



Full wwPDB EM Validation Report ⓘ

Apr 18, 2023 – 06:19 PM JST

PDB ID : 8HG6
EMDB ID : EMD-34736
Title : Cryo-EM structure of the prasinophyte-specific light-harvesting complex (Lhcp) from *Ostreococcus tauri*
Authors : Shan, J.; Sheng, X.; Ishii, A.; Watanabe, A.; Song, C.; Murata, K.; Minagawa, J.; Liu, Z.
Deposited on : 2022-11-13
Resolution : 3.44 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:

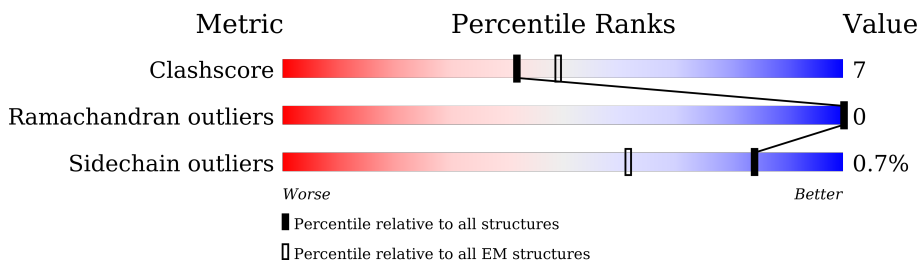
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

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 3.44 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	V	233	
1	W	233	
1	X	233	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CLA	V	301	X	-	-	-
2	CLA	V	302	X	-	-	-
2	CLA	V	303	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CLA	V	309	X	-	-	-
2	CLA	V	310	X	-	-	-
2	CLA	V	311	X	-	-	-
2	CLA	V	313	X	-	-	-
2	CLA	W	301	X	-	-	-
2	CLA	W	302	X	-	-	-
2	CLA	W	303	X	-	-	-
2	CLA	W	309	X	-	-	-
2	CLA	W	310	X	-	-	-
2	CLA	W	311	X	-	-	-
2	CLA	W	312	X	-	-	-
2	CLA	W	313	X	-	-	-
2	CLA	X	302	X	-	-	-
2	CLA	X	303	X	-	-	-
2	CLA	X	304	X	-	-	-
2	CLA	X	310	X	-	-	-
2	CLA	X	311	X	-	-	-
2	CLA	X	312	X	-	-	-
2	CLA	X	313	X	-	-	-
2	CLA	X	314	X	-	-	-
3	CHL	V	304	X	-	-	-
3	CHL	V	305	X	-	-	-
3	CHL	V	306	X	-	-	-
3	CHL	V	307	X	-	-	-
3	CHL	V	314	X	-	-	-
3	CHL	W	304	X	-	-	-
3	CHL	W	305	X	-	-	-
3	CHL	W	306	X	-	-	-
3	CHL	W	307	X	-	-	-
3	CHL	W	314	X	-	-	-
3	CHL	X	305	X	-	-	-
3	CHL	X	306	X	-	-	-
3	CHL	X	307	X	-	-	-
3	CHL	X	308	X	-	-	-
3	CHL	X	315	X	-	-	-

2 Entry composition [i](#)

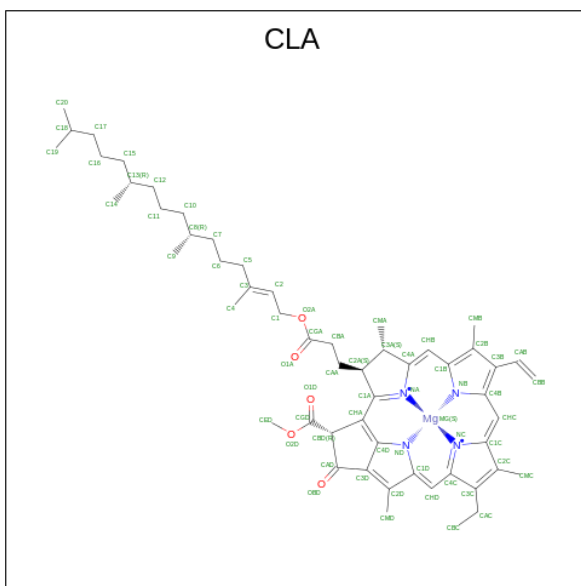
There are 7 unique types of molecules in this entry. The entry contains 7259 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	V	197	Total	C	N	O	S	0	0
			1484	956	242	280	6		
1	W	200	Total	C	N	O	S	0	0
			1499	964	245	284	6		
1	X	196	Total	C	N	O	S	0	0
			1474	949	241	278	6		

- Molecule 2 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



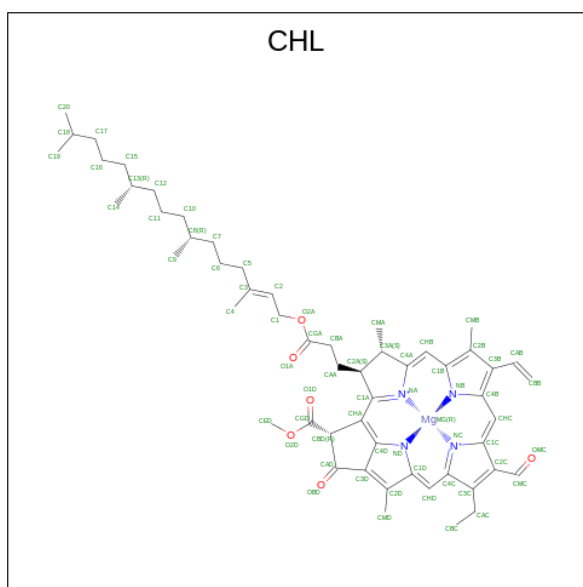
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
2	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
2	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
2	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
2	V	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

Continued on next page...

Continued from previous page...

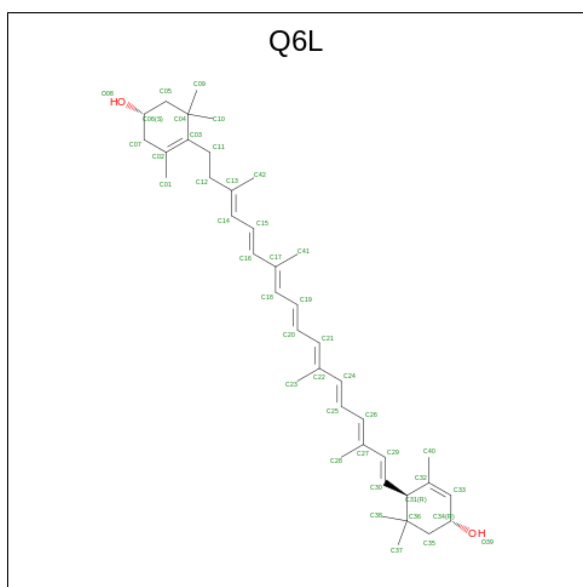
Mol	Chain	Residues	Atoms					AltConf
2	V	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
2	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
2	V	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
2	V	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
2	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
2	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
2	W	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
2	W	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
2	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
2	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
2	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
2	W	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
2	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
2	X	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
2	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
2	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
2	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
2	X	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
2	X	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
2	X	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 3 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
3	V	1	46	35	1	4	6	0
3	V	1	43	34	1	4	4	0
3	V	1	44	35	1	4	4	0
3	V	1	44	35	1	4	4	0
3	V	1	44	35	1	4	4	0
3	W	1	42	33	1	4	4	0
3	W	1	42	33	1	4	4	0
3	W	1	52	41	1	4	6	0
3	W	1	66	55	1	4	6	0
3	W	1	41	32	1	4	4	0
3	X	1	42	33	1	4	4	0
3	X	1	42	33	1	4	4	0
3	X	1	52	41	1	4	6	0
3	X	1	44	35	1	4	4	0

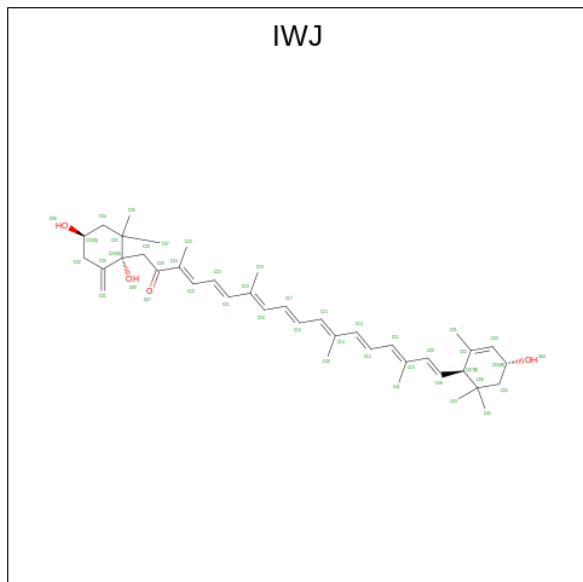
Continued on next page...



Mol	Chain	Residues	Atoms		AltConf
5	V	1	Total	C O	0
			42	40 2	
5	V	1	Total	C O	0
			42	40 2	
5	V	1	Total	C O	0
			42	40 2	
5	V	1	Total	C O	0
			42	40 2	
5	W	1	Total	C O	0
			42	40 2	
5	W	1	Total	C O	0
			42	40 2	
5	W	1	Total	C O	0
			42	40 2	
5	W	1	Total	C O	0
			42	40 2	
5	X	1	Total	C O	0
			42	40 2	
5	X	1	Total	C	0
			40	40	
5	X	1	Total	C O	0
			42	40 2	
5	X	1	Total	C O	0
			42	40 2	

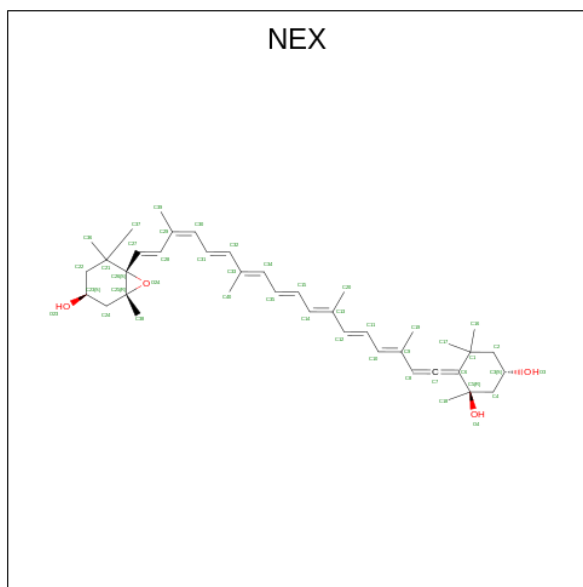
- Molecule 6 is (3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-1-[(1 {S},4 {S})-2,2-dimethyl-6-methylidene-1,4-bis(oxidanyl)cyclohexyl]-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octa

en-2-one (three-letter code: IWJ) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	V	1	Total	C	O	0
			44	40	4	
6	V	1	Total	C	O	0
			44	40	4	
6	V	1	Total	C	O	0
			44	40	4	
6	W	1	Total	C	O	0
			44	40	4	
6	X	1	Total	C	O	0
			44	40	4	

- Molecule 7 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).

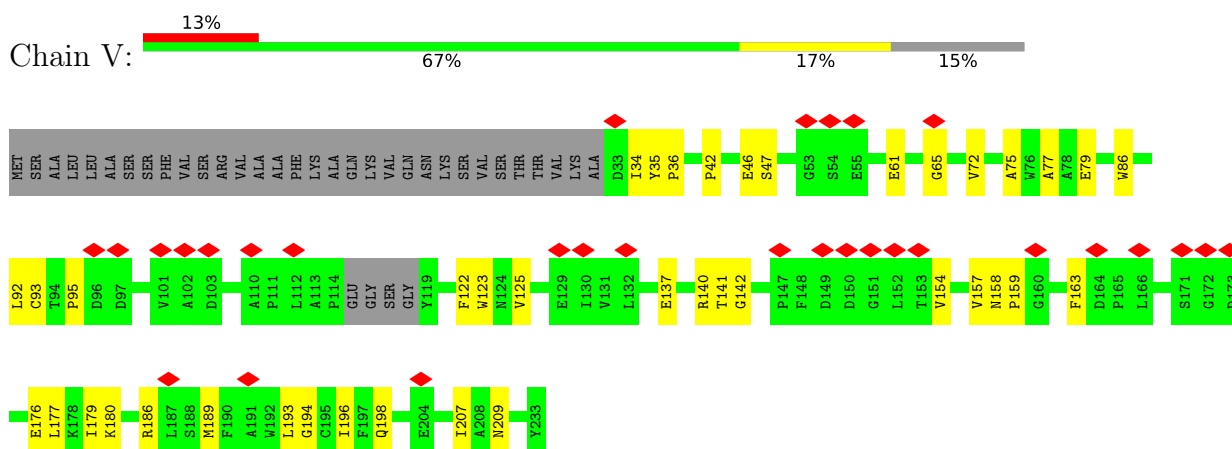


Mol	Chain	Residues	Atoms		AltConf
7	W	1	Total	C O	0
			44	40 4	

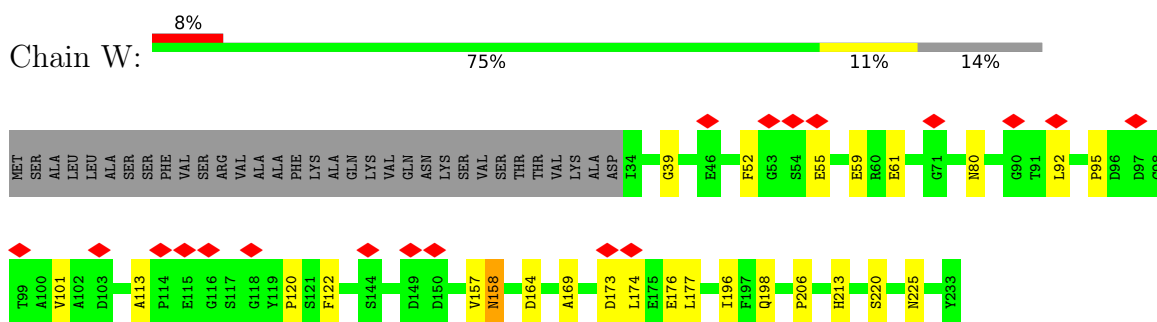
3 Residue-property plots [i](#)

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

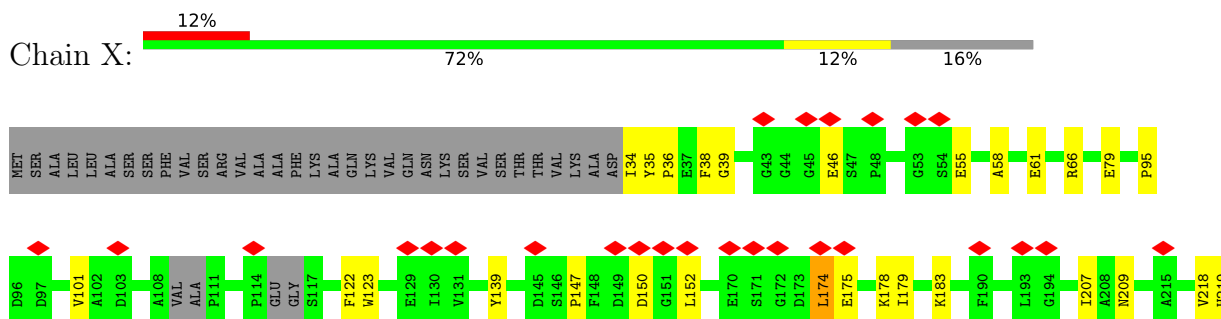
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

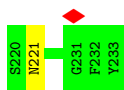


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein, chloroplastic





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80573	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0154	Depositor
Map size (\AA)	399.36, 399.36, 399.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	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: IWJ, Q6L, NEX, CLA, KC2, CHL

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	V	0.55	1/1529 (0.1%)	0.70	2/2089 (0.1%)
1	W	0.56	1/1545 (0.1%)	0.67	1/2111 (0.0%)
1	X	0.50	0/1518	0.68	1/2070 (0.0%)
All	All	0.54	2/4592 (0.0%)	0.68	4/6270 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	55	GLU	CB-CG	5.45	1.62	1.52
1	V	93	CYS	CB-SG	-5.04	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	55	GLU	OE1-CD-OE2	-6.73	115.22	123.30
1	X	174	LEU	CA-CB-CG	5.33	127.56	115.30
1	V	36	PRO	CA-N-CD	-5.28	104.11	111.50
1	V	92	LEU	CB-CG-CD1	-5.25	102.07	111.00

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	V	1484	0	1411	35	0
1	W	1499	0	1425	22	0
1	X	1474	0	1401	26	0
2	V	412	0	347	15	0
2	W	427	0	379	11	0
2	X	373	0	290	9	0
3	V	221	0	153	2	0
3	W	243	0	189	0	0
3	X	225	0	155	2	0
4	V	45	0	0	1	0
4	W	45	0	0	0	0
4	X	45	0	0	0	0
5	V	168	0	0	1	0
5	W	168	0	0	2	0
5	X	166	0	0	1	0
6	V	132	0	0	2	0
6	W	44	0	0	2	0
6	X	44	0	0	0	0
7	W	44	0	56	0	0
All	All	7259	0	5806	93	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 7.

