDL	OB8-CB7-C71	2.32	119.19	111.91
25	i	303	UQ8	C46-C44-C45	2.31	119.70	114.60
22	k	202	CDL	OB8-CB7-C71	2.29	119.11	111.91
25	I	303	UQ8	C12-C13-C14	-2.29	122.14	127.66
23	d	301	PC1	O31-C31-C32	2.29	119.10	111.91
25	i	303	UQ8	C1M-C1-C6	-2.29	120.67	124.40
22	b	401	CDL	OB8-CB7-C71	2.27	119.02	111.91
25	I	303	UQ8	C41-C39-C38	-2.26	116.55	121.12
22	J	302	CDL	OA8-CA7-C31	2.25	118.97	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	l	304	CDL	OB8-CB7-C71	2.25	118.97	111.91
25	i	303	UQ8	C40-C39-C38	-2.22	117.97	123.68
25	I	303	UQ8	C35-C34-C33	-2.22	117.98	123.68
22	f	303	CDL	OA6-CA5-OA7	-2.19	118.40	123.70
22	B	402	CDL	OA8-CA7-C31	2.19	118.78	111.91
28	J	304	PEE	C17-C18-C19	-2.19	107.94	124.73
29	e	900	NAD	C6N-N1N-C2N	-2.19	119.98	121.97
22	B	404	CDL	OB8-CB7-C71	2.16	118.69	111.91
22	k	201	CDL	OA6-CA5-OA7	-2.15	118.50	123.70
22	k	203	CDL	OB8-CB7-C71	2.15	118.66	111.91
29	E	900	NAD	C6N-N1N-C2N	-2.14	120.02	121.97
22	B	402	CDL	OB8-CB7-C71	2.14	118.61	111.91
22	l	301	CDL	OB8-CB7-C71	2.12	118.57	111.91
25	I	303	UQ8	C42-C43-C44	-2.12	120.50	127.75
28	J	303	PEE	C17-C18-C19	-2.12	108.48	124.73
29	e	900	NAD	C3B-C2B-C1B	2.11	104.16	100.98
22	B	405	CDL	OA6-CA5-OA7	-2.11	118.60	123.70
22	A	501	CDL	OB8-CB7-C71	2.11	118.53	111.91
25	i	303	UQ8	C37-C38-C39	-2.08	122.65	127.66
28	l	302	PEE	C37-C38-C39	-2.08	108.78	124.73
25	i	303	UQ8	C32-C33-C34	-2.04	122.74	127.66
28	J	303	PEE	C40-C39-C38	-2.03	109.12	124.73
22	f	302	CDL	OB8-CB7-C71	2.02	118.26	111.91
22	B	401	CDL	CB4-OB6-CB5	-2.02	112.81	117.79
25	I	303	UQ8	C30-C29-C31	2.02	118.67	115.27
28	l	303	PEE	C17-C18-C19	-2.01	109.27	124.73
22	P	201	CDL	CA4-OA6-CA5	-2.01	112.84	117.79
23	d	301	PC1	O21-C21-O22	-2.01	118.85	123.70

There are no chirality outliers.

