



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 11:03 AM JST

PDB ID : 7XQD
EMDB ID : EMD-33393
Title : Structure of C-terminal truncated connexin43/Cx43/GJA1 gap junction inter-cellular channel in POPE/CHS nanodiscs (C1 symmetry)
Authors : Lee, H.J.; Cha, H.J.; Jeong, H.; Lee, S.N.; Lee, C.W.; Woo, J.S.
Deposited on : 2022-05-07
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

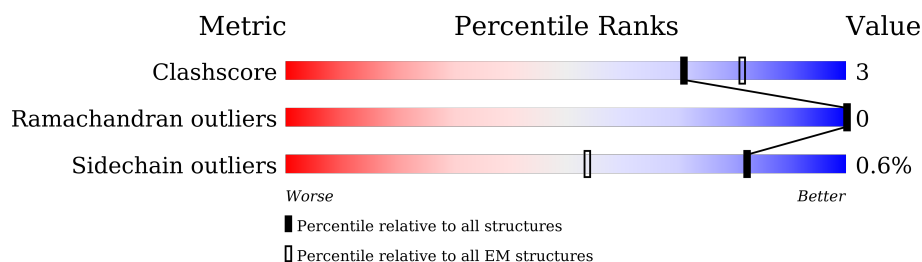
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.



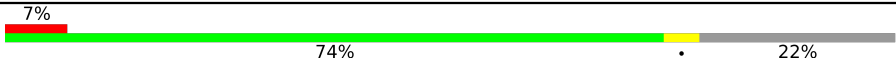

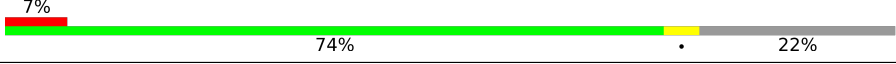

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	257	
1	B	257	
1	C	257	
1	D	257	
1	E	257	
1	F	257	
1	G	257	
1	H	257	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	257	
1	J	257	
1	K	257	
1	L	257	

2 Entry composition

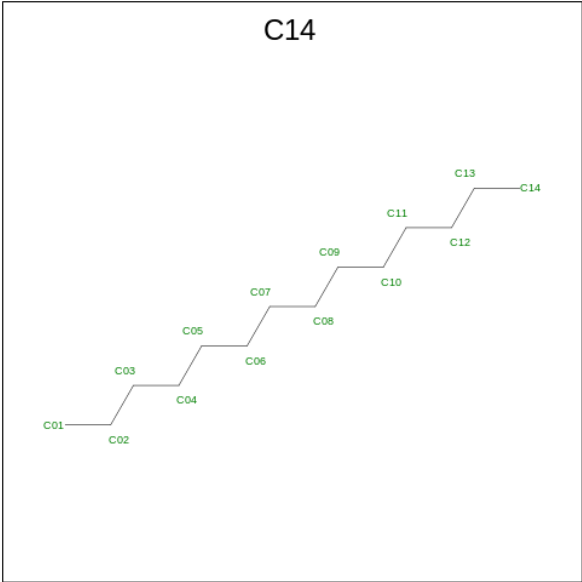
There are 5 unique types of molecules in this entry. The entry contains 48020 atoms, of which 25008 are hydrogens and 0 are deuteriums.

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 Gap junction alpha-1 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		
1	B	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		
1	C	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		
1	D	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		
1	E	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		
1	F	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		
1	G	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		
1	H	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		
1	I	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		
1	J	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		
1	K	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		
1	L	201	Total	C	H	N	O	S	0	0
			3300	1090	1664	260	278	8		

- Molecule 2 is TETRADECANE (three-letter code: C14) (formula: C₁₄H₃₀).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	H	0
			35	12	23	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			39	13	26	
2	A	1	Total	C	H	0
			41	14	27	
2	B	1	Total	C	H	0
			41	14	27	
2	B	1	Total	C	H	0
			41	14	27	
2	B	1	Total	C	H	0
			41	14	27	
2	B	1	Total	C	H	0
			39	13	26	
2	B	1	Total	C	H	0
			41	14	27	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
2	B	1	Total 35	C 12	H 23	0
2	B	1	Total 41	C 14	H 27	0
2	B	1	Total 41	C 14	H 27	0
2	B	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 39	C 13	H 26	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 35	C 12	H 23	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	C	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 39	C 13	H 26	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 35	C 12	H 23	0
2	D	1	Total 41	C 14	H 27	0
2	D	1	Total 41	C 14	H 27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
2	D	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 39	C 13	H 26	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 35	C 12	H 23	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	E	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 39	C 13	H 26	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 35	C 12	H 23	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	F	1	Total 41	C 14	H 27	0
2	G	1	Total 35	C 12	H 23	0
2	G	1	Total 41	C 14	H 27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
2	G	1	Total 41	C 14	H 27	0
2	G	1	Total 41	C 14	H 27	0
2	G	1	Total 41	C 14	H 27	0
2	G	1	Total 41	C 14	H 27	0
2	G	1	Total 41	C 14	H 27	0
2	G	1	Total 39	C 13	H 26	0
2	G	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 39	C 13	H 26	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 35	C 12	H 23	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	H	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 39	C 13	H 26	0
2	I	1	Total 41	C 14	H 27	0

Continued on next page...

Continued from previous page...

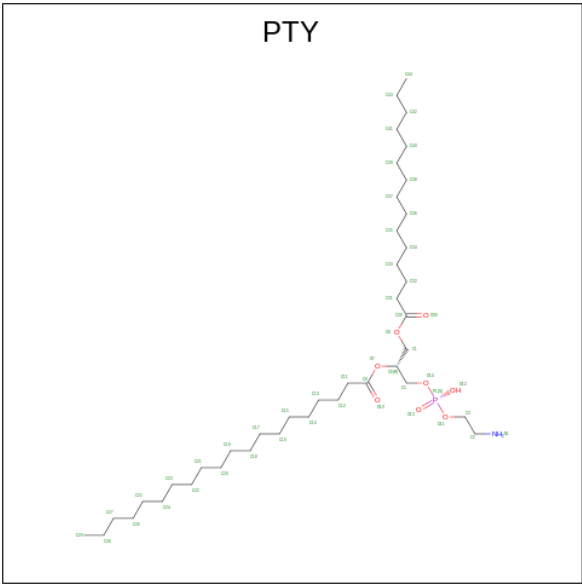
Mol	Chain	Residues	Atoms			AltConf
2	I	1	Total 35	C 12	H 23	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	I	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 39	C 13	H 26	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 35	C 12	H 23	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	J	1	Total 41	C 14	H 27	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 39	C 13	H 26	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 35	C 12	H 23	0
2	K	1	Total 41	C 14	H 27	0
2	K	1	Total 41	C 14	H 27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
2	K	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			39	13	26	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			35	12	23	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	
2	L	1	Total	C	H	0
			41	14	27	

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	E	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	E	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	F	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	F	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	G	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	G	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	H	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	H	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	I	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	I	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	J	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	J	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	K	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	
3	K	1	Total	C	H	N	O	P	0
			75	23	42	1	8	1	

Continued on next page...

Mol	Chain	Residues	Atoms						AltConf
3	L	1	Total 75	C 23	H 42	N 1	O 8	P 1	0
3	L	1	Total 75	C 23	H 42	N 1	O 8	P 1	0

- # Y01

Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 84	C 31	H 49	O 4	0
4	A	1	Total 84	C 31	H 49	O 4	0
4	B	1	Total 84	C 31	H 49	O 4	0
4	B	1	Total 84	C 31	H 49	O 4	0
4	C	1	Total 84	C 31	H 49	O 4	0
4	C	1	Total 84	C 31	H 49	O 4	0
4	D	1	Total 84	C 31	H 49	O 4	0
4	D	1	Total 84	C 31	H 49	O 4	0
4	E	1	Total 84	C 31	H 49	O 4	0



Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
4	E	1	Total	C	H	O	0
			84	31	49	4	
4	F	1	Total	C	H	O	0
			84	31	49	4	
4	F	1	Total	C	H	O	0
			84	31	49	4	
4	G	1	Total	C	H	O	0
			84	31	49	4	
4	G	1	Total	C	H	O	0
			84	31	49	4	
4	H	1	Total	C	H	O	0
			84	31	49	4	
4	H	1	Total	C	H	O	0
			84	31	49	4	
4	I	1	Total	C	H	O	0
			84	31	49	4	
4	I	1	Total	C	H	O	0
			84	31	49	4	
4	J	1	Total	C	H	O	0
			84	31	49	4	
4	J	1	Total	C	H	O	0
			84	31	49	4	
4	K	1	Total	C	H	O	0
			84	31	49	4	
4	K	1	Total	C	H	O	0
			84	31	49	4	
4	L	1	Total	C	H	O	0
			84	31	49	4	
4	L	1	Total	C	H	O	0
			84	31	49	4	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	21	Total	O	0
			21	21	
5	B	25	Total	O	0
			25	25	
5	C	23	Total	O	0
			23	23	
5	D	22	Total	O	0
			22	22	

Continued on next page...

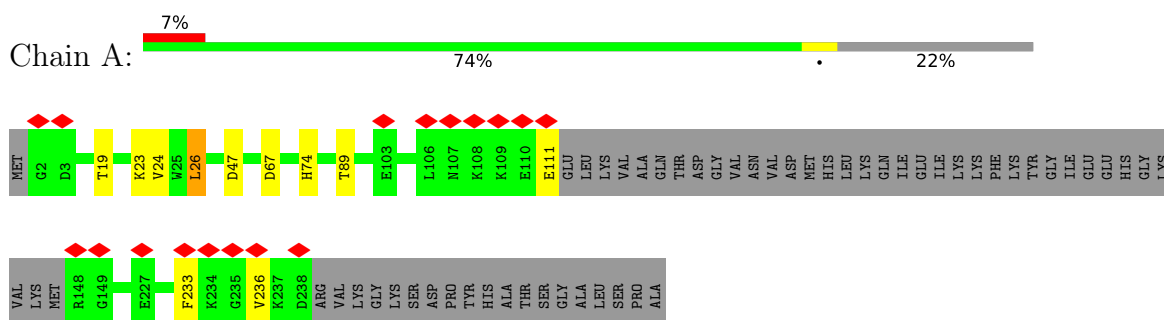
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
5	E	24	Total 24	O 24	0
5	F	23	Total 23	O 23	0
5	G	21	Total 21	O 21	0
5	H	22	Total 22	O 22	0
5	I	21	Total 21	O 21	0
5	J	22	Total 22	O 22	0
5	K	24	Total 24	O 24	0
5	L	24	Total 24	O 24	0

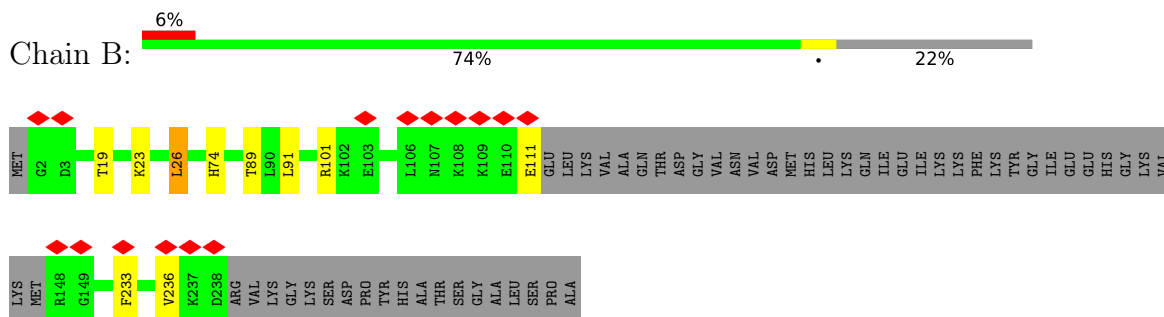
3 Residue-property plots [i](#)

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

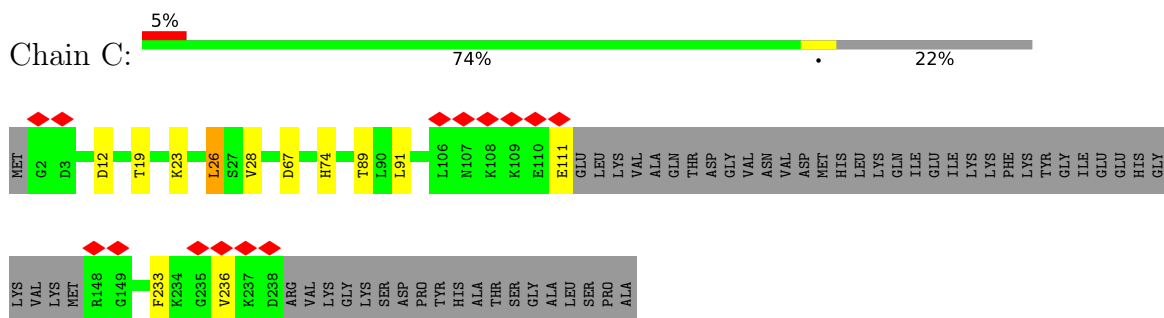
- Molecule 1: Gap junction alpha-1 protein



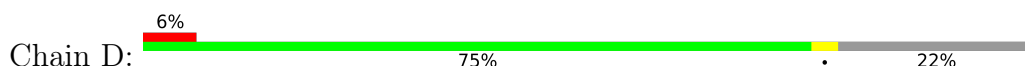
- Molecule 1: Gap junction alpha-1 protein

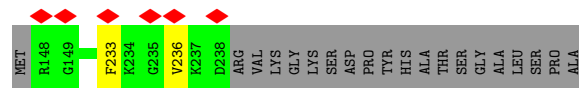
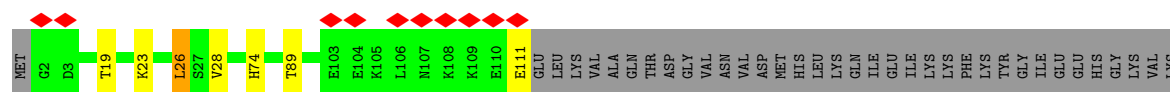


- Molecule 1: Gap junction alpha-1 protein

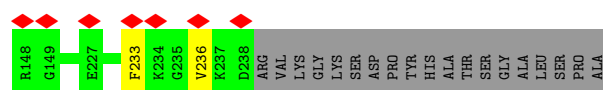
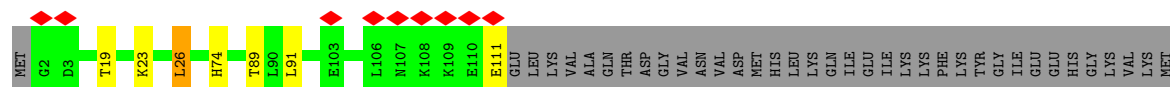
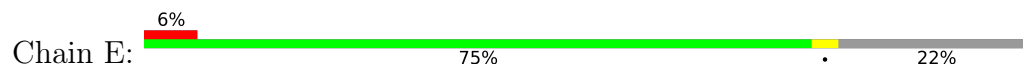


- Molecule 1: Gap junction alpha-1 protein

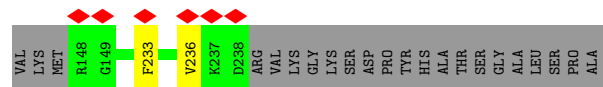
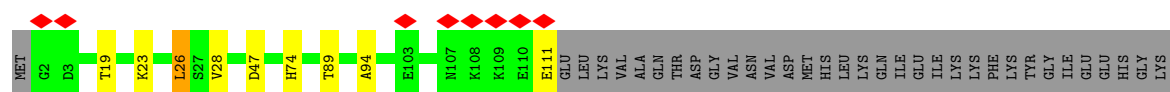
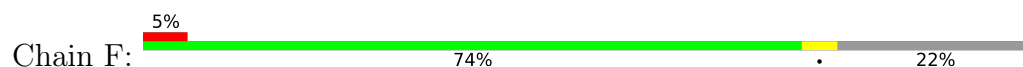




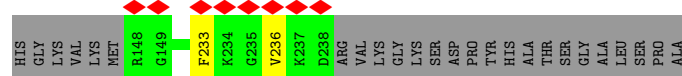
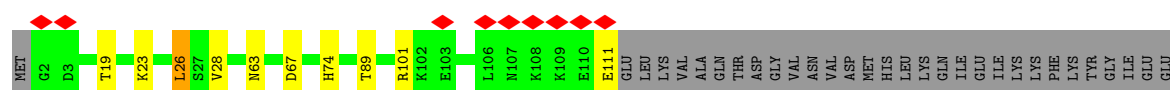
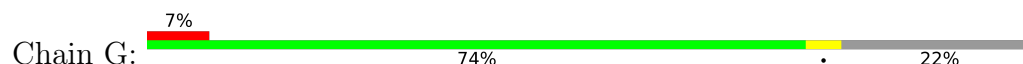
- Molecule 1: Gap junction alpha-1 protein



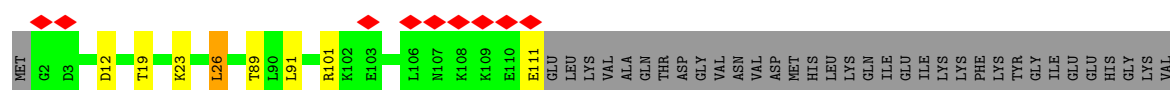
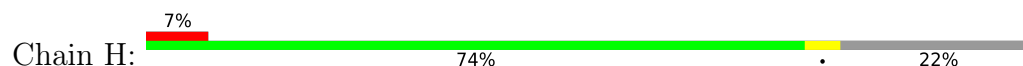
- Molecule 1: Gap junction alpha-1 protein

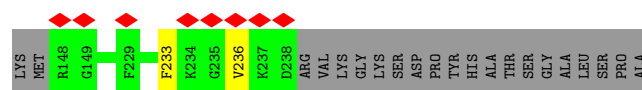


- Molecule 1: Gap junction alpha-1 protein

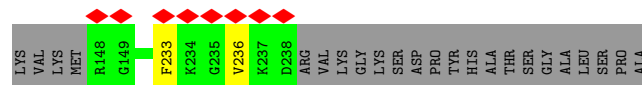
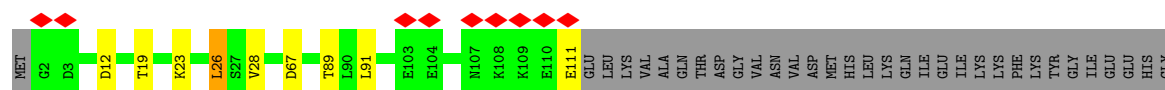
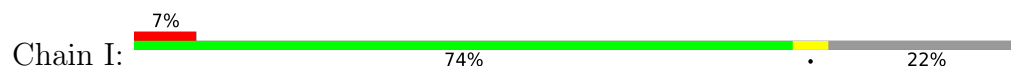


- Molecule 1: Gap junction alpha-1 protein

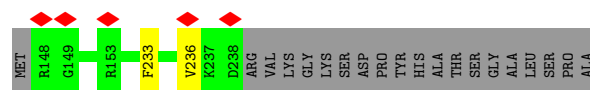
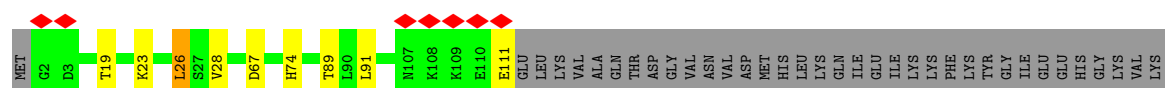
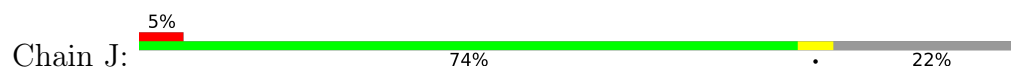




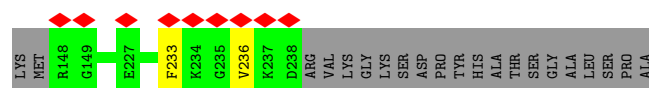
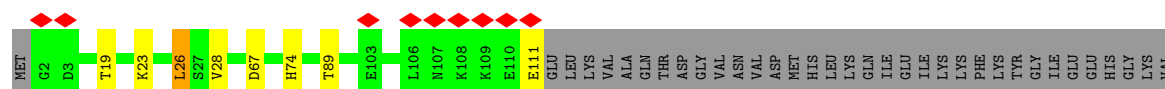
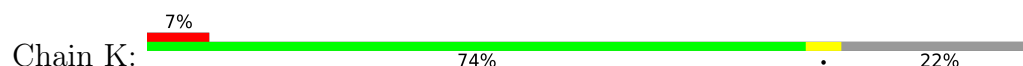
- Molecule 1: Gap junction alpha-1 protein



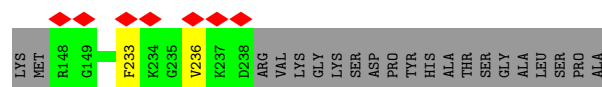
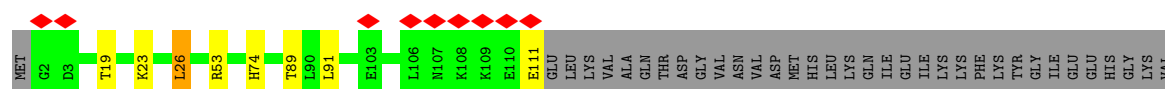
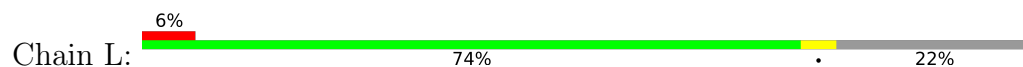
- Molecule 1: Gap junction alpha-1 protein



- Molecule 1: Gap junction alpha-1 protein



- Molecule 1: Gap junction alpha-1 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	325564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72.42	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (\AA)	271.36, 271.36, 271.36	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.84799993, 0.84799993, 0.84799993	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C14, Y01, PTY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/1679	0.43	0/2274
1	B	0.26	0/1679	0.43	0/2274
1	C	0.26	0/1679	0.43	0/2274
1	D	0.26	0/1679	0.43	0/2274
1	E	0.26	0/1679	0.43	0/2274
1	F	0.26	0/1679	0.43	0/2274
1	G	0.26	0/1679	0.43	0/2274
1	H	0.26	0/1679	0.43	0/2274
1	I	0.26	0/1679	0.43	0/2274
1	J	0.26	0/1679	0.43	0/2274
1	K	0.26	0/1679	0.43	0/2274
1	L	0.26	0/1679	0.43	0/2274
All	All	0.26	0/20148	0.43	0/27288

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1636	1664	1664	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1636	1664	1664	9	0
1	C	1636	1664	1664	11	0
1	D	1636	1664	1664	8	0
1	E	1636	1664	1664	8	0
1	F	1636	1664	1664	10	0
1	G	1636	1664	1664	11	0
1	H	1636	1664	1664	9	0
1	I	1636	1664	1664	10	0
1	J	1636	1664	1664	10	0
1	K	1636	1664	1664	9	0
1	L	1636	1664	1664	9	0
2	A	123	238	255	0	0
2	B	123	238	255	0	0
2	C	123	238	255	0	0
2	D	123	238	255	0	0
2	E	123	238	255	0	0
2	F	123	238	255	0	0
2	G	123	238	255	0	0
2	H	123	238	255	0	0
2	I	123	238	255	0	0
2	J	123	238	255	0	0
2	K	123	238	255	0	0
2	L	123	238	255	0	0
3	A	66	84	78	1	0
3	B	66	84	78	0	0
3	C	66	84	78	0	0
3	D	66	84	78	0	0
3	E	66	84	78	0	0
3	F	66	84	78	1	0
3	G	66	84	78	1	0
3	H	66	84	78	1	0
3	I	66	84	78	0	0
3	J	66	84	78	0	0
3	K	66	84	78	0	0
3	L	66	84	78	1	0
4	A	70	98	98	8	0
4	B	70	98	98	8	0
4	C	70	98	98	7	0
4	D	70	98	98	7	0
4	E	70	98	98	7	0
4	F	70	98	98	7	0
4	G	70	98	98	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	70	98	98	8	0
4	I	70	98	98	8	0
4	J	70	98	98	7	0
4	K	70	98	98	7	0
4	L	70	98	98	7	0
5	A	21	0	0	3	0
5	B	25	0	0	1	0
5	C	23	0	0	2	0
5	D	22	0	0	1	0
5	E	24	0	0	1	0
5	F	23	0	0	2	0
5	G	21	0	0	3	0
5	H	22	0	0	0	0
5	I	21	0	0	1	0
5	J	22	0	0	2	0
5	K	24	0	0	2	0
5	L	24	0	0	2	0
All	All	23012	25008	25140	156	0

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

All (156) 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:D:74:HIS:ND1	5:D:401:HOH:O	2.18	0.76
1:C:74:HIS:ND1	5:C:402:HOH:O	2.18	0.76
1:E:74:HIS:ND1	5:E:401:HOH:O	2.18	0.76
1:K:74:HIS:ND1	5:K:402:HOH:O	2.19	0.75
1:J:74:HIS:ND1	5:J:402:HOH:O	2.20	0.73
1:F:74:HIS:ND1	5:F:402:HOH:O	2.22	0.72
1:G:63:ASN:OD1	5:G:401:HOH:O	2.07	0.72
1:L:74:HIS:ND1	5:L:401:HOH:O	2.23	0.72
1:G:74:HIS:ND1	5:G:403:HOH:O	2.24	0.71
1:B:74:HIS:ND1	5:B:401:HOH:O	2.24	0.70
1:F:47:ASP:OD1	5:F:401:HOH:O	2.09	0.69
1:A:67:ASP:OD1	5:A:401:HOH:O	2.11	0.69
1:A:74:HIS:ND1	5:A:403:HOH:O	2.25	0.68
1:C:67:ASP:OD1	5:C:401:HOH:O	2.12	0.68
1:K:67:ASP:OD1	5:K:401:HOH:O	2.13	0.66
1:I:67:ASP:OD1	5:I:401:HOH:O	2.14	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:ASP:OD1	5:G:402:HOH:O	2.14	0.63
1:G:111:GLU:N	1:G:111:GLU:OE1	2.32	0.62
1:F:111:GLU:OE1	1:F:111:GLU:N	2.32	0.62
1:E:91:LEU:HD23	1:F:28:VAL:HG21	1.81	0.61
1:A:111:GLU:N	1:A:111:GLU:OE1	2.32	0.61
1:J:91:LEU:HD23	1:K:28:VAL:HG21	1.82	0.61
1:B:111:GLU:OE1	1:B:111:GLU:N	2.32	0.60
1:H:111:GLU:N	1:H:111:GLU:OE1	2.32	0.60
1:L:111:GLU:N	1:L:111:GLU:OE1	2.32	0.60
1:B:89:THR:HG21	4:B:312:Y01:CAD	2.32	0.60
1:E:111:GLU:N	1:E:111:GLU:OE1	2.32	0.60
1:E:89:THR:HG21	4:E:312:Y01:CAD	2.32	0.60
1:F:89:THR:HG21	4:F:313:Y01:CAD	2.32	0.60
1:I:111:GLU:N	1:I:111:GLU:OE1	2.32	0.60
1:L:89:THR:HG21	4:L:313:Y01:CAD	2.32	0.60
1:I:89:THR:HG21	4:I:312:Y01:CAD	2.32	0.60
1:J:67:ASP:OD1	5:J:401:HOH:O	2.16	0.60
4:D:311:Y01:HAE2	4:D:311:Y01:HAC1	1.84	0.60
1:G:89:THR:HG21	4:G:307:Y01:CAD	2.32	0.60
1:D:89:THR:HG21	4:D:312:Y01:CAD	2.32	0.60
4:I:311:Y01:HAC1	4:I:311:Y01:HAE2	1.84	0.60
4:K:311:Y01:HAE2	4:K:311:Y01:HAC1	1.84	0.60
1:K:89:THR:HG21	4:K:312:Y01:CAD	2.32	0.60
1:A:89:THR:HG21	4:A:307:Y01:CAD	2.32	0.59
4:A:306:Y01:HAE2	4:A:306:Y01:HAC1	1.84	0.59
4:B:311:Y01:HAE2	4:B:311:Y01:HAC1	1.84	0.59
1:H:89:THR:HG21	4:H:312:Y01:CAD	2.32	0.59
4:H:311:Y01:HAE2	4:H:311:Y01:HAC1	1.84	0.59
4:L:312:Y01:HAE2	4:L:312:Y01:HAC1	1.84	0.59
1:J:89:THR:HG21	4:J:312:Y01:CAD	2.32	0.59
1:J:111:GLU:OE1	1:J:111:GLU:N	2.32	0.59
4:E:311:Y01:HAC1	4:E:311:Y01:HAE2	1.84	0.59
1:C:89:THR:HG21	4:C:312:Y01:CAD	2.32	0.58
1:C:111:GLU:N	1:C:111:GLU:OE1	2.32	0.58
4:F:312:Y01:HAE2	4:F:312:Y01:HAC1	1.84	0.58
4:C:311:Y01:HAE2	4:C:311:Y01:HAC1	1.84	0.58
4:J:311:Y01:HAE2	4:J:311:Y01:HAC1	1.84	0.58
4:G:306:Y01:HAE2	4:G:306:Y01:HAC1	1.84	0.58
1:C:26:LEU:HD23	4:C:312:Y01:HAM2	1.86	0.57
1:D:26:LEU:HD23	4:D:312:Y01:HAM2	1.86	0.57
1:J:26:LEU:HD23	4:J:312:Y01:HAM2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:26:LEU:HD23	4:K:312:Y01:HAM2	1.86	0.57
1:K:111:GLU:N	1:K:111:GLU:OE1	2.32	0.57
1:I:26:LEU:HD23	4:I:312:Y01:HAM2	1.86	0.57
1:B:26:LEU:HD23	4:B:312:Y01:HAM2	1.86	0.57
4:B:312:Y01:HAO1	4:B:312:Y01:HAA1	1.87	0.57
1:D:111:GLU:N	1:D:111:GLU:OE1	2.32	0.57
4:A:307:Y01:HAA1	4:A:307:Y01:HAO1	1.87	0.57
4:H:312:Y01:HAA1	4:H:312:Y01:HAO1	1.87	0.57
4:I:312:Y01:HAA1	4:I:312:Y01:HAO1	1.87	0.57
1:E:26:LEU:HD23	4:E:312:Y01:HAM2	1.86	0.57
1:L:26:LEU:HD23	4:L:313:Y01:HAM2	1.86	0.57
4:G:307:Y01:HAO1	4:G:307:Y01:HAA1	1.87	0.56
4:F:313:Y01:HAO1	4:F:313:Y01:HAA1	1.87	0.56
1:H:26:LEU:HD23	4:H:312:Y01:HAM2	1.86	0.56
1:F:26:LEU:HD23	4:F:313:Y01:HAM2	1.86	0.56
1:A:26:LEU:HD23	4:A:307:Y01:HAM2	1.86	0.56
4:D:312:Y01:HAA1	4:D:312:Y01:HAO1	1.87	0.56
4:E:312:Y01:HAA1	4:E:312:Y01:HAO1	1.87	0.56
1:G:26:LEU:HD23	4:G:307:Y01:HAM2	1.86	0.56
4:J:312:Y01:HAO1	4:J:312:Y01:HAA1	1.87	0.56
4:C:312:Y01:HAO1	4:C:312:Y01:HAA1	1.87	0.56
4:K:312:Y01:HAA1	4:K:312:Y01:HAO1	1.87	0.56
4:L:313:Y01:HAA1	4:L:313:Y01:HAO1	1.87	0.56
1:A:89:THR:HG21	4:A:307:Y01:HAD3	1.88	0.55
1:H:89:THR:HG21	4:H:312:Y01:HAD3	1.89	0.55
1:D:89:THR:HG21	4:D:312:Y01:HAD3	1.89	0.55
1:E:89:THR:HG21	4:E:312:Y01:HAD3	1.88	0.55
1:L:89:THR:HG21	4:L:313:Y01:HAD3	1.88	0.55
1:K:89:THR:HG21	4:K:312:Y01:HAD3	1.88	0.55
1:F:89:THR:HG21	4:F:313:Y01:HAD3	1.88	0.55
1:I:89:THR:HG21	4:I:312:Y01:HAD3	1.88	0.55
1:B:89:THR:HG21	4:B:312:Y01:HAD3	1.88	0.55
1:C:89:THR:HG21	4:C:312:Y01:HAD3	1.88	0.55
1:G:89:THR:HG21	4:G:307:Y01:HAD3	1.89	0.55
1:J:89:THR:HG21	4:J:312:Y01:HAD3	1.88	0.55
1:H:91:LEU:HD23	1:I:28:VAL:HG21	1.90	0.53
1:B:19:THR:O	1:B:23:LYS:NZ	2.41	0.53
1:L:19:THR:O	1:L:23:LYS:NZ	2.42	0.53
1:I:19:THR:O	1:I:23:LYS:NZ	2.42	0.52
1:J:19:THR:O	1:J:23:LYS:NZ	2.41	0.52
1:H:101:ARG:NH2	1:I:12:ASP:OD1	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:O	1:A:23:LYS:NZ	2.41	0.51
1:H:19:THR:O	1:H:23:LYS:NZ	2.42	0.51
1:B:91:LEU:HD23	1:C:28:VAL:HG21	1.93	0.51
1:C:19:THR:O	1:C:23:LYS:NZ	2.41	0.50
1:E:19:THR:O	1:E:23:LYS:NZ	2.41	0.49
1:D:19:THR:O	1:D:23:LYS:NZ	2.42	0.48
1:I:91:LEU:HD23	1:J:28:VAL:HG21	1.96	0.48
1:K:19:THR:O	1:K:23:LYS:NZ	2.41	0.48
1:F:19:THR:O	1:F:23:LYS:NZ	2.41	0.47
1:G:19:THR:O	1:G:23:LYS:NZ	2.41	0.47
1:A:47:ASP:OD1	5:A:402:HOH:O	2.20	0.47
4:B:312:Y01:HAE2	4:B:312:Y01:HAC1	1.98	0.46
4:F:313:Y01:HAE2	4:F:313:Y01:HAC1	1.98	0.46
4:G:307:Y01:HAE2	4:G:307:Y01:HAC1	1.98	0.46
4:H:312:Y01:HAE2	4:H:312:Y01:HAC1	1.98	0.46
4:I:312:Y01:HAE2	4:I:312:Y01:HAC1	1.98	0.46
4:A:307:Y01:HAC1	4:A:307:Y01:HAE2	1.98	0.46
4:L:313:Y01:HAE2	4:L:313:Y01:HAC1	1.98	0.46
4:E:312:Y01:HAC1	4:E:312:Y01:HAE2	1.98	0.46
4:L:313:Y01:HAD1	4:L:313:Y01:OAW	2.17	0.45
1:B:101:ARG:NH2	1:C:12:ASP:OD1	2.49	0.45
4:D:312:Y01:HAD1	4:D:312:Y01:OAW	2.16	0.45
4:D:312:Y01:HAE2	4:D:312:Y01:HAC1	1.98	0.45
4:K:312:Y01:HAE2	4:K:312:Y01:HAC1	1.98	0.45
4:E:312:Y01:HAD1	4:E:312:Y01:OAW	2.17	0.45
4:K:312:Y01:HAD1	4:K:312:Y01:OAW	2.17	0.45
4:C:312:Y01:HAD1	4:C:312:Y01:OAW	2.17	0.45
4:J:312:Y01:HAE2	4:J:312:Y01:HAC1	1.98	0.45
4:C:312:Y01:HAE2	4:C:312:Y01:HAC1	1.98	0.45
4:J:312:Y01:OAW	4:J:312:Y01:HAD1	2.17	0.45
4:F:313:Y01:HAD1	4:F:313:Y01:OAW	2.16	0.45
4:G:307:Y01:OAW	4:G:307:Y01:HAD1	2.17	0.45
4:B:312:Y01:OAW	4:B:312:Y01:HAD1	2.17	0.45
4:H:312:Y01:HAD1	4:H:312:Y01:OAW	2.17	0.44
4:I:312:Y01:HAD1	4:I:312:Y01:OAW	2.16	0.44
4:A:307:Y01:HAD1	4:A:307:Y01:OAW	2.17	0.44
1:C:91:LEU:HD23	1:D:28:VAL:HG21	2.00	0.43
1:B:233:PHE:O	1:B:236:VAL:HG12	2.19	0.43
1:L:53:ARG:NH1	5:L:403:HOH:O	2.51	0.43
1:I:233:PHE:O	1:I:236:VAL:HG12	2.19	0.43
1:J:233:PHE:O	1:J:236:VAL:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:PHE:O	1:C:236:VAL:HG12	2.19	0.42
1:L:233:PHE:O	1:L:236:VAL:HG12	2.19	0.42
1:E:233:PHE:O	1:E:236:VAL:HG12	2.19	0.42
1:G:101:ARG:NH2	1:H:12:ASP:OD1	2.53	0.42
1:A:233:PHE:O	1:A:236:VAL:HG12	2.19	0.42
1:G:233:PHE:O	1:G:236:VAL:HG12	2.19	0.41
1:F:233:PHE:O	1:F:236:VAL:HG12	2.19	0.41
1:D:233:PHE:O	1:D:236:VAL:HG12	2.19	0.41
1:H:233:PHE:O	1:H:236:VAL:HG12	2.19	0.41
1:K:233:PHE:O	1:K:236:VAL:HG12	2.19	0.41
1:G:28:VAL:HG21	1:L:91:LEU:HD23	2.02	0.41
3:G:308:PTY:H332	4:H:311:Y01:HAT2	2.03	0.40
4:A:306:Y01:HAT2	3:F:301:PTY:H332	2.03	0.40
4:G:306:Y01:HAT2	3:L:301:PTY:H332	2.04	0.40
1:A:24:VAL:HG13	1:F:94:ALA:HB3	2.03	0.40
3:A:308:PTY:H332	4:B:311:Y01:HAT2	2.04	0.40
3:H:313:PTY:H332	4:I:311:Y01:HAT2	2.04	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	A	197/257 (77%)	193 (98%)	4 (2%)	0	100	100
1	B	197/257 (77%)	193 (98%)	4 (2%)	0	100	100
1	C	197/257 (77%)	193 (98%)	4 (2%)	0	100	100
1	D	197/257 (77%)	193 (98%)	4 (2%)	0	100	100
1	E	197/257 (77%)	193 (98%)	4 (2%)	0	100	100
1	F	197/257 (77%)	193 (98%)	4 (2%)	0	100	100
1	G	197/257 (77%)	193 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	197/257 (77%)	193 (98%)	4 (2%)	0	100	100
1	I	197/257 (77%)	193 (98%)	4 (2%)	0	100	100
1	J	197/257 (77%)	193 (98%)	4 (2%)	0	100	100
1	K	197/257 (77%)	193 (98%)	4 (2%)	0	100	100
1	L	197/257 (77%)	193 (98%)	4 (2%)	0	100	100
All	All	2364/3084 (77%)	2316 (98%)	48 (2%)	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	A	180/227 (79%)	179 (99%)	1 (1%)	84	94
1	B	180/227 (79%)	179 (99%)	1 (1%)	84	94
1	C	180/227 (79%)	179 (99%)	1 (1%)	84	94
1	D	180/227 (79%)	179 (99%)	1 (1%)	84	94
1	E	180/227 (79%)	179 (99%)	1 (1%)	84	94
1	F	180/227 (79%)	179 (99%)	1 (1%)	84	94
1	G	180/227 (79%)	179 (99%)	1 (1%)	84	94
1	H	180/227 (79%)	179 (99%)	1 (1%)	84	94
1	I	180/227 (79%)	179 (99%)	1 (1%)	84	94
1	J	180/227 (79%)	179 (99%)	1 (1%)	84	94
1	K	180/227 (79%)	179 (99%)	1 (1%)	84	94
1	L	180/227 (79%)	179 (99%)	1 (1%)	84	94
All	All	2160/2724 (79%)	2148 (99%)	12 (1%)	82	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	B	26	LEU
1	C	26	LEU
1	D	26	LEU
1	E	26	LEU
1	F	26	LEU
1	G	26	LEU
1	H	26	LEU
1	I	26	LEU
1	J	26	LEU
1	K	26	LEU
1	L	26	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

