



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:04 PM UTC

PDB ID : 8Z82 / pdb_00008z82
EMDB ID : EMD-39836
Title : Photosynthetic LH1-RC-HiPIP complex from the purple bacterium Halorhodospira halophila
Authors : Tani, K.; Kanno, R.; Nagashima, K.V.P.; Hiwatashi, N.; Kawakami, M.; Nakata, K.; Nagashima, S.; Inoue, K.; Takaichi, S.; Purba, E.R.; Hall, M.; Yu, L.-J.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Kimura, Y.; Wang-Otomo, Z.-Y.
Deposited on : 2024-04-21
Resolution : 2.40 Å (reported)
Based on initial models : 5D8V, 5Y5S

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

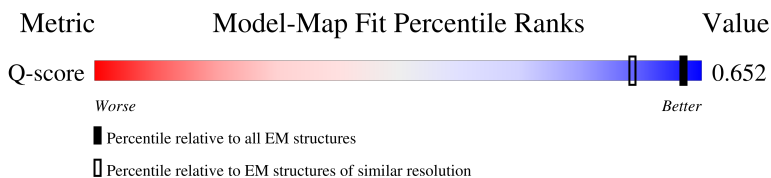
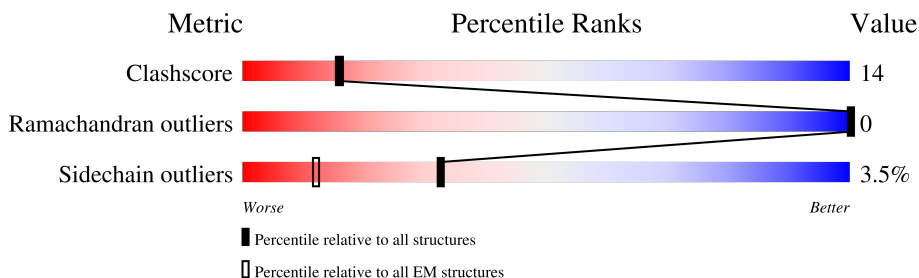
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

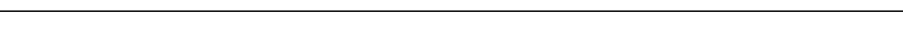
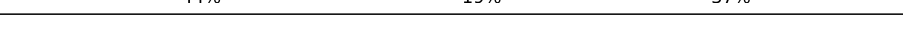
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment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

Mol	Chain	Length	Quality of chain
1	C	362	
2	L	276	

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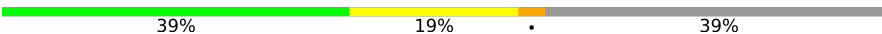
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
3	M	323	
4	H	278	
5	3	64	
5	7	64	
5	A	64	
5	F	64	
5	K	64	
5	Q	64	
5	U	64	
5	Y	64	
6	4	75	
6	8	75	
6	B	75	
6	G	75	
6	N	75	
6	R	75	
6	V	75	
6	Z	75	
7	1	67	
7	5	67	
7	9	67	
7	D	67	
7	I	67	
7	O	67	
7	S	67	

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Mol	Chain	Length	Quality of chain
7	W	67	
8	0	74	
8	2	74	
8	6	74	
8	E	74	
8	J	74	
8	P	74	
8	T	74	
8	X	74	
9	a	142	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 29045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	336	Total	C	N	O	S	0	0
			2642	1616	453	549	24		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	33	THR	SER	conflict	UNP A1WXF5
C	47	ASN	THR	conflict	UNP A1WXF5
C	72	ARG	LYS	conflict	UNP A1WXF5
C	84	ASP	THR	conflict	UNP A1WXF5
C	103	SER	ALA	conflict	UNP A1WXF5
C	143	ASP	GLU	conflict	UNP A1WXF5
C	172	THR	GLU	conflict	UNP A1WXF5
C	173	PRO	LEU	conflict	UNP A1WXF5
C	175	VAL	PHE	conflict	UNP A1WXF5
C	177	MET	VAL	conflict	UNP A1WXF5
C	178	ALA	HIS	conflict	UNP A1WXF5
C	183	THR	ASP	conflict	UNP A1WXF5
C	184	MET	GLN	conflict	UNP A1WXF5
C	193	THR	VAL	conflict	UNP A1WXF5
C	194	GLU	GLY	conflict	UNP A1WXF5
C	195	TYR	PHE	conflict	UNP A1WXF5
C	202	ALA	VAL	conflict	UNP A1WXF5
C	223	HIS	ASN	conflict	UNP A1WXF5
C	239	SER	GLY	conflict	UNP A1WXF5
C	246	ALA	ASP	conflict	UNP A1WXF5
C	269	GLU	VAL	conflict	UNP A1WXF5
C	289	ILE	MET	conflict	UNP A1WXF5
C	298	GLU	ASP	conflict	UNP A1WXF5
C	341	ALA	GLU	conflict	UNP A1WXF5
C	354	ASP	GLU	conflict	UNP A1WXF5
C	360	ASN	ASP	conflict	UNP A1WXF5

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	274	Total	C	N	O	S	0	0
			2170	1461	348	353	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	99	THR	ALA	conflict	UNP A0A2L1K3P0
L	205	PRO	SER	conflict	UNP A0A2L1K3P0
L	220	ILE	VAL	conflict	UNP A0A2L1K3P0
L	241	GLY	ALA	conflict	UNP A0A2L1K3P0

- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	318	Total	C	N	O	S	0	0
			2518	1679	410	420	9		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	34	ALA	SER	conflict	UNP A0A2L1K3T5
M	65	ILE	LEU	conflict	UNP A0A2L1K3T5
M	66	VAL	LEU	conflict	UNP A0A2L1K3T5
M	84	LEU	ILE	conflict	UNP A0A2L1K3T5
M	86	PHE	TRP	conflict	UNP A0A2L1K3T5
M	126	VAL	ILE	conflict	UNP A0A2L1K3T5
M	130	PHE	TRP	conflict	UNP A0A2L1K3T5
M	131	ALA	VAL	conflict	UNP A0A2L1K3T5
M	236	GLU	ASP	conflict	UNP A0A2L1K3T5

- Molecule 4 is a protein called Photosynthetic reaction centre, H-chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	278	Total	C	N	O	S	0	0
			2174	1379	374	410	11		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	69	VAL	THR	conflict	UNP A1WXI3
H	97	GLU	ALA	conflict	UNP A1WXI3
H	118	LEU	VAL	conflict	UNP A1WXI3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	135	GLY	ALA	conflict	UNP A1WXI3
H	137	LYS	ASN	conflict	UNP A1WXI3
H	141	CYS	ALA	conflict	UNP A1WXI3
H	158	ALA	ARG	conflict	UNP A1WXI3
H	163	GLU	GLN	conflict	UNP A1WXI3
H	164	ILE	LEU	conflict	UNP A1WXI3
H	171	TYR	ASP	conflict	UNP A1WXI3
H	179	LYS	THR	conflict	UNP A1WXI3
H	210	GLY	SER	conflict	UNP A1WXI3
H	226	SER	GLY	conflict	UNP A1WXI3
H	236	GLN	LYS	conflict	UNP A1WXI3
H	247	ALA	SER	conflict	UNP A1WXI3
H	262	PHE	TYR	conflict	UNP A1WXI3

- Molecule 5 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	F	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	K	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	Q	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	U	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	Y	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	3	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	7	46	Total	C	N	O	S	0	0
			385	263	66	55	1		

- Molecule 6 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	48	Total	C	N	O	S	0	0
			386	259	60	66	1		
6	G	47	Total	C	N	O	S	0	0
			380	256	59	64	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
6	R	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
6	V	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
6	Z	48	Total	C	N	O	S	0	0
			386	259	60	66	1		
6	4	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
6	8	47	Total	C	N	O	S	0	0
			380	256	59	64	1		

- Molecule 7 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	I	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	O	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	S	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	W	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	1	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	5	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	9	46	Total	C	N	O	S	0	0
			390	261	67	59	3		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	37	ASN	SER	conflict	UNP A1WXF8
D	42	GLN	GLU	conflict	UNP A1WXF8
D	48	ASP	ASN	conflict	UNP A1WXF8
D	57	ASP	GLU	conflict	UNP A1WXF8
I	37	ASN	SER	conflict	UNP A1WXF8
I	42	GLN	GLU	conflict	UNP A1WXF8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	48	ASP	ASN	conflict	UNP A1WXF8
I	57	ASP	GLU	conflict	UNP A1WXF8
O	37	ASN	SER	conflict	UNP A1WXF8
O	42	GLN	GLU	conflict	UNP A1WXF8
O	48	ASP	ASN	conflict	UNP A1WXF8
O	57	ASP	GLU	conflict	UNP A1WXF8
S	37	ASN	SER	conflict	UNP A1WXF8
S	42	GLN	GLU	conflict	UNP A1WXF8
S	48	ASP	ASN	conflict	UNP A1WXF8
S	57	ASP	GLU	conflict	UNP A1WXF8
W	37	ASN	SER	conflict	UNP A1WXF8
W	42	GLN	GLU	conflict	UNP A1WXF8
W	48	ASP	ASN	conflict	UNP A1WXF8
W	57	ASP	GLU	conflict	UNP A1WXF8
1	37	ASN	SER	conflict	UNP A1WXF8
1	42	GLN	GLU	conflict	UNP A1WXF8
1	48	ASP	ASN	conflict	UNP A1WXF8
1	57	ASP	GLU	conflict	UNP A1WXF8
5	37	ASN	SER	conflict	UNP A1WXF8
5	42	GLN	GLU	conflict	UNP A1WXF8
5	48	ASP	ASN	conflict	UNP A1WXF8
5	57	ASP	GLU	conflict	UNP A1WXF8
9	37	ASN	SER	conflict	UNP A1WXF8
9	42	GLN	GLU	conflict	UNP A1WXF8
9	48	ASP	ASN	conflict	UNP A1WXF8
9	57	ASP	GLU	conflict	UNP A1WXF8

- Molecule 8 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	J	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	P	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	T	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	X	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	2	45	Total	C	N	O	S	0	0
			362	240	58	63	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	0	45	Total	C	N	O	S	0	0
			362	240	58	63	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	30	ILE	VAL	conflict	UNP A1WXF9
J	30	ILE	VAL	conflict	UNP A1WXF9
P	30	ILE	VAL	conflict	UNP A1WXF9
T	30	ILE	VAL	conflict	UNP A1WXF9
X	30	ILE	VAL	conflict	UNP A1WXF9
2	30	ILE	VAL	conflict	UNP A1WXF9
6	30	ILE	VAL	conflict	UNP A1WXF9
0	30	ILE	VAL	conflict	UNP A1WXF9

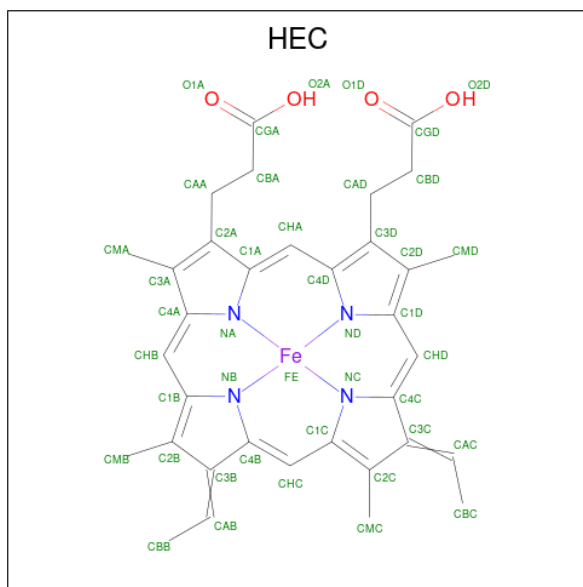
- Molecule 9 is a protein called High-potential iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	97	Total	C	N	O	S	0	0
			763	471	135	151	6		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	3	LYS	ASN	conflict	UNP A1WXH6
a	38	ASP	ASN	conflict	UNP A1WXH6
a	?	-	GLY	deletion	UNP A1WXH6
a	?	-	ASN	deletion	UNP A1WXH6
a	45	ARG	GLN	conflict	UNP A1WXH6
a	114	ASN	SER	conflict	UNP A1WXH6
a	129	VAL	ILE	conflict	UNP A1WXH6
a	136	ALA	GLU	conflict	UNP A1WXH6

- Molecule 10 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

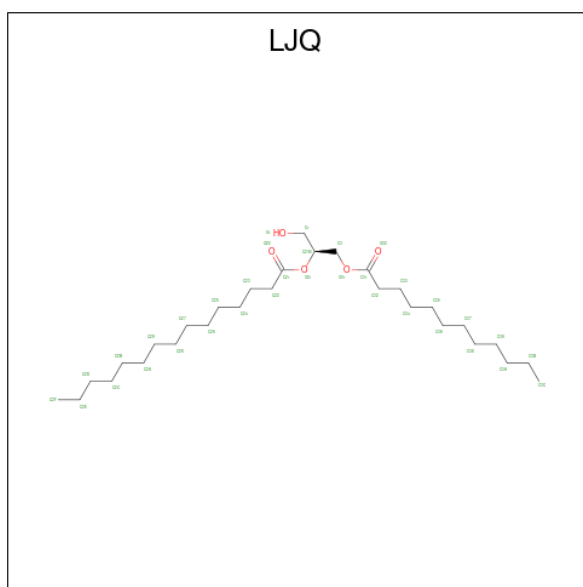


Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

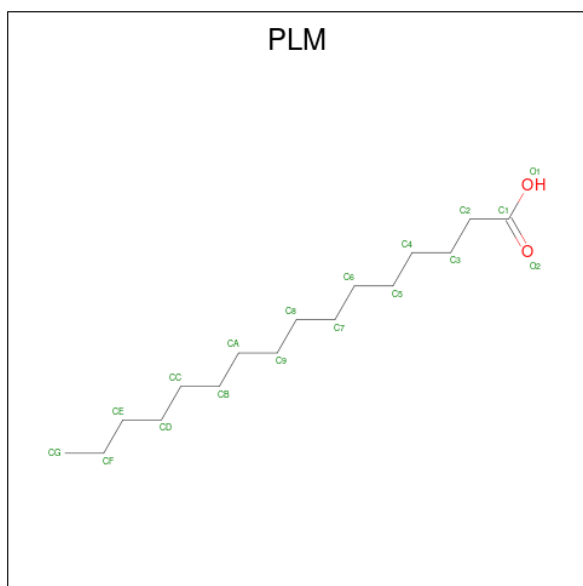
Mol	Chain	Residues	Atoms		AltConf
11	C	1	Total	Mg	0
			1	1	

- Molecule 12 is [(2 {S})-1-dodecanoyloxy-3-oxidanyl-propan-2-yl] pentadecanoate (CCD ID: LJQ) (formula: C₃₀H₅₈O₅).



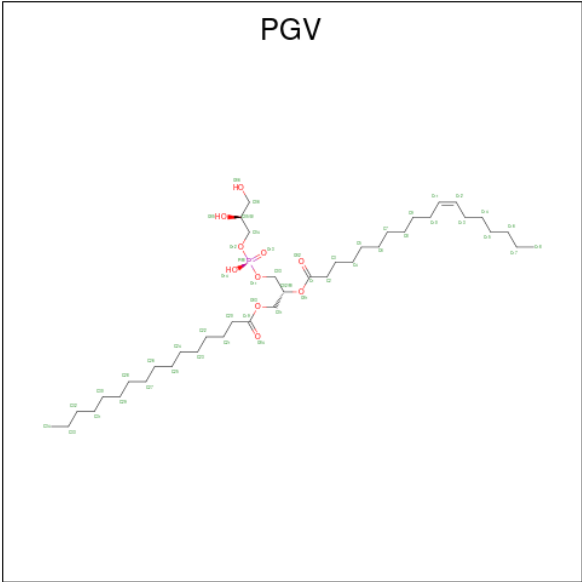
Mol	Chain	Residues	Atoms			AltConf
12	C	1	Total	C	O	0
			31	27	4	

- Molecule 13 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	C	O	0
			12	11	1	

- Molecule 14 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	O	P	0
			32	21	10	1	
14	L	1	Total	C	O	P	0
			43	32	10	1	
14	L	1	Total	C	O	P	0
			36	27	8	1	
14	L	1	Total	C	O	P	0
			41	30	10	1	
14	M	1	Total	C	O	P	0
			51	40	10	1	
14	H	1	Total	C	O	P	0
			36	25	10	1	
14	H	1	Total	C	O	P	0
			42	31	10	1	
14	B	1	Total	C	O	P	0
			44	33	10	1	
14	B	1	Total	C	O	P	0
			41	32	8	1	
14	E	1	Total	C	O	P	0
			38	27	10	1	
14	F	1	Total	C	O	P	0
			50	39	10	1	
14	G	1	Total	C	O	P	0
			49	38	10	1	
14	G	1	Total	C	O	P	0
			50	39	10	1	
14	G	1	Total	C	O	P	0
			42	33	8	1	

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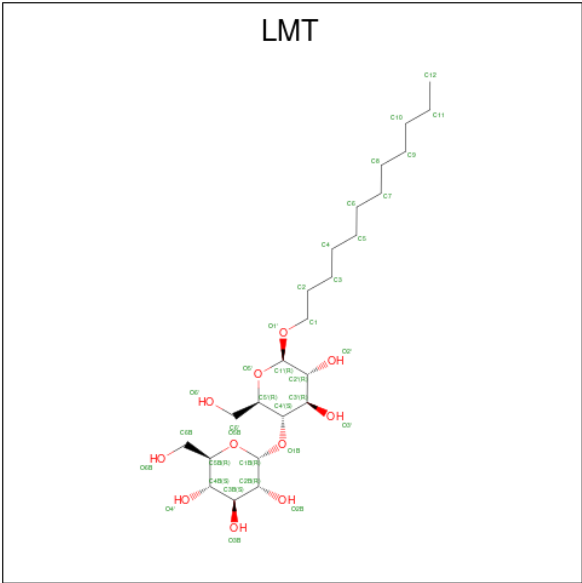
Mol	Chain	Residues	Atoms				AltConf
14	J	1	Total	C	O	P	0
			33	24	8	1	
14	N	1	Total	C	O	P	0
			50	39	10	1	
14	N	1	Total	C	O	P	0
			47	36	10	1	
14	N	1	Total	C	O	P	0
			37	26	10	1	
14	P	1	Total	C	O	P	0
			47	36	10	1	
14	P	1	Total	C	O	P	0
			40	31	8	1	
14	R	1	Total	C	O	P	0
			43	32	10	1	
14	R	1	Total	C	O	P	0
			41	32	8	1	
14	T	1	Total	C	O	P	0
			46	35	10	1	
14	T	1	Total	C	O	P	0
			47	36	10	1	
14	V	1	Total	C	O	P	0
			44	33	10	1	
14	X	1	Total	C	O	P	0
			43	32	10	1	
14	X	1	Total	C	O	P	0
			45	34	10	1	
14	Z	1	Total	C	O	P	0
			46	35	10	1	
14	Z	1	Total	C	O	P	0
			44	33	10	1	
14	Z	1	Total	C	O	P	0
			43	34	8	1	
14	1	1	Total	C	O	P	0
			45	34	10	1	
14	2	1	Total	C	O	P	0
			46	36	9	1	
14	2	1	Total	C	O	P	0
			37	27	9	1	
14	3	1	Total	C	O	P	0
			30	21	8	1	
14	4	1	Total	C	O	P	0
			44	34	9	1	

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Mol	Chain	Residues	Atoms				AltConf
14	6	1	Total	C	O	P	0
			46	35	10	1	
14	6	1	Total	C	O	P	0
			44	34	9	1	
14	6	1	Total	C	O	P	0
			43	32	10	1	
14	8	1	Total	C	O	P	0
			43	32	10	1	
14	0	1	Total	C	O	P	0
			41	30	10	1	
14	0	1	Total	C	O	P	0
			44	33	10	1	
14	0	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 15 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



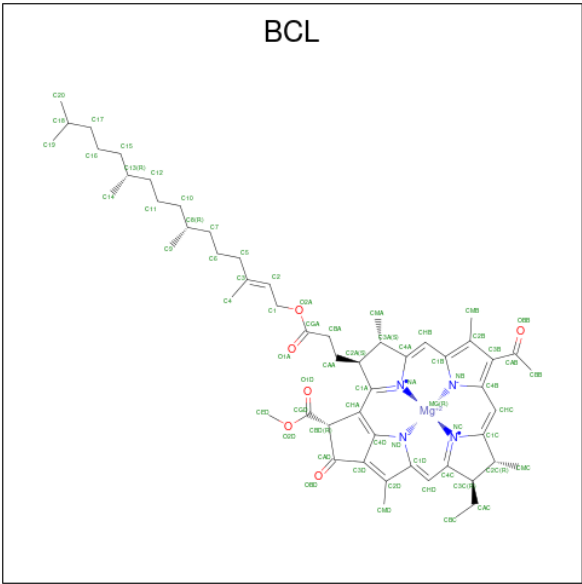
Mol	Chain	Residues	Atoms			AltConf
15	L	1	Total	C	O	0
			25	14	11	
15	L	1	Total	C	O	0
			35	24	11	
15	M	1	Total	C	O	0
			35	24	11	
15	H	1	Total	C	O	0
			30	19	11	

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Mol	Chain	Residues	Atoms			AltConf
15	H	1	Total	C	O	0
			35	24	11	
15	H	1	Total	C	O	0
			26	15	11	
15	F	1	Total	C	O	0
			33	22	11	
15	I	1	Total	C	O	0
			25	14	11	
15	O	1	Total	C	O	0
			29	18	11	
15	Q	1	Total	C	O	0
			32	21	11	
15	5	1	Total	C	O	0
			35	24	11	
15	5	1	Total	C	O	0
			24	13	11	
15	7	1	Total	C	O	0
			25	14	11	

- Molecule 16 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	L	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
16	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	S	1	Total 66	C 55	Mg 1	N 4	O 6	0

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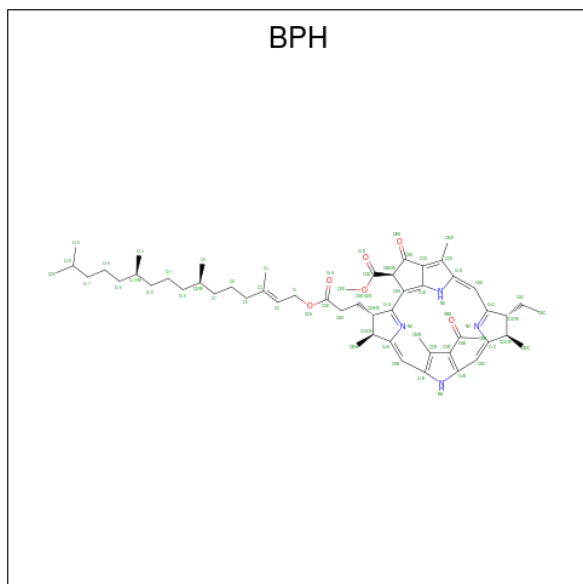
Mol	Chain	Residues	Atoms					AltConf
16	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	9	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	0	1	66	55	1	4	6	0

- Molecule 17 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
17	L	1	65	55	4	6	0
17	M	1	65	55	4	6	0

- Molecule 18 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).

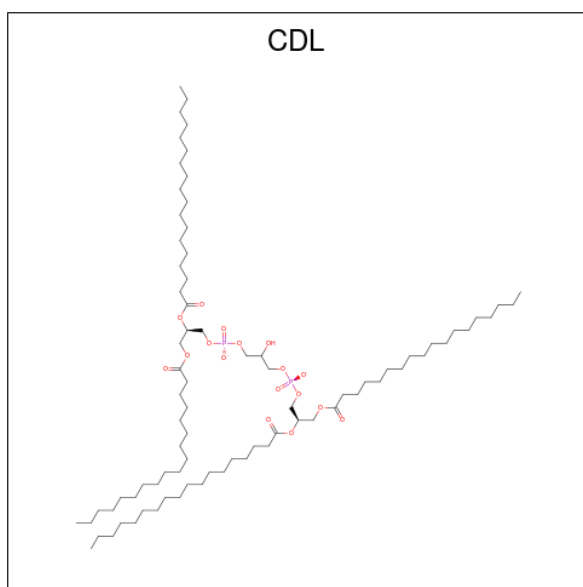


Mol	Chain	Residues	Atoms			AltConf
18	L	1	Total 33	C 29	O 4	0
18	L	1	Total 38	C 34	O 4	0
18	L	1	Total 17	C 13	O 4	0

- Molecule 19 is FE (III) ION (CCD ID: FE) (formula: Fe).

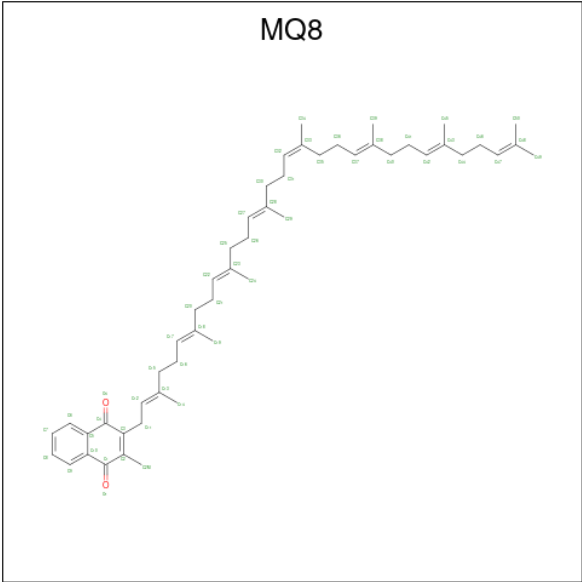
Mol	Chain	Residues	Atoms	AltConf
19	M	1	Total Fe 1 1	0

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



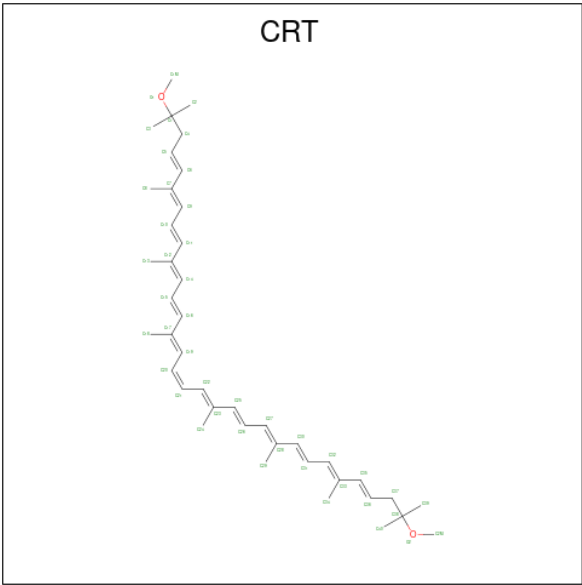
Mol	Chain	Residues	Atoms				AltConf
20	M	1	Total	C	O	P	0
			82	63	17	2	
20	M	1	Total	C	O	P	0
			80	61	17	2	
20	M	1	Total	C	O	P	0
			56	37	17	2	
20	M	1	Total	C	O	P	0
			50	31	17	2	
20	H	1	Total	C	O	P	0
			64	45	17	2	
20	H	1	Total	C	O	P	0
			75	56	17	2	
20	O	1	Total	C	O	P	0
			73	54	17	2	
20	U	1	Total	C	O	P	0
			51	32	17	2	
20	U	1	Total	C	O	P	0
			46	27	17	2	

- Molecule 21 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$).



Mol	Chain	Residues	Atoms			AltConf
21	M	1	Total	C	O	0
			53	51	2	

- Molecule 22 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



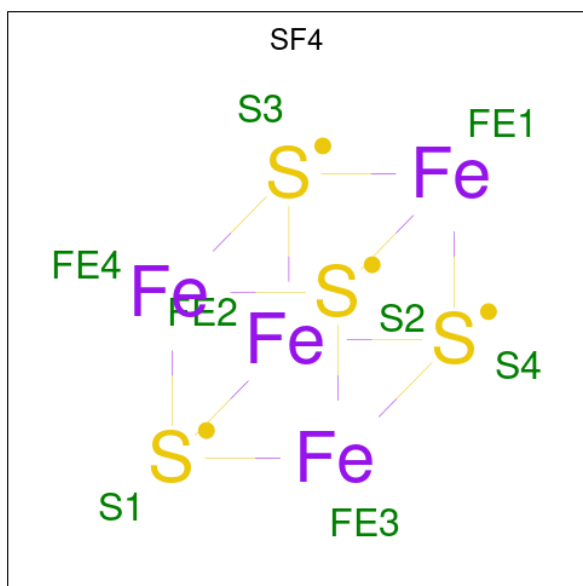
Mol	Chain	Residues	Atoms			AltConf
22	M	1	Total	C	O	0
			44	42	2	
22	B	1	Total	C	O	0
			44	42	2	
22	G	1	Total	C	O	0
			44	42	2	

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Mol	Chain	Residues	Atoms			AltConf
22	N	1	Total	C	O	0
			44	42	2	
22	R	1	Total	C	O	0
			44	42	2	
22	V	1	Total	C	O	0
			44	42	2	
22	Y	1	Total	C	O	0
			44	42	2	
22	4	1	Total	C	O	0
			44	42	2	
22	8	1	Total	C	O	0
			44	42	2	

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
23	a	1	Total	Fe	S	0
			8	4	4	

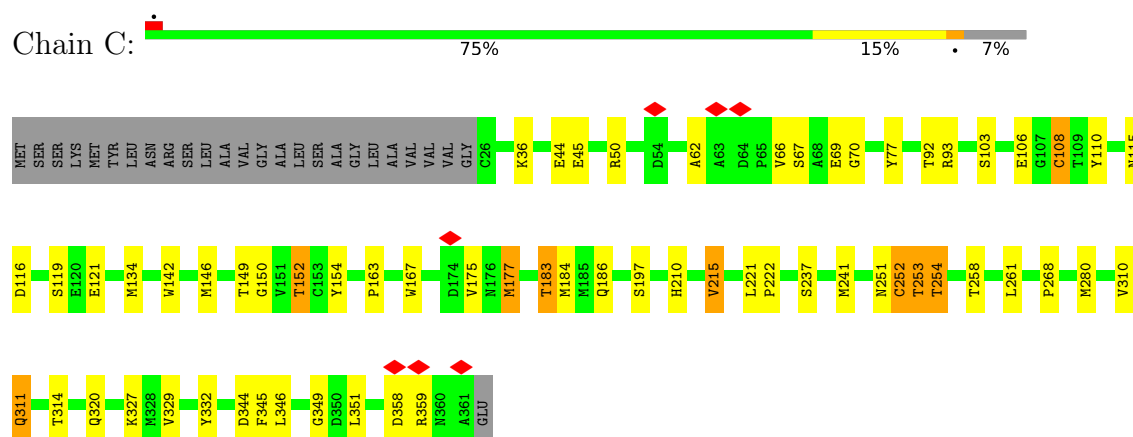
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		AltConf
24	C	4	Total	O	0
			4	4	
24	M	1	Total	O	0
			1	1	

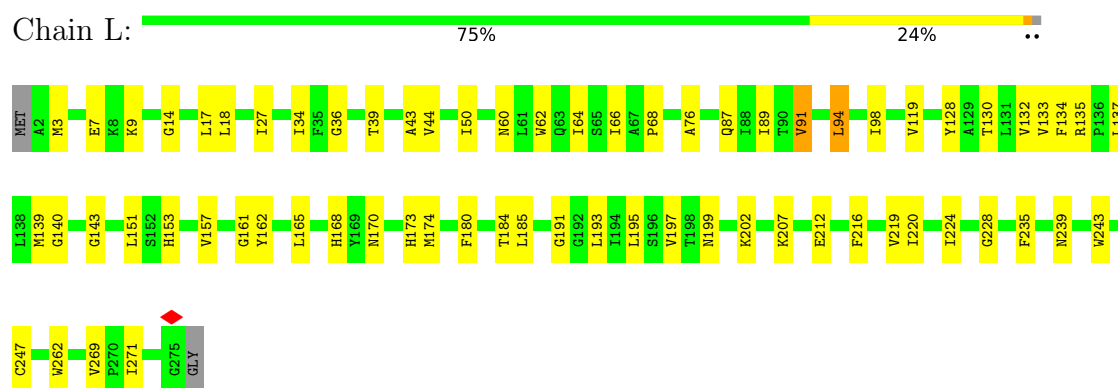
3 Residue-property plots

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

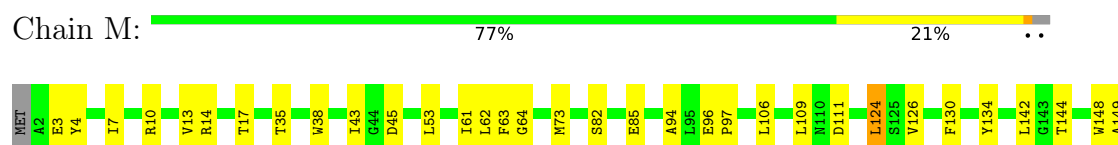
- Molecule 1: Photosynthetic reaction center cytochrome c subunit

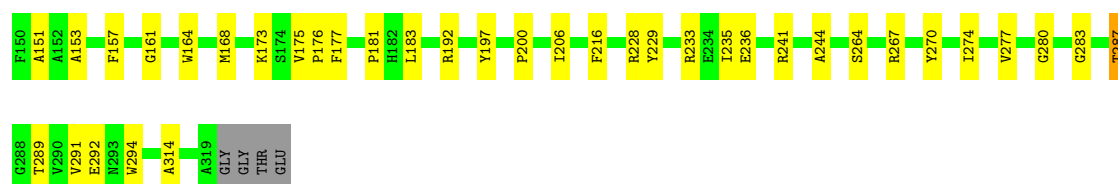


- Molecule 2: Reaction center protein L chain



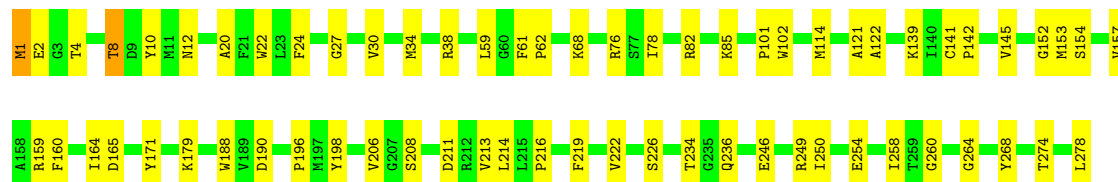
- Molecule 3: Reaction center protein M chain





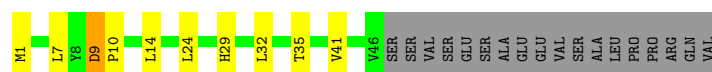
- Molecule 4: Photosynthetic reaction centre, H-chain

Chain H: 77% 23% .



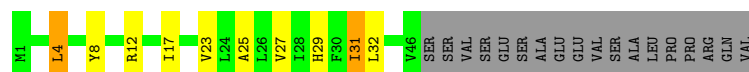
- Molecule 5: Antenna complex, alpha/beta subunit

Chain A: 56% 14% . 28%



- Molecule 5: Antenna complex, alpha/beta subunit

Chain F: 56% 12% . 28%



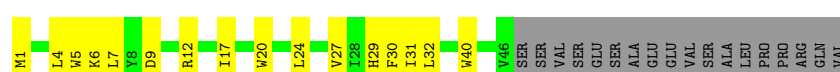
- Molecule 5: Antenna complex, alpha/beta subunit

Chain K: 53% 17% . 28%



- Molecule 5: Antenna complex, alpha/beta subunit

Chain Q: 47% 25% 28%



- Molecule 5: Antenna complex, alpha/beta subunit

Chain U: 52% 19% . 28%



- Molecule 5: Antenna complex, alpha/beta subunit



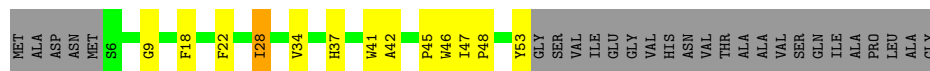
- Molecule 5: Antenna complex, alpha/beta subunit



- Molecule 5: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit

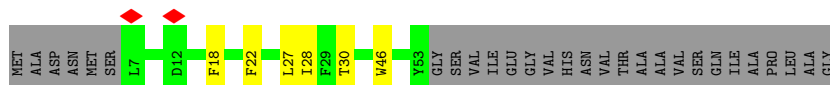


- Molecule 6: Antenna complex, alpha/beta subunit

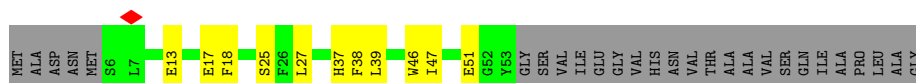




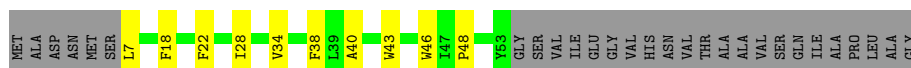
- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



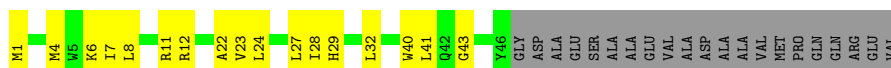
- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 7: Antenna complex, alpha/beta subunit

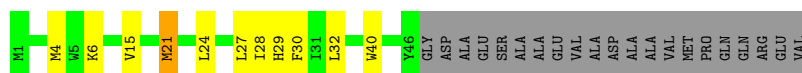


- Molecule 7: Antenna complex, alpha/beta subunit



- Molecule 7: Antenna complex, alpha/beta subunit

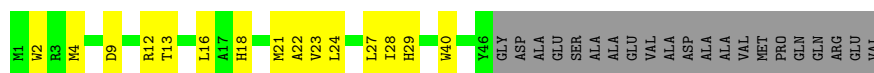




- Molecule 7: Antenna complex, alpha/beta subunit



- Molecule 7: Antenna complex, alpha/beta subunit



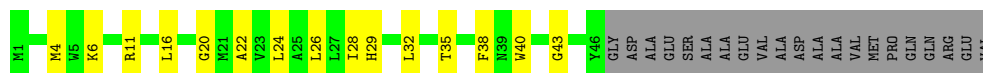
- Molecule 7: Antenna complex, alpha/beta subunit



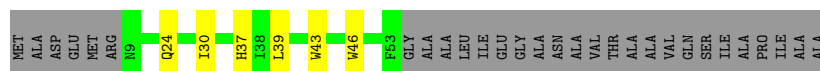
- Molecule 7: Antenna complex, alpha/beta subunit



- Molecule 7: Antenna complex, alpha/beta subunit



- Molecule 8: Antenna complex, alpha/beta subunit



- Molecule 8: Antenna complex, alpha/beta subunit

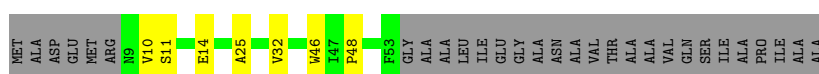




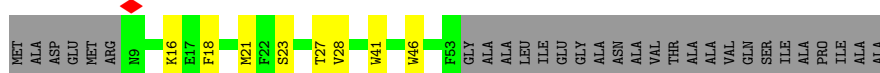
- Molecule 8: Antenna complex, alpha/beta subunit



- Molecule 8: Antenna complex, alpha/beta subunit



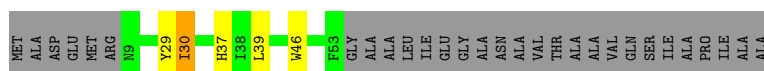
- Molecule 8: Antenna complex, alpha/beta subunit



- Molecule 8: Antenna complex, alpha/beta subunit



- Molecule 8: Antenna complex, alpha/beta subunit

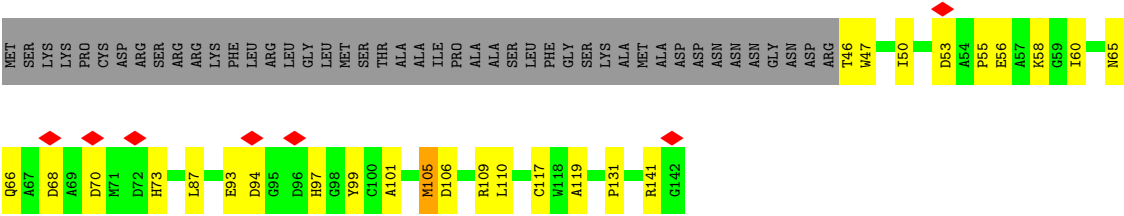


- Molecule 8: Antenna complex, alpha/beta subunit



- Molecule 9: High-potential iron-sulfur protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90126	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.213	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, UQ8, MG, SF4, BCL, HEC, FE, MQ8, PGV, CRT, LMT, BPH, LJQ, PLM

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	C	0.25	0/2702	0.40	0/3674
2	L	0.25	0/2252	0.36	0/3082
3	M	0.25	0/2613	0.35	0/3582
4	H	0.21	0/2229	0.33	0/3027
5	3	0.21	0/398	0.30	0/543
5	7	0.22	0/398	0.28	0/543
5	A	0.24	0/398	0.31	0/543
5	F	0.22	0/398	0.31	0/543
5	K	0.20	0/398	0.28	0/543
5	Q	0.20	0/398	0.29	0/543
5	U	0.22	0/398	0.29	0/543
5	Y	0.21	0/398	0.34	0/543
6	4	0.18	0/395	0.25	0/539
6	8	0.19	0/395	0.29	0/539
6	B	0.22	0/401	0.33	0/547
6	G	0.21	0/395	0.25	0/539
6	N	0.19	0/395	0.28	0/539
6	R	0.21	0/395	0.32	0/539
6	V	0.19	0/395	0.27	0/539
6	Z	0.18	0/401	0.29	0/547
7	1	0.21	0/402	0.29	0/547
7	5	0.21	0/402	0.30	0/547
7	9	0.23	0/402	0.31	0/547
7	D	0.25	0/402	0.33	0/547
7	I	0.23	0/402	0.31	0/547
7	O	0.21	0/402	0.31	0/547
7	S	0.23	0/402	0.36	0/547
7	W	0.22	0/402	0.33	0/547
8	0	0.20	0/376	0.24	0/514
8	2	0.19	0/376	0.24	0/514
8	6	0.20	0/376	0.25	0/514
8	E	0.21	0/376	0.26	0/514

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	J	0.19	0/376	0.25	0/514
8	P	0.22	0/376	0.25	0/514
8	T	0.20	0/376	0.29	0/514
8	X	0.20	0/376	0.25	0/514
9	a	0.18	0/786	0.46	0/1068
All	All	0.22	0/23162	0.33	0/31593

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2642	0	2401	52	0
2	L	2170	0	2145	59	0
3	M	2518	0	2465	63	0
4	H	2174	0	2131	49	0
5	3	385	0	403	15	0
5	7	385	0	403	18	0
5	A	385	0	403	10	0
5	F	385	0	403	12	0
5	K	385	0	403	12	0
5	Q	385	0	403	18	0
5	U	385	0	403	16	0
5	Y	385	0	403	8	0
6	4	380	0	359	12	0
6	8	380	0	359	14	0
6	B	386	0	364	16	0
6	G	380	0	359	11	0
6	N	380	0	359	11	0
6	R	380	0	359	11	0
6	V	380	0	359	4	0
6	Z	386	0	364	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	1	390	0	401	23	0
7	5	390	0	401	17	0
7	9	390	0	401	17	0
7	D	390	0	401	21	0
7	I	390	0	401	20	0
7	O	390	0	401	12	0
7	S	390	0	401	19	0
7	W	390	0	401	15	0
8	0	362	0	333	16	0
8	2	362	0	333	12	0
8	6	362	0	333	5	0
8	E	362	0	333	6	0
8	J	362	0	333	15	0
8	P	362	0	333	8	0
8	T	362	0	333	5	0
8	X	362	0	333	9	0
9	a	763	0	666	14	0
10	C	172	0	121	14	0
11	C	1	0	0	0	0
12	C	31	0	0	0	0
13	C	12	0	18	5	0
14	0	128	0	161	16	0
14	1	45	0	58	12	0
14	2	83	0	106	6	0
14	3	30	0	31	4	0
14	4	44	0	59	4	0
14	6	133	0	173	9	0
14	8	43	0	54	8	0
14	B	85	0	107	12	0
14	C	32	0	34	3	0
14	E	38	0	44	2	0
14	F	50	0	71	6	0
14	G	141	0	193	16	0
14	H	78	0	99	8	0
14	J	33	0	37	4	0
14	L	120	0	150	15	0
14	M	51	0	76	5	0
14	N	134	0	178	10	0
14	P	87	0	116	9	0
14	R	84	0	107	8	0
14	T	93	0	128	9	0
14	V	44	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	X	88	0	116	8	0
14	Z	133	0	177	14	0
15	5	59	0	67	7	0
15	7	25	0	23	4	0
15	F	33	0	39	4	0
15	H	91	0	104	9	0
15	I	25	0	23	5	0
15	L	60	0	69	5	0
15	M	35	0	46	4	0
15	O	29	0	31	1	0
15	Q	32	0	37	3	0
16	0	66	0	74	9	0
16	1	132	0	148	17	0
16	2	66	0	74	10	0
16	3	66	0	74	8	0
16	4	66	0	74	5	0
16	5	132	0	148	20	0
16	6	66	0	74	7	0
16	7	66	0	74	3	0
16	8	66	0	74	11	0
16	9	132	0	148	11	0
16	A	66	0	74	4	0
16	B	66	0	74	11	0
16	D	132	0	148	10	0
16	E	66	0	74	6	0
16	F	66	0	74	2	0
16	G	66	0	74	10	0
16	I	132	0	148	20	0
16	J	66	0	74	8	0
16	K	66	0	74	7	0
16	L	198	0	221	13	0
16	M	66	0	74	7	0
16	N	66	0	74	8	0
16	O	132	0	148	11	0
16	P	66	0	74	9	0
16	Q	66	0	74	7	0
16	R	66	0	74	10	0
16	S	132	0	148	21	0
16	T	66	0	74	6	0
16	U	66	0	74	5	0
16	V	66	0	74	9	0
16	W	132	0	148	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	X	66	0	74	5	0
16	Y	132	0	148	8	0
16	Z	66	0	74	8	0
17	L	65	0	76	6	0
17	M	65	0	76	8	0
18	L	88	0	98	10	0
19	M	1	0	0	0	0
20	H	139	0	169	12	0
20	M	268	0	318	20	0
20	O	73	0	90	3	0
20	U	97	0	82	6	0
21	M	53	0	72	3	0
22	4	44	0	60	12	0
22	8	44	0	60	6	0
22	B	44	0	60	4	0
22	G	44	0	60	6	0
22	M	44	0	60	11	0
22	N	44	0	60	11	0
22	R	44	0	60	9	0
22	V	44	0	60	9	0
22	Y	44	0	60	9	0
23	a	8	0	0	0	0
24	C	4	0	0	0	0
24	M	1	0	0	0	0
All	All	29045	0	29545	844	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (844) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:CYS:SG	10:C:401:HEC:HAB	1.39	1.58
1:C:108:CYS:CB	10:C:401:HEC:HAB	1.51	1.40
1:C:108:CYS:SG	10:C:401:HEC:CAB	2.11	1.37
1:C:108:CYS:CB	10:C:401:HEC:CAB	2.27	1.11
1:C:108:CYS:HB3	10:C:401:HEC:CAB	1.86	1.05
1:C:108:CYS:HB3	10:C:401:HEC:C3B	1.86	1.05
1:C:152:THR:HG22	1:C:154:TYR:H	1.43	0.84
14:B:103:PGV:H131	14:B:104:PGV:H51	1.59	0.83
3:M:97:PRO:HD3	3:M:176:PRO:HB3	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:34:SER:HB3	14:3:101:PGV:H22	1.60	0.82
16:5:104:BCL:H143	5:7:26:LEU:HD11	1.62	0.80
4:H:8:THR:HG21	7:I:35:THR:HG22	1.64	0.80
7:S:7:ILE:HD11	22:V:101:CRT:H32A	1.64	0.79
14:Z:101:PGV:H71	14:Z:101:PGV:H032	1.63	0.78
5:F:8:TYR:HD1	15:F:102:LMT:H5'	1.50	0.76
7:1:21:MET:HE3	16:1:103:BCL:H72	1.67	0.76
3:M:287:THR:HB	3:M:294:TRP:HE1	1.49	0.76
6:N:18:PHE:HA	22:N:102:CRT:H6	1.66	0.76
3:M:64:GLY:HA3	17:M:404:BPH:H5C1	1.66	0.75
14:2:102:PGV:H012	14:2:102:PGV:H51	1.67	0.75
2:L:119:VAL:HG21	20:M:402:CDL:H512	1.69	0.74
1:C:108:CYS:SG	10:C:401:HEC:CBB	2.76	0.73
14:0:103:PGV:H12	14:0:104:PGV:H32	1.70	0.73
7:W:9:ASP:HB3	7:W:12:ARG:HG2	1.71	0.73
22:8:101:CRT:H292	16:9:102:BCL:HBB3	1.71	0.72
5:7:32:LEU:HD11	16:8:102:BCL:HHD	1.70	0.72
8:P:49:GLY:H	14:P:102:PGV:H05	1.55	0.71
15:I:101:LMT:H5'	20:O:101:CDL:H121	1.72	0.70
16:Q:102:BCL:H91	6:R:25:SER:HB3	1.74	0.70
8:2:30:ILE:HD11	16:2:101:BCL:H11	1.71	0.70
18:L:307:UQ8:H3M	16:L:312:BCL:H161	1.73	0.70
22:Y:403:CRT:H292	16:1:103:BCL:HBB3	1.73	0.70
7:S:32:LEU:HD11	16:T:101:BCL:HHD	1.73	0.70
16:Z:102:BCL:H121	8:2:32:VAL:HG11	1.72	0.70
20:M:409:CDL:HB61	15:M:411:LMT:H6D	1.74	0.69
14:6:104:PGV:H061	14:6:104:PGV:H012	1.73	0.69
7:5:15:VAL:HG22	16:5:103:BCL:H18	1.74	0.69
8:0:10:VAL:HG23	8:0:14:GLU:HG3	1.75	0.69
7:O:24:LEU:HD23	16:P:101:BCL:HED3	1.73	0.69
3:M:161:GLY:HA3	22:M:406:CRT:H292	1.74	0.69
3:M:94:ALA:HB2	3:M:181:PRO:HG2	1.75	0.68
14:B:104:PGV:H252	14:B:104:PGV:H91	1.75	0.68
14:J:102:PGV:H51	14:N:101:PGV:H142	1.74	0.68
9:a:70:ASP:HB3	9:a:73:HIS:HB2	1.75	0.67
14:C:408:PGV:H42	15:5:101:LMT:H81	1.76	0.67
3:M:264:SER:HA	3:M:267:ARG:HG3	1.75	0.67
15:H:305:LMT:H4B	7:I:12:ARG:HD2	1.75	0.67
7:I:21:MET:HE2	16:I:103:BCL:H2	1.77	0.67
6:4:18:PHE:HB2	22:4:101:CRT:H31A	1.76	0.66
5:Q:4:LEU:HD11	16:S:102:BCL:HHD	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:0:103:PGV:H141	14:0:104:PGV:H72	1.77	0.66
16:V:102:BCL:H141	8:X:28:VAL:HG12	1.76	0.66
7:S:22:ALA:HB2	16:S:101:BCL:H43	1.77	0.66
20:H:301:CDL:H512	7:D:8:LEU:HD13	1.78	0.66
6:N:39:LEU:HB3	14:N:101:PGV:H222	1.78	0.66
20:M:409:CDL:HA4	16:Y:401:BCL:HMC3	1.76	0.66
3:M:7:ILE:HD12	20:M:402:CDL:H591	1.78	0.65
3:M:200:PRO:HB3	14:H:302:PGV:H22	1.76	0.65
7:5:22:ALA:HA	16:5:103:BCL:H11	1.78	0.65
6:N:47:ILE:HG21	14:N:104:PGV:H202	1.76	0.65
7:O:32:LEU:HD11	16:P:101:BCL:HHD	1.78	0.65
1:C:146:MET:HE3	1:C:150:GLY:HA2	1.78	0.65
22:N:102:CRT:H292	16:O:104:BCL:HBB3	1.79	0.65
7:D:7:ILE:HD11	22:G:102:CRT:H32A	1.79	0.65
22:B:101:CRT:H1M1	7:9:6:LYS:HB2	1.78	0.64
5:U:19:SER:HB3	16:W:101:BCL:H192	1.78	0.64
2:L:140:GLY:HA3	15:L:301:LMT:H3B	1.80	0.64
3:M:10:ARG:HG2	4:H:222:VAL:HB	1.79	0.64
18:L:306:UQ8:H1M	15:L:308:LMT:H72	1.80	0.64
5:U:7:LEU:HD11	8:X:21:MET:HE1	1.80	0.64
1:C:251:ASN:HA	2:L:165:LEU:HD21	1.80	0.63
3:M:280:GLY:HA2	16:M:403:BCL:HED2	1.81	0.63
3:M:289:THR:HB	14:M:410:PGV:H32	1.79	0.63
14:6:103:PGV:H202	6:8:43:TRP:HB2	1.80	0.63
7:9:20:GLY:HA3	16:9:102:BCL:H93	1.80	0.63
7:1:27:LEU:HD12	14:1:101:PGV:H261	1.81	0.63
7:W:29:HIS:CE1	16:X:102:BCL:HMD3	2.33	0.63
2:L:193:LEU:HD22	2:L:216:PHE:HE2	1.64	0.63
2:L:197:VAL:HG21	2:L:212:GLU:HG3	1.79	0.63
1:C:177:MET:HE2	3:M:111:ASP:HB2	1.80	0.63
4:H:20:ALA:HB2	14:H:304:PGV:H321	1.81	0.63
6:8:41:TRP:HE1	14:8:103:PGV:H061	1.63	0.63
14:0:104:PGV:H251	14:0:104:PGV:H101	1.81	0.63
14:B:103:PGV:H132	8:E:39:LEU:HD13	1.80	0.62
7:D:32:LEU:HD11	16:E:101:BCL:HHD	1.81	0.62
5:U:20:TRP:HB2	16:W:101:BCL:H152	1.81	0.62
22:V:101:CRT:H372	7:W:29:HIS:CG	2.34	0.62
8:J:46:TRP:CD2	16:J:101:BCL:H2C	2.34	0.62
5:3:3:ARG:HA	5:3:6:LYS:HG3	1.81	0.62
6:Z:46:TRP:CD2	16:Z:102:BCL:H2C	2.34	0.62
20:M:409:CDL:HB32	15:M:411:LMT:H4'	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:32:LEU:HD11	16:V:102:BCL:HHD	1.82	0.62
16:V:102:BCL:H143	16:V:102:BCL:H91	1.82	0.62
3:M:241:ARG:HB3	4:H:85:LYS:HE2	1.81	0.62
6:G:36:ALA:HB1	14:G:101:PGV:H282	1.82	0.62
7:I:32:LEU:HD11	16:J:101:BCL:HHD	1.81	0.61
16:9:101:BCL:H3C	14:0:101:PGV:H231	1.82	0.61
1:C:108:CYS:CA	10:C:401:HEC:HAB	2.29	0.61
14:G:104:PGV:H142	14:G:105:PGV:H82	1.82	0.61
16:R:102:BCL:H93	8:T:32:VAL:HG11	1.82	0.61
3:M:61:ILE:HD12	17:M:404:BPH:H102	1.83	0.61
3:M:229:TYR:HB2	3:M:244:ALA:HB2	1.81	0.61
14:B:104:PGV:H82	14:B:104:PGV:H222	1.81	0.61
7:D:29:HIS:CE1	16:E:101:BCL:HMD3	2.36	0.61
7:1:21:MET:HE1	16:2:101:BCL:H91	1.81	0.61
2:L:219:VAL:HG12	2:L:220:ILE:HG23	1.82	0.61
5:7:34:SER:HA	15:7:101:LMT:H1B	1.82	0.61
1:C:103:SER:HB2	1:C:106:GLU:HB2	1.83	0.61
14:G:105:PGV:H301	14:G:105:PGV:H252	1.83	0.61
16:8:102:BCL:H122	8:0:29:TYR:HD1	1.65	0.61
2:L:17:LEU:HB3	18:L:306:UQ8:H30	1.81	0.61
7:W:22:ALA:HB2	16:W:101:BCL:H43	1.83	0.60
1:C:258:THR:HA	1:C:261:LEU:HD13	1.83	0.60
3:M:153:ALA:HA	3:M:277:VAL:HG21	1.82	0.60
14:E:102:PGV:H91	14:E:102:PGV:H221	1.83	0.60
22:M:406:CRT:H2M3	5:Q:31:ILE:HG12	1.82	0.60
7:W:27:LEU:HD11	5:Y:30:PHE:HZ	1.67	0.60
6:R:46:TRP:CD2	16:R:102:BCL:H2C	2.37	0.60
16:3:102:BCL:H18	6:4:28:ILE:HD12	1.83	0.60
6:8:46:TRP:CD2	16:8:102:BCL:H2C	2.36	0.60
7:9:32:LEU:HD11	16:0:102:BCL:HHD	1.84	0.60
3:M:168:MET:HE3	3:M:289:THR:HG22	1.83	0.60
16:5:104:BCL:H51	16:6:102:BCL:H61	1.82	0.60
8:0:42:ALA:HB1	14:0:101:PGV:H32	1.83	0.60
17:L:303:BPH:HBB3	17:L:303:BPH:HHC	1.83	0.60
4:H:61:PHE:HZ	15:H:305:LMT:H12	1.66	0.60
7:5:32:LEU:HD11	16:6:102:BCL:HHD	1.83	0.59
7:W:21:MET:HE2	16:W:102:BCL:H2	1.85	0.59
16:Z:102:BCL:H3A	16:Z:102:BCL:H2	1.84	0.59
6:G:46:TRP:CD2	16:G:103:BCL:H2C	2.38	0.59
8:J:34:VAL:HG13	14:J:102:PGV:H242	1.84	0.59
8:X:46:TRP:CD2	16:X:102:BCL:H2C	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:101:PGV:H61	14:3:101:PGV:H42	1.85	0.59
9:a:106:ASP:HB3	9:a:109:ARG:HB2	1.85	0.59
6:4:46:TRP:CD2	16:4:102:BCL:H2C	2.38	0.59
14:C:408:PGV:H52	14:3:101:PGV:H82	1.85	0.59
7:S:21:MET:HE3	16:S:102:BCL:H51	1.85	0.59
16:2:101:BCL:H102	16:3:102:BCL:H11	1.84	0.59
14:L:309:PGV:H102	5:F:23:VAL:HG13	1.84	0.59
7:W:18:HIS:HD2	16:W:101:BCL:H51	1.68	0.59
16:K:101:BCL:HMA3	14:N:101:PGV:H322	1.84	0.59
3:M:7:ILE:HG23	20:M:402:CDL:H611	1.85	0.58
3:M:73:MET:HE1	5:U:31:ILE:HG13	1.85	0.58
7:D:23:VAL:HG12	16:D:102:BCL:H161	1.83	0.58
14:T:103:PGV:H281	14:T:103:PGV:H201	1.85	0.58
14:R:103:PGV:H151	14:R:104:PGV:H21	1.86	0.58
2:L:199:ASN:HB3	20:M:407:CDL:HA21	1.84	0.58
14:L:310:PGV:H202	14:1:101:PGV:H251	1.85	0.58
22:8:101:CRT:H393	7:9:26:LEU:HD23	1.85	0.58
14:G:104:PGV:H012	8:J:43:TRP:HD1	1.69	0.58
16:Y:401:BCL:H192	7:1:23:VAL:HG21	1.86	0.58
7:1:21:MET:HB3	16:1:102:BCL:H12	1.86	0.58
5:U:17:ILE:HA	16:W:101:BCL:H91	1.86	0.57
2:L:235:PHE:HB2	20:M:402:CDL:H601	1.86	0.57
16:8:102:BCL:H203	16:9:102:BCL:HAC2	1.86	0.57
22:Y:403:CRT:H6	6:Z:18:PHE:HA	1.85	0.57
5:A:32:LEU:HD11	16:B:102:BCL:HHD	1.86	0.57
7:S:18:HIS:HB3	16:S:101:BCL:H62	1.87	0.57
8:T:46:TRP:CD2	16:T:101:BCL:H2C	2.40	0.57
2:L:220:ILE:HD11	18:L:304:UQ8:H10B	1.86	0.57
5:K:7:LEU:HD11	8:P:21:MET:HE1	1.87	0.57
5:Y:32:LEU:HD11	16:Z:102:BCL:HHD	1.87	0.57
7:1:18:HIS:CE1	16:1:102:BCL:H192	2.39	0.57
2:L:50:ILE:HG13	2:L:89:ILE:HD13	1.86	0.57
2:L:132:VAL:HG23	2:L:133:VAL:HG23	1.86	0.57
16:G:103:BCL:H102	8:J:32:VAL:HG11	1.86	0.57
14:0:101:PGV:H011	14:0:101:PGV:H31	1.86	0.57
7:5:24:LEU:HD23	16:6:102:BCL:HED3	1.87	0.56
16:J:101:BCL:H8	16:K:101:BCL:H2	1.87	0.56
16:R:102:BCL:H193	16:S:102:BCL:HAC2	1.86	0.56
5:7:7:LEU:HB3	7:9:11:ARG:HG2	1.86	0.56
7:9:24:LEU:HD23	16:0:102:BCL:HED3	1.87	0.56
14:L:305:PGV:H61	14:L:309:PGV:H241	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:102:CRT:H35	16:O:103:BCL:HMB2	1.88	0.56
2:L:44:VAL:HG11	16:D:101:BCL:H201	1.87	0.56
5:7:34:SER:HA	15:7:101:LMT:H4'	1.87	0.56
8:0:46:TRP:CD2	16:0:102:BCL:H2C	2.41	0.56
2:L:193:LEU:HD22	2:L:216:PHE:CE2	2.40	0.56
3:M:109:LEU:HD11	7:S:31:ILE:HG23	1.87	0.56
14:L:310:PGV:H11	14:1:101:PGV:H272	1.88	0.56
5:A:14:LEU:HD13	7:9:4:MET:HE1	1.86	0.56
5:K:32:LEU:HD11	16:N:103:BCL:HHD	1.87	0.56
6:4:34:VAL:HG13	14:4:103:PGV:H271	1.88	0.56
7:D:24:LEU:HD12	7:D:27:LEU:HD23	1.88	0.56
5:Q:32:LEU:HD11	16:R:102:BCL:HHD	1.87	0.55
6:Z:37:HIS:CD2	14:Z:104:PGV:H11	2.41	0.55
8:P:49:GLY:N	14:P:102:PGV:H05	2.20	0.55
8:2:46:TRP:CD2	16:2:101:BCL:H2C	2.42	0.55
8:0:41:TRP:CD1	14:0:104:PGV:H05	2.41	0.55
15:I:101:LMT:H4'	5:K:11:ARG:HH22	1.71	0.55
14:N:104:PGV:H171	8:P:35:VAL:HG13	1.89	0.55
7:5:24:LEU:HD13	16:5:104:BCL:H142	1.89	0.55
1:C:149:THR:HA	1:C:327:LYS:HG2	1.88	0.55
6:B:46:TRP:CD2	16:B:102:BCL:H2C	2.41	0.55
7:I:1:MET:HG2	16:K:101:BCL:H192	1.88	0.55
8:E:46:TRP:CD2	16:E:101:BCL:H2C	2.41	0.55
14:2:102:PGV:H222	6:4:43:TRP:HB2	1.88	0.55
16:8:102:BCL:H8	8:0:32:VAL:HG11	1.89	0.55
5:F:4:LEU:HD12	16:I:103:BCL:HAC1	1.88	0.55
7:O:6:LYS:HG2	8:P:10:VAL:HG12	1.87	0.54
14:G:104:PGV:H142	14:G:105:PGV:H51	1.88	0.54
22:M:406:CRT:H2M2	5:Q:30:PHE:HD1	1.72	0.54
4:H:250:ILE:HG13	4:H:254:GLU:HB2	1.87	0.54
6:R:18:PHE:HB2	22:R:101:CRT:H31A	1.90	0.54
16:L:302:BCL:H2	17:L:303:BPH:HHC	1.90	0.54
5:A:10:PRO:HB3	6:B:18:PHE:CE1	2.42	0.54
8:P:46:TRP:CD2	16:P:101:BCL:H2C	2.42	0.54
14:Z:104:PGV:H252	14:Z:104:PGV:H91	1.88	0.54
7:1:6:LYS:HB2	22:4:101:CRT:H1M1	1.88	0.54
14:1:101:PGV:H82	14:3:101:PGV:H51	1.88	0.54
2:L:195:LEU:HD21	3:M:267:ARG:HG2	1.90	0.54
7:I:6:LYS:HD3	22:N:102:CRT:H1M1	1.89	0.54
3:M:168:MET:HA	3:M:168:MET:HE2	1.89	0.54
7:O:6:LYS:HB2	22:R:101:CRT:H1M1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:403:CRT:H293	16:1:102:BCL:H72	1.89	0.54
3:M:13:VAL:HG13	4:H:196:PRO:HG3	1.90	0.53
14:Z:103:PGV:H232	8:2:39:LEU:HB3	1.90	0.53
22:4:101:CRT:H35	16:5:103:BCL:HMB1	1.90	0.53
2:L:66:ILE:HG21	2:L:89:ILE:HD12	1.89	0.53
2:L:68:PRO:HB2	2:L:143:GLY:HA2	1.90	0.53
3:M:43:ILE:HG12	20:M:402:CDL:H651	1.90	0.53
7:D:27:LEU:HD22	16:D:102:BCL:H171	1.89	0.53
22:R:101:CRT:H35	16:S:101:BCL:HMB2	1.90	0.53
14:R:104:PGV:H301	14:R:104:PGV:H242	1.90	0.53
16:5:103:BCL:H111	16:5:104:BCL:HMC3	1.90	0.53
1:C:251:ASN:O	1:C:254:THR:HG23	2.09	0.53
2:L:44:VAL:HG21	16:D:101:BCL:H201	1.91	0.53
22:4:101:CRT:H35	16:5:103:BCL:CMB	2.38	0.53
20:M:407:CDL:H192	4:H:24:PHE:HA	1.90	0.53
14:G:104:PGV:H282	8:J:36:ALA:HB1	1.91	0.53
2:L:168:HIS:HB3	3:M:183:LEU:HD13	1.89	0.53
22:Y:403:CRT:H372	7:1:29:HIS:CG	2.43	0.53
22:4:101:CRT:H32	16:5:103:BCL:HMB1	1.91	0.53
1:C:50:ARG:HG2	15:5:101:LMT:H6'1	1.91	0.53
2:L:170:ASN:O	2:L:174:MET:HG3	2.08	0.53
16:B:102:BCL:HAA1	14:B:104:PGV:H132	1.89	0.53
5:F:8:TYR:CD1	15:F:102:LMT:H5'	2.39	0.53
5:Q:6:LYS:O	6:R:7:LEU:HB2	2.09	0.53
21:M:405:MQ8:H411	21:M:405:MQ8:H471	1.91	0.53
17:L:303:BPH:HHC	17:L:303:BPH:CBB	2.39	0.53
16:5:103:BCL:H3C	14:6:101:PGV:H242	1.90	0.53
5:7:9:ASP:OD2	5:7:12:ARG:HD2	2.09	0.53
2:L:170:ASN:HB3	2:L:173:HIS:HB3	1.90	0.52
5:Q:24:LEU:HD23	16:R:102:BCL:HED3	1.90	0.52
8:0:30:ILE:HG12	16:0:102:BCL:H11	1.91	0.52
5:A:41:VAL:HB	7:9:35:THR:HG21	1.92	0.52
2:L:137:LEU:O	15:L:301:LMT:H3'	2.10	0.52
3:M:164:TRP:CZ3	3:M:173:LYS:HB3	2.45	0.52
16:B:102:BCL:H203	8:E:24:GLN:HG2	1.92	0.52
5:Q:5:TRP:O	6:R:10:LEU:HD12	2.09	0.52
5:Q:20:TRP:HZ2	22:R:101:CRT:H31	1.74	0.52
16:S:102:BCL:H191	5:U:23:VAL:HG22	1.92	0.52
7:1:20:GLY:HA3	16:1:103:BCL:H93	1.90	0.52
7:1:24:LEU:HD13	16:1:103:BCL:H142	1.91	0.52
22:8:101:CRT:H372	7:9:29:HIS:CG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:154:SER:HB3	4:H:157:VAL:HB	1.92	0.52
6:B:42:ALA:HB1	14:O:103:PGV:H41	1.92	0.52
16:I:103:BCL:H203	5:K:15:ILE:HG12	1.91	0.52
6:N:22:PHE:CD2	22:N:102:CRT:H14	2.45	0.52
6:G:48:PRO:HG3	7:I:43:GLY:HA2	1.92	0.52
22:G:102:CRT:H372	7:I:29:HIS:CG	2.44	0.52
14:1:101:PGV:H21	5:3:33:LEU:HD22	1.91	0.52
6:V:18:PHE:HA	22:V:101:CRT:H6	1.92	0.52
2:L:14:GLY:HA3	4:H:274:THR:HG23	1.92	0.52
2:L:98:ILE:HD13	20:M:402:CDL:H202	1.91	0.52
2:L:119:VAL:HG11	20:M:402:CDL:H532	1.91	0.52
3:M:228:ARG:HB3	4:H:219:PHE:CZ	2.45	0.52
17:M:404:BPH:HBC3	17:M:404:BPH:HHD	1.92	0.52
5:Q:29:HIS:CE1	16:R:102:BCL:HMD1	2.45	0.52
16:Y:401:BCL:H91	7:1:19:VAL:HG11	1.91	0.52
22:M:406:CRT:H2M2	5:Q:30:PHE:CD1	2.44	0.52
6:Z:47:ILE:HG13	14:Z:104:PGV:H41	1.91	0.51
3:M:38:TRP:HB2	4:H:154:SER:HB2	1.91	0.51
16:I:103:BCL:HBA1	8:J:26:PHE:HA	1.92	0.51
5:U:9:ASP:HB3	5:U:12:ARG:HE	1.75	0.51
16:Z:102:BCL:H141	16:1:103:BCL:HMB3	1.91	0.51
14:Z:104:PGV:H011	14:Z:104:PGV:H341	1.90	0.51
2:L:130:THR:HA	2:L:134:PHE:HB2	1.92	0.51
4:H:102:TRP:CD1	5:A:9:ASP:HB2	2.46	0.51
16:J:101:BCL:H61	16:K:101:BCL:H2	1.93	0.51
16:8:102:BCL:H192	8:O:25:ALA:HA	1.91	0.51
14:E:102:PGV:H72	14:G:101:PGV:H141	1.93	0.51
7:I:1:MET:HE1	22:N:102:CRT:H133	1.92	0.51
6:N:46:TRP:CD2	16:N:103:BCL:H2C	2.46	0.51
14:X:103:PGV:H252	14:X:103:PGV:H92	1.92	0.51
2:L:62:TRP:HB3	2:L:151:LEU:HD23	1.93	0.51
5:F:32:LEU:HD11	16:G:103:BCL:HHD	1.92	0.51
7:5:40:TRP:CE3	16:5:103:BCL:HBC3	2.45	0.51
16:L:311:BCL:H92	20:H:303:CDL:H831	1.93	0.51
4:H:61:PHE:CE1	15:H:305:LMT:H6D	2.46	0.51
16:I:103:BCL:HBA2	16:I:103:BCL:HBD	1.92	0.51
14:R:104:PGV:H222	14:R:104:PGV:H91	1.93	0.51
6:V:30:THR:HG23	16:V:102:BCL:H11	1.93	0.51
1:C:310:VAL:HG13	1:C:314:THR:HB	1.92	0.51
13:C:407:PLM:H82	14:L:310:PGV:H102	1.93	0.51
16:P:101:BCL:H8	16:Q:102:BCL:H11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:102:PGV:H151	14:T:103:PGV:H21	1.92	0.51
16:2:101:BCL:H93	16:2:101:BCL:HMA2	1.92	0.51
6:B:37:HIS:HB3	14:B:104:PGV:H232	1.93	0.51
7:S:6:LYS:HB2	22:V:101:CRT:H1M1	1.93	0.51
7:1:22:ALA:HA	16:1:102:BCL:H43	1.92	0.51
14:V:103:PGV:H21	14:X:101:PGV:H132	1.93	0.50
5:3:10:PRO:HB3	6:4:18:PHE:CE1	2.45	0.50
8:6:37:HIS:CD2	14:6:104:PGV:H101	2.46	0.50
5:F:17:ILE:HG12	16:I:102:BCL:H101	1.93	0.50
6:G:7:LEU:HD22	6:G:10:LEU:HD21	1.94	0.50
5:Q:20:TRP:HB2	16:S:101:BCL:H122	1.93	0.50
14:G:104:PGV:H211	8:J:43:TRP:HB2	1.94	0.50
8:X:46:TRP:CE2	16:X:102:BCL:H2C	2.46	0.50
7:5:18:HIS:CD2	16:5:103:BCL:H72	2.46	0.50
16:6:102:BCL:H101	16:7:102:BCL:H3A	1.92	0.50
16:L:302:BCL:H2	17:L:303:BPH:HBB3	1.93	0.50
3:M:7:ILE:HD11	20:M:402:CDL:H562	1.93	0.50
17:M:404:BPH:HHC	17:M:404:BPH:HBB3	1.92	0.50
16:2:101:BCL:H13	16:3:102:BCL:HBA2	1.93	0.50
1:C:142:TRP:CD1	1:C:280:MET:HG3	2.47	0.50
14:P:102:PGV:H142	14:P:103:PGV:H42	1.92	0.50
7:S:12:ARG:HD2	20:U:101:CDL:OB3	2.12	0.50
16:Z:102:BCL:H102	8:2:32:VAL:HG11	1.93	0.50
5:7:7:LEU:HD22	7:9:11:ARG:HD2	1.93	0.50
2:L:207:LYS:HG3	3:M:142:LEU:HD23	1.94	0.50
6:B:34:VAL:HG13	14:B:104:PGV:H251	1.93	0.50
14:X:103:PGV:H71	14:Z:101:PGV:H171	1.93	0.50
16:8:102:BCL:HBB2	14:0:101:PGV:H281	1.93	0.50
14:F:101:PGV:H101	7:I:30:PHE:HB3	1.94	0.49
5:Q:9:ASP:HB3	5:Q:12:ARG:HG3	1.93	0.49
6:V:46:TRP:CD2	16:V:102:BCL:H2C	2.47	0.49
5:Y:20:TRP:CD1	16:1:102:BCL:H93	2.46	0.49
7:5:18:HIS:HD2	16:5:103:BCL:H72	1.78	0.49
14:6:103:PGV:H221	6:8:39:LEU:HB3	1.94	0.49
14:6:103:PGV:H272	6:8:36:ALA:HB1	1.93	0.49
1:C:251:ASN:H	1:C:254:THR:HG23	1.77	0.49
2:L:212:GLU:HB3	18:L:304:UQ8:H4MB	1.93	0.49
4:H:278:LEU:HD13	5:7:12:ARG:HB3	1.94	0.49
5:Q:27:VAL:O	5:Q:31:ILE:HG13	2.12	0.49
7:1:4:MET:HE2	7:1:8:LEU:HG	1.95	0.49
4:H:142:PRO:HA	4:H:188:TRP:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:102:PGV:H162	14:T:103:PGV:H301	1.93	0.49
5:U:40:TRP:CD2	16:U:103:BCL:H2C	2.47	0.49
16:G:103:BCL:H13	16:I:103:BCL:C2B	2.43	0.49
16:G:103:BCL:H13	16:I:103:BCL:C3B	2.42	0.49
7:1:38:PHE:HZ	8:2:46:TRP:HA	1.78	0.49
5:U:29:HIS:CE1	16:V:102:BCL:HMD1	2.47	0.49
5:U:40:TRP:CE3	16:U:103:BCL:HAC2	2.47	0.49
6:8:41:TRP:CE2	14:8:103:PGV:H012	2.48	0.49
14:8:103:PGV:H71	14:8:103:PGV:H231	1.95	0.49
14:0:101:PGV:H011	14:0:101:PGV:H62	1.95	0.49
6:4:38:PHE:CE2	14:4:103:PGV:H212	2.47	0.49
22:4:101:CRT:H25	16:4:102:BCL:O1A	2.12	0.49
4:H:159:ARG:HD2	4:H:160:PHE:CZ	2.48	0.49
14:G:104:PGV:H141	14:G:105:PGV:H282	1.95	0.49
5:Q:7:LEU:HB3	7:S:11:ARG:HG2	1.94	0.49
14:L:305:PGV:H201	14:L:305:PGV:H31	1.95	0.49
4:H:121:ALA:HB2	4:H:264:GLY:HA3	1.94	0.49
7:5:35:THR:HA	15:5:102:LMT:H1B	1.95	0.49
1:C:67:SER:HB2	1:C:69:GLU:HG2	1.96	0.48
7:O:24:LEU:HA	16:O:104:BCL:H142	1.95	0.48
7:S:21:MET:HG3	16:S:102:BCL:HMA3	1.95	0.48
2:L:18:LEU:HB2	2:L:34:ILE:HG21	1.94	0.48
20:H:303:CDL:H772	20:H:303:CDL:H542	1.96	0.48
16:D:101:BCL:HMD3	8:E:37:HIS:CE1	2.48	0.48
5:3:32:LEU:HD11	16:4:102:BCL:HHD	1.94	0.48
9:a:99:TYR:HB3	9:a:105:MET:HG3	1.95	0.48
4:H:27:GLY:HA2	20:O:101:CDL:H202	1.94	0.48
14:R:103:PGV:H221	16:S:101:BCL:H3C	1.96	0.48
7:5:1:MET:HE1	16:7:102:BCL:H202	1.96	0.48
2:L:9:LYS:HE2	4:H:122:ALA:HB1	1.95	0.48
6:B:18:PHE:HB2	22:B:101:CRT:H31A	1.95	0.48
8:0:34:VAL:O	8:0:38:ILE:HG13	2.14	0.48
16:A:101:BCL:HMB2	16:0:102:BCL:H162	1.95	0.48
16:4:102:BCL:H142	8:6:29:TYR:HD1	1.78	0.48
2:L:239:ASN:HD22	2:L:243:TRP:NE1	2.12	0.48
15:M:411:LMT:O2B	15:M:411:LMT:H6E	2.14	0.48
16:P:101:BCL:HBB2	14:P:102:PGV:H291	1.95	0.48
5:7:10:PRO:HB3	6:8:18:PHE:CZ	2.49	0.48
4:H:114:MET:HE2	4:H:268:TYR:HB2	1.96	0.48
7:D:28:ILE:HD12	16:E:101:BCL:O1D	2.14	0.48
8:J:46:TRP:NE1	16:J:101:BCL:HHC	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:40:TRP:CE3	16:O:103:BCL:HBC2	2.48	0.48
5:3:9:ASP:HB3	5:3:12:ARG:HG3	1.96	0.48
2:L:36:GLY:HA2	2:L:39:THR:HG22	1.95	0.48
2:L:212:GLU:OE2	3:M:235:ILE:HG13	2.14	0.48
16:L:312:BCL:H162	22:M:406:CRT:H133	1.95	0.48
22:4:101:CRT:H342	16:5:103:BCL:HBA2	1.96	0.48
4:H:34:MET:HE1	15:H:305:LMT:O4'	2.14	0.48
6:B:41:TRP:CZ2	14:B:104:PGV:H02	2.48	0.48
7:I:22:ALA:HA	16:I:102:BCL:H43	1.95	0.48
5:3:6:LYS:O	6:4:7:LEU:HD22	2.14	0.48
1:C:152:THR:HG22	1:C:154:TYR:N	2.22	0.47
1:C:167:TRP:HD1	1:C:311:GLN:HG2	1.79	0.47
8:J:46:TRP:CE2	16:J:101:BCL:H2C	2.49	0.47
6:G:43:TRP:HB2	14:G:101:PGV:H201	1.95	0.47
5:K:20:TRP:HB2	16:O:103:BCL:H151	1.95	0.47
22:R:101:CRT:H292	16:S:102:BCL:HBB3	1.96	0.47
16:1:102:BCL:HMD3	8:2:37:HIS:CE1	2.49	0.47
8:0:39:LEU:HB3	14:0:101:PGV:H212	1.96	0.47
2:L:191:GLY:O	2:L:195:LEU:HG	2.14	0.47
2:L:269:VAL:HG12	2:L:271:ILE:H	1.78	0.47
16:B:102:BCL:H93	16:B:102:BCL:H61	1.67	0.47
16:R:102:BCL:H203	8:T:25:ALA:HA	1.96	0.47
7:S:16:LEU:HD23	20:U:101:CDL:H512	1.95	0.47
3:M:233:ARG:O	3:M:236:GLU:HG2	2.15	0.47
3:M:287:THR:HB	3:M:294:TRP:NE1	2.23	0.47
4:H:10:TYR:CE2	14:F:101:PGV:H61	2.50	0.47
3:M:197:TYR:CE1	16:M:403:BCL:HMC2	2.49	0.47
5:A:29:HIS:CE1	16:B:102:BCL:HMD1	2.49	0.47
16:B:102:BCL:H162	16:B:102:BCL:H141	1.64	0.47
22:G:102:CRT:H292	16:I:103:BCL:HBB3	1.96	0.47
22:V:101:CRT:H35	16:W:101:BCL:HMB2	1.96	0.47
1:C:184:MET:HG3	3:M:96:GLU:HG2	1.97	0.47
1:C:241:MET:HB3	10:C:403:HEC:C4B	2.45	0.47
2:L:91:VAL:HG12	18:L:306:UQ8:H8	1.97	0.47
14:L:309:PGV:H21	5:F:31:ILE:HG13	1.95	0.47
3:M:3:GLU:HG2	3:M:228:ARG:NH2	2.30	0.47
16:F:103:BCL:H203	6:G:21:ILE:HG23	1.95	0.47
6:G:17:GLU:HG2	22:G:102:CRT:H22A	1.96	0.47
16:G:103:BCL:H141	8:J:29:TYR:CD1	2.50	0.47
20:U:101:CDL:OB3	20:U:101:CDL:HB62	2.15	0.47
14:V:103:PGV:H272	14:V:103:PGV:H72	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:2:TRP:HZ3	5:3:6:LYS:HD2	1.80	0.47
5:7:29:HIS:CE1	16:8:102:BCL:HMD1	2.49	0.47
7:9:40:TRP:CE3	16:9:101:BCL:HBC3	2.49	0.47
3:M:10:ARG:HD3	20:M:408:CDL:H1	1.96	0.47
5:F:25:ALA:HB2	16:G:103:BCL:HED2	1.95	0.47
22:N:102:CRT:H35	16:O:103:BCL:CMB	2.44	0.47
2:L:94:LEU:HG	2:L:128:TYR:HE2	1.79	0.47
14:2:102:PGV:H152	14:2:103:PGV:H22	1.97	0.47
22:N:102:CRT:H372	7:O:29:HIS:CG	2.50	0.47
7:W:12:ARG:HG3	7:W:13:THR:N	2.29	0.47
16:W:101:BCL:H62	16:W:101:BCL:H41	1.53	0.47
5:Y:7:LEU:HD21	8:2:18:PHE:CE1	2.50	0.47
6:Z:38:PHE:CE1	14:Z:104:PGV:H261	2.50	0.47
2:L:3:MET:HB3	2:L:7:GLU:HB3	1.96	0.46
20:M:409:CDL:OA4	5:Y:12:ARG:HD3	2.15	0.46
4:H:62:PRO:HB3	15:H:305:LMT:H6E	1.96	0.46
15:H:305:LMT:H3'	7:I:16:LEU:HD21	1.96	0.46
6:B:47:ILE:HG13	14:B:104:PGV:H31	1.97	0.46
7:I:20:GLY:HA3	16:I:103:BCL:H101	1.95	0.46
5:K:29:HIS:CE1	16:N:103:BCL:HMD1	2.51	0.46
14:4:103:PGV:H232	14:4:103:PGV:H261	1.71	0.46
16:5:104:BCL:H143	16:5:104:BCL:H161	1.75	0.46
9:a:47:TRP:HB2	9:a:110:LEU:HD11	1.96	0.46
16:L:311:BCL:HMD2	3:M:206:ILE:HD13	1.96	0.46
3:M:4:TYR:CE1	20:M:408:CDL:HA21	2.50	0.46
17:M:404:BPH:H3A	17:M:404:BPH:HBA2	1.70	0.46
7:D:22:ALA:HA	16:D:101:BCL:H43	1.96	0.46
6:N:24:GLN:O	6:N:28:ILE:HG12	2.15	0.46
7:S:29:HIS:CE1	16:T:101:BCL:HMD1	2.50	0.46
22:V:101:CRT:H20	22:V:101:CRT:H181	1.77	0.46
1:C:163:PRO:HD2	10:C:402:HEC:HBD1	1.96	0.46
16:A:101:BCL:H143	16:O:102:BCL:H122	1.96	0.46
7:D:1:MET:HE2	16:F:103:BCL:H143	1.96	0.46
7:I:28:ILE:HD12	16:J:101:BCL:O1D	2.16	0.46
14:X:103:PGV:H231	14:X:103:PGV:H72	1.97	0.46
16:Z:102:BCL:H192	16:Z:102:BCL:H162	1.74	0.46
6:8:41:TRP:NE1	14:8:103:PGV:H061	2.28	0.46
2:L:239:ASN:HD22	2:L:243:TRP:HE1	1.61	0.46
4:H:30:VAL:O	4:H:34:MET:HG3	2.15	0.46
15:H:305:LMT:H6'1	15:I:101:LMT:H3'	1.96	0.46
6:N:30:THR:O	6:N:34:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:6:101:PGV:H51	14:6:101:PGV:H82	1.76	0.46
15:O:102:LMT:H6D	15:Q:101:LMT:H11	1.97	0.46
16:1:102:BCL:H41	16:1:102:BCL:H61	1.50	0.46
1:C:237:SER:O	1:C:241:MET:HG2	2.16	0.46
1:C:345:PHE:CD1	1:C:345:PHE:C	2.94	0.46
3:M:148:TRP:HB3	20:M:407:CDL:H732	1.97	0.46
14:1:101:PGV:H32	5:3:33:LEU:HD13	1.96	0.46
7:5:19:VAL:O	7:5:23:VAL:HG23	2.16	0.46
1:C:251:ASN:H	1:C:254:THR:CG2	2.28	0.46
2:L:202:LYS:HB2	2:L:202:LYS:HE2	1.78	0.46
5:7:40:TRP:CD1	5:7:41:VAL:HG13	2.51	0.46
2:L:60:ASN:O	2:L:64:ILE:HG13	2.16	0.46
6:R:37:HIS:HB3	14:R:104:PGV:H232	1.98	0.46
1:C:210:HIS:HB2	1:C:349:GLY:HA3	1.96	0.46
22:V:101:CRT:H372	7:W:29:HIS:CD2	2.51	0.46
16:Y:402:BCL:H41	16:Y:402:BCL:H62	1.59	0.46
16:1:103:BCL:O1A	8:2:26:PHE:HD1	1.99	0.46
6:B:47:ILE:HD12	14:B:103:PGV:H221	1.98	0.45
22:Y:403:CRT:H20	22:Y:403:CRT:H181	1.82	0.45
5:Q:40:TRP:CE3	16:Q:102:BCL:HBC2	2.50	0.45
7:9:28:ILE:HD12	16:O:102:BCL:O1D	2.16	0.45
8:0:41:TRP:CH2	14:O:104:PGV:H41	2.51	0.45
4:H:246:GLU:OE1	4:H:249:ARG:HD3	2.16	0.45
20:H:303:CDL:H792	20:H:303:CDL:H821	1.82	0.45
22:G:102:CRT:H20	22:G:102:CRT:H181	1.75	0.45
5:Q:30:PHE:CD2	15:Q:101:LMT:H72	2.51	0.45
7:S:24:LEU:HD22	16:T:101:BCL:H102	1.98	0.45
2:L:44:VAL:HG22	21:M:405:MQ8:H421	1.98	0.45
2:L:153:HIS:O	2:L:157:VAL:HG23	2.17	0.45
16:Q:102:BCL:H61	16:Q:102:BCL:H41	1.77	0.45
14:R:104:PGV:H241	14:R:104:PGV:H272	1.89	0.45
16:Y:401:BCL:H52	16:Y:401:BCL:CHC	2.46	0.45
15:L:308:LMT:H82	5:7:27:VAL:HG21	1.97	0.45
21:M:405:MQ8:H352	21:M:405:MQ8:H312	1.72	0.45
6:R:46:TRP:CE2	16:R:102:BCL:H2C	2.52	0.45
22:R:101:CRT:H372	7:S:29:HIS:CG	2.52	0.45
1:C:77:TYR:HB3	10:C:401:HEC:CGA	2.47	0.45
16:B:102:BCL:H13	16:D:102:BCL:C4B	2.47	0.45
14:G:104:PGV:H012	8:J:43:TRP:CD1	2.50	0.45
4:H:121:ALA:HA	4:H:260:GLY:O	2.17	0.45
4:H:171:TYR:CZ	4:H:226:SER:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:234:THR:HG22	4:H:236:GLN:H	1.82	0.45
7:D:40:TRP:CE3	16:D:101:BCL:HBC2	2.52	0.45
16:T:101:BCL:H61	16:T:101:BCL:H2	1.65	0.45
7:W:18:HIS:CD2	16:W:101:BCL:H51	2.51	0.45
7:1:35:THR:HA	14:1:101:PGV:H031	1.98	0.45
5:3:22:ALA:HA	16:3:102:BCL:H12	1.98	0.45
9:a:60:ILE:O	9:a:117:CYS:HB2	2.17	0.45
1:C:66:VAL:HG13	1:C:93:ARG:HD2	1.99	0.45
1:C:108:CYS:SG	10:C:401:HEC:HBB1	2.55	0.45
14:N:101:PGV:H102	14:N:101:PGV:H131	1.71	0.45
16:S:101:BCL:H61	16:S:101:BCL:H41	1.57	0.45
16:9:102:BCL:H141	16:9:102:BCL:H162	1.78	0.45
8:0:47:ILE:HD12	14:0:103:PGV:H201	1.97	0.45
1:C:70:GLY:HA3	9:a:55:PRO:HB2	1.99	0.45
14:C:408:PGV:H21	5:3:31:ILE:HG12	1.99	0.45
3:M:62:LEU:HD22	16:S:102:BCL:H171	1.99	0.45
5:7:5:TRP:CD1	6:8:19:HIS:HB2	2.52	0.45
16:V:102:BCL:HMB3	14:X:101:PGV:H271	1.99	0.45
8:X:41:TRP:HE1	14:X:103:PGV:H062	1.81	0.45
14:X:103:PGV:H332	14:Z:101:PGV:H142	1.99	0.45
16:A:101:BCL:H152	6:B:28:ILE:HD13	1.98	0.44
7:S:1:MET:HA	7:S:1:MET:HE2	1.99	0.44
3:M:153:ALA:HB2	17:M:404:BPH:HAC1	1.99	0.44
5:A:35:THR:HG21	7:D:41:LEU:HB3	2.00	0.44
7:D:24:LEU:HB2	16:D:102:BCL:H13	1.99	0.44
8:E:46:TRP:CE2	16:E:101:BCL:H2C	2.53	0.44
15:I:101:LMT:H4'	5:K:11:ARG:NH2	2.33	0.44
14:P:102:PGV:H12	14:P:102:PGV:H151	1.63	0.44
5:Q:30:PHE:HD2	15:Q:101:LMT:H72	1.80	0.44
6:R:53:TYR:CE2	7:S:43:GLY:HA3	2.52	0.44
5:U:15:ILE:HD11	20:U:101:CDL:OB6	2.17	0.44
16:L:312:BCL:H91	16:L:312:BCL:H112	1.75	0.44
3:M:82:SER:HB3	3:M:85:GLU:HB3	2.00	0.44
7:W:23:VAL:HG11	16:W:102:BCL:H161	1.98	0.44
5:3:32:LEU:HD13	16:3:102:BCL:HBC1	2.00	0.44
6:8:18:PHE:HB2	22:8:101:CRT:H31A	2.00	0.44
14:8:103:PGV:H91	14:8:103:PGV:H62	1.68	0.44
14:0:104:PGV:H281	14:0:104:PGV:H252	1.78	0.44
1:C:44:GLU:N	1:C:253:THR:HG21	2.31	0.44
2:L:224:ILE:HG12	2:L:228:GLY:HA3	1.98	0.44
14:L:305:PGV:H21	14:L:309:PGV:H011	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:402:CDL:H422	20:M:402:CDL:H391	1.87	0.44
5:U:23:VAL:HG21	16:W:101:BCL:H193	2.00	0.44
5:Y:40:TRP:CD2	16:Y:402:BCL:H2C	2.53	0.44
22:Y:403:CRT:H22A	6:Z:17:GLU:HG2	2.00	0.44
1:C:108:CYS:HB3	10:C:401:HEC:C4B	2.46	0.44
1:C:110:TYR:CE1	9:a:131:PRO:HA	2.53	0.44
17:L:303:BPH:H202	16:L:311:BCL:C1B	2.47	0.44
14:L:310:PGV:H82	14:1:101:PGV:H252	1.98	0.44
3:M:106:LEU:HD21	22:M:406:CRT:H2M1	1.99	0.44
20:M:407:CDL:H182	4:H:27:GLY:HA3	1.98	0.44
15:M:411:LMT:H71	5:Y:19:SER:OG	2.17	0.44
15:I:101:LMT:H2'	16:I:103:BCL:H202	2.00	0.44
6:Z:46:TRP:HZ2	14:Z:104:PGV:H81	1.83	0.44
3:M:63:PHE:CZ	3:M:124:LEU:HD23	2.53	0.44
15:H:306:LMT:H71	15:H:306:LMT:H102	1.88	0.44
6:R:37:HIS:CD2	14:R:104:PGV:H131	2.52	0.44
14:T:102:PGV:H131	14:T:102:PGV:H102	1.79	0.44
5:U:12:ARG:HG3	20:U:101:CDL:HA32	1.99	0.44
6:Z:39:LEU:HD22	14:Z:101:PGV:H132	1.99	0.44
16:1:102:BCL:HBC3	16:1:102:BCL:H2C	1.80	0.44
8:6:46:TRP:CD2	16:6:102:BCL:H2C	2.51	0.44
18:L:304:UQ8:H7	18:L:304:UQ8:H10	1.55	0.44
16:G:103:BCL:H143	16:G:103:BCL:H111	1.68	0.44
16:U:103:BCL:H151	16:U:103:BCL:H18	1.79	0.44
5:Y:29:HIS:CE1	16:Z:102:BCL:HMD1	2.53	0.44
7:1:32:LEU:HD11	16:2:101:BCL:HHD	1.99	0.44
2:L:174:MET:SD	16:L:312:BCL:HED3	2.58	0.44
18:L:306:UQ8:H20	18:L:306:UQ8:H17A	1.68	0.44
22:4:101:CRT:H20	22:4:101:CRT:H181	1.80	0.44
1:C:50:ARG:HB3	15:5:101:LMT:H6'1	1.98	0.44
1:C:358:ASP:OD1	1:C:359:ARG:HD2	2.18	0.44
4:H:179:LYS:HE3	4:H:206:VAL:HG12	1.98	0.44
5:F:29:HIS:CE1	16:G:103:BCL:HMD1	2.53	0.44
16:I:102:BCL:H41	16:I:102:BCL:H61	1.38	0.44
16:Q:102:BCL:H162	16:Q:102:BCL:H141	1.74	0.44
7:S:28:ILE:HD12	16:T:101:BCL:O1D	2.18	0.44
14:T:103:PGV:H231	14:T:103:PGV:H202	1.81	0.44
7:W:2:TRP:CE2	8:X:16:LYS:HE2	2.53	0.44
2:L:161:GLY:HA3	16:L:302:BCL:HAC1	2.00	0.43
16:L:311:BCL:H3A	16:L:311:BCL:HBA2	1.72	0.43
4:H:152:GLY:HA2	4:H:165:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:302:PGV:H05	14:F:101:PGV:H232	1.99	0.43
5:A:1:MET:HE3	16:B:102:BCL:H202	1.99	0.43
15:F:102:LMT:H42	16:I:102:BCL:H143	1.99	0.43
8:X:18:PHE:HA	8:X:21:MET:HE2	2.00	0.43
3:M:228:ARG:HB3	4:H:219:PHE:CE2	2.54	0.43
14:P:102:PGV:H242	16:Q:102:BCL:H3C	2.00	0.43
7:W:24:LEU:HD21	16:X:102:BCL:H121	2.00	0.43
16:W:102:BCL:H52	16:W:102:BCL:H8	1.48	0.43
16:1:103:BCL:H162	16:1:103:BCL:H141	1.59	0.43
16:9:101:BCL:H61	16:9:101:BCL:H41	1.44	0.43
8:0:41:TRP:CZ2	14:0:104:PGV:H02	2.53	0.43
1:C:116:ASP:OD2	1:C:119:SER:HB2	2.18	0.43
1:C:222:PRO:HA	3:M:292:GLU:HB2	2.01	0.43
3:M:38:TRP:CH2	4:H:164:ILE:HD12	2.53	0.43
22:M:406:CRT:H20	22:M:406:CRT:H181	1.71	0.43
4:H:139:LYS:HE2	4:H:190:ASP:OD1	2.18	0.43
16:K:101:BCL:H141	16:K:101:BCL:H161	1.78	0.43
7:O:29:HIS:CE1	16:P:101:BCL:HMD1	2.52	0.43
14:Z:103:PGV:H251	14:Z:104:PGV:H42	2.00	0.43
14:Z:104:PGV:H272	14:Z:104:PGV:H241	1.82	0.43
14:2:102:PGV:H62	14:2:102:PGV:H91	1.73	0.43
7:9:29:HIS:CE1	16:0:102:BCL:HMD1	2.54	0.43
8:0:11:SER:OG	8:0:14:GLU:HG2	2.18	0.43
9:a:53:ASP:O	9:a:58:LYS:HE2	2.19	0.43
1:C:252:CYS:HB2	2:L:162:TYR:HB3	1.99	0.43
13:C:407:PLM:H42	14:L:310:PGV:H41	2.00	0.43
13:C:407:PLM:H62	14:L:310:PGV:H61	2.00	0.43
3:M:283:GLY:O	3:M:287:THR:HG22	2.19	0.43
16:S:101:BCL:H41	16:S:101:BCL:H102	1.99	0.43
2:L:180:PHE:O	2:L:184:THR:HG22	2.18	0.43
14:B:103:PGV:H242	14:B:103:PGV:H211	1.69	0.43
6:G:17:GLU:O	6:G:21:ILE:HG13	2.18	0.43
14:G:105:PGV:H102	14:G:105:PGV:H251	2.00	0.43
7:S:40:TRP:CE3	16:S:101:BCL:HBC3	2.53	0.43
16:2:101:BCL:H91	16:2:101:BCL:H112	1.70	0.43
14:2:102:PGV:H131	14:2:102:PGV:H102	1.71	0.43
5:3:29:HIS:NE2	16:3:102:BCL:NB	2.65	0.43
6:4:22:PHE:CD1	22:4:101:CRT:H14	2.54	0.43
22:4:101:CRT:H241	16:5:103:BCL:H91	2.01	0.43
7:5:34:SER:HB2	15:5:102:LMT:H6D	1.99	0.43
9:a:87:LEU:HB3	9:a:101:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:302:PGV:H262	20:H:303:CDL:H842	2.00	0.43
6:B:22:PHE:CD2	22:B:101:CRT:H14	2.54	0.43
5:F:23:VAL:O	5:F:27:VAL:HG23	2.19	0.43
22:N:102:CRT:H35	16:O:103:BCL:C2B	2.49	0.43
16:N:103:BCL:H192	16:N:103:BCL:H161	1.74	0.43
14:P:102:PGV:H32	14:P:103:PGV:O13	2.19	0.43
16:V:102:BCL:H142	16:V:102:BCL:H112	1.82	0.43
4:H:61:PHE:CD2	20:H:301:CDL:H162	2.54	0.43
6:G:34:VAL:HG22	14:G:105:PGV:H141	2.00	0.43
14:R:103:PGV:H131	14:R:103:PGV:H102	1.64	0.43
16:S:101:BCL:H61	16:S:101:BCL:H102	1.41	0.43
7:1:21:MET:HE2	7:1:21:MET:HA	2.00	0.43
9:a:141:ARG:HA	9:a:141:ARG:NE	2.34	0.43
2:L:43:ALA:HB1	17:L:303:BPH:H4C2	2.01	0.43
22:M:406:CRT:H10	22:M:406:CRT:H81	1.77	0.43
6:B:46:TRP:CE2	16:B:102:BCL:H2C	2.54	0.43
16:R:102:BCL:H13	16:S:102:BCL:C3B	2.49	0.43
14:L:310:PGV:H81	14:1:101:PGV:H11	2.00	0.43
4:H:208:SER:OG	4:H:211:ASP:HB2	2.19	0.43
1:C:150:GLY:HA3	1:C:329:VAL:HG21	2.01	0.43
2:L:76:ALA:HA	15:L:308:LMT:H3'	2.01	0.43
5:7:5:TRP:O	6:8:10:LEU:HD12	2.19	0.43
3:M:291:VAL:HG21	3:M:294:TRP:CH2	2.53	0.42
6:N:36:ALA:HB1	14:N:101:PGV:H292	2.01	0.42
14:N:101:PGV:H252	14:N:101:PGV:H282	1.93	0.42
16:R:102:BCL:H61	16:R:102:BCL:H41	1.45	0.42
16:5:103:BCL:HBA1	16:5:103:BCL:H3A	1.63	0.42
13:C:407:PLM:H72	2:L:262:TRP:CZ2	2.54	0.42
16:M:403:BCL:H192	16:M:403:BCL:H162	1.92	0.42
6:G:46:TRP:CE2	16:G:103:BCL:H2C	2.54	0.42
22:N:102:CRT:H20	22:N:102:CRT:H181	1.85	0.42
5:7:33:LEU:O	15:7:101:LMT:H6E	2.18	0.42
14:L:309:PGV:H012	14:H:302:PGV:H061	2.02	0.42
3:M:134:TYR:CZ	3:M:144:THR:HG21	2.54	0.42
16:M:403:BCL:H202	22:M:406:CRT:H16	2.01	0.42
7:D:4:MET:HE3	7:D:4:MET:HA	2.02	0.42
16:S:102:BCL:H161	16:S:102:BCL:H193	1.76	0.42
7:W:40:TRP:CZ3	16:W:101:BCL:HBC3	2.55	0.42
8:6:39:LEU:HB3	14:6:101:PGV:H211	2.01	0.42
16:6:102:BCL:H8	16:6:102:BCL:H51	1.88	0.42
1:C:344:ASP:C	1:C:346:LEU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:137:LEU:HD23	2:L:137:LEU:HA	1.77	0.42
3:M:177:PHE:CE1	22:M:406:CRT:H25	2.54	0.42
14:M:410:PGV:H252	14:M:410:PGV:H52	2.01	0.42
20:H:301:CDL:HB32	7:D:12:ARG:HB2	2.00	0.42
14:F:101:PGV:H262	14:F:101:PGV:H291	1.69	0.42
14:G:101:PGV:H201	14:G:101:PGV:H232	1.65	0.42
8:2:46:TRP:CE2	16:2:101:BCL:H2C	2.55	0.42
8:2:51:GLU:H	8:2:51:GLU:CD	2.28	0.42
7:5:28:ILE:HD12	16:6:102:BCL:O1D	2.19	0.42
16:5:104:BCL:H161	5:7:26:LEU:HD11	2.01	0.42
1:C:221:LEU:HB2	4:H:2:GLU:O	2.20	0.42
4:H:188:TRP:HB2	4:H:198:TYR:HB2	2.02	0.42
7:O:21:MET:SD	16:O:104:BCL:H2	2.59	0.42
14:P:102:PGV:H82	14:P:102:PGV:H52	1.79	0.42
6:R:18:PHE:HD1	22:R:101:CRT:H33	1.84	0.42
22:V:101:CRT:H10	22:V:101:CRT:H81	1.85	0.42
8:0:26:PHE:O	8:0:30:ILE:HB	2.19	0.42
3:M:4:TYR:HE1	20:M:408:CDL:HA21	1.83	0.42
14:F:101:PGV:H322	14:F:101:PGV:H292	1.86	0.42
16:N:103:BCL:H161	16:N:103:BCL:H141	1.78	0.42
22:R:101:CRT:H10	22:R:101:CRT:H81	1.88	0.42
8:X:41:TRP:CD1	14:X:103:PGV:H202	2.55	0.42
7:5:21:MET:SD	16:5:104:BCL:H72	2.59	0.42
15:5:102:LMT:H3B	5:7:42:GLY:HA2	2.01	0.42
17:M:404:BPH:H4C1	17:M:404:BPH:H6C1	1.73	0.42
4:H:216:PRO:HB2	4:H:219:PHE:HD2	1.84	0.42
6:B:53:TYR:CD2	7:D:43:GLY:HA3	2.55	0.42
16:I:102:BCL:H8	16:I:102:BCL:H122	1.87	0.42
5:K:1:MET:HE3	5:K:4:LEU:HB2	2.01	0.42
16:N:103:BCL:H93	16:N:103:BCL:H111	1.76	0.42
8:T:48:PRO:HG3	5:U:43:GLY:HA2	2.00	0.42
16:3:102:BCL:HBC2	6:4:43:TRP:HZ3	1.84	0.42
7:9:22:ALA:HA	16:9:101:BCL:H43	2.01	0.42
1:C:215:VAL:O	3:M:192:ARG:HD2	2.20	0.42
4:H:38:ARG:NH2	4:H:68:LYS:HB2	2.34	0.42
4:H:59:LEU:HB2	5:F:12:ARG:NH1	2.35	0.42
16:A:101:BCL:H41	16:A:101:BCL:H61	1.83	0.42
15:F:102:LMT:H2B	7:I:11:ARG:HD2	2.02	0.42
5:K:40:TRP:CD2	16:K:101:BCL:H2C	2.55	0.42
16:N:103:BCL:H111	16:N:103:BCL:H142	1.69	0.42
16:O:103:BCL:H72	16:O:103:BCL:H112	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:102:PGV:H241	14:P:102:PGV:H272	1.80	0.42
14:T:102:PGV:H171	14:T:103:PGV:H42	2.02	0.42
5:7:21:LEU:HD22	16:8:102:BCL:HED1	2.02	0.42
2:L:135:ARG:O	2:L:139:MET:HG3	2.20	0.42
18:L:304:UQ8:H21A	18:L:304:UQ8:H17	1.82	0.42
4:H:214:LEU:HB2	4:H:258:ILE:HD13	2.01	0.42
5:A:7:LEU:HD13	7:D:11:ARG:HG3	2.01	0.42
5:A:24:LEU:HD23	16:B:102:BCL:HED3	2.02	0.42
16:S:101:BCL:HAC2	16:S:101:BCL:HHD	1.87	0.42
2:L:87:GLN:O	2:L:91:VAL:HG13	2.19	0.42
18:L:304:UQ8:H15	18:L:304:UQ8:H12	1.75	0.42
3:M:149:ALA:HB2	3:M:270:TYR:CE1	2.55	0.42
16:D:102:BCL:H142	16:D:102:BCL:H112	1.73	0.42
16:I:103:BCL:H141	16:I:103:BCL:H162	1.74	0.42
16:O:104:BCL:HHD	16:O:104:BCL:HAC2	1.77	0.42
6:4:48:PRO:HG3	7:5:43:GLY:HA2	2.02	0.42
7:5:31:ILE:O	7:5:35:THR:HG23	2.20	0.42
2:L:185:LEU:HD13	17:M:404:BPH:ND	2.35	0.41
3:M:130:PHE:CE1	3:M:151:ALA:HB2	2.55	0.41
20:H:303:CDL:H511	20:H:303:CDL:H741	2.02	0.41
16:N:103:BCL:H112	16:O:104:BCL:C3B	2.50	0.41
8:P:47:ILE:HD13	8:P:47:ILE:HA	1.90	0.41
7:W:28:ILE:HD12	16:X:102:BCL:O1D	2.20	0.41
22:Y:403:CRT:H392	7:1:29:HIS:HB3	2.02	0.41
8:2:41:TRP:CZ2	8:2:45:PRO:HB3	2.55	0.41
5:3:6:LYS:HE2	5:3:6:LYS:HB3	1.91	0.41
5:3:15:ILE:HD13	5:3:15:ILE:HA	1.87	0.41
20:H:301:CDL:H141	20:H:303:CDL:HB4	2.01	0.41
16:Q:102:BCL:H152	16:Q:102:BCL:H112	1.96	0.41
14:T:103:PGV:H72	14:T:103:PGV:H101	1.75	0.41
7:1:6:LYS:HE2	22:4:101:CRT:H1M1	2.01	0.41
9:a:68:ASP:OD1	9:a:68:ASP:C	2.63	0.41
1:C:183:THR:HB	1:C:186:GLN:O	2.20	0.41
13:C:407:PLM:HA2	14:L:310:PGV:H131	2.03	0.41
3:M:291:VAL:HG11	3:M:294:TRP:CE3	2.56	0.41
4:H:1:MET:HE3	4:H:12:ASN:HB3	2.02	0.41
20:H:301:CDL:H161	20:H:303:CDL:OB7	2.21	0.41
14:H:304:PGV:H042	5:K:36:ASP:OD2	2.21	0.41
7:D:24:LEU:HD23	16:E:101:BCL:HED3	2.02	0.41
16:P:101:BCL:H13	16:P:101:BCL:H102	1.83	0.41
16:3:102:BCL:H162	16:3:102:BCL:H192	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:117:CYS:SG	9:a:119:ALA:HB3	2.60	0.41
14:L:305:PGV:H291	14:L:305:PGV:H262	1.81	0.41
16:L:312:BCL:HBB1	3:M:157:PHE:CE1	2.56	0.41
6:B:48:PRO:HG3	7:D:43:GLY:HA2	2.03	0.41
7:1:40:TRP:CE3	16:1:102:BCL:HBC3	2.56	0.41
16:8:102:BCL:C3B	14:8:103:PGV:H82	2.50	0.41
9:a:94:ASP:OD2	9:a:97:HIS:HB2	2.20	0.41
2:L:197:VAL:HG13	2:L:207:LYS:HB2	2.03	0.41
5:F:4:LEU:HA	5:F:4:LEU:HD23	1.77	0.41
7:I:13:THR:HG23	16:I:103:BCL:H141	2.00	0.41
22:Y:403:CRT:H35	16:1:102:BCL:HMB1	2.02	0.41
16:7:102:BCL:H62	16:7:102:BCL:H41	1.62	0.41
4:H:30:VAL:HG11	15:H:305:LMT:O3'	2.20	0.41
6:N:17:GLU:HB3	22:N:102:CRT:H22A	2.01	0.41
7:1:31:ILE:HG12	14:1:101:PGV:H51	2.01	0.41
14:6:104:PGV:H281	14:6:104:PGV:H241	2.03	0.41
14:M:410:PGV:H282	14:M:410:PGV:H312	1.85	0.41
14:F:101:PGV:H211	7:I:30:PHE:HE1	1.85	0.41
7:I:29:HIS:CE1	16:J:101:BCL:HMD1	2.55	0.41
8:J:37:HIS:ND1	14:J:102:PGV:H132	2.36	0.41
8:P:46:TRP:CE3	16:P:101:BCL:HAC2	2.56	0.41
7:S:40:TRP:CZ2	16:S:101:BCL:HHC	2.56	0.41
16:U:103:BCL:H141	16:U:103:BCL:H162	1.90	0.41
15:5:101:LMT:H121	15:5:101:LMT:H92	1.86	0.41
15:7:101:LMT:H2'	15:7:101:LMT:H11	1.75	0.41
6:8:10:LEU:HA	6:8:10:LEU:HD23	1.80	0.41
10:C:403:HEC:HBB1	2:L:165:LEU:HD22	2.02	0.41
8:J:41:TRP:CH2	14:J:102:PGV:H32	2.55	0.41
16:V:102:BCL:HBB3	16:W:101:BCL:C1C	2.51	0.41
14:0:103:PGV:H51	14:0:103:PGV:H011	2.03	0.41
1:C:268:PRO:O	3:M:314:ALA:HB2	2.21	0.41
16:M:403:BCL:HAA2	16:M:403:BCL:HBD	2.02	0.41
14:M:410:PGV:H242	7:O:30:PHE:HB3	2.01	0.41
4:H:101:PRO:HG3	6:B:9:GLY:HA3	2.03	0.41
4:H:157:VAL:HG12	4:H:165:ASP:HB2	2.02	0.41
22:B:101:CRT:H372	7:D:29:HIS:CD2	2.56	0.41
14:B:103:PGV:H201	8:E:43:TRP:HB2	2.03	0.41
7:I:2:TRP:CE2	8:J:16:LYS:HE3	2.55	0.41
5:Q:17:ILE:HA	16:S:101:BCL:H91	2.02	0.41
6:R:22:PHE:CD2	22:R:101:CRT:H14	2.55	0.41
16:Y:401:BCL:H162	16:Y:401:BCL:H202	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:403:CRT:H372	7:1:29:HIS:CD2	2.56	0.41
7:1:24:LEU:HD22	16:2:101:BCL:H112	2.03	0.41
14:1:101:PGV:H202	14:1:101:PGV:H52	2.02	0.41
14:2:102:PGV:H232	6:4:40:ALA:HA	2.02	0.41
7:5:6:LYS:HE2	7:5:6:LYS:HB3	1.86	0.41
8:6:30:ILE:HA	8:6:30:ILE:HD13	1.83	0.41
16:8:102:BCL:H121	16:9:102:BCL:C3B	2.50	0.41
3:M:126:VAL:HG12	16:M:403:BCL:H142	2.03	0.41
14:M:410:PGV:H211	14:H:304:PGV:H21	2.02	0.41
3:M:35:THR:HB	20:U:102:CDL:HB62	2.03	0.40
3:M:197:TYR:CZ	16:M:403:BCL:HMC2	2.56	0.40
22:M:406:CRT:H403	22:M:406:CRT:H36	1.87	0.40
5:K:9:ASP:HB3	5:K:12:ARG:HB2	2.02	0.40
14:Z:103:PGV:H201	14:Z:103:PGV:H42	2.03	0.40
22:4:101:CRT:H26	16:5:103:BCL:H91	2.02	0.40
14:4:103:PGV:H261	14:4:103:PGV:H291	1.84	0.40
16:9:102:BCL:H62	16:9:102:BCL:H41	1.76	0.40
1:C:36:LYS:HD3	1:C:45:GLU:OE1	2.21	0.40
7:I:17:ALA:HA	16:I:103:BCL:H112	2.02	0.40
5:K:40:TRP:CE3	16:K:101:BCL:HAC2	2.56	0.40
6:N:26:PHE:HD2	6:N:27:LEU:HD22	1.87	0.40
14:N:101:PGV:H262	14:N:101:PGV:H232	1.85	0.40
7:O:15:VAL:HG11	20:O:101:CDL:HB32	2.03	0.40
7:O:28:ILE:HD12	16:P:101:BCL:O1D	2.21	0.40
14:T:102:PGV:H142	14:T:103:PGV:H301	2.03	0.40
22:8:101:CRT:H402	16:9:101:BCL:HBB2	2.03	0.40
1:C:62:ALA:HA	1:C:332:TYR:OH	2.22	0.40
1:C:134:MET:HE2	1:C:134:MET:HB3	1.99	0.40
16:L:312:BCL:HBC3	16:L:312:BCL:H2C	1.92	0.40
4:H:22:TRP:CZ2	14:H:302:PGV:H232	2.55	0.40
6:B:41:TRP:CZ2	6:B:45:PRO:HB3	2.56	0.40
22:G:102:CRT:H36	22:G:102:CRT:H341	1.95	0.40
16:I:102:BCL:HED2	8:J:33:ALA:HB2	2.04	0.40
8:T:10:VAL:O	8:T:14:GLU:HB3	2.21	0.40
8:X:23:SER:O	8:X:27:THR:HG22	2.21	0.40
14:8:103:PGV:H202	14:8:103:PGV:H232	1.74	0.40
9:a:50:ILE:HD11	9:a:56:GLU:HG3	2.02	0.40
6:G:43:TRP:HD1	14:G:101:PGV:H012	1.85	0.40
16:I:103:BCL:H162	16:I:103:BCL:H192	1.73	0.40
6:N:39:LEU:O	14:N:101:PGV:H221	2.22	0.40
14:T:102:PGV:H31	14:T:102:PGV:H61	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:41:TRP:NE1	14:8:103:PGV:H012	2.36	0.40
22:8:101:CRT:H392	7:9:29:HIS:HB3	2.02	0.40
7:9:38:PHE:HZ	8:0:46:TRP:HA	1.86	0.40
16:0:102:BCL:H92	16:0:102:BCL:H62	1.80	0.40
1:C:167:TRP:CD1	1:C:311:GLN:HG2	2.56	0.40
2:L:27:ILE:HG23	20:H:303:CDL:H311	2.02	0.40
3:M:14:ARG:HB2	4:H:153:MET:SD	2.61	0.40
20:H:303:CDL:H171	20:H:303:CDL:H202	1.94	0.40
7:D:6:LYS:HE3	7:D:6:LYS:HB3	1.91	0.40
14:G:101:PGV:H12	14:G:101:PGV:H151	1.84	0.40
5:U:32:LEU:HD13	16:U:103:BCL:HBC1	2.02	0.40
6:V:22:PHE:CD2	22:V:101:CRT:H14	2.57	0.40
16:Y:402:BCL:H152	6:Z:25:SER:HA	2.04	0.40
16:4:102:BCL:H161	16:4:102:BCL:H141	1.88	0.40
6:8:53:TYR:CD2	7:9:43:GLY:HA3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	C	334/362 (92%)	316 (95%)	18 (5%)	0	100	100
2	L	272/276 (99%)	261 (96%)	11 (4%)	0	100	100
3	M	316/323 (98%)	304 (96%)	12 (4%)	0	100	100
4	H	276/278 (99%)	272 (99%)	4 (1%)	0	100	100
5	3	44/64 (69%)	44 (100%)	0	0	100	100
5	7	44/64 (69%)	44 (100%)	0	0	100	100
5	A	44/64 (69%)	44 (100%)	0	0	100	100
5	F	44/64 (69%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K	44/64 (69%)	44 (100%)	0	0	100	100
5	Q	44/64 (69%)	44 (100%)	0	0	100	100
5	U	44/64 (69%)	44 (100%)	0	0	100	100
5	Y	44/64 (69%)	44 (100%)	0	0	100	100
6	4	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
6	8	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
6	B	46/75 (61%)	44 (96%)	2 (4%)	0	100	100
6	G	45/75 (60%)	44 (98%)	1 (2%)	0	100	100
6	N	45/75 (60%)	44 (98%)	1 (2%)	0	100	100
6	R	45/75 (60%)	44 (98%)	1 (2%)	0	100	100
6	V	45/75 (60%)	44 (98%)	1 (2%)	0	100	100
6	Z	46/75 (61%)	43 (94%)	3 (6%)	0	100	100
7	1	44/67 (66%)	44 (100%)	0	0	100	100
7	5	44/67 (66%)	44 (100%)	0	0	100	100
7	9	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
7	D	44/67 (66%)	44 (100%)	0	0	100	100
7	I	44/67 (66%)	44 (100%)	0	0	100	100
7	O	44/67 (66%)	44 (100%)	0	0	100	100
7	S	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
7	W	44/67 (66%)	44 (100%)	0	0	100	100
8	0	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	2	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	6	43/74 (58%)	41 (95%)	2 (5%)	0	100	100
8	E	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	J	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	P	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	T	43/74 (58%)	41 (95%)	2 (5%)	0	100	100
8	X	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
9	a	95/142 (67%)	86 (90%)	9 (10%)	0	100	100
All	All	2703/3621 (75%)	2624 (97%)	79 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	287/306 (94%)	271 (94%)	16 (6%)	19	33
2	L	218/219 (100%)	215 (99%)	3 (1%)	59	79
3	M	252/255 (99%)	244 (97%)	8 (3%)	34	56
4	H	228/228 (100%)	219 (96%)	9 (4%)	28	48
5	3	39/55 (71%)	39 (100%)	0	100	100
5	7	39/55 (71%)	38 (97%)	1 (3%)	40	63
5	A	39/55 (71%)	38 (97%)	1 (3%)	40	63
5	F	39/55 (71%)	37 (95%)	2 (5%)	21	37
5	K	39/55 (71%)	38 (97%)	1 (3%)	40	63
5	Q	39/55 (71%)	38 (97%)	1 (3%)	40	63
5	U	39/55 (71%)	38 (97%)	1 (3%)	40	63
5	Y	39/55 (71%)	38 (97%)	1 (3%)	40	63
6	4	37/57 (65%)	37 (100%)	0	100	100
6	8	37/57 (65%)	36 (97%)	1 (3%)	39	62
6	B	38/57 (67%)	37 (97%)	1 (3%)	40	63
6	G	37/57 (65%)	35 (95%)	2 (5%)	20	35
6	N	37/57 (65%)	36 (97%)	1 (3%)	39	62
6	R	37/57 (65%)	36 (97%)	1 (3%)	39	62
6	V	37/57 (65%)	35 (95%)	2 (5%)	20	35
6	Z	38/57 (67%)	35 (92%)	3 (8%)	11	19
7	1	41/55 (74%)	40 (98%)	1 (2%)	43	65
7	5	41/55 (74%)	41 (100%)	0	100	100
7	9	41/55 (74%)	40 (98%)	1 (2%)	43	65
7	D	41/55 (74%)	41 (100%)	0	100	100
7	I	41/55 (74%)	38 (93%)	3 (7%)	13	22
7	O	41/55 (74%)	38 (93%)	3 (7%)	13	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	S	41/55 (74%)	40 (98%)	1 (2%)	43	65
7	W	41/55 (74%)	39 (95%)	2 (5%)	22	39
8	0	35/52 (67%)	32 (91%)	3 (9%)	10	16
8	2	35/52 (67%)	35 (100%)	0	100	100
8	6	35/52 (67%)	34 (97%)	1 (3%)	37	60
8	E	35/52 (67%)	34 (97%)	1 (3%)	37	60
8	J	35/52 (67%)	34 (97%)	1 (3%)	37	60
8	P	35/52 (67%)	33 (94%)	2 (6%)	18	33
8	T	35/52 (67%)	34 (97%)	1 (3%)	37	60
8	X	35/52 (67%)	35 (100%)	0	100	100
9	a	75/111 (68%)	70 (93%)	5 (7%)	15	26
All	All	2278/2871 (79%)	2198 (96%)	80 (4%)	32	53