All (1517) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	a	501	CDL	CB3-OB5-PB2-OB3
22	a	501	CDL	CB3-OB5-PB2-OB4
22	a	501	CDL	OB7-CB5-OB6-CB4
22	a	501	CDL	C51-CB5-OB6-CB4
22	b	401	CDL	C1-CA2-OA2-PA1
22	b	401	CDL	CA4-CA3-OA5-PA1
22	b	401	CDL	C11-CA5-OA6-CA4
22	b	401	CDL	CB2-OB2-PB2-OB5
22	b	402	CDL	CA3-OA5-PA1-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	f	302	CDL	CA3-OA5-PA1-OA3
22	f	302	CDL	CA3-OA5-PA1-OA4
22	f	302	CDL	C11-CA5-OA6-CA4
22	f	302	CDL	CB3-OB5-PB2-OB3
22	f	302	CDL	CB3-OB5-PB2-OB4
22	f	302	CDL	OB7-CB5-OB6-CB4
22	f	302	CDL	C51-CB5-OB6-CB4
22	f	303	CDL	CA2-C1-CB2-OB2
22	f	303	CDL	OA7-CA5-OA6-CA4
22	f	303	CDL	C11-CA5-OA6-CA4
22	f	303	CDL	OA9-CA7-OA8-CA6
22	f	303	CDL	C31-CA7-OA8-CA6
22	f	303	CDL	CB2-OB2-PB2-OB3
22	f	303	CDL	CB3-OB5-PB2-OB3
22	f	303	CDL	CB3-OB5-PB2-OB4
22	f	303	CDL	OB6-CB4-CB6-OB8
22	f	304	CDL	CB2-C1-CA2-OA2
22	f	304	CDL	CA2-C1-CB2-OB2
22	f	304	CDL	CB2-OB2-PB2-OB3
22	f	304	CDL	CB3-OB5-PB2-OB3
22	f	304	CDL	CB3-OB5-PB2-OB4
22	f	304	CDL	OB7-CB5-OB6-CB4
22	i	302	CDL	CB3-OB5-PB2-OB2
22	i	302	CDL	CB3-OB5-PB2-OB3
22	i	302	CDL	CB3-OB5-PB2-OB4
22	i	302	CDL	OB7-CB5-OB6-CB4
22	i	302	CDL	C51-CB5-OB6-CB4
22	k	201	CDL	OA7-CA5-OA6-CA4
22	k	201	CDL	C11-CA5-OA6-CA4
22	k	201	CDL	CB2-OB2-PB2-OB3
22	k	201	CDL	CB3-OB5-PB2-OB3
22	k	202	CDL	C11-CA5-OA6-CA4
22	k	202	CDL	CB3-OB5-PB2-OB2
22	k	202	CDL	CB3-OB5-PB2-OB3
22	k	202	CDL	CB3-OB5-PB2-OB4
22	k	203	CDL	CB3-OB5-PB2-OB3
22	j	301	CDL	C51-CB5-OB6-CB4
22	j	302	CDL	CA3-OA5-PA1-OA2
22	j	302	CDL	CA3-OA5-PA1-OA3
22	j	302	CDL	CA3-OA5-PA1-OA4
22	j	302	CDL	CB3-OB5-PB2-OB3
22	j	302	CDL	CB3-OB5-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	l	301	CDL	CA3-OA5-PA1-OA4
22	p	201	CDL	CB2-OB2-PB2-OB3
22	p	201	CDL	CB3-OB5-PB2-OB3
22	p	201	CDL	CB3-OB5-PB2-OB4
22	r	201	CDL	CB2-OB2-PB2-OB3
22	A	501	CDL	CB2-C1-CA2-OA2
22	A	501	CDL	C1-CA2-OA2-PA1
22	A	501	CDL	CA2-OA2-PA1-OA3
22	A	501	CDL	CB3-OB5-PB2-OB3
22	A	501	CDL	CB3-OB5-PB2-OB4
22	A	501	CDL	C51-CB5-OB6-CB4
22	B	401	CDL	CB2-C1-CA2-OA2
22	B	401	CDL	O1-C1-CB2-OB2
22	B	401	CDL	CB3-OB5-PB2-OB3
22	B	401	CDL	C51-CB5-OB6-CB4
22	B	402	CDL	CA4-CA3-OA5-PA1
22	B	402	CDL	C11-CA5-OA6-CA4
22	B	402	CDL	CB3-OB5-PB2-OB3
22	B	403	CDL	OA7-CA5-OA6-CA4
22	B	403	CDL	CB3-OB5-PB2-OB3
22	B	403	CDL	CB3-OB5-PB2-OB4
22	B	403	CDL	OB7-CB5-OB6-CB4
22	B	404	CDL	CA3-OA5-PA1-OA2
22	B	405	CDL	CA2-C1-CB2-OB2
22	B	405	CDL	OA7-CA5-OA6-CA4
22	B	405	CDL	OA9-CA7-OA8-CA6
22	B	405	CDL	C31-CA7-OA8-CA6
22	B	405	CDL	CB2-OB2-PB2-OB3
22	B	405	CDL	CB3-OB5-PB2-OB3
22	B	405	CDL	CB3-OB5-PB2-OB4
22	I	301	CDL	CB3-OB5-PB2-OB3
22	I	301	CDL	CB3-OB5-PB2-OB4
22	I	302	CDL	CB2-C1-CA2-OA2
22	I	302	CDL	O1-C1-CB2-OB2
22	I	302	CDL	CB3-OB5-PB2-OB2
22	I	302	CDL	CB3-OB5-PB2-OB3
22	I	302	CDL	CB3-OB5-PB2-OB4
22	I	302	CDL	OB7-CB5-OB6-CB4
22	I	302	CDL	C51-CB5-OB6-CB4
22	K	201	CDL	CB2-C1-CA2-OA2
22	K	201	CDL	CA3-OA5-PA1-OA3
22	K	201	CDL	OA7-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	K	201	CDL	C11-CA5-OA6-CA4
22	K	201	CDL	CB2-OB2-PB2-OB3
22	K	201	CDL	CB3-OB5-PB2-OB3
22	K	202	CDL	OA5-CA3-CA4-OA6
22	K	202	CDL	OA7-CA5-OA6-CA4
22	K	202	CDL	C11-CA5-OA6-CA4
22	K	202	CDL	CB3-OB5-PB2-OB2
22	K	202	CDL	CB3-OB5-PB2-OB3
22	K	202	CDL	CB3-OB5-PB2-OB4
22	J	301	CDL	OB7-CB5-OB6-CB4
22	J	302	CDL	CA3-OA5-PA1-OA4
22	J	302	CDL	CB3-OB5-PB2-OB3
22	J	302	CDL	CB3-OB5-PB2-OB4
22	L	301	CDL	O1-C1-CA2-OA2
22	L	301	CDL	CA3-OA5-PA1-OA2
22	P	201	CDL	CB2-OB2-PB2-OB3
22	P	201	CDL	CB2-OB2-PB2-OB5
22	P	201	CDL	CB3-OB5-PB2-OB2
22	P	201	CDL	CB3-OB5-PB2-OB3
22	P	201	CDL	CB3-OB5-PB2-OB4
23	d	301	PC1	O22-C21-O21-C2
23	d	301	PC1	C22-C21-O21-C2
23	g	303	PC1	O22-C21-O21-C2
23	g	303	PC1	C22-C21-O21-C2
23	D	301	PC1	O13-C11-C12-N
23	D	301	PC1	O22-C21-O21-C2
23	D	301	PC1	C22-C21-O21-C2
23	G	303	PC1	C1-O11-P-O12
23	G	303	PC1	C1-O11-P-O14
23	G	304	PC1	O22-C21-O21-C2
25	i	303	UQ8	C34-C36-C37-C38
25	i	303	UQ8	C29-C31-C32-C33
25	I	303	UQ8	C40-C39-C41-C42
25	I	303	UQ8	C38-C39-C41-C42
28	l	302	PEE	C1-O3P-P-O1P
28	l	302	PEE	C4-O4P-P-O2P
28	l	302	PEE	C4-O4P-P-O1P
28	l	303	PEE	C4-O4P-P-O2P
28	l	303	PEE	C4-O4P-P-O1P
28	J	303	PEE	C1-O3P-P-O2P
28	J	303	PEE	C1-O3P-P-O1P
28	J	303	PEE	C1-O3P-P-O4P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	J	304	PEE	C17-C18-C19-C20
28	J	304	PEE	C4-O4P-P-O2P
28	J	304	PEE	C4-O4P-P-O1P
29	e	900	NAD	C5B-O5B-PA-O2A
29	E	900	NAD	C5D-O5D-PN-O3
28	J	303	PEE	O5-C30-O3-C3
22	f	303	CDL	OB9-CB7-OB8-CB6
22	k	201	CDL	OB9-CB7-OB8-CB6
22	k	202	CDL	OA9-CA7-OA8-CA6
22	l	304	CDL	OB9-CB7-OB8-CB6
22	r	201	CDL	OA9-CA7-OA8-CA6
22	r	201	CDL	OB9-CB7-OB8-CB6
22	B	404	CDL	OB9-CB7-OB8-CB6
22	B	405	CDL	OB9-CB7-OB8-CB6
22	I	301	CDL	OA9-CA7-OA8-CA6
22	I	301	CDL	OB9-CB7-OB8-CB6
22	J	302	CDL	OA9-CA7-OA8-CA6
28	l	302	PEE	O5-C30-O3-C3
28	l	303	PEE	O5-C30-O3-C3
22	b	401	CDL	OA7-CA5-OA6-CA4
22	f	302	CDL	OA7-CA5-OA6-CA4
22	k	202	CDL	OA7-CA5-OA6-CA4
22	j	301	CDL	OB7-CB5-OB6-CB4
22	p	201	CDL	OA7-CA5-OA6-CA4
22	A	501	CDL	OB7-CB5-OB6-CB4
22	B	401	CDL	OB7-CB5-OB6-CB4
22	B	404	CDL	OA7-CA5-OA6-CA4
22	P	201	CDL	OA7-CA5-OA6-CA4
22	j	302	CDL	OA9-CA7-OA8-CA6
22	k	201	CDL	C71-CB7-OB8-CB6
22	k	203	CDL	C71-CB7-OB8-CB6
22	r	201	CDL	C31-CA7-OA8-CA6
22	B	405	CDL	C71-CB7-OB8-CB6
22	I	301	CDL	C31-CA7-OA8-CA6
28	l	303	PEE	C31-C30-O3-C3
28	J	303	PEE	C31-C30-O3-C3
22	f	304	CDL	C51-CB5-OB6-CB4
22	p	201	CDL	C11-CA5-OA6-CA4
22	B	403	CDL	C11-CA5-OA6-CA4
22	B	403	CDL	C51-CB5-OB6-CB4
22	B	405	CDL	C11-CA5-OA6-CA4
22	J	301	CDL	C51-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	P	201	CDL	C11-CA5-OA6-CA4
23	G	304	PC1	C22-C21-O21-C2
22	f	303	CDL	C71-CB7-OB8-CB6
22	k	202	CDL	C31-CA7-OA8-CA6
22	j	302	CDL	C31-CA7-OA8-CA6
22	l	304	CDL	C71-CB7-OB8-CB6
22	r	201	CDL	C71-CB7-OB8-CB6
22	B	401	CDL	C31-CA7-OA8-CA6
22	B	404	CDL	C71-CB7-OB8-CB6
22	I	301	CDL	C71-CB7-OB8-CB6
22	K	202	CDL	C31-CA7-OA8-CA6
22	J	302	CDL	C31-CA7-OA8-CA6
28	l	302	PEE	C31-C30-O3-C3
22	B	402	CDL	OA7-CA5-OA6-CA4
22	b	402	CDL	OB9-CB7-OB8-CB6
22	k	203	CDL	OB9-CB7-OB8-CB6
22	K	201	CDL	OB9-CB7-OB8-CB6
22	K	202	CDL	OA9-CA7-OA8-CA6
22	f	303	CDL	O1-C1-CB2-OB2
22	f	304	CDL	O1-C1-CB2-OB2
22	k	201	CDL	O1-C1-CA2-OA2
22	k	202	CDL	O1-C1-CA2-OA2
22	B	405	CDL	O1-C1-CB2-OB2
22	I	301	CDL	O1-C1-CA2-OA2
22	K	201	CDL	O1-C1-CA2-OA2
23	d	301	PC1	C32-C31-O31-C3
22	B	401	CDL	OA9-CA7-OA8-CA6
22	a	501	CDL	C11-CA5-OA6-CA4
22	b	402	CDL	C11-CA5-OA6-CA4
22	j	302	CDL	C11-CA5-OA6-CA4
22	l	304	CDL	C11-CA5-OA6-CA4
22	r	201	CDL	C11-CA5-OA6-CA4
22	B	404	CDL	C11-CA5-OA6-CA4
22	I	301	CDL	C11-CA5-OA6-CA4
22	J	302	CDL	C11-CA5-OA6-CA4
28	J	303	PEE	C34-C35-C36-C37
29	E	900	NAD	O4D-C4D-C5D-O5D
22	b	402	CDL	C71-CB7-OB8-CB6
22	K	201	CDL	C71-CB7-OB8-CB6
23	D	301	PC1	C32-C31-O31-C3
22	a	501	CDL	OA7-CA5-OA6-CA4
22	b	402	CDL	OA7-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	r	201	CDL	OA7-CA5-OA6-CA4
22	I	301	CDL	OA7-CA5-OA6-CA4
23	d	301	PC1	O32-C31-O31-C3
28	l	302	PEE	C34-C35-C36-C37
23	D	301	PC1	O32-C31-O31-C3
25	I	303	UQ8	C39-C41-C42-C43
25	I	303	UQ8	C34-C36-C37-C38
25	I	303	UQ8	C29-C31-C32-C33
22	k	203	CDL	C11-CA5-OA6-CA4
22	b	402	CDL	CB2-C1-CA2-OA2
22	i	302	CDL	CB2-C1-CA2-OA2
22	k	201	CDL	CB2-C1-CA2-OA2
22	B	401	CDL	CA2-C1-CB2-OB2
22	B	402	CDL	CA2-C1-CB2-OB2
22	B	404	CDL	CB2-C1-CA2-OA2
22	I	301	CDL	CB2-C1-CA2-OA2
22	I	302	CDL	CA2-C1-CB2-OB2
22	L	301	CDL	CB2-C1-CA2-OA2
22	j	302	CDL	OA7-CA5-OA6-CA4
22	l	304	CDL	OA7-CA5-OA6-CA4
22	J	302	CDL	OA7-CA5-OA6-CA4
22	B	401	CDL	C71-CB7-OB8-CB6
22	L	301	CDL	CA7-C31-C32-C33
22	B	401	CDL	OA5-CA3-CA4-OA6
22	b	402	CDL	O1-C1-CA2-OA2
22	f	302	CDL	O1-C1-CB2-OB2
22	A	501	CDL	O1-C1-CA2-OA2
22	B	401	CDL	O1-C1-CA2-OA2
22	B	402	CDL	O1-C1-CB2-OB2
22	B	403	CDL	O1-C1-CB2-OB2
22	B	404	CDL	O1-C1-CA2-OA2
22	b	402	CDL	CA5-C11-C12-C13
22	B	405	CDL	OB6-CB4-CB6-OB8
28	J	304	PEE	O2-C2-C3-O3
22	f	304	CDL	C11-CA5-OA6-CA4
22	A	501	CDL	C11-CA5-OA6-CA4
22	B	405	CDL	CB5-C51-C52-C53
22	f	303	CDL	CA5-C11-C12-C13
22	f	303	CDL	CB7-C71-C72-C73
22	i	302	CDL	CB5-C51-C52-C53
22	k	201	CDL	CA5-C11-C12-C13
22	l	301	CDL	CB5-C51-C52-C53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	B	401	CDL	CB5-C51-C52-C53
22	B	404	CDL	CA5-C11-C12-C13
22	J	302	CDL	CA5-C11-C12-C13
22	B	401	CDL	OB9-CB7-OB8-CB6
22	f	304	CDL	CB5-C51-C52-C53
22	B	403	CDL	CA5-C11-C12-C13
22	B	404	CDL	CB7-C71-C72-C73
22	B	405	CDL	CA5-C11-C12-C13
22	l	301	CDL	C71-CB7-OB8-CB6
22	k	203	CDL	OA7-CA5-OA6-CA4
22	k	203	CDL	CA5-C11-C12-C13
22	r	201	CDL	CA5-C11-C12-C13
22	i	302	CDL	O1-C1-CA2-OA2
22	I	302	CDL	O1-C1-CA2-OA2
22	A	501	CDL	OA7-CA5-OA6-CA4
22	b	402	CDL	CA7-C31-C32-C33
22	i	302	CDL	CB7-C71-C72-C73
22	j	301	CDL	C11-CA5-OA6-CA4
22	B	401	CDL	C11-CA5-OA6-CA4
22	a	501	CDL	CB3-OB5-PB2-OB2
22	b	401	CDL	CB3-OB5-PB2-OB2
22	f	302	CDL	CA3-OA5-PA1-OA2
22	f	302	CDL	CB3-OB5-PB2-OB2
22	f	303	CDL	CB3-OB5-PB2-OB2
22	f	304	CDL	CB3-OB5-PB2-OB2
22	k	201	CDL	CB2-OB2-PB2-OB5
22	k	201	CDL	CB3-OB5-PB2-OB2
22	k	202	CDL	CB2-OB2-PB2-OB5
22	j	301	CDL	CB3-OB5-PB2-OB2
22	j	302	CDL	CB3-OB5-PB2-OB2
22	l	301	CDL	CA3-OA5-PA1-OA2
22	l	301	CDL	CB3-OB5-PB2-OB2
22	p	201	CDL	CB3-OB5-PB2-OB2
22	r	201	CDL	CA3-OA5-PA1-OA2
22	r	201	CDL	CB2-OB2-PB2-OB5
22	A	501	CDL	CB3-OB5-PB2-OB2
22	B	403	CDL	CB3-OB5-PB2-OB2
22	B	405	CDL	CB3-OB5-PB2-OB2
22	I	301	CDL	CA3-OA5-PA1-OA2
22	I	301	CDL	CB3-OB5-PB2-OB2
22	K	201	CDL	CB2-OB2-PB2-OB5
22	K	201	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	J	301	CDL	CB3-OB5-PB2-OB2
22	J	302	CDL	CA3-OA5-PA1-OA2
22	J	302	CDL	CB3-OB5-PB2-OB2
22	L	301	CDL	CB3-OB5-PB2-OB2
23	i	301	PC1	C11-O13-P-O11
23	G	303	PC1	C11-O13-P-O11
23	G	303	PC1	C1-O11-P-O13
28	l	302	PEE	C1-O3P-P-O4P
28	l	302	PEE	C4-O4P-P-O3P
28	l	303	PEE	C4-O4P-P-O3P
28	J	304	PEE	C1-O3P-P-O4P
28	J	304	PEE	C4-O4P-P-O3P
22	b	401	CDL	CB5-C51-C52-C53
22	j	302	CDL	CA5-C11-C12-C13
22	A	501	CDL	CA7-C31-C32-C33
22	k	202	CDL	CB2-C1-CA2-OA2
22	f	304	CDL	OA7-CA5-OA6-CA4
22	j	301	CDL	OA7-CA5-OA6-CA4
22	B	401	CDL	OA7-CA5-OA6-CA4
22	k	202	CDL	C74-C75-C76-C77
22	I	302	CDL	C19-C20-C21-C22
22	J	301	CDL	C33-C34-C35-C36
22	a	501	CDL	C33-C34-C35-C36
22	b	401	CDL	C77-C78-C79-C80
22	f	304	CDL	C79-C80-C81-C82
22	k	203	CDL	C15-C16-C17-C18
22	j	301	CDL	C14-C15-C16-C17
22	j	302	CDL	C72-C73-C74-C75
22	l	304	CDL	C78-C79-C80-C81
22	r	201	CDL	C20-C21-C22-C23
22	A	501	CDL	C16-C17-C18-C19
22	A	501	CDL	C36-C37-C38-C39
22	B	403	CDL	C51-C52-C53-C54
22	B	403	CDL	C81-C82-C83-C84
22	B	404	CDL	C51-C52-C53-C54
22	B	404	CDL	C74-C75-C76-C77
22	B	405	CDL	C16-C17-C18-C19
23	d	301	PC1	C28-C29-C2A-C2B
28	l	302	PEE	C42-C43-C44-C45
22	l	301	CDL	OB9-CB7-OB8-CB6
22	b	401	CDL	C35-C36-C37-C38
22	f	304	CDL	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	k	203	CDL	C78-C79-C80-C81
22	r	201	CDL	C53-C54-C55-C56
22	A	501	CDL	C13-C14-C15-C16
22	A	501	CDL	C74-C75-C76-C77
22	B	403	CDL	C72-C73-C74-C75
22	I	301	CDL	C43-C44-C45-C46
22	K	201	CDL	C72-C73-C74-C75
22	J	302	CDL	C21-C22-C23-C24
22	B	402	CDL	CA3-CA4-OA6-CA5
22	A	501	CDL	C55-C56-C57-C58
22	k	203	CDL	C79-C80-C81-C82
22	j	301	CDL	C20-C21-C22-C23
22	l	301	CDL	C72-C73-C74-C75
22	B	402	CDL	C38-C39-C40-C41
22	B	404	CDL	C82-C83-C84-C85
22	I	302	CDL	C12-C13-C14-C15
22	J	301	CDL	C20-C21-C22-C23
22	J	302	CDL	C72-C73-C74-C75
22	f	304	CDL	O1-C1-CA2-OA2
22	i	302	CDL	O1-C1-CB2-OB2
22	l	301	CDL	O1-C1-CA2-OA2
22	K	202	CDL	O1-C1-CA2-OA2
22	a	501	CDL	C74-C75-C76-C77
22	f	303	CDL	C43-C44-C45-C46
22	k	203	CDL	C52-C53-C54-C55
22	j	301	CDL	C31-C32-C33-C34
22	B	401	CDL	C18-C19-C20-C21
22	K	202	CDL	C78-C79-C80-C81
22	L	301	CDL	C57-C58-C59-C60
22	B	402	CDL	CB5-C51-C52-C53
22	B	404	CDL	CA7-C31-C32-C33
22	K	201	CDL	CA5-C11-C12-C13
22	b	402	CDL	C73-C74-C75-C76
22	f	304	CDL	C38-C39-C40-C41
22	f	304	CDL	C63-C64-C65-C66
22	p	201	CDL	C57-C58-C59-C60
22	A	501	CDL	C14-C15-C16-C17
22	B	405	CDL	C51-C52-C53-C54
22	J	302	CDL	C31-C32-C33-C34
22	L	301	CDL	C61-C62-C63-C64
22	P	201	CDL	C23-C24-C25-C26
22	a	501	CDL	C55-C56-C57-C58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	f	303	CDL	C35-C36-C37-C38
22	f	304	CDL	C82-C83-C84-C85
22	k	203	CDL	C31-C32-C33-C34
22	r	201	CDL	C82-C83-C84-C85
22	B	401	CDL	C74-C75-C76-C77
22	B	402	CDL	C18-C19-C20-C21
23	d	301	PC1	C2D-C2E-C2F-C2G
28	l	302	PEE	C43-C44-C45-C46
22	k	203	CDL	C16-C17-C18-C19
22	j	302	CDL	C31-C32-C33-C34
22	l	304	CDL	C76-C77-C78-C79
22	B	401	CDL	C39-C40-C41-C42
22	B	405	CDL	C35-C36-C37-C38
22	I	301	CDL	C81-C82-C83-C84
23	i	301	PC1	C35-C36-C37-C38
22	a	501	CDL	C36-C37-C38-C39
22	p	201	CDL	C74-C75-C76-C77
22	r	201	CDL	C18-C19-C20-C21
22	B	401	CDL	C63-C64-C65-C66
22	b	402	CDL	C51-C52-C53-C54
22	f	303	CDL	C79-C80-C81-C82
22	f	304	CDL	C22-C23-C24-C25
22	k	203	CDL	C71-C72-C73-C74
22	B	401	CDL	C11-C12-C13-C14
22	I	301	CDL	C18-C19-C20-C21
22	I	302	CDL	C74-C75-C76-C77
22	P	201	CDL	C52-C53-C54-C55
28	l	302	PEE	C32-C33-C34-C35
28	J	304	PEE	C19-C20-C21-C22
22	I	301	CDL	CA5-C11-C12-C13
22	a	501	CDL	C51-C52-C53-C54
22	b	401	CDL	C31-C32-C33-C34
22	b	401	CDL	C74-C75-C76-C77
22	b	402	CDL	C75-C76-C77-C78
22	f	302	CDL	C53-C54-C55-C56
22	j	301	CDL	C13-C14-C15-C16
22	p	201	CDL	C23-C24-C25-C26
22	p	201	CDL	C54-C55-C56-C57
22	B	401	CDL	C21-C22-C23-C24
22	B	402	CDL	C78-C79-C80-C81
22	B	405	CDL	C43-C44-C45-C46
22	I	301	CDL	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	J	302	CDL	C74-C75-C76-C77
28	J	303	PEE	C42-C43-C44-C45
22	a	501	CDL	C42-C43-C44-C45
22	j	301	CDL	C33-C34-C35-C36
22	B	402	CDL	C41-C42-C43-C44
22	J	301	CDL	C31-C32-C33-C34
22	b	402	CDL	C82-C83-C84-C85
22	k	202	CDL	C78-C79-C80-C81
22	p	201	CDL	C58-C59-C60-C61
22	B	403	CDL	C19-C20-C21-C22
22	B	404	CDL	C75-C76-C77-C78
22	J	301	CDL	C72-C73-C74-C75
22	f	304	CDL	CA5-C11-C12-C13
22	f	304	CDL	CB7-C71-C72-C73
22	l	304	CDL	CA5-C11-C12-C13
22	L	301	CDL	CA5-C11-C12-C13
23	G	303	PC1	C31-C32-C33-C34
28	J	303	PEE	C10-C11-C12-C13
22	b	401	CDL	C53-C54-C55-C56
22	P	201	CDL	C37-C38-C39-C40
28	J	304	PEE	C23-C24-C25-C26
23	G	304	PC1	C32-C31-O31-C3
22	b	402	CDL	C12-C13-C14-C15
22	j	301	CDL	C37-C38-C39-C40
22	A	501	CDL	C56-C57-C58-C59
22	B	405	CDL	C79-C80-C81-C82
28	l	302	PEE	C40-C41-C42-C43
22	f	303	CDL	C12-C13-C14-C15
22	k	201	CDL	C39-C40-C41-C42
22	k	203	CDL	C33-C34-C35-C36
22	j	302	CDL	C21-C22-C23-C24
22	B	403	CDL	C76-C77-C78-C79
23	d	301	PC1	C37-C38-C39-C3A
22	j	301	CDL	C78-C79-C80-C81
22	r	201	CDL	C16-C17-C18-C19
22	B	401	CDL	C72-C73-C74-C75
22	B	405	CDL	C12-C13-C14-C15
28	l	302	PEE	C41-C42-C43-C44
22	i	302	CDL	C31-CA7-OA8-CA6
22	b	401	CDL	C32-C33-C34-C35
22	k	202	CDL	C53-C54-C55-C56
22	k	203	CDL	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	B	404	CDL	C11-C12-C13-C14
22	P	201	CDL	C76-C77-C78-C79
22	a	501	CDL	C21-C22-C23-C24
22	i	302	CDL	C74-C75-C76-C77
22	k	203	CDL	C74-C75-C76-C77
22	k	203	CDL	C75-C76-C77-C78
22	j	301	CDL	C60-C61-C62-C63
22	B	402	CDL	C22-C23-C24-C25
22	K	202	CDL	C56-C57-C58-C59
29	E	900	NAD	C3B-C4B-C5B-O5B
29	E	900	NAD	C3D-C4D-C5D-O5D
22	l	304	CDL	C61-C62-C63-C64
22	P	201	CDL	C80-C81-C82-C83
23	d	301	PC1	C22-C23-C24-C25
22	a	501	CDL	C61-C62-C63-C64
22	B	401	CDL	C13-C14-C15-C16
22	K	202	CDL	C77-C78-C79-C80
28	l	302	PEE	C12-C13-C14-C15
22	r	201	CDL	CB2-C1-CA2-OA2
22	k	201	CDL	C56-C57-C58-C59
22	l	301	CDL	C11-C12-C13-C14
22	B	405	CDL	C56-C57-C58-C59
22	k	203	CDL	C53-C54-C55-C56
22	l	301	CDL	C21-C22-C23-C24
22	K	201	CDL	C60-C61-C62-C63
23	D	301	PC1	C28-C29-C2A-C2B
22	b	401	CDL	C22-C23-C24-C25
22	b	402	CDL	C58-C59-C60-C61
22	k	203	CDL	C54-C55-C56-C57
22	j	301	CDL	C72-C73-C74-C75
22	A	501	CDL	C75-C76-C77-C78
22	K	201	CDL	C71-C72-C73-C74
23	G	304	PC1	C27-C28-C29-C2A
22	j	302	CDL	C12-C13-C14-C15
22	K	202	CDL	C40-C41-C42-C43
28	J	304	PEE	C41-C42-C43-C44
22	k	202	CDL	C71-CB7-OB8-CB6
22	j	302	CDL	C51-CB5-OB6-CB4
22	J	301	CDL	C11-CA5-OA6-CA4
22	b	401	CDL	C33-C34-C35-C36
22	f	304	CDL	C81-C82-C83-C84
22	i	302	CDL	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	p	201	CDL	C80-C81-C82-C83
22	K	202	CDL	C74-C75-C76-C77
22	L	301	CDL	C52-C53-C54-C55
28	l	303	PEE	C20-C21-C22-C23
28	J	303	PEE	C40-C41-C42-C43
22	K	202	CDL	CA5-C11-C12-C13
28	l	303	PEE	C30-C31-C32-C33
28	J	303	PEE	C32-C33-C34-C35
22	L	301	CDL	C11-C12-C13-C14
25	i	303	UQ8	C30-C29-C31-C32
25	I	303	UQ8	C15-C14-C16-C17
25	i	303	UQ8	C13-C14-C16-C17
28	l	303	PEE	C17-C18-C19-C20
22	i	302	CDL	OA9-CA7-OA8-CA6
23	G	304	PC1	O32-C31-O31-C3
22	a	501	CDL	C12-C13-C14-C15
22	I	301	CDL	C17-C18-C19-C20
22	f	303	CDL	OB7-CB5-OB6-CB4
22	b	402	CDL	CB7-C71-C72-C73
22	l	301	CDL	C31-CA7-OA8-CA6
22	B	402	CDL	C31-CA7-OA8-CA6
22	B	403	CDL	C71-CB7-OB8-CB6
22	I	302	CDL	C31-CA7-OA8-CA6
22	b	402	CDL	C52-C53-C54-C55
22	k	201	CDL	C72-C73-C74-C75
22	k	202	CDL	C11-C12-C13-C14
22	J	302	CDL	C14-C15-C16-C17
22	f	302	CDL	C71-C72-C73-C74
22	J	301	CDL	C12-C13-C14-C15
22	J	301	CDL	C21-C22-C23-C24
22	k	201	CDL	CA7-C31-C32-C33
28	J	304	PEE	C10-C11-C12-C13
22	p	201	CDL	C11-C12-C13-C14
22	B	405	CDL	C74-C75-C76-C77
22	I	302	CDL	C14-C15-C16-C17
22	j	302	CDL	C22-C23-C24-C25
22	B	404	CDL	C12-C13-C14-C15
22	a	501	CDL	C22-C23-C24-C25
22	f	304	CDL	C62-C63-C64-C65
22	f	304	CDL	C83-C84-C85-C86
22	K	202	CDL	C13-C14-C15-C16
22	J	301	CDL	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	l	301	CDL	CA5-C11-C12-C13
22	f	303	CDL	C51-CB5-OB6-CB4
22	I	302	CDL	C11-CA5-OA6-CA4
22	a	501	CDL	OA5-CA3-CA4-OA6
22	i	302	CDL	OB5-CB3-CB4-OB6
22	k	202	CDL	OA5-CA3-CA4-OA6
22	f	304	CDL	C17-C18-C19-C20
22	j	301	CDL	C52-C53-C54-C55
22	f	304	CDL	C60-C61-C62-C63
22	A	501	CDL	C78-C79-C80-C81
22	J	301	CDL	OA7-CA5-OA6-CA4
22	i	302	CDL	C57-C58-C59-C60
22	B	403	CDL	C53-C54-C55-C56
22	f	304	CDL	C76-C77-C78-C79
22	i	302	CDL	C76-C77-C78-C79
22	B	403	CDL	C22-C23-C24-C25
28	J	304	PEE	C40-C41-C42-C43
22	f	303	CDL	C19-C20-C21-C22
22	B	402	CDL	C39-C40-C41-C42
22	B	404	CDL	C76-C77-C78-C79
22	J	301	CDL	C35-C36-C37-C38
28	l	303	PEE	C19-C20-C21-C22
28	l	303	PEE	C35-C36-C37-C38
25	i	303	UQ8	C15-C14-C16-C17
25	I	303	UQ8	C13-C14-C16-C17
22	a	501	CDL	C56-C57-C58-C59
22	k	203	CDL	C77-C78-C79-C80
22	B	401	CDL	C35-C36-C37-C38
22	B	405	CDL	C13-C14-C15-C16
22	L	301	CDL	C81-C82-C83-C84
29	e	900	NAD	O4B-C4B-C5B-O5B
29	e	900	NAD	O4D-C4D-C5D-O5D
22	f	303	CDL	C13-C14-C15-C16
22	J	301	CDL	C57-C58-C59-C60
28	l	302	PEE	C33-C34-C35-C36
28	l	303	PEE	C11-C12-C13-C14
22	B	404	CDL	C79-C80-C81-C82
22	I	302	CDL	C15-C16-C17-C18
22	k	201	CDL	C76-C77-C78-C79
22	l	301	CDL	C80-C81-C82-C83
22	k	202	CDL	OB9-CB7-OB8-CB6
22	j	302	CDL	OB7-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	B	403	CDL	C71-C72-C73-C74
22	B	405	CDL	C59-C60-C61-C62
22	P	201	CDL	C72-C73-C74-C75
23	G	304	PC1	C3B-C3C-C3D-C3E
22	b	401	CDL	CA2-OA2-PA1-OA5
22	f	303	CDL	CB2-OB2-PB2-OB5
22	k	203	CDL	CB3-OB5-PB2-OB2
22	I	301	CDL	CB2-OB2-PB2-OB5
22	K	202	CDL	CB2-OB2-PB2-OB5
28	l	303	PEE	C1-O3P-P-O4P
22	J	302	CDL	C12-C13-C14-C15
22	j	301	CDL	CB5-C51-C52-C53
22	l	301	CDL	CA7-C31-C32-C33
22	l	304	CDL	CB7-C71-C72-C73
22	L	301	CDL	C19-C20-C21-C22
28	J	303	PEE	C14-C15-C16-C17
22	b	401	CDL	C71-CB7-OB8-CB6
22	f	302	CDL	OA5-CA3-CA4-CA6
22	f	304	CDL	OB5-CB3-CB4-CB6
22	k	202	CDL	OA5-CA3-CA4-CA6
22	B	402	CDL	OA5-CA3-CA4-CA6
22	K	202	CDL	OA5-CA3-CA4-CA6
23	G	304	PC1	O11-C1-C2-C3
22	j	301	CDL	C74-C75-C76-C77
22	I	301	CDL	C79-C80-C81-C82
22	J	302	CDL	C23-C24-C25-C26
22	b	401	CDL	C14-C15-C16-C17
22	f	303	CDL	C38-C39-C40-C41
22	k	203	CDL	C32-C33-C34-C35
22	j	302	CDL	C74-C75-C76-C77
22	k	202	CDL	C15-C16-C17-C18
22	B	405	CDL	C78-C79-C80-C81
22	L	301	CDL	C21-C22-C23-C24
23	D	301	PC1	C37-C38-C39-C3A
22	J	302	CDL	C13-C14-C15-C16
22	L	301	CDL	C80-C81-C82-C83
22	k	202	CDL	C52-C53-C54-C55
22	l	304	CDL	C15-C16-C17-C18
22	l	304	CDL	C17-C18-C19-C20
22	r	201	CDL	C62-C63-C64-C65
22	B	404	CDL	C78-C79-C80-C81
22	B	402	CDL	OA9-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	b	402	CDL	C43-C44-C45-C46
22	f	304	CDL	C77-C78-C79-C80
22	b	401	CDL	CB3-CB4-CB6-OB8
22	f	303	CDL	CB3-CB4-CB6-OB8
22	f	303	CDL	C56-C57-C58-C59
22	j	301	CDL	CB3-CB4-CB6-OB8
22	r	201	CDL	CB3-CB4-CB6-OB8
22	B	401	CDL	CA3-CA4-CA6-OA8
22	B	402	CDL	C15-C16-C17-C18
22	B	405	CDL	CB3-CB4-CB6-OB8
22	I	301	CDL	CB3-CB4-CB6-OB8
22	I	302	CDL	CB3-CB4-CB6-OB8
22	J	302	CDL	CA3-CA4-CA6-OA8
22	J	302	CDL	CB3-CB4-CB6-OB8
23	d	301	PC1	C1-C2-C3-O31
28	l	303	PEE	C1-C2-C3-O3
22	l	301	CDL	C62-C63-C64-C65
22	B	402	CDL	C13-C14-C15-C16
22	f	302	CDL	CB5-C51-C52-C53
22	I	302	CDL	OA9-CA7-OA8-CA6
22	f	304	CDL	C36-C37-C38-C39
22	r	201	CDL	C14-C15-C16-C17
22	A	501	CDL	C15-C16-C17-C18
22	J	301	CDL	C78-C79-C80-C81
22	B	402	CDL	C76-C77-C78-C79
22	l	304	CDL	C32-C31-CA7-OA8
22	B	403	CDL	OB9-CB7-OB8-CB6
22	K	201	CDL	C74-C75-C76-C77
22	K	202	CDL	C22-C23-C24-C25
22	J	301	CDL	C71-C72-C73-C74
22	L	301	CDL	C53-C54-C55-C56
22	l	304	CDL	C32-C33-C34-C35
22	b	401	CDL	C24-C25-C26-C27
22	B	404	CDL	C43-C44-C45-C46
22	K	202	CDL	C53-C54-C55-C56
28	l	302	PEE	C35-C36-C37-C38
28	J	303	PEE	C19-C20-C21-C22
28	J	303	PEE	C35-C36-C37-C38
28	J	304	PEE	C35-C36-C37-C38
22	l	301	CDL	OA9-CA7-OA8-CA6
22	b	401	CDL	C23-C24-C25-C26
22	B	403	CDL	C54-C55-C56-C57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	K	201	CDL	C22-C23-C24-C25
22	K	202	CDL	C80-C81-C82-C83
22	B	402	CDL	C57-C58-C59-C60
22	b	401	CDL	CA5-C11-C12-C13
22	k	202	CDL	CA5-C11-C12-C13
22	P	201	CDL	CA7-C31-C32-C33
23	i	301	PC1	C31-C32-C33-C34
22	P	201	CDL	C58-C59-C60-C61
22	b	402	CDL	CA6-CA4-OA6-CA5
22	B	404	CDL	CA6-CA4-OA6-CA5
22	I	301	CDL	CA6-CA4-OA6-CA5
22	I	302	CDL	OA7-CA5-OA6-CA4
22	j	301	CDL	C34-C35-C36-C37
22	f	303	CDL	C76-C77-C78-C79
22	j	302	CDL	C14-C15-C16-C17
22	K	202	CDL	C79-C80-C81-C82
22	J	301	CDL	C22-C23-C24-C25
22	K	202	CDL	C71-CB7-OB8-CB6
22	a	501	CDL	OB5-CB3-CB4-OB6
22	B	401	CDL	OB5-CB3-CB4-OB6
22	I	302	CDL	OB5-CB3-CB4-OB6
22	k	201	CDL	C80-C81-C82-C83
22	k	203	CDL	C41-C42-C43-C44
22	j	301	CDL	C54-C55-C56-C57
22	B	401	CDL	C41-C42-C43-C44
22	B	403	CDL	C43-C44-C45-C46
22	K	202	CDL	C52-C53-C54-C55
22	P	201	CDL	C11-C12-C13-C14
22	f	302	CDL	C16-C17-C18-C19
22	f	303	CDL	C16-C17-C18-C19
22	K	202	CDL	C43-C44-C45-C46
22	k	203	CDL	CB5-C51-C52-C53
22	k	202	CDL	C76-C77-C78-C79
22	k	201	CDL	OB6-CB4-CB6-OB8
22	A	501	CDL	OB6-CB4-CB6-OB8
22	l	304	CDL	C74-C75-C76-C77
22	I	301	CDL	C77-C78-C79-C80
22	b	401	CDL	OB9-CB7-OB8-CB6
22	b	401	CDL	C81-C82-C83-C84
22	B	404	CDL	C52-C53-C54-C55
23	g	303	PC1	C38-C39-C3A-C3B
23	D	301	PC1	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	r	201	CDL	C83-C84-C85-C86
22	i	302	CDL	C17-C18-C19-C20
22	k	201	CDL	C54-C55-C56-C57
22	B	403	CDL	C56-C57-C58-C59
22	J	302	CDL	C54-C55-C56-C57
28	J	303	PEE	C12-C13-C14-C15
23	g	303	PC1	C29-C2A-C2B-C2C
22	f	302	CDL	C71-CB7-OB8-CB6
22	b	401	CDL	C16-C17-C18-C19
22	I	302	CDL	C52-C53-C54-C55
28	J	303	PEE	C41-C42-C43-C44
22	j	302	CDL	C13-C14-C15-C16
22	A	501	CDL	C44-C45-C46-C47
22	B	404	CDL	C24-C25-C26-C27
22	B	405	CDL	C38-C39-C40-C41
22	K	202	CDL	CB2-C1-CA2-OA2
22	f	302	CDL	C76-C77-C78-C79
22	i	302	CDL	C56-C57-C58-C59
22	r	201	CDL	C35-C36-C37-C38
28	J	304	PEE	C37-C38-C39-C40
22	J	302	CDL	CA7-C31-C32-C33
22	f	302	CDL	C79-C80-C81-C82
23	i	301	PC1	C3E-C3F-C3G-C3H
29	E	900	NAD	O4B-C4B-C5B-O5B
22	a	501	CDL	OA5-CA3-CA4-CA6
22	a	501	CDL	OB5-CB3-CB4-CB6
22	b	401	CDL	OA5-CA3-CA4-CA6
22	i	302	CDL	OB5-CB3-CB4-CB6
22	j	301	CDL	OA5-CA3-CA4-CA6
22	p	201	CDL	OB5-CB3-CB4-CB6
22	B	401	CDL	OA5-CA3-CA4-CA6
22	I	301	CDL	OA5-CA3-CA4-CA6
22	I	301	CDL	OB5-CB3-CB4-CB6
22	I	302	CDL	OB5-CB3-CB4-CB6
22	J	301	CDL	OA5-CA3-CA4-CA6
23	g	303	PC1	O11-C1-C2-C3
28	J	304	PEE	O3P-C1-C2-C3
22	A	501	CDL	C61-C62-C63-C64
22	B	402	CDL	CA5-C11-C12-C13
22	r	201	CDL	C76-C77-C78-C79
22	k	203	CDL	C31-CA7-OA8-CA6
22	B	401	CDL	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	B	401	CDL	C38-C39-C40-C41
22	K	201	CDL	C58-C59-C60-C61
22	a	501	CDL	CB7-C71-C72-C73
22	l	301	CDL	C37-C38-C39-C40
22	p	201	CDL	C22-C23-C24-C25
22	f	304	CDL	C19-C20-C21-C22
23	i	301	PC1	C24-C25-C26-C27
28	l	302	PEE	C13-C14-C15-C16
22	p	201	CDL	C31-CA7-OA8-CA6
23	g	303	PC1	C32-C31-O31-C3
22	B	402	CDL	C32-C31-CA7-OA8
22	L	301	CDL	C72-C71-CB7-OB8
22	j	302	CDL	CA7-C31-C32-C33
22	B	402	CDL	CB7-C71-C72-C73
22	k	203	CDL	C37-C38-C39-C40
22	A	501	CDL	C32-C33-C34-C35
22	a	501	CDL	C1-CB2-OB2-PB2
22	i	302	CDL	C31-C32-C33-C34
22	B	404	CDL	C73-C74-C75-C76
22	I	302	CDL	C41-C42-C43-C44
22	p	201	CDL	C76-C77-C78-C79
22	B	402	CDL	C80-C81-C82-C83
22	I	301	CDL	C36-C37-C38-C39
22	b	402	CDL	C77-C78-C79-C80
22	f	304	CDL	C35-C36-C37-C38
22	k	202	CDL	C13-C14-C15-C16
22	I	301	CDL	C44-C45-C46-C47
22	b	402	CDL	C76-C77-C78-C79
22	k	202	CDL	C31-C32-C33-C34
22	f	302	CDL	CB3-CB4-CB6-OB8
22	f	304	CDL	CA3-CA4-CA6-OA8
22	i	302	CDL	CB3-CB4-CB6-OB8
22	j	302	CDL	CB3-CB4-CB6-OB8
22	A	501	CDL	CB3-CB4-CB6-OB8
22	J	301	CDL	CA3-CA4-CA6-OA8
28	J	304	PEE	C1-C2-C3-O3
22	f	302	CDL	C83-C84-C85-C86
22	k	201	CDL	C22-C23-C24-C25
22	a	501	CDL	C38-C39-C40-C41
22	k	202	CDL	C72-C73-C74-C75
22	l	301	CDL	C23-C24-C25-C26
22	J	301	CDL	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	b	402	CDL	C79-C80-C81-C82
22	k	203	CDL	C76-C77-C78-C79
25	i	303	UQ8	C40-C39-C41-C42
22	j	301	CDL	C11-C12-C13-C14
22	A	501	CDL	CA3-OA5-PA1-OA2
22	B	401	CDL	CB3-OB5-PB2-OB2
22	B	402	CDL	CA2-OA2-PA1-OA5
22	B	402	CDL	CB3-OB5-PB2-OB2
22	B	405	CDL	CB2-OB2-PB2-OB5
22	K	202	CDL	CA3-OA5-PA1-OA2
22	B	402	CDL	C77-C78-C79-C80
22	b	401	CDL	OB5-CB3-CB4-OB6
22	f	302	CDL	OA5-CA3-CA4-OA6
22	p	201	CDL	OB5-CB3-CB4-OB6
22	r	201	CDL	OA5-CA3-CA4-OA6
22	A	501	CDL	OB5-CB3-CB4-OB6
23	d	301	PC1	O11-C1-C2-O21
28	J	304	PEE	O3P-C1-C2-O2
22	K	201	CDL	C31-CA7-OA8-CA6
22	K	202	CDL	OB9-CB7-OB8-CB6
22	B	403	CDL	C32-C31-CA7-OA8
22	K	201	CDL	C39-C40-C41-C42
22	j	302	CDL	C11-C12-C13-C14
22	B	402	CDL	C63-C64-C65-C66
22	b	401	CDL	OB6-CB4-CB6-OB8
22	i	302	CDL	OB6-CB4-CB6-OB8
22	j	302	CDL	OB6-CB4-CB6-OB8
22	B	402	CDL	OB6-CB4-CB6-OB8
22	B	405	CDL	OA6-CA4-CA6-OA8
22	J	302	CDL	OA6-CA4-CA6-OA8
22	J	302	CDL	OB6-CB4-CB6-OB8
23	d	301	PC1	O21-C2-C3-O31
22	B	402	CDL	C73-C74-C75-C76
22	b	401	CDL	C42-C43-C44-C45
25	I	303	UQ8	C14-C16-C17-C18
22	b	401	CDL	C11-C12-C13-C14
22	A	501	CDL	C33-C34-C35-C36
22	B	404	CDL	C39-C40-C41-C42
22	f	303	CDL	C44-C45-C46-C47
22	f	302	CDL	C84-C85-C86-C87
22	k	202	CDL	C80-C81-C82-C83
22	r	201	CDL	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	P	201	CDL	C22-C23-C24-C25
22	k	201	CDL	C36-C37-C38-C39
22	p	201	CDL	C71-C72-C73-C74
22	b	402	CDL	C1-CB2-OB2-PB2
22	L	301	CDL	C1-CB2-OB2-PB2
22	r	201	CDL	C58-C59-C60-C61
22	k	203	CDL	C12-C13-C14-C15
23	g	303	PC1	C27-C28-C29-C2A
22	J	302	CDL	C51-CB5-OB6-CB4
22	a	501	CDL	C14-C15-C16-C17
22	f	302	CDL	OB9-CB7-OB8-CB6
22	b	401	CDL	OB5-CB3-CB4-CB6
22	r	201	CDL	OA5-CA3-CA4-CA6
22	B	401	CDL	OB5-CB3-CB4-CB6
22	f	303	CDL	C58-C59-C60-C61
22	A	501	CDL	C72-C73-C74-C75
28	J	303	PEE	C37-C38-C39-C40
22	f	302	CDL	C41-C42-C43-C44
22	b	402	CDL	C34-C35-C36-C37
22	J	302	CDL	C16-C17-C18-C19
22	B	404	CDL	C55-C56-C57-C58
22	f	303	CDL	C59-C60-C61-C62
22	l	301	CDL	C34-C35-C36-C37
22	l	304	CDL	C31-CA7-OA8-CA6
22	I	302	CDL	C71-CB7-OB8-CB6
22	i	302	CDL	C78-C79-C80-C81
22	l	304	CDL	C41-C42-C43-C44
23	G	304	PC1	C21-C22-C23-C24
22	b	401	CDL	C76-C77-C78-C79
22	k	203	CDL	C42-C43-C44-C45
22	p	201	CDL	C37-C38-C39-C40
22	B	404	CDL	C81-C82-C83-C84
22	j	302	CDL	CA6-CA4-OA6-CA5
22	l	304	CDL	CA6-CA4-OA6-CA5
22	r	201	CDL	CA6-CA4-OA6-CA5
22	B	403	CDL	CB6-CB4-OB6-CB5
22	J	302	CDL	CA6-CA4-OA6-CA5
22	B	404	CDL	C35-C36-C37-C38
22	B	401	CDL	C32-C33-C34-C35
22	B	402	CDL	C81-C82-C83-C84
22	k	202	CDL	C56-C57-C58-C59
22	f	304	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	k	201	CDL	C1-CB2-OB2-PB2
22	j	301	CDL	C1-CB2-OB2-PB2
22	j	302	CDL	CA3-CA4-CA6-OA8
22	p	201	CDL	CA3-CA4-CA6-OA8
22	B	402	CDL	CB3-CB4-CB6-OB8
22	B	404	CDL	C1-CB2-OB2-PB2
22	B	404	CDL	CB4-CB3-OB5-PB2
22	B	405	CDL	CA3-CA4-CA6-OA8
22	I	301	CDL	CA3-CA4-CA6-OA8
22	J	301	CDL	C1-CB2-OB2-PB2
22	P	201	CDL	CA3-CA4-CA6-OA8
23	i	301	PC1	C2-C1-O11-P
23	D	301	PC1	C1-C2-C3-O31
22	K	201	CDL	OA9-CA7-OA8-CA6
22	B	402	CDL	C71-C72-C73-C74
22	j	301	CDL	OA5-CA3-CA4-OA6
22	j	302	CDL	OB5-CB3-CB4-OB6
22	l	304	CDL	OB5-CB3-CB4-OB6
22	B	402	CDL	OA5-CA3-CA4-OA6
22	B	403	CDL	OB5-CB3-CB4-OB6
22	I	301	CDL	OB5-CB3-CB4-OB6
23	g	303	PC1	O11-C1-C2-O21
28	l	302	PEE	O3P-C1-C2-O2
22	B	403	CDL	C75-C76-C77-C78
28	J	304	PEE	C31-C32-C33-C34
22	A	501	CDL	C63-C64-C65-C66
22	B	403	CDL	C33-C34-C35-C36
22	B	403	CDL	CA2-C1-CB2-OB2
22	J	302	CDL	OB7-CB5-OB6-CB4
22	r	201	CDL	C72-C73-C74-C75
23	g	303	PC1	C21-C22-C23-C24
22	k	203	CDL	OA9-CA7-OA8-CA6
22	p	201	CDL	OA9-CA7-OA8-CA6
22	B	404	CDL	C15-C16-C17-C18
22	f	302	CDL	OB6-CB4-CB6-OB8
22	f	304	CDL	OA6-CA4-CA6-OA8
22	j	301	CDL	OB6-CB4-CB6-OB8
22	r	201	CDL	OB6-CB4-CB6-OB8
22	I	301	CDL	OA6-CA4-CA6-OA8
22	I	302	CDL	OB6-CB4-CB6-OB8
22	J	301	CDL	OA6-CA4-CA6-OA8
23	D	301	PC1	O21-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	j	301	CDL	C55-C56-C57-C58
28	J	304	PEE	C21-C22-C23-C24
23	g	303	PC1	O32-C31-O31-C3
29	e	900	NAD	C5B-O5B-PA-O3
22	k	202	CDL	C40-C41-C42-C43
22	J	301	CDL	C74-C75-C76-C77
25	I	303	UQ8	C30-C29-C31-C32
22	B	405	CDL	C17-C18-C19-C20
22	I	302	CDL	C60-C61-C62-C63
22	L	301	CDL	CB7-C71-C72-C73
22	f	304	CDL	C71-CB7-OB8-CB6
22	f	302	CDL	C77-C78-C79-C80
22	l	304	CDL	C51-C52-C53-C54
22	B	401	CDL	C76-C77-C78-C79
23	G	304	PC1	C24-C25-C26-C27
22	K	202	CDL	C44-C45-C46-C47
29	e	900	NAD	C3B-C4B-C5B-O5B
22	b	401	CDL	CA7-C31-C32-C33
22	K	201	CDL	CB5-C51-C52-C53
22	k	201	CDL	C44-C45-C46-C47
22	I	302	CDL	OB9-CB7-OB8-CB6
28	l	303	PEE	C12-C13-C14-C15
22	r	201	CDL	C21-C22-C23-C24
22	I	301	CDL	C74-C75-C76-C77
23	G	304	PC1	C38-C39-C3A-C3B
22	f	304	CDL	C14-C15-C16-C17
22	b	402	CDL	CB2-OB2-PB2-OB5
22	f	304	CDL	CA2-OA2-PA1-OA5
22	i	302	CDL	CA3-OA5-PA1-OA2
22	l	304	CDL	CB3-OB5-PB2-OB2
22	p	201	CDL	CB2-OB2-PB2-OB5
22	k	203	CDL	C17-C18-C19-C20
22	a	501	CDL	C1-CA2-OA2-PA1
22	b	402	CDL	CB4-CB3-OB5-PB2
22	l	301	CDL	CA4-CA3-OA5-PA1
22	l	304	CDL	C1-CA2-OA2-PA1
22	L	301	CDL	C1-CA2-OA2-PA1
22	L	301	CDL	CA4-CA3-OA5-PA1
23	G	303	PC1	C2-C1-O11-P
25	i	303	UQ8	C28-C29-C31-C32
22	i	302	CDL	C80-C81-C82-C83
22	k	201	CDL	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	B	402	CDL	C43-C44-C45-C46
22	a	501	CDL	CA2-OA2-PA1-OA4
22	b	401	CDL	CA2-OA2-PA1-OA4
22	b	401	CDL	CB2-OB2-PB2-OB4
22	b	401	CDL	CB3-OB5-PB2-OB3
22	b	401	CDL	CB3-OB5-PB2-OB4
22	f	304	CDL	CA2-OA2-PA1-OA3
22	f	304	CDL	CA2-OA2-PA1-OA4
22	f	304	CDL	CA3-OA5-PA1-OA3
22	k	201	CDL	CB3-OB5-PB2-OB4
22	k	202	CDL	CB2-OB2-PB2-OB4
22	k	203	CDL	CA3-OA5-PA1-OA4
22	k	203	CDL	CB3-OB5-PB2-OB4
22	j	301	CDL	CB3-OB5-PB2-OB3
22	j	301	CDL	CB3-OB5-PB2-OB4
22	l	301	CDL	CB3-OB5-PB2-OB3
22	l	301	CDL	CB3-OB5-PB2-OB4
22	l	304	CDL	CA3-OA5-PA1-OA4
22	l	304	CDL	CB3-OB5-PB2-OB3
22	l	304	CDL	CB3-OB5-PB2-OB4
22	r	201	CDL	CA3-OA5-PA1-OA4
22	r	201	CDL	CB3-OB5-PB2-OB3
22	B	401	CDL	CB3-OB5-PB2-OB4
22	I	301	CDL	CA3-OA5-PA1-OA4
22	I	301	CDL	CB2-OB2-PB2-OB3
22	I	301	CDL	CB2-OB2-PB2-OB4
22	K	201	CDL	CB3-OB5-PB2-OB4
22	K	202	CDL	CB2-OB2-PB2-OB4
22	J	301	CDL	CB2-OB2-PB2-OB3
22	J	301	CDL	CB3-OB5-PB2-OB3
22	J	301	CDL	CB3-OB5-PB2-OB4
22	L	301	CDL	CA3-OA5-PA1-OA4
22	L	301	CDL	CB3-OB5-PB2-OB3
22	L	301	CDL	CB3-OB5-PB2-OB4
23	i	301	PC1	C11-O13-P-O12
23	i	301	PC1	C11-O13-P-O14
23	i	301	PC1	C1-O11-P-O14
23	G	303	PC1	C11-O13-P-O12
23	G	303	PC1	C11-O13-P-O14
28	l	303	PEE	C1-O3P-P-O2P
28	J	303	PEE	C4-O4P-P-O2P
28	J	304	PEE	C1-O3P-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	e	900	NAD	C5B-O5B-PA-O1A
29	E	900	NAD	C5D-O5D-PN-O2N
22	I	301	CDL	CB5-C51-C52-C53
22	a	501	CDL	C31-C32-C33-C34
22	b	402	CDL	OB5-CB3-CB4-CB6
22	B	404	CDL	OB5-CB3-CB4-CB6
22	P	201	CDL	OB5-CB3-CB4-CB6
23	d	301	PC1	O11-C1-C2-C3
28	l	302	PEE	O3P-C1-C2-C3
28	l	303	PEE	O3P-C1-C2-C3
22	f	303	CDL	C64-C65-C66-C67
22	l	301	CDL	C17-C18-C19-C20
22	r	201	CDL	C11-C12-C13-C14
22	l	304	CDL	OA9-CA7-OA8-CA6
22	b	402	CDL	C61-C62-C63-C64
22	L	301	CDL	C76-C77-C78-C79
22	l	304	CDL	C82-C83-C84-C85
23	G	304	PC1	C2B-C2C-C2D-C2E
22	B	402	CDL	C84-C85-C86-C87
22	f	304	CDL	OB9-CB7-OB8-CB6
22	b	402	CDL	C22-C23-C24-C25
22	r	201	CDL	CB7-C71-C72-C73
22	f	302	CDL	CA2-C1-CB2-OB2
22	B	402	CDL	C54-C55-C56-C57
22	B	405	CDL	C39-C40-C41-C42
22	I	302	CDL	C34-C35-C36-C37
22	b	401	CDL	OA5-CA3-CA4-OA6
22	I	301	CDL	OA5-CA3-CA4-OA6
22	J	301	CDL	OA5-CA3-CA4-OA6
22	P	201	CDL	OB5-CB3-CB4-OB6
23	G	304	PC1	O11-C1-C2-O21
22	B	403	CDL	C79-C80-C81-C82
22	l	301	CDL	C72-C71-CB7-OB8
22	k	202	CDL	C23-C24-C25-C26
22	P	201	CDL	C74-C75-C76-C77
22	i	302	CDL	C11-CA5-OA6-CA4
22	L	301	CDL	C11-CA5-OA6-CA4
22	a	501	CDL	C75-C76-C77-C78
22	r	201	CDL	O1-C1-CA2-OA2
22	l	301	CDL	C74-C75-C76-C77
22	B	404	CDL	C22-C23-C24-C25
22	B	405	CDL	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	J	301	CDL	C72-C71-CB7-OB8
22	k	201	CDL	CB3-CB4-CB6-OB8
22	r	201	CDL	CA3-CA4-CA6-OA8
22	B	403	CDL	C32-C33-C34-C35
23	d	301	PC1	O13-C11-C12-N
23	g	303	PC1	O13-C11-C12-N
23	G	304	PC1	O13-C11-C12-N
22	L	301	CDL	OA7-CA5-OA6-CA4
22	f	304	CDL	OB6-CB4-CB6-OB8
22	k	201	CDL	OA6-CA4-CA6-OA8
22	j	302	CDL	OA6-CA4-CA6-OA8
22	r	201	CDL	OA6-CA4-CA6-OA8
22	B	401	CDL	OA6-CA4-CA6-OA8
22	B	403	CDL	OB6-CB4-CB6-OB8
22	J	301	CDL	OB6-CB4-CB6-OB8
23	i	301	PC1	O21-C2-C3-O31
28	l	303	PEE	O2-C2-C3-O3
22	B	401	CDL	C75-C76-C77-C78
22	f	304	CDL	C11-C12-C13-C14
22	b	401	CDL	C17-C18-C19-C20
22	b	402	CDL	C37-C38-C39-C40
22	f	304	CDL	C71-C72-C73-C74
22	k	203	CDL	C1-CA2-OA2-PA1
22	l	304	CDL	C44-C45-C46-C47
22	b	401	CDL	C31-CA7-OA8-CA6
22	B	403	CDL	C80-C81-C82-C83
22	a	501	CDL	C34-C35-C36-C37
22	B	404	CDL	C34-C35-C36-C37
22	I	302	CDL	C76-C77-C78-C79
22	K	201	CDL	C59-C60-C61-C62
22	K	202	CDL	C54-C55-C56-C57
22	i	302	CDL	C58-C59-C60-C61
22	I	302	CDL	CB7-C71-C72-C73
22	b	402	CDL	C39-C40-C41-C42
22	k	202	CDL	C16-C17-C18-C19
23	i	301	PC1	C23-C24-C25-C26
22	J	302	CDL	C33-C34-C35-C36
22	J	302	CDL	C77-C78-C79-C80
22	a	501	CDL	CA5-C11-C12-C13
22	b	402	CDL	C31-C32-C33-C34
22	k	203	CDL	C44-C45-C46-C47
22	I	301	CDL	C82-C83-C84-C85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	P	201	CDL	C54-C55-C56-C57
22	p	201	CDL	C72-C71-CB7-OB8
23	G	304	PC1	C3C-C3D-C3E-C3F
22	f	304	CDL	C12-C13-C14-C15
22	I	302	CDL	C72-C71-CB7-OB8
22	k	203	CDL	C13-C14-C15-C16
22	a	501	CDL	CA7-C31-C32-C33
22	k	201	CDL	CB5-C51-C52-C53
22	j	301	CDL	C15-C16-C17-C18
28	l	303	PEE	C14-C15-C16-C17
22	b	401	CDL	OA9-CA7-OA8-CA6
22	f	302	CDL	C32-C33-C34-C35
22	b	401	CDL	CA6-CA4-OA6-CA5
22	k	203	CDL	CA6-CA4-OA6-CA5
22	i	302	CDL	OA7-CA5-OA6-CA4
22	B	403	CDL	C18-C19-C20-C21
22	f	304	CDL	C78-C79-C80-C81
22	i	302	CDL	C71-C72-C73-C74
22	P	201	CDL	C81-C82-C83-C84
22	B	401	CDL	C71-C72-C73-C74
22	K	201	CDL	C1-CB2-OB2-PB2
22	K	202	CDL	CB4-CB3-OB5-PB2
22	L	301	CDL	CB4-CB3-OB5-PB2
22	k	202	CDL	C12-C13-C14-C15
22	P	201	CDL	C13-C14-C15-C16
22	j	301	CDL	C31-CA7-OA8-CA6
22	j	301	CDL	OA9-CA7-OA8-CA6
22	b	402	CDL	OB5-CB3-CB4-OB6
22	f	304	CDL	OB5-CB3-CB4-OB6
22	B	404	CDL	OB5-CB3-CB4-OB6
22	l	301	CDL	C19-C20-C21-C22
22	f	302	CDL	C32-C31-CA7-OA8
22	i	302	CDL	C72-C71-CB7-OB8
22	j	301	CDL	C72-C71-CB7-OB8
25	I	303	UQ8	C28-C29-C31-C32
22	l	304	CDL	C12-C13-C14-C15
22	P	201	CDL	C31-CA7-OA8-CA6
22	i	302	CDL	C22-C23-C24-C25
22	L	301	CDL	C51-CB5-OB6-CB4
22	p	201	CDL	CA7-C31-C32-C33
25	I	303	UQ8	C19-C21-C22-C23
22	P	201	CDL	OA9-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	f	303	CDL	OA6-CA4-CA6-OA8
22	I	301	CDL	OB6-CB4-CB6-OB8
22	l	304	CDL	C39-C40-C41-C42
22	I	301	CDL	C32-C33-C34-C35
22	L	301	CDL	C71-CB7-OB8-CB6
22	k	202	CDL	CA3-OA5-PA1-OA2
22	k	203	CDL	CB2-OB2-PB2-OB5
22	l	304	CDL	CB2-OB2-PB2-OB5
22	B	401	CDL	CA2-OA2-PA1-OA5
22	B	403	CDL	CA3-OA5-PA1-OA2
22	B	404	CDL	CB2-OB2-PB2-OB5
22	I	302	CDL	CA3-OA5-PA1-OA2
22	I	302	CDL	CB2-OB2-PB2-OB5
22	J	302	CDL	C11-C12-C13-C14
22	I	302	CDL	C31-C32-C33-C34
22	B	403	CDL	CB3-CB4-CB6-OB8
23	i	301	PC1	C1-C2-C3-O31
22	f	302	CDL	C62-C63-C64-C65
22	L	301	CDL	C74-C75-C76-C77
23	D	301	PC1	C39-C3A-C3B-C3C
22	b	401	CDL	C80-C81-C82-C83
22	i	302	CDL	C14-C15-C16-C17
22	L	301	CDL	OB7-CB5-OB6-CB4
22	f	303	CDL	CB5-C51-C52-C53
22	b	402	CDL	C11-C12-C13-C14
22	b	402	CDL	C55-C56-C57-C58
22	k	202	CDL	C38-C39-C40-C41
22	k	202	CDL	CB4-CB3-OB5-PB2
22	B	401	CDL	C1-CB2-OB2-PB2
22	B	405	CDL	CA4-CA3-OA5-PA1
22	I	302	CDL	CB4-CB3-OB5-PB2
22	f	304	CDL	C74-C75-C76-C77
22	K	201	CDL	C16-C17-C18-C19
23	g	303	PC1	C36-C37-C38-C39
22	p	201	CDL	C52-C53-C54-C55
22	f	304	CDL	C75-C76-C77-C78
22	a	501	CDL	C71-CB7-OB8-CB6
22	L	301	CDL	OB9-CB7-OB8-CB6
23	d	301	PC1	C35-C36-C37-C38
22	b	401	CDL	C72-C71-CB7-OB8
22	b	401	CDL	C78-C79-C80-C81
22	f	302	CDL	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	A	501	CDL	C11-C12-C13-C14
22	P	201	CDL	C36-C37-C38-C39
22	f	304	CDL	C37-C38-C39-C40
22	k	203	CDL	C21-C22-C23-C24
22	B	403	CDL	C41-C42-C43-C44
22	j	302	CDL	C16-C17-C18-C19
22	B	401	CDL	C78-C79-C80-C81
22	I	301	CDL	C34-C35-C36-C37
22	k	202	CDL	C79-C80-C81-C82
22	a	501	CDL	OB9-CB7-OB8-CB6
22	p	201	CDL	C13-C14-C15-C16
22	k	203	CDL	O1-C1-CA2-OA2
22	a	501	CDL	C16-C17-C18-C19
22	f	302	CDL	C23-C24-C25-C26
22	f	302	CDL	C33-C34-C35-C36
22	f	304	CDL	C52-C53-C54-C55
22	I	302	CDL	C22-C23-C24-C25
22	a	501	CDL	OA6-CA4-CA6-OA8
22	K	201	CDL	OA6-CA4-CA6-OA8
22	P	201	CDL	C43-C44-C45-C46
22	a	501	CDL	CB4-CB3-OB5-PB2
22	j	302	CDL	CB4-CB3-OB5-PB2
22	l	301	CDL	C1-CA2-OA2-PA1
22	B	401	CDL	C1-CA2-OA2-PA1
22	l	304	CDL	C32-C31-CA7-OA9
22	i	302	CDL	C24-C25-C26-C27
22	I	301	CDL	C71-C72-C73-C74
22	A	501	CDL	C32-C31-CA7-OA8
22	A	501	CDL	C73-C74-C75-C76
22	L	301	CDL	C79-C80-C81-C82
22	b	402	CDL	C31-CA7-OA8-CA6
22	l	301	CDL	C63-C64-C65-C66
22	l	304	CDL	C75-C76-C77-C78
22	B	403	CDL	C64-C65-C66-C67
23	d	301	PC1	C36-C37-C38-C39
22	b	401	CDL	CB7-C71-C72-C73
22	B	401	CDL	C40-C41-C42-C43
22	B	402	CDL	C32-C33-C34-C35
22	I	301	CDL	C22-C23-C24-C25
22	i	302	CDL	CA2-C1-CB2-OB2
22	k	202	CDL	CB3-CB4-CB6-OB8
28	l	302	PEE	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	a	501	CDL	C77-C78-C79-C80
28	l	303	PEE	C23-C24-C25-C26
22	P	201	CDL	C71-CB7-OB8-CB6
22	B	402	CDL	C52-C53-C54-C55
23	d	301	PC1	C34-C35-C36-C37
22	a	501	CDL	C17-C18-C19-C20
22	l	301	CDL	C59-C60-C61-C62
22	B	402	CDL	C74-C75-C76-C77
22	B	403	CDL	C74-C75-C76-C77
22	f	304	CDL	CA6-CA4-OA6-CA5
22	k	201	CDL	C58-C59-C60-C61
22	B	405	CDL	C77-C78-C79-C80
22	L	301	CDL	C44-C45-C46-C47
22	B	402	CDL	C37-C38-C39-C40
22	B	403	CDL	C77-C78-C79-C80
23	G	304	PC1	C11-O13-P-O11
28	J	303	PEE	C4-O4P-P-O3P
22	B	402	CDL	C72-C71-CB7-OB8
22	J	302	CDL	C72-C71-CB7-OB8
22	B	404	CDL	C71-C72-C73-C74
22	f	303	CDL	CA4-CA3-OA5-PA1
22	i	302	CDL	CB4-CB3-OB5-PB2
23	D	301	PC1	O11-C1-C2-O21
22	k	201	CDL	C31-CA7-OA8-CA6
22	j	302	CDL	C18-C19-C20-C21
22	l	301	CDL	C54-C55-C56-C57
22	A	501	CDL	OB5-CB3-CB4-CB6
28	J	304	PEE	C36-C37-C38-C39
22	f	302	CDL	C73-C74-C75-C76
22	j	301	CDL	C53-C54-C55-C56
23	i	301	PC1	C3D-C3E-C3F-C3G
22	l	301	CDL	C22-C23-C24-C25
22	I	301	CDL	C72-C73-C74-C75
22	b	402	CDL	OA9-CA7-OA8-CA6
23	G	303	PC1	O22-C21-O21-C2
22	j	302	CDL	C24-C25-C26-C27
22	l	304	CDL	C77-C78-C79-C80
22	I	301	CDL	C60-C61-C62-C63
22	I	302	CDL	C64-C65-C66-C67
22	A	501	CDL	C31-CA7-OA8-CA6
22	B	402	CDL	C71-CB7-OB8-CB6
22	b	401	CDL	C73-C74-C75-C76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	A	501	CDL	C80-C81-C82-C83
22	k	202	CDL	C77-C78-C79-C80
22	P	201	CDL	OB9-CB7-OB8-CB6
22	l	301	CDL	CB2-C1-CA2-OA2
22	b	402	CDL	C41-C42-C43-C44
22	l	301	CDL	C44-C45-C46-C47
22	B	402	CDL	OB9-CB7-OB8-CB6
23	G	303	PC1	C23-C24-C25-C26
22	B	401	CDL	C19-C20-C21-C22
22	k	201	CDL	OA9-CA7-OA8-CA6
22	A	501	CDL	C60-C61-C62-C63
22	b	401	CDL	C44-C45-C46-C47
22	K	201	CDL	C20-C21-C22-C23
22	a	501	CDL	C19-C20-C21-C22
22	f	302	CDL	C72-C73-C74-C75
22	f	304	CDL	C16-C17-C18-C19
22	B	402	CDL	C35-C36-C37-C38
22	A	501	CDL	OA9-CA7-OA8-CA6
22	l	304	CDL	C83-C84-C85-C86
22	K	202	CDL	C24-C25-C26-C27
22	j	302	CDL	C72-C71-CB7-OB8
22	P	201	CDL	C72-C71-CB7-OB8
23	G	304	PC1	O31-C31-C32-C33
22	r	201	CDL	C44-C45-C46-C47
28	l	302	PEE	C37-C38-C39-C40
22	b	402	CDL	C38-C39-C40-C41
22	f	302	CDL	C54-C55-C56-C57
22	f	304	CDL	C18-C19-C20-C21
22	B	402	CDL	C56-C57-C58-C59
23	G	304	PC1	C33-C34-C35-C36
22	r	201	CDL	C12-C13-C14-C15
22	K	201	CDL	OB5-CB3-CB4-OB6
22	B	404	CDL	C41-C42-C43-C44
23	d	301	PC1	C25-C26-C27-C28
22	j	302	CDL	OB5-CB3-CB4-CB6
22	l	304	CDL	OB5-CB3-CB4-CB6
22	B	403	CDL	OB5-CB3-CB4-CB6
22	A	501	CDL	OB9-CB7-OB8-CB6
28	l	302	PEE	C44-C45-C46-C47
22	A	501	CDL	C71-CB7-OB8-CB6
22	f	302	CDL	C14-C15-C16-C17
22	B	405	CDL	C41-C42-C43-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	j	301	CDL	C83-C84-C85-C86
22	B	402	CDL	C16-C17-C18-C19
22	B	402	CDL	C32-C31-CA7-OA9
22	J	301	CDL	CA4-CA3-OA5-PA1
22	r	201	CDL	C43-C44-C45-C46
23	g	303	PC1	C39-C3A-C3B-C3C
22	l	304	CDL	C59-C60-C61-C62
23	g	303	PC1	O31-C31-C32-C33
29	e	900	NAD	C3D-C4D-C5D-O5D
22	B	403	CDL	C62-C63-C64-C65
22	I	302	CDL	C78-C79-C80-C81
22	a	501	CDL	CB5-C51-C52-C53
22	f	304	CDL	CB2-OB2-PB2-OB5
22	A	501	CDL	CA2-OA2-PA1-OA5
25	i	303	UQ8	C38-C39-C41-C42
22	p	201	CDL	C43-C44-C45-C46
22	r	201	CDL	C32-C33-C34-C35
22	J	301	CDL	C54-C55-C56-C57
22	f	303	CDL	C32-C31-CA7-OA8
23	G	303	PC1	O31-C31-C32-C33
28	J	304	PEE	C16-C17-C18-C19
22	p	201	CDL	C15-C16-C17-C18
22	J	302	CDL	C41-C42-C43-C44
22	k	201	CDL	C78-C79-C80-C81
22	L	301	CDL	C42-C43-C44-C45
22	L	301	CDL	C75-C76-C77-C78
22	a	501	CDL	C32-C31-CA7-OA8
22	f	302	CDL	C52-C51-CB5-OB6
22	B	401	CDL	C72-C71-CB7-OB8
22	k	201	CDL	C24-C25-C26-C27
22	k	201	CDL	C11-C12-C13-C14
22	K	202	CDL	C31-C32-C33-C34
22	L	301	CDL	C72-C71-CB7-OB9
22	b	401	CDL	C12-C11-CA5-OA6
22	l	304	CDL	C52-C51-CB5-OB6
28	l	302	PEE	C36-C37-C38-C39
22	K	201	CDL	C12-C13-C14-C15
22	k	201	CDL	CA3-CA4-CA6-OA8
22	j	302	CDL	C1-CB2-OB2-PB2
22	K	201	CDL	CA3-CA4-CA6-OA8
22	J	301	CDL	CB3-CB4-CB6-OB8
23	G	303	PC1	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	i	302	CDL	C51-C52-C53-C54
22	k	203	CDL	C59-C60-C61-C62
22	J	302	CDL	OB5-CB3-CB4-OB6
22	P	201	CDL	OA5-CA3-CA4-OA6
22	K	202	CDL	C12-C11-CA5-OA6
28	l	303	PEE	O2-C10-C11-C12
28	J	304	PEE	O2-C10-C11-C12
22	k	203	CDL	C39-C40-C41-C42
22	b	401	CDL	C72-C73-C74-C75
23	g	303	PC1	C2D-C2E-C2F-C2G
22	k	202	CDL	C72-C71-CB7-OB8
22	l	301	CDL	C56-C57-C58-C59
22	a	501	CDL	C72-C73-C74-C75
22	L	301	CDL	C71-C72-C73-C74
22	k	202	CDL	C19-C20-C21-C22
23	G	304	PC1	C36-C37-C38-C39
22	B	403	CDL	C32-C31-CA7-OA9
22	I	301	CDL	C72-C71-CB7-OB8
22	K	202	CDL	C72-C71-CB7-OB8
28	l	302	PEE	O2-C10-C11-C12
22	P	201	CDL	OA5-CA3-CA4-CA6
22	j	301	CDL	C16-C17-C18-C19
22	B	402	CDL	C42-C43-C44-C45
28	l	302	PEE	C31-C32-C33-C34
22	f	303	CDL	C72-C71-CB7-OB8
22	k	203	CDL	C32-C31-CA7-OA8
22	P	201	CDL	C12-C11-CA5-OA6
22	l	304	CDL	CA7-C31-C32-C33
22	j	301	CDL	OB9-CB7-OB8-CB6
22	f	302	CDL	C64-C65-C66-C67
22	B	404	CDL	C20-C21-C22-C23
22	B	401	CDL	C36-C37-C38-C39
22	L	301	CDL	C32-C31-CA7-OA8
23	i	301	PC1	O31-C31-C32-C33
28	J	303	PEE	O2-C10-C11-C12
29	e	900	NAD	C5D-O5D-PN-O3
22	p	201	CDL	C12-C11-CA5-OA6
22	B	405	CDL	C72-C71-CB7-OB8
22	a	501	CDL	C79-C80-C81-C82
28	l	303	PEE	C36-C37-C38-C39
22	k	202	CDL	C12-C11-CA5-OA6
22	A	501	CDL	C52-C51-CB5-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	l	304	CDL	CB5-C51-C52-C53
22	I	301	CDL	CB7-C71-C72-C73
22	l	301	CDL	C81-C82-C83-C84
22	A	501	CDL	O1-C1-CB2-OB2
22	i	302	CDL	C64-C65-C66-C67
22	r	201	CDL	C56-C57-C58-C59
22	A	501	CDL	C18-C19-C20-C21
22	B	401	CDL	C54-C55-C56-C57
22	J	301	CDL	C17-C18-C19-C20
22	j	301	CDL	C71-CB7-OB8-CB6
22	f	304	CDL	C52-C51-CB5-OB6
22	p	201	CDL	C32-C31-CA7-OA8
22	b	401	CDL	C12-C13-C14-C15
22	b	401	CDL	C13-C14-C15-C16
23	G	303	PC1	C22-C21-O21-C2
22	I	302	CDL	C39-C40-C41-C42
22	j	302	CDL	C59-C60-C61-C62
28	J	303	PEE	C36-C37-C38-C39
22	K	202	CDL	C12-C11-CA5-OA7
23	G	303	PC1	O32-C31-C32-C33
22	A	501	CDL	C51-C52-C53-C54
22	j	301	CDL	C32-C33-C34-C35
23	G	303	PC1	O21-C21-C22-C23
22	j	301	CDL	C22-C23-C24-C25
22	B	403	CDL	C16-C17-C18-C19
22	A	501	CDL	C76-C77-C78-C79
22	f	302	CDL	C55-C56-C57-C58
22	i	302	CDL	C44-C45-C46-C47
22	r	201	CDL	C34-C35-C36-C37
22	a	501	CDL	C32-C31-CA7-OA9
22	f	304	CDL	C52-C51-CB5-OB7
22	B	401	CDL	C72-C71-CB7-OB9
28	J	303	PEE	C20-C21-C22-C23
28	J	303	PEE	C31-C32-C33-C34
28	l	303	PEE	O4-C10-C11-C12
22	f	303	CDL	C36-C37-C38-C39
22	r	201	CDL	CB3-OB5-PB2-OB2
22	B	401	CDL	CA4-CA3-OA5-PA1
22	k	202	CDL	C12-C11-CA5-OA7
22	K	202	CDL	C72-C71-CB7-OB9
28	l	303	PEE	C16-C17-C18-C19
22	B	405	CDL	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	I	301	CDL	C52-C53-C54-C55
22	P	201	CDL	C75-C76-C77-C78
22	k	202	CDL	CB2-OB2-PB2-OB3
22	k	203	CDL	CB2-OB2-PB2-OB3
22	j	301	CDL	CA2-OA2-PA1-OA3
22	j	301	CDL	CB2-OB2-PB2-OB3
22	l	301	CDL	CB2-OB2-PB2-OB3
22	l	304	CDL	CB2-OB2-PB2-OB3
22	A	501	CDL	CB2-OB2-PB2-OB3
22	B	401	CDL	CA2-OA2-PA1-OA3
22	B	401	CDL	CA3-OA5-PA1-OA3
22	B	404	CDL	CA3-OA5-PA1-OA4
22	K	202	CDL	CA2-OA2-PA1-OA3
22	L	301	CDL	CB2-OB2-PB2-OB3
23	D	301	PC1	C1-O11-P-O14
28	J	304	PEE	C1-O3P-P-O1P
29	E	900	NAD	C5B-O5B-PA-O1A
22	f	303	CDL	C72-C71-CB7-OB9
22	B	405	CDL	C72-C71-CB7-OB9
22	P	201	CDL	C12-C11-CA5-OA7
23	i	301	PC1	O32-C31-C32-C33
28	J	304	PEE	O4-C10-C11-C12
22	r	201	CDL	C36-C37-C38-C39
22	L	301	CDL	C78-C79-C80-C81
22	f	302	CDL	C52-C51-CB5-OB7
22	f	303	CDL	C32-C31-CA7-OA9
22	l	304	CDL	C52-C51-CB5-OB7
28	l	302	PEE	O4-C10-C11-C12
28	J	303	PEE	O4-C10-C11-C12
22	p	201	CDL	C12-C13-C14-C15
22	r	201	CDL	C79-C80-C81-C82
22	f	304	CDL	CA7-C31-C32-C33
22	I	301	CDL	C72-C71-CB7-OB9
22	J	302	CDL	C60-C61-C62-C63
22	L	301	CDL	C52-C51-CB5-OB6
22	k	202	CDL	C72-C71-CB7-OB9
22	i	302	CDL	C79-C80-C81-C82
28	l	303	PEE	C43-C44-C45-C46
23	g	303	PC1	C12-C11-O13-P
22	k	203	CDL	C32-C31-CA7-OA9
22	p	201	CDL	C12-C11-CA5-OA7
22	a	501	CDL	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	P	201	CDL	C42-C43-C44-C45
22	f	303	CDL	C37-C38-C39-C40
23	G	304	PC1	C26-C27-C28-C29
22	I	302	CDL	C36-C37-C38-C39
23	g	303	PC1	C26-C27-C28-C29
22	P	201	CDL	C32-C31-CA7-OA8
22	A	501	CDL	C34-C35-C36-C37
22	P	201	CDL	C15-C16-C17-C18
22	A	501	CDL	C52-C51-CB5-OB7
22	J	301	CDL	C32-C31-CA7-OA8
22	p	201	CDL	C32-C31-CA7-OA9
22	b	402	CDL	C33-C34-C35-C36
22	i	302	CDL	C32-C33-C34-C35
22	b	402	CDL	C1-CA2-OA2-PA1
22	K	201	CDL	C56-C57-C58-C59
22	B	402	CDL	OB5-CB3-CB4-OB6
22	L	301	CDL	C32-C31-CA7-OA9
22	B	402	CDL	C60-C61-C62-C63
22	B	402	CDL	C83-C84-C85-C86
22	b	402	CDL	C32-C31-CA7-OA8
22	l	301	CDL	C12-C11-CA5-OA6
22	B	401	CDL	C12-C11-CA5-OA6
22	b	401	CDL	C62-C63-C64-C65
22	b	401	CDL	C84-C85-C86-C87
22	I	301	CDL	C39-C40-C41-C42
22	b	402	CDL	C32-C31-CA7-OA9
23	G	303	PC1	O22-C21-C22-C23
22	L	301	CDL	C24-C25-C26-C27
22	f	302	CDL	C72-C71-CB7-OB8
22	r	201	CDL	C72-C71-CB7-OB8
23	D	301	PC1	C36-C37-C38-C39
22	b	401	CDL	C56-C57-C58-C59
22	I	301	CDL	C55-C56-C57-C58
22	J	302	CDL	C32-C33-C34-C35
23	i	301	PC1	O21-C21-C22-C23
22	K	201	CDL	C75-C76-C77-C78
22	J	301	CDL	C32-C31-CA7-OA9
22	I	302	CDL	C32-C31-CA7-OA8