All (93) 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:V:177:LEU:HG	2:V:309:CLA:H3A	1.62	0.80
1:W:174:LEU:HD12	2:W:309:CLA:HMA2	1.65	0.78
1:V:137:GLU:OE1	4:V:308:KC2:C4C	2.34	0.73
1:W:169:ALA:HB1	1:W:174:LEU:HD13	1.70	0.72
3:V:307:CHL:HBB1	3:V:307:CHL:HMB1	1.75	0.68
1:X:36:PRO:HD2	1:X:183:LYS:NZ	2.09	0.68
1:W:169:ALA:CB	1:W:174:LEU:HD13	2.24	0.67
1:V:180:LYS:HZ1	2:V:311:CLA:HBD	1.59	0.66
1:X:39:GLY:HA3	2:X:302:CLA:HMD1	1.78	0.65
1:W:92:LEU:CD2	2:W:303:CLA:H2A	2.26	0.65
1:X:36:PRO:HD2	1:X:183:LYS:HZ1	1.60	0.65
1:V:198:GLN:HE21	1:V:209:ASN:HD22	1.44	0.64
1:W:61:GLU:OE1	2:W:301:CLA:C4A	2.46	0.63
1:X:35:TYR:CD2	1:X:183:LYS:HE2	2.34	0.63
1:X:35:TYR:HD2	1:X:183:LYS:HE2	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:301:CLA:H72	2:V:302:CLA:HMD1	1.82	0.62
1:V:163:PHE:CD2	2:V:309:CLA:HMD1	2.34	0.62
6:W:318:IWJ:O27	6:W:318:IWJ:O39	2.15	0.60
1:W:92:LEU:HG	1:W:101:VAL:HG22	1.84	0.59
1:X:174:LEU:HG	1:X:178:LYS:HZ2	1.68	0.59
1:V:194:GLY:O	1:V:198:GLN:HG3	2.03	0.58
1:W:39:GLY:HA3	2:W:301:CLA:HMD1	1.85	0.58
1:W:173:ASP:HB2	1:W:176:GLU:HB2	1.85	0.57
1:W:206:PRO:O	5:W:315:Q6L:O08	2.23	0.57
1:X:34:ILE:HG12	1:X:36:PRO:HD3	1.87	0.57
1:X:209:ASN:N	1:X:209:ASN:OD1	2.36	0.56
2:V:301:CLA:O1A	2:V:301:CLA:H3A	2.06	0.56
1:X:61:GLU:OE1	2:X:302:CLA:C4A	2.53	0.56
1:V:86:TRP:CH2	1:V:196:ILE:HG22	2.41	0.56
2:X:304:CLA:H2A	2:X:304:CLA:HED3	1.87	0.56
1:X:101:VAL:HG11	3:X:306:CHL:HBC1	1.88	0.55
1:W:80:ASN:ND2	6:W:318:IWJ:O44	2.39	0.55
1:X:218:VAL:O	1:X:221:ASN:ND2	2.39	0.55
1:V:86:TRP:HH2	1:V:196:ILE:HG22	1.70	0.54
1:V:61:GLU:OE2	1:V:186:ARG:NE	2.40	0.54
1:V:35:TYR:OH	1:V:186:ARG:NH1	2.41	0.53
1:V:177:LEU:CG	2:V:309:CLA:H3A	2.35	0.53
1:W:52:PHE:HA	2:W:301:CLA:HBA1	1.90	0.53
1:V:79:GLU:OE1	1:V:207:ILE:HB	2.10	0.52
1:V:176:GLU:O	1:V:180:LYS:HG3	2.11	0.51
1:V:198:GLN:HG2	2:V:312:CLA:ND	2.26	0.50
1:V:34:ILE:HD11	1:V:179:ILE:HG21	1.94	0.50
2:X:311:CLA:HED3	2:X:311:CLA:H2A	1.93	0.50
1:X:36:PRO:HG3	2:X:311:CLA:HMA3	1.93	0.49
1:V:42:PRO:HD3	1:V:186:ARG:NH2	2.27	0.49
1:V:46:GLU:OE2	1:V:47:SER:OG	2.30	0.49
6:V:317:IWJ:O39	6:V:317:IWJ:O27	2.30	0.49
2:W:309:CLA:H2A	2:W:309:CLA:O1D	2.12	0.49
1:V:189:MET:HB3	2:V:301:CLA:HMC3	1.94	0.48
1:W:158:ASN:HB2	2:W:309:CLA:CGD	2.44	0.48
1:X:66:ARG:NH1	3:X:308:CHL:OBD	2.45	0.48
1:V:125:VAL:HG21	3:V:305:CHL:C3D	2.44	0.47
1:V:142:GLY:HA2	1:V:154:VAL:HG11	1.95	0.47
1:X:36:PRO:HG3	2:X:311:CLA:CMA	2.45	0.47
1:V:61:GLU:OE1	2:V:301:CLA:C4A	2.57	0.47
1:V:142:GLY:CA	1:V:154:VAL:HG11	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:72:VAL:O	1:V:75:ALA:HB3	2.15	0.46
1:W:198:GLN:HG2	2:W:312:CLA:ND	2.30	0.46
1:W:113:ALA:HB3	1:W:120:PRO:HG3	1.96	0.46
1:W:164:ASP:OD1	5:W:315:Q6L:O39	2.33	0.46
6:V:320:IWJ:O27	6:V:320:IWJ:O39	2.34	0.46
1:W:213:HIS:HA	1:W:220:SER:HB2	1.98	0.46
1:W:95:PRO:HA	1:W:122:PHE:HB3	1.97	0.46
1:X:34:ILE:N	1:X:179:ILE:HG21	2.31	0.45
1:X:79:GLU:OE2	1:X:207:ILE:N	2.46	0.45
1:V:123:TRP:HZ2	1:X:218:VAL:HG21	1.82	0.45
1:V:137:GLU:HA	1:V:140:ARG:HG2	1.98	0.45
1:X:174:LEU:HD11	2:X:310:CLA:HED2	1.98	0.45
1:X:46:GLU:HA	2:X:302:CLA:HED1	1.99	0.44
1:X:175:GLU:HA	1:X:178:LYS:HZ3	1.83	0.44
1:V:65:GLY:HA2	1:V:189:MET:HG3	1.99	0.44
1:W:59:GLU:OE2	1:W:157:VAL:HG13	2.18	0.44
1:X:139:TYR:CE2	1:X:147:PRO:HB3	2.53	0.44
1:X:175:GLU:HA	1:X:178:LYS:NZ	2.33	0.44
2:V:301:CLA:H3A	2:V:301:CLA:CGA	2.48	0.43
1:W:225:ASN:ND2	2:W:312:CLA:OBD	2.51	0.43
1:V:158:ASN:ND2	2:V:309:CLA:O1D	2.51	0.43
1:V:193:LEU:O	1:V:196:ILE:HG12	2.18	0.43
5:V:321:Q6L:C28	1:W:196:ILE:HG23	2.48	0.43
1:V:95:PRO:HA	1:V:122:PHE:CD2	2.54	0.42
1:V:140:ARG:HG3	1:V:141:THR:HG23	2.01	0.42
1:X:150:ASP:HB3	1:X:152:LEU:HD23	2.02	0.42
1:X:95:PRO:HA	1:X:122:PHE:HB3	2.01	0.42
1:V:198:GLN:HG2	2:V:312:CLA:C1D	2.50	0.42
1:V:180:LYS:NZ	2:V:311:CLA:HAA2	2.35	0.42
2:X:313:CLA:H2A	2:X:313:CLA:O2D	2.20	0.41
1:W:177:LEU:HD13	2:W:309:CLA:O1A	2.21	0.41
1:X:38:PHE:O	5:X:319:Q6L:O39	2.38	0.41
1:V:77:ALA:O	2:V:303:CLA:HMD3	2.20	0.41
1:W:177:LEU:HB3	2:W:309:CLA:H3A	2.03	0.41
1:X:55:GLU:O	1:X:58:ALA:N	2.54	0.41
1:V:157:VAL:C	1:V:159:PRO:HD3	2.42	0.40
1:V:180:LYS:NZ	2:V:311:CLA:HBD	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	193/233 (83%)	188 (97%)	5 (3%)	0	100	100
1	W	198/233 (85%)	188 (95%)	10 (5%)	0	100	100
1	X	190/233 (82%)	184 (97%)	6 (3%)	0	100	100
All	All	581/699 (83%)	560 (96%)	21 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	151/179 (84%)	151 (100%)	0	100	100
1	W	152/179 (85%)	151 (99%)	1 (1%)	84	93
1	X	150/179 (84%)	148 (99%)	2 (1%)	69	86
All	All	453/537 (84%)	450 (99%)	3 (1%)	84	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	158	ASN
1	X	123	TRP
1	X	219	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	V	209	ASN
1	W	209	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

60 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
3	CHL	W	314	1	40,49,74	1.84	6 (15%)	42,83,114	1.99	10 (23%)
5	Q6L	X	319	-	42,43,43	1.92	6 (14%)	47,60,60	1.77	7 (14%)
3	CHL	V	314	1	44,52,74	1.79	7 (15%)	46,87,114	1.66	10 (21%)
2	CLA	X	313	1	41,49,73	1.86	8 (19%)	47,84,113	1.60	9 (19%)
5	Q6L	X	317	-	42,43,43	1.86	7 (16%)	47,60,60	1.57	5 (10%)
3	CHL	X	308	-	44,52,74	1.72	6 (13%)	46,87,114	1.77	10 (21%)
5	Q6L	W	315	-	42,43,43	1.84	7 (16%)	47,60,60	1.54	7 (14%)
3	CHL	V	305	1	43,51,74	1.74	7 (16%)	45,86,114	1.76	7 (15%)
3	CHL	V	307	-	44,52,74	1.74	5 (11%)	46,87,114	1.53	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CLA	X	304	-	42,50,73	1.86	8 (19%)	48,85,113	1.74	9 (18%)
2	CLA	X	303	-	51,59,73	1.72	8 (15%)	59,96,113	1.32	7 (11%)
2	CLA	W	313	-	43,51,73	1.77	6 (13%)	49,86,113	1.41	7 (14%)
2	CLA	V	302	-	50,58,73	1.70	9 (18%)	58,95,113	1.47	11 (18%)
2	CLA	V	301	1	60,68,73	1.48	5 (8%)	70,107,113	1.74	11 (15%)
2	CLA	X	314	-	41,49,73	1.85	7 (17%)	47,84,113	1.55	8 (17%)
3	CHL	W	307	-	66,74,74	1.46	6 (9%)	73,114,114	1.53	10 (13%)
6	IWJ	V	320	-	43,45,45	1.16	5 (11%)	43,65,65	1.13	2 (4%)
2	CLA	V	312	1	55,63,73	1.60	9 (16%)	64,101,113	1.47	9 (14%)
4	KC2	V	308	1	48,53,53	2.53	16 (33%)	54,89,89	2.21	19 (35%)
2	CLA	V	311	-	60,68,73	1.51	7 (11%)	70,107,113	1.40	11 (15%)
6	IWJ	V	317	-	43,45,45	1.17	4 (9%)	43,65,65	1.20	2 (4%)
2	CLA	X	311	1	50,58,73	1.65	7 (14%)	58,95,113	1.41	8 (13%)
3	CHL	V	306	-	44,52,74	1.75	7 (15%)	46,87,114	1.96	12 (26%)
3	CHL	X	305	1	42,50,74	1.85	5 (11%)	44,85,114	1.43	8 (18%)
5	Q6L	V	321	-	42,43,43	1.86	7 (16%)	47,60,60	1.57	4 (8%)
5	Q6L	X	316	-	40,41,43	1.86	5 (12%)	46,56,60	1.61	6 (13%)
6	IWJ	V	318	-	43,45,45	1.14	4 (9%)	43,65,65	1.43	8 (18%)
6	IWJ	W	318	-	43,45,45	1.15	4 (9%)	43,65,65	1.36	6 (13%)
3	CHL	W	305	-	42,50,74	1.81	6 (14%)	44,85,114	1.83	10 (22%)
4	KC2	X	309	1	48,53,53	2.57	16 (33%)	54,89,89	2.54	21 (38%)
2	CLA	W	310	1	60,68,73	1.55	6 (10%)	70,107,113	1.30	8 (11%)
2	CLA	W	301	1	55,63,73	1.59	9 (16%)	64,101,113	1.53	9 (14%)
5	Q6L	V	316	-	42,43,43	1.94	7 (16%)	47,60,60	1.60	5 (10%)
2	CLA	V	309	1	42,50,73	2.12	9 (21%)	48,85,113	2.06	14 (29%)
5	Q6L	X	301	-	42,43,43	1.90	7 (16%)	47,60,60	1.52	5 (10%)
5	Q6L	V	319	-	42,43,43	1.81	7 (16%)	47,60,60	1.79	12 (25%)
3	CHL	X	307	-	52,60,74	1.58	10 (19%)	56,97,114	2.51	18 (32%)
2	CLA	X	302	1	55,63,73	1.64	10 (18%)	64,101,113	1.48	13 (20%)
2	CLA	V	310	1	47,55,73	1.74	8 (17%)	54,91,113	1.48	10 (18%)
4	KC2	W	308	1	48,53,53	2.57	16 (33%)	54,89,89	2.32	20 (37%)
5	Q6L	V	315	-	42,43,43	1.91	7 (16%)	47,60,60	1.45	6 (12%)
2	CLA	W	312	1	55,63,73	1.60	7 (12%)	64,101,113	1.79	13 (20%)
2	CLA	W	311	-	45,53,73	1.68	6 (13%)	52,89,113	1.62	8 (15%)
2	CLA	W	302	-	55,63,73	1.61	8 (14%)	64,101,113	1.34	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CLA	V	313	-	48,56,73	1.70	7 (14%)	55,92,113	1.37	8 (14%)
2	CLA	X	312	-	51,59,73	1.66	8 (15%)	59,96,113	1.56	11 (18%)
3	CHL	X	315	1	45,53,74	1.83	6 (13%)	46,88,114	1.36	5 (10%)
3	CHL	W	304	1	42,50,74	1.88	5 (11%)	44,85,114	1.58	7 (15%)
3	CHL	X	306	-	42,50,74	1.79	6 (14%)	44,85,114	1.84	8 (18%)
3	CHL	W	306	-	52,60,74	1.60	8 (15%)	56,97,114	2.11	14 (25%)
7	NEX	W	317	-	38,46,46	1.13	4 (10%)	50,70,70	2.59	13 (26%)
2	CLA	X	310	1	42,50,73	1.82	7 (16%)	48,85,113	1.58	9 (18%)
3	CHL	V	304	1	46,54,74	1.78	8 (17%)	49,90,114	1.49	8 (16%)
5	Q6L	W	316	-	42,43,43	1.91	9 (21%)	47,60,60	1.54	6 (12%)
2	CLA	W	303	-	50,58,73	1.65	8 (16%)	58,95,113	1.68	11 (18%)
5	Q6L	W	320	-	42,43,43	1.88	7 (16%)	47,60,60	1.72	5 (10%)
5	Q6L	W	319	-	42,43,43	1.88	7 (16%)	47,60,60	1.45	7 (14%)
6	IWJ	X	318	-	43,45,45	1.18	7 (16%)	43,65,65	1.39	7 (16%)
2	CLA	W	309	1	64,72,73	1.51	6 (9%)	74,111,113	1.59	14 (18%)
2	CLA	V	303	-	50,58,73	1.72	8 (16%)	58,95,113	1.73	8 (13%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CHL	W	314	1	3/3/14/26	5/10/104/137	-
5	Q6L	X	319	-	-	10/29/67/67	0/2/2/2
3	CHL	V	314	1	3/3/15/26	5/13/111/137	-
2	CLA	X	313	1	1/1/10/20	3/8/86/115	-
5	Q6L	X	317	-	-	2/29/67/67	0/2/2/2
3	CHL	X	308	-	3/3/15/26	8/13/111/137	-
5	Q6L	W	315	-	-	4/29/67/67	0/2/2/2
3	CHL	V	305	1	3/3/15/26	2/12/110/137	-
3	CHL	V	307	-	3/3/15/26	5/13/111/137	-
2	CLA	X	304	-	1/1/10/20	5/10/88/115	-
2	CLA	X	303	-	1/1/12/20	9/21/99/115	-
2	CLA	W	313	-	1/1/10/20	2/11/89/115	-
2	CLA	V	302	-	1/1/12/20	9/19/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLA	V	301	1	1/1/14/20	10/31/109/115	-
2	CLA	X	314	-	1/1/10/20	5/8/86/115	-
3	CHL	W	307	-	3/3/20/26	13/39/137/137	-
6	IWJ	V	320	-	-	5/33/76/76	1/2/2/2
2	CLA	V	312	1	-	7/25/103/115	-
4	KC2	V	308	1	-	10/15/71/71	-
2	CLA	V	311	-	1/1/14/20	10/31/109/115	-
6	IWJ	V	317	-	-	6/33/76/76	0/2/2/2
2	CLA	X	311	1	1/1/12/20	8/19/97/115	-
3	CHL	V	306	-	3/3/15/26	0/13/111/137	-
3	CHL	X	305	1	3/3/15/26	1/10/108/137	-
5	Q6L	V	321	-	-	6/29/67/67	0/2/2/2
5	Q6L	X	316	-	-	7/29/63/67	0/2/2/2
6	IWJ	V	318	-	-	4/33/76/76	0/2/2/2
6	IWJ	W	318	-	-	10/33/76/76	0/2/2/2
3	CHL	W	305	-	3/3/15/26	2/10/108/137	-
4	KC2	X	309	1	-	10/15/71/71	-
2	CLA	W	310	1	1/1/14/20	9/31/109/115	-
2	CLA	W	301	1	1/1/13/20	10/25/103/115	-
5	Q6L	V	316	-	-	8/29/67/67	0/2/2/2
2	CLA	V	309	1	1/1/10/20	4/10/88/115	-
5	Q6L	X	301	-	-	8/29/67/67	0/2/2/2
5	Q6L	V	319	-	-	9/29/67/67	0/2/2/2
3	CHL	X	307	-	3/3/17/26	10/23/121/137	-
2	CLA	X	302	1	1/1/13/20	8/25/103/115	-
2	CLA	V	310	1	1/1/11/20	8/16/94/115	-
4	KC2	W	308	1	-	10/15/71/71	-
5	Q6L	V	315	-	-	11/29/67/67	0/2/2/2
2	CLA	W	312	1	1/1/13/20	9/25/103/115	-
2	CLA	W	311	-	1/1/11/20	5/13/91/115	-
2	CLA	W	302	-	1/1/13/20	5/25/103/115	-
2	CLA	V	313	-	1/1/11/20	4/17/95/115	-
2	CLA	X	312	-	1/1/12/20	4/21/99/115	-
3	CHL	X	315	1	3/3/15/26	4/13/112/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CHL	W	304	1	3/3/15/26	0/10/108/137	-
3	CHL	X	306	-	3/3/15/26	2/10/108/137	-
3	CHL	W	306	-	3/3/17/26	5/23/121/137	-
7	NEX	W	317	-	-	2/27/83/83	0/3/3/3
2	CLA	X	310	1	1/1/10/20	3/10/88/115	-
3	CHL	V	304	1	3/3/16/26	8/15/113/137	-
5	Q6L	W	316	-	-	5/29/67/67	0/2/2/2
2	CLA	W	303	-	1/1/12/20	4/19/97/115	-
5	Q6L	W	320	-	-	7/29/67/67	0/2/2/2
5	Q6L	W	319	-	-	9/29/67/67	0/2/2/2
6	IWJ	X	318	-	-	6/33/76/76	1/2/2/2
2	CLA	W	309	1	1/1/14/20	7/36/114/115	-
2	CLA	V	303	-	1/1/12/20	5/19/97/115	-