156 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C14	C	302	-	13,13,13	0.29	0	12,12,12	0.83	0
2	C14	G	304	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	E	306	-	11,11,13	0.28	0	10,10,12	0.81	0
4	Y01	C	311	-	38,38,38	0.68	0	57,57,57	0.95	1 (1%)
2	C14	B	308	-	13,13,13	0.27	0	12,12,12	0.84	0
2	C14	D	307	-	13,13,13	0.30	0	12,12,12	0.76	0
2	C14	J	306	-	11,11,13	0.28	0	10,10,12	0.81	0
2	C14	L	302	-	13,13,13	0.29	0	12,12,12	0.80	0
2	C14	D	308	-	13,13,13	0.27	0	12,12,12	0.84	0
4	Y01	A	306	-	38,38,38	0.68	0	57,57,57	0.95	1 (1%)
2	C14	D	305	-	13,13,13	0.29	0	12,12,12	0.81	0
3	PTY	E	313	-	32,32,49	1.06	4 (12%)	35,37,54	0.97	2 (5%)
4	Y01	G	307	-	38,38,38	0.68	0	57,57,57	1.05	4 (7%)
2	C14	C	309	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	J	309	-	13,13,13	0.29	0	12,12,12	0.81	0
3	PTY	A	305	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
4	Y01	K	311	-	38,38,38	0.68	0	57,57,57	0.95	1 (1%)
2	C14	E	301	-	13,13,13	0.29	0	12,12,12	0.80	0
4	Y01	C	312	-	38,38,38	0.68	0	57,57,57	1.05	4 (7%)
4	Y01	K	312	-	38,38,38	0.68	0	57,57,57	1.05	4 (7%)
2	C14	J	305	-	13,13,13	0.29	0	12,12,12	0.81	0
4	Y01	J	312	-	38,38,38	0.68	0	57,57,57	1.05	4 (7%)
2	C14	F	308	-	13,13,13	0.30	0	12,12,12	0.76	0
2	C14	E	309	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	D	303	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	C	301	-	13,13,13	0.29	0	12,12,12	0.80	0
2	C14	A	311	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	B	305	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	C	303	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	G	311	-	13,13,13	0.29	0	12,12,12	0.81	0
3	PTY	C	313	-	32,32,49	1.06	4 (12%)	35,37,54	0.97	2 (5%)
3	PTY	L	301	-	32,32,49	1.06	4 (12%)	35,37,54	0.97	2 (5%)
2	C14	I	301	-	13,13,13	0.29	0	12,12,12	0.80	0
3	PTY	C	310	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
2	C14	I	306	-	11,11,13	0.27	0	10,10,12	0.81	0
2	C14	G	313	-	13,13,13	0.30	0	12,12,12	0.81	0
3	PTY	B	310	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
2	C14	A	309	-	13,13,13	0.29	0	12,12,12	0.80	0
3	PTY	D	310	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
2	C14	A	303	-	13,13,13	0.27	0	12,12,12	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PTY	I	310	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
3	PTY	F	311	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
3	PTY	J	313	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
2	C14	B	303	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	K	303	-	13,13,13	0.29	0	12,12,12	0.81	0
3	PTY	G	308	-	32,32,49	1.06	4 (12%)	35,37,54	0.97	2 (5%)
2	C14	L	310	-	13,13,13	0.29	0	12,12,12	0.81	0
3	PTY	G	305	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
2	C14	B	301	-	13,13,13	0.29	0	12,12,12	0.80	0
2	C14	K	308	-	13,13,13	0.27	0	12,12,12	0.84	0
4	Y01	J	311	-	38,38,38	0.68	0	57,57,57	0.95	1 (1%)
2	C14	H	302	-	13,13,13	0.29	0	12,12,12	0.83	0
2	C14	C	304	-	12,12,13	0.29	0	11,11,12	0.81	0
2	C14	J	307	-	13,13,13	0.30	0	12,12,12	0.76	0
3	PTY	B	313	-	32,32,49	1.05	4 (12%)	35,37,54	0.97	2 (5%)
2	C14	B	304	-	12,12,13	0.29	0	11,11,12	0.81	0
3	PTY	K	310	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
2	C14	I	303	-	13,13,13	0.29	0	12,12,12	0.81	0
4	Y01	B	312	-	38,38,38	0.67	0	57,57,57	1.05	4 (7%)
4	Y01	H	311	-	38,38,38	0.68	0	57,57,57	0.95	1 (1%)
2	C14	H	308	-	13,13,13	0.27	0	12,12,12	0.84	0
2	C14	F	306	-	13,13,13	0.29	0	12,12,12	0.81	0
4	Y01	A	307	-	38,38,38	0.68	0	57,57,57	1.04	4 (7%)
3	PTY	I	313	-	32,32,49	1.06	4 (12%)	35,37,54	0.97	2 (5%)
2	C14	H	304	-	12,12,13	0.29	0	11,11,12	0.81	0
2	C14	F	310	-	13,13,13	0.29	0	12,12,12	0.81	0
4	Y01	F	312	-	38,38,38	0.68	0	57,57,57	0.95	1 (1%)
2	C14	A	302	-	13,13,13	0.30	0	12,12,12	0.76	0
2	C14	F	309	-	13,13,13	0.27	0	12,12,12	0.84	0
2	C14	E	304	-	12,12,13	0.29	0	11,11,12	0.82	0
2	C14	H	307	-	13,13,13	0.30	0	12,12,12	0.76	0
2	C14	E	303	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	A	310	-	13,13,13	0.29	0	12,12,12	0.83	0
2	C14	B	306	-	11,11,13	0.28	0	10,10,12	0.81	0
2	C14	K	305	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	K	309	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	C	306	-	11,11,13	0.27	0	10,10,12	0.81	0
2	C14	F	305	-	12,12,13	0.29	0	11,11,12	0.81	0
2	C14	D	301	-	13,13,13	0.29	0	12,12,12	0.80	0
2	C14	K	304	-	12,12,13	0.29	0	11,11,12	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	Y01	E	311	-	38,38,38	0.68	0	57,57,57	0.95	1 (1%)
2	C14	L	306	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	F	303	-	13,13,13	0.29	0	12,12,12	0.83	0
3	PTY	F	301	-	32,32,49	1.06	4 (12%)	35,37,54	0.97	2 (5%)
2	C14	D	302	-	13,13,13	0.29	0	12,12,12	0.83	0
2	C14	H	305	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	L	309	-	13,13,13	0.27	0	12,12,12	0.84	0
2	C14	J	302	-	13,13,13	0.28	0	12,12,12	0.82	0
4	Y01	L	313	-	38,38,38	0.67	0	57,57,57	1.05	4 (7%)
2	C14	H	303	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	H	309	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	E	307	-	13,13,13	0.30	0	12,12,12	0.76	0
3	PTY	A	308	-	32,32,49	1.06	4 (12%)	35,37,54	0.97	2 (5%)
2	C14	G	302	-	13,13,13	0.30	0	12,12,12	0.76	0
2	C14	D	306	-	11,11,13	0.27	0	10,10,12	0.81	0
3	PTY	H	310	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
2	C14	J	301	-	13,13,13	0.29	0	12,12,12	0.80	0
2	C14	D	304	-	12,12,13	0.29	0	11,11,12	0.81	0
2	C14	D	309	-	13,13,13	0.29	0	12,12,12	0.81	0
4	Y01	H	312	-	38,38,38	0.68	0	57,57,57	1.05	4 (7%)
2	C14	F	302	-	13,13,13	0.29	0	12,12,12	0.80	0
2	C14	A	312	-	12,12,13	0.29	0	11,11,12	0.81	0
4	Y01	I	311	-	38,38,38	0.67	0	57,57,57	0.95	1 (1%)
4	Y01	D	312	-	38,38,38	0.68	0	57,57,57	1.05	4 (7%)
2	C14	L	308	-	13,13,13	0.30	0	12,12,12	0.76	0
2	C14	I	309	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	E	305	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	H	301	-	13,13,13	0.29	0	12,12,12	0.80	0
2	C14	K	302	-	13,13,13	0.29	0	12,12,12	0.83	0
2	C14	F	304	-	13,13,13	0.29	0	12,12,12	0.81	0
3	PTY	D	313	-	32,32,49	1.06	4 (12%)	35,37,54	0.97	2 (5%)
2	C14	L	304	-	13,13,13	0.29	0	12,12,12	0.81	0
3	PTY	E	310	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
3	PTY	L	311	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
2	C14	J	303	-	13,13,13	0.29	0	12,12,12	0.81	0
3	PTY	H	313	-	32,32,49	1.06	4 (12%)	35,37,54	0.97	2 (5%)
2	C14	B	307	-	13,13,13	0.31	0	12,12,12	0.76	0
2	C14	A	313	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	K	301	-	13,13,13	0.29	0	12,12,12	0.80	0
2	C14	G	312	-	12,12,13	0.29	0	11,11,12	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C14	I	307	-	13,13,13	0.30	0	12,12,12	0.76	0
2	C14	G	303	-	13,13,13	0.27	0	12,12,12	0.84	0
3	PTY	K	313	-	32,32,49	1.06	4 (12%)	35,37,54	0.97	2 (5%)
2	C14	G	310	-	13,13,13	0.29	0	12,12,12	0.83	0
2	C14	L	307	-	11,11,13	0.27	0	10,10,12	0.81	0
4	Y01	E	312	-	38,38,38	0.68	0	57,57,57	1.05	4 (7%)
2	C14	I	302	-	13,13,13	0.29	0	12,12,12	0.83	0
2	C14	B	309	-	13,13,13	0.29	0	12,12,12	0.81	0
4	Y01	D	311	-	38,38,38	0.68	0	57,57,57	0.95	1 (1%)
2	C14	E	302	-	13,13,13	0.29	0	12,12,12	0.83	0
2	C14	I	308	-	13,13,13	0.27	0	12,12,12	0.84	0
2	C14	I	305	-	13,13,13	0.29	0	12,12,12	0.81	0
4	Y01	G	306	-	38,38,38	0.68	0	57,57,57	0.95	1 (1%)
2	C14	C	305	-	13,13,13	0.29	0	12,12,12	0.81	0
2	C14	L	303	-	13,13,13	0.29	0	12,12,12	0.83	0
4	Y01	B	311	-	38,38,38	0.68	0	57,57,57	0.95	1 (1%)
2	C14	K	306	-	11,11,13	0.27	0	10,10,12	0.81	0
2	C14	G	309	-	13,13,13	0.29	0	12,12,12	0.80	0
2	C14	L	305	-	12,12,13	0.29	0	11,11,12	0.82	0
2	C14	B	302	-	13,13,13	0.29	0	12,12,12	0.83	0
2	C14	F	307	-	11,11,13	0.27	0	10,10,12	0.81	0
3	PTY	J	310	-	32,32,49	1.06	4 (12%)	35,37,54	0.96	2 (5%)
4	Y01	I	312	-	38,38,38	0.68	0	57,57,57	1.05	4 (7%)
4	Y01	F	313	-	38,38,38	0.68	0	57,57,57	1.05	4 (7%)
2	C14	H	306	-	11,11,13	0.27	0	10,10,12	0.81	0
2	C14	C	308	-	13,13,13	0.27	0	12,12,12	0.84	0
2	C14	J	308	-	13,13,13	0.27	0	12,12,12	0.84	0
2	C14	J	304	-	12,12,13	0.29	0	11,11,12	0.82	0
2	C14	K	307	-	13,13,13	0.30	0	12,12,12	0.76	0
2	C14	A	301	-	11,11,13	0.28	0	10,10,12	0.81	0
4	Y01	L	312	-	38,38,38	0.68	0	57,57,57	0.95	1 (1%)
2	C14	C	307	-	13,13,13	0.30	0	12,12,12	0.76	0
2	C14	G	301	-	11,11,13	0.28	0	10,10,12	0.81	0
2	C14	E	308	-	13,13,13	0.27	0	12,12,12	0.84	0
2	C14	I	304	-	12,12,13	0.29	0	11,11,12	0.82	0
2	C14	A	304	-	13,13,13	0.29	0	12,12,12	0.81	0

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
2	C14	C	302	-	-	2/11/11/11	-
2	C14	G	304	-	-	2/11/11/11	-
2	C14	E	306	-	-	0/9/9/11	-
4	Y01	C	311	-	-	8/19/77/77	0/4/4/4
2	C14	B	308	-	-	1/11/11/11	-
2	C14	D	307	-	-	4/11/11/11	-
2	C14	J	306	-	-	0/9/9/11	-
2	C14	L	302	-	-	1/11/11/11	-
2	C14	D	308	-	-	1/11/11/11	-
4	Y01	A	306	-	-	8/19/77/77	0/4/4/4
2	C14	D	305	-	-	6/11/11/11	-
3	PTY	E	313	-	-	18/36/36/53	-
4	Y01	G	307	-	-	12/19/77/77	0/4/4/4
2	C14	C	309	-	-	2/11/11/11	-
2	C14	J	309	-	-	2/11/11/11	-
3	PTY	A	305	-	-	17/36/36/53	-
4	Y01	K	311	-	-	8/19/77/77	0/4/4/4
2	C14	E	301	-	-	1/11/11/11	-
4	Y01	C	312	-	-	12/19/77/77	0/4/4/4
4	Y01	K	312	-	-	12/19/77/77	0/4/4/4
2	C14	J	305	-	-	6/11/11/11	-
4	Y01	J	312	-	-	12/19/77/77	0/4/4/4
2	C14	F	308	-	-	4/11/11/11	-
2	C14	E	309	-	-	2/11/11/11	-
2	C14	D	303	-	-	2/11/11/11	-
2	C14	C	301	-	-	1/11/11/11	-
2	C14	A	311	-	-	2/11/11/11	-
2	C14	B	305	-	-	6/11/11/11	-
2	C14	C	303	-	-	2/11/11/11	-
2	C14	G	311	-	-	2/11/11/11	-
3	PTY	C	313	-	-	18/36/36/53	-
3	PTY	L	301	-	-	18/36/36/53	-
2	C14	I	301	-	-	1/11/11/11	-
3	PTY	C	310	-	-	17/36/36/53	-
2	C14	I	306	-	-	0/9/9/11	-
2	C14	G	313	-	-	6/11/11/11	-
3	PTY	B	310	-	-	17/36/36/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C14	A	309	-	-	1/11/11/11	-
3	PTY	D	310	-	-	17/36/36/53	-
2	C14	A	303	-	-	1/11/11/11	-
3	PTY	I	310	-	-	17/36/36/53	-
3	PTY	F	311	-	-	17/36/36/53	-
3	PTY	J	313	-	-	18/36/36/53	-
2	C14	B	303	-	-	2/11/11/11	-
2	C14	K	303	-	-	2/11/11/11	-
3	PTY	G	308	-	-	18/36/36/53	-
2	C14	L	310	-	-	2/11/11/11	-
3	PTY	G	305	-	-	17/36/36/53	-
2	C14	B	301	-	-	1/11/11/11	-
2	C14	K	308	-	-	1/11/11/11	-
4	Y01	J	311	-	-	8/19/77/77	0/4/4/4
2	C14	H	302	-	-	2/11/11/11	-
2	C14	C	304	-	-	2/10/10/11	-
2	C14	J	307	-	-	4/11/11/11	-
3	PTY	B	313	-	-	18/36/36/53	-
2	C14	B	304	-	-	2/10/10/11	-
3	PTY	K	310	-	-	17/36/36/53	-
2	C14	I	303	-	-	2/11/11/11	-
4	Y01	B	312	-	-	12/19/77/77	0/4/4/4
4	Y01	H	311	-	-	8/19/77/77	0/4/4/4
2	C14	H	308	-	-	1/11/11/11	-
2	C14	F	306	-	-	6/11/11/11	-
4	Y01	A	307	-	-	12/19/77/77	0/4/4/4
3	PTY	I	313	-	-	18/36/36/53	-
2	C14	H	304	-	-	2/10/10/11	-
2	C14	F	310	-	-	2/11/11/11	-
4	Y01	F	312	-	-	8/19/77/77	0/4/4/4
2	C14	A	302	-	-	4/11/11/11	-
2	C14	F	309	-	-	1/11/11/11	-
2	C14	E	304	-	-	2/10/10/11	-
2	C14	H	307	-	-	4/11/11/11	-
2	C14	E	303	-	-	2/11/11/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C14	A	310	-	-	2/11/11/11	-
2	C14	B	306	-	-	0/9/9/11	-
2	C14	K	305	-	-	6/11/11/11	-
2	C14	K	309	-	-	2/11/11/11	-
2	C14	C	306	-	-	0/9/9/11	-
2	C14	F	305	-	-	2/10/10/11	-
2	C14	D	301	-	-	1/11/11/11	-
2	C14	K	304	-	-	2/10/10/11	-
4	Y01	E	311	-	-	8/19/77/77	0/4/4/4
2	C14	L	306	-	-	6/11/11/11	-
2	C14	F	303	-	-	2/11/11/11	-
3	PTY	F	301	-	-	18/36/36/53	-
2	C14	D	302	-	-	2/11/11/11	-
2	C14	H	305	-	-	6/11/11/11	-
2	C14	L	309	-	-	1/11/11/11	-
2	C14	J	302	-	-	2/11/11/11	-
4	Y01	L	313	-	-	12/19/77/77	0/4/4/4
2	C14	H	303	-	-	2/11/11/11	-
2	C14	H	309	-	-	2/11/11/11	-
2	C14	E	307	-	-	4/11/11/11	-
3	PTY	A	308	-	-	18/36/36/53	-
2	C14	G	302	-	-	4/11/11/11	-
2	C14	D	306	-	-	0/9/9/11	-
3	PTY	H	310	-	-	17/36/36/53	-
2	C14	J	301	-	-	1/11/11/11	-
2	C14	D	304	-	-	2/10/10/11	-
2	C14	D	309	-	-	2/11/11/11	-
4	Y01	H	312	-	-	12/19/77/77	0/4/4/4
2	C14	F	302	-	-	1/11/11/11	-
2	C14	A	312	-	-	2/10/10/11	-
4	Y01	I	311	-	-	8/19/77/77	0/4/4/4
4	Y01	D	312	-	-	12/19/77/77	0/4/4/4
2	C14	L	308	-	-	4/11/11/11	-
2	C14	I	309	-	-	2/11/11/11	-
2	C14	E	305	-	-	6/11/11/11	-
2	C14	H	301	-	-	1/11/11/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C14	K	302	-	-	2/11/11/11	-
2	C14	F	304	-	-	2/11/11/11	-
3	PTY	D	313	-	-	18/36/36/53	-
2	C14	L	304	-	-	2/11/11/11	-
3	PTY	E	310	-	-	17/36/36/53	-
3	PTY	L	311	-	-	17/36/36/53	-
2	C14	J	303	-	-	2/11/11/11	-
3	PTY	H	313	-	-	18/36/36/53	-
2	C14	B	307	-	-	4/11/11/11	-
2	C14	A	313	-	-	6/11/11/11	-
2	C14	K	301	-	-	1/11/11/11	-
2	C14	G	312	-	-	2/10/10/11	-
2	C14	I	307	-	-	4/11/11/11	-
2	C14	G	303	-	-	1/11/11/11	-
3	PTY	K	313	-	-	18/36/36/53	-
2	C14	G	310	-	-	2/11/11/11	-
2	C14	L	307	-	-	0/9/9/11	-
4	Y01	E	312	-	-	12/19/77/77	0/4/4/4
2	C14	I	302	-	-	2/11/11/11	-
2	C14	B	309	-	-	2/11/11/11	-
4	Y01	D	311	-	-	8/19/77/77	0/4/4/4
2	C14	E	302	-	-	2/11/11/11	-
2	C14	I	308	-	-	1/11/11/11	-
2	C14	I	305	-	-	6/11/11/11	-
4	Y01	G	306	-	-	8/19/77/77	0/4/4/4
2	C14	C	305	-	-	6/11/11/11	-
2	C14	L	303	-	-	2/11/11/11	-
4	Y01	B	311	-	-	8/19/77/77	0/4/4/4
2	C14	K	306	-	-	0/9/9/11	-
2	C14	G	309	-	-	1/11/11/11	-
2	C14	L	305	-	-	2/10/10/11	-
2	C14	B	302	-	-	2/11/11/11	-
2	C14	F	307	-	-	0/9/9/11	-
3	PTY	J	310	-	-	17/36/36/53	-
4	Y01	I	312	-	-	12/19/77/77	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Y01	F	313	-	-	12/19/77/77	0/4/4/4
2	C14	H	306	-	-	0/9/9/11	-
2	C14	C	308	-	-	1/11/11/11	-
2	C14	J	308	-	-	1/11/11/11	-
2	C14	J	304	-	-	2/10/10/11	-
2	C14	K	307	-	-	4/11/11/11	-
2	C14	A	301	-	-	0/9/9/11	-
4	Y01	L	312	-	-	8/19/77/77	0/4/4/4
2	C14	C	307	-	-	4/11/11/11	-
2	C14	G	301	-	-	0/9/9/11	-
2	C14	E	308	-	-	1/11/11/11	-
2	C14	I	304	-	-	2/10/10/11	-
2	C14	A	304	-	-	2/11/11/11	-

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	310	PTY	O7-C6	-2.61	1.40	1.46
3	J	310	PTY	O7-C6	-2.60	1.40	1.46
3	H	310	PTY	O7-C6	-2.59	1.40	1.46
3	D	310	PTY	O7-C6	-2.58	1.40	1.46
3	I	310	PTY	O7-C6	-2.57	1.40	1.46
3	A	305	PTY	O7-C6	-2.57	1.40	1.46
3	C	310	PTY	O7-C6	-2.57	1.40	1.46
3	F	311	PTY	O7-C6	-2.57	1.40	1.46
3	G	305	PTY	O7-C6	-2.56	1.40	1.46
3	G	308	PTY	O7-C6	-2.56	1.40	1.46
3	L	311	PTY	O7-C6	-2.55	1.40	1.46
3	K	310	PTY	O7-C6	-2.55	1.40	1.46
3	K	313	PTY	O7-C6	-2.54	1.40	1.46
3	B	310	PTY	O7-C6	-2.54	1.40	1.46
3	E	313	PTY	O7-C6	-2.54	1.40	1.46
3	L	301	PTY	O7-C6	-2.54	1.40	1.46
3	J	313	PTY	O7-C6	-2.53	1.40	1.46
3	A	308	PTY	O7-C6	-2.53	1.40	1.46
3	D	313	PTY	O7-C6	-2.53	1.40	1.46
3	F	301	PTY	O7-C6	-2.53	1.40	1.46
3	C	313	PTY	O7-C6	-2.52	1.40	1.46
3	B	313	PTY	O7-C6	-2.52	1.40	1.46
3	H	313	PTY	O7-C6	-2.51	1.40	1.46
3	I	313	PTY	O7-C6	-2.51	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	310	PTY	O4-C30	2.41	1.40	1.33
3	J	313	PTY	O4-C30	2.41	1.40	1.33
3	L	311	PTY	O4-C30	2.41	1.40	1.33
3	C	313	PTY	O4-C30	2.40	1.40	1.33
3	G	308	PTY	O4-C30	2.40	1.40	1.33
3	G	305	PTY	O4-C30	2.40	1.40	1.33
3	A	308	PTY	O4-C30	2.40	1.40	1.33
3	K	310	PTY	O4-C30	2.39	1.40	1.33
3	F	311	PTY	O4-C30	2.39	1.40	1.33
3	J	310	PTY	O4-C30	2.39	1.40	1.33
3	E	310	PTY	O4-C30	2.39	1.40	1.33
3	I	310	PTY	O4-C30	2.39	1.40	1.33
3	I	313	PTY	O4-C30	2.39	1.40	1.33
3	B	310	PTY	O4-C30	2.39	1.40	1.33
3	K	313	PTY	O4-C30	2.39	1.40	1.33
3	D	313	PTY	O4-C30	2.39	1.40	1.33
3	L	301	PTY	O4-C30	2.38	1.40	1.33
3	B	313	PTY	O4-C30	2.38	1.40	1.33
3	H	310	PTY	O4-C30	2.37	1.40	1.33
3	F	301	PTY	O4-C30	2.37	1.40	1.33
3	E	313	PTY	O4-C30	2.37	1.40	1.33
3	H	313	PTY	O4-C30	2.37	1.40	1.33
3	A	305	PTY	O4-C30	2.37	1.40	1.33
3	C	310	PTY	O4-C30	2.36	1.40	1.33
3	A	308	PTY	O7-C8	2.16	1.40	1.34
3	I	313	PTY	O7-C8	2.15	1.40	1.34
3	F	301	PTY	O7-C8	2.15	1.40	1.34
3	A	308	PTY	O4-C1	-2.15	1.40	1.45
3	G	308	PTY	O7-C8	2.15	1.40	1.34
3	H	313	PTY	O7-C8	2.14	1.40	1.34
3	L	301	PTY	O7-C8	2.14	1.40	1.34
3	E	313	PTY	O7-C8	2.14	1.40	1.34
3	J	313	PTY	O4-C1	-2.14	1.40	1.45
3	K	313	PTY	O7-C8	2.14	1.40	1.34
3	I	313	PTY	O4-C1	-2.13	1.40	1.45
3	J	313	PTY	O7-C8	2.13	1.40	1.34
3	K	313	PTY	O4-C1	-2.13	1.40	1.45
3	L	301	PTY	O4-C1	-2.13	1.40	1.45
3	C	310	PTY	O7-C8	2.13	1.40	1.34
3	D	313	PTY	O7-C8	2.13	1.40	1.34
3	H	313	PTY	O4-C1	-2.12	1.40	1.45
3	B	313	PTY	O7-C8	2.12	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	313	PTY	O4-C1	-2.12	1.40	1.45
3	L	311	PTY	O4-C1	-2.12	1.40	1.45
3	A	305	PTY	O4-C1	-2.11	1.40	1.45
3	F	301	PTY	O4-C1	-2.11	1.40	1.45
3	C	313	PTY	O7-C8	2.11	1.40	1.34
3	E	313	PTY	O4-C1	-2.11	1.40	1.45
3	G	305	PTY	O4-C1	-2.11	1.40	1.45
3	C	313	PTY	O4-C1	-2.11	1.40	1.45
3	E	310	PTY	O7-C8	2.11	1.40	1.34
3	G	305	PTY	O7-C8	2.11	1.40	1.34
3	G	308	PTY	O4-C1	-2.11	1.40	1.45
3	D	310	PTY	O7-C8	2.10	1.40	1.34
3	I	310	PTY	O7-C8	2.10	1.40	1.34
3	I	310	PTY	O4-C1	-2.10	1.40	1.45
3	B	313	PTY	O4-C1	-2.10	1.40	1.45
3	E	310	PTY	O4-C1	-2.10	1.40	1.45
3	F	311	PTY	O4-C1	-2.10	1.40	1.45
3	J	310	PTY	O7-C8	2.10	1.40	1.34
3	J	310	PTY	O4-C1	-2.09	1.40	1.45
3	H	310	PTY	O7-C8	2.09	1.40	1.34
3	B	310	PTY	O7-C8	2.09	1.40	1.34
3	K	310	PTY	O7-C8	2.09	1.40	1.34
3	A	305	PTY	O7-C8	2.08	1.40	1.34
3	D	310	PTY	O4-C1	-2.08	1.40	1.45
3	H	310	PTY	O4-C1	-2.08	1.40	1.45
3	F	311	PTY	O7-C8	2.08	1.40	1.34
3	K	310	PTY	O4-C1	-2.08	1.40	1.45
3	L	311	PTY	O7-C8	2.07	1.40	1.34
3	C	310	PTY	O4-C1	-2.07	1.40	1.45
3	B	310	PTY	O4-C1	-2.07	1.40	1.45

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	301	PTY	O7-C8-C11	3.62	119.31	111.50
3	C	313	PTY	O7-C8-C11	3.62	119.30	111.50
3	G	308	PTY	O7-C8-C11	3.61	119.29	111.50
3	B	313	PTY	O7-C8-C11	3.61	119.28	111.50
3	K	313	PTY	O7-C8-C11	3.61	119.28	111.50
3	D	313	PTY	O7-C8-C11	3.61	119.28	111.50
3	E	313	PTY	O7-C8-C11	3.60	119.25	111.50
3	I	313	PTY	O7-C8-C11	3.60	119.25	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	PTY	O7-C8-C11	3.59	119.25	111.50
3	A	308	PTY	O7-C8-C11	3.59	119.24	111.50
3	H	313	PTY	O7-C8-C11	3.59	119.24	111.50
3	J	313	PTY	O7-C8-C11	3.59	119.23	111.50
3	B	310	PTY	O7-C8-C11	3.58	119.22	111.50
3	F	311	PTY	O7-C8-C11	3.58	119.21	111.50
3	J	310	PTY	O7-C8-C11	3.58	119.21	111.50
3	I	310	PTY	O7-C8-C11	3.57	119.20	111.50
3	G	305	PTY	O7-C8-C11	3.57	119.20	111.50
3	D	310	PTY	O7-C8-C11	3.57	119.19	111.50
3	C	310	PTY	O7-C8-C11	3.57	119.19	111.50
3	A	305	PTY	O7-C8-C11	3.57	119.19	111.50
3	L	311	PTY	O7-C8-C11	3.57	119.19	111.50
3	H	310	PTY	O7-C8-C11	3.56	119.18	111.50
3	E	310	PTY	O7-C8-C11	3.56	119.17	111.50
3	K	310	PTY	O7-C8-C11	3.56	119.17	111.50
4	F	313	Y01	CAT-CBH-CBF	2.83	112.68	108.73
4	C	312	Y01	CAT-CBH-CBF	2.81	112.66	108.73
4	L	313	Y01	CAT-CBH-CBF	2.81	112.65	108.73
4	D	312	Y01	CAT-CBH-CBF	2.80	112.64	108.73
4	K	312	Y01	CAT-CBH-CBF	2.80	112.64	108.73
4	G	307	Y01	CAT-CBH-CBF	2.80	112.63	108.73
4	J	312	Y01	CAT-CBH-CBF	2.79	112.63	108.73
4	H	312	Y01	CAT-CBH-CBF	2.79	112.63	108.73
4	B	312	Y01	CAT-CBH-CBF	2.78	112.62	108.73
4	E	312	Y01	CAT-CBH-CBF	2.78	112.61	108.73
4	I	312	Y01	CAT-CBH-CBF	2.78	112.61	108.73
4	A	307	Y01	CAT-CBH-CBF	2.77	112.59	108.73
3	F	301	PTY	O4-C30-C31	2.65	120.24	111.91
3	H	313	PTY	O4-C30-C31	2.64	120.21	111.91
3	C	310	PTY	O4-C30-C31	2.64	120.20	111.91
3	F	311	PTY	O4-C30-C31	2.64	120.19	111.91
3	K	313	PTY	O4-C30-C31	2.64	120.19	111.91
3	E	310	PTY	O4-C30-C31	2.64	120.19	111.91
3	E	313	PTY	O4-C30-C31	2.64	120.19	111.91
3	L	311	PTY	O4-C30-C31	2.64	120.19	111.91
3	G	308	PTY	O4-C30-C31	2.64	120.18	111.91
3	L	301	PTY	O4-C30-C31	2.64	120.18	111.91
3	I	310	PTY	O4-C30-C31	2.64	120.18	111.91
3	B	313	PTY	O4-C30-C31	2.64	120.18	111.91
3	H	310	PTY	O4-C30-C31	2.63	120.18	111.91
3	A	305	PTY	O4-C30-C31	2.63	120.17	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	310	PTY	O4-C30-C31	2.63	120.17	111.91
3	J	310	PTY	O4-C30-C31	2.63	120.17	111.91
3	G	305	PTY	O4-C30-C31	2.63	120.16	111.91
3	D	310	PTY	O4-C30-C31	2.63	120.15	111.91
3	I	313	PTY	O4-C30-C31	2.63	120.15	111.91
3	C	313	PTY	O4-C30-C31	2.62	120.14	111.91
3	A	308	PTY	O4-C30-C31	2.62	120.14	111.91
3	J	313	PTY	O4-C30-C31	2.62	120.14	111.91
3	D	313	PTY	O4-C30-C31	2.62	120.14	111.91
3	B	310	PTY	O4-C30-C31	2.61	120.11	111.91
4	H	311	Y01	CAV-CAZ-CAI	-2.48	117.04	120.61
4	D	311	Y01	CAV-CAZ-CAI	-2.46	117.06	120.61
4	G	306	Y01	CAV-CAZ-CAI	-2.45	117.07	120.61
4	L	312	Y01	CAV-CAZ-CAI	-2.45	117.08	120.61
4	C	312	Y01	CAV-CAZ-CAI	-2.44	117.09	120.61
4	H	312	Y01	CAV-CAZ-CAI	-2.44	117.09	120.61
4	J	311	Y01	CAV-CAZ-CAI	-2.44	117.09	120.61
4	E	311	Y01	CAV-CAZ-CAI	-2.44	117.09	120.61
4	G	307	Y01	CAV-CAZ-CAI	-2.44	117.09	120.61
4	C	311	Y01	CAV-CAZ-CAI	-2.44	117.10	120.61
4	K	311	Y01	CAV-CAZ-CAI	-2.44	117.10	120.61
4	B	311	Y01	CAV-CAZ-CAI	-2.43	117.10	120.61
4	I	311	Y01	CAV-CAZ-CAI	-2.43	117.10	120.61
4	D	312	Y01	CAV-CAZ-CAI	-2.43	117.11	120.61
4	I	312	Y01	CAV-CAZ-CAI	-2.43	117.11	120.61
4	F	312	Y01	CAV-CAZ-CAI	-2.42	117.11	120.61
4	J	312	Y01	CAV-CAZ-CAI	-2.42	117.12	120.61
4	B	312	Y01	CAV-CAZ-CAI	-2.42	117.12	120.61
4	K	312	Y01	CAV-CAZ-CAI	-2.41	117.13	120.61
4	E	312	Y01	CAV-CAZ-CAI	-2.41	117.13	120.61
4	A	306	Y01	CAV-CAZ-CAI	-2.41	117.13	120.61
4	A	307	Y01	CAV-CAZ-CAI	-2.41	117.14	120.61
4	L	313	Y01	CAV-CAZ-CAI	-2.40	117.14	120.61
4	K	312	Y01	CAD-CBH-CAZ	2.39	112.21	108.34
4	I	312	Y01	CAD-CBH-CAZ	2.38	112.20	108.34
4	F	313	Y01	CAV-CAZ-CAI	-2.38	117.18	120.61
4	B	312	Y01	CAD-CBH-CAZ	2.38	112.19	108.34
4	A	307	Y01	CAD-CBH-CAZ	2.37	112.18	108.34
4	J	312	Y01	CAD-CBH-CAZ	2.37	112.18	108.34
4	E	312	Y01	CAD-CBH-CAZ	2.37	112.17	108.34
4	L	313	Y01	CAD-CBH-CAZ	2.37	112.17	108.34
4	C	312	Y01	CAD-CBH-CAZ	2.36	112.16	108.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	307	Y01	CAD-CBH-CAZ	2.36	112.16	108.34
4	D	312	Y01	CAD-CBH-CAZ	2.36	112.16	108.34
4	H	312	Y01	CAD-CBH-CAZ	2.36	112.16	108.34
4	F	313	Y01	CAD-CBH-CAZ	2.35	112.14	108.34
4	H	312	Y01	CAD-CBH-CBF	-2.32	108.92	111.68
4	K	312	Y01	CAD-CBH-CBF	-2.31	108.92	111.68
4	F	313	Y01	CAD-CBH-CBF	-2.30	108.94	111.68
4	L	313	Y01	CAD-CBH-CBF	-2.30	108.94	111.68
4	C	312	Y01	CAD-CBH-CBF	-2.30	108.94	111.68
4	D	312	Y01	CAD-CBH-CBF	-2.29	108.95	111.68
4	G	307	Y01	CAD-CBH-CBF	-2.29	108.95	111.68
4	E	312	Y01	CAD-CBH-CBF	-2.29	108.95	111.68
4	J	312	Y01	CAD-CBH-CBF	-2.28	108.96	111.68
4	B	312	Y01	CAD-CBH-CBF	-2.28	108.97	111.68
4	A	307	Y01	CAD-CBH-CBF	-2.27	108.97	111.68
4	I	312	Y01	CAD-CBH-CBF	-2.27	108.97	111.68

There are no chirality outliers.