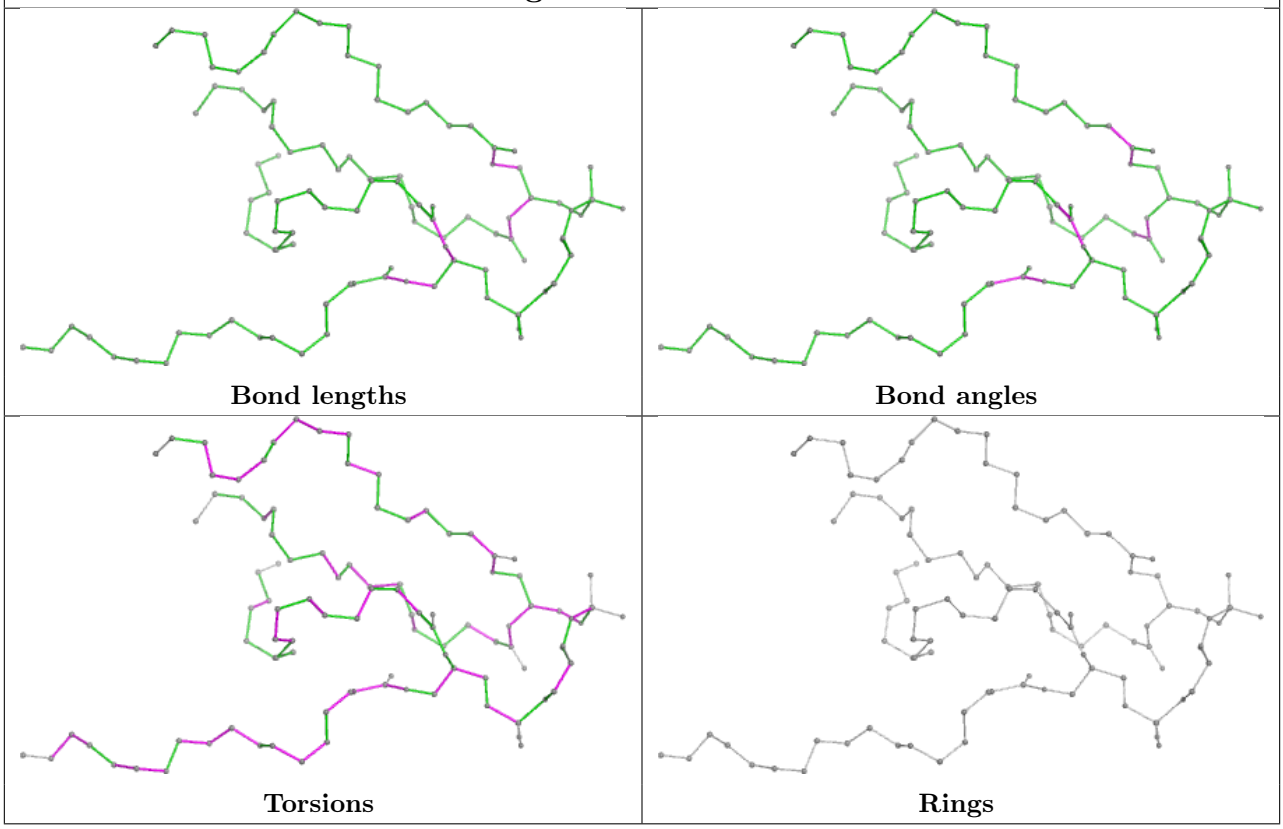
There are no ring outliers.

No monomer is involved in short contacts.

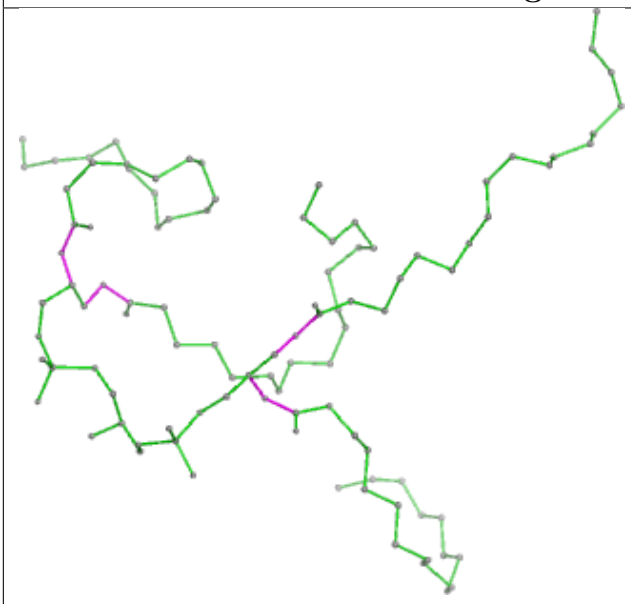
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