All (438) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	309	CLA	C4B-NB	10.02	1.44	1.35
5	V	316	Q6L	C29-C30	8.77	1.53	1.32
4	V	308	KC2	C2A-C3A	8.64	1.54	1.37
4	X	309	KC2	C2A-C3A	8.61	1.54	1.37
5	X	319	Q6L	C29-C30	8.50	1.52	1.32
5	X	301	Q6L	C29-C30	8.42	1.52	1.32
5	W	319	Q6L	C29-C30	8.41	1.52	1.32
5	W	316	Q6L	C29-C30	8.39	1.52	1.32
5	X	316	Q6L	C29-C30	8.38	1.52	1.32
5	X	317	Q6L	C29-C30	8.37	1.52	1.32
5	W	320	Q6L	C29-C30	8.31	1.51	1.32
5	V	321	Q6L	C29-C30	8.29	1.51	1.32
3	X	305	CHL	C4B-NB	8.25	1.42	1.35
5	V	315	Q6L	C29-C30	8.17	1.51	1.32
5	W	315	Q6L	C29-C30	8.06	1.51	1.32
3	W	304	CHL	C4B-NB	8.05	1.42	1.35
4	W	308	KC2	C2A-C3A	7.90	1.53	1.37
3	X	315	CHL	C4B-NB	7.80	1.42	1.35
3	X	308	CHL	C4B-NB	7.71	1.42	1.35
3	W	307	CHL	C4B-NB	7.70	1.42	1.35
3	W	314	CHL	C4B-NB	7.67	1.42	1.35
5	V	319	Q6L	C29-C30	7.59	1.50	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	305	CHL	C4B-NB	7.59	1.42	1.35
3	V	314	CHL	C4B-NB	7.52	1.41	1.35
2	X	313	CLA	C4B-NB	7.51	1.41	1.35
2	W	309	CLA	C4B-NB	7.47	1.41	1.35
2	W	312	CLA	C4B-NB	7.46	1.41	1.35
3	V	307	CHL	C4B-NB	7.35	1.41	1.35
2	X	310	CLA	C4B-NB	7.33	1.41	1.35
2	W	310	CLA	C4B-NB	7.32	1.41	1.35
3	W	306	CHL	C4B-NB	7.31	1.41	1.35
3	V	306	CHL	C4B-NB	7.30	1.41	1.35
2	X	314	CLA	C4B-NB	7.17	1.41	1.35
3	V	304	CHL	C4B-NB	7.12	1.41	1.35
2	V	302	CLA	C4B-NB	7.11	1.41	1.35
2	X	312	CLA	C4B-NB	7.11	1.41	1.35
2	V	303	CLA	C4B-NB	7.06	1.41	1.35
2	V	313	CLA	C4B-NB	7.04	1.41	1.35
2	X	303	CLA	C4B-NB	7.03	1.41	1.35
3	X	306	CHL	C4B-NB	7.03	1.41	1.35
3	V	305	CHL	C4B-NB	6.90	1.41	1.35
2	X	304	CLA	C4B-NB	6.85	1.41	1.35
4	X	309	KC2	C3D-C4D	6.80	1.46	1.40
2	V	311	CLA	C4B-NB	6.78	1.41	1.35
2	W	313	CLA	C4B-NB	6.78	1.41	1.35
2	W	302	CLA	C4B-NB	6.77	1.41	1.35
2	V	312	CLA	C4B-NB	6.70	1.41	1.35
4	W	308	KC2	C1D-ND	6.68	1.41	1.35
2	V	310	CLA	C4B-NB	6.65	1.41	1.35
2	W	311	CLA	C4B-NB	6.56	1.41	1.35
4	W	308	KC2	C3D-C4D	6.56	1.46	1.40
2	X	311	CLA	C4B-NB	6.51	1.41	1.35
2	V	301	CLA	C4B-NB	6.39	1.40	1.35
2	W	303	CLA	C4B-NB	6.37	1.40	1.35
4	V	308	KC2	CBA-CAA	6.28	1.52	1.33
4	X	309	KC2	C1D-ND	6.24	1.40	1.35
2	W	301	CLA	C4B-NB	6.14	1.40	1.35
4	W	308	KC2	CBA-CAA	6.05	1.51	1.33
3	X	307	CHL	C4B-NB	6.04	1.40	1.35
4	X	309	KC2	CBA-CAA	5.98	1.51	1.33
2	X	302	CLA	C4B-NB	5.83	1.40	1.35
5	V	315	Q6L	C12-C11	-5.73	1.33	1.52
5	W	320	Q6L	C12-C11	-5.53	1.34	1.52
5	W	315	Q6L	C12-C11	-5.51	1.34	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	319	Q6L	C12-C11	-5.51	1.34	1.52
5	V	316	Q6L	C12-C11	-5.47	1.34	1.52
5	W	316	Q6L	C12-C11	-5.46	1.34	1.52
5	V	321	Q6L	C12-C11	-5.45	1.34	1.52
5	V	319	Q6L	C12-C11	-5.44	1.34	1.52
5	W	319	Q6L	C12-C11	-5.40	1.34	1.52
5	X	301	Q6L	C12-C11	-5.40	1.34	1.52
4	V	308	KC2	C1D-ND	5.26	1.39	1.35
5	X	316	Q6L	C12-C11	-5.24	1.35	1.52
5	X	317	Q6L	C12-C11	-5.16	1.35	1.52
4	V	308	KC2	C3D-C4D	4.97	1.44	1.40
2	X	302	CLA	C4D-ND	-4.43	1.31	1.37
4	X	309	KC2	CMD-C2D	-4.19	1.42	1.51
4	W	308	KC2	C4A-C3A	4.11	1.52	1.44
4	V	308	KC2	CMD-C2D	-4.07	1.43	1.51
2	V	309	CLA	CHC-C1C	4.03	1.45	1.35
2	V	301	CLA	C4D-ND	-4.03	1.32	1.37
2	X	303	CLA	C1D-ND	3.94	1.42	1.37
3	W	304	CHL	C1D-ND	3.93	1.42	1.37
3	V	304	CHL	C1D-ND	3.92	1.42	1.37
2	W	303	CLA	C4D-ND	-3.91	1.32	1.37
2	W	302	CLA	C1D-ND	3.90	1.42	1.37
3	X	306	CHL	C1D-ND	3.86	1.42	1.37
2	W	312	CLA	C4D-ND	-3.84	1.32	1.37
2	W	310	CLA	C1D-ND	3.83	1.42	1.37
2	X	304	CLA	CMB-C2B	-3.83	1.43	1.51
2	V	311	CLA	C1D-ND	3.82	1.42	1.37
4	V	308	KC2	C4A-C3A	3.81	1.51	1.44
2	W	313	CLA	C1D-ND	3.81	1.42	1.37
2	X	314	CLA	C1D-ND	3.80	1.42	1.37
2	W	301	CLA	C1D-ND	3.79	1.42	1.37
4	X	309	KC2	C4A-C3A	3.76	1.51	1.44
3	W	314	CHL	C1D-ND	3.74	1.42	1.37
3	X	315	CHL	C1D-ND	3.73	1.42	1.37
2	V	310	CLA	C1D-ND	3.70	1.42	1.37
2	W	309	CLA	C1D-ND	3.67	1.42	1.37
2	X	303	CLA	C4D-ND	-3.64	1.32	1.37
4	W	308	KC2	CMD-C2D	-3.62	1.44	1.51
3	X	307	CHL	C1D-ND	3.61	1.42	1.37
3	X	306	CHL	C4D-ND	-3.61	1.32	1.37
2	X	311	CLA	C1D-ND	3.60	1.42	1.37
3	V	307	CHL	C1D-ND	3.60	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	301	CLA	C1D-ND	3.58	1.42	1.37
2	V	313	CLA	C1D-ND	3.57	1.42	1.37
2	X	312	CLA	C1D-ND	3.56	1.42	1.37
2	W	301	CLA	C4D-ND	-3.55	1.32	1.37
3	W	304	CHL	CHC-C1C	3.54	1.44	1.35
3	V	305	CHL	C1D-ND	3.45	1.42	1.37
3	V	314	CHL	C4D-ND	-3.45	1.33	1.37
2	X	313	CLA	C1D-ND	3.44	1.42	1.37
2	W	311	CLA	C1D-ND	3.44	1.42	1.37
3	V	314	CHL	C1D-ND	3.43	1.42	1.37
2	V	302	CLA	C1D-ND	3.43	1.42	1.37
2	X	304	CLA	C3B-C2B	-3.40	1.35	1.40
2	W	313	CLA	C4D-ND	-3.40	1.33	1.37
3	W	307	CHL	C1D-ND	3.39	1.41	1.37
6	V	317	IWJ	C09-C10	3.38	1.53	1.45
3	V	306	CHL	CHC-C1C	3.38	1.43	1.35
2	X	304	CLA	C1D-ND	3.37	1.41	1.37
3	W	306	CHL	C4D-ND	-3.37	1.33	1.37
6	V	320	IWJ	C09-C10	3.35	1.53	1.45
5	V	315	Q6L	C12-C13	-3.35	1.44	1.51
3	V	306	CHL	C1D-ND	3.35	1.41	1.37
3	X	308	CHL	C1D-ND	3.34	1.41	1.37
6	V	318	IWJ	C09-C10	3.33	1.53	1.45
2	V	303	CLA	CHC-C1C	3.33	1.43	1.35
3	V	307	CHL	C4D-ND	-3.30	1.33	1.37
2	V	309	CLA	C1D-ND	3.30	1.41	1.37
6	W	318	IWJ	C09-C10	3.30	1.53	1.45
2	X	310	CLA	C1D-ND	3.30	1.41	1.37
2	V	302	CLA	C4D-ND	-3.29	1.33	1.37
3	X	305	CHL	CHC-C1C	3.25	1.43	1.35
2	V	312	CLA	C4D-ND	-3.22	1.33	1.37
3	V	304	CHL	CHC-C1C	3.21	1.43	1.35
3	X	315	CHL	C4D-ND	-3.19	1.33	1.37
4	V	308	KC2	MG-NA	3.19	2.13	2.06
3	X	308	CHL	CHC-C1C	3.18	1.43	1.35
3	X	305	CHL	C4D-ND	-3.18	1.33	1.37
3	W	304	CHL	C4D-ND	-3.16	1.33	1.37
3	W	307	CHL	CHC-C1C	3.16	1.43	1.35
3	W	305	CHL	C4D-ND	-3.14	1.33	1.37
2	X	314	CLA	C4D-ND	-3.13	1.33	1.37
2	V	303	CLA	C4D-ND	-3.13	1.33	1.37
4	V	308	KC2	C4D-ND	-3.12	1.32	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	310	CLA	CHC-C1C	3.12	1.43	1.35
2	X	311	CLA	C4D-ND	-3.12	1.33	1.37
3	V	306	CHL	C4D-ND	-3.11	1.33	1.37
3	W	305	CHL	C1D-ND	3.10	1.41	1.37
3	W	314	CHL	C4D-ND	-3.10	1.33	1.37
2	W	309	CLA	CHC-C1C	3.10	1.42	1.35
2	X	302	CLA	C3B-CAB	-3.08	1.41	1.47
2	W	302	CLA	C4D-ND	-3.08	1.33	1.37
2	V	310	CLA	C4D-ND	-3.07	1.33	1.37
2	X	312	CLA	C4D-ND	-3.07	1.33	1.37
3	X	315	CHL	CHC-C1C	3.07	1.42	1.35
2	W	311	CLA	C4D-ND	-3.07	1.33	1.37
2	X	303	CLA	C3B-C2B	-3.06	1.36	1.40
2	X	302	CLA	C1D-ND	3.05	1.41	1.37
6	X	318	IWJ	C09-C10	3.05	1.52	1.45
2	W	301	CLA	CHC-C1C	3.05	1.42	1.35
2	V	312	CLA	C1D-ND	3.04	1.41	1.37
2	V	303	CLA	C3B-C2B	-3.04	1.36	1.40
2	V	313	CLA	CHC-C1C	3.03	1.42	1.35
4	W	308	KC2	C4B-NB	3.02	1.41	1.37
2	V	303	CLA	CMB-C2B	-3.02	1.45	1.51
5	V	319	Q6L	C34-C33	3.02	1.54	1.50
2	W	303	CLA	C1D-ND	3.01	1.41	1.37
2	W	310	CLA	CHC-C1C	3.01	1.42	1.35
2	W	303	CLA	CMB-C2B	-3.01	1.45	1.51
5	X	319	Q6L	C34-C33	3.01	1.54	1.50
2	X	311	CLA	CHC-C1C	3.00	1.42	1.35
2	X	313	CLA	CHC-C1C	3.00	1.42	1.35
2	X	313	CLA	C4D-ND	-2.99	1.33	1.37
2	X	302	CLA	CHC-C1C	2.99	1.42	1.35
2	V	313	CLA	C4D-ND	-2.99	1.33	1.37
3	V	304	CHL	C4D-ND	-2.99	1.33	1.37
2	X	304	CLA	C4D-ND	-2.98	1.33	1.37
6	V	317	IWJ	C29-C35	-2.97	1.51	1.56
2	W	313	CLA	CHC-C1C	2.97	1.42	1.35
4	X	309	KC2	C2A-C1A	2.96	1.53	1.44
3	X	308	CHL	C4D-ND	-2.95	1.33	1.37
6	X	318	IWJ	C04-C03	2.95	1.54	1.50
3	V	314	CHL	CHC-C1C	2.95	1.42	1.35
2	V	311	CLA	CHC-C1C	2.94	1.42	1.35
3	V	305	CHL	CHC-C1C	2.93	1.42	1.35
3	W	314	CHL	CHC-C1C	2.92	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	306	CHL	CHC-C1C	2.91	1.42	1.35
7	W	317	NEX	C7-C8	-2.90	1.27	1.32
3	V	305	CHL	C4D-ND	-2.89	1.33	1.37
6	V	320	IWJ	C04-C03	2.89	1.54	1.50
4	V	308	KC2	C4B-NB	2.89	1.41	1.37
3	V	307	CHL	CHC-C1C	2.89	1.42	1.35
4	V	308	KC2	C2A-C1A	2.88	1.53	1.44
2	V	312	CLA	CMB-C2B	-2.87	1.45	1.51
2	V	312	CLA	CHC-C1C	2.87	1.42	1.35
2	V	310	CLA	C3B-C2B	-2.87	1.36	1.40
5	X	319	Q6L	C12-C13	-2.87	1.45	1.51
2	V	301	CLA	CMB-C2B	-2.87	1.45	1.51
2	W	302	CLA	CHC-C1C	2.86	1.42	1.35
2	X	314	CLA	CHC-C1C	2.86	1.42	1.35
2	V	311	CLA	C4D-ND	-2.86	1.33	1.37
2	V	310	CLA	CMB-C2B	-2.85	1.45	1.51
5	W	316	Q6L	C12-C13	-2.83	1.45	1.51
4	W	308	KC2	C2A-C1A	2.83	1.53	1.44
2	W	310	CLA	C4D-ND	-2.81	1.33	1.37
4	W	308	KC2	CMC-C2C	-2.81	1.44	1.50
2	X	313	CLA	CMB-C2B	-2.80	1.45	1.51
2	X	310	CLA	C4D-ND	-2.77	1.33	1.37
2	X	312	CLA	CHC-C1C	2.77	1.42	1.35
6	V	318	IWJ	C04-C03	2.77	1.54	1.50
3	W	305	CHL	CHC-C1C	2.76	1.42	1.35
2	W	312	CLA	C1D-ND	2.76	1.41	1.37
2	V	302	CLA	CMB-C2B	-2.76	1.45	1.51
3	X	305	CHL	C1D-ND	2.76	1.41	1.37
3	W	307	CHL	C4D-ND	-2.74	1.33	1.37
5	V	321	Q6L	C12-C13	-2.74	1.45	1.51
3	X	307	CHL	C4D-ND	-2.74	1.33	1.37
5	W	315	Q6L	C12-C13	-2.73	1.45	1.51
5	W	320	Q6L	C34-C33	2.73	1.54	1.50
5	W	320	Q6L	C12-C13	-2.73	1.45	1.51
6	V	317	IWJ	C04-C03	2.72	1.54	1.50
5	V	316	Q6L	C34-C33	2.71	1.54	1.50
5	X	301	Q6L	C33-C32	2.71	1.36	1.33
2	X	314	CLA	CMB-C2B	-2.71	1.46	1.51
5	W	319	Q6L	C12-C13	-2.70	1.45	1.51
2	X	311	CLA	CMB-C2B	-2.70	1.46	1.51
2	W	303	CLA	CHC-C1C	2.69	1.41	1.35
2	W	302	CLA	C3B-C2B	-2.69	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	316	Q6L	C34-C33	2.68	1.54	1.50
6	W	318	IWJ	C04-C03	2.68	1.54	1.50
3	W	305	CHL	CMD-C2D	-2.67	1.45	1.50
5	X	301	Q6L	C34-C33	2.67	1.54	1.50
2	X	310	CLA	CMB-C2B	-2.67	1.46	1.51
3	V	305	CHL	CMD-C2D	-2.67	1.45	1.50
2	W	312	CLA	CMB-C2B	-2.67	1.46	1.51
5	V	319	Q6L	C12-C13	-2.66	1.45	1.51
2	V	312	CLA	CMD-C2D	-2.66	1.45	1.50
5	X	316	Q6L	C02-C03	2.66	1.37	1.34
5	X	317	Q6L	C02-C03	2.65	1.37	1.34
2	V	310	CLA	C4B-CHC	-2.65	1.33	1.41
4	X	309	KC2	CMC-C2C	-2.65	1.45	1.50
3	X	307	CHL	CMB-C2B	-2.64	1.46	1.51
2	W	311	CLA	CHC-C1C	2.64	1.41	1.35
4	X	309	KC2	C4B-NB	2.64	1.41	1.37
6	W	318	IWJ	C03-C02	2.63	1.36	1.33
2	W	309	CLA	C4D-ND	-2.62	1.34	1.37
2	X	312	CLA	CMB-C2B	-2.62	1.46	1.51
4	V	308	KC2	CMC-C2C	-2.62	1.45	1.50
5	X	317	Q6L	C34-C33	2.62	1.53	1.50
3	V	314	CHL	CMD-C2D	-2.61	1.45	1.50
2	V	302	CLA	C3B-C2B	-2.60	1.36	1.40
5	X	301	Q6L	C12-C13	-2.59	1.45	1.51
3	W	306	CHL	C1D-ND	2.58	1.41	1.37
5	W	319	Q6L	C34-C33	2.58	1.53	1.50
3	V	304	CHL	C3B-C2B	-2.58	1.36	1.40
2	V	311	CLA	CMB-C2B	-2.58	1.46	1.51
5	V	316	Q6L	C12-C13	-2.58	1.45	1.51
2	X	303	CLA	CHC-C1C	2.58	1.41	1.35
2	W	302	CLA	CMB-C2B	-2.58	1.46	1.51
2	V	303	CLA	C1D-ND	2.57	1.40	1.37
5	V	315	Q6L	C34-C33	2.57	1.53	1.50
5	W	316	Q6L	C02-C03	2.56	1.37	1.34
2	X	304	CLA	CHC-C1C	2.56	1.41	1.35
5	V	319	Q6L	C02-C03	2.55	1.37	1.34
2	W	309	CLA	CMB-C2B	-2.55	1.46	1.51
2	W	310	CLA	CMB-C2B	-2.55	1.46	1.51
6	W	318	IWJ	C29-C35	-2.54	1.52	1.56
2	W	313	CLA	CMB-C2B	-2.54	1.46	1.51
3	W	306	CHL	CHC-C1C	2.53	1.41	1.35
5	W	315	Q6L	C34-C33	2.53	1.53	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	304	CHL	C3B-CAB	-2.53	1.42	1.47
2	W	311	CLA	CMB-C2B	-2.52	1.46	1.51
2	X	310	CLA	CMD-C2D	-2.52	1.45	1.50
6	V	320	IWJ	C03-C02	2.52	1.36	1.33
3	X	315	CHL	CMB-C2B	-2.52	1.46	1.51
6	X	318	IWJ	C29-C35	-2.52	1.52	1.56
6	V	318	IWJ	C03-C02	2.51	1.36	1.33
3	W	306	CHL	CMB-C2B	-2.51	1.46	1.51
3	W	304	CHL	CMB-C2B	-2.51	1.46	1.51
4	V	308	KC2	O2A-CGA	2.50	1.36	1.30
4	V	308	KC2	CHD-C4C	2.50	1.41	1.35
4	X	309	KC2	CMB-C2B	-2.49	1.45	1.50
5	X	319	Q6L	C02-C03	2.49	1.37	1.34
5	V	321	Q6L	C34-C33	2.48	1.53	1.50
5	W	320	Q6L	C02-C03	2.48	1.37	1.34
3	W	306	CHL	CAC-C3C	-2.48	1.44	1.51
3	X	307	CHL	CHC-C1C	2.48	1.41	1.35
3	X	307	CHL	C4B-CHC	-2.48	1.34	1.41
5	V	315	Q6L	C11-C03	-2.48	1.47	1.51
5	V	315	Q6L	C02-C03	2.47	1.37	1.34
5	W	315	Q6L	C02-C03	2.47	1.37	1.34
2	X	302	CLA	C3B-C2B	-2.47	1.36	1.40
5	V	316	Q6L	C02-C03	2.46	1.37	1.34
2	X	302	CLA	CMB-C2B	-2.46	1.46	1.51
3	X	305	CHL	CMB-C2B	-2.46	1.46	1.51
3	W	314	CHL	CMD-C2D	-2.46	1.45	1.50
2	V	313	CLA	CMB-C2B	-2.45	1.46	1.51
2	V	309	CLA	C1A-CHA	-2.45	1.32	1.43
5	X	316	Q6L	C12-C13	-2.44	1.46	1.51
5	X	319	Q6L	C33-C32	2.43	1.36	1.33
6	X	318	IWJ	C03-C02	2.43	1.36	1.33
2	V	312	CLA	C3B-C2B	-2.43	1.37	1.40
2	W	301	CLA	C3B-C2B	-2.43	1.37	1.40
2	W	309	CLA	C3B-C2B	-2.42	1.37	1.40
5	V	316	Q6L	C33-C32	2.42	1.36	1.33
2	X	303	CLA	CMB-C2B	-2.41	1.46	1.51
2	V	302	CLA	C4B-CHC	-2.41	1.34	1.41
4	W	308	KC2	C4D-ND	-2.41	1.33	1.35
2	V	309	CLA	C1C-C2C	2.41	1.49	1.44
4	X	309	KC2	C1B-NB	-2.40	1.34	1.37
5	V	315	Q6L	C01-C02	2.39	1.54	1.50
5	X	301	Q6L	C02-C03	2.39	1.37	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	307	CHL	CMB-C2B	-2.39	1.46	1.51
2	V	302	CLA	CHC-C1C	2.39	1.41	1.35
3	V	306	CHL	CMB-C2B	-2.38	1.46	1.51
5	W	319	Q6L	C01-C02	2.38	1.54	1.50
4	X	309	KC2	O2A-CGA	2.38	1.36	1.30
2	W	312	CLA	C4B-CHC	-2.37	1.34	1.41
5	V	316	Q6L	C29-C27	2.37	1.51	1.45
2	X	312	CLA	C3B-C2B	-2.37	1.37	1.40
4	W	308	KC2	O2A-CGA	2.37	1.36	1.30
5	V	321	Q6L	C02-C03	2.37	1.37	1.34
5	X	317	Q6L	C12-C13	-2.36	1.46	1.51
2	X	303	CLA	C3B-CAB	-2.35	1.43	1.47
5	W	316	Q6L	C33-C32	2.35	1.36	1.33
2	X	314	CLA	C3B-C2B	-2.35	1.37	1.40
2	V	309	CLA	CMB-C2B	-2.34	1.46	1.51
5	X	301	Q6L	C01-C02	2.32	1.54	1.50
3	V	305	CHL	CMB-C2B	-2.32	1.46	1.51
5	W	319	Q6L	C02-C03	2.32	1.37	1.34
2	W	303	CLA	O2D-CED	-2.32	1.39	1.45
4	V	308	KC2	CAA-C2A	2.31	1.53	1.46
3	W	305	CHL	CMB-C2B	-2.31	1.46	1.51
2	V	301	CLA	CHC-C1C	2.30	1.40	1.35
5	V	319	Q6L	C01-C02	2.29	1.54	1.50
5	X	316	Q6L	C01-C02	2.28	1.54	1.50
2	V	310	CLA	CHC-C1C	2.27	1.40	1.35
4	W	308	KC2	CMB-C2B	-2.27	1.46	1.50
2	W	303	CLA	C3B-C2B	-2.27	1.37	1.40
3	X	307	CHL	CAC-C3C	-2.26	1.45	1.51
3	V	314	CHL	MG-ND	-2.26	2.01	2.05
5	W	316	Q6L	C01-C02	2.25	1.54	1.50
5	W	319	Q6L	C33-C32	2.25	1.35	1.33
3	W	314	CHL	CMB-C2B	-2.25	1.47	1.51
3	V	304	CHL	CMB-C2B	-2.25	1.47	1.51
2	W	301	CLA	CMC-C2C	-2.24	1.46	1.50
2	V	309	CLA	CMD-C2D	-2.24	1.46	1.50
6	V	320	IWJ	C29-C35	-2.23	1.53	1.56
2	V	303	CLA	C3B-CAB	-2.23	1.43	1.47
4	V	308	KC2	MG-NC	2.23	2.11	2.06
2	W	312	CLA	CHC-C1C	2.23	1.40	1.35
2	V	313	CLA	C3B-C2B	-2.23	1.37	1.40
2	X	302	CLA	CMD-C2D	-2.22	1.46	1.50
2	V	311	CLA	C3B-C2B	-2.22	1.37	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	314	CHL	CMB-C2B	-2.22	1.47	1.51
3	V	306	CHL	CMD-C2D	-2.22	1.46	1.50
6	V	317	IWJ	C03-C02	2.22	1.35	1.33
7	W	317	NEX	C35-C15	-2.21	1.30	1.36
3	X	315	CHL	CMD-C2D	-2.21	1.46	1.50
2	X	304	CLA	C4B-CHC	-2.21	1.34	1.41
3	W	307	CHL	CMD-C2D	-2.20	1.46	1.50
2	W	302	CLA	C4B-CHC	-2.20	1.34	1.41
3	X	307	CHL	CMD-C2D	-2.20	1.46	1.50
4	V	308	KC2	CMB-C2B	-2.20	1.46	1.50
3	W	306	CHL	CMD-C2D	-2.19	1.46	1.50
4	X	309	KC2	MG-NB	-2.19	2.01	2.05
2	X	312	CLA	C4B-CHC	-2.18	1.34	1.41
5	W	320	Q6L	C01-C02	2.18	1.54	1.50
4	X	309	KC2	C4D-ND	-2.18	1.33	1.35
2	W	301	CLA	C3B-CAB	-2.18	1.43	1.47
5	X	317	Q6L	C01-C02	2.18	1.54	1.50
3	X	308	CHL	CMB-C2B	-2.18	1.47	1.51
2	V	312	CLA	C4B-CHC	-2.18	1.34	1.41
2	V	302	CLA	C3B-CAB	-2.18	1.43	1.47
6	V	318	IWJ	C29-C35	-2.17	1.53	1.56
2	V	309	CLA	C1B-NB	2.17	1.37	1.35
5	W	315	Q6L	C01-C02	2.17	1.54	1.50
3	W	306	CHL	MG-ND	-2.16	2.01	2.05
2	W	312	CLA	MG-NC	2.16	2.11	2.06
2	X	302	CLA	CMC-C2C	-2.16	1.46	1.50
5	V	321	Q6L	C01-C02	2.16	1.54	1.50
2	W	301	CLA	CMB-C2B	-2.15	1.47	1.51
3	V	304	CHL	CMD-C2D	-2.15	1.46	1.50
3	V	307	CHL	CMB-C2B	-2.15	1.47	1.51
2	W	303	CLA	CMD-C2D	-2.15	1.46	1.50
5	V	319	Q6L	C33-C32	2.14	1.35	1.33
6	X	318	IWJ	O39-C29	-2.14	1.39	1.43
2	X	313	CLA	CMC-C2C	-2.14	1.46	1.50
3	X	308	CHL	CMD-C2D	-2.14	1.46	1.50
3	V	305	CHL	MG-ND	-2.13	2.01	2.05
4	X	309	KC2	MG-NA	2.13	2.11	2.06
3	X	306	CHL	CMB-C2B	-2.13	1.47	1.51
2	X	303	CLA	C4B-CHC	-2.13	1.35	1.41
4	W	308	KC2	MG-NB	-2.13	2.01	2.05
6	X	318	IWJ	C26-C24	-2.13	1.45	1.49
4	W	308	KC2	MG-NA	2.12	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	W	317	NEX	O24-C25	-2.12	1.43	1.46
2	X	313	CLA	C3B-C2B	-2.11	1.37	1.40
3	X	306	CHL	CMD-C2D	-2.11	1.46	1.50
2	V	303	CLA	CMC-C2C	-2.11	1.46	1.50
3	V	306	CHL	MG-ND	-2.10	2.01	2.05
5	W	316	Q6L	C29-C27	2.09	1.50	1.45
4	W	308	KC2	MG-NC	2.08	2.11	2.06
2	X	312	CLA	CMD-C2D	-2.08	1.46	1.50
4	X	309	KC2	MG-NC	2.08	2.11	2.06
5	X	317	Q6L	C33-C32	2.07	1.35	1.33
2	W	302	CLA	C3B-CAB	-2.06	1.43	1.47
2	V	310	CLA	C3B-CAB	-2.06	1.43	1.47
2	V	313	CLA	C4B-CHC	-2.05	1.35	1.41
2	W	310	CLA	C3B-C2B	-2.05	1.37	1.40
5	W	316	Q6L	C11-C03	-2.05	1.48	1.51
2	W	311	CLA	C4B-CHC	-2.05	1.35	1.41
6	X	318	IWJ	C32-C30	2.05	1.55	1.51
2	X	311	CLA	C3B-C2B	-2.05	1.37	1.40
2	X	314	CLA	C4B-CHC	-2.04	1.35	1.41
5	V	321	Q6L	C33-C32	2.04	1.35	1.33
2	V	311	CLA	C4B-CHC	-2.04	1.35	1.41
2	X	311	CLA	C4B-CHC	-2.04	1.35	1.41
2	V	309	CLA	C4D-ND	-2.04	1.34	1.37
2	X	302	CLA	CMA-C3A	-2.04	1.48	1.53
7	W	317	NEX	C22-C21	-2.03	1.51	1.54
4	W	308	KC2	C1A-NA	2.03	1.42	1.38
5	W	315	Q6L	C33-C32	2.03	1.35	1.33
5	W	320	Q6L	C33-C32	2.03	1.35	1.33
2	V	302	CLA	MG-NC	2.02	2.11	2.06
6	V	320	IWJ	C32-C30	2.02	1.55	1.51
2	W	301	CLA	CMD-C2D	-2.02	1.46	1.50
2	W	313	CLA	C3B-C2B	-2.01	1.37	1.40
3	X	307	CHL	O2A-CGA	2.01	1.39	1.33
2	X	310	CLA	C3B-C2B	-2.01	1.37	1.40
2	V	312	CLA	MG-ND	-2.01	2.01	2.05
3	X	307	CHL	C4C-C3C	2.01	1.48	1.45
2	X	313	CLA	CMD-C2D	-2.01	1.46	1.50
2	X	304	CLA	C3B-CAB	-2.01	1.43	1.47