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	92	THR
1	C	108	CYS
1	C	115	ASN
1	C	121	GLU
1	C	152	THR
1	C	175	VAL
1	C	177	MET
1	C	183	THR
1	C	197	SER
1	C	215	VAL
1	C	252	CYS
1	C	253	THR
1	C	254	THR
1	C	311	GLN
1	C	320	GLN
1	C	351	LEU
2	L	91	VAL
2	L	94	LEU
2	L	247	CYS
3	M	17	THR
3	M	45	ASP
3	M	53	LEU

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Mol	Chain	Res	Type
3	M	124	LEU
3	M	175	VAL
3	M	216	PHE
3	M	274	ILE
3	M	287	THR
4	H	1	MET
4	H	4	THR
4	H	8	THR
4	H	76	ARG
4	H	78	ILE
4	H	82	ARG
4	H	141	CYS
4	H	145	VAL
4	H	213	VAL
5	A	9	ASP
6	B	28	ILE
8	E	30	ILE
5	F	4	LEU
5	F	31	ILE
6	G	7	LEU
6	G	13	GLU
7	I	1	MET
7	I	8	LEU
7	I	21	MET
8	J	30	ILE
5	K	4	LEU
6	N	10	LEU
7	O	4	MET
7	O	21	MET
7	O	27	LEU
8	P	27	THR
8	P	50	ASP
5	Q	1	MET
6	R	7	LEU
7	S	1	MET
8	T	11	SER
5	U	15	ILE
6	V	27	LEU
6	V	28	ILE
7	W	4	MET
7	W	16	LEU
5	Y	46	VAL

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Mol	Chain	Res	Type
6	Z	13	GLU
6	Z	27	LEU
6	Z	51	GLU
7	1	16	LEU
8	6	30	ILE
5	7	12	ARG
6	8	7	LEU
7	9	16	LEU
8	0	10	VAL
8	0	17	GLU
8	0	30	ILE
9	a	46	THR
9	a	65	ASN
9	a	66	GLN
9	a	93	GLU
9	a	105	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	78	GLN
1	C	96	GLN
2	L	239	ASN
4	H	48	ASN
4	H	138	GLN
8	E	19	HIS
6	G	24	GLN
7	I	37	ASN
6	N	24	GLN
8	T	24	GLN
7	1	39	ASN
8	6	9	ASN
8	6	24	GLN
8	0	24	GLN
9	a	66	GLN
9	a	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 133 ligands modelled in this entry, 2 are monoatomic - leaving 131 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	$\# Z > 2$
14	PGV	4	103	-	43,43,50	1.00	2 (4%)	46,48,56	1.10	3 (6%)
14	PGV	H	302	-	35,35,50	1.09	2 (5%)	38,41,56	1.18	3 (7%)
14	PGV	X	101	-	42,42,50	0.99	2 (4%)	45,48,56	1.11	3 (6%)
20	CDL	U	101	-	50,50,99	1.29	4 (8%)	56,62,111	1.31	6 (10%)
16	BCL	3	102	5	69,74,74	1.79	17 (24%)	79,115,115	2.23	24 (30%)
14	PGV	V	103	-	43,43,50	0.99	2 (4%)	46,49,56	1.09	2 (4%)
14	PGV	0	103	-	43,43,50	0.97	2 (4%)	46,49,56	0.97	3 (6%)
14	PGV	T	102	-	45,45,50	0.94	2 (4%)	48,51,56	1.00	3 (6%)
20	CDL	M	407	-	79,79,99	1.00	4 (5%)	85,91,111	1.07	7 (8%)
16	BCL	1	103	7	69,74,74	1.81	18 (26%)	79,115,115	2.34	27 (34%)
14	PGV	6	104	-	42,42,50	1.01	2 (4%)	45,48,56	1.02	2 (4%)
20	CDL	M	408	-	55,55,99	1.24	4 (7%)	61,67,111	1.32	7 (11%)
14	PGV	F	101	-	49,49,50	0.94	2 (4%)	52,55,56	1.04	4 (7%)
14	PGV	L	305	-	42,42,50	0.99	2 (4%)	45,48,56	1.08	3 (6%)
16	BCL	8	102	6	69,74,74	1.76	18 (26%)	79,115,115	2.23	22 (27%)
14	PGV	H	304	-	41,41,50	0.99	2 (4%)	44,47,56	1.15	4 (9%)
16	BCL	L	311	2	69,74,74	1.77	17 (24%)	79,115,115	2.22	21 (26%)
14	PGV	G	101	-	48,48,50	0.93	2 (4%)	51,54,56	0.95	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PGV	0	101	-	40,40,50	1.02	2 (5%)	43,46,56	1.14	3 (6%)
20	CDL	H	303	-	74,74,99	1.05	4 (5%)	80,86,111	1.16	8 (10%)
16	BCL	Y	401	20	69,74,74	1.76	18 (26%)	79,115,115	2.25	22 (27%)
14	PGV	8	103	-	42,42,50	1.00	2 (4%)	45,48,56	1.04	3 (6%)
16	BCL	9	102	7	69,74,74	1.80	18 (26%)	79,115,115	2.17	24 (30%)
15	LMT	O	102	-	30,30,36	0.43	0	41,41,47	1.00	3 (7%)
18	UQ8	L	304	-	33,33,53	1.50	2 (6%)	42,43,67	1.71	9 (21%)
14	PGV	P	102	-	46,46,50	0.95	2 (4%)	49,52,56	1.16	4 (8%)
14	PGV	B	104	-	40,40,50	1.00	2 (5%)	43,45,56	1.16	4 (9%)
16	BCL	S	101	7	69,74,74	1.79	18 (26%)	79,115,115	2.26	27 (34%)
16	BCL	7	102	5	69,74,74	1.78	17 (24%)	79,115,115	2.24	24 (30%)
17	BPH	M	404	-	59,70,70	0.78	3 (5%)	59,101,101	0.84	2 (3%)
16	BCL	V	102	6	69,74,74	1.76	18 (26%)	79,115,115	2.12	24 (30%)
12	LJQ	C	406	-	30,30,34	0.31	0	32,32,36	0.42	0
16	BCL	0	102	8	69,74,74	1.81	17 (24%)	79,115,115	2.21	22 (27%)
18	UQ8	L	306	-	38,38,53	1.44	2 (5%)	48,49,67	1.60	11 (22%)
16	BCL	Z	102	6	69,74,74	1.77	17 (24%)	79,115,115	2.16	22 (27%)
14	PGV	Z	101	-	45,45,50	0.99	2 (4%)	48,51,56	1.09	3 (6%)
16	BCL	W	101	7	69,74,74	1.78	16 (23%)	79,115,115	2.25	25 (31%)
15	LMT	L	308	-	36,36,36	0.42	0	47,47,47	0.81	1 (2%)
14	PGV	N	101	-	49,49,50	0.91	2 (4%)	52,55,56	1.02	2 (3%)
15	LMT	5	101	-	36,36,36	0.34	0	47,47,47	0.92	2 (4%)
16	BCL	G	103	6	69,74,74	1.80	17 (24%)	79,115,115	2.15	21 (26%)
16	BCL	R	102	6	69,74,74	1.77	18 (26%)	79,115,115	2.21	22 (27%)
14	PGV	R	104	-	40,40,50	1.04	2 (5%)	43,45,56	1.13	3 (6%)
15	LMT	H	306	-	36,36,36	0.41	0	47,47,47	0.98	3 (6%)
10	HEC	C	401	1	46,50,50	1.76	11 (23%)	58,82,82	1.68	12 (20%)
13	PLM	C	407	-	10,11,17	0.38	0	9,10,17	0.39	0
16	BCL	W	102	7	69,74,74	1.81	17 (24%)	79,115,115	2.22	25 (31%)
22	CRT	G	102	-	43,43,43	0.68	0	48,54,54	2.16	19 (39%)
14	PGV	6	103	-	43,43,50	0.97	2 (4%)	47,49,56	0.98	3 (6%)
16	BCL	T	101	8	69,74,74	1.79	17 (24%)	79,115,115	2.13	22 (27%)
10	HEC	C	403	1	46,50,50	1.79	11 (23%)	58,82,82	1.65	14 (24%)
22	CRT	4	101	-	43,43,43	0.68	0	48,54,54	2.16	13 (27%)
10	HEC	C	404	1	46,50,50	1.77	10 (21%)	58,82,82	1.60	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PGV	L	310	-	40,40,50	1.02	2 (5%)	43,46,56	1.09	3 (6%)
14	PGV	C	408	-	31,31,50	1.13	2 (6%)	34,37,56	1.26	3 (8%)
16	BCL	P	101	8	69,74,74	1.76	18 (26%)	79,115,115	2.17	20 (25%)
16	BCL	L	302	2	69,74,74	1.76	16 (23%)	79,115,115	2.28	24 (30%)
14	PGV	L	309	-	35,35,50	1.06	2 (5%)	38,40,56	1.11	1 (2%)
16	BCL	S	102	7	69,74,74	1.79	17 (24%)	79,115,115	2.17	23 (29%)
15	LMT	I	101	-	26,26,36	0.52	0	37,37,47	1.30	4 (10%)
15	LMT	M	411	-	36,36,36	0.40	0	47,47,47	0.93	0
14	PGV	T	103	-	46,46,50	0.95	2 (4%)	49,52,56	0.94	3 (6%)
16	BCL	I	102	7	69,74,74	1.79	18 (26%)	79,115,115	2.23	25 (31%)
16	BCL	L	312	3	69,74,74	1.78	16 (23%)	79,115,115	2.33	25 (31%)
22	CRT	M	406	-	43,43,43	0.63	0	48,54,54	2.34	15 (31%)
14	PGV	G	104	-	49,49,50	0.93	2 (4%)	52,55,56	0.94	3 (5%)
16	BCL	F	103	5	69,74,74	1.75	17 (24%)	79,115,115	2.30	22 (27%)
20	CDL	U	102	-	45,45,99	1.42	4 (8%)	51,57,111	1.45	6 (11%)
16	BCL	I	103	7	69,74,74	1.80	17 (24%)	79,115,115	2.20	22 (27%)
16	BCL	D	101	7	69,74,74	1.79	19 (27%)	79,115,115	2.33	27 (34%)
16	BCL	4	102	6	69,74,74	1.79	18 (26%)	79,115,115	2.20	20 (25%)
17	BPH	L	303	-	59,70,70	0.83	3 (5%)	59,101,101	1.02	4 (6%)
14	PGV	2	103	-	36,36,50	1.08	2 (5%)	39,41,56	1.11	2 (5%)
21	MQ8	M	405	-	54,54,54	1.28	2 (3%)	67,69,69	1.61	15 (22%)
15	LMT	H	307	-	27,27,36	0.48	0	38,38,47	0.87	1 (2%)
16	BCL	9	101	7	69,74,74	1.78	17 (24%)	79,115,115	2.21	23 (29%)
16	BCL	1	102	7	69,74,74	1.81	17 (24%)	79,115,115	2.27	26 (32%)
15	LMT	H	305	-	31,31,36	0.43	0	42,42,47	1.05	2 (4%)
22	CRT	B	101	-	43,43,43	0.64	0	48,54,54	2.33	15 (31%)
14	PGV	6	101	-	45,45,50	0.95	2 (4%)	48,51,56	1.12	3 (6%)
14	PGV	P	103	-	39,39,50	1.08	2 (5%)	42,44,56	1.20	4 (9%)
14	PGV	X	103	-	44,44,50	0.97	2 (4%)	47,50,56	1.14	4 (8%)
22	CRT	8	101	-	43,43,43	0.69	0	48,54,54	2.09	17 (35%)
16	BCL	5	103	7	69,74,74	1.76	17 (24%)	79,115,115	2.23	27 (34%)
15	LMT	5	102	-	25,25,36	0.49	0	36,36,47	0.68	1 (2%)
16	BCL	M	403	3	69,74,74	1.78	16 (23%)	79,115,115	2.28	26 (32%)
14	PGV	2	102	-	45,45,50	0.98	2 (4%)	48,50,56	1.04	2 (4%)
14	PGV	Z	104	-	42,42,50	1.00	2 (4%)	45,47,56	1.12	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCL	O	103	7	69,74,74	1.79	19 (27%)	79,115,115	2.29	22 (27%)
15	LMT	F	102	-	34,34,36	0.49	0	45,45,47	1.15	3 (6%)
16	BCL	2	101	8	69,74,74	1.77	17 (24%)	79,115,115	2.20	19 (24%)
14	PGV	R	103	-	42,42,50	1.01	2 (4%)	45,48,56	1.15	3 (6%)
16	BCL	E	101	8	69,74,74	1.77	16 (23%)	79,115,115	2.18	23 (29%)
16	BCL	Y	402	5	69,74,74	1.78	17 (24%)	79,115,115	2.15	21 (26%)
15	LMT	Q	101	-	33,33,36	0.45	0	44,44,47	1.05	4 (9%)
16	BCL	K	101	5	69,74,74	1.79	18 (26%)	79,115,115	2.22	19 (24%)
14	PGV	N	105	-	36,36,50	1.05	2 (5%)	39,42,56	1.17	3 (7%)
14	PGV	0	104	-	42,42,50	1.00	2 (4%)	45,48,56	1.13	3 (6%)
16	BCL	A	101	5	69,74,74	1.79	19 (27%)	79,115,115	2.15	21 (26%)
16	BCL	Q	102	5	69,74,74	1.76	18 (26%)	79,115,115	2.27	23 (29%)
20	CDL	M	409	16	49,49,99	1.30	4 (8%)	55,61,111	1.26	5 (9%)
14	PGV	B	103	-	43,43,50	0.97	2 (4%)	46,49,56	1.16	3 (6%)
14	PGV	1	101	-	44,44,50	0.99	2 (4%)	47,50,56	1.04	3 (6%)
16	BCL	J	101	8	69,74,74	1.77	20 (28%)	79,115,115	2.26	25 (31%)
16	BCL	N	103	6	69,74,74	1.77	19 (27%)	79,115,115	2.14	21 (26%)
23	SF4	a	201	9	0,12,12	-	-	-	-	-
14	PGV	3	101	-	29,29,50	1.21	2 (6%)	32,34,56	1.16	2 (6%)
16	BCL	X	102	8	69,74,74	1.75	18 (26%)	79,115,115	2.21	23 (29%)
16	BCL	O	104	7	69,74,74	1.80	17 (24%)	79,115,115	2.17	24 (30%)
20	CDL	H	301	-	63,63,99	1.07	4 (6%)	69,75,111	1.23	5 (7%)
14	PGV	G	105	-	41,41,50	1.01	2 (4%)	44,46,56	1.14	4 (9%)
16	BCL	6	102	8	69,74,74	1.77	17 (24%)	79,115,115	2.16	23 (29%)
22	CRT	V	101	-	43,43,43	0.68	0	48,54,54	2.35	18 (37%)
16	BCL	D	102	7	69,74,74	1.80	18 (26%)	79,115,115	2.15	24 (30%)
16	BCL	5	104	7	69,74,74	1.81	17 (24%)	79,115,115	2.13	23 (29%)
22	CRT	Y	403	-	43,43,43	0.63	0	48,54,54	2.20	17 (35%)
14	PGV	Z	103	-	43,43,50	0.99	2 (4%)	46,49,56	1.06	3 (6%)
22	CRT	R	101	-	43,43,43	0.62	0	48,54,54	2.21	19 (39%)
14	PGV	N	104	-	46,46,50	0.95	2 (4%)	49,52,56	0.95	2 (4%)
22	CRT	N	102	-	43,43,43	0.66	0	48,54,54	2.15	14 (29%)
14	PGV	J	102	-	32,32,50	1.21	2 (6%)	35,37,56	1.25	3 (8%)
15	LMT	7	101	-	26,26,36	0.52	0	37,37,47	1.04	1 (2%)
15	LMT	L	301	-	26,26,36	0.43	0	37,37,47	0.93	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PGV	M	410	-	50,50,50	0.92	2 (4%)	53,56,56	1.12	3 (5%)
20	CDL	M	402	-	81,81,99	1.03	4 (4%)	87,93,111	0.98	4 (4%)
20	CDL	O	101	-	72,72,99	1.07	4 (5%)	78,84,111	1.16	5 (6%)
14	PGV	E	102	-	37,37,50	1.07	2 (5%)	40,43,56	1.09	4 (10%)
16	BCL	U	103	5	69,74,74	1.81	19 (27%)	79,115,115	2.28	22 (27%)
16	BCL	B	102	6	69,74,74	1.79	19 (27%)	79,115,115	2.15	21 (26%)
10	HEC	C	402	1	46,50,50	1.75	11 (23%)	58,82,82	1.61	13 (22%)
18	UQ8	L	307	-	17,17,53	2.15	2 (11%)	22,23,67	1.30	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PGV	4	103	-	-	13/47/47/55	-
14	PGV	H	302	-	-	19/40/40/55	-
14	PGV	X	101	-	-	17/47/47/55	-
20	CDL	U	101	-	-	24/61/61/110	-
16	BCL	3	102	5	-	14/41/137/137	-
14	PGV	V	103	-	-	17/48/48/55	-
14	PGV	0	103	-	-	15/48/48/55	-
14	PGV	T	102	-	-	18/50/50/55	-
20	CDL	M	407	-	-	39/90/90/110	-
16	BCL	1	103	7	-	17/41/137/137	-
14	PGV	6	104	-	-	10/47/47/55	-
20	CDL	M	408	-	-	26/66/66/110	-
14	PGV	F	101	-	-	16/54/54/55	-
14	PGV	L	305	-	-	16/47/47/55	-
16	BCL	8	102	6	-	9/41/137/137	-
14	PGV	H	304	-	-	17/46/46/55	-
16	BCL	L	311	2	-	10/41/137/137	-
14	PGV	G	101	-	-	23/53/53/55	-
14	PGV	0	101	-	-	20/45/45/55	-
20	CDL	H	303	-	-	41/85/85/110	-
16	BCL	Y	401	20	-	12/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PGV	8	103	-	-	17/47/47/55	-
16	BCL	9	102	7	-	7/41/137/137	-
15	LMT	O	102	-	-	7/15/55/61	0/2/2/2
18	UQ8	L	304	-	-	6/27/51/75	0/1/1/1
14	PGV	P	102	-	-	22/51/51/55	-
14	PGV	B	104	-	-	15/44/44/55	-
16	BCL	S	101	7	-	17/41/137/137	-
16	BCL	7	102	5	-	17/41/137/137	-
17	BPH	M	404	-	-	4/37/105/105	0/5/6/6
16	BCL	V	102	6	-	17/41/137/137	-
12	LJQ	C	406	-	-	2/31/31/36	-
16	BCL	0	102	8	-	5/41/137/137	-
18	UQ8	L	306	-	-	7/33/57/75	0/1/1/1
16	BCL	Z	102	6	-	18/41/137/137	-
14	PGV	Z	101	-	-	22/50/50/55	-
16	BCL	W	101	7	-	15/41/137/137	-
15	LMT	L	308	-	-	6/21/61/61	0/2/2/2
14	PGV	N	101	-	-	22/54/54/55	-
15	LMT	5	101	-	-	11/21/61/61	0/2/2/2
16	BCL	G	103	6	-	19/41/137/137	-
16	BCL	R	102	6	-	18/41/137/137	-
14	PGV	R	104	-	-	17/42/42/55	-
15	LMT	H	306	-	-	7/21/61/61	0/2/2/2
10	HEC	C	401	1	-	8/14/54/54	-
13	PLM	C	407	-	-	0/9/9/15	-
16	BCL	W	102	7	-	16/41/137/137	-
22	CRT	G	102	-	-	5/51/51/51	-
14	PGV	6	103	-	-	15/47/47/55	-
16	BCL	T	101	8	-	16/41/137/137	-
10	HEC	C	403	1	-	6/14/54/54	-
22	CRT	4	101	-	-	6/51/51/51	-
10	HEC	C	404	1	-	5/14/54/54	-
14	PGV	L	310	-	-	20/45/45/55	-
14	PGV	C	408	-	-	9/36/36/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCL	P	101	8	-	14/41/137/137	-
16	BCL	L	302	2	-	8/41/137/137	-
14	PGV	L	309	-	-	11/39/39/55	-
16	BCL	S	102	7	-	12/41/137/137	-
15	LMT	I	101	-	-	8/11/51/61	0/2/2/2
15	LMT	M	411	-	-	7/21/61/61	0/2/2/2
14	PGV	T	103	-	-	21/51/51/55	-
16	BCL	I	102	7	-	15/41/137/137	-
16	BCL	L	312	3	-	17/41/137/137	-
22	CRT	M	406	-	-	11/51/51/51	-
14	PGV	G	104	-	-	20/54/54/55	-
16	BCL	F	103	5	-	16/41/137/137	-
20	CDL	U	102	-	-	17/55/55/110	-
16	BCL	I	103	7	-	18/41/137/137	-
16	BCL	D	101	7	-	14/41/137/137	-
16	BCL	4	102	6	-	11/41/137/137	-
17	BPH	L	303	-	-	8/37/105/105	0/5/6/6
14	PGV	2	103	-	-	15/40/40/55	-
21	MQ8	M	405	-	-	4/47/67/67	0/2/2/2
15	LMT	H	307	-	-	3/12/52/61	0/2/2/2
16	BCL	9	101	7	-	11/41/137/137	-
16	BCL	1	102	7	-	12/41/137/137	-
15	LMT	H	305	-	-	7/16/56/61	0/2/2/2
22	CRT	B	101	-	-	7/51/51/51	-
14	PGV	6	101	-	-	14/50/50/55	-
14	PGV	P	103	-	-	10/41/41/55	-
14	PGV	X	103	-	-	14/49/49/55	-
22	CRT	8	101	-	-	5/51/51/51	-
16	BCL	5	103	7	-	11/41/137/137	-
15	LMT	5	102	-	-	4/10/50/61	0/2/2/2
16	BCL	M	403	3	-	13/41/137/137	-
14	PGV	2	102	-	-	15/49/49/55	-
14	PGV	Z	104	-	-	19/46/46/55	-
16	BCL	O	103	7	-	14/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	F	102	-	-	8/19/59/61	0/2/2/2
16	BCL	2	101	8	-	11/41/137/137	-
14	PGV	R	103	-	-	13/47/47/55	-
16	BCL	E	101	8	-	9/41/137/137	-
16	BCL	Y	402	5	-	14/41/137/137	-
15	LMT	Q	101	-	-	10/18/58/61	0/2/2/2
16	BCL	K	101	5	-	19/41/137/137	-
14	PGV	N	105	-	-	14/41/41/55	-
14	PGV	0	104	-	-	11/47/47/55	-
16	BCL	A	101	5	-	16/41/137/137	-
16	BCL	Q	102	5	-	12/41/137/137	-
20	CDL	M	409	16	-	20/60/60/110	-
14	PGV	B	103	-	-	21/48/48/55	-
14	PGV	1	101	-	-	17/49/49/55	-
16	BCL	J	101	8	-	9/41/137/137	-
16	BCL	N	103	6	-	15/41/137/137	-
23	SF4	a	201	9	-	-	0/6/5/5
14	PGV	3	101	-	-	10/33/33/55	-
16	BCL	X	102	8	-	14/41/137/137	-
16	BCL	O	104	7	-	15/41/137/137	-
20	CDL	H	301	-	-	22/73/73/110	-
14	PGV	G	105	-	-	19/45/45/55	-
16	BCL	6	102	8	-	9/41/137/137	-
22	CRT	V	101	-	-	7/51/51/51	-
16	BCL	D	102	7	-	16/41/137/137	-
16	BCL	5	104	7	-	20/41/137/137	-
22	CRT	Y	403	-	-	2/51/51/51	-
14	PGV	Z	103	-	-	23/48/48/55	-
22	CRT	R	101	-	-	9/51/51/51	-
14	PGV	N	104	-	-	12/51/51/55	-
22	CRT	N	102	-	-	5/51/51/51	-
14	PGV	J	102	-	-	6/34/34/55	-
15	LMT	7	101	-	-	4/11/51/61	0/2/2/2
15	LMT	L	301	-	-	3/11/51/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PGV	M	410	-	-	23/55/55/55	-
20	CDL	M	402	-	-	39/92/92/110	-
20	CDL	O	101	-	-	24/83/83/110	-
14	PGV	E	102	-	-	8/42/42/55	-
16	BCL	U	103	5	-	15/41/137/137	-
16	BCL	B	102	6	-	13/41/137/137	-
10	HEC	C	402	1	-	6/14/54/54	-
18	UQ8	L	307	-	-	1/8/32/75	0/1/1/1

All (966) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	307	UQ8	C6-C1	7.79	1.49	1.35
18	L	306	UQ8	C6-C1	7.60	1.48	1.35
21	M	405	MQ8	C3-C2	7.60	1.48	1.35
18	L	304	UQ8	C6-C1	7.54	1.48	1.35
16	Y	402	BCL	O2D-CGD	5.12	1.45	1.33
20	U	102	CDL	OA6-CA5	5.09	1.46	1.35
16	L	302	BCL	O2D-CGD	5.08	1.45	1.33
16	I	103	BCL	O2D-CGD	5.03	1.45	1.33
16	1	102	BCL	O2D-CGD	5.03	1.45	1.33
16	B	102	BCL	O2D-CGD	5.02	1.45	1.33
16	9	101	BCL	O2D-CGD	5.02	1.45	1.33
16	D	101	BCL	O2D-CGD	5.02	1.45	1.33
16	W	102	BCL	O2D-CGD	5.01	1.45	1.33
16	M	403	BCL	O2D-CGD	5.00	1.45	1.33
16	A	101	BCL	O2D-CGD	4.97	1.45	1.33
16	S	102	BCL	O2D-CGD	4.96	1.45	1.33
16	3	102	BCL	O2D-CGD	4.95	1.45	1.33
16	1	103	BCL	O2D-CGD	4.95	1.45	1.33
16	5	103	BCL	O2D-CGD	4.93	1.45	1.33
16	O	104	BCL	O2D-CGD	4.93	1.45	1.33
16	J	101	BCL	C3D-C4D	-4.93	1.33	1.44
16	0	102	BCL	O2D-CGD	4.93	1.45	1.33
16	Z	102	BCL	O2D-CGD	4.92	1.45	1.33
16	D	102	BCL	O2D-CGD	4.92	1.45	1.33
16	S	101	BCL	C3D-C4D	-4.91	1.33	1.44
16	G	103	BCL	O2D-CGD	4.90	1.45	1.33
16	K	101	BCL	O2D-CGD	4.89	1.45	1.33
16	9	102	BCL	O2D-CGD	4.89	1.45	1.33
16	7	102	BCL	O2D-CGD	4.89	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	312	BCL	C3D-C4D	-4.89	1.33	1.44
16	W	101	BCL	C3D-C4D	-4.88	1.33	1.44
16	2	101	BCL	O2D-CGD	4.88	1.45	1.33
16	0	102	BCL	C3D-C4D	-4.87	1.33	1.44
16	Q	102	BCL	O2D-CGD	4.86	1.45	1.33
16	O	103	BCL	O2D-CGD	4.86	1.45	1.33
16	5	104	BCL	O2D-CGD	4.86	1.45	1.33
16	1	103	BCL	C3D-C4D	-4.85	1.33	1.44
16	Y	401	BCL	C3D-C4D	-4.84	1.33	1.44
16	L	311	BCL	O2D-CGD	4.84	1.45	1.33
16	I	102	BCL	O2D-CGD	4.83	1.45	1.33
16	8	102	BCL	O2D-CGD	4.83	1.45	1.33
16	M	403	BCL	C3D-C4D	-4.83	1.33	1.44
16	R	102	BCL	O2D-CGD	4.83	1.45	1.33
16	7	102	BCL	C3D-C4D	-4.83	1.33	1.44
16	9	101	BCL	C3D-C4D	-4.82	1.33	1.44
16	T	101	BCL	O2D-CGD	4.81	1.45	1.33
16	V	102	BCL	O2D-CGD	4.81	1.45	1.33
16	L	311	BCL	C3D-C4D	-4.81	1.33	1.44
21	M	405	MQ8	C10-C5	4.80	1.48	1.40
16	V	102	BCL	C3D-C4D	-4.80	1.33	1.44
16	Z	102	BCL	C3D-C4D	-4.80	1.33	1.44
16	T	101	BCL	C3D-C4D	-4.79	1.33	1.44
16	4	102	BCL	C3D-C4D	-4.79	1.33	1.44
16	S	102	BCL	C3D-C4D	-4.79	1.33	1.44
16	4	102	BCL	O2D-CGD	4.79	1.45	1.33
16	U	103	BCL	O2D-CGD	4.79	1.45	1.33
16	X	102	BCL	O2D-CGD	4.79	1.45	1.33
16	F	103	BCL	O2D-CGD	4.79	1.45	1.33
16	D	102	BCL	C3D-C4D	-4.78	1.33	1.44
16	W	101	BCL	O2D-CGD	4.77	1.45	1.33
16	S	101	BCL	O2D-CGD	4.77	1.45	1.33
16	Y	401	BCL	O2D-CGD	4.77	1.45	1.33
16	2	101	BCL	C3D-C4D	-4.77	1.33	1.44
16	5	104	BCL	C3D-C4D	-4.76	1.33	1.44
16	E	101	BCL	O2D-CGD	4.76	1.44	1.33
16	B	102	BCL	C3D-C4D	-4.75	1.33	1.44
16	6	102	BCL	C3D-C4D	-4.74	1.33	1.44
16	W	102	BCL	C3D-C4D	-4.74	1.33	1.44
16	I	103	BCL	C3D-C4D	-4.73	1.33	1.44
16	6	102	BCL	O2D-CGD	4.73	1.44	1.33
16	D	101	BCL	C3D-C4D	-4.73	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	103	BCL	O2D-CGD	4.71	1.44	1.33
16	K	101	BCL	C3D-C4D	-4.71	1.33	1.44
16	1	102	BCL	C3D-C4D	-4.71	1.33	1.44
16	3	102	BCL	C3D-C4D	-4.71	1.33	1.44
16	9	102	BCL	C3D-C4D	-4.71	1.33	1.44
16	O	104	BCL	C3D-C4D	-4.70	1.33	1.44
16	P	101	BCL	C3D-C4D	-4.70	1.33	1.44
16	P	101	BCL	O2D-CGD	4.70	1.44	1.33
16	F	103	BCL	C3D-C4D	-4.68	1.33	1.44
16	O	103	BCL	C3D-C4D	-4.67	1.33	1.44
16	J	101	BCL	O2D-CGD	4.67	1.44	1.33
16	8	102	BCL	C3D-C4D	-4.67	1.33	1.44
16	G	103	BCL	C3D-C4D	-4.67	1.33	1.44
16	X	102	BCL	C3D-C4D	-4.66	1.33	1.44
16	U	103	BCL	C3D-C4D	-4.66	1.33	1.44
16	Q	102	BCL	C3D-C4D	-4.66	1.33	1.44
16	Y	402	BCL	C3D-C4D	-4.65	1.33	1.44
16	E	101	BCL	C3D-C4D	-4.64	1.33	1.44
16	5	103	BCL	C3D-C4D	-4.63	1.33	1.44
16	L	302	BCL	C3D-C4D	-4.63	1.33	1.44
16	R	102	BCL	C3D-C4D	-4.62	1.33	1.44
16	N	103	BCL	C3D-C4D	-4.61	1.33	1.44
16	7	102	BCL	O2A-CGA	4.58	1.46	1.33
16	I	102	BCL	C3D-C4D	-4.57	1.33	1.44
16	A	101	BCL	C3D-C4D	-4.56	1.33	1.44
16	L	312	BCL	O2D-CGD	4.56	1.44	1.33
10	C	402	HEC	CBC-CAC	-4.53	1.32	1.49
16	A	101	BCL	O2A-CGA	4.51	1.46	1.33
20	U	101	CDL	OA6-CA5	4.46	1.46	1.34
10	C	401	HEC	CBC-CAC	-4.43	1.33	1.49
10	C	404	HEC	CBB-CAB	-4.42	1.33	1.49
10	C	402	HEC	CBB-CAB	-4.41	1.33	1.49
10	C	404	HEC	CBC-CAC	-4.39	1.33	1.49
20	U	101	CDL	OA8-CA7	4.39	1.46	1.33
14	2	102	PGV	O03-C19	4.38	1.46	1.33
14	3	101	PGV	O03-C19	4.37	1.46	1.33
20	M	408	CDL	OB6-CB5	4.37	1.46	1.34
10	C	403	HEC	CBC-CAC	-4.37	1.33	1.49
10	C	401	HEC	CBB-CAB	-4.36	1.33	1.49
14	J	102	PGV	O01-C1	4.35	1.46	1.34
16	O	104	BCL	O2A-CGA	4.34	1.46	1.33
16	E	101	BCL	O2A-CGA	4.34	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	101	PGV	O03-C19	4.33	1.46	1.33
10	C	403	HEC	CBB-CAB	-4.33	1.33	1.49
14	H	302	PGV	O01-C1	4.32	1.46	1.34
16	W	101	BCL	O2A-CGA	4.32	1.45	1.33
16	2	101	BCL	O2A-CGA	4.32	1.45	1.33
14	Z	101	PGV	O03-C19	4.31	1.45	1.33
20	U	102	CDL	OB8-CB7	4.31	1.45	1.33
16	B	102	BCL	O2A-CGA	4.31	1.45	1.33
20	M	402	CDL	OB6-CB5	4.31	1.46	1.34
14	6	104	PGV	O03-C19	4.30	1.45	1.33
16	D	102	BCL	O2A-CGA	4.29	1.45	1.33
20	M	408	CDL	OA8-CA7	4.29	1.45	1.33
14	M	410	PGV	O03-C19	4.29	1.45	1.33
14	4	103	PGV	O01-C1	4.29	1.46	1.34
16	Y	401	BCL	O2A-CGA	4.29	1.45	1.33
14	J	102	PGV	O03-C19	4.29	1.45	1.33
16	T	101	BCL	O2A-CGA	4.29	1.45	1.33
14	T	103	PGV	O03-C19	4.29	1.45	1.33
14	P	103	PGV	O01-C1	4.28	1.46	1.34
14	N	104	PGV	O03-C19	4.28	1.45	1.33
16	Q	102	BCL	O2A-CGA	4.28	1.45	1.33
20	O	101	CDL	OA8-CA7	4.27	1.45	1.33
14	G	105	PGV	O01-C1	4.27	1.46	1.34
14	E	102	PGV	O03-C19	4.27	1.45	1.33
16	9	102	BCL	O2A-CGA	4.26	1.45	1.33
20	H	301	CDL	OB8-CB7	4.26	1.45	1.33
16	K	101	BCL	O2A-CGA	4.26	1.45	1.33
16	N	103	BCL	O2A-CGA	4.25	1.45	1.33
20	M	402	CDL	OA6-CA5	4.25	1.46	1.34
14	C	408	PGV	O03-C19	4.25	1.45	1.33
14	P	102	PGV	O03-C19	4.24	1.45	1.33
20	M	409	CDL	OA8-CA7	4.24	1.45	1.33
14	V	103	PGV	O01-C1	4.24	1.46	1.34
14	F	101	PGV	O01-C1	4.24	1.46	1.34
20	M	402	CDL	OB8-CB7	4.24	1.45	1.33
20	H	301	CDL	OA6-CA5	4.23	1.46	1.34
14	8	103	PGV	O03-C19	4.23	1.45	1.33
16	3	102	BCL	O2A-CGA	4.23	1.45	1.33
20	O	101	CDL	OB8-CB7	4.23	1.45	1.33
20	M	409	CDL	OB8-CB7	4.22	1.45	1.33
20	M	409	CDL	OA6-CA5	4.22	1.46	1.34
16	W	102	BCL	C3B-C4B	4.22	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	102	BCL	O2A-CGA	4.21	1.45	1.33
14	2	102	PGV	O01-C1	4.21	1.46	1.34
14	Z	103	PGV	O03-C19	4.21	1.45	1.33
20	H	303	CDL	OA8-CA7	4.21	1.45	1.33
14	0	104	PGV	O03-C19	4.21	1.45	1.33
14	F	101	PGV	O03-C19	4.21	1.45	1.33
14	R	103	PGV	O03-C19	4.20	1.45	1.33
16	V	102	BCL	O2A-CGA	4.20	1.45	1.33
16	S	101	BCL	O2A-CGA	4.20	1.45	1.33
20	M	402	CDL	OA8-CA7	4.20	1.45	1.33
14	P	103	PGV	O03-C19	4.20	1.45	1.33
14	2	103	PGV	O03-C19	4.20	1.45	1.33
14	L	310	PGV	O03-C19	4.20	1.45	1.33
16	Y	402	BCL	O2A-CGA	4.20	1.45	1.33
14	Z	104	PGV	O01-C1	4.19	1.46	1.34
16	G	103	BCL	O2A-CGA	4.18	1.45	1.33
16	4	102	BCL	O2A-CGA	4.18	1.45	1.33
20	M	407	CDL	OB8-CB7	4.18	1.45	1.33
14	H	304	PGV	O03-C19	4.18	1.45	1.33
14	Z	101	PGV	O01-C1	4.17	1.46	1.34
14	R	103	PGV	O01-C1	4.17	1.46	1.34
14	0	101	PGV	O03-C19	4.17	1.45	1.33
14	G	101	PGV	O03-C19	4.17	1.45	1.33
16	R	102	BCL	O2A-CGA	4.17	1.45	1.33
16	L	302	BCL	O2A-CGA	4.17	1.45	1.33
16	O	103	BCL	O2A-CGA	4.16	1.45	1.33
14	L	305	PGV	O03-C19	4.16	1.45	1.33
20	M	408	CDL	OB8-CB7	4.16	1.45	1.33
14	4	103	PGV	O03-C19	4.15	1.45	1.33
14	N	105	PGV	O01-C1	4.15	1.46	1.34
14	M	410	PGV	O01-C1	4.15	1.46	1.34
16	L	311	BCL	O2A-CGA	4.14	1.45	1.33
14	0	104	PGV	O01-C1	4.14	1.46	1.34
16	0	102	BCL	O2A-CGA	4.14	1.45	1.33
14	G	104	PGV	O01-C1	4.14	1.46	1.34
16	Z	102	BCL	O2A-CGA	4.14	1.45	1.33
14	G	104	PGV	O03-C19	4.14	1.45	1.33
16	L	312	BCL	C3B-C4B	4.14	1.49	1.41
16	J	101	BCL	O2A-CGA	4.13	1.45	1.33
16	S	102	BCL	O2A-CGA	4.13	1.45	1.33
20	U	102	CDL	OB6-CB5	4.13	1.45	1.34
16	I	102	BCL	O2A-CGA	4.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Z	103	PGV	O01-C1	4.13	1.45	1.34
14	1	101	PGV	O01-C1	4.12	1.45	1.34
14	X	101	PGV	O01-C1	4.12	1.45	1.34
14	6	103	PGV	O03-C19	4.12	1.45	1.33
20	H	303	CDL	OB6-CB5	4.11	1.45	1.34
16	F	103	BCL	O2A-CGA	4.11	1.45	1.33
16	1	103	BCL	C3B-C4B	4.11	1.49	1.41
14	3	101	PGV	O01-C1	4.11	1.45	1.34
14	6	101	PGV	O03-C19	4.11	1.45	1.33
14	R	104	PGV	O01-C1	4.10	1.45	1.34
16	M	403	BCL	C3B-C4B	4.10	1.49	1.41
20	H	303	CDL	OA6-CA5	4.10	1.45	1.34
16	I	103	BCL	O2A-CGA	4.10	1.45	1.33
16	5	103	BCL	C3B-C4B	4.10	1.49	1.41
14	X	103	PGV	O01-C1	4.10	1.45	1.34
14	B	103	PGV	O01-C1	4.10	1.45	1.34
14	G	105	PGV	O03-C19	4.10	1.45	1.33
14	N	101	PGV	O03-C19	4.10	1.45	1.33
14	B	104	PGV	O01-C1	4.10	1.45	1.34
16	5	104	BCL	O2A-CGA	4.10	1.45	1.33
14	0	101	PGV	O01-C1	4.10	1.45	1.34
14	6	101	PGV	O01-C1	4.10	1.45	1.34
16	6	102	BCL	O2A-CGA	4.09	1.45	1.33
16	8	102	BCL	O2A-CGA	4.09	1.45	1.33
14	P	102	PGV	O01-C1	4.09	1.45	1.34
16	U	103	BCL	O2A-CGA	4.09	1.45	1.33
10	C	403	HEC	CAC-C3C	4.09	1.48	1.35
20	O	101	CDL	OB6-CB5	4.09	1.45	1.34
14	T	102	PGV	O03-C19	4.09	1.45	1.33
16	P	101	BCL	O2A-CGA	4.09	1.45	1.33
14	6	104	PGV	O01-C1	4.08	1.45	1.34
16	L	312	BCL	O2A-CGA	4.08	1.45	1.33
20	M	409	CDL	OB6-CB5	4.08	1.45	1.34
16	W	102	BCL	O2A-CGA	4.08	1.45	1.33
20	U	101	CDL	OB8-CB7	4.07	1.45	1.33
20	M	408	CDL	OA6-CA5	4.07	1.45	1.34
14	L	305	PGV	O01-C1	4.07	1.45	1.34
14	B	103	PGV	O03-C19	4.07	1.45	1.33
20	H	303	CDL	OB8-CB7	4.07	1.45	1.33
16	W	101	BCL	C3B-C4B	4.07	1.49	1.41
20	U	102	CDL	OA8-CA7	4.07	1.45	1.33
14	E	102	PGV	O01-C1	4.07	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	9	101	BCL	O2A-CGA	4.06	1.45	1.33
16	1	103	BCL	O2A-CGA	4.06	1.45	1.33
20	O	101	CDL	OA6-CA5	4.06	1.45	1.34
14	Z	104	PGV	O03-C19	4.06	1.45	1.33
20	M	407	CDL	OA8-CA7	4.05	1.45	1.33
14	0	103	PGV	O01-C1	4.04	1.45	1.34
14	R	104	PGV	O03-C19	4.04	1.45	1.33
20	M	407	CDL	OB6-CB5	4.04	1.45	1.34
14	X	101	PGV	O03-C19	4.03	1.45	1.33
14	L	310	PGV	O01-C1	4.03	1.45	1.34
16	1	102	BCL	C3B-C4B	4.02	1.49	1.41
14	V	103	PGV	O03-C19	4.02	1.45	1.33
16	I	102	BCL	C3B-C4B	4.02	1.49	1.41
14	X	103	PGV	O03-C19	4.02	1.45	1.33
14	8	103	PGV	O01-C1	4.02	1.45	1.34
10	C	404	HEC	CAC-C3C	4.01	1.48	1.35
16	D	101	BCL	O2A-CGA	4.01	1.45	1.33
14	L	309	PGV	O01-C1	4.01	1.45	1.34
14	0	103	PGV	O03-C19	4.00	1.45	1.33
14	6	103	PGV	O01-C1	4.00	1.45	1.34
14	N	101	PGV	O01-C1	3.99	1.45	1.34
16	5	104	BCL	CHD-C1D	3.99	1.46	1.38
20	H	301	CDL	OB6-CB5	3.98	1.45	1.34
14	T	102	PGV	O01-C1	3.97	1.45	1.34
10	C	402	HEC	CAC-C3C	3.97	1.47	1.35
14	H	302	PGV	O03-C19	3.97	1.44	1.33
16	M	403	BCL	O2A-CGA	3.96	1.44	1.33
14	G	101	PGV	O01-C1	3.96	1.45	1.34
14	2	103	PGV	O01-C1	3.96	1.45	1.34
14	B	104	PGV	O03-C19	3.95	1.44	1.33
16	U	103	BCL	C3B-C4B	3.93	1.48	1.41
16	E	101	BCL	C3B-C4B	3.91	1.48	1.41
14	N	105	PGV	O03-C19	3.91	1.44	1.33
14	L	309	PGV	O03-C19	3.91	1.44	1.33
14	N	104	PGV	O01-C1	3.91	1.45	1.34
14	T	103	PGV	O01-C1	3.91	1.45	1.34
16	S	101	BCL	C3B-C4B	3.90	1.48	1.41
16	Q	102	BCL	C3B-C4B	3.90	1.48	1.41
16	1	102	BCL	O2A-CGA	3.90	1.44	1.33
20	M	407	CDL	OA6-CA5	3.90	1.45	1.34
14	H	304	PGV	O01-C1	3.89	1.45	1.34
16	5	103	BCL	O2A-CGA	3.88	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	401	HEC	CAC-C3C	3.87	1.47	1.35
10	C	404	HEC	CAB-C3B	3.87	1.47	1.35
16	O	102	BCL	C3B-C4B	3.87	1.48	1.41
14	C	408	PGV	O01-C1	3.86	1.45	1.34
20	U	101	CDL	OB6-CB5	3.86	1.45	1.34
16	J	101	BCL	C3B-C4B	3.86	1.48	1.41
16	K	101	BCL	C3B-C4B	3.86	1.48	1.41
16	F	103	BCL	C3B-C4B	3.85	1.48	1.41
16	D	101	BCL	C3B-C4B	3.84	1.48	1.41
16	O	103	BCL	C3B-C4B	3.82	1.48	1.41
16	L	302	BCL	C3B-C4B	3.82	1.48	1.41
16	A	101	BCL	C3B-C4B	3.82	1.48	1.41
16	9	101	BCL	C3B-C4B	3.81	1.48	1.41
16	T	101	BCL	C3B-C4B	3.81	1.48	1.41
16	8	102	BCL	C3B-C4B	3.80	1.48	1.41
16	Y	402	BCL	C3B-C4B	3.80	1.48	1.41
16	4	102	BCL	C3B-C4B	3.79	1.48	1.41
16	O	104	BCL	CHD-C1D	3.79	1.45	1.38
16	9	102	BCL	CHD-C1D	3.78	1.45	1.38
16	Y	401	BCL	CHD-C1D	3.78	1.45	1.38
16	S	102	BCL	C3B-C4B	3.78	1.48	1.41
16	6	102	BCL	C3B-C4B	3.78	1.48	1.41
16	K	101	BCL	CHD-C1D	3.76	1.45	1.38
16	7	102	BCL	C3B-C4B	3.75	1.48	1.41
16	X	102	BCL	C3B-C4B	3.73	1.48	1.41
10	C	401	HEC	CAB-C3B	3.73	1.47	1.35
16	1	102	BCL	CHD-C1D	3.72	1.45	1.38
10	C	402	HEC	CAB-C3B	3.72	1.47	1.35
16	D	102	BCL	CHD-C1D	3.71	1.45	1.38
16	N	103	BCL	C3B-C4B	3.71	1.48	1.41
16	D	102	BCL	CHB-C1B	3.71	1.47	1.39
16	O	104	BCL	C3B-C4B	3.71	1.48	1.41
10	C	403	HEC	CAB-C3B	3.70	1.47	1.35
16	3	102	BCL	C3B-C4B	3.69	1.48	1.41
16	4	102	BCL	OBD-CAD	3.67	1.28	1.22
16	R	102	BCL	C3B-C4B	3.67	1.48	1.41
16	U	103	BCL	OBD-CAD	3.67	1.28	1.22
16	I	103	BCL	CHD-C1D	3.65	1.45	1.38
16	T	101	BCL	C1D-ND	-3.65	1.33	1.37
16	A	101	BCL	CHD-C1D	3.65	1.45	1.38
16	6	102	BCL	OBD-CAD	3.64	1.28	1.22
16	1	103	BCL	CHD-C1D	3.64	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	102	BCL	CHD-C1D	3.63	1.45	1.38
16	G	103	BCL	C3B-C4B	3.63	1.48	1.41
16	L	311	BCL	C3B-C4B	3.63	1.48	1.41
16	2	101	BCL	C3B-C4B	3.63	1.48	1.41
16	Y	401	BCL	C3B-C4B	3.62	1.48	1.41
16	W	102	BCL	CHD-C1D	3.62	1.45	1.38
16	Y	402	BCL	CHB-C1B	3.61	1.47	1.39
16	O	103	BCL	CHB-C1B	3.61	1.47	1.39
16	P	101	BCL	C3B-C4B	3.60	1.48	1.41
16	5	104	BCL	CHB-C1B	3.60	1.47	1.39
16	5	104	BCL	C3B-C4B	3.60	1.48	1.41
16	9	102	BCL	C3B-C4B	3.60	1.48	1.41
16	S	102	BCL	CHD-C1D	3.59	1.45	1.38
16	1	103	BCL	CHC-C4B	3.59	1.47	1.39
18	L	307	UQ8	C4-C3	3.58	1.49	1.36
16	W	102	BCL	CHB-C1B	3.57	1.47	1.39
16	N	103	BCL	CHB-C1B	3.56	1.47	1.39
16	O	104	BCL	CHB-C1B	3.56	1.47	1.39
16	Z	102	BCL	C3B-C4B	3.56	1.48	1.41
16	N	103	BCL	OBD-CAD	3.55	1.28	1.22
16	I	103	BCL	CHB-C1B	3.55	1.47	1.39
16	2	101	BCL	CHB-C1B	3.54	1.47	1.39
16	I	102	BCL	OBD-CAD	3.53	1.28	1.22
16	L	312	BCL	CHD-C1D	3.53	1.45	1.38
16	M	403	BCL	CHC-C4B	3.52	1.47	1.39
16	B	102	BCL	C3B-C4B	3.52	1.48	1.41
16	I	102	BCL	CHB-C1B	3.52	1.47	1.39
16	W	101	BCL	CHD-C1D	3.51	1.45	1.38
18	L	306	UQ8	C4-C3	3.51	1.49	1.36
16	3	102	BCL	CHD-C1D	3.51	1.45	1.38
16	7	102	BCL	CHD-C1D	3.51	1.45	1.38
16	L	311	BCL	CHD-C1D	3.50	1.45	1.38
16	L	311	BCL	OBD-CAD	3.50	1.28	1.22
16	E	101	BCL	OBD-CAD	3.50	1.28	1.22
16	9	102	BCL	CHB-C1B	3.50	1.47	1.39
16	R	102	BCL	OBD-CAD	3.50	1.28	1.22
16	1	102	BCL	OBD-CAD	3.50	1.28	1.22
16	0	102	BCL	C1D-ND	-3.49	1.33	1.37
16	I	103	BCL	C3B-C4B	3.49	1.48	1.41
16	W	102	BCL	OBD-CAD	3.49	1.28	1.22
16	U	103	BCL	CHD-C1D	3.48	1.45	1.38
16	G	103	BCL	CHD-C1D	3.48	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	312	BCL	CHB-C1B	3.47	1.47	1.39
16	V	102	BCL	CHB-C1B	3.46	1.47	1.39
16	9	102	BCL	OBD-CAD	3.46	1.28	1.22
16	3	102	BCL	OBD-CAD	3.46	1.28	1.22
16	S	101	BCL	CHD-C1D	3.45	1.45	1.38
16	T	101	BCL	OBD-CAD	3.45	1.28	1.22
16	0	102	BCL	OBD-CAD	3.45	1.28	1.22
16	X	102	BCL	OBD-CAD	3.44	1.28	1.22
16	G	103	BCL	OBD-CAD	3.44	1.28	1.22
16	D	101	BCL	OBD-CAD	3.44	1.28	1.22
16	Y	402	BCL	CHD-C1D	3.44	1.45	1.38
16	9	101	BCL	CHD-C1D	3.44	1.45	1.38
16	L	302	BCL	CHB-C1B	3.44	1.47	1.39
16	Y	402	BCL	OBD-CAD	3.44	1.28	1.22
16	L	311	BCL	CHB-C1B	3.43	1.47	1.39
16	9	101	BCL	CHB-C1B	3.43	1.47	1.39
16	S	101	BCL	OBD-CAD	3.42	1.28	1.22
16	B	102	BCL	CHB-C1B	3.42	1.47	1.39
16	S	102	BCL	CHB-C1B	3.42	1.47	1.39
16	D	102	BCL	C3B-C4B	3.42	1.47	1.41
16	P	101	BCL	OBD-CAD	3.42	1.28	1.22
16	B	102	BCL	OBD-CAD	3.41	1.28	1.22
16	1	103	BCL	OBD-CAD	3.41	1.28	1.22
16	J	101	BCL	OBD-CAD	3.40	1.28	1.22
16	L	312	BCL	OBD-CAD	3.40	1.28	1.22
16	S	101	BCL	CHB-C1B	3.40	1.47	1.39
16	3	102	BCL	CHB-C1B	3.40	1.47	1.39
16	L	302	BCL	OBD-CAD	3.40	1.28	1.22
16	V	102	BCL	OBD-CAD	3.39	1.28	1.22
16	8	102	BCL	OBD-CAD	3.39	1.28	1.22
16	S	102	BCL	OBD-CAD	3.38	1.28	1.22
16	4	102	BCL	CHB-C1B	3.38	1.47	1.39
16	8	102	BCL	CHB-C1B	3.38	1.47	1.39
16	5	103	BCL	CHC-C4B	3.38	1.47	1.39
16	6	102	BCL	CHD-C1D	3.38	1.45	1.38
16	L	302	BCL	CHD-C1D	3.38	1.45	1.38
16	T	101	BCL	CHC-C4B	3.38	1.47	1.39
16	I	103	BCL	OBD-CAD	3.37	1.28	1.22
16	5	103	BCL	OBD-CAD	3.37	1.28	1.22
16	5	104	BCL	OBD-CAD	3.37	1.28	1.22
16	D	101	BCL	CHB-C1B	3.37	1.47	1.39
16	O	103	BCL	OBD-CAD	3.37	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	4	102	BCL	CHD-C1D	3.37	1.45	1.38
16	5	103	BCL	CHB-C1B	3.37	1.47	1.39
16	A	101	BCL	OBD-CAD	3.37	1.28	1.22
16	O	104	BCL	OBD-CAD	3.36	1.28	1.22
16	R	102	BCL	CHB-C1B	3.36	1.47	1.39
16	7	102	BCL	CHB-C1B	3.36	1.46	1.39
16	X	102	BCL	CHB-C1B	3.35	1.46	1.39
16	K	101	BCL	OBD-CAD	3.35	1.28	1.22
16	0	102	BCL	CHC-C4B	3.34	1.46	1.39
16	2	101	BCL	OBD-CAD	3.34	1.28	1.22
16	V	102	BCL	C1D-ND	-3.34	1.33	1.37
16	Z	102	BCL	CHB-C1B	3.33	1.46	1.39
16	Z	102	BCL	OBD-CAD	3.33	1.28	1.22
16	1	103	BCL	CHB-C1B	3.32	1.46	1.39
17	M	404	BPH	C4D-CHA	3.32	1.44	1.39
16	D	102	BCL	OBD-CAD	3.31	1.28	1.22
16	5	104	BCL	CHC-C4B	3.31	1.46	1.39
16	Q	102	BCL	CHB-C1B	3.31	1.46	1.39
16	O	104	BCL	CHC-C4B	3.30	1.46	1.39
16	6	102	BCL	CHB-C1B	3.30	1.46	1.39
16	2	101	BCL	CHC-C4B	3.30	1.46	1.39
16	I	103	BCL	CHC-C4B	3.29	1.46	1.39
16	W	101	BCL	CHB-C1B	3.29	1.46	1.39
16	M	403	BCL	CHD-C1D	3.29	1.44	1.38
16	N	103	BCL	CHD-C1D	3.29	1.44	1.38
16	8	102	BCL	CHC-C4B	3.28	1.46	1.39
16	Q	102	BCL	CHD-C1D	3.28	1.44	1.38
16	0	102	BCL	CHB-C1B	3.28	1.46	1.39
16	G	103	BCL	CHB-C1B	3.28	1.46	1.39
16	5	104	BCL	C4B-NB	-3.28	1.33	1.37
16	K	101	BCL	CHB-C1B	3.27	1.46	1.39
16	S	102	BCL	CHC-C4B	3.27	1.46	1.39
16	V	102	BCL	C3B-C4B	3.26	1.47	1.41
16	D	101	BCL	CHC-C4B	3.26	1.46	1.39
16	9	101	BCL	OBD-CAD	3.26	1.28	1.22
16	R	102	BCL	CHC-C4B	3.26	1.46	1.39
16	P	101	BCL	C1D-ND	-3.25	1.33	1.37
16	G	103	BCL	C4B-NB	-3.25	1.33	1.37
16	W	102	BCL	CHC-C4B	3.25	1.46	1.39
16	Y	401	BCL	CHB-C1B	3.25	1.46	1.39
16	L	302	BCL	CHC-C4B	3.24	1.46	1.39
16	L	312	BCL	CHC-C4B	3.24	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	101	BCL	CHD-C1D	3.23	1.44	1.38
16	Q	102	BCL	OBD-CAD	3.23	1.28	1.22
16	K	101	BCL	CHC-C4B	3.23	1.46	1.39
16	J	101	BCL	CHB-C1B	3.23	1.46	1.39
16	U	103	BCL	CHC-C4B	3.22	1.46	1.39
16	6	102	BCL	CHC-C4B	3.22	1.46	1.39
16	W	101	BCL	CHC-C4B	3.22	1.46	1.39
18	L	304	UQ8	C4-C3	3.22	1.48	1.36
16	X	102	BCL	C1D-ND	-3.22	1.33	1.37
16	B	102	BCL	CHC-C4B	3.22	1.46	1.39
16	5	103	BCL	CHD-C1D	3.22	1.44	1.38
16	8	102	BCL	C1D-ND	-3.22	1.33	1.37
16	D	102	BCL	CHC-C4B	3.22	1.46	1.39
16	R	102	BCL	C1D-ND	-3.22	1.33	1.37
16	1	102	BCL	CHC-C4B	3.21	1.46	1.39
16	P	101	BCL	CHD-C1D	3.21	1.44	1.38
16	O	103	BCL	CHD-C1D	3.21	1.44	1.38
16	P	101	BCL	CHC-C4B	3.20	1.46	1.39
16	Z	102	BCL	C4B-NB	-3.20	1.33	1.37
16	R	102	BCL	CHD-C1D	3.20	1.44	1.38
16	L	311	BCL	CHC-C4B	3.20	1.46	1.39
16	E	101	BCL	CHB-C1B	3.20	1.46	1.39
16	9	102	BCL	C4B-NB	-3.20	1.33	1.37
16	E	101	BCL	CHC-C4B	3.19	1.46	1.39
16	A	101	BCL	CHB-C1B	3.19	1.46	1.39
16	Z	102	BCL	CHC-C4B	3.19	1.46	1.39
16	J	101	BCL	CHC-C4B	3.19	1.46	1.39
16	M	403	BCL	OBD-CAD	3.18	1.28	1.22
16	V	102	BCL	CHC-C4B	3.18	1.46	1.39
16	0	102	BCL	CHD-C1D	3.18	1.44	1.38
16	7	102	BCL	OBD-CAD	3.18	1.28	1.22
16	1	102	BCL	CHB-C1B	3.17	1.46	1.39
16	P	101	BCL	CHB-C1B	3.17	1.46	1.39
16	F	103	BCL	CHB-C1B	3.17	1.46	1.39
16	F	103	BCL	OBD-CAD	3.17	1.27	1.22
16	Z	102	BCL	CHD-C1D	3.16	1.44	1.38
16	U	103	BCL	CHB-C1B	3.16	1.46	1.39
16	Y	401	BCL	CHC-C4B	3.16	1.46	1.39
16	Q	102	BCL	CHC-C4B	3.16	1.46	1.39
16	A	101	BCL	C3D-C2D	3.15	1.47	1.39
16	N	103	BCL	CHC-C4B	3.15	1.46	1.39
16	J	101	BCL	CHD-C1D	3.15	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	9	102	BCL	CHC-C4B	3.15	1.46	1.39
16	V	102	BCL	CHD-C1D	3.15	1.44	1.38
16	9	101	BCL	CHC-C4B	3.14	1.46	1.39
16	T	101	BCL	CHB-C1B	3.14	1.46	1.39
16	S	101	BCL	C4B-NB	-3.14	1.33	1.37
16	M	403	BCL	CHB-C1B	3.14	1.46	1.39
16	J	101	BCL	C1D-ND	-3.14	1.33	1.37
16	A	101	BCL	CHC-C4B	3.13	1.46	1.39
16	G	103	BCL	CHC-C4B	3.13	1.46	1.39
16	E	101	BCL	CHD-C1D	3.12	1.44	1.38
16	6	102	BCL	C1D-ND	-3.11	1.33	1.37
16	2	101	BCL	CHD-C1D	3.11	1.44	1.38
16	T	101	BCL	CHD-C1D	3.11	1.44	1.38
16	E	101	BCL	C1D-ND	-3.11	1.33	1.37
16	4	102	BCL	C3D-C2D	3.11	1.47	1.39
16	9	101	BCL	C4B-NB	-3.10	1.33	1.37
16	L	312	BCL	C4B-NB	-3.10	1.33	1.37
16	5	104	BCL	C3D-C2D	3.10	1.47	1.39
17	L	303	BPH	C4D-CHA	3.10	1.44	1.39
16	I	102	BCL	C3D-C2D	3.10	1.47	1.39
16	F	103	BCL	CHD-C1D	3.09	1.44	1.38
16	3	102	BCL	C3D-C2D	3.07	1.47	1.39
16	6	102	BCL	C3D-C2D	3.07	1.47	1.39
16	N	103	BCL	C1D-ND	-3.07	1.33	1.37
16	S	101	BCL	CHC-C4B	3.07	1.46	1.39
16	I	102	BCL	CHC-C4B	3.07	1.46	1.39
16	F	103	BCL	CHC-C4B	3.06	1.46	1.39
16	N	103	BCL	C3D-C2D	3.06	1.47	1.39
16	X	102	BCL	CHC-C4B	3.06	1.46	1.39
16	4	102	BCL	CHC-C4B	3.06	1.46	1.39
16	G	103	BCL	C3D-C2D	3.06	1.47	1.39
16	W	101	BCL	OBD-CAD	3.06	1.27	1.22
16	Y	402	BCL	C3D-C2D	3.05	1.47	1.39
16	I	103	BCL	C3D-C2D	3.05	1.47	1.39
16	V	102	BCL	C3D-C2D	3.05	1.47	1.39
16	I	103	BCL	C4B-NB	-3.04	1.33	1.37
16	1	102	BCL	C3D-C2D	3.04	1.47	1.39
16	O	103	BCL	CHC-C4B	3.04	1.46	1.39
16	D	102	BCL	C4B-NB	-3.03	1.33	1.37
16	9	102	BCL	C3D-C2D	3.03	1.47	1.39
16	W	101	BCL	C4B-NB	-3.03	1.33	1.37
16	2	101	BCL	C1D-ND	-3.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	101	BCL	C3D-C2D	3.03	1.47	1.39
16	O	103	BCL	C3D-C2D	3.03	1.47	1.39
16	Y	402	BCL	CHC-C4B	3.03	1.46	1.39
16	P	101	BCL	C3D-C2D	3.03	1.47	1.39
16	E	101	BCL	C3D-C2D	3.03	1.47	1.39
16	Q	102	BCL	C3D-C2D	3.02	1.47	1.39
16	G	103	BCL	C1D-ND	-3.02	1.33	1.37
16	7	102	BCL	C4B-NB	-3.02	1.33	1.37
16	B	102	BCL	C3D-C2D	3.01	1.47	1.39
16	O	103	BCL	C1D-ND	-3.01	1.33	1.37
16	1	102	BCL	C4B-NB	-3.01	1.33	1.37
16	D	102	BCL	C3D-C2D	3.00	1.47	1.39
16	3	102	BCL	CHC-C4B	3.00	1.46	1.39
16	B	102	BCL	CHD-C1D	3.00	1.44	1.38
10	C	403	HEC	C1B-NB	-3.00	1.34	1.39
10	C	404	HEC	C1B-NB	-3.00	1.34	1.39
16	B	102	BCL	C4B-NB	-3.00	1.33	1.37
16	7	102	BCL	CHC-C4B	3.00	1.46	1.39
16	E	101	BCL	C4B-NB	-2.99	1.33	1.37
16	Y	401	BCL	OBD-CAD	2.99	1.27	1.22
16	F	103	BCL	C1D-ND	-2.99	1.33	1.37
16	8	102	BCL	CHD-C1D	2.99	1.44	1.38
16	0	102	BCL	C3D-C2D	2.99	1.47	1.39
16	L	311	BCL	C3D-C2D	2.99	1.47	1.39
16	U	103	BCL	C4B-NB	-2.99	1.33	1.37
16	O	103	BCL	C4B-NB	-2.99	1.33	1.37
16	F	103	BCL	C4B-NB	-2.98	1.33	1.37
16	3	102	BCL	C1D-ND	-2.98	1.33	1.37
16	4	102	BCL	C1D-ND	-2.98	1.33	1.37
16	X	102	BCL	CHD-C1D	2.97	1.44	1.38
16	8	102	BCL	C3D-C2D	2.95	1.47	1.39
16	W	102	BCL	C3D-C2D	2.95	1.47	1.39
16	Z	102	BCL	C3D-C2D	2.94	1.47	1.39
16	O	104	BCL	C3D-C2D	2.94	1.47	1.39
16	I	102	BCL	C1D-ND	-2.94	1.34	1.37
10	C	403	HEC	C4B-NB	-2.94	1.34	1.39
16	S	102	BCL	C3D-C2D	2.93	1.47	1.39
16	2	101	BCL	C4B-NB	-2.93	1.34	1.37
16	S	101	BCL	C1D-ND	-2.93	1.34	1.37
16	A	101	BCL	C4B-NB	-2.93	1.34	1.37
16	2	101	BCL	C3D-C2D	2.93	1.47	1.39
16	9	101	BCL	C3D-C2D	2.93	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	102	BCL	C1D-ND	-2.92	1.34	1.37
16	W	101	BCL	C3D-C2D	2.92	1.47	1.39
16	6	102	BCL	C4B-NB	-2.92	1.34	1.37
10	C	404	HEC	C4B-NB	-2.92	1.34	1.39
16	T	101	BCL	C3D-C2D	2.92	1.46	1.39
16	R	102	BCL	C3D-C2D	2.92	1.46	1.39
16	K	101	BCL	C3D-C2D	2.91	1.46	1.39
16	L	311	BCL	C4B-NB	-2.91	1.34	1.37
16	L	312	BCL	C1D-ND	-2.91	1.34	1.37
16	F	103	BCL	C3D-C2D	2.90	1.46	1.39
16	5	103	BCL	C3D-C2D	2.90	1.46	1.39
16	O	104	BCL	CHD-C4C	2.90	1.47	1.39
16	J	101	BCL	C3D-C2D	2.90	1.46	1.39
16	1	102	BCL	C1D-ND	-2.89	1.34	1.37
16	D	101	BCL	C1D-ND	-2.89	1.34	1.37
16	Z	102	BCL	C1D-ND	-2.89	1.34	1.37
10	C	401	HEC	C1B-NB	-2.89	1.34	1.39
16	V	102	BCL	C4B-NB	-2.89	1.34	1.37
16	Y	401	BCL	C4B-NB	-2.89	1.34	1.37
16	S	101	BCL	C3D-C2D	2.88	1.46	1.39
16	D	101	BCL	C4B-NB	-2.88	1.34	1.37
16	S	102	BCL	C1D-ND	-2.87	1.34	1.37
16	0	102	BCL	C4B-NB	-2.87	1.34	1.37
16	3	102	BCL	C4B-NB	-2.87	1.34	1.37
16	Y	401	BCL	CHD-C4C	2.87	1.47	1.39
16	Q	102	BCL	C4B-NB	-2.86	1.34	1.37
16	I	103	BCL	C1D-ND	-2.85	1.34	1.37
16	7	102	BCL	C3D-C2D	2.85	1.46	1.39
16	U	103	BCL	C3D-C2D	2.85	1.46	1.39
16	I	102	BCL	C4B-NB	-2.85	1.34	1.37
16	X	102	BCL	C3D-C2D	2.84	1.46	1.39
16	P	101	BCL	C4B-NB	-2.84	1.34	1.37
16	L	312	BCL	C3D-C2D	2.84	1.46	1.39
16	5	104	BCL	CHD-C4C	2.83	1.47	1.39
16	U	103	BCL	C1D-ND	-2.83	1.34	1.37
16	M	403	BCL	C4B-NB	-2.83	1.34	1.37
10	C	402	HEC	C4B-NB	-2.83	1.34	1.39
16	W	101	BCL	C1D-ND	-2.83	1.34	1.37
16	S	102	BCL	C4B-NB	-2.83	1.34	1.37
16	Y	402	BCL	C1D-ND	-2.82	1.34	1.37
16	M	403	BCL	C1D-ND	-2.82	1.34	1.37
16	U	103	BCL	C1B-NB	-2.82	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	103	BCL	C4B-NB	-2.82	1.34	1.37
16	1	103	BCL	C3D-C2D	2.81	1.46	1.39
16	X	102	BCL	C4B-NB	-2.81	1.34	1.37
16	W	101	BCL	CHD-C4C	2.81	1.47	1.39
16	L	312	BCL	CHD-C4C	2.81	1.47	1.39
16	0	102	BCL	C1B-NB	-2.81	1.34	1.37
16	9	101	BCL	C1D-ND	-2.81	1.34	1.37
16	Y	401	BCL	C1D-C2D	2.81	1.50	1.45
16	1	103	BCL	CHD-C4C	2.80	1.47	1.39
16	K	101	BCL	CHD-C4C	2.80	1.47	1.39
10	C	402	HEC	C4D-ND	-2.80	1.34	1.39
16	D	102	BCL	C1D-ND	-2.80	1.34	1.37
16	L	311	BCL	C1D-ND	-2.79	1.34	1.37
16	9	102	BCL	CHD-C4C	2.79	1.47	1.39
16	D	102	BCL	CHD-C4C	2.78	1.47	1.39
16	L	302	BCL	C3D-C2D	2.78	1.46	1.39
16	L	302	BCL	C1B-C2B	2.78	1.49	1.43
16	1	102	BCL	CHD-C4C	2.77	1.47	1.39
16	A	101	BCL	CHD-C4C	2.77	1.47	1.39
16	U	103	BCL	CHD-C4C	2.77	1.47	1.39
16	A	101	BCL	C1B-NB	-2.76	1.34	1.37
16	K	101	BCL	C4B-NB	-2.76	1.34	1.37
16	Y	401	BCL	C3D-C2D	2.76	1.46	1.39
16	W	102	BCL	CHD-C4C	2.76	1.47	1.39
16	J	101	BCL	C4B-NB	-2.76	1.34	1.37
16	T	101	BCL	C4B-NB	-2.75	1.34	1.37
16	M	403	BCL	C3D-C2D	2.75	1.46	1.39
16	K	101	BCL	C1D-C2D	2.75	1.50	1.45
16	L	302	BCL	C4B-NB	-2.75	1.34	1.37
16	O	104	BCL	C1D-C2D	2.74	1.50	1.45
10	C	403	HEC	C1A-C2A	-2.73	1.40	1.45
10	C	403	HEC	C1D-ND	-2.73	1.34	1.39
16	Y	402	BCL	CHD-C4C	2.73	1.46	1.39
16	W	102	BCL	MG-NC	-2.72	1.99	2.06
16	A	101	BCL	C1D-ND	-2.72	1.34	1.37
10	C	401	HEC	C4B-NB	-2.72	1.34	1.39
16	Q	102	BCL	C1D-ND	-2.72	1.34	1.37
16	K	101	BCL	C1D-ND	-2.72	1.34	1.37
16	4	102	BCL	C4B-NB	-2.71	1.34	1.37
10	C	402	HEC	C1B-NB	-2.71	1.34	1.39
16	1	102	BCL	C1D-C2D	2.71	1.50	1.45
16	I	103	BCL	CHD-C4C	2.70	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	103	BCL	C4B-NB	-2.70	1.34	1.37
16	5	103	BCL	CHD-C4C	2.70	1.46	1.39
16	3	102	BCL	CHD-C4C	2.69	1.46	1.39
10	C	403	HEC	C4D-ND	-2.69	1.34	1.39
16	5	103	BCL	C4B-NB	-2.69	1.34	1.37
16	5	103	BCL	C1D-ND	-2.68	1.34	1.37
16	N	103	BCL	C1B-NB	-2.68	1.34	1.37
16	I	102	BCL	CHD-C4C	2.68	1.46	1.39
16	S	102	BCL	CHD-C4C	2.68	1.46	1.39
10	C	404	HEC	C1D-ND	-2.67	1.34	1.39
16	W	102	BCL	C1D-ND	-2.67	1.34	1.37
16	O	104	BCL	C4B-NB	-2.67	1.34	1.37
16	Y	402	BCL	C4B-NB	-2.66	1.34	1.37
16	L	302	BCL	C1D-ND	-2.66	1.34	1.37
16	7	102	BCL	CHD-C4C	2.66	1.46	1.39
16	L	312	BCL	C1D-C2D	2.65	1.50	1.45
16	W	101	BCL	C1D-C2D	2.65	1.50	1.45
16	L	311	BCL	CHD-C4C	2.65	1.46	1.39
16	D	102	BCL	MG-NC	-2.64	2.00	2.06
16	9	101	BCL	CHD-C4C	2.63	1.46	1.39
16	M	403	BCL	C1B-NB	-2.63	1.34	1.37
16	O	104	BCL	MG-NC	-2.63	2.00	2.06
16	S	101	BCL	CHD-C4C	2.63	1.46	1.39
16	1	103	BCL	MG-NC	-2.63	2.00	2.06
16	1	103	BCL	C1D-C2D	2.63	1.50	1.45
16	S	102	BCL	C1B-NB	-2.62	1.34	1.37
16	5	104	BCL	C1D-ND	-2.62	1.34	1.37
16	F	103	BCL	CHD-C4C	2.62	1.46	1.39
16	W	102	BCL	C1B-C2B	2.62	1.49	1.43
16	R	102	BCL	C4B-NB	-2.61	1.34	1.37
16	L	302	BCL	CHD-C4C	2.61	1.46	1.39
10	C	402	HEC	C1D-ND	-2.61	1.34	1.39
16	3	102	BCL	C1D-C2D	2.60	1.50	1.45
16	W	102	BCL	C1D-C2D	2.60	1.50	1.45
16	J	101	BCL	C1B-NB	-2.60	1.34	1.37
16	9	102	BCL	C1B-C2B	2.59	1.49	1.43
16	D	102	BCL	C1B-C2B	2.59	1.49	1.43
16	5	104	BCL	C1D-C2D	2.59	1.50	1.45
16	U	103	BCL	C1D-C2D	2.59	1.50	1.45
16	9	102	BCL	MG-NC	-2.58	2.00	2.06
16	D	102	BCL	MG-NA	-2.58	2.00	2.06
10	C	401	HEC	C1D-ND	-2.57	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	103	BCL	CHD-C4C	2.55	1.46	1.39
16	O	103	BCL	CHD-C4C	2.55	1.46	1.39
16	P	101	BCL	CHD-C4C	2.55	1.46	1.39
10	C	404	HEC	C4A-C3A	-2.55	1.40	1.45
16	Q	102	BCL	CHD-C4C	2.55	1.46	1.39
16	5	104	BCL	MG-NC	-2.54	2.00	2.06
10	C	404	HEC	C4D-ND	-2.53	1.34	1.39
16	6	102	BCL	CHD-C4C	2.53	1.46	1.39
16	I	102	BCL	C1D-C2D	2.53	1.50	1.45
16	1	102	BCL	MG-NA	-2.53	2.00	2.06
16	1	103	BCL	C1D-ND	-2.52	1.34	1.37
16	4	102	BCL	C1B-NB	-2.51	1.34	1.37
10	C	403	HEC	C4A-C3A	-2.51	1.40	1.45
16	8	102	BCL	C4B-NB	-2.50	1.34	1.37
16	5	104	BCL	C1B-C2B	2.50	1.49	1.43
16	K	101	BCL	C1B-NB	-2.50	1.34	1.37
16	I	103	BCL	MG-NC	-2.50	2.00	2.06
16	M	403	BCL	CHD-C4C	2.50	1.46	1.39
16	2	101	BCL	C1B-C2B	2.50	1.49	1.43
16	I	103	BCL	MG-NA	-2.50	2.00	2.06
16	D	101	BCL	CHD-C4C	2.49	1.46	1.39
16	O	103	BCL	MG-NA	-2.49	2.00	2.06
16	S	101	BCL	C1B-NB	-2.49	1.34	1.37
16	W	102	BCL	MG-NA	-2.49	2.00	2.06
16	4	102	BCL	CHD-C4C	2.49	1.46	1.39
16	S	101	BCL	C1D-C2D	2.49	1.50	1.45
16	3	102	BCL	MG-NA	-2.49	2.00	2.06
16	9	101	BCL	MG-NA	-2.48	2.00	2.06
16	T	101	BCL	C1B-NB	-2.48	1.34	1.37
16	5	103	BCL	C1D-C2D	2.48	1.50	1.45
16	7	102	BCL	C1D-ND	-2.48	1.34	1.37
16	S	101	BCL	MG-NA	-2.48	2.00	2.06
16	B	102	BCL	C1B-C2B	2.48	1.48	1.43
16	7	102	BCL	C1B-NB	-2.47	1.34	1.37
16	X	102	BCL	C1B-NB	-2.47	1.34	1.37
16	O	104	BCL	MG-NA	-2.47	2.00	2.06
16	7	102	BCL	C1D-C2D	2.47	1.50	1.45
17	L	303	BPH	C3A-C2A	-2.46	1.52	1.54
16	0	102	BCL	MG-NC	-2.46	2.00	2.06
16	R	102	BCL	CHD-C4C	2.46	1.46	1.39
16	O	104	BCL	C1B-C2B	2.46	1.48	1.43
16	E	101	BCL	C1B-NB	-2.46	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	9	102	BCL	C1D-C2D	2.46	1.50	1.45
16	F	103	BCL	MG-NA	-2.45	2.00	2.06
16	U	103	BCL	MG-NA	-2.45	2.00	2.06
16	G	103	BCL	C1B-NB	-2.45	1.34	1.37
16	2	101	BCL	MG-NA	-2.45	2.00	2.06
16	N	103	BCL	C1B-C2B	2.45	1.48	1.43
16	9	102	BCL	C1D-ND	-2.44	1.34	1.37
16	L	312	BCL	MG-NA	-2.44	2.00	2.06
16	Y	401	BCL	C1B-C2B	2.44	1.48	1.43
16	L	311	BCL	MG-NA	-2.44	2.00	2.06
20	H	301	CDL	OA8-CA7	2.44	1.45	1.33
16	I	103	BCL	C1B-C2B	2.44	1.48	1.43
16	W	101	BCL	C1B-NB	-2.44	1.34	1.37
16	R	102	BCL	C1B-C2B	2.44	1.48	1.43
16	V	102	BCL	CHD-C4C	2.44	1.46	1.39
16	S	102	BCL	C1B-C2B	2.43	1.48	1.43
16	D	101	BCL	MG-NA	-2.43	2.00	2.06
16	5	104	BCL	C1B-NB	-2.43	1.34	1.37
16	F	103	BCL	C1B-NB	-2.43	1.34	1.37
16	1	102	BCL	C1B-NB	-2.43	1.34	1.37
10	C	401	HEC	C4A-C3A	-2.43	1.40	1.45
16	O	104	BCL	C1D-ND	-2.42	1.34	1.37
16	3	102	BCL	C1B-C2B	2.42	1.48	1.43
16	8	102	BCL	C1B-C2B	2.42	1.48	1.43
16	9	101	BCL	C1B-NB	-2.42	1.34	1.37
16	X	102	BCL	C1B-C2B	2.42	1.48	1.43
10	C	401	HEC	C4D-ND	-2.42	1.35	1.39
16	D	101	BCL	C1D-C2D	2.42	1.50	1.45
16	Q	102	BCL	C1B-NB	-2.41	1.34	1.37
16	J	101	BCL	CHD-C4C	2.41	1.46	1.39
16	1	103	BCL	MG-NA	-2.41	2.00	2.06
16	D	102	BCL	C1D-C2D	2.41	1.50	1.45
16	G	103	BCL	C1B-C2B	2.41	1.48	1.43
16	M	403	BCL	C1D-C2D	2.41	1.50	1.45
16	T	101	BCL	CHD-C4C	2.40	1.45	1.39
16	B	102	BCL	CHD-C4C	2.40	1.45	1.39
16	9	102	BCL	C1B-NB	-2.40	1.34	1.37
16	A	101	BCL	C1D-C2D	2.40	1.50	1.45
16	I	102	BCL	MG-NA	-2.40	2.00	2.06
16	0	102	BCL	MG-NA	-2.40	2.00	2.06
16	I	102	BCL	C1B-NB	-2.40	1.34	1.37
16	N	103	BCL	CHD-C4C	2.39	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	103	BCL	C1B-NB	-2.39	1.34	1.37
16	W	101	BCL	MG-NA	-2.39	2.00	2.06
16	Z	102	BCL	C1B-NB	-2.39	1.34	1.37
16	2	101	BCL	CHD-C4C	2.39	1.45	1.39
16	5	104	BCL	MG-NA	-2.39	2.00	2.06
16	8	102	BCL	CHD-C4C	2.38	1.45	1.39
16	4	102	BCL	C1B-C2B	2.38	1.48	1.43
16	1	102	BCL	MG-NC	-2.37	2.00	2.06
16	F	103	BCL	C1D-C2D	2.37	1.50	1.45
16	I	103	BCL	C1B-NB	-2.37	1.34	1.37
16	I	103	BCL	C1D-C2D	2.37	1.50	1.45
16	D	101	BCL	C1B-NB	-2.36	1.34	1.37
16	8	102	BCL	C3C-C4C	-2.36	1.48	1.51
16	Y	401	BCL	C1D-ND	-2.36	1.34	1.37
16	9	102	BCL	MG-NA	-2.36	2.00	2.06
16	L	311	BCL	C1B-NB	-2.36	1.34	1.37
16	5	103	BCL	C1B-C2B	2.36	1.48	1.43
16	W	102	BCL	C1B-NB	-2.36	1.34	1.37
16	6	102	BCL	C1B-NB	-2.35	1.34	1.37
16	V	102	BCL	C1B-C2B	2.35	1.48	1.43
10	C	404	HEC	C1A-C2A	-2.35	1.41	1.45
16	5	103	BCL	MG-NA	-2.35	2.00	2.06
16	S	102	BCL	C1D-C2D	2.35	1.50	1.45
16	Z	102	BCL	CHD-C4C	2.35	1.45	1.39
16	O	103	BCL	C1D-C2D	2.34	1.50	1.45
16	Y	402	BCL	C1B-NB	-2.34	1.34	1.37
16	7	102	BCL	MG-NA	-2.34	2.00	2.06
16	B	102	BCL	MG-NA	-2.34	2.00	2.06
16	0	102	BCL	C1B-C2B	2.33	1.48	1.43
16	O	103	BCL	C1B-C2B	2.33	1.48	1.43
16	7	102	BCL	C1B-C2B	2.33	1.48	1.43
16	E	101	BCL	CHD-C4C	2.33	1.45	1.39
16	1	103	BCL	C1B-NB	-2.33	1.34	1.37
17	L	303	BPH	C1B-C2B	2.33	1.42	1.39
16	Y	402	BCL	C1B-C2B	2.33	1.48	1.43
16	Q	102	BCL	C1B-C2B	2.33	1.48	1.43
16	E	101	BCL	C1B-C2B	2.32	1.48	1.43
16	0	102	BCL	CHD-C4C	2.32	1.45	1.39
16	M	403	BCL	MG-NA	-2.32	2.00	2.06
16	I	102	BCL	C1B-C2B	2.31	1.48	1.43
16	L	302	BCL	C1D-C2D	2.31	1.49	1.45
16	8	102	BCL	C1B-NB	-2.31	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	311	BCL	C1D-C2D	2.31	1.49	1.45
16	3	102	BCL	C1B-NB	-2.30	1.34	1.37
16	D	102	BCL	C1B-NB	-2.30	1.34	1.37
16	W	102	BCL	C4B-NB	-2.30	1.34	1.37
16	T	101	BCL	MG-NA	-2.30	2.00	2.06
16	V	102	BCL	C1B-NB	-2.30	1.34	1.37
16	P	101	BCL	C1B-C2B	2.30	1.48	1.43
17	M	404	BPH	C3A-C2A	-2.30	1.52	1.54
16	Y	402	BCL	C1D-C2D	2.30	1.49	1.45
16	T	101	BCL	MG-NC	-2.29	2.00	2.06
16	U	103	BCL	MG-NC	-2.29	2.00	2.06
16	4	102	BCL	MG-NA	-2.29	2.00	2.06
16	X	102	BCL	CHD-C4C	2.28	1.45	1.39
16	P	101	BCL	MG-NA	-2.28	2.00	2.06
16	G	103	BCL	C1D-C2D	2.27	1.49	1.45
16	T	101	BCL	C1B-C2B	2.27	1.48	1.43
16	Z	102	BCL	C1B-C2B	2.27	1.48	1.43
16	9	101	BCL	C1D-C2D	2.27	1.49	1.45
16	L	312	BCL	C1B-NB	-2.27	1.34	1.37
16	R	102	BCL	MG-NA	-2.26	2.00	2.06
10	C	402	HEC	C1A-C2A	-2.26	1.41	1.45
16	O	103	BCL	C3C-C4C	-2.26	1.48	1.51
10	C	402	HEC	C4A-C3A	-2.25	1.40	1.45
16	R	102	BCL	MG-NC	-2.25	2.00	2.06
16	O	103	BCL	C1B-NB	-2.25	1.34	1.37
16	Y	401	BCL	MG-NC	-2.25	2.00	2.06
16	8	102	BCL	MG-NC	-2.25	2.00	2.06
16	R	102	BCL	C1B-NB	-2.24	1.34	1.37
16	Q	102	BCL	MG-NA	-2.24	2.00	2.06
16	L	311	BCL	C1B-C2B	2.24	1.48	1.43
16	D	101	BCL	MG-NC	-2.23	2.01	2.06
16	6	102	BCL	C1B-C2B	2.23	1.48	1.43
16	Y	401	BCL	C1B-NB	-2.23	1.34	1.37
16	O	103	BCL	MG-NC	-2.23	2.01	2.06
16	Q	102	BCL	C1D-C2D	2.23	1.49	1.45
16	J	101	BCL	MG-NC	-2.22	2.01	2.06
16	K	101	BCL	MG-NC	-2.21	2.01	2.06
16	D	101	BCL	C1B-C2B	2.20	1.48	1.43
16	T	101	BCL	C3C-C4C	-2.19	1.48	1.51
16	E	101	BCL	MG-NA	-2.19	2.01	2.06
16	L	302	BCL	C1B-NB	-2.19	1.35	1.37
16	9	101	BCL	C1B-C2B	2.19	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	101	BCL	C1B-C2B	2.19	1.48	1.43
16	S	102	BCL	MG-NC	-2.19	2.01	2.06
16	V	102	BCL	MG-NA	-2.18	2.01	2.06
16	J	101	BCL	MG-NA	-2.18	2.01	2.06
16	Y	402	BCL	MG-NA	-2.18	2.01	2.06
16	8	102	BCL	C1D-C2D	2.18	1.49	1.45
16	B	102	BCL	MG-NC	-2.18	2.01	2.06
16	P	101	BCL	MG-NC	-2.17	2.01	2.06
16	S	102	BCL	MG-NA	-2.17	2.01	2.06
16	5	103	BCL	MG-NC	-2.17	2.01	2.06
16	G	103	BCL	CHC-C1C	-2.17	1.32	1.37
16	U	103	BCL	CHB-C4A	-2.17	1.32	1.37
16	4	102	BCL	C1D-C2D	2.17	1.49	1.45
16	L	311	BCL	MG-NC	-2.17	2.01	2.06
16	O	104	BCL	C1B-NB	-2.16	1.35	1.37
16	1	102	BCL	C1B-C2B	2.16	1.48	1.43
16	N	103	BCL	MG-NA	-2.15	2.01	2.06
16	7	102	BCL	CHC-C1C	-2.15	1.32	1.37
16	9	101	BCL	MG-NC	-2.15	2.01	2.06
16	X	102	BCL	MG-NA	-2.14	2.01	2.06
16	K	101	BCL	C1B-C2B	2.14	1.48	1.43
16	Z	102	BCL	CHC-C1C	-2.14	1.32	1.37
16	4	102	BCL	MG-NC	-2.13	2.01	2.06
16	R	102	BCL	C1D-C2D	2.13	1.49	1.45
16	6	102	BCL	C1D-C2D	2.13	1.49	1.45
16	A	101	BCL	CHB-C4A	-2.13	1.32	1.37
16	B	102	BCL	C3C-C4C	-2.13	1.48	1.51
16	S	101	BCL	CHC-C1C	-2.13	1.32	1.37
16	6	102	BCL	MG-NC	-2.13	2.01	2.06
16	K	101	BCL	MG-NA	-2.12	2.01	2.06
16	R	102	BCL	C3C-C4C	-2.12	1.48	1.51
16	B	102	BCL	CHC-C1C	-2.12	1.32	1.37
16	1	103	BCL	C1B-C2B	2.11	1.48	1.43
16	I	102	BCL	CHC-C1C	-2.11	1.32	1.37
16	2	101	BCL	MG-NC	-2.10	2.01	2.06
16	2	101	BCL	C3C-C4C	-2.10	1.48	1.51
16	G	103	BCL	MG-NC	-2.10	2.01	2.06
16	X	102	BCL	MG-NC	-2.10	2.01	2.06
16	9	102	BCL	CHC-C1C	-2.10	1.32	1.37
16	P	101	BCL	C1B-NB	-2.10	1.35	1.37
16	L	312	BCL	C1B-C2B	2.10	1.48	1.43
16	8	102	BCL	MG-NA	-2.09	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	401	HEC	C1A-C2A	-2.09	1.41	1.45
16	M	403	BCL	MG-NC	-2.09	2.01	2.06
10	C	401	HEC	C3C-C4C	-2.09	1.42	1.46
16	D	101	BCL	C3C-C4C	-2.09	1.49	1.51
16	X	102	BCL	C3C-C4C	-2.09	1.49	1.51
16	E	101	BCL	MG-NC	-2.09	2.01	2.06
16	6	102	BCL	MG-NA	-2.08	2.01	2.06
16	Z	102	BCL	MG-NC	-2.08	2.01	2.06
16	3	102	BCL	CHC-C1C	-2.08	1.32	1.37
16	Z	102	BCL	MG-NA	-2.08	2.01	2.06
16	W	101	BCL	C1B-C2B	2.08	1.48	1.43
16	N	103	BCL	MG-NC	-2.07	2.01	2.06
16	S	101	BCL	C1B-C2B	2.07	1.48	1.43
16	Y	401	BCL	MG-NA	-2.07	2.01	2.06
16	2	101	BCL	C1D-C2D	2.07	1.49	1.45
10	C	402	HEC	C3C-C4C	-2.07	1.42	1.46
16	A	101	BCL	C4D-CHA	2.06	1.45	1.38
16	Y	402	BCL	CHC-C1C	-2.06	1.32	1.37
16	F	103	BCL	C1B-C2B	2.06	1.48	1.43
16	P	101	BCL	C1D-C2D	2.06	1.49	1.45
16	B	102	BCL	C1B-NB	-2.06	1.35	1.37
16	D	101	BCL	CHC-C1C	-2.06	1.32	1.37
17	M	404	BPH	CBD-CGD	-2.06	1.49	1.52
16	V	102	BCL	MG-NC	-2.05	2.01	2.06
16	D	102	BCL	CHC-C1C	-2.05	1.32	1.37
16	I	102	BCL	MG-NC	-2.05	2.01	2.06
16	J	101	BCL	C1D-C2D	2.03	1.49	1.45
16	N	103	BCL	CHC-C1C	-2.03	1.32	1.37
16	U	103	BCL	C3C-C4C	-2.03	1.49	1.51
16	P	101	BCL	C3C-C4C	-2.03	1.49	1.51
16	Y	401	BCL	CHB-C4A	-2.03	1.32	1.37
16	F	103	BCL	CHC-C1C	-2.03	1.32	1.37
16	V	102	BCL	C3C-C4C	-2.03	1.49	1.51
16	U	103	BCL	C1B-C2B	2.03	1.47	1.43
16	Q	102	BCL	C3C-C4C	-2.03	1.49	1.51
16	S	101	BCL	MG-NC	-2.03	2.01	2.06
16	0	102	BCL	C3C-C4C	-2.02	1.49	1.51
16	A	101	BCL	C1B-C2B	2.02	1.47	1.43
16	J	101	BCL	C3C-C4C	-2.02	1.49	1.51
16	K	101	BCL	CHC-C1C	-2.02	1.32	1.37
16	N	103	BCL	C3C-C4C	-2.02	1.49	1.51
16	V	102	BCL	CHC-C1C	-2.02	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	102	BCL	MG-NC	-2.02	2.01	2.06
16	B	102	BCL	C1D-C2D	2.02	1.49	1.45
16	A	101	BCL	CHC-C1C	-2.02	1.32	1.37
16	X	102	BCL	CHC-C1C	-2.02	1.32	1.37
16	4	102	BCL	C3C-C4C	-2.01	1.49	1.51
16	O	103	BCL	C4D-CHA	2.01	1.45	1.38
16	A	101	BCL	MG-NA	-2.01	2.01	2.06
10	C	403	HEC	O2D-CGD	-2.01	1.24	1.30
16	J	101	BCL	CHB-C4A	-2.01	1.32	1.37
16	N	103	BCL	C1D-C2D	2.01	1.49	1.45
16	J	101	BCL	CHC-C1C	-2.00	1.32	1.37
16	1	103	BCL	C3C-C4C	-2.00	1.49	1.51
16	L	302	BCL	MG-NA	-2.00	2.01	2.06