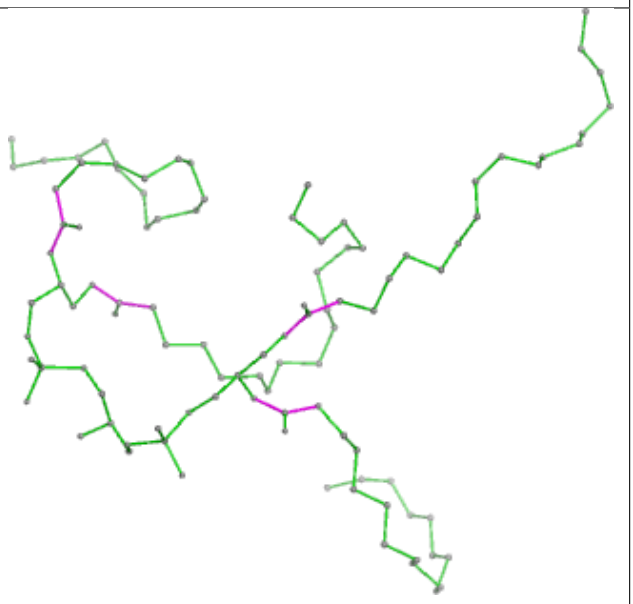
Ligand CDL B 402



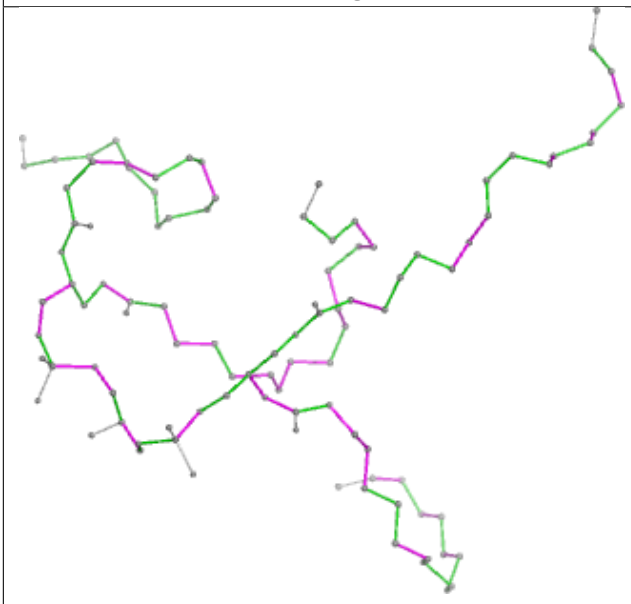
Ligand CDL B 404



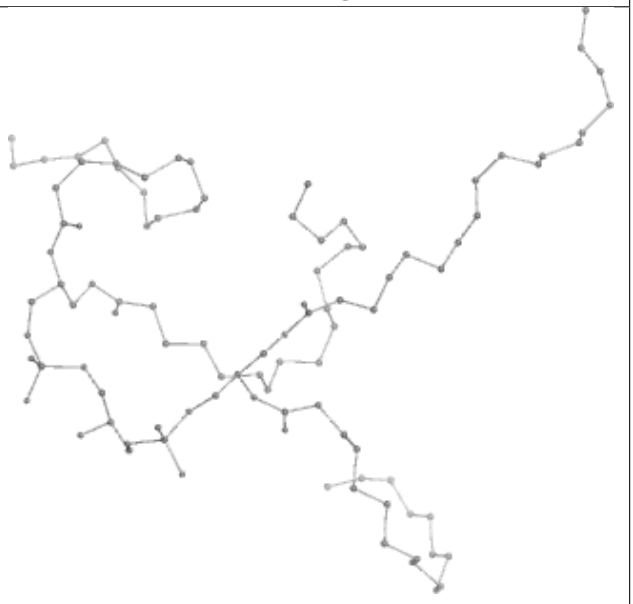
Bond lengths



Bond angles



Torsions

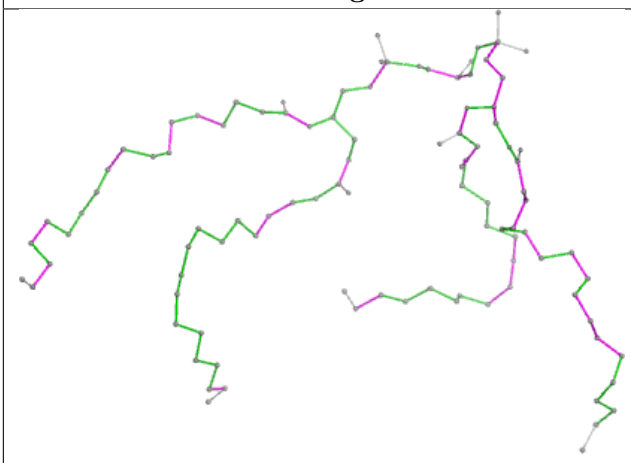


Rings

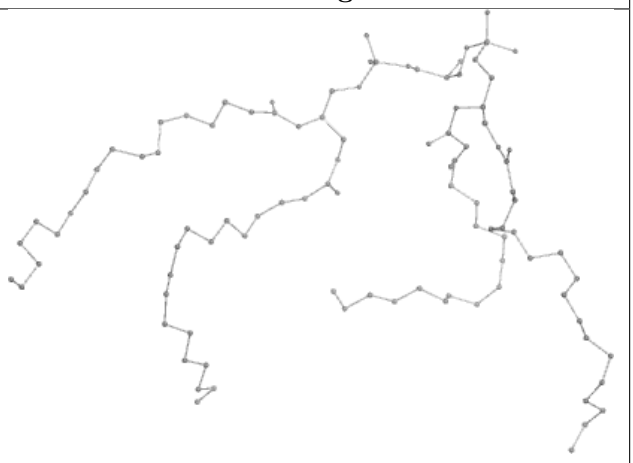
Ligand CDL i 302

Bond lengths

Bond angles

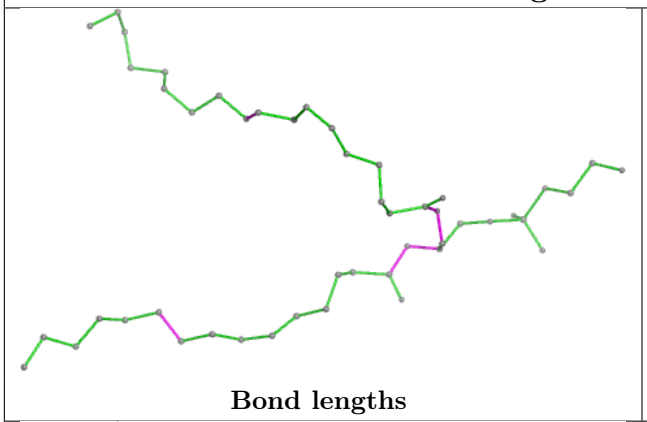


Torsions

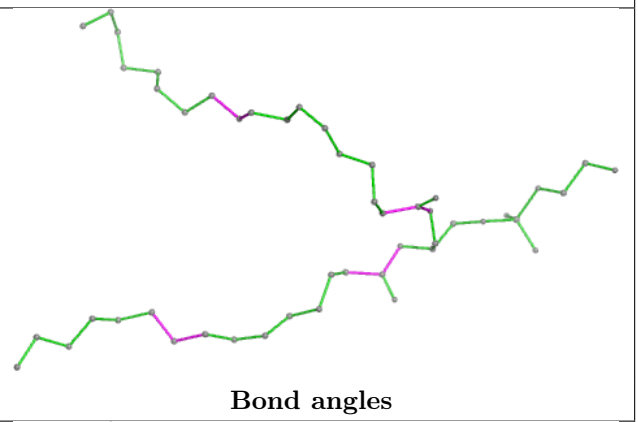


Rings

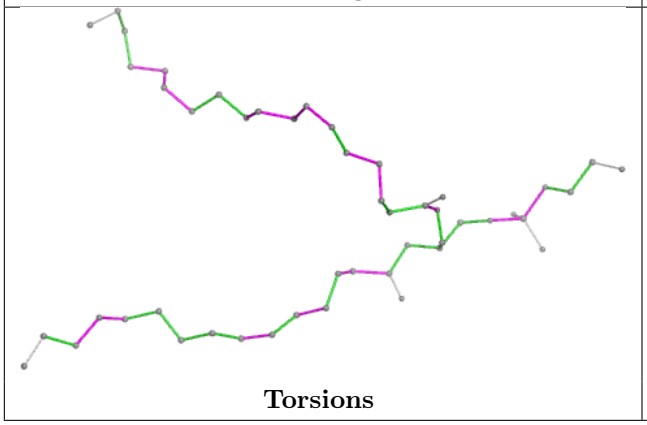
Ligand PEE J 303



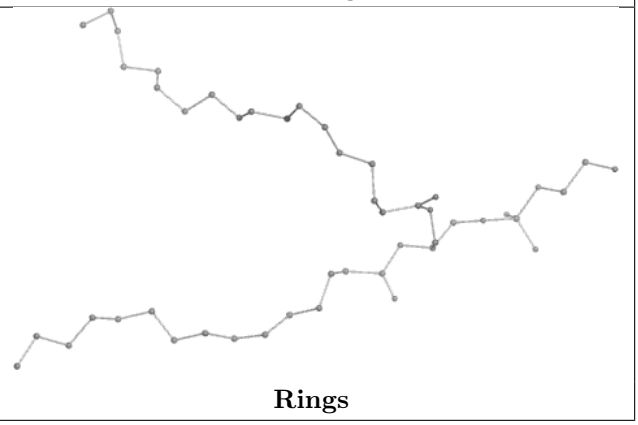
Bond lengths



Bond angles

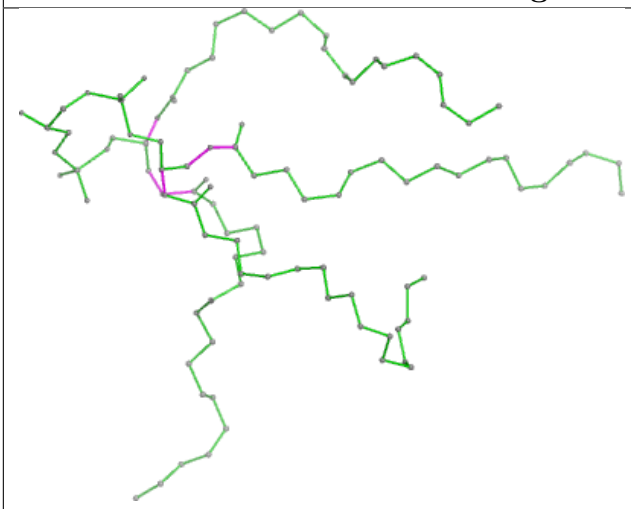


Torsions



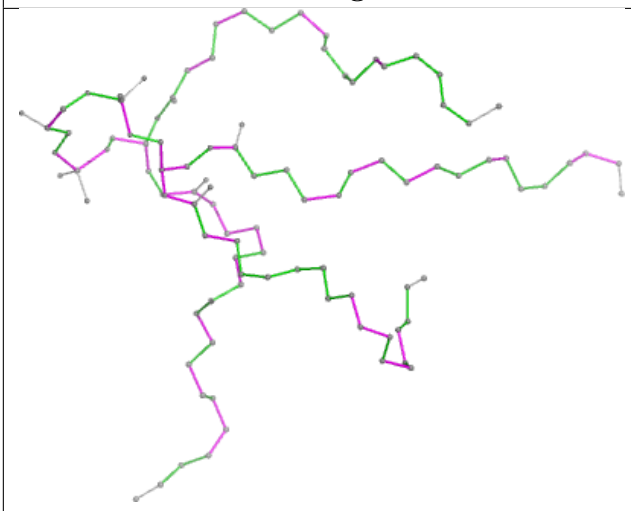
Rings

Ligand CDL I 301

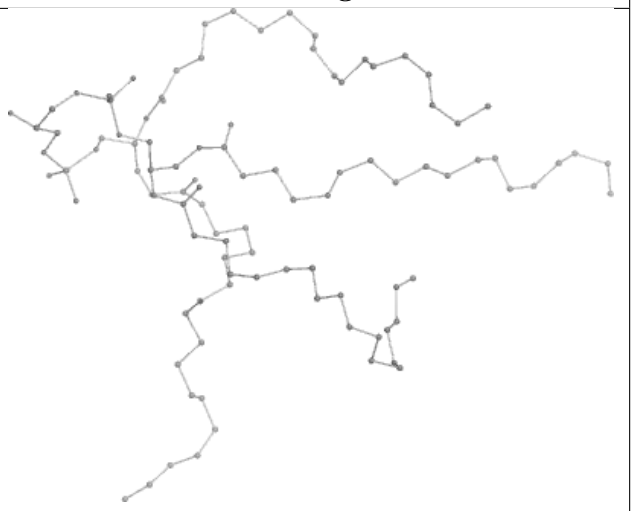


Bond lengths

Bond angles

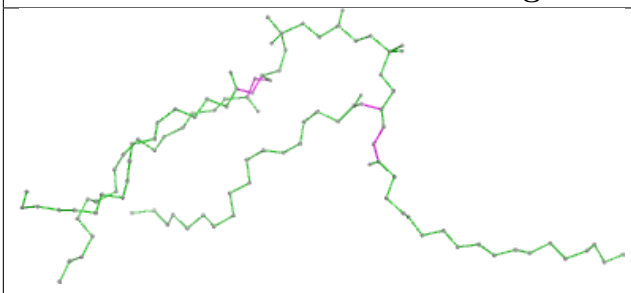


Torsions

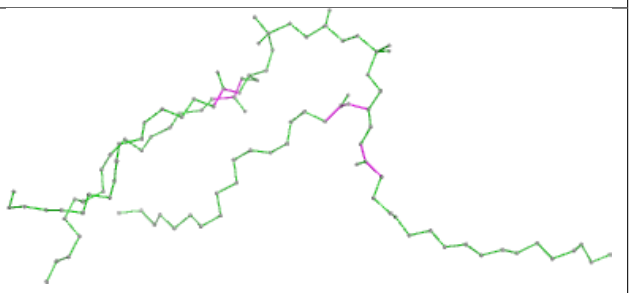


Rings

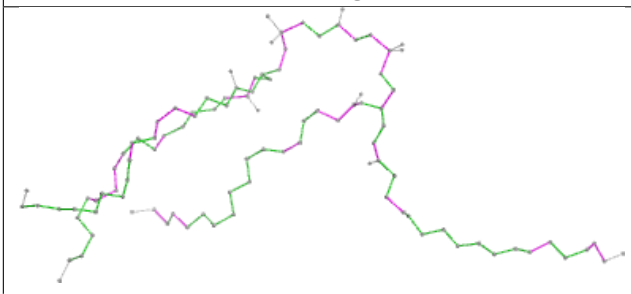
Ligand CDL K 202



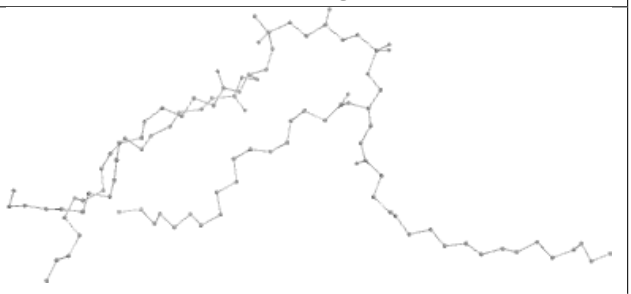
Bond lengths



Bond angles

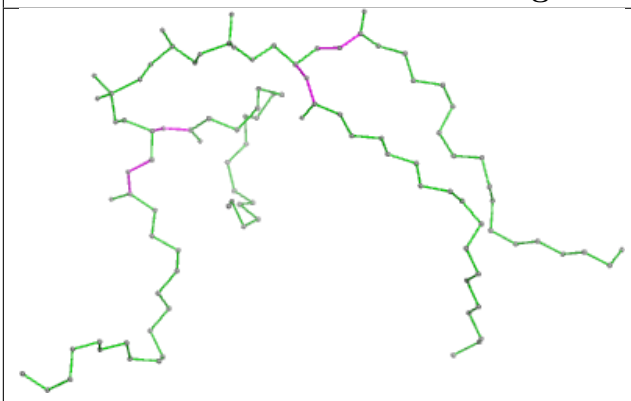


Torsions

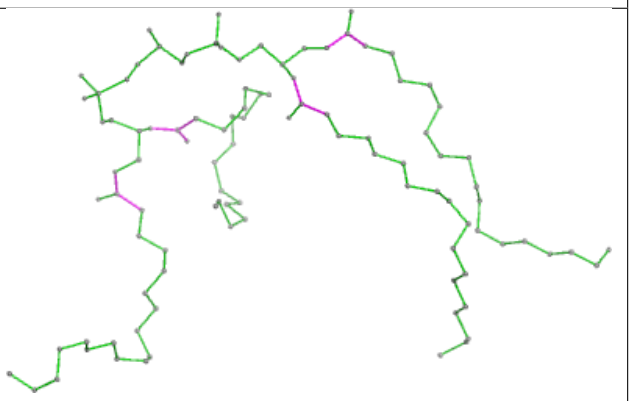


Rings

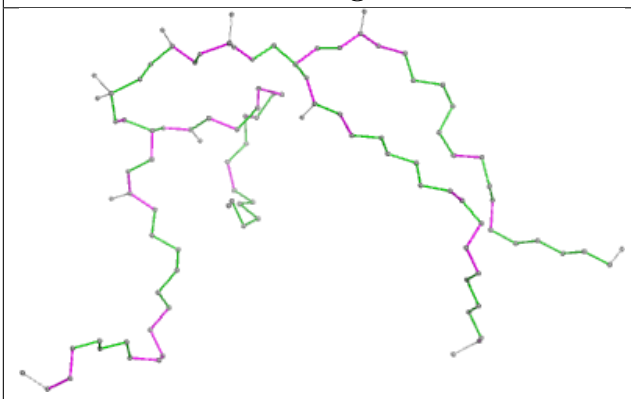
Ligand CDL f 303



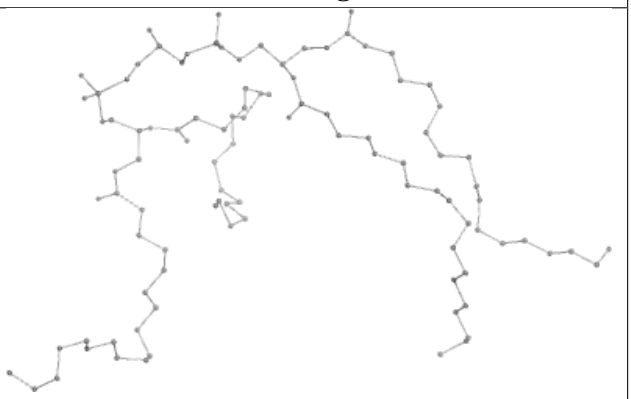
Bond lengths



Bond angles

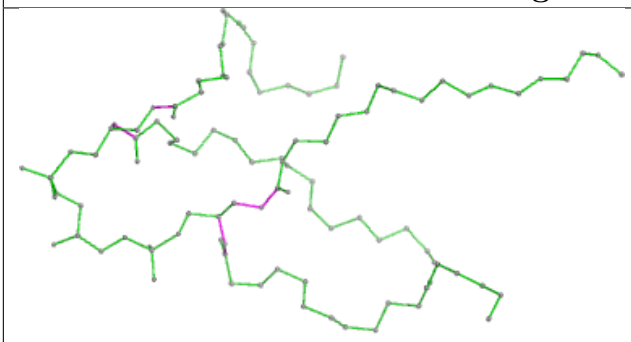


Torsions

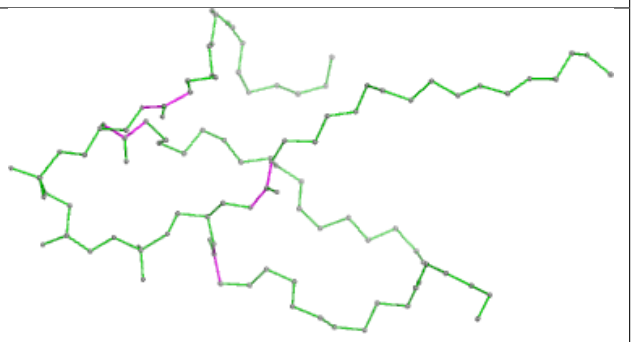


Rings

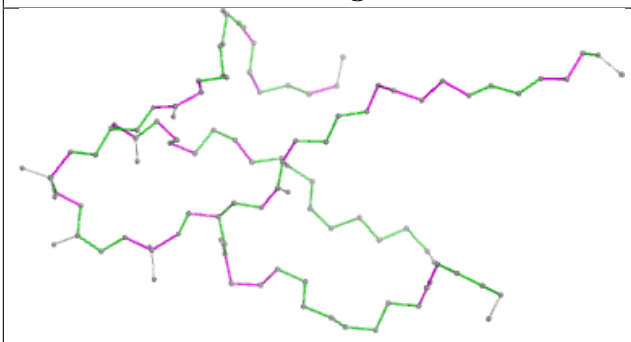
Ligand CDL l 304



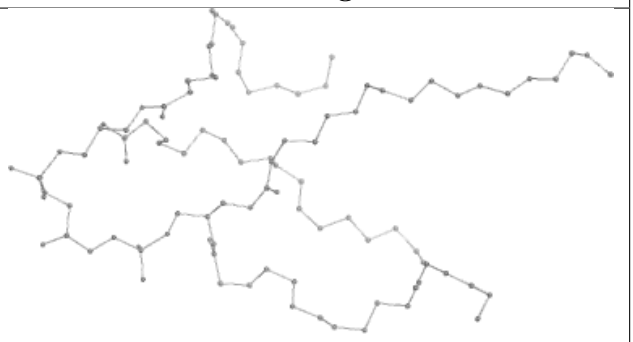
Bond lengths



Bond angles

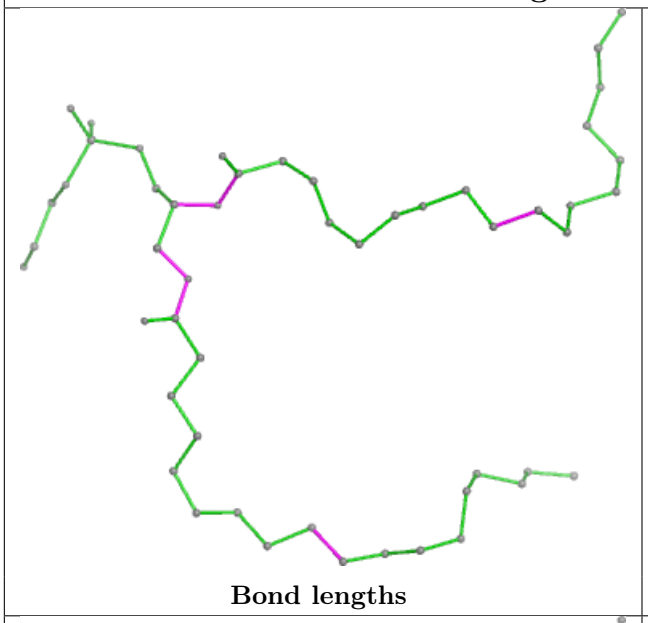


Torsions

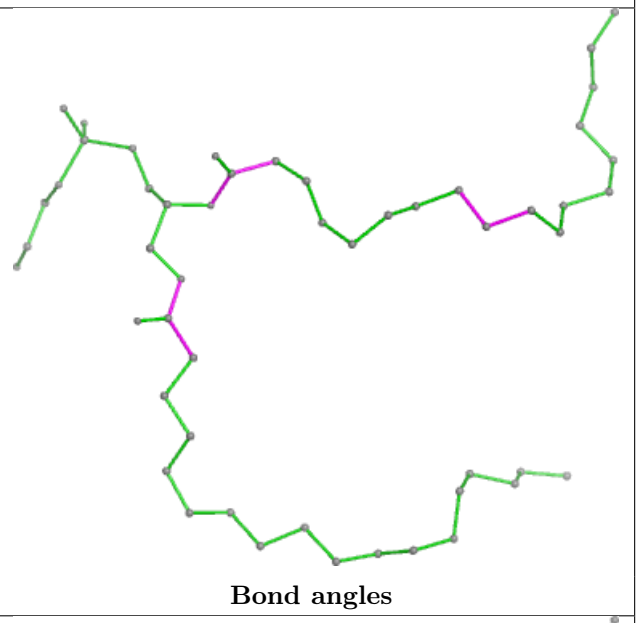


Rings

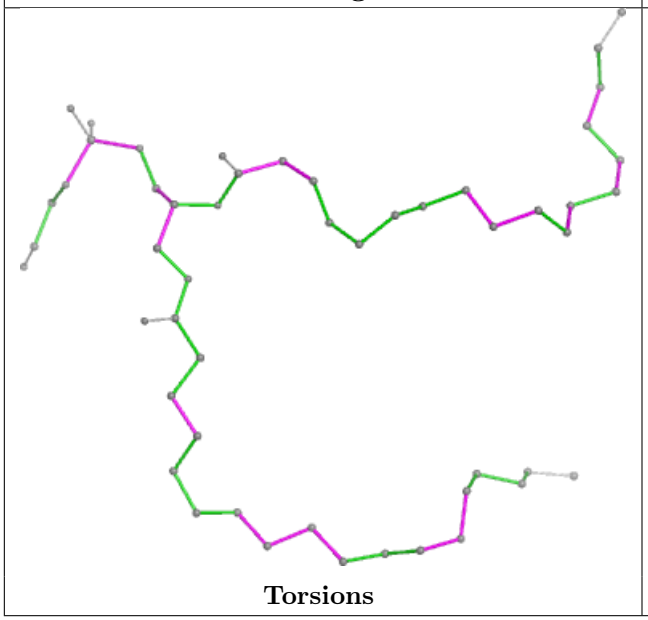
Ligand PEE J 304



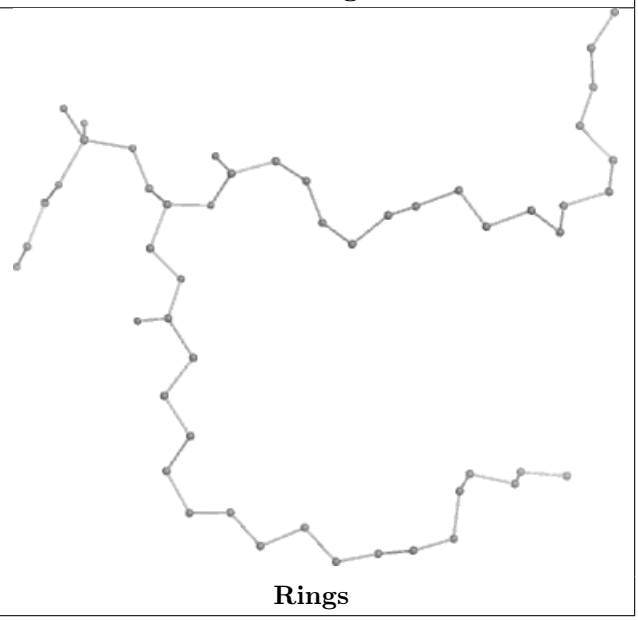
Bond lengths



Bond angles

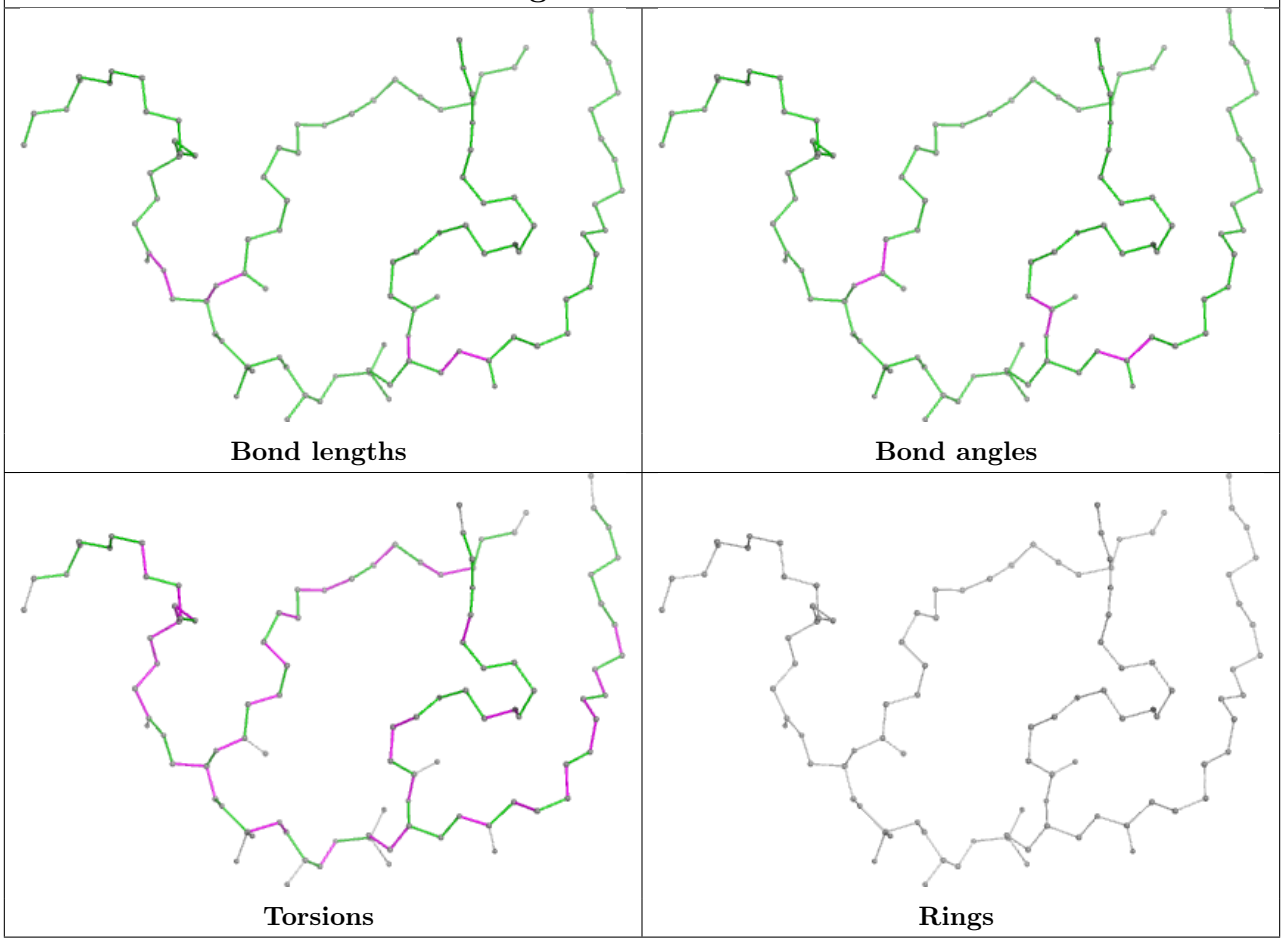


Torsions

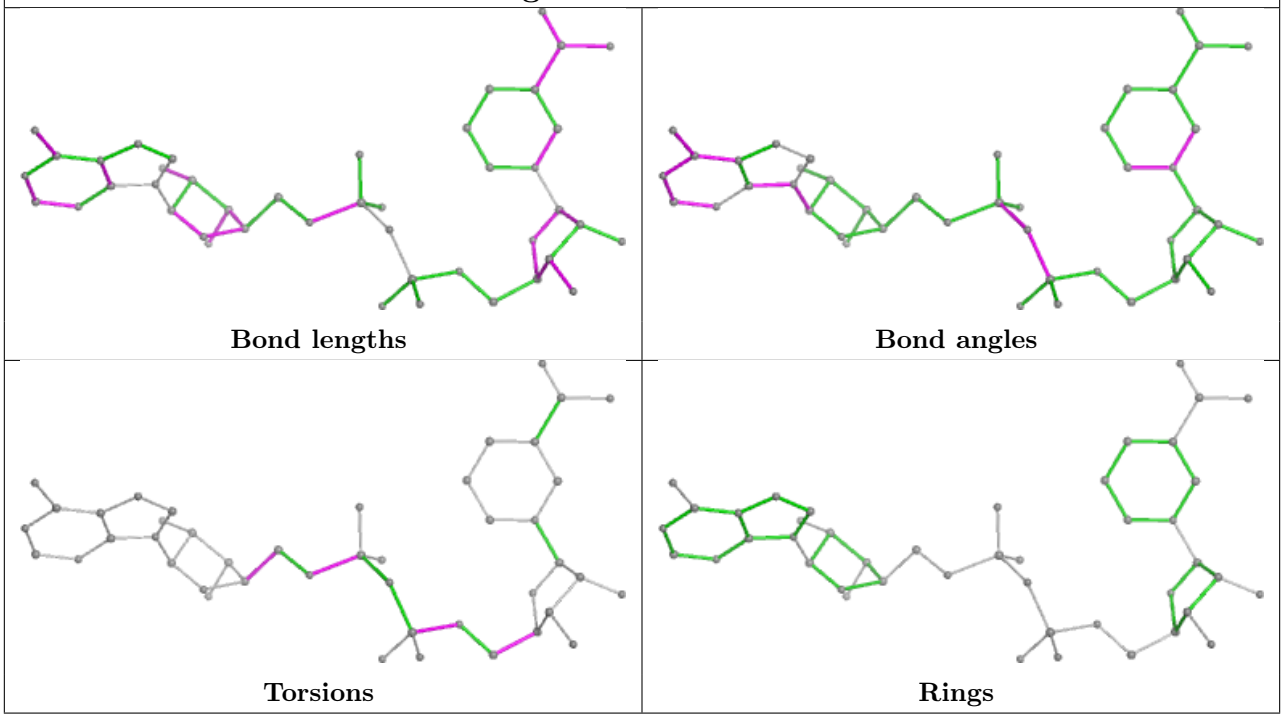


Rings

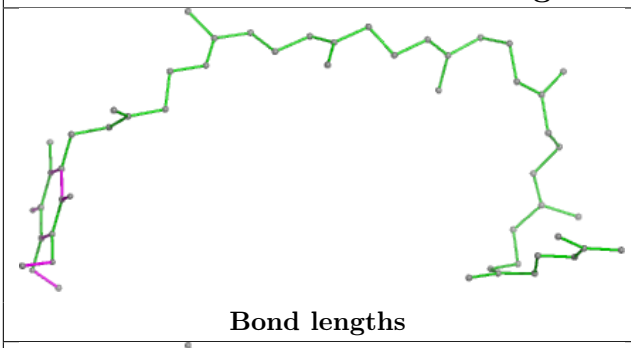
Ligand CDL a 501



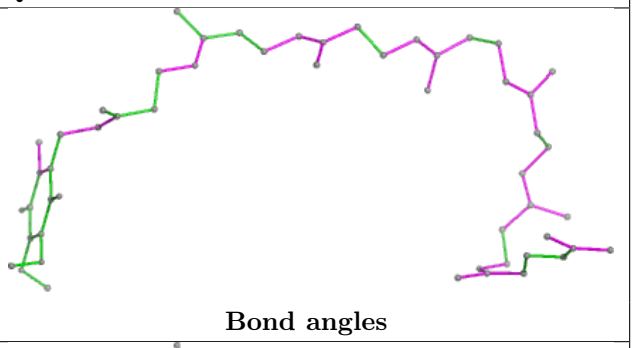
Ligand NAD E 900



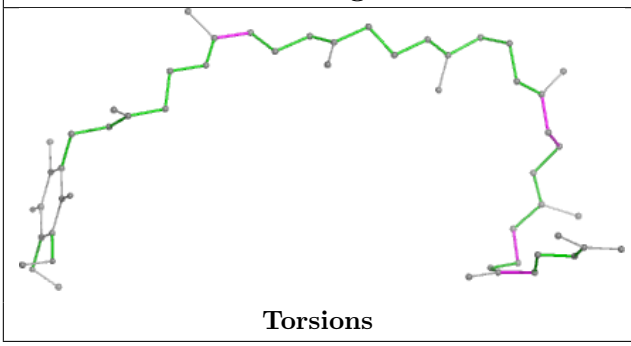
Ligand UQ8 i 303



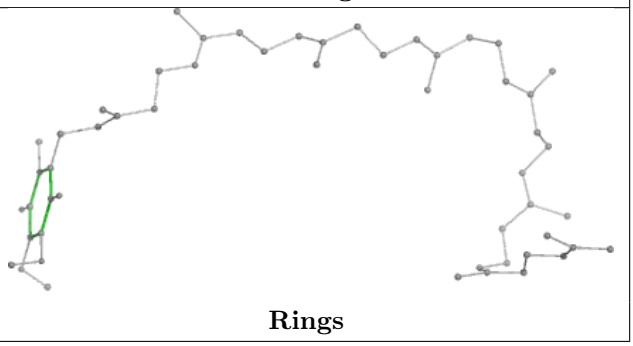
Bond lengths



Bond angles

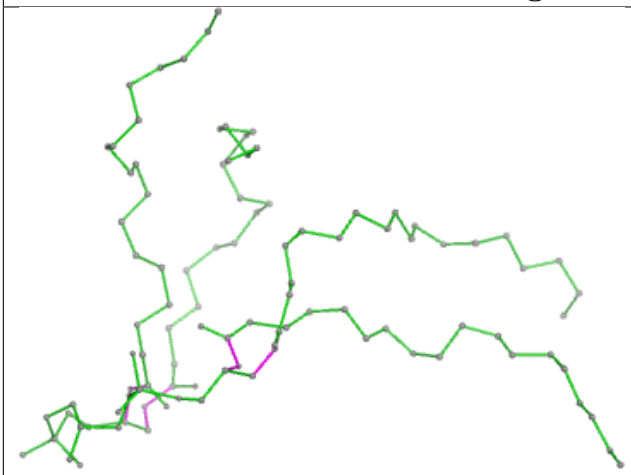