All (553) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	317	NEX	O24-C25-C24	13.18	123.28	113.38
4	X	309	KC2	CMA-C3A-C4A	-8.51	112.08	125.04
3	X	307	CHL	C4A-NA-C1A	7.68	110.16	106.71
4	W	308	KC2	C1A-C2A-C3A	-7.54	101.13	107.11
3	X	307	CHL	OMC-CMC-C2C	-7.18	109.46	125.69
5	W	320	Q6L	C11-C12-C13	6.89	132.26	112.69
3	W	314	CHL	CMB-C2B-C1B	-6.79	118.03	128.46
4	X	309	KC2	C1A-NA-C4A	6.72	109.73	106.71
5	X	319	Q6L	C11-C12-C13	6.72	131.77	112.69
5	V	316	Q6L	C11-C12-C13	6.53	131.23	112.69
5	V	319	Q6L	C11-C12-C13	6.45	131.02	112.69
5	V	321	Q6L	C11-C12-C13	6.44	130.98	112.69
2	V	301	CLA	CMB-C2B-C1B	-6.40	118.63	128.46
2	X	312	CLA	C4A-NA-C1A	6.37	109.57	106.71
3	W	306	CHL	C4A-NA-C1A	6.32	109.55	106.71
3	X	308	CHL	CMB-C2B-C1B	-6.32	118.75	128.46
2	W	303	CLA	CMB-C2B-C1B	-6.31	118.77	128.46
5	W	315	Q6L	C11-C12-C13	6.18	130.25	112.69
4	V	308	KC2	C1A-C2A-C3A	-6.09	102.28	107.11
3	W	305	CHL	C4A-NA-C1A	6.01	109.41	106.71
2	W	312	CLA	C4A-NA-C1A	5.98	109.39	106.71
2	X	304	CLA	CMB-C2B-C1B	-5.95	119.33	128.46
4	W	308	KC2	C1A-NA-C4A	5.92	109.37	106.71
3	W	306	CHL	CMB-C2B-C1B	-5.88	119.42	128.46
5	X	301	Q6L	C11-C12-C13	5.87	129.37	112.69
3	W	307	CHL	CMB-C2B-C1B	-5.85	119.48	128.46
2	V	309	CLA	CMC-C2C-C1C	5.73	133.77	125.04
4	X	309	KC2	CMD-C2D-C1D	-5.69	119.72	128.46
2	V	303	CLA	CMB-C2B-C1B	-5.60	119.86	128.46
2	V	303	CLA	CAC-C3C-C4C	5.53	131.98	124.81
3	V	306	CHL	CMB-C2B-C1B	-5.49	120.03	128.46
5	X	316	Q6L	C11-C12-C13	5.49	128.28	112.69
2	X	314	CLA	C4A-NA-C1A	5.45	109.16	106.71
3	V	314	CHL	CMB-C2B-C1B	-5.37	120.21	128.46
3	V	306	CHL	C4A-NA-C1A	5.35	109.11	106.71
7	W	317	NEX	C26-C27-C28	-5.31	114.76	125.99
4	W	308	KC2	CMA-C3A-C2A	-5.22	115.52	128.30
2	W	311	CLA	C4A-NA-C1A	5.21	109.05	106.71
2	V	311	CLA	C4A-NA-C1A	5.14	109.02	106.71
3	W	306	CHL	C2C-C3C-C4C	5.11	110.13	106.49
5	X	317	Q6L	C11-C12-C13	5.06	127.06	112.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	301	CLA	CMB-C2B-C3B	5.05	134.12	124.68
3	W	314	CHL	CMB-C2B-C3B	5.04	134.12	124.68
2	W	312	CLA	CMB-C2B-C1B	-5.04	120.72	128.46
2	V	312	CLA	C4A-NA-C1A	5.03	108.97	106.71
5	W	316	Q6L	C11-C12-C13	5.03	126.98	112.69
4	V	308	KC2	CMA-C3A-C2A	-5.03	115.99	128.30
2	W	303	CLA	CMB-C2B-C3B	5.02	134.08	124.68
3	X	306	CHL	CMB-C2B-C1B	-5.01	120.76	128.46
2	W	309	CLA	O2D-CGD-O1D	-5.00	114.07	123.84
4	X	309	KC2	CMA-C3A-C2A	-4.93	116.24	128.30
3	V	305	CHL	CMB-C2B-C1B	-4.90	120.94	128.46
2	W	301	CLA	C4A-NA-C1A	4.83	108.88	106.71
5	V	321	Q6L	C40-C32-C33	-4.82	113.25	123.56
3	X	308	CHL	CMB-C2B-C3B	4.74	133.54	124.68
2	V	313	CLA	C4A-NA-C1A	4.74	108.83	106.71
3	V	305	CHL	C4A-NA-C1A	4.70	108.82	106.71
3	X	306	CHL	CMA-C3A-C2A	-4.68	105.17	116.10
2	V	303	CLA	CMB-C2B-C3B	4.67	133.42	124.68
2	W	311	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
5	V	315	Q6L	C11-C12-C13	4.66	125.93	112.69
5	X	301	Q6L	C40-C32-C33	-4.66	113.60	123.56
3	W	305	CHL	CMB-C2B-C1B	-4.64	121.33	128.46
5	W	319	Q6L	C11-C12-C13	4.60	125.76	112.69
5	W	316	Q6L	C40-C32-C33	-4.57	113.78	123.56
2	W	313	CLA	C4A-NA-C1A	4.53	108.74	106.71
4	W	308	KC2	CMA-C3A-C4A	-4.49	118.19	125.04
2	X	313	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
4	X	309	KC2	C1A-C2A-C3A	-4.43	103.59	107.11
4	V	308	KC2	CMD-C2D-C1D	-4.43	121.65	128.46
2	X	313	CLA	C4A-NA-C1A	4.43	108.70	106.71
5	W	320	Q6L	C40-C32-C33	-4.42	114.10	123.56
3	X	307	CHL	CHB-C4A-NA	4.40	130.59	124.51
2	V	309	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
3	X	307	CHL	C2C-C3C-C4C	4.37	109.61	106.49
2	X	304	CLA	CMB-C2B-C3B	4.36	132.83	124.68
6	V	317	IWJ	C01-C02-C03	-4.33	114.29	123.56
3	X	306	CHL	CMA-C3A-C4A	4.33	123.42	111.77
3	W	304	CHL	C4A-NA-C1A	4.33	108.65	106.71
3	X	307	CHL	C1-O2A-CGA	4.32	127.79	116.44
4	V	308	KC2	C2A-C3A-C4A	-4.32	103.28	106.49
5	V	316	Q6L	C40-C32-C33	-4.32	114.32	123.56
2	V	309	CLA	C1D-ND-C4D	-4.28	103.30	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	310	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
3	W	306	CHL	CMB-C2B-C3B	4.25	132.64	124.68
3	W	307	CHL	CMB-C2B-C3B	4.23	132.59	124.68
6	W	318	IWJ	C01-C02-C03	-4.22	114.54	123.56
6	V	320	IWJ	C01-C02-C03	-4.20	114.56	123.56
6	V	318	IWJ	C01-C02-C03	-4.20	114.57	123.56
3	V	306	CHL	CMB-C2B-C3B	4.20	132.54	124.68
6	X	318	IWJ	C01-C02-C03	-4.19	114.59	123.56
2	V	309	CLA	CMB-C2B-C3B	4.18	132.50	124.68
4	X	309	KC2	C2A-C3A-C4A	-4.15	103.41	106.49
2	V	309	CLA	O2D-CGD-O1D	-4.14	115.74	123.84
2	W	301	CLA	C1B-CHB-C4A	-4.14	121.92	130.12
5	X	317	Q6L	C40-C32-C33	-4.13	114.72	123.56
2	V	301	CLA	C4A-NA-C1A	4.12	108.56	106.71
4	V	308	KC2	CMA-C3A-C4A	-4.11	118.78	125.04
3	W	306	CHL	C1C-C2C-C3C	-4.11	103.85	107.11
3	V	314	CHL	CMB-C2B-C3B	4.08	132.30	124.68
2	X	302	CLA	C1B-CHB-C4A	-4.05	122.09	130.12
3	V	306	CHL	C1B-CHB-C4A	-4.04	122.11	130.12
5	X	316	Q6L	C05-C04-C03	4.04	116.28	109.92
2	V	301	CLA	C4-C3-C5	4.04	122.06	115.27
2	W	311	CLA	CMB-C2B-C3B	4.03	132.22	124.68
3	X	307	CHL	CMB-C2B-C1B	-4.02	122.29	128.46
2	V	312	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
3	X	307	CHL	C1C-C2C-C3C	-3.99	103.94	107.11
5	X	319	Q6L	C05-C06-C07	3.98	115.75	110.30
3	V	305	CHL	CMB-C2B-C3B	3.98	132.12	124.68
4	X	309	KC2	CMD-C2D-C3D	3.97	132.11	124.68
5	V	316	Q6L	C38-C36-C31	-3.95	103.55	109.55
5	X	316	Q6L	C34-C33-C32	-3.94	121.07	124.85
3	W	304	CHL	CMB-C2B-C1B	-3.93	122.43	128.46
2	W	301	CLA	CHB-C4A-NA	3.92	129.94	124.51
2	W	310	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
2	X	311	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
2	W	312	CLA	CMB-C2B-C3B	3.90	131.97	124.68
7	W	317	NEX	C38-C25-C26	-3.88	115.77	122.26
2	V	301	CLA	C1B-CHB-C4A	-3.87	122.45	130.12
2	W	309	CLA	O2D-CGD-CBD	3.87	118.14	111.27
5	W	319	Q6L	C40-C32-C33	-3.86	115.30	123.56
2	W	313	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
2	W	310	CLA	C4A-NA-C1A	3.85	108.44	106.71
4	W	308	KC2	CMD-C2D-C1D	-3.85	122.55	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	307	CHL	C3C-C4C-NC	-3.81	106.30	110.57
5	W	315	Q6L	C40-C32-C33	-3.81	115.41	123.56
2	W	309	CLA	C4-C3-C5	3.80	121.67	115.27
3	V	304	CHL	C1B-CHB-C4A	-3.80	122.59	130.12
5	W	320	Q6L	C38-C36-C35	-3.79	102.26	109.44
3	X	306	CHL	CMB-C2B-C3B	3.78	131.75	124.68
3	V	314	CHL	C1B-CHB-C4A	-3.77	122.65	130.12
3	X	315	CHL	CMB-C2B-C1B	-3.77	122.67	128.46
3	V	307	CHL	C4A-NA-C1A	3.76	108.40	106.71
6	X	318	IWJ	C16-C15-C14	-3.75	121.96	127.31
3	W	306	CHL	C3C-C4C-NC	-3.73	106.39	110.57
5	X	319	Q6L	C40-C32-C33	-3.72	115.61	123.56
7	W	317	NEX	C39-C29-C30	-3.69	117.75	122.92
5	V	315	Q6L	C40-C32-C33	-3.68	115.68	123.56
4	V	308	KC2	CBA-CAA-C2A	-3.67	111.26	125.27
3	W	307	CHL	C4A-NA-C1A	3.65	108.35	106.71
5	X	317	Q6L	C19-C18-C17	-3.63	122.13	127.31
4	V	308	KC2	O2D-CGD-O1D	-3.63	116.74	123.84
2	X	313	CLA	CMB-C2B-C3B	3.58	131.37	124.68
2	X	304	CLA	C4A-NA-C1A	3.57	108.31	106.71
2	X	310	CLA	CMB-C2B-C3B	3.55	131.31	124.68
2	W	309	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
4	X	309	KC2	O2D-CGD-O1D	-3.54	116.92	123.84
3	X	305	CHL	C1B-CHB-C4A	-3.54	123.11	130.12
7	W	317	NEX	C28-C29-C30	3.53	124.36	118.94
3	W	306	CHL	C1B-CHB-C4A	-3.52	123.14	130.12
3	X	307	CHL	O2D-CGD-O1D	-3.52	116.95	123.84
4	V	308	KC2	C3A-C4A-NA	3.48	114.37	110.57
2	V	311	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
2	W	309	CLA	C4A-NA-C1A	3.46	108.26	106.71
3	X	308	CHL	C4A-NA-C1A	3.44	108.25	106.71
3	X	315	CHL	C1B-CHB-C4A	-3.43	123.32	130.12
3	X	307	CHL	CAA-C2A-C3A	3.43	122.17	112.78
2	V	309	CLA	C1B-CHB-C4A	-3.42	123.33	130.12
3	W	304	CHL	C1B-CHB-C4A	-3.42	123.34	130.12
2	X	302	CLA	C4A-NA-C1A	3.40	108.23	106.71
4	V	308	KC2	O2D-CGD-CBD	3.40	117.30	111.27
2	W	302	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
2	V	302	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
2	X	312	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
2	W	302	CLA	C4A-NA-C1A	3.37	108.22	106.71
3	X	305	CHL	CMB-C2B-C1B	-3.37	123.28	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	307	CHL	O2D-CGD-CBD	3.37	117.25	111.27
3	X	307	CHL	C1B-CHB-C4A	-3.37	123.45	130.12
5	X	316	Q6L	C25-C26-C27	3.36	132.10	127.31
4	W	308	KC2	O2D-CGD-O1D	-3.36	117.28	123.84
3	V	307	CHL	CHB-C4A-NA	3.35	129.15	124.51
2	V	309	CLA	O2D-CGD-CBD	3.34	117.20	111.27
2	X	310	CLA	C4A-NA-C1A	3.34	108.21	106.71
2	W	303	CLA	C1B-CHB-C4A	-3.34	123.51	130.12
2	W	302	CLA	C1B-CHB-C4A	-3.33	123.51	130.12
3	W	306	CHL	CHB-C4A-NA	3.32	129.11	124.51
2	X	310	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
5	W	320	Q6L	C35-C34-C33	3.31	115.51	111.74
2	W	310	CLA	CMB-C2B-C3B	3.29	130.84	124.68
3	X	307	CHL	C2D-C1D-ND	-3.29	107.68	110.10
2	X	303	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
3	W	304	CHL	O2D-CGD-O1D	-3.28	117.43	123.84
2	V	310	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
2	X	311	CLA	CMB-C2B-C3B	3.25	130.76	124.68
4	V	308	KC2	CHB-C4A-C3A	-3.25	119.90	124.98
2	V	302	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
7	W	317	NEX	C15-C35-C34	-3.23	116.85	123.47
2	X	311	CLA	C4A-NA-C1A	3.23	108.16	106.71
2	V	301	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
2	W	303	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
3	V	306	CHL	O2D-CGD-O1D	-3.21	117.56	123.84
2	X	302	CLA	CMB-C2B-C3B	3.21	130.68	124.68
2	W	312	CLA	C1D-ND-C4D	-3.21	104.06	106.33
3	V	304	CHL	CHB-C4A-NA	3.20	128.94	124.51
2	X	314	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
2	V	302	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
2	V	312	CLA	C1B-CHB-C4A	-3.18	123.83	130.12
2	W	309	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
2	V	309	CLA	C3A-C2A-C1A	-3.17	96.59	101.34
2	V	309	CLA	CHD-C1D-ND	-3.16	121.55	124.45
3	V	305	CHL	C1B-CHB-C4A	-3.16	123.86	130.12
3	W	306	CHL	O2D-CGD-O1D	-3.16	117.67	123.84
3	X	307	CHL	CHD-C4C-C3C	3.16	129.48	124.84
3	W	314	CHL	C4A-NA-C1A	3.15	108.12	106.71
2	W	313	CLA	CMB-C2B-C3B	3.14	130.56	124.68
3	W	314	CHL	C1B-CHB-C4A	-3.14	123.91	130.12
2	V	312	CLA	O2A-CGA-O1A	-3.13	115.69	123.59
3	X	306	CHL	O2D-CGD-O1D	-3.10	117.78	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	314	CHL	C4A-NA-C1A	3.10	108.10	106.71
2	V	310	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
3	W	305	CHL	CMB-C2B-C3B	3.08	130.44	124.68
5	X	319	Q6L	C42-C13-C12	3.08	120.45	115.27
4	W	308	KC2	C3C-C2C-C1C	3.08	108.77	106.49
2	X	302	CLA	C4D-CHA-C1A	3.08	124.99	121.25
2	X	310	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
2	W	301	CLA	CMB-C2B-C3B	3.07	130.43	124.68
2	X	312	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
3	W	314	CHL	CBD-CHA-C1A	3.07	132.12	128.50
5	V	319	Q6L	C28-C27-C26	3.06	127.21	122.92
2	V	302	CLA	C1-C2-C3	-3.06	121.80	126.75
2	V	311	CLA	CMB-C2B-C3B	3.06	130.40	124.68
2	V	303	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
3	X	307	CHL	CAC-C3C-C4C	3.06	128.78	124.81
2	V	303	CLA	CAC-C3C-C2C	-3.05	122.31	127.53
2	V	312	CLA	CMB-C2B-C3B	3.04	130.37	124.68
3	X	307	CHL	O2A-CGA-O1A	-3.04	115.92	123.59
2	X	304	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
3	X	308	CHL	C1B-CHB-C4A	-3.03	124.11	130.12
3	V	304	CHL	CMB-C2B-C1B	-3.02	123.82	128.46
2	W	312	CLA	CAC-C3C-C4C	3.02	128.72	124.81
2	V	301	CLA	CAA-C2A-C1A	-3.02	102.09	111.97
2	V	313	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
4	W	308	KC2	CMD-C2D-C3D	3.01	130.31	124.68
2	W	303	CLA	C1-C2-C3	-3.00	121.89	126.75
4	X	309	KC2	CAA-C2A-C1A	-3.00	110.96	124.75
3	W	305	CHL	C1C-C2C-C3C	-3.00	104.73	107.11
2	W	309	CLA	CMB-C2B-C3B	3.00	130.29	124.68
2	V	302	CLA	C4A-NA-C1A	2.99	108.05	106.71
3	V	305	CHL	CHB-C4A-NA	2.98	128.64	124.51
2	W	310	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
5	V	319	Q6L	C26-C25-C24	-2.97	113.94	123.22
3	V	307	CHL	C2C-C3C-C4C	2.96	108.60	106.49
2	W	312	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
2	V	311	CLA	CHB-C4A-NA	2.95	128.59	124.51
2	X	303	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
2	V	303	CLA	CHD-C1D-ND	-2.94	121.75	124.45
4	W	308	KC2	CAC-C3C-C2C	-2.93	118.96	128.60
2	V	311	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
7	W	317	NEX	C16-C1-C6	2.92	113.09	110.47
5	X	319	Q6L	C12-C13-C14	-2.92	113.14	121.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	304	CHL	O2A-CGA-O1A	-2.91	116.06	123.30
3	X	306	CHL	C4A-NA-C1A	2.90	108.01	106.71
2	V	303	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
5	V	319	Q6L	C40-C32-C33	-2.90	117.36	123.56
3	V	305	CHL	O2D-CGD-O1D	-2.89	118.18	123.84
2	X	313	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
4	W	308	KC2	CBA-CAA-C2A	-2.89	114.25	125.27
5	W	320	Q6L	C01-C02-C07	-2.89	109.00	114.36
5	X	301	Q6L	C19-C18-C17	-2.89	123.19	127.31
2	W	302	CLA	CMB-C2B-C3B	2.88	130.07	124.68
4	W	308	KC2	CMC-C2C-C1C	2.88	129.43	125.04
3	V	307	CHL	C1B-CHB-C4A	-2.88	124.42	130.12
3	X	307	CHL	CMB-C2B-C3B	2.88	130.06	124.68
3	V	304	CHL	CMB-C2B-C3B	2.87	130.05	124.68
7	W	317	NEX	C19-C9-C10	2.87	126.94	122.92
2	X	311	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
3	W	314	CHL	O2D-CGD-O1D	-2.86	118.25	123.84
2	V	312	CLA	CHB-C4A-NA	2.86	128.46	124.51
3	W	307	CHL	CHB-C4A-NA	2.86	128.46	124.51
3	V	306	CHL	CHB-C4A-NA	2.86	128.46	124.51
5	V	319	Q6L	C29-C27-C26	-2.85	114.57	118.94
2	X	314	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
2	X	302	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