All (1482) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	401	BCL	CMD-C2D-C1D	8.69	140.03	124.73
16	L	312	BCL	CMD-C2D-C1D	8.31	139.36	124.73
16	M	403	BCL	CMD-C2D-C1D	8.29	139.32	124.73
16	O	104	BCL	CMD-C2D-C1D	8.28	139.32	124.73
16	S	101	BCL	CMD-C2D-C1D	8.21	139.19	124.73
16	W	101	BCL	CMD-C2D-C1D	8.13	139.05	124.73
16	1	103	BCL	CMD-C2D-C1D	8.09	138.98	124.73
16	L	302	BCL	CMD-C2D-C1D	8.07	138.94	124.73
16	7	102	BCL	CMD-C2D-C1D	8.02	138.85	124.73
16	K	101	BCL	CMD-C2D-C1D	8.02	138.85	124.73
16	U	103	BCL	CMD-C2D-C1D	7.94	138.71	124.73
16	W	102	BCL	CMD-C2D-C1D	7.87	138.59	124.73
16	5	103	BCL	CMD-C2D-C1D	7.82	138.50	124.73
16	9	101	BCL	CMD-C2D-C1D	7.70	138.29	124.73
16	1	102	BCL	CMD-C2D-C1D	7.67	138.23	124.73
16	D	102	BCL	CMD-C2D-C1D	7.61	138.12	124.73
16	I	103	BCL	CMD-C2D-C1D	7.58	138.08	124.73
16	9	102	BCL	CMD-C2D-C1D	7.58	138.08	124.73
16	Q	102	BCL	CMD-C2D-C1D	7.53	137.98	124.73
16	F	103	BCL	CMD-C2D-C1D	7.49	137.92	124.73
16	5	104	BCL	CMD-C2D-C1D	7.47	137.88	124.73
16	3	102	BCL	CMD-C2D-C1D	7.45	137.85	124.73
16	O	103	BCL	CMD-C2D-C1D	7.41	137.77	124.73
16	D	101	BCL	CMD-C2D-C1D	7.37	137.71	124.73
16	Y	402	BCL	CMD-C2D-C1D	7.34	137.66	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	S	102	BCL	CMD-C2D-C1D	7.33	137.64	124.73
16	A	101	BCL	CMD-C2D-C1D	7.31	137.61	124.73
16	J	101	BCL	CMD-C2D-C1D	7.11	137.25	124.73
16	I	102	BCL	CMD-C2D-C1D	7.11	137.24	124.73
16	L	311	BCL	CMD-C2D-C1D	7.10	137.23	124.73
16	G	103	BCL	CMD-C2D-C1D	7.05	137.14	124.73
16	2	101	BCL	CMD-C2D-C1D	6.98	137.03	124.73
16	1	102	BCL	C2B-C1B-NB	6.97	117.55	110.33
16	8	102	BCL	CMD-C2D-C1D	6.85	136.80	124.73
16	R	102	BCL	CMD-C2D-C1D	6.85	136.79	124.73
22	M	406	CRT	C37-C36-C35	-6.73	115.46	124.91
16	E	101	BCL	C2B-C1B-NB	6.73	117.31	110.33
16	4	102	BCL	CMD-C2D-C1D	6.70	136.52	124.73
16	L	312	BCL	C2B-C1B-NB	6.67	117.24	110.33
16	B	102	BCL	CMD-C2D-C1D	6.63	136.40	124.73
16	Z	102	BCL	CMD-C2D-C1D	6.61	136.37	124.73
16	W	101	BCL	C2B-C1B-NB	6.61	117.18	110.33
16	U	103	BCL	C2B-C1B-NB	6.61	117.18	110.33
16	L	312	BCL	O2D-CGD-CBD	6.61	122.79	111.23
16	M	403	BCL	C2B-C1B-NB	6.60	117.17	110.33
16	F	103	BCL	C2B-C1B-NB	6.60	117.17	110.33
16	1	103	BCL	C2B-C1B-NB	6.58	117.15	110.33
16	A	101	BCL	C2B-C1B-NB	6.58	117.15	110.33
16	6	102	BCL	CMD-C2D-C1D	6.54	136.24	124.73
16	Q	102	BCL	C2B-C1B-NB	6.51	117.08	110.33
16	X	102	BCL	C2B-C1B-NB	6.50	117.07	110.33
16	6	102	BCL	C2B-C1B-NB	6.50	117.06	110.33
16	N	103	BCL	CMD-C2D-C1D	6.50	136.17	124.73
16	5	103	BCL	C2B-C1B-NB	6.47	117.04	110.33
16	P	101	BCL	CMD-C2D-C1D	6.47	136.12	124.73
16	3	102	BCL	C2B-C1B-NB	6.46	117.02	110.33
16	G	103	BCL	C2B-C1B-NB	6.44	117.00	110.33
16	K	101	BCL	C2B-C1B-NB	6.41	116.98	110.33
16	T	101	BCL	C2B-C1B-NB	6.39	116.96	110.33
16	4	102	BCL	C2B-C1B-NB	6.39	116.95	110.33
16	J	101	BCL	C2B-C1B-NB	6.39	116.95	110.33
16	P	101	BCL	C2B-C1B-NB	6.38	116.95	110.33
16	R	102	BCL	C2B-C1B-NB	6.38	116.95	110.33
16	E	101	BCL	CMD-C2D-C1D	6.35	135.91	124.73
16	X	102	BCL	CMD-C2D-C1D	6.34	135.90	124.73
16	Z	102	BCL	C2B-C1B-NB	6.32	116.89	110.33
16	D	101	BCL	C2B-C1B-NB	6.30	116.86	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	101	BCL	CMD-C2D-C1D	6.28	135.80	124.73
16	8	102	BCL	C2B-C1B-NB	6.28	116.84	110.33
16	7	102	BCL	C2B-C1B-NB	6.28	116.84	110.33
16	V	102	BCL	CMD-C2D-C1D	6.28	135.78	124.73
16	L	302	BCL	C2B-C1B-NB	6.26	116.82	110.33
16	S	102	BCL	C2B-C1B-NB	6.22	116.78	110.33
16	0	102	BCL	CMD-C2D-C1D	6.22	135.68	124.73
16	I	102	BCL	C2B-C1B-NB	6.18	116.73	110.33
16	Y	402	BCL	C2B-C1B-NB	6.17	116.73	110.33
16	0	102	BCL	C2B-C1B-NB	6.17	116.72	110.33
16	S	101	BCL	C2B-C1B-NB	6.14	116.70	110.33
16	N	103	BCL	C2B-C1B-NB	6.14	116.69	110.33
16	L	311	BCL	C2B-C1B-NB	6.12	116.67	110.33
16	B	102	BCL	C2B-C1B-NB	6.12	116.67	110.33
16	O	103	BCL	C2B-C1B-NB	6.09	116.65	110.33
16	Y	401	BCL	C2B-C1B-NB	6.08	116.63	110.33
16	L	312	BCL	CHD-C1D-ND	-6.05	116.28	124.80
16	L	311	BCL	O2D-CGD-CBD	6.03	121.77	111.23
16	U	103	BCL	CHD-C1D-ND	-6.02	116.33	124.80
16	9	101	BCL	C2B-C1B-NB	6.01	116.56	110.33
22	V	101	CRT	C21-C22-C23	-6.01	118.85	127.28
16	2	101	BCL	C2B-C1B-NB	6.00	116.55	110.33
16	1	102	BCL	CHD-C1D-ND	-5.99	116.38	124.80
22	B	101	CRT	C4-C5-C6	-5.99	116.51	124.91
16	I	103	BCL	C2B-C1B-NB	5.98	116.53	110.33
16	W	102	BCL	C2B-C1B-NB	5.98	116.53	110.33
16	W	101	BCL	CHD-C1D-ND	-5.98	116.39	124.80
16	O	104	BCL	CHD-C1D-ND	-5.96	116.42	124.80
16	I	102	BCL	CHD-C1D-ND	-5.94	116.45	124.80
16	3	102	BCL	CHD-C1D-ND	-5.93	116.46	124.80
16	S	101	BCL	CHD-C1D-ND	-5.90	116.49	124.80
16	K	101	BCL	CHD-C1D-ND	-5.89	116.51	124.80
22	4	101	CRT	C37-C36-C35	-5.89	116.64	124.91
16	W	102	BCL	CHD-C1D-ND	-5.85	116.56	124.80
16	9	102	BCL	C2B-C1B-NB	5.84	116.38	110.33
16	O	103	BCL	CHD-C1D-ND	-5.81	116.62	124.80
16	0	102	BCL	O2D-CGD-CBD	5.80	121.37	111.23
16	O	104	BCL	C2B-C1B-NB	5.79	116.33	110.33
16	1	103	BCL	CHD-C1D-ND	-5.78	116.67	124.80
16	Y	401	BCL	CHD-C1D-ND	-5.77	116.67	124.80
16	9	101	BCL	CHD-C1D-ND	-5.74	116.72	124.80
16	5	104	BCL	C2B-C1B-NB	5.72	116.26	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	311	BCL	CHD-C1D-ND	-5.71	116.77	124.80
10	C	403	HEC	CHC-C4B-NB	5.70	130.66	124.45
16	D	101	BCL	CHD-C1D-ND	-5.69	116.79	124.80
16	V	102	BCL	C2B-C1B-NB	5.67	116.20	110.33
16	5	103	BCL	CHD-C1D-ND	-5.66	116.83	124.80
16	A	101	BCL	CHD-C1D-ND	-5.66	116.83	124.80
16	E	101	BCL	O2D-CGD-CBD	5.66	121.13	111.23
16	7	102	BCL	CHD-C1D-ND	-5.65	116.85	124.80
16	5	104	BCL	CHD-C1D-ND	-5.64	116.86	124.80
16	M	403	BCL	CHD-C1D-ND	-5.64	116.87	124.80
22	B	101	CRT	C3-C1-C2	5.61	120.69	110.43
16	F	103	BCL	CHD-C1D-ND	-5.60	116.92	124.80
22	V	101	CRT	C37-C36-C35	-5.59	117.06	124.91
22	G	102	CRT	C21-C22-C23	-5.58	119.45	127.28
22	R	101	CRT	C3-C1-C2	5.55	120.57	110.43
16	Y	402	BCL	CHD-C1D-ND	-5.54	117.01	124.80
16	Q	102	BCL	CHD-C1D-ND	-5.53	117.02	124.80
16	D	102	BCL	CHD-C1D-ND	-5.51	117.05	124.80
22	N	102	CRT	C3-C1-C2	5.50	120.48	110.43
16	D	102	BCL	O2D-CGD-CBD	5.50	120.84	111.23
22	8	101	CRT	C3-C1-C2	5.48	120.45	110.43
22	8	101	CRT	C37-C36-C35	-5.47	117.23	124.91
16	D	102	BCL	C2B-C1B-NB	5.43	115.95	110.33
16	9	102	BCL	CHD-C1D-ND	-5.40	117.20	124.80
22	4	101	CRT	C3-C1-C2	5.39	120.29	110.43
16	9	102	BCL	O2D-CGD-CBD	5.37	120.62	111.23
22	N	102	CRT	C37-C36-C35	-5.36	117.39	124.91
22	M	406	CRT	C20-C19-C17	-5.33	119.80	127.28
16	8	102	BCL	CHD-C1D-ND	-5.31	117.33	124.80
16	R	102	BCL	CHD-C1D-ND	-5.30	117.34	124.80
16	N	103	BCL	O2D-CGD-CBD	5.29	120.48	111.23
10	C	402	HEC	CHC-C4B-NB	5.29	130.21	124.45
16	1	103	BCL	O2D-CGD-CBD	5.28	120.47	111.23
16	I	103	BCL	CHD-C1D-ND	-5.28	117.37	124.80
16	L	302	BCL	CHD-C1D-ND	-5.27	117.39	124.80
16	L	302	BCL	C3D-C2D-C1D	-5.26	98.65	105.83
22	B	101	CRT	C21-C22-C23	-5.26	119.90	127.28
22	M	406	CRT	C21-C22-C23	-5.25	119.91	127.28
16	4	102	BCL	CHD-C1D-ND	-5.25	117.41	124.80
16	F	103	BCL	O2D-CGD-CBD	5.22	120.36	111.23
16	P	101	BCL	CHD-C1D-ND	-5.22	117.46	124.80
16	J	101	BCL	O2D-CGD-CBD	5.21	120.34	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	403	CRT	C37-C36-C35	-5.21	117.60	124.91
16	O	104	BCL	O2D-CGD-CBD	5.20	120.33	111.23
16	S	102	BCL	CHD-C1D-ND	-5.19	117.50	124.80
22	B	101	CRT	C37-C36-C35	-5.18	117.64	124.91
16	T	101	BCL	CHD-C1D-ND	-5.17	117.53	124.80
16	F	103	BCL	C3D-C2D-C1D	-5.16	98.79	105.83
22	G	102	CRT	C37-C36-C35	-5.16	117.67	124.91
16	Y	401	BCL	O2D-CGD-CBD	5.16	120.24	111.23
10	C	401	HEC	CHC-C4B-NB	5.15	130.06	124.45
22	Y	403	CRT	C3-C1-C2	5.14	119.83	110.43
16	I	103	BCL	O2D-CGD-CBD	5.10	120.14	111.23
16	J	101	BCL	CHD-C1D-ND	-5.09	117.64	124.80
22	4	101	CRT	C4-C5-C6	-5.07	117.79	124.91
16	W	101	BCL	O2D-CGD-CBD	5.07	120.09	111.23
16	2	101	BCL	CHD-C1D-ND	-5.06	117.68	124.80
16	D	101	BCL	O2D-CGD-CBD	5.04	120.05	111.23
16	G	103	BCL	CHD-C1D-ND	-5.04	117.71	124.80
22	N	102	CRT	C4-C5-C6	-5.02	117.86	124.91
16	O	103	BCL	C3D-C2D-C1D	-5.01	99.00	105.83
16	6	102	BCL	O2D-CGD-CBD	4.99	119.95	111.23
16	5	103	BCL	C3D-C2D-C1D	-4.99	99.02	105.83
16	X	102	BCL	O2D-CGD-CBD	4.97	119.92	111.23
16	M	403	BCL	C3D-C2D-C1D	-4.97	99.05	105.83
22	R	101	CRT	C37-C36-C35	-4.97	117.94	124.91
16	O	103	BCL	O2D-CGD-CBD	4.96	119.91	111.23
16	5	104	BCL	O2D-CGD-CBD	4.96	119.90	111.23
16	9	101	BCL	C3D-C2D-C1D	-4.95	99.07	105.83
16	N	103	BCL	CHD-C1D-ND	-4.95	117.83	124.80
22	Y	403	CRT	C21-C22-C23	-4.95	120.34	127.28
16	B	102	BCL	CHD-C1D-ND	-4.95	117.84	124.80
16	Q	102	BCL	C3D-C2D-C1D	-4.95	99.08	105.83
16	Y	401	BCL	C3D-C2D-C1D	-4.93	99.11	105.83
16	2	101	BCL	O2D-CGD-CBD	4.91	119.82	111.23
22	R	101	CRT	C21-C22-C23	-4.91	120.39	127.28
16	Z	102	BCL	C3D-C2D-C1D	-4.91	99.13	105.83
16	X	102	BCL	C3C-C4C-CHD	-4.90	113.05	123.39
16	S	102	BCL	O2D-CGD-CBD	4.90	119.80	111.23
16	D	101	BCL	C3D-C2D-C1D	-4.90	99.14	105.83
16	Q	102	BCL	C3C-C4C-CHD	-4.88	113.09	123.39
16	W	101	BCL	C3D-C2D-C1D	-4.87	99.19	105.83
16	7	102	BCL	C3D-C2D-C1D	-4.86	99.19	105.83
20	H	301	CDL	OA6-CA5-C11	4.86	122.00	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	8	102	BCL	C3D-C2D-C1D	-4.86	99.20	105.83
16	X	102	BCL	C3D-C2D-C1D	-4.85	99.21	105.83
16	D	101	BCL	C1-C2-C3	-4.85	118.25	126.20
16	4	102	BCL	C3C-C4C-CHD	-4.85	113.17	123.39
16	Z	102	BCL	C3C-C4C-CHD	-4.84	113.19	123.39
16	I	103	BCL	C3D-C2D-C1D	-4.84	99.23	105.83
16	8	102	BCL	C3C-C4C-CHD	-4.83	113.20	123.39
16	T	101	BCL	O2D-CGD-CBD	4.83	119.68	111.23
16	1	103	BCL	C3D-C2D-C1D	-4.83	99.24	105.83
22	G	102	CRT	C20-C19-C17	-4.83	120.51	127.28
16	U	103	BCL	C3D-C2D-C1D	-4.82	99.25	105.83
16	W	102	BCL	O2D-CGD-CBD	4.82	119.65	111.23
16	2	101	BCL	C3D-C2D-C1D	-4.82	99.26	105.83
16	E	101	BCL	C3C-C4C-CHD	-4.81	113.26	123.39
16	W	102	BCL	C3D-C2D-C1D	-4.80	99.29	105.83
16	K	101	BCL	C3D-C2D-C1D	-4.79	99.29	105.83
16	B	102	BCL	C3D-C2D-C1D	-4.79	99.30	105.83
16	8	102	BCL	O2D-CGD-CBD	4.78	119.59	111.23
16	9	102	BCL	C3D-C2D-C1D	-4.78	99.31	105.83
16	L	311	BCL	C3D-C2D-C1D	-4.78	99.31	105.83
16	6	102	BCL	CHD-C1D-ND	-4.78	118.08	124.80
16	A	101	BCL	O2D-CGD-CBD	4.77	119.58	111.23
16	P	101	BCL	O2D-CGD-CBD	4.77	119.58	111.23
10	C	404	HEC	CHC-C4B-NB	4.77	129.65	124.45
22	V	101	CRT	C3-C1-C2	4.77	119.14	110.43
16	O	103	BCL	C3C-C4C-CHD	-4.76	113.35	123.39
16	Q	102	BCL	O2D-CGD-CBD	4.76	119.56	111.23
16	V	102	BCL	C3C-C4C-CHD	-4.76	113.36	123.39
16	S	101	BCL	C3D-C2D-C1D	-4.76	99.34	105.83
16	9	101	BCL	O2D-CGD-CBD	4.75	119.54	111.23
22	N	102	CRT	C21-C22-C23	-4.75	120.62	127.28
16	X	102	BCL	CHD-C1D-ND	-4.75	118.12	124.80
16	Z	102	BCL	CHD-C1D-ND	-4.75	118.12	124.80
16	I	102	BCL	C3D-C2D-C1D	-4.74	99.36	105.83
20	U	102	CDL	OA6-CA5-C11	4.73	119.53	111.09
16	O	104	BCL	C3D-C2D-C1D	-4.73	99.37	105.83
16	K	101	BCL	O2D-CGD-CBD	4.73	119.50	111.23
16	E	101	BCL	CHD-C1D-ND	-4.72	118.16	124.80
16	R	102	BCL	C3D-C2D-C1D	-4.71	99.40	105.83
16	G	103	BCL	C3D-C2D-C1D	-4.71	99.40	105.83
16	B	102	BCL	C3C-C4C-CHD	-4.71	113.46	123.39
16	A	101	BCL	C3D-C2D-C1D	-4.71	99.40	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	0	102	BCL	CHD-C1D-ND	-4.71	118.18	124.80
16	1	102	BCL	O2D-CGD-CBD	4.71	119.46	111.23
16	Y	402	BCL	C3D-C2D-C1D	-4.70	99.42	105.83
16	V	102	BCL	C3D-C2D-C1D	-4.70	99.42	105.83
16	M	403	BCL	C3C-C4C-CHD	-4.69	113.50	123.39
16	2	101	BCL	C3C-C4C-CHD	-4.69	113.50	123.39
16	J	101	BCL	C3C-C4C-CHD	-4.68	113.52	123.39
20	U	101	CDL	OB6-CB5-C51	4.67	121.59	111.48
22	M	406	CRT	C10-C9-C7	-4.67	120.73	127.28
22	V	101	CRT	C26-C27-C28	-4.66	120.74	127.28
16	4	102	BCL	C3D-C2D-C1D	-4.66	99.47	105.83
16	N	103	BCL	C3D-C2D-C1D	-4.66	99.47	105.83
16	I	103	BCL	C1-C2-C3	-4.66	118.57	126.20
16	D	102	BCL	C3D-C2D-C1D	-4.65	99.48	105.83
16	N	103	BCL	C3C-C4C-CHD	-4.65	113.58	123.39
16	V	102	BCL	CHD-C1D-ND	-4.64	118.27	124.80
22	G	102	CRT	C3-C1-C2	4.64	118.90	110.43
16	R	102	BCL	C3C-C4C-CHD	-4.64	113.62	123.39
16	P	101	BCL	C1D-ND-C4D	-4.63	103.06	106.31
16	L	302	BCL	C3C-C4C-CHD	-4.63	113.63	123.39
16	P	101	BCL	C3D-C2D-C1D	-4.63	99.52	105.83
16	S	101	BCL	O2D-CGD-CBD	4.62	119.31	111.23
16	L	312	BCL	C3D-C2D-C1D	-4.61	99.54	105.83
16	5	104	BCL	C3D-C2D-C1D	-4.60	99.56	105.83
16	1	102	BCL	C3D-C2D-C1D	-4.60	99.56	105.83
16	3	102	BCL	C3D-C2D-C1D	-4.59	99.57	105.83
16	J	101	BCL	C3D-C2D-C1D	-4.59	99.57	105.83
16	V	102	BCL	C1-C2-C3	-4.57	118.71	126.20
16	U	103	BCL	O2D-CGD-CBD	4.56	119.21	111.23
16	E	101	BCL	C3D-C2D-C1D	-4.56	99.61	105.83
16	6	102	BCL	C3D-C2D-C1D	-4.55	99.62	105.83
16	8	102	BCL	C1D-ND-C4D	-4.51	103.15	106.31
16	P	101	BCL	C3C-C4C-CHD	-4.51	113.89	123.39
16	S	102	BCL	C3D-C2D-C1D	-4.51	99.68	105.83
18	L	304	UQ8	C7-C8-C9	-4.50	119.08	126.83
16	R	102	BCL	C1D-ND-C4D	-4.50	103.15	106.31
16	B	102	BCL	O2D-CGD-CBD	4.50	119.09	111.23
16	R	102	BCL	O2D-CGD-CBD	4.47	119.04	111.23
16	4	102	BCL	C1-C2-C3	-4.46	118.90	126.20
16	0	102	BCL	C3C-C4C-CHD	-4.45	114.01	123.39
16	F	103	BCL	C3C-C4C-CHD	-4.43	114.05	123.39
16	T	101	BCL	C3C-C4C-CHD	-4.41	114.09	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	101	BCL	C3D-C2D-C1D	-4.40	99.82	105.83
16	U	103	BCL	C1D-ND-C4D	-4.40	103.22	106.31
16	G	103	BCL	C3C-C4C-CHD	-4.40	114.11	123.39
16	U	103	BCL	C3C-C4C-CHD	-4.40	114.12	123.39
16	3	102	BCL	O2D-CGD-CBD	4.39	118.91	111.23
22	V	101	CRT	C20-C19-C17	-4.39	121.12	127.28
20	H	303	CDL	OB6-CB5-C51	4.39	120.97	111.48
22	4	101	CRT	C21-C22-C23	-4.38	121.14	127.28
16	T	101	BCL	C1D-ND-C4D	-4.37	103.24	106.31
20	M	408	CDL	OA6-CA5-C11	4.37	120.94	111.48
16	Y	402	BCL	C3C-C4C-CHD	-4.37	114.18	123.39
14	G	105	PGV	O01-C1-C2	4.36	120.92	111.48
16	L	311	BCL	C1D-ND-C4D	-4.35	103.26	106.31
16	I	102	BCL	O2D-CGD-CBD	4.35	118.83	111.23
16	X	102	BCL	C1D-ND-C4D	-4.33	103.27	106.31
10	C	401	HEC	CBB-CAB-C3B	-4.33	118.78	127.43
16	1	103	BCL	C1D-ND-C4D	-4.32	103.28	106.31
16	6	102	BCL	C3C-C4C-CHD	-4.32	114.29	123.39
20	U	102	CDL	OB6-CB5-C51	4.31	120.81	111.48
16	Z	102	BCL	O2D-CGD-CBD	4.31	118.76	111.23
14	X	103	PGV	O01-C1-C2	4.30	120.79	111.48
16	5	103	BCL	O2D-CGD-CBD	4.30	118.75	111.23
22	8	101	CRT	C21-C22-C23	-4.30	121.25	127.28
16	A	101	BCL	C3C-C4C-CHD	-4.29	114.34	123.39
16	0	102	BCL	C3D-C2D-C1D	-4.29	99.98	105.83
22	4	101	CRT	C20-C19-C17	-4.28	121.27	127.28
16	7	102	BCL	O2D-CGD-CBD	4.28	118.72	111.23
16	L	302	BCL	C1D-ND-C4D	-4.28	103.31	106.31
14	H	302	PGV	O01-C1-C2	4.28	120.74	111.48
16	D	101	BCL	C3C-C4C-CHD	-4.27	114.39	123.39
16	L	302	BCL	C2D-C1D-ND	4.27	114.35	110.13
16	7	102	BCL	C3C-C4C-CHD	-4.27	114.40	123.39
16	4	102	BCL	C1D-ND-C4D	-4.26	103.32	106.31
22	Y	403	CRT	C4-C5-C6	-4.26	118.93	124.91
22	Y	403	CRT	C20-C19-C17	-4.26	121.31	127.28
16	J	101	BCL	C1D-ND-C4D	-4.25	103.33	106.31
16	X	102	BCL	C2D-C1D-ND	4.25	114.33	110.13
16	V	102	BCL	O2D-CGD-CBD	4.24	118.64	111.23
16	G	103	BCL	O2D-CGD-CBD	4.24	118.64	111.23
14	P	102	PGV	O01-C1-C2	4.22	120.61	111.48
16	3	102	BCL	C3B-C4B-NB	4.21	115.32	109.76
14	Z	104	PGV	O01-C1-C2	4.21	120.59	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	101	CRT	C4-C5-C6	-4.21	119.00	124.91
16	8	102	BCL	C2D-C1D-ND	4.20	114.28	110.13
16	M	403	BCL	O2D-CGD-CBD	4.20	118.57	111.23
16	I	102	BCL	C1-C2-C3	-4.20	119.32	126.20
16	O	103	BCL	C1-C2-C3	-4.18	119.35	126.20
14	X	101	PGV	O01-C1-C2	4.18	120.52	111.48
14	6	101	PGV	O01-C1-C2	4.17	120.51	111.48
16	6	102	BCL	C1-C2-C3	-4.17	119.36	126.20
14	B	103	PGV	O01-C1-C2	4.17	120.50	111.48
16	O	103	BCL	C1D-ND-C4D	-4.16	103.39	106.31
16	N	103	BCL	C1D-ND-C4D	-4.14	103.41	106.31
14	N	105	PGV	O01-C1-C2	4.14	120.43	111.48
16	Y	402	BCL	C3B-C4B-NB	4.13	115.21	109.76
16	Q	102	BCL	C1D-ND-C4D	-4.12	103.42	106.31
20	O	101	CDL	OB6-CB5-C51	4.12	120.39	111.48
16	O	103	BCL	C2D-C1D-ND	4.12	114.20	110.13
14	V	103	PGV	O01-C1-C2	4.12	120.39	111.48
16	D	101	BCL	C1D-ND-C4D	-4.11	103.43	106.31
14	R	103	PGV	O01-C1-C2	4.10	120.35	111.48
16	S	102	BCL	C3C-C4C-CHD	-4.10	114.75	123.39
16	2	101	BCL	C1D-ND-C4D	-4.10	103.44	106.31
22	8	101	CRT	C4-C5-C6	-4.09	119.17	124.91
16	3	102	BCL	C3C-C4C-CHD	-4.09	114.77	123.39
14	F	101	PGV	O01-C1-C2	4.09	120.32	111.48
14	2	103	PGV	O01-C1-C2	4.09	120.32	111.48
22	M	406	CRT	C26-C27-C28	-4.08	121.56	127.28
16	R	102	BCL	C2D-C1D-ND	4.08	114.16	110.13
22	M	406	CRT	C4-C5-C6	-4.08	119.19	124.91
16	L	312	BCL	C3C-C4C-CHD	-4.07	114.80	123.39
16	F	103	BCL	C2D-C1D-ND	4.07	114.16	110.13
16	P	101	BCL	C2D-C1D-ND	4.07	114.16	110.13
16	M	403	BCL	C1D-ND-C4D	-4.06	103.46	106.31
10	C	403	HEC	CBB-CAB-C3B	-4.05	119.33	127.43
10	C	401	HEC	CBC-CAC-C3C	-4.04	119.35	127.43
16	Q	102	BCL	C3B-C4B-NB	4.03	115.08	109.76
16	N	103	BCL	C3B-C4B-NB	4.03	115.08	109.76
16	9	101	BCL	C1-C2-C3	-4.03	119.60	126.20
16	K	101	BCL	C1D-ND-C4D	-4.02	103.49	106.31
17	L	303	BPH	C4D-CHA-CBD	-4.02	106.53	108.45
16	5	103	BCL	C1D-ND-C4D	-4.02	103.49	106.31
14	H	304	PGV	O01-C1-C2	4.02	120.17	111.48
16	L	312	BCL	C1D-ND-C4D	-4.01	103.50	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	0	102	BCL	C1D-ND-C4D	-4.01	103.50	106.31
16	E	101	BCL	C1D-ND-C4D	-4.00	103.51	106.31
20	M	407	CDL	OB6-CB5-C51	3.99	120.11	111.48
16	Q	102	BCL	C2D-C1D-ND	3.99	114.07	110.13
14	Z	101	PGV	O01-C1-C2	3.98	120.10	111.48
16	7	102	BCL	C3B-C4B-NB	3.98	115.01	109.76
16	9	102	BCL	C3B-C4B-NB	3.98	115.01	109.76
16	S	101	BCL	C1-C2-C3	-3.97	119.69	126.20
14	0	104	PGV	O01-C1-C2	3.96	120.05	111.48
16	N	103	BCL	C2D-C1D-ND	3.96	114.05	110.13
16	K	101	BCL	C3C-C4C-CHD	-3.96	115.04	123.39
16	1	103	BCL	C1-C2-C3	-3.96	119.71	126.20
16	Z	102	BCL	C3B-C4B-NB	3.96	114.98	109.76
16	V	102	BCL	C2D-C1D-ND	3.95	114.03	110.13
14	Z	103	PGV	O01-C1-C2	3.95	120.02	111.48
16	4	102	BCL	C3B-C4B-NB	3.95	114.97	109.76
16	F	103	BCL	C1-C2-C3	-3.94	119.74	126.20
14	J	102	PGV	O01-C1-C2	3.93	119.99	111.48
14	4	103	PGV	O01-C1-C2	3.93	119.98	111.48
16	8	102	BCL	C1-C2-C3	-3.93	119.76	126.20
16	L	311	BCL	C3C-C4C-CHD	-3.93	115.11	123.39
16	0	102	BCL	C1-C2-C3	-3.92	119.77	126.20
16	B	102	BCL	C1D-ND-C4D	-3.92	103.56	106.31
16	2	101	BCL	C2D-C1D-ND	3.92	114.01	110.13
14	C	408	PGV	O01-C1-C2	3.92	119.96	111.48
16	Z	102	BCL	C1D-ND-C4D	-3.92	103.56	106.31
16	R	102	BCL	C3B-C4B-NB	3.92	114.93	109.76
20	M	408	CDL	OB6-CB5-C51	3.92	119.95	111.48
16	Y	402	BCL	O2D-CGD-CBD	3.91	118.07	111.23
16	Z	102	BCL	C2D-C1D-ND	3.91	114.00	110.13
16	I	102	BCL	C3B-C4B-NB	3.91	114.92	109.76
20	M	407	CDL	OA6-CA5-C11	3.91	119.94	111.48
20	U	101	CDL	OA6-CA5-C11	3.91	119.94	111.48
16	B	102	BCL	C3B-C4B-NB	3.91	114.92	109.76
16	F	103	BCL	C3B-C4B-NB	3.90	114.91	109.76
16	3	102	BCL	C1D-ND-C4D	-3.89	103.58	106.31
16	P	101	BCL	C3D-C4D-ND	3.89	116.31	109.99
16	W	102	BCL	C3B-C4B-NB	3.89	114.89	109.76
16	X	102	BCL	C3B-C4B-NB	3.89	114.89	109.76
16	O	103	BCL	C3B-C4B-NB	3.89	114.89	109.76
16	F	103	BCL	C1D-ND-C4D	-3.87	103.59	106.31
16	I	102	BCL	C1D-ND-C4D	-3.87	103.60	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	102	BCL	C1D-ND-C4D	-3.86	103.60	106.31
22	N	102	CRT	C26-C27-C28	-3.85	121.87	127.28
16	D	101	BCL	C2D-C1D-ND	3.85	113.94	110.13
16	G	103	BCL	C3B-C4B-NB	3.85	114.84	109.76
16	T	101	BCL	C3D-C4D-ND	3.85	116.24	109.99
16	T	101	BCL	C2D-C1D-ND	3.84	113.93	110.13
16	J	101	BCL	C3B-C4B-NB	3.84	114.83	109.76
16	S	102	BCL	C1D-ND-C4D	-3.84	103.62	106.31
16	Q	102	BCL	C1-C2-C3	-3.84	119.90	126.20
16	4	102	BCL	C2D-C1D-ND	3.83	113.92	110.13
16	5	103	BCL	C2D-C1D-ND	3.83	113.91	110.13
14	3	101	PGV	O01-C1-C2	3.83	119.76	111.48
16	E	101	BCL	C2D-C1D-ND	3.82	113.91	110.13
14	L	305	PGV	O01-C1-C2	3.82	119.75	111.48
16	B	102	BCL	C2D-C1D-ND	3.82	113.90	110.13
16	U	103	BCL	C2D-C1D-ND	3.81	113.90	110.13
16	K	101	BCL	C3B-C4B-NB	3.81	114.78	109.76
16	5	104	BCL	C1-C2-C3	-3.80	119.97	126.20
16	L	312	BCL	C1-C2-C3	-3.80	119.97	126.20
16	Y	401	BCL	C1-C2-C3	-3.80	119.97	126.20
14	1	101	PGV	O01-C1-C2	3.80	119.70	111.48
14	R	104	PGV	O01-C1-C2	3.79	119.69	111.48
16	L	311	BCL	C2D-C1D-ND	3.79	113.88	110.13
10	C	404	HEC	CBB-CAB-C3B	-3.78	119.87	127.43
22	V	101	CRT	C4-C5-C6	-3.78	119.61	124.91
16	5	103	BCL	C1-C2-C3	-3.78	120.01	126.20
14	M	410	PGV	O01-C1-C2	3.77	119.64	111.48
16	T	101	BCL	C3B-C4B-NB	3.77	114.73	109.76
15	H	305	LMT	C4B-C3B-C2B	-3.76	104.22	110.83
16	1	103	BCL	C3C-C4C-CHD	-3.76	115.46	123.39
16	7	102	BCL	C1D-ND-C4D	-3.76	103.67	106.31
14	2	102	PGV	O01-C1-C2	3.76	119.61	111.48
16	U	103	BCL	C3B-C4B-NB	3.75	114.71	109.76
16	L	302	BCL	C3B-C4B-NB	3.75	114.70	109.76
14	6	104	PGV	O01-C1-C2	3.74	119.58	111.48
15	F	102	LMT	C1B-O5B-C5B	3.74	121.03	113.72
16	J	101	BCL	C1-C2-C3	-3.74	120.07	126.20
16	W	102	BCL	C1D-ND-C4D	-3.74	103.69	106.31
16	1	102	BCL	C1D-ND-C4D	-3.74	103.69	106.31
16	Y	402	BCL	C1D-ND-C4D	-3.73	103.69	106.31
20	M	409	CDL	OB6-CB5-C51	3.73	119.55	111.48
20	M	409	CDL	OA6-CA5-C11	3.73	119.54	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	303	CDL	OA6-CA5-C11	3.72	119.53	111.48
16	M	403	BCL	C2D-C1D-ND	3.72	113.81	110.13
16	W	101	BCL	C3B-C4B-NB	3.72	114.67	109.76
16	J	101	BCL	C2D-C1D-ND	3.72	113.81	110.13
16	6	102	BCL	C1D-ND-C4D	-3.72	103.70	106.31
22	B	101	CRT	C20-C19-C17	-3.72	122.07	127.28
16	4	102	BCL	O2D-CGD-CBD	3.71	117.71	111.23
16	S	101	BCL	C3B-C4B-NB	3.71	114.65	109.76
16	R	102	BCL	C3D-C4D-ND	3.70	116.01	109.99
14	P	103	PGV	O01-C1-C2	3.70	119.49	111.48
16	4	102	BCL	C3D-C4D-ND	3.70	116.00	109.99
16	3	102	BCL	C3D-C4D-ND	3.69	115.99	109.99
16	6	102	BCL	C3B-C4B-NB	3.69	114.63	109.76
16	I	102	BCL	C2D-C1D-ND	3.69	113.78	110.13
14	0	101	PGV	O01-C1-C2	3.69	119.47	111.48
16	1	102	BCL	C1-C2-C3	-3.68	120.17	126.20
16	9	101	BCL	C2D-C1D-ND	3.68	113.77	110.13
16	0	102	BCL	C3B-C4B-NB	3.68	114.61	109.76
14	N	101	PGV	O01-C1-C2	3.68	119.44	111.48
14	8	103	PGV	O01-C1-C2	3.68	119.44	111.48
18	L	306	UQ8	C10-C9-C11	3.67	121.60	115.23
16	1	103	BCL	C3D-C4D-ND	3.67	115.95	109.99
16	9	101	BCL	C1D-ND-C4D	-3.67	103.74	106.31
16	L	311	BCL	C3D-C4D-ND	3.67	115.95	109.99
16	D	101	BCL	C3B-C4B-NB	3.67	114.60	109.76
16	0	102	BCL	C3D-C4D-ND	3.66	115.94	109.99
16	0	102	BCL	C2D-C1D-ND	3.66	113.75	110.13
14	B	104	PGV	O01-C1-C2	3.66	119.39	111.48
17	M	404	BPH	C4D-CHA-CBD	-3.65	106.70	108.45
10	C	404	HEC	CBC-CAC-C3C	-3.65	120.14	127.43
20	O	101	CDL	OA6-CA5-C11	3.64	119.37	111.48
16	J	101	BCL	C3D-C4D-ND	3.64	115.91	109.99
16	Y	402	BCL	C2D-C1D-ND	3.64	113.73	110.13
16	U	103	BCL	C3D-C4D-ND	3.64	115.90	109.99
16	P	101	BCL	C3B-C4B-NB	3.63	114.55	109.76
16	E	101	BCL	C3B-C4B-NB	3.63	114.55	109.76
16	8	102	BCL	C3B-C4B-NB	3.63	114.55	109.76
20	M	402	CDL	OA6-CA5-C11	3.62	119.31	111.48
16	S	102	BCL	C3B-C4B-NB	3.62	114.54	109.76
16	L	312	BCL	C3D-C4D-ND	3.62	115.87	109.99
16	K	101	BCL	C3D-C4D-ND	3.62	115.87	109.99
16	8	102	BCL	C3D-C4D-ND	3.62	115.87	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	309	PGV	O01-C1-C2	3.61	119.30	111.48
10	C	402	HEC	CBB-CAB-C3B	-3.61	120.21	127.43
16	B	102	BCL	C1-C2-C3	-3.61	120.28	126.20
16	S	102	BCL	C3D-C4D-ND	3.60	115.84	109.99
16	1	102	BCL	C3D-C4D-ND	3.59	115.82	109.99
16	O	104	BCL	C1D-ND-C4D	-3.58	103.80	106.31
22	R	101	CRT	C20-C19-C17	-3.57	122.27	127.28
16	A	101	BCL	C3B-C4B-NB	3.57	114.47	109.76
16	1	102	BCL	C3B-C4B-NB	3.57	114.47	109.76
16	6	102	BCL	C3D-C4D-ND	3.57	115.78	109.99
16	0	102	BCL	C4-C3-C5	3.57	121.42	115.23
16	D	102	BCL	C1-C2-C3	-3.56	120.36	126.20
16	Y	401	BCL	C3C-C4C-CHD	-3.56	115.89	123.39
16	R	102	BCL	C1-C2-C3	-3.56	120.37	126.20
16	G	103	BCL	C2D-C1D-ND	3.55	113.64	110.13
16	I	103	BCL	C3B-C4B-NB	3.55	114.45	109.76
20	H	301	CDL	OB6-CB5-C51	3.54	119.14	111.48
16	1	103	BCL	C2D-C1D-ND	3.54	113.63	110.13
16	G	103	BCL	C1D-ND-C4D	-3.53	103.83	106.31
16	6	102	BCL	C2D-C1D-ND	3.53	113.62	110.13
16	W	101	BCL	C1D-ND-C4D	-3.53	103.83	106.31
16	S	101	BCL	C1D-ND-C4D	-3.52	103.84	106.31
16	E	101	BCL	C3D-C4D-ND	3.52	115.71	109.99
16	N	103	BCL	C3D-C4D-ND	3.52	115.71	109.99
16	S	101	BCL	O2A-CGA-CBA	3.52	122.56	111.83
16	9	101	BCL	C3B-C4B-NB	3.52	114.40	109.76
16	D	101	BCL	C3D-C4D-ND	3.51	115.70	109.99
16	L	302	BCL	C1-C2-C3	-3.51	120.44	126.20
16	I	102	BCL	C3D-C4D-ND	3.51	115.69	109.99
16	D	102	BCL	C3B-C4B-NB	3.50	114.38	109.76
21	M	405	MQ8	C26-C27-C28	-3.49	119.62	127.62
16	5	103	BCL	C3B-C4B-NB	3.49	114.37	109.76
14	R	103	PGV	O03-C19-C20	3.49	122.49	111.83
14	T	102	PGV	O01-C1-C2	3.49	119.04	111.48
16	O	104	BCL	C3D-C4D-ND	3.49	115.66	109.99
18	L	306	UQ8	C22-C23-C24	-3.49	119.64	127.62
14	L	310	PGV	O01-C1-C2	3.48	119.01	111.48
16	2	101	BCL	C3B-C4B-NB	3.48	114.35	109.76
16	V	102	BCL	C3B-C4B-NB	3.47	114.34	109.76
14	6	103	PGV	O01-C1-C2	3.47	118.99	111.48
16	I	103	BCL	O2A-CGA-CBA	3.47	122.42	111.83
16	L	302	BCL	O2D-CGD-CBD	3.47	117.30	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	X	102	BCL	C1-C2-C3	-3.47	120.51	126.20
16	7	102	BCL	C2D-C1D-ND	3.47	113.56	110.13
16	K	101	BCL	C2D-C1D-ND	3.47	113.56	110.13
16	L	311	BCL	C3B-C4B-NB	3.46	114.33	109.76
16	Y	401	BCL	C3B-C4B-NB	3.46	114.33	109.76
16	A	101	BCL	C2D-C1D-ND	3.46	113.55	110.13
16	1	103	BCL	C3B-C4B-NB	3.45	114.32	109.76
16	3	102	BCL	C2D-C1D-ND	3.45	113.54	110.13
16	B	102	BCL	C3D-C4D-ND	3.44	115.59	109.99
16	Y	401	BCL	C1D-ND-C4D	-3.44	103.90	106.31
16	L	312	BCL	O2D-CGD-O1D	-3.44	117.15	123.85
16	W	102	BCL	C3D-C4D-ND	3.44	115.57	109.99
20	M	408	CDL	CA4-OA6-CA5	-3.43	109.59	117.80
16	W	102	BCL	C2D-C1D-ND	3.43	113.52	110.13
15	Q	101	LMT	C1B-O5B-C5B	3.42	120.41	113.72
16	2	101	BCL	C3D-C4D-ND	3.42	115.55	109.99
16	S	101	BCL	C1C-NC-C4C	-3.42	105.12	106.68
16	E	101	BCL	O2D-CGD-O1D	-3.42	117.19	123.85
16	O	103	BCL	CAC-C3C-C4C	-3.42	105.00	112.58
16	W	101	BCL	O2A-CGA-CBA	3.41	122.24	111.83
16	I	103	BCL	C3C-C4C-CHD	-3.41	116.20	123.39
16	I	103	BCL	C2D-C1D-ND	3.41	113.50	110.13
22	M	406	CRT	C32-C31-C30	-3.41	113.32	123.20
16	O	104	BCL	C3B-C4B-NB	3.41	114.26	109.76
16	W	102	BCL	C3C-C4C-CHD	-3.41	116.21	123.39
14	E	102	PGV	O01-C1-C2	3.41	118.85	111.48
16	5	104	BCL	C3D-C4D-ND	3.40	115.52	109.99
16	G	103	BCL	C3D-C4D-ND	3.40	115.51	109.99
14	M	410	PGV	C02-O01-C1	-3.39	109.69	117.80
16	V	102	BCL	C4-C3-C5	3.39	121.11	115.23
16	O	103	BCL	C3D-C4D-ND	3.38	115.49	109.99
16	Q	102	BCL	C3D-C4D-ND	3.38	115.48	109.99
16	W	101	BCL	C2D-C1D-ND	3.38	113.47	110.13
16	W	101	BCL	C3C-C4C-CHD	-3.38	116.27	123.39
16	S	101	BCL	C3D-C4D-ND	3.37	115.47	109.99
16	V	102	BCL	C3D-C4D-ND	3.37	115.47	109.99
10	C	402	HEC	CBC-CAC-C3C	-3.37	120.70	127.43
18	L	304	UQ8	C1M-C1-C6	-3.37	118.92	124.45
16	5	103	BCL	C3D-C4D-ND	3.36	115.46	109.99
16	L	302	BCL	CED-O2D-CGD	3.36	123.53	115.92
16	A	101	BCL	C1D-ND-C4D	-3.36	103.96	106.31
16	W	101	BCL	O2D-CGD-O1D	-3.35	117.32	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	104	PGV	O01-C1-C2	3.35	118.73	111.48
16	M	403	BCL	C3D-C4D-ND	3.35	115.43	109.99
16	S	101	BCL	C3C-C4C-CHD	-3.35	116.33	123.39
16	Y	402	BCL	C3D-C4D-ND	3.35	115.43	109.99
16	S	102	BCL	C2D-C1D-ND	3.35	113.44	110.13
16	X	102	BCL	C3D-C4D-ND	3.34	115.42	109.99
16	I	102	BCL	C3C-C4C-CHD	-3.32	116.40	123.39
22	V	101	CRT	C10-C9-C7	-3.31	122.63	127.28
16	R	102	BCL	C4-C3-C5	3.31	120.98	115.23
16	9	101	BCL	C3C-C4C-CHD	-3.31	116.41	123.39
16	9	102	BCL	C1D-ND-C4D	-3.31	103.99	106.31
16	5	104	BCL	O2A-CGA-CBA	3.31	121.93	111.83
16	L	312	BCL	C2D-C1D-ND	3.31	113.40	110.13
16	N	103	BCL	C1-C2-C3	-3.31	120.78	126.20
16	1	102	BCL	C2D-C1D-ND	3.30	113.39	110.13
14	H	304	PGV	C02-O01-C1	-3.30	109.90	117.80
15	I	101	LMT	C1B-C2B-C3B	3.30	116.95	110.01
16	S	101	BCL	C2D-C1D-ND	3.30	113.39	110.13
14	0	103	PGV	O01-C1-C2	3.30	118.61	111.48
16	Y	401	BCL	C3D-C4D-ND	3.29	115.33	109.99
16	0	102	BCL	O2D-CGD-O1D	-3.29	117.45	123.85
14	N	104	PGV	O01-C1-C2	3.29	118.59	111.48
16	2	101	BCL	C1-C2-C3	-3.29	120.81	126.20
16	D	102	BCL	C3D-C4D-ND	3.28	115.33	109.99
16	L	302	BCL	O2A-CGA-CBA	3.28	121.84	111.83
14	C	408	PGV	O03-C19-C20	3.27	121.82	111.83
18	L	307	UQ8	C7-C6-C1	-3.27	119.28	124.89
16	9	102	BCL	C2D-C1D-ND	3.27	113.36	110.13
16	Z	102	BCL	C3D-C4D-ND	3.27	115.30	109.99
22	G	102	CRT	C4-C5-C6	-3.26	120.34	124.91
16	9	102	BCL	C3D-C4D-ND	3.26	115.28	109.99
22	R	101	CRT	C26-C27-C28	-3.25	122.72	127.28
22	4	101	CRT	C10-C9-C7	-3.25	122.72	127.28
16	W	101	BCL	C3D-C4D-ND	3.25	115.27	109.99
16	1	102	BCL	C3C-C4C-CHD	-3.25	116.54	123.39
16	A	101	BCL	C3D-C4D-ND	3.24	115.25	109.99
16	I	102	BCL	C4A-NA-C1A	3.23	108.15	106.68
16	O	104	BCL	O2A-CGA-CBA	3.23	121.69	111.83
18	L	304	UQ8	C17-C18-C19	-3.23	120.23	127.62
16	3	102	BCL	C1-C2-C3	-3.23	120.91	126.20
16	K	101	BCL	C1-C2-C3	-3.22	120.93	126.20
16	9	102	BCL	C3C-C4C-CHD	-3.21	116.62	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	103	BCL	C3D-C4D-ND	3.21	115.21	109.99
16	A	101	BCL	C1-O2A-CGA	3.20	124.40	116.65
16	I	103	BCL	C1D-ND-C4D	-3.20	104.06	106.31
21	M	405	MQ8	C39-C38-C40	3.20	120.78	115.23
16	K	101	BCL	C4-C3-C5	3.20	120.78	115.23
15	O	102	LMT	C1B-O1B-C4'	-3.20	110.40	117.98
16	9	101	BCL	C3D-C4D-ND	3.20	115.18	109.99
17	L	303	BPH	C1-C2-C3	-3.19	120.96	126.20
16	5	103	BCL	C3C-C4C-CHD	-3.19	116.66	123.39
16	M	403	BCL	C3B-C4B-NB	3.19	113.97	109.76
16	7	102	BCL	C3D-C4D-ND	3.19	115.17	109.99
14	L	310	PGV	O03-C19-C20	3.19	121.55	111.83
18	L	306	UQ8	C17-C18-C19	-3.18	120.33	127.62
22	B	101	CRT	C32-C31-C30	-3.18	113.98	123.20
14	P	102	PGV	O03-C19-C20	3.18	121.53	111.83
16	O	103	BCL	O2A-CGA-CBA	3.18	121.53	111.83
14	Z	101	PGV	O03-C19-C20	3.17	121.49	111.83
16	8	102	BCL	O2A-CGA-CBA	3.16	121.47	111.83
16	D	102	BCL	O2A-CGA-CBA	3.15	121.44	111.83
16	O	104	BCL	C2D-C1D-ND	3.15	113.24	110.13
16	9	102	BCL	C1-C2-C3	-3.14	121.05	126.20
16	J	101	BCL	O2D-CGD-O1D	-3.14	117.74	123.85
22	B	101	CRT	C9-C10-C11	-3.13	114.12	123.20
16	F	103	BCL	C3D-C4D-ND	3.13	115.08	109.99
16	L	302	BCL	C3D-C4D-ND	3.13	115.07	109.99
17	M	404	BPH	C2B-C1B-NB	-3.13	107.17	109.43
16	5	104	BCL	C3C-C4C-CHD	-3.12	116.81	123.39
16	W	102	BCL	C1-C2-C3	-3.12	121.08	126.20
16	U	103	BCL	C4-C3-C5	3.12	120.64	115.23
16	D	102	BCL	C2D-C1D-ND	3.12	113.21	110.13
16	Y	402	BCL	O2A-CGA-CBA	3.11	121.33	111.83
16	Y	401	BCL	C2D-C1D-ND	3.11	113.20	110.13
16	D	101	BCL	O2A-CGA-CBA	3.11	121.32	111.83
16	Q	102	BCL	C4-C3-C5	3.11	120.62	115.23
16	5	104	BCL	CHB-C1B-NB	-3.11	119.39	124.05
16	L	311	BCL	C6-C5-C3	-3.10	105.91	113.47
16	Z	102	BCL	C1C-NC-C4C	-3.10	105.27	106.68
21	M	405	MQ8	C41-C42-C43	-3.10	120.53	127.62
16	D	102	BCL	C1D-ND-C4D	-3.09	104.14	106.31
16	3	102	BCL	C4-C3-C5	3.09	120.59	115.23
16	P	101	BCL	C1-C2-C3	-3.09	121.14	126.20
16	G	103	BCL	C4-C3-C5	3.08	120.58	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	M	406	CRT	C5-C6-C7	-3.08	121.24	125.89
20	U	102	CDL	OB8-CB7-C71	3.07	121.21	111.83
18	L	306	UQ8	C7-C6-C1	-3.07	119.63	124.89
16	W	101	BCL	CHC-C4B-NB	-3.06	119.46	124.05
16	4	102	BCL	C2A-C1A-CHA	-3.06	118.56	123.87
16	5	104	BCL	C3B-C4B-NB	3.05	113.78	109.76
22	8	101	CRT	C13-C12-C11	3.05	122.74	118.09
22	M	406	CRT	C14-C15-C16	-3.04	114.38	123.20
16	I	102	BCL	O2A-CGA-CBA	3.04	121.09	111.83
22	V	101	CRT	C14-C15-C16	-3.02	114.45	123.20
16	1	103	BCL	O2A-CGA-CBA	3.02	121.03	111.83
16	0	102	BCL	C4D-CHA-C1A	-3.01	117.65	121.24
16	E	101	BCL	C1-C2-C3	-3.01	121.27	126.20
18	L	304	UQ8	C15-C14-C16	3.00	120.44	115.23
16	Z	102	BCL	C4-C3-C5	3.00	120.44	115.23
16	W	101	BCL	C1-C2-C3	-3.00	121.28	126.20
22	G	102	CRT	C14-C15-C16	-3.00	114.52	123.20
16	L	312	BCL	C3B-C4B-NB	3.00	113.71	109.76
16	W	102	BCL	C4-C3-C5	2.99	120.42	115.23
16	9	101	BCL	C4-C3-C5	2.99	120.42	115.23
14	E	102	PGV	O03-C19-C20	2.99	120.94	111.83
22	B	101	CRT	C21-C20-C19	-2.98	117.41	123.52
21	M	405	MQ8	C45-C43-C44	2.98	120.41	115.23
21	M	405	MQ8	C14-C13-C15	2.98	120.41	115.23
14	M	410	PGV	O03-C19-C20	2.98	120.93	111.83
16	5	103	BCL	O2A-CGA-CBA	2.98	120.93	111.83
16	Y	401	BCL	CMD-C2D-C3D	-2.98	120.86	127.69
16	I	102	BCL	C1C-NC-C4C	-2.98	105.32	106.68
14	H	304	PGV	O03-C19-C20	2.98	120.92	111.83
10	C	401	HEC	CHD-C1D-ND	2.98	129.26	123.86
16	L	312	BCL	C4-C3-C5	2.98	120.39	115.23
16	U	103	BCL	O2A-CGA-CBA	2.98	120.91	111.83
22	N	102	CRT	C20-C19-C17	-2.97	123.11	127.28
20	H	301	CDL	OB8-CB7-C71	2.97	120.88	111.83
16	T	101	BCL	O2A-CGA-CBA	2.96	120.87	111.83
16	5	104	BCL	C1D-ND-C4D	-2.96	104.23	106.31
14	B	104	PGV	C02-O01-C1	-2.96	110.71	117.80
16	K	101	BCL	CHC-C1C-NC	2.96	128.67	124.40
16	S	102	BCL	C1-C2-C3	-2.96	121.35	126.20
22	B	101	CRT	C34-C33-C35	2.96	122.61	118.09
16	R	102	BCL	O2A-CGA-CBA	2.96	120.86	111.83
16	7	102	BCL	C1-O2A-CGA	2.96	123.81	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	301	CDL	CA4-OA6-CA5	-2.95	110.73	117.80
16	L	312	BCL	O2A-CGA-CBA	2.95	120.83	111.83
20	M	402	CDL	OA8-CA7-C31	2.95	120.83	111.83
16	7	102	BCL	C1-C2-C3	-2.95	121.37	126.20
16	4	102	BCL	O2A-CGA-CBA	2.95	120.82	111.83
16	D	102	BCL	O2D-CGD-O1D	-2.94	118.12	123.85
20	M	409	CDL	OA8-CA7-C31	2.94	120.79	111.83
20	U	101	CDL	OA8-CA7-C31	2.94	120.79	111.83
16	Y	402	BCL	CHC-C1C-NC	2.94	128.64	124.40
21	M	405	MQ8	C36-C37-C38	-2.93	120.93	127.62
16	B	102	BCL	O2A-CGA-CBA	2.92	120.75	111.83
21	M	405	MQ8	C34-C33-C35	2.92	120.30	115.23
22	R	101	CRT	C32-C31-C30	-2.92	114.75	123.20
14	C	408	PGV	C02-O01-C1	-2.92	110.82	117.80
16	F	103	BCL	CHC-C4B-NB	-2.91	119.68	124.05
16	I	102	BCL	CHC-C4B-NB	-2.91	119.68	124.05
22	Y	403	CRT	C13-C12-C11	2.91	122.53	118.09
16	G	103	BCL	O2A-CGA-CBA	2.91	120.70	111.83
15	H	306	LMT	C1'-C2'-C3'	2.90	116.12	110.01
14	0	101	PGV	C02-O01-C1	-2.90	110.85	117.80
16	J	101	BCL	O2A-CGA-CBA	2.90	120.69	111.83
10	C	403	HEC	CHA-C4D-ND	2.90	129.12	123.86
22	4	101	CRT	C14-C15-C16	-2.90	114.80	123.20
16	F	103	BCL	CHC-C1C-NC	2.90	128.58	124.40
16	Y	402	BCL	C4-C3-C5	2.90	120.26	115.23
14	B	103	PGV	O03-C19-C20	2.90	120.67	111.83
16	5	104	BCL	C2D-C1D-ND	2.90	112.99	110.13
16	9	101	BCL	CHC-C4B-NB	-2.90	119.71	124.05
10	C	403	HEC	CHA-C1A-NA	2.89	127.61	124.45
16	W	102	BCL	O2A-CGA-CBA	2.89	120.65	111.83
16	X	102	BCL	C1C-NC-C4C	-2.89	105.36	106.68
22	8	101	CRT	C15-C14-C12	-2.89	123.23	127.28
20	H	303	CDL	CB4-OB6-CB5	-2.89	110.88	117.80
16	O	103	BCL	CHC-C1C-NC	2.88	128.56	124.40
14	P	102	PGV	C02-O01-C1	-2.88	110.90	117.80
16	5	104	BCL	CHC-C4B-NB	-2.88	119.73	124.05
21	M	405	MQ8	C31-C32-C33	-2.87	121.05	127.62
16	L	312	BCL	CMD-C2D-C3D	-2.87	121.10	127.69
16	Z	102	BCL	C6-C5-C3	-2.87	106.47	113.47
16	M	403	BCL	C1-C2-C3	-2.87	121.50	126.20
16	X	102	BCL	O2D-CGD-O1D	-2.87	118.27	123.85
16	P	101	BCL	O2D-CGD-O1D	-2.86	118.28	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	102	BCL	O2A-CGA-CBA	2.86	120.56	111.83
16	0	102	BCL	O2A-CGA-CBA	2.86	120.55	111.83
16	U	103	BCL	C1-C2-C3	-2.86	121.51	126.20
16	L	311	BCL	C4-C3-C5	2.86	120.19	115.23
10	C	403	HEC	CBC-CAC-C3C	-2.86	121.72	127.43
22	G	102	CRT	C13-C12-C11	2.86	122.45	118.09
16	1	102	BCL	CHC-C4B-NB	-2.86	119.76	124.05
16	9	101	BCL	O2A-CGA-CBA	2.85	120.53	111.83
14	G	105	PGV	O03-C19-C20	2.85	120.53	111.83
16	1	103	BCL	CHC-C4B-NB	-2.85	119.78	124.05
10	C	402	HEC	CHA-C4D-ND	2.85	129.02	123.86
16	1	103	BCL	CAC-C3C-C4C	-2.85	106.27	112.58
20	O	101	CDL	CB4-OB6-CB5	-2.85	110.99	117.80
16	N	103	BCL	O2D-CGD-O1D	-2.84	118.32	123.85
16	S	102	BCL	C4-C3-C5	2.84	120.16	115.23
16	1	103	BCL	C2A-C1A-CHA	-2.84	118.94	123.87
16	8	102	BCL	O2D-CGD-O1D	-2.84	118.32	123.85
16	2	101	BCL	O2A-CGA-CBA	2.84	120.49	111.83
14	T	103	PGV	O01-C1-C2	2.83	117.60	111.48
16	P	101	BCL	C4-C3-C5	2.83	120.14	115.23
16	M	403	BCL	CHC-C4B-NB	-2.83	119.81	124.05
16	Q	102	BCL	O2D-CGD-O1D	-2.83	118.35	123.85
14	G	101	PGV	O01-C1-C2	2.82	117.58	111.48
15	I	101	LMT	O5B-C1B-C2B	2.82	116.17	110.37
16	3	102	BCL	CHC-C1C-NC	2.82	128.47	124.40
16	R	102	BCL	CHB-C4A-NA	2.82	128.47	124.40
10	C	403	HEC	CHD-C1D-ND	2.82	128.97	123.86
16	U	103	BCL	CHC-C4B-NB	-2.82	119.83	124.05
16	U	103	BCL	CHC-C1C-NC	2.81	128.46	124.40
16	2	101	BCL	C4-C3-C5	2.81	120.11	115.23
22	G	102	CRT	C9-C10-C11	-2.81	115.05	123.20
16	6	102	BCL	O2A-CGA-CBA	2.81	120.41	111.83
16	9	102	BCL	CHB-C1B-NB	-2.81	119.83	124.05
22	V	101	CRT	C32-C31-C30	-2.81	115.05	123.20
22	B	101	CRT	C26-C27-C28	-2.81	123.34	127.28
14	G	101	PGV	O03-C19-C20	2.80	120.38	111.83
16	D	102	BCL	C4A-NA-C1A	2.80	107.96	106.68
16	J	101	BCL	C2A-C1A-CHA	-2.80	119.01	123.87
16	T	101	BCL	O2D-CGD-O1D	-2.79	118.41	123.85
16	3	102	BCL	CHB-C4A-NA	2.79	128.43	124.40
20	O	101	CDL	OA8-CA7-C31	2.79	120.34	111.83
16	2	101	BCL	O2D-CGD-O1D	-2.79	118.42	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	306	UQ8	C7-C8-C9	-2.79	122.03	126.83
16	E	101	BCL	CHB-C4A-NA	2.79	128.43	124.40
16	L	312	BCL	CHC-C4B-NB	-2.79	119.87	124.05
16	N	103	BCL	C4-C3-C5	2.79	120.07	115.23
14	N	104	PGV	O03-C19-C20	2.79	120.33	111.83
16	E	101	BCL	C4-C3-C5	2.79	120.06	115.23
16	O	104	BCL	CMD-C2D-C3D	-2.78	121.31	127.69
16	L	311	BCL	C1-C2-C3	-2.78	121.64	126.20
10	C	402	HEC	CHD-C1D-ND	2.78	128.90	123.86
16	7	102	BCL	CHB-C4A-NA	2.78	128.41	124.40
16	F	103	BCL	O2D-CGD-O1D	-2.78	118.44	123.85
22	R	101	CRT	C10-C9-C7	-2.78	123.39	127.28
16	1	103	BCL	C6-C5-C3	-2.77	106.71	113.47
20	M	407	CDL	OB8-CB7-C71	2.77	120.29	111.83
16	T	101	BCL	CHB-C4A-NA	2.77	128.40	124.40
16	J	101	BCL	C4-C3-C5	2.77	120.04	115.23
16	1	103	BCL	O2D-CGD-O1D	-2.77	118.46	123.85
16	Q	102	BCL	O2A-CGA-CBA	2.77	120.28	111.83
16	1	102	BCL	C4-C3-C5	2.77	120.03	115.23
16	9	102	BCL	CHC-C4B-NB	-2.77	119.90	124.05
16	P	101	BCL	O2A-CGA-CBA	2.77	120.27	111.83
16	9	102	BCL	O2D-CGD-O1D	-2.76	118.47	123.85
16	Y	401	BCL	O2A-CGA-CBA	2.76	120.26	111.83
22	M	406	CRT	C36-C35-C33	-2.76	121.72	125.89
16	9	102	BCL	O2A-CGA-CBA	2.76	120.25	111.83
16	F	103	BCL	C1C-NC-C4C	-2.76	105.42	106.68
15	7	101	LMT	C1B-O1B-C4'	-2.76	111.44	117.98
16	6	102	BCL	O2D-CGD-O1D	-2.76	118.48	123.85
16	4	102	BCL	C4-C3-C5	2.75	120.01	115.23
14	2	102	PGV	O03-C19-C20	2.75	120.23	111.83
16	O	104	BCL	C3C-C4C-CHD	-2.75	117.59	123.39
16	F	103	BCL	O2A-CGA-CBA	2.75	120.22	111.83
16	L	302	BCL	C4-C3-C5	2.75	120.00	115.23
22	M	406	CRT	C9-C10-C11	-2.75	115.23	123.20
16	I	102	BCL	CHC-C1C-NC	2.75	128.37	124.40
16	Z	102	BCL	O2A-CGA-CBA	2.75	120.21	111.83
21	M	405	MQ8	C29-C28-C30	2.74	119.99	115.23
16	Q	102	BCL	CHC-C4B-NB	-2.74	119.93	124.05
16	E	101	BCL	O2A-CGA-CBA	2.74	120.20	111.83
14	P	103	PGV	C03-C02-C01	-2.74	105.39	111.78
16	3	102	BCL	C1C-NC-C4C	-2.74	105.43	106.68
16	D	101	BCL	C4-C3-C5	2.74	119.98	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	M	408	CDL	OA8-CA7-C31	2.73	120.17	111.83
14	O	101	PGV	O03-C19-C20	2.73	120.17	111.83
14	N	105	PGV	C02-O01-C1	-2.73	111.25	117.80
22	V	101	CRT	C21-C20-C19	-2.73	117.93	123.52
22	B	101	CRT	C15-C14-C12	-2.73	123.45	127.28
22	Y	403	CRT	C9-C10-C11	-2.73	115.28	123.20
18	L	304	UQ8	C12-C13-C14	-2.73	121.37	127.62
16	M	403	BCL	CED-O2D-CGD	2.73	122.11	115.92
16	5	103	BCL	C4-C3-C5	2.73	119.96	115.23
14	V	103	PGV	C02-O01-C1	-2.73	111.27	117.80
16	X	102	BCL	O2A-CGA-CBA	2.73	120.15	111.83
22	Y	403	CRT	C5-C6-C7	-2.73	121.77	125.89
14	G	104	PGV	O03-C19-C20	2.73	120.15	111.83
15	Q	101	LMT	O5B-C1B-C2B	2.72	115.96	110.37
16	J	101	BCL	C4D-CHA-C1A	-2.72	118.00	121.24
16	S	101	BCL	CHC-C4B-NB	-2.72	119.97	124.05
16	V	102	BCL	C1C-NC-C4C	-2.71	105.44	106.68
21	M	405	MQ8	C24-C23-C25	2.71	119.94	115.23
16	U	103	BCL	CMB-C2B-C3B	2.71	134.23	125.67
20	M	402	CDL	OB6-CB5-C51	2.71	117.35	111.48
16	S	101	BCL	CMD-C2D-C3D	-2.71	121.47	127.69
14	6	101	PGV	O03-C19-C20	2.71	120.09	111.83
16	9	101	BCL	O2D-CGD-O1D	-2.71	118.58	123.85
10	C	403	HEC	CBA-CAA-C2A	-2.71	105.05	112.53
16	9	101	BCL	C4A-NA-C1A	2.70	107.91	106.68
17	L	303	BPH	C2B-C1B-NB	-2.70	107.48	109.43
22	N	102	CRT	C14-C15-C16	-2.70	115.38	123.20
22	Y	403	CRT	C14-C15-C16	-2.70	115.38	123.20
16	5	104	BCL	C4-C3-C5	2.70	119.91	115.23
10	C	404	HEC	CHA-C4D-ND	2.69	128.75	123.86
14	3	101	PGV	O03-C19-C20	2.69	120.05	111.83
16	L	302	BCL	CHB-C4A-NA	2.69	128.29	124.40
16	9	101	BCL	C1D-CHD-C4C	-2.69	120.13	126.62
16	7	102	BCL	C1C-NC-C4C	-2.69	105.45	106.68
16	P	101	BCL	C2A-C1A-CHA	-2.69	119.20	123.87
10	C	404	HEC	CHD-C1D-ND	2.69	128.74	123.86
16	2	101	BCL	C1C-NC-C4C	-2.69	105.45	106.68
16	X	102	BCL	C4-C3-C5	2.69	119.90	115.23
10	C	401	HEC	CHB-C1B-NB	2.69	128.73	123.86
16	L	302	BCL	C1C-NC-C4C	-2.69	105.45	106.68
14	P	103	PGV	O03-C19-C20	2.68	120.01	111.83
14	6	104	PGV	O03-C19-C20	2.68	120.01	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	101	BCL	CHB-C4A-NA	2.68	128.27	124.40
16	J	101	BCL	CHC-C4B-NB	-2.68	120.03	124.05
22	Y	403	CRT	C10-C9-C7	-2.68	123.53	127.28
16	6	102	BCL	C4-C3-C5	2.67	119.87	115.23
14	H	302	PGV	O03-C19-C20	2.67	119.98	111.83
16	R	102	BCL	O2D-CGD-O1D	-2.67	118.65	123.85
15	L	301	LMT	C1B-O1B-C4'	-2.67	111.65	117.98
16	M	403	BCL	CMB-C2B-C3B	2.67	134.09	125.67
16	0	102	BCL	CHC-C4B-NB	-2.67	120.05	124.05
16	Y	401	BCL	C4-C3-C5	2.66	119.85	115.23
16	N	103	BCL	CHC-C4B-NB	-2.66	120.06	124.05
20	M	409	CDL	OB8-CB7-C71	2.66	119.94	111.83
16	S	102	BCL	CHC-C4B-NB	-2.66	120.06	124.05
16	Y	402	BCL	C1-C2-C3	-2.66	121.84	126.20
22	8	101	CRT	C20-C19-C17	-2.65	123.56	127.28
16	5	103	BCL	CAA-CBA-CGA	-2.65	105.67	113.21
16	2	101	BCL	C2A-C1A-CHA	-2.65	119.26	123.87
22	N	102	CRT	C21-C20-C19	-2.65	118.09	123.52
16	O	104	BCL	C4-C3-C5	2.65	119.83	115.23
16	F	103	BCL	CMB-C2B-C3B	2.65	134.03	125.67
16	D	101	BCL	O2D-CGD-O1D	-2.65	118.69	123.85
16	M	403	BCL	CMD-C2D-C3D	-2.65	121.61	127.69
16	D	101	BCL	CAC-C3C-C4C	-2.65	106.70	112.58
16	F	103	BCL	C4-C3-C5	2.65	119.83	115.23
16	A	101	BCL	CMB-C2B-C3B	2.65	134.02	125.67
16	7	102	BCL	CHC-C4B-NB	-2.64	120.08	124.05
16	X	102	BCL	CHC-C1C-NC	2.64	128.22	124.40
18	L	307	UQ8	C1M-C1-C6	-2.64	120.11	124.45
20	M	408	CDL	OB8-CB7-C71	2.64	119.89	111.83
14	Z	103	PGV	O03-C19-C20	2.64	119.88	111.83
14	2	103	PGV	O03-C19-C20	2.64	119.88	111.83
22	N	102	CRT	C32-C31-C30	-2.64	115.55	123.20
20	O	101	CDL	OB8-CB7-C71	2.64	119.88	111.83
16	W	102	BCL	CHC-C4B-NB	-2.64	120.09	124.05
16	M	403	BCL	CHB-C4A-NA	2.64	128.20	124.40
16	8	102	BCL	CHC-C1C-NC	2.64	128.20	124.40
14	0	104	PGV	O03-C19-C20	2.64	119.87	111.83
16	7	102	BCL	C4-C3-C5	2.63	119.80	115.23
21	M	405	MQ8	C21-C22-C23	-2.63	121.60	127.62
16	O	103	BCL	CHC-C4B-NB	-2.63	120.10	124.05
16	1	103	BCL	C4-C3-C5	2.63	119.79	115.23
16	1	102	BCL	CHB-C4A-NA	2.63	128.19	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	S	102	BCL	O2A-CGA-CBA	2.63	119.85	111.83
16	L	311	BCL	O2D-CGD-O1D	-2.63	118.73	123.85
16	W	101	BCL	CMB-C2B-C3B	2.62	133.94	125.67
16	S	102	BCL	C2A-C1A-CHA	-2.62	119.32	123.87
16	A	101	BCL	CHC-C1C-NC	2.62	128.18	124.40
16	M	403	BCL	C4-C3-C5	2.61	119.77	115.23
14	O	103	PGV	O03-C19-C20	2.61	119.81	111.83
16	G	103	BCL	C2A-C1A-CHA	-2.61	119.33	123.87
16	R	102	BCL	C2A-C1A-CHA	-2.61	119.33	123.87
16	4	102	BCL	CHC-C1C-NC	2.61	128.17	124.40
14	6	103	PGV	O03-C19-C20	2.61	119.79	111.83
15	H	307	LMT	C1B-O1B-C4'	-2.61	111.80	117.98
16	Q	102	BCL	CAC-C3C-C4C	-2.61	106.80	112.58
16	D	102	BCL	CHB-C1B-NB	-2.61	120.14	124.05
16	L	311	BCL	CHC-C1C-NC	2.60	128.16	124.40
14	B	104	PGV	O03-C19-C20	2.60	119.77	111.83
15	H	306	LMT	C2'-C3'-C4'	2.60	115.58	109.68
16	1	103	BCL	CMB-C2B-C3B	2.60	133.87	125.67
22	4	101	CRT	C26-C27-C28	-2.60	123.63	127.28
16	J	101	BCL	CMB-C2B-C3B	2.60	133.87	125.67
16	U	103	BCL	CAC-C3C-C4C	-2.60	106.82	112.58
16	V	102	BCL	C2A-C1A-CHA	-2.59	119.37	123.87
16	M	403	BCL	C4A-NA-C1A	2.59	107.86	106.68
10	C	402	HEC	CHB-C1B-NB	2.59	128.56	123.86
16	7	102	BCL	O2D-CGD-O1D	-2.59	118.80	123.85
22	8	101	CRT	C32-C31-C30	-2.59	115.69	123.20
10	C	404	HEC	CHA-C1A-NA	2.59	127.27	124.45
16	I	102	BCL	C4-C3-C5	2.59	119.72	115.23
16	G	103	BCL	CHB-C4A-NA	2.59	128.13	124.40
16	W	101	BCL	CMD-C2D-C3D	-2.59	121.76	127.69
16	Y	402	BCL	CED-O2D-CGD	2.58	121.78	115.92
18	L	306	UQ8	C1M-C1-C6	-2.58	120.20	124.45
16	O	103	BCL	C4-C3-C5	2.58	119.71	115.23
16	6	102	BCL	CHC-C1C-NC	2.58	128.13	124.40
10	C	401	HEC	CHA-C4D-ND	2.58	128.54	123.86
16	Y	402	BCL	CHC-C4B-NB	-2.58	120.17	124.05
16	1	103	BCL	CMD-C2D-C3D	-2.58	121.78	127.69
16	8	102	BCL	CHB-C4A-NA	2.58	128.12	124.40
16	T	101	BCL	C2A-C1A-CHA	-2.58	119.40	123.87
16	5	104	BCL	C4A-NA-C1A	2.58	107.85	106.68
14	L	305	PGV	O03-C19-C20	2.57	119.69	111.83
16	B	102	BCL	CHB-C4A-NA	2.57	128.11	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	403	BCL	CAA-C2A-C3A	-2.57	106.05	113.00
16	1	102	BCL	CMB-C2B-C3B	2.57	133.77	125.67
20	U	102	CDL	OA8-CA7-C31	2.57	119.67	111.83
16	6	102	BCL	C2A-C1A-CHA	-2.57	119.41	123.87
16	2	101	BCL	C1D-CHD-C4C	-2.57	120.43	126.62
14	J	102	PGV	O03-C19-C20	2.57	119.66	111.83
16	S	101	BCL	C4-C3-C5	2.56	119.68	115.23
16	5	103	BCL	CHC-C4B-NB	-2.56	120.21	124.05
14	6	101	PGV	C02-O01-C1	-2.56	111.67	117.80
22	R	101	CRT	C34-C33-C35	2.56	122.00	118.09
10	C	403	HEC	CBD-CAD-C3D	-2.56	105.45	112.53
16	T	101	BCL	CHC-C1C-NC	2.56	128.09	124.40
14	Z	104	PGV	C02-O01-C1	-2.56	111.68	117.80
14	N	105	PGV	O03-C19-C20	2.56	119.63	111.83
14	1	101	PGV	C02-O01-C1	-2.56	111.68	117.80
20	U	101	CDL	CB4-OB6-CB5	-2.56	111.68	117.80
16	D	102	BCL	C4-C3-C5	2.56	119.66	115.23
22	V	101	CRT	C18-C17-C16	2.55	121.99	118.09
20	U	102	CDL	CB4-OB6-CB5	-2.55	111.69	117.80
16	J	101	BCL	CHC-C1C-NC	2.55	128.08	124.40
16	L	311	BCL	O1D-CGD-CBD	-2.55	119.49	124.52
22	Y	403	CRT	C21-C20-C19	-2.55	118.30	123.52
16	9	102	BCL	C4A-NA-C1A	2.55	107.84	106.68
21	M	405	MQ8	C19-C18-C20	2.55	119.65	115.23
14	N	101	PGV	O03-C19-C20	2.55	119.60	111.83
16	G	103	BCL	C1-C2-C3	-2.55	122.03	126.20
16	1	102	BCL	CHC-C1C-NC	2.54	128.07	124.40
16	K	101	BCL	CMD-C2D-C3D	-2.54	121.86	127.69
16	Q	102	BCL	C2A-C1A-CHA	-2.54	119.46	123.87
22	8	101	CRT	C26-C27-C28	-2.54	123.72	127.28
16	L	311	BCL	O2A-CGA-CBA	2.54	119.57	111.83
16	8	102	BCL	C6-C5-C3	-2.53	107.30	113.47
16	R	102	BCL	CHC-C1C-NC	2.53	128.06	124.40
16	K	101	BCL	O2A-CGA-CBA	2.53	119.56	111.83
16	Z	102	BCL	C1D-CHD-C4C	-2.53	120.51	126.62
14	X	101	PGV	O03-C19-C20	2.53	119.55	111.83
22	Y	403	CRT	C26-C27-C28	-2.53	123.73	127.28
18	L	304	UQ8	C20-C19-C21	2.53	119.62	115.23
22	8	101	CRT	C9-C10-C11	-2.53	115.87	123.20
15	5	101	LMT	O1B-C4'-C5'	2.53	116.11	109.48
22	R	101	CRT	C21-C20-C19	-2.53	118.35	123.52
20	M	402	CDL	OB8-CB7-C71	2.53	119.54	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	101	CRT	C9-C10-C11	-2.53	115.88	123.20
16	Z	102	BCL	CHB-C4A-NA	2.53	128.04	124.40
14	F	101	PGV	O03-C19-C20	2.53	119.53	111.83
16	Q	102	BCL	CHB-C4A-NA	2.53	128.04	124.40
14	E	102	PGV	C02-O01-C1	-2.52	111.76	117.80
16	A	101	BCL	CHC-C4B-NB	-2.52	120.27	124.05
22	B	101	CRT	C8-C7-C6	2.52	121.94	118.09
16	W	101	BCL	C4-C3-C5	2.52	119.60	115.23
16	3	102	BCL	CHC-C4B-NB	-2.52	120.28	124.05
16	B	102	BCL	C2A-C1A-CHA	-2.52	119.50	123.87
16	D	101	BCL	C1C-NC-C4C	-2.51	105.53	106.68
16	2	101	BCL	CHC-C1C-NC	2.51	128.03	124.40
22	R	101	CRT	C14-C15-C16	-2.51	115.93	123.20
10	C	404	HEC	C2A-C1A-NA	-2.51	107.90	110.32
14	Z	104	PGV	O03-C19-C20	2.50	119.47	111.83
16	G	103	BCL	O2D-CGD-O1D	-2.50	118.97	123.85
16	3	102	BCL	O2A-CGA-CBA	2.50	119.47	111.83
14	Z	103	PGV	C02-O01-C1	-2.50	111.80	117.80
16	T	101	BCL	CHC-C4B-NB	-2.50	120.29	124.05
10	C	403	HEC	CHB-C1B-NB	2.50	128.40	123.86
16	7	102	BCL	CMD-C2D-C3D	-2.50	121.95	127.69
16	8	102	BCL	C2A-C1A-CHA	-2.50	119.53	123.87
16	3	102	BCL	C4A-NA-C1A	2.50	107.82	106.68
21	M	405	MQ8	C16-C17-C18	-2.50	121.91	127.62
16	5	103	BCL	CHB-C4A-NA	2.50	128.00	124.40
22	V	101	CRT	C9-C10-C11	-2.50	115.97	123.20
16	I	103	BCL	O2A-CGA-O1A	-2.50	117.39	123.63
14	X	103	PGV	C02-O01-C1	-2.49	111.83	117.80
16	W	101	BCL	CHC-C1C-NC	2.49	128.00	124.40
16	D	101	BCL	CHC-C4B-NB	-2.49	120.31	124.05
16	5	104	BCL	O2D-CGD-O1D	-2.49	119.01	123.85
16	U	103	BCL	O2D-CGD-O1D	-2.48	119.02	123.85
16	L	302	BCL	CMB-C2B-C1B	2.48	129.20	125.42
14	R	104	PGV	C02-O01-C1	-2.48	111.86	117.80
22	4	101	CRT	C9-C10-C11	-2.48	116.01	123.20
21	M	405	MQ8	C50-C48-C49	2.48	120.30	114.59
16	9	102	BCL	C4-C3-C5	2.48	119.53	115.23
22	V	101	CRT	C29-C28-C30	2.48	121.87	118.09
16	W	102	BCL	CHC-C1C-NC	2.48	127.97	124.40
16	X	102	BCL	C2A-C1A-CHA	-2.48	119.57	123.87
14	T	102	PGV	O03-C19-C20	2.48	119.38	111.83
16	A	101	BCL	O2D-CGD-O1D	-2.47	119.04	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	102	BCL	CHC-C1C-NC	2.47	127.97	124.40
22	N	102	CRT	C18-C17-C16	2.47	121.86	118.09
14	L	305	PGV	C02-O01-C1	-2.47	111.89	117.80
16	6	102	BCL	C6-C5-C3	-2.47	107.46	113.47
16	0	102	BCL	C2A-C1A-CHA	-2.47	119.59	123.87
16	E	101	BCL	CMB-C2B-C3B	2.46	133.44	125.67
16	U	103	BCL	CMD-C2D-C3D	-2.46	122.04	127.69
16	O	104	BCL	CHB-C4A-NA	2.46	127.95	124.40
22	N	102	CRT	C10-C9-C7	-2.46	123.83	127.28
14	X	103	PGV	O03-C19-C20	2.46	119.34	111.83
20	U	101	CDL	OB6-CB5-OB7	-2.46	117.95	123.70
16	S	102	BCL	O2D-CGD-O1D	-2.46	119.06	123.85
14	1	101	PGV	O03-C19-C20	2.46	119.33	111.83
16	I	103	BCL	CHB-C1B-NB	-2.46	120.36	124.05
22	Y	403	CRT	C36-C35-C33	-2.46	122.18	125.89
16	L	302	BCL	O2A-CGA-O1A	-2.46	117.49	123.63
16	5	104	BCL	O2A-CGA-O1A	-2.45	117.49	123.63
16	L	302	BCL	CHB-C1B-NB	-2.45	120.37	124.05
16	W	102	BCL	C1D-CHD-C4C	-2.45	120.70	126.62
16	G	103	BCL	CMB-C2B-C3B	2.45	133.40	125.67
16	V	102	BCL	CHB-C4A-NA	2.45	127.94	124.40
16	Y	401	BCL	CHC-C4B-NB	-2.45	120.38	124.05
16	Z	102	BCL	CMB-C2B-C3B	2.45	133.39	125.67
22	M	406	CRT	C13-C12-C11	2.45	121.83	118.09
16	D	101	BCL	CAA-CBA-CGA	-2.45	106.26	113.21
16	Y	401	BCL	C2A-C1A-CHA	-2.45	119.62	123.87
16	1	103	BCL	C4D-CHA-C1A	-2.44	118.33	121.24
22	V	101	CRT	C8-C7-C6	2.44	121.82	118.09
16	B	102	BCL	C1D-CHD-C4C	-2.44	120.73	126.62
22	8	101	CRT	C21-C20-C19	-2.44	118.52	123.52
16	W	101	BCL	C1D-CHD-C4C	-2.44	120.73	126.62
16	Z	102	BCL	C2A-C1A-CHA	-2.44	119.63	123.87
16	5	103	BCL	C1D-CHD-C4C	-2.44	120.74	126.62
16	Y	401	BCL	C1D-CHD-C4C	-2.44	120.74	126.62
16	V	102	BCL	C1-O2A-CGA	2.44	122.55	116.65
16	V	102	BCL	O2A-CGA-CBA	2.44	119.27	111.83
16	B	102	BCL	C1C-NC-C4C	-2.44	105.57	106.68
16	F	103	BCL	C6-C5-C3	-2.44	107.53	113.47
20	H	303	CDL	OB8-CB7-C71	2.44	119.27	111.83
20	H	303	CDL	OA8-CA7-C31	2.43	119.26	111.83
16	V	102	BCL	C1D-CHD-C4C	-2.43	120.75	126.62
16	D	101	BCL	C6-C5-C3	-2.43	107.54	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	6	102	BCL	CMB-C2B-C3B	2.43	133.34	125.67
10	C	402	HEC	CHA-C1A-NA	2.43	127.10	124.45
22	V	101	CRT	C34-C33-C35	2.43	121.80	118.09
16	W	102	BCL	CMD-C2D-C3D	-2.43	122.11	127.69
16	5	103	BCL	C6-C5-C3	-2.43	107.55	113.47
22	B	101	CRT	C10-C9-C7	-2.43	123.87	127.28
16	W	101	BCL	C1C-NC-C4C	-2.43	105.57	106.68
16	D	101	BCL	CHB-C4A-NA	2.42	127.90	124.40
16	A	101	BCL	C1C-NC-C4C	-2.42	105.57	106.68
16	S	101	BCL	CMB-C2B-C3B	2.42	133.31	125.67
16	4	102	BCL	CHB-C4A-NA	2.42	127.90	124.40
16	S	101	BCL	C1D-CHD-C4C	-2.42	120.78	126.62
16	K	101	BCL	CMB-C2B-C3B	2.42	133.30	125.67
17	L	303	BPH	CMA-C3A-C4A	-2.42	109.40	114.61
16	6	102	BCL	C1D-CHD-C4C	-2.42	120.79	126.62
22	Y	403	CRT	C27-C26-C25	-2.42	116.19	123.20
22	R	101	CRT	C8-C7-C6	2.42	121.78	118.09
16	0	102	BCL	CHB-C1B-NB	-2.42	120.42	124.05
16	M	403	BCL	CHC-C1C-NC	2.42	127.89	124.40
16	0	102	BCL	CMB-C2B-C3B	2.41	133.28	125.67
18	L	304	UQ8	C25-C24-C26	2.41	120.14	114.59
14	4	103	PGV	O03-C19-C20	2.41	119.19	111.83
16	9	102	BCL	CHB-C4A-NA	2.41	127.88	124.40
22	Y	403	CRT	C32-C31-C30	-2.41	116.22	123.20
16	K	101	BCL	O2D-CGD-O1D	-2.41	119.16	123.85
16	9	102	BCL	C1D-CHD-C4C	-2.41	120.82	126.62
16	I	103	BCL	O2D-CGD-O1D	-2.40	119.17	123.85
14	J	102	PGV	O14-P-O13	2.40	120.19	110.83
16	5	103	BCL	CHC-C1C-NC	2.40	127.86	124.40
16	Y	401	BCL	O2D-CGD-O1D	-2.40	119.18	123.85
16	O	104	BCL	CHC-C4B-NB	-2.40	120.45	124.05
16	W	102	BCL	O2D-CGD-O1D	-2.40	119.18	123.85
18	L	304	UQ8	C10-C9-C11	2.40	119.39	115.23
16	O	103	BCL	O2D-CGD-O1D	-2.40	119.18	123.85
22	B	101	CRT	C27-C26-C25	-2.40	116.26	123.20
16	U	103	BCL	CAA-CBA-CGA	-2.39	106.41	113.21
16	L	312	BCL	CHC-C1C-NC	2.39	127.86	124.40
16	O	104	BCL	C1D-CHD-C4C	-2.39	120.84	126.62
16	I	103	BCL	CAC-C3C-C4C	-2.39	107.27	112.58
20	U	101	CDL	OB8-CB7-C71	2.39	119.14	111.83
16	D	101	BCL	C1D-CHD-C4C	-2.39	120.84	126.62
16	P	101	BCL	CHC-C1C-NC	2.39	127.85	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	103	BCL	CHB-C4A-NA	2.39	127.85	124.40
22	8	101	CRT	C18-C17-C16	2.39	121.74	118.09
16	E	101	BCL	CHC-C1C-NC	2.39	127.84	124.40
16	1	102	BCL	CMD-C2D-C3D	-2.39	122.22	127.69
16	N	103	BCL	CHB-C4A-NA	2.39	127.84	124.40
16	E	101	BCL	CHC-C4B-NB	-2.39	120.47	124.05
16	O	103	BCL	C1D-CHD-C4C	-2.39	120.87	126.62
22	R	101	CRT	C27-C26-C25	-2.38	116.29	123.20
16	W	102	BCL	C4D-CHA-C1A	-2.38	118.40	121.24
16	4	102	BCL	CMB-C2B-C3B	2.38	133.19	125.67
16	L	311	BCL	C1D-CHD-C4C	-2.38	120.88	126.62
16	G	103	BCL	C1C-NC-C4C	-2.38	105.59	106.68
10	C	401	HEC	CHD-C4C-NC	2.38	127.04	124.45
22	M	406	CRT	C18-C17-C16	2.38	121.72	118.09
16	K	101	BCL	CHC-C4B-NB	-2.38	120.48	124.05
16	I	103	BCL	CHB-C4A-NA	2.38	127.83	124.40
22	8	101	CRT	C14-C15-C16	-2.37	116.32	123.20
16	0	102	BCL	C11-C12-C13	-2.37	108.08	115.97
16	1	102	BCL	C2A-C1A-CHA	-2.37	119.75	123.87
16	6	102	BCL	CHC-C4B-NB	-2.37	120.50	124.05
16	1	102	BCL	CED-O2D-CGD	2.37	121.28	115.92
16	4	102	BCL	C1D-CHD-C4C	-2.37	120.91	126.62
16	9	101	BCL	CMB-C2B-C3B	2.36	133.13	125.67
16	E	101	BCL	C1D-CHD-C4C	-2.36	120.92	126.62
16	2	101	BCL	CHB-C4A-NA	2.36	127.81	124.40
16	X	102	BCL	C1D-CHD-C4C	-2.36	120.92	126.62
16	Z	102	BCL	O2D-CGD-O1D	-2.36	119.25	123.85
16	M	403	BCL	C1D-CHD-C4C	-2.36	120.92	126.62
16	D	101	BCL	C4A-NA-C1A	2.36	107.76	106.68
16	O	104	BCL	O2D-CGD-O1D	-2.36	119.25	123.85
16	4	102	BCL	O2D-CGD-O1D	-2.36	119.26	123.85
16	T	101	BCL	C1-C2-C3	-2.36	122.33	126.20
16	Q	102	BCL	CHC-C1C-NC	2.36	127.80	124.40
14	R	103	PGV	O03-C19-O04	-2.36	117.73	123.63
15	O	102	LMT	O1'-C1'-C2'	2.36	111.85	108.27
16	D	102	BCL	C2A-C1A-CHA	-2.36	119.78	123.87
16	O	103	BCL	C1C-NC-C4C	-2.35	105.61	106.68
16	N	103	BCL	CHB-C1B-NB	-2.35	120.52	124.05
16	S	101	BCL	CAA-CBA-CGA	-2.35	106.53	113.21
15	L	308	LMT	C1B-O1B-C4'	-2.35	112.41	117.98
16	Y	402	BCL	C1D-CHD-C4C	-2.34	120.97	126.62
15	H	306	LMT	C1B-O1B-C4'	-2.34	112.43	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	X	102	BCL	CHB-C4A-NA	2.34	127.78	124.40
18	L	306	UQ8	C25-C24-C26	2.34	119.29	115.23
16	T	101	BCL	CMB-C2B-C3B	2.34	133.05	125.67
16	S	101	BCL	O2D-CGD-O1D	-2.34	119.30	123.85
15	Q	101	LMT	C1B-O1B-C4'	-2.34	112.44	117.98
14	4	103	PGV	C02-O01-C1	-2.34	112.21	117.80
16	S	102	BCL	CHB-C1B-NB	-2.33	120.55	124.05
16	L	302	BCL	C1D-CHD-C4C	-2.33	120.99	126.62
16	Q	102	BCL	C1D-CHD-C4C	-2.33	121.00	126.62
16	X	102	BCL	CMB-C2B-C3B	2.33	133.02	125.67
22	4	101	CRT	C32-C31-C30	-2.33	116.45	123.20
16	J	101	BCL	CHB-C4A-NA	2.33	127.76	124.40
16	I	102	BCL	C1D-CHD-C4C	-2.33	121.01	126.62
16	Q	102	BCL	CMB-C2B-C3B	2.33	133.01	125.67
16	4	102	BCL	CHC-C4B-NB	-2.33	120.56	124.05
16	D	101	BCL	CMB-C2B-C3B	2.33	133.01	125.67
16	1	102	BCL	O2D-CGD-O1D	-2.33	119.32	123.85
16	O	104	BCL	CHD-C1D-C2D	2.33	130.32	125.49
16	A	101	BCL	C1-C2-C3	-2.32	122.39	126.20
15	H	305	LMT	O5'-C5'-C6'	2.32	112.20	106.44
16	F	103	BCL	CHB-C1B-C2B	-2.32	120.69	127.43
20	H	303	CDL	OB6-CB5-OB7	-2.32	118.28	123.70
16	Z	102	BCL	CHC-C1C-NC	2.32	127.75	124.40
22	Y	403	CRT	C11-C12-C14	-2.32	115.36	119.01
16	Y	401	BCL	CHB-C1B-NB	-2.32	120.57	124.05
14	P	103	PGV	O14-P-O13	2.32	119.87	110.83
16	G	103	BCL	CHC-C1C-NC	2.32	127.75	124.40
16	I	103	BCL	CHC-C4B-NB	-2.32	120.57	124.05
16	G	103	BCL	C1D-CHD-C4C	-2.32	121.03	126.62
16	1	102	BCL	CAA-CBA-CGA	-2.32	106.63	113.21
16	L	312	BCL	CHD-C1D-C2D	2.31	130.30	125.49
14	X	101	PGV	C02-O01-C1	-2.31	112.26	117.80
16	Y	402	BCL	CMB-C2B-C3B	2.31	132.96	125.67
10	C	401	HEC	CHB-C1B-C2B	-2.31	120.72	127.43
16	9	101	BCL	C1C-NC-C4C	-2.31	105.63	106.68
16	D	102	BCL	CMD-C2D-C3D	-2.31	122.40	127.69
15	F	102	LMT	O5B-C1B-C2B	2.31	115.11	110.37
20	H	303	CDL	CB6-CB4-CB3	-2.31	106.41	111.78
16	7	102	BCL	C2A-C1A-CHA	-2.31	119.86	123.87
16	L	302	BCL	CMD-C2D-C3D	-2.30	122.41	127.69
16	O	103	BCL	O2A-CGA-O1A	-2.30	117.87	123.63
16	N	103	BCL	C1D-CHD-C4C	-2.30	121.08	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	W	102	BCL	CHB-C1B-NB	-2.30	120.61	124.05
16	F	103	BCL	CHB-C4A-NA	2.30	127.71	124.40
22	G	102	CRT	C27-C26-C25	-2.30	116.55	123.20
16	O	103	BCL	CMB-C2B-C3B	2.29	132.91	125.67
16	T	101	BCL	C4-C3-C5	2.29	119.21	115.23
16	P	101	BCL	C1D-CHD-C4C	-2.29	121.10	126.62
16	R	102	BCL	CHC-C4B-NB	-2.29	120.62	124.05
16	7	102	BCL	O2A-CGA-CBA	2.29	118.81	111.83
22	8	101	CRT	C31-C32-C33	-2.29	124.07	127.28
20	M	407	CDL	OA8-CA7-C31	2.28	118.80	111.83
16	3	102	BCL	O2D-CGD-O1D	-2.28	119.40	123.85
16	W	101	BCL	O2A-CGA-O1A	-2.28	117.92	123.63
10	C	404	HEC	CHB-C1B-NB	2.28	128.00	123.86
16	X	102	BCL	C4D-CHA-C1A	-2.28	118.52	121.24
16	W	101	BCL	CHB-C4A-NA	2.28	127.69	124.40
14	R	104	PGV	O14-P-O13	2.28	119.71	110.83
16	D	101	BCL	C2A-C1A-CHA	-2.28	119.91	123.87
22	R	101	CRT	C5-C6-C7	-2.28	122.45	125.89
16	W	101	BCL	CHB-C1B-C2B	-2.28	120.82	127.43
22	V	101	CRT	C13-C12-C11	2.27	121.56	118.09
16	W	102	BCL	CAC-C3C-C4C	-2.27	107.54	112.58
16	5	103	BCL	CMD-C2D-C3D	-2.27	122.48	127.69
16	N	103	BCL	C2A-C1A-CHA	-2.27	119.92	123.87
16	7	102	BCL	CHC-C1C-NC	2.27	127.68	124.40
16	L	302	BCL	C2A-C1A-CHA	-2.27	119.93	123.87
16	Y	402	BCL	C1C-NC-C4C	-2.27	105.64	106.68
16	S	102	BCL	C1D-CHD-C4C	-2.27	121.14	126.62
16	1	102	BCL	CHD-C1D-C2D	2.27	130.21	125.49
16	D	102	BCL	C3C-C4C-CHD	-2.27	118.61	123.39
16	L	311	BCL	CMB-C2B-C3B	2.27	132.82	125.67
22	G	102	CRT	C21-C20-C19	-2.27	118.88	123.52
16	S	101	BCL	C4A-NA-C1A	2.27	107.71	106.68
16	B	102	BCL	CMB-C2B-C3B	2.27	132.82	125.67
16	R	102	BCL	C1D-CHD-C4C	-2.26	121.16	126.62
15	I	101	LMT	O3'-C3'-C2'	-2.26	105.04	110.38
16	I	102	BCL	CHB-C4A-NA	2.26	127.66	124.40
16	M	403	BCL	O2A-CGA-CBA	2.26	118.73	111.83
16	L	312	BCL	O1D-CGD-CBD	-2.26	120.06	124.52
16	7	102	BCL	C1D-CHD-C4C	-2.26	121.17	126.62
16	A	101	BCL	CHB-C1B-C2B	-2.26	120.87	127.43
16	F	103	BCL	C1D-CHD-C4C	-2.26	121.18	126.62
16	5	103	BCL	CMB-C2B-C3B	2.26	132.79	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	312	BCL	CHB-C1B-C2B	-2.26	120.88	127.43
16	L	312	BCL	CMB-C2B-C3B	2.26	132.78	125.67
16	X	102	BCL	CHC-C4B-NB	-2.26	120.67	124.05
14	B	103	PGV	C02-O01-C1	-2.26	112.40	117.80
16	1	102	BCL	C1D-CHD-C4C	-2.25	121.18	126.62
16	O	104	BCL	C2A-C1A-CHA	-2.25	119.95	123.87
16	Y	402	BCL	O2A-CGA-O1A	-2.25	117.99	123.63
16	D	102	BCL	CHB-C4A-NA	2.25	127.65	124.40
22	N	102	CRT	C34-C33-C35	2.25	121.53	118.09
16	V	102	BCL	O2D-CGD-O1D	-2.25	119.47	123.85
22	8	101	CRT	C27-C26-C25	-2.25	116.68	123.20
18	L	306	UQ8	C20-C19-C21	2.25	119.13	115.23
16	L	302	BCL	CHC-C1C-NC	2.25	127.64	124.40
22	G	102	CRT	C10-C9-C7	-2.25	124.13	127.28
16	Z	102	BCL	C1-C2-C3	-2.24	122.52	126.20
16	8	102	BCL	C4-C3-C5	2.24	119.12	115.23
14	0	104	PGV	C02-O01-C1	-2.24	112.43	117.80
16	7	102	BCL	CMB-C2B-C3B	2.24	132.74	125.67
22	4	101	CRT	C21-C20-C19	-2.24	118.94	123.52
16	5	103	BCL	O2D-CGD-O1D	-2.24	119.49	123.85
16	P	101	BCL	CHC-C4B-NB	-2.24	120.69	124.05
16	5	104	BCL	CHD-C1D-C2D	2.24	130.14	125.49
16	W	101	BCL	CHD-C1D-C2D	2.23	130.13	125.49
16	I	102	BCL	CMB-C2B-C3B	2.23	132.72	125.67
16	N	103	BCL	C1C-NC-C4C	-2.23	105.66	106.68
16	5	104	BCL	CMD-C2D-C3D	-2.23	122.57	127.69
16	D	101	BCL	CHC-C1C-NC	2.23	127.62	124.40
16	1	103	BCL	C1D-CHD-C4C	-2.23	121.24	126.62
16	L	311	BCL	C2A-C1A-CHA	-2.23	120.00	123.87
16	3	102	BCL	CMD-C2D-C3D	-2.23	122.58	127.69
16	Y	401	BCL	CHD-C1D-C2D	2.23	130.12	125.49
16	O	104	BCL	O2A-CGA-O1A	-2.23	118.06	123.63
15	I	101	LMT	C2'-C3'-C4'	2.22	114.73	109.68
22	G	102	CRT	C32-C31-C30	-2.22	116.76	123.20
16	S	101	BCL	CHD-C1D-C2D	2.22	130.11	125.49
16	A	101	BCL	O2A-CGA-CBA	2.22	118.61	111.83
16	D	102	BCL	CHC-C4B-NB	-2.22	120.72	124.05
20	H	301	CDL	OA6-CA5-OA7	-2.22	118.52	123.70
22	G	102	CRT	C26-C27-C28	-2.22	124.17	127.28
20	M	407	CDL	CB4-OB6-CB5	-2.21	112.50	117.80
16	6	102	BCL	CHB-C4A-NA	2.21	127.59	124.40
16	9	102	BCL	CAC-C3C-C4C	-2.21	107.67	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	9	102	BCL	CMD-C2D-C3D	-2.21	122.62	127.69
16	8	102	BCL	O2A-CGA-O1A	-2.21	118.10	123.63
16	9	102	BCL	C1C-NC-C4C	-2.21	105.67	106.68
16	U	103	BCL	CHB-C1B-C2B	-2.21	121.01	127.43
22	N	102	CRT	C9-C10-C11	-2.21	116.80	123.20
22	M	406	CRT	C15-C14-C12	-2.21	124.18	127.28
16	6	102	BCL	C1C-NC-C4C	-2.21	105.67	106.68
22	G	102	CRT	C5-C6-C7	-2.21	122.56	125.89
16	M	403	BCL	CHB-C1B-C2B	-2.20	121.03	127.43
16	9	101	BCL	CMD-C2D-C3D	-2.20	122.64	127.69
14	H	302	PGV	C03-C02-C01	-2.20	106.65	111.78
16	S	101	BCL	CHC-C1C-NC	2.20	127.58	124.40
22	R	101	CRT	C29-C28-C30	2.20	121.45	118.09
16	3	102	BCL	CMB-C2B-C3B	2.20	132.61	125.67
16	D	102	BCL	C1D-CHD-C4C	-2.20	121.32	126.62
16	Q	102	BCL	C1C-NC-C4C	-2.20	105.68	106.68
15	5	102	LMT	C1B-O1B-C4'	-2.20	112.77	117.98
10	C	402	HEC	CHD-C4C-NC	2.19	126.84	124.45
16	V	102	BCL	CHC-C1C-NC	2.19	127.56	124.40
16	P	101	BCL	CMB-C2B-C3B	2.19	132.59	125.67
16	O	104	BCL	C4A-NA-C1A	2.19	107.68	106.68
10	C	401	HEC	CHD-C1D-C2D	-2.19	121.06	127.43
14	H	304	PGV	O03-C19-O04	-2.19	118.15	123.63
16	B	102	BCL	O2D-CGD-O1D	-2.19	119.58	123.85
16	8	102	BCL	CHC-C4B-NB	-2.19	120.76	124.05
14	8	103	PGV	C02-O01-C1	-2.19	112.56	117.80
16	0	102	BCL	C1D-CHD-C4C	-2.19	121.34	126.62
16	1	102	BCL	CHB-C1B-C2B	-2.19	121.07	127.43
14	8	103	PGV	O03-C19-C20	2.19	118.51	111.83
16	Y	401	BCL	C16-C15-C13	-2.19	108.69	115.97
22	B	101	CRT	C13-C12-C11	2.19	121.43	118.09
16	S	102	BCL	CMD-C2D-C3D	-2.19	122.67	127.69
16	S	102	BCL	CMB-C2B-C3B	2.18	132.56	125.67
16	N	103	BCL	CHC-C1C-NC	2.18	127.55	124.40
16	I	103	BCL	CMD-C2D-C3D	-2.18	122.68	127.69
16	N	103	BCL	CMB-C2B-C3B	2.18	132.55	125.67
14	T	103	PGV	O03-C19-C20	2.18	118.48	111.83
16	I	102	BCL	O2D-CGD-O1D	-2.18	119.61	123.85
22	N	102	CRT	C29-C28-C30	2.18	121.41	118.09
16	5	103	BCL	CED-O2D-CGD	2.18	120.85	115.92
16	J	101	BCL	C11-C12-C13	-2.18	108.73	115.97
10	C	402	HEC	CHB-C1B-C2B	-2.17	121.12	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	102	CRT	C38-C37-C36	-2.17	107.34	112.98
14	Z	101	PGV	O03-C19-O04	-2.17	118.19	123.63
16	8	102	BCL	C4D-CHA-C1A	-2.17	118.65	121.24
22	R	101	CRT	C38-C37-C36	-2.17	107.35	112.98
16	I	103	BCL	C1D-CHD-C4C	-2.17	121.39	126.62
16	L	302	BCL	C4D-CHA-C1A	-2.17	118.66	121.24
10	C	404	HEC	CAD-CBD-CGD	-2.17	107.92	113.67
16	3	102	BCL	CHD-C1D-C2D	2.17	129.99	125.49
18	L	306	UQ8	C15-C14-C13	-2.16	118.07	123.63
22	8	101	CRT	C10-C9-C7	-2.16	124.24	127.28
16	L	312	BCL	C2A-C1A-CHA	-2.16	120.12	123.87
16	X	102	BCL	CHB-C1B-NB	-2.16	120.81	124.05
16	D	102	BCL	C11-C12-C13	-2.16	108.80	115.97
16	E	101	BCL	C2A-C1A-CHA	-2.16	120.13	123.87
16	B	102	BCL	CHC-C4B-NB	-2.15	120.82	124.05
16	3	102	BCL	C2A-C1A-CHA	-2.15	120.13	123.87
16	5	104	BCL	C1D-CHD-C4C	-2.15	121.43	126.62
14	X	103	PGV	O01-C1-O02	-2.15	118.68	123.70
10	C	401	HEC	O2D-CGD-CBD	2.15	120.78	114.00
16	S	102	BCL	CHB-C4A-NA	2.15	127.50	124.40
16	5	103	BCL	C4A-NA-C1A	2.15	107.66	106.68
16	A	101	BCL	C1D-CHD-C4C	-2.14	121.45	126.62
16	Z	102	BCL	CHC-C4B-NB	-2.14	120.83	124.05
16	7	102	BCL	C4A-NA-C1A	2.14	107.66	106.68
10	C	401	HEC	CHB-C4A-NA	2.14	126.78	124.45
16	0	102	BCL	C6-C7-C8	-2.14	108.85	115.97
16	M	403	BCL	CAA-CBA-CGA	-2.14	107.14	113.21
16	L	311	BCL	C1C-NC-C4C	-2.13	105.70	106.68
10	C	401	HEC	CHA-C1A-NA	2.13	126.77	124.45
16	I	102	BCL	C6-C7-C8	-2.13	108.89	115.97
20	M	409	CDL	CB4-OB6-CB5	-2.13	112.71	117.80
16	1	103	BCL	CHB-C1B-C2B	-2.13	121.26	127.43
22	V	101	CRT	C24-C23-C25	2.12	121.33	118.09
16	K	101	BCL	CHD-C1D-C2D	2.12	129.91	125.49
20	M	408	CDL	CB6-CB4-CB3	-2.12	106.83	111.78
14	0	103	PGV	O03-C19-O04	-2.12	118.31	123.63
10	C	402	HEC	O2A-CGA-CBA	2.12	120.71	114.00
16	W	102	BCL	CHD-C1D-C2D	2.12	129.90	125.49
16	I	103	BCL	C4-C3-C5	2.12	118.91	115.23
16	R	102	BCL	CHB-C1B-NB	-2.12	120.87	124.05
16	S	101	BCL	O2A-CGA-O1A	-2.12	118.33	123.63
14	G	105	PGV	O03-C19-O04	-2.12	118.33	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	102	BCL	C6-C5-C3	-2.11	108.32	113.47
20	U	102	CDL	OB6-CB5-OB7	-2.11	118.77	123.70
16	I	103	BCL	CED-O2D-CGD	2.11	120.70	115.92
14	G	101	PGV	O03-C19-O04	-2.11	118.35	123.63
16	9	101	BCL	CHC-C1C-NC	2.11	127.45	124.40
16	8	102	BCL	C1D-CHD-C4C	-2.11	121.53	126.62
22	G	102	CRT	C18-C17-C16	2.11	121.31	118.09
14	P	102	PGV	O01-C1-O02	-2.11	118.77	123.70
16	J	101	BCL	C1D-CHD-C4C	-2.11	121.54	126.62
16	W	102	BCL	CHB-C4A-NA	2.11	127.44	124.40
22	4	101	CRT	C34-C33-C35	2.11	121.31	118.09
16	O	104	BCL	CMB-C2B-C3B	2.11	132.31	125.67
22	G	102	CRT	O1-C1-C3	2.10	123.44	108.97
16	1	103	BCL	O2A-CGA-O1A	-2.10	118.37	123.63
16	S	101	BCL	CHB-C4A-NA	2.10	127.44	124.40
16	J	101	BCL	CHB-C1B-C2B	-2.10	121.32	127.43
16	S	101	BCL	C2A-C1A-CHA	-2.10	120.22	123.87
18	L	306	UQ8	C17-C16-C14	-2.10	106.23	113.19
16	R	102	BCL	CMB-C2B-C3B	2.10	132.29	125.67
16	W	101	BCL	C4A-NA-C1A	2.10	107.64	106.68
15	Q	101	LMT	C1B-C2B-C3B	2.10	114.42	110.01
15	O	102	LMT	C1-O1'-C1'	-2.09	110.10	113.68
15	5	101	LMT	C6B-C5B-C4B	-2.09	107.88	113.02
16	5	104	BCL	C2A-C1A-CHA	-2.09	120.24	123.87
16	O	104	BCL	O1D-CGD-CBD	-2.09	120.39	124.52
16	L	312	BCL	O2A-CGA-O1A	-2.09	118.40	123.63
22	G	102	CRT	C36-C35-C33	-2.09	122.74	125.89
10	C	404	HEC	C4B-NB-C1B	2.09	109.22	105.82
16	5	103	BCL	CHB-C1B-C2B	-2.09	121.37	127.43
14	G	104	PGV	O03-C19-O04	-2.09	118.41	123.63
16	I	102	BCL	O2A-CGA-O1A	-2.08	118.42	123.63
22	V	101	CRT	C38-C37-C36	-2.08	107.58	112.98
16	E	101	BCL	C4D-CHA-C1A	-2.08	118.76	121.24
16	9	101	BCL	O2A-CGA-O1A	-2.08	118.42	123.63
14	E	102	PGV	O03-C19-O04	-2.08	118.42	123.63
16	Y	402	BCL	CMD-C2D-C3D	-2.08	122.92	127.69
14	Z	104	PGV	O01-C1-O02	-2.08	118.85	123.70
14	T	103	PGV	C02-O01-C1	-2.08	112.83	117.80
14	B	104	PGV	O03-C19-O04	-2.08	118.44	123.63
16	Q	102	BCL	CMD-C2D-C3D	-2.07	122.93	127.69
10	C	402	HEC	CHB-C4A-NA	2.07	126.71	124.45
14	G	105	PGV	C03-C02-C01	-2.07	106.96	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	6	103	PGV	C02-O01-C1	-2.07	112.84	117.80
16	B	102	BCL	CHB-C1B-NB	-2.07	120.95	124.05
16	W	102	BCL	CMB-C2B-C3B	2.07	132.19	125.67
16	T	101	BCL	CHB-C1B-C2B	-2.07	121.42	127.43
16	1	102	BCL	C11-C12-C13	-2.07	109.09	115.97
18	L	304	UQ8	C7-C6-C1	-2.07	121.35	124.89
10	C	402	HEC	CHD-C1D-C2D	-2.07	121.43	127.43
10	C	403	HEC	C4B-NB-C1B	2.06	109.18	105.82
16	W	102	BCL	O2A-CGA-O1A	-2.06	118.47	123.63
20	M	407	CDL	OB8-CB7-OB9	-2.06	118.47	123.63
20	M	407	CDL	OB6-CB5-OB7	-2.06	118.89	123.70
16	L	312	BCL	C1D-CHD-C4C	-2.06	121.65	126.62
10	C	403	HEC	CHD-C1D-C2D	-2.06	121.44	127.43
16	E	101	BCL	C1C-NC-C4C	-2.06	105.74	106.68
16	J	101	BCL	CAA-CBA-CGA	-2.06	107.36	113.21
16	D	102	BCL	O2A-CGA-O1A	-2.06	118.48	123.63
10	C	403	HEC	CHD-C4C-NC	2.06	126.69	124.45
16	U	103	BCL	CHD-C1D-C2D	2.06	129.76	125.49
16	V	102	BCL	C4-C3-C2	-2.06	118.35	123.63
16	9	101	BCL	CHB-C4A-NA	2.05	127.36	124.40
16	5	104	BCL	CAC-C3C-C4C	-2.05	108.03	112.58
16	A	101	BCL	CMD-C2D-C3D	-2.05	122.99	127.69
16	1	103	BCL	C6-C7-C8	-2.05	109.15	115.97
16	9	102	BCL	CMB-C2B-C3B	2.05	132.13	125.67
22	R	101	CRT	C35-C33-C32	-2.05	115.79	119.01
20	H	303	CDL	OB8-CB7-OB9	-2.05	118.50	123.63
21	M	405	MQ8	C2M-C2-C3	-2.05	121.09	124.45
16	E	101	BCL	CHB-C1B-C2B	-2.05	121.48	127.43
16	D	102	BCL	CHD-C1D-C2D	2.05	129.74	125.49
10	C	402	HEC	CBA-CAA-C2A	-2.05	106.88	112.53
22	4	101	CRT	C18-C17-C16	2.04	121.21	118.09
16	I	102	BCL	CHD-C1D-C2D	2.04	129.74	125.49
16	V	102	BCL	CHB-C1B-NB	-2.04	120.99	124.05
16	5	103	BCL	O2A-CGA-O1A	-2.04	118.52	123.63
16	O	104	BCL	CHB-C1B-NB	-2.04	120.99	124.05
16	D	101	BCL	O2A-CGA-O1A	-2.04	118.52	123.63
10	C	403	HEC	CHC-C4B-C3B	-2.04	121.78	125.21
22	G	102	CRT	C34-C33-C35	2.04	121.20	118.09
16	9	102	BCL	CED-O2D-CGD	2.04	120.53	115.92
16	Y	401	BCL	O1D-CGD-CBD	-2.03	120.50	124.52
22	M	406	CRT	C26-C25-C23	-2.03	120.78	126.36
22	8	101	CRT	C13-C12-C14	-2.03	119.52	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	306	UQ8	C27-C28-C29	-2.03	120.87	127.64
16	M	403	BCL	C1-O2A-CGA	2.03	121.56	116.65
16	M	403	BCL	O2D-CGD-O1D	-2.03	119.90	123.85
14	L	310	PGV	O14-P-O13	2.03	121.87	112.44
16	1	103	BCL	CHD-C1D-C2D	2.02	129.70	125.49
16	V	102	BCL	CHC-C4B-C3B	-2.02	123.68	131.72
16	R	102	BCL	O2A-CGA-O1A	-2.02	118.57	123.63
16	T	101	BCL	C1D-CHD-C4C	-2.02	121.74	126.62
16	D	101	BCL	C6-C7-C8	-2.02	109.24	115.97
16	S	102	BCL	CED-O2D-CGD	2.02	120.50	115.92
10	C	403	HEC	CHB-C1B-C2B	-2.02	121.56	127.43
16	L	312	BCL	CHB-C4A-NA	2.02	127.31	124.40
16	S	101	BCL	CHB-C1B-C2B	-2.02	121.57	127.43
16	5	103	BCL	C1C-NC-C4C	-2.02	105.76	106.68
20	M	408	CDL	OA6-CA5-OA7	-2.02	118.99	123.70
16	G	103	BCL	CHC-C4B-NB	-2.02	121.03	124.05
16	S	102	BCL	C16-C15-C13	-2.01	109.27	115.97
14	F	101	PGV	O01-C1-O02	-2.01	119.00	123.70
22	Y	403	CRT	C18-C17-C16	2.01	121.16	118.09
14	T	102	PGV	C02-O01-C1	-2.01	112.99	117.80
15	F	102	LMT	C1B-C2B-C3B	2.01	114.24	110.01
22	R	101	CRT	C13-C12-C11	2.01	121.15	118.09
14	F	101	PGV	C03-C02-C01	-2.00	107.11	111.78
16	V	102	BCL	CMB-C2B-C3B	2.00	131.99	125.67
16	J	101	BCL	C6-C7-C8	-2.00	109.31	115.97
16	T	101	BCL	O2A-CGA-O1A	-2.00	118.62	123.63
16	O	103	BCL	C4A-NA-C1A	2.00	107.59	106.68
16	6	102	BCL	O2A-CGA-O1A	-2.00	118.62	123.63
16	I	102	BCL	C2A-C1A-CHA	-2.00	120.40	123.87