Torsions

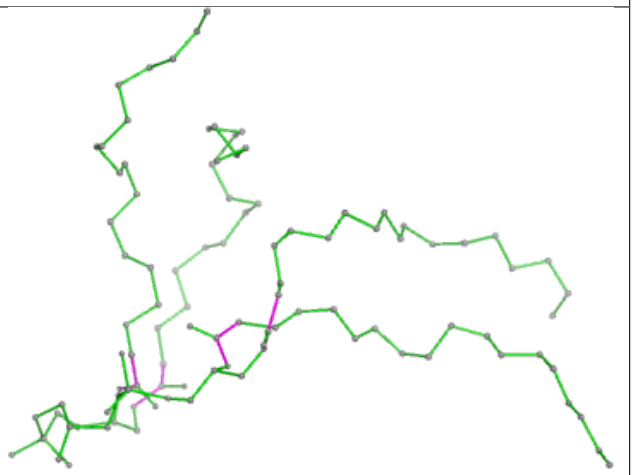


Rings

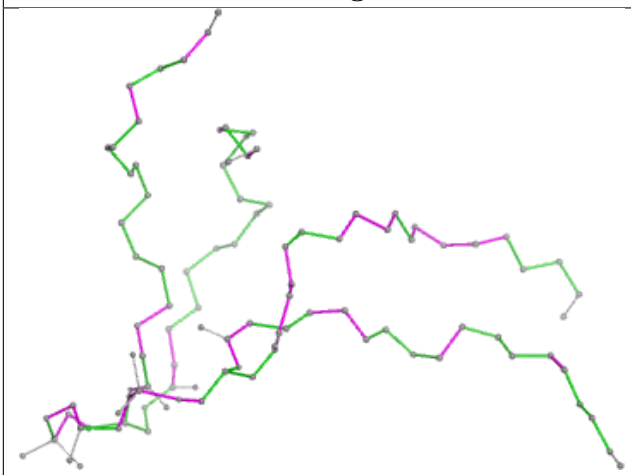
Ligand CDL L 301



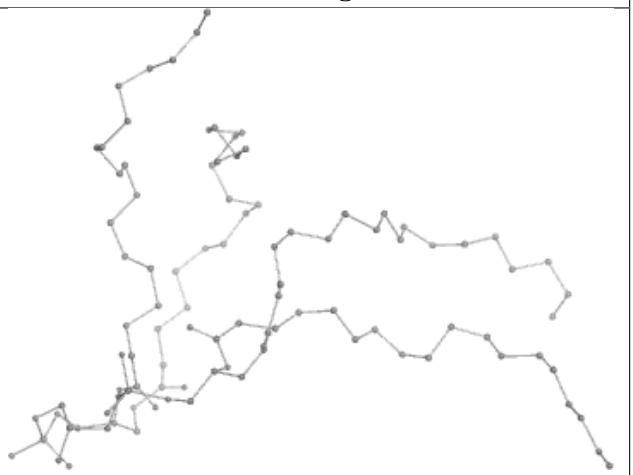
Bond lengths



Bond angles

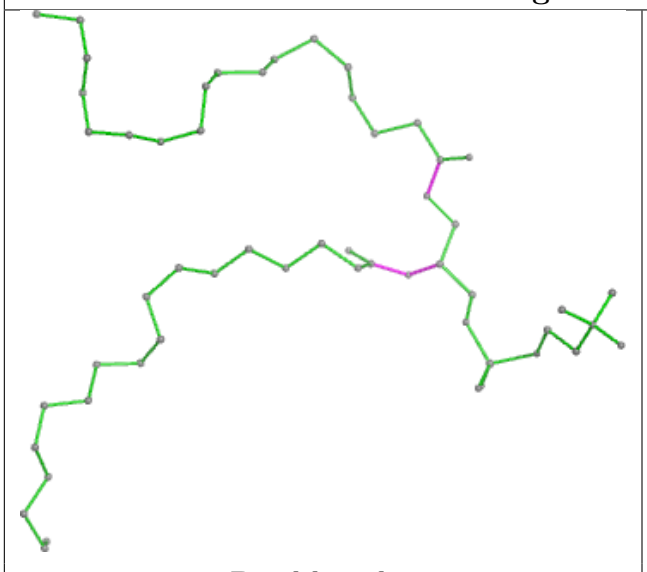


Torsions

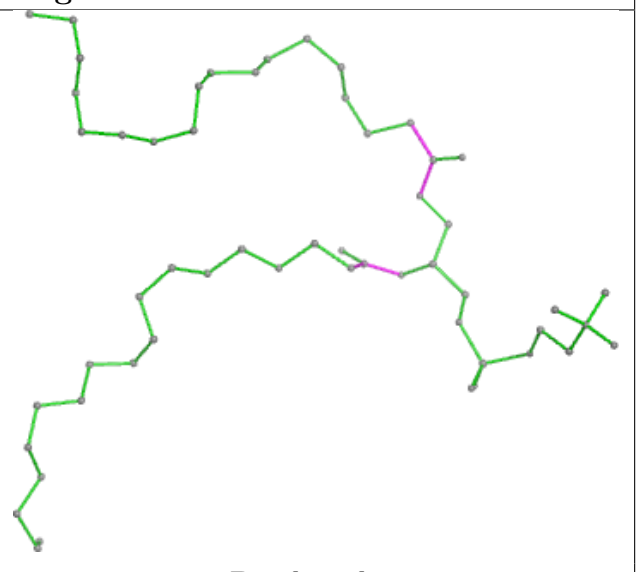


Rings

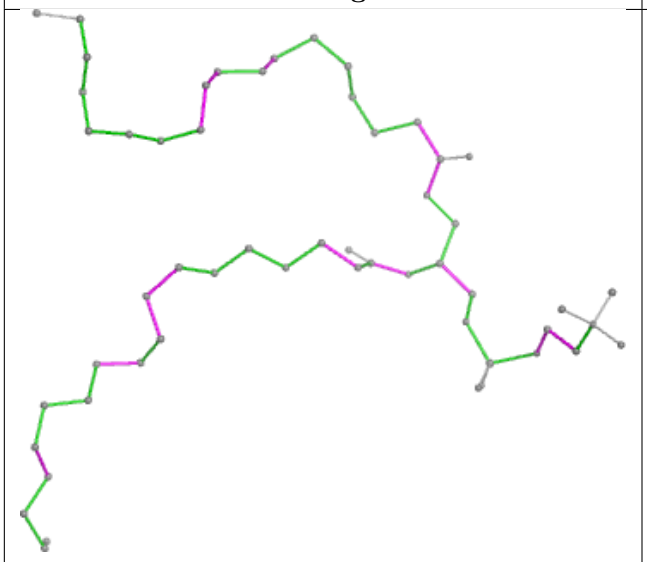
Ligand PC1 g 303



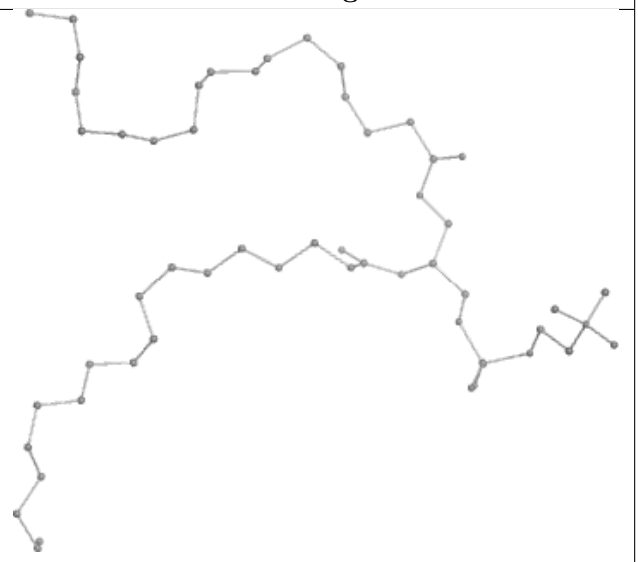
Bond lengths



Bond angles

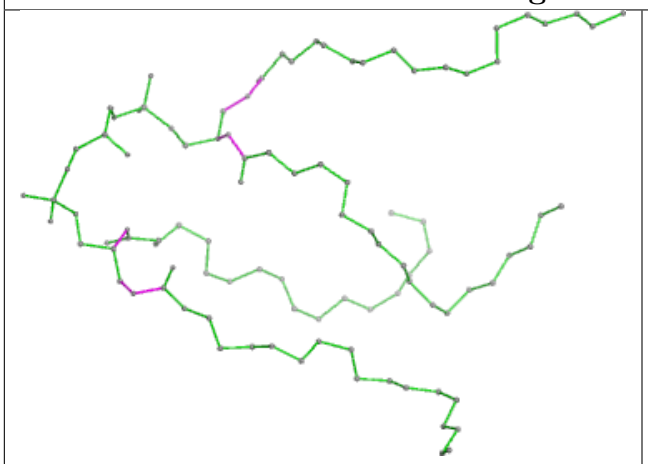


Torsions

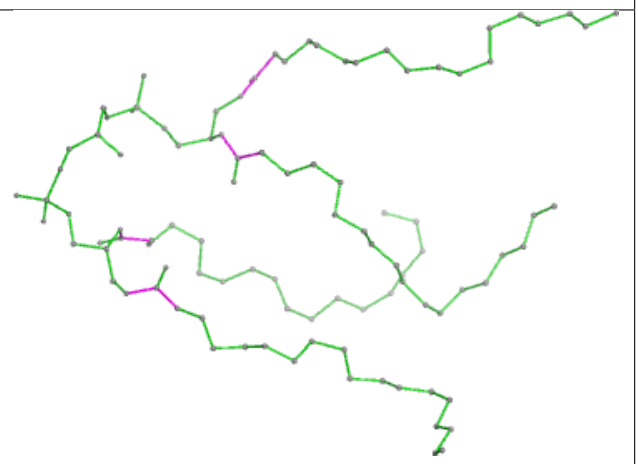


Rings

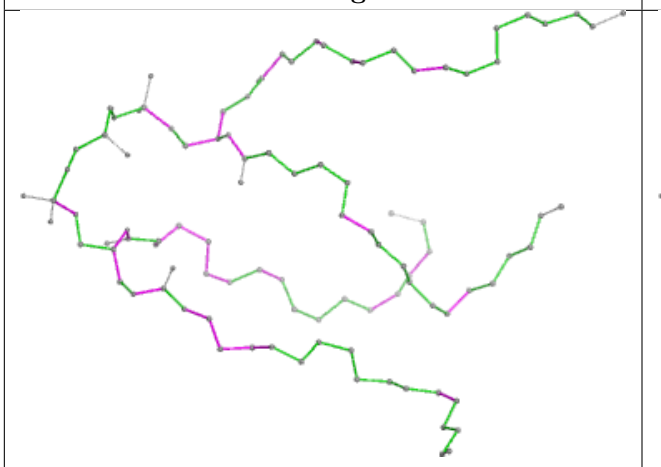
Ligand CDL J 302



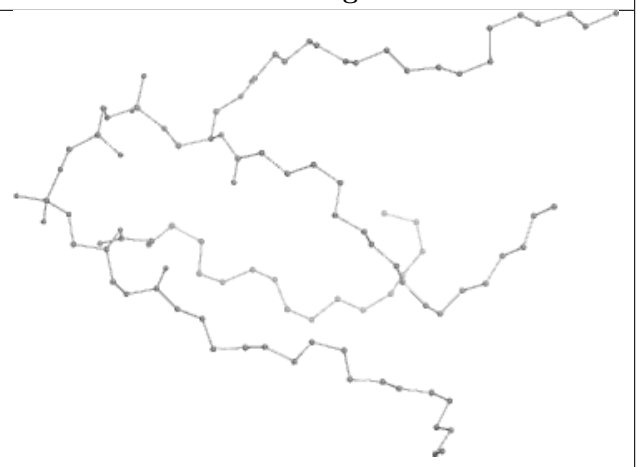
Bond lengths



Bond angles

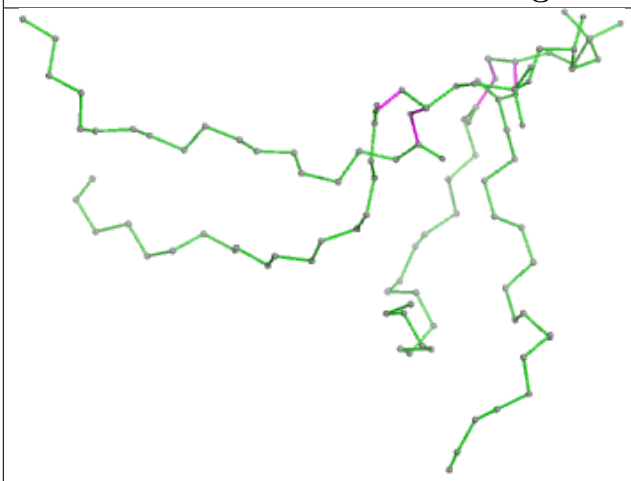


Torsions



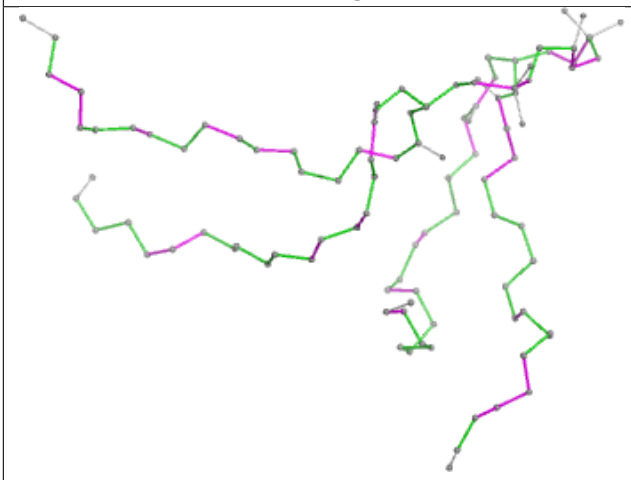
Rings

Ligand CDL l 301

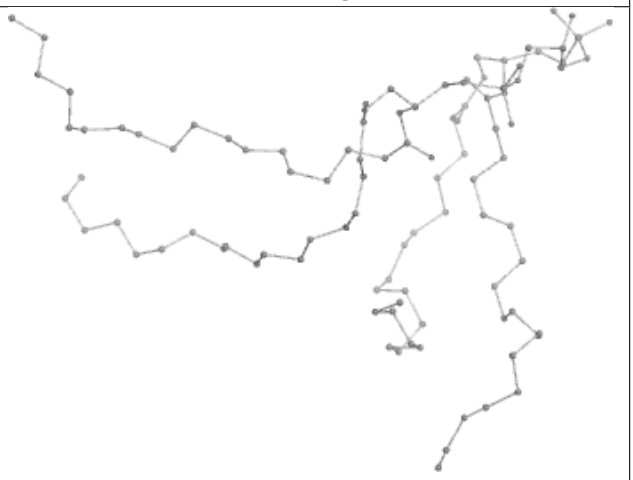


Bond lengths

Bond angles

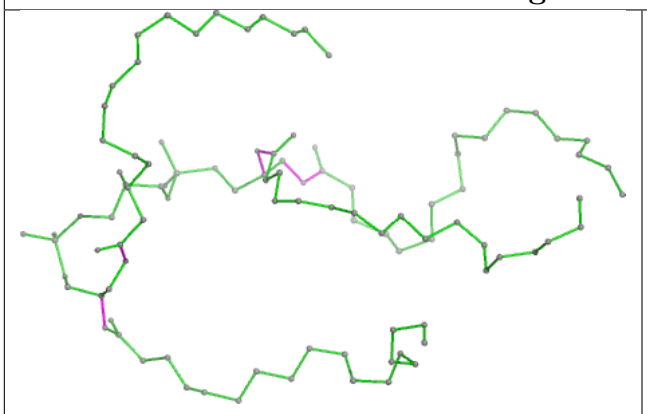


Torsions

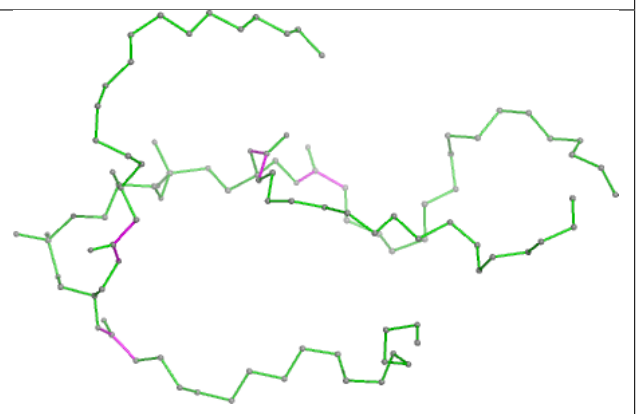


Rings

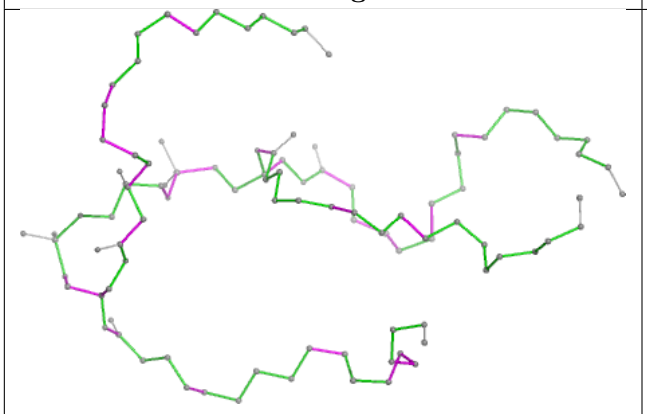
Ligand CDL J 301



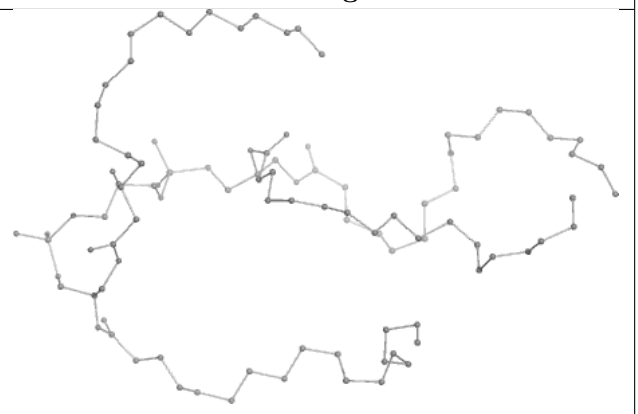
Bond lengths



Bond angles

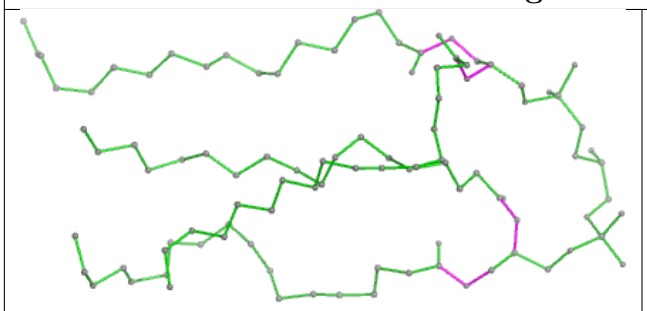


Torsions

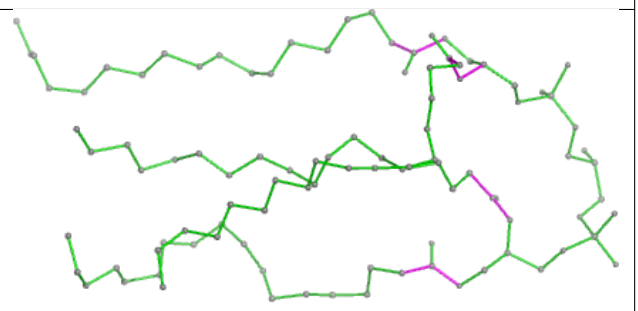


Rings

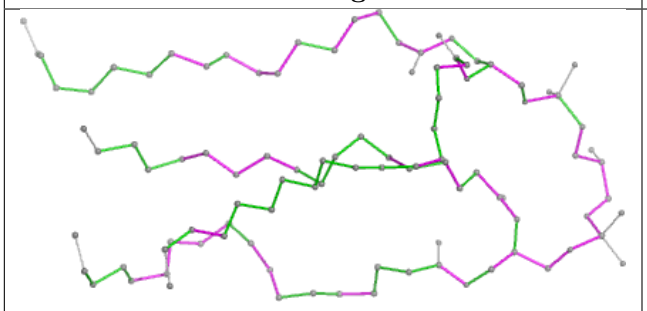
Ligand CDL B 401



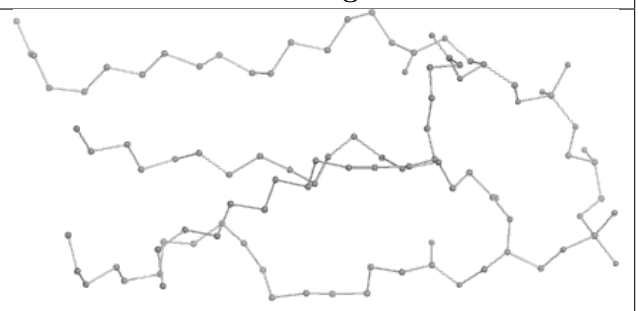
Bond lengths



Bond angles

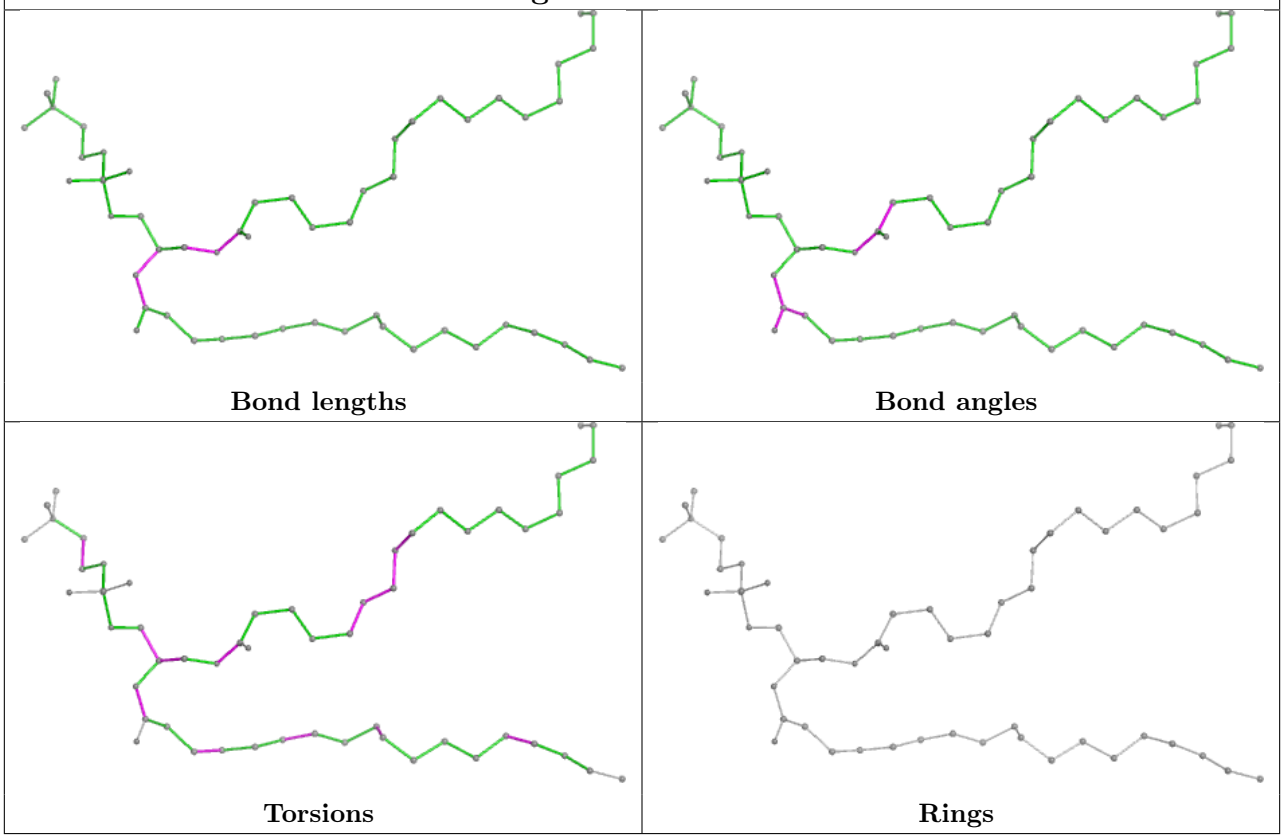


Torsions

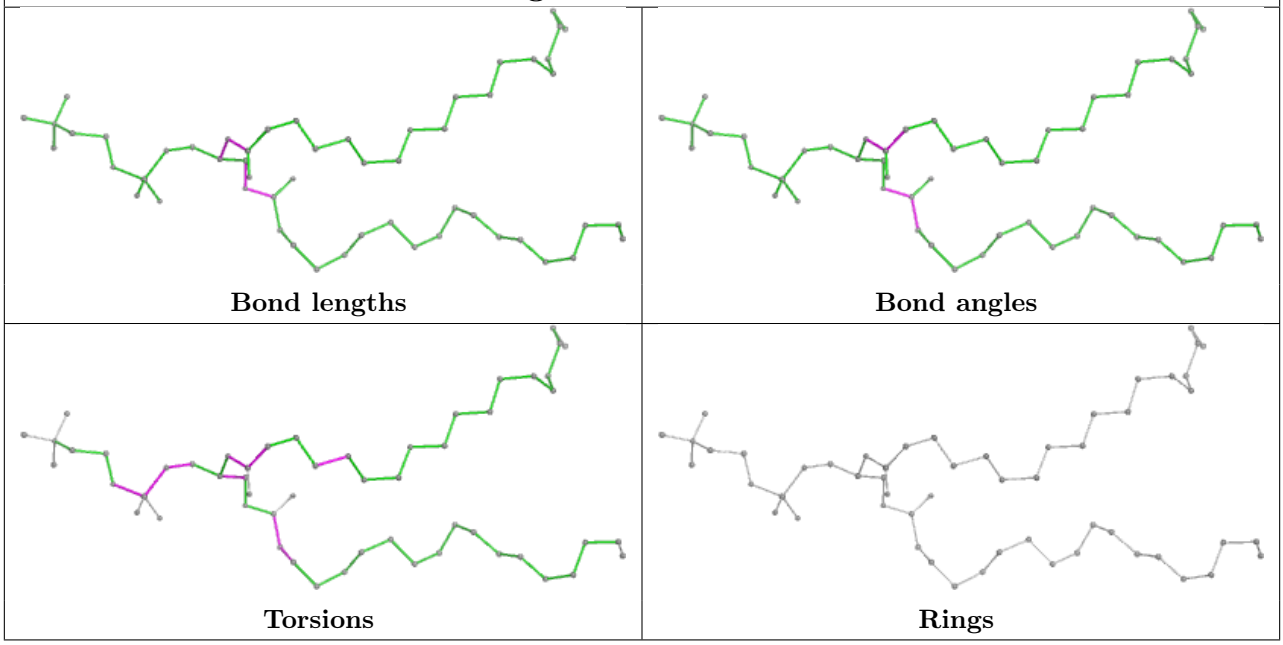


Rings

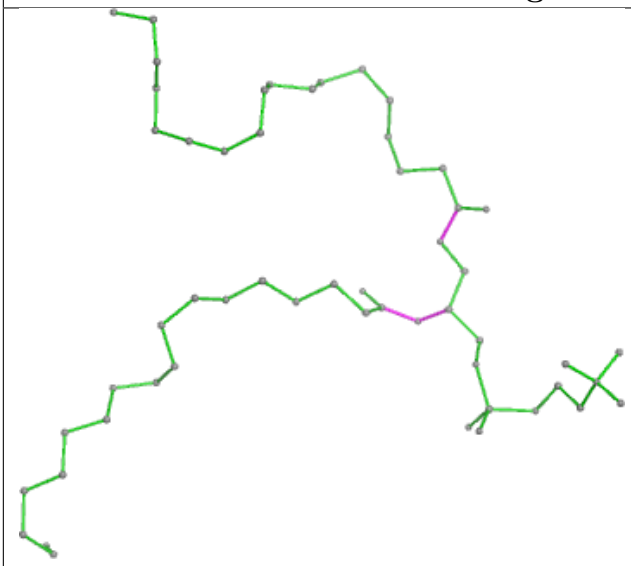
Ligand PC1 d 301



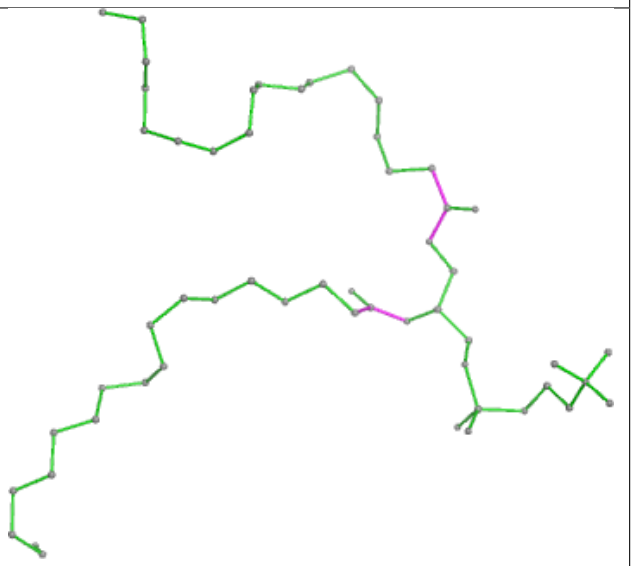
Ligand PC1 G 303



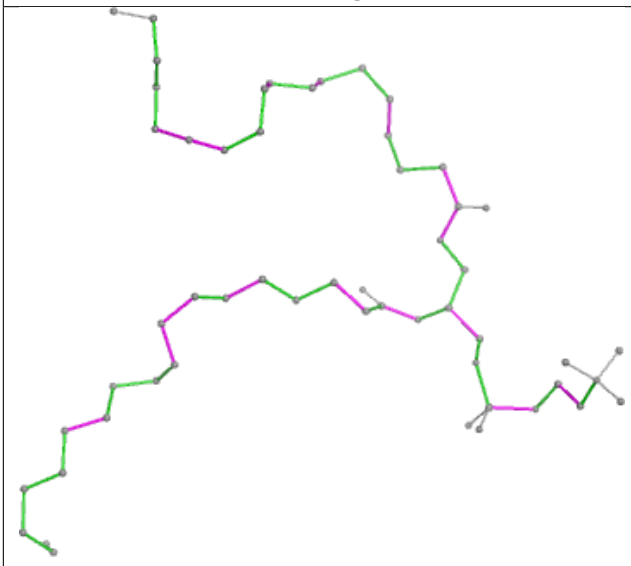
Ligand PC1 G 304



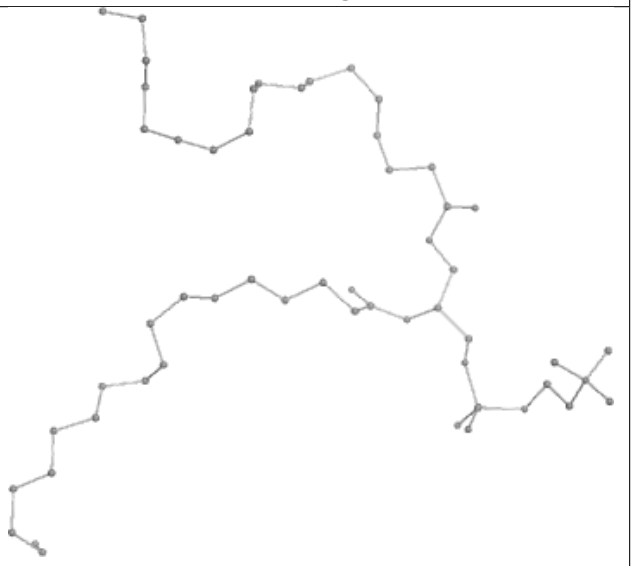
Bond lengths



Bond angles

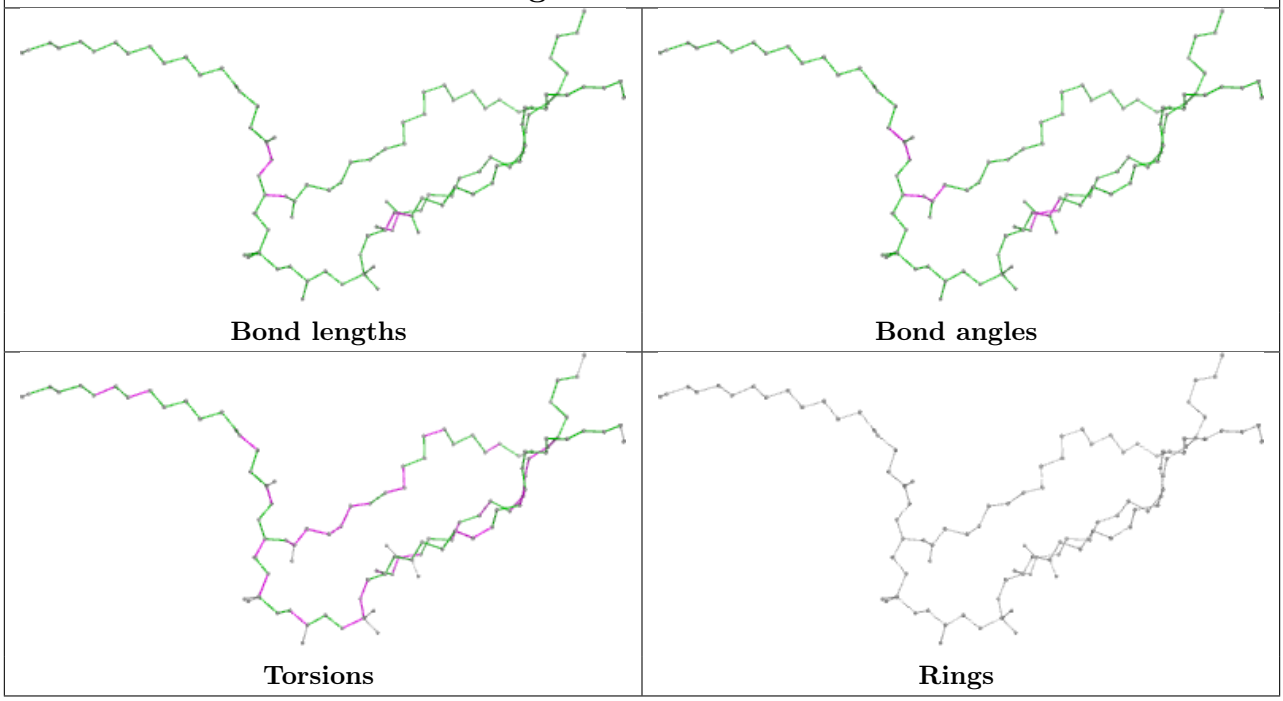


Torsions

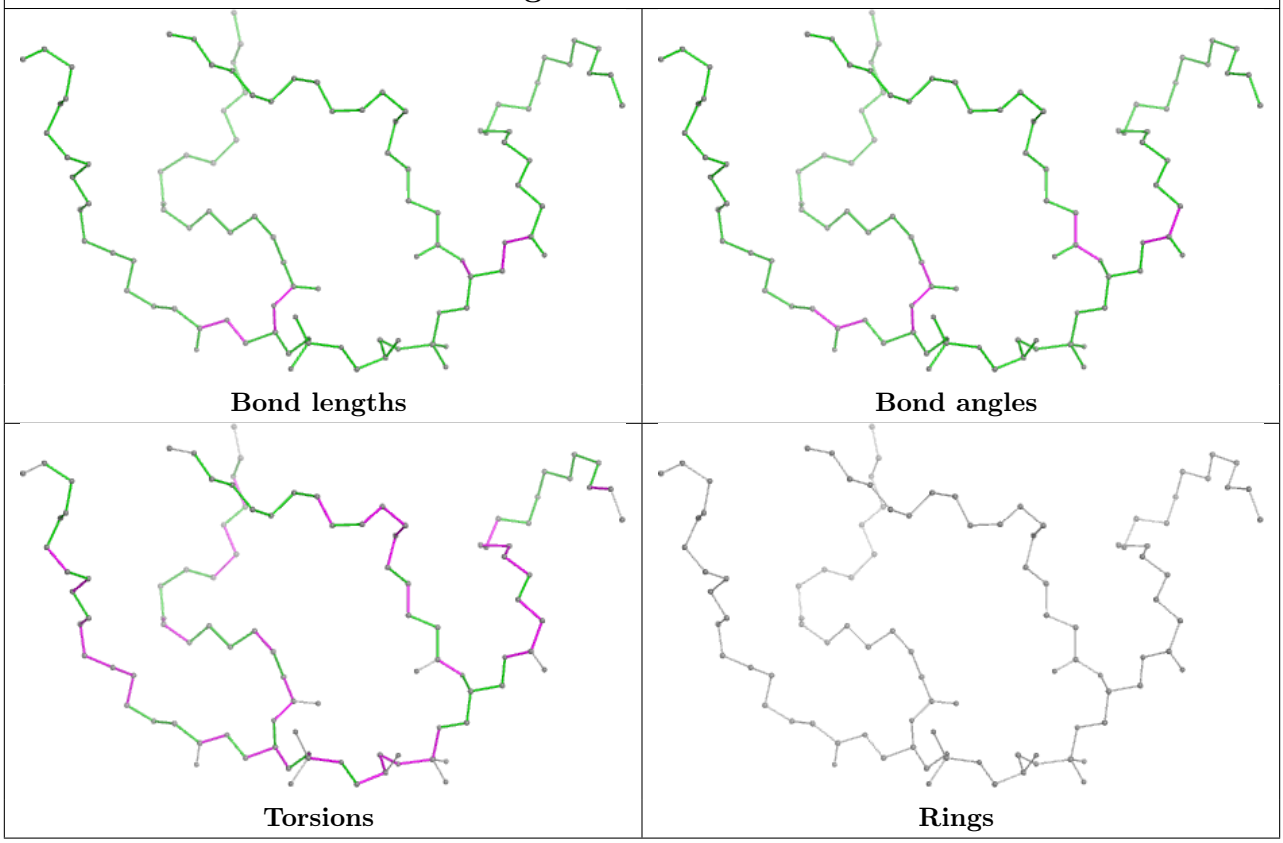


Rings

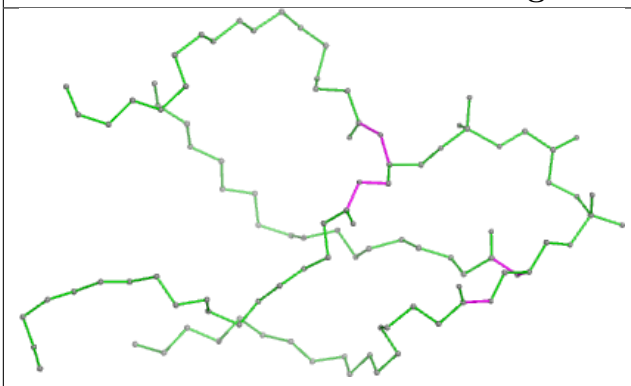
Ligand CDL k 202



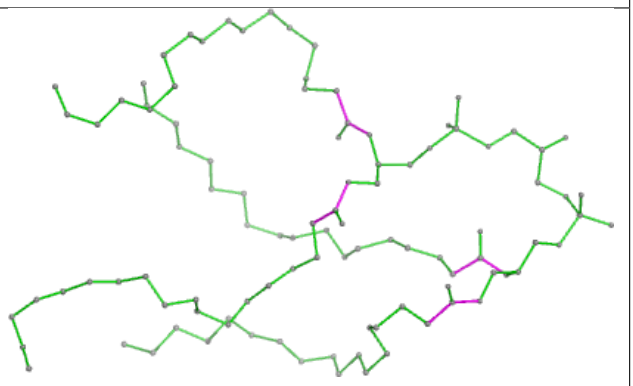
Ligand CDL A 501



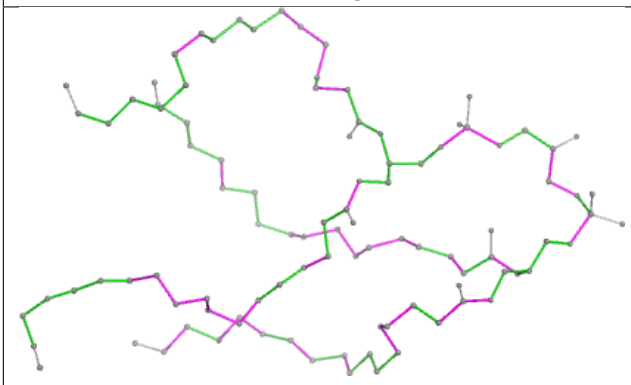
Ligand CDL k 203



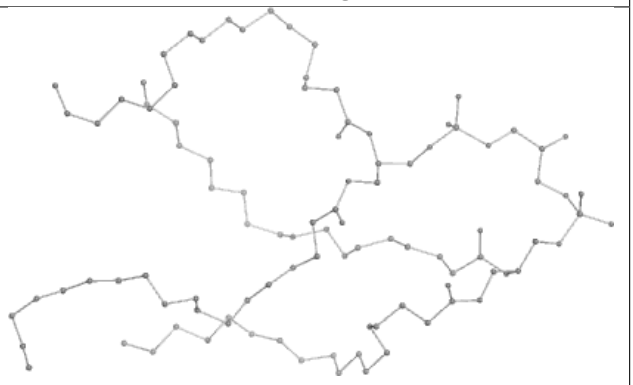
Bond lengths



Bond angles

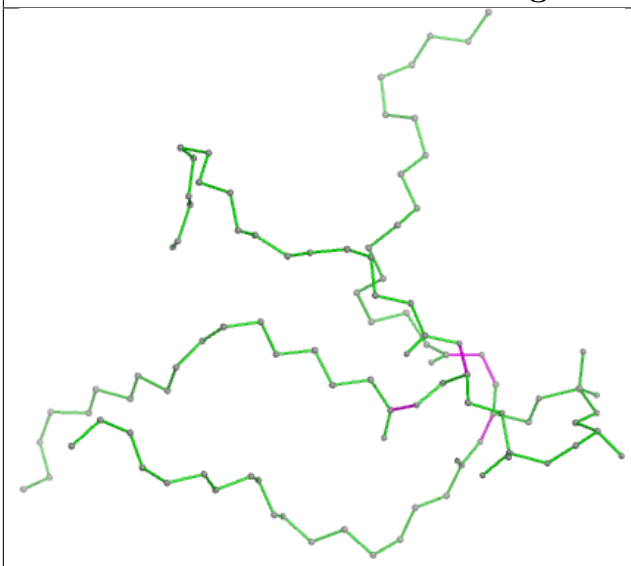