All (900) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	305	PTY	C5-O14-P1-O12
3	A	305	PTY	C5-O14-P1-O13
3	A	308	PTY	N1-C2-C3-O11
3	A	308	PTY	C5-O14-P1-O11
3	A	308	PTY	C5-O14-P1-O12
3	A	308	PTY	C5-O14-P1-O13
3	B	310	PTY	C5-O14-P1-O12
3	B	310	PTY	C5-O14-P1-O13
3	B	313	PTY	N1-C2-C3-O11
3	B	313	PTY	C5-O14-P1-O11
3	B	313	PTY	C5-O14-P1-O12
3	B	313	PTY	C5-O14-P1-O13
3	C	310	PTY	C5-O14-P1-O12
3	C	310	PTY	C5-O14-P1-O13
3	C	313	PTY	N1-C2-C3-O11
3	C	313	PTY	C5-O14-P1-O11
3	C	313	PTY	C5-O14-P1-O12
3	C	313	PTY	C5-O14-P1-O13
3	D	310	PTY	C5-O14-P1-O12
3	D	310	PTY	C5-O14-P1-O13
3	D	313	PTY	N1-C2-C3-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	313	PTY	C5-O14-P1-O11
3	D	313	PTY	C5-O14-P1-O12
3	D	313	PTY	C5-O14-P1-O13
3	E	310	PTY	C5-O14-P1-O12
3	E	310	PTY	C5-O14-P1-O13
3	E	313	PTY	N1-C2-C3-O11
3	E	313	PTY	C5-O14-P1-O11
3	E	313	PTY	C5-O14-P1-O12
3	E	313	PTY	C5-O14-P1-O13
3	F	301	PTY	N1-C2-C3-O11
3	F	301	PTY	C5-O14-P1-O11
3	F	301	PTY	C5-O14-P1-O12
3	F	301	PTY	C5-O14-P1-O13
3	F	311	PTY	C5-O14-P1-O12
3	F	311	PTY	C5-O14-P1-O13
3	G	305	PTY	C5-O14-P1-O12
3	G	305	PTY	C5-O14-P1-O13
3	G	308	PTY	N1-C2-C3-O11
3	G	308	PTY	C5-O14-P1-O11
3	G	308	PTY	C5-O14-P1-O12
3	G	308	PTY	C5-O14-P1-O13
3	H	310	PTY	C5-O14-P1-O12
3	H	310	PTY	C5-O14-P1-O13
3	H	313	PTY	N1-C2-C3-O11
3	H	313	PTY	C5-O14-P1-O11
3	H	313	PTY	C5-O14-P1-O12
3	H	313	PTY	C5-O14-P1-O13
3	I	310	PTY	C5-O14-P1-O12
3	I	310	PTY	C5-O14-P1-O13
3	I	313	PTY	N1-C2-C3-O11
3	I	313	PTY	C5-O14-P1-O11
3	I	313	PTY	C5-O14-P1-O12
3	I	313	PTY	C5-O14-P1-O13
3	J	310	PTY	C5-O14-P1-O12
3	J	310	PTY	C5-O14-P1-O13
3	J	313	PTY	N1-C2-C3-O11
3	J	313	PTY	C5-O14-P1-O11
3	J	313	PTY	C5-O14-P1-O12
3	J	313	PTY	C5-O14-P1-O13
3	K	310	PTY	C5-O14-P1-O12
3	K	310	PTY	C5-O14-P1-O13
3	K	313	PTY	N1-C2-C3-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	K	313	PTY	C5-O14-P1-O11
3	K	313	PTY	C5-O14-P1-O12
3	K	313	PTY	C5-O14-P1-O13
3	L	301	PTY	N1-C2-C3-O11
3	L	301	PTY	C5-O14-P1-O11
3	L	301	PTY	C5-O14-P1-O12
3	L	301	PTY	C5-O14-P1-O13
3	L	311	PTY	C5-O14-P1-O12
3	L	311	PTY	C5-O14-P1-O13
4	A	306	Y01	CAC-CBB-CBE-CBI
4	A	306	Y01	CAM-CAY-OAW-CBC
4	A	307	Y01	OAG-CAY-OAW-CBC
4	B	311	Y01	CAC-CBB-CBE-CBI
4	B	311	Y01	CAM-CAY-OAW-CBC
4	B	312	Y01	OAG-CAY-OAW-CBC
4	C	311	Y01	CAC-CBB-CBE-CBI
4	C	311	Y01	CAM-CAY-OAW-CBC
4	C	312	Y01	OAG-CAY-OAW-CBC
4	D	311	Y01	CAC-CBB-CBE-CBI
4	D	311	Y01	CAM-CAY-OAW-CBC
4	D	312	Y01	OAG-CAY-OAW-CBC
4	E	311	Y01	CAC-CBB-CBE-CBI
4	E	311	Y01	CAM-CAY-OAW-CBC
4	E	312	Y01	OAG-CAY-OAW-CBC
4	F	312	Y01	CAC-CBB-CBE-CBI
4	F	312	Y01	CAM-CAY-OAW-CBC
4	F	313	Y01	OAG-CAY-OAW-CBC
4	G	306	Y01	CAC-CBB-CBE-CBI
4	G	306	Y01	CAM-CAY-OAW-CBC
4	G	307	Y01	OAG-CAY-OAW-CBC
4	H	311	Y01	CAC-CBB-CBE-CBI
4	H	311	Y01	CAM-CAY-OAW-CBC
4	H	312	Y01	OAG-CAY-OAW-CBC
4	I	311	Y01	CAC-CBB-CBE-CBI
4	I	311	Y01	CAM-CAY-OAW-CBC
4	I	312	Y01	OAG-CAY-OAW-CBC
4	J	311	Y01	CAC-CBB-CBE-CBI
4	J	311	Y01	CAM-CAY-OAW-CBC
4	J	312	Y01	OAG-CAY-OAW-CBC
4	K	311	Y01	CAC-CBB-CBE-CBI
4	K	311	Y01	CAM-CAY-OAW-CBC
4	K	312	Y01	OAG-CAY-OAW-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	L	312	Y01	CAC-CBB-CBE-CBI
4	L	312	Y01	CAM-CAY-OAW-CBC
4	L	313	Y01	OAG-CAY-OAW-CBC
3	A	305	PTY	O30-C30-O4-C1
3	B	310	PTY	O30-C30-O4-C1
3	C	310	PTY	O30-C30-O4-C1
3	D	310	PTY	O30-C30-O4-C1
3	E	310	PTY	O30-C30-O4-C1
3	F	311	PTY	O30-C30-O4-C1
3	G	305	PTY	O30-C30-O4-C1
3	H	310	PTY	O30-C30-O4-C1
3	I	310	PTY	O30-C30-O4-C1
3	J	310	PTY	O30-C30-O4-C1
3	K	310	PTY	O30-C30-O4-C1
3	L	311	PTY	O30-C30-O4-C1
4	A	306	Y01	CAO-CBB-CBE-CAP
4	C	311	Y01	CAO-CBB-CBE-CAP
4	D	311	Y01	CAO-CBB-CBE-CAP
4	E	311	Y01	CAO-CBB-CBE-CAP
4	F	312	Y01	CAO-CBB-CBE-CAP
4	H	311	Y01	CAO-CBB-CBE-CAP
4	J	311	Y01	CAO-CBB-CBE-CAP
4	K	311	Y01	CAO-CBB-CBE-CAP
4	A	306	Y01	OAG-CAY-OAW-CBC
4	B	311	Y01	OAG-CAY-OAW-CBC
4	C	311	Y01	OAG-CAY-OAW-CBC
4	D	311	Y01	OAG-CAY-OAW-CBC
4	E	311	Y01	OAG-CAY-OAW-CBC
4	F	312	Y01	OAG-CAY-OAW-CBC
4	G	306	Y01	OAG-CAY-OAW-CBC
4	H	311	Y01	OAG-CAY-OAW-CBC
4	I	311	Y01	OAG-CAY-OAW-CBC
4	J	311	Y01	OAG-CAY-OAW-CBC
4	K	311	Y01	OAG-CAY-OAW-CBC
4	L	312	Y01	OAG-CAY-OAW-CBC
4	A	307	Y01	CAM-CAY-OAW-CBC
4	B	312	Y01	CAM-CAY-OAW-CBC
4	C	312	Y01	CAM-CAY-OAW-CBC
4	D	312	Y01	CAM-CAY-OAW-CBC
4	E	312	Y01	CAM-CAY-OAW-CBC
4	F	313	Y01	CAM-CAY-OAW-CBC
4	G	307	Y01	CAM-CAY-OAW-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	H	312	Y01	CAM-CAY-OAW-CBC
4	I	312	Y01	CAM-CAY-OAW-CBC
4	J	312	Y01	CAM-CAY-OAW-CBC
4	K	312	Y01	CAM-CAY-OAW-CBC
4	L	313	Y01	CAM-CAY-OAW-CBC
4	A	306	Y01	CAC-CBB-CBE-CAP
4	B	311	Y01	CAC-CBB-CBE-CAP
4	C	311	Y01	CAC-CBB-CBE-CAP
4	D	311	Y01	CAC-CBB-CBE-CAP
4	E	311	Y01	CAC-CBB-CBE-CAP
4	F	312	Y01	CAC-CBB-CBE-CAP
4	G	306	Y01	CAC-CBB-CBE-CAP
4	H	311	Y01	CAC-CBB-CBE-CAP
4	I	311	Y01	CAC-CBB-CBE-CAP
4	J	311	Y01	CAC-CBB-CBE-CAP
4	K	311	Y01	CAC-CBB-CBE-CAP
4	L	312	Y01	CAC-CBB-CBE-CAP
4	B	311	Y01	CAO-CBB-CBE-CAP
4	G	306	Y01	CAO-CBB-CBE-CAP
4	I	311	Y01	CAO-CBB-CBE-CAP
4	L	312	Y01	CAO-CBB-CBE-CAP
3	A	305	PTY	C31-C30-O4-C1
3	B	310	PTY	C31-C30-O4-C1
3	C	310	PTY	C31-C30-O4-C1
3	D	310	PTY	C31-C30-O4-C1
3	E	310	PTY	C31-C30-O4-C1
3	F	311	PTY	C31-C30-O4-C1
3	G	305	PTY	C31-C30-O4-C1
3	H	310	PTY	C31-C30-O4-C1
3	I	310	PTY	C31-C30-O4-C1
3	J	310	PTY	C31-C30-O4-C1
3	J	313	PTY	C31-C30-O4-C1
3	K	310	PTY	C31-C30-O4-C1
3	L	301	PTY	C31-C30-O4-C1
3	L	311	PTY	C31-C30-O4-C1
3	A	308	PTY	C31-C30-O4-C1
3	B	313	PTY	C31-C30-O4-C1
3	C	313	PTY	C31-C30-O4-C1
3	D	313	PTY	C31-C30-O4-C1
3	E	313	PTY	C31-C30-O4-C1
3	F	301	PTY	C31-C30-O4-C1
3	G	308	PTY	C31-C30-O4-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	H	313	PTY	C31-C30-O4-C1
3	I	313	PTY	C31-C30-O4-C1
3	K	313	PTY	C31-C30-O4-C1
4	A	306	Y01	CAO-CBB-CBE-CBI
4	B	311	Y01	CAO-CBB-CBE-CBI
4	C	311	Y01	CAO-CBB-CBE-CBI
4	D	311	Y01	CAO-CBB-CBE-CBI
4	E	311	Y01	CAO-CBB-CBE-CBI
4	F	312	Y01	CAO-CBB-CBE-CBI
4	G	306	Y01	CAO-CBB-CBE-CBI
4	H	311	Y01	CAO-CBB-CBE-CBI
4	I	311	Y01	CAO-CBB-CBE-CBI
4	J	311	Y01	CAO-CBB-CBE-CBI
4	K	311	Y01	CAO-CBB-CBE-CBI
4	L	312	Y01	CAO-CBB-CBE-CBI
3	F	301	PTY	O30-C30-O4-C1
3	H	313	PTY	O30-C30-O4-C1
3	K	313	PTY	O30-C30-O4-C1
3	A	308	PTY	O30-C30-O4-C1
3	B	313	PTY	O30-C30-O4-C1
3	C	313	PTY	O30-C30-O4-C1
3	D	313	PTY	O30-C30-O4-C1
3	E	313	PTY	O30-C30-O4-C1
3	G	308	PTY	O30-C30-O4-C1
3	I	313	PTY	O30-C30-O4-C1
3	J	313	PTY	O30-C30-O4-C1
3	L	301	PTY	O30-C30-O4-C1
4	A	307	Y01	CAJ-CAO-CBB-CBE
4	B	312	Y01	CAJ-CAO-CBB-CBE
4	C	312	Y01	CAJ-CAO-CBB-CBE
4	D	312	Y01	CAJ-CAO-CBB-CBE
4	E	312	Y01	CAJ-CAO-CBB-CBE
4	F	313	Y01	CAJ-CAO-CBB-CBE
4	G	307	Y01	CAJ-CAO-CBB-CBE
4	H	312	Y01	CAJ-CAO-CBB-CBE
4	I	312	Y01	CAJ-CAO-CBB-CBE
4	J	312	Y01	CAJ-CAO-CBB-CBE
4	K	312	Y01	CAJ-CAO-CBB-CBE
4	L	313	Y01	CAJ-CAO-CBB-CBE
4	A	307	Y01	CAJ-CAO-CBB-CAC
4	B	312	Y01	CAJ-CAO-CBB-CAC
4	C	312	Y01	CAJ-CAO-CBB-CAC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	312	Y01	CAJ-CAO-CBB-CAC
4	E	312	Y01	CAJ-CAO-CBB-CAC
4	F	313	Y01	CAJ-CAO-CBB-CAC
4	G	307	Y01	CAJ-CAO-CBB-CAC
4	H	312	Y01	CAJ-CAO-CBB-CAC
4	I	312	Y01	CAJ-CAO-CBB-CAC
4	J	312	Y01	CAJ-CAO-CBB-CAC
4	K	312	Y01	CAJ-CAO-CBB-CAC
4	L	313	Y01	CAJ-CAO-CBB-CAC
3	A	308	PTY	C8-C11-C12-C13
3	B	313	PTY	C8-C11-C12-C13
3	C	313	PTY	C8-C11-C12-C13
3	D	313	PTY	C8-C11-C12-C13
3	E	313	PTY	C8-C11-C12-C13
3	F	301	PTY	C8-C11-C12-C13
3	G	308	PTY	C8-C11-C12-C13
3	H	313	PTY	C8-C11-C12-C13
3	I	313	PTY	C8-C11-C12-C13
3	J	313	PTY	C8-C11-C12-C13
3	K	313	PTY	C8-C11-C12-C13
3	L	301	PTY	C8-C11-C12-C13
4	A	306	Y01	CAX-CAL-CAM-CAY
4	B	311	Y01	CAX-CAL-CAM-CAY
4	C	311	Y01	CAX-CAL-CAM-CAY
4	D	311	Y01	CAX-CAL-CAM-CAY
4	E	311	Y01	CAX-CAL-CAM-CAY
4	F	312	Y01	CAX-CAL-CAM-CAY
4	G	306	Y01	CAX-CAL-CAM-CAY
4	H	311	Y01	CAX-CAL-CAM-CAY
4	I	311	Y01	CAX-CAL-CAM-CAY
4	J	311	Y01	CAX-CAL-CAM-CAY
4	K	311	Y01	CAX-CAL-CAM-CAY
4	L	312	Y01	CAX-CAL-CAM-CAY
3	A	305	PTY	C3-O11-P1-O14
3	A	305	PTY	C5-O14-P1-O11
3	B	310	PTY	C3-O11-P1-O14
3	B	310	PTY	C5-O14-P1-O11
3	C	310	PTY	C3-O11-P1-O14
3	C	310	PTY	C5-O14-P1-O11
3	D	310	PTY	C3-O11-P1-O14
3	D	310	PTY	C5-O14-P1-O11
3	E	310	PTY	C3-O11-P1-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	310	PTY	C5-O14-P1-O11
3	F	311	PTY	C3-O11-P1-O14
3	F	311	PTY	C5-O14-P1-O11
3	G	305	PTY	C3-O11-P1-O14
3	G	305	PTY	C5-O14-P1-O11
3	H	310	PTY	C3-O11-P1-O14
3	H	310	PTY	C5-O14-P1-O11
3	I	310	PTY	C3-O11-P1-O14
3	I	310	PTY	C5-O14-P1-O11
3	J	310	PTY	C3-O11-P1-O14
3	J	310	PTY	C5-O14-P1-O11
3	K	310	PTY	C3-O11-P1-O14
3	K	310	PTY	C5-O14-P1-O11
3	L	311	PTY	C3-O11-P1-O14
3	L	311	PTY	C5-O14-P1-O11
2	E	307	C14	C08-C09-C10-C11
2	F	308	C14	C08-C09-C10-C11
2	A	302	C14	C08-C09-C10-C11
2	B	307	C14	C08-C09-C10-C11
2	C	307	C14	C08-C09-C10-C11
2	D	307	C14	C08-C09-C10-C11
2	G	302	C14	C08-C09-C10-C11
2	H	307	C14	C08-C09-C10-C11
2	I	307	C14	C08-C09-C10-C11
2	J	307	C14	C08-C09-C10-C11
2	K	307	C14	C08-C09-C10-C11
2	L	308	C14	C08-C09-C10-C11
3	A	305	PTY	C37-C38-C39-C40
3	B	310	PTY	C37-C38-C39-C40
3	C	310	PTY	C37-C38-C39-C40
3	D	310	PTY	C37-C38-C39-C40
3	E	310	PTY	C37-C38-C39-C40
3	F	311	PTY	C37-C38-C39-C40
3	G	305	PTY	C37-C38-C39-C40
3	H	310	PTY	C37-C38-C39-C40
3	I	310	PTY	C37-C38-C39-C40
3	J	310	PTY	C37-C38-C39-C40
3	K	310	PTY	C37-C38-C39-C40
3	L	311	PTY	C37-C38-C39-C40
3	A	305	PTY	C11-C8-O7-C6
3	B	310	PTY	C11-C8-O7-C6
3	C	310	PTY	C11-C8-O7-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	310	PTY	C11-C8-O7-C6
3	E	310	PTY	C11-C8-O7-C6
3	F	311	PTY	C11-C8-O7-C6
3	G	305	PTY	C11-C8-O7-C6
3	H	310	PTY	C11-C8-O7-C6
3	I	310	PTY	C11-C8-O7-C6
3	J	310	PTY	C11-C8-O7-C6
3	K	310	PTY	C11-C8-O7-C6
3	L	311	PTY	C11-C8-O7-C6
3	A	308	PTY	C33-C34-C35-C36
3	C	313	PTY	C33-C34-C35-C36
3	D	313	PTY	C33-C34-C35-C36
3	E	313	PTY	C33-C34-C35-C36
3	G	308	PTY	C33-C34-C35-C36
3	H	313	PTY	C33-C34-C35-C36
3	K	313	PTY	C33-C34-C35-C36
3	L	301	PTY	C33-C34-C35-C36
3	B	313	PTY	C33-C34-C35-C36
3	F	301	PTY	C33-C34-C35-C36
3	I	313	PTY	C33-C34-C35-C36
3	J	313	PTY	C33-C34-C35-C36
2	A	303	C14	C10-C11-C12-C13
2	B	308	C14	C10-C11-C12-C13
2	D	307	C14	C06-C07-C08-C09
2	D	308	C14	C10-C11-C12-C13
2	E	307	C14	C06-C07-C08-C09
2	E	308	C14	C10-C11-C12-C13
2	F	308	C14	C06-C07-C08-C09
2	F	309	C14	C10-C11-C12-C13
2	G	302	C14	C06-C07-C08-C09
2	G	303	C14	C10-C11-C12-C13
2	H	307	C14	C06-C07-C08-C09
2	H	308	C14	C10-C11-C12-C13
2	I	307	C14	C06-C07-C08-C09
2	I	308	C14	C10-C11-C12-C13
2	J	307	C14	C06-C07-C08-C09
2	J	308	C14	C10-C11-C12-C13
2	K	307	C14	C06-C07-C08-C09
2	K	308	C14	C10-C11-C12-C13
2	L	308	C14	C06-C07-C08-C09
2	L	309	C14	C10-C11-C12-C13
2	A	302	C14	C06-C07-C08-C09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	307	C14	C06-C07-C08-C09
2	C	307	C14	C06-C07-C08-C09
2	C	308	C14	C10-C11-C12-C13
2	D	303	C14	C10-C11-C12-C13
2	H	303	C14	C10-C11-C12-C13
2	J	303	C14	C10-C11-C12-C13
2	K	303	C14	C10-C11-C12-C13
3	A	305	PTY	O10-C8-O7-C6
3	B	310	PTY	O10-C8-O7-C6
3	C	310	PTY	O10-C8-O7-C6
3	D	310	PTY	O10-C8-O7-C6
3	E	310	PTY	O10-C8-O7-C6
3	F	311	PTY	O10-C8-O7-C6
3	G	305	PTY	O10-C8-O7-C6
3	H	310	PTY	O10-C8-O7-C6
3	I	310	PTY	O10-C8-O7-C6
3	J	310	PTY	O10-C8-O7-C6
3	K	310	PTY	O10-C8-O7-C6
3	L	311	PTY	O10-C8-O7-C6
2	A	311	C14	C10-C11-C12-C13
2	B	303	C14	C10-C11-C12-C13
2	C	303	C14	C10-C11-C12-C13
2	E	303	C14	C10-C11-C12-C13
2	F	304	C14	C10-C11-C12-C13
2	G	311	C14	C10-C11-C12-C13
2	I	303	C14	C10-C11-C12-C13
2	L	304	C14	C10-C11-C12-C13
3	B	310	PTY	C38-C39-C40-C41
3	A	305	PTY	C38-C39-C40-C41
3	C	310	PTY	C38-C39-C40-C41
3	D	310	PTY	C38-C39-C40-C41
3	E	310	PTY	C38-C39-C40-C41
3	F	311	PTY	C38-C39-C40-C41
3	G	305	PTY	C38-C39-C40-C41
3	H	310	PTY	C38-C39-C40-C41
3	I	310	PTY	C38-C39-C40-C41
3	J	310	PTY	C38-C39-C40-C41
3	K	310	PTY	C38-C39-C40-C41
3	L	311	PTY	C38-C39-C40-C41
4	A	307	Y01	CAJ-CAN-CBA-CAB
4	B	312	Y01	CAJ-CAN-CBA-CAB
4	C	312	Y01	CAJ-CAN-CBA-CAB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	312	Y01	CAJ-CAN-CBA-CAB
4	E	312	Y01	CAJ-CAN-CBA-CAB
4	F	313	Y01	CAJ-CAN-CBA-CAB
4	G	307	Y01	CAJ-CAN-CBA-CAB
4	H	312	Y01	CAJ-CAN-CBA-CAB
4	I	312	Y01	CAJ-CAN-CBA-CAB
4	J	312	Y01	CAJ-CAN-CBA-CAB
4	K	312	Y01	CAJ-CAN-CBA-CAB
4	L	313	Y01	CAJ-CAN-CBA-CAB
2	A	302	C14	C04-C05-C06-C07
2	B	307	C14	C04-C05-C06-C07
2	C	307	C14	C04-C05-C06-C07
2	D	307	C14	C04-C05-C06-C07
2	E	307	C14	C04-C05-C06-C07
2	F	308	C14	C04-C05-C06-C07
2	H	307	C14	C04-C05-C06-C07
2	I	307	C14	C04-C05-C06-C07
2	J	307	C14	C04-C05-C06-C07
2	K	307	C14	C04-C05-C06-C07
2	L	308	C14	C04-C05-C06-C07
2	G	302	C14	C04-C05-C06-C07
3	C	310	PTY	C35-C36-C37-C38
3	A	305	PTY	C35-C36-C37-C38
3	B	310	PTY	C35-C36-C37-C38
3	D	310	PTY	C35-C36-C37-C38
3	E	310	PTY	C35-C36-C37-C38
3	F	311	PTY	C35-C36-C37-C38
3	G	305	PTY	C35-C36-C37-C38
3	H	310	PTY	C35-C36-C37-C38
3	I	310	PTY	C35-C36-C37-C38
3	J	310	PTY	C35-C36-C37-C38
3	K	310	PTY	C35-C36-C37-C38
3	L	311	PTY	C35-C36-C37-C38
4	A	307	Y01	CAJ-CAN-CBA-CAA
4	B	312	Y01	CAJ-CAN-CBA-CAA
4	C	312	Y01	CAJ-CAN-CBA-CAA
4	D	312	Y01	CAJ-CAN-CBA-CAA
4	E	312	Y01	CAJ-CAN-CBA-CAA
4	F	313	Y01	CAJ-CAN-CBA-CAA
4	G	307	Y01	CAJ-CAN-CBA-CAA
4	H	312	Y01	CAJ-CAN-CBA-CAA
4	I	312	Y01	CAJ-CAN-CBA-CAA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	J	312	Y01	CAJ-CAN-CBA-CAA
4	K	312	Y01	CAJ-CAN-CBA-CAA
4	L	313	Y01	CAJ-CAN-CBA-CAA
2	K	305	C14	C03-C04-C05-C06
2	A	313	C14	C03-C04-C05-C06
2	B	305	C14	C03-C04-C05-C06
2	C	305	C14	C03-C04-C05-C06
2	D	305	C14	C03-C04-C05-C06
2	E	305	C14	C03-C04-C05-C06
2	F	306	C14	C03-C04-C05-C06
2	G	313	C14	C03-C04-C05-C06
2	H	305	C14	C03-C04-C05-C06
2	I	305	C14	C03-C04-C05-C06
2	L	306	C14	C03-C04-C05-C06
2	J	305	C14	C03-C04-C05-C06
3	A	308	PTY	O4-C1-C6-C5
3	B	313	PTY	O4-C1-C6-C5
3	C	313	PTY	O4-C1-C6-C5
3	D	313	PTY	O4-C1-C6-C5
3	E	313	PTY	O4-C1-C6-C5
3	F	301	PTY	O4-C1-C6-C5
3	G	308	PTY	O4-C1-C6-C5
3	H	313	PTY	O4-C1-C6-C5
3	I	313	PTY	O4-C1-C6-C5
3	J	313	PTY	O4-C1-C6-C5
3	K	313	PTY	O4-C1-C6-C5
3	L	301	PTY	O4-C1-C6-C5
3	A	308	PTY	C11-C12-C13-C14
3	B	313	PTY	C11-C12-C13-C14
3	C	313	PTY	C11-C12-C13-C14
3	D	313	PTY	C11-C12-C13-C14
3	E	313	PTY	C11-C12-C13-C14
3	F	301	PTY	C11-C12-C13-C14
3	G	308	PTY	C11-C12-C13-C14
3	H	313	PTY	C11-C12-C13-C14
3	I	313	PTY	C11-C12-C13-C14
3	J	313	PTY	C11-C12-C13-C14
3	K	313	PTY	C11-C12-C13-C14
3	L	301	PTY	C11-C12-C13-C14
2	B	301	C14	C11-C12-C13-C14
2	D	301	C14	C11-C12-C13-C14
2	F	302	C14	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	I	301	C14	C11-C12-C13-C14
2	J	301	C14	C11-C12-C13-C14
2	L	302	C14	C11-C12-C13-C14
2	A	309	C14	C11-C12-C13-C14
2	C	301	C14	C11-C12-C13-C14
2	E	301	C14	C11-C12-C13-C14
2	G	309	C14	C11-C12-C13-C14
2	H	301	C14	C11-C12-C13-C14
2	K	301	C14	C11-C12-C13-C14
4	A	307	Y01	CAN-CAJ-CAO-CBB
4	B	312	Y01	CAN-CAJ-CAO-CBB
4	C	312	Y01	CAN-CAJ-CAO-CBB
4	D	312	Y01	CAN-CAJ-CAO-CBB
4	E	312	Y01	CAN-CAJ-CAO-CBB
4	F	313	Y01	CAN-CAJ-CAO-CBB
4	G	307	Y01	CAN-CAJ-CAO-CBB
4	H	312	Y01	CAN-CAJ-CAO-CBB
4	I	312	Y01	CAN-CAJ-CAO-CBB
4	J	312	Y01	CAN-CAJ-CAO-CBB
4	K	312	Y01	CAN-CAJ-CAO-CBB
4	L	313	Y01	CAN-CAJ-CAO-CBB
3	A	308	PTY	O14-C5-C6-C1
3	B	313	PTY	O14-C5-C6-C1
3	C	313	PTY	O14-C5-C6-C1
3	D	313	PTY	O14-C5-C6-C1
3	E	313	PTY	O14-C5-C6-C1
3	F	301	PTY	O14-C5-C6-C1
3	G	308	PTY	O14-C5-C6-C1
3	H	313	PTY	O14-C5-C6-C1
3	I	313	PTY	O14-C5-C6-C1
3	J	313	PTY	O14-C5-C6-C1
3	K	313	PTY	O14-C5-C6-C1
3	L	301	PTY	O14-C5-C6-C1
2	A	312	C14	C04-C05-C06-C07
2	C	304	C14	C04-C05-C06-C07
2	D	304	C14	C04-C05-C06-C07
2	E	304	C14	C04-C05-C06-C07
2	F	305	C14	C04-C05-C06-C07
2	J	304	C14	C04-C05-C06-C07
2	K	304	C14	C04-C05-C06-C07
2	L	305	C14	C04-C05-C06-C07
2	A	313	C14	C09-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	304	C14	C04-C05-C06-C07
2	B	305	C14	C09-C10-C11-C12
2	F	306	C14	C09-C10-C11-C12
2	G	312	C14	C04-C05-C06-C07
2	H	304	C14	C04-C05-C06-C07
2	H	305	C14	C09-C10-C11-C12
2	I	304	C14	C04-C05-C06-C07
2	J	305	C14	C09-C10-C11-C12
2	L	306	C14	C09-C10-C11-C12
2	C	305	C14	C09-C10-C11-C12
2	D	305	C14	C09-C10-C11-C12
2	E	305	C14	C09-C10-C11-C12
2	G	313	C14	C09-C10-C11-C12
2	K	305	C14	C09-C10-C11-C12
2	I	305	C14	C09-C10-C11-C12
3	A	308	PTY	O14-C5-C6-O7
3	B	313	PTY	O14-C5-C6-O7
3	C	313	PTY	O14-C5-C6-O7
3	D	313	PTY	O14-C5-C6-O7
3	E	313	PTY	O14-C5-C6-O7
3	F	301	PTY	O14-C5-C6-O7
3	G	308	PTY	O14-C5-C6-O7
3	H	313	PTY	O14-C5-C6-O7
3	I	313	PTY	O14-C5-C6-O7
3	J	313	PTY	O14-C5-C6-O7
3	K	313	PTY	O14-C5-C6-O7
3	L	301	PTY	O14-C5-C6-O7
3	A	305	PTY	C11-C12-C13-C14
3	C	310	PTY	C11-C12-C13-C14
3	D	310	PTY	C11-C12-C13-C14
3	E	310	PTY	C11-C12-C13-C14
3	F	311	PTY	C11-C12-C13-C14
3	H	310	PTY	C11-C12-C13-C14
3	J	310	PTY	C11-C12-C13-C14
3	B	310	PTY	C11-C12-C13-C14
3	G	305	PTY	C11-C12-C13-C14
3	I	310	PTY	C11-C12-C13-C14
3	K	310	PTY	C11-C12-C13-C14
3	L	311	PTY	C11-C12-C13-C14
2	A	302	C14	C07-C08-C09-C10
2	B	307	C14	C07-C08-C09-C10
2	C	307	C14	C07-C08-C09-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	307	C14	C07-C08-C09-C10
2	E	307	C14	C07-C08-C09-C10
2	F	308	C14	C07-C08-C09-C10
2	G	302	C14	C07-C08-C09-C10
2	H	307	C14	C07-C08-C09-C10
2	I	307	C14	C07-C08-C09-C10
2	J	307	C14	C07-C08-C09-C10
2	K	307	C14	C07-C08-C09-C10
2	L	308	C14	C07-C08-C09-C10
2	F	310	C14	C05-C06-C07-C08
2	G	304	C14	C05-C06-C07-C08
2	L	310	C14	C05-C06-C07-C08
2	A	304	C14	C05-C06-C07-C08
2	B	309	C14	C05-C06-C07-C08
2	C	309	C14	C05-C06-C07-C08
2	D	309	C14	C05-C06-C07-C08
2	E	309	C14	C05-C06-C07-C08
2	I	309	C14	C05-C06-C07-C08
2	J	309	C14	C05-C06-C07-C08
2	K	309	C14	C05-C06-C07-C08
2	H	309	C14	C05-C06-C07-C08
2	A	304	C14	C09-C10-C11-C12
2	B	309	C14	C09-C10-C11-C12
2	C	309	C14	C09-C10-C11-C12
2	D	309	C14	C09-C10-C11-C12
2	E	309	C14	C09-C10-C11-C12
2	F	310	C14	C09-C10-C11-C12
2	G	304	C14	C09-C10-C11-C12
2	H	309	C14	C09-C10-C11-C12
2	K	309	C14	C09-C10-C11-C12
2	L	310	C14	C09-C10-C11-C12
2	I	309	C14	C09-C10-C11-C12
2	J	309	C14	C09-C10-C11-C12
3	A	308	PTY	O4-C1-C6-O7
3	B	313	PTY	O4-C1-C6-O7
3	C	313	PTY	O4-C1-C6-O7
3	D	313	PTY	O4-C1-C6-O7
3	E	313	PTY	O4-C1-C6-O7
3	F	301	PTY	O4-C1-C6-O7
3	G	308	PTY	O4-C1-C6-O7
3	H	313	PTY	O4-C1-C6-O7
3	I	313	PTY	O4-C1-C6-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	J	313	PTY	O4-C1-C6-O7
3	K	313	PTY	O4-C1-C6-O7
3	L	301	PTY	O4-C1-C6-O7
2	H	303	C14	C06-C07-C08-C09
3	A	305	PTY	C3-O11-P1-O12
3	B	310	PTY	C3-O11-P1-O12
3	C	310	PTY	C3-O11-P1-O12
3	D	310	PTY	C3-O11-P1-O12
3	E	310	PTY	C3-O11-P1-O12
3	F	311	PTY	C3-O11-P1-O12
3	G	305	PTY	C3-O11-P1-O12
3	H	310	PTY	C3-O11-P1-O12
3	I	310	PTY	C3-O11-P1-O12
3	J	310	PTY	C3-O11-P1-O12
3	K	310	PTY	C3-O11-P1-O12
3	L	311	PTY	C3-O11-P1-O12
3	A	308	PTY	C30-C31-C32-C33
3	E	313	PTY	C30-C31-C32-C33
3	F	301	PTY	C30-C31-C32-C33
3	G	308	PTY	C30-C31-C32-C33
3	H	313	PTY	C30-C31-C32-C33
3	J	313	PTY	C30-C31-C32-C33
3	K	313	PTY	C30-C31-C32-C33
2	A	311	C14	C06-C07-C08-C09
2	B	303	C14	C06-C07-C08-C09
2	F	304	C14	C06-C07-C08-C09
2	I	303	C14	C06-C07-C08-C09
2	L	304	C14	C06-C07-C08-C09
2	D	303	C14	C06-C07-C08-C09
2	J	303	C14	C06-C07-C08-C09
2	K	303	C14	C06-C07-C08-C09
2	C	303	C14	C06-C07-C08-C09
2	G	311	C14	C06-C07-C08-C09
3	B	313	PTY	C30-C31-C32-C33
3	C	313	PTY	C30-C31-C32-C33
3	D	313	PTY	C30-C31-C32-C33
3	I	313	PTY	C30-C31-C32-C33
3	L	301	PTY	C30-C31-C32-C33
2	E	303	C14	C06-C07-C08-C09
2	B	304	C14	C07-C08-C09-C10
2	C	304	C14	C07-C08-C09-C10
2	D	304	C14	C07-C08-C09-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	304	C14	C07-C08-C09-C10
2	F	305	C14	C07-C08-C09-C10
2	G	312	C14	C07-C08-C09-C10
2	H	304	C14	C07-C08-C09-C10
2	I	304	C14	C07-C08-C09-C10
2	J	304	C14	C07-C08-C09-C10
2	K	304	C14	C07-C08-C09-C10
2	L	305	C14	C07-C08-C09-C10
2	A	312	C14	C07-C08-C09-C10
2	A	313	C14	C04-C05-C06-C07
2	F	306	C14	C04-C05-C06-C07
2	H	305	C14	C04-C05-C06-C07
2	J	305	C14	C04-C05-C06-C07
2	K	305	C14	C04-C05-C06-C07
2	B	305	C14	C04-C05-C06-C07
2	C	305	C14	C04-C05-C06-C07
2	D	305	C14	C04-C05-C06-C07
2	E	305	C14	C04-C05-C06-C07
2	I	305	C14	C04-C05-C06-C07
2	L	306	C14	C04-C05-C06-C07
2	G	313	C14	C04-C05-C06-C07
4	B	312	Y01	CAX-CAL-CAM-CAY
4	D	312	Y01	CAX-CAL-CAM-CAY
4	F	313	Y01	CAX-CAL-CAM-CAY
4	G	307	Y01	CAX-CAL-CAM-CAY
4	L	313	Y01	CAX-CAL-CAM-CAY
4	A	307	Y01	CAX-CAL-CAM-CAY
4	C	312	Y01	CAX-CAL-CAM-CAY
4	E	312	Y01	CAX-CAL-CAM-CAY
4	H	312	Y01	CAX-CAL-CAM-CAY
4	I	312	Y01	CAX-CAL-CAM-CAY
4	J	312	Y01	CAX-CAL-CAM-CAY
4	K	312	Y01	CAX-CAL-CAM-CAY
2	A	313	C14	C08-C09-C10-C11
2	B	305	C14	C08-C09-C10-C11
2	C	305	C14	C08-C09-C10-C11
2	L	306	C14	C08-C09-C10-C11
2	A	310	C14	C03-C04-C05-C06
2	B	302	C14	C03-C04-C05-C06
2	C	302	C14	C03-C04-C05-C06
2	D	302	C14	C03-C04-C05-C06
2	D	305	C14	C08-C09-C10-C11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	305	C14	C08-C09-C10-C11
2	F	306	C14	C08-C09-C10-C11
2	G	313	C14	C08-C09-C10-C11
2	H	305	C14	C08-C09-C10-C11
2	I	302	C14	C03-C04-C05-C06
2	I	305	C14	C08-C09-C10-C11
2	J	305	C14	C08-C09-C10-C11
2	K	305	C14	C08-C09-C10-C11
2	E	302	C14	C03-C04-C05-C06
2	F	303	C14	C03-C04-C05-C06
2	G	310	C14	C03-C04-C05-C06
2	H	302	C14	C03-C04-C05-C06
2	L	303	C14	C03-C04-C05-C06
2	J	302	C14	C03-C04-C05-C06
2	K	302	C14	C03-C04-C05-C06
3	A	305	PTY	C6-C5-O14-P1
3	B	310	PTY	C6-C5-O14-P1
3	C	310	PTY	C6-C5-O14-P1
3	D	310	PTY	C6-C5-O14-P1
3	E	310	PTY	C6-C5-O14-P1
3	F	311	PTY	C6-C5-O14-P1
3	G	305	PTY	C6-C5-O14-P1
3	H	310	PTY	C6-C5-O14-P1
3	I	310	PTY	C6-C5-O14-P1
3	J	310	PTY	C6-C5-O14-P1
3	K	310	PTY	C6-C5-O14-P1
3	L	311	PTY	C6-C5-O14-P1
3	L	311	PTY	C34-C35-C36-C37
3	J	310	PTY	C34-C35-C36-C37
3	H	310	PTY	C34-C35-C36-C37
3	F	311	PTY	C34-C35-C36-C37
3	B	310	PTY	C34-C35-C36-C37
3	G	305	PTY	C34-C35-C36-C37
3	D	310	PTY	C34-C35-C36-C37
3	K	310	PTY	C34-C35-C36-C37
3	A	305	PTY	C34-C35-C36-C37
3	C	310	PTY	C34-C35-C36-C37
3	E	310	PTY	C34-C35-C36-C37
3	I	310	PTY	C34-C35-C36-C37
2	G	310	C14	C05-C06-C07-C08
2	L	303	C14	C05-C06-C07-C08
2	D	302	C14	C05-C06-C07-C08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	302	C14	C05-C06-C07-C08
2	F	303	C14	C05-C06-C07-C08
2	I	302	C14	C05-C06-C07-C08
2	K	302	C14	C05-C06-C07-C08
2	A	310	C14	C05-C06-C07-C08
2	B	302	C14	C05-C06-C07-C08
2	H	302	C14	C05-C06-C07-C08
2	J	302	C14	C05-C06-C07-C08
2	C	302	C14	C05-C06-C07-C08
3	A	305	PTY	C8-C11-C12-C13
3	B	310	PTY	C8-C11-C12-C13
3	I	310	PTY	C8-C11-C12-C13
3	L	311	PTY	C8-C11-C12-C13
3	C	310	PTY	C8-C11-C12-C13
3	D	310	PTY	C8-C11-C12-C13
3	E	310	PTY	C8-C11-C12-C13
3	F	311	PTY	C8-C11-C12-C13
3	G	305	PTY	C8-C11-C12-C13
3	H	310	PTY	C8-C11-C12-C13
3	J	310	PTY	C8-C11-C12-C13
3	K	310	PTY	C8-C11-C12-C13
3	B	313	PTY	C34-C35-C36-C37
3	I	313	PTY	C34-C35-C36-C37
3	A	308	PTY	C34-C35-C36-C37
3	F	301	PTY	C34-C35-C36-C37
3	G	308	PTY	C34-C35-C36-C37
3	L	301	PTY	C34-C35-C36-C37
3	C	313	PTY	C34-C35-C36-C37
3	D	313	PTY	C34-C35-C36-C37
3	H	313	PTY	C34-C35-C36-C37
3	J	313	PTY	C34-C35-C36-C37
3	K	313	PTY	C34-C35-C36-C37
3	E	313	PTY	C34-C35-C36-C37
2	I	305	C14	C10-C11-C12-C13
2	G	313	C14	C10-C11-C12-C13
2	H	305	C14	C10-C11-C12-C13
2	A	313	C14	C10-C11-C12-C13
2	B	305	C14	C10-C11-C12-C13
2	E	305	C14	C10-C11-C12-C13
2	F	306	C14	C10-C11-C12-C13
2	C	305	C14	C10-C11-C12-C13
2	D	305	C14	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	K	305	C14	C10-C11-C12-C13
2	L	306	C14	C10-C11-C12-C13
2	J	305	C14	C10-C11-C12-C13
4	A	307	Y01	CAL-CAM-CAY-OAW
4	B	312	Y01	CAL-CAM-CAY-OAW
4	D	312	Y01	CAL-CAM-CAY-OAW
4	E	312	Y01	CAL-CAM-CAY-OAW
4	F	313	Y01	CAL-CAM-CAY-OAW
4	G	307	Y01	CAL-CAM-CAY-OAW
4	I	312	Y01	CAL-CAM-CAY-OAW
4	J	312	Y01	CAL-CAM-CAY-OAW
4	K	312	Y01	CAL-CAM-CAY-OAW
4	L	313	Y01	CAL-CAM-CAY-OAW
4	C	312	Y01	CAL-CAM-CAY-OAW
4	H	312	Y01	CAL-CAM-CAY-OAW
4	H	311	Y01	CAJ-CAO-CBB-CAC
4	K	312	Y01	CAM-CAL-CAX-OAH
4	A	306	Y01	CAJ-CAO-CBB-CAC
4	B	311	Y01	CAJ-CAO-CBB-CAC
4	D	311	Y01	CAJ-CAO-CBB-CAC
4	E	311	Y01	CAJ-CAO-CBB-CAC
4	G	306	Y01	CAJ-CAO-CBB-CAC
4	I	311	Y01	CAJ-CAO-CBB-CAC
4	J	311	Y01	CAJ-CAO-CBB-CAC
4	K	311	Y01	CAJ-CAO-CBB-CAC
4	L	312	Y01	CAJ-CAO-CBB-CAC
2	C	305	C14	C07-C08-C09-C10
2	F	306	C14	C07-C08-C09-C10
2	G	313	C14	C07-C08-C09-C10
2	I	305	C14	C07-C08-C09-C10
2	K	305	C14	C07-C08-C09-C10
4	A	307	Y01	CAM-CAL-CAX-OAH
4	B	312	Y01	CAM-CAL-CAX-OAH
4	C	312	Y01	CAM-CAL-CAX-OAH
4	D	312	Y01	CAM-CAL-CAX-OAH
4	E	312	Y01	CAM-CAL-CAX-OAH
4	F	313	Y01	CAM-CAL-CAX-OAH
4	G	307	Y01	CAM-CAL-CAX-OAH
4	H	312	Y01	CAM-CAL-CAX-OAH
4	I	312	Y01	CAM-CAL-CAX-OAH
4	J	312	Y01	CAM-CAL-CAX-OAH
4	L	313	Y01	CAM-CAL-CAX-OAH