There are no chirality outliers.

All (1747) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	401	HEC	C2B-C3B-CAB-CBB
10	C	401	HEC	C2C-C3C-CAC-CBC
10	C	401	HEC	C4C-C3C-CAC-CBC
10	C	402	HEC	C2B-C3B-CAB-CBB
10	C	402	HEC	C4B-C3B-CAB-CBB
10	C	402	HEC	C2C-C3C-CAC-CBC
10	C	402	HEC	C4C-C3C-CAC-CBC
10	C	403	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
10	C	403	HEC	C4B-C3B-CAB-CBB
10	C	403	HEC	C2C-C3C-CAC-CBC
10	C	403	HEC	C4C-C3C-CAC-CBC
10	C	404	HEC	C2B-C3B-CAB-CBB
10	C	404	HEC	C4B-C3B-CAB-CBB
10	C	404	HEC	C2C-C3C-CAC-CBC
10	C	404	HEC	C4C-C3C-CAC-CBC
14	L	305	PGV	C03-O11-P-O12
14	L	305	PGV	C03-O11-P-O13
14	L	309	PGV	C04-O12-P-O11
14	L	309	PGV	C04-O12-P-O13
14	L	310	PGV	C03-O11-P-O12
14	L	310	PGV	C03-O11-P-O13
14	L	310	PGV	C03-O11-P-O14
14	L	310	PGV	C04-O12-P-O11
14	M	410	PGV	C04-O12-P-O11
14	M	410	PGV	C04-O12-P-O13
14	M	410	PGV	O12-C04-C05-O05
14	M	410	PGV	O02-C1-O01-C02
14	H	302	PGV	C03-O11-P-O13
14	H	302	PGV	C04-O12-P-O11
14	H	302	PGV	C04-O12-P-O13
14	H	302	PGV	C04-O12-P-O14
14	H	302	PGV	O12-C04-C05-C06
14	H	304	PGV	C04-O12-P-O11
14	H	304	PGV	C04-O12-P-O13
14	H	304	PGV	C04-O12-P-O14
14	H	304	PGV	C2-C1-O01-C02
14	B	103	PGV	C03-O11-P-O12
14	B	103	PGV	C03-O11-P-O13
14	B	103	PGV	C03-O11-P-O14
14	B	103	PGV	C04-O12-P-O11
14	B	103	PGV	C04-O12-P-O13
14	B	103	PGV	C04-O12-P-O14
14	B	103	PGV	O12-C04-C05-O05
14	B	104	PGV	C03-O11-P-O12
14	B	104	PGV	C03-O11-P-O13
14	B	104	PGV	C03-O11-P-O14
14	F	101	PGV	C03-O11-P-O12
14	F	101	PGV	C03-O11-P-O13
14	F	101	PGV	C03-O11-P-O14
14	F	101	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
14	F	101	PGV	C04-O12-P-O14
14	G	101	PGV	C04-O12-P-O13
14	G	101	PGV	O03-C01-C02-O01
14	G	104	PGV	C03-O11-P-O12
14	G	104	PGV	C03-O11-P-O13
14	G	104	PGV	C03-O11-P-O14
14	G	105	PGV	C03-O11-P-O12
14	G	105	PGV	C2-C1-O01-C02
14	N	101	PGV	C04-O12-P-O11
14	N	101	PGV	C04-O12-P-O13
14	N	101	PGV	C04-C05-C06-O06
14	N	104	PGV	C03-O11-P-O13
14	N	104	PGV	C04-O12-P-O13
14	N	105	PGV	C03-O11-P-O12
14	N	105	PGV	C03-O11-P-O13
14	N	105	PGV	C03-O11-P-O14
14	P	102	PGV	C03-O11-P-O12
14	P	102	PGV	C03-O11-P-O13
14	P	102	PGV	C03-O11-P-O14
14	P	102	PGV	C04-O12-P-O13
14	P	102	PGV	O04-C19-O03-C01
14	P	102	PGV	C20-C19-O03-C01
14	R	103	PGV	C04-O12-P-O13
14	R	104	PGV	C03-O11-P-O12
14	R	104	PGV	C03-O11-P-O14
14	T	102	PGV	C03-O11-P-O12
14	T	102	PGV	C03-O11-P-O14
14	T	103	PGV	C03-O11-P-O12
14	T	103	PGV	C03-O11-P-O13
14	T	103	PGV	C03-O11-P-O14
14	V	103	PGV	C03-O11-P-O12
14	V	103	PGV	C03-O11-P-O13
14	V	103	PGV	C03-O11-P-O14
14	V	103	PGV	C04-C05-C06-O06
14	X	101	PGV	C03-O11-P-O13
14	X	103	PGV	C03-O11-P-O12
14	X	103	PGV	C03-O11-P-O14
14	Z	101	PGV	C03-O11-P-O12
14	Z	101	PGV	C03-O11-P-O13
14	Z	101	PGV	C03-O11-P-O14
14	Z	101	PGV	C04-O12-P-O13
14	Z	101	PGV	C04-C05-C06-O06

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Mol	Chain	Res	Type	Atoms
14	Z	103	PGV	C03-O11-P-O13
14	Z	103	PGV	C03-O11-P-O14
14	Z	103	PGV	C04-O12-P-O11
14	Z	103	PGV	C04-O12-P-O13
14	Z	104	PGV	C2-C1-O01-C02
14	1	101	PGV	C03-O11-P-O12
14	1	101	PGV	C03-O11-P-O14
14	1	101	PGV	C04-O12-P-O11
14	1	101	PGV	C04-O12-P-O14
14	1	101	PGV	C04-C05-C06-O06
14	2	102	PGV	C04-O12-P-O11
14	2	102	PGV	C04-O12-P-O14
14	2	102	PGV	C2-C1-O01-C02
14	2	103	PGV	C03-O11-P-O12
14	2	103	PGV	C03-O11-P-O13
14	2	103	PGV	C04-O12-P-O11
14	2	103	PGV	O12-C04-C05-O05
14	3	101	PGV	C03-O11-P-O12
14	3	101	PGV	C03-O11-P-O13
14	3	101	PGV	C03-O11-P-O14
14	4	103	PGV	C03-O11-P-O12
14	4	103	PGV	C03-O11-P-O14
14	4	103	PGV	C2-C1-O01-C02
14	6	101	PGV	C03-O11-P-O12
14	6	101	PGV	C03-O11-P-O13
14	6	101	PGV	C03-O11-P-O14
14	6	103	PGV	C04-O12-P-O11
14	6	103	PGV	C04-O12-P-O14
14	6	104	PGV	C04-O12-P-O11
14	6	104	PGV	C04-O12-P-O13
14	6	104	PGV	C2-C1-O01-C02
14	8	103	PGV	C03-O11-P-O12
14	8	103	PGV	C03-O11-P-O13
14	8	103	PGV	C03-O11-P-O14
14	8	103	PGV	O03-C01-C02-O01
14	8	103	PGV	C2-C1-O01-C02
14	0	101	PGV	C03-O11-P-O12
14	0	101	PGV	C03-O11-P-O13
14	0	101	PGV	C03-O11-P-O14
14	0	101	PGV	C04-O12-P-O11
14	0	101	PGV	C04-O12-P-O14
14	0	103	PGV	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
14	0	104	PGV	C2-C1-O01-C02
15	O	102	LMT	C2-C1-O1'-C1'
15	7	101	LMT	O5'-C1'-O1'-C1
16	L	311	BCL	C1A-C2A-CAA-CBA
16	L	311	BCL	C3A-C2A-CAA-CBA
16	L	311	BCL	C4C-C3C-CAC-CBC
16	A	101	BCL	C4C-C3C-CAC-CBC
16	B	102	BCL	C1A-C2A-CAA-CBA
16	B	102	BCL	C3A-C2A-CAA-CBA
16	B	102	BCL	C2C-C3C-CAC-CBC
16	B	102	BCL	C4C-C3C-CAC-CBC
16	D	101	BCL	C1A-C2A-CAA-CBA
16	D	101	BCL	C3A-C2A-CAA-CBA
16	E	101	BCL	C2C-C3C-CAC-CBC
16	E	101	BCL	C4C-C3C-CAC-CBC
16	F	103	BCL	C2C-C3C-CAC-CBC
16	F	103	BCL	C4C-C3C-CAC-CBC
16	G	103	BCL	C1A-C2A-CAA-CBA
16	G	103	BCL	C2C-C3C-CAC-CBC
16	G	103	BCL	C4C-C3C-CAC-CBC
16	I	103	BCL	C1A-C2A-CAA-CBA
16	I	103	BCL	C2C-C3C-CAC-CBC
16	I	103	BCL	C4C-C3C-CAC-CBC
16	J	101	BCL	C4C-C3C-CAC-CBC
16	K	101	BCL	C1A-C2A-CAA-CBA
16	K	101	BCL	C3A-C2A-CAA-CBA
16	K	101	BCL	C4C-C3C-CAC-CBC
16	N	103	BCL	C1A-C2A-CAA-CBA
16	N	103	BCL	C3A-C2A-CAA-CBA
16	O	104	BCL	C2C-C3C-CAC-CBC
16	O	104	BCL	C11-C10-C8-C9
16	P	101	BCL	C2C-C3C-CAC-CBC
16	P	101	BCL	C4C-C3C-CAC-CBC
16	R	102	BCL	C1A-C2A-CAA-CBA
16	R	102	BCL	C2C-C3C-CAC-CBC
16	R	102	BCL	C4C-C3C-CAC-CBC
16	S	101	BCL	C1A-C2A-CAA-CBA
16	U	103	BCL	C4C-C3C-CAC-CBC
16	V	102	BCL	C11-C12-C13-C14
16	X	102	BCL	C2C-C3C-CAC-CBC
16	X	102	BCL	C4C-C3C-CAC-CBC
16	Y	401	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
16	Y	401	BCL	C4C-C3C-CAC-CBC
16	Y	402	BCL	C1A-C2A-CAA-CBA
16	Y	402	BCL	C2C-C3C-CAC-CBC
16	Y	402	BCL	C4C-C3C-CAC-CBC
16	1	102	BCL	C2C-C3C-CAC-CBC
16	1	103	BCL	C4C-C3C-CAC-CBC
16	2	101	BCL	C2C-C3C-CAC-CBC
16	2	101	BCL	C4C-C3C-CAC-CBC
16	3	102	BCL	C4C-C3C-CAC-CBC
16	5	103	BCL	C1A-C2A-CAA-CBA
16	5	103	BCL	C3A-C2A-CAA-CBA
16	5	104	BCL	C2C-C3C-CAC-CBC
16	5	104	BCL	C4C-C3C-CAC-CBC
16	6	102	BCL	C2C-C3C-CAC-CBC
16	6	102	BCL	C4C-C3C-CAC-CBC
16	7	102	BCL	C2C-C3C-CAC-CBC
16	7	102	BCL	C4C-C3C-CAC-CBC
16	8	102	BCL	C1A-C2A-CAA-CBA
16	8	102	BCL	C3A-C2A-CAA-CBA
16	8	102	BCL	C2C-C3C-CAC-CBC
16	8	102	BCL	C4C-C3C-CAC-CBC
16	9	101	BCL	C1A-C2A-CAA-CBA
16	0	102	BCL	C1A-C2A-CAA-CBA
17	L	303	BPH	C1-C2-C3-C4
17	L	303	BPH	C1-C2-C3-C5
20	M	402	CDL	CA3-OA5-PA1-OA2
20	M	402	CDL	CA3-OA5-PA1-OA3
20	M	402	CDL	CB2-OB2-PB2-OB4
20	M	402	CDL	CB2-OB2-PB2-OB5
20	M	402	CDL	CB3-OB5-PB2-OB2
20	M	407	CDL	O1-C1-CA2-OA2
20	M	407	CDL	CA3-OA5-PA1-OA2
20	M	407	CDL	CA3-OA5-PA1-OA3
20	M	407	CDL	CA3-OA5-PA1-OA4
20	M	407	CDL	C11-CA5-OA6-CA4
20	M	408	CDL	CA2-OA2-PA1-OA3
20	M	408	CDL	CA2-OA2-PA1-OA5
20	M	408	CDL	CA3-OA5-PA1-OA4
20	M	408	CDL	C11-CA5-OA6-CA4
20	M	408	CDL	CB2-OB2-PB2-OB3
20	M	408	CDL	CB2-OB2-PB2-OB4
20	M	408	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
20	M	408	CDL	CB3-OB5-PB2-OB3
20	M	408	CDL	C51-CB5-OB6-CB4
20	M	409	CDL	CA2-OA2-PA1-OA3
20	M	409	CDL	CB2-OB2-PB2-OB5
20	M	409	CDL	CB3-OB5-PB2-OB2
20	M	409	CDL	CB3-OB5-PB2-OB3
20	H	301	CDL	OA7-CA5-OA6-CA4
20	H	301	CDL	C11-CA5-OA6-CA4
20	H	301	CDL	CB2-OB2-PB2-OB3
20	H	301	CDL	CB2-OB2-PB2-OB4
20	H	301	CDL	CB2-OB2-PB2-OB5
20	H	301	CDL	CB3-OB5-PB2-OB3
20	H	303	CDL	CA2-OA2-PA1-OA3
20	H	303	CDL	CA2-OA2-PA1-OA4
20	H	303	CDL	CA2-OA2-PA1-OA5
20	H	303	CDL	CA3-OA5-PA1-OA2
20	H	303	CDL	CB2-OB2-PB2-OB3
20	H	303	CDL	CB2-OB2-PB2-OB5
20	O	101	CDL	CA2-OA2-PA1-OA3
20	O	101	CDL	CA2-OA2-PA1-OA4
20	O	101	CDL	CA2-OA2-PA1-OA5
20	O	101	CDL	CA3-OA5-PA1-OA2
20	O	101	CDL	CA3-OA5-PA1-OA4
20	O	101	CDL	C11-CA5-OA6-CA4
20	O	101	CDL	CB3-OB5-PB2-OB2
20	O	101	CDL	OB7-CB5-OB6-CB4
20	U	101	CDL	CB2-OB2-PB2-OB4
20	U	101	CDL	CB2-OB2-PB2-OB5
20	U	102	CDL	CA2-OA2-PA1-OA5
20	U	102	CDL	CA3-OA5-PA1-OA2
20	U	102	CDL	C11-CA5-OA6-CA4
20	U	102	CDL	CB2-OB2-PB2-OB5
22	M	406	CRT	O1-C1-C4-C5
22	M	406	CRT	C2-C1-C4-C5
22	M	406	CRT	C3-C1-C4-C5
22	M	406	CRT	C32-C33-C35-C36
22	M	406	CRT	C34-C33-C35-C36
22	M	406	CRT	C35-C36-C37-C38
22	M	406	CRT	C36-C37-C38-C39
22	M	406	CRT	C36-C37-C38-C40
22	M	406	CRT	C36-C37-C38-O2
22	B	101	CRT	C2-C1-O1-C1M

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Mol	Chain	Res	Type	Atoms
22	B	101	CRT	C15-C16-C17-C19
22	N	102	CRT	C2-C1-O1-C1M
22	N	102	CRT	C3-C1-O1-C1M
22	N	102	CRT	C40-C38-O2-C2M
22	R	101	CRT	C27-C28-C30-C31
22	V	101	CRT	C4-C1-O1-C1M
22	4	101	CRT	C5-C6-C7-C8
22	4	101	CRT	C5-C6-C7-C9
22	8	101	CRT	C15-C16-C17-C19
20	U	102	CDL	OA7-CA5-OA6-CA4
15	M	411	LMT	O5B-C1B-O1B-C4'
15	H	305	LMT	O5B-C1B-O1B-C4'
14	N	101	PGV	O04-C19-O03-C01
16	Z	102	BCL	O1A-CGA-O2A-C1
14	H	304	PGV	O02-C1-O01-C02
14	B	104	PGV	O02-C1-O01-C02
14	G	105	PGV	O02-C1-O01-C02
14	X	103	PGV	O02-C1-O01-C02
14	Z	104	PGV	O02-C1-O01-C02
14	2	102	PGV	O02-C1-O01-C02
14	4	103	PGV	O02-C1-O01-C02
14	6	104	PGV	O02-C1-O01-C02
14	8	103	PGV	O02-C1-O01-C02
20	M	407	CDL	OA7-CA5-OA6-CA4
20	M	408	CDL	OA7-CA5-OA6-CA4
20	M	408	CDL	OB7-CB5-OB6-CB4
20	O	101	CDL	OA7-CA5-OA6-CA4
16	B	102	BCL	C3-C5-C6-C7
16	D	101	BCL	C3-C5-C6-C7
16	I	102	BCL	C3-C5-C6-C7
16	O	103	BCL	C3-C5-C6-C7
16	R	102	BCL	C3-C5-C6-C7
16	T	101	BCL	C3-C5-C6-C7
16	1	102	BCL	C3-C5-C6-C7
16	4	102	BCL	C3-C5-C6-C7
16	9	101	BCL	C3-C5-C6-C7
14	N	101	PGV	C20-C19-O03-C01
16	L	302	BCL	CBD-CGD-O2D-CED
16	Y	401	BCL	CBD-CGD-O2D-CED
14	M	410	PGV	C2-C1-O01-C02
14	B	104	PGV	C2-C1-O01-C02
14	X	103	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
20	O	101	CDL	C51-CB5-OB6-CB4
14	N	104	PGV	O04-C19-O03-C01
16	D	101	BCL	C4-C3-C5-C6
16	F	103	BCL	C4-C3-C5-C6
16	K	101	BCL	C4-C3-C5-C6
16	Q	102	BCL	C4-C3-C5-C6
16	S	101	BCL	C4-C3-C5-C6
16	W	101	BCL	C4-C3-C5-C6
16	W	102	BCL	C4-C3-C5-C6
16	Y	402	BCL	C4-C3-C5-C6
16	7	102	BCL	C4-C3-C5-C6
16	9	102	BCL	C4-C3-C5-C6
16	F	103	BCL	C2-C3-C5-C6
16	K	101	BCL	C2-C3-C5-C6
16	Q	102	BCL	C2-C3-C5-C6
16	S	101	BCL	C2-C3-C5-C6
16	Y	402	BCL	C2-C3-C5-C6
16	7	102	BCL	C2-C3-C5-C6
16	9	102	BCL	C2-C3-C5-C6
16	S	101	BCL	CBD-CGD-O2D-CED
16	S	101	BCL	C3-C5-C6-C7
16	1	103	BCL	C3-C5-C6-C7
14	N	104	PGV	C20-C19-O03-C01
16	Z	102	BCL	CBA-CGA-O2A-C1
20	M	402	CDL	C31-CA7-OA8-CA6
15	F	102	LMT	C2B-C1B-O1B-C4'
14	Z	103	PGV	O04-C19-O03-C01
16	3	102	BCL	O1A-CGA-O2A-C1
14	J	102	PGV	O02-C1-O01-C02
14	0	104	PGV	O02-C1-O01-C02
15	L	308	LMT	O5'-C5'-C6'-O6'
16	L	302	BCL	C3-C5-C6-C7
16	I	102	BCL	CBD-CGD-O2D-CED
16	3	102	BCL	CBD-CGD-O2D-CED
14	H	302	PGV	O12-C04-C05-O05
20	H	303	CDL	O1-C1-CB2-OB2
14	3	101	PGV	C20-C19-O03-C01
20	U	101	CDL	C31-CA7-OA8-CA6
16	W	102	BCL	C5-C6-C7-C8
14	J	102	PGV	C2-C1-O01-C02
20	M	409	CDL	C11-CA5-OA6-CA4
20	U	102	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
15	I	101	LMT	O5B-C5B-C6B-O6B
14	Z	103	PGV	C20-C19-O03-C01
16	3	102	BCL	CBA-CGA-O2A-C1
16	A	101	BCL	C4-C3-C5-C6
16	I	102	BCL	C4-C3-C5-C6
16	O	103	BCL	C4-C3-C5-C6
16	5	103	BCL	C4-C3-C5-C6
18	L	306	UQ8	C25-C24-C26-C27
16	I	102	BCL	C2-C3-C5-C6
16	R	102	BCL	C2-C3-C5-C6
16	W	101	BCL	C2-C3-C5-C6
16	5	103	BCL	C2-C3-C5-C6
16	9	101	BCL	C2-C3-C5-C6
18	L	304	UQ8	C14-C16-C17-C18
18	L	306	UQ8	C14-C16-C17-C18
21	M	405	MQ8	C38-C40-C41-C42
15	L	308	LMT	C4'-C5'-C6'-O6'
14	3	101	PGV	O04-C19-O03-C01
20	M	402	CDL	OA9-CA7-OA8-CA6
20	U	101	CDL	OA9-CA7-OA8-CA6
15	L	308	LMT	O5'-C1'-O1'-C1
15	I	101	LMT	O5'-C1'-O1'-C1
16	K	101	BCL	CBD-CGD-O2D-CED
20	M	409	CDL	OA7-CA5-OA6-CA4
14	M	410	PGV	O12-C04-C05-C06
14	B	103	PGV	O12-C04-C05-C06
20	M	407	CDL	CB2-C1-CA2-OA2
14	C	408	PGV	C20-C19-O03-C01
14	L	310	PGV	C20-C19-O03-C01
16	W	102	BCL	CBA-CGA-O2A-C1
20	M	402	CDL	C71-CB7-OB8-CB6
20	M	408	CDL	C71-CB7-OB8-CB6
20	H	301	CDL	C71-CB7-OB8-CB6
20	U	101	CDL	C71-CB7-OB8-CB6
14	G	101	PGV	C26-C27-C28-C29
16	R	102	BCL	C4-C3-C5-C6
16	1	102	BCL	C4-C3-C5-C6
16	9	101	BCL	C4-C3-C5-C6
16	A	101	BCL	C2-C3-C5-C6
16	D	101	BCL	C2-C3-C5-C6
16	O	103	BCL	C2-C3-C5-C6
16	W	102	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	1	102	BCL	C2-C3-C5-C6
17	M	404	BPH	C2-C3-C5-C6
16	O	104	BCL	C3-C5-C6-C7
16	9	102	BCL	C3-C5-C6-C7
16	D	102	BCL	CBD-CGD-O2D-CED
16	L	312	BCL	C11-C10-C8-C9
16	A	101	BCL	C11-C10-C8-C9
16	B	102	BCL	C11-C10-C8-C9
16	F	103	BCL	C6-C7-C8-C9
16	G	103	BCL	C11-C10-C8-C9
16	J	101	BCL	C11-C10-C8-C9
16	N	103	BCL	C11-C12-C13-C14
16	P	101	BCL	C6-C7-C8-C9
16	P	101	BCL	C11-C10-C8-C9
16	Q	102	BCL	C6-C7-C8-C9
16	S	102	BCL	C11-C10-C8-C9
16	T	101	BCL	C6-C7-C8-C9
16	U	103	BCL	C6-C7-C8-C9
16	3	102	BCL	C6-C7-C8-C9
16	4	102	BCL	C14-C13-C15-C16
16	5	103	BCL	C6-C7-C8-C9
16	7	102	BCL	C11-C10-C8-C9
15	L	308	LMT	C2'-C1'-O1'-C1
14	P	102	PGV	C1-C2-C3-C4
14	G	101	PGV	O12-C04-C05-O05
14	R	103	PGV	O12-C04-C05-O05
14	T	103	PGV	O12-C04-C05-O05
15	Q	101	LMT	O5'-C5'-C6'-O6'
22	B	101	CRT	C15-C16-C17-C18
22	R	101	CRT	C29-C28-C30-C31
22	8	101	CRT	C15-C16-C17-C18
16	F	103	BCL	C2A-CAA-CBA-CGA
14	C	408	PGV	O04-C19-O03-C01
16	W	102	BCL	O1A-CGA-O2A-C1
20	U	101	CDL	OB9-CB7-OB8-CB6
20	H	303	CDL	OA6-CA4-CA6-OA8
16	Z	102	BCL	C2-C1-O2A-CGA
16	L	302	BCL	O1D-CGD-O2D-CED
15	I	101	LMT	C4B-C5B-C6B-O6B
16	D	102	BCL	C13-C15-C16-C17
16	Y	401	BCL	C10-C11-C12-C13
16	5	104	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	N	101	PGV	O05-C05-C06-O06
14	V	103	PGV	O05-C05-C06-O06
16	1	103	BCL	CBD-CGD-O2D-CED
16	K	101	BCL	C6-C7-C8-C10
16	S	101	BCL	C6-C7-C8-C10
16	T	101	BCL	C11-C10-C8-C7
16	W	102	BCL	C11-C10-C8-C7
16	Z	102	BCL	C11-C10-C8-C7
16	1	102	BCL	C6-C7-C8-C10
16	A	101	BCL	CBA-CGA-O2A-C1
15	O	102	LMT	O1'-C1-C2-C3
16	O	104	BCL	C4-C3-C5-C6
17	M	404	BPH	C4-C3-C5-C6
15	L	301	LMT	O5'-C5'-C6'-O6'
16	G	103	BCL	C10-C11-C12-C13
16	O	104	BCL	C5-C6-C7-C8
16	V	102	BCL	C5-C6-C7-C8
14	G	105	PGV	C19-C20-C21-C22
14	J	102	PGV	C19-C20-C21-C22
14	Z	101	PGV	C19-C20-C21-C22
20	H	303	CDL	C73-C74-C75-C76
18	L	304	UQ8	C19-C21-C22-C23
16	N	103	BCL	C5-C6-C7-C8
16	1	102	BCL	C10-C11-C12-C13
15	5	101	LMT	C5'-C4'-O1B-C1B
14	L	309	PGV	C1-C2-C3-C4
14	G	101	PGV	C1-C2-C3-C4
14	G	104	PGV	C1-C2-C3-C4
14	1	101	PGV	C19-C20-C21-C22
14	0	104	PGV	C1-C2-C3-C4
20	M	408	CDL	CA5-C11-C12-C13
14	L	310	PGV	O04-C19-O03-C01
16	I	103	BCL	CBA-CGA-O2A-C1
16	O	103	BCL	C8-C10-C11-C12
16	Q	102	BCL	C15-C16-C17-C18
16	R	102	BCL	C5-C6-C7-C8
16	U	103	BCL	C8-C10-C11-C12
16	Z	102	BCL	C13-C15-C16-C17
16	1	103	BCL	C5-C6-C7-C8
16	9	101	BCL	C13-C15-C16-C17
16	S	101	BCL	C2A-CAA-CBA-CGA
16	W	101	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	3	102	BCL	C2A-CAA-CBA-CGA
16	7	102	BCL	C2A-CAA-CBA-CGA
15	I	101	LMT	C5'-C4'-O1B-C1B
16	M	403	BCL	C5-C6-C7-C8
16	G	103	BCL	C5-C6-C7-C8
16	1	102	BCL	C5-C6-C7-C8
16	5	103	BCL	C15-C16-C17-C18
16	5	104	BCL	C10-C11-C12-C13
15	7	101	LMT	O5'-C5'-C6'-O6'
15	M	411	LMT	O1'-C1-C2-C3
14	H	304	PGV	C1-C2-C3-C4
14	E	102	PGV	C19-C20-C21-C22
14	F	101	PGV	C1-C2-C3-C4
14	G	105	PGV	C1-C2-C3-C4
14	T	102	PGV	C1-C2-C3-C4
20	M	402	CDL	CA7-C31-C32-C33
20	H	301	CDL	CB7-C71-C72-C73
20	O	101	CDL	CA7-C31-C32-C33
20	M	402	CDL	OB9-CB7-OB8-CB6
16	K	101	BCL	C3-C5-C6-C7
14	B	103	PGV	C21-C22-C23-C24
16	B	102	BCL	C10-C11-C12-C13
16	F	103	BCL	C15-C16-C17-C18
16	N	103	BCL	C15-C16-C17-C18
16	T	101	BCL	C10-C11-C12-C13
16	Z	102	BCL	C5-C6-C7-C8
16	Z	102	BCL	C10-C11-C12-C13
14	L	310	PGV	O12-C04-C05-O05
15	H	305	LMT	O1'-C1-C2-C3
16	S	102	BCL	CBA-CGA-O2A-C1
15	I	101	LMT	C3'-C4'-O1B-C1B
20	H	301	CDL	OB9-CB7-OB8-CB6
14	L	305	PGV	C19-C20-C21-C22
14	L	310	PGV	C1-C2-C3-C4
14	2	102	PGV	C1-C2-C3-C4
16	L	312	BCL	C8-C10-C11-C12
16	A	101	BCL	C15-C16-C17-C18
16	T	101	BCL	C5-C6-C7-C8
20	U	102	CDL	OB7-CB5-OB6-CB4
15	5	102	LMT	O5B-C5B-C6B-O6B
15	L	301	LMT	C4'-C5'-C6'-O6'
16	J	101	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	W	101	BCL	C15-C16-C17-C18
16	X	102	BCL	C5-C6-C7-C8
16	M	403	BCL	CBD-CGD-O2D-CED
14	T	103	PGV	C19-C20-C21-C22
20	M	407	CDL	CB7-C71-C72-C73
20	M	408	CDL	CA7-C31-C32-C33
16	3	102	BCL	O1D-CGD-O2D-CED
14	2	103	PGV	C20-C19-O03-C01
16	L	311	BCL	CBA-CGA-O2A-C1
16	K	101	BCL	CBA-CGA-O2A-C1
16	N	103	BCL	CBA-CGA-O2A-C1
16	O	104	BCL	CBA-CGA-O2A-C1
14	E	102	PGV	C2-C1-O01-C02
14	T	102	PGV	C2-C1-O01-C02
14	0	101	PGV	C2-C1-O01-C02
20	H	303	CDL	C11-CA5-OA6-CA4
20	H	303	CDL	C51-CB5-OB6-CB4
16	A	101	BCL	O1A-CGA-O2A-C1
20	M	408	CDL	OB9-CB7-OB8-CB6
16	S	101	BCL	C10-C11-C12-C13
14	E	102	PGV	O02-C1-O01-C02
14	T	102	PGV	O02-C1-O01-C02
14	0	101	PGV	O02-C1-O01-C02
14	L	310	PGV	O12-C04-C05-C06
16	Y	401	BCL	O1D-CGD-O2D-CED
16	P	101	BCL	CBA-CGA-O2A-C1
16	B	102	BCL	C13-C15-C16-C17
16	W	102	BCL	C8-C10-C11-C12
16	2	101	BCL	C5-C6-C7-C8
16	4	102	BCL	C5-C6-C7-C8
16	7	102	BCL	C5-C6-C7-C8
16	7	102	BCL	C15-C16-C17-C18
16	9	102	BCL	C10-C11-C12-C13
16	J	101	BCL	C10-C11-C12-C13
14	G	104	PGV	C26-C27-C28-C29
14	P	102	PGV	C28-C29-C30-C31
15	I	101	LMT	O5'-C5'-C6'-O6'
16	U	103	BCL	C10-C11-C12-C13
16	V	102	BCL	C10-C11-C12-C13
16	W	102	BCL	C10-C11-C12-C13
16	9	101	BCL	C8-C10-C11-C12
16	S	102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	S	101	BCL	O1D-CGD-O2D-CED
16	8	102	BCL	C10-C11-C12-C13
14	R	104	PGV	C2-C1-O01-C02
15	F	102	LMT	O5B-C1B-O1B-C4'
14	R	104	PGV	O02-C1-O01-C02
20	H	303	CDL	OA7-CA5-OA6-CA4
20	H	303	CDL	OB7-CB5-OB6-CB4
15	I	101	LMT	C2'-C1'-O1'-C1
14	3	101	PGV	C1-C2-C3-C4
18	L	306	UQ8	C19-C21-C22-C23
14	P	103	PGV	C20-C19-O03-C01
16	A	101	BCL	C16-C17-C18-C19
16	R	102	BCL	C16-C17-C18-C19
22	B	101	CRT	C5-C6-C7-C8
22	R	101	CRT	C5-C6-C7-C8
22	8	101	CRT	C5-C6-C7-C8
16	G	103	BCL	C2A-CAA-CBA-CGA
16	R	102	BCL	C15-C16-C17-C18
14	H	302	PGV	C04-C05-C06-O06
14	B	103	PGV	C04-C05-C06-O06
14	T	103	PGV	C04-C05-C06-O06
14	0	101	PGV	C04-C05-C06-O06
14	2	102	PGV	C01-C02-O01-C1
14	E	102	PGV	C5-C6-C7-C8
16	D	102	BCL	C16-C17-C18-C19
16	D	102	BCL	C16-C17-C18-C20
16	I	103	BCL	O1A-CGA-O2A-C1
16	K	101	BCL	O1A-CGA-O2A-C1
16	O	104	BCL	O1A-CGA-O2A-C1
16	U	103	BCL	C3-C5-C6-C7
15	5	101	LMT	O5'-C1'-O1'-C1
14	V	103	PGV	C2-C1-O01-C02
18	L	306	UQ8	C23-C24-C26-C27
16	I	102	BCL	O1D-CGD-O2D-CED
16	P	101	BCL	O1A-CGA-O2A-C1
14	G	105	PGV	C22-C23-C24-C25
14	2	102	PGV	C4-C5-C6-C7
14	M	410	PGV	C20-C19-O03-C01
16	D	101	BCL	C5-C6-C7-C8
16	O	103	BCL	C16-C17-C18-C20
16	R	102	BCL	C16-C17-C18-C20
16	7	102	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	Z	101	PGV	C21-C22-C23-C24
16	L	311	BCL	O1A-CGA-O2A-C1
16	S	102	BCL	O1A-CGA-O2A-C1
14	X	101	PGV	C7-C8-C9-C10
14	X	103	PGV	C27-C28-C29-C30
20	M	407	CDL	C15-C16-C17-C18
20	M	407	CDL	C75-C76-C77-C78
14	H	302	PGV	C21-C22-C23-C24
14	8	103	PGV	C4-C5-C6-C7
20	M	407	CDL	C11-C12-C13-C14
14	2	102	PGV	C19-C20-C21-C22
16	D	102	BCL	C8-C10-C11-C12
16	W	101	BCL	C8-C10-C11-C12
16	2	101	BCL	C8-C10-C11-C12
14	B	103	PGV	C7-C8-C9-C10
14	B	104	PGV	C4-C5-C6-C7
14	G	104	PGV	C3-C4-C5-C6
14	Z	103	PGV	C22-C23-C24-C25
14	6	103	PGV	C23-C24-C25-C26
14	Z	101	PGV	O05-C05-C06-O06
14	1	101	PGV	O05-C05-C06-O06
15	M	411	LMT	C2-C1-O1'-C1'
15	F	102	LMT	C2-C1-O1'-C1'
15	5	101	LMT	C2-C1-O1'-C1'
14	R	104	PGV	C26-C27-C28-C29
20	M	408	CDL	C32-C33-C34-C35
14	N	101	PGV	C19-C20-C21-C22
14	L	309	PGV	C7-C8-C9-C10
16	O	103	BCL	C16-C17-C18-C19
16	5	104	BCL	C16-C17-C18-C19
16	L	311	BCL	C2A-CAA-CBA-CGA
16	W	102	BCL	C2A-CAA-CBA-CGA
14	T	102	PGV	C4-C5-C6-C7
20	M	402	CDL	C11-CA5-OA6-CA4
20	M	409	CDL	C51-CB5-OB6-CB4
20	U	101	CDL	C51-CB5-OB6-CB4
14	B	103	PGV	C20-C21-C22-C23
14	P	102	PGV	C7-C8-C9-C10
14	X	103	PGV	C30-C31-C32-C33
16	D	102	BCL	C11-C10-C8-C7
16	O	103	BCL	C11-C10-C8-C7
14	T	103	PGV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
14	6	101	PGV	C13-C14-C15-C16
14	B	103	PGV	C19-C20-C21-C22
14	V	103	PGV	C19-C20-C21-C22
20	H	303	CDL	CA5-C11-C12-C13
20	O	101	CDL	CB5-C51-C52-C53
14	2	102	PGV	C13-C14-C15-C16
14	3	101	PGV	C4-C5-C6-C7
16	N	103	BCL	O1A-CGA-O2A-C1
15	H	306	LMT	C4B-C5B-C6B-O6B
16	F	103	BCL	C3A-C2A-CAA-CBA
16	G	103	BCL	C3A-C2A-CAA-CBA
16	I	102	BCL	C3A-C2A-CAA-CBA
16	O	103	BCL	C3A-C2A-CAA-CBA
16	Q	102	BCL	C3A-C2A-CAA-CBA
16	R	102	BCL	C3A-C2A-CAA-CBA
16	S	101	BCL	C3A-C2A-CAA-CBA
16	U	103	BCL	C3A-C2A-CAA-CBA
16	V	102	BCL	C3A-C2A-CAA-CBA
16	Y	402	BCL	C3A-C2A-CAA-CBA
16	Z	102	BCL	C3A-C2A-CAA-CBA
16	4	102	BCL	C3A-C2A-CAA-CBA
16	7	102	BCL	C3A-C2A-CAA-CBA
16	9	101	BCL	C3A-C2A-CAA-CBA
16	0	102	BCL	C3A-C2A-CAA-CBA
14	R	104	PGV	C3-C4-C5-C6
16	O	104	BCL	C2-C3-C5-C6
14	G	101	PGV	C20-C21-C22-C23
14	P	102	PGV	C20-C21-C22-C23
17	M	404	BPH	C5-C6-C7-C8
16	K	101	BCL	O1D-CGD-O2D-CED
15	Q	101	LMT	C1-C2-C3-C4
14	2	103	PGV	O04-C19-O03-C01
14	8	103	PGV	C21-C22-C23-C24
16	D	102	BCL	CBA-CGA-O2A-C1
16	5	104	BCL	CBA-CGA-O2A-C1
20	H	303	CDL	C31-CA7-OA8-CA6
14	3	101	PGV	C3-C4-C5-C6
20	M	407	CDL	C74-C75-C76-C77
16	N	103	BCL	C3-C5-C6-C7
16	6	102	BCL	C3-C5-C6-C7
14	0	103	PGV	C1-C2-C3-C4
14	L	309	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	B	104	PGV	C27-C28-C29-C30
14	T	102	PGV	C22-C23-C24-C25
14	6	101	PGV	C23-C24-C25-C26
20	H	303	CDL	C80-C81-C82-C83
14	X	101	PGV	C21-C22-C23-C24
14	Z	101	PGV	C7-C8-C9-C10
14	6	104	PGV	C25-C26-C27-C28
15	5	101	LMT	C3-C4-C5-C6
20	H	303	CDL	C76-C77-C78-C79
14	M	410	PGV	C19-C20-C21-C22
14	2	103	PGV	C19-C20-C21-C22
14	0	101	PGV	C22-C23-C24-C25
14	N	105	PGV	C2-C1-O01-C02
14	6	101	PGV	C2-C1-O01-C02
16	S	102	BCL	C3-C5-C6-C7
14	G	101	PGV	C21-C22-C23-C24
14	N	101	PGV	C26-C27-C28-C29
20	H	303	CDL	C17-C18-C19-C20
14	X	103	PGV	C26-C27-C28-C29
16	Q	102	BCL	C2A-CAA-CBA-CGA
14	V	103	PGV	C1-C2-C3-C4
14	J	102	PGV	C3-C4-C5-C6
14	P	103	PGV	O04-C19-O03-C01
14	N	105	PGV	O02-C1-O01-C02
14	V	103	PGV	O02-C1-O01-C02
20	M	409	CDL	OB7-CB5-OB6-CB4
20	U	101	CDL	OB7-CB5-OB6-CB4
14	8	103	PGV	C24-C25-C26-C27
16	W	101	BCL	C10-C11-C12-C13
16	4	102	BCL	C8-C10-C11-C12
16	S	102	BCL	C2-C3-C5-C6
20	O	101	CDL	C18-C19-C20-C21
16	2	101	BCL	C11-C10-C8-C9
16	5	104	BCL	C14-C13-C15-C16
14	P	103	PGV	C6-C7-C8-C9
15	5	101	LMT	C6-C7-C8-C9
16	B	102	BCL	C5-C6-C7-C8
14	Z	104	PGV	C26-C27-C28-C29
20	H	301	CDL	C60-C61-C62-C63
20	O	101	CDL	C19-C20-C21-C22
14	M	410	PGV	O04-C19-O03-C01
16	D	102	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	H	303	CDL	OA9-CA7-OA8-CA6
14	X	101	PGV	C22-C23-C24-C25
20	M	407	CDL	C16-C17-C18-C19
14	J	102	PGV	C4-C5-C6-C7
14	B	104	PGV	C11-C12-C13-C14
14	T	103	PGV	C11-C12-C13-C14
15	F	102	LMT	O1'-C1-C2-C3
16	A	101	BCL	C16-C17-C18-C20
14	P	102	PGV	C2-C1-O01-C02
14	P	103	PGV	C2-C1-O01-C02
14	T	103	PGV	C2-C1-O01-C02
14	Z	103	PGV	C2-C1-O01-C02
15	O	102	LMT	C4B-C5B-C6B-O6B
14	P	102	PGV	C19-C20-C21-C22
20	M	402	CDL	C36-C37-C38-C39
16	K	101	BCL	C15-C16-C17-C18
14	P	102	PGV	O02-C1-O01-C02
20	M	402	CDL	OA7-CA5-OA6-CA4
14	M	410	PGV	C29-C30-C31-C32
14	H	304	PGV	C3-C4-C5-C6
14	G	104	PGV	C28-C29-C30-C31
14	2	103	PGV	C11-C10-C9-C8
15	5	101	LMT	C3'-C4'-O1B-C1B
14	G	105	PGV	C24-C25-C26-C27
15	M	411	LMT	C2-C3-C4-C5
14	N	104	PGV	C1-C2-C3-C4
14	X	101	PGV	C19-C20-C21-C22
20	H	303	CDL	C18-C19-C20-C21
14	L	305	PGV	C6-C7-C8-C9
14	N	104	PGV	C20-C21-C22-C23
14	X	101	PGV	C26-C27-C28-C29
15	5	101	LMT	C1-C2-C3-C4
20	H	303	CDL	C51-C52-C53-C54
16	5	104	BCL	O1A-CGA-O2A-C1
20	H	303	CDL	CB7-C71-C72-C73
20	U	102	CDL	CB7-C71-C72-C73
14	N	104	PGV	C2-C3-C4-C5
14	0	101	PGV	C20-C21-C22-C23
14	6	101	PGV	O02-C1-O01-C02
14	6	101	PGV	O01-C02-C03-O11
14	Z	103	PGV	C02-C01-O03-C19
20	M	402	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
20	U	101	CDL	C11-CA5-OA6-CA4
15	H	307	LMT	O1'-C1-C2-C3
15	H	306	LMT	C2-C3-C4-C5
14	4	103	PGV	C1-C2-C3-C4
14	4	103	PGV	C19-C20-C21-C22
16	F	103	BCL	C13-C15-C16-C17
16	V	102	BCL	CBD-CGD-O2D-CED
14	T	103	PGV	O03-C01-C02-O01
20	M	407	CDL	OB6-CB4-CB6-OB8
14	G	101	PGV	C3-C4-C5-C6
15	5	102	LMT	C4'-C5'-C6'-O6'
14	N	101	PGV	C3-C4-C5-C6
14	F	101	PGV	C23-C24-C25-C26
15	Q	101	LMT	O5B-C5B-C6B-O6B
14	N	101	PGV	C13-C14-C15-C16
15	5	101	LMT	O5'-C5'-C6'-O6'
14	G	104	PGV	C25-C26-C27-C28
14	P	103	PGV	O02-C1-O01-C02
14	Z	103	PGV	O02-C1-O01-C02
20	H	303	CDL	CA2-C1-CB2-OB2
14	8	103	PGV	C5-C6-C7-C8
16	L	302	BCL	C2A-CAA-CBA-CGA
16	J	101	BCL	C2A-CAA-CBA-CGA
16	X	102	BCL	C2A-CAA-CBA-CGA
14	G	105	PGV	C20-C19-O03-C01
14	P	102	PGV	C21-C22-C23-C24
14	L	305	PGV	C2-C1-O01-C02
16	W	101	BCL	C16-C17-C18-C19
16	G	103	BCL	C8-C10-C11-C12
14	T	103	PGV	O05-C05-C06-O06
14	0	101	PGV	O05-C05-C06-O06
16	V	102	BCL	C3-C5-C6-C7
14	T	103	PGV	C2-C3-C4-C5
14	H	302	PGV	C23-C24-C25-C26
20	M	402	CDL	C13-C14-C15-C16
16	F	103	BCL	C1A-C2A-CAA-CBA
16	I	102	BCL	C1A-C2A-CAA-CBA
16	O	103	BCL	C1A-C2A-CAA-CBA
16	Q	102	BCL	C1A-C2A-CAA-CBA
16	U	103	BCL	C1A-C2A-CAA-CBA
16	Z	102	BCL	C1A-C2A-CAA-CBA
16	4	102	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	7	102	BCL	C1A-C2A-CAA-CBA
16	S	102	BCL	C15-C16-C17-C18
16	9	101	BCL	C5-C6-C7-C8
14	B	104	PGV	C2-C3-C4-C5
14	G	105	PGV	C11-C10-C9-C8
14	6	103	PGV	C11-C10-C9-C8
14	0	103	PGV	C11-C10-C9-C8
14	G	104	PGV	C2-C3-C4-C5
16	D	102	BCL	C15-C16-C17-C18
14	M	410	PGV	C01-C02-C03-O11
15	L	301	LMT	O5B-C5B-C6B-O6B
14	H	304	PGV	C29-C30-C31-C32
14	N	104	PGV	C13-C14-C15-C16
16	E	101	BCL	C11-C10-C8-C7
16	F	103	BCL	C6-C7-C8-C10
16	G	103	BCL	C6-C7-C8-C10
16	G	103	BCL	C11-C10-C8-C7
16	I	102	BCL	C6-C7-C8-C10
16	O	103	BCL	C6-C7-C8-C10
16	P	101	BCL	C11-C10-C8-C7
16	Q	102	BCL	C11-C10-C8-C7
16	S	102	BCL	C11-C10-C8-C7
16	T	101	BCL	C6-C7-C8-C10
16	W	101	BCL	C11-C10-C8-C7
16	5	104	BCL	C11-C12-C13-C15
16	9	101	BCL	C11-C10-C8-C7
14	H	302	PGV	C20-C21-C22-C23
14	N	101	PGV	C4-C5-C6-C7
16	1	102	BCL	C16-C17-C18-C19
16	A	101	BCL	C2C-C3C-CAC-CBC
16	J	101	BCL	C2C-C3C-CAC-CBC
16	K	101	BCL	C2C-C3C-CAC-CBC
16	T	101	BCL	C2C-C3C-CAC-CBC
16	U	103	BCL	C2C-C3C-CAC-CBC
16	1	103	BCL	C2C-C3C-CAC-CBC
16	3	102	BCL	C2C-C3C-CAC-CBC
22	V	101	CRT	C2-C1-C4-C5
22	V	101	CRT	C3-C1-C4-C5
15	Q	101	LMT	O5B-C1B-O1B-C4'
14	V	103	PGV	C2-C3-C4-C5
14	G	105	PGV	C26-C27-C28-C29
15	F	102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
14	6	103	PGV	C20-C21-C22-C23
16	D	101	BCL	C13-C15-C16-C17
16	L	311	BCL	C3-C5-C6-C7
16	I	102	BCL	C2A-CAA-CBA-CGA
16	T	101	BCL	C2A-CAA-CBA-CGA
16	D	101	BCL	C6-C7-C8-C9
16	I	103	BCL	C6-C7-C8-C9
16	K	101	BCL	C11-C10-C8-C9
16	S	102	BCL	C6-C7-C8-C9
16	5	104	BCL	C11-C12-C13-C14
16	9	101	BCL	C11-C10-C8-C9
16	9	102	BCL	C11-C10-C8-C9
14	X	103	PGV	C22-C23-C24-C25
14	B	104	PGV	C22-C23-C24-C25
14	Z	104	PGV	C20-C19-O03-C01
14	8	103	PGV	C20-C19-O03-C01
16	X	102	BCL	CBA-CGA-O2A-C1
15	H	305	LMT	O5'-C5'-C6'-O6'
15	O	102	LMT	C3-C4-C5-C6
15	F	102	LMT	C2'-C1'-O1'-C1
20	M	407	CDL	C34-C35-C36-C37
14	C	408	PGV	O03-C01-C02-C03
14	G	105	PGV	O03-C01-C02-C03
14	T	102	PGV	O03-C01-C02-C03
14	T	103	PGV	O03-C01-C02-C03
14	X	101	PGV	O03-C01-C02-C03
14	Z	103	PGV	O03-C01-C02-C03
14	Z	104	PGV	O03-C01-C02-C03
20	M	402	CDL	CA3-CA4-CA6-OA8
20	M	407	CDL	CA3-CA4-CA6-OA8
20	M	409	CDL	CA3-CA4-CA6-OA8
20	H	303	CDL	CA3-CA4-CA6-OA8
20	U	102	CDL	CA3-CA4-CA6-OA8
14	0	101	PGV	C27-C28-C29-C30
14	L	305	PGV	C20-C19-O03-C01
16	Y	402	BCL	CBA-CGA-O2A-C1
16	1	102	BCL	C16-C17-C18-C20
14	M	410	PGV	C7-C8-C9-C10
20	M	407	CDL	CA5-C11-C12-C13
18	L	304	UQ8	C12-C11-C9-C8
16	L	312	BCL	C10-C11-C12-C13
14	R	104	PGV	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
14	H	302	PGV	C3-C4-C5-C6
16	S	101	BCL	C8-C10-C11-C12
14	C	408	PGV	C5-C6-C7-C8
14	P	102	PGV	C23-C24-C25-C26
14	R	103	PGV	C20-C21-C22-C23
14	3	101	PGV	C04-O12-P-O13
20	M	407	CDL	CA6-CA4-OA6-CA5
20	O	101	CDL	CA6-CA4-OA6-CA5
14	1	101	PGV	C25-C26-C27-C28
14	F	101	PGV	C27-C28-C29-C30
14	Z	104	PGV	C3-C4-C5-C6
15	Q	101	LMT	C4'-C5'-C6'-O6'
14	R	104	PGV	O01-C02-C03-O11
14	0	104	PGV	O01-C02-C03-O11
12	C	406	LJQ	C32-C31-O31-C3
14	6	103	PGV	C20-C19-O03-C01
14	X	101	PGV	C23-C24-C25-C26
14	Z	104	PGV	C25-C26-C27-C28
14	6	101	PGV	C14-C15-C16-C17
14	8	103	PGV	C6-C7-C8-C9
20	M	402	CDL	C58-C59-C60-C61
14	N	101	PGV	C25-C26-C27-C28
20	M	407	CDL	C32-C33-C34-C35
16	G	103	BCL	C16-C17-C18-C19
14	1	101	PGV	C7-C8-C9-C10
14	4	103	PGV	C2-C3-C4-C5
15	O	102	LMT	O5B-C5B-C6B-O6B
14	V	103	PGV	C21-C22-C23-C24
20	M	402	CDL	C12-C13-C14-C15
15	O	102	LMT	C1-C2-C3-C4
14	T	102	PGV	O03-C01-C02-O01
14	Z	101	PGV	O03-C01-C02-O01
20	H	301	CDL	OA6-CA4-CA6-OA8
20	M	408	CDL	O1-C1-CB2-OB2
20	H	301	CDL	C11-C12-C13-C14
14	R	104	PGV	C7-C8-C9-C10
20	M	407	CDL	C31-C32-C33-C34
20	H	303	CDL	C14-C15-C16-C17
14	N	101	PGV	C15-C16-C17-C18
20	M	408	CDL	C34-C35-C36-C37
20	O	101	CDL	C36-C37-C38-C39
17	L	303	BPH	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	0	101	PGV	C20-C19-O03-C01
16	U	103	BCL	CBA-CGA-O2A-C1
16	2	101	BCL	CBA-CGA-O2A-C1
22	B	101	CRT	C3-C1-O1-C1M
22	G	102	CRT	C3-C1-O1-C1M
22	R	101	CRT	C2-C1-O1-C1M
22	R	101	CRT	C40-C38-O2-C2M
22	V	101	CRT	C3-C1-O1-C1M
22	Y	403	CRT	C2-C1-O1-C1M
22	Y	403	CRT	C3-C1-O1-C1M
22	4	101	CRT	C2-C1-O1-C1M
22	4	101	CRT	C3-C1-O1-C1M
22	8	101	CRT	C2-C1-O1-C1M
14	T	103	PGV	C31-C32-C33-C34
14	B	103	PGV	C22-C23-C24-C25
14	R	103	PGV	C6-C7-C8-C9
14	Z	103	PGV	C29-C30-C31-C32
14	0	101	PGV	C1-C2-C3-C4
14	H	304	PGV	C24-C25-C26-C27
16	V	102	BCL	C13-C15-C16-C17
16	1	103	BCL	C15-C16-C17-C18
16	M	403	BCL	O1D-CGD-O2D-CED
16	W	101	BCL	C16-C17-C18-C20
16	P	101	BCL	C4-C3-C5-C6
18	L	304	UQ8	C15-C14-C16-C17
18	L	304	UQ8	C12-C11-C9-C10
16	I	103	BCL	C2-C3-C5-C6
14	G	104	PGV	C19-C20-C21-C22
14	0	103	PGV	C2-C3-C4-C5
14	G	105	PGV	C4-C5-C6-C7
14	1	101	PGV	C28-C29-C30-C31
20	U	101	CDL	C71-C72-C73-C74
14	T	103	PGV	O02-C1-O01-C02
14	H	302	PGV	O05-C05-C06-O06
14	B	103	PGV	O05-C05-C06-O06
16	G	103	BCL	C6-C7-C8-C9
16	I	102	BCL	C6-C7-C8-C9
16	I	103	BCL	C14-C13-C15-C16
16	O	103	BCL	C6-C7-C8-C9
16	O	104	BCL	C14-C13-C15-C16
16	Q	102	BCL	C11-C10-C8-C9
16	R	102	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
16	S	101	BCL	C11-C10-C8-C9
16	W	101	BCL	C11-C10-C8-C9
16	Y	401	BCL	C11-C12-C13-C14
16	2	101	BCL	C6-C7-C8-C9
14	N	105	PGV	C7-C8-C9-C10
14	0	104	PGV	C5-C6-C7-C8
20	M	402	CDL	C42-C43-C44-C45
16	1	102	BCL	C8-C10-C11-C12
14	L	310	PGV	C4-C5-C6-C7
14	0	104	PGV	C25-C26-C27-C28
20	M	407	CDL	C38-C39-C40-C41
14	1	101	PGV	C2-C3-C4-C5
16	5	104	BCL	C16-C17-C18-C20
15	7	101	LMT	C2'-C1'-O1'-C1
14	M	410	PGV	C26-C27-C28-C29
14	P	103	PGV	C2-C3-C4-C5
14	0	104	PGV	C3-C4-C5-C6
20	H	301	CDL	C74-C75-C76-C77
14	L	305	PGV	C01-C02-C03-O11
14	6	101	PGV	C01-C02-C03-O11
14	6	103	PGV	C01-C02-C03-O11
14	6	104	PGV	C01-C02-C03-O11
20	M	407	CDL	OA5-CA3-CA4-CA6
16	L	312	BCL	C6-C7-C8-C10
16	L	312	BCL	C11-C10-C8-C7
16	A	101	BCL	C11-C10-C8-C7
16	B	102	BCL	C11-C10-C8-C7
16	D	101	BCL	C6-C7-C8-C10
16	E	101	BCL	C6-C7-C8-C10
16	I	103	BCL	C6-C7-C8-C10
16	K	101	BCL	C11-C10-C8-C7
16	N	103	BCL	C11-C12-C13-C15
16	O	104	BCL	C11-C10-C8-C7
16	P	101	BCL	C6-C7-C8-C10
16	S	101	BCL	C11-C10-C8-C7
16	S	102	BCL	C6-C7-C8-C10
16	V	102	BCL	C11-C12-C13-C15
16	V	102	BCL	C12-C13-C15-C16
16	W	101	BCL	C11-C12-C13-C15
16	W	102	BCL	C11-C12-C13-C15
16	Y	401	BCL	C11-C12-C13-C15
16	Y	402	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	2	101	BCL	C6-C7-C8-C10
16	3	102	BCL	C6-C7-C8-C10
16	7	102	BCL	C11-C10-C8-C7
16	A	101	BCL	C10-C11-C12-C13
16	Q	102	BCL	C10-C11-C12-C13
16	5	103	BCL	C5-C6-C7-C8
20	M	402	CDL	C18-C19-C20-C21
14	8	103	PGV	C1-C2-C3-C4
16	7	102	BCL	C16-C17-C18-C19
20	H	303	CDL	C19-C20-C21-C22
14	G	105	PGV	O04-C19-O03-C01
16	X	102	BCL	O1A-CGA-O2A-C1
16	Y	402	BCL	C3-C5-C6-C7
16	W	101	BCL	C3A-C2A-CAA-CBA
16	3	102	BCL	C3A-C2A-CAA-CBA
21	M	405	MQ8	C29-C28-C30-C31
14	0	103	PGV	C5-C6-C7-C8
15	F	102	LMT	C3-C4-C5-C6
20	M	402	CDL	C38-C39-C40-C41
16	Y	402	BCL	O1A-CGA-O2A-C1
22	4	101	CRT	C24-C23-C25-C26
14	Z	103	PGV	C4-C5-C6-C7
14	L	305	PGV	O04-C19-O03-C01
14	Z	104	PGV	O04-C19-O03-C01
14	8	103	PGV	O04-C19-O03-C01
14	Z	104	PGV	C22-C23-C24-C25
15	5	101	LMT	C4'-C5'-C6'-O6'
20	M	407	CDL	C18-C19-C20-C21
20	M	402	CDL	C35-C36-C37-C38
14	V	103	PGV	O03-C01-C02-C03
14	8	103	PGV	O03-C01-C02-C03
20	M	407	CDL	CB3-CB4-CB6-OB8
20	H	301	CDL	CA3-CA4-CA6-OA8
20	H	301	CDL	CB3-CB4-CB6-OB8
14	X	101	PGV	C3-C4-C5-C6
16	G	103	BCL	C16-C17-C18-C20
16	L	312	BCL	C5-C6-C7-C8
20	M	408	CDL	C71-C72-C73-C74
15	H	305	LMT	O5B-C5B-C6B-O6B
16	I	103	BCL	C4-C3-C5-C6
16	T	101	BCL	C4-C3-C5-C6
16	X	102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	F	102	LMT	C4-C5-C6-C7
16	T	101	BCL	C2-C3-C5-C6
14	H	302	PGV	C6-C7-C8-C9
16	E	101	BCL	C16-C17-C18-C19
16	1	103	BCL	C16-C17-C18-C19
14	L	305	PGV	O02-C1-O01-C02
20	M	402	CDL	OB7-CB5-OB6-CB4
20	U	101	CDL	OA7-CA5-OA6-CA4
14	6	104	PGV	O01-C02-C03-O11
14	0	101	PGV	O01-C02-C03-O11
20	M	407	CDL	OA5-CA3-CA4-OA6
14	0	104	PGV	C20-C21-C22-C23
14	X	101	PGV	O12-C04-C05-O05
14	4	103	PGV	C3-C4-C5-C6
15	Q	101	LMT	C5-C6-C7-C8
20	M	402	CDL	C43-C44-C45-C46
20	M	407	CDL	C40-C41-C42-C43
16	I	103	BCL	C15-C16-C17-C18
14	C	408	PGV	O03-C01-C02-O01
14	N	101	PGV	O03-C01-C02-O01
14	X	103	PGV	O03-C01-C02-O01
14	Z	103	PGV	O03-C01-C02-O01
14	6	103	PGV	O03-C01-C02-O01
20	M	407	CDL	OA6-CA4-CA6-OA8
20	M	408	CDL	OB6-CB4-CB6-OB8
20	M	409	CDL	OA6-CA4-CA6-OA8
14	L	310	PGV	C25-C26-C27-C28
16	1	103	BCL	O1D-CGD-O2D-CED
14	6	103	PGV	C7-C8-C9-C10
16	1	103	BCL	C13-C15-C16-C17
15	5	102	LMT	C4B-C5B-C6B-O6B
14	0	101	PGV	C23-C24-C25-C26
15	5	101	LMT	O1'-C1-C2-C3
16	P	101	BCL	C2-C3-C5-C6
16	X	102	BCL	C2-C3-C5-C6
18	L	304	UQ8	C13-C14-C16-C17
21	M	405	MQ8	C27-C28-C30-C31
15	M	411	LMT	C4-C5-C6-C7
20	M	402	CDL	CB7-C71-C72-C73
16	N	103	BCL	C14-C13-C15-C16
16	Y	402	BCL	C11-C10-C8-C9
14	T	102	PGV	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
14	R	104	PGV	C25-C26-C27-C28
16	D	102	BCL	O1D-CGD-O2D-CED
14	H	304	PGV	C31-C32-C33-C34
16	D	101	BCL	C16-C17-C18-C19
18	L	306	UQ8	C9-C11-C12-C13
16	T	101	BCL	C4C-C3C-CAC-CBC
14	2	103	PGV	C5-C6-C7-C8
14	N	105	PGV	C11-C12-C13-C14
16	L	302	BCL	C13-C15-C16-C17
16	V	102	BCL	O1D-CGD-O2D-CED
14	T	103	PGV	C23-C24-C25-C26
16	K	101	BCL	C13-C15-C16-C17
16	8	102	BCL	C8-C10-C11-C12
14	L	309	PGV	C11-C10-C9-C8
14	Z	101	PGV	C20-C19-O03-C01
16	6	102	BCL	CBA-CGA-O2A-C1
14	N	104	PGV	C19-C20-C21-C22
16	O	103	BCL	C5-C6-C7-C8
16	R	102	BCL	C10-C11-C12-C13
14	1	101	PGV	C29-C30-C31-C32
14	N	105	PGV	C01-C02-C03-O11
14	Z	104	PGV	C01-C02-C03-O11
15	5	102	LMT	O5'-C5'-C6'-O6'
16	U	103	BCL	O1A-CGA-O2A-C1
16	D	101	BCL	C10-C11-C12-C13
16	J	101	BCL	C11-C10-C8-C7
16	Q	102	BCL	C6-C7-C8-C10
16	R	102	BCL	C6-C7-C8-C10
16	X	102	BCL	C11-C10-C8-C7
16	4	102	BCL	C6-C7-C8-C10
16	0	102	BCL	C11-C10-C8-C7
14	C	408	PGV	C2-C3-C4-C5
20	U	102	CDL	C72-C73-C74-C75
16	8	102	BCL	C3-C5-C6-C7
16	F	103	BCL	C8-C10-C11-C12
22	B	101	CRT	C5-C6-C7-C9
22	R	101	CRT	C5-C6-C7-C9
22	8	101	CRT	C5-C6-C7-C9
14	H	304	PGV	C27-C28-C29-C30
14	0	101	PGV	O04-C19-O03-C01
16	2	101	BCL	O1A-CGA-O2A-C1
18	L	307	UQ8	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	R	103	PGV	C24-C25-C26-C27
14	P	102	PGV	C4-C5-C6-C7
12	C	406	LJQ	O32-C31-O31-C3
20	H	303	CDL	C71-CB7-OB8-CB6
14	N	104	PGV	C25-C26-C27-C28
17	L	303	BPH	O2A-C1-C2-C3
20	U	101	CDL	CA6-CA4-OA6-CA5
14	6	103	PGV	O04-C19-O03-C01
14	J	102	PGV	C2-C3-C4-C5
14	6	103	PGV	C2-C3-C4-C5
20	M	409	CDL	C31-C32-C33-C34
22	M	406	CRT	C25-C26-C27-C28
20	O	101	CDL	C35-C36-C37-C38
15	H	305	LMT	C2-C3-C4-C5
14	M	410	PGV	O01-C02-C03-O11
14	V	103	PGV	O01-C02-C03-O11
20	H	301	CDL	OB5-CB3-CB4-OB6
14	T	103	PGV	C24-C25-C26-C27
14	G	101	PGV	O03-C01-C02-C03
14	R	103	PGV	O03-C01-C02-C03
14	6	103	PGV	O03-C01-C02-C03
16	4	102	BCL	C15-C16-C17-C18
16	E	101	BCL	C16-C17-C18-C20
14	T	103	PGV	C6-C7-C8-C9
16	D	102	BCL	C4-C3-C5-C6
14	6	103	PGV	C24-C25-C26-C27
14	6	101	PGV	C15-C16-C17-C18
14	G	105	PGV	O03-C01-C02-O01
14	P	102	PGV	C12-C13-C14-C15
14	R	103	PGV	O03-C01-C02-O01
14	V	103	PGV	O03-C01-C02-O01
14	X	101	PGV	O03-C01-C02-O01
20	M	402	CDL	OA6-CA4-CA6-OA8
20	H	301	CDL	OB6-CB4-CB6-OB8
20	H	303	CDL	OB6-CB4-CB6-OB8
20	U	102	CDL	OA6-CA4-CA6-OA8
16	L	312	BCL	C6-C7-C8-C9
16	G	103	BCL	C11-C12-C13-C14
16	V	102	BCL	C14-C13-C15-C16
16	X	102	BCL	C11-C10-C8-C9
14	0	103	PGV	C6-C7-C8-C9
14	L	310	PGV	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	U	102	CDL	C71-C72-C73-C74
16	6	102	BCL	O1A-CGA-O2A-C1
14	L	310	PGV	C19-C20-C21-C22
14	Z	104	PGV	C27-C28-C29-C30
20	M	402	CDL	C60-C61-C62-C63
14	G	101	PGV	C20-C19-O03-C01
16	W	102	BCL	C16-C17-C18-C19
15	7	101	LMT	C4'-C5'-C6'-O6'
15	H	306	LMT	O5B-C5B-C6B-O6B
14	R	103	PGV	O12-C04-C05-C06
14	X	101	PGV	O12-C04-C05-C06
16	1	103	BCL	C16-C17-C18-C20
14	Z	101	PGV	C11-C10-C9-C8
20	M	408	CDL	OA9-CA7-OA8-CA6
16	X	102	BCL	CBD-CGD-O2D-CED
14	L	310	PGV	C20-C21-C22-C23
14	E	102	PGV	C2-C3-C4-C5
20	M	408	CDL	C31-CA7-OA8-CA6
14	G	101	PGV	C23-C24-C25-C26
14	G	104	PGV	C7-C8-C9-C10
15	H	305	LMT	C3'-C4'-O1B-C1B
16	7	102	BCL	C3-C5-C6-C7
15	Q	101	LMT	C4-C5-C6-C7
16	L	312	BCL	C1A-C2A-CAA-CBA
16	V	102	BCL	C1A-C2A-CAA-CBA
16	3	102	BCL	C1A-C2A-CAA-CBA
16	D	102	BCL	C2-C3-C5-C6
16	U	103	BCL	C15-C16-C17-C18
14	Z	101	PGV	O04-C19-O03-C01
14	L	310	PGV	C01-C02-C03-O11
14	R	104	PGV	C01-C02-C03-O11
14	2	102	PGV	C01-C02-C03-O11
20	H	301	CDL	OB5-CB3-CB4-CB6
16	L	302	BCL	C15-C16-C17-C18
16	L	312	BCL	C11-C12-C13-C15
16	L	312	BCL	C12-C13-C15-C16
16	A	101	BCL	C11-C12-C13-C15
16	J	101	BCL	C6-C7-C8-C10
16	T	101	BCL	C11-C12-C13-C15
16	1	102	BCL	C11-C12-C13-C15
16	5	103	BCL	C6-C7-C8-C10
14	G	101	PGV	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
16	V	102	BCL	C15-C16-C17-C18
14	2	103	PGV	C1-C2-C3-C4
20	H	301	CDL	C54-C55-C56-C57
16	4	102	BCL	C2C-C3C-CAC-CBC
14	6	101	PGV	C02-C03-O11-P
20	O	101	CDL	C1-CA2-OA2-PA1
20	U	102	CDL	CB4-CB3-OB5-PB2
14	Z	104	PGV	C31-C32-C33-C34
10	C	401	HEC	C4B-C3B-CAB-CBB
14	L	305	PGV	O01-C02-C03-O11
14	L	310	PGV	O01-C02-C03-O11
14	N	105	PGV	O01-C02-C03-O11
14	6	103	PGV	O01-C02-C03-O11
20	U	101	CDL	OA5-CA3-CA4-OA6
20	U	101	CDL	OB5-CB3-CB4-OB6
14	2	102	PGV	C12-C13-C14-C15
16	E	101	BCL	C2A-CAA-CBA-CGA
16	E	101	BCL	C11-C10-C8-C9
16	R	102	BCL	C6-C7-C8-C9
16	T	101	BCL	C11-C10-C8-C9
16	W	102	BCL	C11-C12-C13-C14
16	Z	102	BCL	C11-C10-C8-C9
16	4	102	BCL	C6-C7-C8-C9
16	0	102	BCL	C11-C10-C8-C9
14	M	410	PGV	C23-C24-C25-C26
14	T	102	PGV	C21-C22-C23-C24
14	1	101	PGV	C22-C23-C24-C25
14	L	309	PGV	C9-C10-C11-C12
14	G	101	PGV	O04-C19-O03-C01
14	Z	104	PGV	O03-C01-C02-O01
14	0	103	PGV	O03-C01-C02-O01
20	H	303	CDL	C79-C80-C81-C82
16	L	312	BCL	C15-C16-C17-C18
16	I	102	BCL	C13-C15-C16-C17
14	N	101	PGV	O03-C01-C02-C03
14	X	103	PGV	O03-C01-C02-C03
14	R	103	PGV	O01-C1-C2-C3
14	Z	101	PGV	C22-C23-C24-C25
20	H	301	CDL	C73-C74-C75-C76
14	M	410	PGV	C15-C16-C17-C18
22	G	102	CRT	C4-C1-O1-C1M
14	6	101	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
20	H	303	CDL	OB9-CB7-OB8-CB6
14	Z	103	PGV	C27-C28-C29-C30
20	H	303	CDL	C72-C73-C74-C75
16	D	101	BCL	C16-C17-C18-C20
16	B	102	BCL	C15-C16-C17-C18
17	M	404	BPH	C15-C16-C17-C18
14	Z	101	PGV	O02-C1-O01-C02
14	Z	101	PGV	C23-C24-C25-C26
14	E	102	PGV	C6-C7-C8-C9
14	C	408	PGV	C04-O12-P-O13
14	L	305	PGV	C04-O12-P-O13
14	L	310	PGV	C04-O12-P-O13
14	H	302	PGV	C03-O11-P-O12
14	H	302	PGV	C03-O11-P-O14
14	G	105	PGV	C03-O11-P-O13
14	N	101	PGV	C03-O11-P-O12
14	N	101	PGV	C03-O11-P-O13
14	N	101	PGV	C03-O11-P-O14
14	R	103	PGV	C03-O11-P-O14
14	R	103	PGV	C04-O12-P-O11
14	X	103	PGV	C03-O11-P-O13
14	Z	101	PGV	C04-O12-P-O11
14	Z	103	PGV	C03-O11-P-O12
14	Z	104	PGV	C04-O12-P-O14
14	2	103	PGV	C04-O12-P-O13
14	4	103	PGV	C03-O11-P-O13
14	0	103	PGV	C03-O11-P-O14
16	M	403	BCL	CHA-CBD-CGD-O1D
16	M	403	BCL	CHA-CBD-CGD-O2D
17	L	303	BPH	CHA-CBD-CGD-O1D
17	L	303	BPH	CHA-CBD-CGD-O2D
20	M	402	CDL	CA3-OA5-PA1-OA4
20	M	402	CDL	CB3-OB5-PB2-OB3
20	M	407	CDL	CB2-OB2-PB2-OB3
20	M	408	CDL	CA3-OA5-PA1-OA2
20	M	409	CDL	CA2-OA2-PA1-OA5
20	M	409	CDL	CB2-OB2-PB2-OB3
20	M	409	CDL	CB3-OB5-PB2-OB4
20	H	303	CDL	CA3-OA5-PA1-OA3
20	H	303	CDL	CB3-OB5-PB2-OB3
20	O	101	CDL	CB3-OB5-PB2-OB3
20	U	101	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
20	U	101	CDL	CB3-OB5-PB2-OB3
20	U	102	CDL	CA2-OA2-PA1-OA3
20	U	102	CDL	CA3-OA5-PA1-OA3
20	U	102	CDL	CB2-OB2-PB2-OB3
14	Z	103	PGV	C1-C2-C3-C4
14	Z	103	PGV	C25-C26-C27-C28
15	H	305	LMT	C5'-C4'-O1B-C1B
14	P	102	PGV	C3-C4-C5-C6
14	F	101	PGV	C02-C03-O11-P
14	R	104	PGV	C02-C03-O11-P
20	O	101	CDL	CA4-CA3-OA5-PA1
16	Q	102	BCL	C8-C10-C11-C12
16	R	102	BCL	C13-C15-C16-C17
14	L	310	PGV	C22-C23-C24-C25
14	E	102	PGV	C3-C4-C5-C6
14	R	104	PGV	C27-C28-C29-C30
14	G	104	PGV	C24-C25-C26-C27
16	L	302	BCL	C16-C17-C18-C19
14	P	103	PGV	C11-C12-C13-C14
14	R	104	PGV	C19-C20-C21-C22
16	K	101	BCL	C8-C10-C11-C12
16	5	103	BCL	C8-C10-C11-C12
14	Z	101	PGV	C2-C1-O01-C02
20	M	402	CDL	CA6-CA4-OA6-CA5
20	M	402	CDL	CB6-CB4-OB6-CB5
20	H	303	CDL	CA3-CA4-OA6-CA5
20	U	102	CDL	CA6-CA4-OA6-CA5
14	N	101	PGV	C2-C3-C4-C5
14	6	101	PGV	C1-C2-C3-C4
14	2	103	PGV	C3-C4-C5-C6
22	M	406	CRT	C20-C21-C22-C23
14	0	101	PGV	C01-C02-C03-O11
14	0	104	PGV	C01-C02-C03-O11
20	M	402	CDL	OB5-CB3-CB4-CB6
20	U	101	CDL	OB5-CB3-CB4-CB6
16	L	311	BCL	C6-C7-C8-C9
16	E	101	BCL	C6-C7-C8-C9
16	O	104	BCL	C6-C7-C8-C9
16	R	102	BCL	C14-C13-C15-C16
16	S	102	BCL	C14-C13-C15-C16
16	T	101	BCL	C11-C12-C13-C14
16	W	101	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
16	Z	102	BCL	C6-C7-C8-C9
17	L	303	BPH	C11-C10-C8-C9
16	M	403	BCL	C6-C7-C8-C10
16	S	102	BCL	C12-C13-C15-C16
16	7	102	BCL	C11-C12-C13-C15
14	B	103	PGV	C9-C10-C11-C12
16	N	103	BCL	C10-C11-C12-C13
16	3	102	BCL	C4-C3-C5-C6
18	L	306	UQ8	C15-C14-C16-C17
14	2	102	PGV	C21-C22-C23-C24
14	0	104	PGV	C22-C23-C24-C25
14	H	304	PGV	O03-C01-C02-O01
14	Z	101	PGV	O01-C1-C2-C3
20	M	402	CDL	C56-C57-C58-C59
14	X	103	PGV	C24-C25-C26-C27
14	Z	101	PGV	O03-C01-C02-C03
14	G	101	PGV	C4-C5-C6-C7
22	N	102	CRT	C15-C16-C17-C18
22	V	101	CRT	C5-C6-C7-C8
16	B	102	BCL	C16-C17-C18-C19
22	N	102	CRT	C39-C38-O2-C2M
22	R	101	CRT	C39-C38-O2-C2M
22	V	101	CRT	C39-C38-O2-C2M
22	V	101	CRT	C40-C38-O2-C2M
14	R	104	PGV	C9-C10-C11-C12
20	M	407	CDL	CA7-C31-C32-C33
20	M	409	CDL	CA5-C11-C12-C13
14	N	104	PGV	O01-C1-C2-C3
20	O	101	CDL	C54-C55-C56-C57
14	G	104	PGV	C27-C28-C29-C30
16	6	102	BCL	C2A-CAA-CBA-CGA
15	H	306	LMT	C3-C4-C5-C6
16	G	103	BCL	C4-C3-C5-C6
16	3	102	BCL	C2-C3-C5-C6
14	P	103	PGV	C21-C22-C23-C24
14	G	101	PGV	O12-C04-C05-C06
16	L	312	BCL	C11-C12-C13-C14
16	L	312	BCL	C14-C13-C15-C16
16	I	102	BCL	C14-C13-C15-C16
16	W	102	BCL	C11-C10-C8-C9
16	5	103	BCL	C11-C10-C8-C9
10	C	401	HEC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
16	I	103	BCL	C16-C17-C18-C19
14	G	104	PGV	C20-C19-O03-C01
16	5	104	BCL	C4-C3-C5-C6
14	G	105	PGV	C11-C12-C13-C14
14	F	101	PGV	C3-C4-C5-C6
16	M	403	BCL	C11-C10-C8-C7
17	L	303	BPH	C11-C10-C8-C7
14	N	105	PGV	C4-C5-C6-C7
14	N	105	PGV	C21-C22-C23-C24
14	M	410	PGV	C2-C3-C4-C5
14	P	102	PGV	C22-C23-C24-C25
14	M	410	PGV	C13-C14-C15-C16
14	G	105	PGV	C6-C7-C8-C9
14	X	101	PGV	C6-C7-C8-C9
20	H	303	CDL	C74-C75-C76-C77
14	G	101	PGV	C22-C23-C24-C25
14	B	104	PGV	C7-C8-C9-C10
14	T	103	PGV	C3-C4-C5-C6
16	A	101	BCL	C3A-C2A-CAA-CBA
16	I	103	BCL	C3A-C2A-CAA-CBA
14	L	309	PGV	C23-C24-C25-C26
14	N	101	PGV	C24-C25-C26-C27
14	8	103	PGV	C20-C21-C22-C23
16	R	102	BCL	C2-C1-O2A-CGA
16	B	102	BCL	C8-C10-C11-C12
16	D	102	BCL	C5-C6-C7-C8
14	H	302	PGV	C02-C03-O11-P
14	G	101	PGV	C05-C04-O12-P
20	M	402	CDL	C61-C62-C63-C64
16	Z	102	BCL	C4-C3-C5-C6
20	M	407	CDL	C78-C79-C80-C81
14	P	102	PGV	C11-C12-C13-C14
14	3	101	PGV	O03-C01-C02-C03
16	M	403	BCL	C6-C7-C8-C9
16	A	101	BCL	C11-C12-C13-C14
16	D	101	BCL	C11-C12-C13-C14
16	F	103	BCL	C11-C10-C8-C9
16	K	101	BCL	C14-C13-C15-C16
16	5	104	BCL	C11-C10-C8-C9
16	9	101	BCL	C11-C12-C13-C14
14	V	103	PGV	C7-C8-C9-C10
14	Z	104	PGV	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	C	403	HEC	CAA-CBA-CGA-O2A
15	Q	101	LMT	C2B-C1B-O1B-C4'
14	T	102	PGV	O01-C1-C2-C3
20	H	301	CDL	CA5-C11-C12-C13
15	Q	101	LMT	C2-C3-C4-C5
14	B	103	PGV	C11-C10-C9-C8
14	6	104	PGV	C1-C2-C3-C4
14	0	101	PGV	C24-C25-C26-C27
16	G	103	BCL	C2-C3-C5-C6
16	Z	102	BCL	C2-C3-C5-C6
14	0	103	PGV	C22-C23-C24-C25
14	G	104	PGV	O04-C19-O03-C01
20	U	101	CDL	C11-C12-C13-C14
16	A	101	BCL	C1A-C2A-CAA-CBA
16	W	101	BCL	C1A-C2A-CAA-CBA
16	2	101	BCL	C1A-C2A-CAA-CBA
14	Z	104	PGV	O01-C02-C03-O11
20	M	409	CDL	OB5-CB3-CB4-OB6
15	M	411	LMT	C3'-C4'-O1B-C1B
15	H	307	LMT	C2B-C1B-O1B-C4'
14	B	103	PGV	C02-C03-O11-P
14	G	104	PGV	C02-C03-O11-P
20	M	409	CDL	CB4-CB3-OB5-PB2
20	U	101	CDL	CB4-CB3-OB5-PB2
20	H	303	CDL	C31-C32-C33-C34
16	6	102	BCL	C4-C3-C5-C6
20	M	402	CDL	C34-C35-C36-C37
14	R	103	PGV	C25-C26-C27-C28
16	I	102	BCL	C12-C13-C15-C16
16	O	104	BCL	C6-C7-C8-C10
16	S	101	BCL	C12-C13-C15-C16
16	Z	102	BCL	C6-C7-C8-C10
16	1	103	BCL	C6-C7-C8-C10
16	5	103	BCL	C11-C10-C8-C7
16	6	102	BCL	C11-C10-C8-C7
16	Y	401	BCL	C2A-CAA-CBA-CGA
14	L	310	PGV	O03-C01-C02-O01
16	N	103	BCL	C2C-C3C-CAC-CBC
16	Y	402	BCL	C8-C10-C11-C12
20	O	101	CDL	C14-C15-C16-C17
16	N	103	BCL	C13-C15-C16-C17
14	G	104	PGV	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
16	3	102	BCL	C16-C17-C18-C19
20	H	303	CDL	C77-C78-C79-C80
14	T	102	PGV	C19-C20-C21-C22
22	G	102	CRT	C15-C16-C17-C18
14	M	410	PGV	C3-C4-C5-C6
20	M	407	CDL	C76-C77-C78-C79
10	C	401	HEC	CAA-CBA-CGA-O1A
16	4	102	BCL	C4-C3-C5-C6
14	0	101	PGV	C2-C3-C4-C5
14	0	103	PGV	O01-C1-C2-C3
16	5	104	BCL	C2-C3-C5-C6
15	L	308	LMT	C11-C10-C9-C8
16	P	101	BCL	C2-C1-O2A-CGA
14	H	302	PGV	C22-C23-C24-C25
22	4	101	CRT	C22-C23-C25-C26
14	R	103	PGV	C1-C2-C3-C4
14	F	101	PGV	C7-C8-C9-C10
10	C	403	HEC	CAA-CBA-CGA-O1A
16	D	102	BCL	C11-C10-C8-C9
16	U	103	BCL	C11-C10-C8-C9
14	C	408	PGV	O02-C1-O01-C02
14	0	103	PGV	O02-C1-O01-C02
14	L	305	PGV	C28-C29-C30-C31
14	4	103	PGV	C4-C5-C6-C7
14	6	103	PGV	C19-C20-C21-C22
20	M	402	CDL	C59-C60-C61-C62
16	V	102	BCL	C4-C3-C5-C6
16	S	101	BCL	C13-C15-C16-C17
10	C	401	HEC	CAA-CBA-CGA-O2A
14	M	410	PGV	C02-C03-O11-P
14	6	104	PGV	C05-C04-O12-P
16	V	102	BCL	C8-C10-C11-C12
16	I	103	BCL	C8-C10-C11-C12
20	O	101	CDL	CB7-C71-C72-C73
14	X	103	PGV	O03-C19-C20-C21
14	L	305	PGV	C5-C6-C7-C8
14	2	102	PGV	C7-C8-C9-C10
14	0	103	PGV	O03-C01-C02-C03
20	H	303	CDL	CB3-CB4-CB6-OB8
15	M	411	LMT	C5'-C4'-O1B-C1B
16	P	101	BCL	C2A-CAA-CBA-CGA
16	Y	402	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	2	102	PGV	C6-C7-C8-C9
16	N	103	BCL	C16-C17-C18-C19
14	G	105	PGV	C3-C4-C5-C6
20	M	407	CDL	C80-C81-C82-C83
22	R	101	CRT	C37-C38-O2-C2M
14	H	304	PGV	C4-C5-C6-C7
14	2	102	PGV	C14-C15-C16-C17
14	B	104	PGV	O01-C02-C03-O11
14	L	310	PGV	C9-C10-C11-C12
14	0	104	PGV	C9-C10-C11-C12
14	B	104	PGV	O03-C19-C20-C21
15	H	306	LMT	C3'-C4'-O1B-C1B
16	Z	102	BCL	C16-C17-C18-C19
16	9	102	BCL	C15-C16-C17-C18
20	M	408	CDL	CB2-C1-CA2-OA2
14	4	103	PGV	C11-C10-C9-C8
16	L	312	BCL	O1A-CGA-O2A-C1
14	V	103	PGV	C01-C02-C03-O11
14	X	101	PGV	C01-C02-C03-O11
14	8	103	PGV	C01-C02-C03-O11
20	U	101	CDL	OA5-CA3-CA4-CA6
14	G	105	PGV	C28-C29-C30-C31
14	N	105	PGV	C9-C10-C11-C12
14	0	103	PGV	C9-C10-C11-C12
16	F	103	BCL	C11-C10-C8-C7
16	W	102	BCL	C6-C7-C8-C10
14	1	101	PGV	C23-C24-C25-C26
14	4	103	PGV	C23-C24-C25-C26
16	O	103	BCL	O1D-CGD-O2D-CED
14	B	104	PGV	C25-C26-C27-C28
14	X	101	PGV	O01-C1-C2-C3
16	V	102	BCL	CAA-CBA-CGA-O2A
16	J	101	BCL	C6-C7-C8-C9
16	8	102	BCL	C14-C13-C15-C16
20	H	301	CDL	C55-C56-C57-C58
14	X	103	PGV	C1-C2-C3-C4
14	P	103	PGV	C22-C23-C24-C25
20	O	101	CDL	C32-C33-C34-C35
14	B	103	PGV	C11-C12-C13-C14
16	U	103	BCL	C2A-CAA-CBA-CGA
16	0	102	BCL	C2A-CAA-CBA-CGA
16	T	101	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
16	1	103	BCL	C2-C1-O2A-CGA
16	6	102	BCL	C2-C1-O2A-CGA
16	7	102	BCL	C2-C1-O2A-CGA
20	M	409	CDL	OB9-CB7-OB8-CB6
16	Y	401	BCL	C13-C15-C16-C17
16	P	101	BCL	C3A-C2A-CAA-CBA
16	2	101	BCL	C3A-C2A-CAA-CBA
16	L	312	BCL	CBA-CGA-O2A-C1
20	M	409	CDL	C71-CB7-OB8-CB6
14	Z	104	PGV	C7-C8-C9-C10
14	T	102	PGV	C01-C02-O01-C1
14	G	101	PGV	C11-C12-C13-C14
20	M	407	CDL	C39-C40-C41-C42
14	P	102	PGV	C26-C27-C28-C29
14	B	103	PGV	C20-C19-O03-C01
14	N	105	PGV	C6-C7-C8-C9
14	F	101	PGV	C9-C10-C11-C12
20	U	101	CDL	C1-CA2-OA2-PA1
14	G	101	PGV	O01-C1-C2-C3
20	M	409	CDL	OA5-CA3-CA4-OA6
20	H	303	CDL	OA5-CA3-CA4-OA6
15	Q	101	LMT	O5'-C1'-O1'-C1
21	M	405	MQ8	C18-C20-C21-C22
16	I	103	BCL	C5-C6-C7-C8
14	Z	101	PGV	C11-C12-C13-C14
14	N	105	PGV	C20-C21-C22-C23
20	M	402	CDL	C39-C40-C41-C42
20	M	407	CDL	C17-C18-C19-C20
16	Y	401	BCL	C16-C17-C18-C20
20	M	407	CDL	C72-C73-C74-C75
16	I	102	BCL	C5-C6-C7-C8
14	1	101	PGV	O01-C1-C2-C3
16	5	104	BCL	CAA-CBA-CGA-O2A
16	M	403	BCL	C11-C10-C8-C9
16	X	102	BCL	C6-C7-C8-C9
16	Y	401	BCL	C11-C10-C8-C9
14	L	309	PGV	O01-C1-C2-C3
14	H	302	PGV	O01-C1-C2-C3
14	B	104	PGV	C01-C02-C03-O11
20	M	408	CDL	OA5-CA3-CA4-CA6
15	H	307	LMT	O5'-C5'-C6'-O6'
20	H	303	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
16	M	403	BCL	C11-C12-C13-C15
16	G	103	BCL	C12-C13-C15-C16
16	U	103	BCL	C6-C7-C8-C10
16	U	103	BCL	C11-C10-C8-C7
16	Y	401	BCL	C11-C10-C8-C7
16	W	101	BCL	C3-C5-C6-C7
14	N	101	PGV	C1-C2-C3-C4
14	C	408	PGV	C2-C1-O01-C02
14	O	103	PGV	C2-C1-O01-C02
14	F	101	PGV	C11-C12-C13-C14
14	G	104	PGV	C11-C12-C13-C14
14	X	101	PGV	C9-C10-C11-C12
14	G	104	PGV	C15-C16-C17-C18
14	Z	104	PGV	C28-C29-C30-C31
14	F	101	PGV	C14-C15-C16-C17
14	M	410	PGV	O01-C1-C2-C3
14	Z	103	PGV	O03-C19-C20-C21
16	1	103	BCL	CAA-CBA-CGA-O2A
14	G	101	PGV	C28-C29-C30-C31
16	1	103	BCL	O1A-CGA-O2A-C1
22	G	102	CRT	C39-C38-O2-C2M
16	K	101	BCL	C2A-CAA-CBA-CGA
16	I	103	BCL	C13-C15-C16-C17
14	B	103	PGV	O04-C19-O03-C01
16	Z	102	BCL	CAA-CBA-CGA-O2A
14	2	103	PGV	C6-C7-C8-C9
10	C	402	HEC	CAA-CBA-CGA-O1A
14	R	104	PGV	C24-C25-C26-C27
16	O	103	BCL	C15-C16-C17-C18
16	M	403	BCL	C11-C12-C13-C14
16	1	102	BCL	C11-C12-C13-C14
16	8	102	BCL	C6-C7-C8-C9
16	O	104	BCL	CAA-CBA-CGA-O2A
14	2	103	PGV	O03-C01-C02-C03
20	M	408	CDL	CB3-CB4-CB6-OB8
20	U	101	CDL	CA3-CA4-CA6-OA8
14	L	305	PGV	C26-C27-C28-C29
14	F	101	PGV	C29-C30-C31-C32
16	P	101	BCL	C1A-C2A-CAA-CBA
20	U	101	CDL	OB6-CB4-CB6-OB8
14	6	104	PGV	C21-C22-C23-C24
16	O	104	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	5	104	BCL	C8-C10-C11-C12
16	T	101	BCL	O1A-CGA-O2A-C1
14	L	305	PGV	O01-C1-C2-C3
14	Z	103	PGV	C04-C05-C06-O06
18	L	306	UQ8	C26-C27-C28-C29
14	L	309	PGV	C21-C22-C23-C24
16	M	403	BCL	C3-C5-C6-C7
16	X	102	BCL	C2-C1-O2A-CGA
16	5	104	BCL	C2-C1-O2A-CGA
16	D	102	BCL	C6-C7-C8-C10
16	F	103	BCL	C11-C12-C13-C15
16	Y	402	BCL	C11-C12-C13-C15
16	V	102	BCL	C2-C3-C5-C6
14	M	410	PGV	C20-C21-C22-C23
14	T	102	PGV	C6-C7-C8-C9
14	T	102	PGV	C03-C02-O01-C1
14	4	103	PGV	C7-C8-C9-C10
14	G	101	PGV	C6-C7-C8-C9
16	5	104	BCL	C15-C16-C17-C18
16	Z	102	BCL	C2C-C3C-CAC-CBC
22	B	101	CRT	C36-C37-C38-C40
14	G	101	PGV	C14-C15-C16-C17
16	1	103	BCL	CBA-CGA-O2A-C1
14	V	103	PGV	C20-C21-C22-C23
16	D	101	BCL	C2A-CAA-CBA-CGA
16	L	311	BCL	C16-C17-C18-C19
14	G	104	PGV	C21-C22-C23-C24
20	M	407	CDL	C77-C78-C79-C80
16	9	102	BCL	CAA-CBA-CGA-O2A
16	1	103	BCL	CAA-CBA-CGA-O1A
14	N	104	PGV	C5-C6-C7-C8
20	M	402	CDL	C1-CA2-OA2-PA1
10	C	402	HEC	CAA-CBA-CGA-O2A
16	W	102	BCL	CAA-CBA-CGA-O2A
16	Z	102	BCL	CAA-CBA-CGA-O1A
15	H	306	LMT	C5-C6-C7-C8
14	Z	103	PGV	C3-C4-C5-C6
16	F	103	BCL	C11-C12-C13-C14
16	S	101	BCL	C14-C13-C15-C16
16	W	102	BCL	C6-C7-C8-C9
16	1	103	BCL	C6-C7-C8-C9
16	7	102	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	Z	101	PGV	C4-C5-C6-C7
15	L	308	LMT	C3-C4-C5-C6
14	T	102	PGV	C3-C4-C5-C6
14	E	102	PGV	C20-C21-C22-C23
16	N	103	BCL	C8-C10-C11-C12
15	H	306	LMT	C5'-C4'-O1B-C1B
14	M	410	PGV	O02-C1-C2-C3
15	I	101	LMT	C4'-C5'-C6'-O6'
20	M	402	CDL	C44-C45-C46-C47
22	R	101	CRT	C1-C4-C5-C6
14	X	101	PGV	O05-C05-C06-O06
14	Z	104	PGV	C24-C25-C26-C27
14	H	304	PGV	O03-C19-C20-C21
16	G	103	BCL	CAA-CBA-CGA-O2A
16	L	312	BCL	C13-C15-C16-C17
22	G	102	CRT	C15-C16-C17-C19
14	L	305	PGV	O02-C1-C2-C3
14	L	309	PGV	O02-C1-C2-C3
14	H	302	PGV	O02-C1-C2-C3
14	1	101	PGV	O02-C1-C2-C3
16	I	103	BCL	C10-C11-C12-C13
15	5	101	LMT	C9-C10-C11-C12
20	U	101	CDL	OA6-CA4-CA6-OA8
14	H	304	PGV	C28-C29-C30-C31
14	Z	103	PGV	O04-C19-C20-C21
16	O	104	BCL	CAA-CBA-CGA-O1A
16	D	102	BCL	CAA-CBA-CGA-O2A
20	M	407	CDL	C52-C51-CB5-OB6
16	X	102	BCL	C8-C10-C11-C12
14	R	104	PGV	C5-C6-C7-C8
14	1	101	PGV	C26-C27-C28-C29
14	0	103	PGV	C3-C4-C5-C6
16	5	104	BCL	CAA-CBA-CGA-O1A
14	H	304	PGV	C21-C22-C23-C24
16	I	102	BCL	C15-C16-C17-C18
14	T	102	PGV	C15-C16-C17-C18
10	C	401	HEC	CAD-CBD-CGD-O2D
14	G	101	PGV	C19-C20-C21-C22
16	M	403	BCL	CAD-CBD-CGD-O2D
20	M	407	CDL	C72-C71-CB7-OB8
14	Z	103	PGV	C23-C24-C25-C26
20	H	303	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
16	L	302	BCL	C2-C1-O2A-CGA
16	I	103	BCL	C2-C1-O2A-CGA
16	S	101	BCL	C2-C1-O2A-CGA
14	F	101	PGV	C26-C27-C28-C29
16	5	104	BCL	C2A-CAA-CBA-CGA
10	C	404	HEC	CAA-CBA-CGA-O2A
14	P	103	PGV	C5-C6-C7-C8
14	N	101	PGV	O01-C1-C2-C3
14	T	103	PGV	O03-C19-C20-C21
14	2	103	PGV	O03-C19-C20-C21
16	L	311	BCL	CAA-CBA-CGA-O2A
16	L	312	BCL	CAA-CBA-CGA-O2A
14	T	103	PGV	C20-C21-C22-C23
14	P	102	PGV	C9-C10-C11-C12
14	H	304	PGV	O04-C19-C20-C21
20	M	407	CDL	C52-C51-CB5-OB7
15	O	102	LMT	C3'-C4'-O1B-C1B