Torsions

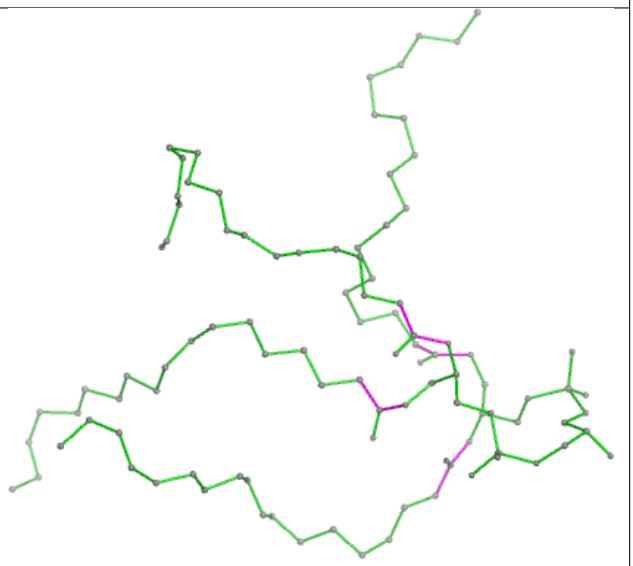


Rings

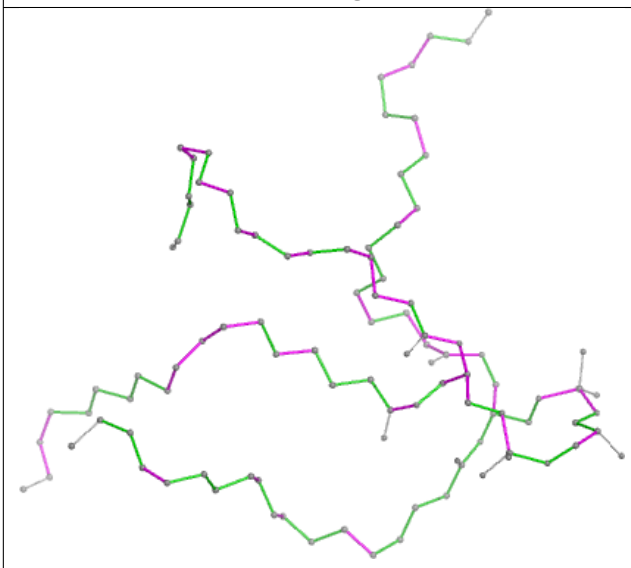
Ligand CDL r 201



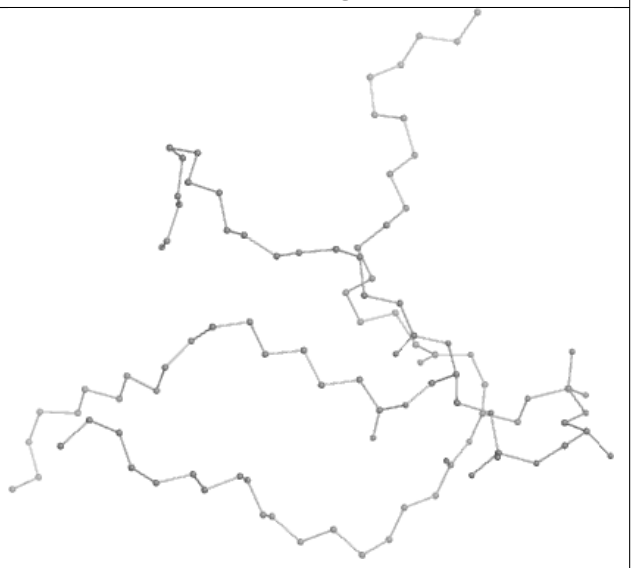
Bond lengths



Bond angles

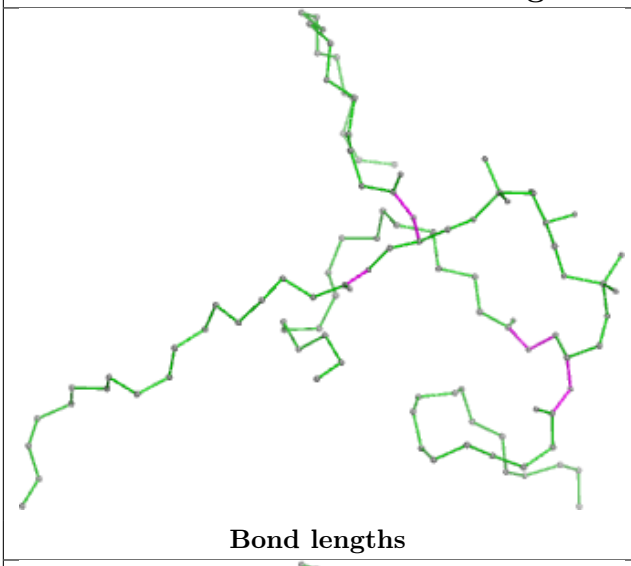


Torsions

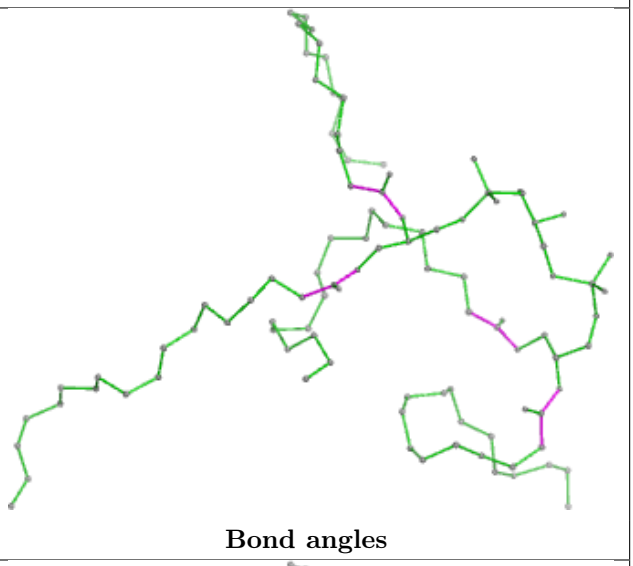


Rings

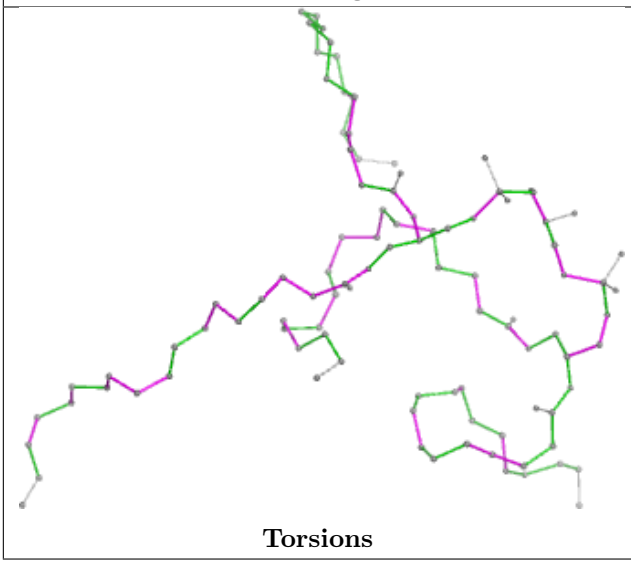
Ligand CDL b 402



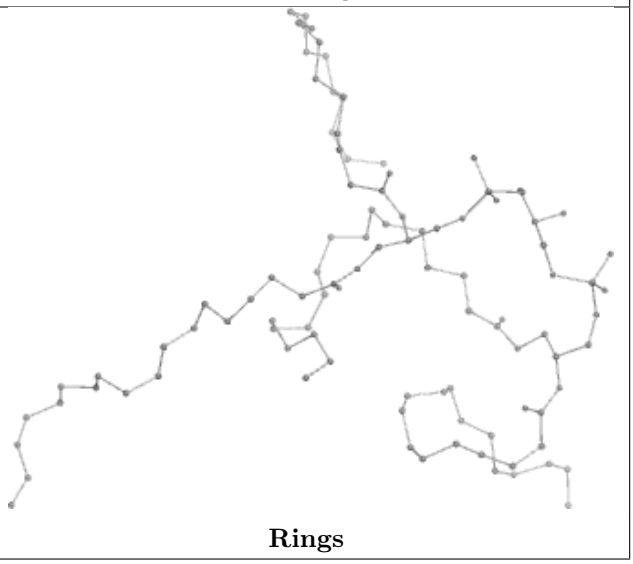
Bond lengths



Bond angles

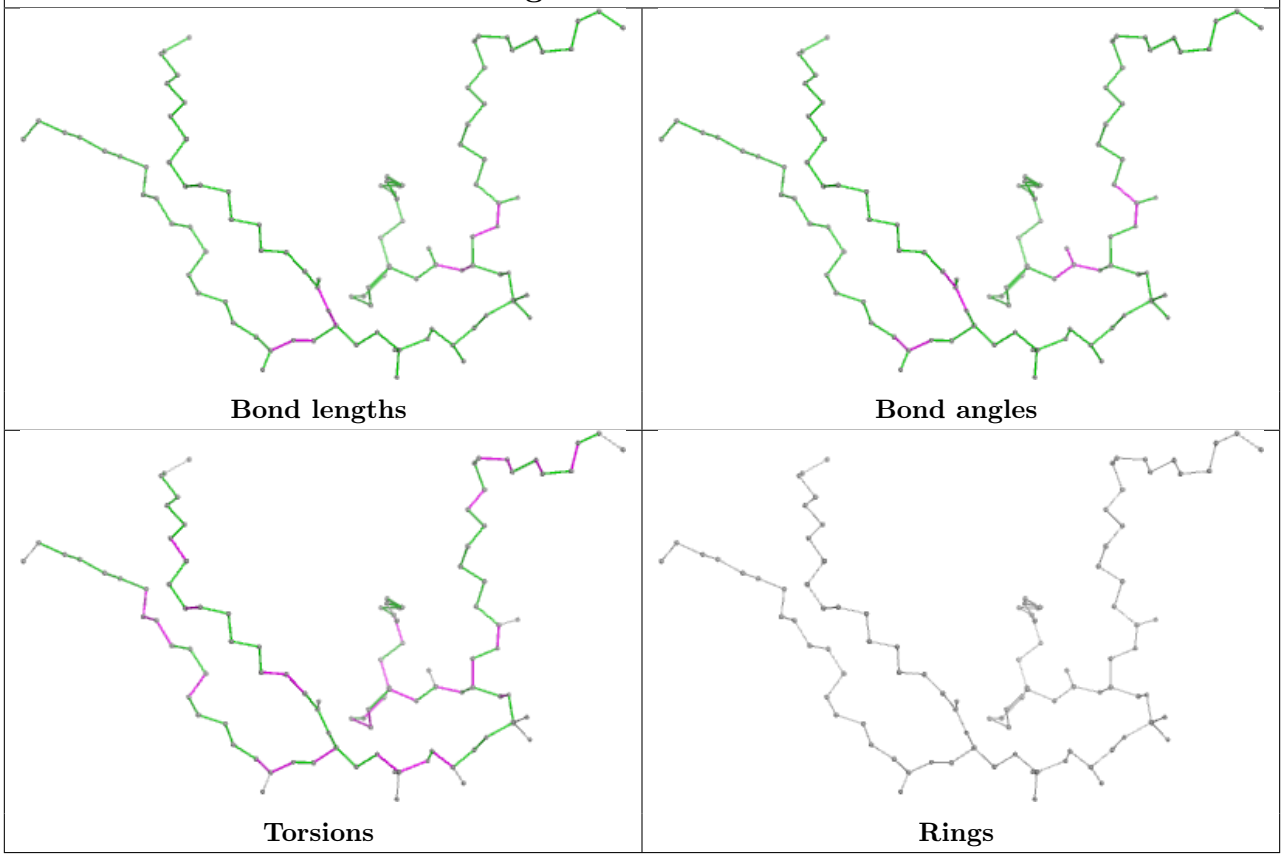


Torsions

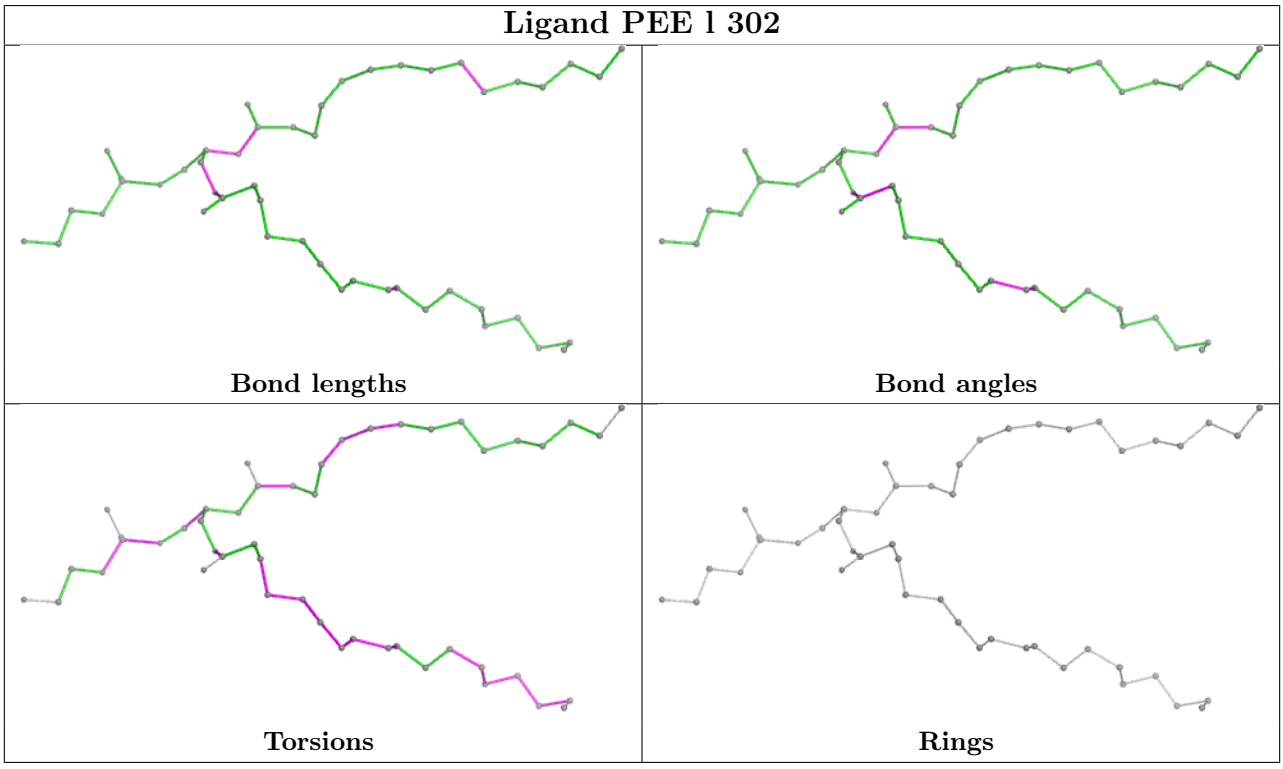


Rings

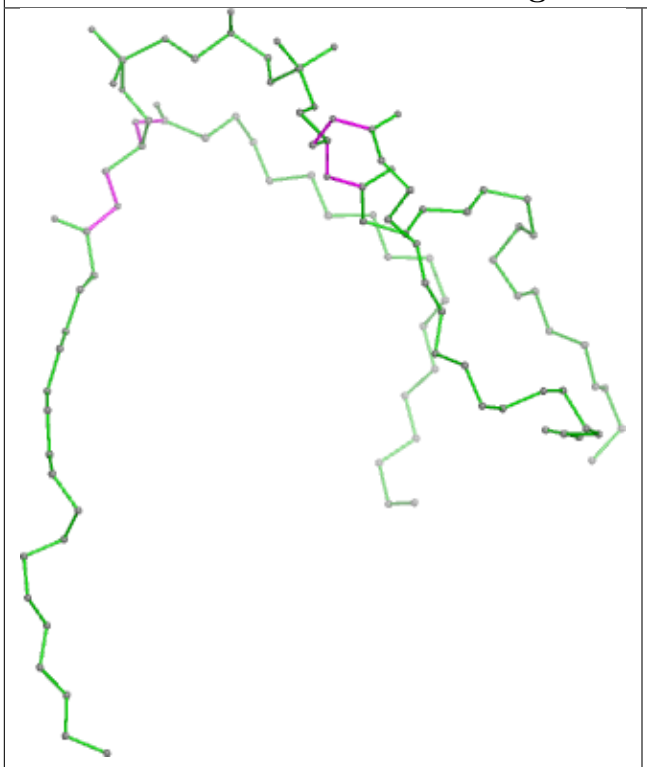
Ligand CDL B 405



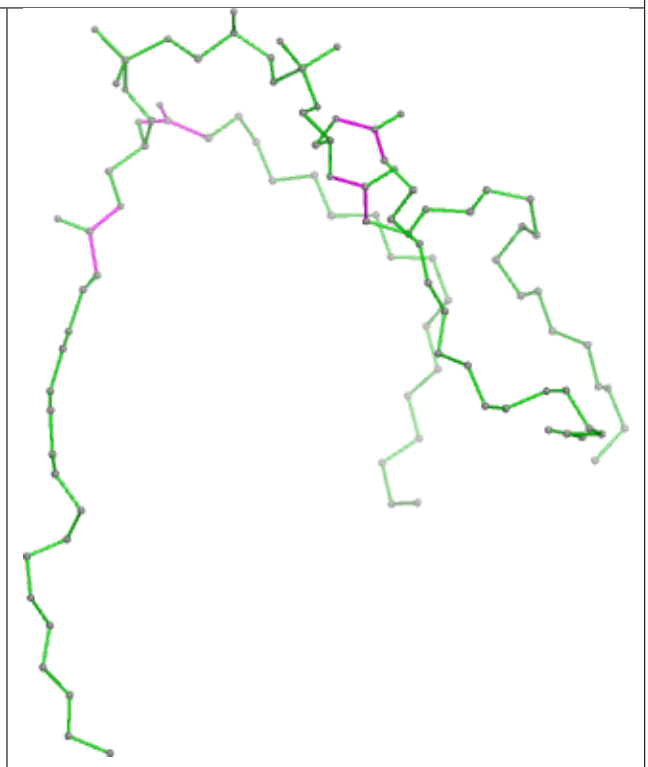
Ligand PEE l 302



Ligand CDL k 201

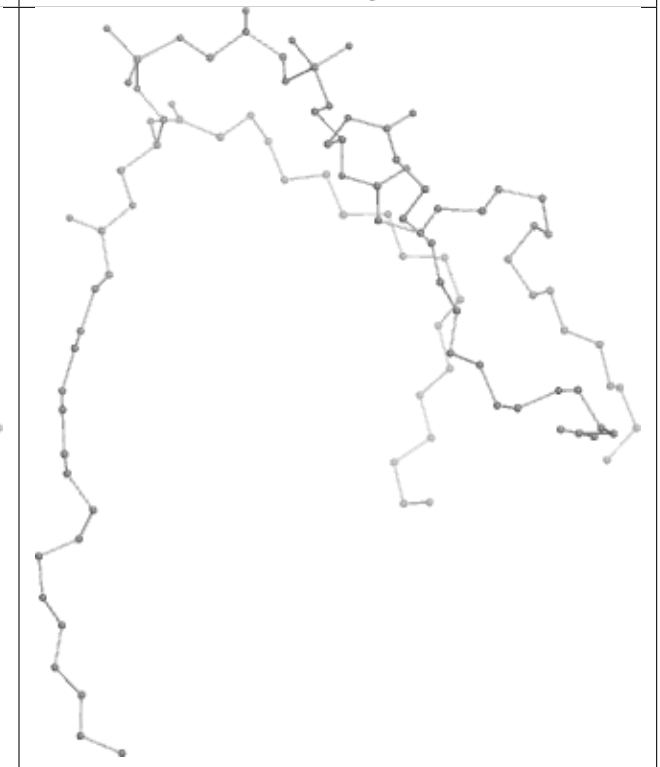


Bond lengths



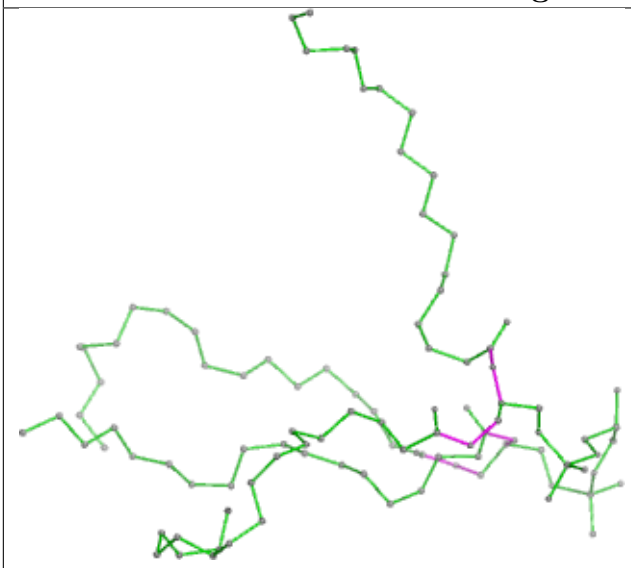
Bond angles

Torsions

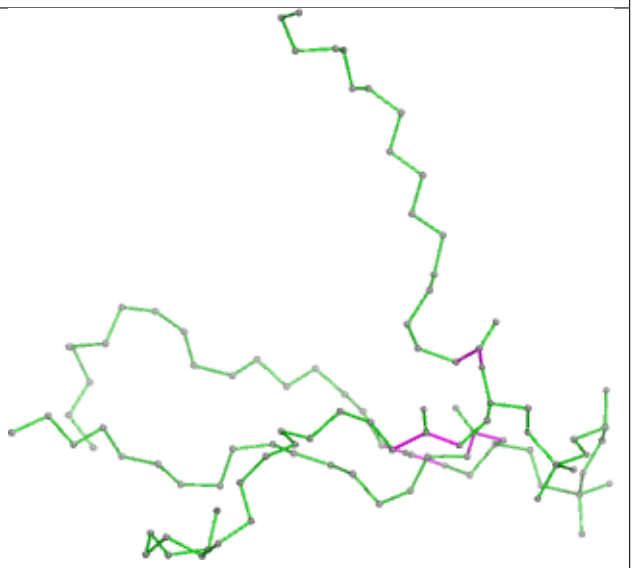


Rings

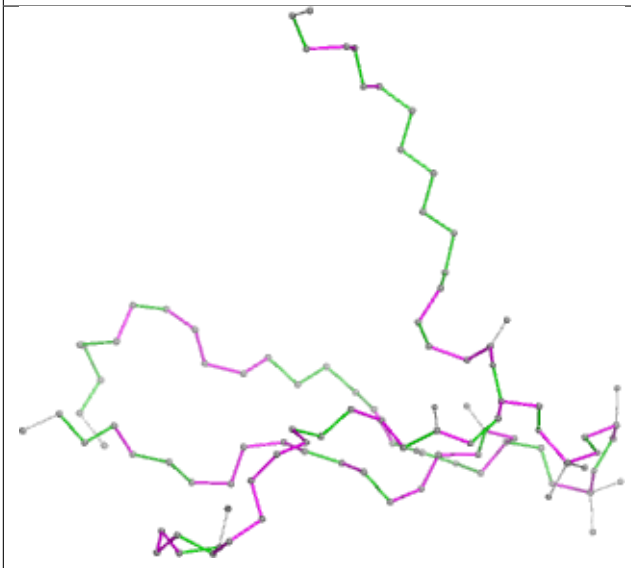
Ligand CDL f 304



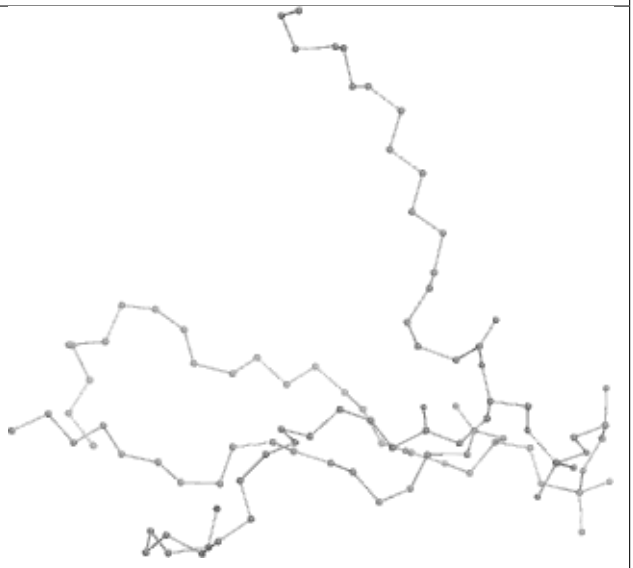
Bond lengths



Bond angles

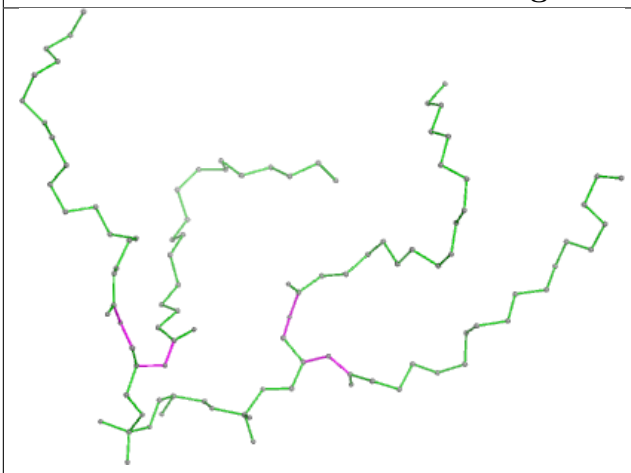


Torsions

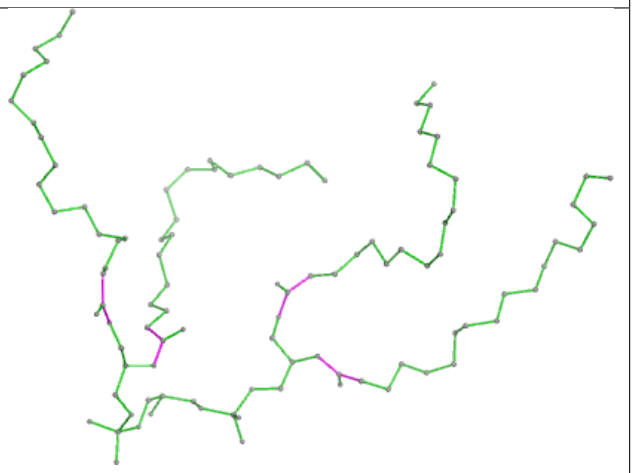


Rings

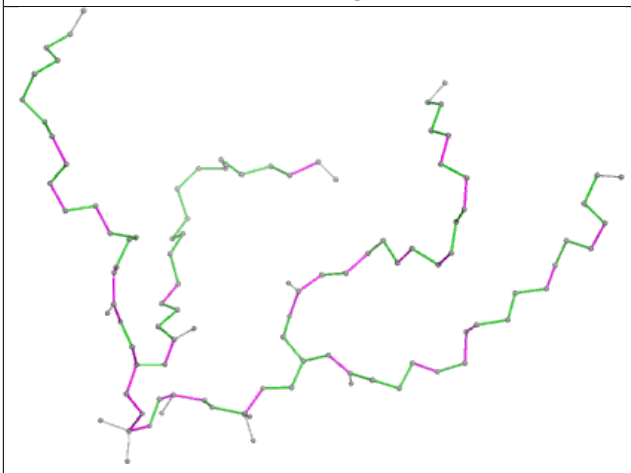
Ligand CDL I 302



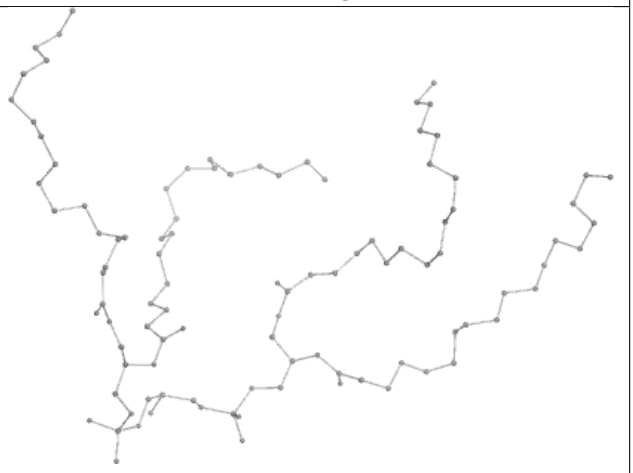
Bond lengths



Bond angles

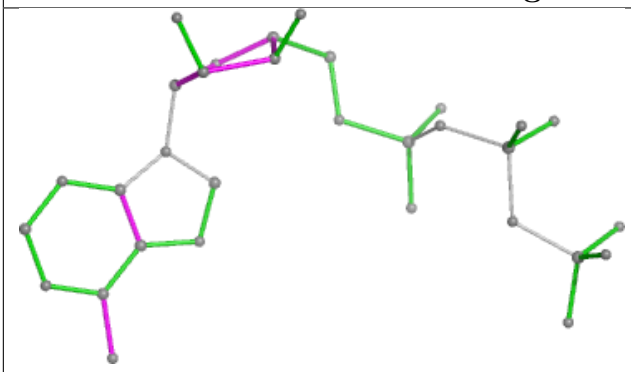


Torsions

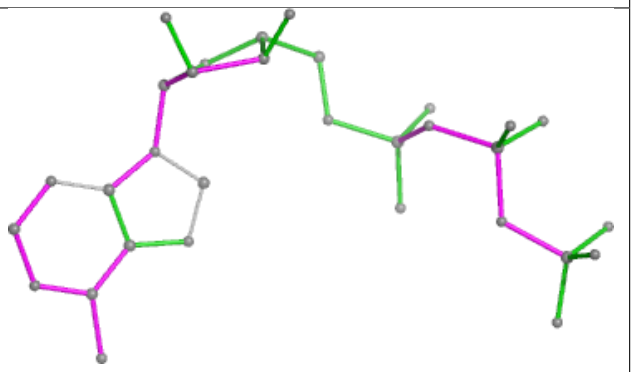


Rings

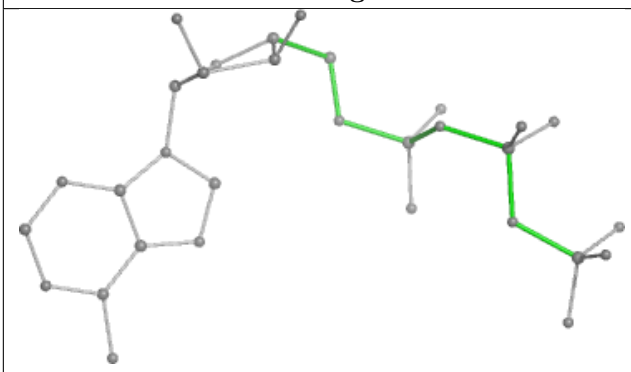
Ligand ATP G 301



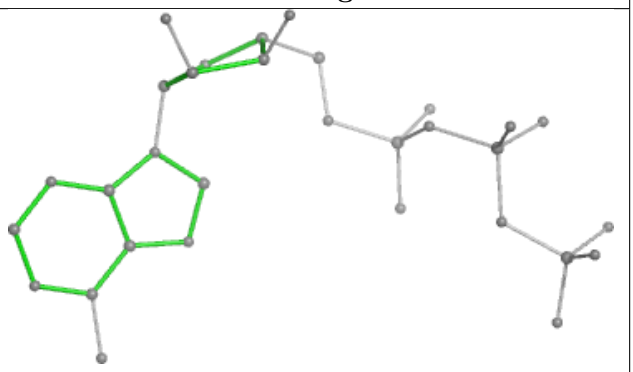
Bond lengths



Bond angles

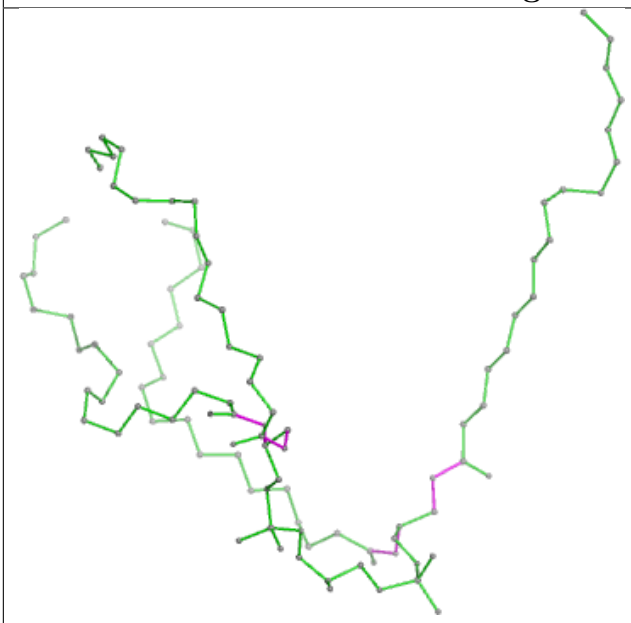


Torsions

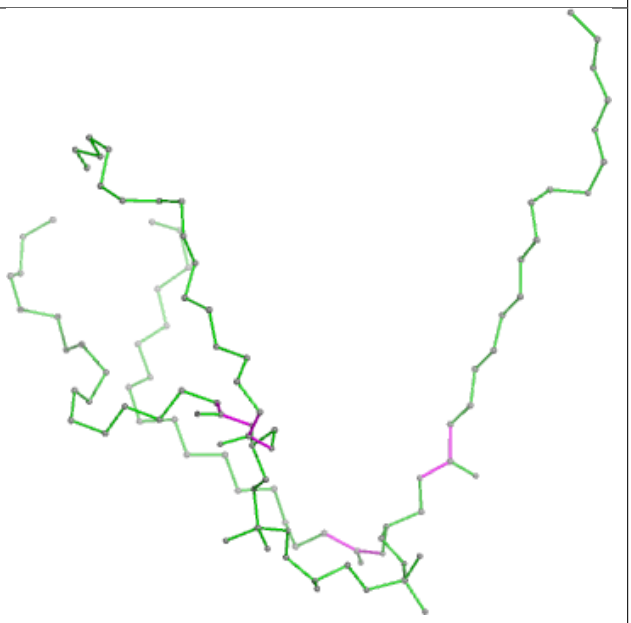


Rings

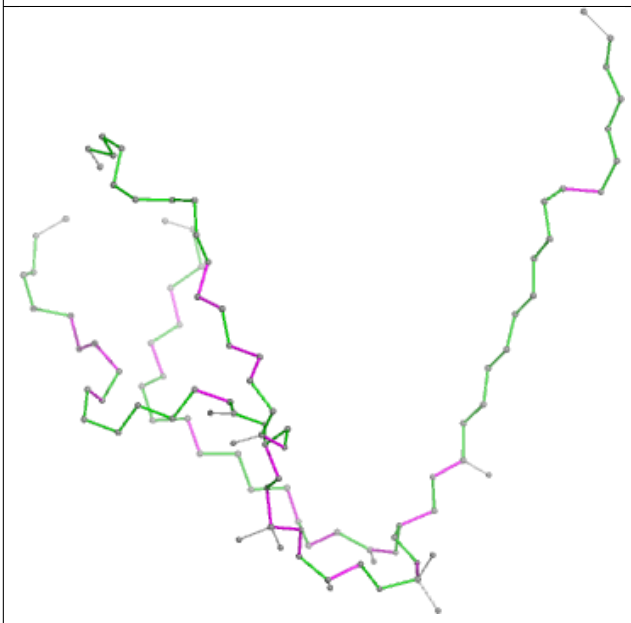
Ligand CDL K 201



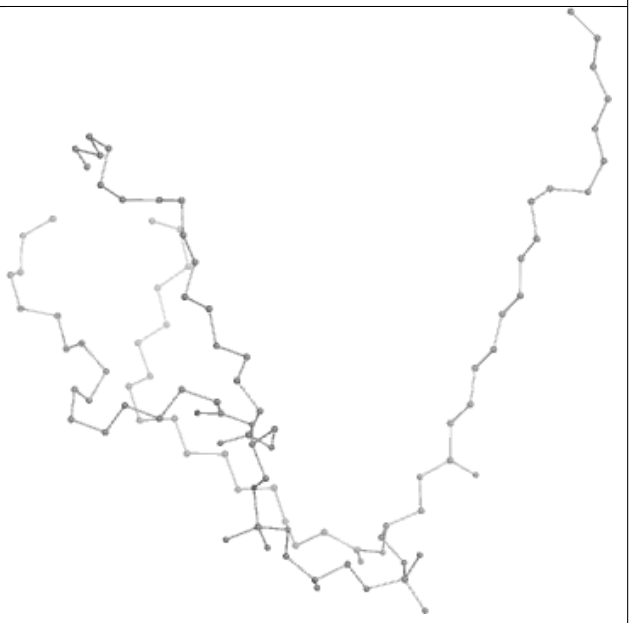
Bond lengths



Bond angles

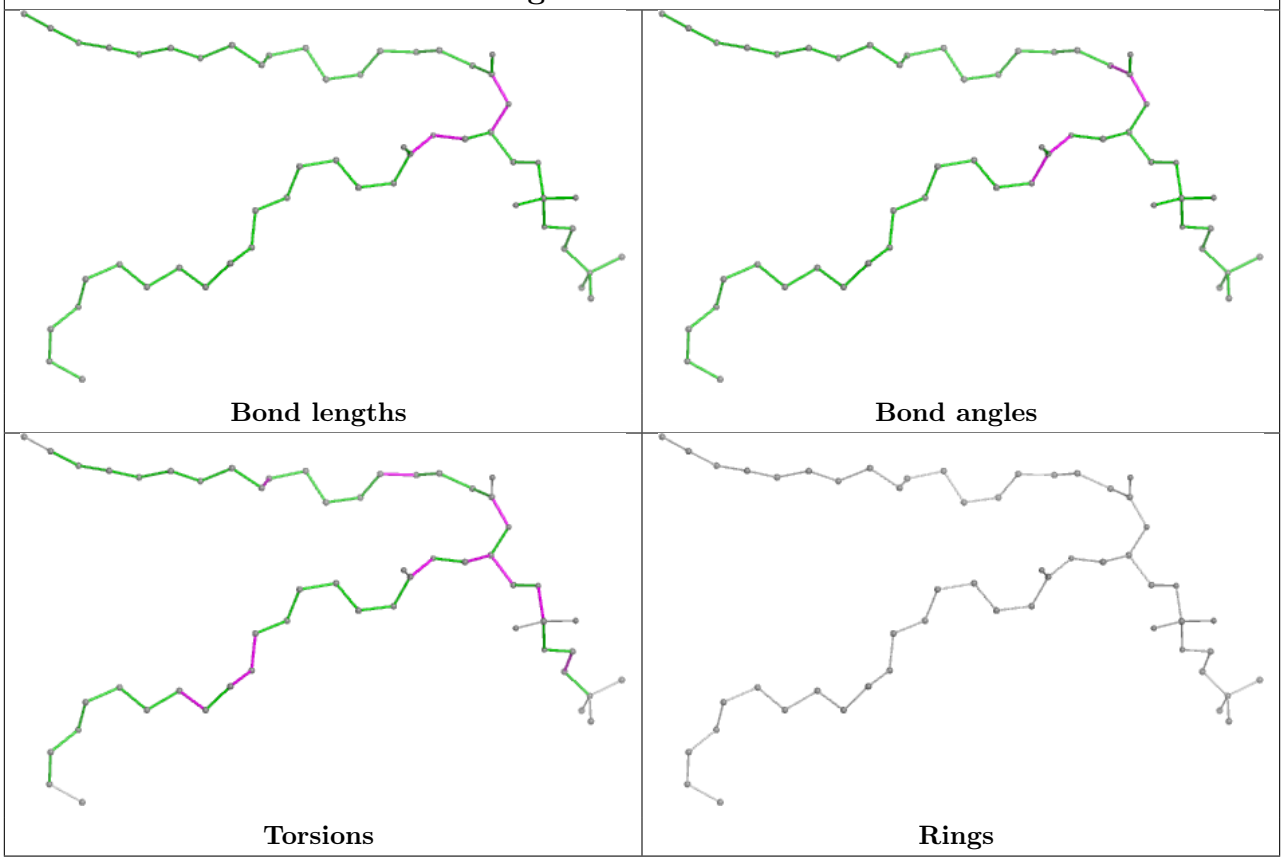


Torsions

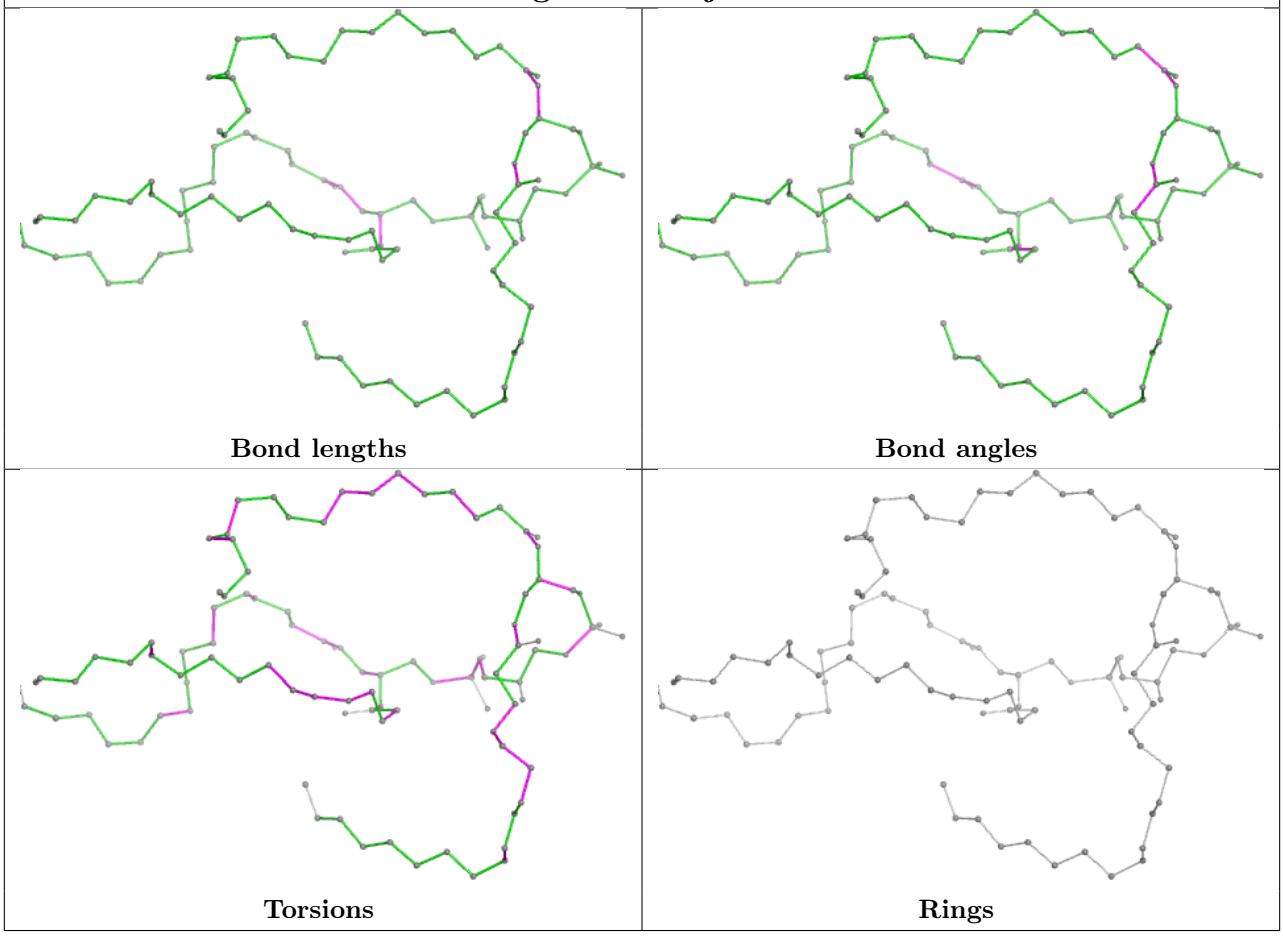


Rings

Ligand PC1 D 301



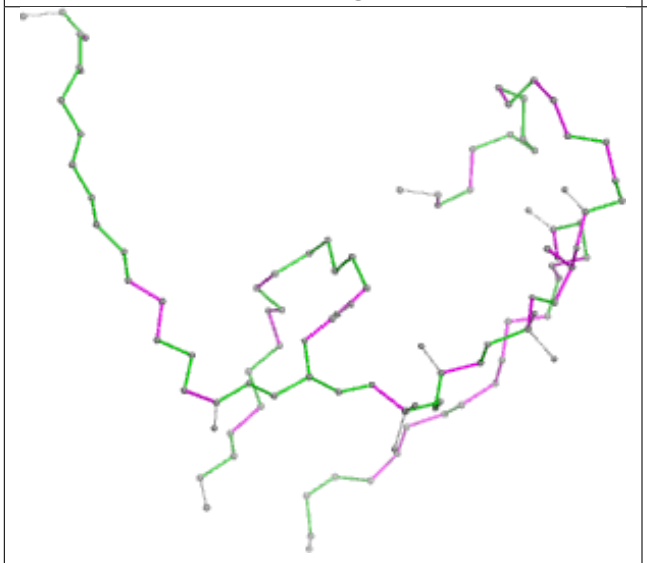
Ligand CDL j 301



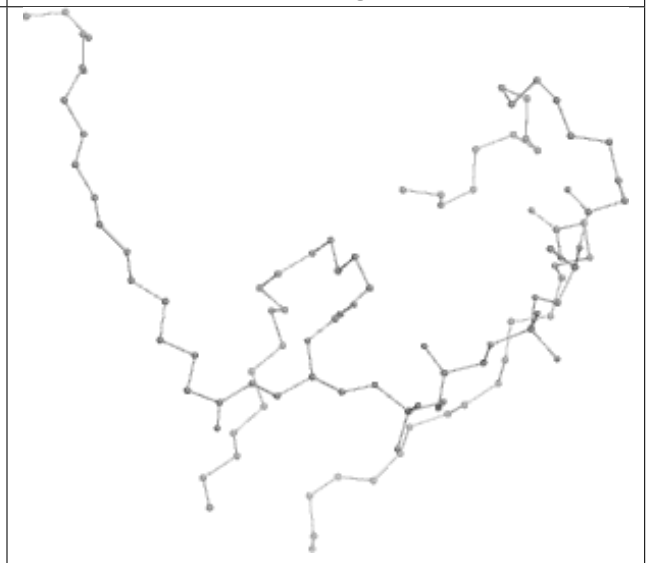
Ligand CDL B 403

Bond lengths

Bond angles

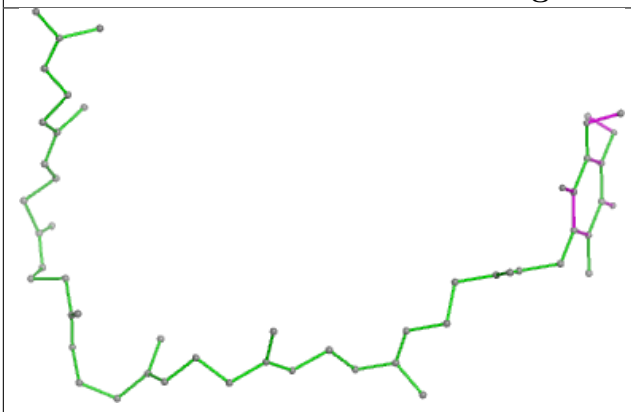


Torsions

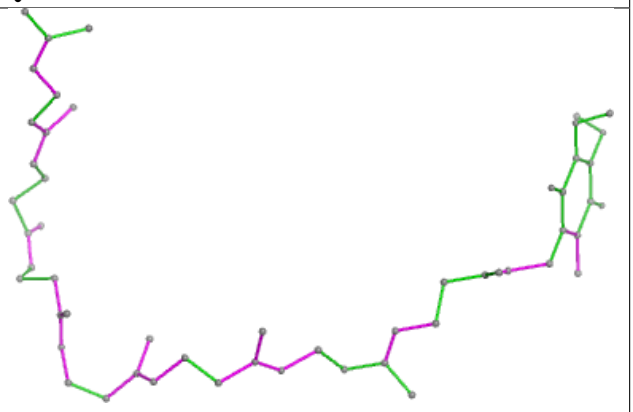


Rings

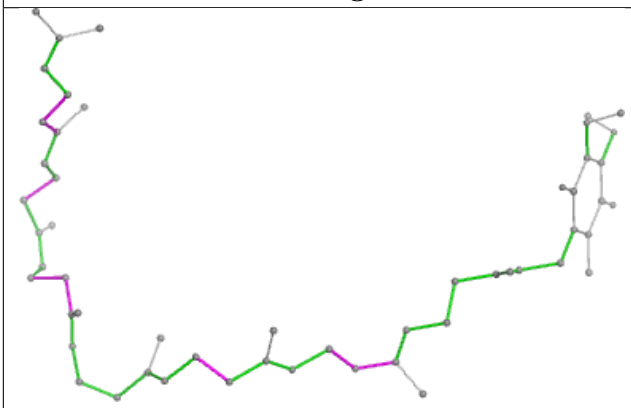