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	311	Y01	CAJ-CAO-CBB-CAC
4	F	312	Y01	CAJ-CAO-CBB-CAC
2	B	305	C14	C07-C08-C09-C10
2	D	305	C14	C07-C08-C09-C10
2	E	305	C14	C07-C08-C09-C10
2	H	305	C14	C07-C08-C09-C10
2	A	313	C14	C07-C08-C09-C10
2	J	305	C14	C07-C08-C09-C10
2	L	306	C14	C07-C08-C09-C10
3	I	310	PTY	C36-C37-C38-C39
3	B	310	PTY	C36-C37-C38-C39
3	K	310	PTY	C36-C37-C38-C39
3	A	305	PTY	C36-C37-C38-C39
3	D	310	PTY	C36-C37-C38-C39
3	F	311	PTY	C36-C37-C38-C39
3	G	305	PTY	C36-C37-C38-C39
3	J	310	PTY	C36-C37-C38-C39
3	C	310	PTY	C36-C37-C38-C39
3	E	310	PTY	C36-C37-C38-C39
3	H	310	PTY	C36-C37-C38-C39
3	L	311	PTY	C36-C37-C38-C39
3	A	308	PTY	C37-C38-C39-C40
3	I	313	PTY	C37-C38-C39-C40
3	D	313	PTY	C37-C38-C39-C40
3	G	308	PTY	C37-C38-C39-C40
3	C	313	PTY	C37-C38-C39-C40
3	L	301	PTY	C37-C38-C39-C40
3	B	313	PTY	C37-C38-C39-C40
3	F	301	PTY	C37-C38-C39-C40
3	H	313	PTY	C37-C38-C39-C40
3	K	313	PTY	C37-C38-C39-C40
3	E	313	PTY	C37-C38-C39-C40
3	J	313	PTY	C37-C38-C39-C40
3	F	301	PTY	C36-C37-C38-C39
3	H	313	PTY	C36-C37-C38-C39
3	G	308	PTY	C36-C37-C38-C39
3	B	313	PTY	C36-C37-C38-C39
3	L	301	PTY	C36-C37-C38-C39
3	C	313	PTY	C36-C37-C38-C39
3	E	313	PTY	C36-C37-C38-C39
3	I	313	PTY	C36-C37-C38-C39
3	J	313	PTY	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	313	PTY	C36-C37-C38-C39
3	K	313	PTY	C36-C37-C38-C39
3	A	308	PTY	C36-C37-C38-C39
3	A	308	PTY	C3-O11-P1-O13
3	B	313	PTY	C3-O11-P1-O13
3	C	313	PTY	C3-O11-P1-O13
3	D	313	PTY	C3-O11-P1-O13
3	E	313	PTY	C3-O11-P1-O13
3	F	301	PTY	C3-O11-P1-O13
3	G	308	PTY	C3-O11-P1-O13
3	H	313	PTY	C3-O11-P1-O13
3	I	313	PTY	C3-O11-P1-O13
3	J	313	PTY	C3-O11-P1-O13
3	K	313	PTY	C3-O11-P1-O13
3	L	301	PTY	C3-O11-P1-O13
4	A	307	Y01	CAL-CAM-CAY-OAG
4	B	312	Y01	CAL-CAM-CAY-OAG
4	C	312	Y01	CAL-CAM-CAY-OAG
4	D	312	Y01	CAL-CAM-CAY-OAG
4	E	312	Y01	CAL-CAM-CAY-OAG
4	F	313	Y01	CAL-CAM-CAY-OAG
4	G	307	Y01	CAL-CAM-CAY-OAG
4	H	312	Y01	CAL-CAM-CAY-OAG
4	I	312	Y01	CAL-CAM-CAY-OAG
4	J	312	Y01	CAL-CAM-CAY-OAG
4	K	312	Y01	CAL-CAM-CAY-OAG
4	L	313	Y01	CAL-CAM-CAY-OAG
4	B	312	Y01	CAM-CAL-CAX-OAF
4	C	312	Y01	CAM-CAL-CAX-OAF
4	D	312	Y01	CAM-CAL-CAX-OAF
4	F	313	Y01	CAM-CAL-CAX-OAF
4	G	307	Y01	CAM-CAL-CAX-OAF
4	H	312	Y01	CAM-CAL-CAX-OAF
4	I	312	Y01	CAM-CAL-CAX-OAF
4	J	312	Y01	CAM-CAL-CAX-OAF
4	K	312	Y01	CAM-CAL-CAX-OAF
4	L	313	Y01	CAM-CAL-CAX-OAF
4	A	307	Y01	CAM-CAL-CAX-OAF
4	E	312	Y01	CAM-CAL-CAX-OAF

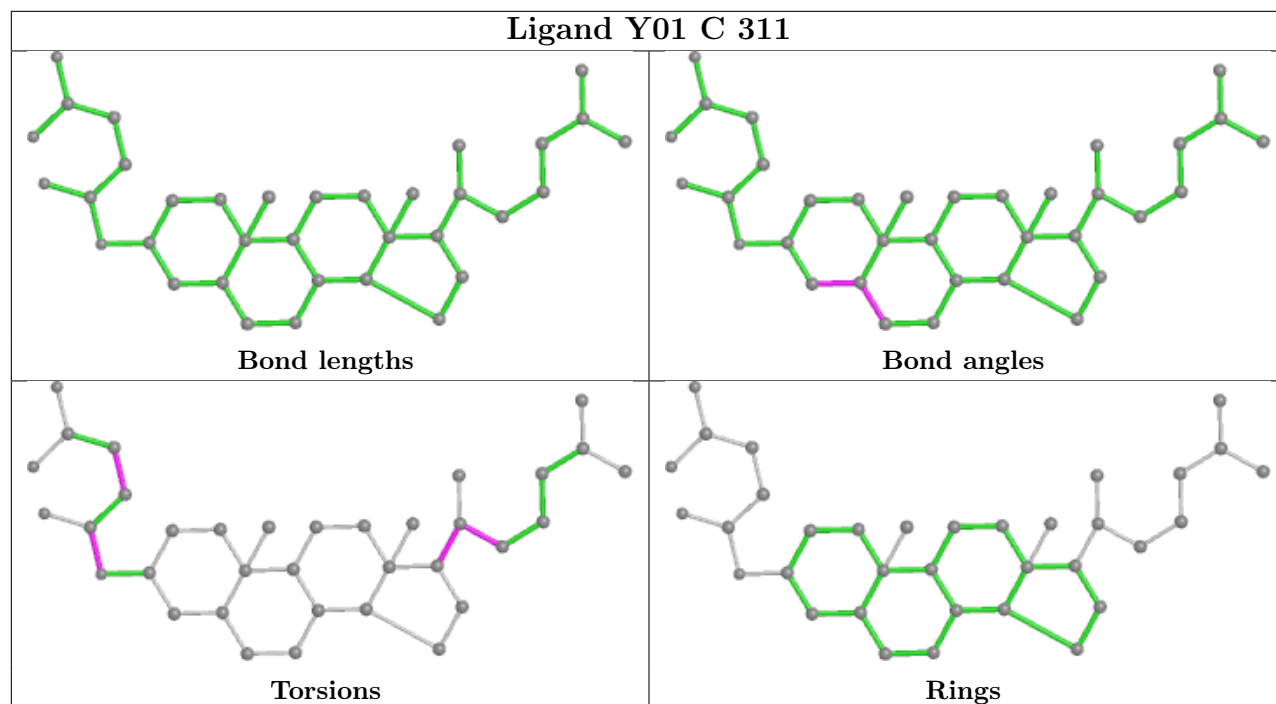
There are no ring outliers.

29 monomers are involved in 89 short contacts:

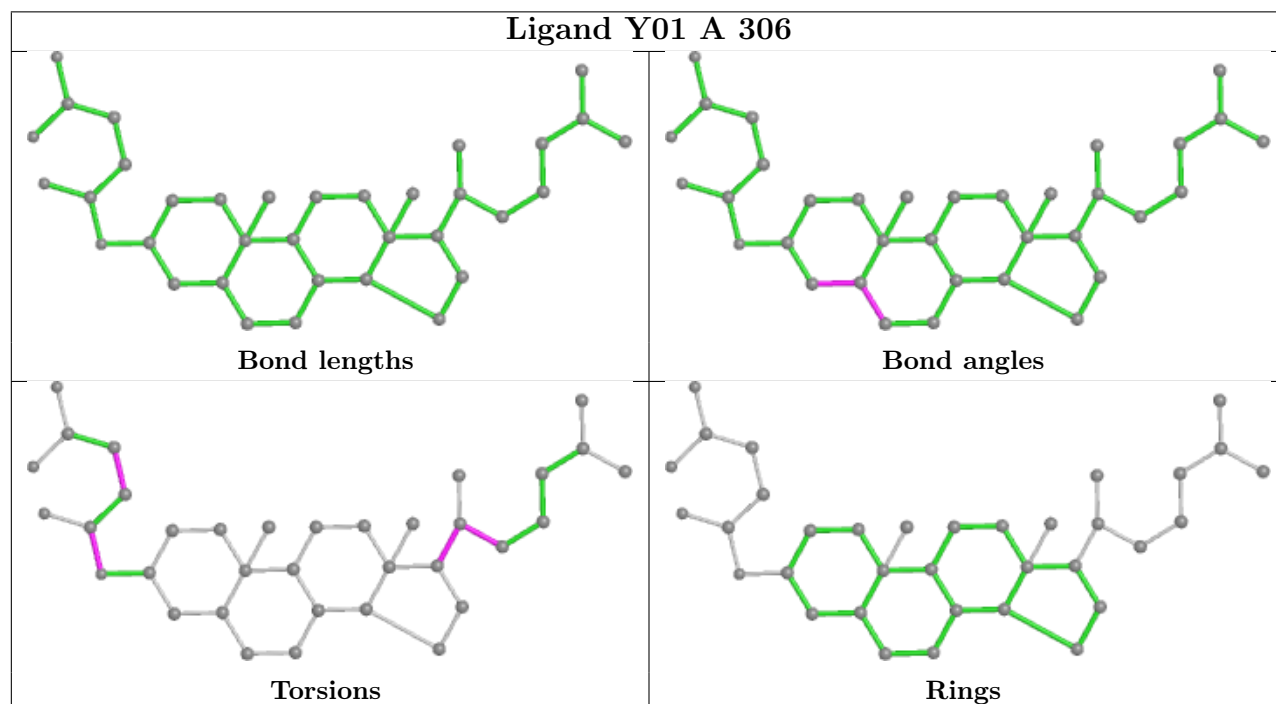
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	311	Y01	1	0
4	A	306	Y01	2	0
4	G	307	Y01	6	0
4	K	311	Y01	1	0
4	C	312	Y01	6	0
4	K	312	Y01	6	0
4	J	312	Y01	6	0
3	L	301	PTY	1	0
3	G	308	PTY	1	0
4	J	311	Y01	1	0
4	B	312	Y01	6	0
4	H	311	Y01	2	0
4	A	307	Y01	6	0
4	F	312	Y01	1	0
4	E	311	Y01	1	0
3	F	301	PTY	1	0
4	L	313	Y01	6	0
3	A	308	PTY	1	0
4	H	312	Y01	6	0
4	I	311	Y01	2	0
4	D	312	Y01	6	0
3	H	313	PTY	1	0
4	E	312	Y01	6	0
4	D	311	Y01	1	0
4	G	306	Y01	2	0
4	B	311	Y01	2	0
4	I	312	Y01	6	0
4	F	313	Y01	6	0
4	L	312	Y01	1	0

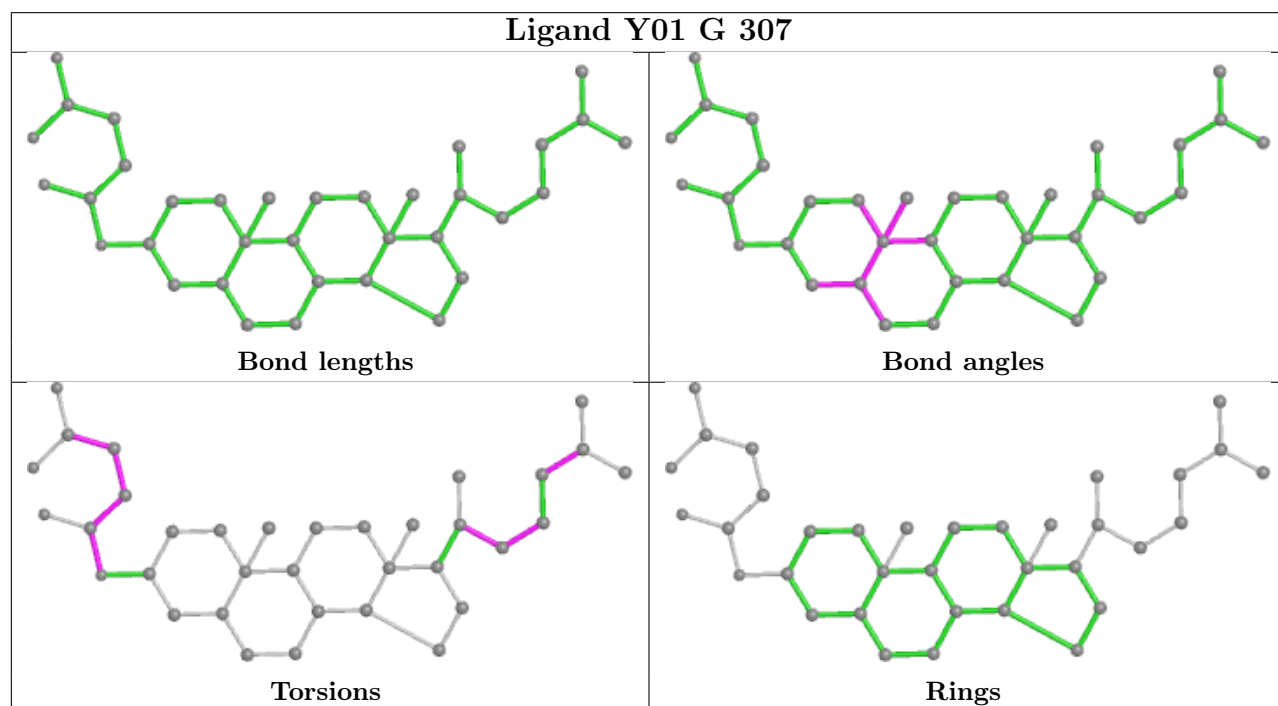
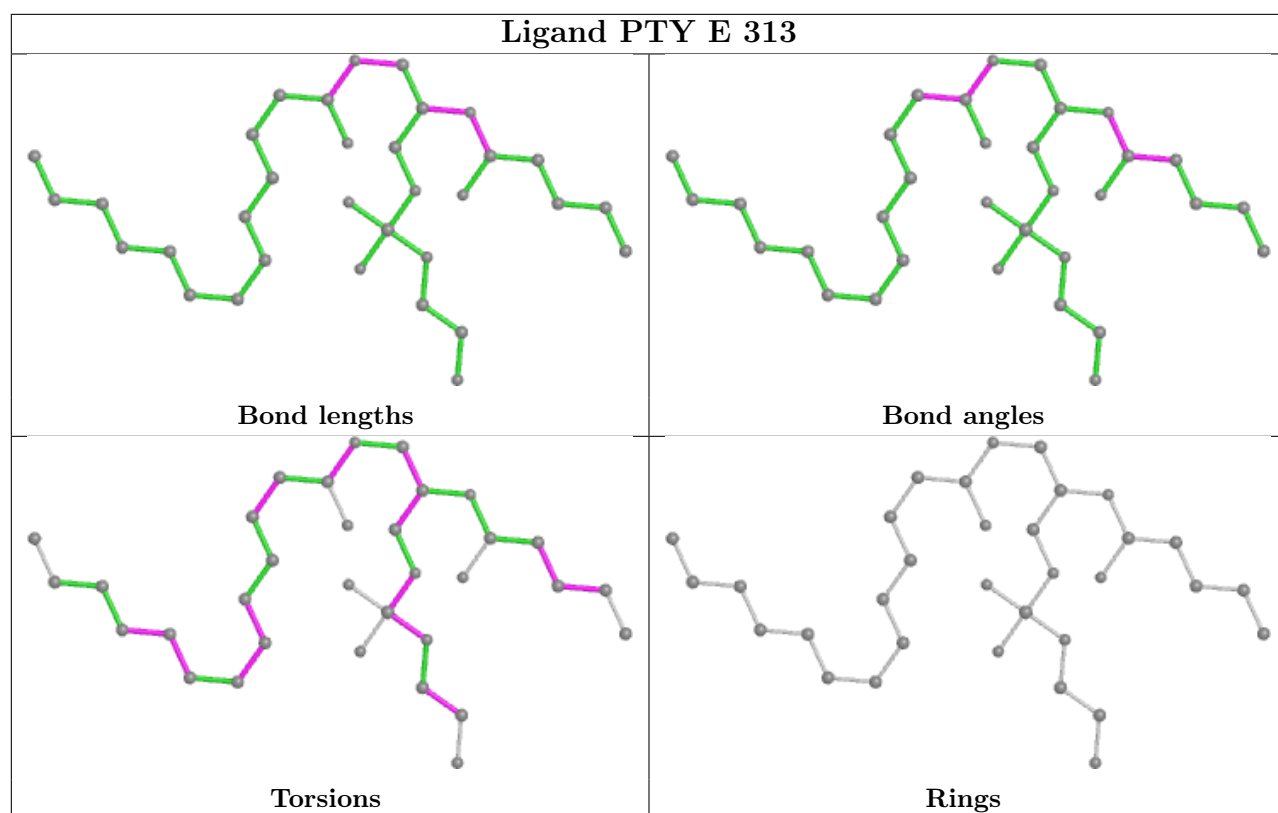
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

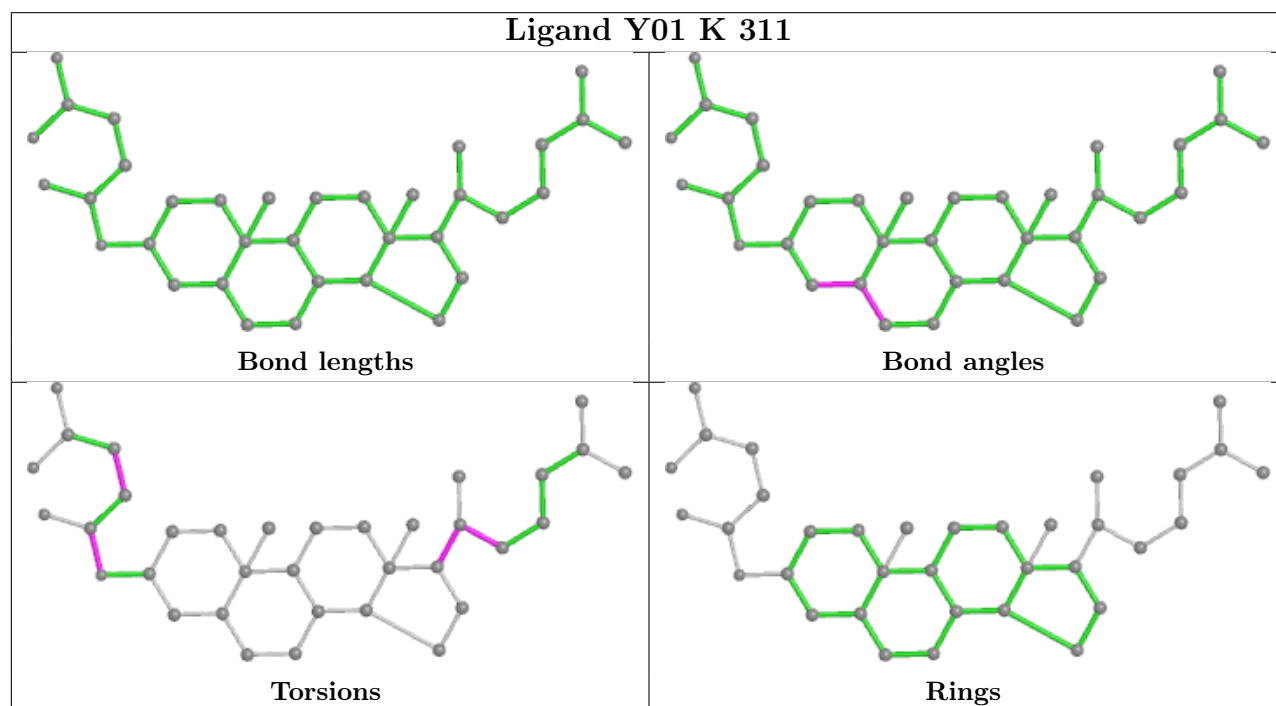
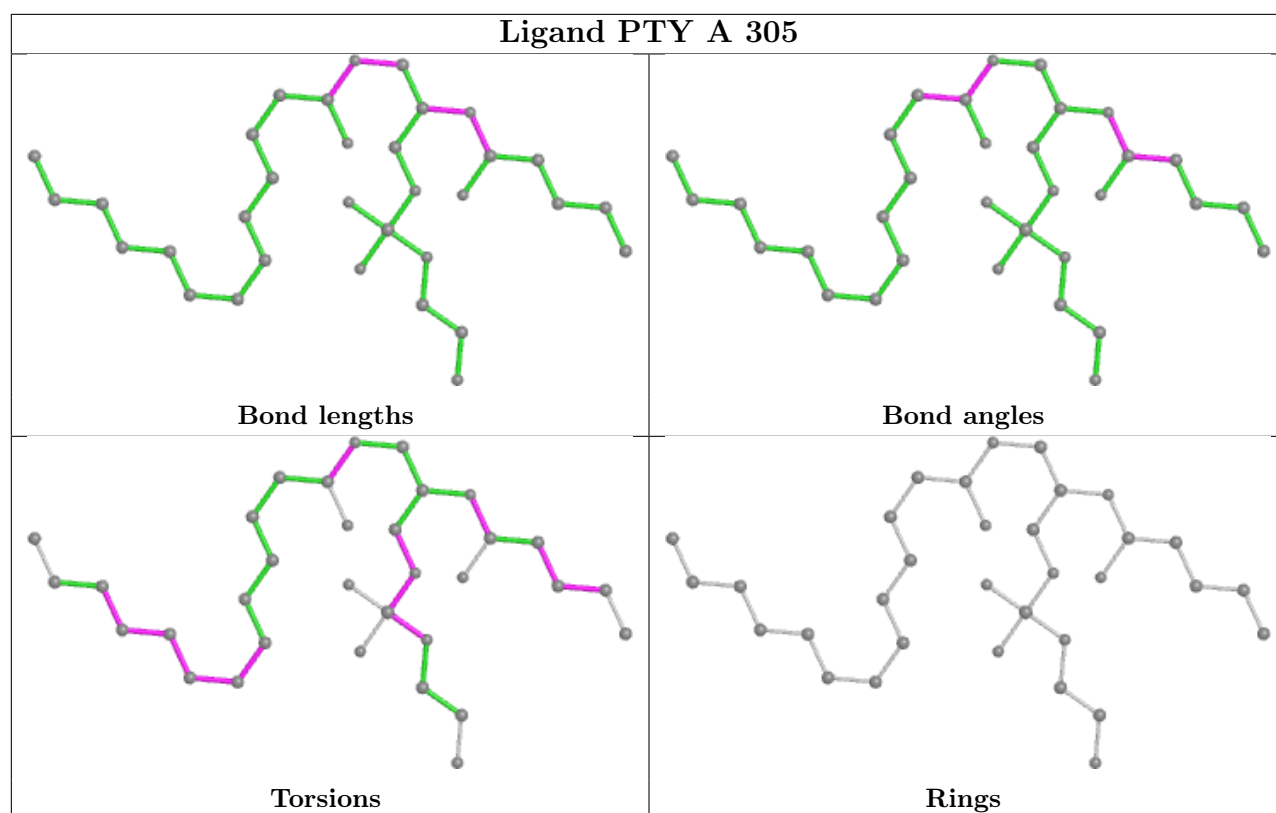
Ligand Y01 C 311



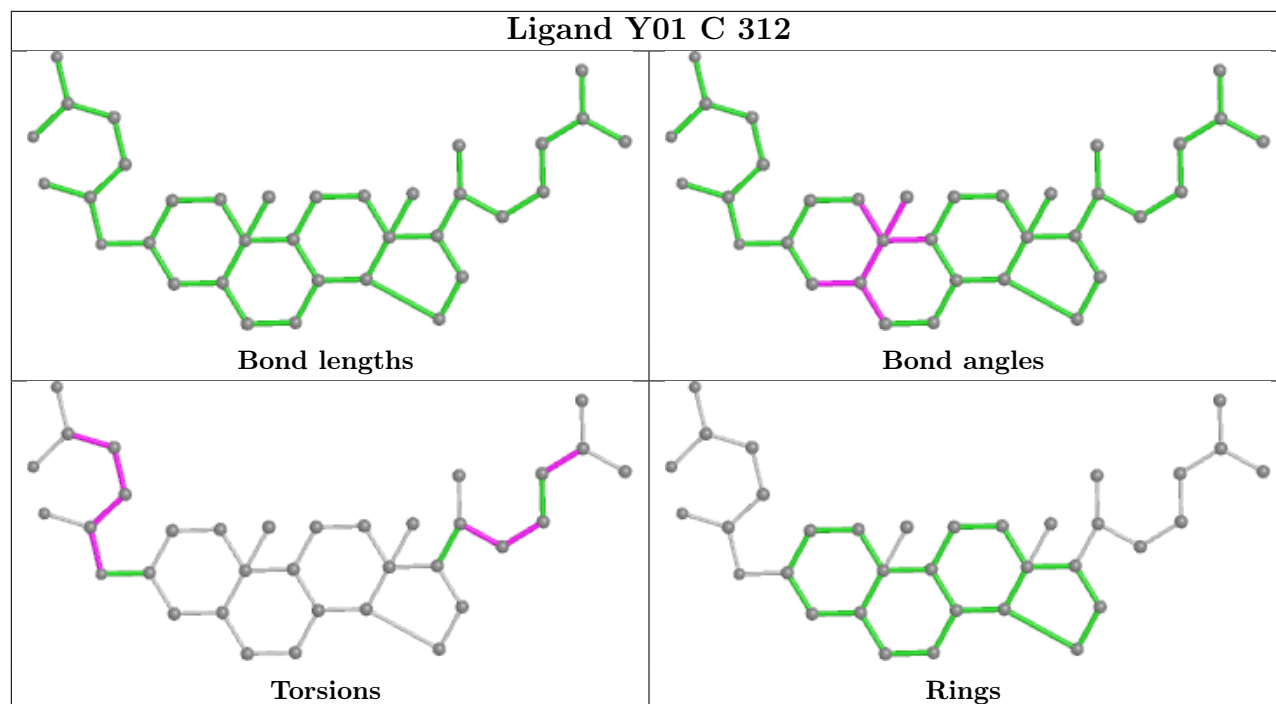
Ligand Y01 A 306



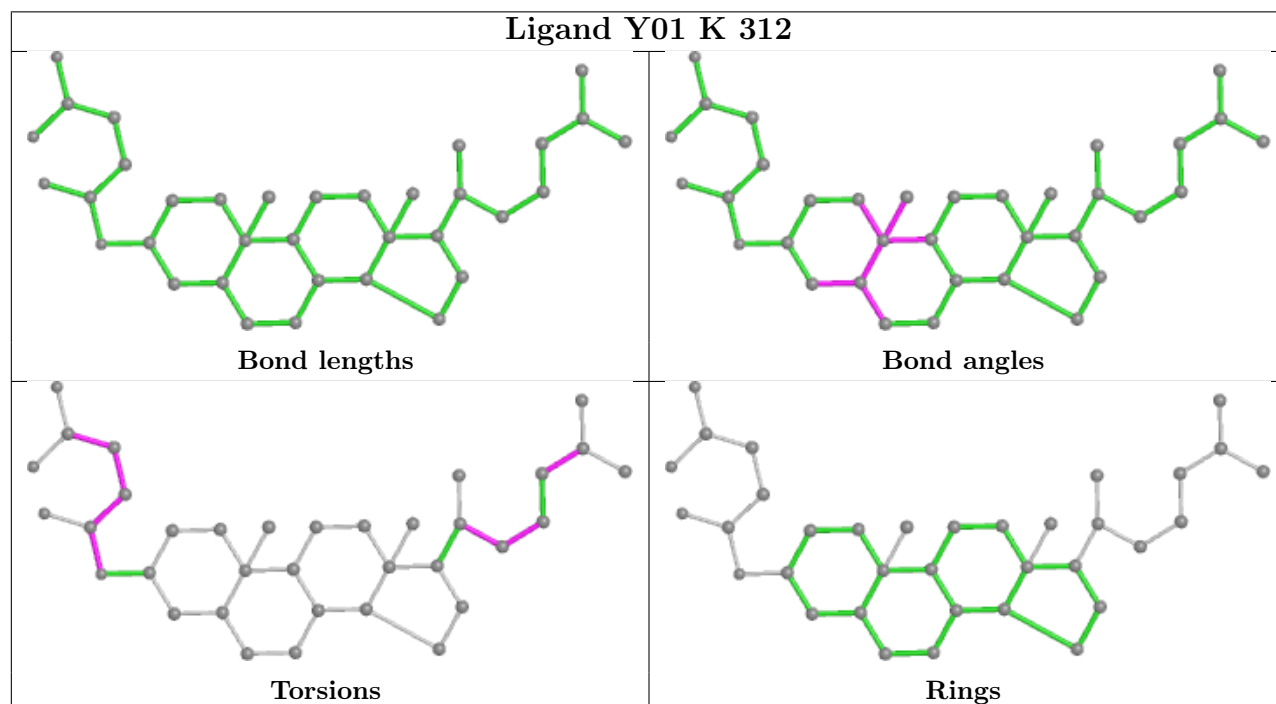


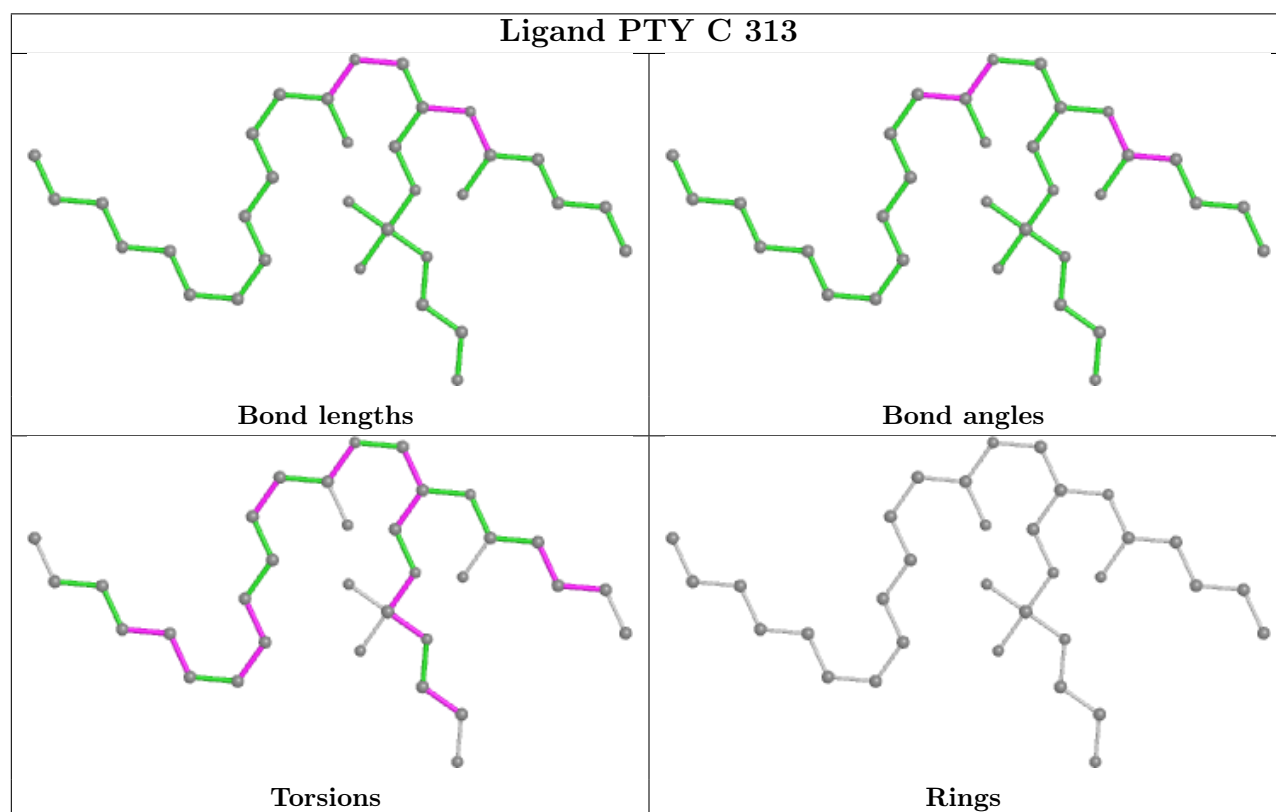
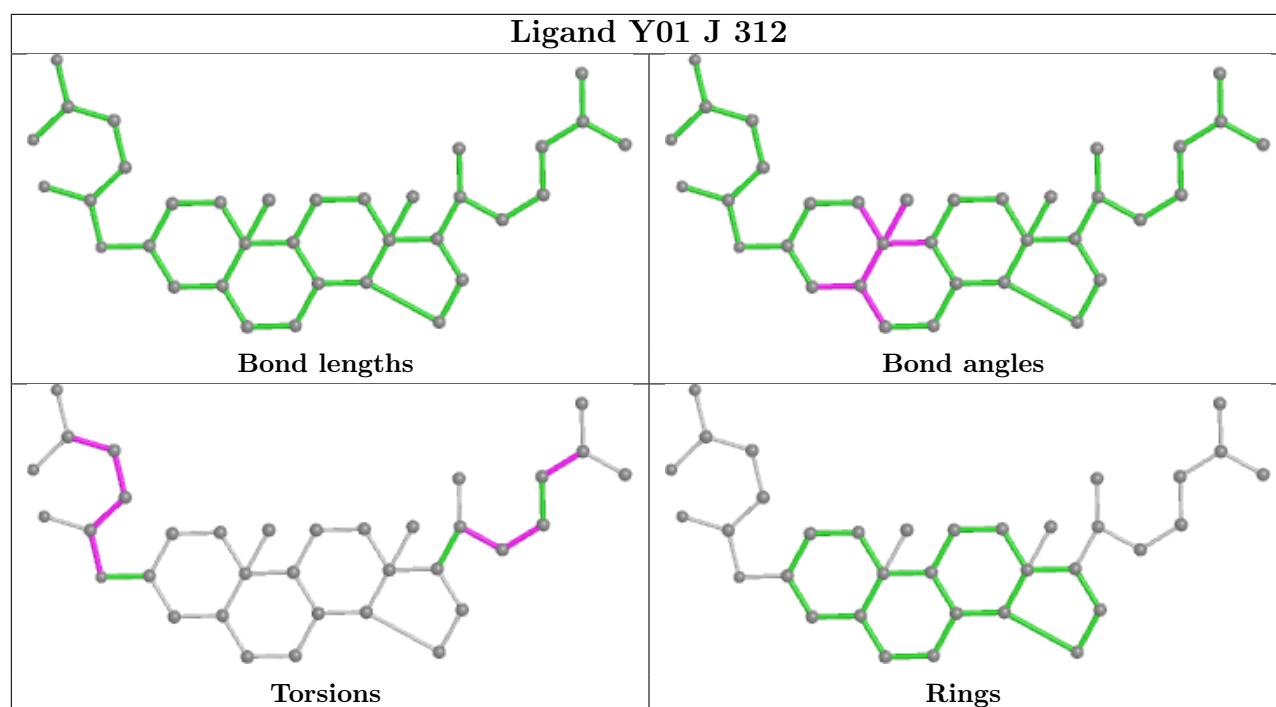