7	W	317	NEX	C15-C14-C13	-2.83	123.27	127.31
5	V	321	Q6L	C38-C36-C35	-2.83	104.08	109.44
2	V	313	CLA	CHD-C1D-ND	-2.82	121.86	124.45
4	X	309	KC2	CBD-CHA-C1A	2.82	134.14	128.88
3	V	305	CHL	C2D-C1D-ND	-2.82	108.03	110.10
3	X	308	CHL	O2D-CGD-O1D	-2.82	118.33	123.84
3	W	305	CHL	CHB-C4A-NA	2.80	128.38	124.51
4	V	308	KC2	CAC-C3C-C2C	-2.79	119.40	128.60
4	X	309	KC2	CBA-CAA-C2A	-2.79	114.62	125.27
3	X	308	CHL	C2A-C1A-CHA	2.79	128.74	123.86
2	W	313	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
5	X	319	Q6L	C35-C34-C33	2.79	114.92	111.74
5	X	301	Q6L	C19-C20-C21	-2.79	117.76	123.47
5	W	316	Q6L	C41-C17-C18	2.79	126.83	122.92
2	W	310	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
3	W	305	CHL	C2C-C3C-C4C	2.78	108.47	106.49
3	W	307	CHL	C1B-CHB-C4A	-2.78	124.61	130.12
5	X	317	Q6L	C19-C20-C21	-2.78	117.78	123.47
5	W	316	Q6L	C19-C20-C21	-2.78	117.78	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	311	CLA	CHB-C4A-NA	2.77	128.35	124.51
2	V	303	CLA	CHB-C4A-NA	2.77	128.34	124.51
3	V	314	CHL	O2D-CGD-O1D	-2.77	118.42	123.84
5	V	319	Q6L	C19-C20-C21	-2.77	117.80	123.47
2	V	302	CLA	O2D-CGD-CBD	2.77	116.18	111.27
2	X	313	CLA	CHB-C4A-NA	2.76	128.33	124.51
5	V	319	Q6L	C42-C13-C12	2.76	119.91	115.27
2	X	312	CLA	CMB-C2B-C3B	2.76	129.84	124.68
2	V	310	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
3	X	306	CHL	C1B-CHB-C4A	-2.75	124.66	130.12
3	V	307	CHL	C3C-C4C-NC	-2.75	107.49	110.57
2	V	313	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
3	X	307	CHL	O2A-CGA-CBA	2.74	120.51	111.91
2	V	313	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
2	W	303	CLA	CHD-C1D-ND	-2.74	121.94	124.45
3	W	305	CHL	C1B-CHB-C4A	-2.74	124.70	130.12
2	W	301	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
4	X	309	KC2	CAA-CBA-CGA	-2.73	113.23	127.26
2	X	311	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
2	X	314	CLA	CHD-C1D-ND	-2.73	121.95	124.45
2	V	302	CLA	CMB-C2B-C3B	2.72	129.76	124.68
2	W	302	CLA	CHB-C4A-NA	2.72	128.27	124.51
2	X	313	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
3	V	304	CHL	O2D-CGD-O1D	-2.71	118.54	123.84
4	W	308	KC2	CAA-CBA-CGA	-2.71	113.34	127.26
3	W	304	CHL	CHB-C4A-NA	2.71	128.26	124.51
6	V	318	IWJ	O27-C26-C28	-2.70	116.17	121.66
2	W	311	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
2	W	312	CLA	C4-C3-C5	2.70	119.82	115.27
3	V	306	CHL	C2D-C1D-ND	-2.70	108.11	110.10
4	V	308	KC2	CMD-C2D-C3D	2.70	129.73	124.68
2	W	303	CLA	CED-O2D-CGD	-2.69	109.84	115.94
5	W	319	Q6L	C05-C06-C07	2.69	113.99	110.30
2	W	310	CLA	CHB-C4A-NA	2.69	128.22	124.51
5	W	319	Q6L	C42-C13-C12	2.68	119.79	115.27
2	V	310	CLA	C4A-NA-C1A	2.68	107.91	106.71
4	V	308	KC2	O2A-CGA-O1A	-2.68	117.10	122.67
3	X	315	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
3	W	305	CHL	CMA-C3A-C2A	-2.67	109.87	116.10
2	W	302	CLA	CHD-C1D-ND	-2.66	122.01	124.45
2	X	303	CLA	CHD-C1D-ND	-2.66	122.01	124.45
4	W	308	KC2	CMC-C2C-C3C	-2.65	121.80	128.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	301	CLA	C4-C3-C5	2.65	119.73	115.27
2	W	312	CLA	CBC-CAC-C3C	2.65	119.74	112.43
6	W	318	IWJ	C21-C19-C18	-2.65	114.88	118.94
2	X	310	CLA	CHB-C4A-NA	2.65	128.18	124.51
3	V	306	CHL	O2D-CGD-CBD	2.65	115.97	111.27
5	W	315	Q6L	C42-C13-C12	2.65	119.72	115.27
4	X	309	KC2	CAC-C3C-C2C	-2.65	119.89	128.60
5	V	315	Q6L	C24-C22-C21	-2.64	114.90	118.94
2	W	312	CLA	CHB-C4A-NA	2.63	128.15	124.51
3	W	307	CHL	C4-C3-C2	-2.63	116.92	123.68
3	V	307	CHL	CHD-C1D-ND	-2.63	122.04	124.45
2	V	309	CLA	CHB-C4A-NA	2.63	128.15	124.51
3	V	314	CHL	C1D-CHD-C4C	-2.63	120.39	126.06
6	V	318	IWJ	C22-C21-C19	2.62	133.77	126.42
2	X	303	CLA	C4A-NA-C1A	2.62	107.88	106.71
2	W	309	CLA	CHB-C4A-NA	2.61	128.12	124.51
3	X	305	CHL	O2D-CGD-O1D	-2.61	118.74	123.84
3	W	307	CHL	C1-C2-C3	-2.60	121.54	126.04
2	V	310	CLA	CMB-C2B-C3B	2.60	129.54	124.68
2	X	302	CLA	CHB-C4A-NA	2.59	128.10	124.51
2	W	303	CLA	C4A-NA-C1A	2.59	107.87	106.71
3	X	306	CHL	CAA-C2A-C3A	-2.59	110.05	116.10
4	X	309	KC2	O1A-CGA-CBA	2.59	129.08	120.99
2	X	304	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
3	W	306	CHL	C1-C2-C3	-2.58	121.59	126.04
5	V	321	Q6L	C01-C02-C07	-2.57	109.59	114.36
5	W	315	Q6L	C12-C13-C14	-2.57	114.19	121.98
5	X	319	Q6L	C01-C02-C07	-2.57	109.59	114.36
4	X	309	KC2	C4C-C3C-C2C	-2.56	105.08	107.11
2	V	311	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
7	W	317	NEX	C31-C30-C29	-2.55	123.66	127.31
4	W	308	KC2	O1A-CGA-CBA	2.55	128.97	120.99
2	W	312	CLA	C2C-C1C-NC	2.55	112.36	109.97
2	X	310	CLA	CHD-C1D-ND	-2.55	122.11	124.45
2	X	302	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
2	W	313	CLA	CHD-C1D-ND	-2.54	122.12	124.45
3	V	307	CHL	C1C-C2C-C3C	-2.54	105.10	107.11
2	V	309	CLA	CMC-C2C-C3C	-2.54	119.23	126.12
2	V	310	CLA	CHB-C4A-NA	2.53	128.02	124.51
3	X	305	CHL	CHD-C1D-ND	-2.53	122.12	124.45
5	V	315	Q6L	C35-C34-C33	2.53	114.62	111.74
3	X	305	CHL	C4A-NA-C1A	2.53	107.84	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	305	CHL	O2D-CGD-O1D	-2.52	118.91	123.84
2	V	301	CLA	CHB-C4A-NA	2.52	127.99	124.51
4	V	308	KC2	CAA-CBA-CGA	-2.51	114.36	127.26
5	V	315	Q6L	C19-C20-C21	-2.50	118.35	123.47
5	V	316	Q6L	C01-C02-C07	-2.50	109.72	114.36
4	X	309	KC2	O2D-CGD-CBD	2.50	115.71	111.27
2	X	312	CLA	CHB-C4A-NA	2.50	127.97	124.51
5	V	316	Q6L	C37-C36-C31	2.49	113.32	109.55
2	W	312	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
3	W	304	CHL	CMB-C2B-C3B	2.49	129.34	124.68
5	X	317	Q6L	C05-C06-C07	2.49	113.71	110.30
2	X	302	CLA	O1D-CGD-CBD	2.48	129.57	124.48
2	W	302	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
5	V	319	Q6L	C12-C13-C14	-2.48	114.48	121.98
6	W	318	IWJ	C17-C18-C19	2.47	130.84	127.31
2	X	314	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
3	V	307	CHL	O2D-CGD-O1D	-2.46	119.02	123.84
3	W	307	CHL	O2D-CGD-O1D	-2.45	119.05	123.84
2	V	311	CLA	C2A-C1A-CHA	2.44	128.13	123.86
5	V	319	Q6L	C24-C22-C21	-2.44	115.19	118.94
3	X	308	CHL	CHB-C4A-NA	2.44	127.89	124.51
2	X	312	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
6	V	318	IWJ	C36-C35-C34	-2.43	104.75	108.98
5	W	319	Q6L	C06-C07-C02	2.43	116.70	111.85
2	X	313	CLA	CAA-C2A-C3A	-2.43	110.43	116.10
2	X	314	CLA	CMB-C2B-C3B	2.43	129.22	124.68
2	V	312	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
7	W	317	NEX	C11-C10-C9	-2.43	123.85	127.31
4	W	308	KC2	CBD-CHA-C1A	2.41	133.38	128.88
3	V	306	CHL	C3C-C4C-NC	-2.41	107.87	110.57
5	W	319	Q6L	C12-C13-C14	-2.41	114.69	121.98
3	W	314	CHL	CHB-C4A-NA	2.40	127.84	124.51
4	W	308	KC2	CAC-C3C-C4C	2.40	135.66	124.47
4	W	308	KC2	C4C-C3C-C2C	-2.40	105.21	107.11
7	W	317	NEX	C32-C33-C34	-2.39	115.27	118.94
2	X	302	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
2	W	301	CLA	CHD-C1D-ND	-2.38	122.26	124.45
4	W	308	KC2	O2D-CGD-CBD	2.38	115.50	111.27
3	W	314	CHL	C2D-C1D-ND	-2.38	108.35	110.10
2	X	311	CLA	CHD-C1D-ND	-2.37	122.27	124.45
3	W	314	CHL	C2A-C1A-CHA	2.37	126.38	122.71
3	X	305	CHL	CHB-C4A-NA	2.37	127.78	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	308	KC2	O1A-CGA-CBA	2.36	128.37	120.99
2	V	313	CLA	CHB-C4A-NA	2.36	127.78	124.51
2	V	313	CLA	CMB-C2B-C3B	2.36	129.10	124.68
4	V	308	KC2	CAA-C2A-C1A	-2.36	113.90	124.75
3	W	306	CHL	CHD-C1D-ND	-2.35	122.29	124.45
3	W	306	CHL	CAA-C2A-C3A	2.35	119.22	112.78
3	X	315	CHL	CMB-C2B-C3B	2.35	129.08	124.68
2	V	310	CLA	C2C-C1C-NC	2.35	112.17	109.97
5	W	319	Q6L	C19-C20-C21	-2.35	118.66	123.47
5	V	319	Q6L	C16-C17-C18	-2.35	115.34	118.94
2	X	312	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
2	X	314	CLA	CHB-C4A-NA	2.34	127.75	124.51
4	V	308	KC2	OBD-CAD-CBD	-2.34	122.56	125.89
5	V	319	Q6L	C23-C22-C21	2.34	126.20	122.92
6	V	318	IWJ	C21-C19-C18	-2.33	115.36	118.94
2	X	302	CLA	CHD-C1D-ND	-2.33	122.31	124.45
3	W	304	CHL	CHD-C1D-ND	-2.33	122.31	124.45
2	X	303	CLA	CHB-C4A-NA	2.33	127.73	124.51
2	X	314	CLA	CAA-C2A-C3A	-2.33	110.67	116.10
2	X	310	CLA	O2D-CGD-CBD	2.32	115.39	111.27
2	W	311	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
6	W	318	IWJ	C25-C24-C26	2.32	119.92	116.02
3	X	315	CHL	CHB-C4A-NA	2.31	127.70	124.51
5	W	315	Q6L	C01-C02-C07	-2.30	110.09	114.36
2	V	301	CLA	C4-C3-C2	-2.30	117.78	123.68
3	W	306	CHL	O2D-CGD-CBD	2.29	115.34	111.27
2	W	310	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
2	W	310	CLA	CHD-C1D-ND	-2.28	122.36	124.45
5	X	316	Q6L	C29-C27-C26	-2.28	115.44	118.94
2	W	309	CLA	CHD-C1D-ND	-2.28	122.36	124.45
2	V	302	CLA	CAC-C3C-C4C	2.27	127.76	124.81
2	X	304	CLA	CHD-C1D-ND	-2.27	122.37	124.45
4	X	309	KC2	CAC-C3C-C4C	2.26	135.01	124.47
3	V	306	CHL	C2C-C3C-C4C	2.26	108.10	106.49
6	V	318	IWJ	C37-C35-C34	-2.26	105.06	108.98
2	W	301	CLA	O2A-C1-C2	-2.25	102.71	108.64
2	V	310	CLA	CHD-C1D-ND	-2.25	122.39	124.45
2	W	312	CLA	O2D-CGD-CBD	2.24	115.25	111.27
3	V	314	CHL	CHB-C4A-NA	2.24	127.61	124.51
2	X	312	CLA	C5-C3-C2	2.24	126.04	120.50
2	V	310	CLA	CAC-C3C-C4C	2.23	127.71	124.81
2	W	309	CLA	C6-C5-C3	2.23	119.31	113.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	313	CLA	CHD-C1D-ND	-2.23	122.40	124.45
2	V	302	CLA	CHB-C4A-NA	2.23	127.60	124.51
4	V	308	KC2	C2A-C1A-NA	2.22	112.97	109.40
5	X	316	Q6L	C28-C27-C26	2.22	126.03	122.92
6	W	318	IWJ	C32-C30-C31	2.21	125.47	121.10
2	V	309	CLA	C4A-NA-C1A	2.21	107.70	106.71
2	V	302	CLA	C2C-C1C-NC	2.21	112.04	109.97
6	W	318	IWJ	C36-C35-C34	-2.21	105.15	108.98
2	W	311	CLA	CHA-C1A-NA	-2.20	121.35	126.40
2	V	310	CLA	CMC-C2C-C1C	2.20	128.39	125.04
5	V	319	Q6L	C01-C02-C07	-2.20	110.28	114.36
6	V	318	IWJ	C23-C22-C21	-2.20	116.35	123.22
2	W	313	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
5	W	315	Q6L	C05-C06-C07	2.20	113.31	110.30
2	V	311	CLA	CHD-C1D-ND	-2.19	122.44	124.45
6	X	318	IWJ	C23-C22-C21	-2.19	116.37	123.22
2	V	301	CLA	CHD-C1D-ND	-2.19	122.44	124.45
2	W	302	CLA	CAC-C3C-C4C	2.18	127.64	124.81
2	X	303	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
2	V	311	CLA	C1-C2-C3	-2.17	122.29	126.04
4	W	308	KC2	O2A-CGA-O1A	-2.17	118.17	122.67
2	V	309	CLA	CAA-C2A-C3A	2.17	119.67	114.26
3	V	304	CHL	C4A-NA-C1A	2.16	107.68	106.71
3	V	314	CHL	C2D-C1D-ND	-2.16	108.51	110.10
4	X	309	KC2	C3C-C2C-C1C	2.16	108.09	106.49
2	V	311	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
4	W	308	KC2	CAA-C2A-C1A	-2.15	114.84	124.75
3	X	308	CHL	OMC-CMC-C2C	-2.15	120.82	125.69
2	W	312	CLA	C3A-C2A-C1A	2.15	104.56	101.34
3	V	314	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
3	W	307	CHL	CBA-CAA-C2A	2.14	120.19	113.86
5	V	315	Q6L	C05-C06-C07	2.14	113.23	110.30
2	X	304	CLA	CAC-C3C-C4C	2.14	127.58	124.81
2	W	303	CLA	C3A-C2A-C1A	2.14	104.54	101.34
2	X	304	CLA	CMA-C3A-C4A	-2.13	106.04	111.77
4	X	309	KC2	CHB-C4A-C3A	-2.13	121.65	124.98
2	X	302	CLA	CMC-C2C-C1C	2.13	128.29	125.04
3	X	305	CHL	CAA-C2A-C3A	-2.13	111.12	116.10
2	W	309	CLA	C2D-C1D-ND	-2.13	108.54	110.10
2	W	309	CLA	C1-C2-C3	-2.13	122.36	126.04
6	V	320	IWJ	C22-C21-C19	2.13	132.39	126.42
3	W	307	CHL	C5-C3-C2	2.12	125.42	121.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	311	CLA	C2A-C1A-CHA	2.12	127.57	123.86
4	V	308	KC2	CAC-C3C-C4C	2.12	134.35	124.47
2	V	312	CLA	O1D-CGD-CBD	2.12	128.82	124.48
2	W	303	CLA	CHB-C4A-NA	2.12	127.44	124.51
2	W	313	CLA	CHB-C4A-NA	2.12	127.44	124.51
2	W	301	CLA	CAA-C2A-C1A	-2.12	105.04	111.97
2	X	302	CLA	CHA-C1A-NA	-2.12	121.55	126.40
2	V	301	CLA	C4D-CHA-C1A	2.11	123.82	121.25
2	X	312	CLA	CHD-C1D-ND	-2.11	122.52	124.45
3	X	308	CHL	C2A-C3A-C4A	-2.11	98.47	101.87
6	V	318	IWJ	C34-C33-C32	2.10	113.18	110.30
3	X	305	CHL	CMB-C2B-C3B	2.10	128.61	124.68
6	X	318	IWJ	C25-C24-C26	2.10	119.55	116.02
2	V	309	CLA	C3D-C4D-ND	2.10	113.63	110.24
4	X	309	KC2	C1B-CHB-C4A	2.10	130.58	126.06
2	X	312	CLA	C2A-C1A-CHA	2.10	127.52	123.86
3	W	314	CHL	OMC-CMC-C2C	-2.10	120.95	125.69
2	V	313	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
2	X	313	CLA	CMA-C3A-C2A	-2.09	111.22	116.10
3	V	306	CHL	C2A-C1A-CHA	2.09	127.51	123.86
2	W	309	CLA	CAA-CBA-CGA	-2.08	107.16	113.25
2	V	311	CLA	CHA-C1A-NA	-2.08	121.63	126.40
5	W	315	Q6L	C19-C20-C21	-2.08	119.21	123.47
2	X	311	CLA	CHB-C4A-NA	2.07	127.38	124.51
2	X	312	CLA	C4-C3-C2	-2.07	118.38	123.68
3	W	306	CHL	CHD-C4C-C3C	2.06	127.87	124.84
7	W	317	NEX	C40-C33-C32	2.06	121.33	118.08
2	W	309	CLA	C5-C3-C2	-2.06	116.96	121.12
2	X	303	CLA	C2C-C1C-NC	2.05	111.89	109.97
2	X	302	CLA	C4-C3-C2	-2.05	118.42	123.68
6	X	318	IWJ	C36-C35-C34	-2.05	105.42	108.98
6	X	318	IWJ	C22-C23-C24	2.04	132.61	126.61
6	X	318	IWJ	C33-C32-C30	2.04	115.53	112.04
5	X	301	Q6L	C24-C22-C21	-2.04	115.82	118.94
2	X	304	CLA	O2D-CGD-CBD	2.03	114.88	111.27
3	V	307	CHL	CMB-C2B-C1B	-2.03	125.35	128.46
2	X	311	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
5	W	316	Q6L	C41-C17-C16	-2.02	114.89	118.08
6	V	317	IWJ	C33-C32-C30	2.02	115.49	112.04
2	V	312	CLA	CBA-CAA-C2A	2.02	119.82	113.86
2	V	302	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
3	V	306	CHL	C1D-CHD-C4C	-2.02	121.71	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	310	CLA	C2D-C1D-ND	-2.01	108.62	110.10
4	X	309	KC2	O2A-CGA-O1A	-2.01	118.50	122.67
3	V	314	CHL	CHA-C1A-NA	-2.00	121.81	126.40
3	X	308	CHL	O1D-CGD-CBD	2.00	128.59	124.48
2	W	303	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
5	W	316	Q6L	C29-C27-C26	-2.00	115.87	118.94
3	V	304	CHL	C2D-C1D-ND	-2.00	108.63	110.10
3	W	305	CHL	C3C-C4C-NC	-2.00	108.33	110.57