There are no ring outliers.

126 monomers are involved in 630 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	4	103	PGV	4	0
14	H	302	PGV	5	0
14	X	101	PGV	2	0
20	U	101	CDL	5	0
16	3	102	BCL	8	0
14	V	103	PGV	2	0
14	0	103	PGV	5	0
14	T	102	PGV	6	0
20	M	407	CDL	4	0
16	1	103	BCL	7	0
14	6	104	PGV	3	0
20	M	408	CDL	3	0
14	F	101	PGV	6	0
14	L	305	PGV	4	0
16	8	102	BCL	11	0
14	H	304	PGV	3	0
16	L	311	BCL	4	0
14	G	101	PGV	6	0
14	0	101	PGV	6	0
20	H	303	CDL	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	401	BCL	5	0
14	8	103	PGV	8	0
16	9	102	BCL	6	0
15	O	102	LMT	1	0
18	L	304	UQ8	5	0
14	P	102	PGV	9	0
14	B	104	PGV	8	0
16	S	101	BCL	12	0
16	7	102	BCL	3	0
17	M	404	BPH	8	0
16	V	102	BCL	9	0
16	0	102	BCL	9	0
18	L	306	UQ8	4	0
16	Z	102	BCL	8	0
14	Z	101	PGV	4	0
16	W	101	BCL	11	0
15	L	308	LMT	3	0
14	N	101	PGV	8	0
15	5	101	LMT	4	0
16	G	103	BCL	10	0
16	R	102	BCL	10	0
14	R	104	PGV	6	0
15	H	306	LMT	1	0
10	C	401	HEC	11	0
13	C	407	PLM	5	0
16	W	102	BCL	3	0
22	G	102	CRT	6	0
14	6	103	PGV	3	0
16	T	101	BCL	6	0
10	C	403	HEC	2	0
22	4	101	CRT	12	0
14	L	310	PGV	8	0
14	C	408	PGV	3	0
16	P	101	BCL	9	0
16	L	302	BCL	3	0
14	L	309	PGV	5	0
16	S	102	BCL	9	0
15	I	101	LMT	5	0
15	M	411	LMT	4	0
14	T	103	PGV	7	0
16	I	102	BCL	6	0
16	L	312	BCL	6	0

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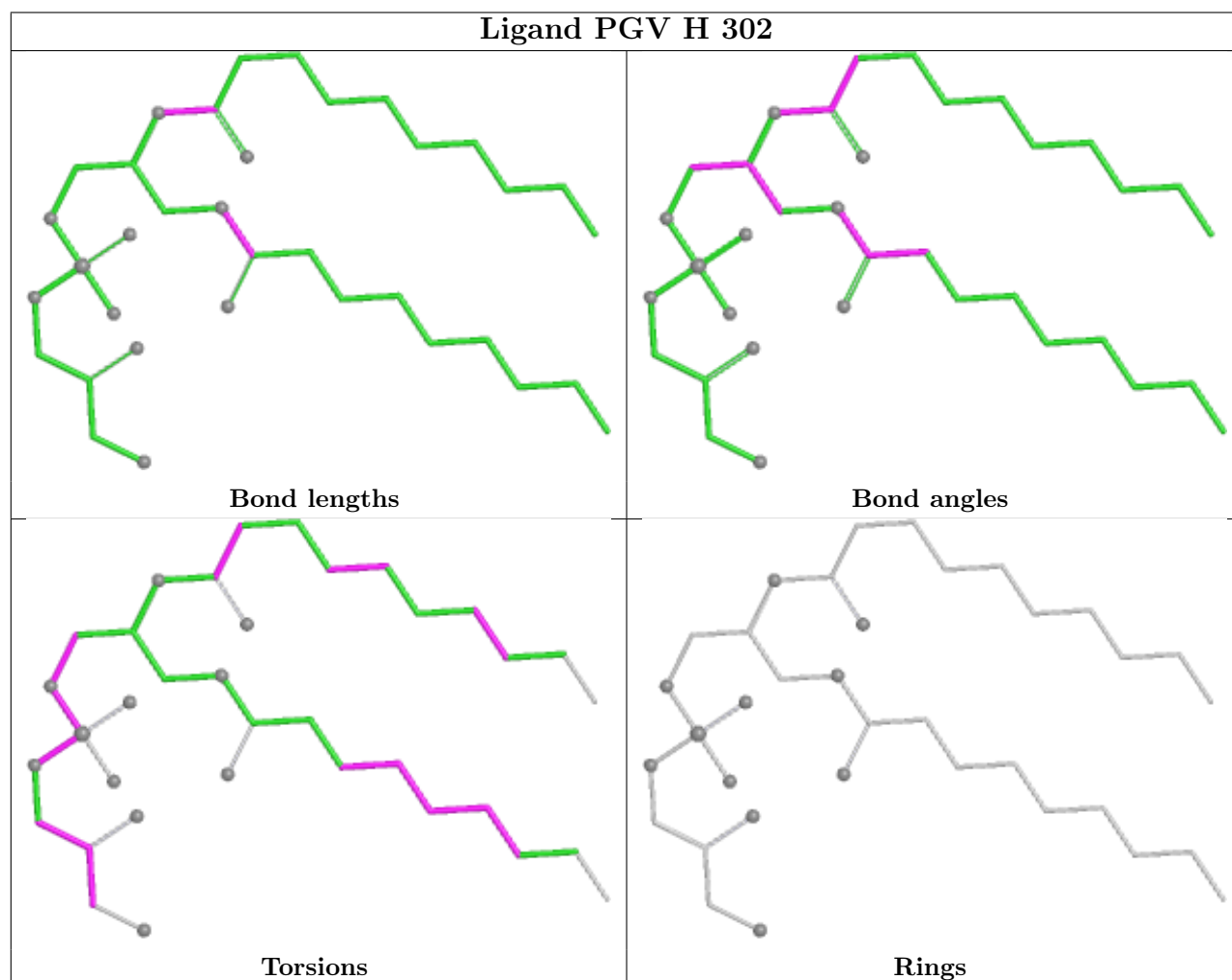
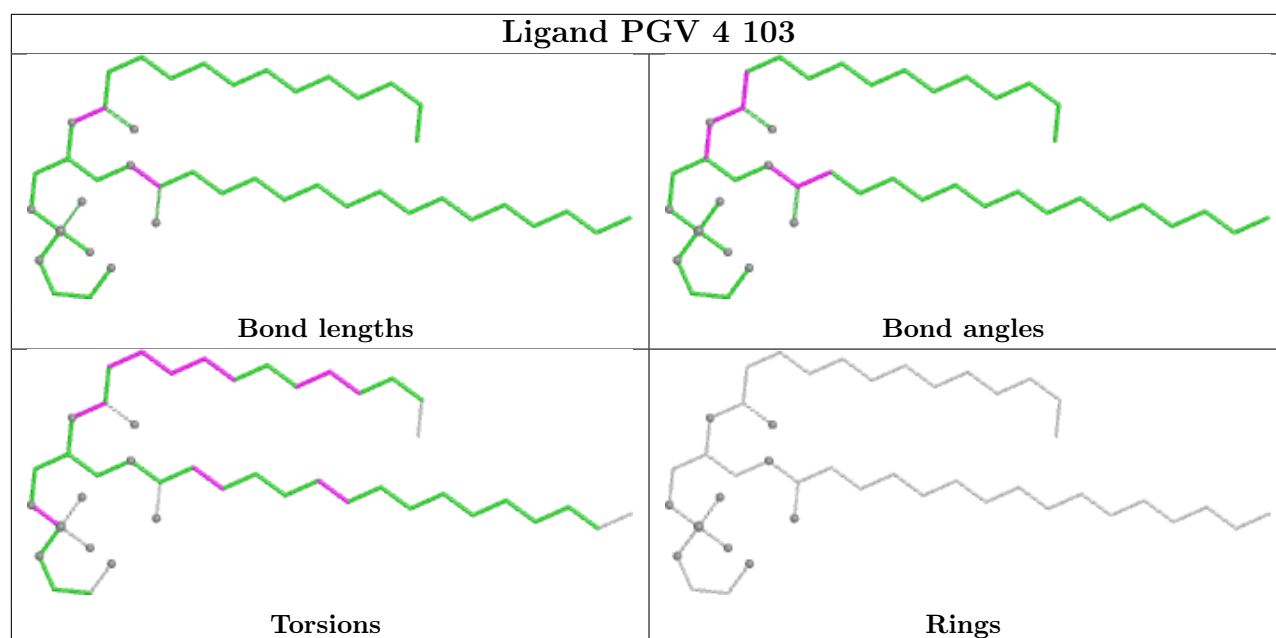
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	M	406	CRT	11	0
14	G	104	PGV	7	0
16	F	103	BCL	2	0
20	U	102	CDL	1	0
16	I	103	BCL	14	0
16	D	101	BCL	5	0
16	4	102	BCL	5	0
17	L	303	BPH	6	0
14	2	103	PGV	1	0
21	M	405	MQ8	3	0
16	9	101	BCL	5	0
16	1	102	BCL	10	0
15	H	305	LMT	8	0
22	B	101	CRT	4	0
14	6	101	PGV	3	0
14	P	103	PGV	2	0
14	X	103	PGV	6	0
22	8	101	CRT	6	0
16	5	103	BCL	14	0
15	5	102	LMT	3	0
16	M	403	BCL	7	0
14	2	102	PGV	6	0
14	Z	104	PGV	8	0
16	O	103	BCL	6	0
15	F	102	LMT	4	0
16	2	101	BCL	10	0
14	R	103	PGV	3	0
16	E	101	BCL	6	0
16	Y	402	BCL	3	0
15	Q	101	LMT	3	0
16	K	101	BCL	7	0
14	0	104	PGV	7	0
16	A	101	BCL	4	0
16	Q	102	BCL	7	0
20	M	409	CDL	4	0
14	B	103	PGV	5	0
14	1	101	PGV	12	0
16	J	101	BCL	8	0
16	N	103	BCL	8	0
14	3	101	PGV	4	0
16	X	102	BCL	5	0
16	O	104	BCL	5	0

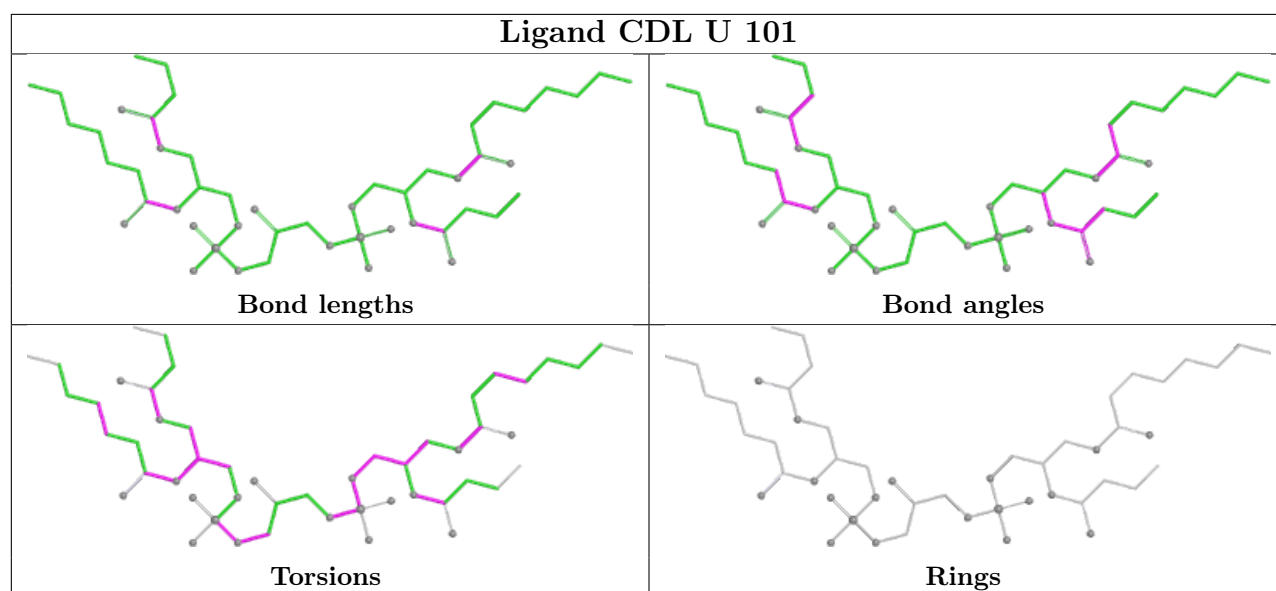
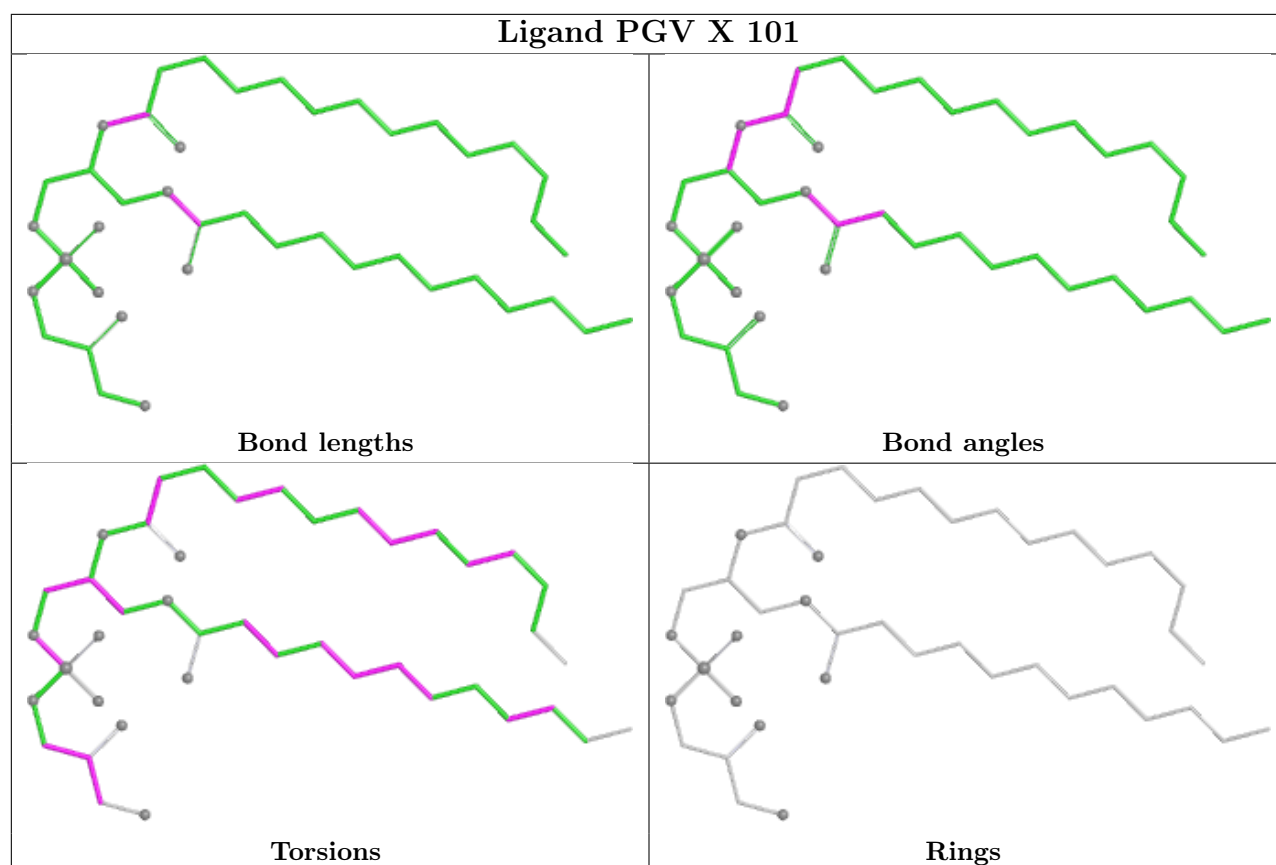
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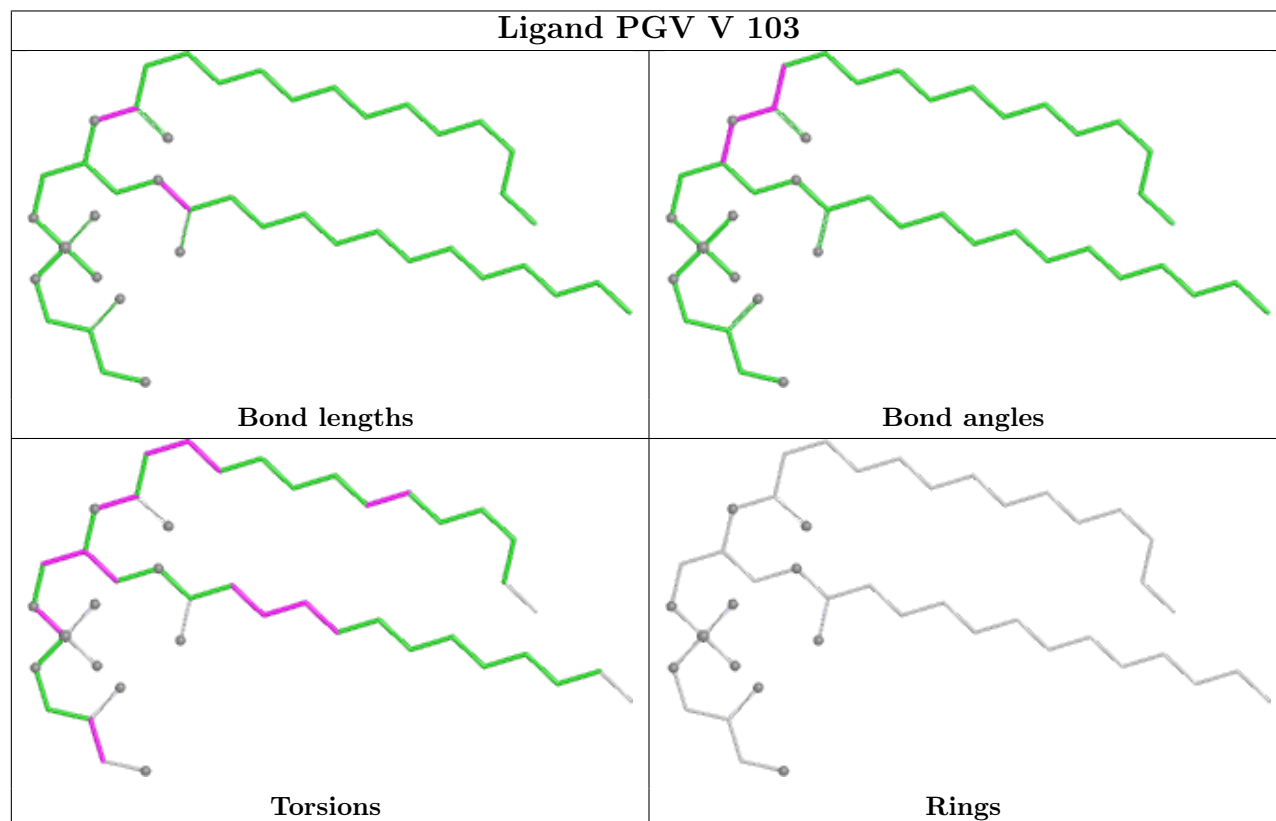
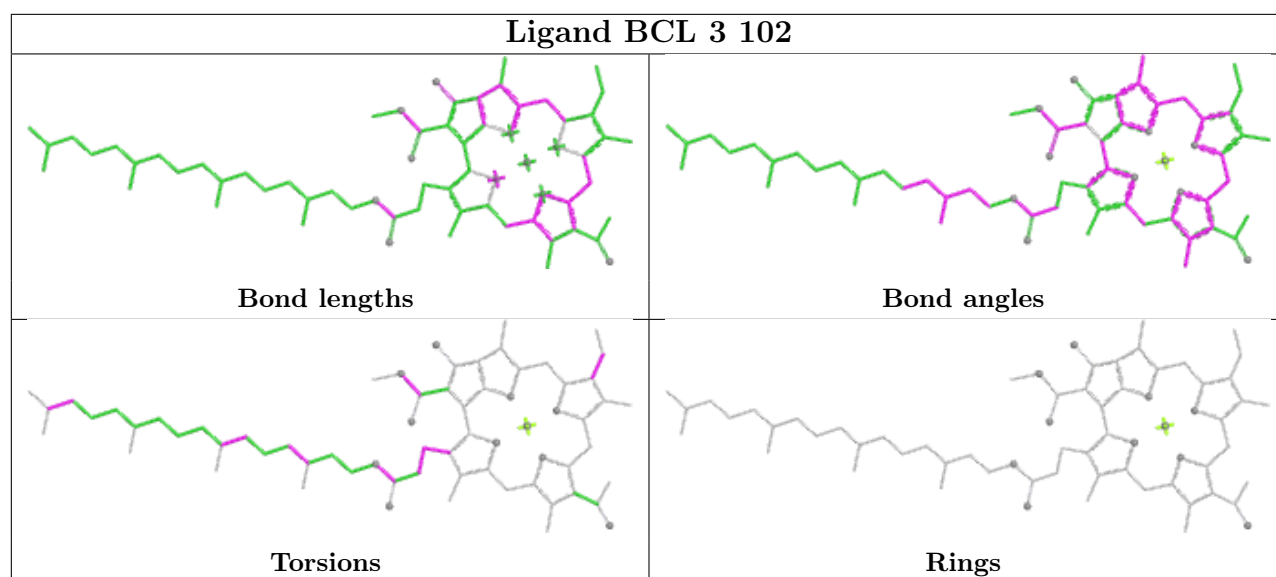
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	H	301	CDL	5	0
14	G	105	PGV	6	0
16	6	102	BCL	7	0
22	V	101	CRT	9	0
16	D	102	BCL	5	0
16	5	104	BCL	7	0
22	Y	403	CRT	9	0
14	Z	103	PGV	3	0
22	R	101	CRT	9	0
14	N	104	PGV	2	0
22	N	102	CRT	11	0
14	J	102	PGV	4	0
15	7	101	LMT	4	0
15	L	301	LMT	2	0
14	M	410	PGV	5	0
20	M	402	CDL	9	0
20	O	101	CDL	3	0
14	E	102	PGV	2	0
16	U	103	BCL	5	0
16	B	102	BCL	11	0
10	C	402	HEC	1	0
18	L	307	UQ8	1	0

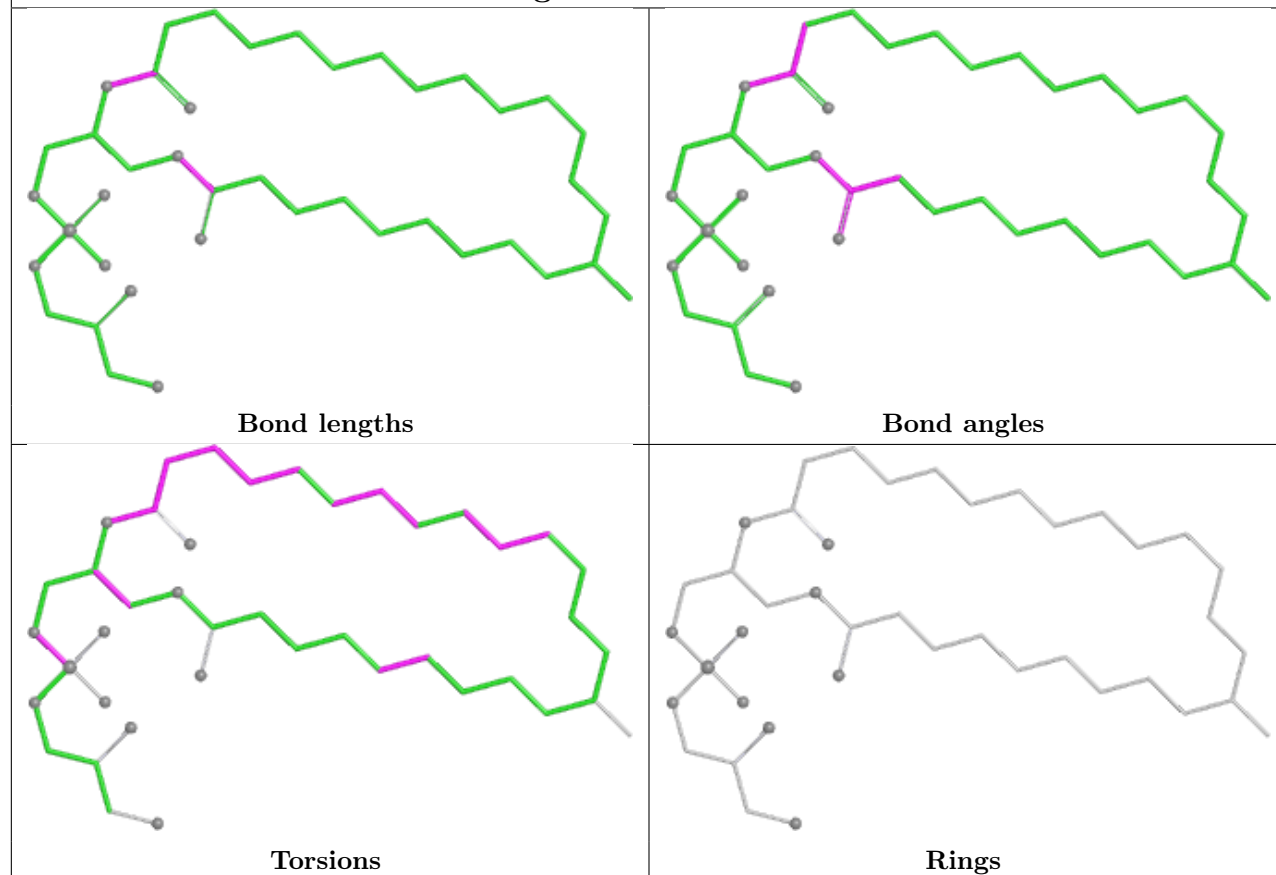
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



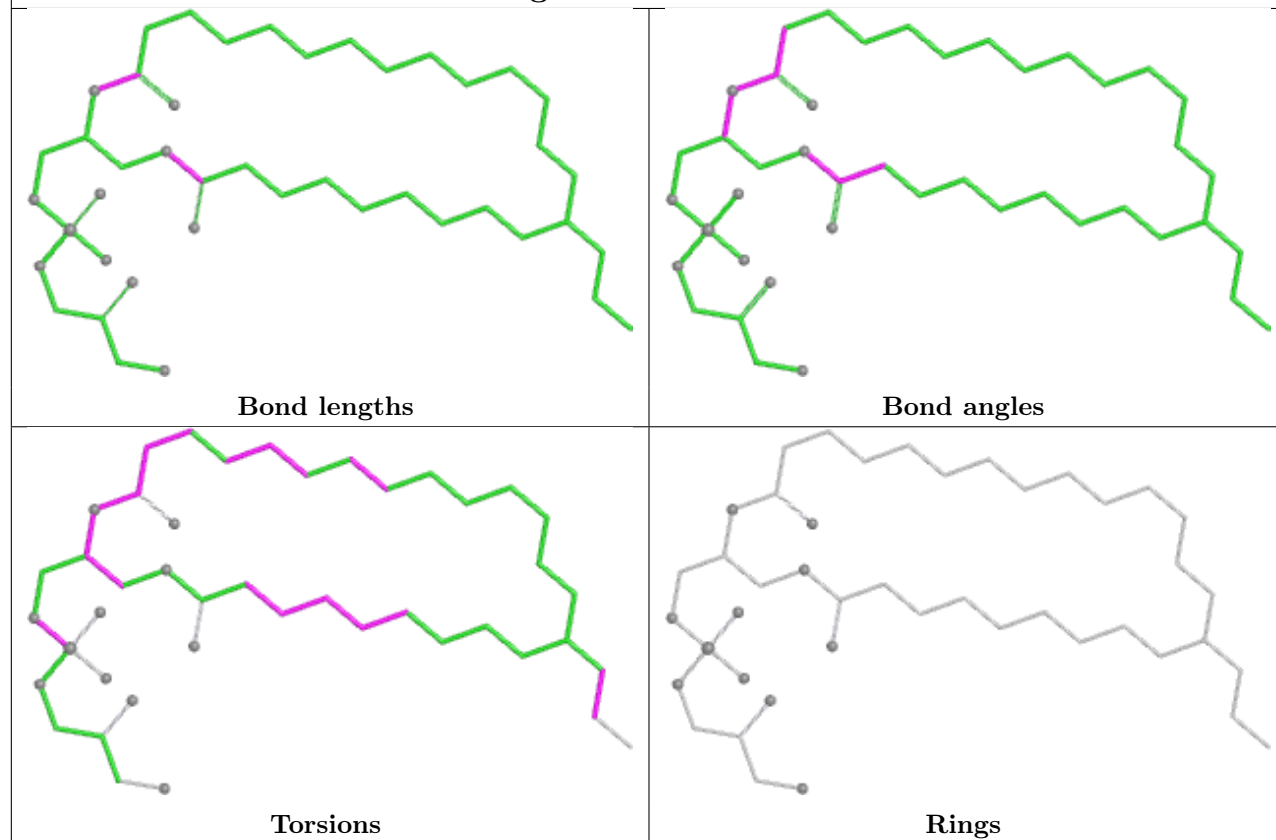


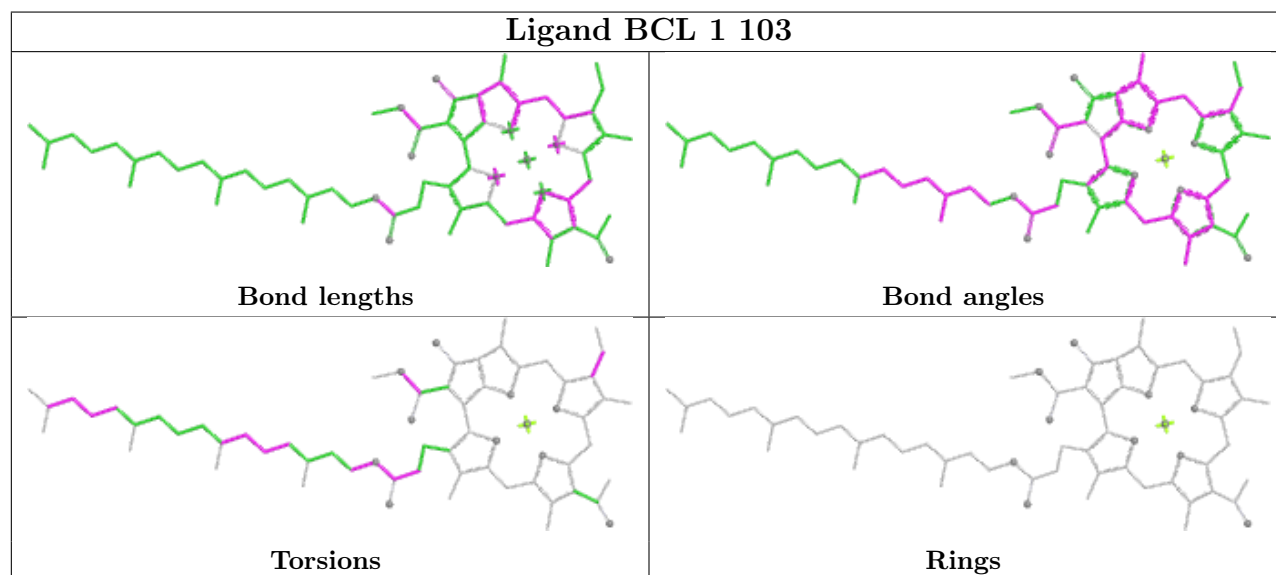
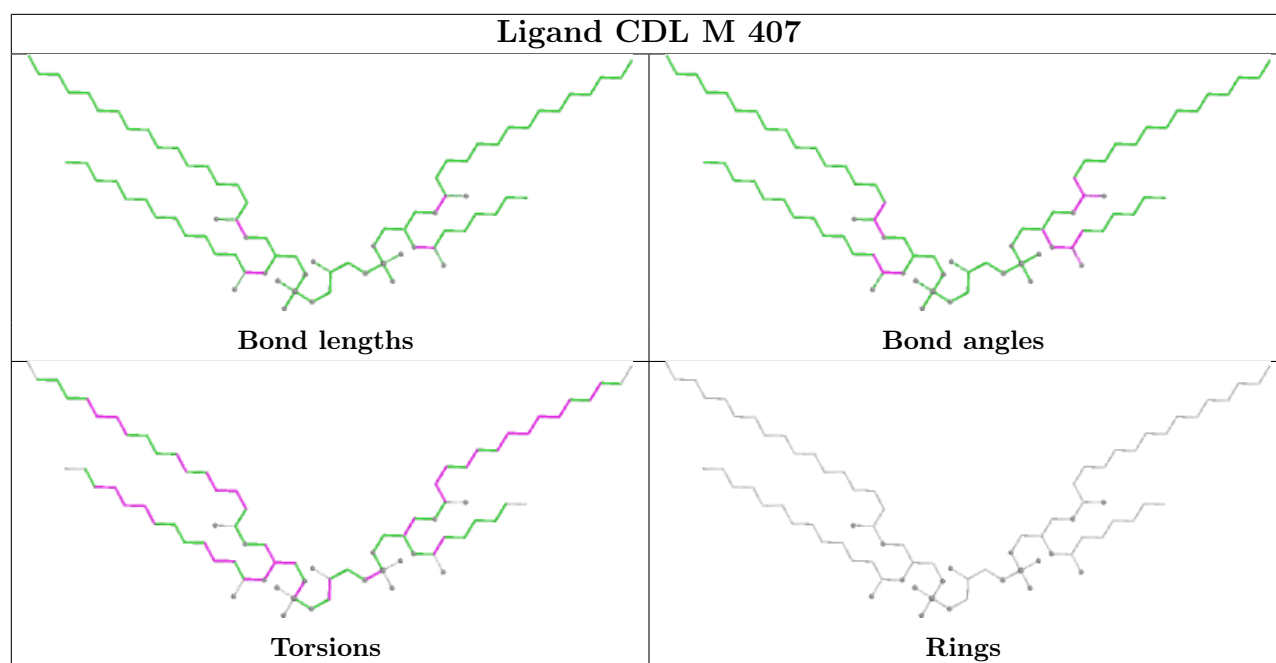


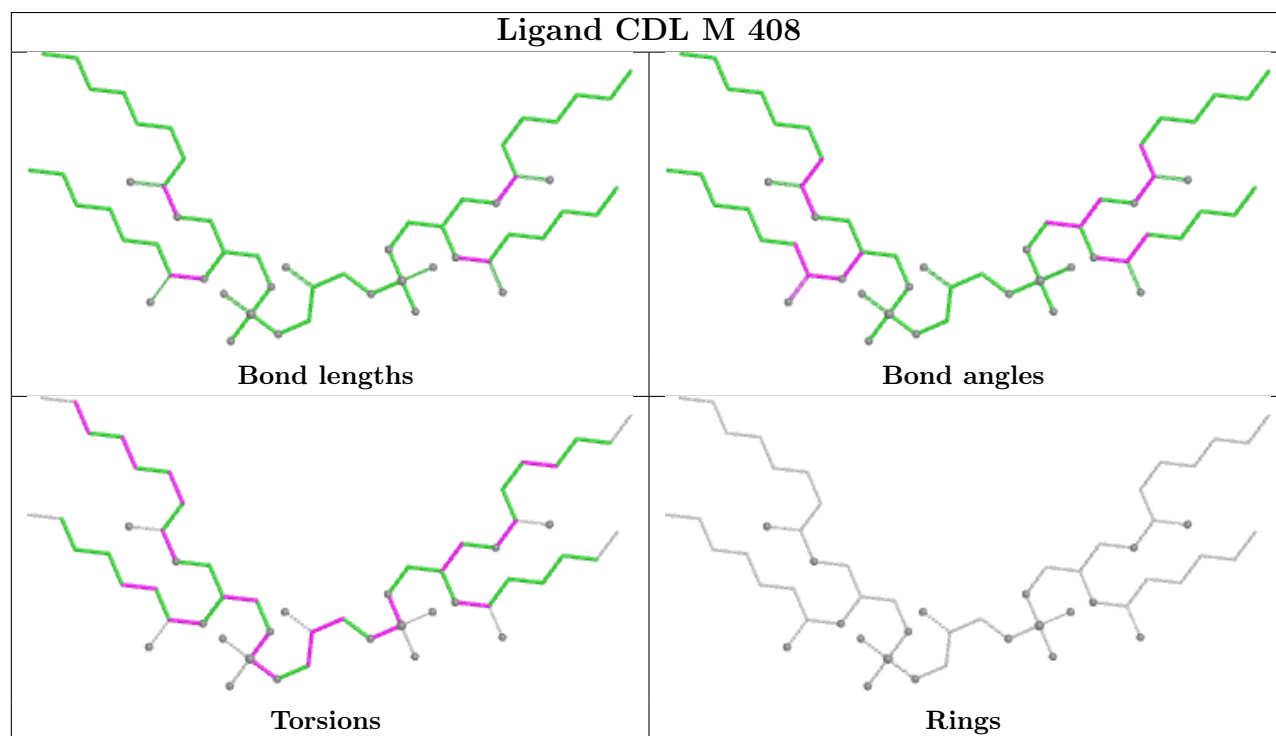
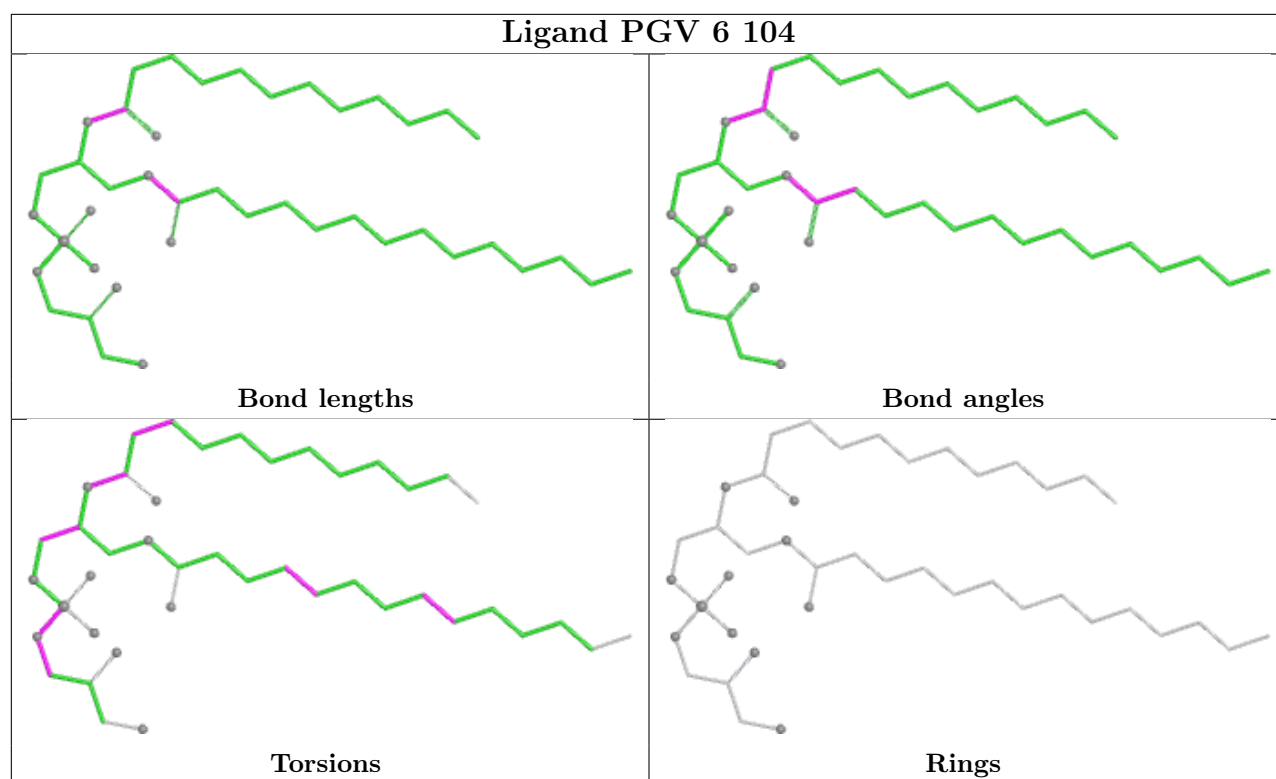
Ligand PGV 0 103

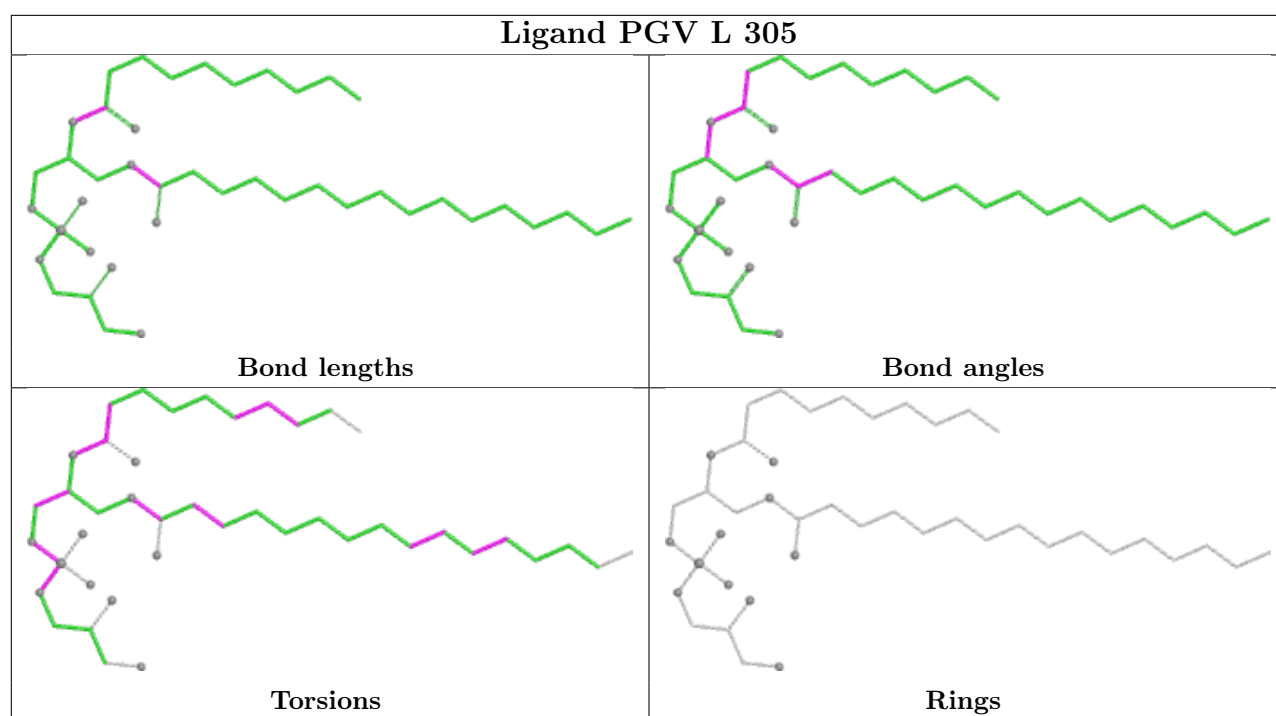
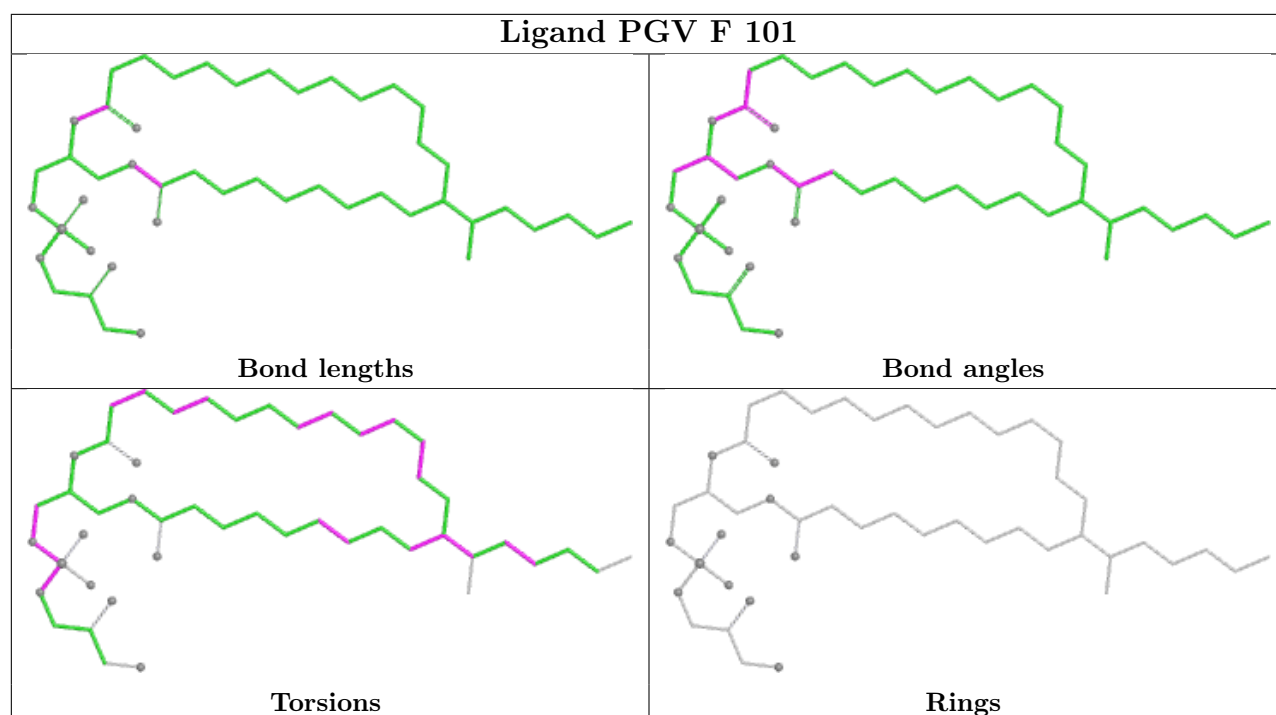


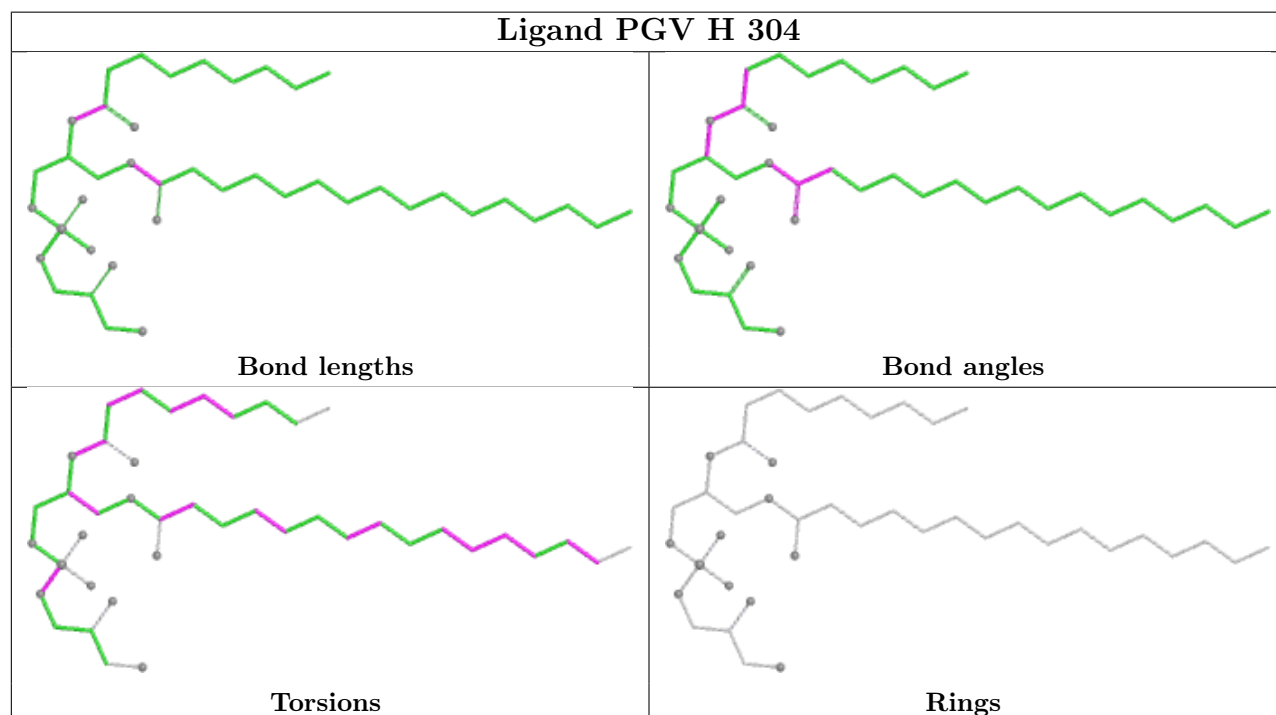
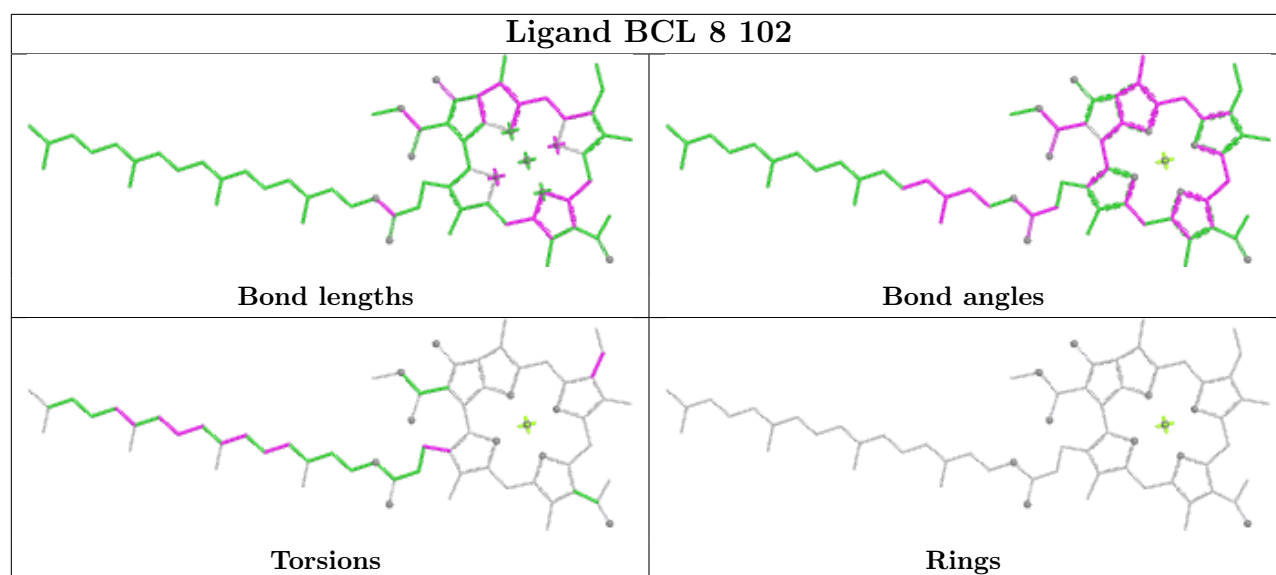
Ligand PGV T 102

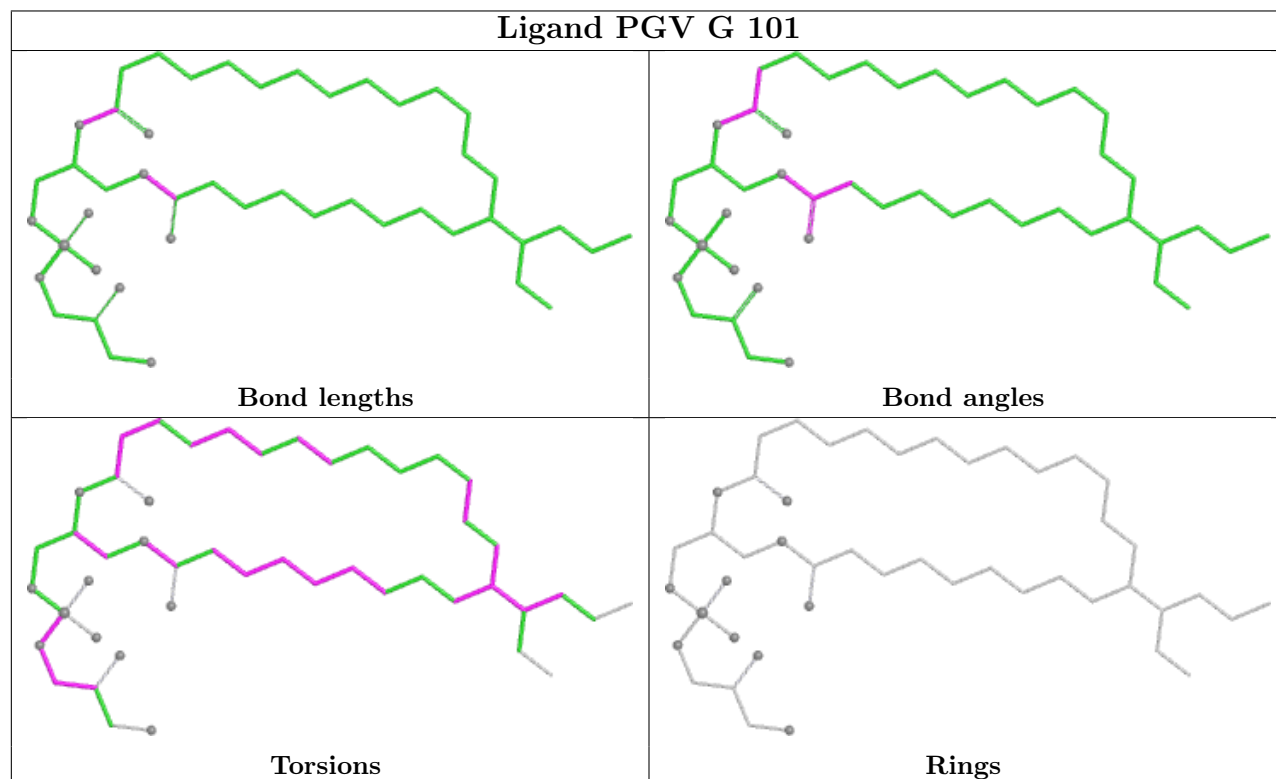
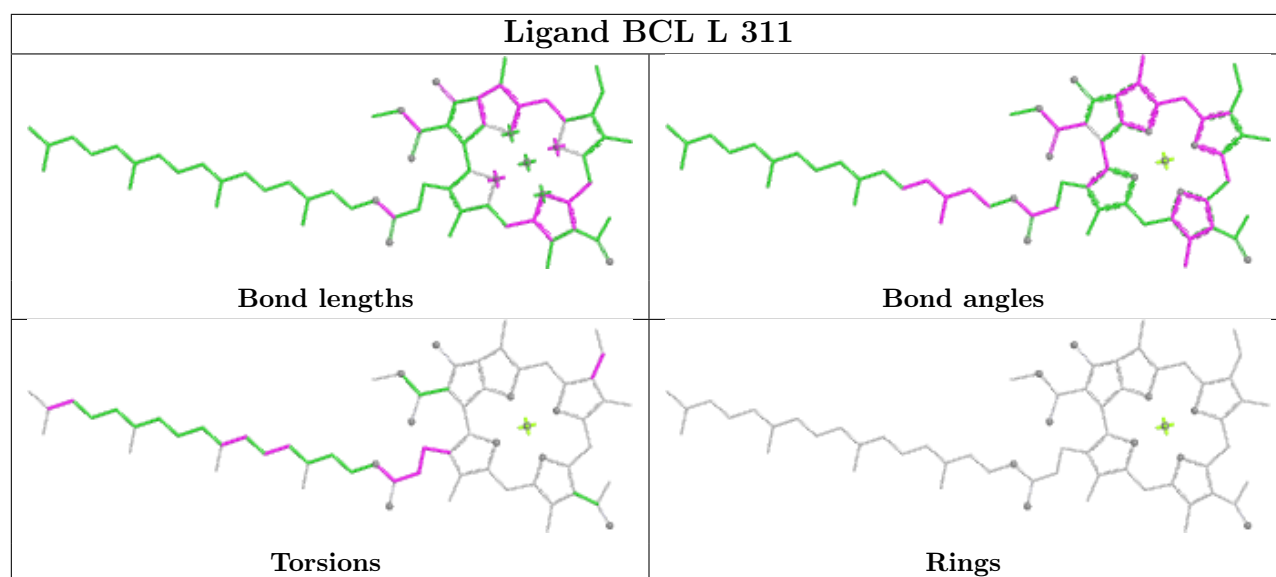


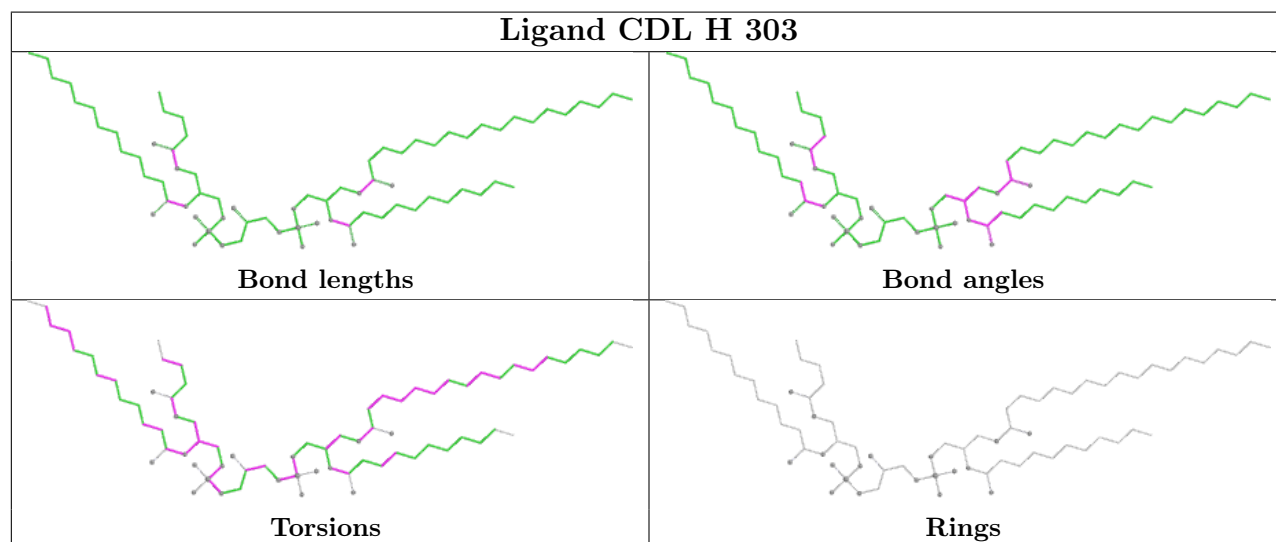
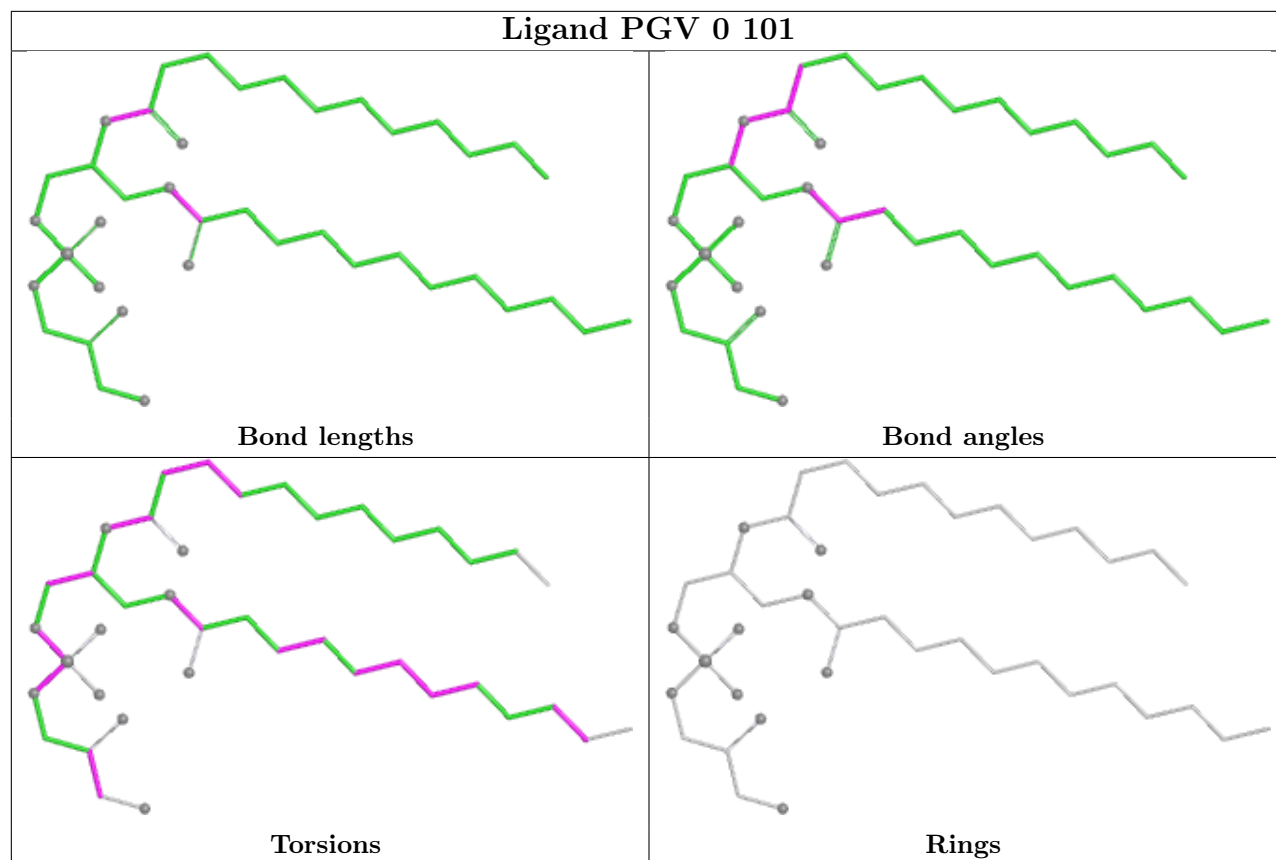


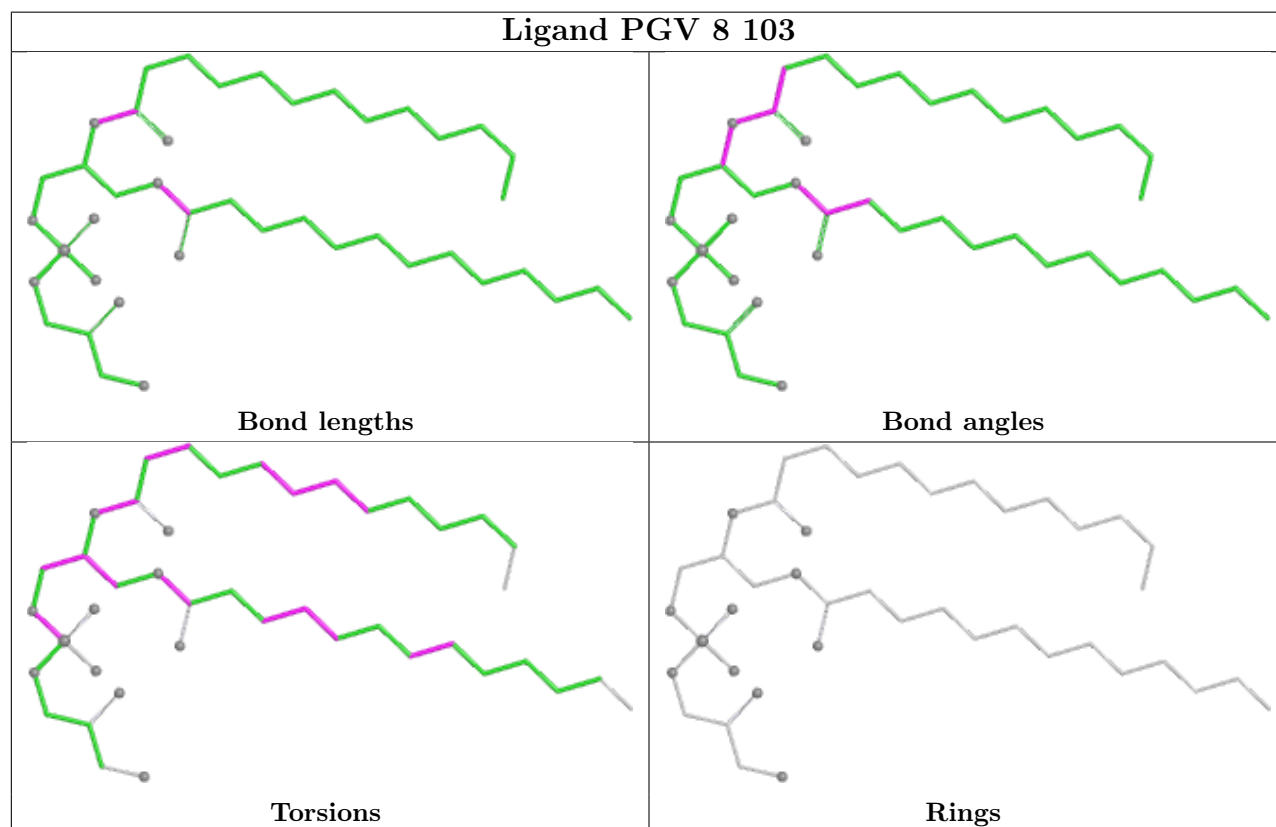
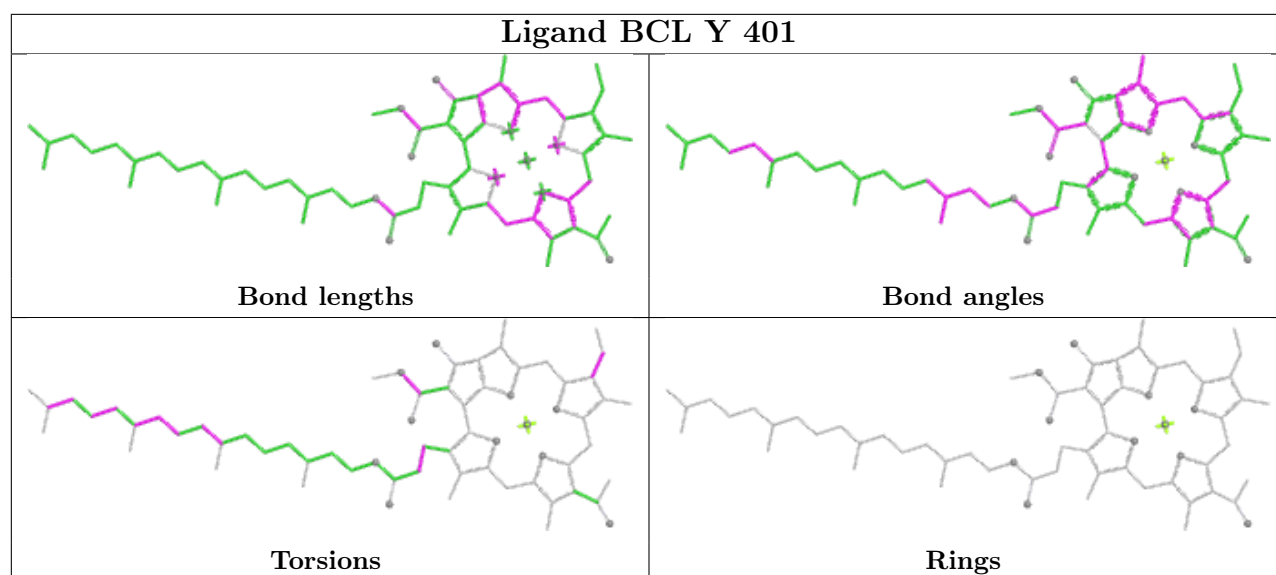