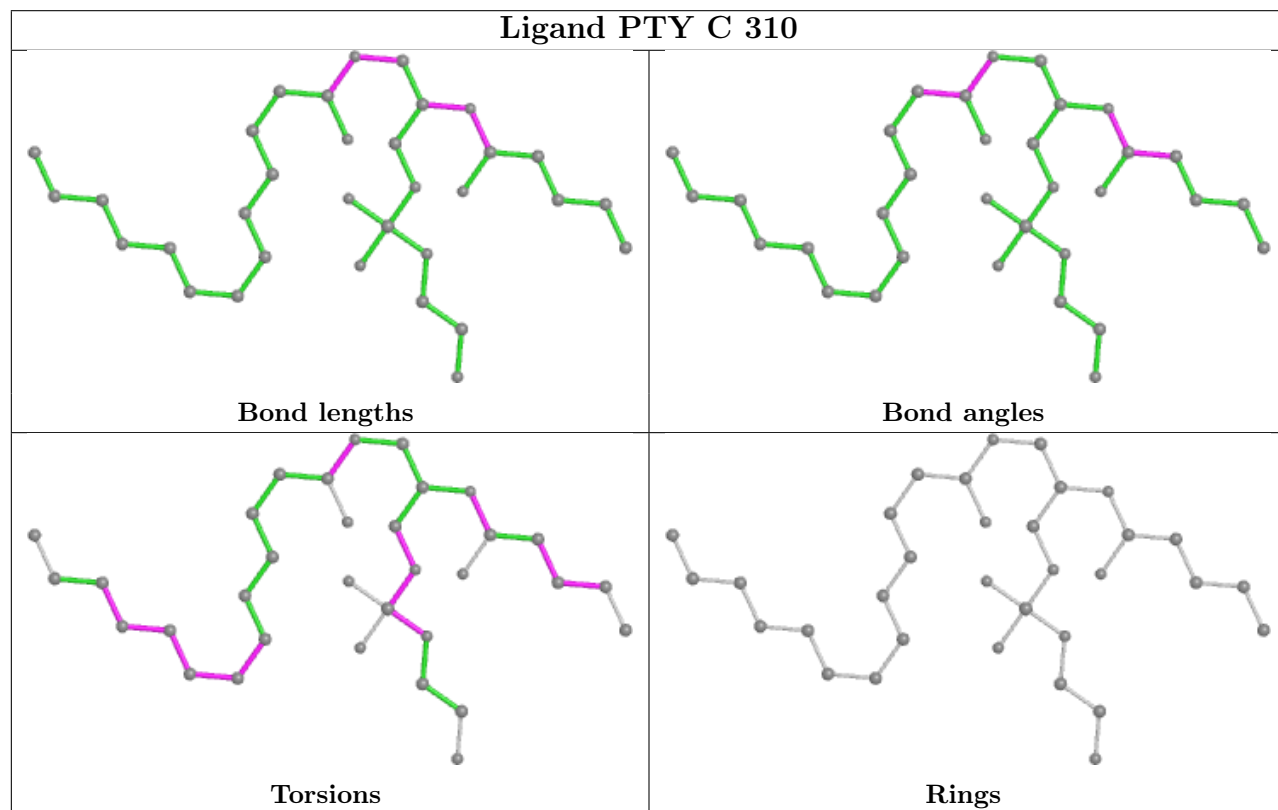
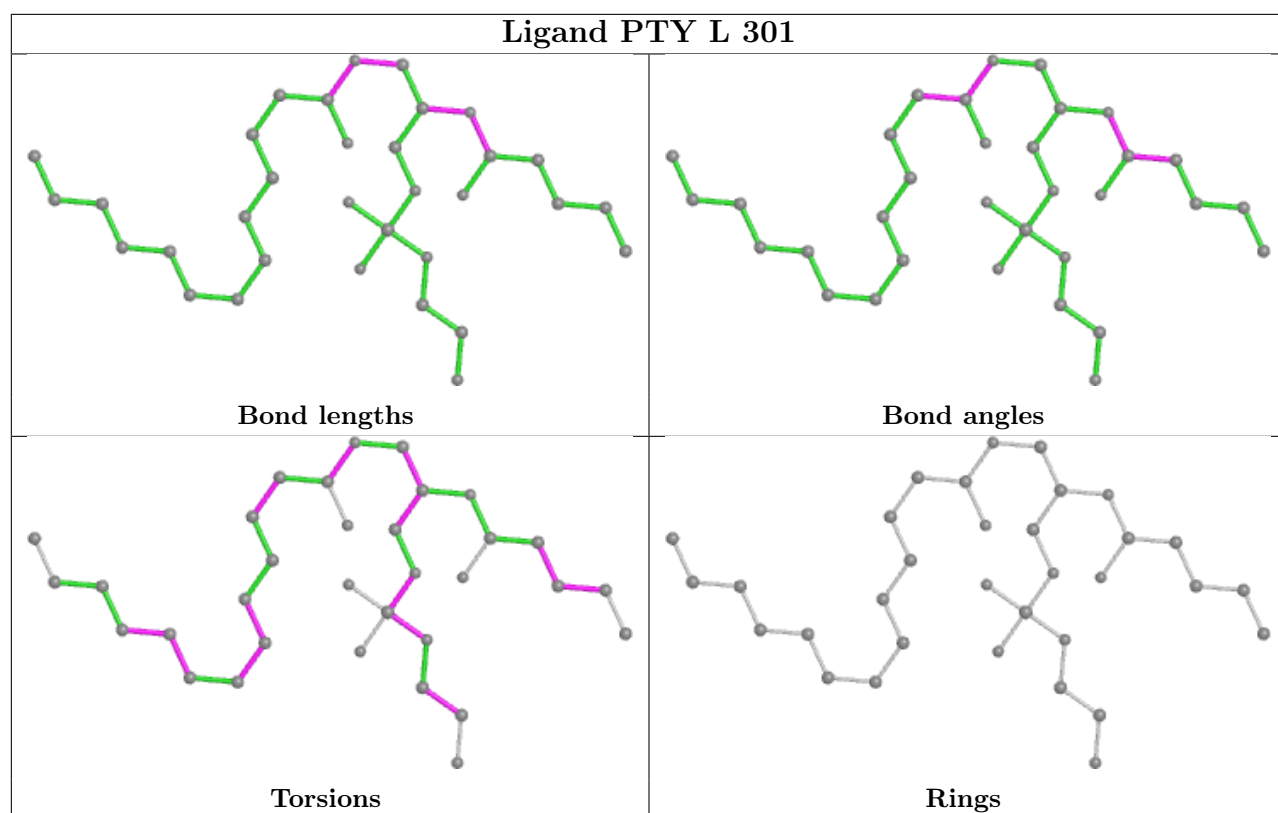
Ligand Y01 C 312

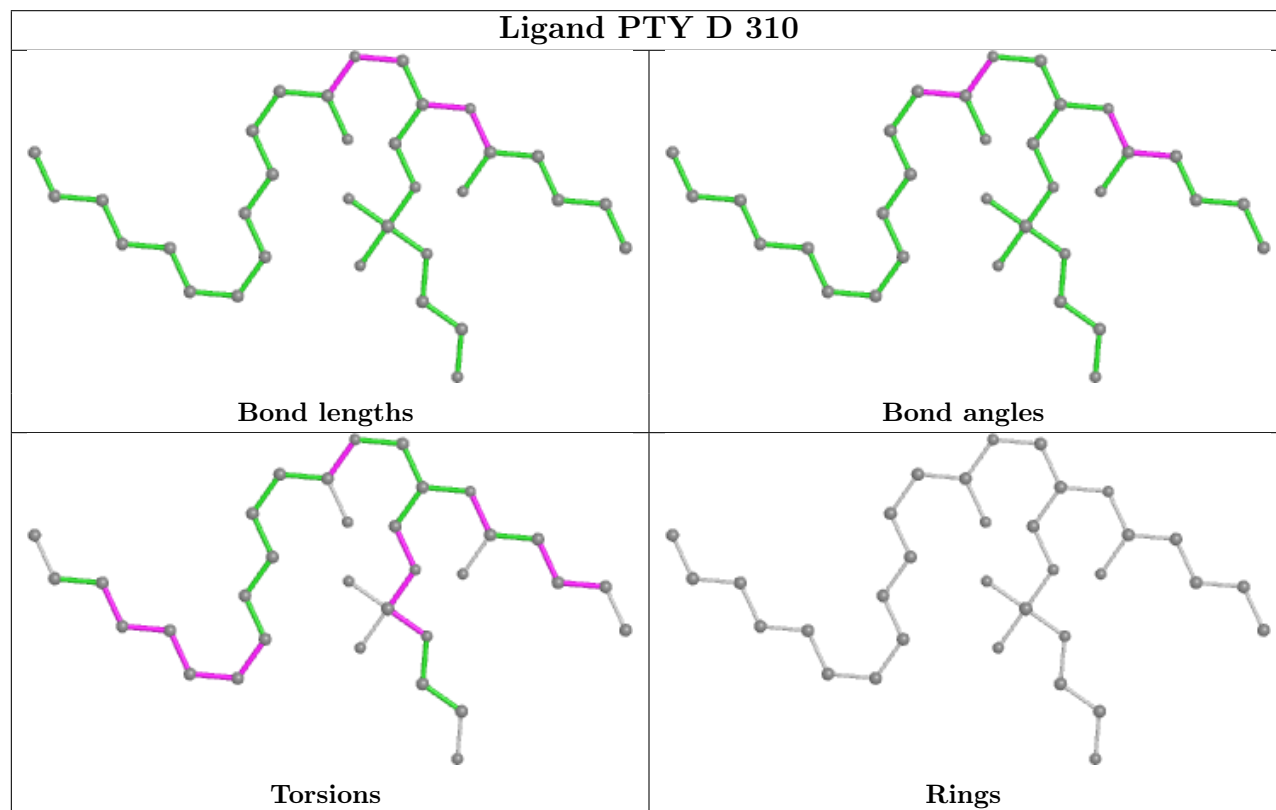
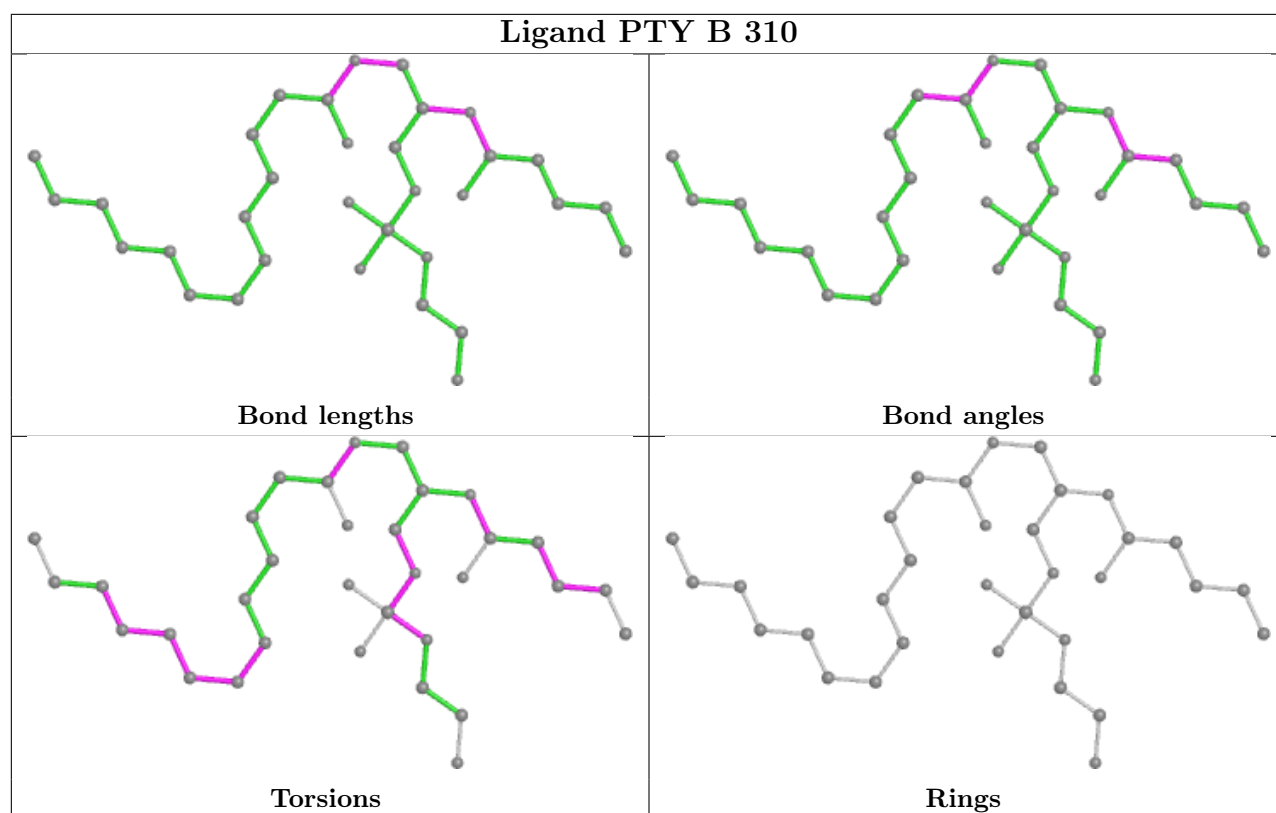


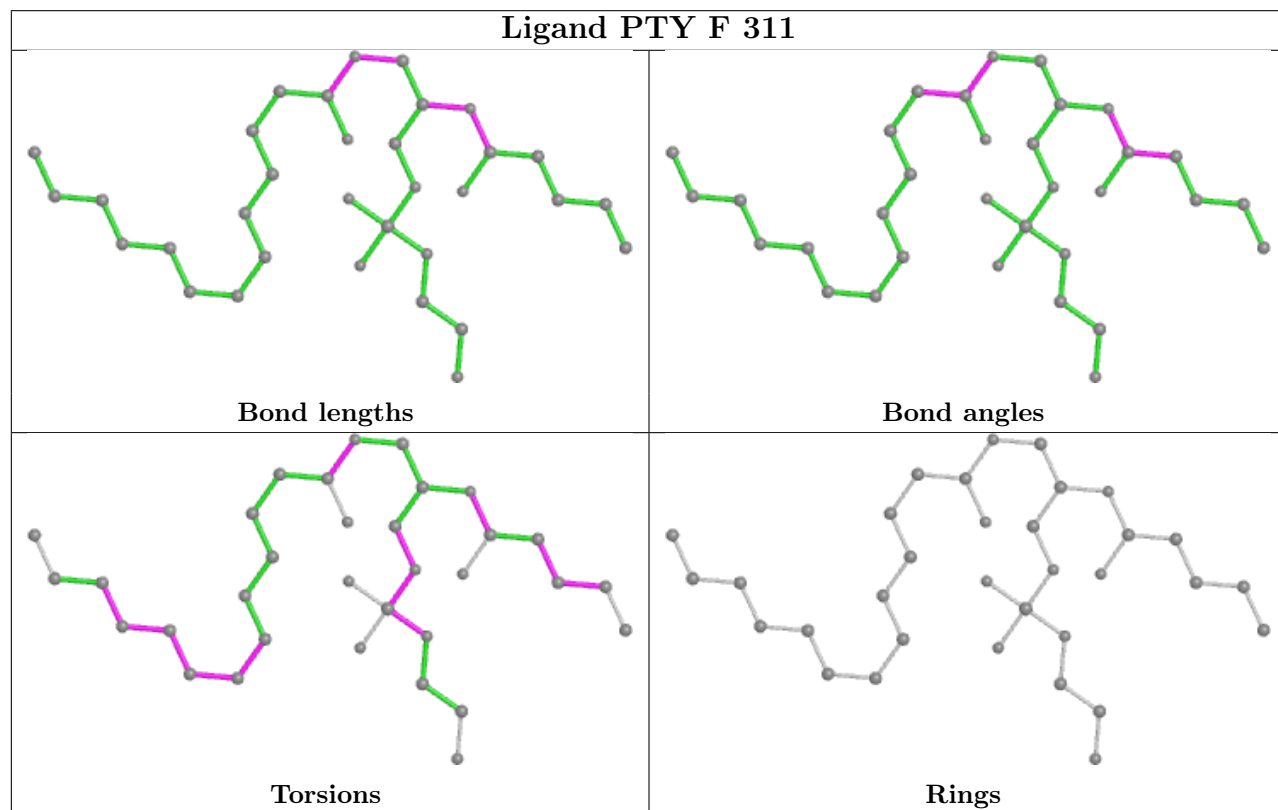
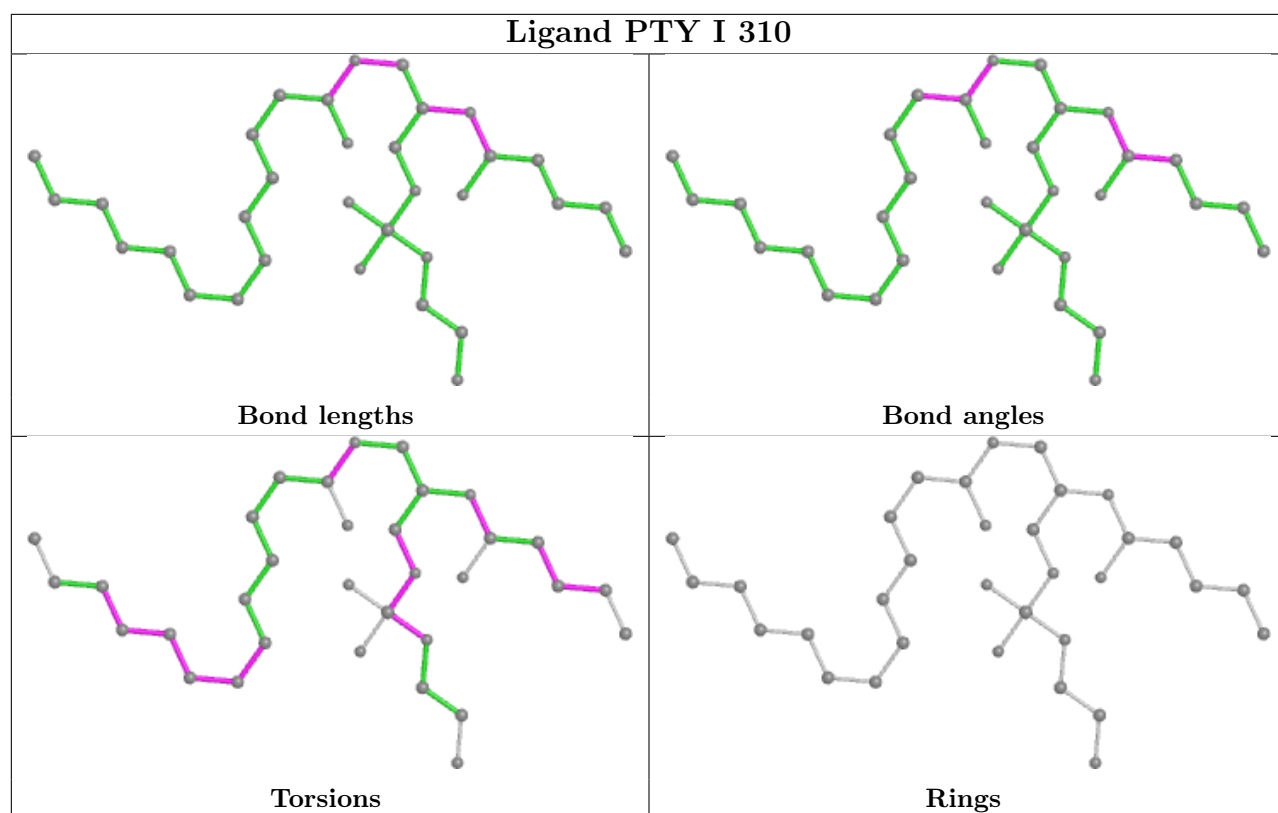
Ligand Y01 K 312

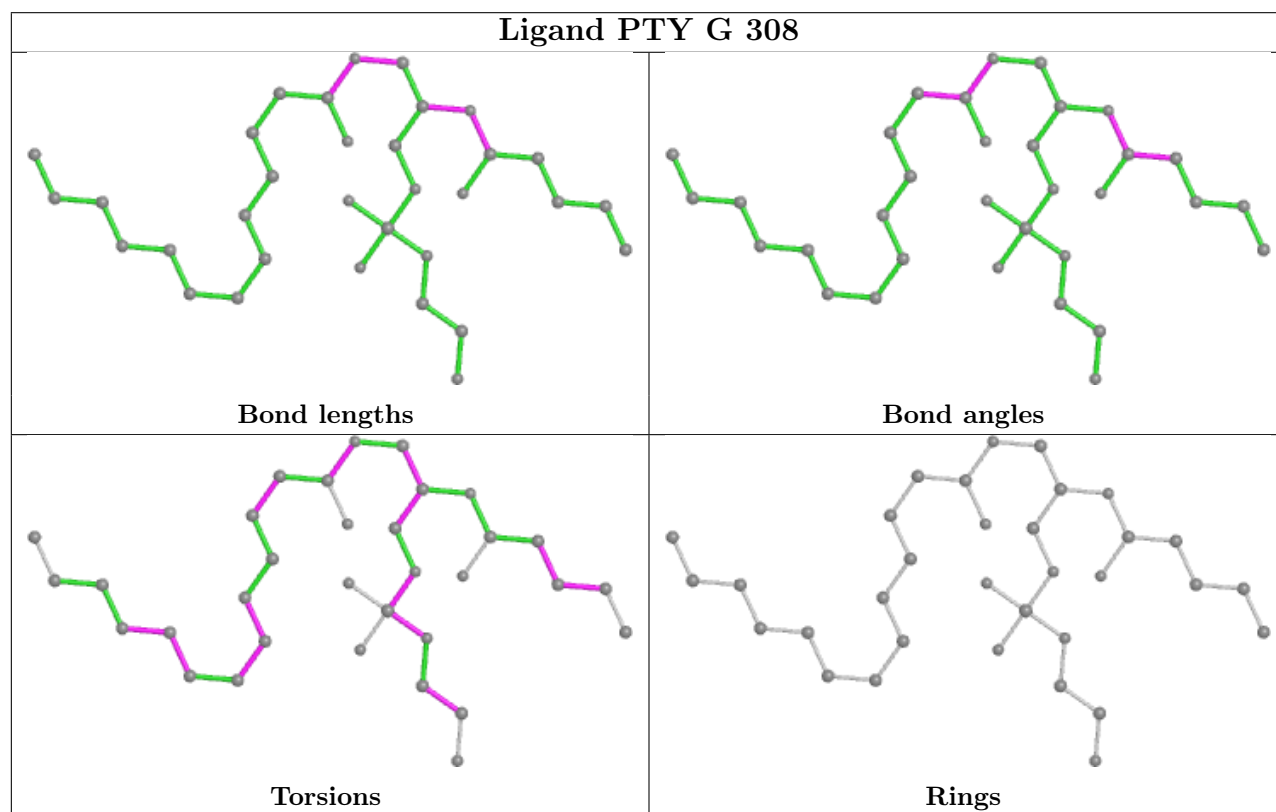
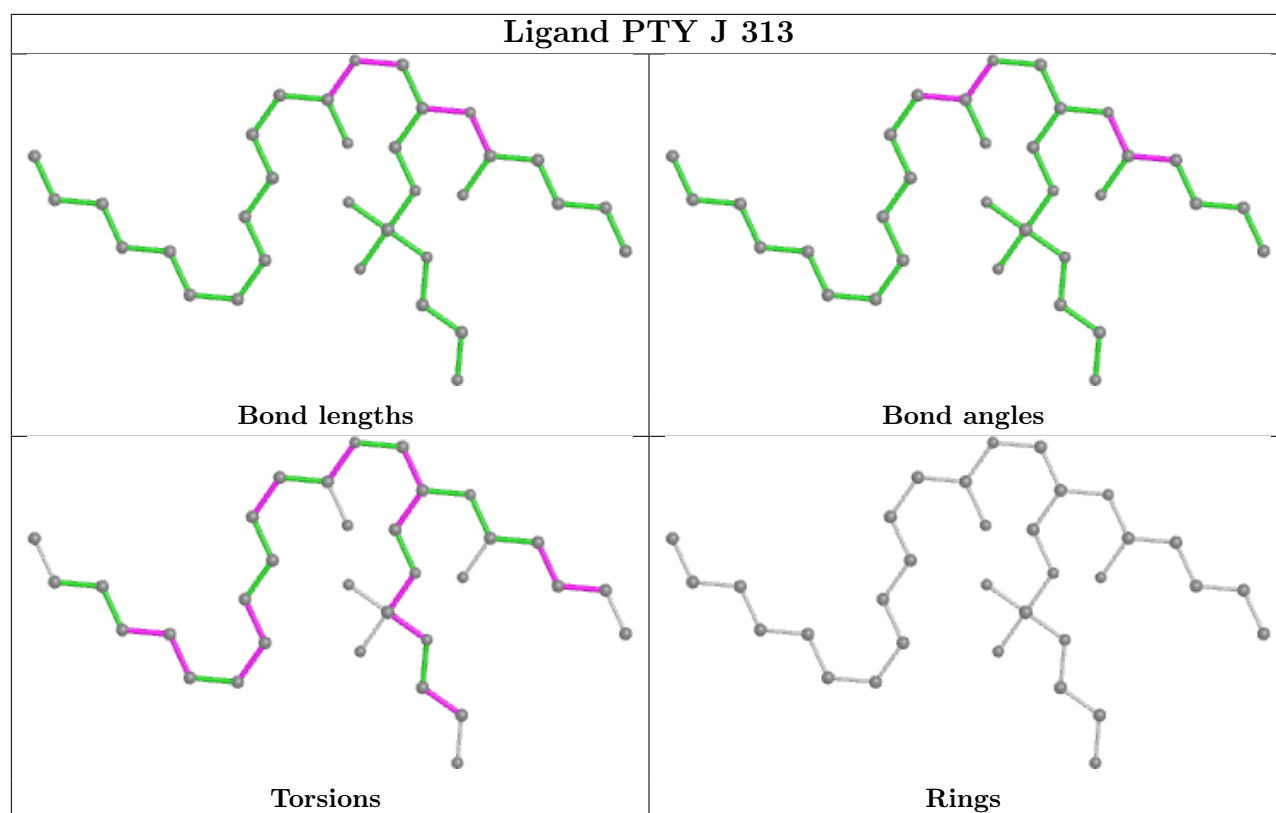


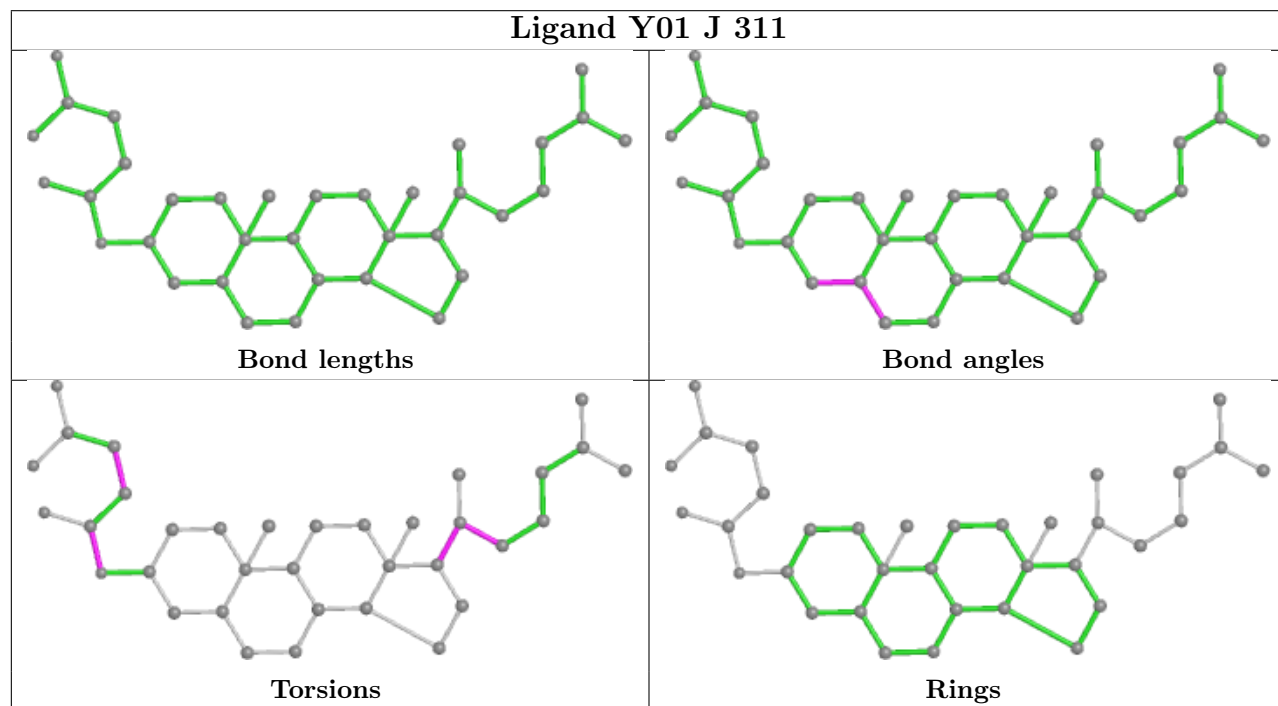
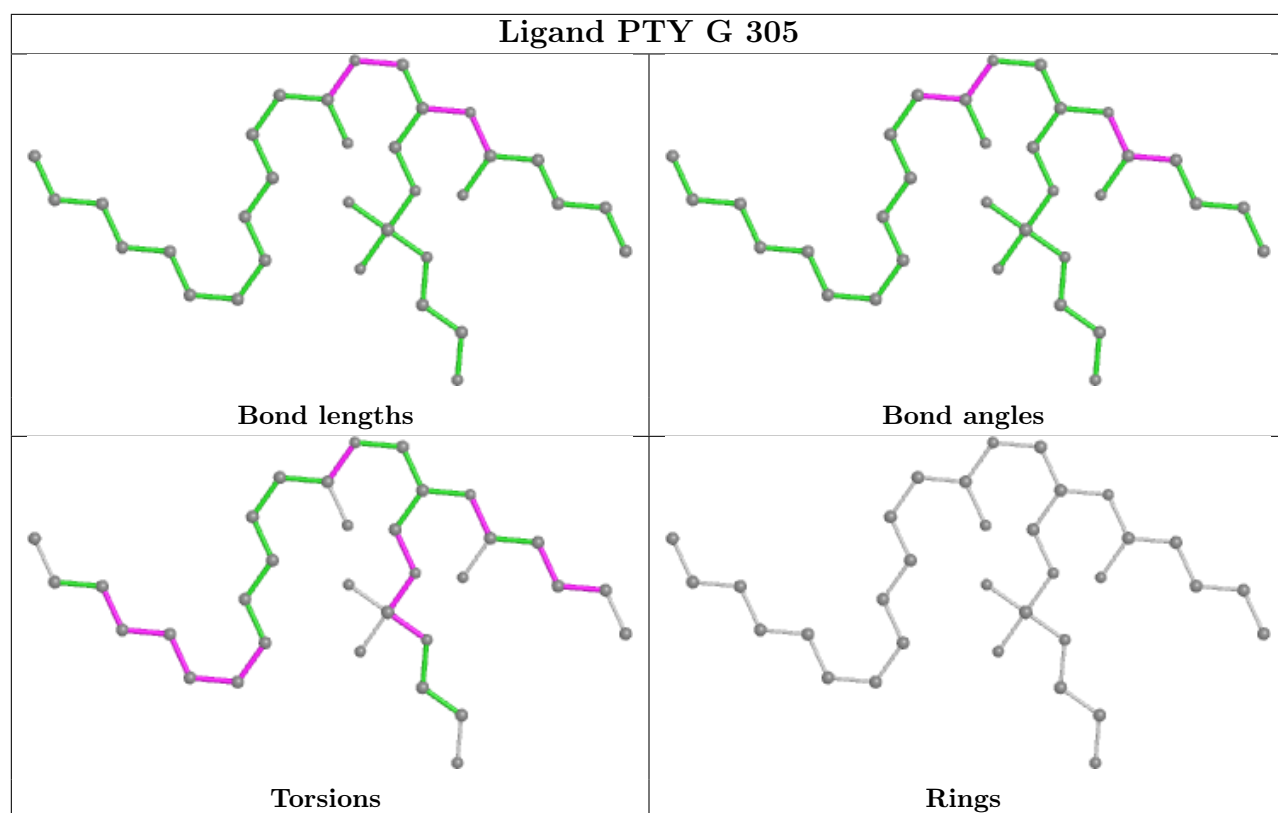


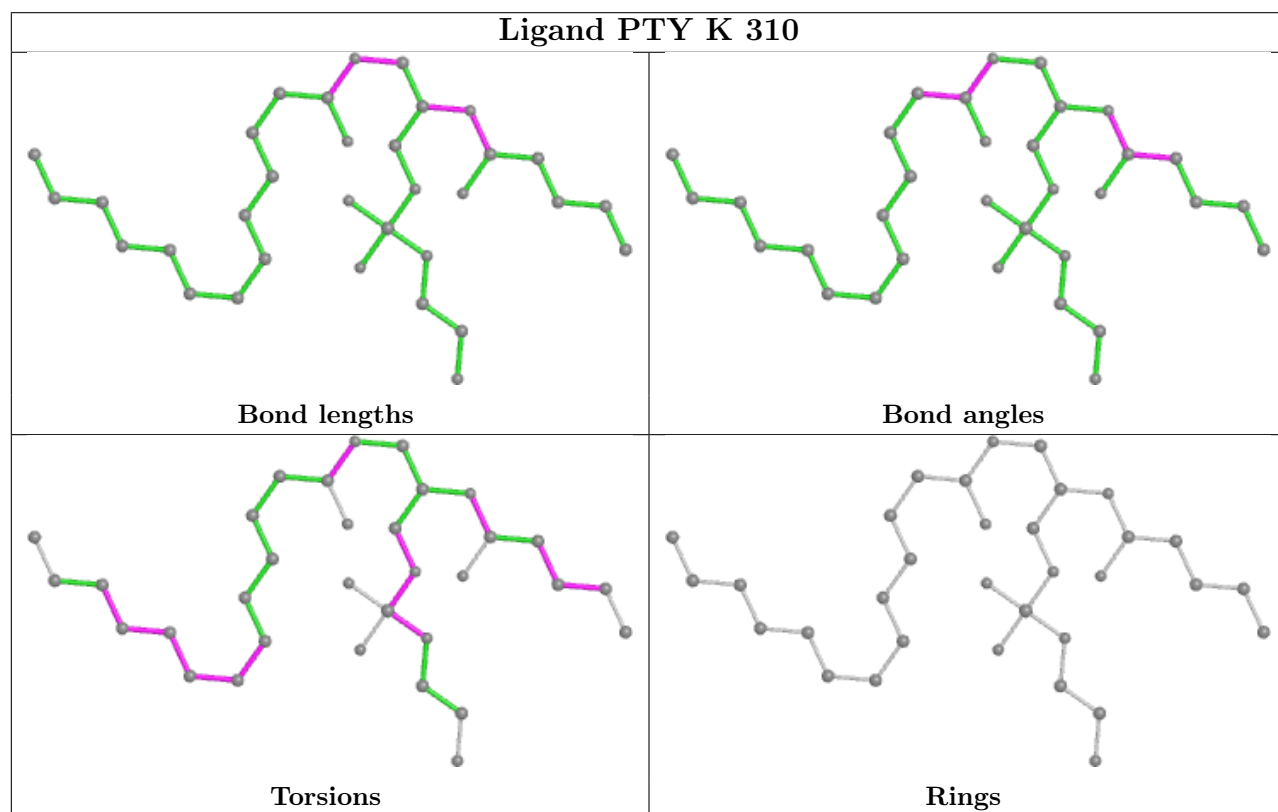
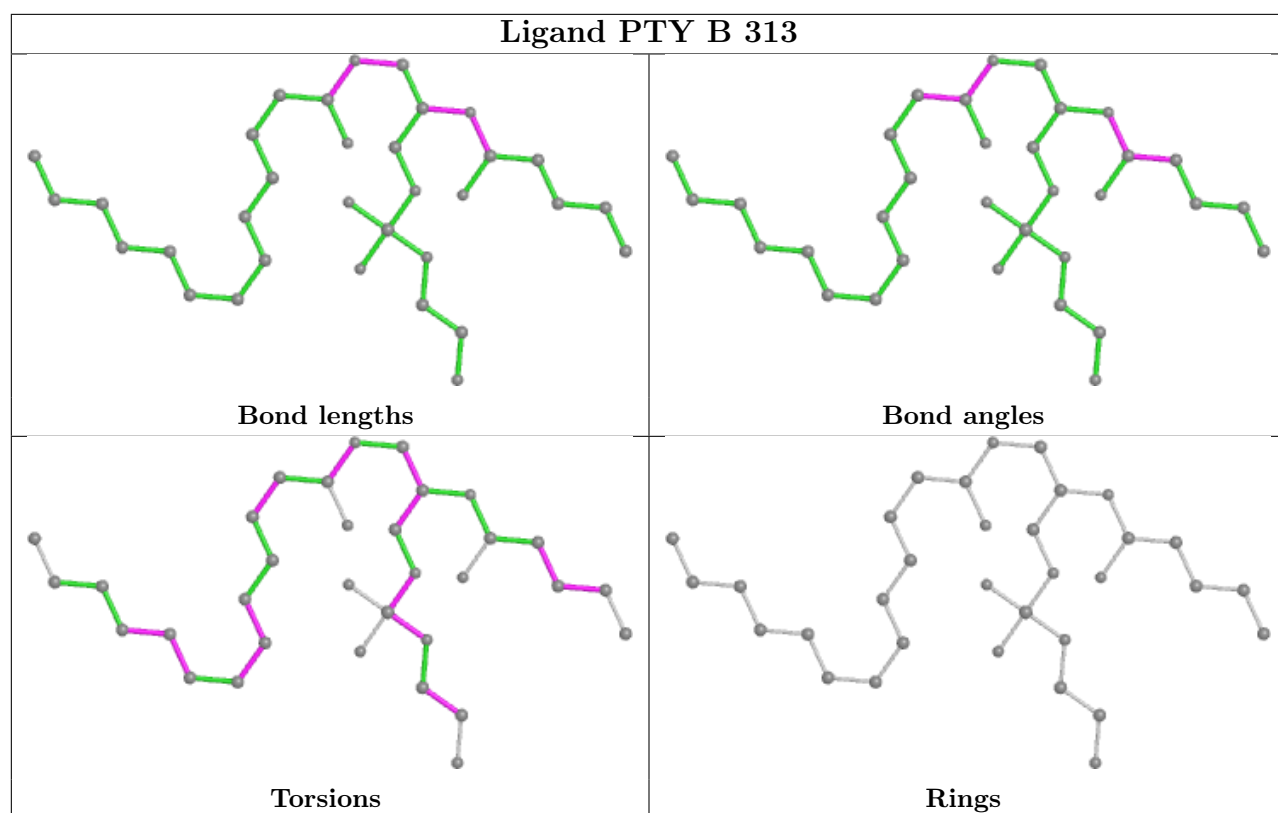