All (68) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	V	301	CLA	ND
2	V	302	CLA	ND
2	V	303	CLA	ND
2	V	309	CLA	ND
2	V	310	CLA	ND
2	V	311	CLA	ND
2	V	313	CLA	ND
2	W	301	CLA	ND
2	W	302	CLA	ND
2	W	303	CLA	ND
2	W	309	CLA	ND
2	W	310	CLA	ND
2	W	311	CLA	ND
2	W	312	CLA	ND
2	W	313	CLA	ND
2	X	302	CLA	ND
2	X	303	CLA	ND
2	X	304	CLA	ND
2	X	310	CLA	ND
2	X	311	CLA	ND
2	X	312	CLA	ND
2	X	313	CLA	ND
2	X	314	CLA	ND
3	V	304	CHL	NC
3	V	304	CHL	ND
3	V	304	CHL	NA
3	V	305	CHL	NC
3	V	305	CHL	ND
3	V	305	CHL	NA
3	V	306	CHL	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	V	306	CHL	ND
3	V	306	CHL	NA
3	V	307	CHL	NC
3	V	307	CHL	ND
3	V	307	CHL	NA
3	V	314	CHL	NC
3	V	314	CHL	ND
3	V	314	CHL	NA
3	W	304	CHL	NC
3	W	304	CHL	ND
3	W	304	CHL	NA
3	W	305	CHL	NC
3	W	305	CHL	ND
3	W	305	CHL	NA
3	W	306	CHL	NC
3	W	306	CHL	ND
3	W	306	CHL	NA
3	W	307	CHL	NC
3	W	307	CHL	ND
3	W	307	CHL	NA
3	W	314	CHL	NC
3	W	314	CHL	ND
3	W	314	CHL	NA
3	X	305	CHL	NC
3	X	305	CHL	ND
3	X	305	CHL	NA
3	X	306	CHL	NC
3	X	306	CHL	ND
3	X	306	CHL	NA
3	X	307	CHL	NC
3	X	307	CHL	ND
3	X	307	CHL	NA
3	X	308	CHL	NC
3	X	308	CHL	ND
3	X	308	CHL	NA
3	X	315	CHL	NC
3	X	315	CHL	ND
3	X	315	CHL	NA