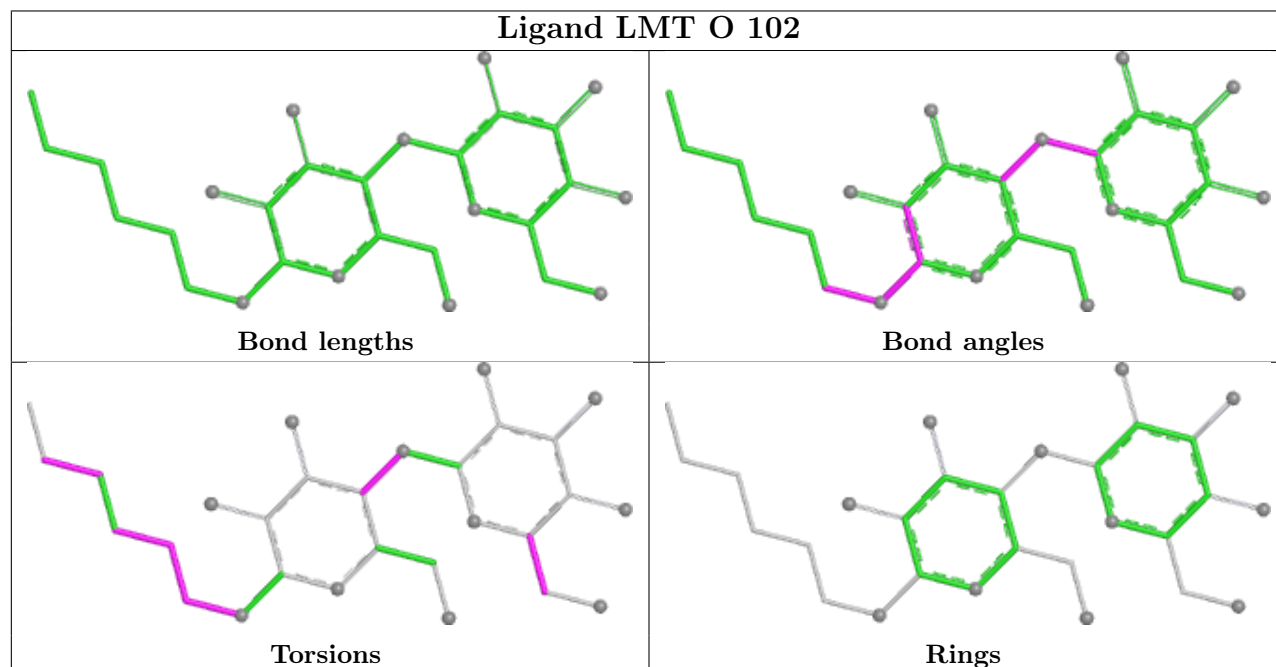
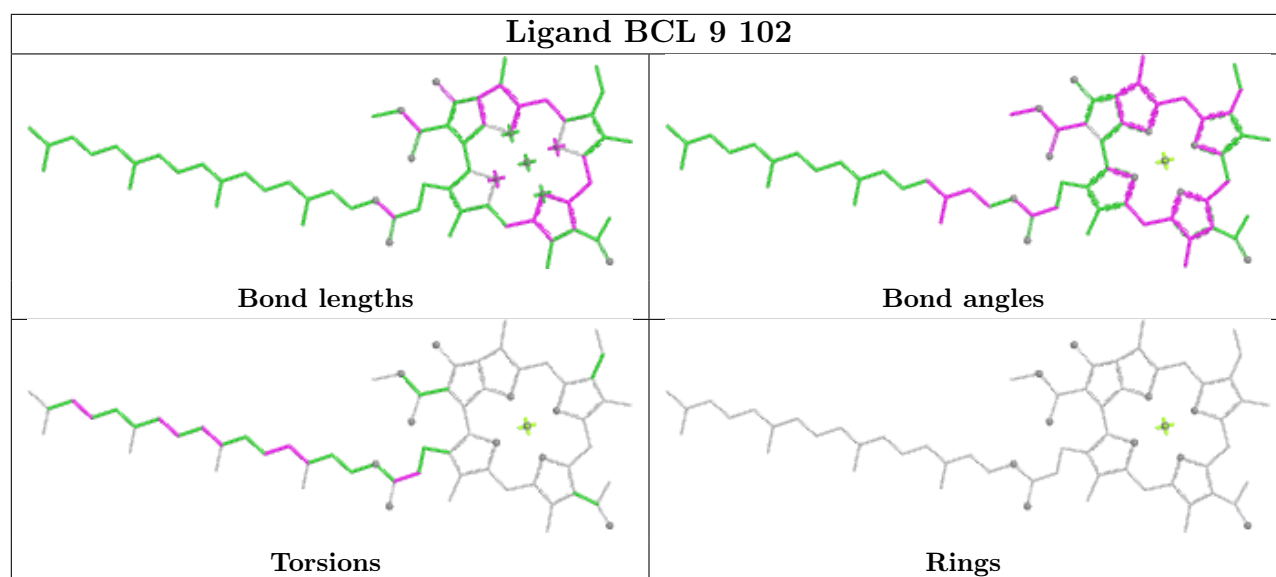


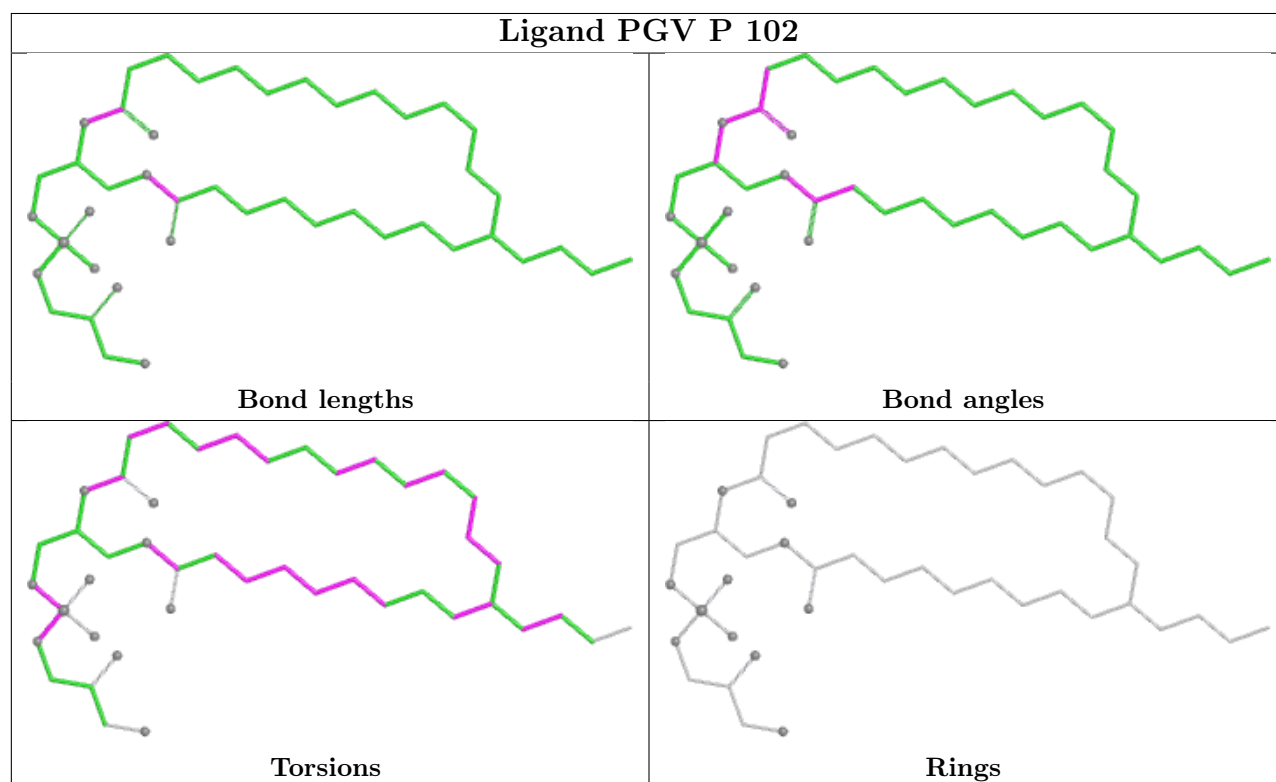
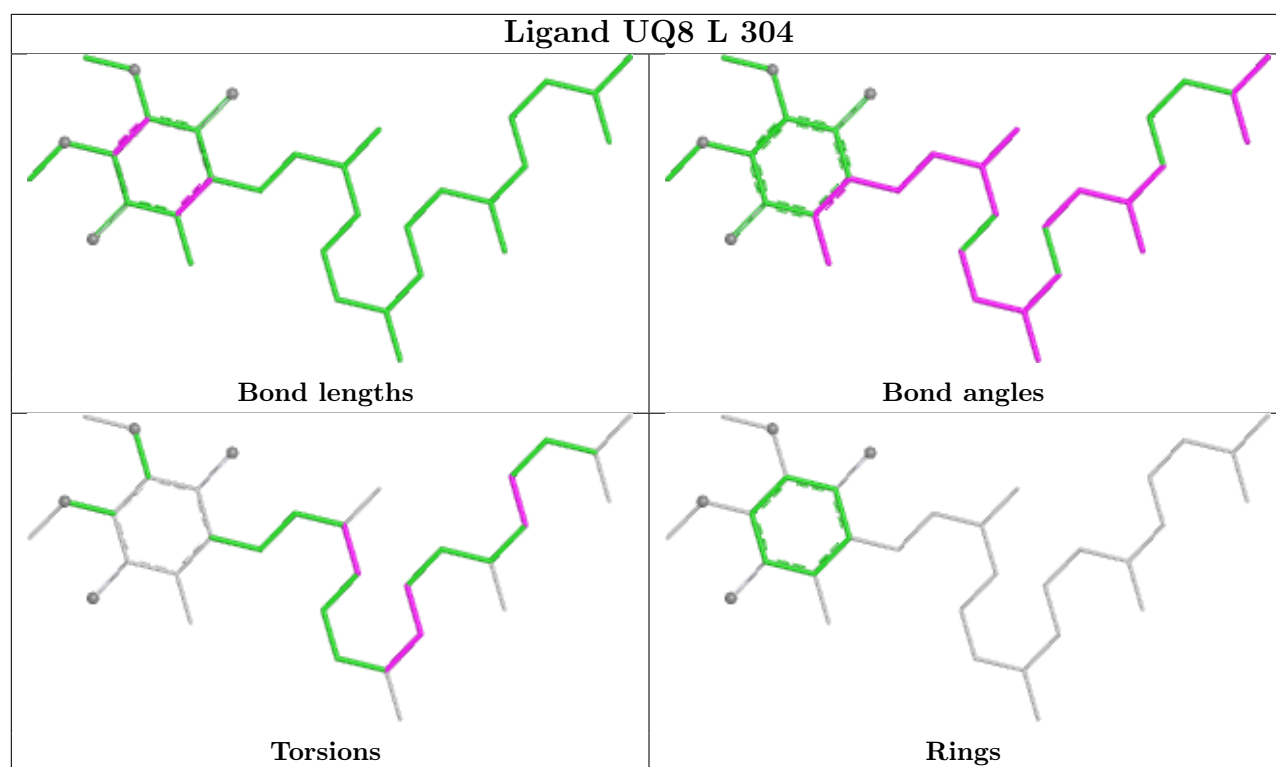


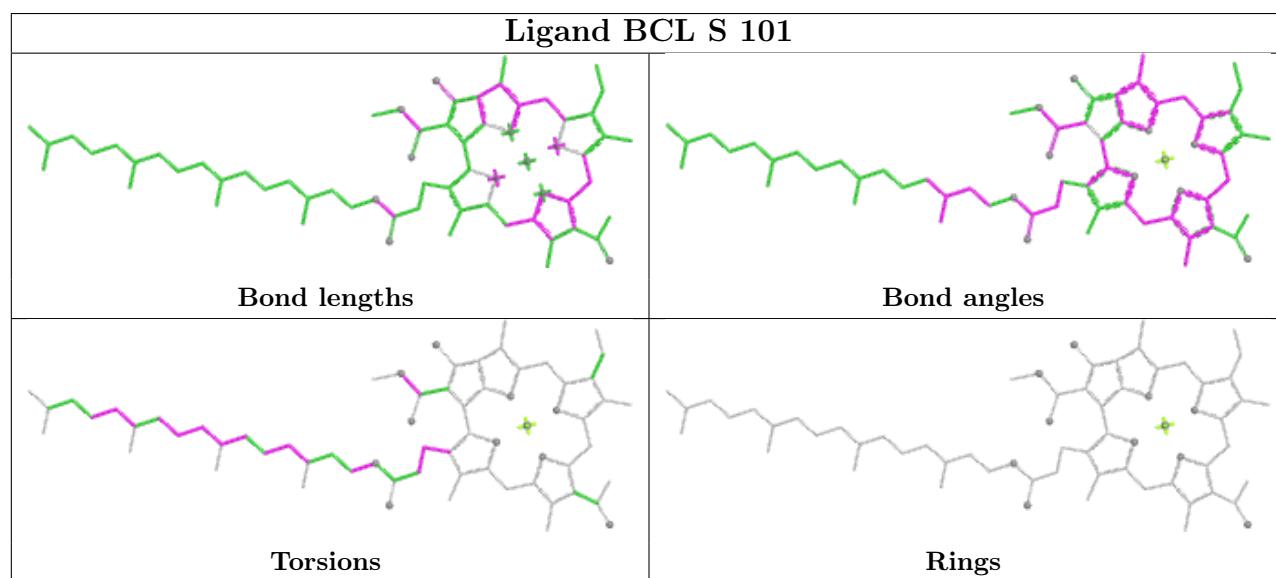
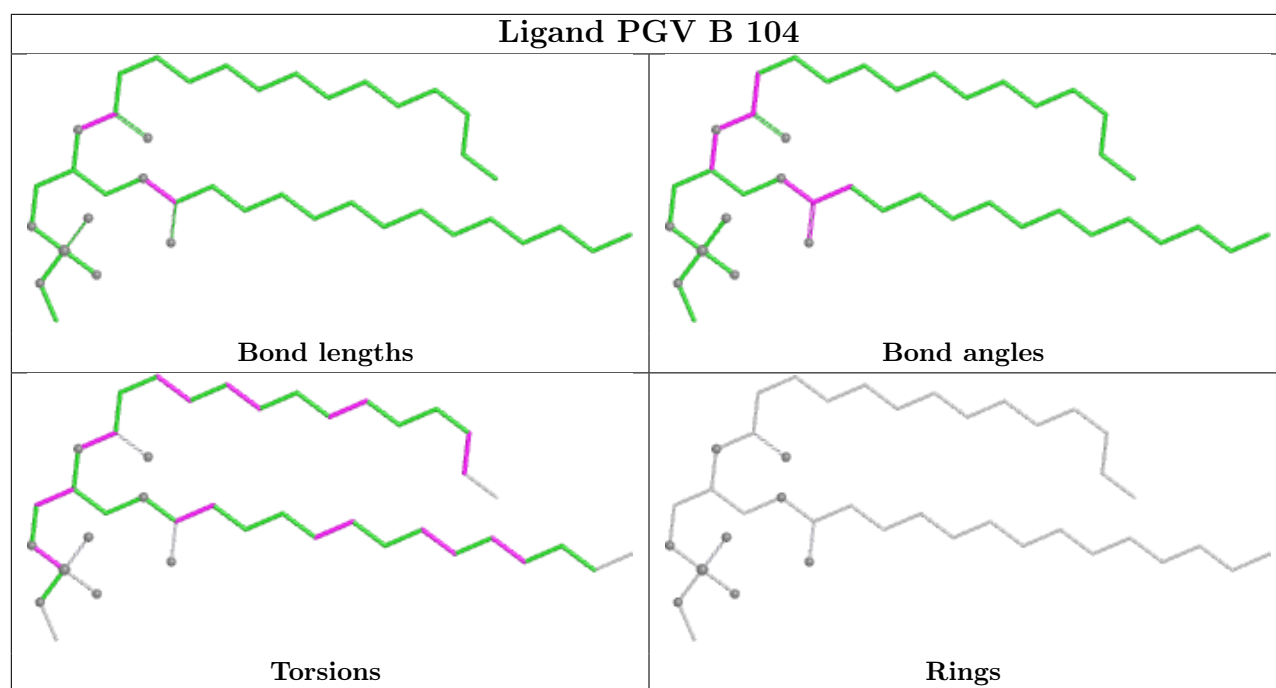


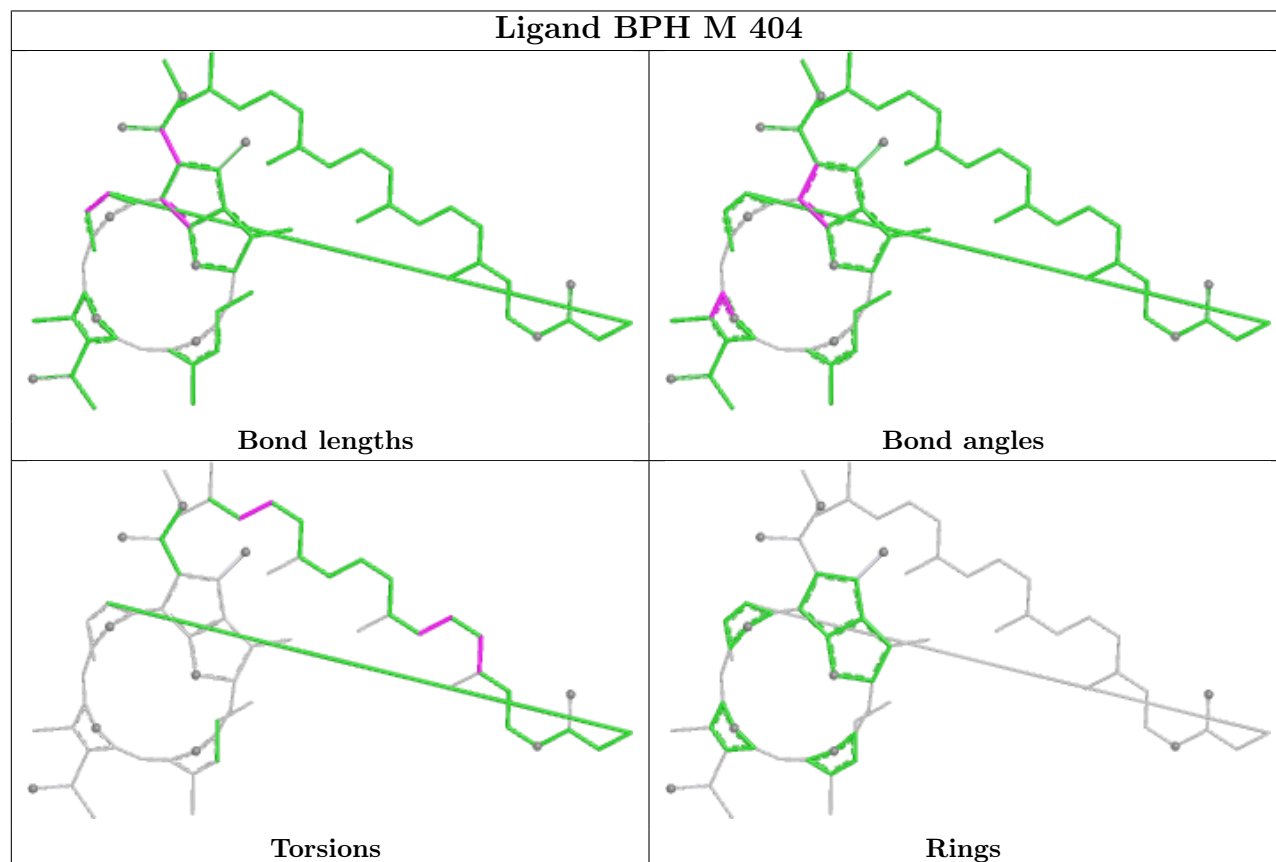
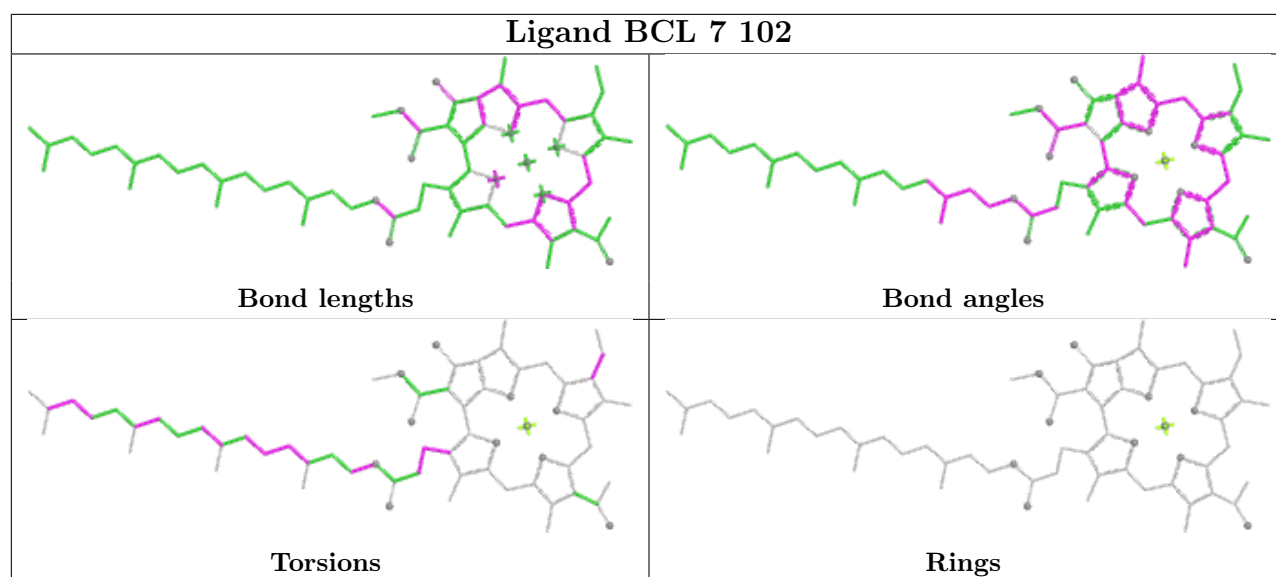


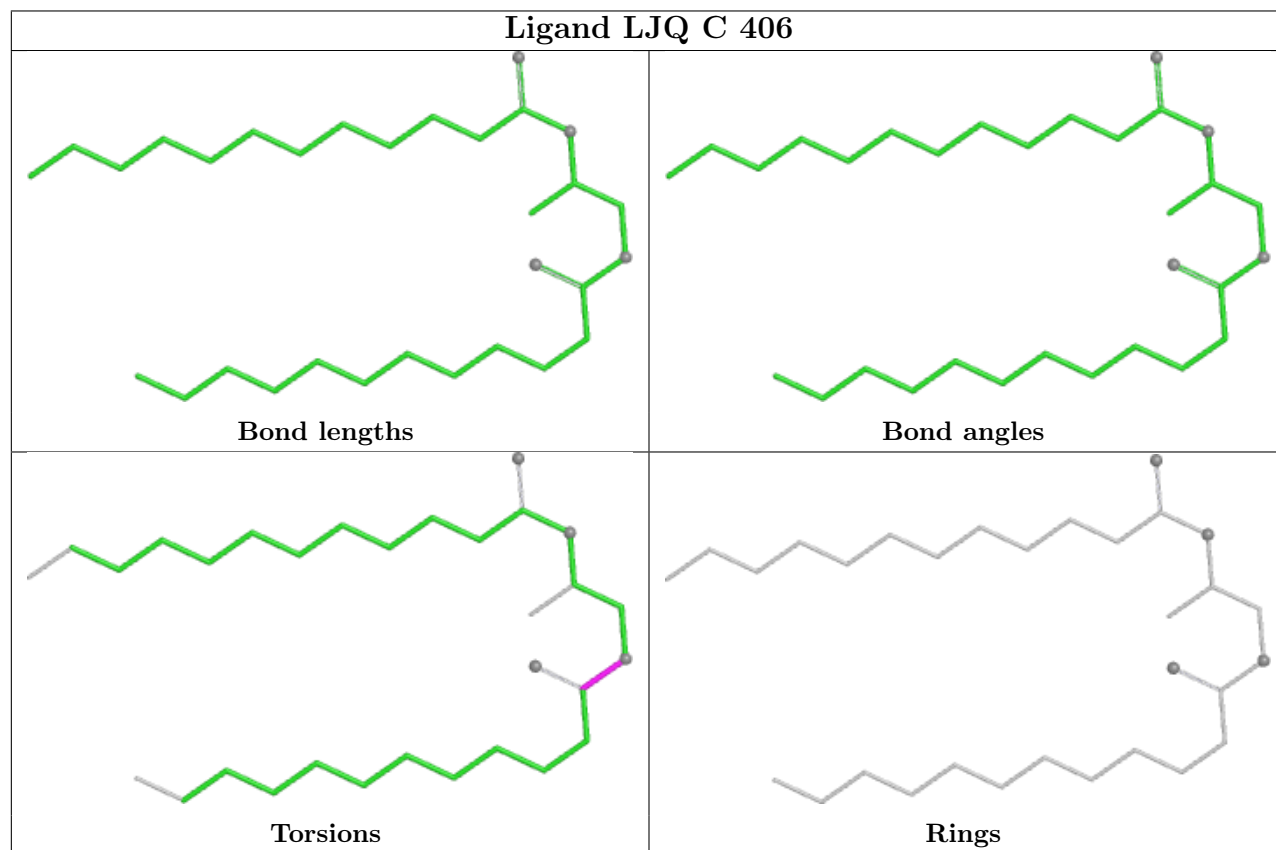
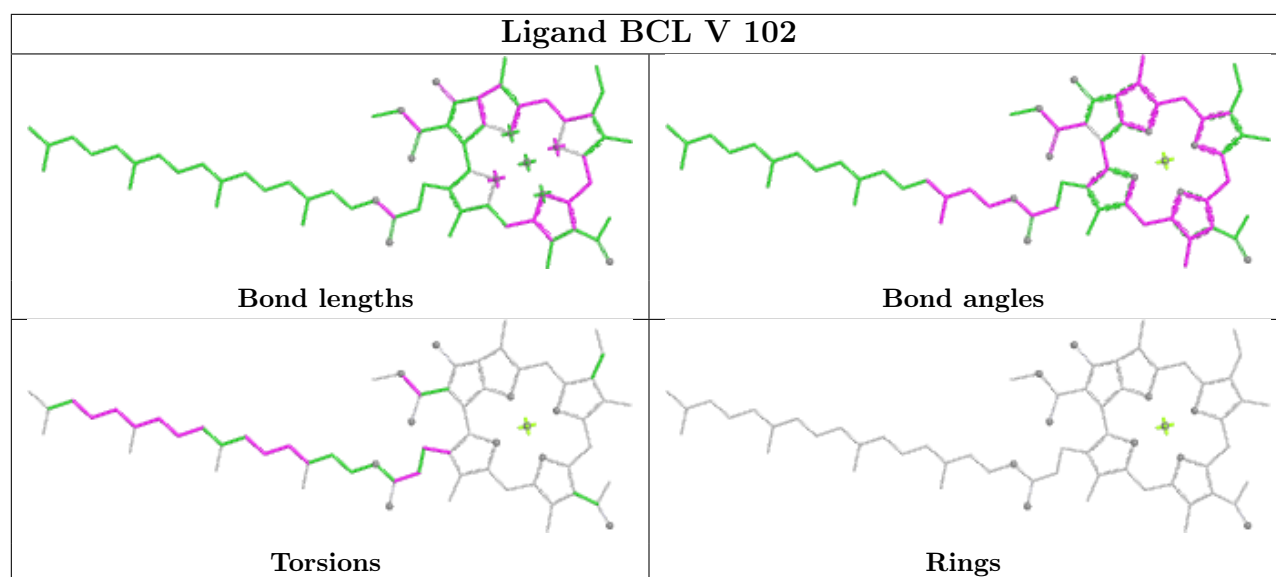


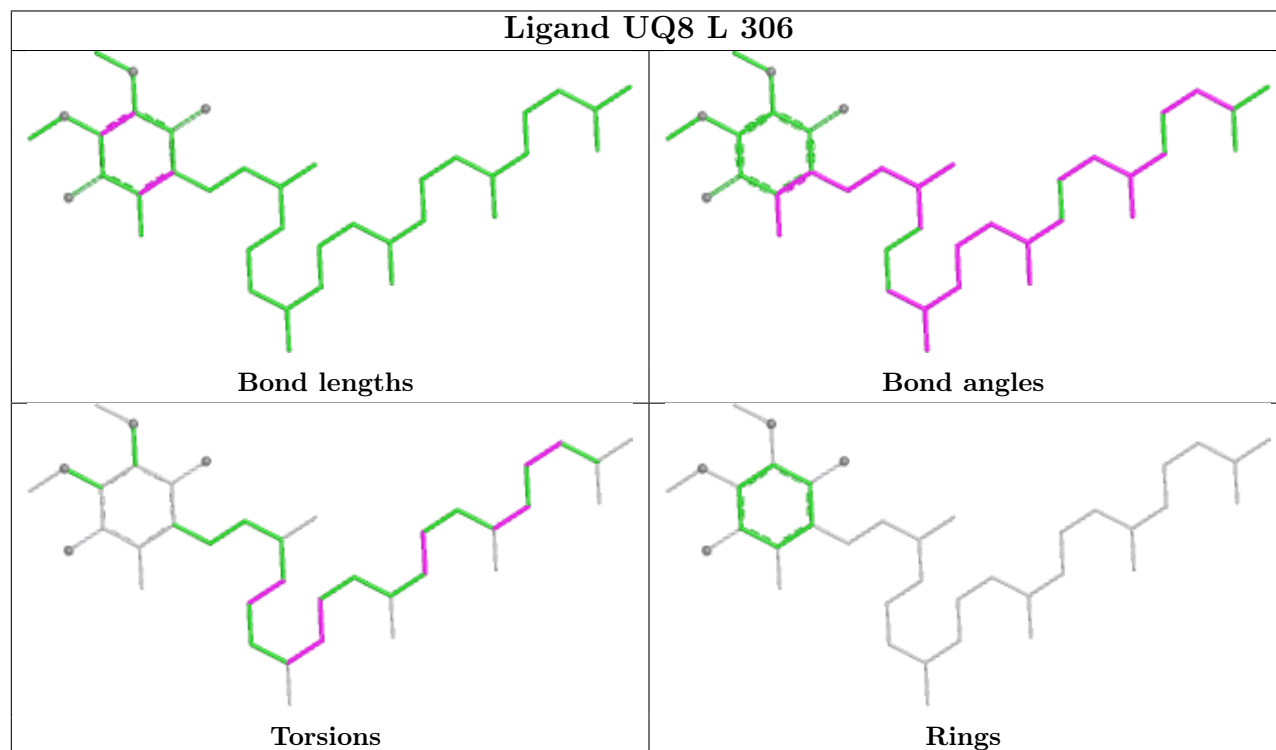
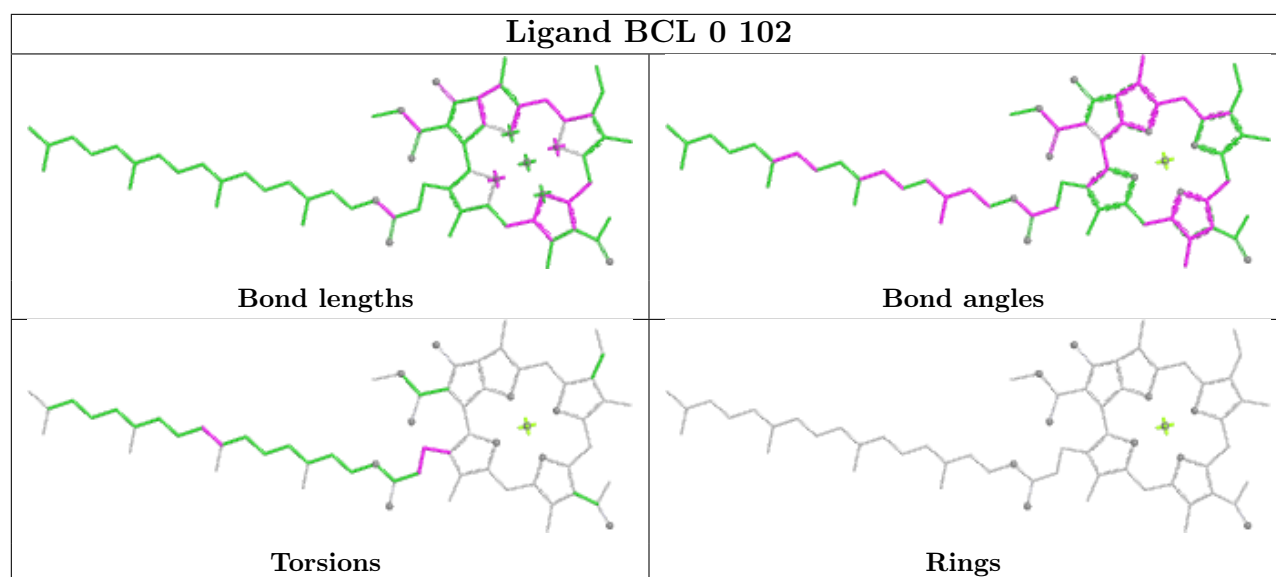


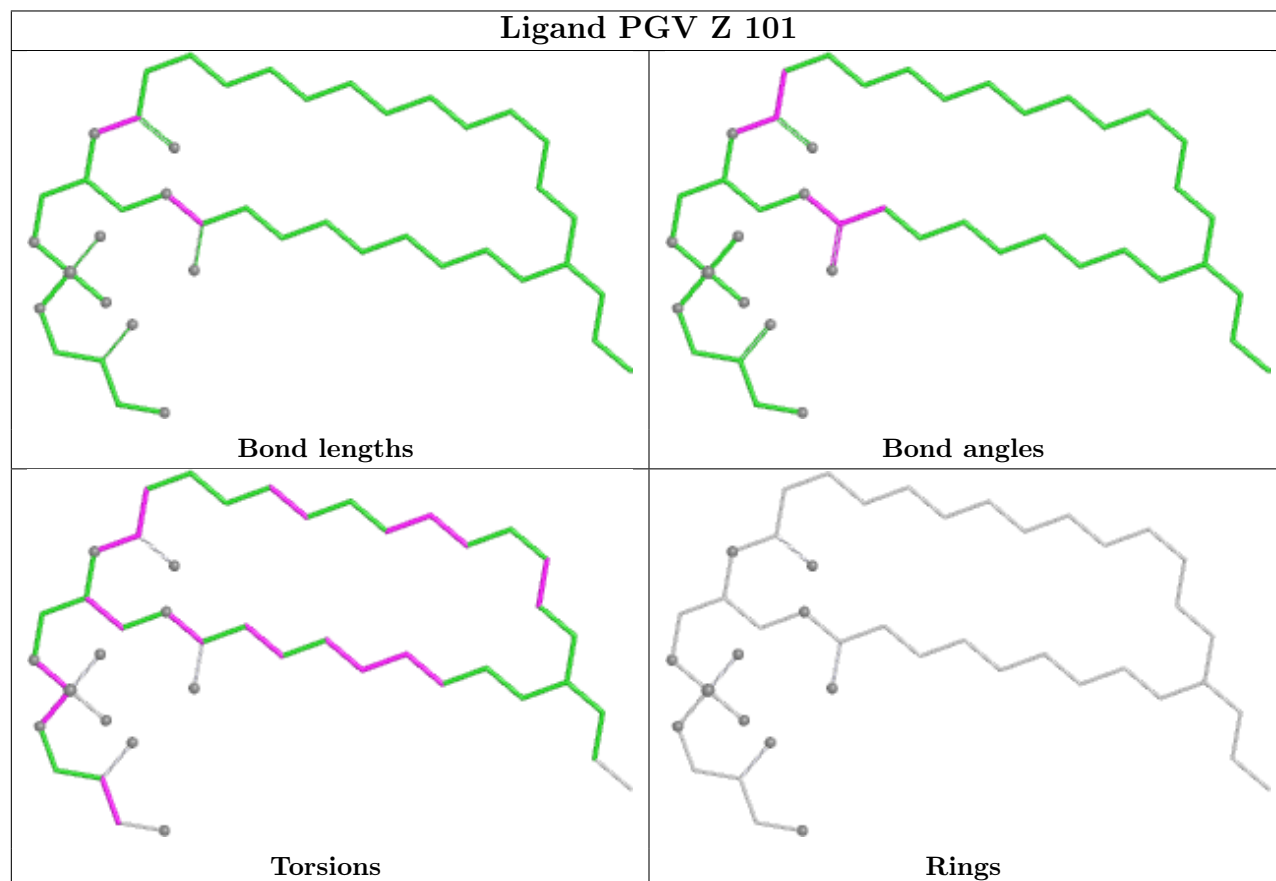
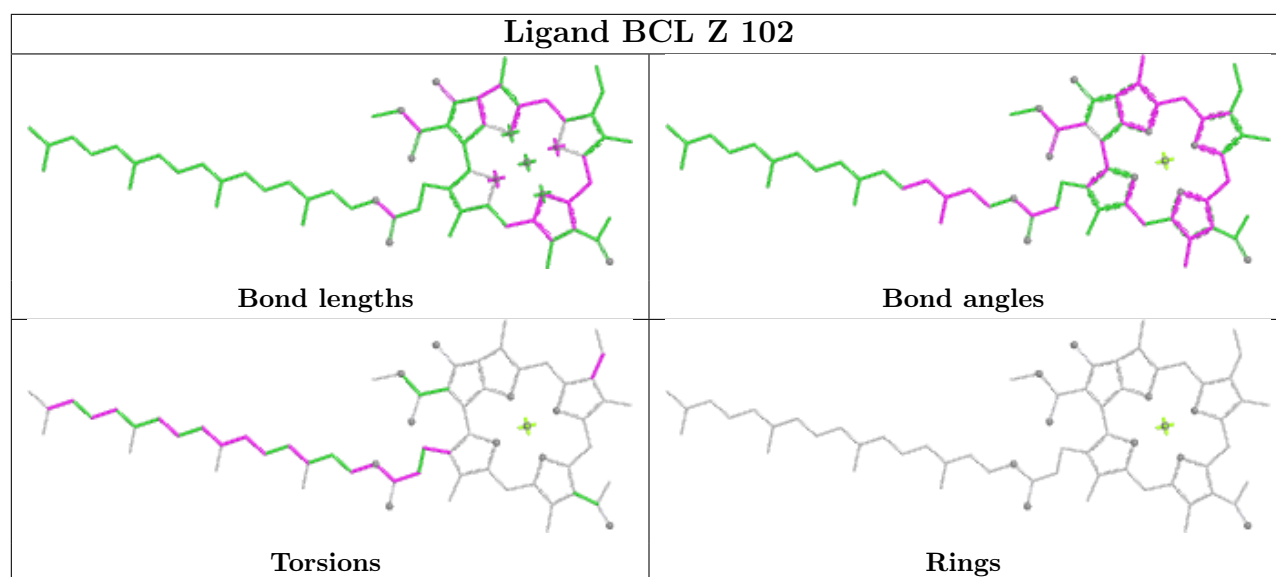


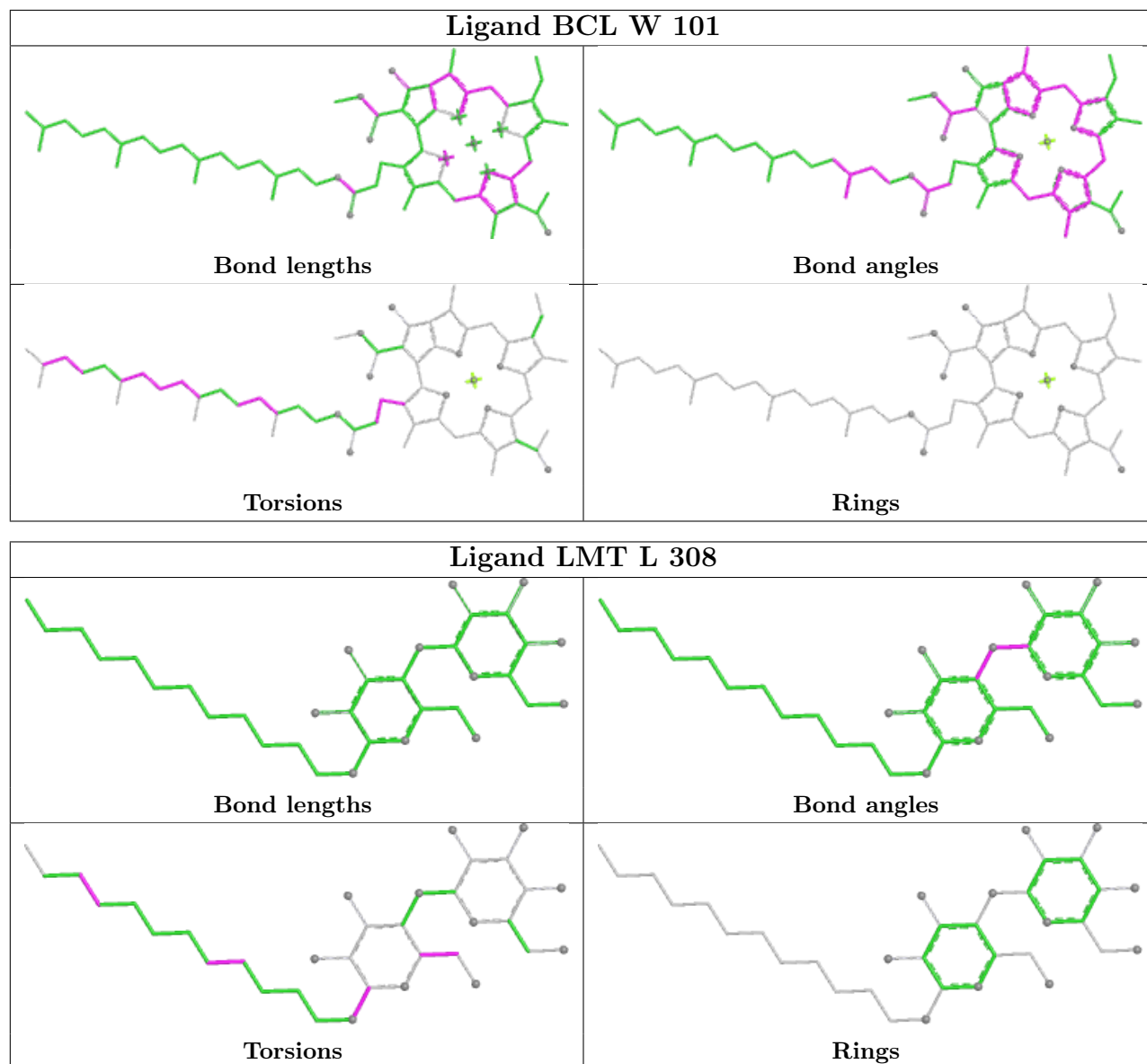


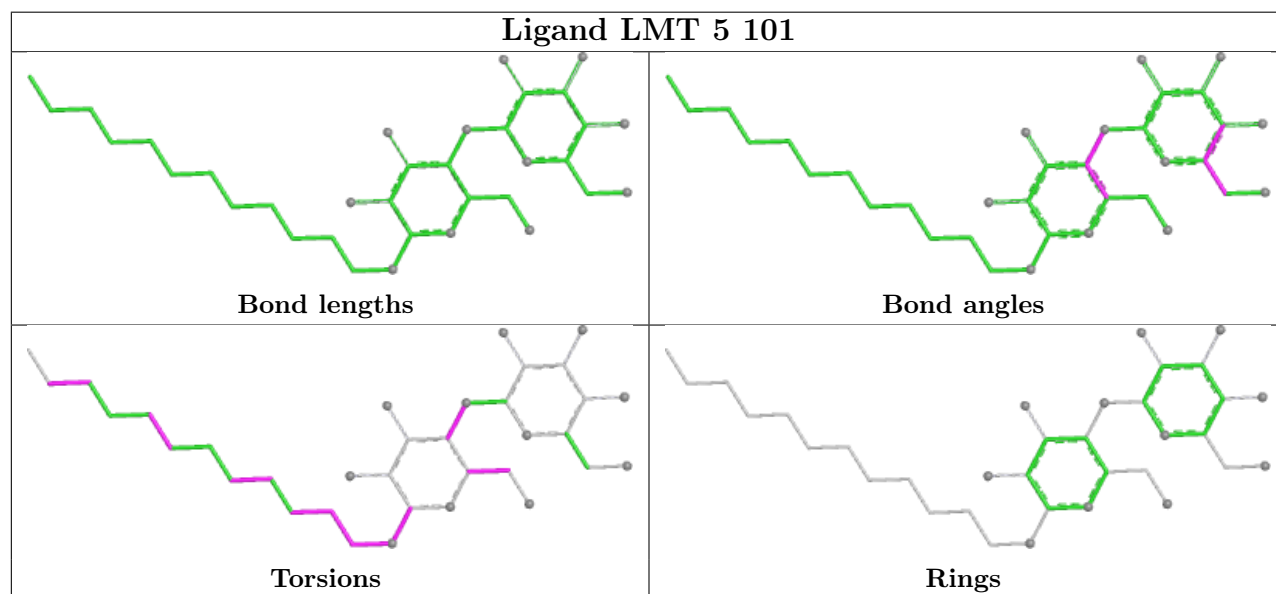
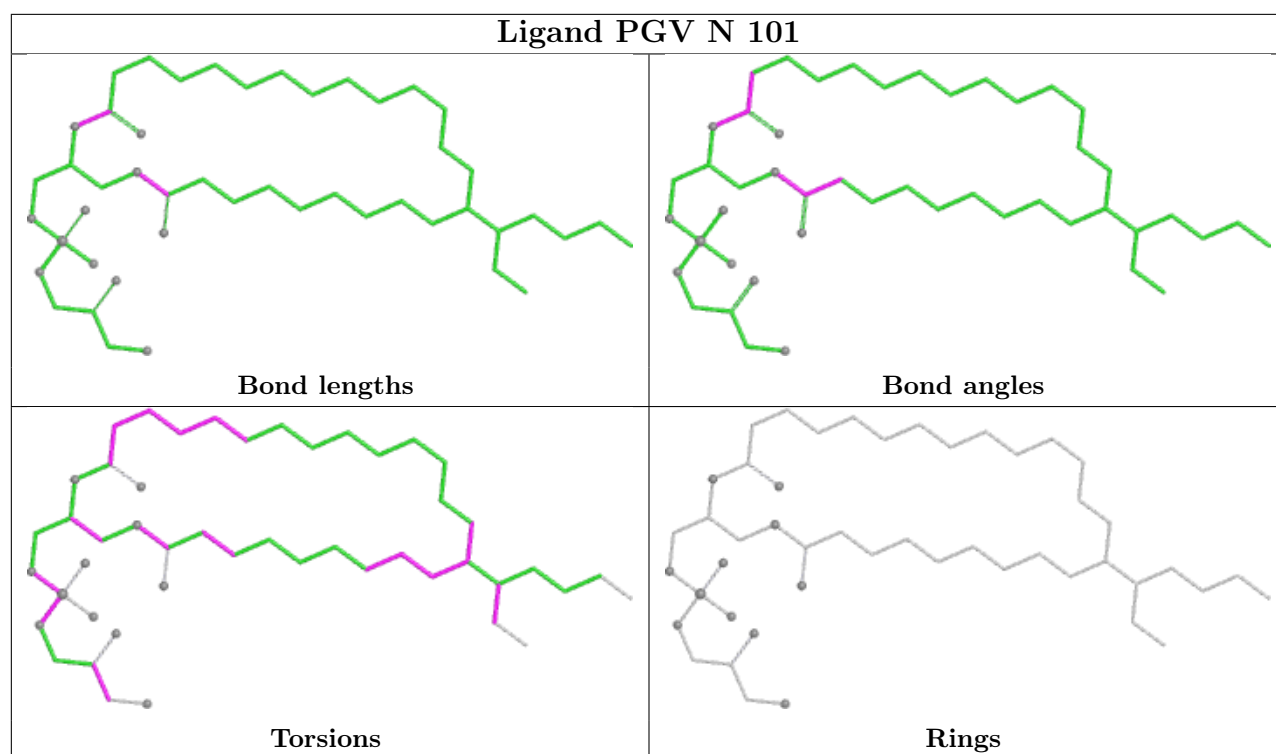


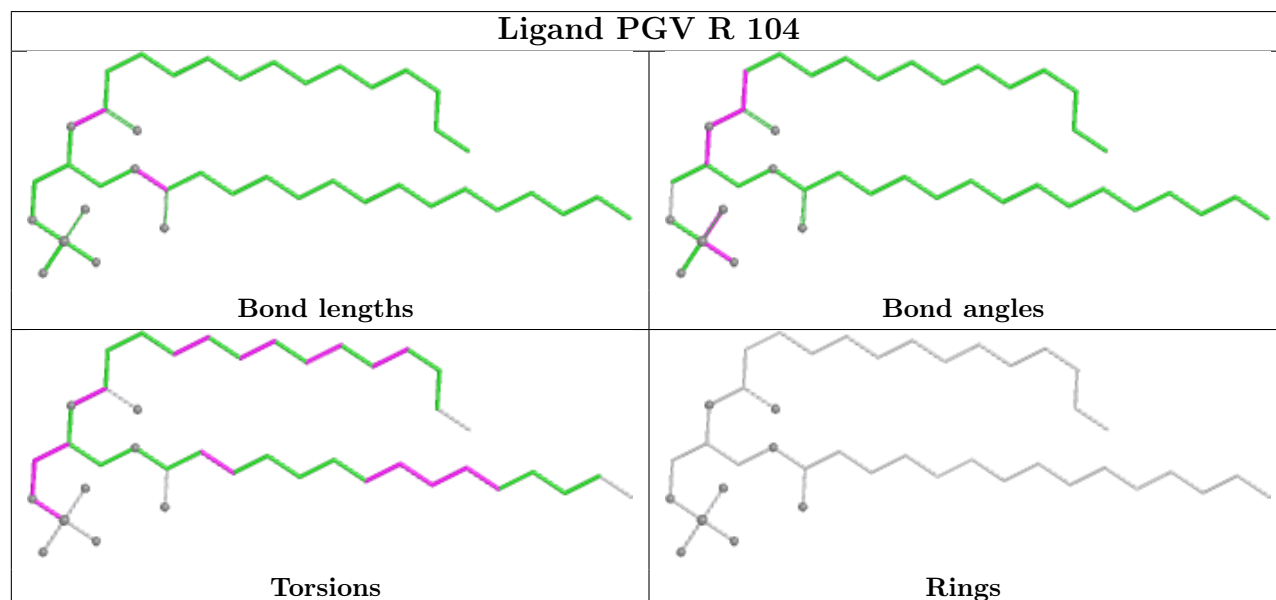
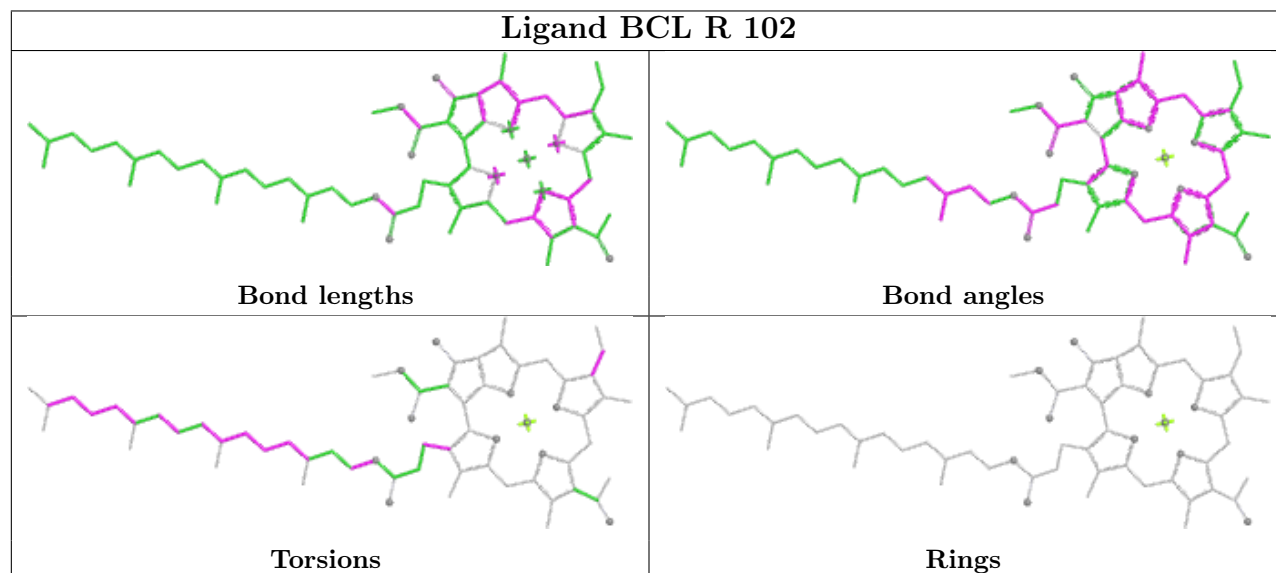
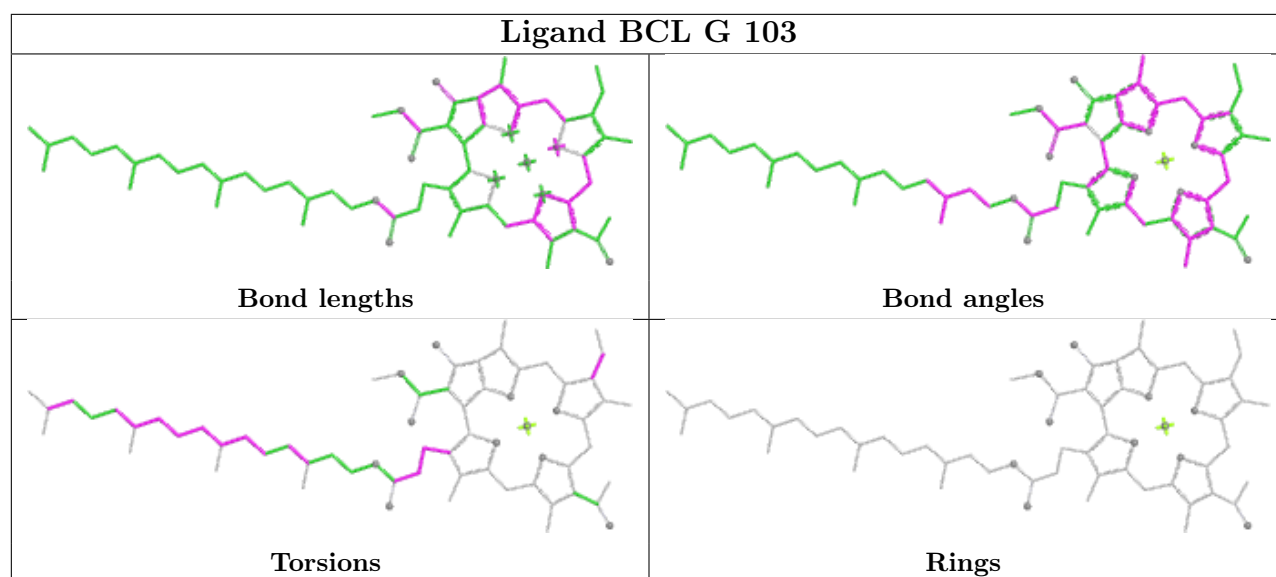


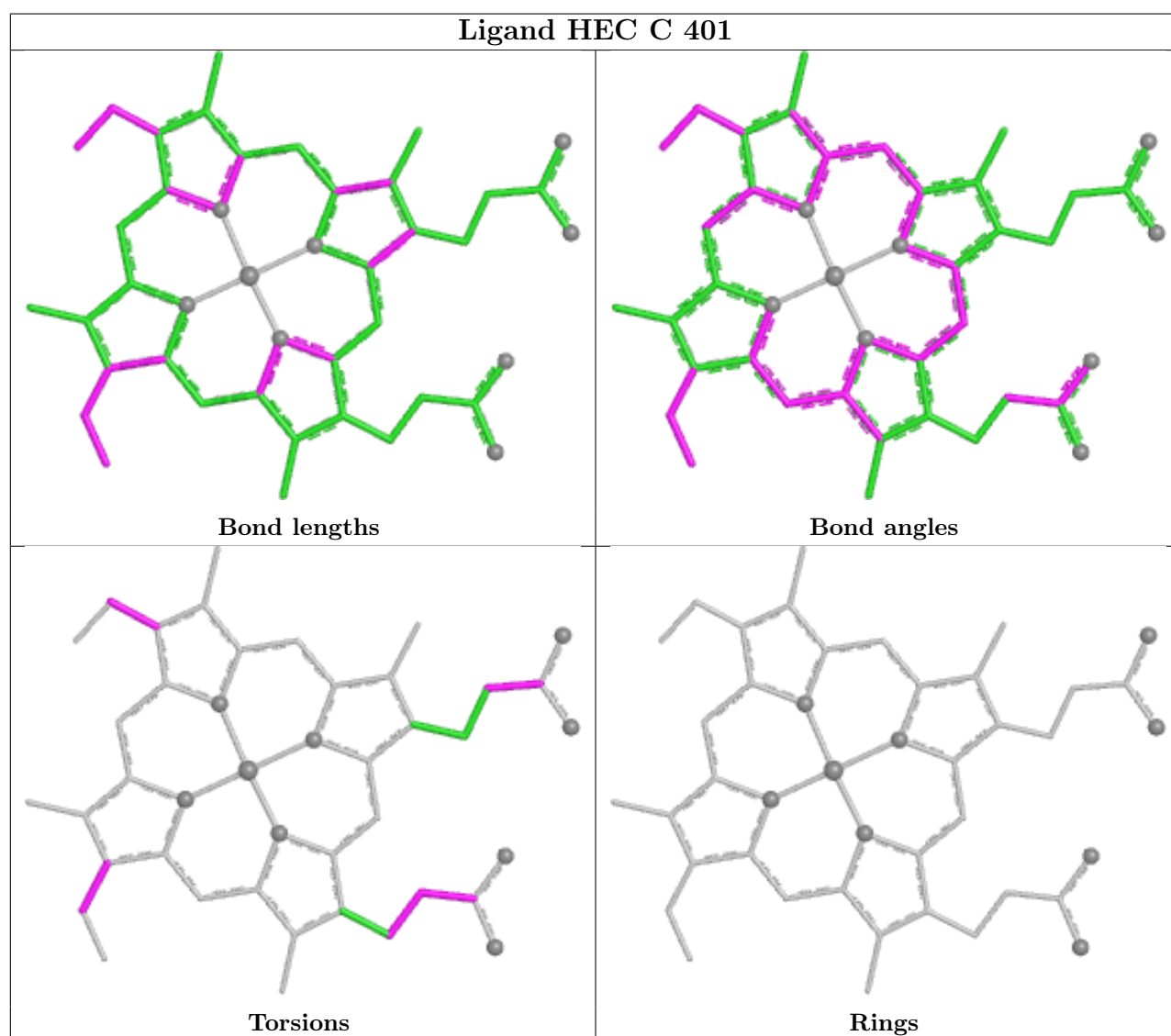
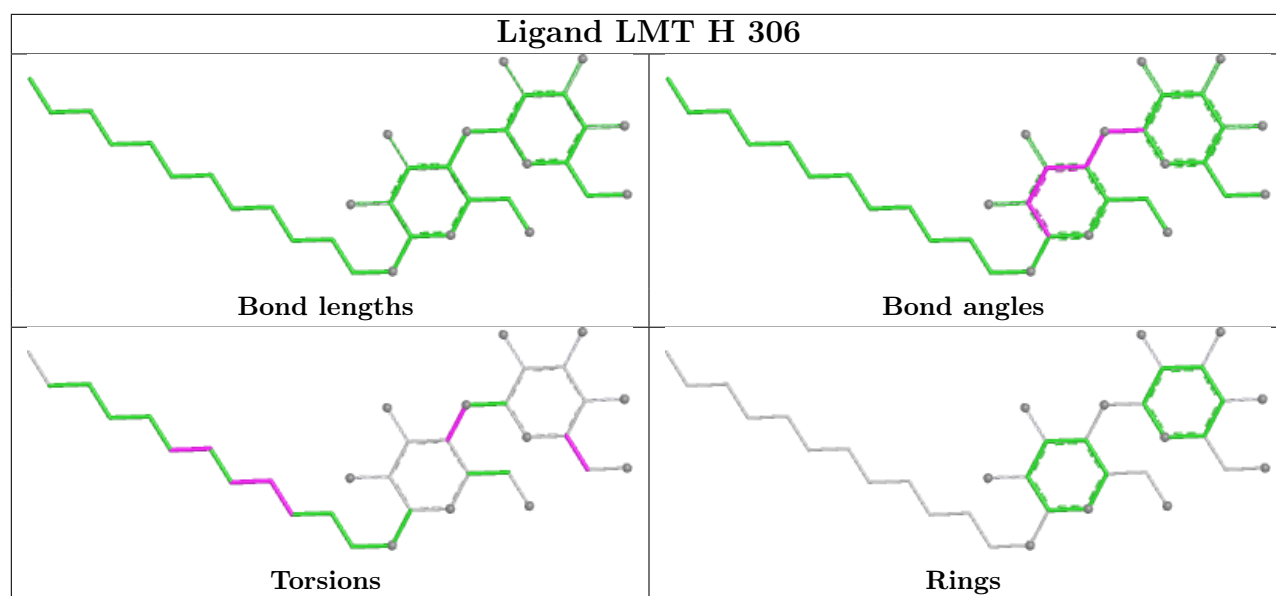


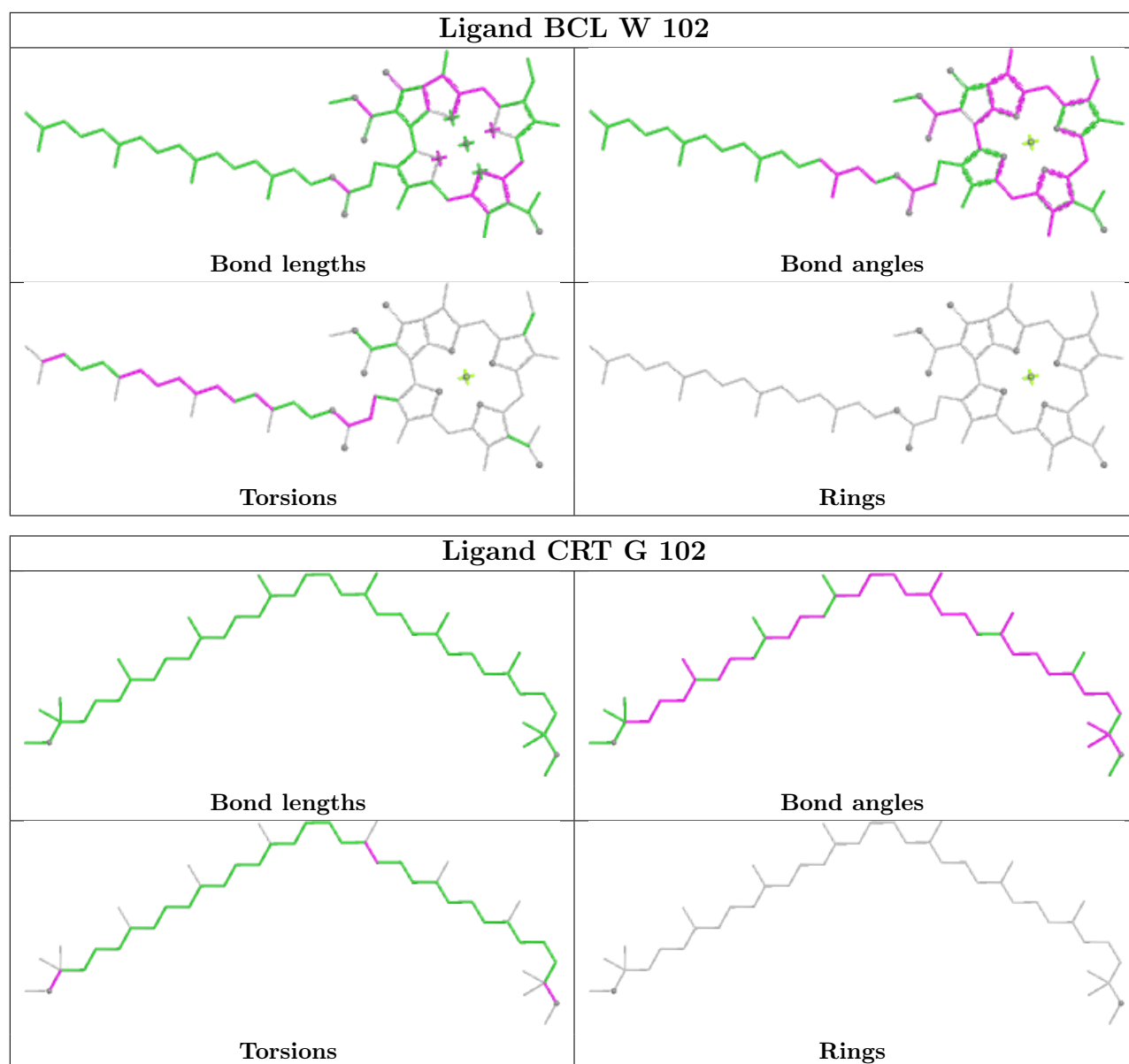




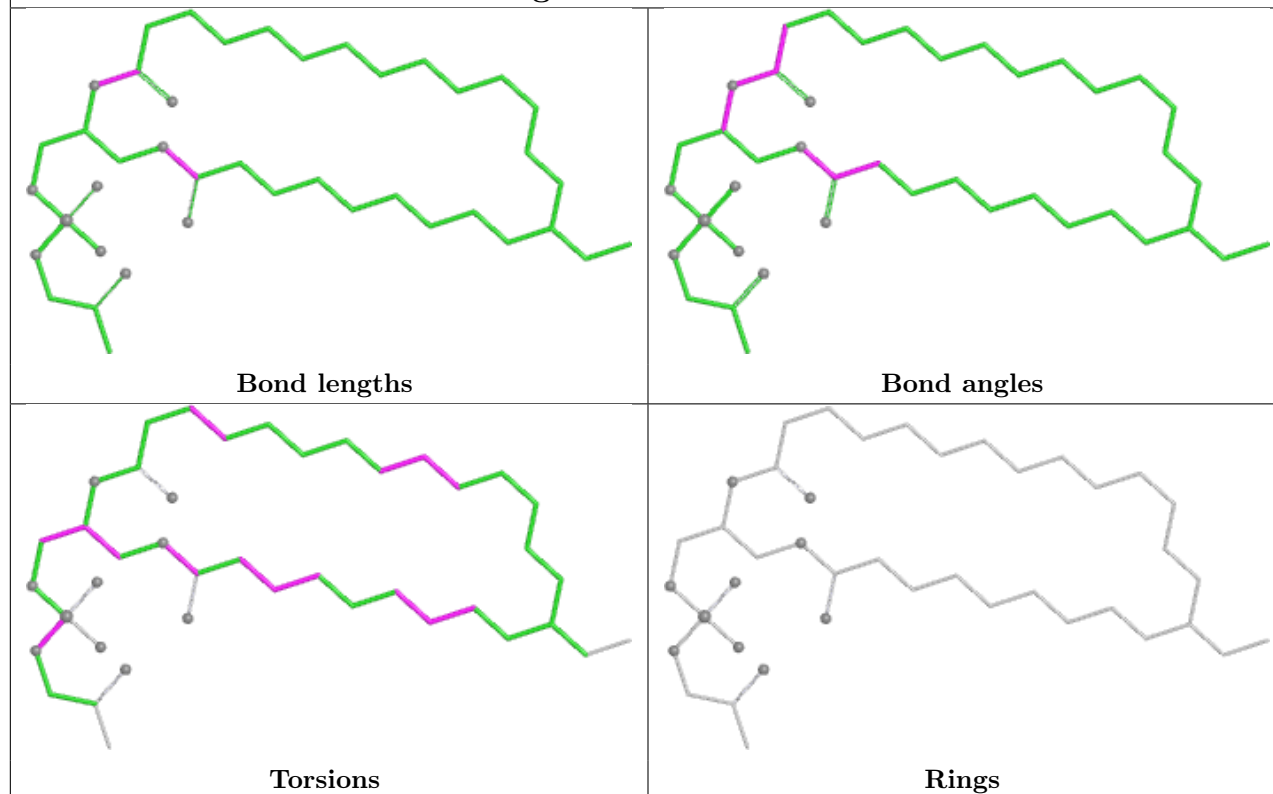




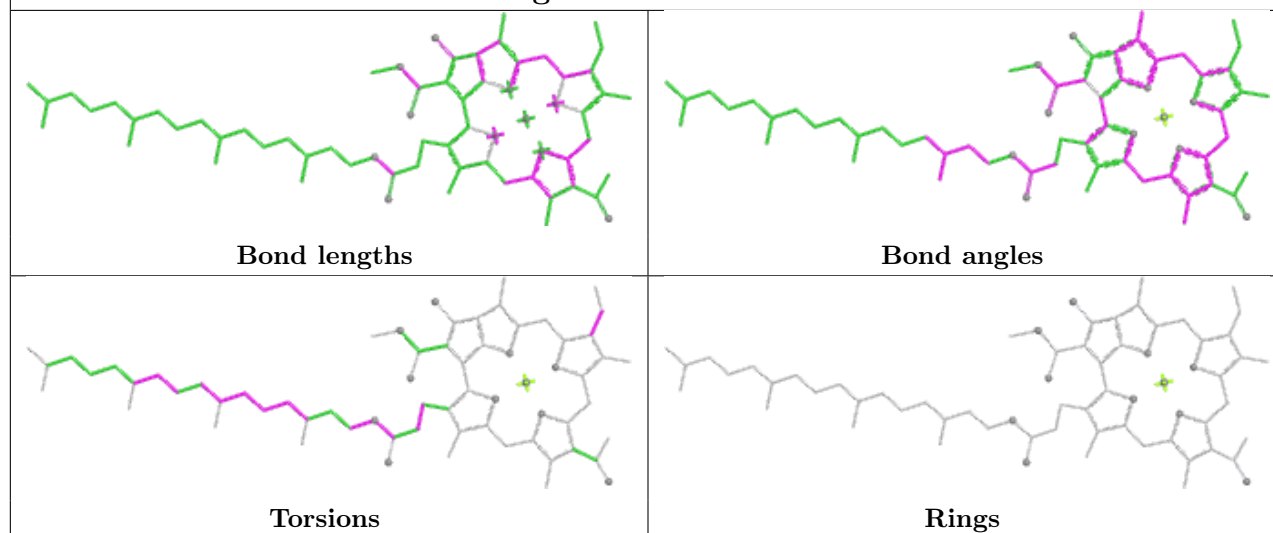


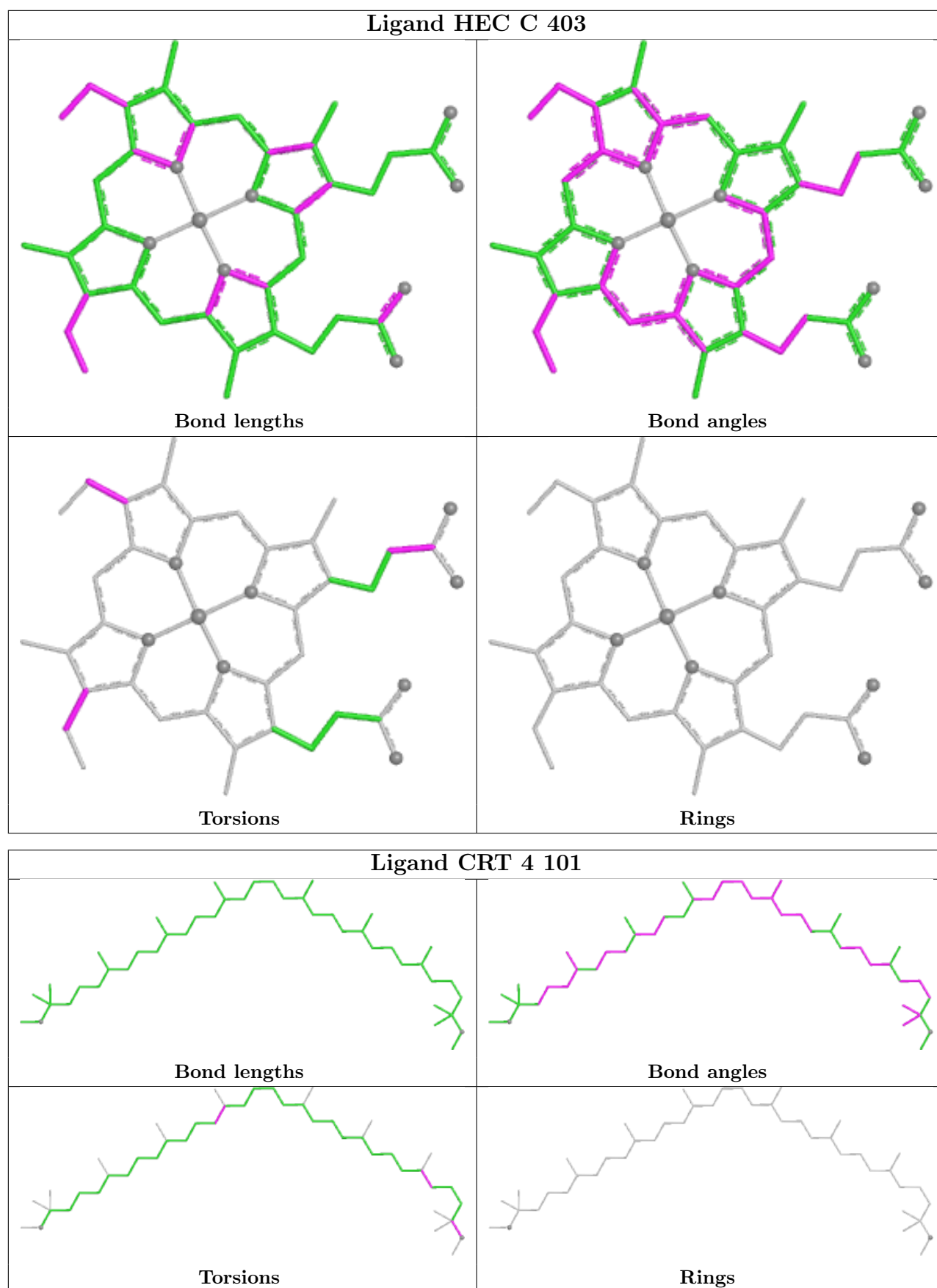


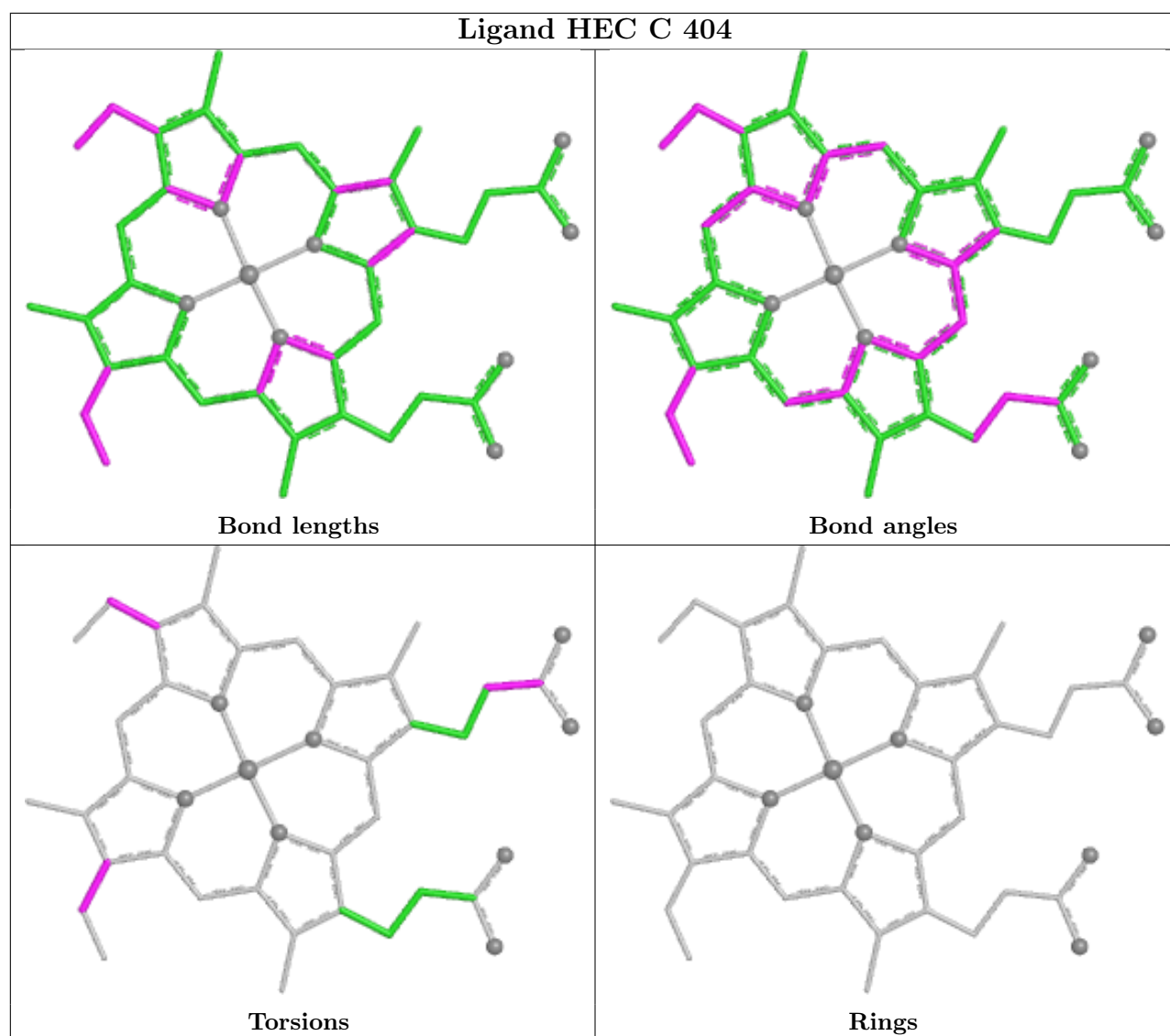
Ligand PGV 6 103

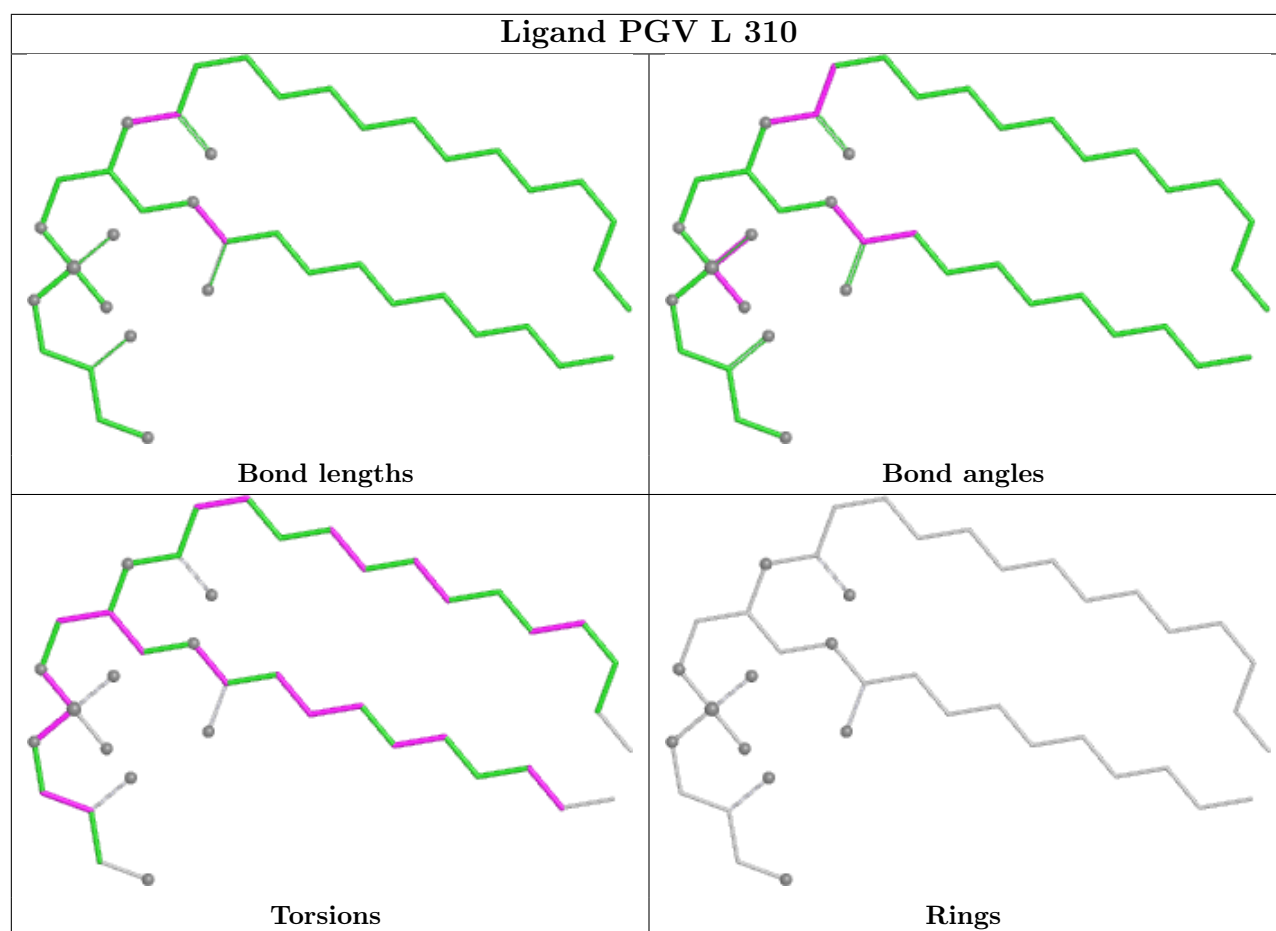


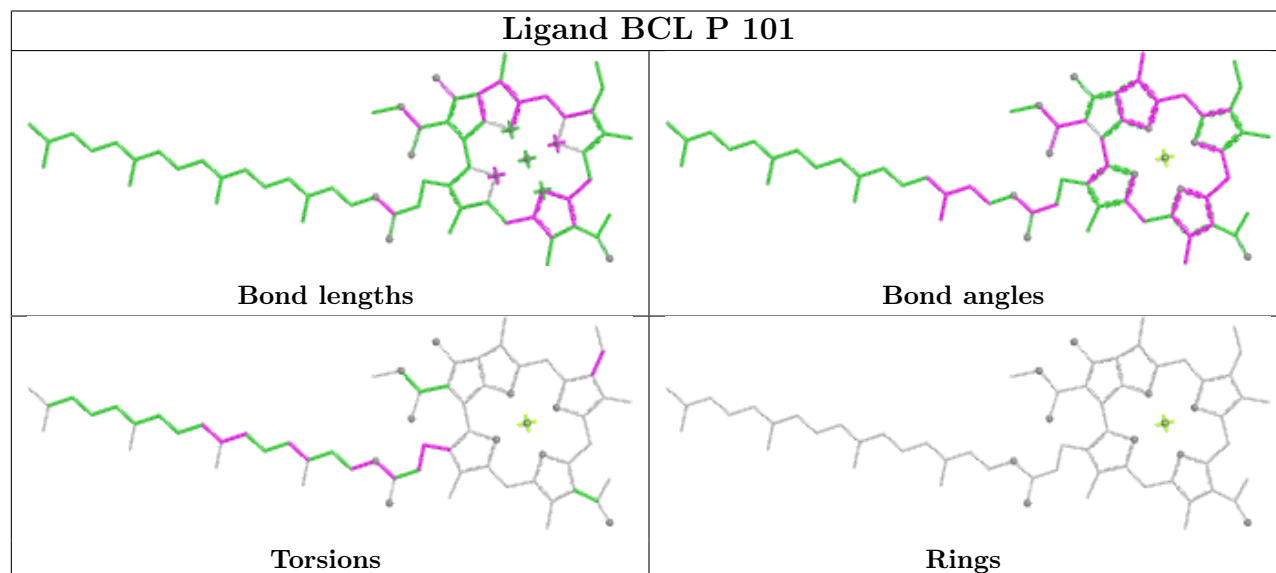
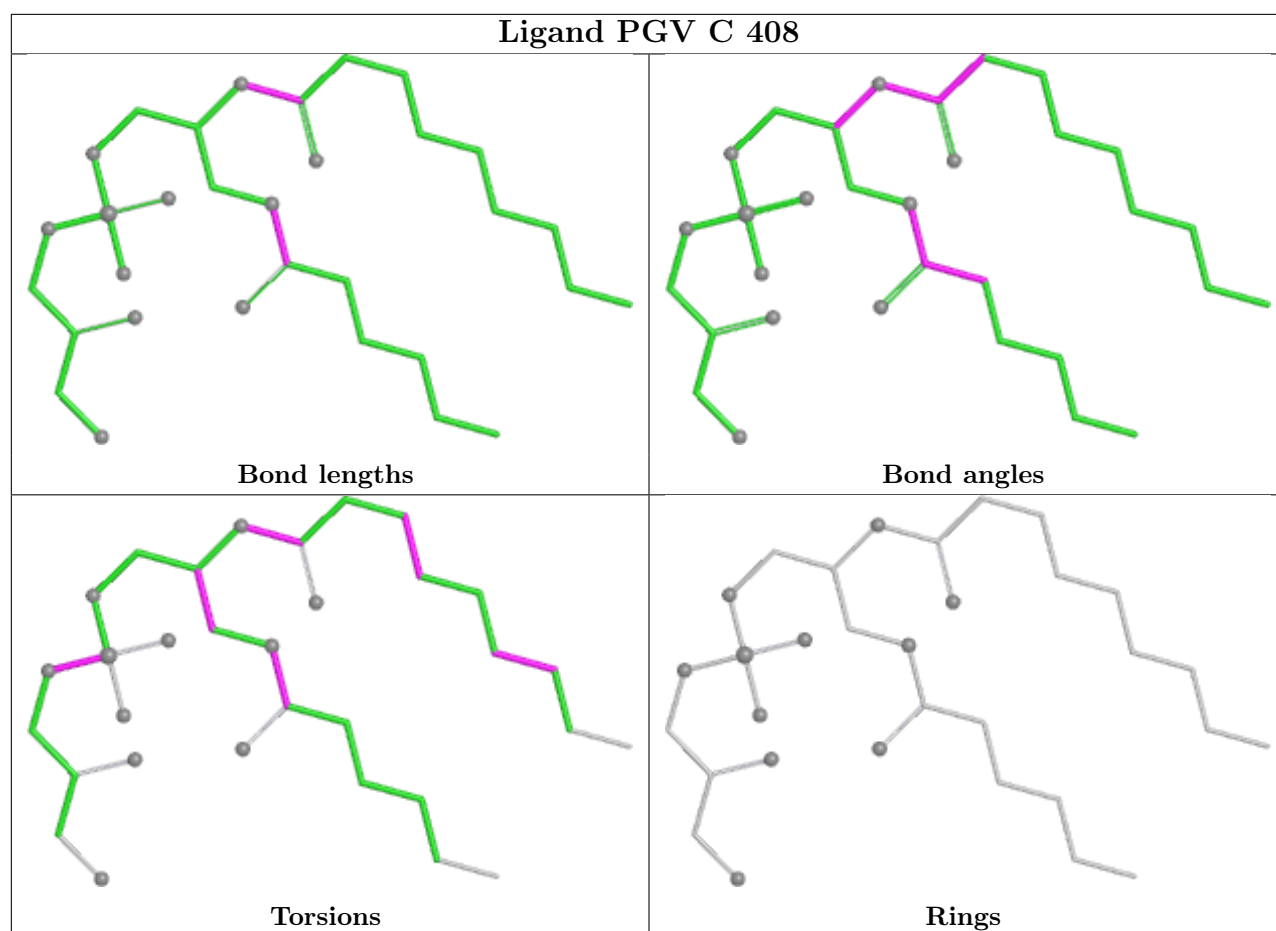
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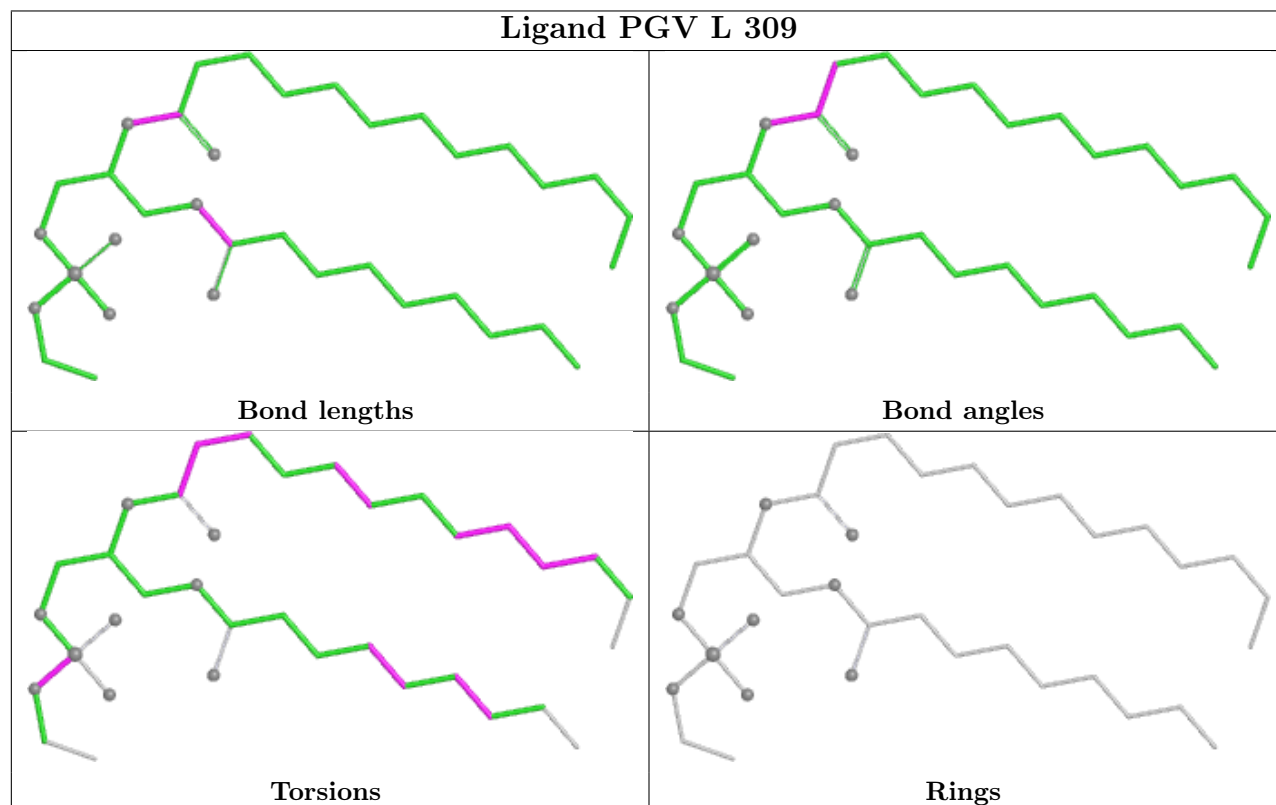
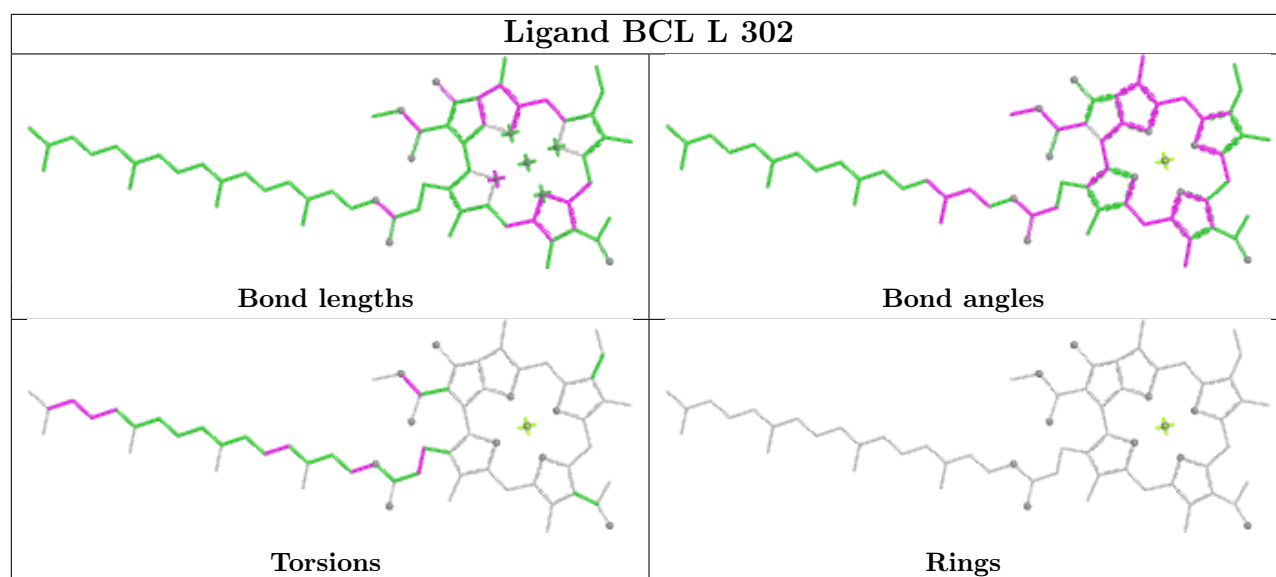


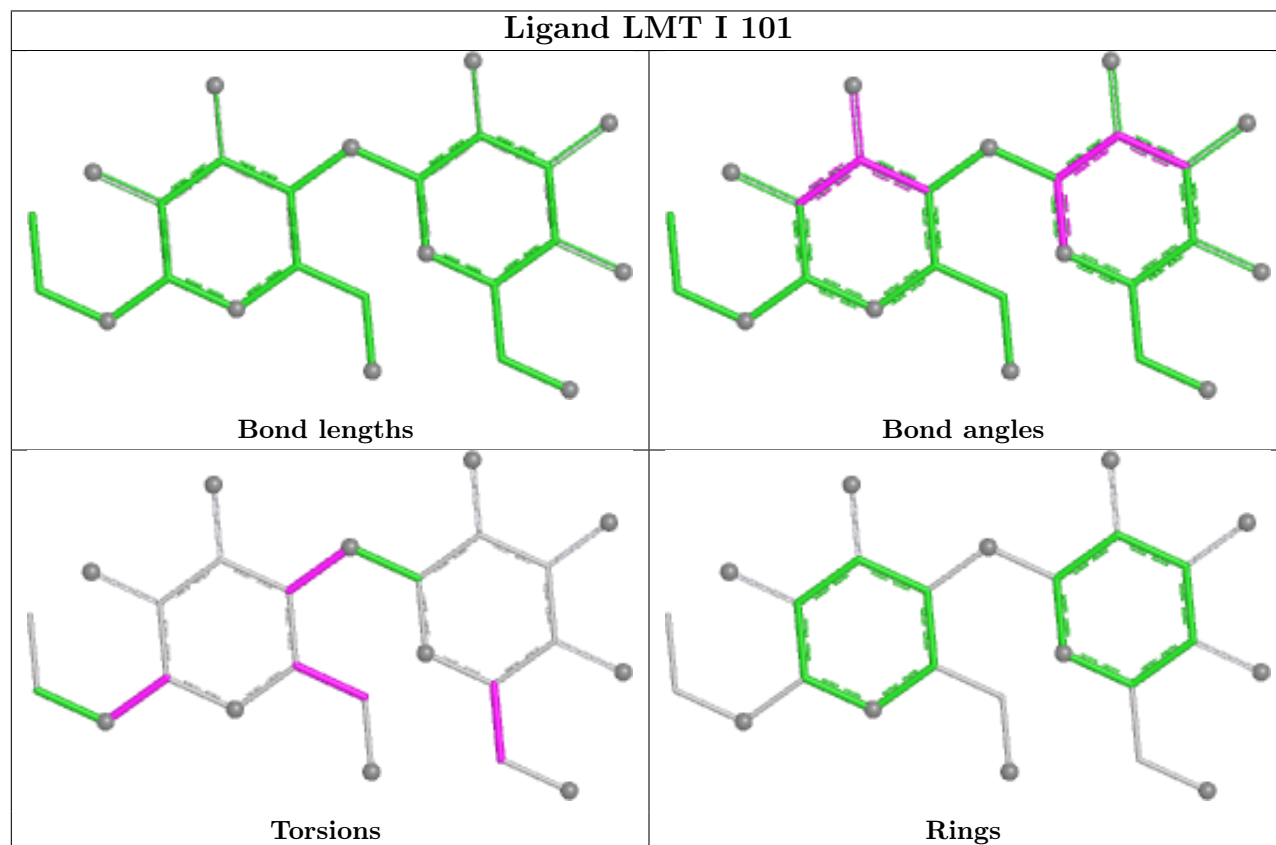
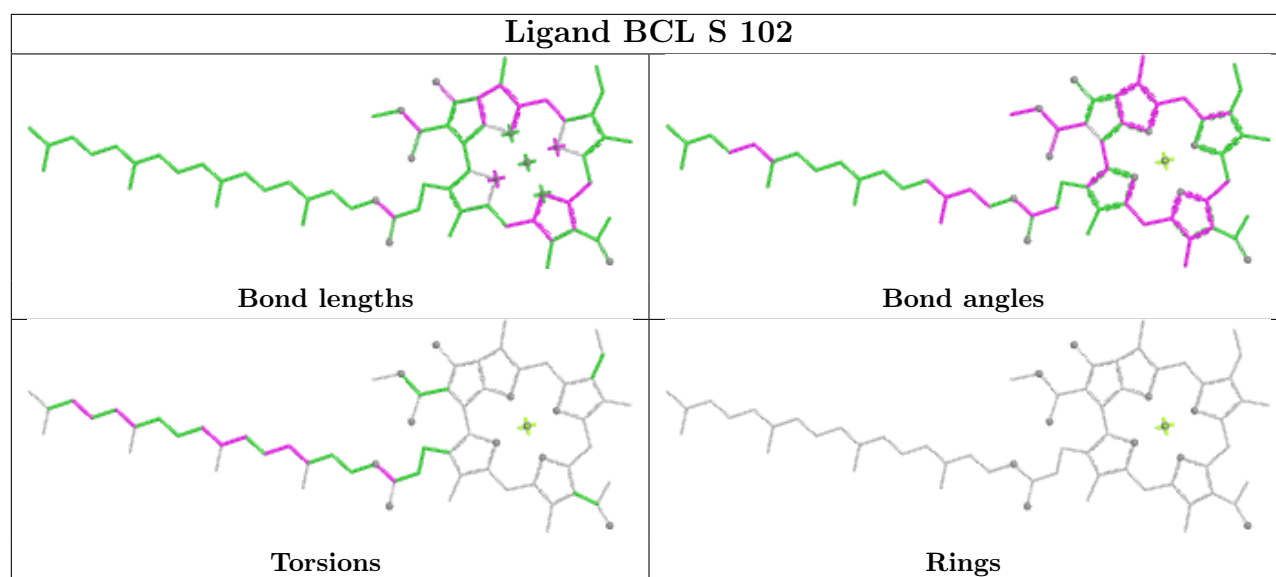


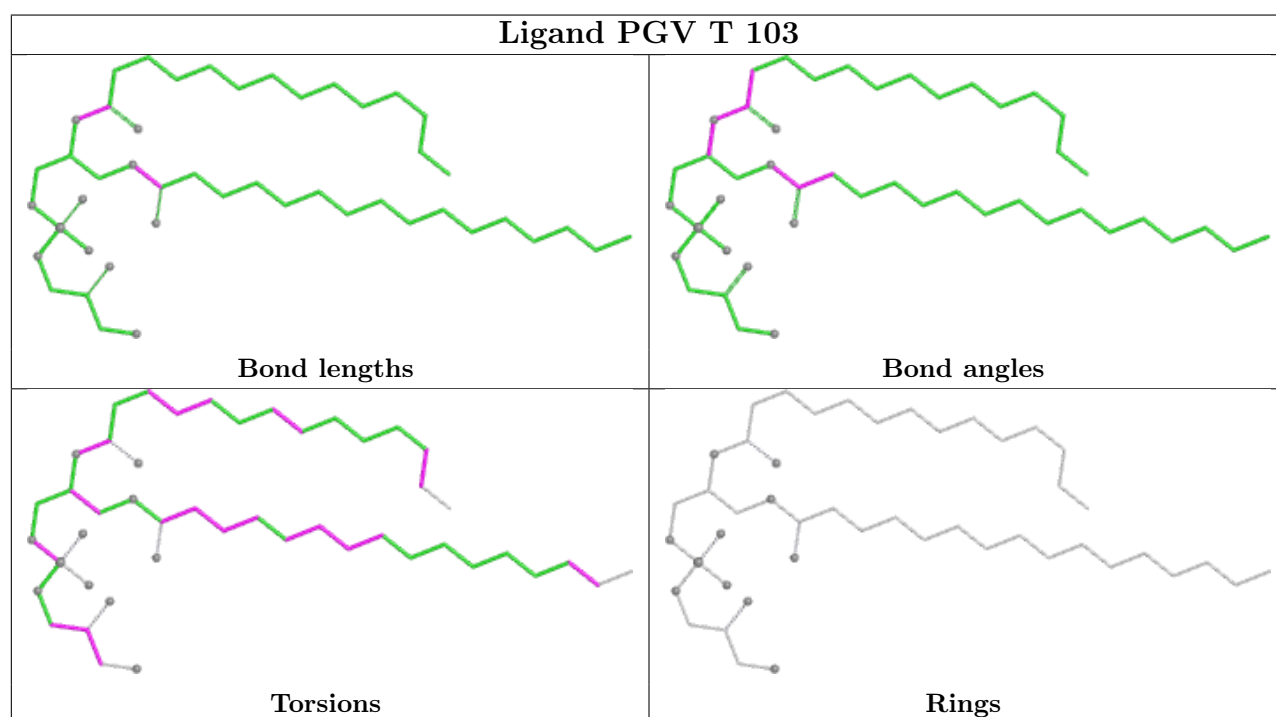
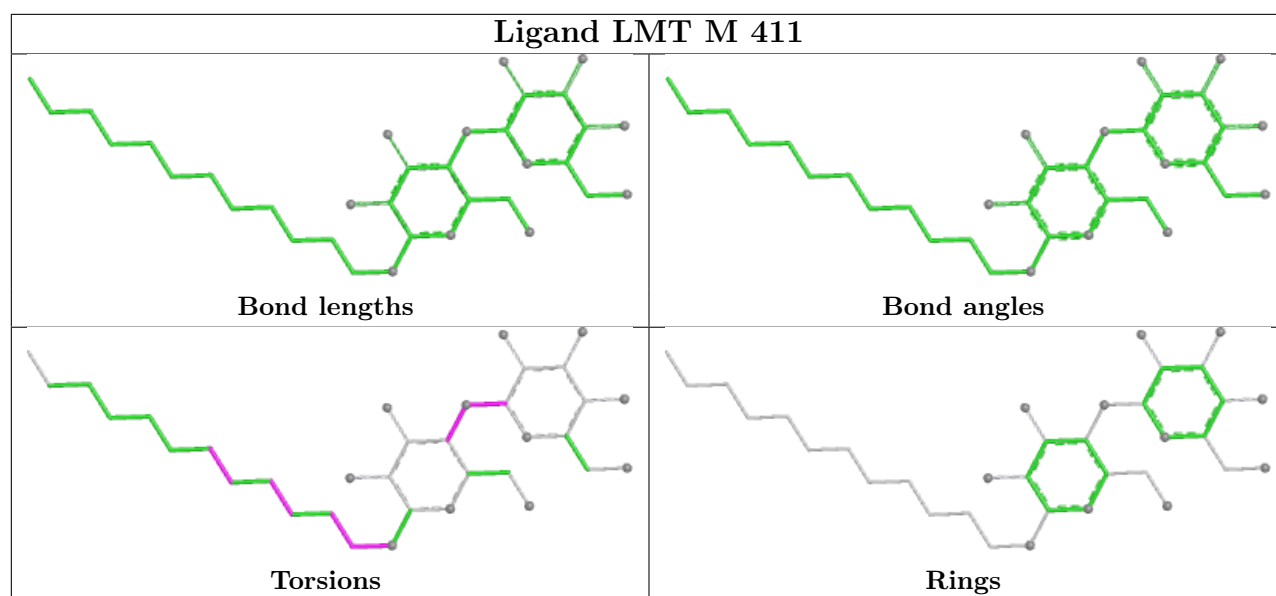