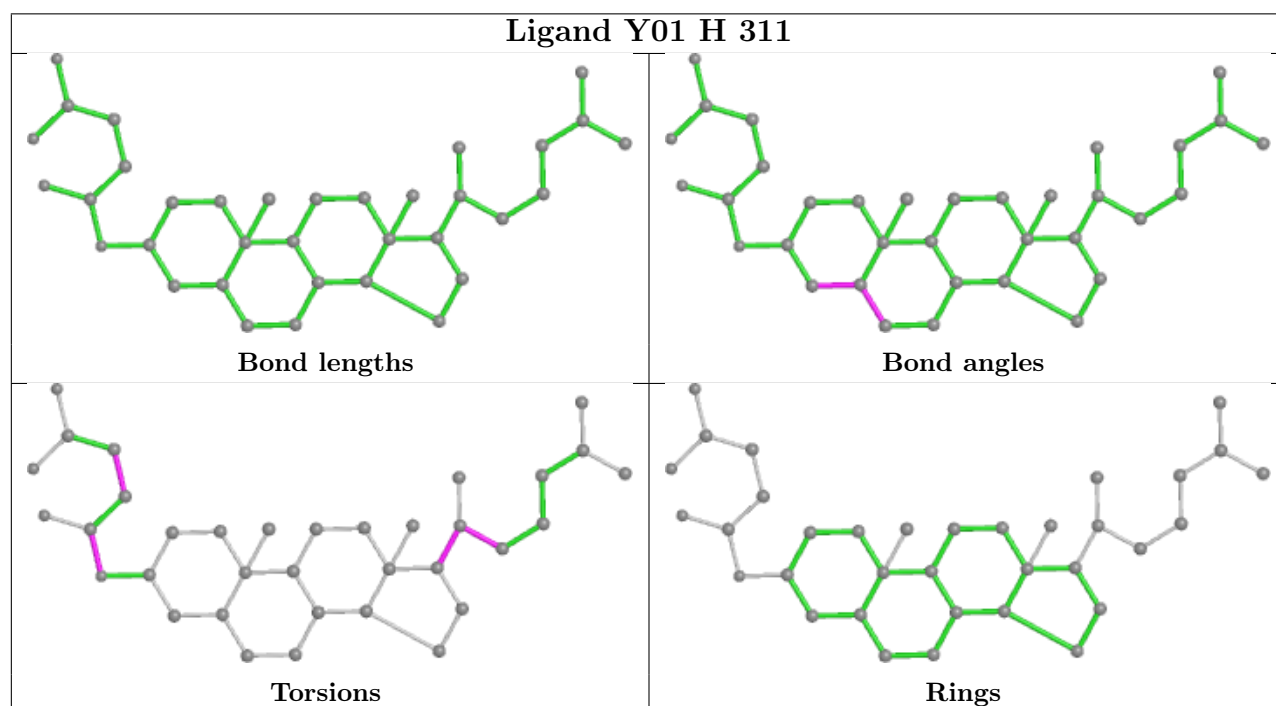
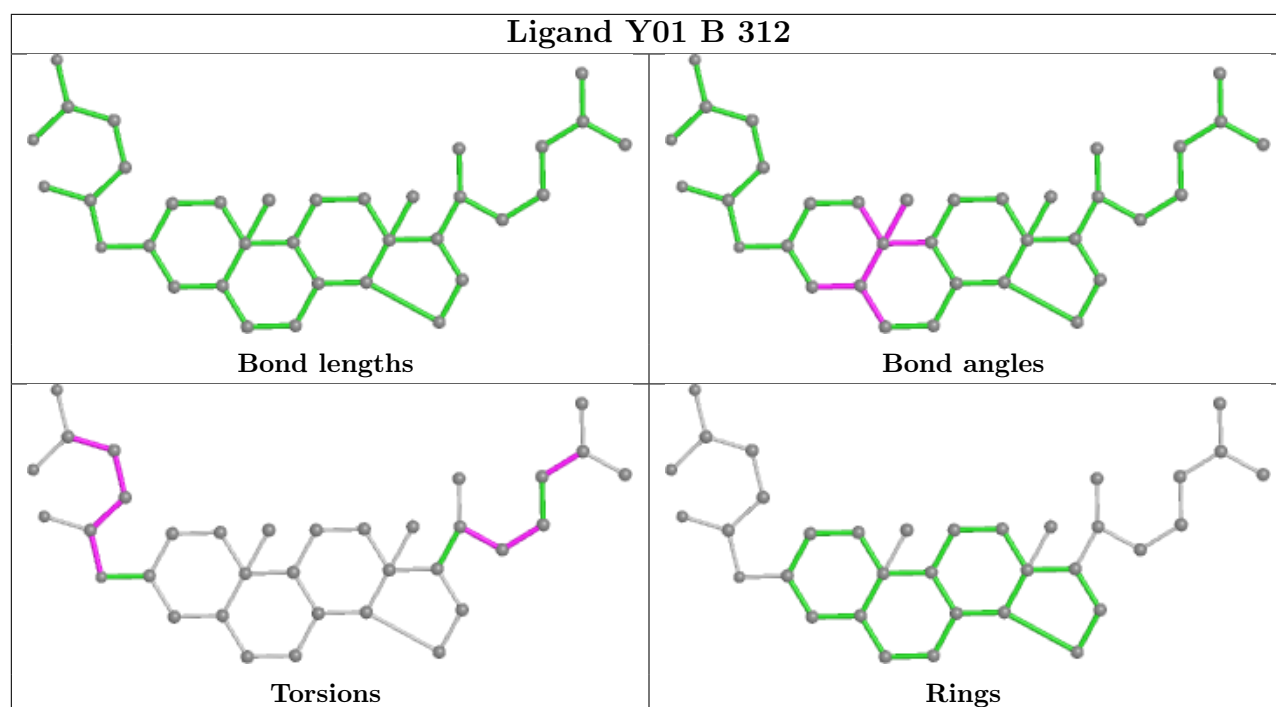


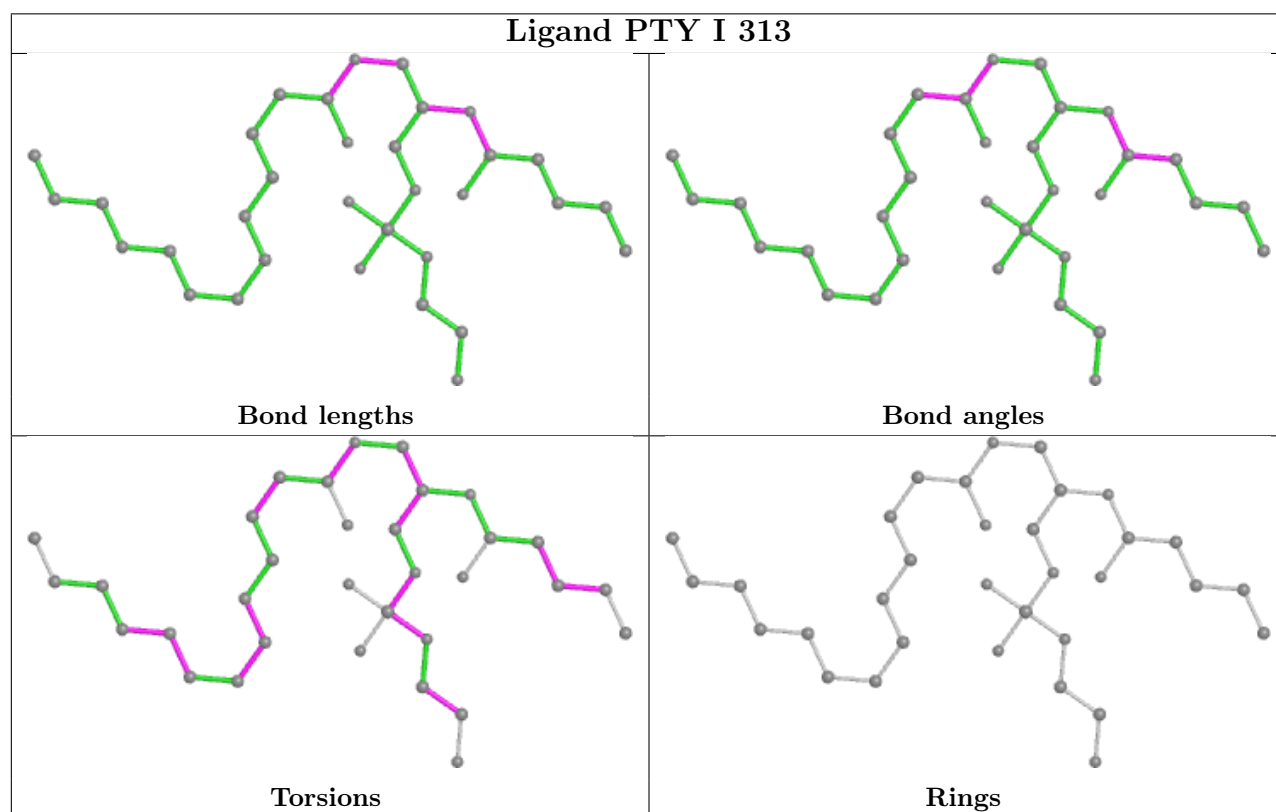
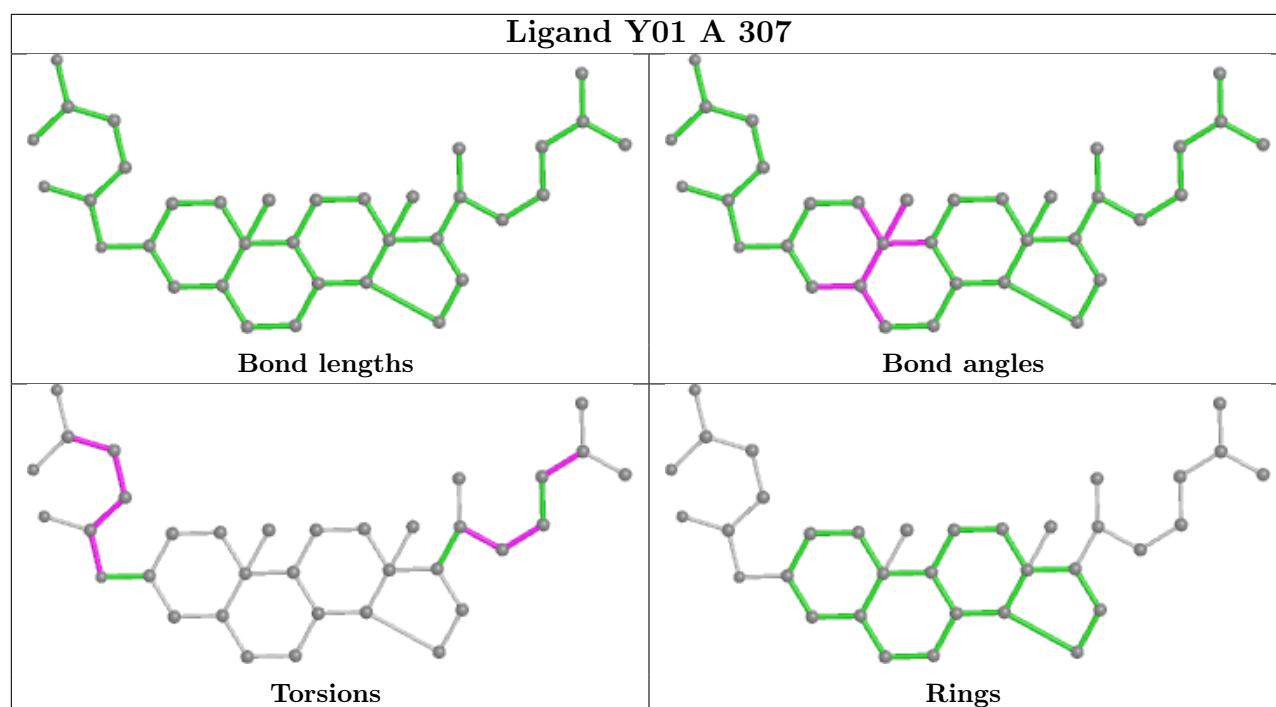




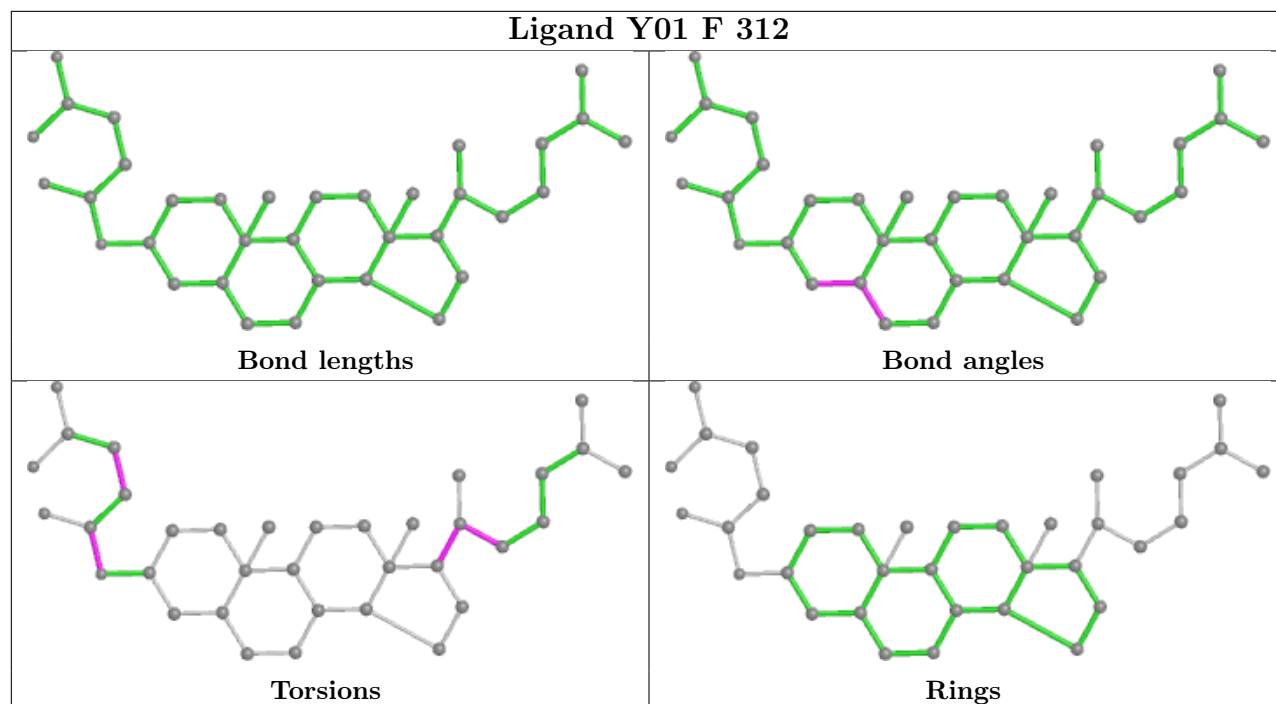




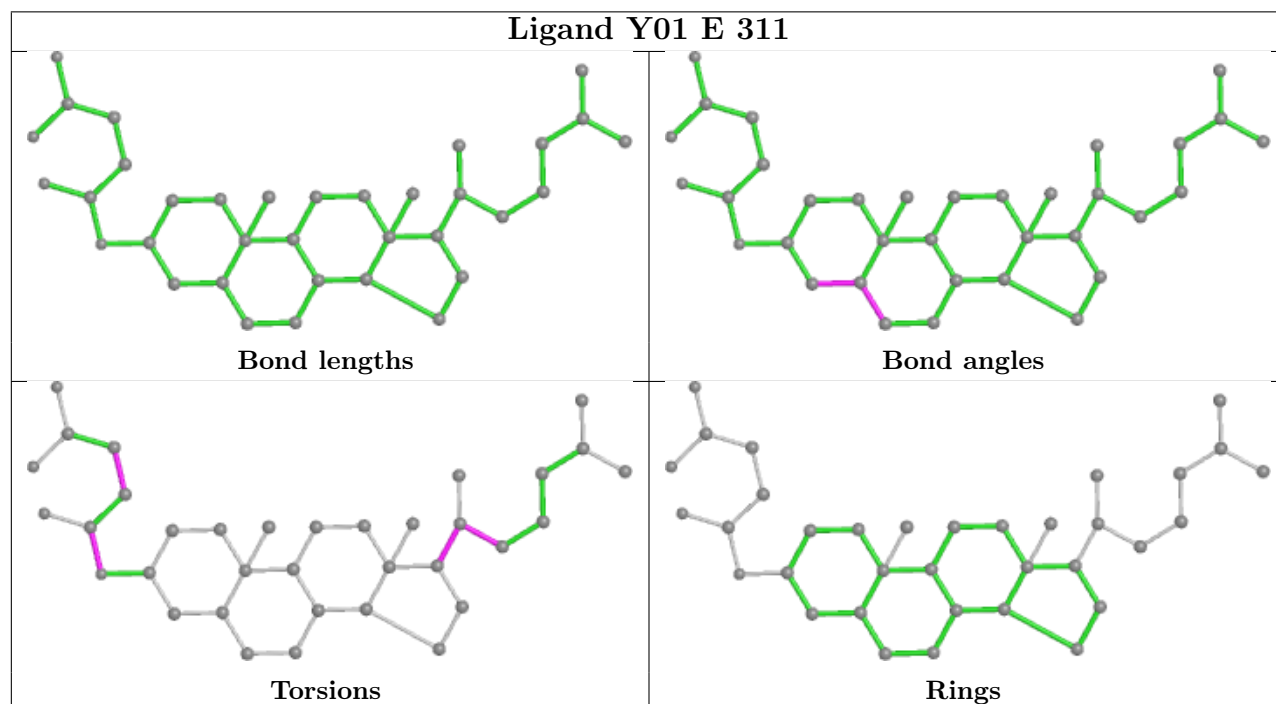


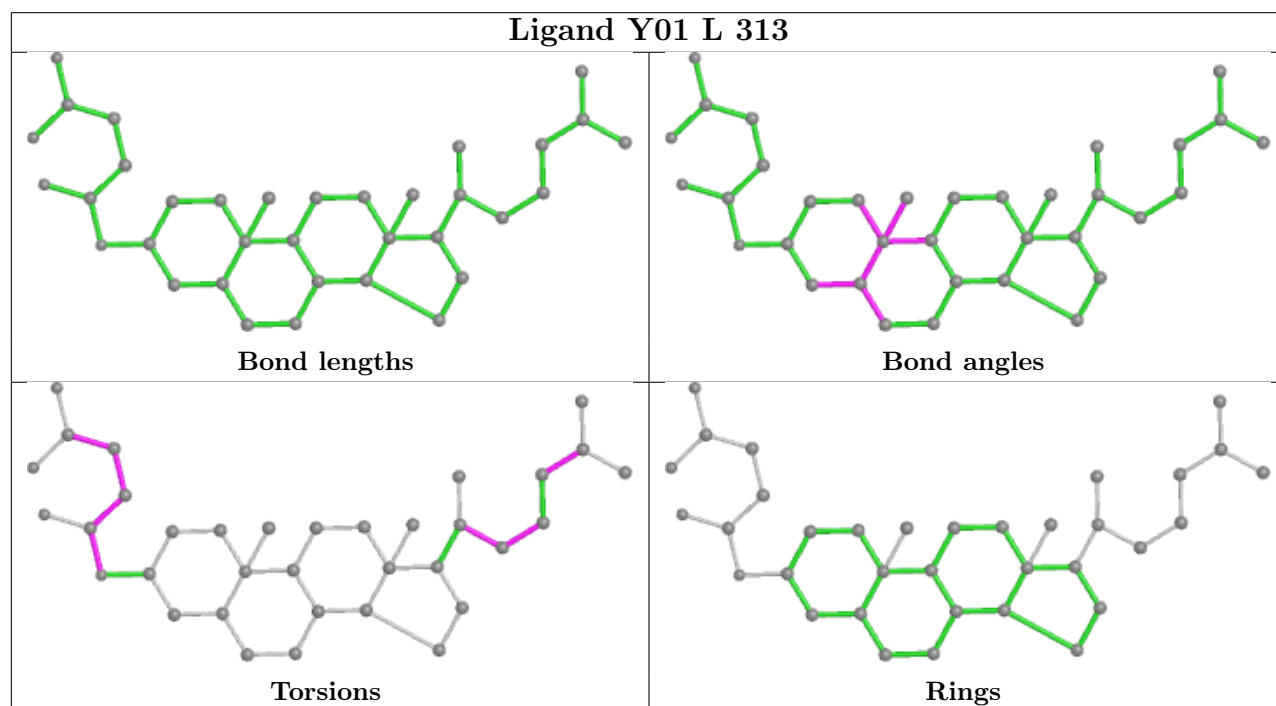
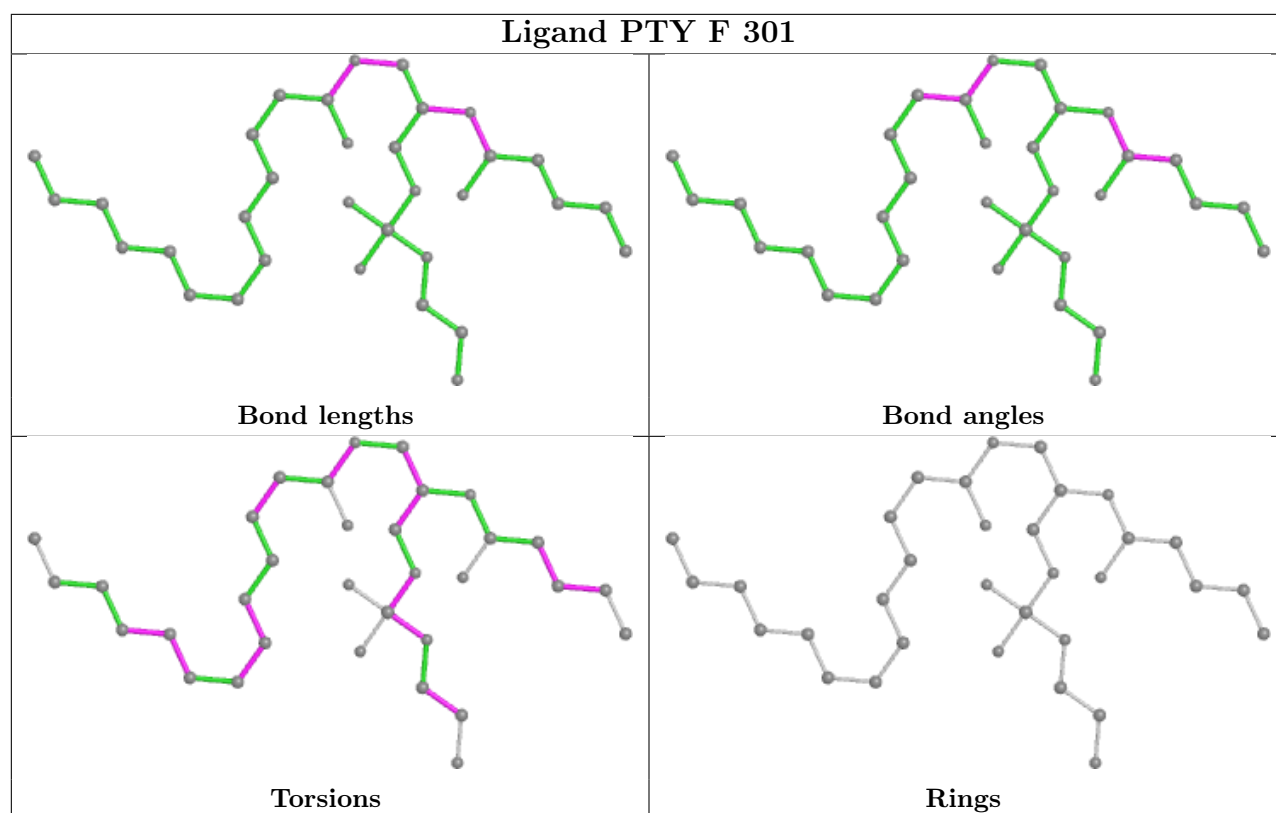


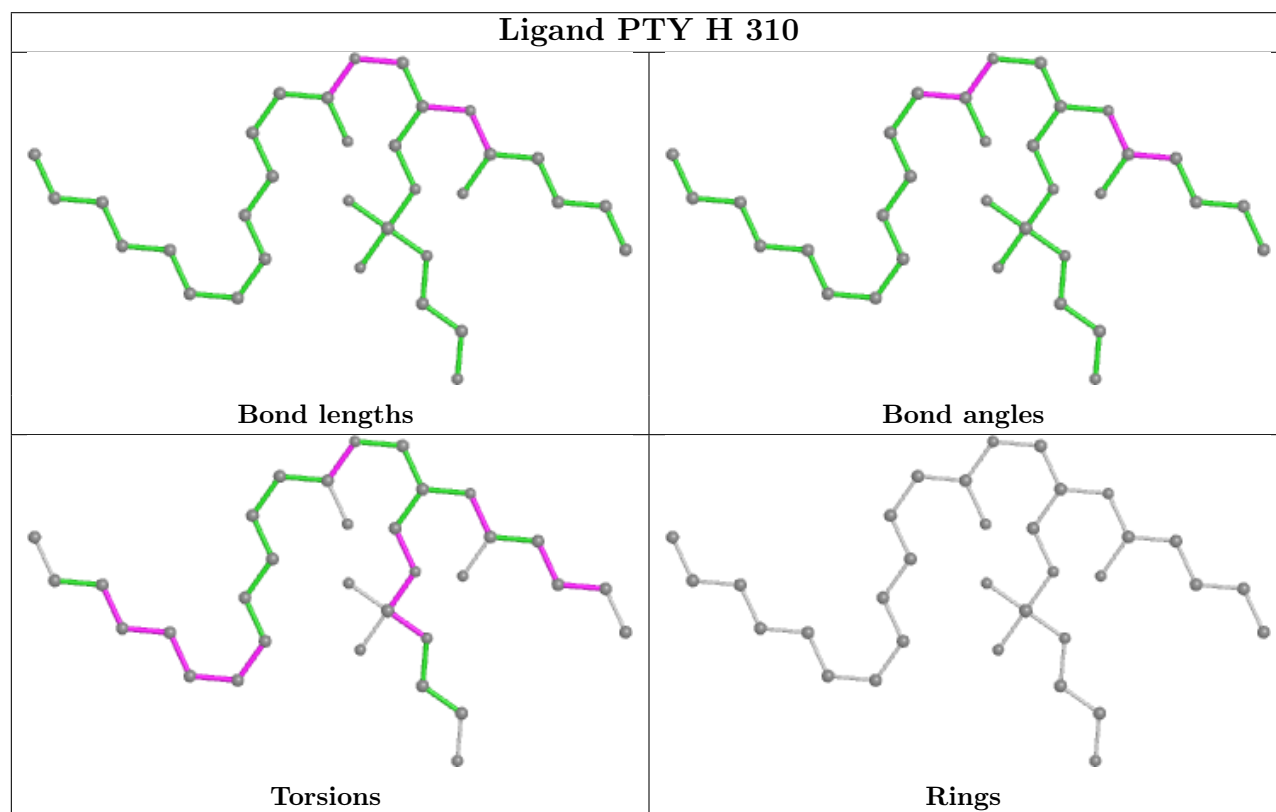
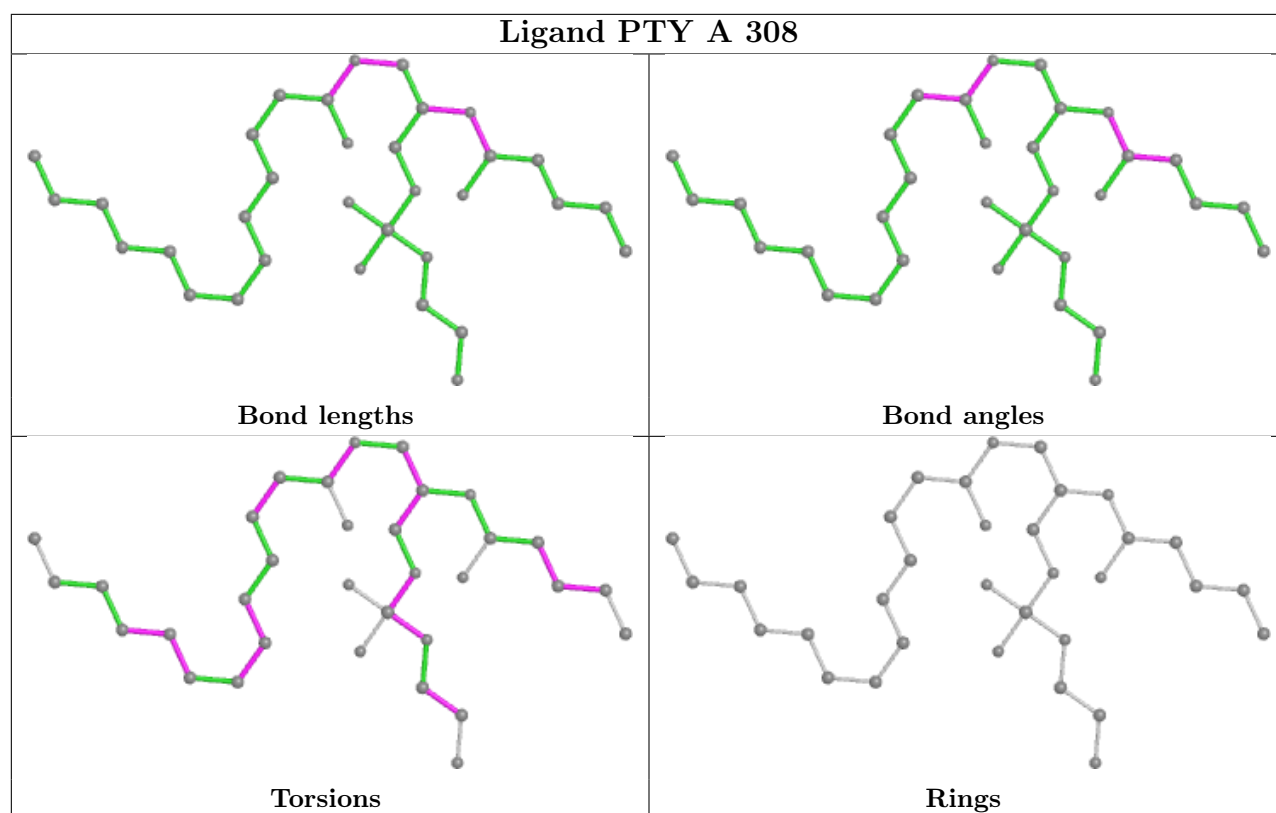
Ligand Y01 F 312