All (372) torsion outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
-----	-------	-----	------	-------

Mol	Chain	Res	Type	Atoms
2	V	302	CLA	CHA-CBD-CGD-O1D
2	V	302	CLA	CHA-CBD-CGD-O2D
2	V	303	CLA	CBD-CGD-O2D-CED
2	V	312	CLA	C1A-C2A-CAA-CBA
2	V	312	CLA	C3A-C2A-CAA-CBA
2	V	312	CLA	CHA-CBD-CGD-O1D
2	V	312	CLA	CHA-CBD-CGD-O2D
2	W	301	CLA	C1A-C2A-CAA-CBA
2	X	303	CLA	C1A-C2A-CAA-CBA
2	X	303	CLA	C3A-C2A-CAA-CBA
2	X	304	CLA	CHA-CBD-CGD-O1D
2	X	304	CLA	CHA-CBD-CGD-O2D
2	X	311	CLA	C1A-C2A-CAA-CBA
2	X	311	CLA	C3A-C2A-CAA-CBA
2	X	311	CLA	CBD-CGD-O2D-CED
2	X	312	CLA	CBD-CGD-O2D-CED
2	X	313	CLA	CBD-CGD-O2D-CED
2	X	314	CLA	CHA-CBD-CGD-O1D
2	X	314	CLA	CHA-CBD-CGD-O2D
2	X	314	CLA	CAD-CBD-CGD-O1D
2	X	314	CLA	CBD-CGD-O2D-CED
3	V	304	CHL	CHA-CBD-CGD-O1D
3	V	304	CHL	CHA-CBD-CGD-O2D
3	V	304	CHL	CBD-CGD-O2D-CED
3	V	305	CHL	C3C-C2C-CMC-OMC
3	W	307	CHL	C1A-C2A-CAA-CBA
3	W	314	CHL	C3C-C2C-CMC-OMC
3	W	314	CHL	CHA-CBD-CGD-O1D
3	W	314	CHL	CHA-CBD-CGD-O2D
3	X	307	CHL	C3A-C2A-CAA-CBA
3	X	307	CHL	CBA-CGA-O2A-C1
3	X	307	CHL	O1A-CGA-O2A-C1
3	X	307	CHL	C1C-C2C-CMC-OMC
3	X	307	CHL	C3C-C2C-CMC-OMC
3	X	307	CHL	O2A-C1-C2-C3
3	X	308	CHL	C1A-C2A-CAA-CBA
3	X	308	CHL	CHA-CBD-CGD-O1D
3	X	308	CHL	CHA-CBD-CGD-O2D
3	X	308	CHL	CAD-CBD-CGD-O1D
3	X	308	CHL	CBD-CGD-O2D-CED
3	X	315	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	V	308	KC2	C3A-C2A-CAA-CBA
4	V	308	KC2	C2A-CAA-CBA-CGA
4	V	308	KC2	CHA-CBD-CGD-O1D
4	V	308	KC2	CHA-CBD-CGD-O2D
4	W	308	KC2	C3A-C2A-CAA-CBA
4	W	308	KC2	C2A-CAA-CBA-CGA
4	X	309	KC2	C1A-C2A-CAA-CBA
4	X	309	KC2	C3A-C2A-CAA-CBA
4	X	309	KC2	C2A-CAA-CBA-CGA
5	V	315	Q6L	C02-C03-C11-C12
5	V	315	Q6L	C21-C22-C24-C25
5	V	315	Q6L	C23-C22-C24-C25
5	V	315	Q6L	C29-C30-C31-C32
5	V	315	Q6L	C27-C29-C30-C31
5	V	315	Q6L	C15-C16-C17-C18
5	V	315	Q6L	C15-C16-C17-C41
5	V	316	Q6L	C04-C03-C11-C12
5	V	316	Q6L	C29-C30-C31-C36
5	V	316	Q6L	C29-C30-C31-C32
5	V	316	Q6L	C27-C29-C30-C31
5	V	316	Q6L	C19-C20-C21-C22
5	V	319	Q6L	C02-C03-C11-C12
5	V	319	Q6L	C28-C27-C29-C30
5	V	319	Q6L	C26-C27-C29-C30
5	V	321	Q6L	C04-C03-C11-C12
5	W	315	Q6L	C15-C16-C17-C18
5	W	315	Q6L	C15-C16-C17-C41
5	W	319	Q6L	C28-C27-C29-C30
5	W	319	Q6L	C26-C27-C29-C30
5	W	320	Q6L	C02-C03-C11-C12
5	W	320	Q6L	C11-C12-C13-C14
5	W	320	Q6L	C11-C12-C13-C42
5	W	320	Q6L	C28-C27-C29-C30
5	W	320	Q6L	C29-C30-C31-C36
5	W	320	Q6L	C29-C30-C31-C32
5	X	301	Q6L	C29-C30-C31-C32
5	X	301	Q6L	C27-C29-C30-C31
5	X	317	Q6L	C04-C03-C11-C12
5	X	319	Q6L	C11-C12-C13-C14
5	X	319	Q6L	C11-C12-C13-C42
5	X	319	Q6L	C21-C22-C24-C25
5	X	319	Q6L	C23-C22-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	X	319	Q6L	C28-C27-C29-C30
5	X	319	Q6L	C26-C27-C29-C30
5	X	319	Q6L	C29-C30-C31-C36
5	X	319	Q6L	C29-C30-C31-C32
5	X	319	Q6L	C27-C29-C30-C31
5	X	319	Q6L	C24-C25-C26-C27
6	V	317	IWJ	C18-C19-C21-C22
6	V	317	IWJ	C20-C19-C21-C22
6	V	317	IWJ	C26-C28-C29-C30
6	V	317	IWJ	C26-C28-C29-C35
6	V	317	IWJ	C26-C28-C29-O39
6	V	318	IWJ	C26-C28-C29-C30
6	V	318	IWJ	C26-C28-C29-C35
6	V	318	IWJ	C26-C28-C29-O39
6	V	320	IWJ	C26-C28-C29-C30
6	V	320	IWJ	C26-C28-C29-C35
6	V	320	IWJ	C26-C28-C29-O39
6	W	318	IWJ	C18-C19-C21-C22
6	W	318	IWJ	C20-C19-C21-C22
6	W	318	IWJ	C26-C28-C29-C30
6	W	318	IWJ	C26-C28-C29-C35
6	W	318	IWJ	C26-C28-C29-O39
6	X	318	IWJ	C18-C19-C21-C22
6	X	318	IWJ	C20-C19-C21-C22
6	X	318	IWJ	C26-C28-C29-C30
6	X	318	IWJ	C26-C28-C29-O39
2	V	310	CLA	O1D-CGD-O2D-CED
2	W	303	CLA	O1D-CGD-O2D-CED
3	V	307	CHL	O1D-CGD-O2D-CED
3	X	308	CHL	O1D-CGD-O2D-CED
3	X	315	CHL	O1D-CGD-O2D-CED
2	W	311	CLA	O1D-CGD-O2D-CED
2	X	312	CLA	O1D-CGD-O2D-CED
2	V	301	CLA	CBD-CGD-O2D-CED
2	V	310	CLA	CBD-CGD-O2D-CED
2	W	301	CLA	CBD-CGD-O2D-CED
2	W	303	CLA	CBD-CGD-O2D-CED
2	W	311	CLA	CBD-CGD-O2D-CED
2	W	313	CLA	CBD-CGD-O2D-CED
2	X	303	CLA	CBD-CGD-O2D-CED
2	X	304	CLA	CBD-CGD-O2D-CED
3	V	307	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	W	307	CHL	CBD-CGD-O2D-CED
4	X	309	KC2	CBD-CGD-O2D-CED
2	V	302	CLA	O1A-CGA-O2A-C1
2	V	303	CLA	O1D-CGD-O2D-CED
2	W	313	CLA	O1D-CGD-O2D-CED
2	X	313	CLA	O1D-CGD-O2D-CED
2	X	314	CLA	O1D-CGD-O2D-CED
3	V	304	CHL	O1D-CGD-O2D-CED
3	W	307	CHL	O1D-CGD-O2D-CED
2	X	303	CLA	O1D-CGD-O2D-CED
2	V	302	CLA	CBA-CGA-O2A-C1
2	V	302	CLA	CBD-CGD-O2D-CED
2	V	309	CLA	CBD-CGD-O2D-CED
3	X	306	CHL	CBD-CGD-O2D-CED
4	W	308	KC2	CBD-CGD-O2D-CED
2	V	313	CLA	O1A-CGA-O2A-C1
2	X	302	CLA	O1A-CGA-O2A-C1
2	X	311	CLA	O1A-CGA-O2A-C1
2	X	312	CLA	O1A-CGA-O2A-C1
3	W	306	CHL	O1A-CGA-O2A-C1
3	W	307	CHL	O1A-CGA-O2A-C1
2	X	311	CLA	O1D-CGD-O2D-CED
2	V	312	CLA	C3-C5-C6-C7
2	W	302	CLA	C3-C5-C6-C7
2	W	312	CLA	C3-C5-C6-C7
2	X	302	CLA	CBA-CGA-O2A-C1
2	X	311	CLA	CBA-CGA-O2A-C1
3	W	307	CHL	CBA-CGA-O2A-C1
2	V	311	CLA	CBD-CGD-O2D-CED
2	V	313	CLA	C2A-CAA-CBA-CGA
2	W	301	CLA	C2A-CAA-CBA-CGA
3	V	304	CHL	C2A-CAA-CBA-CGA
2	W	301	CLA	O1D-CGD-O2D-CED
2	W	301	CLA	C3-C5-C6-C7
2	V	313	CLA	CBA-CGA-O2A-C1
2	X	312	CLA	CBA-CGA-O2A-C1
3	W	306	CHL	CBA-CGA-O2A-C1
2	V	301	CLA	O1D-CGD-O2D-CED
5	V	315	Q6L	C17-C18-C19-C20
6	V	320	IWJ	C10-C11-C12-C13
2	W	310	CLA	CBD-CGD-O2D-CED
3	X	307	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	X	309	KC2	O1D-CGD-O2D-CED
2	W	303	CLA	CBA-CGA-O2A-C1
2	W	310	CLA	CBA-CGA-O2A-C1
2	X	303	CLA	CBA-CGA-O2A-C1
3	W	314	CHL	CBD-CGD-O2D-CED
2	V	311	CLA	C3-C5-C6-C7
2	W	309	CLA	C3-C5-C6-C7
2	X	302	CLA	C3-C5-C6-C7
2	V	301	CLA	C4-C3-C5-C6
5	V	315	Q6L	C11-C12-C13-C42
5	V	319	Q6L	C11-C12-C13-C42
2	V	301	CLA	C2-C3-C5-C6
5	V	315	Q6L	C11-C12-C13-C14
5	V	319	Q6L	C11-C12-C13-C14
2	V	311	CLA	C2A-CAA-CBA-CGA
2	W	303	CLA	O1A-CGA-O2A-C1
2	W	310	CLA	O1A-CGA-O2A-C1
2	X	303	CLA	O1A-CGA-O2A-C1
2	V	311	CLA	CBA-CGA-O2A-C1
2	X	304	CLA	O1D-CGD-O2D-CED
2	V	309	CLA	O1D-CGD-O2D-CED
3	X	306	CHL	O1D-CGD-O2D-CED
4	W	308	KC2	O1D-CGD-O2D-CED
2	V	311	CLA	O1A-CGA-O2A-C1
2	W	301	CLA	CBA-CGA-O2A-C1
2	W	302	CLA	CBA-CGA-O2A-C1
2	W	310	CLA	C8-C10-C11-C12
4	V	308	KC2	CAA-CBA-CGA-O1A
4	V	308	KC2	CAA-CBA-CGA-O2A
4	W	308	KC2	CAA-CBA-CGA-O1A
3	W	307	CHL	C5-C6-C7-C8
2	V	301	CLA	C11-C10-C8-C9
3	W	307	CHL	C6-C7-C8-C9
2	V	302	CLA	O1D-CGD-O2D-CED
5	V	321	Q6L	C28-C27-C29-C30
5	W	319	Q6L	C23-C22-C24-C25
5	X	316	Q6L	C15-C16-C17-C41
5	V	321	Q6L	C26-C27-C29-C30
5	W	319	Q6L	C21-C22-C24-C25
5	W	320	Q6L	C26-C27-C29-C30
4	W	308	KC2	CAA-CBA-CGA-O2A
2	W	310	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	W	312	CLA	CBA-CGA-O2A-C1
2	X	310	CLA	CBD-CGD-O2D-CED
2	W	301	CLA	O1A-CGA-O2A-C1
5	W	319	Q6L	C24-C25-C26-C27
6	V	318	IWJ	C10-C11-C12-C13
2	W	302	CLA	O1A-CGA-O2A-C1
2	V	301	CLA	C10-C11-C12-C13
2	W	312	CLA	O1A-CGA-O2A-C1
5	W	315	Q6L	C11-C12-C13-C42
2	V	311	CLA	O1D-CGD-O2D-CED
2	W	310	CLA	O1D-CGD-O2D-CED
5	W	316	Q6L	C28-C27-C29-C30
5	X	301	Q6L	C28-C27-C29-C30
5	X	301	Q6L	C26-C27-C29-C30
2	W	312	CLA	C6-C7-C8-C9
2	X	302	CLA	C5-C6-C7-C8
2	V	312	CLA	CBA-CGA-O2A-C1
3	V	314	CHL	C3A-C2A-CAA-CBA
3	W	307	CHL	C3A-C2A-CAA-CBA
2	W	312	CLA	C6-C7-C8-C10
5	V	316	Q6L	C11-C12-C13-C14
2	V	312	CLA	O1A-CGA-O2A-C1
2	W	309	CLA	C4-C3-C5-C6
3	W	314	CHL	O1D-CGD-O2D-CED
5	W	319	Q6L	C11-C12-C13-C14
5	V	319	Q6L	C24-C25-C26-C27
5	X	301	Q6L	C24-C25-C26-C27
3	X	307	CHL	O1D-CGD-O2D-CED
4	X	309	KC2	C4C-C3C-CAC-CBC
5	V	316	Q6L	C11-C12-C13-C42
5	W	319	Q6L	C11-C12-C13-C42
5	X	301	Q6L	C11-C12-C13-C42
5	W	315	Q6L	C11-C12-C13-C14
2	W	311	CLA	C2A-CAA-CBA-CGA
3	V	314	CHL	C1A-C2A-CAA-CBA
3	X	307	CHL	C1A-C2A-CAA-CBA
3	X	315	CHL	C1A-C2A-CAA-CBA
5	X	316	Q6L	C17-C18-C19-C20
3	W	307	CHL	C15-C16-C17-C18
2	X	310	CLA	O1D-CGD-O2D-CED
2	X	311	CLA	C4C-C3C-CAC-CBC
2	W	312	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	V	310	CLA	CBA-CGA-O2A-C1
3	W	307	CHL	C11-C12-C13-C15
3	W	307	CHL	C11-C12-C13-C14
3	V	314	CHL	C2A-CAA-CBA-CGA
2	V	313	CLA	O2A-C1-C2-C3
5	X	301	Q6L	C11-C12-C13-C14
2	W	301	CLA	C3A-C2A-CAA-CBA
6	X	318	IWJ	C21-C22-C23-C24
6	V	317	IWJ	O27-C26-C28-C29
6	V	320	IWJ	O27-C26-C28-C29
6	X	318	IWJ	O27-C26-C28-C29
5	V	319	Q6L	C29-C30-C31-C36
2	V	310	CLA	O1A-CGA-O2A-C1
2	X	302	CLA	C6-C7-C8-C10
2	W	309	CLA	C2-C3-C5-C6
3	V	304	CHL	C3C-C2C-CMC-OMC
6	W	318	IWJ	C23-C24-C26-C28
4	W	308	KC2	C1A-C2A-CAA-CBA
2	V	309	CLA	C1A-C2A-CAA-CBA
2	X	304	CLA	C1A-C2A-CAA-CBA
5	X	316	Q6L	C15-C16-C17-C18
2	X	302	CLA	C6-C7-C8-C9
2	W	309	CLA	C11-C10-C8-C7
5	V	316	Q6L	C24-C25-C26-C27
5	W	316	Q6L	C13-C14-C15-C16
5	X	317	Q6L	C13-C14-C15-C16
2	V	309	CLA	CAD-CBD-CGD-O2D
2	W	302	CLA	CAD-CBD-CGD-O2D
2	X	310	CLA	CAD-CBD-CGD-O2D
3	V	307	CHL	CAD-CBD-CGD-O2D
3	V	314	CHL	CAD-CBD-CGD-O2D
3	W	306	CHL	CAD-CBD-CGD-O2D
3	X	308	CHL	CAD-CBD-CGD-O2D
4	V	308	KC2	C2B-C3B-CAB-CBB
4	X	309	KC2	C2B-C3B-CAB-CBB
5	X	316	Q6L	C11-C12-C13-C14
6	W	318	IWJ	C25-C24-C26-O27
4	V	308	KC2	C4C-C3C-CAC-CBC
4	W	308	KC2	C4C-C3C-CAC-CBC
2	V	310	CLA	CHA-CBD-CGD-O1D
6	W	318	IWJ	C23-C24-C26-O27
2	X	311	CLA	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	X	316	Q6L	C11-C12-C13-C42
5	X	316	Q6L	C23-C22-C24-C25
2	V	302	CLA	CAD-CBD-CGD-O1D
2	V	311	CLA	CAD-CBD-CGD-O1D
2	X	303	CLA	C2-C3-C5-C6
3	W	307	CHL	C6-C7-C8-C10
5	V	319	Q6L	C29-C30-C31-C32
5	W	319	Q6L	C29-C30-C31-C32
2	W	310	CLA	CAA-CBA-CGA-O2A
3	V	307	CHL	C2C-C3C-CAC-CBC
3	V	305	CHL	C1C-C2C-CMC-OMC
2	W	309	CLA	C11-C10-C8-C9
2	V	311	CLA	C2-C1-O2A-CGA
5	W	319	Q6L	C27-C29-C30-C31
6	W	318	IWJ	C25-C24-C26-C28
3	W	305	CHL	O1D-CGD-O2D-CED
6	W	318	IWJ	C16-C17-C18-C19
4	V	308	KC2	C4B-C3B-CAB-CBB
4	X	309	KC2	C4B-C3B-CAB-CBB
5	V	321	Q6L	C24-C25-C26-C27
2	W	312	CLA	C5-C6-C7-C8
7	W	317	NEX	C39-C29-C30-C31
2	V	311	CLA	C6-C7-C8-C10
5	X	301	Q6L	C19-C20-C21-C22
2	V	301	CLA	C5-C6-C7-C8
7	W	317	NEX	C28-C29-C30-C31
3	V	304	CHL	CAA-CBA-CGA-O2A
5	V	321	Q6L	C11-C12-C13-C42
5	W	316	Q6L	C26-C27-C29-C30
3	V	307	CHL	C4C-C3C-CAC-CBC
2	W	311	CLA	CAA-CBA-CGA-O2A
2	W	311	CLA	CAA-CBA-CGA-O1A
3	V	314	CHL	O1D-CGD-O2D-CED
4	V	308	KC2	CBD-CGD-O2D-CED
2	V	301	CLA	CAA-CBA-CGA-O2A
3	W	306	CHL	C3A-C2A-CAA-CBA
2	X	302	CLA	CAD-CBD-CGD-O2D
2	X	313	CLA	CAD-CBD-CGD-O2D
3	X	305	CHL	CAD-CBD-CGD-O2D
3	X	307	CHL	CAD-CBD-CGD-O2D
2	V	310	CLA	CAA-CBA-CGA-O2A
3	W	305	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	V	304	CHL	CAA-CBA-CGA-O1A
5	X	316	Q6L	C21-C22-C24-C25
2	V	303	CLA	O2A-C1-C2-C3
2	W	302	CLA	O2A-C1-C2-C3
4	W	308	KC2	C4B-C3B-CAB-CBB
2	X	302	CLA	C2A-CAA-CBA-CGA
2	V	303	CLA	CHA-CBD-CGD-O1D
2	V	303	CLA	CHA-CBD-CGD-O2D
2	V	310	CLA	CHA-CBD-CGD-O2D
2	W	301	CLA	CHA-CBD-CGD-O1D
2	W	301	CLA	CHA-CBD-CGD-O2D
2	W	310	CLA	CHA-CBD-CGD-O1D
2	W	310	CLA	CHA-CBD-CGD-O2D
2	W	312	CLA	CHA-CBD-CGD-O1D
2	W	312	CLA	CHA-CBD-CGD-O2D
4	X	309	KC2	CAA-CBA-CGA-O1A
3	W	306	CHL	C1A-C2A-CAA-CBA
5	V	315	Q6L	C04-C03-C11-C12
5	W	316	Q6L	C04-C03-C11-C12
2	V	301	CLA	CAA-CBA-CGA-O1A
5	W	316	Q6L	C19-C20-C21-C22
2	W	309	CLA	C16-C17-C18-C19
2	V	310	CLA	CAA-CBA-CGA-O1A
3	X	315	CHL	CAD-CBD-CGD-O1D
4	W	308	KC2	CAD-CBD-CGD-O1D
2	V	311	CLA	C6-C7-C8-C9
4	X	309	KC2	CAA-CBA-CGA-O2A
2	X	303	CLA	CAA-CBA-CGA-O2A
2	V	302	CLA	CAA-CBA-CGA-O2A
3	W	307	CHL	C3-C5-C6-C7
2	V	301	CLA	C11-C10-C8-C7
3	X	308	CHL	C3A-C2A-CAA-CBA
5	V	321	Q6L	C29-C30-C31-C32
2	V	302	CLA	CAA-CBA-CGA-O1A
5	V	319	Q6L	C19-C20-C21-C22
2	X	303	CLA	CAA-CBA-CGA-O1A
2	W	309	CLA	O1A-CGA-O2A-C1