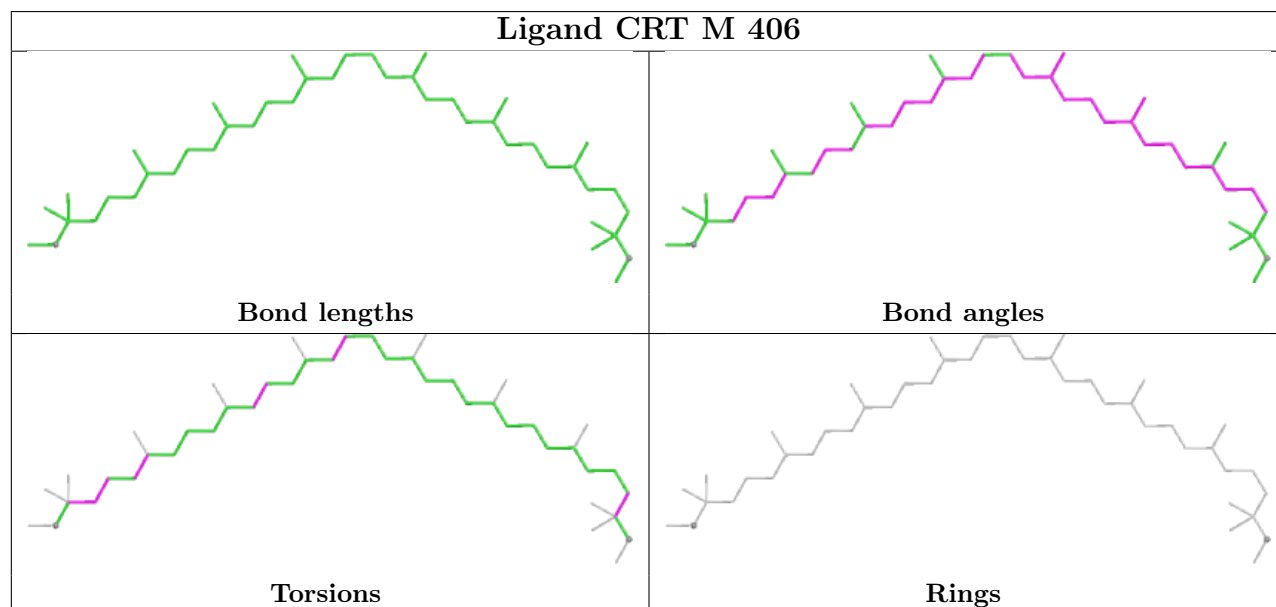
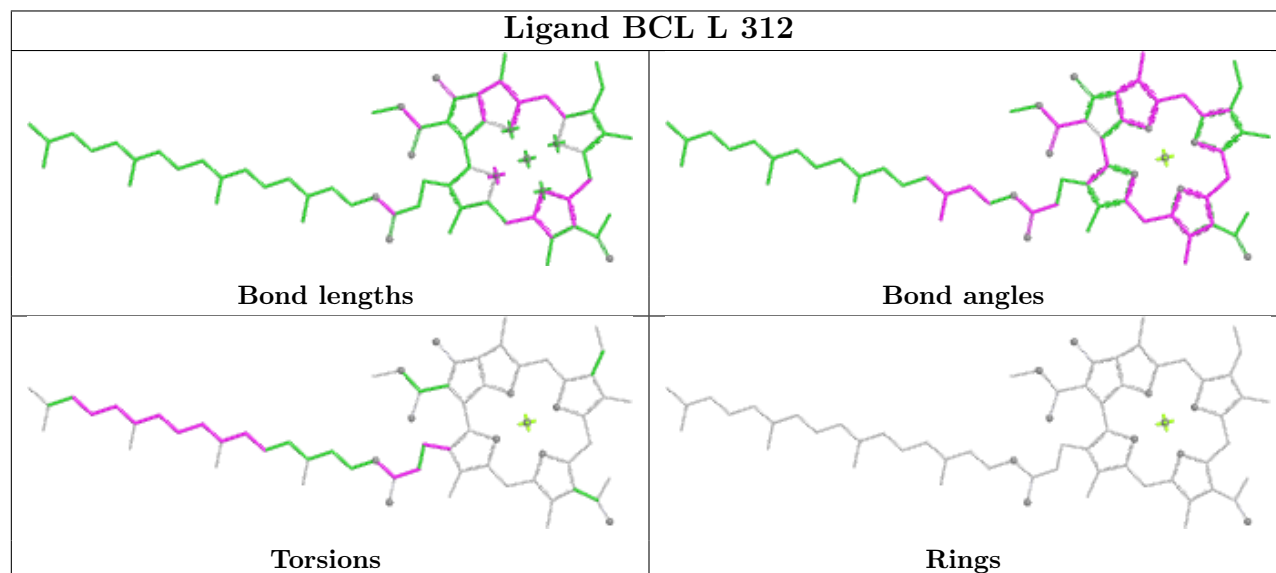
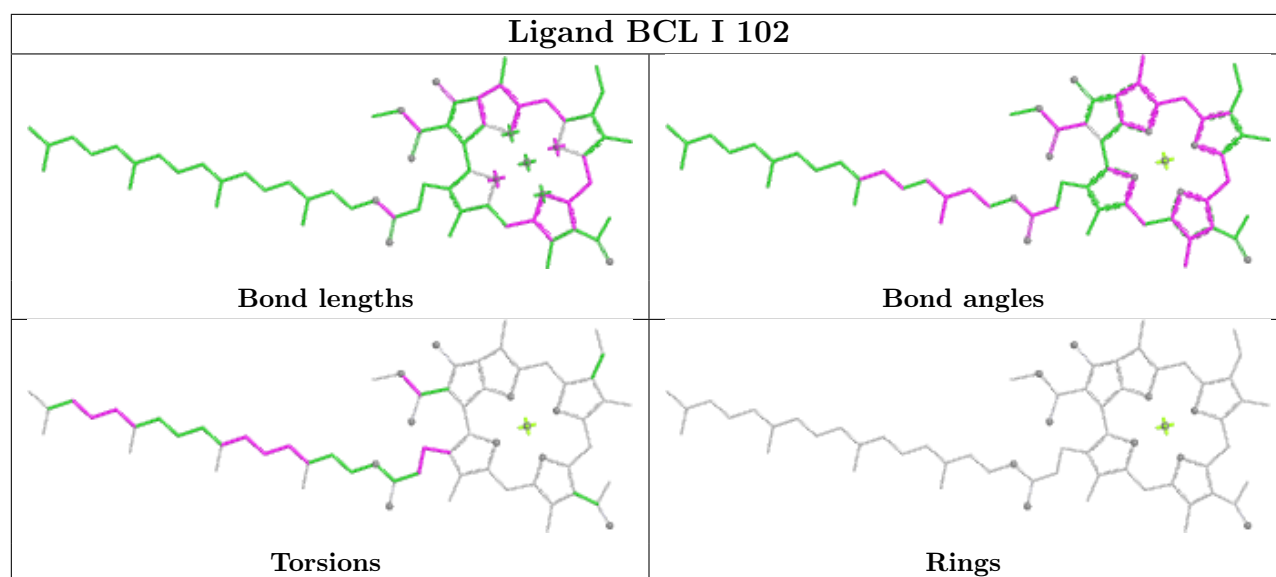


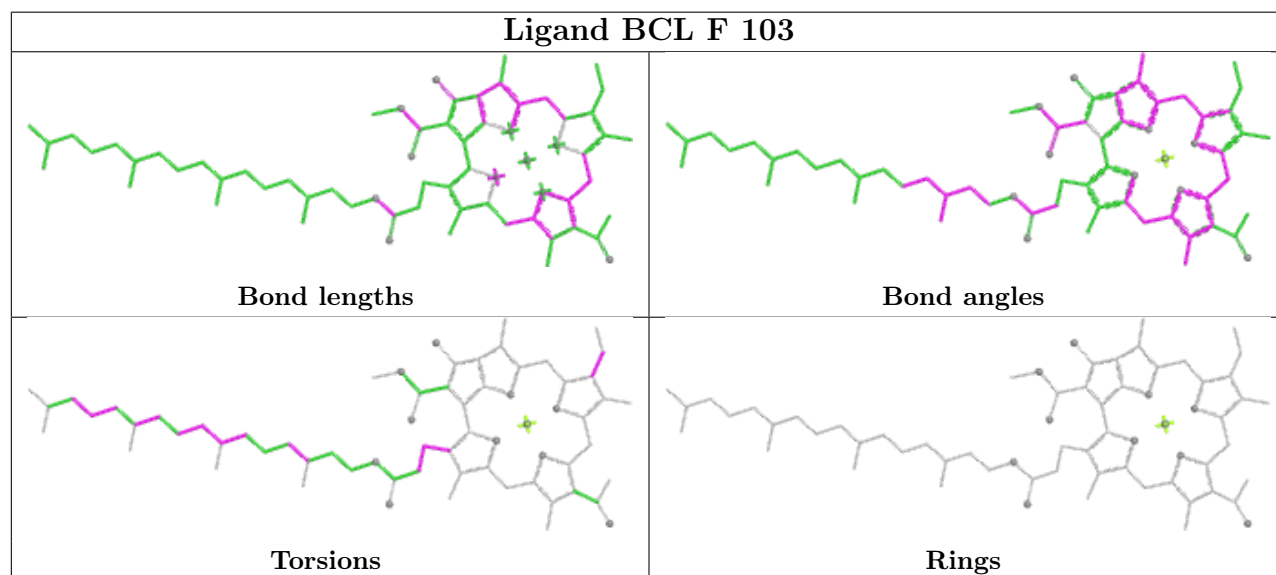
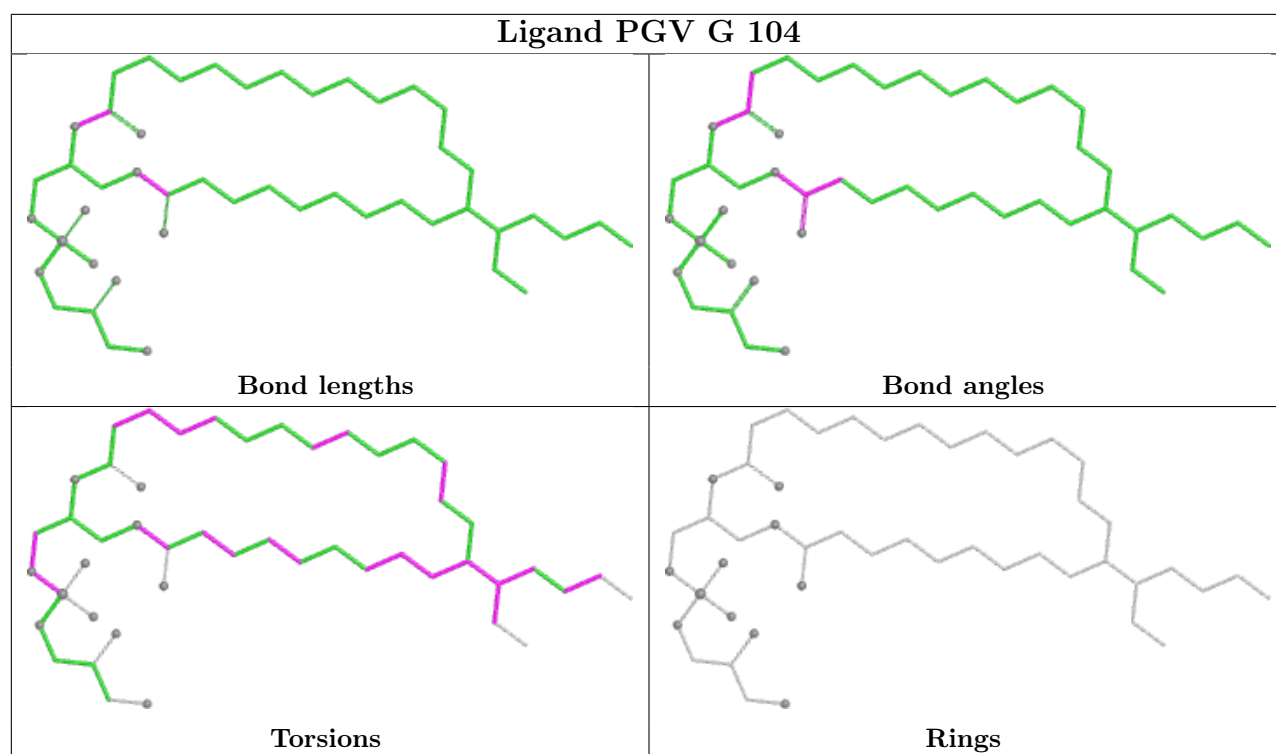


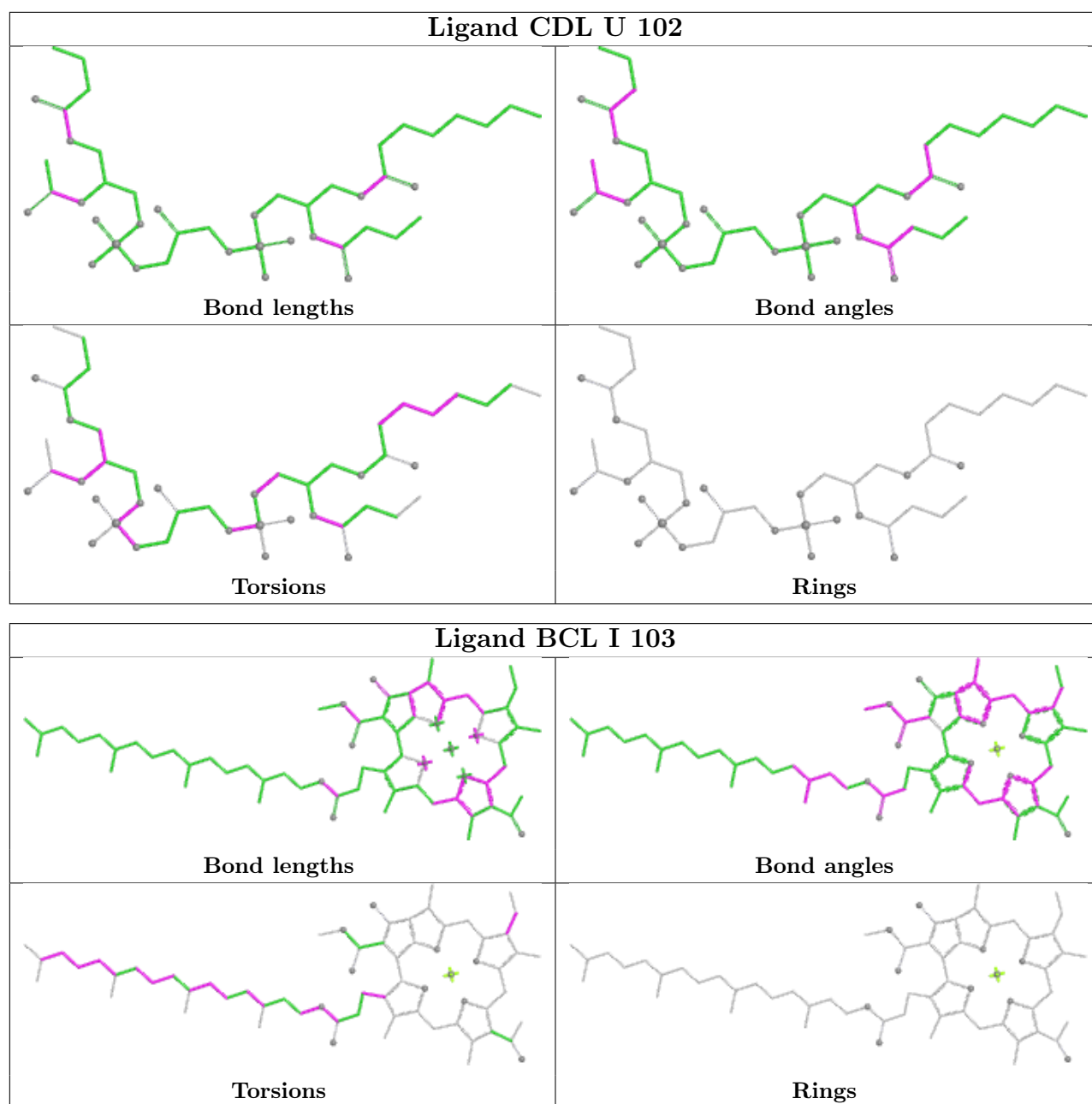


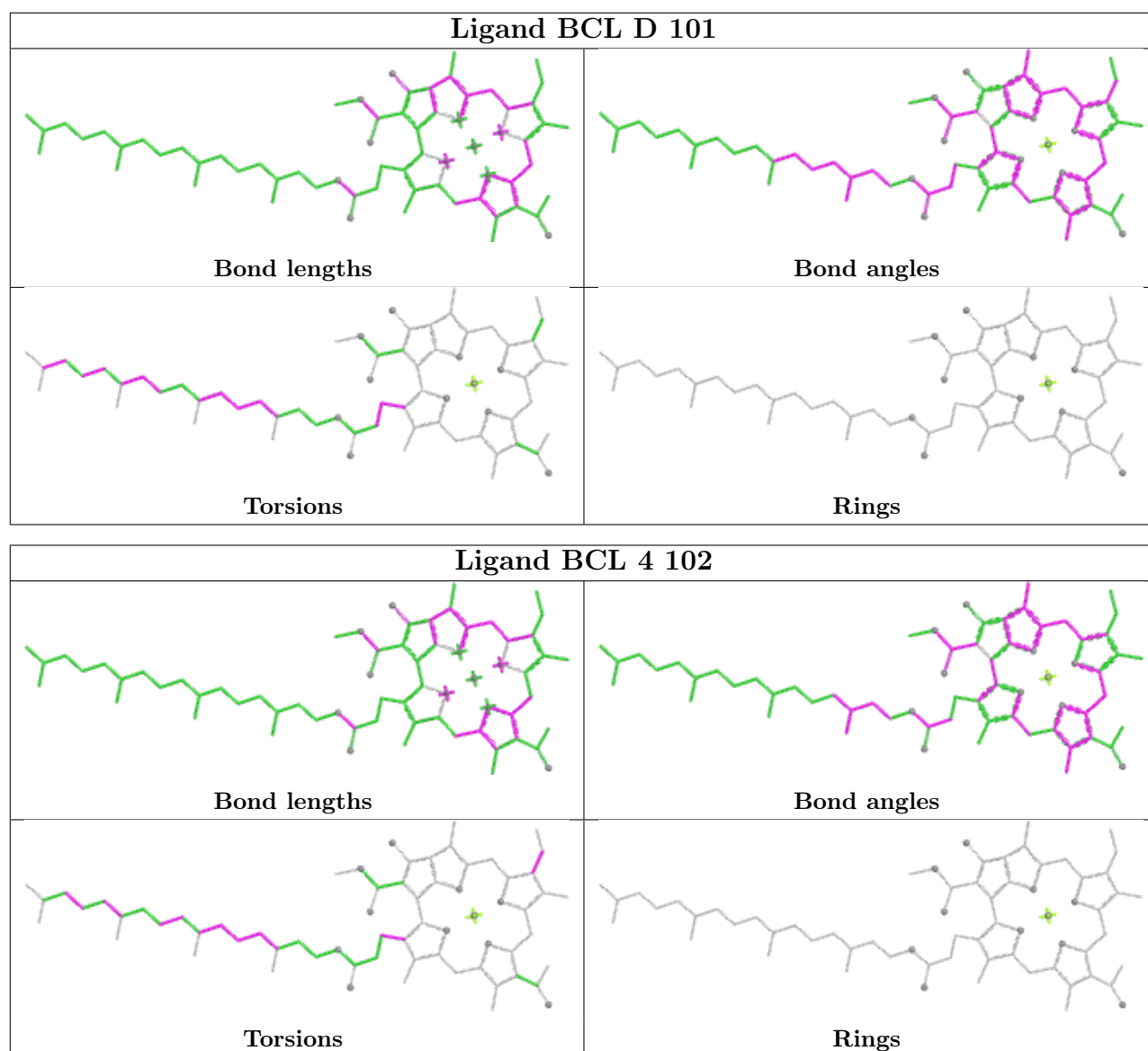




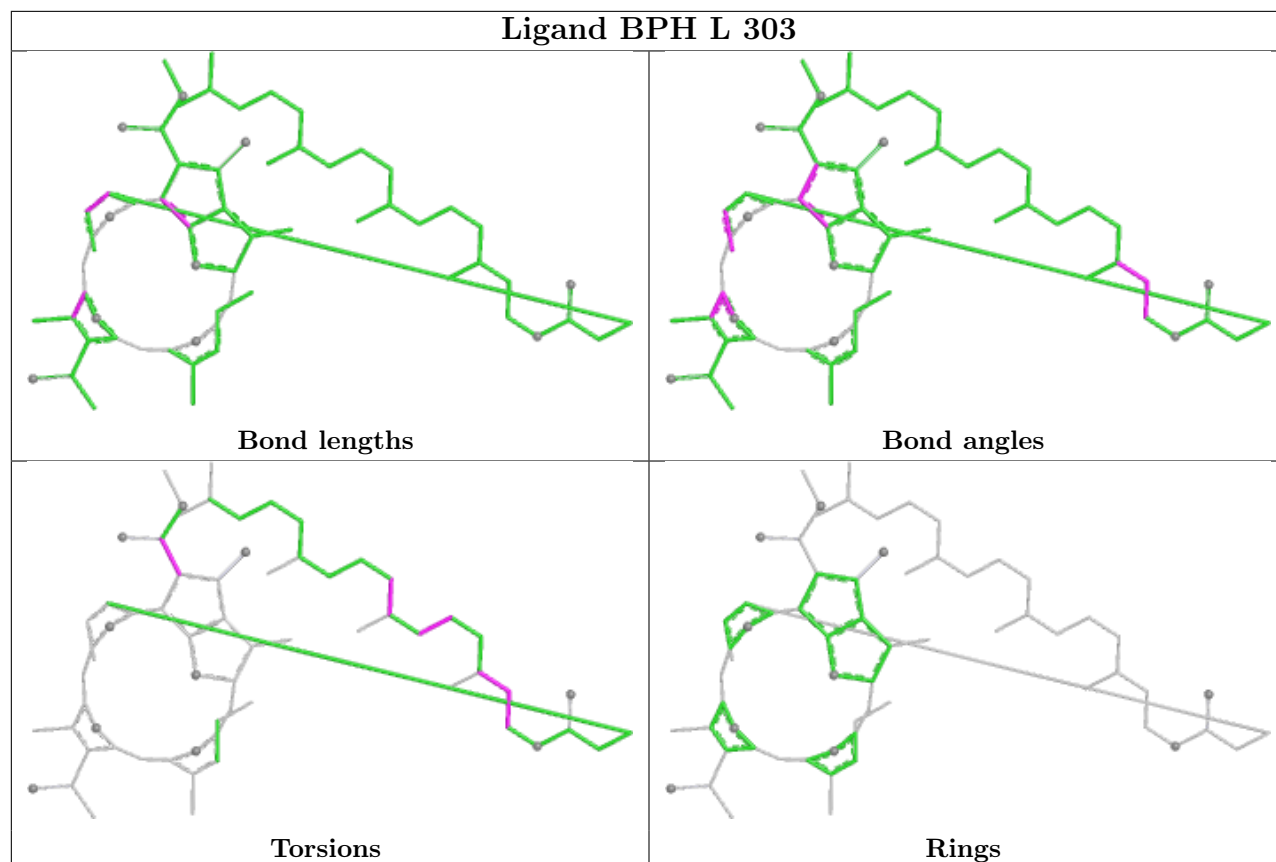




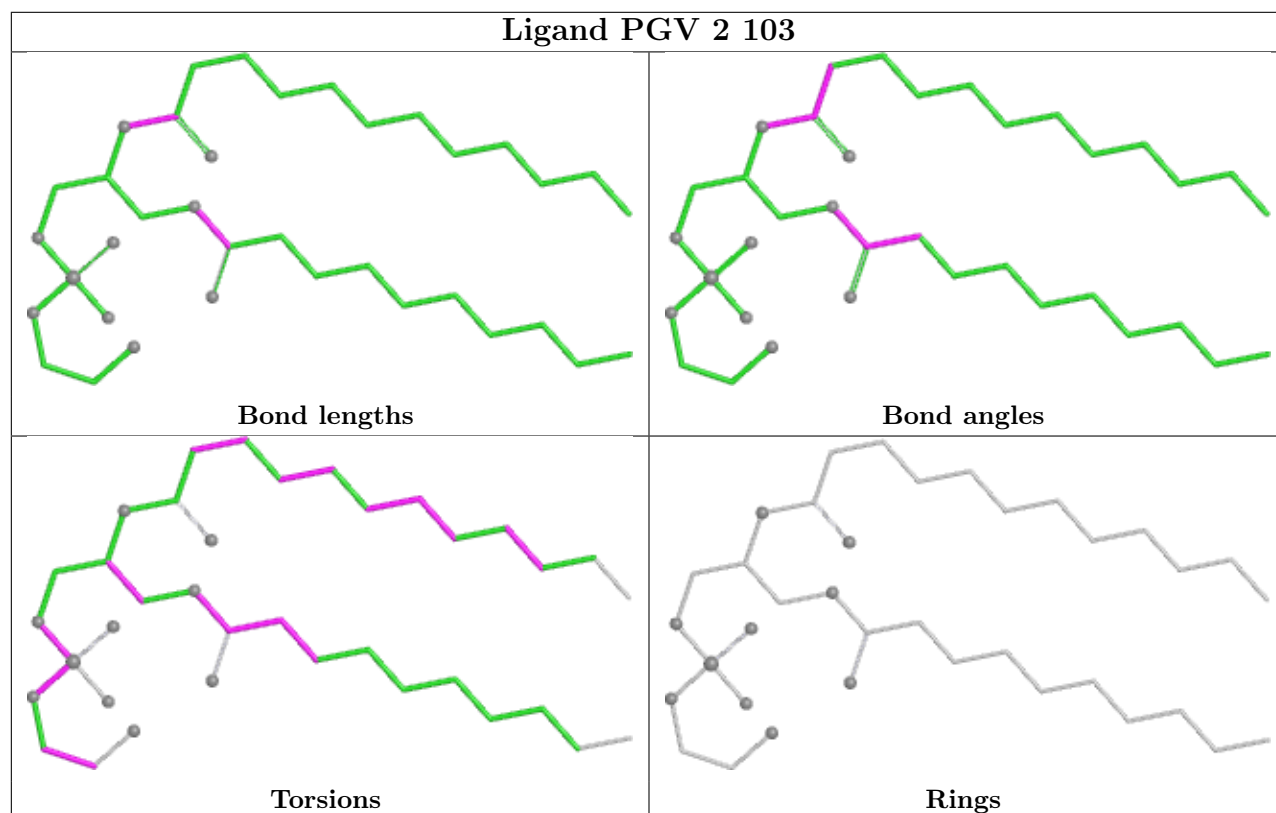


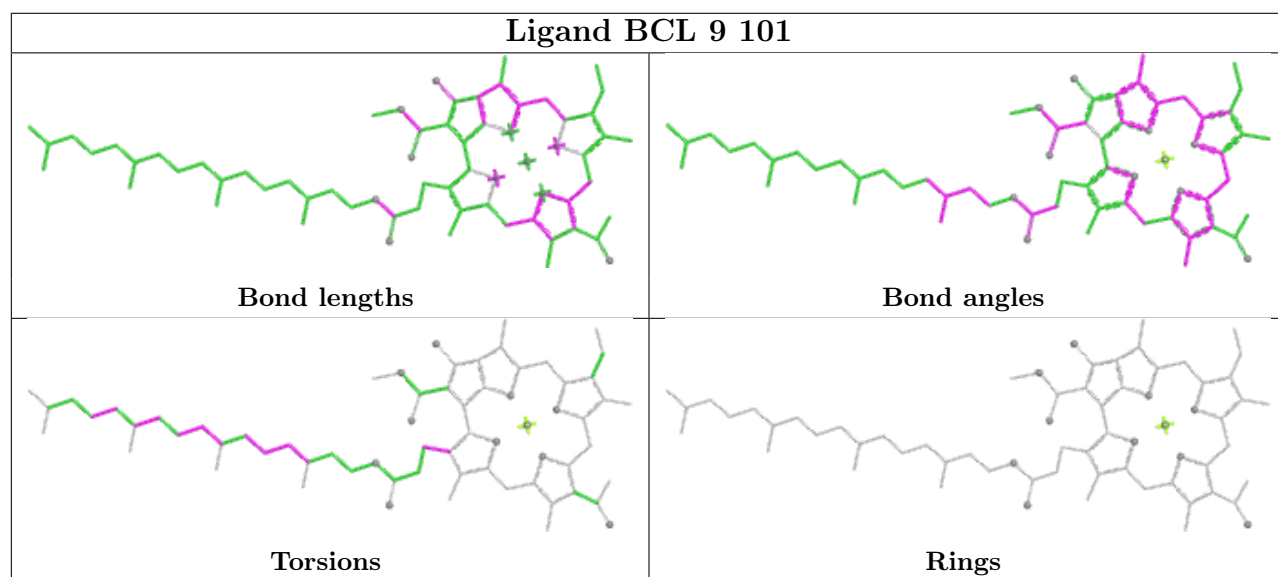
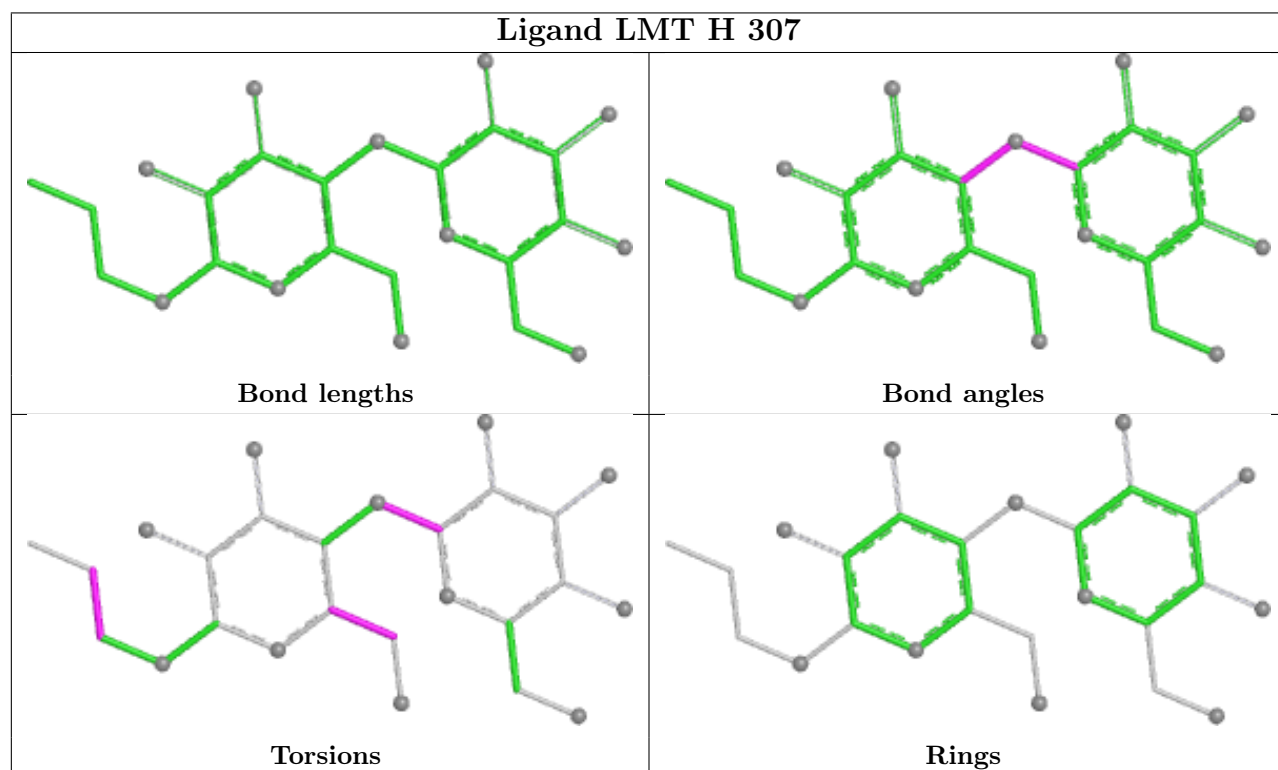
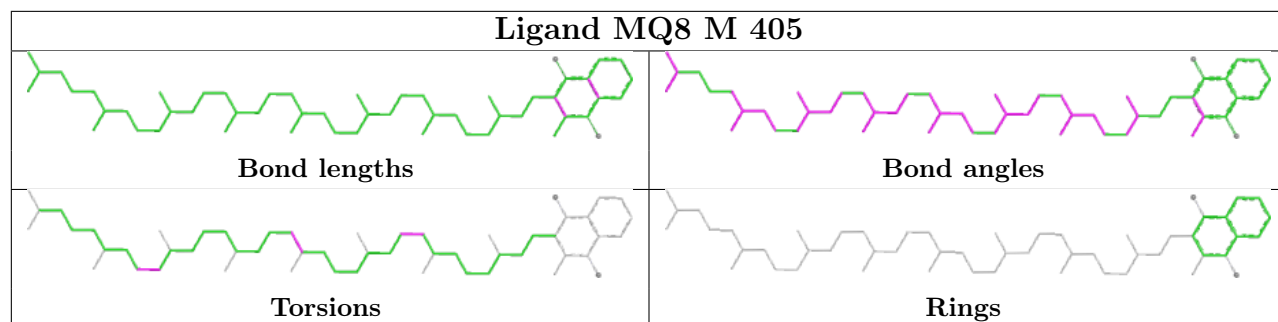


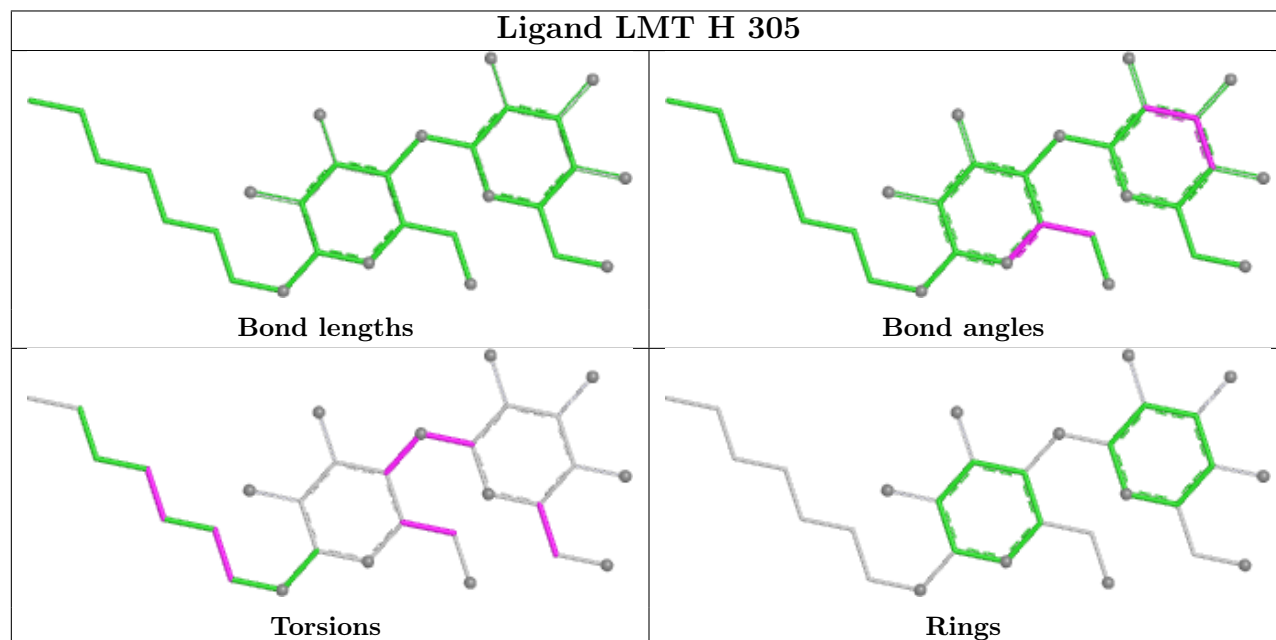
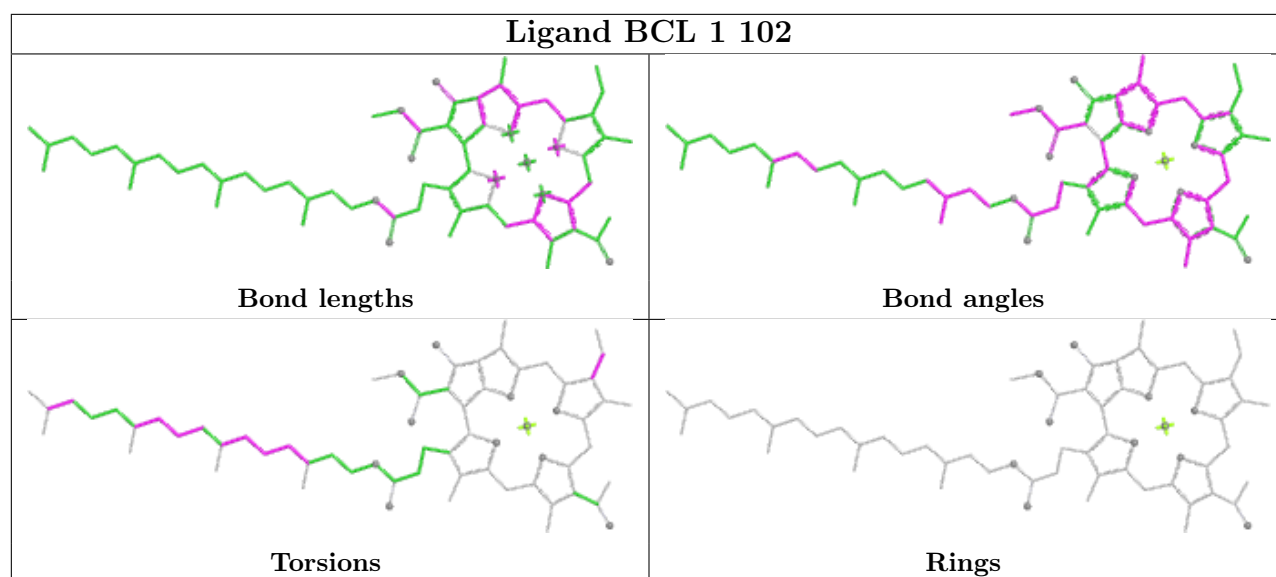
Ligand BPH L 303

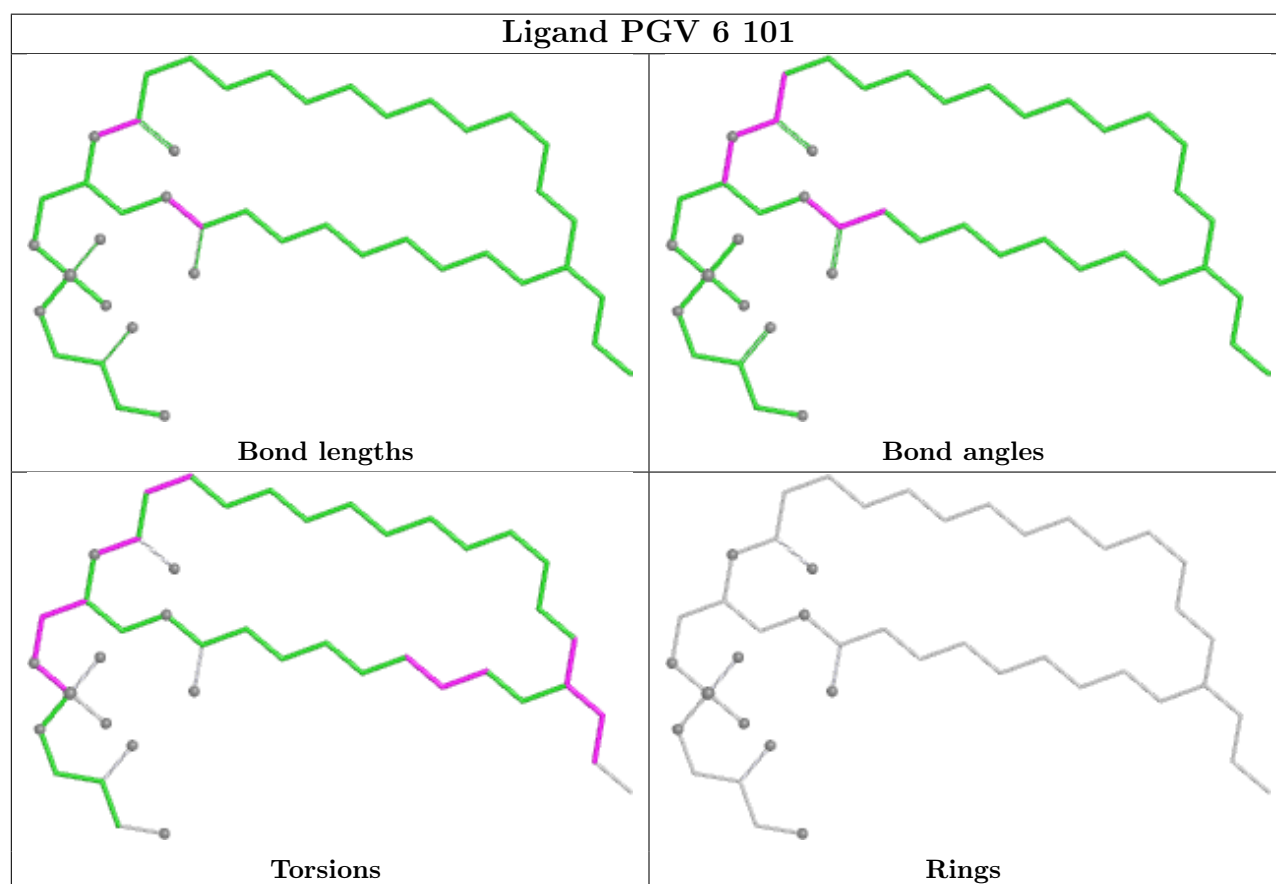
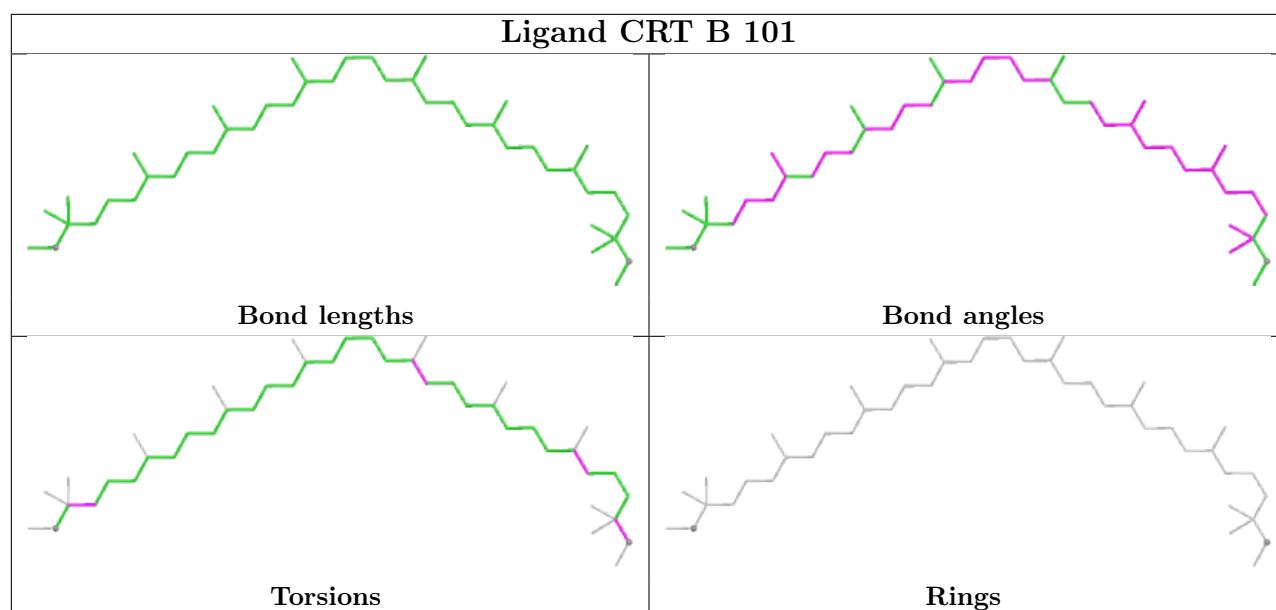


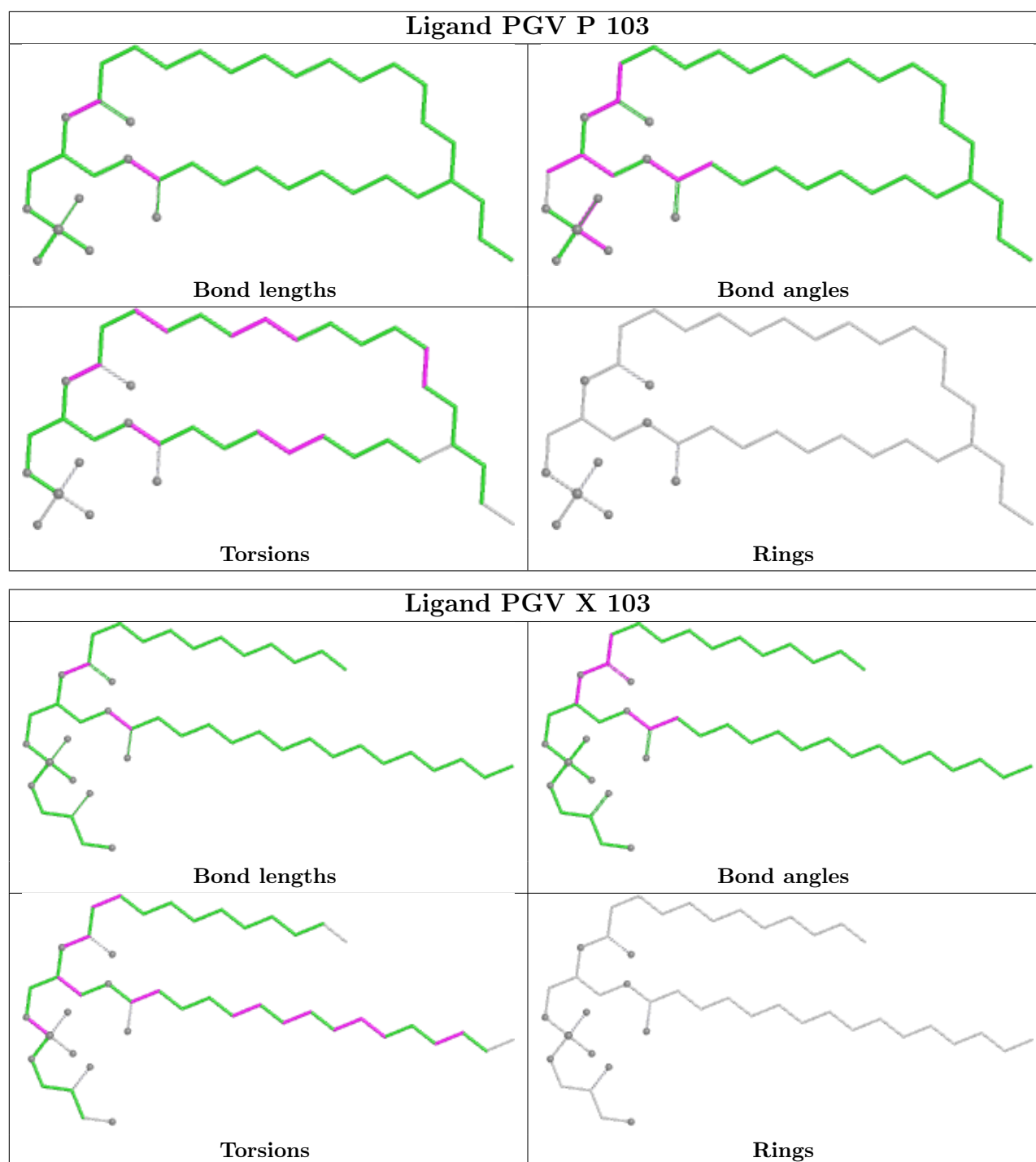
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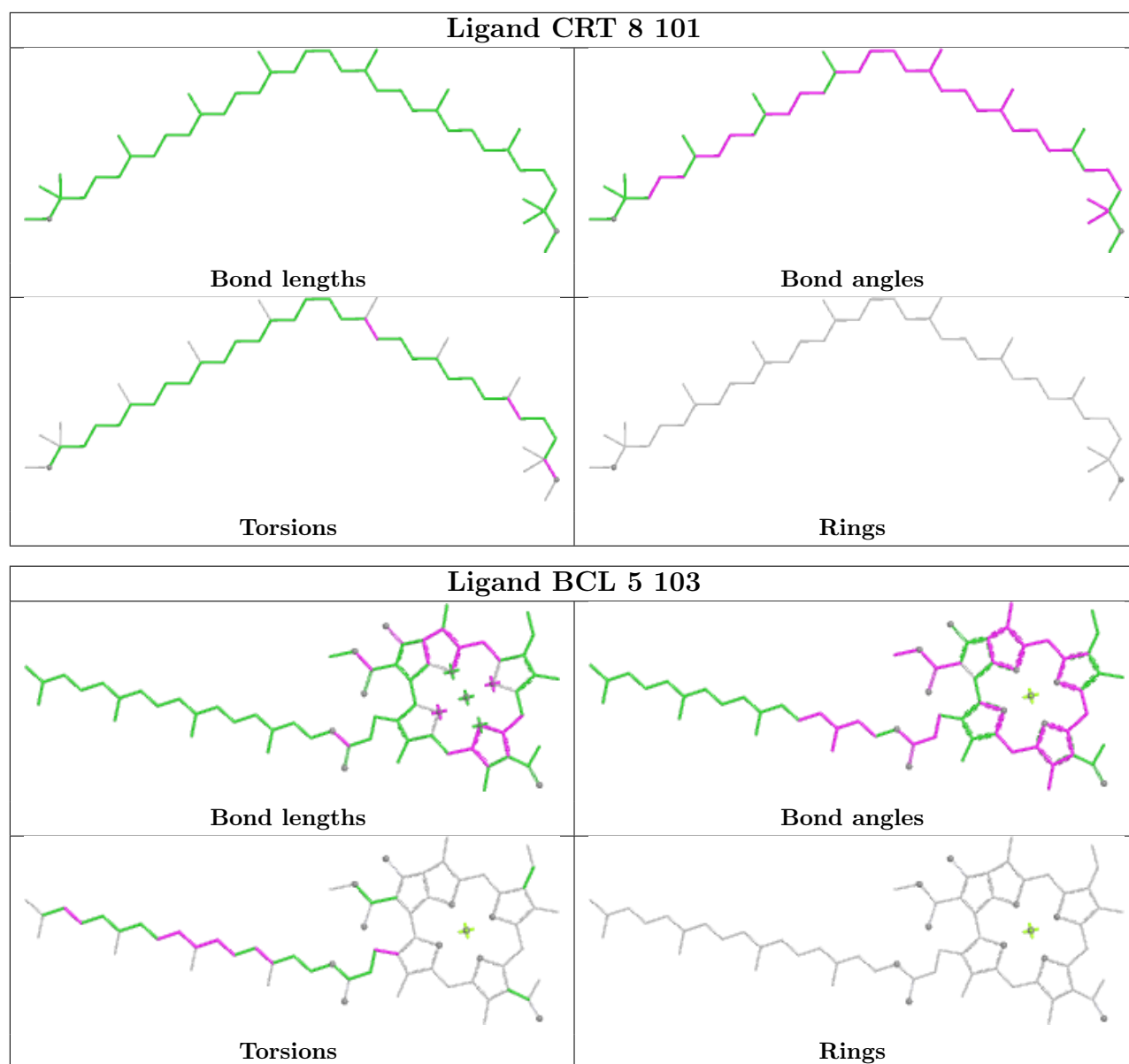


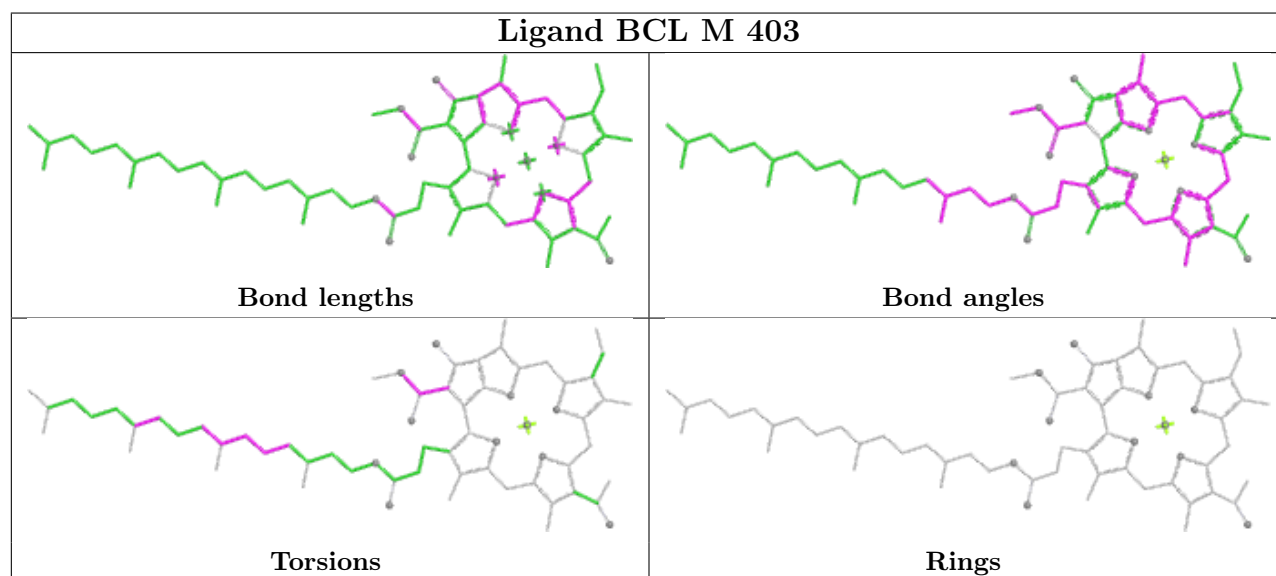
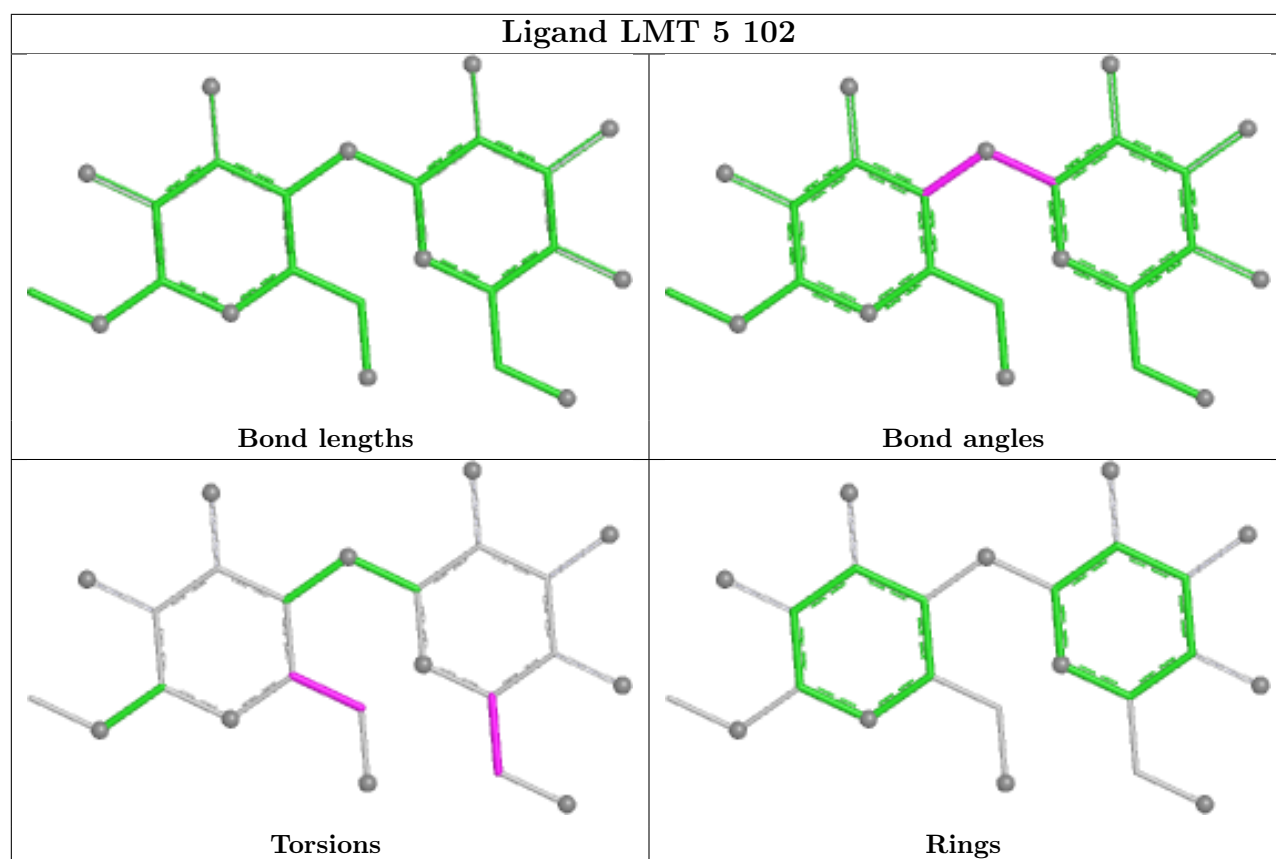


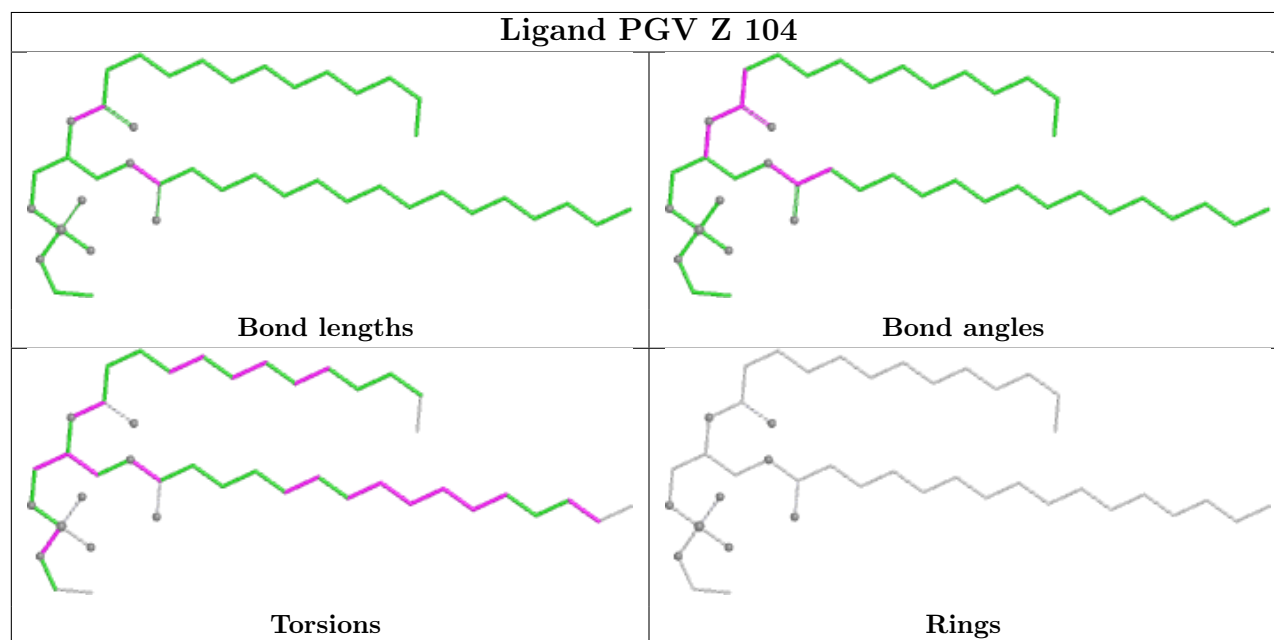
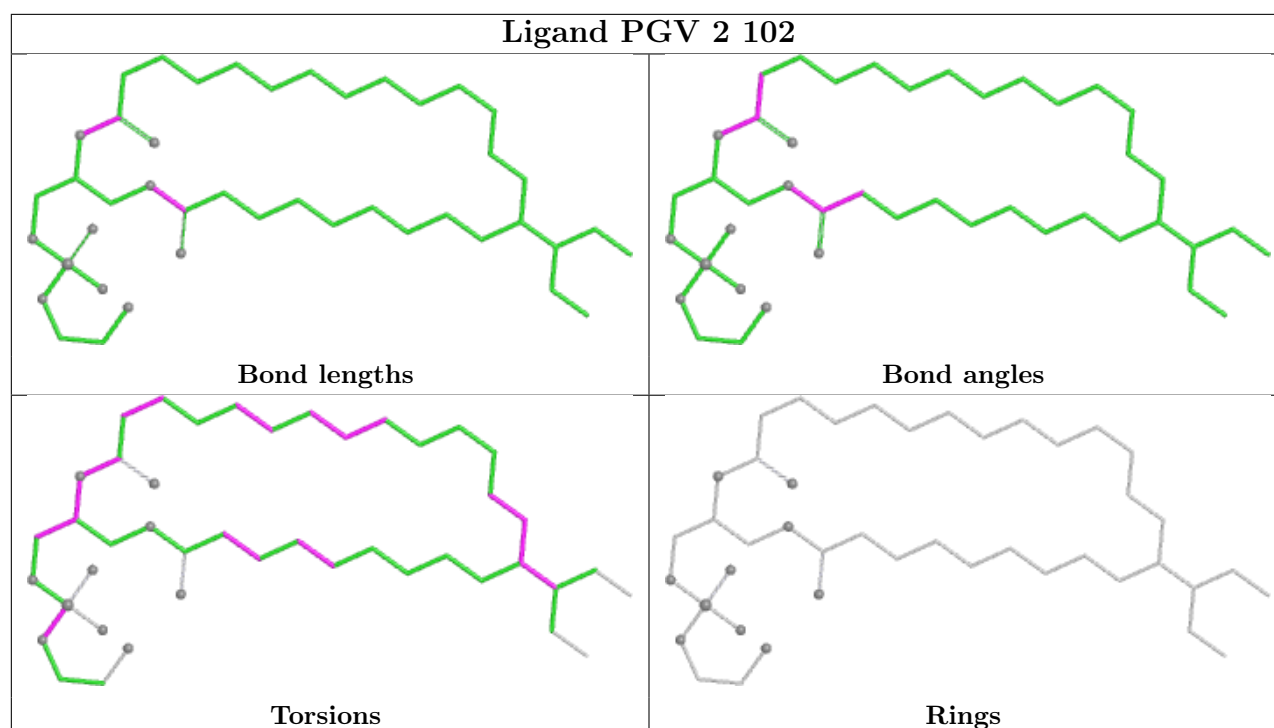


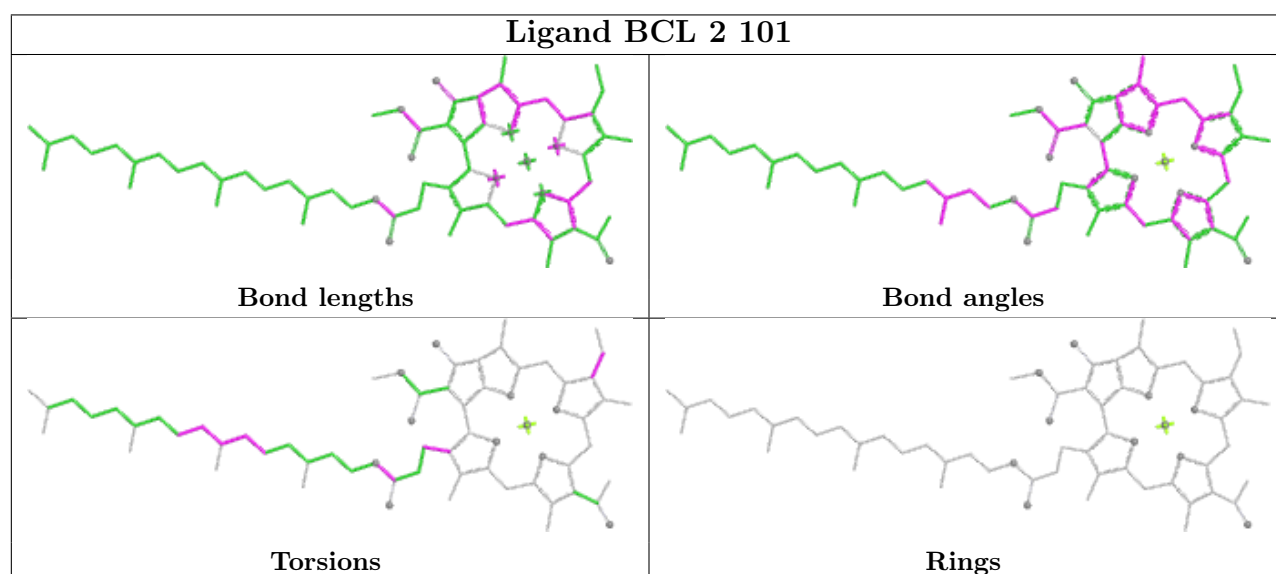
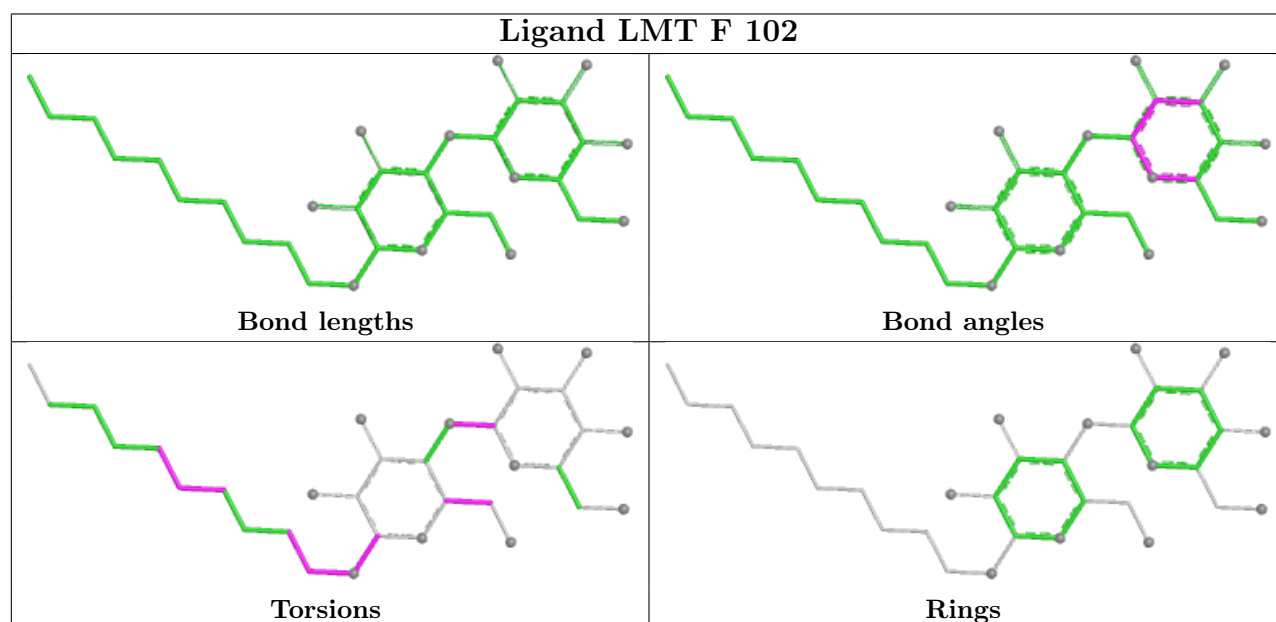
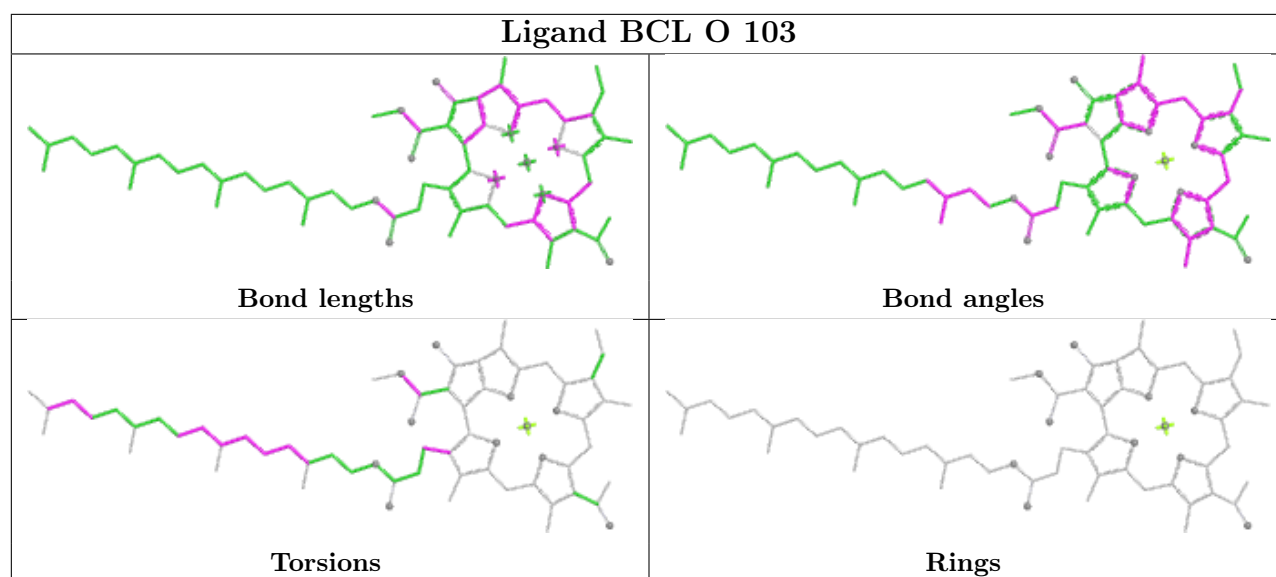


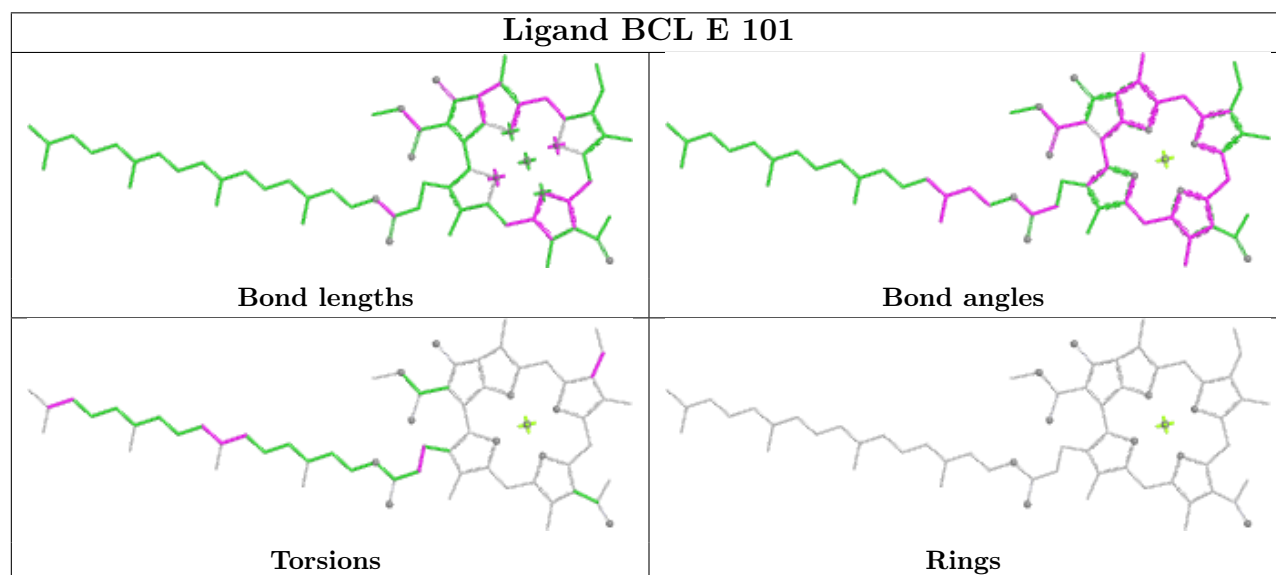
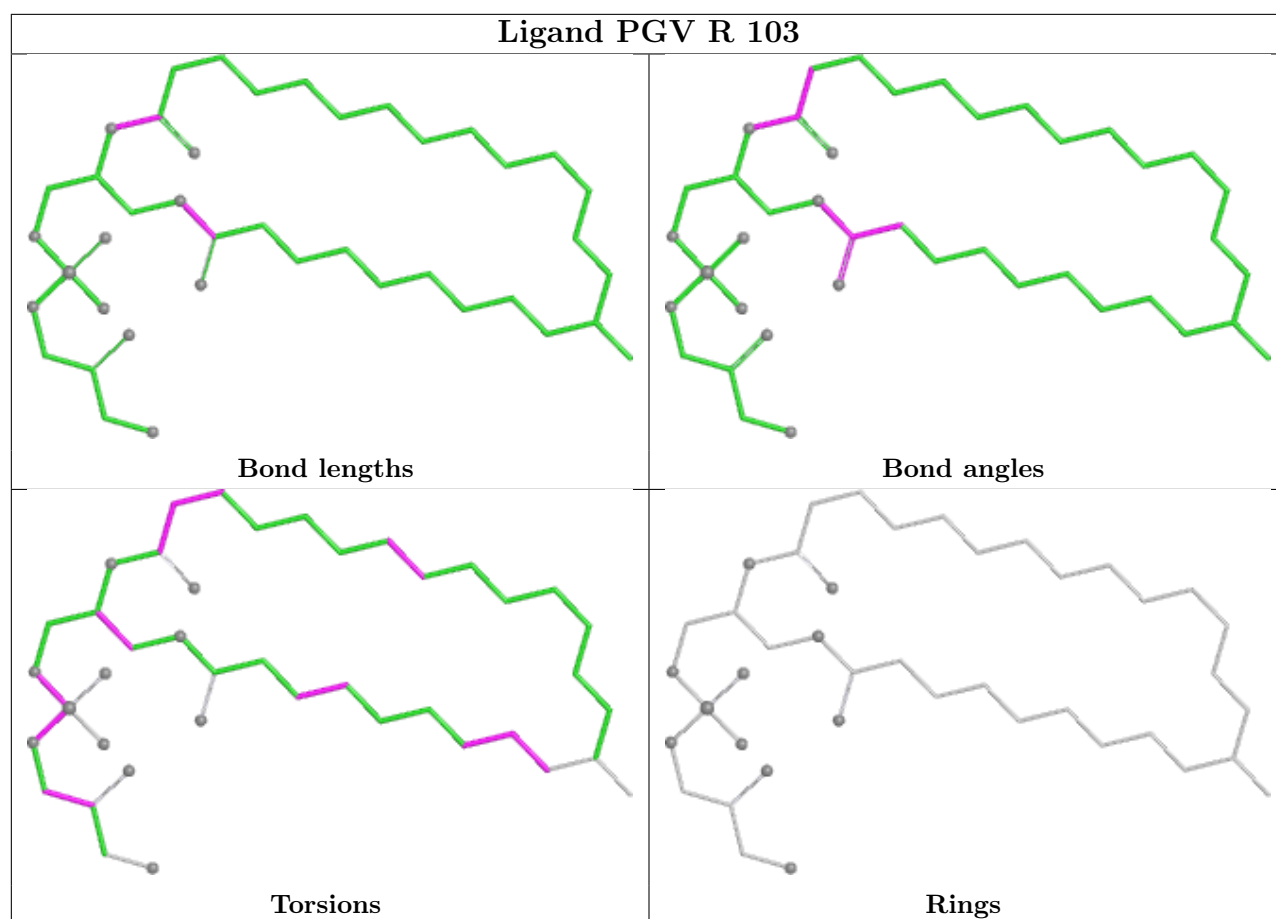


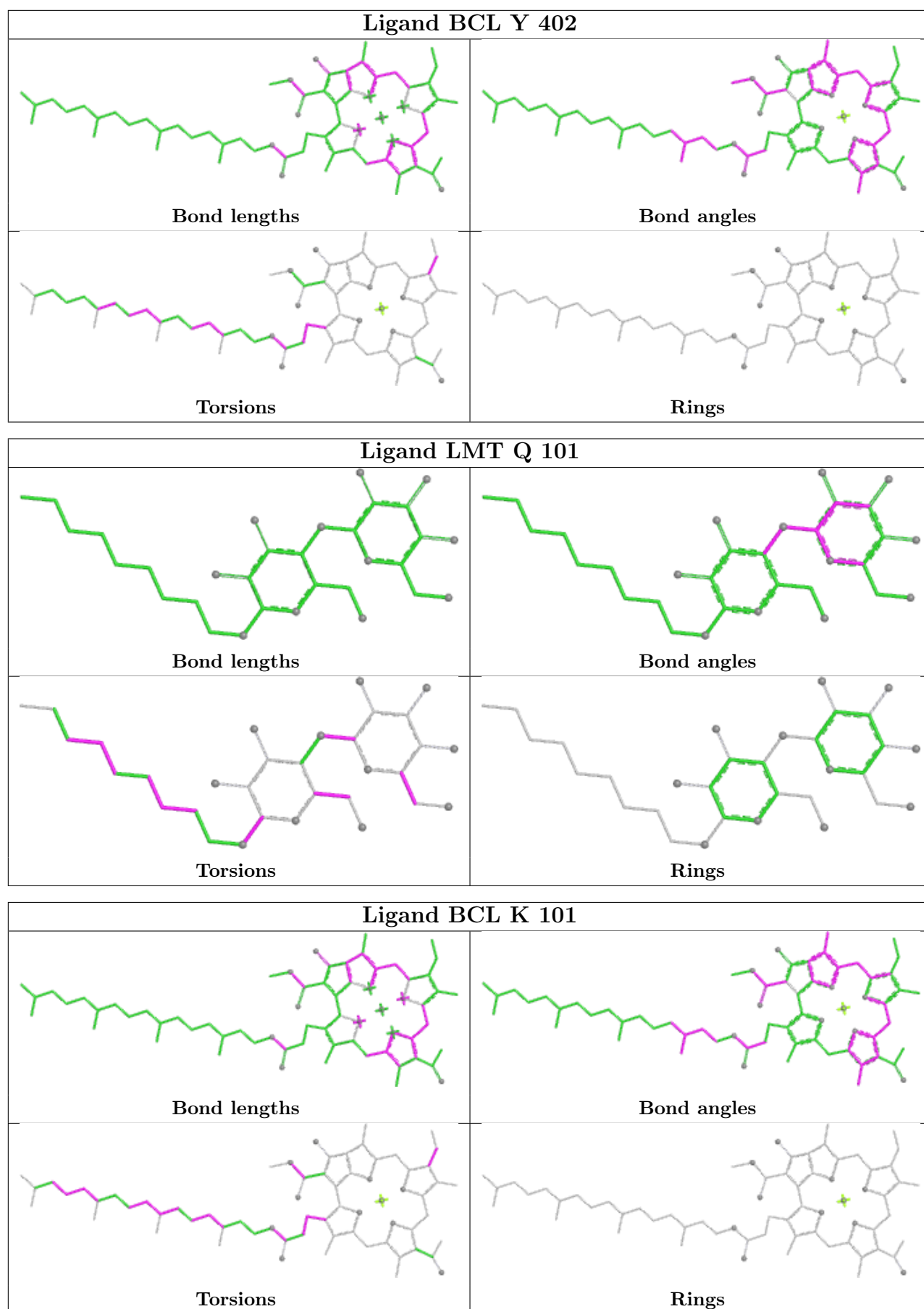


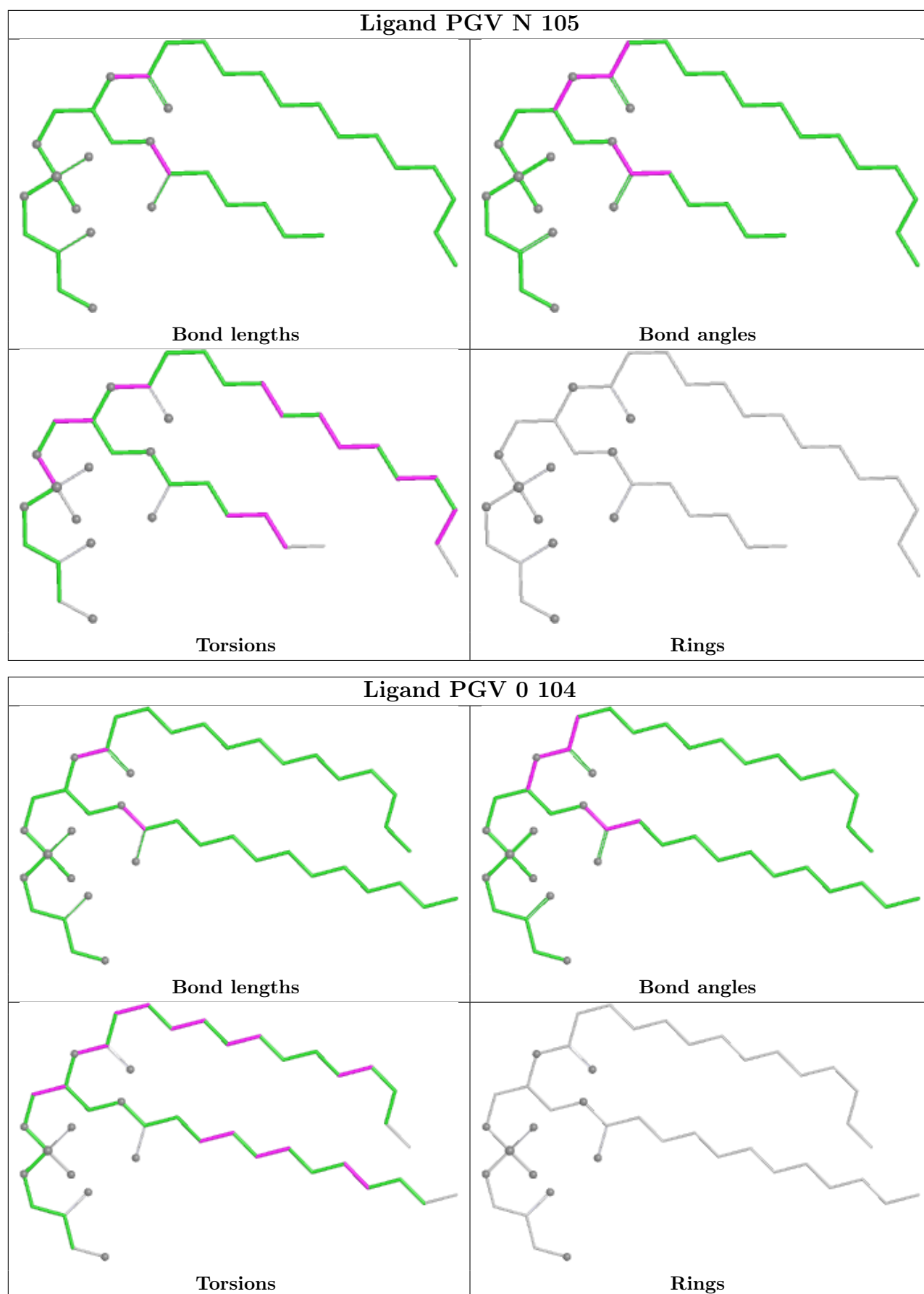


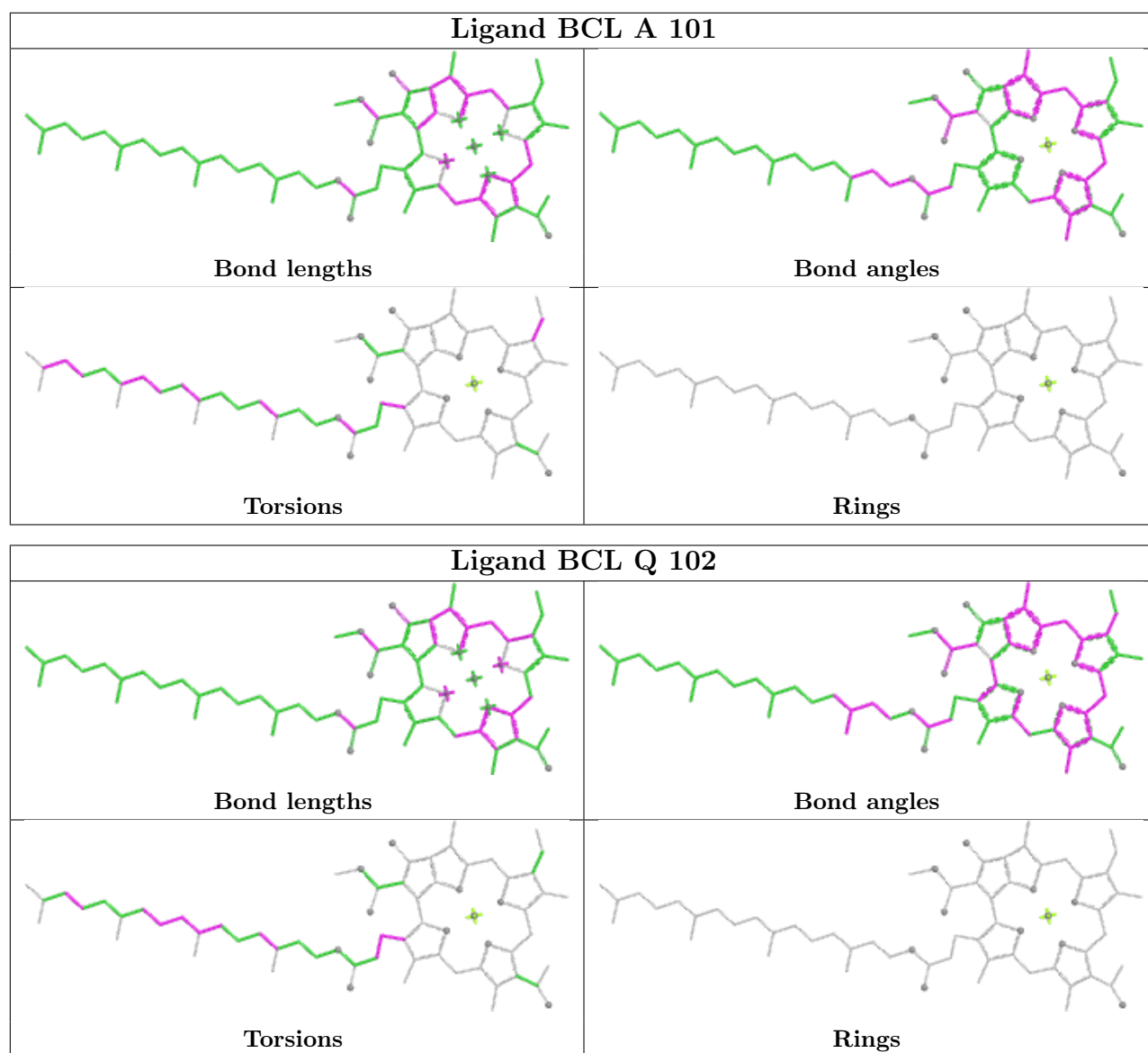


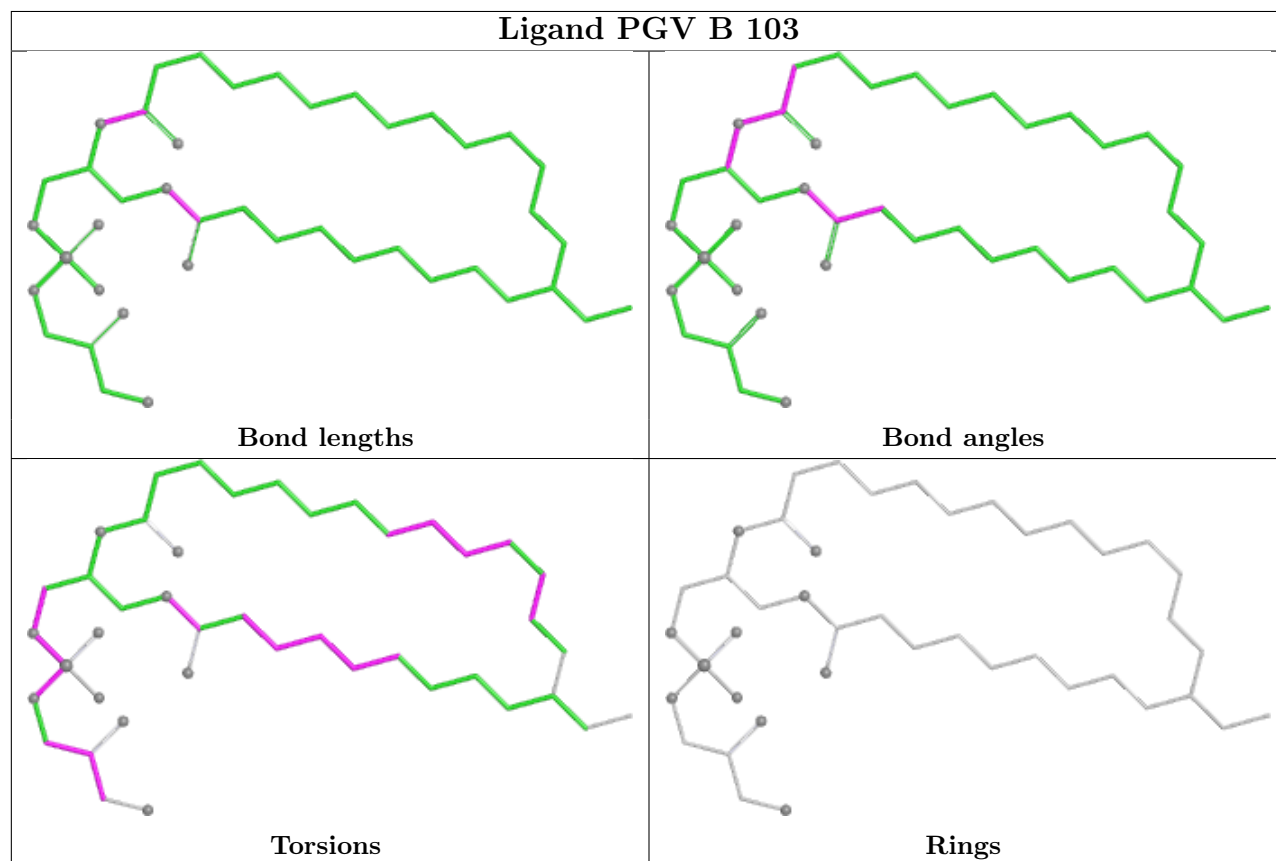
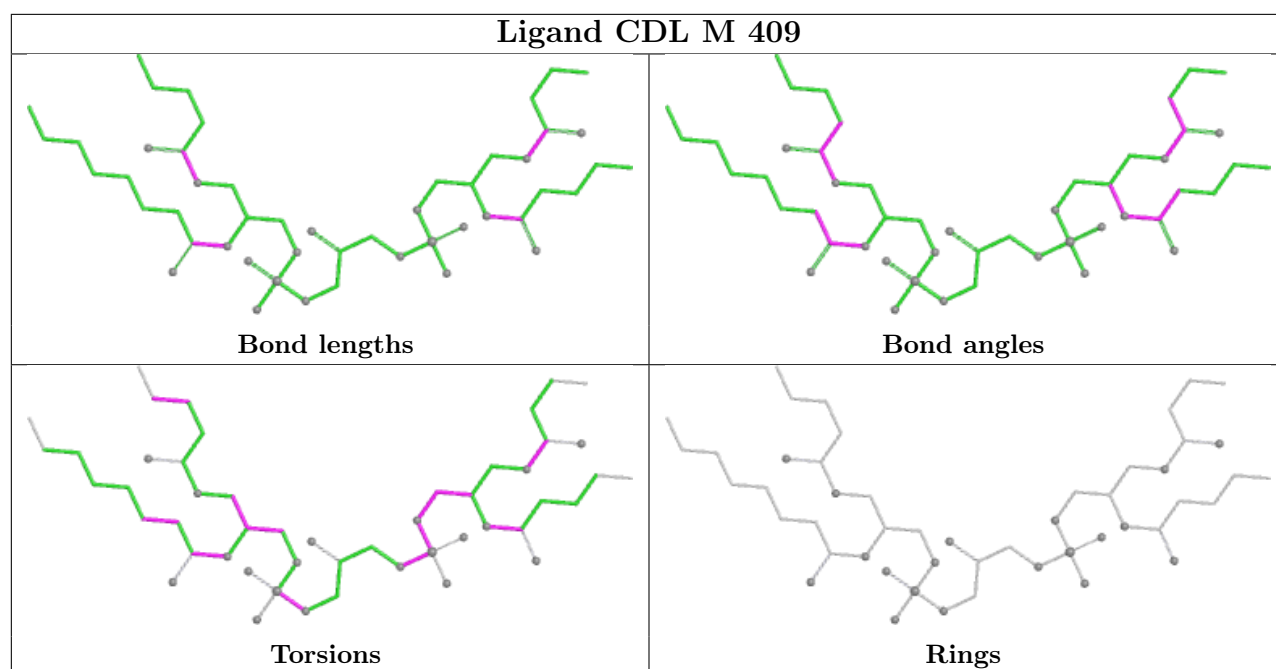


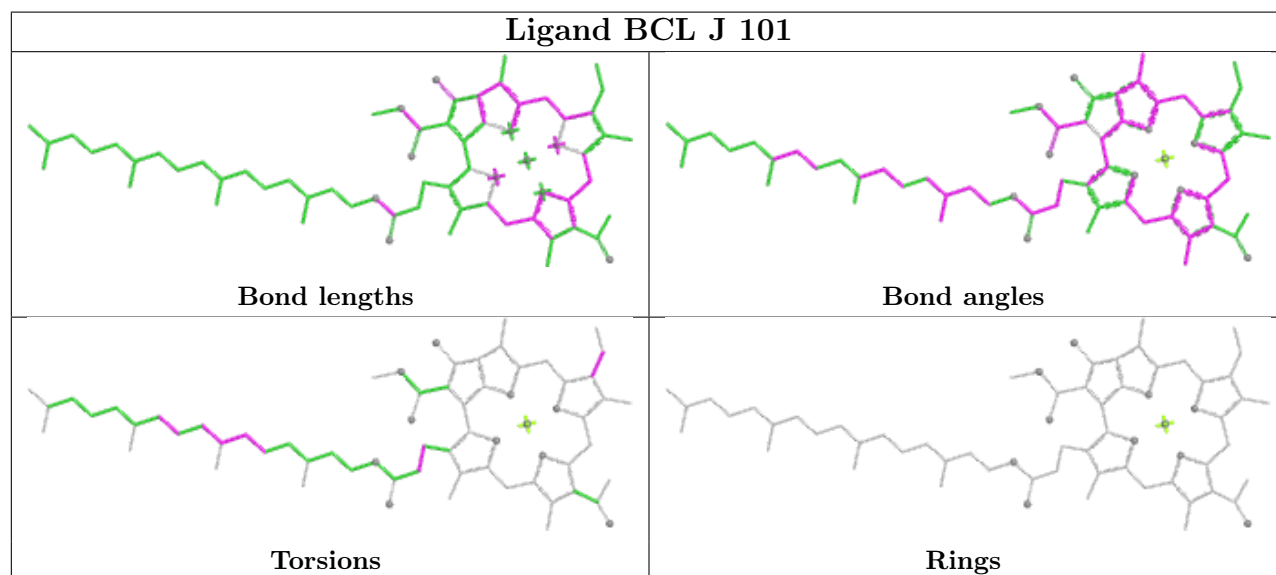
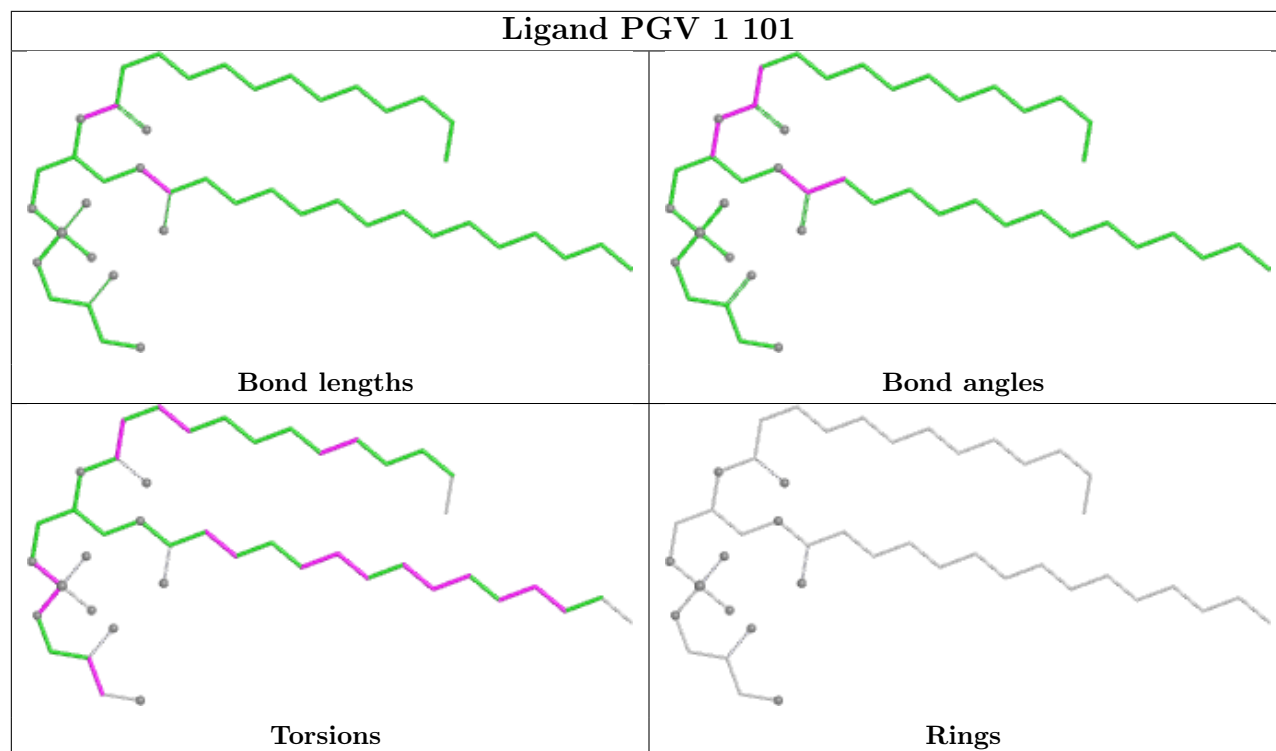