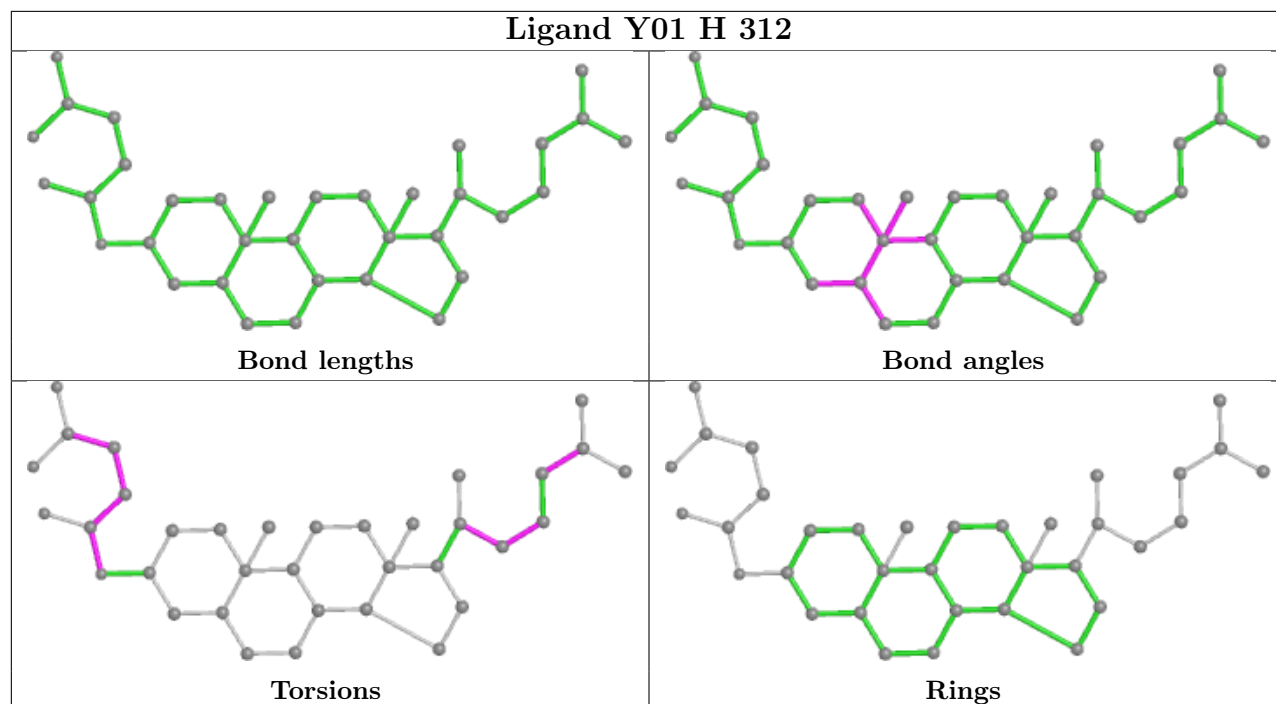
Ligand Y01 E 311



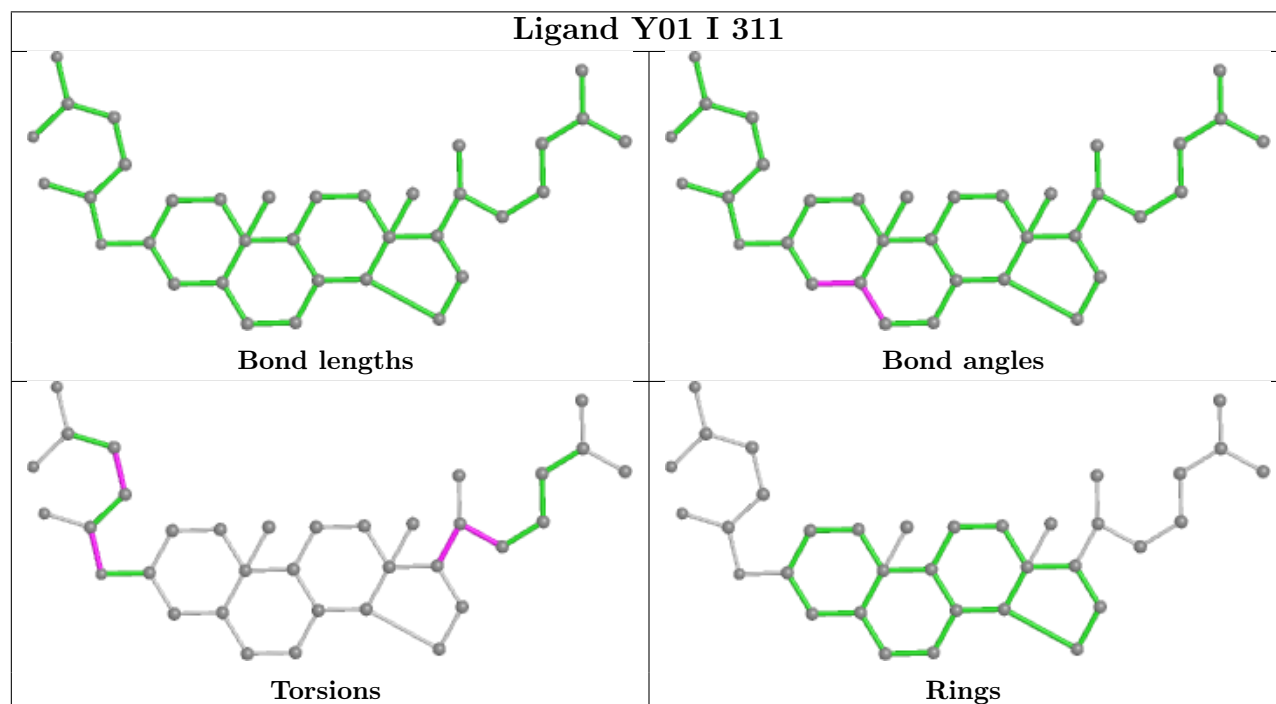




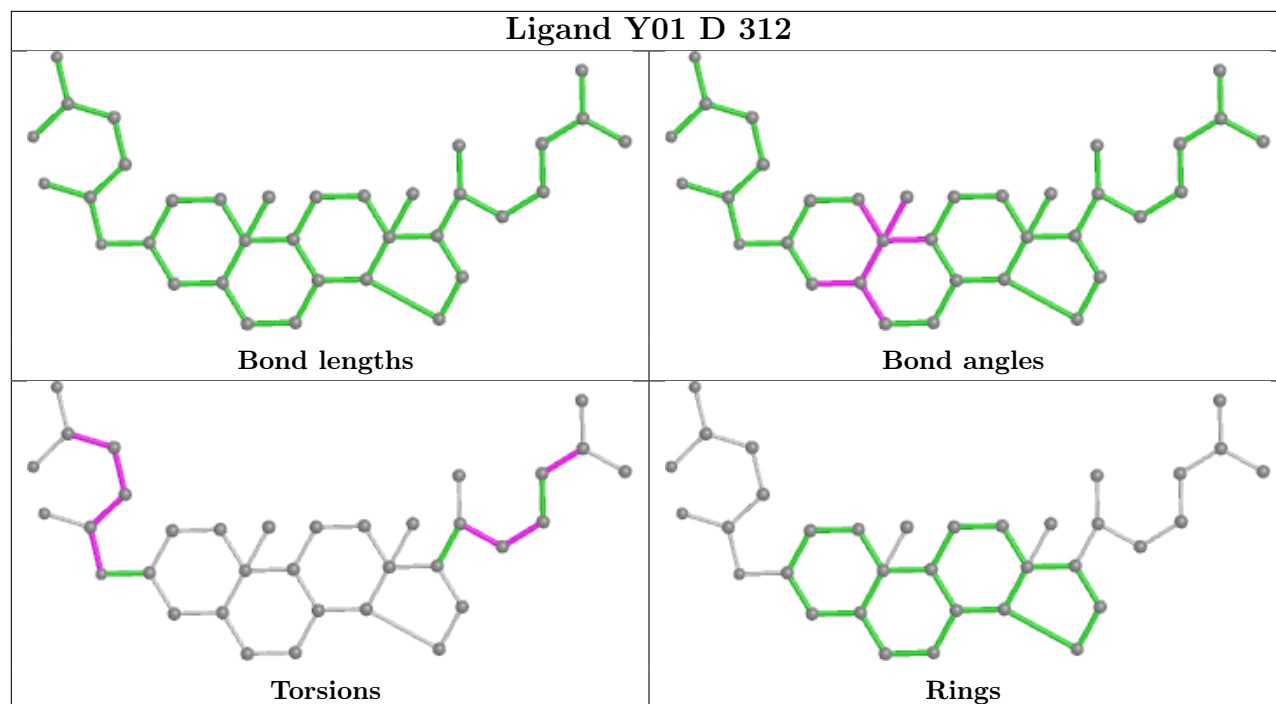
Ligand Y01 H 312



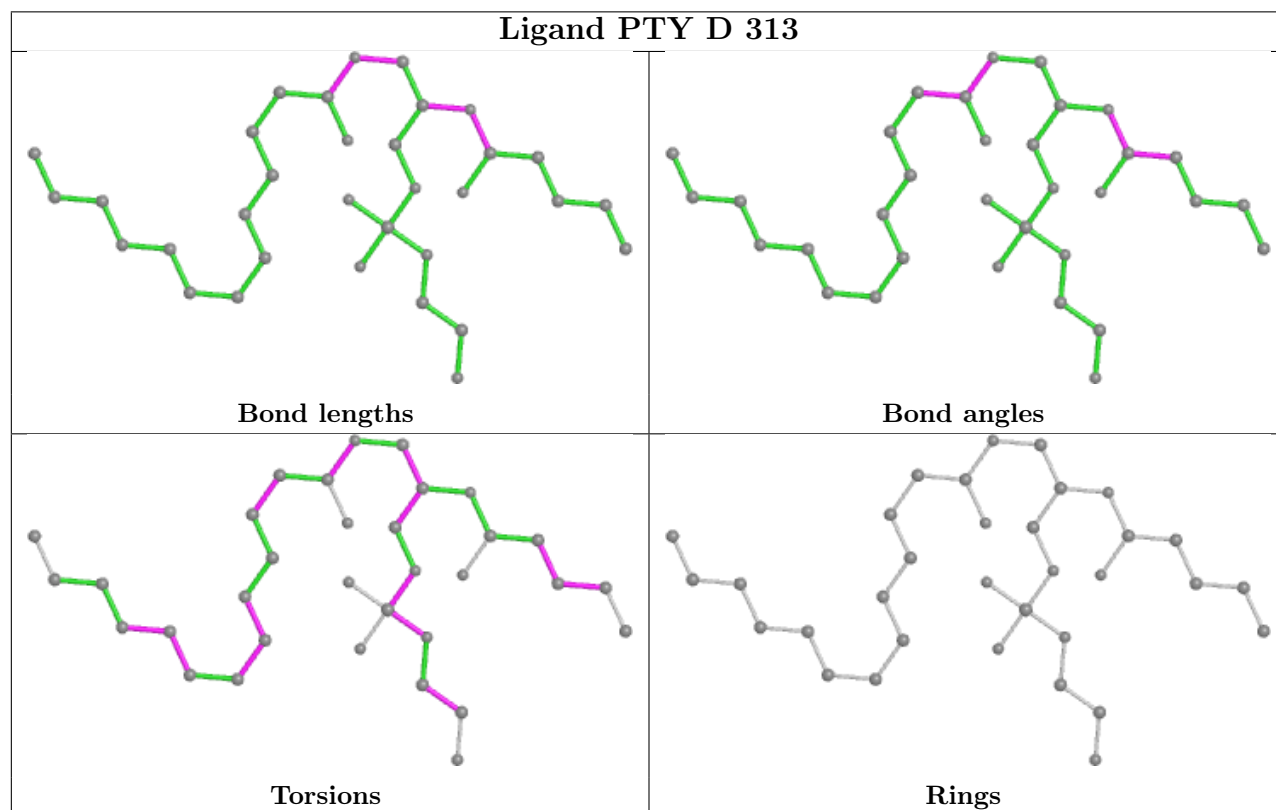
Ligand Y01 I 311

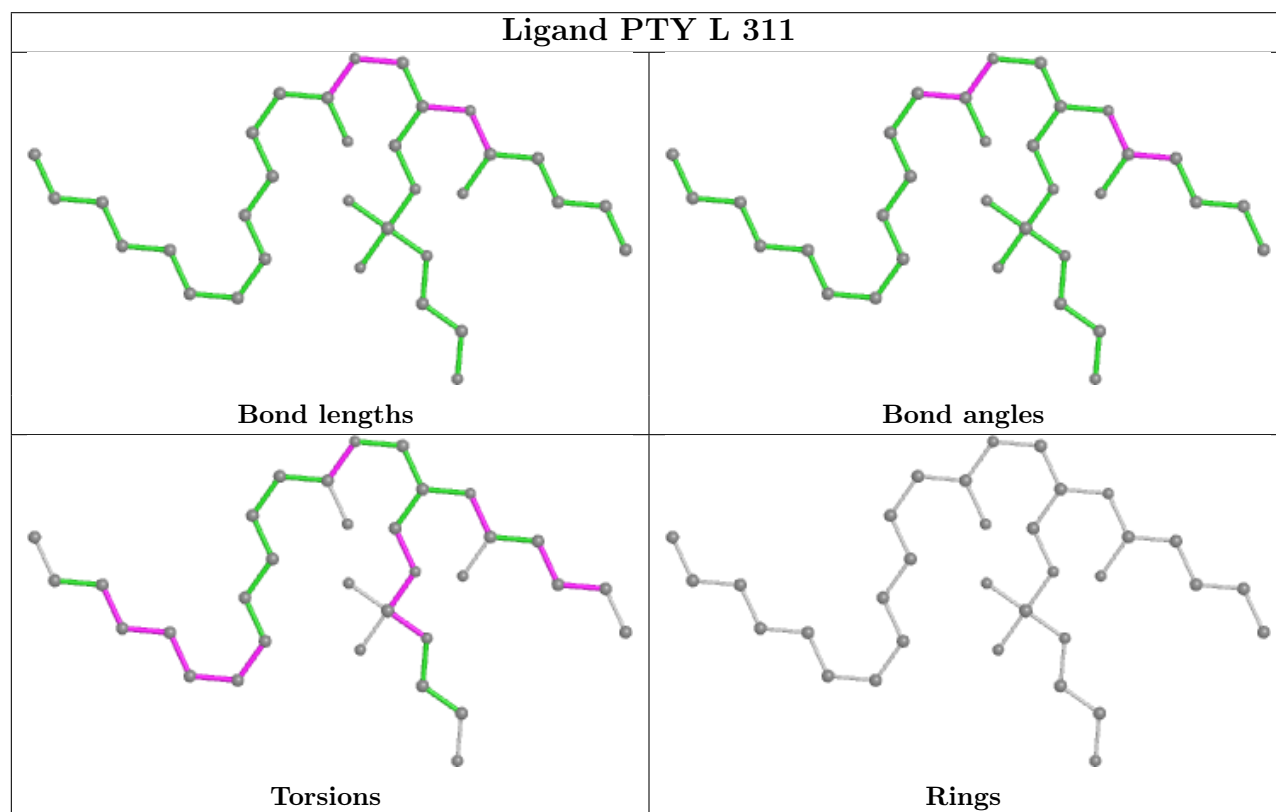
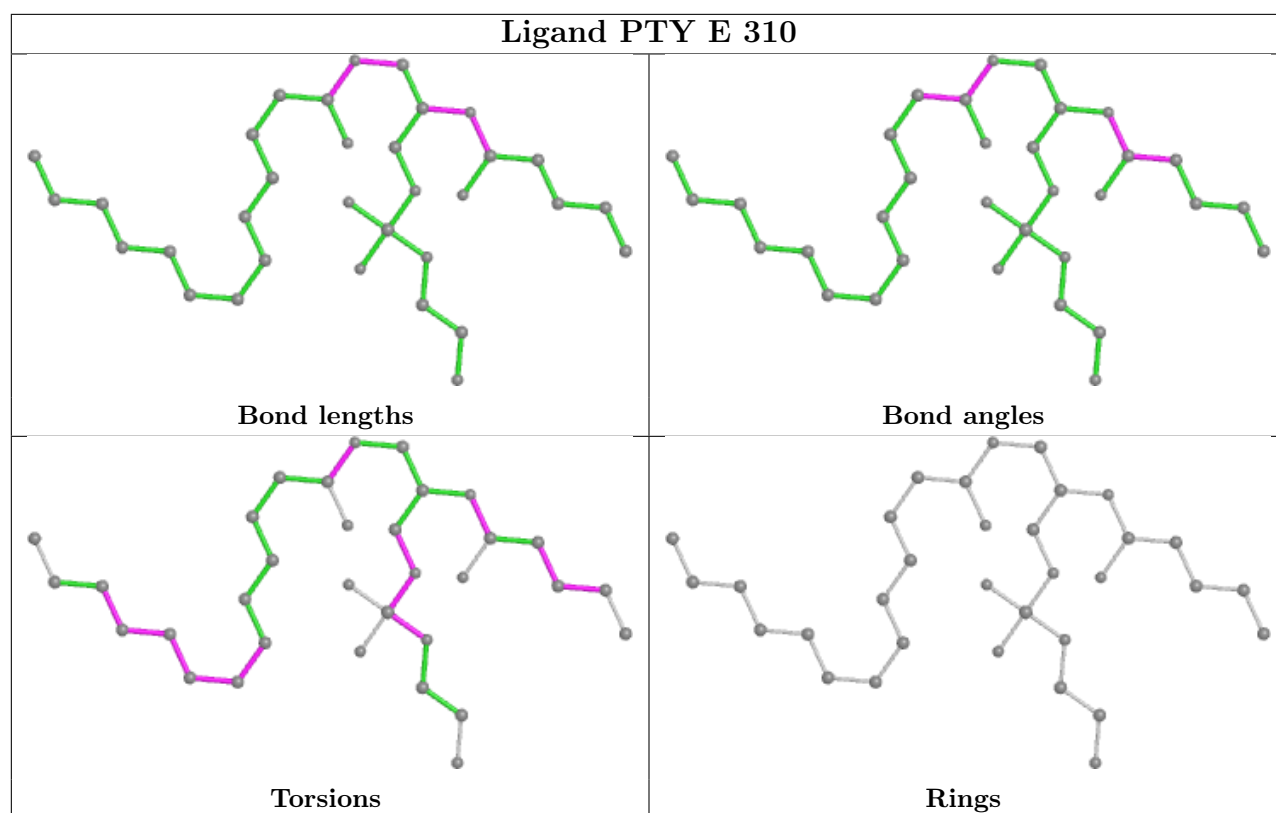


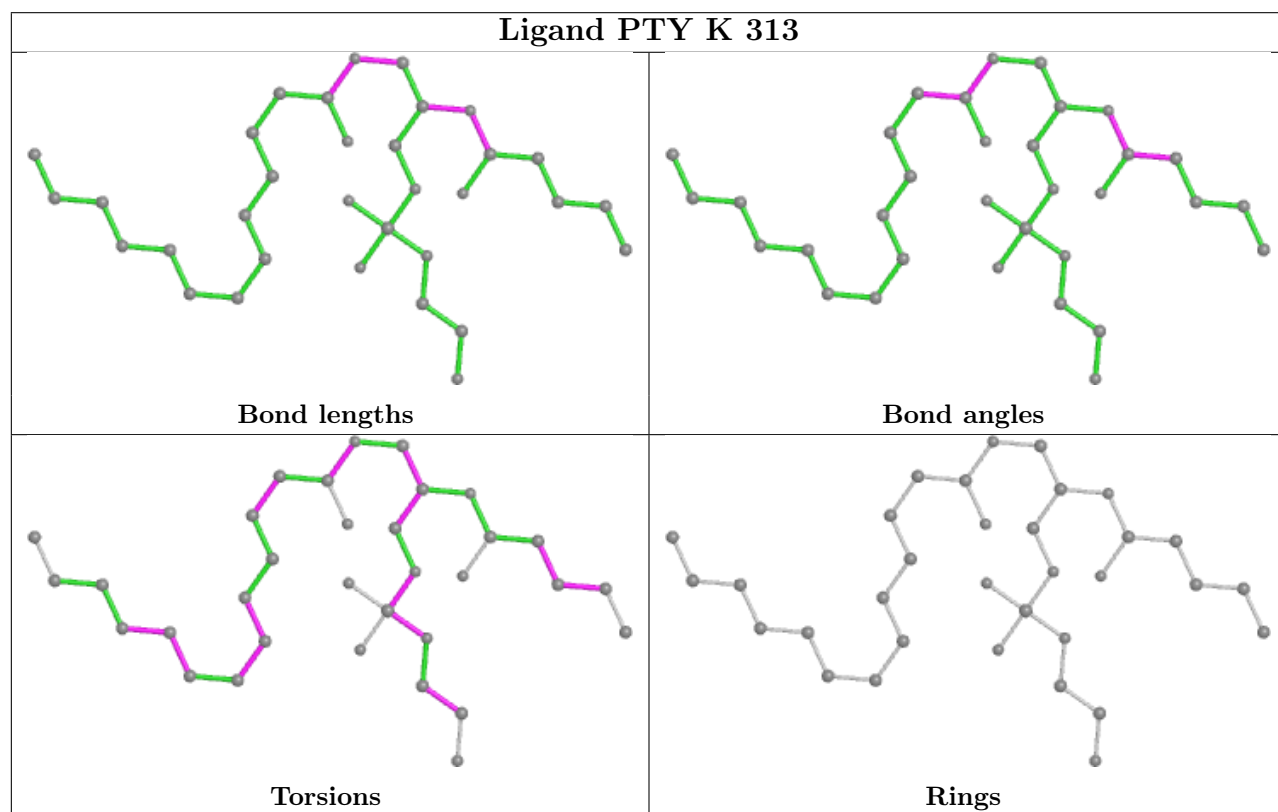
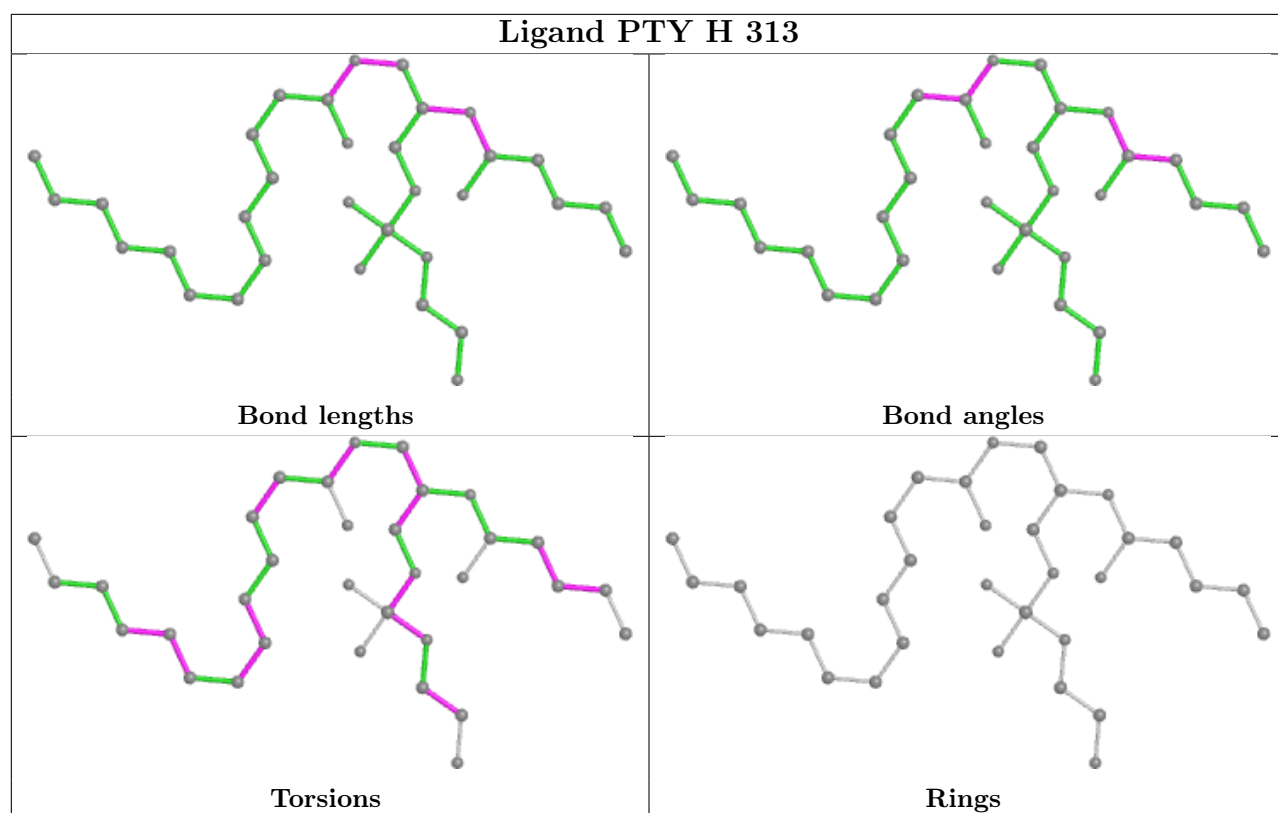
Ligand Y01 D 312



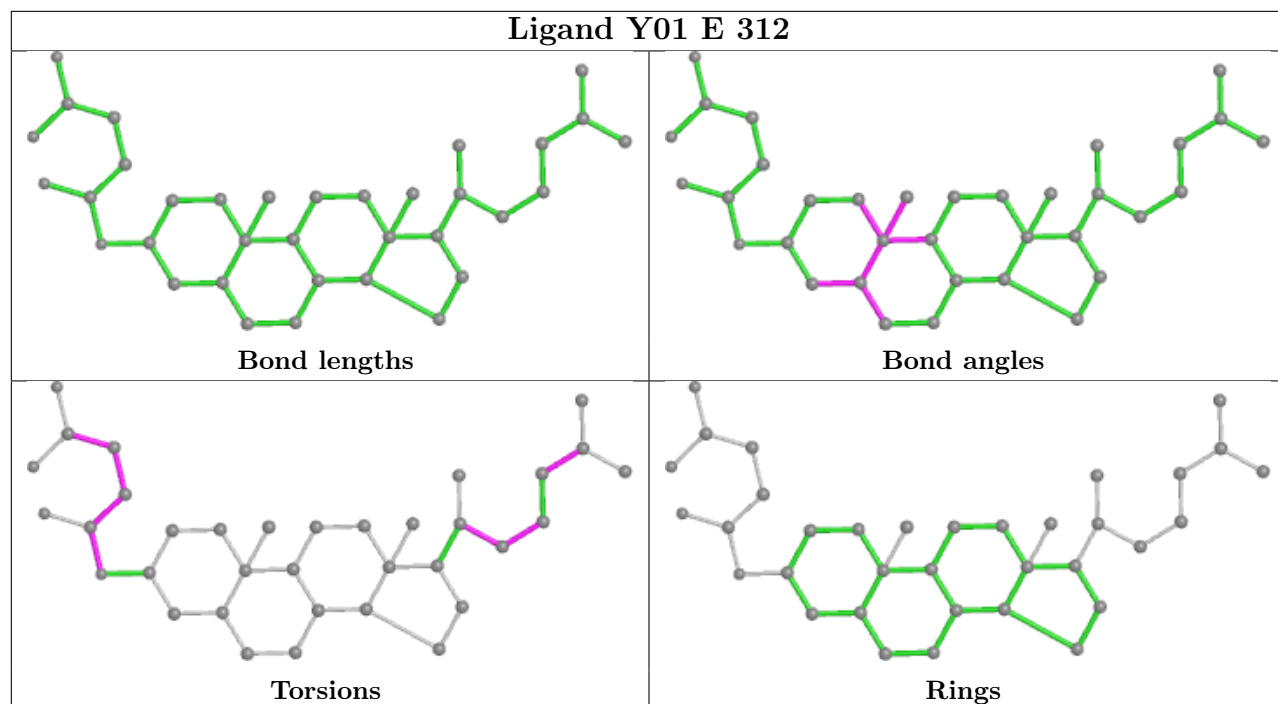
Ligand PTY D 313



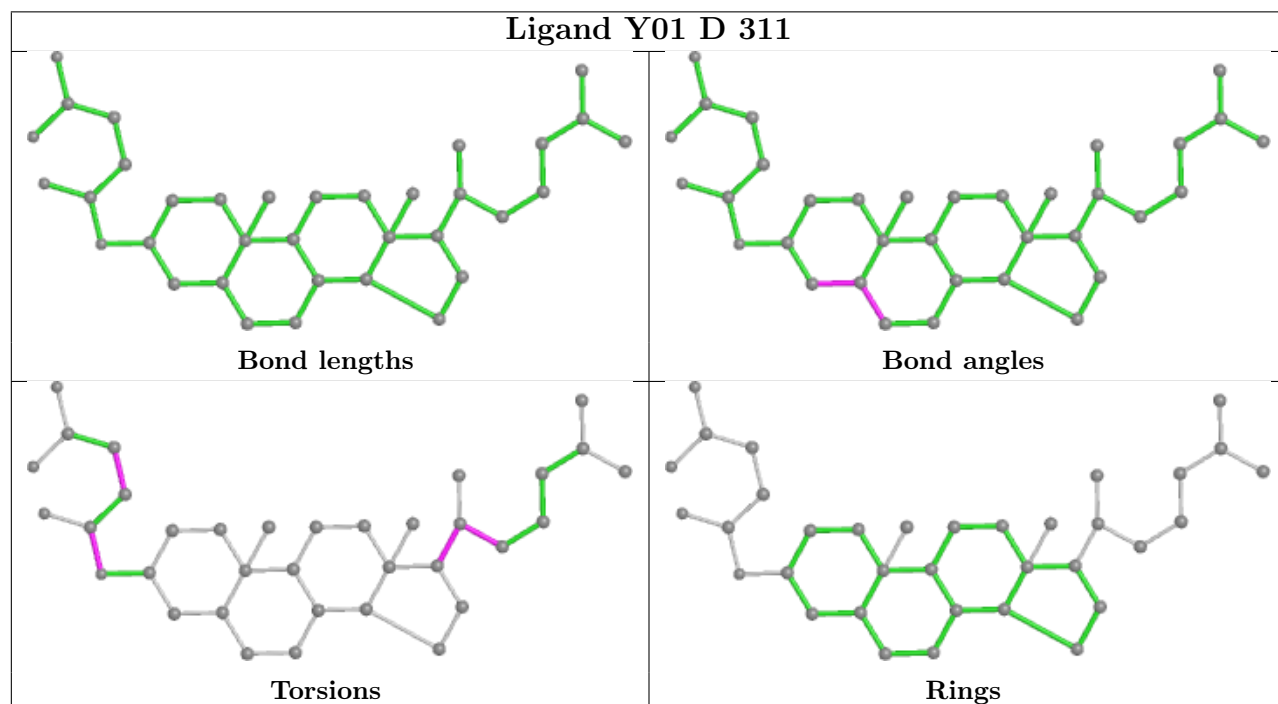




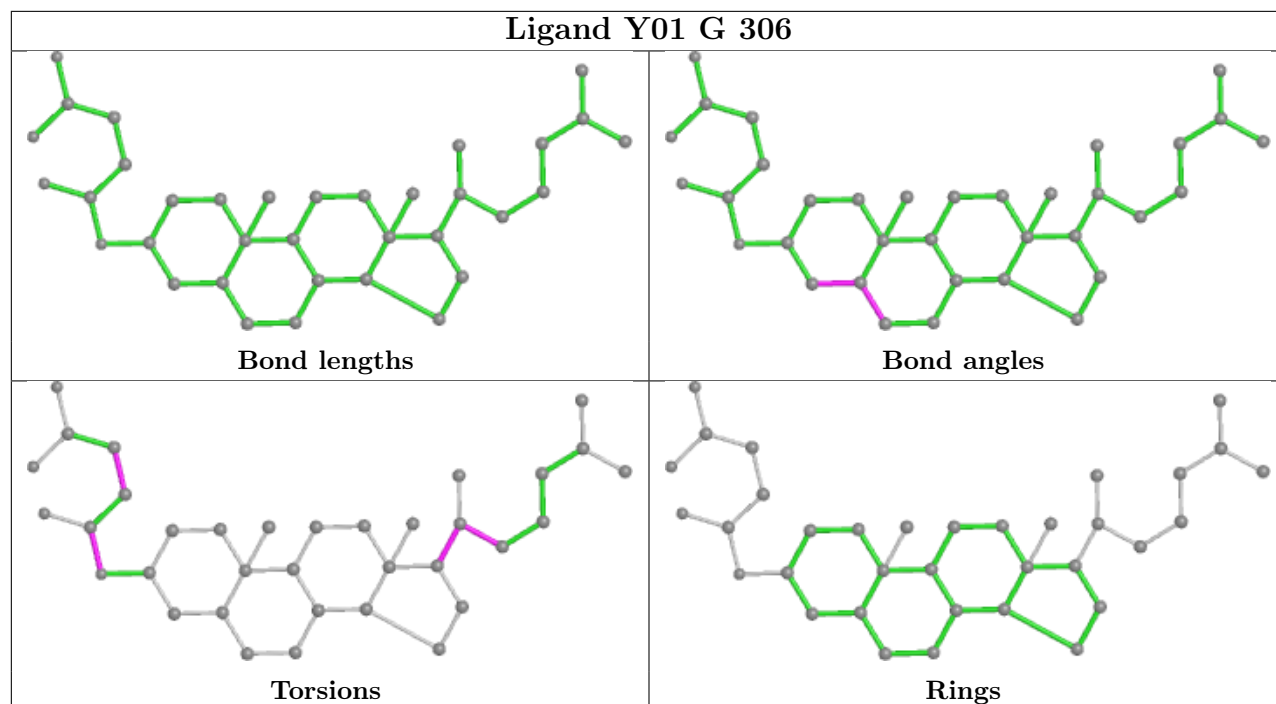
Ligand Y01 E 312



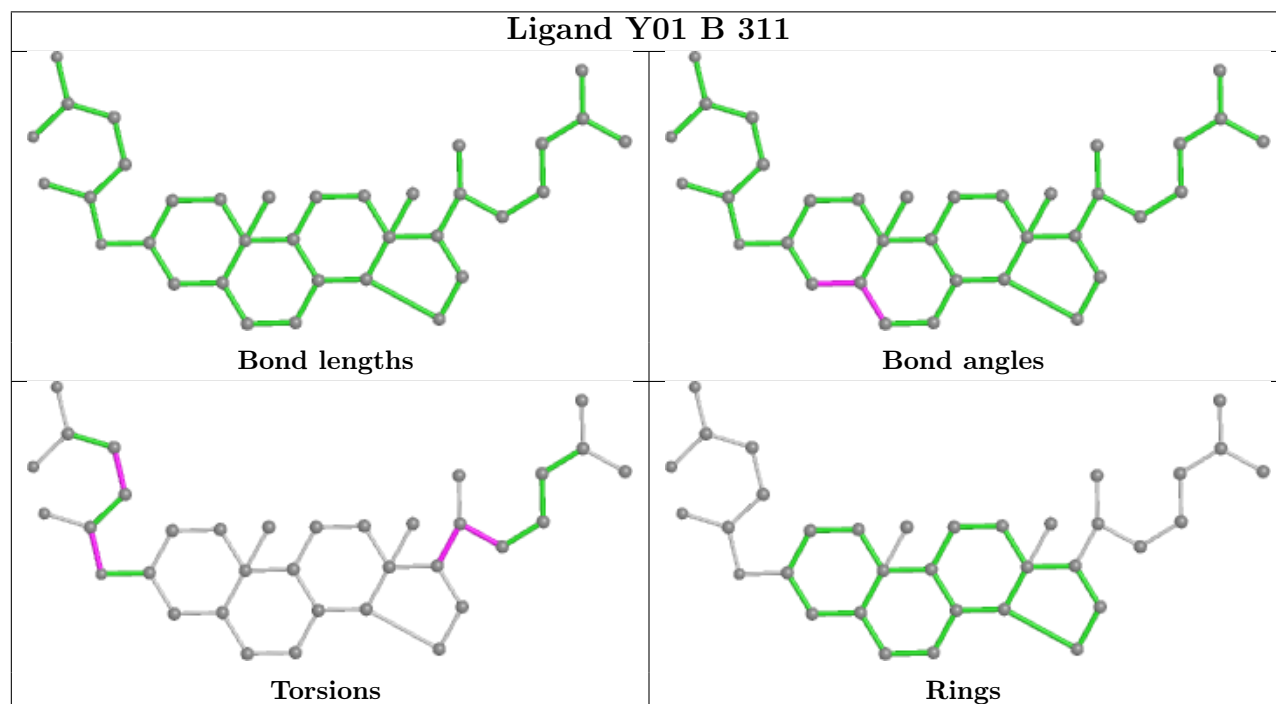
Ligand Y01 D 311

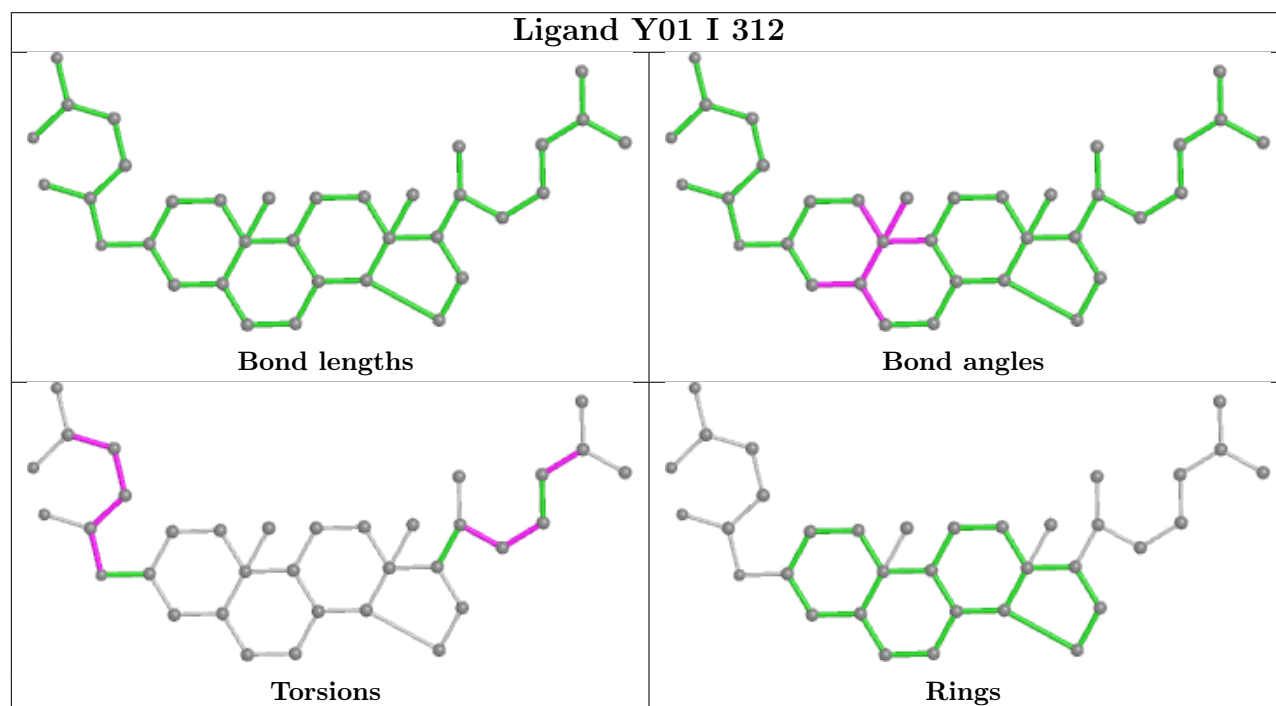
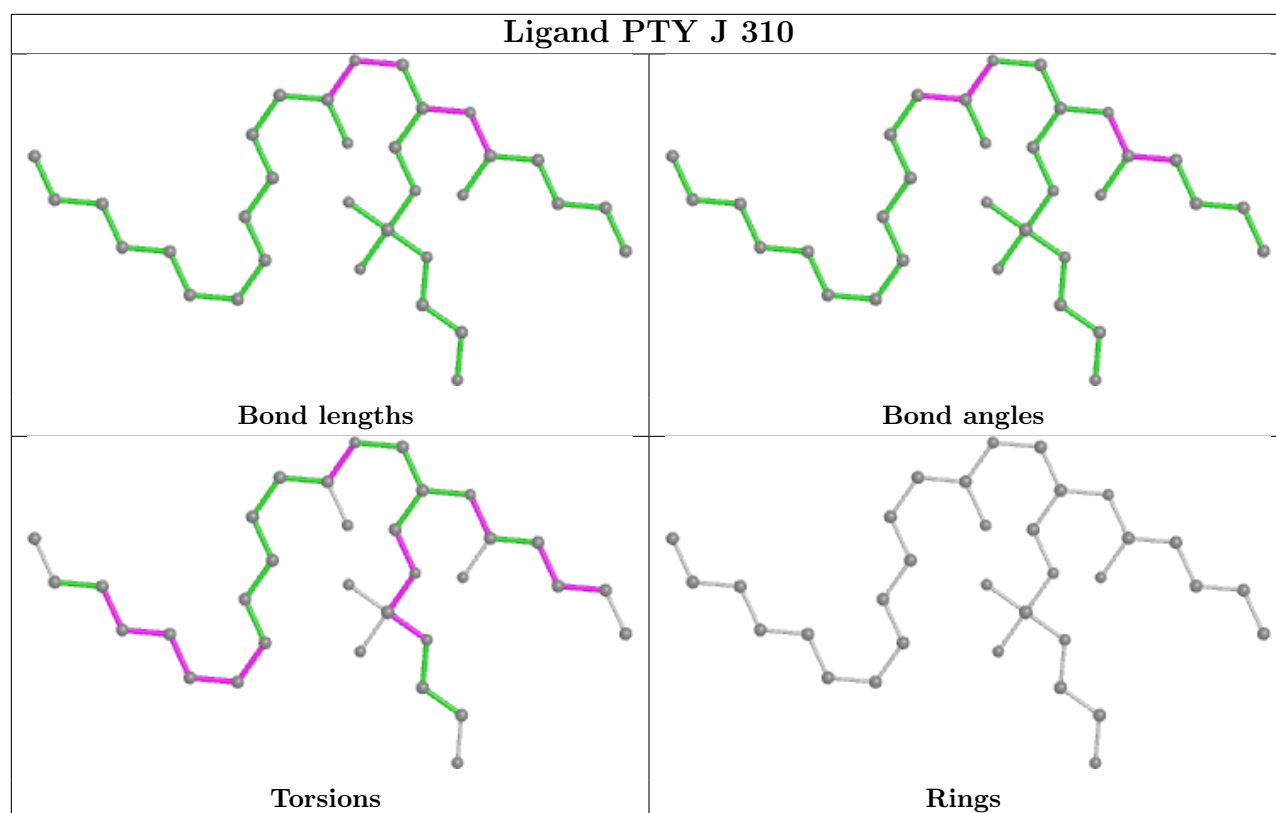


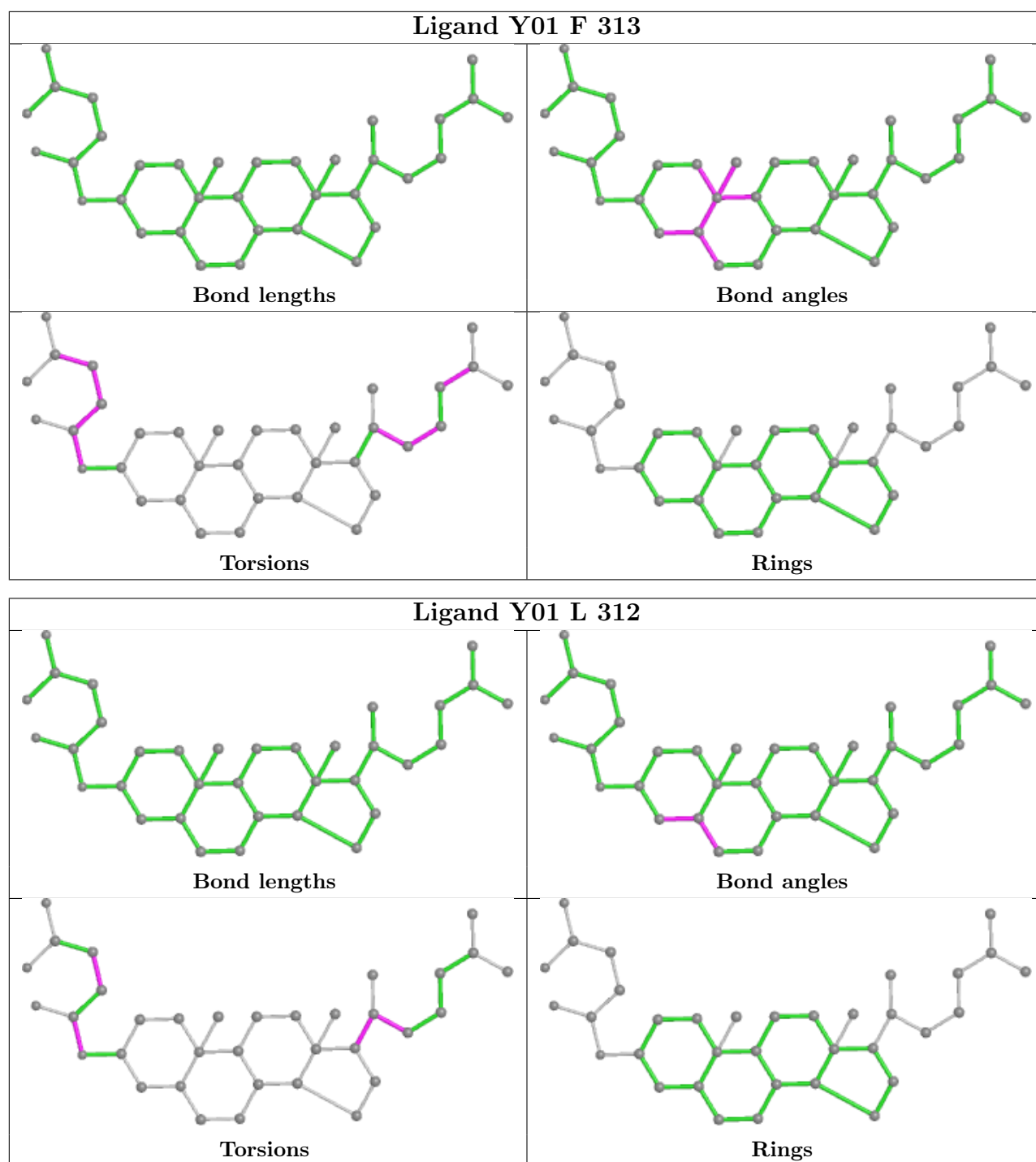
Ligand Y01 G 306



Ligand Y01 B 311







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.

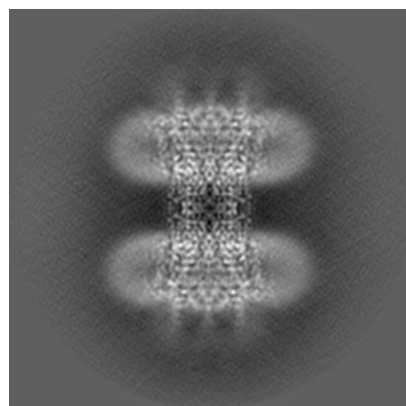
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33393. These allow visual inspection of the internal detail of the map and identification of artifacts.