Ligand UQ8 I 303



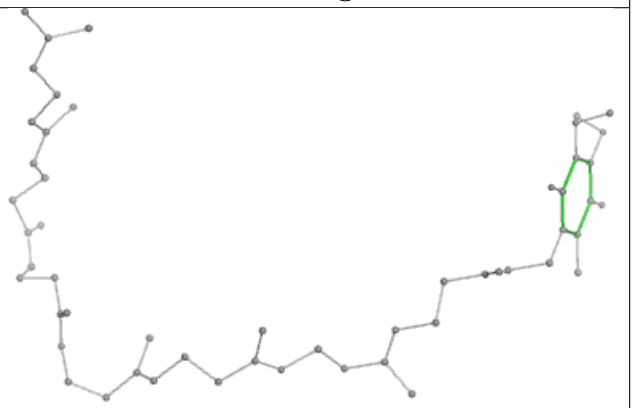
Bond lengths



Bond angles

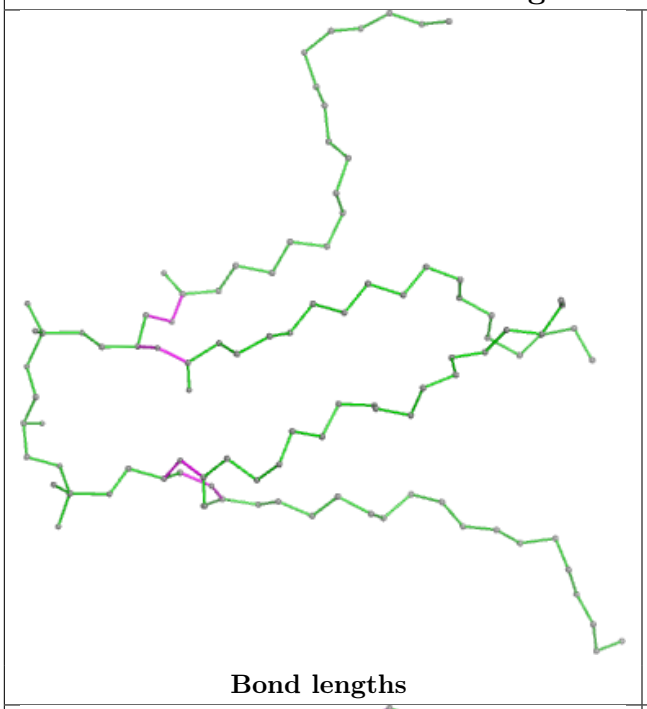


Torsions

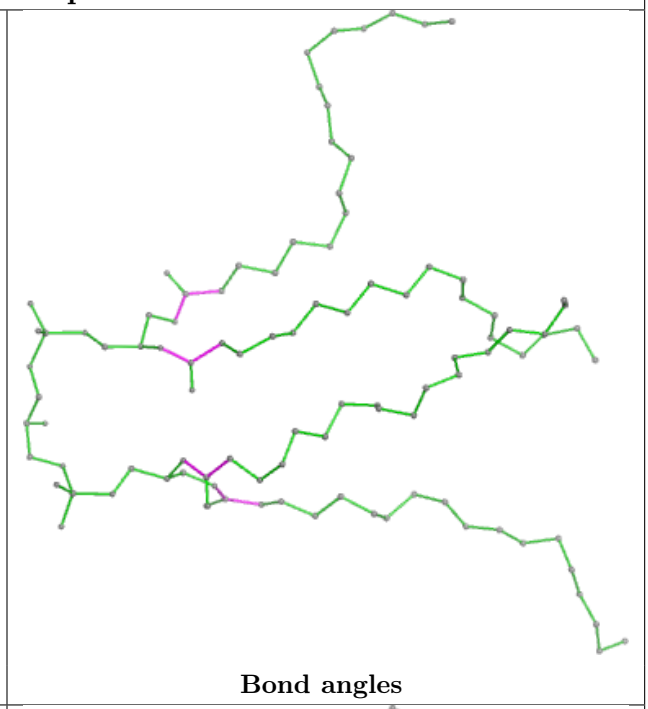


Rings

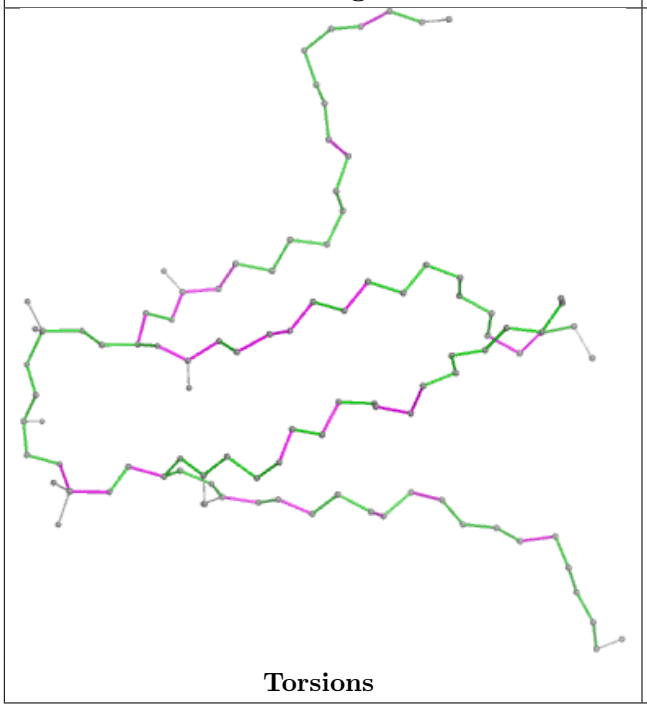
Ligand CDL p 201



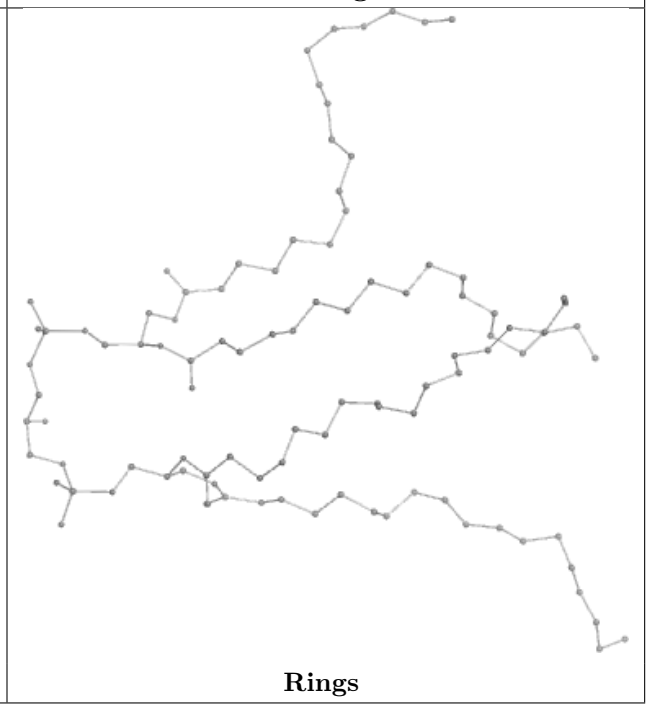
Bond lengths



Bond angles

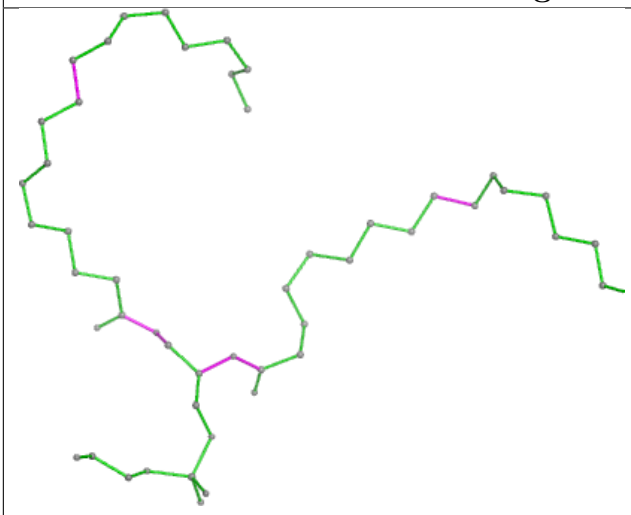


Torsions

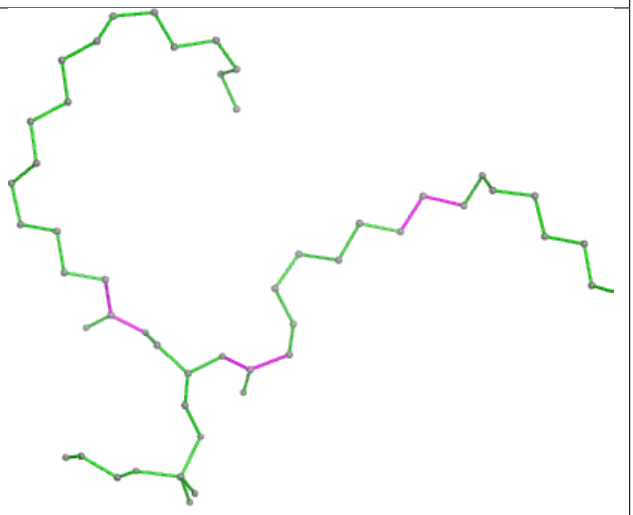


Rings

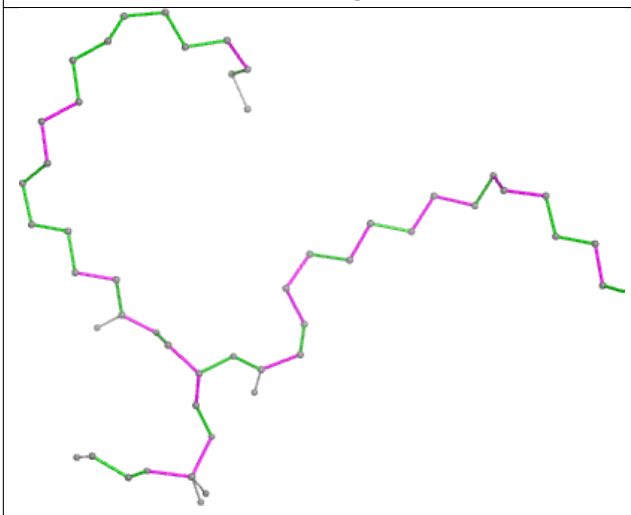
Ligand PEE l 303



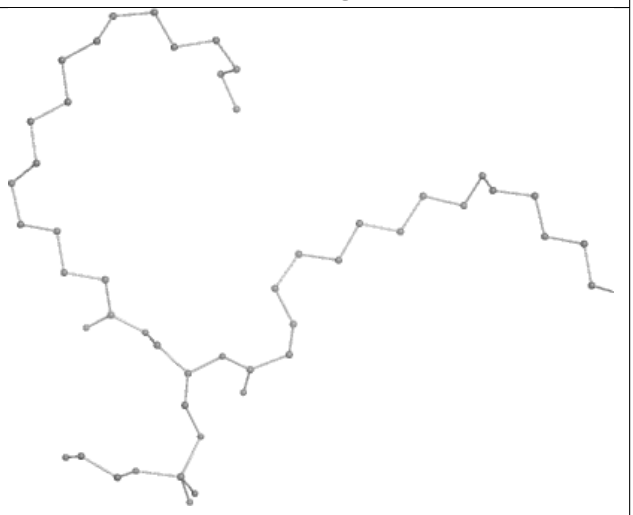
Bond lengths



Bond angles

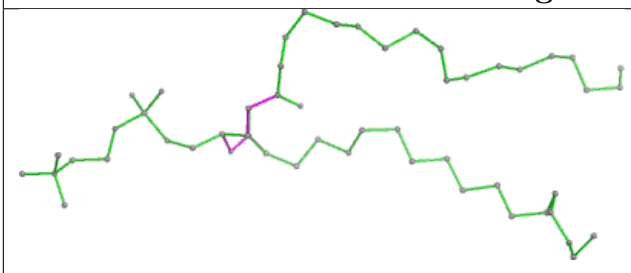


Torsions

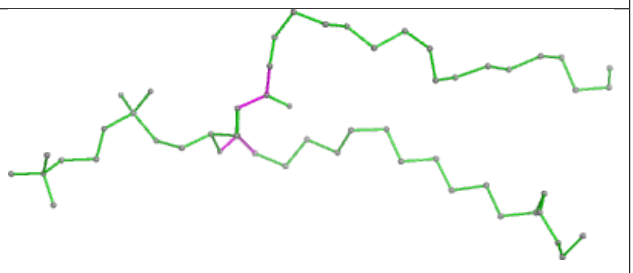


Rings

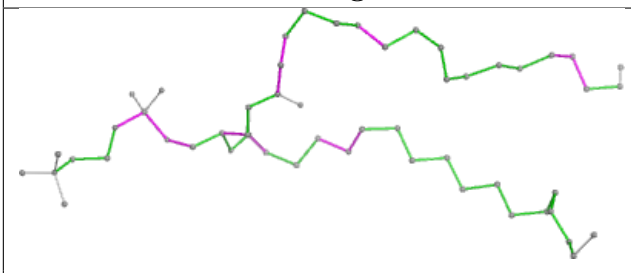
Ligand PC1 i 301



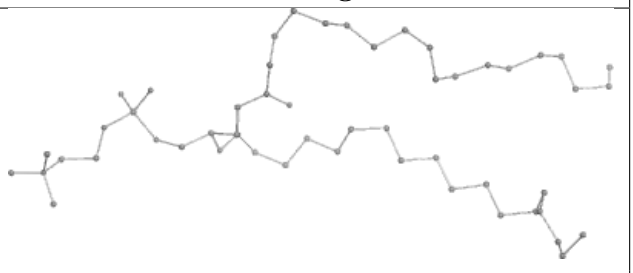
Bond lengths



Bond angles

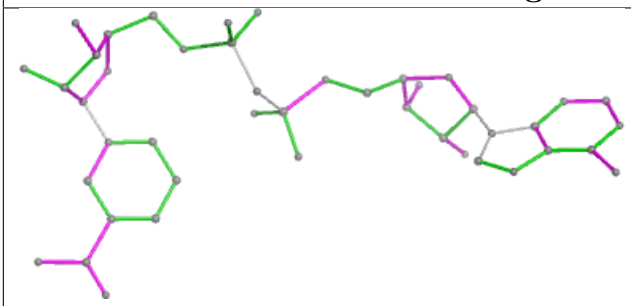


Torsions

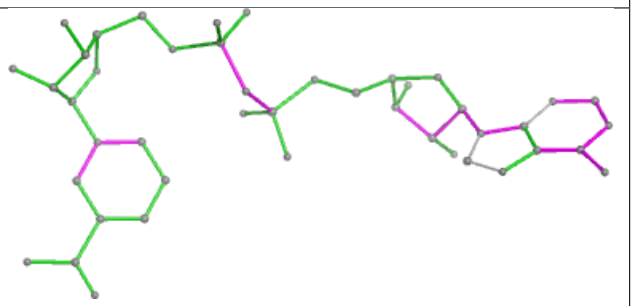


Rings

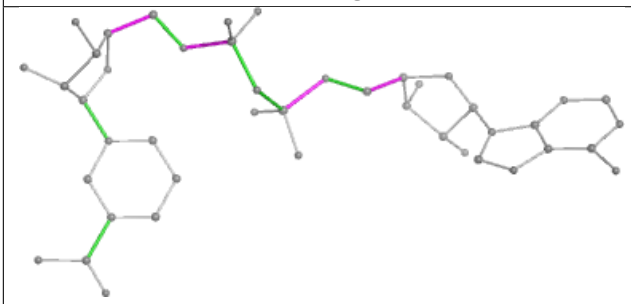
Ligand NAD e 900



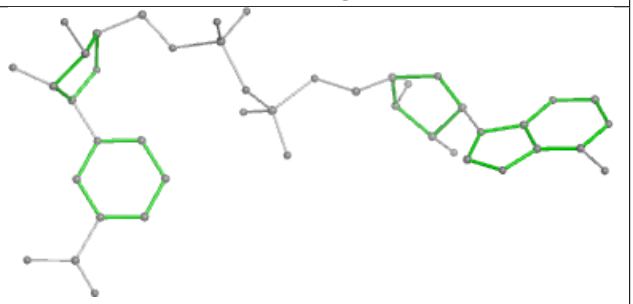
Bond lengths



Bond angles



Torsions

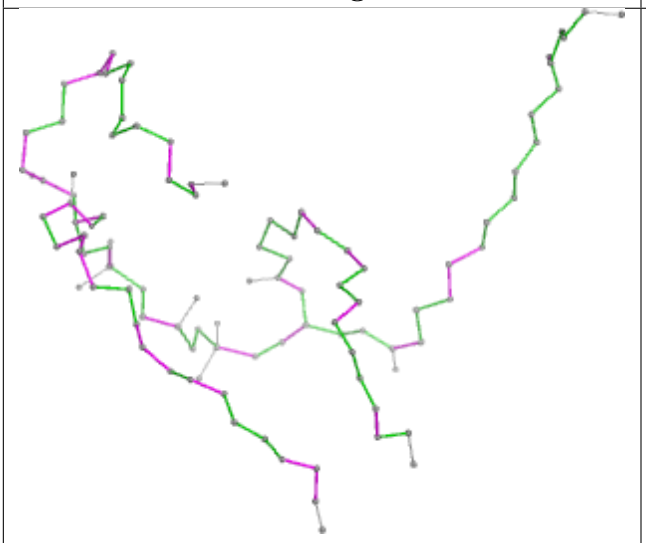


Rings

Ligand CDL f 302

Bond lengths

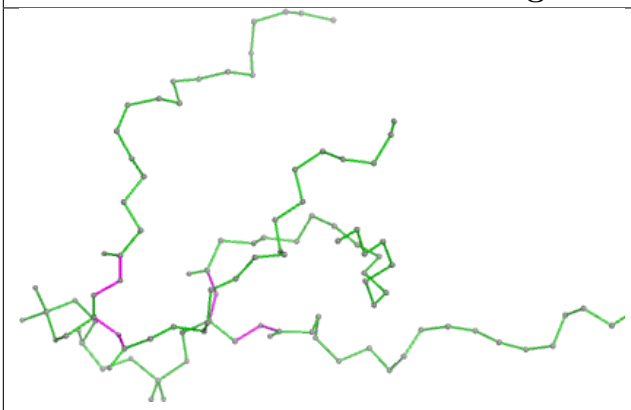
Bond angles



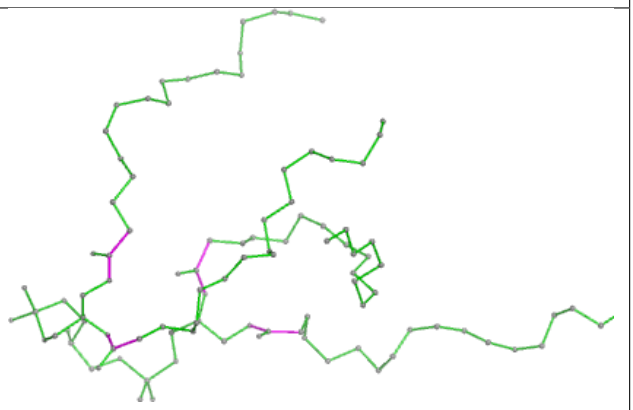
Torsions

Rings

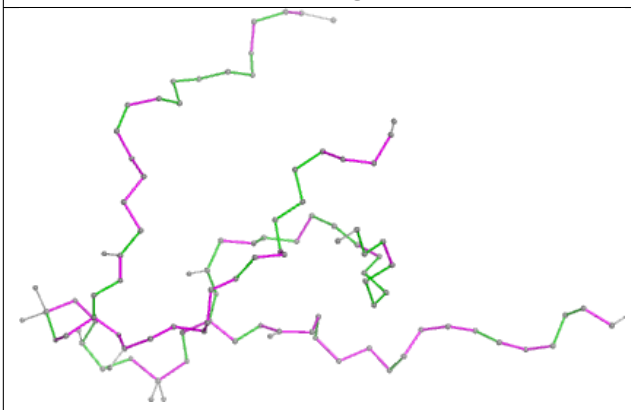
Ligand CDL b 401



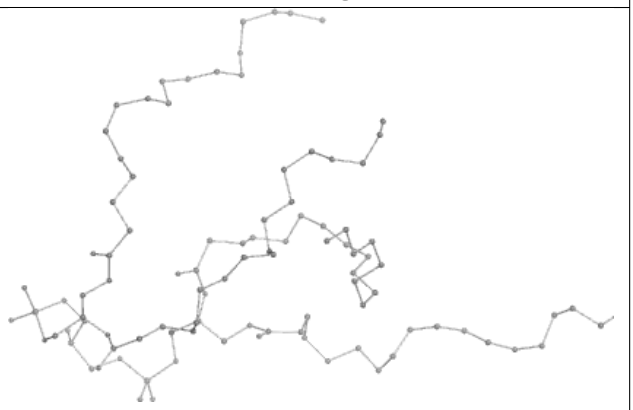
Bond lengths



Bond angles

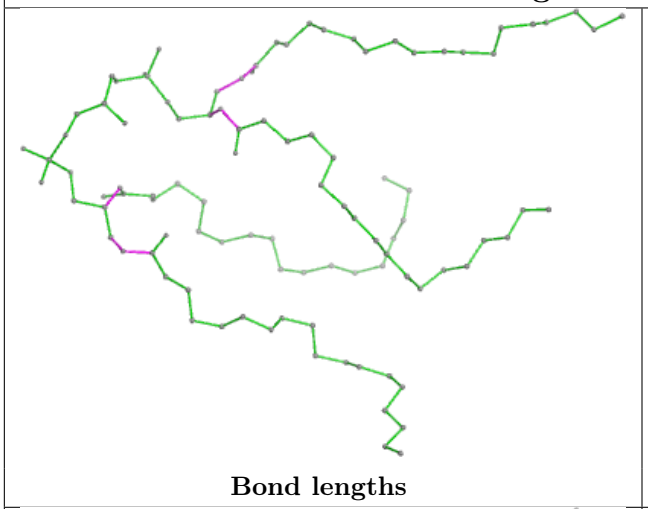


Torsions

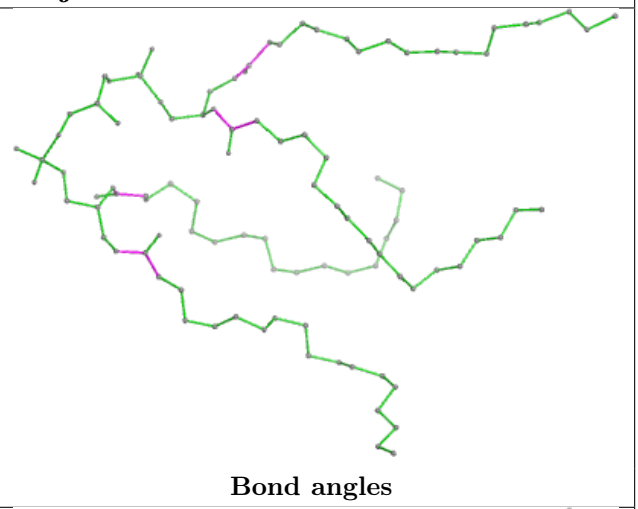


Rings

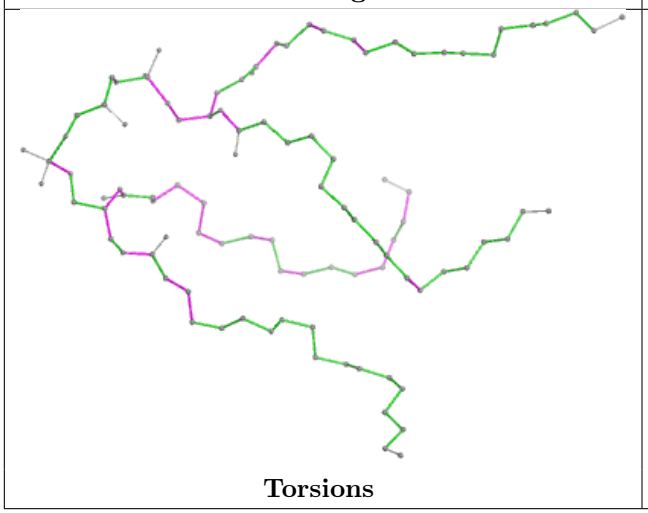
Ligand CDL j 302



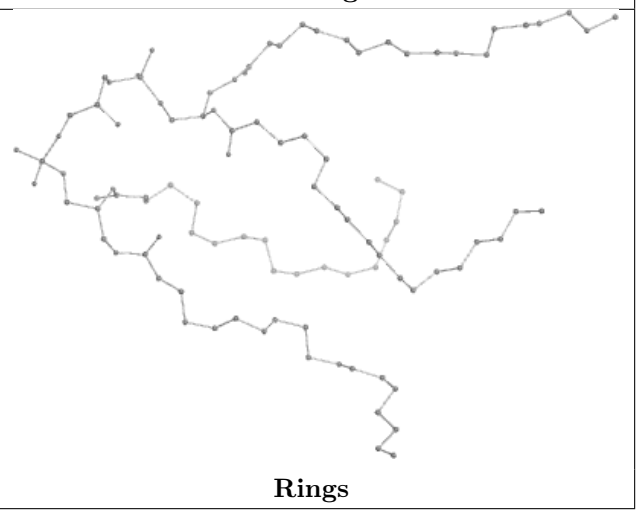
Bond lengths



Bond angles



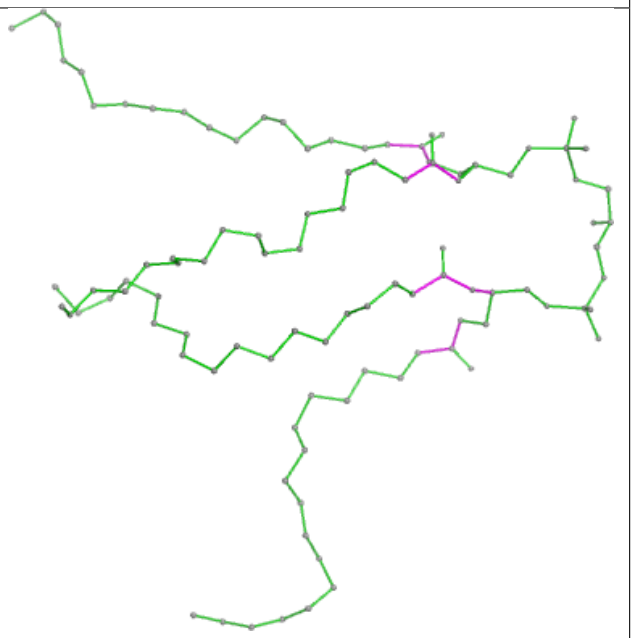
Torsions



Rings

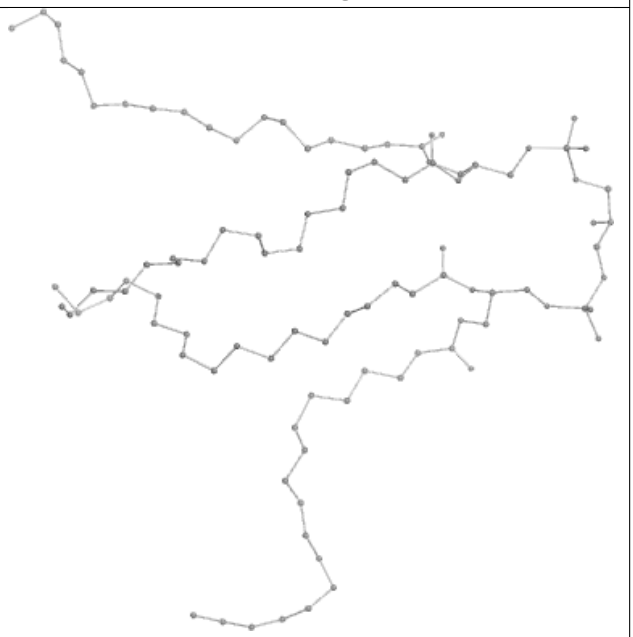
Ligand CDL P 201

Bond lengths



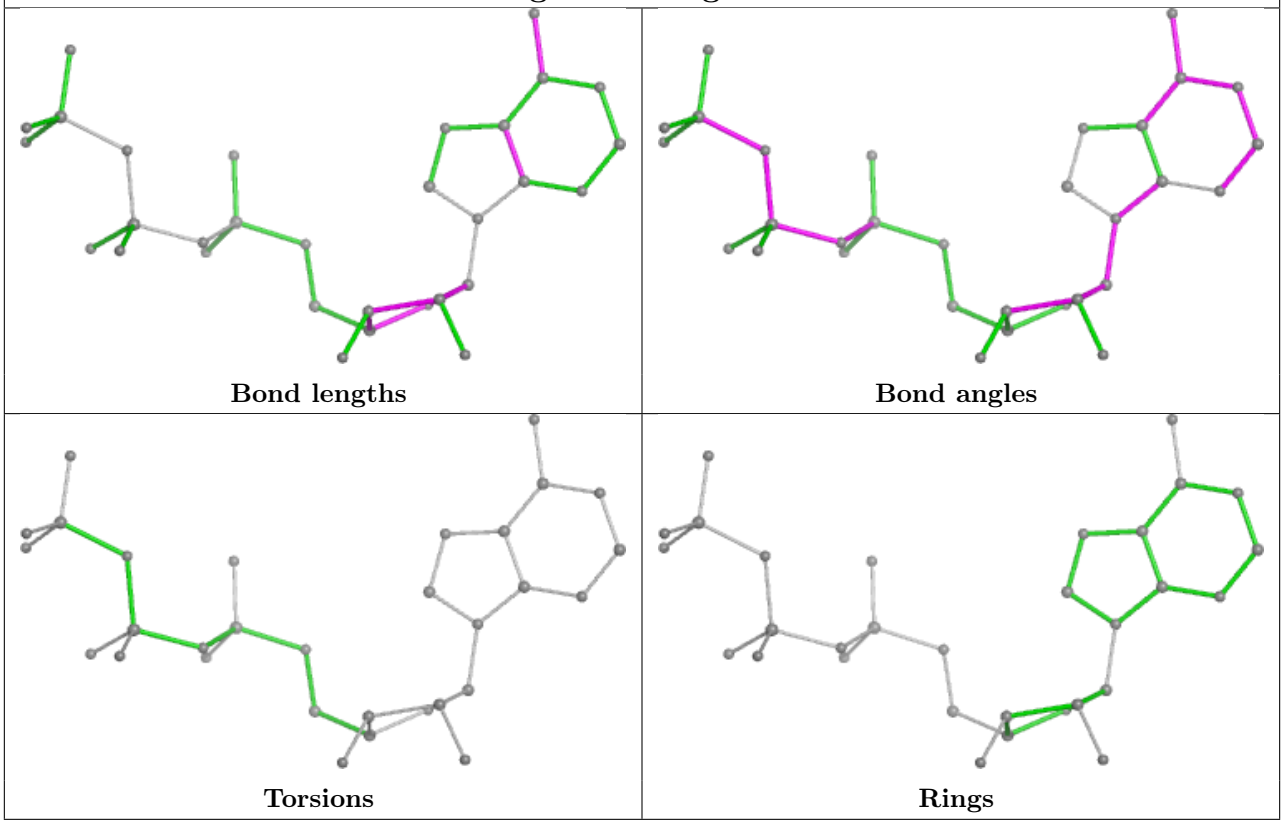
Bond angles

Torsions



Rings

Ligand ATP g 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

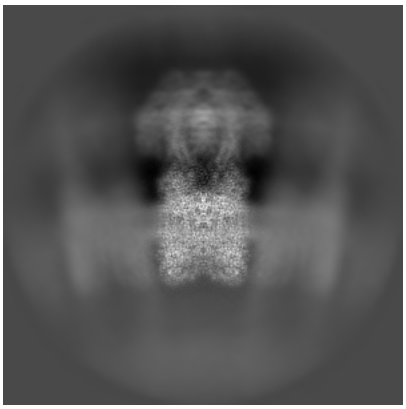
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10859. These allow visual inspection of the internal detail of the map and identification of artifacts.