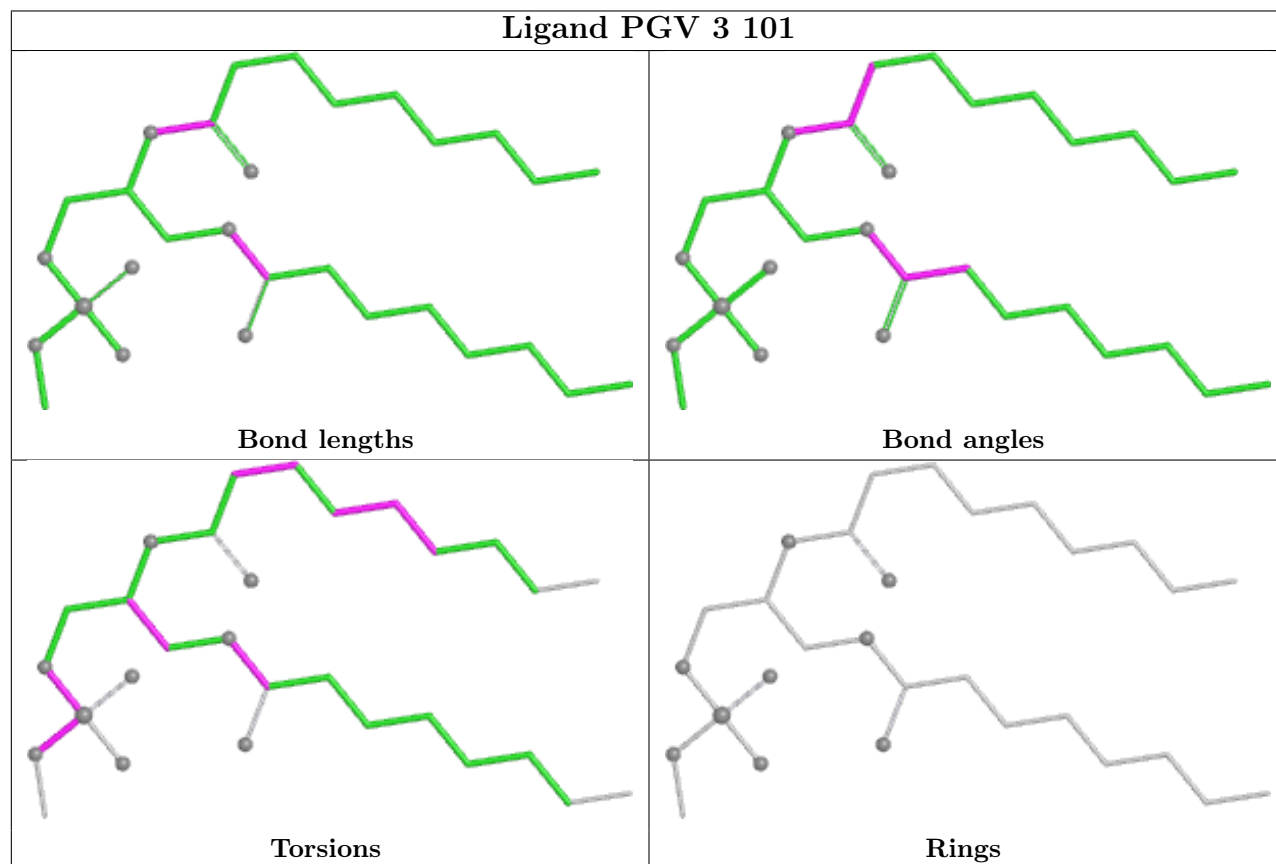
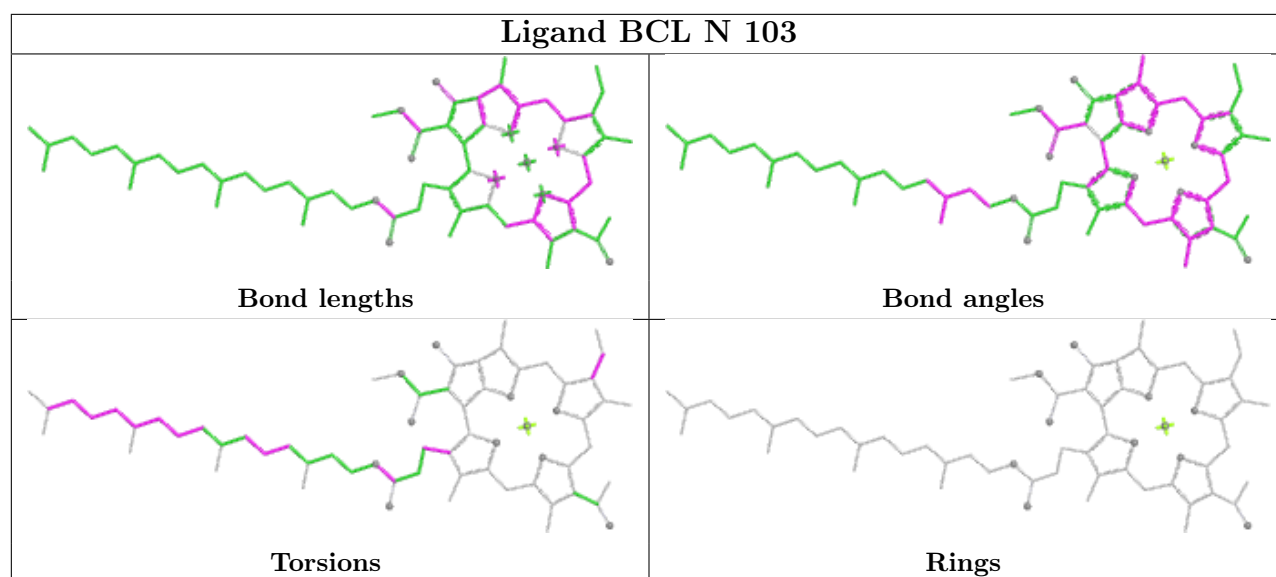


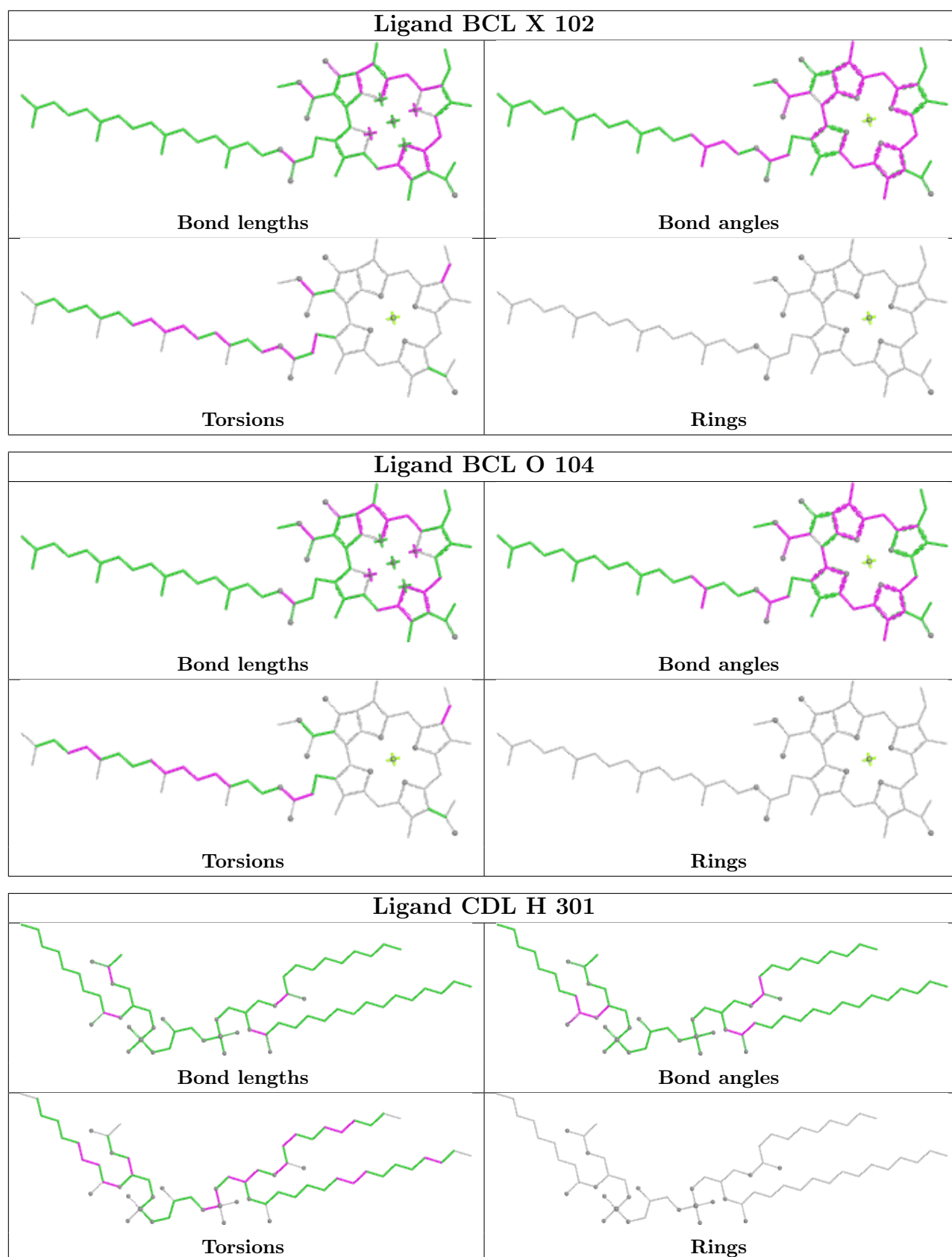


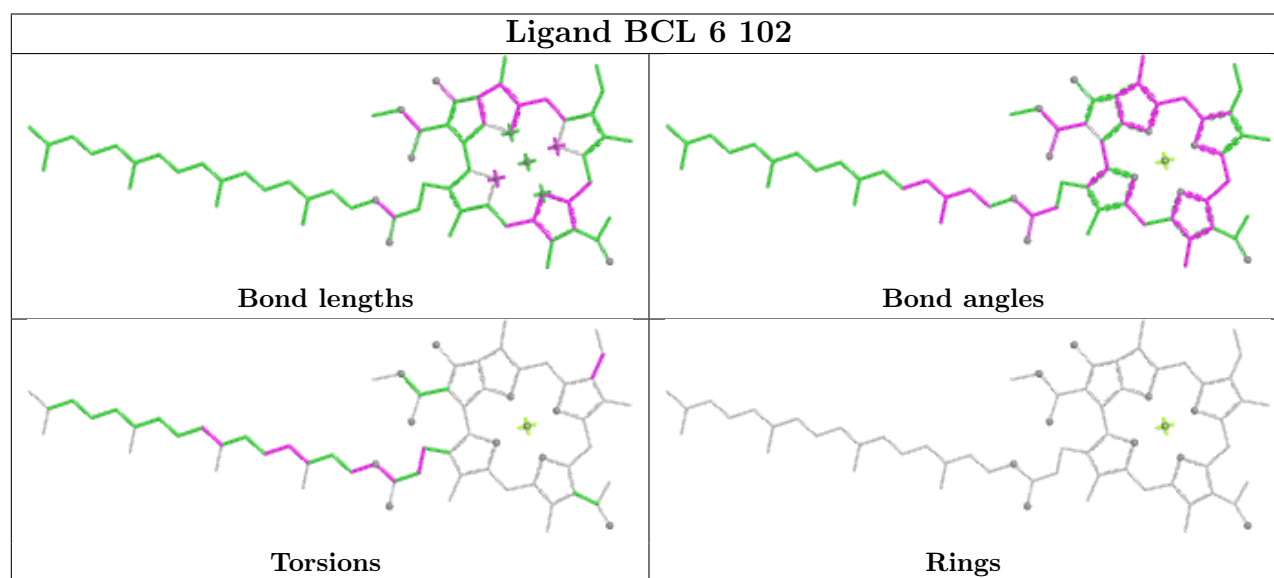
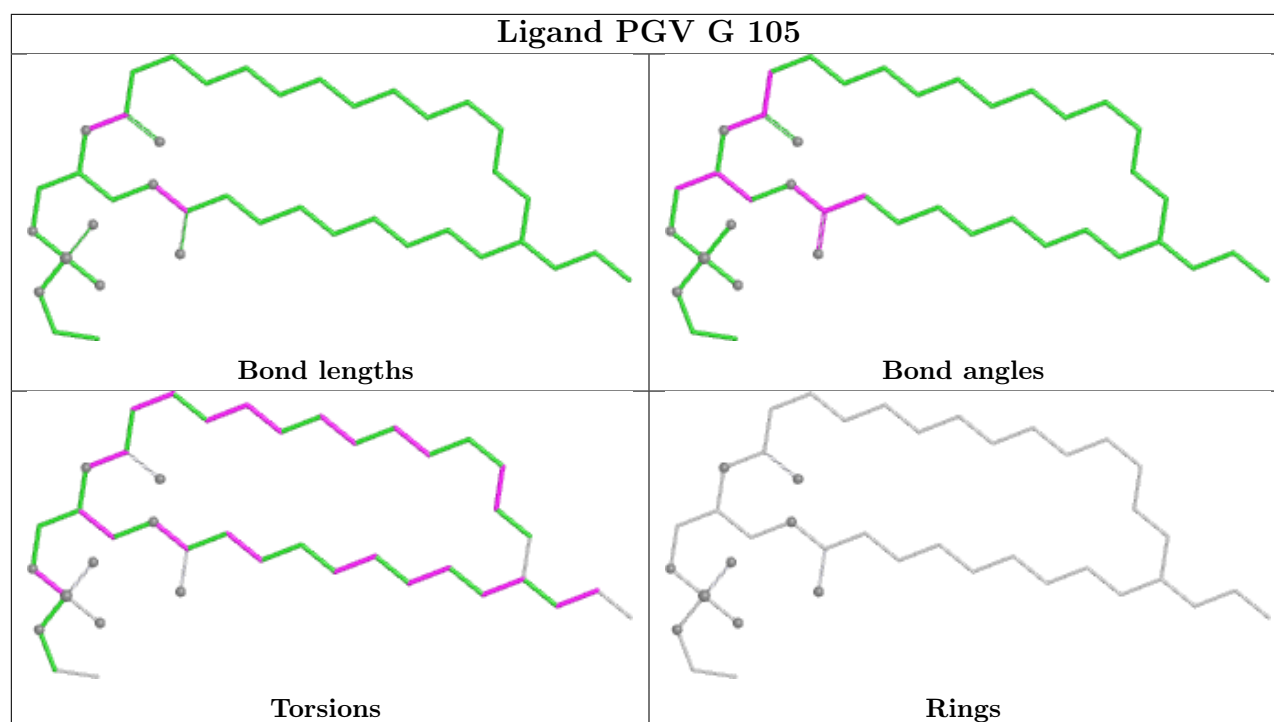


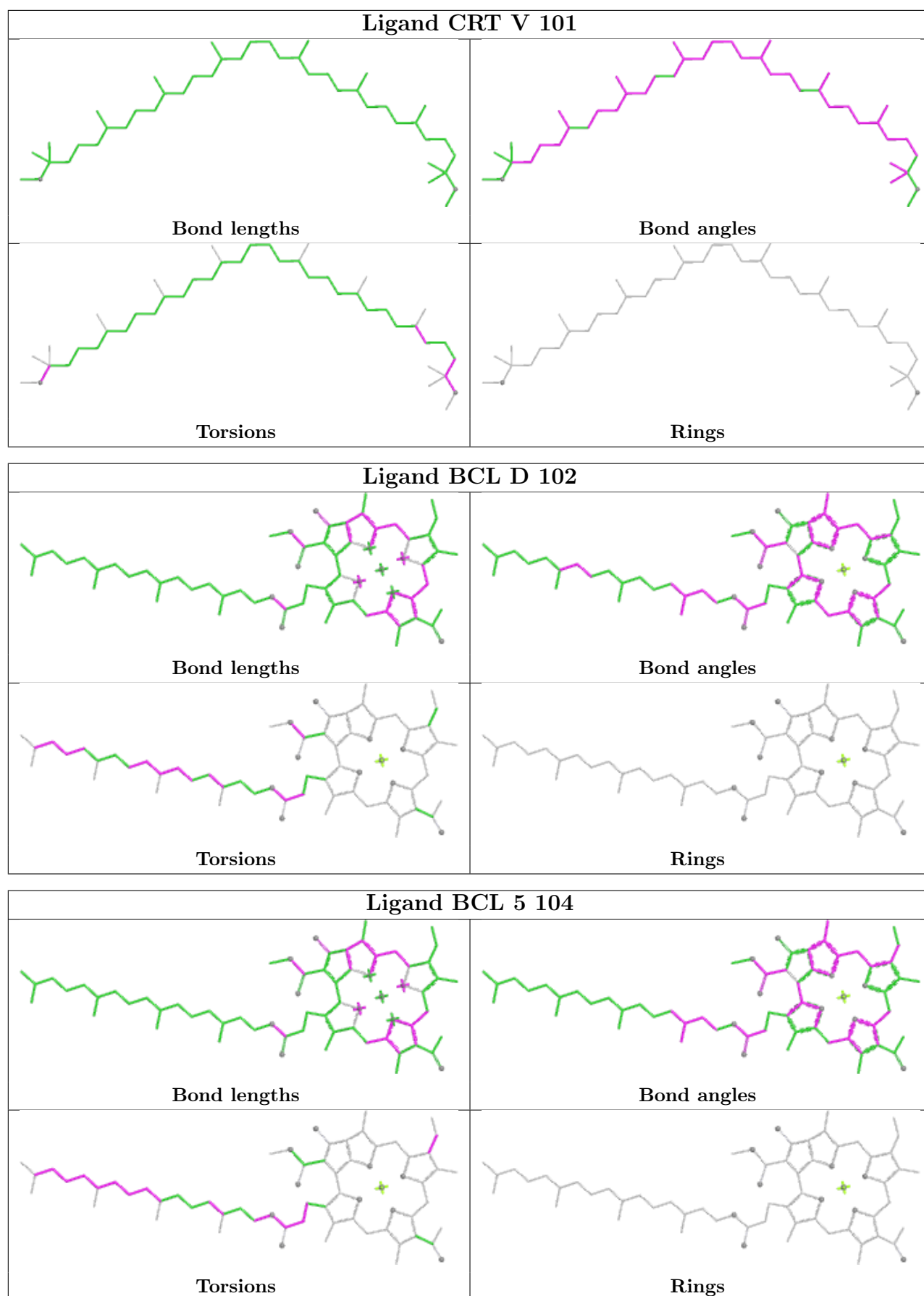


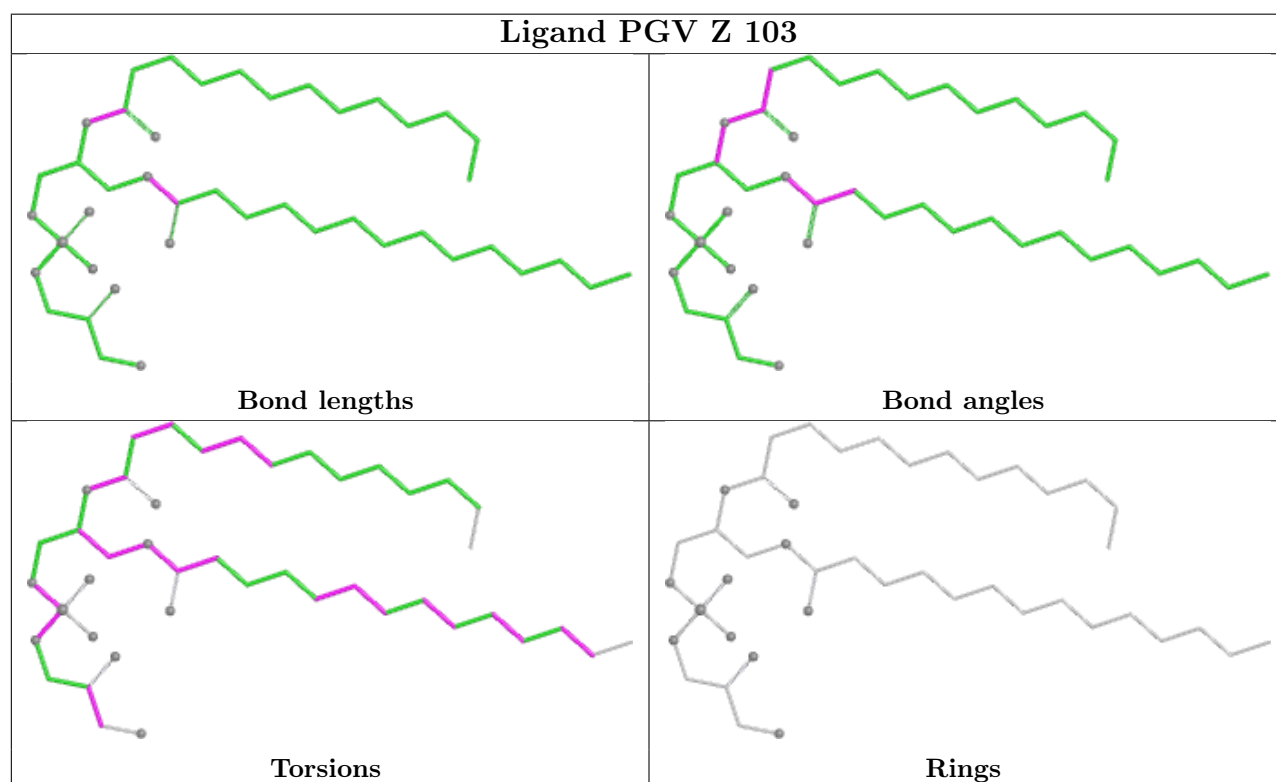
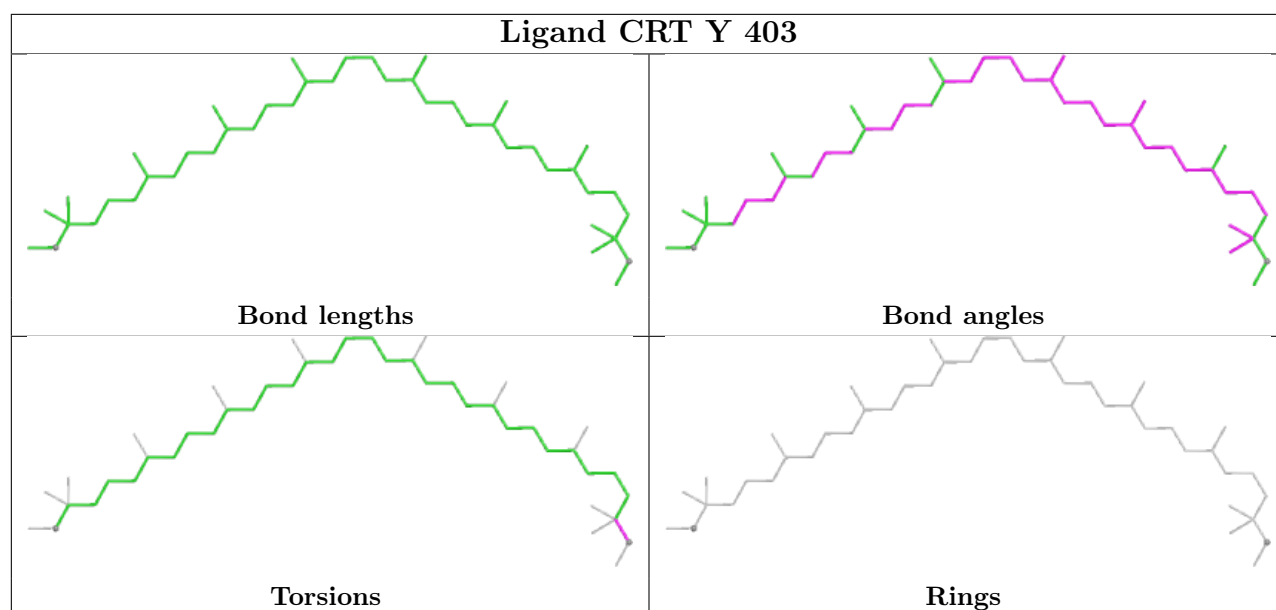


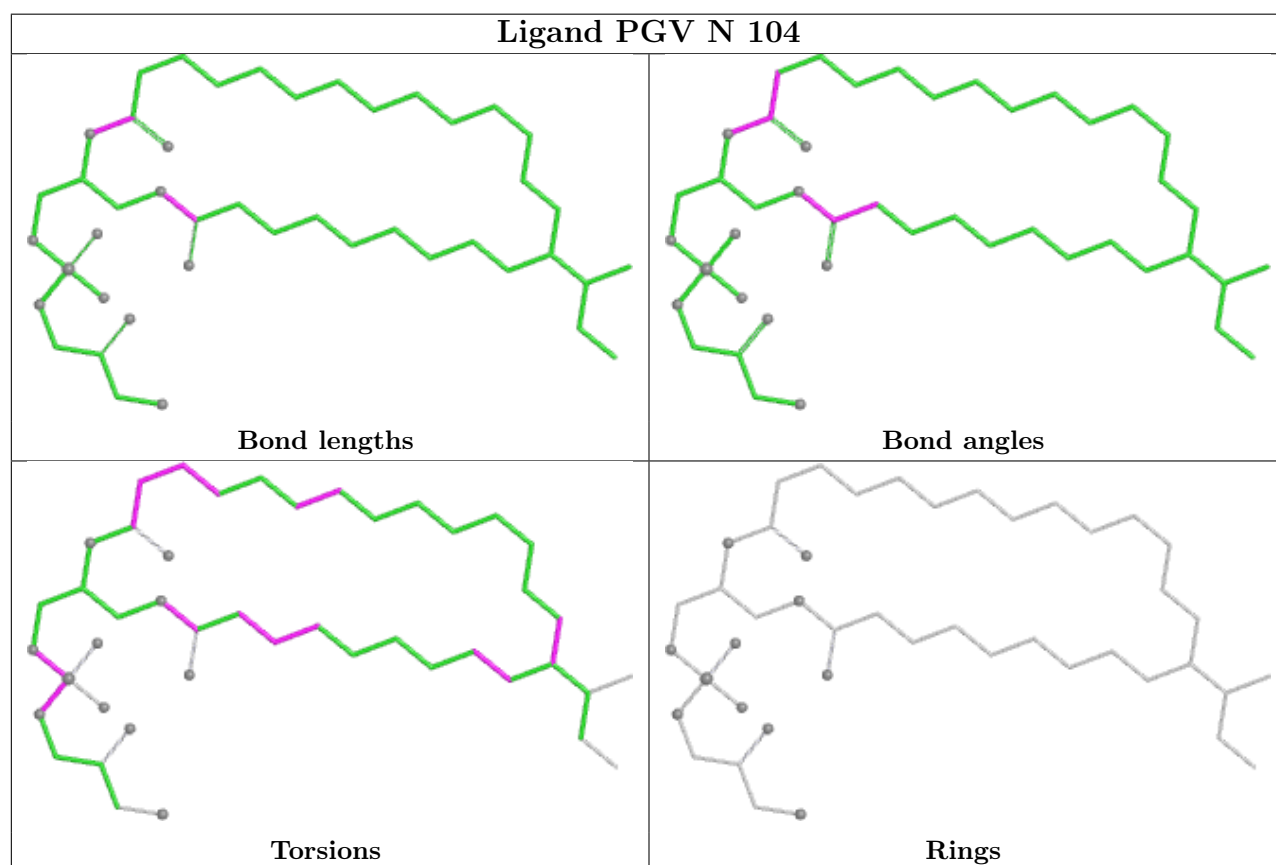
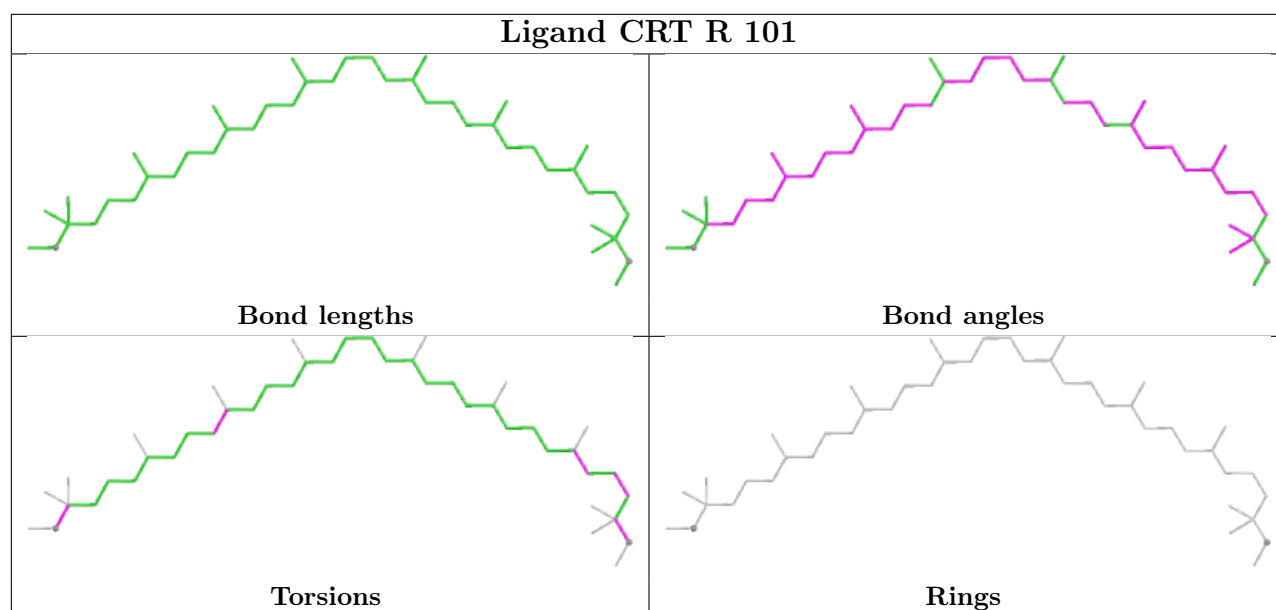


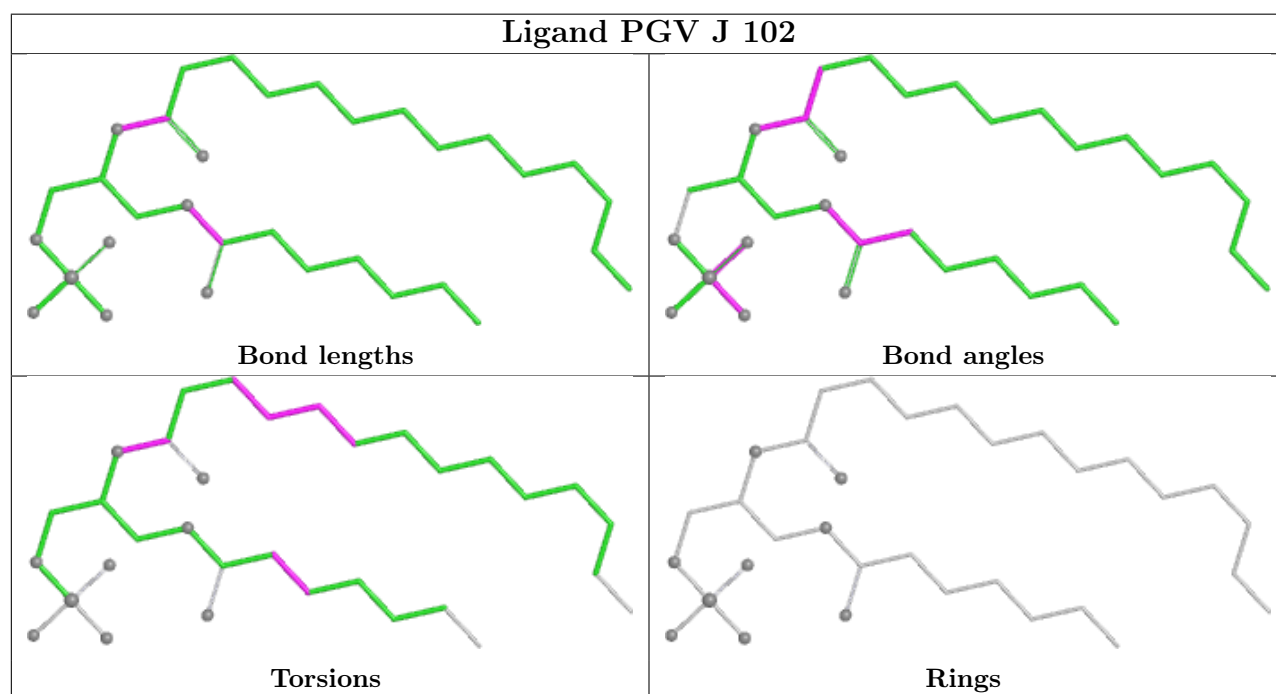
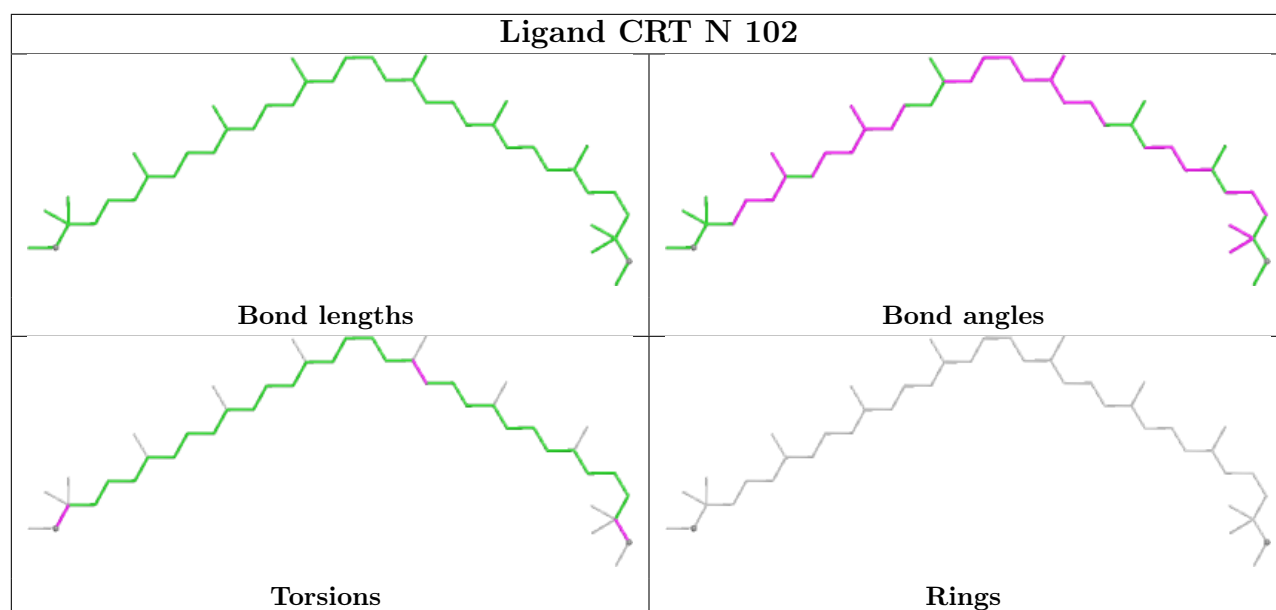


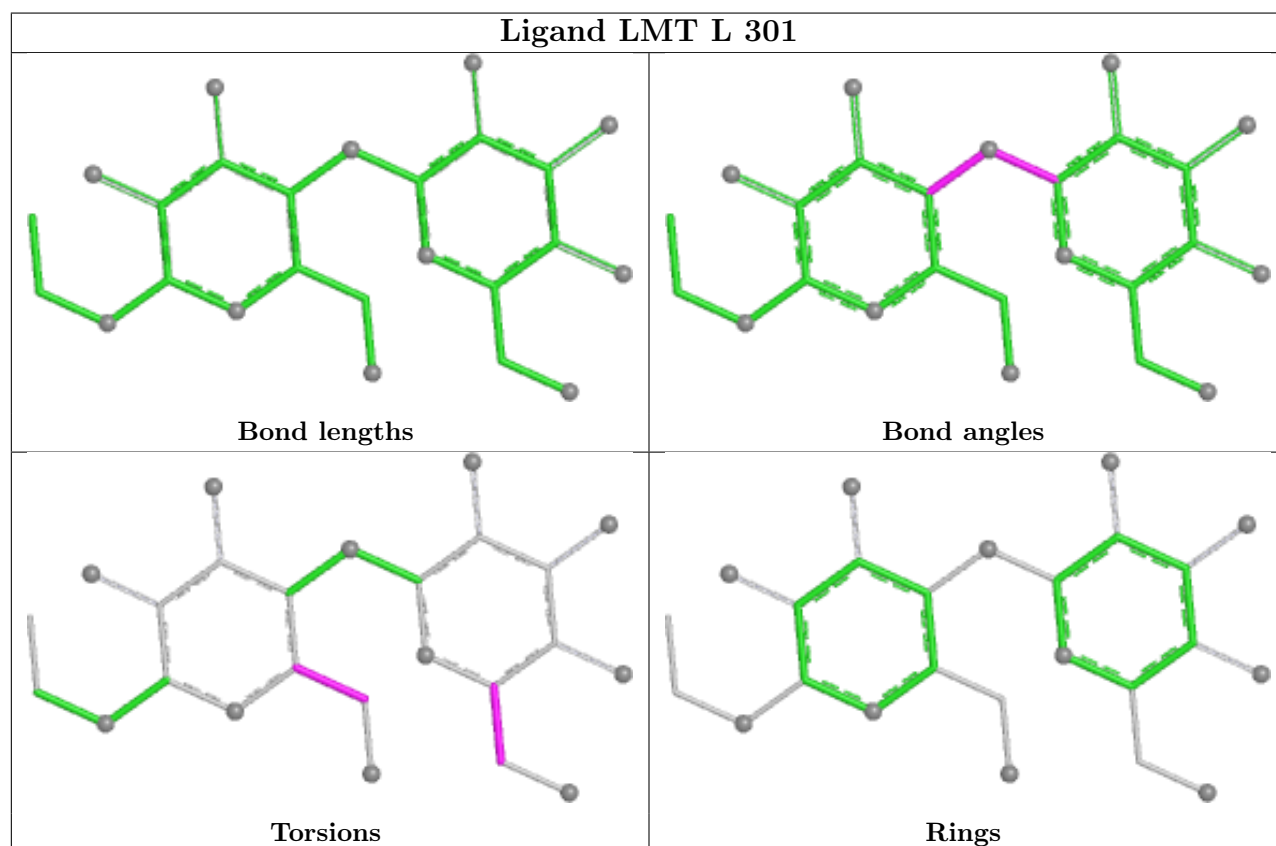
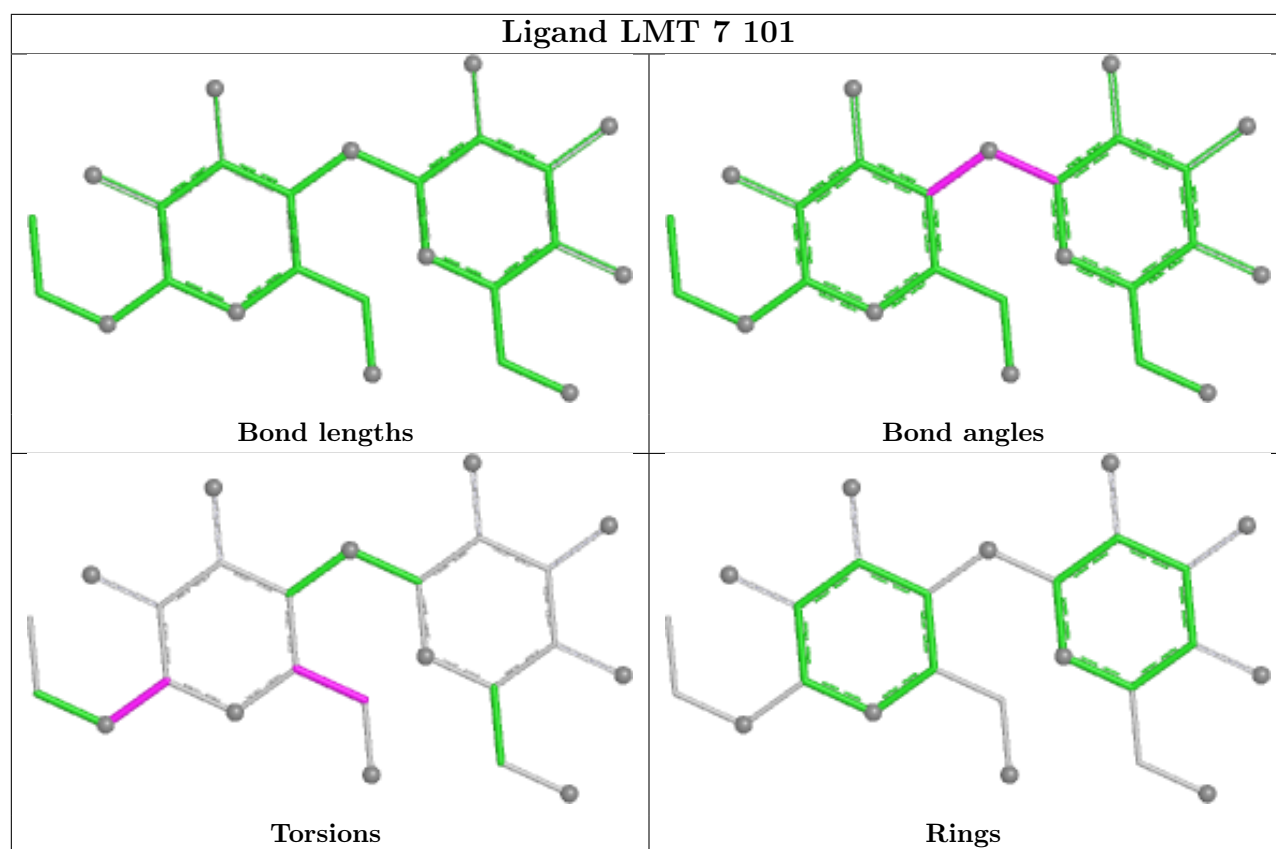


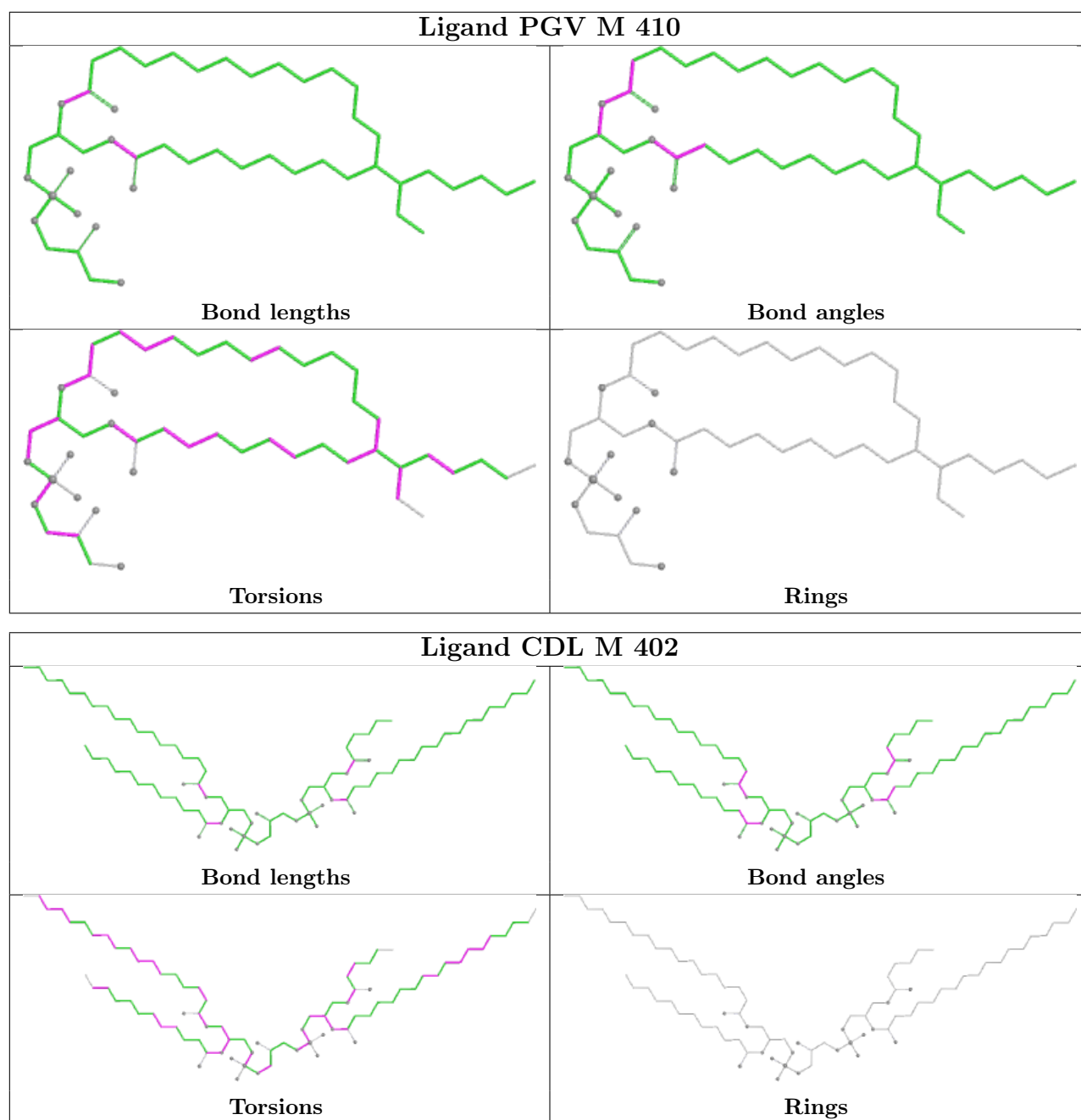


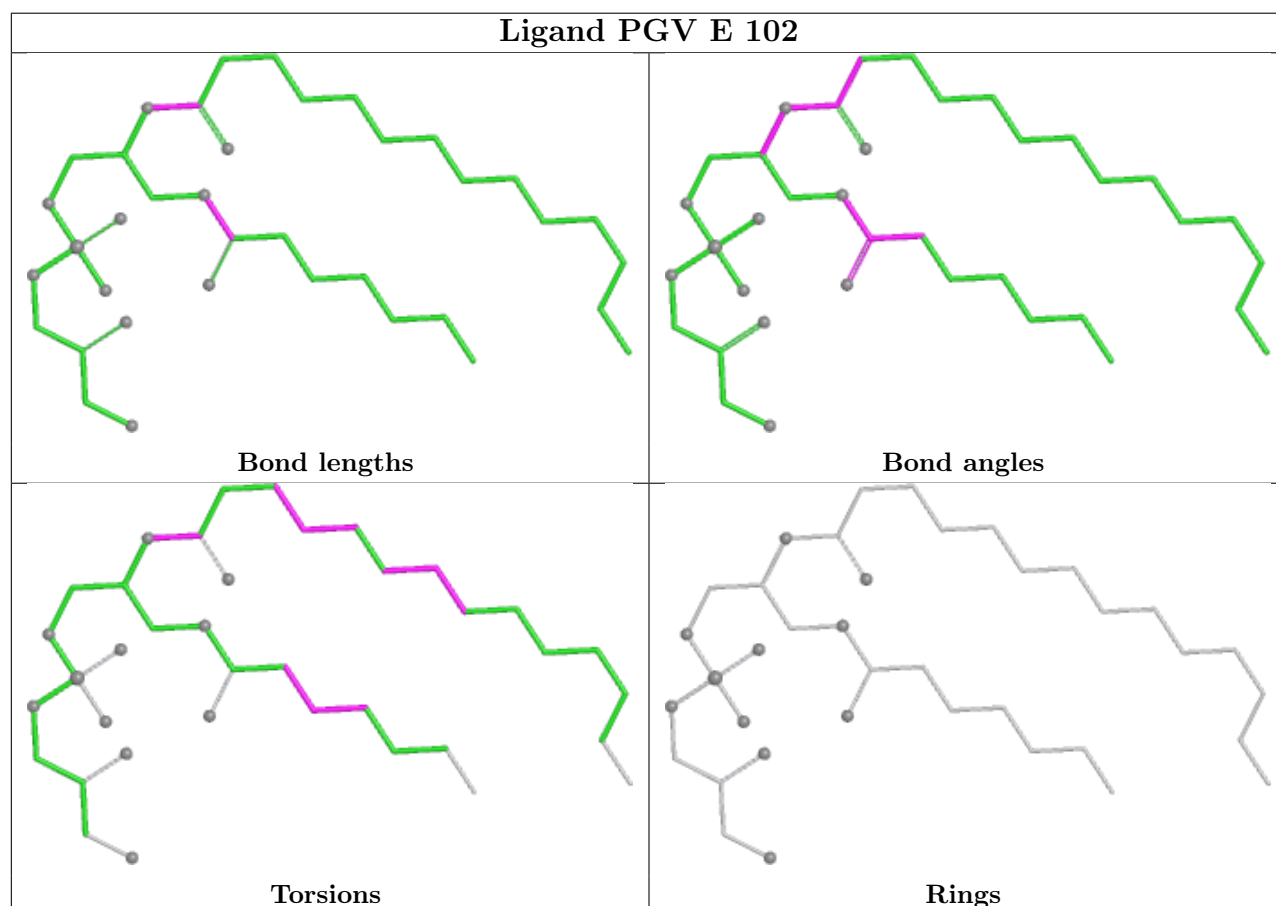
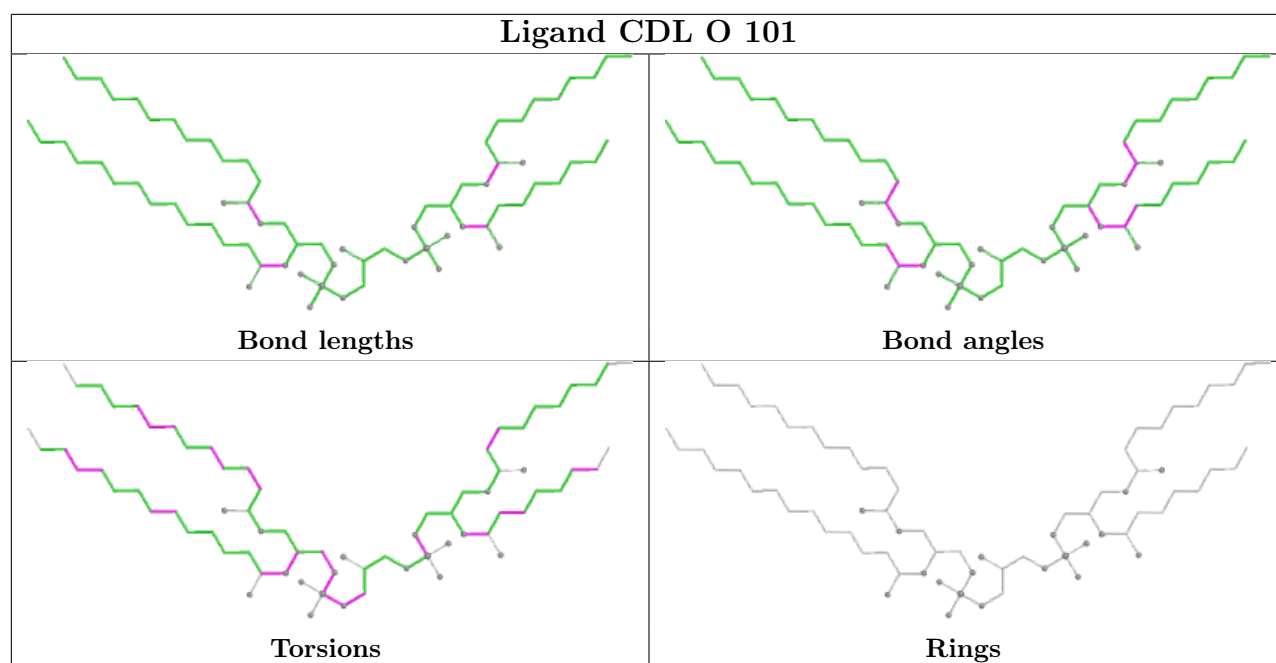


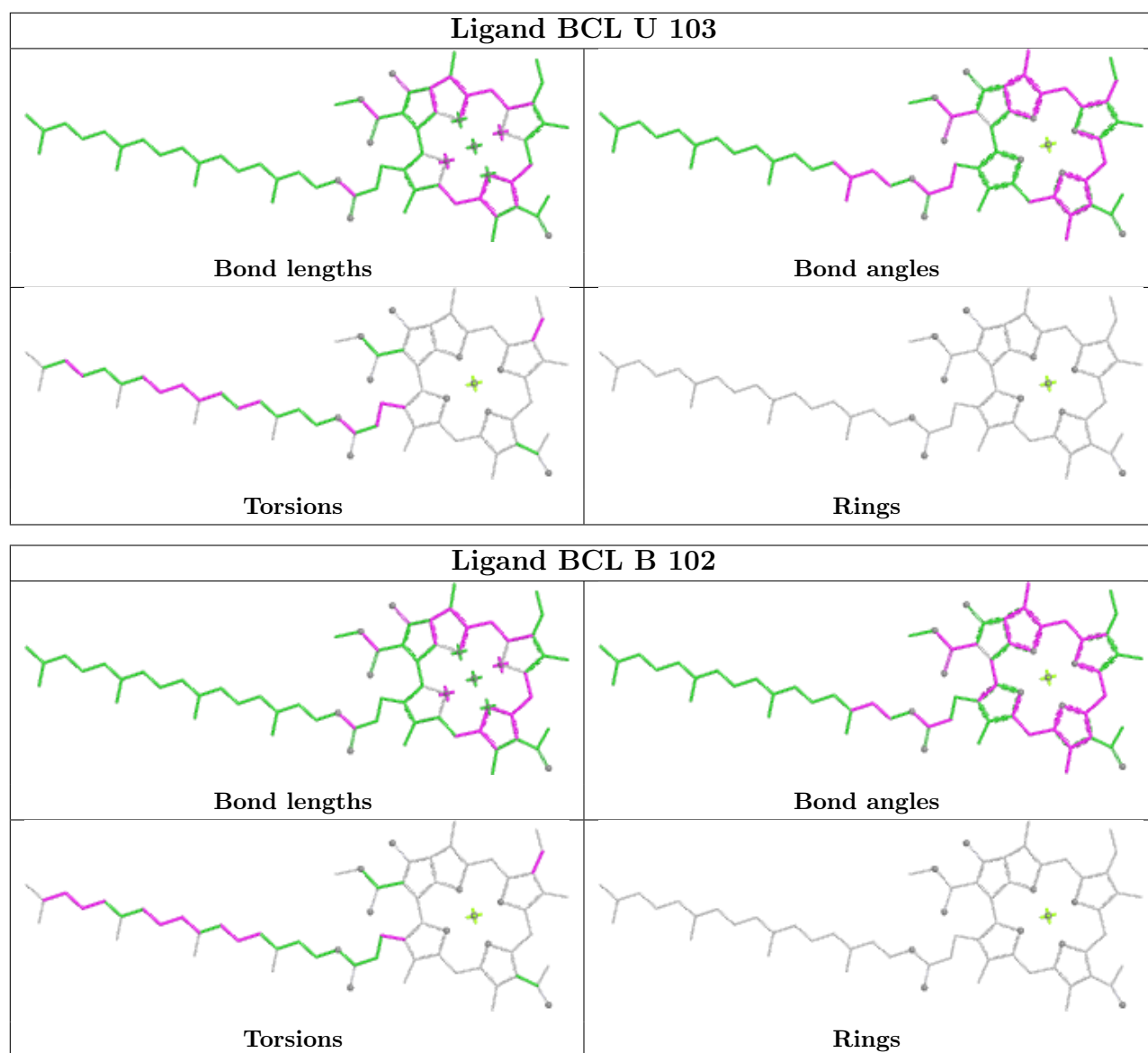


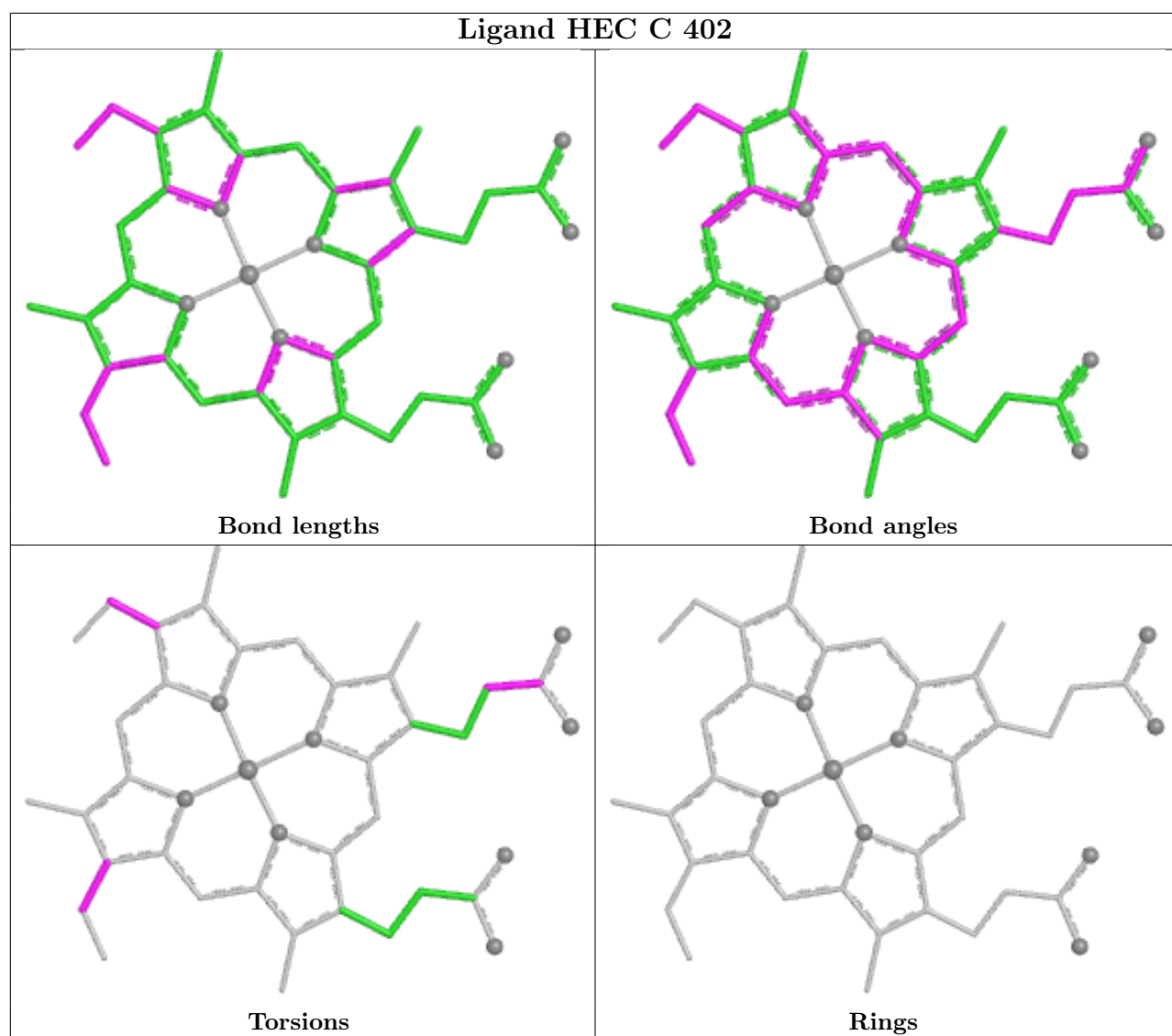


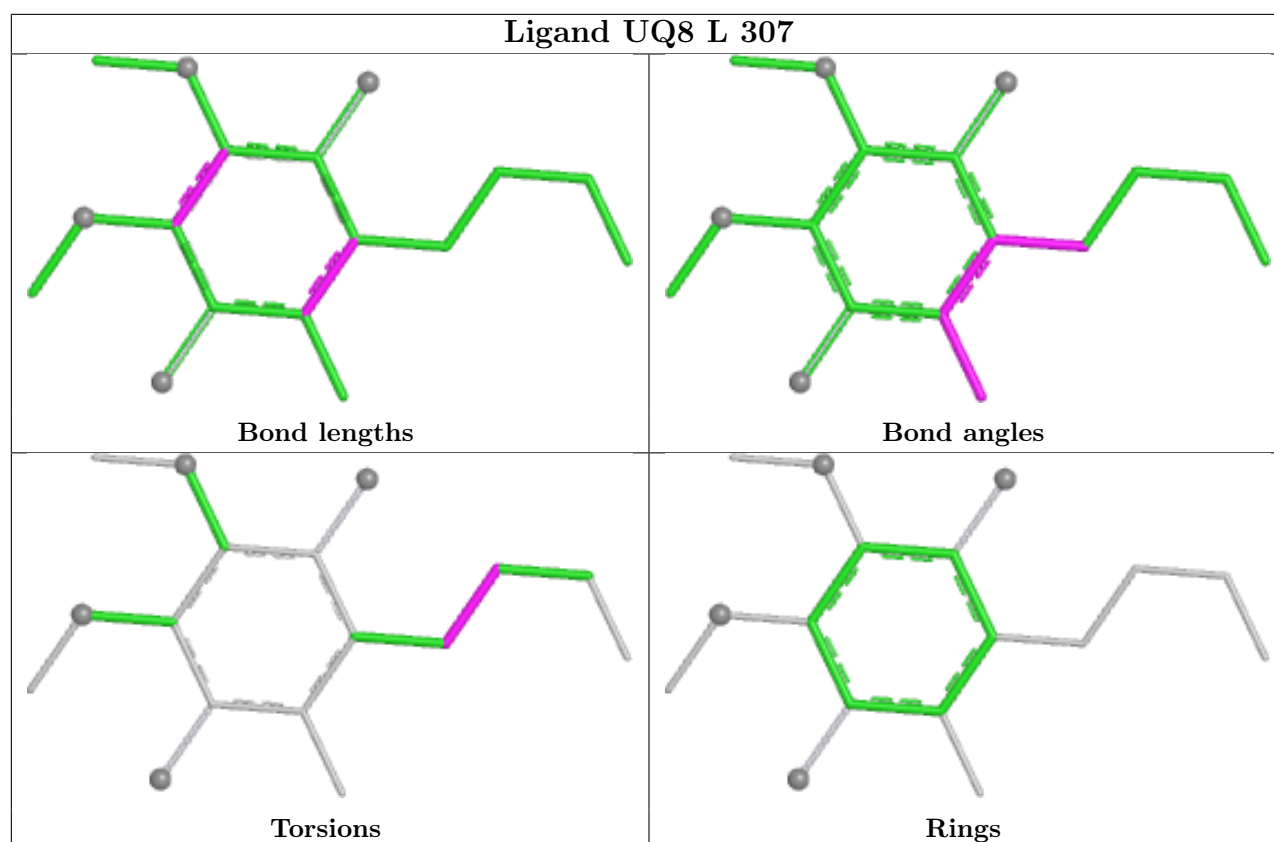












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

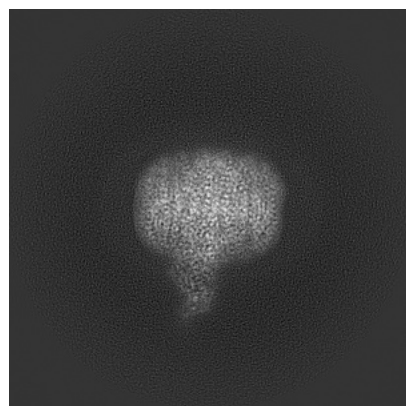
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39836. These allow visual inspection of the internal detail of the map and identification of artifacts.

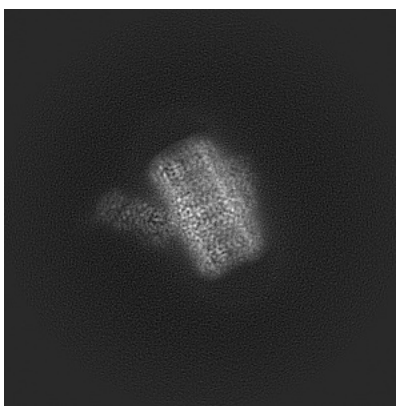
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

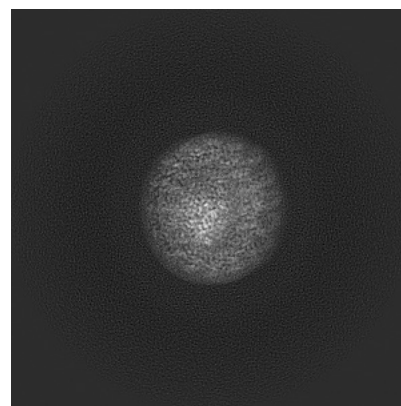
6.1.1 Primary map



X

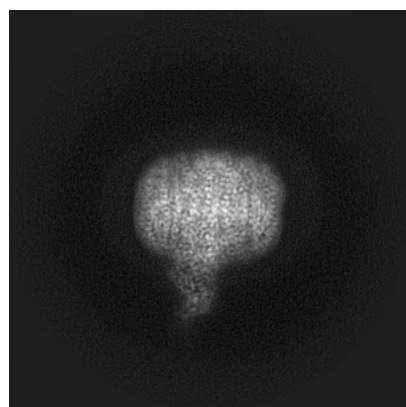


Y

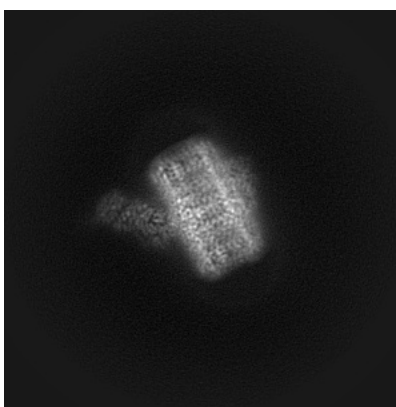


Z

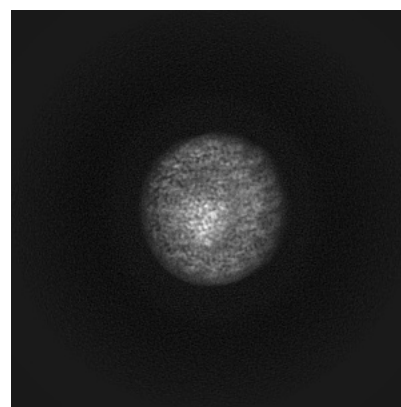
6.1.2 Raw map



X



Y

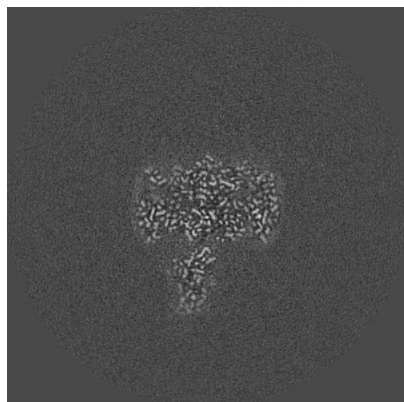


Z

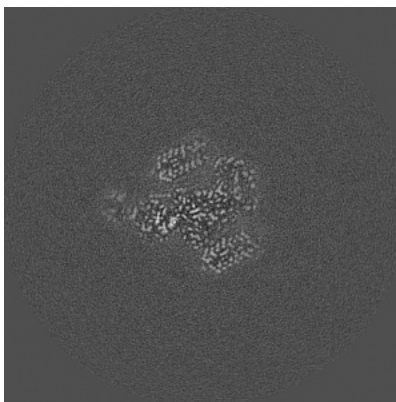
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

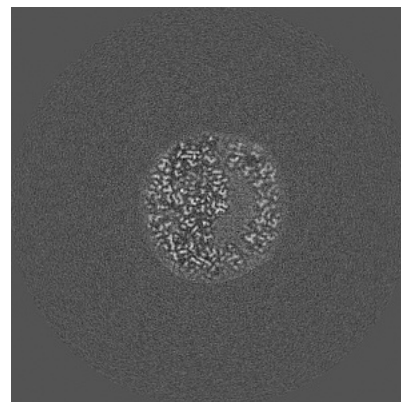
6.2.1 Primary map



X Index: 200

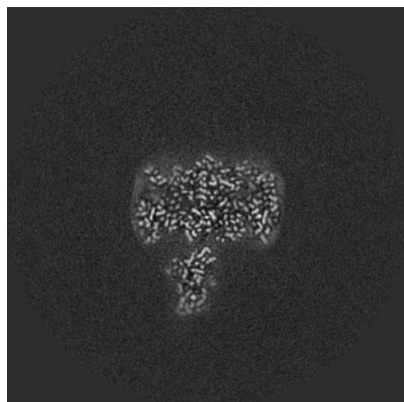


Y Index: 200

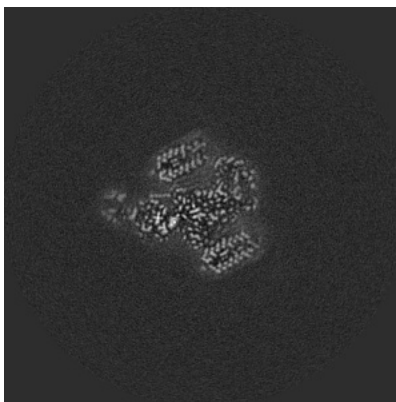


Z Index: 200

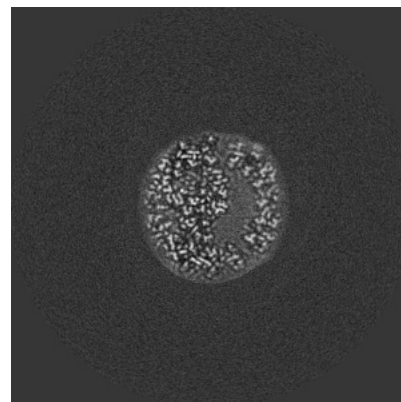
6.2.2 Raw map



X Index: 200



Y Index: 200

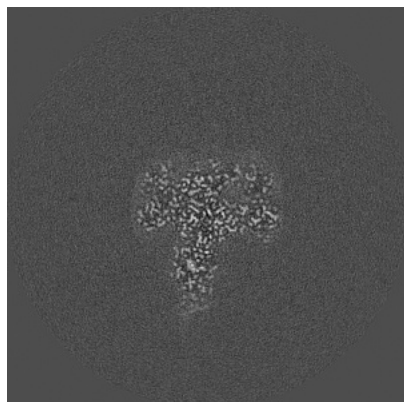


Z Index: 200

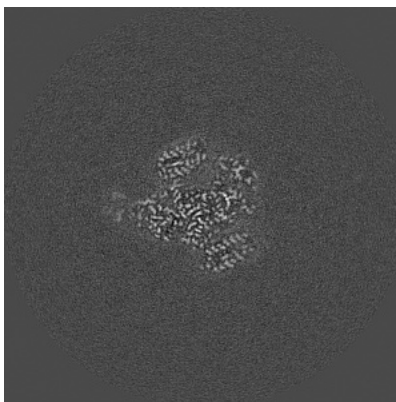
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

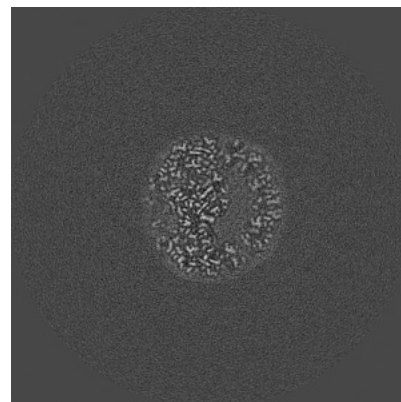
6.3.1 Primary map



X Index: 193

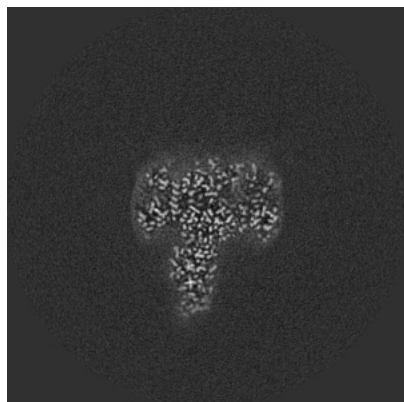


Y Index: 202

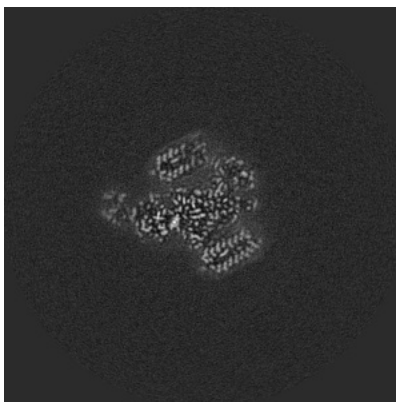


Z Index: 196

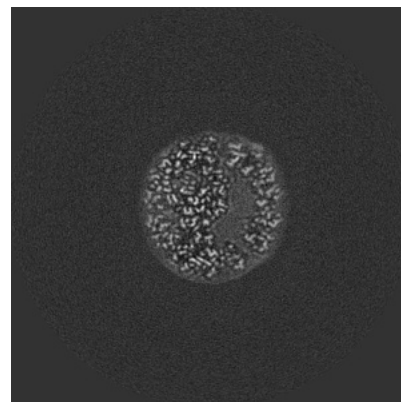
6.3.2 Raw map



X Index: 194



Y Index: 199

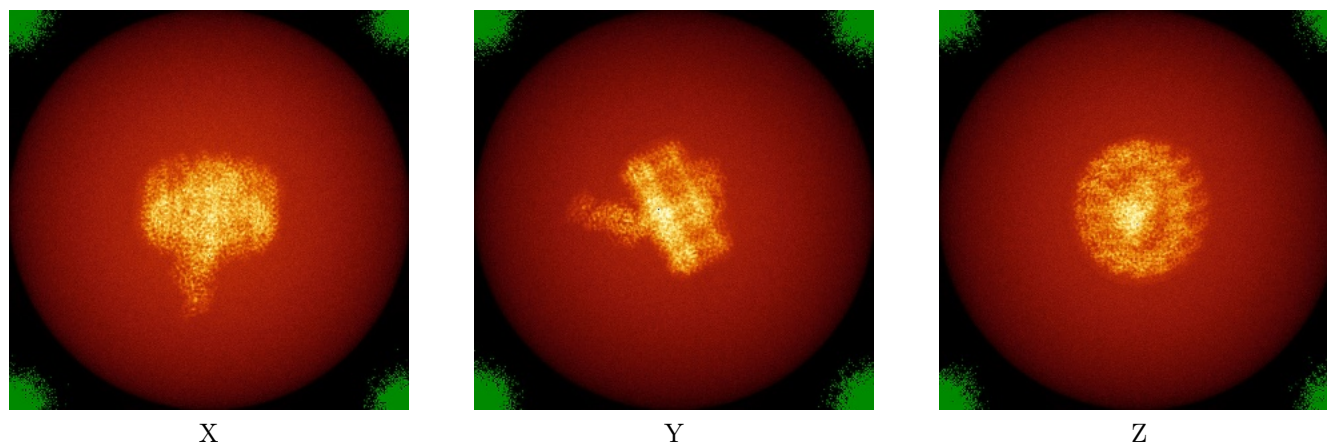


Z Index: 199

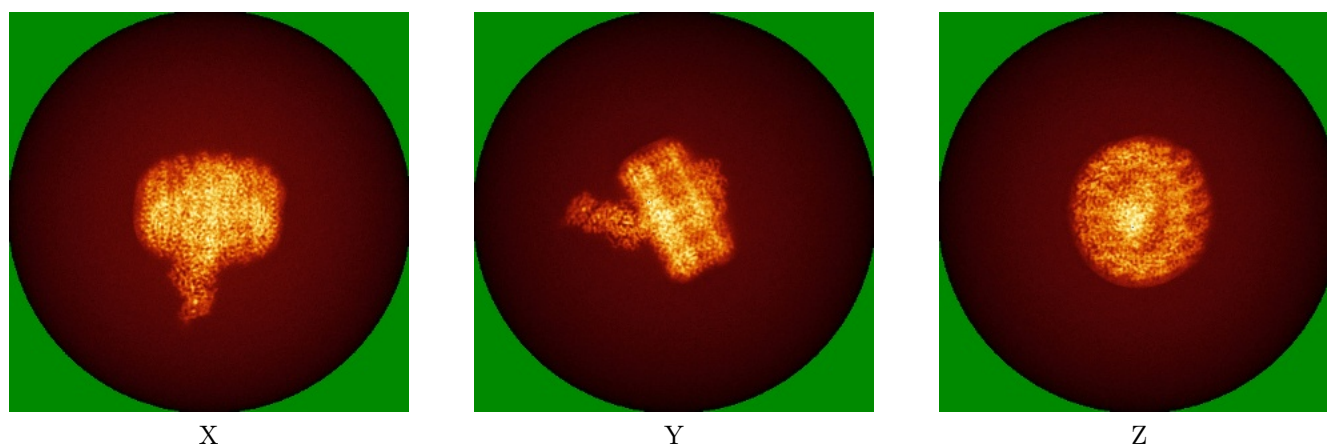
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

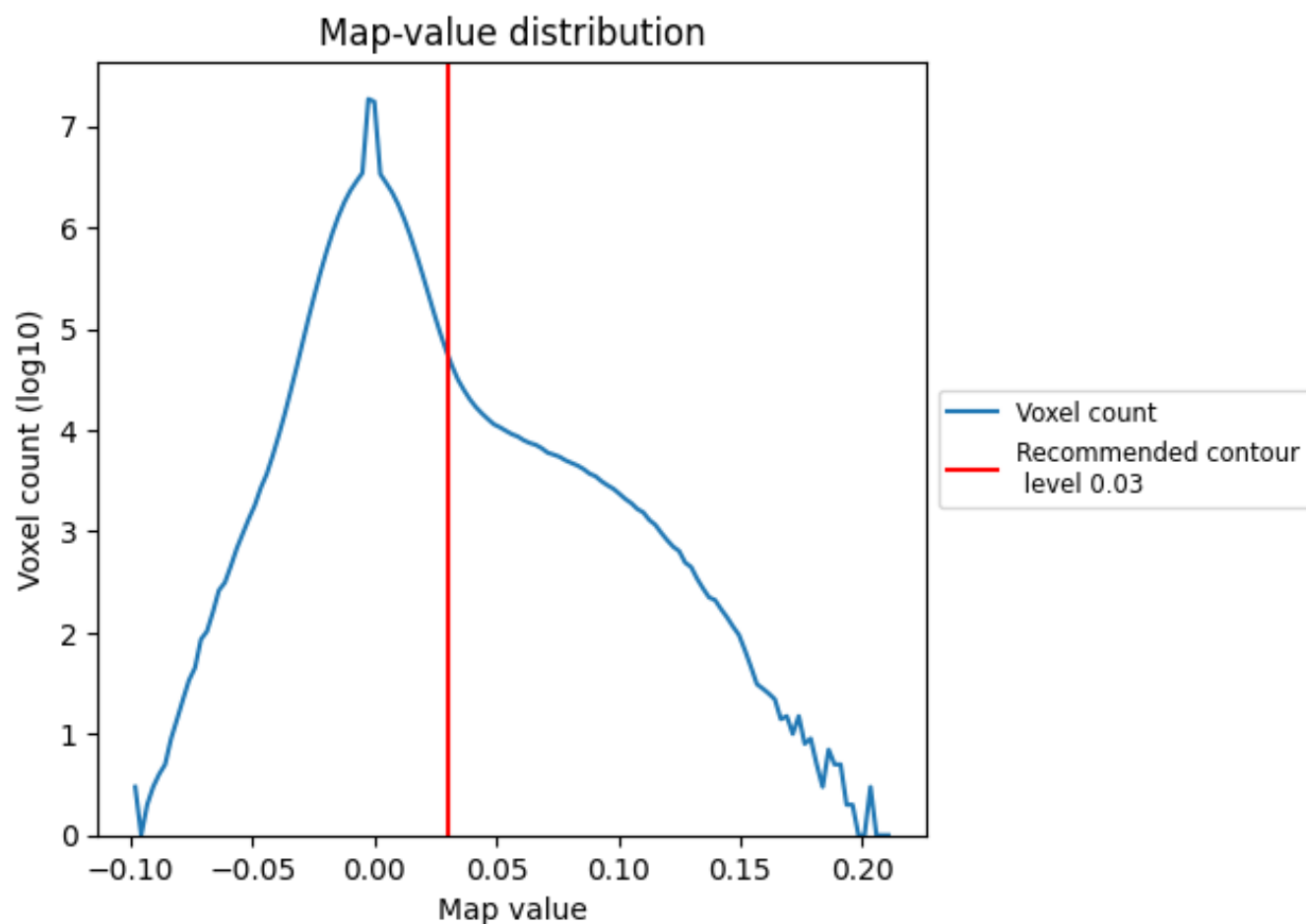
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

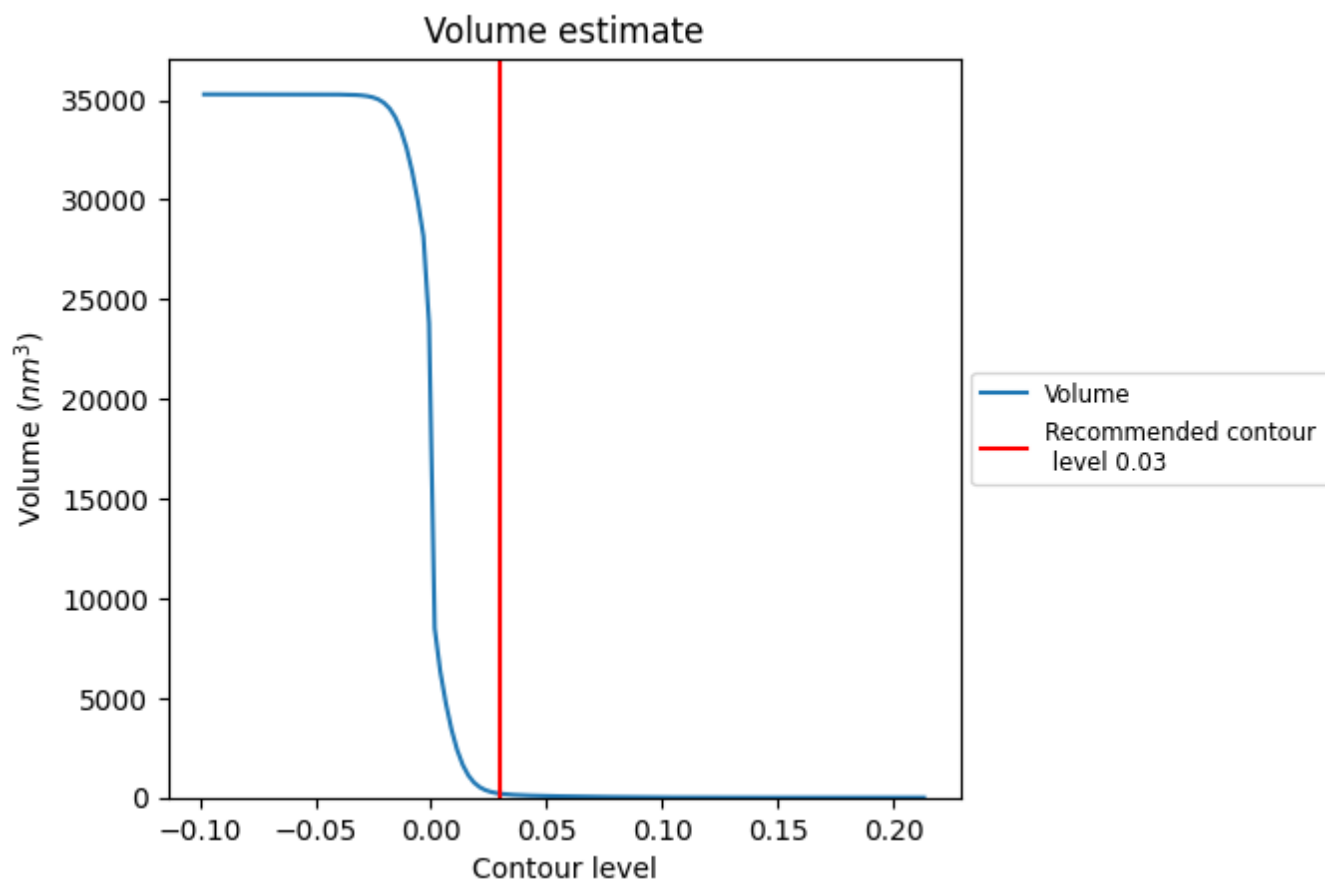
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

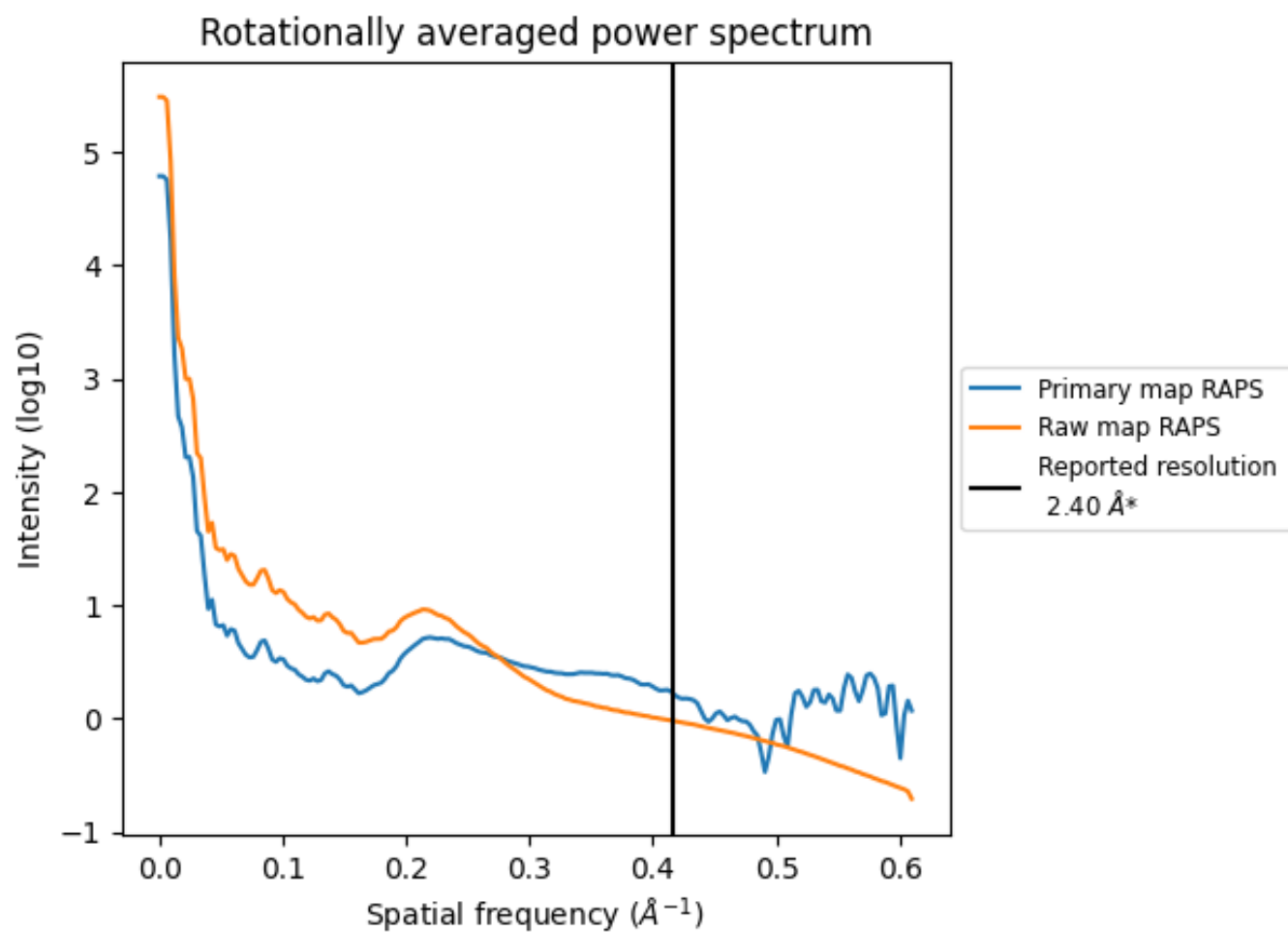
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm^3 ; this corresponds to an approximate mass of 178 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 ⓘ

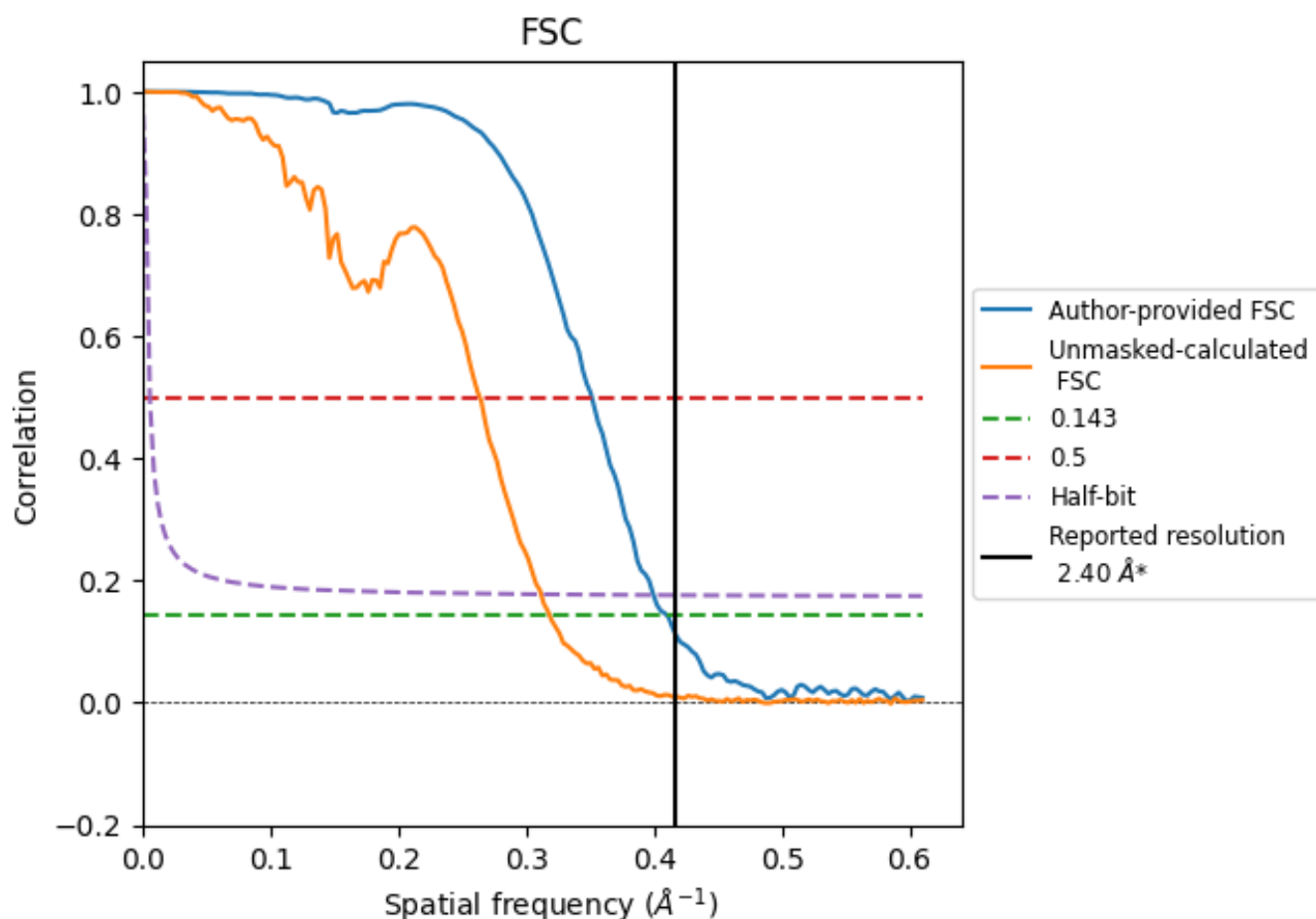


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.44	2.84	2.50
Unmasked-calculated*	3.14	3.79	3.21

*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 3.14 differs from the reported value 2.4 by more than 10 %

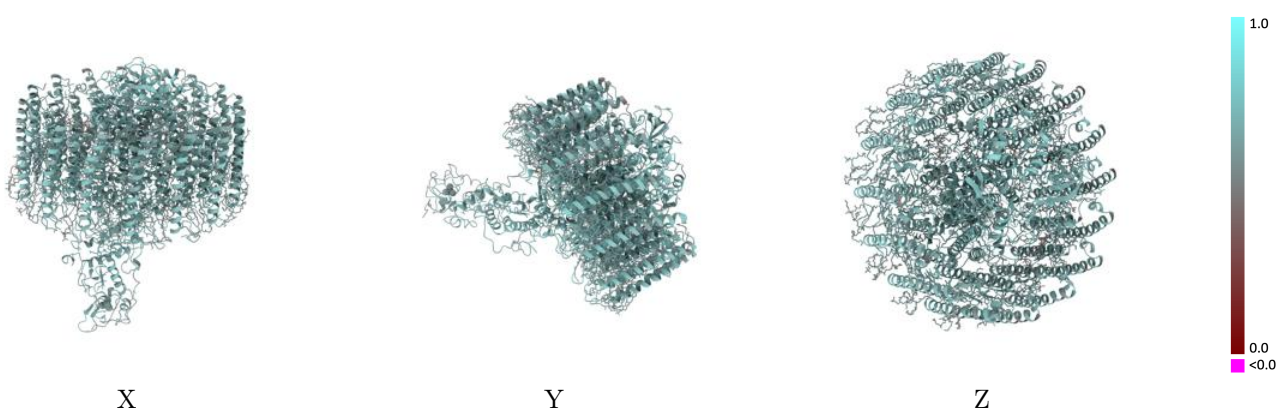
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39836 and PDB model 8Z82. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)

This section was not generated.

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

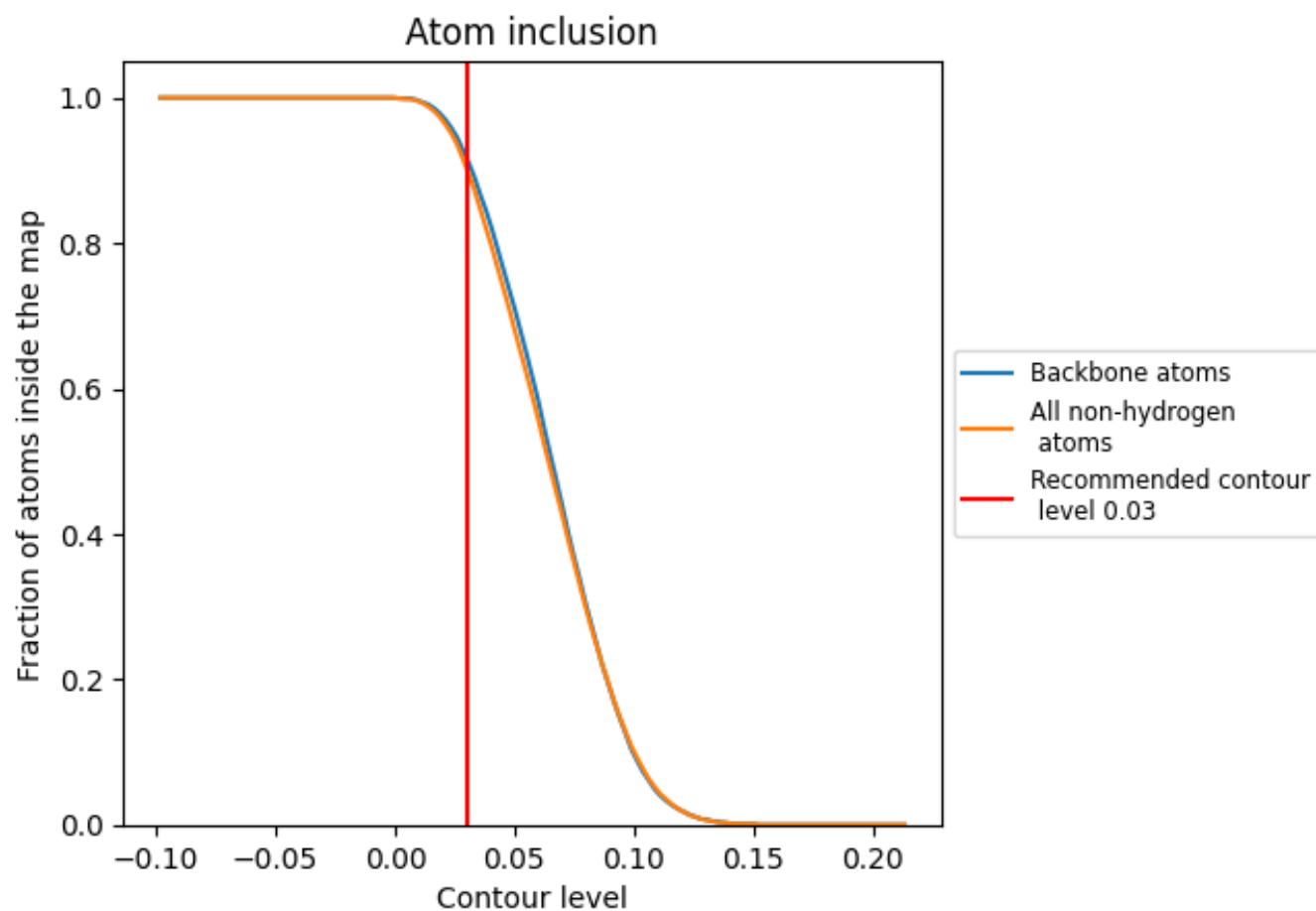


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9030	 0.6520
0	 0.8440	 0.6300
1	 0.9180	 0.6560
2	 0.8800	 0.6360
3	 0.9070	 0.6430
4	 0.8720	 0.6330
5	 0.8750	 0.6290
6	 0.8190	 0.6160
7	 0.9060	 0.6340
8	 0.8640	 0.6330
9	 0.9360	 0.6570
A	 0.9520	 0.6650
B	 0.9050	 0.6510
C	 0.9240	 0.6680
D	 0.9660	 0.6790
E	 0.9060	 0.6520
F	 0.9030	 0.6540
G	 0.8420	 0.6310
H	 0.9110	 0.6530
I	 0.9300	 0.6530
J	 0.8850	 0.6540
K	 0.9350	 0.6540
L	 0.9550	 0.6810
M	 0.9470	 0.6800
N	 0.8470	 0.6270
O	 0.8810	 0.6370
P	 0.8570	 0.6330
Q	 0.9250	 0.6470
R	 0.8920	 0.6400
S	 0.9480	 0.6700
T	 0.8590	 0.6310
U	 0.8830	 0.6340
V	 0.8440	 0.6310
W	 0.9400	 0.6580
X	 0.8540	 0.6400



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Chain	Atom inclusion	Q-score
Y	 0.9330	 0.6570
Z	 0.8400	 0.6180
a	 0.7760	 0.5860