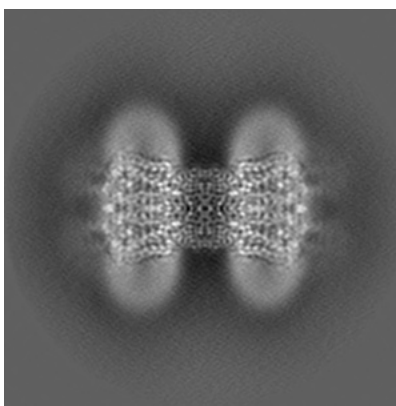
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

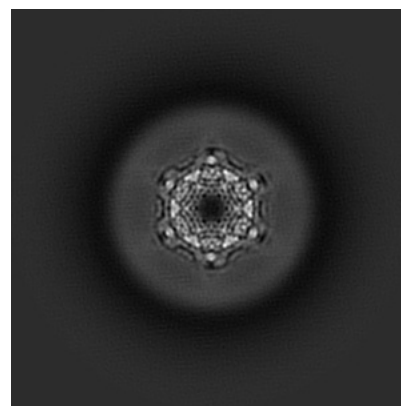
6.1.1 Primary map



X

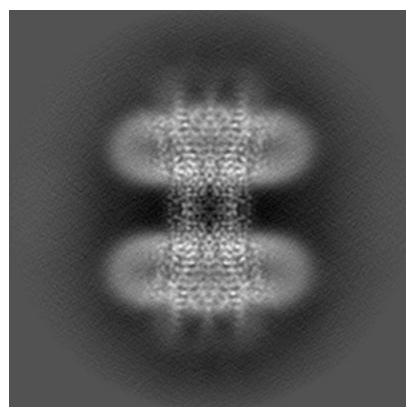


Y

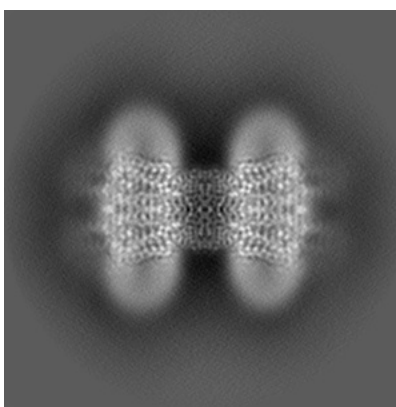


Z

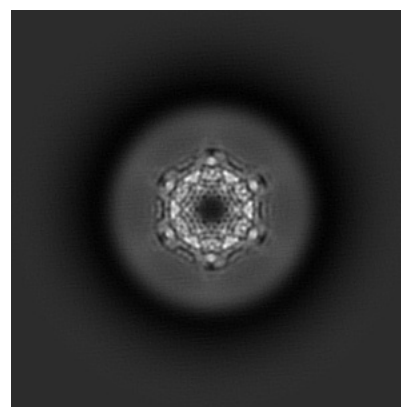
6.1.2 Raw map



X



Y

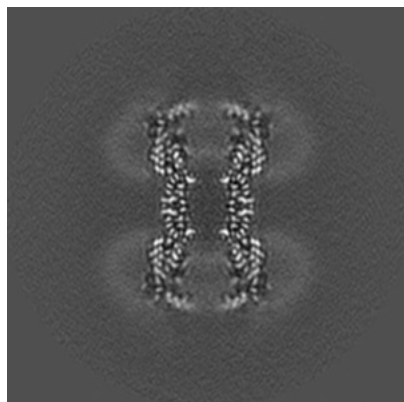


Z

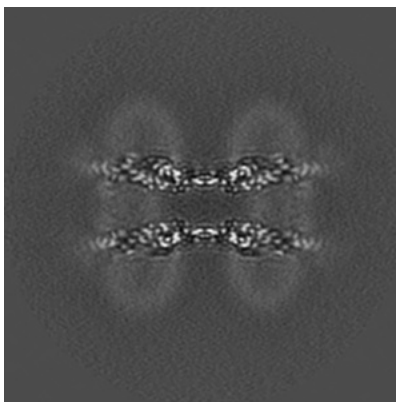
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

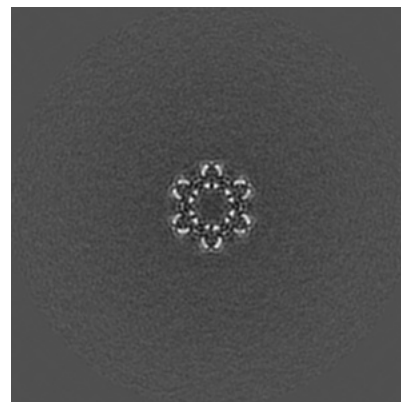
6.2.1 Primary map



X Index: 160

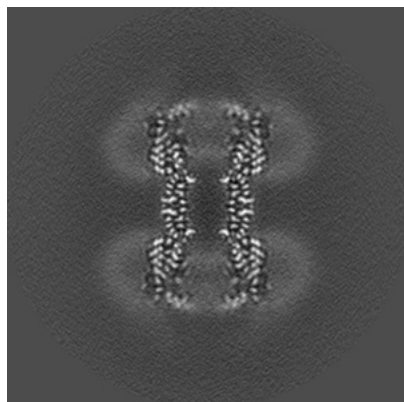


Y Index: 160

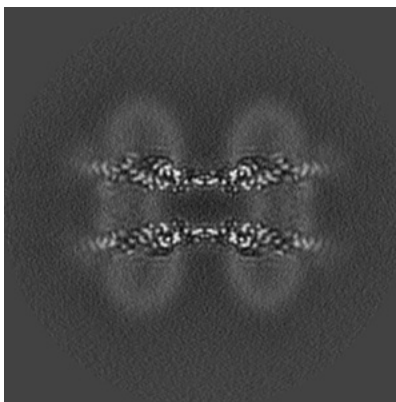


Z Index: 160

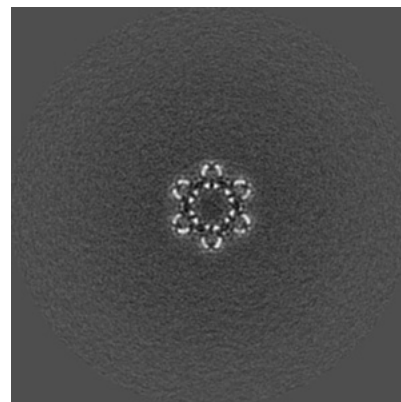
6.2.2 Raw map



X Index: 160



Y Index: 160

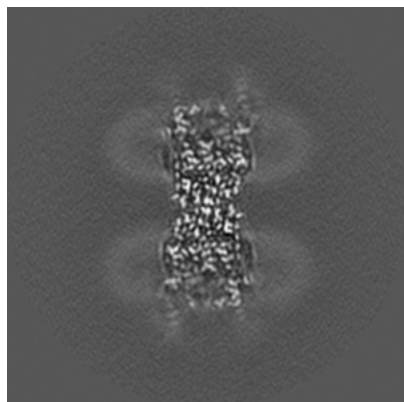


Z Index: 160

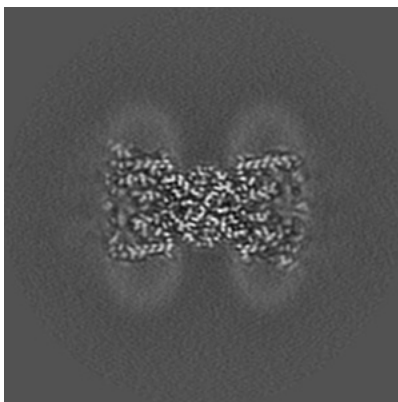
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

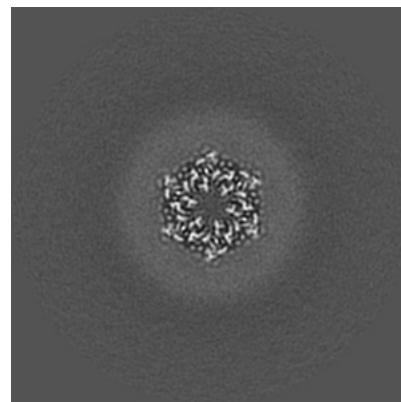
6.3.1 Primary map



X Index: 179

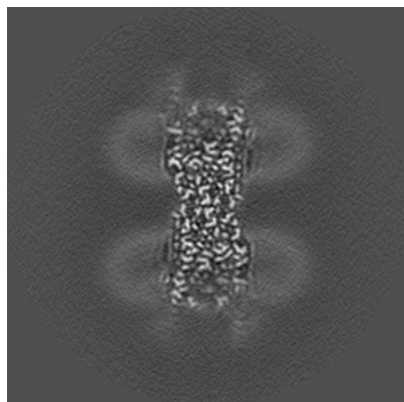


Y Index: 178

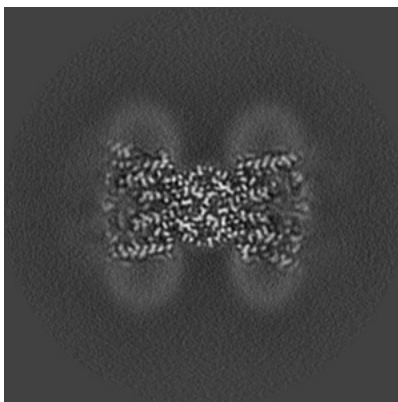


Z Index: 190

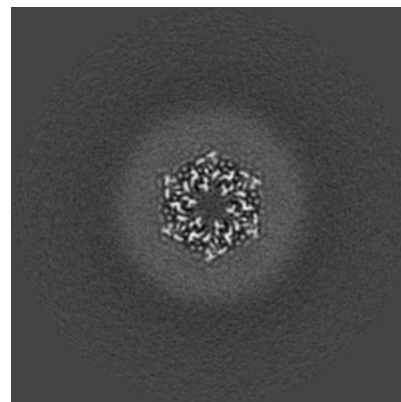
6.3.2 Raw map



X Index: 140



Y Index: 177

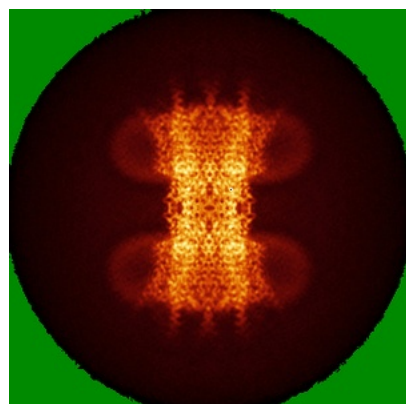


Z Index: 190

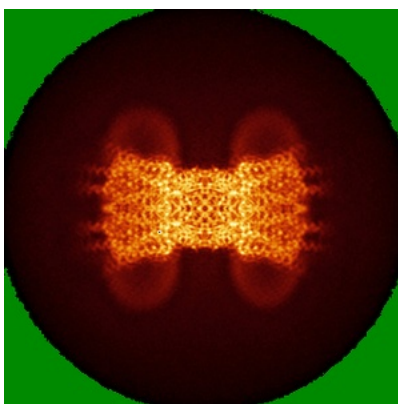
The images above show the largest variance slices of the map in three orthogonal directions.

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

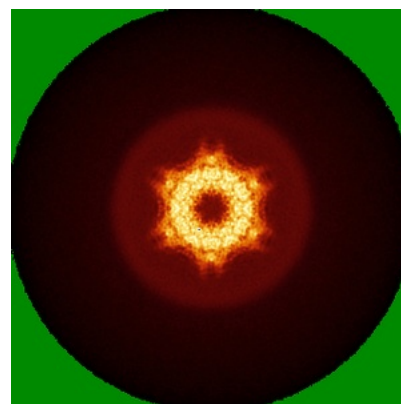
6.4.1 Primary map



X

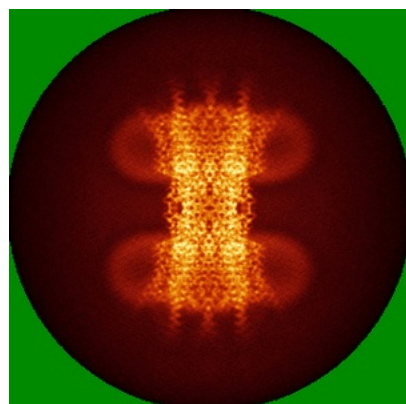


Y

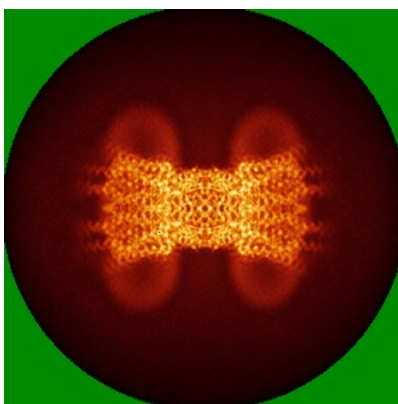


Z

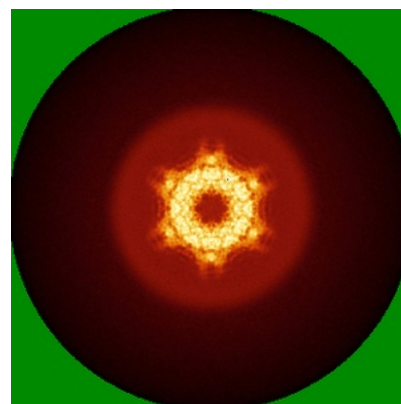
6.4.2 Raw map



X



Y

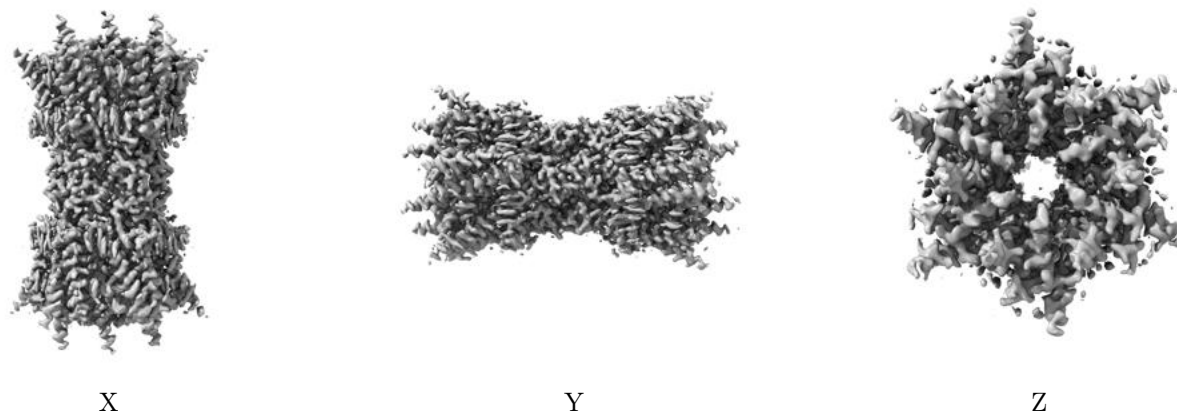


Z

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

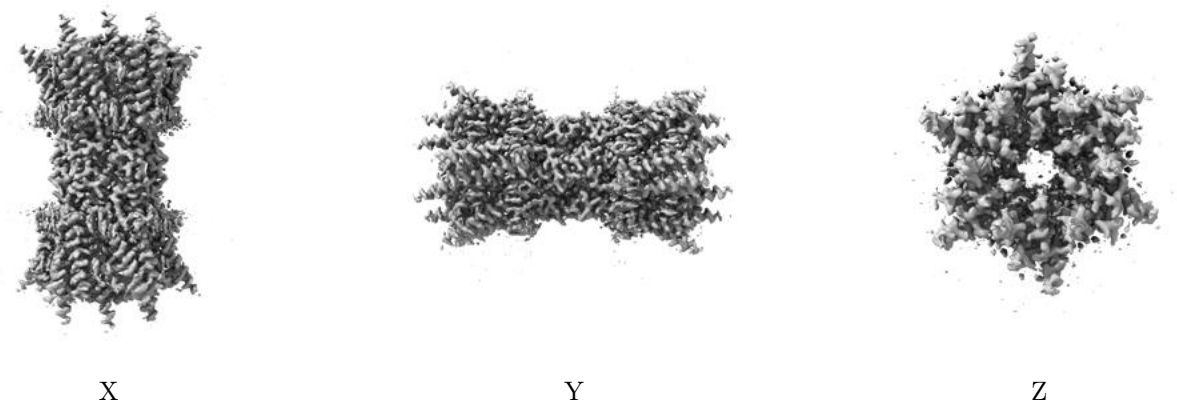
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

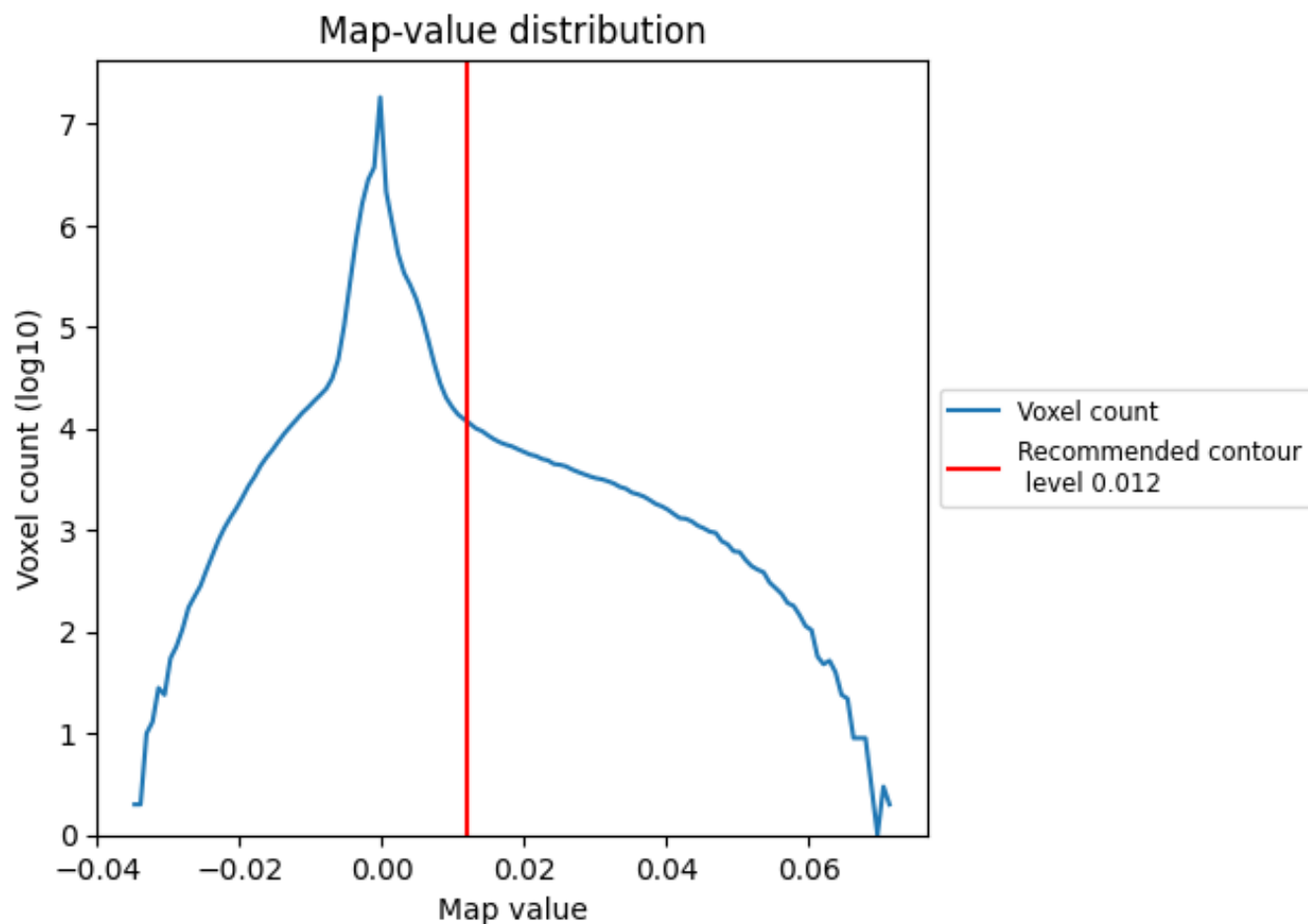
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

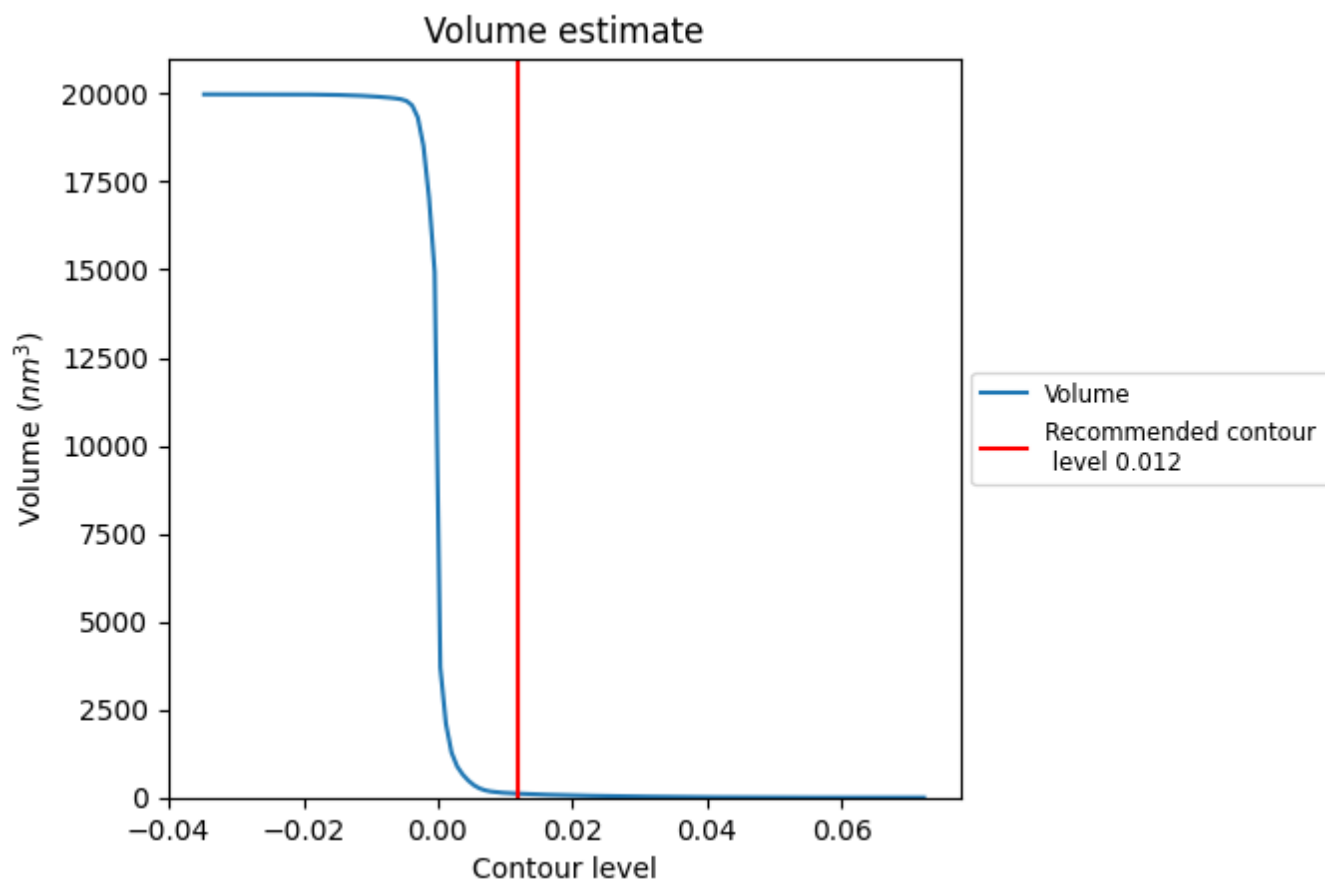
This section contains the results of statistical analysis of the map.

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.

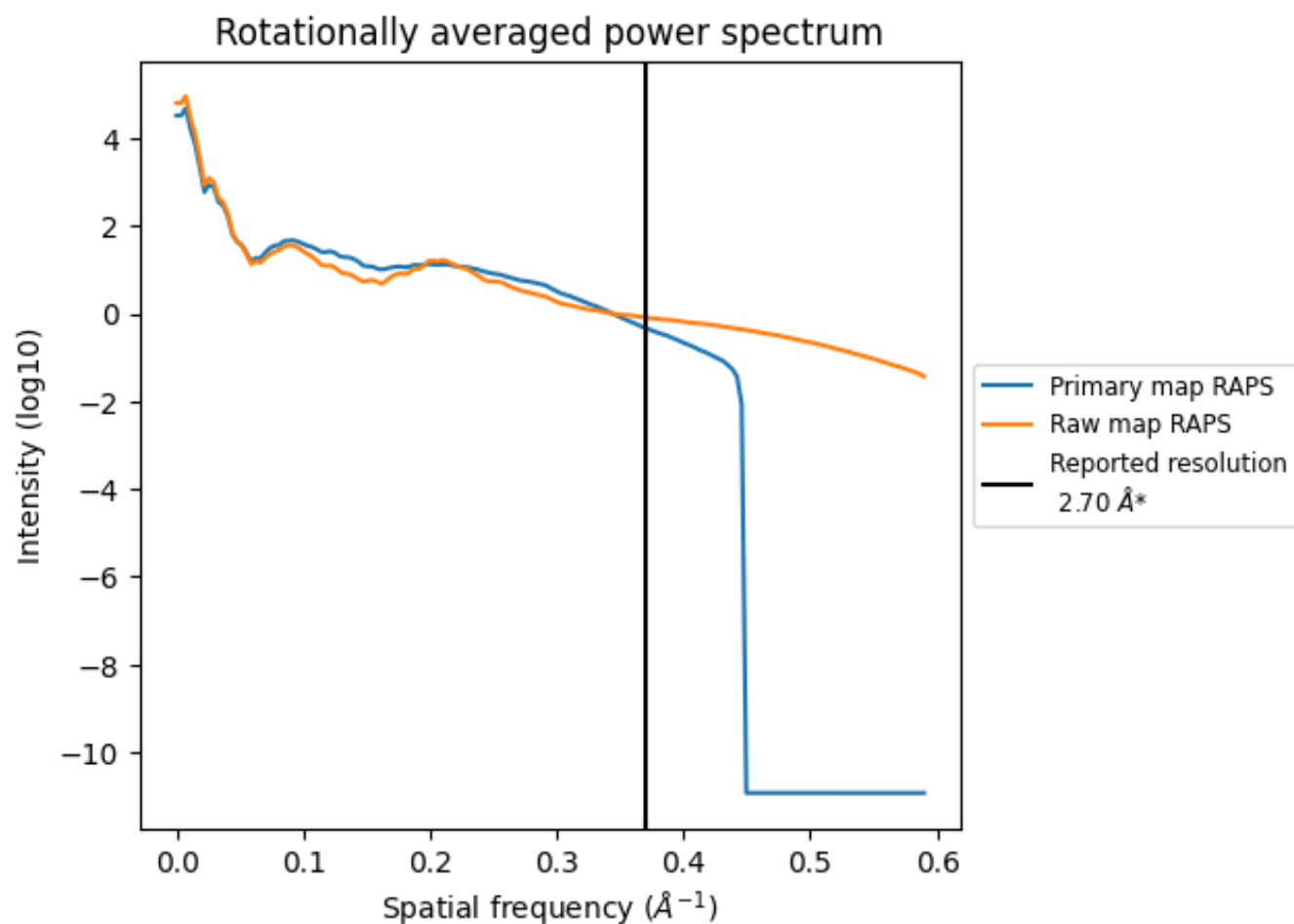
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm³; this corresponds to an approximate mass of 100 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 ⓘ

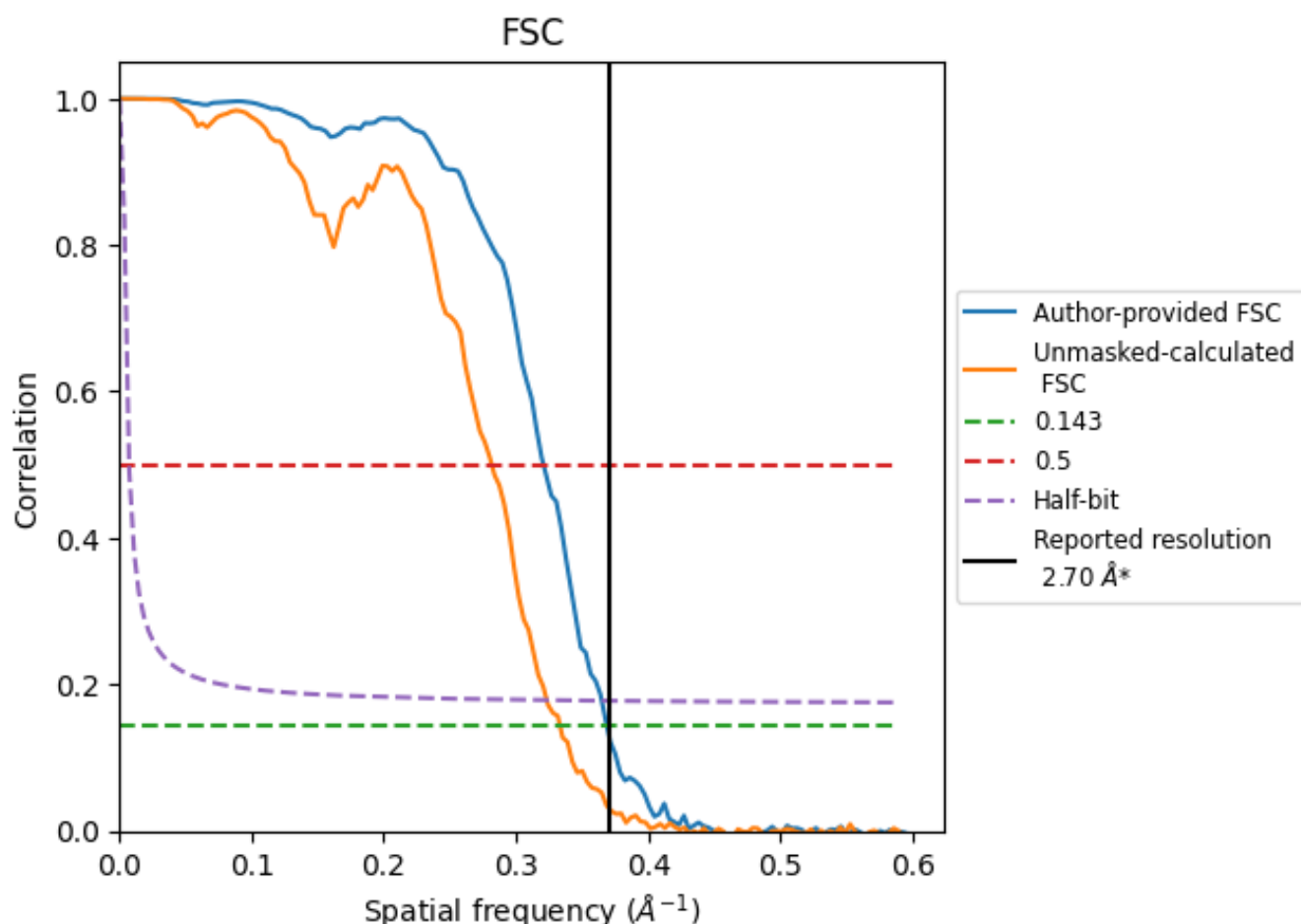


*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

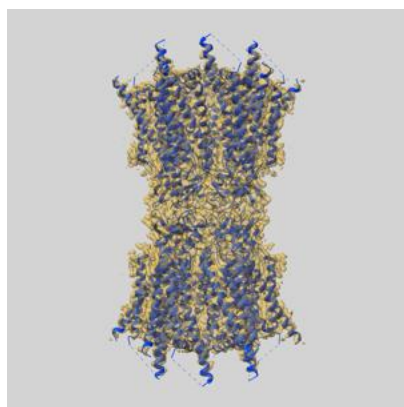
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.12	2.74
Unmasked-calculated*	3.00	3.55	3.09

*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 3.00 differs from the reported value 2.7 by more than 10 %

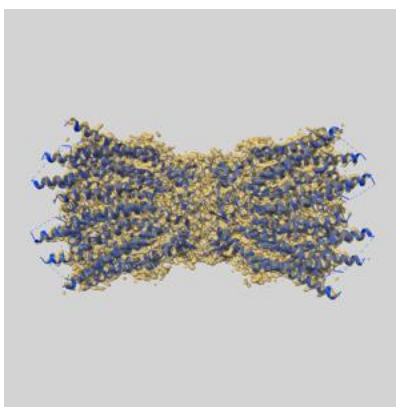
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33393 and PDB model 7XQD. Per-residue inclusion information can be found in section [3](#) on page [15](#).

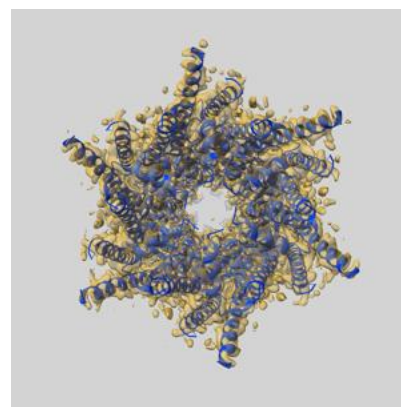
9.1 Map-model overlay [i](#)



X



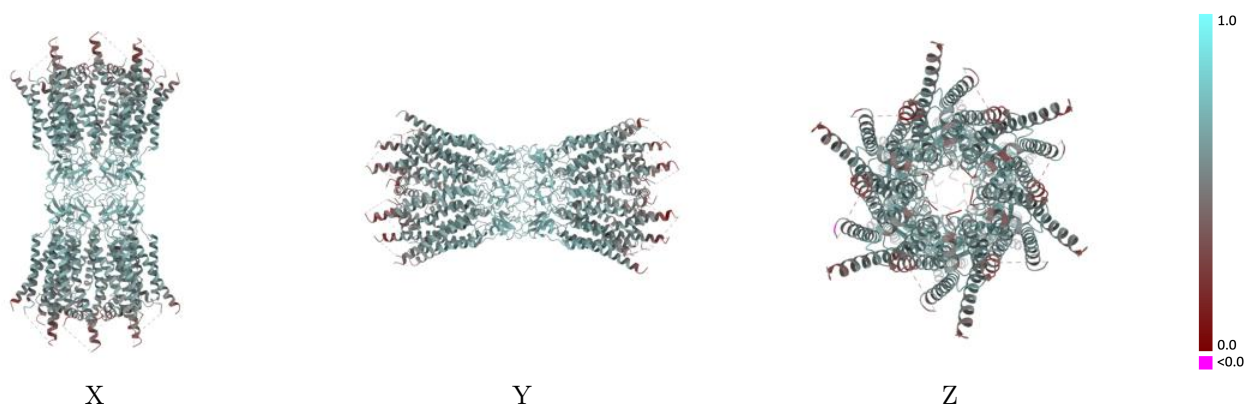
Y



Z

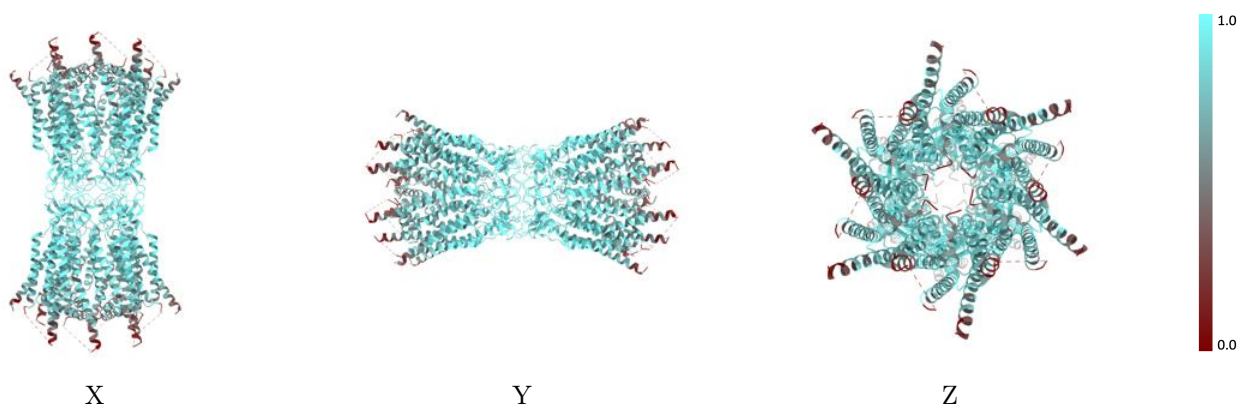
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



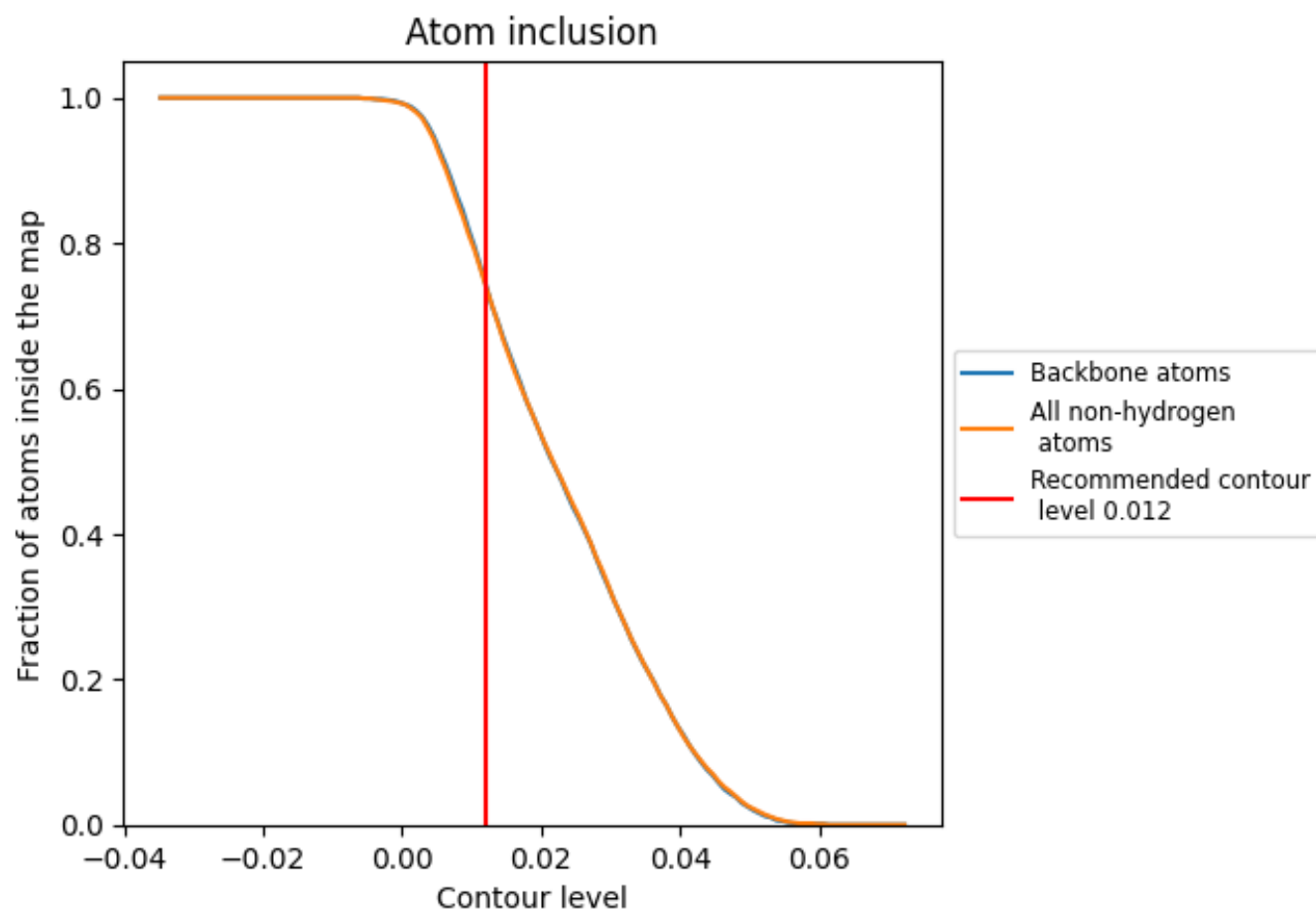
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7420	<div><div></div></div> 0.5580
A	<div><div></div></div> 0.7470	<div><div></div></div> 0.5580
B	<div><div></div></div> 0.7510	<div><div></div></div> 0.5580
C	<div><div></div></div> 0.7420	<div><div></div></div> 0.5580
D	<div><div></div></div> 0.7450	<div><div></div></div> 0.5610
E	<div><div></div></div> 0.7420	<div><div></div></div> 0.5610
F	<div><div></div></div> 0.7390	<div><div></div></div> 0.5510
G	<div><div></div></div> 0.7420	<div><div></div></div> 0.5610
H	<div><div></div></div> 0.7370	<div><div></div></div> 0.5560
I	<div><div></div></div> 0.7450	<div><div></div></div> 0.5550
J	<div><div></div></div> 0.7490	<div><div></div></div> 0.5590
K	<div><div></div></div> 0.7440	<div><div></div></div> 0.5580
L	<div><div></div></div> 0.7490	<div><div></div></div> 0.5610