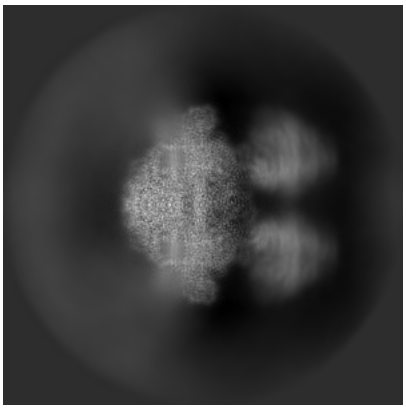
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

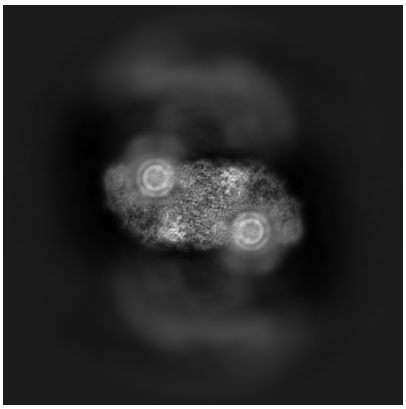
6.1.1 Primary map



X

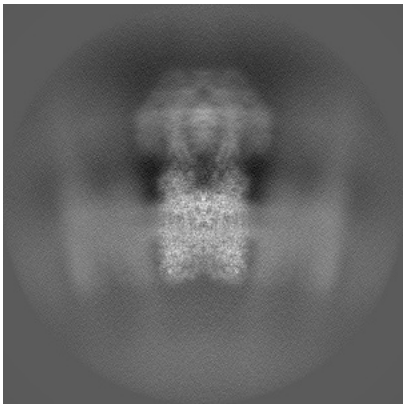


Y

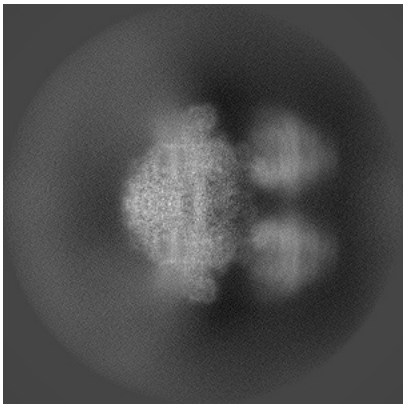


Z

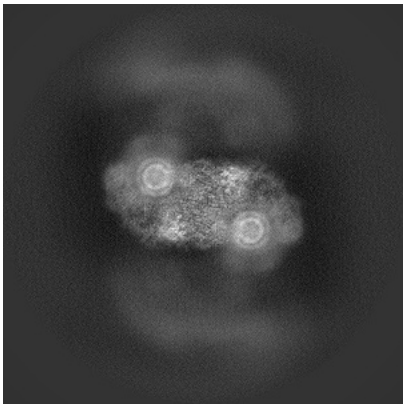
6.1.2 Raw map



X



Y

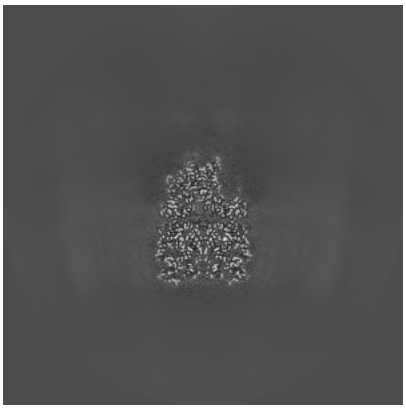


Z

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

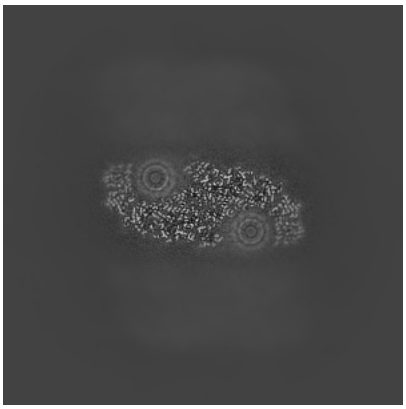
6.2 Central slices (i)

6.2.1 Primary map



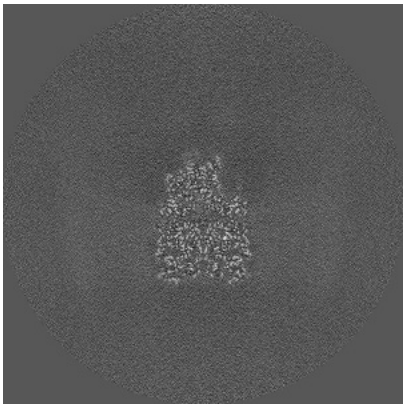
X Index: 300

Y Index: 300

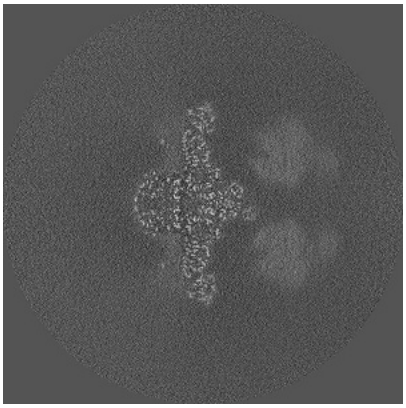


Z Index: 300

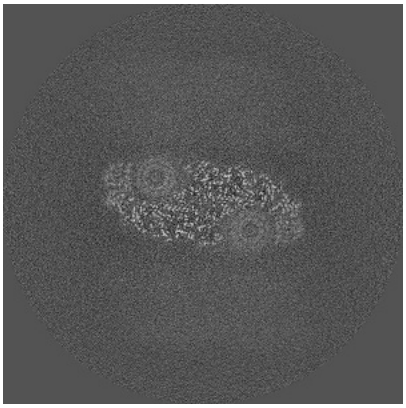
6.2.2 Raw map



X Index: 300



Y Index: 300

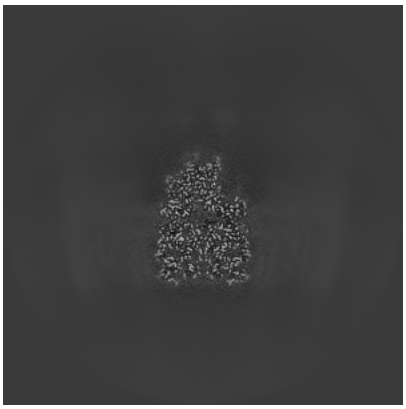


Z Index: 300

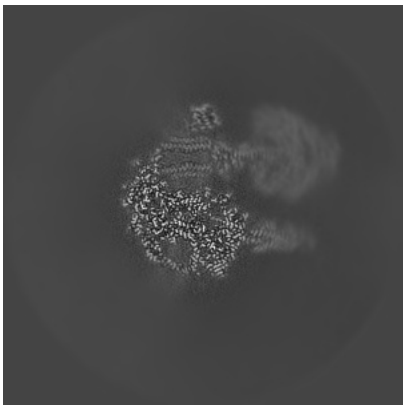
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



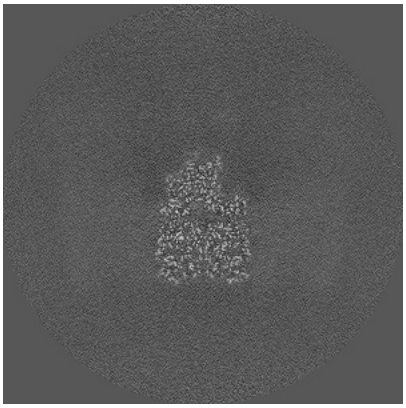
X Index: 299



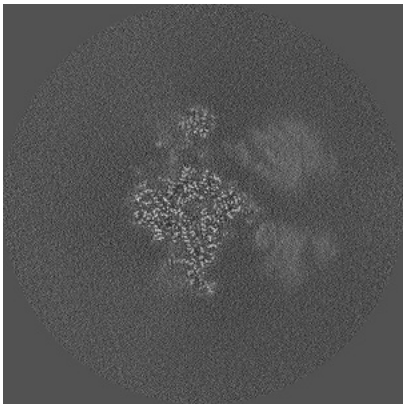
Y Index: 259

Z Index: 292

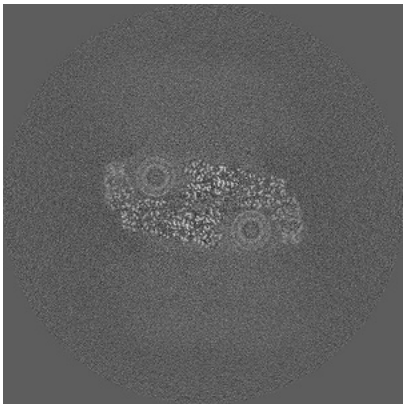
6.3.2 Raw map



X Index: 299



Y Index: 290

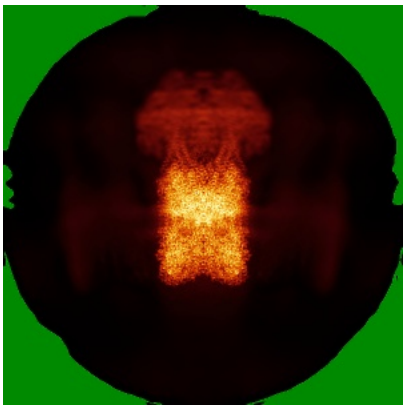


Z Index: 292

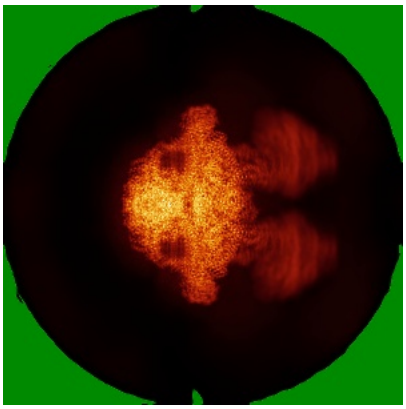
The images above show the largest variance slices of the map in three orthogonal directions.

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

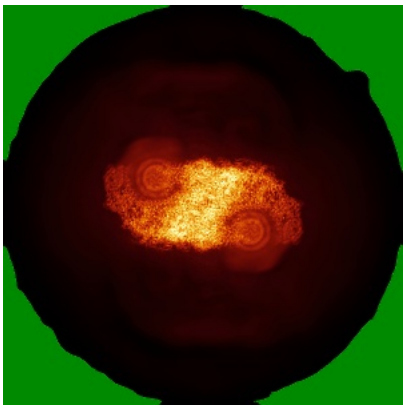
6.4.1 Primary map



X

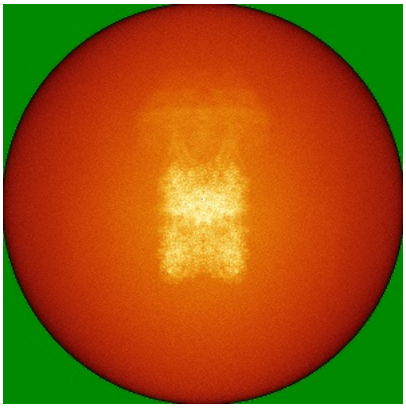


Y

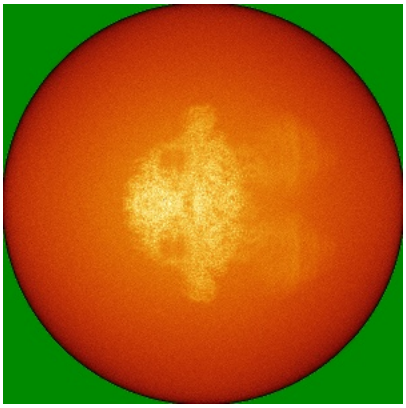


Z

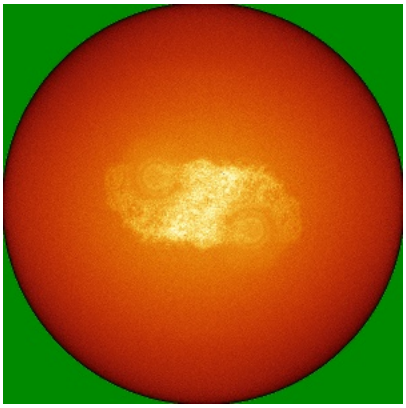
6.4.2 Raw map



X



Y

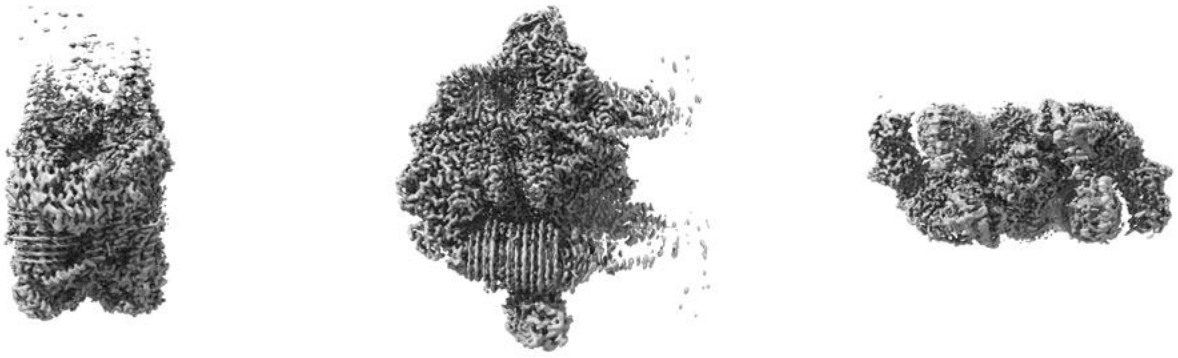


Z

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)

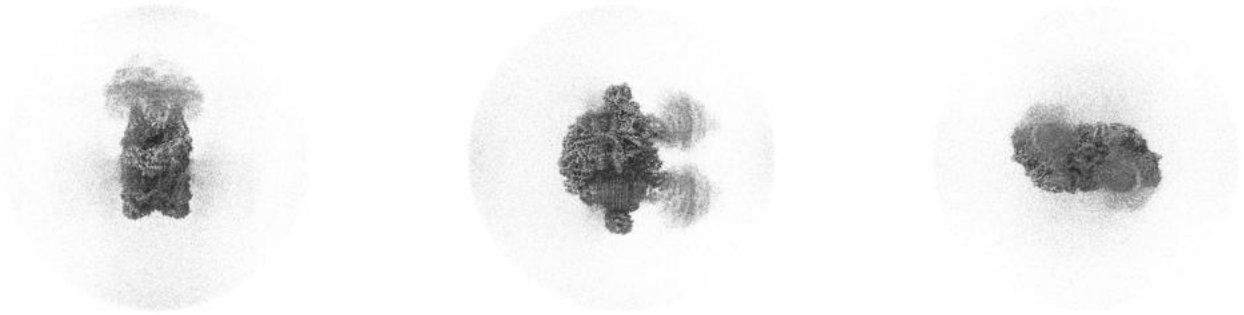
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

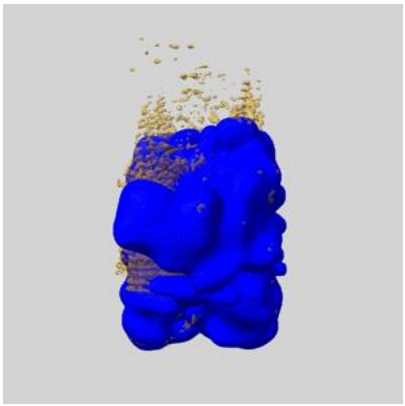
6.6 Mask visualisation (i)

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

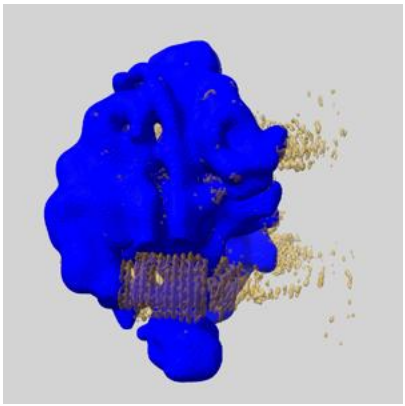
A mask typically either:

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

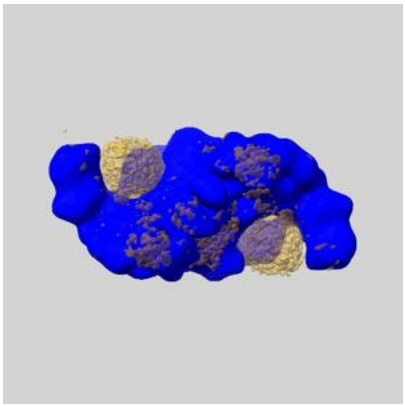
6.6.1 emd_10859_msk_1.map (i)



X



Y

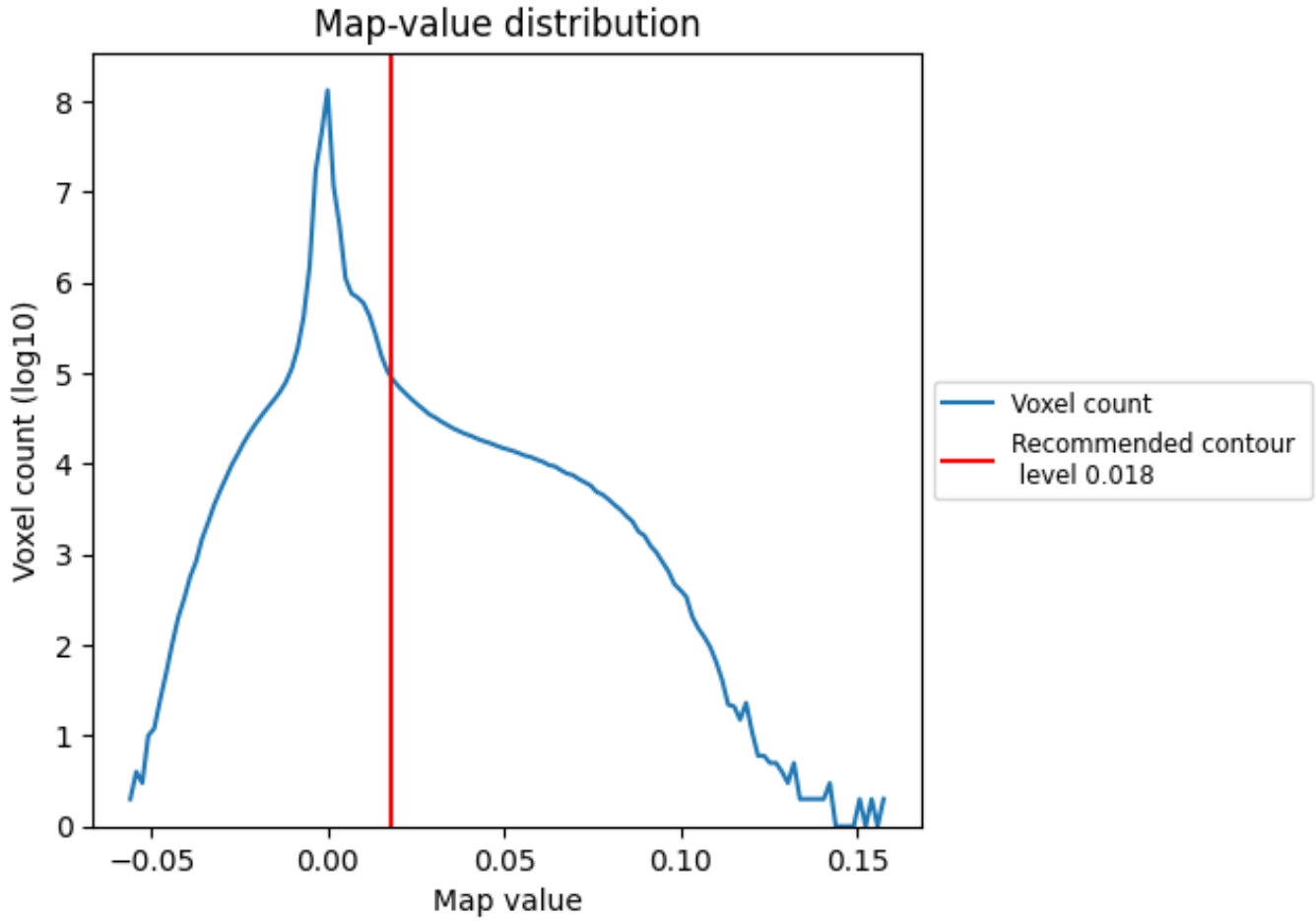


Z

7 Map analysis

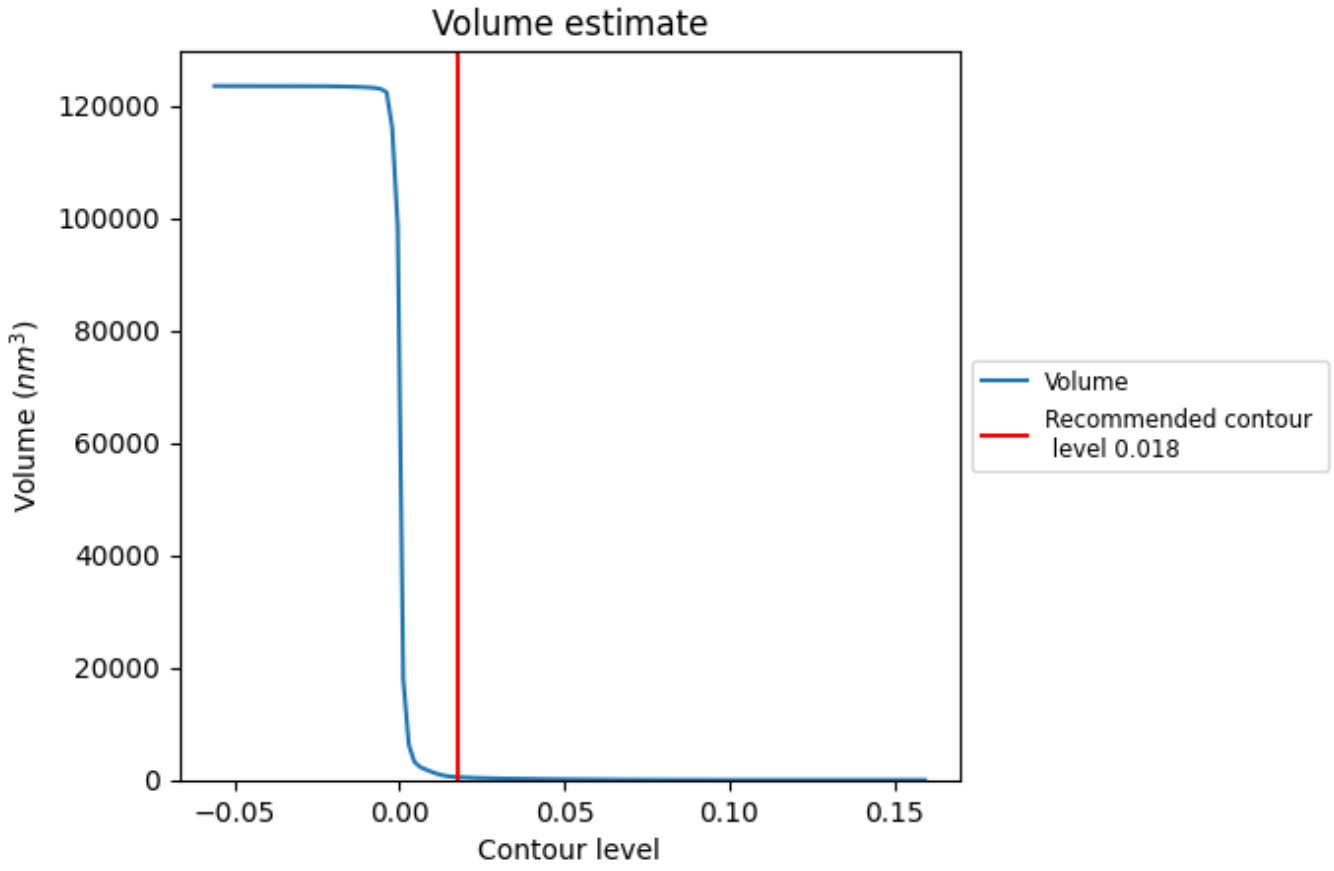
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

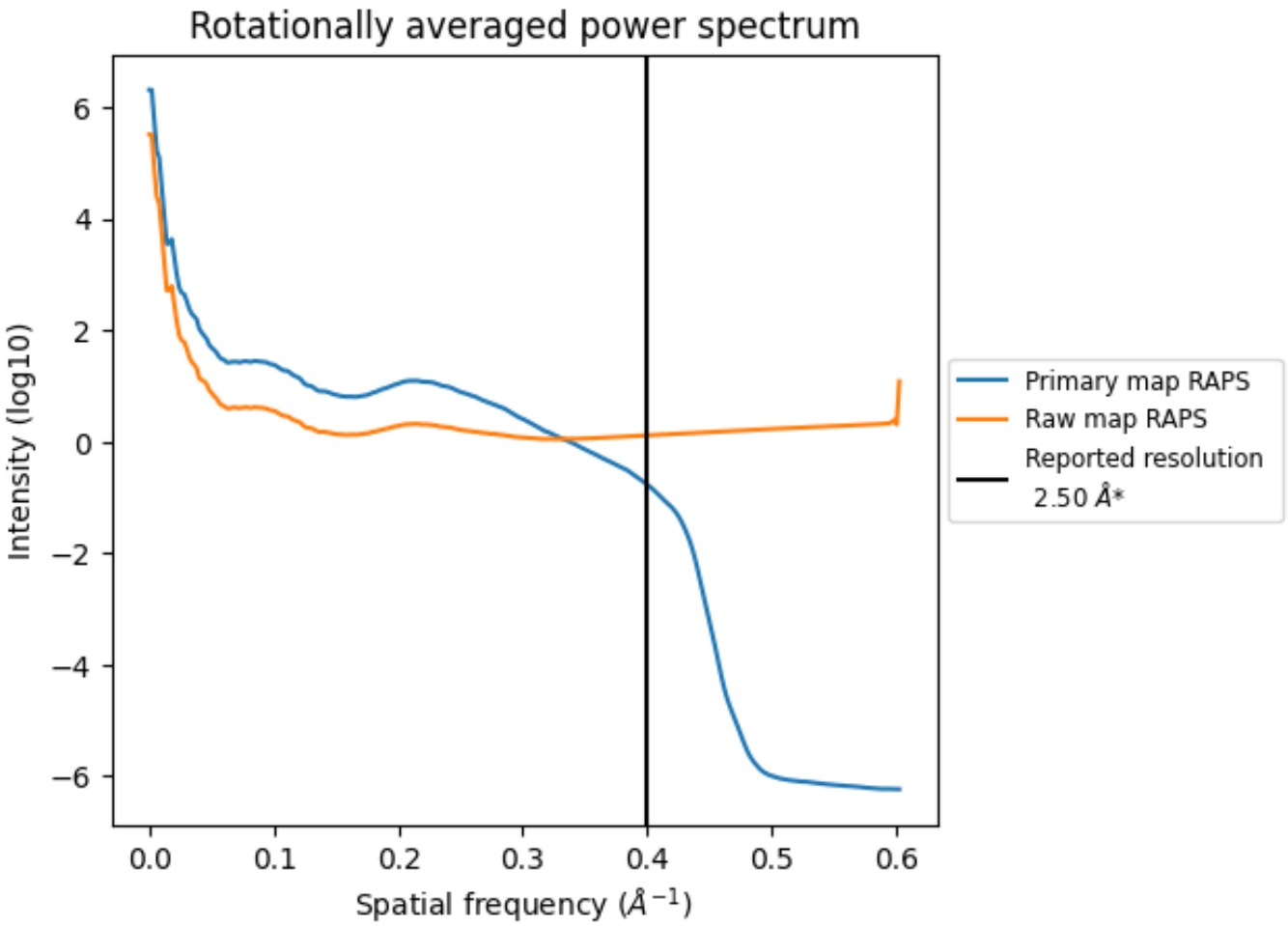
7.2 Volume estimate



The volume at the recommended contour level is 494 nm^3; this corresponds to an approximate mass of 446 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)

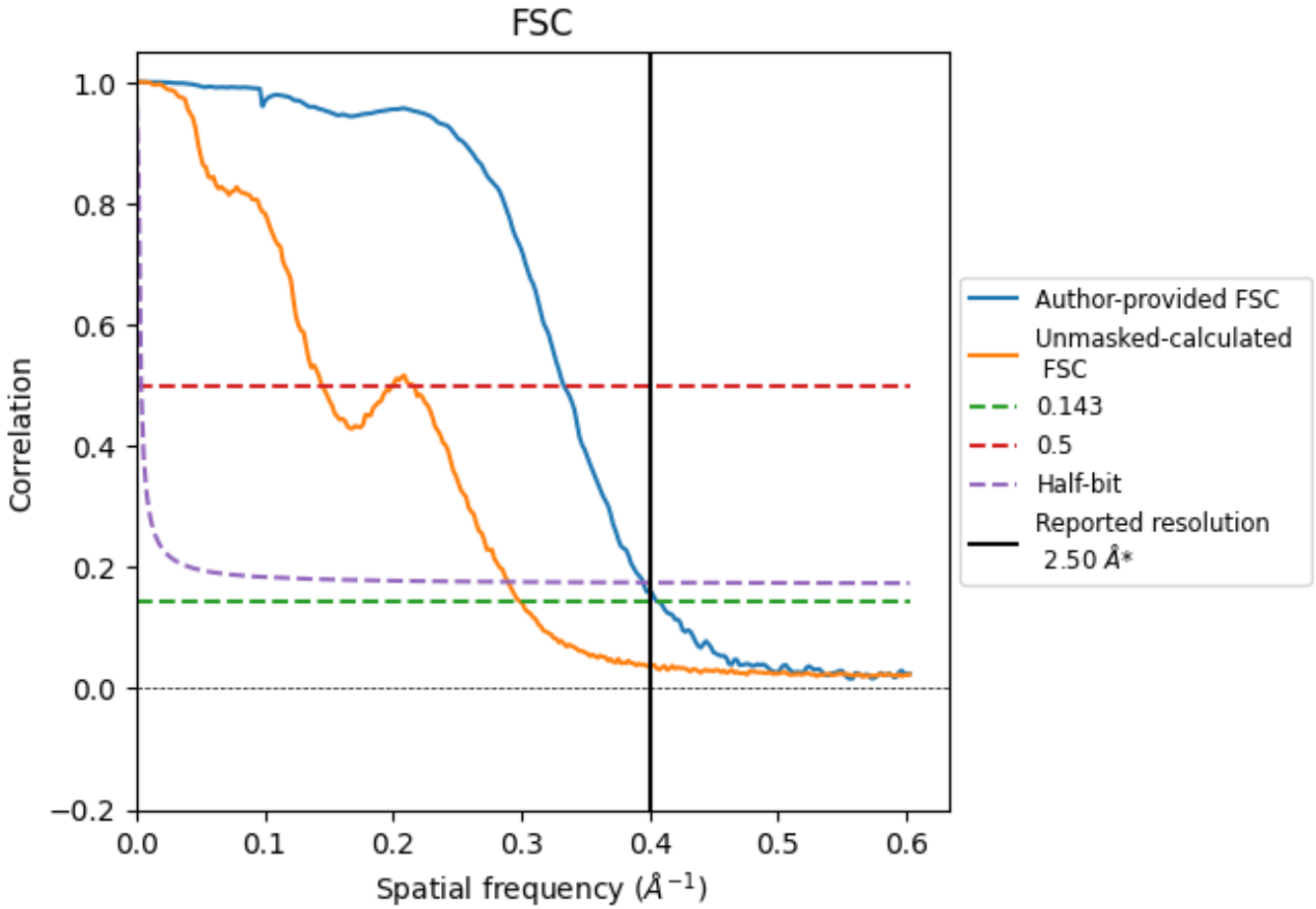


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

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 0.400 Å^{-1}

8.2 Resolution estimates (i)

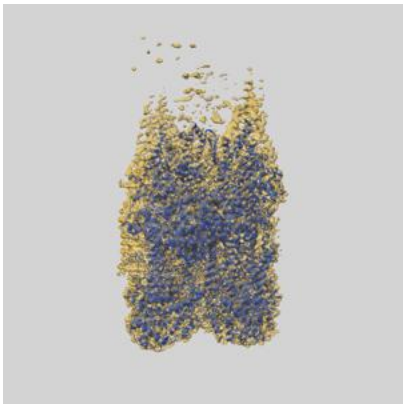
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.46	3.00	2.53
Unmasked-calculated*	3.34	6.92	3.45

*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 3.34 differs from the reported value 2.5 by more than 10 %

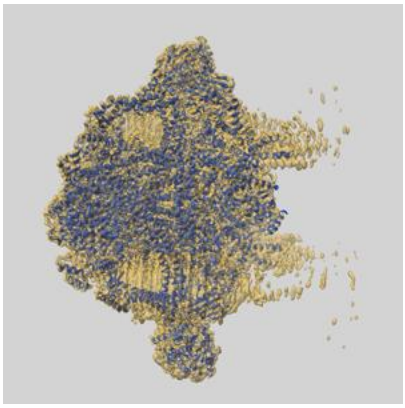
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10859 and PDB model 6YNX. Per-residue inclusion information can be found in section 3 on page 16.

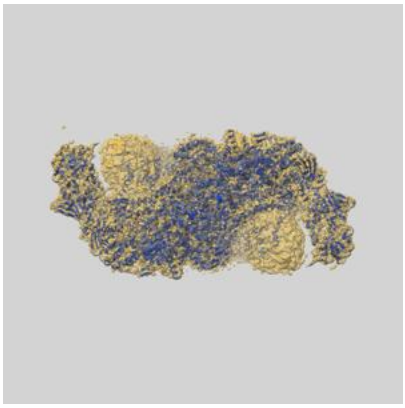
9.1 Map-model overlay



X



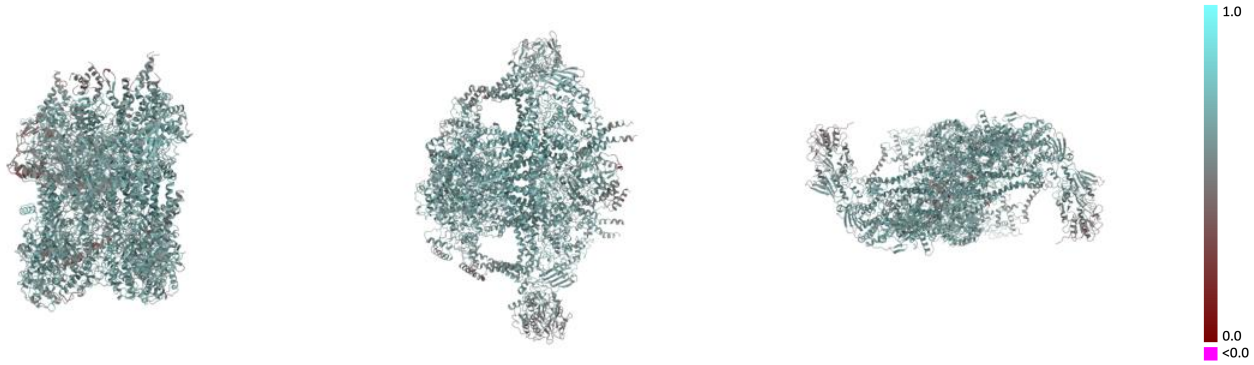
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

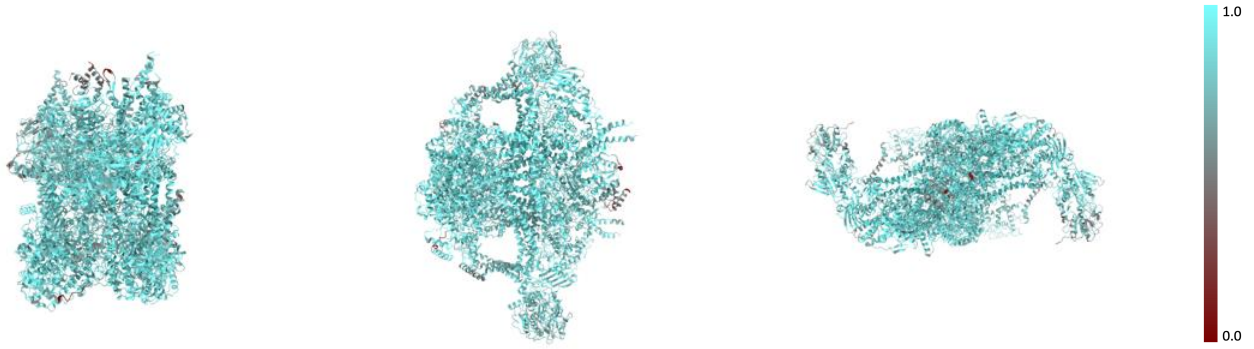
9.2 Q-score mapped to coordinate model (i)



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.

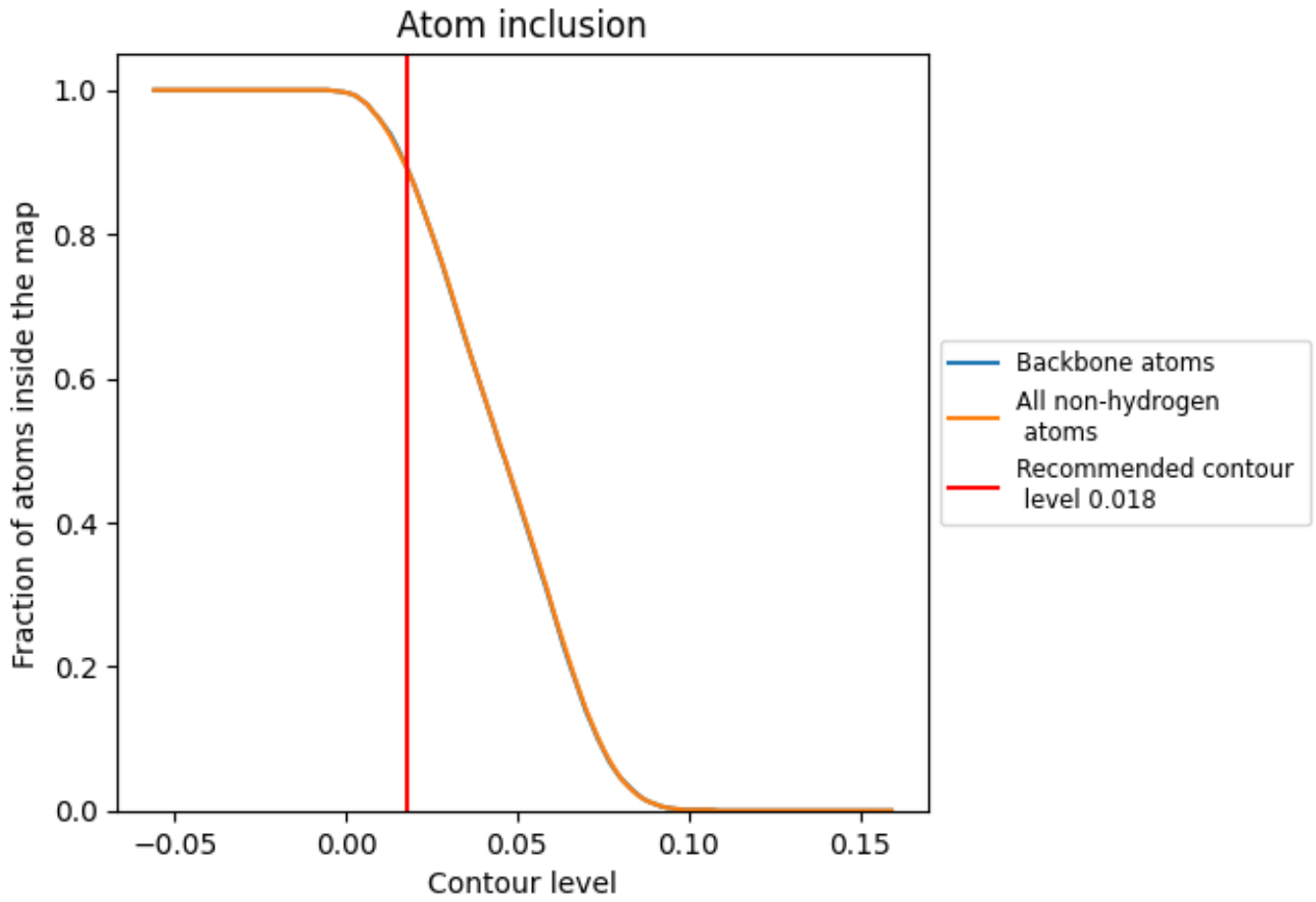
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.6170
A	0.9410	0.6470
B	0.8590	0.6150
C	0.9720	0.6630
D	0.9470	0.6500
E	0.7790	0.5230
F	0.9700	0.6710
G	0.9030	0.6150
H	0.9170	0.6300
I	0.8920	0.6220
J	0.8580	0.6070
K	0.8170	0.5610
L	0.9280	0.6450
M	0.9640	0.6530
N	0.9630	0.6550
O	0.9300	0.6230
P	0.7830	0.5660
Q	0.9060	0.6210
R	0.9350	0.6420
S	0.9270	0.6240
a	0.9430	0.6470
b	0.8970	0.6280
c	0.9710	0.6650
d	0.9510	0.6560
e	0.7880	0.5250
f	0.9220	0.6510
g	0.9170	0.6200
h	0.9230	0.6370
i	0.8890	0.6240
i1	0.5450	0.4790
i2	0.5300	0.4990
j	0.8640	0.6130
k	0.7810	0.5550
l	0.9020	0.6320
m	0.9680	0.6550

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
n	0.9550	0.6560
o	0.9220	0.6200
p	0.7930	0.5660
q	0.9180	0.6240
r	0.9270	0.6350
s	0.9130	0.6170
t	0.9230	0.6310