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	X	318	IWJ	C29-C30-C32-C33-C34-C35

Continued on next page...

Continued from previous page...

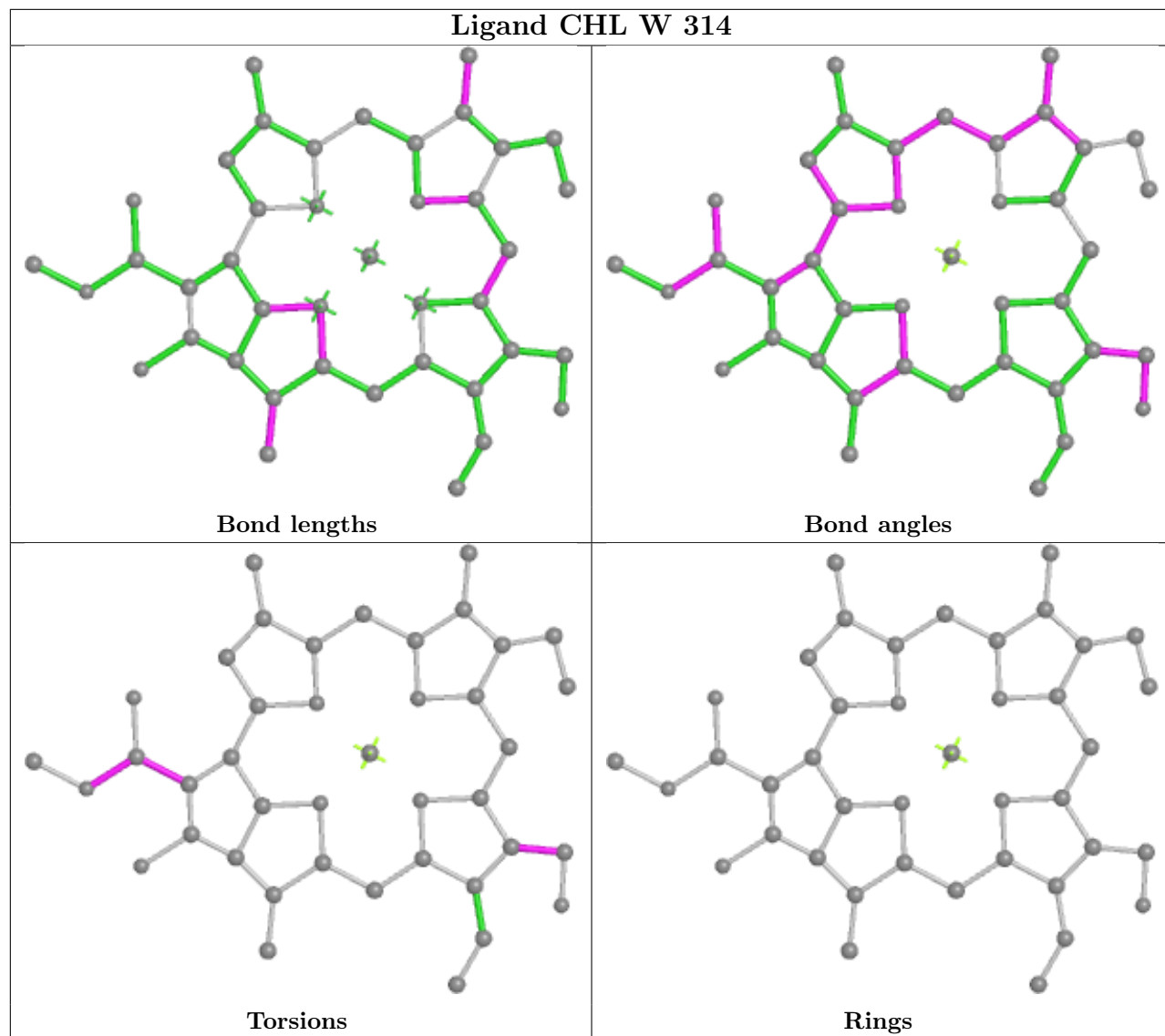
Mol	Chain	Res	Type	Atoms
6	V	320	IWJ	C29-C30-C32-C33-C34-C35

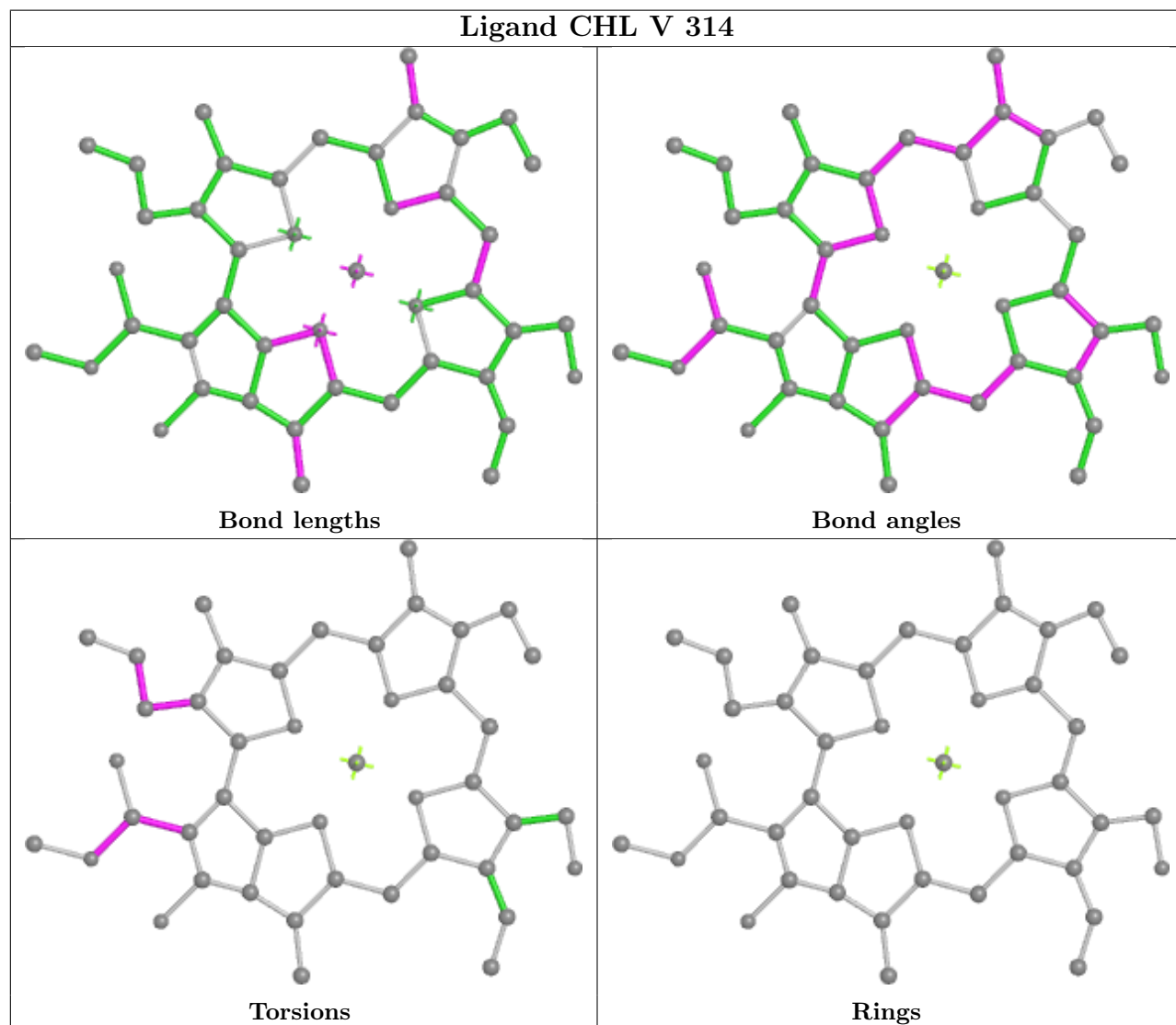
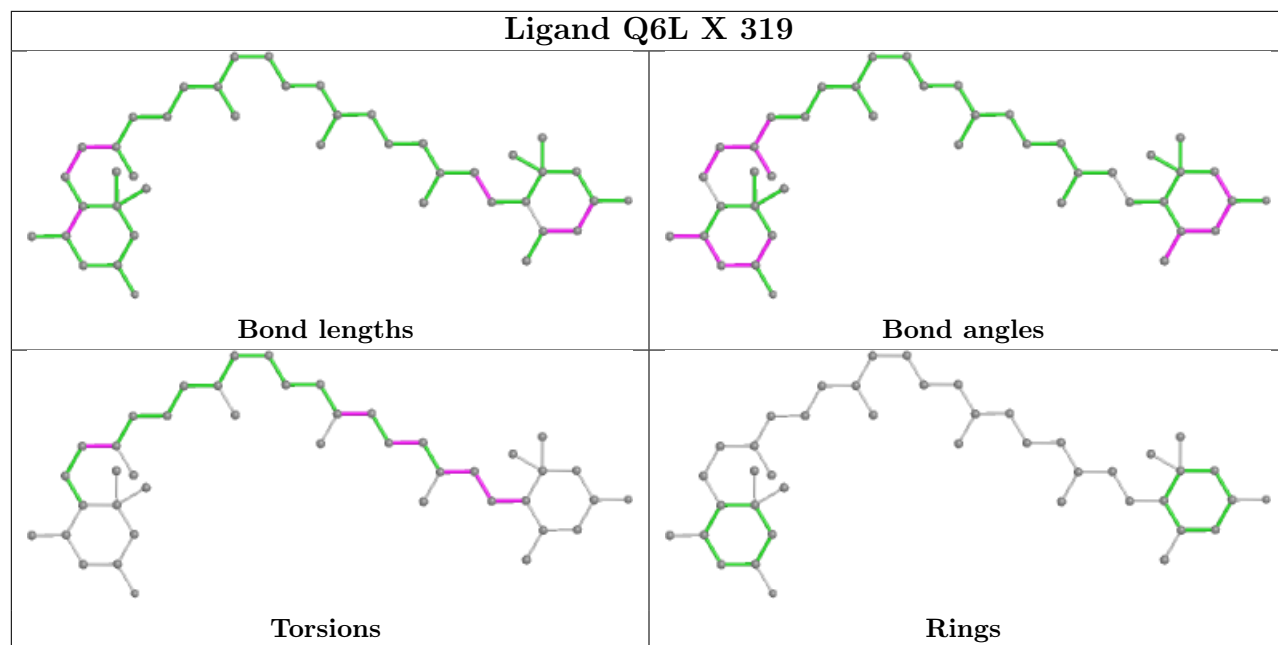
26 monomers are involved in 48 short contacts:

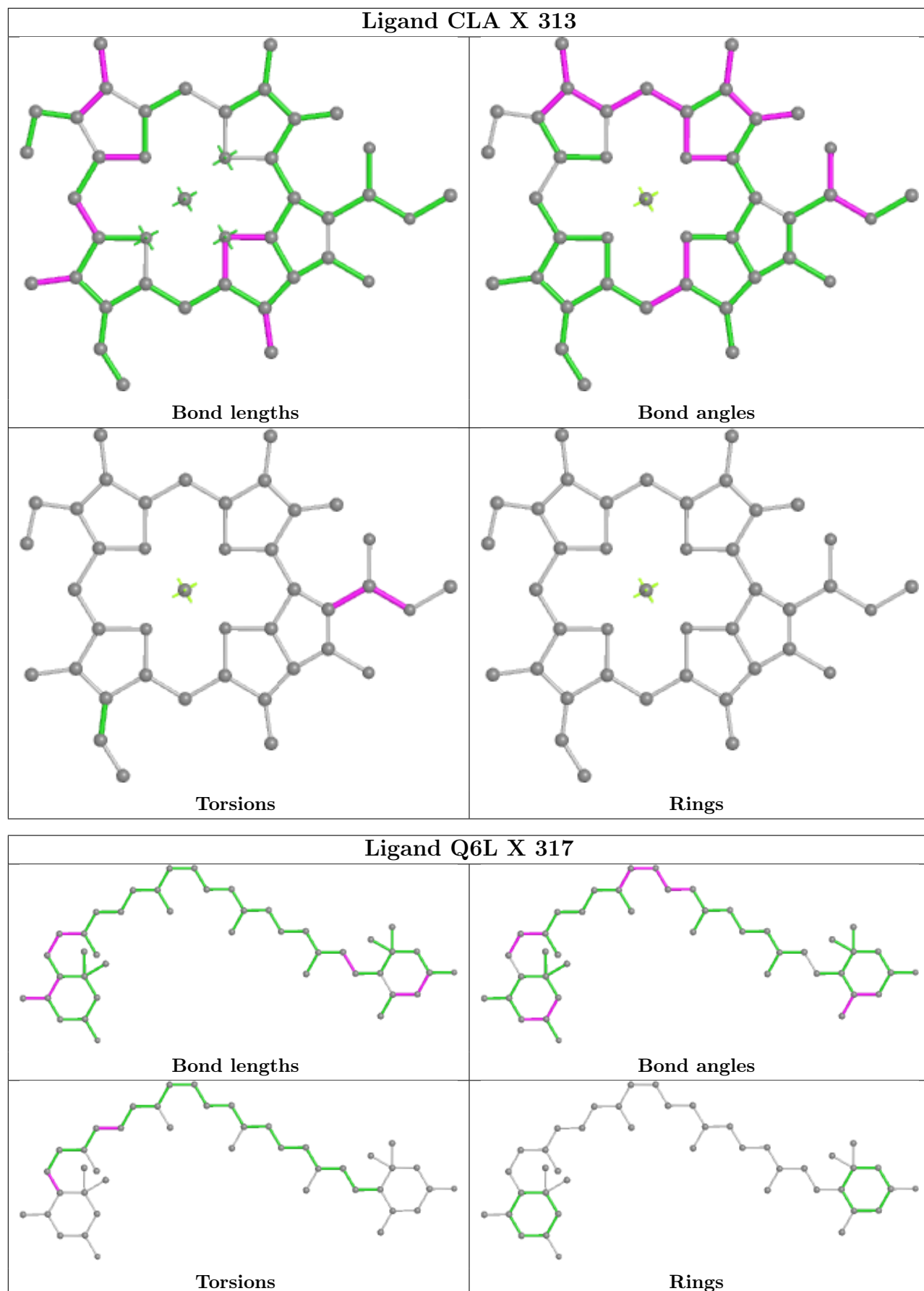
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	X	319	Q6L	1	0
2	X	313	CLA	1	0
3	X	308	CHL	1	0
5	W	315	Q6L	2	0
3	V	305	CHL	1	0
3	V	307	CHL	1	0
2	X	304	CLA	1	0
2	V	302	CLA	1	0
2	V	301	CLA	5	0
6	V	320	IWJ	1	0
2	V	312	CLA	2	0
4	V	308	KC2	1	0
2	V	311	CLA	3	0
6	V	317	IWJ	1	0
2	X	311	CLA	3	0
5	V	321	Q6L	1	0
6	W	318	IWJ	2	0
2	W	301	CLA	3	0
2	V	309	CLA	4	0
2	X	302	CLA	3	0
2	W	312	CLA	2	0
3	X	306	CHL	1	0
2	X	310	CLA	1	0
2	W	303	CLA	1	0
2	W	309	CLA	5	0
2	V	303	CLA	1	0

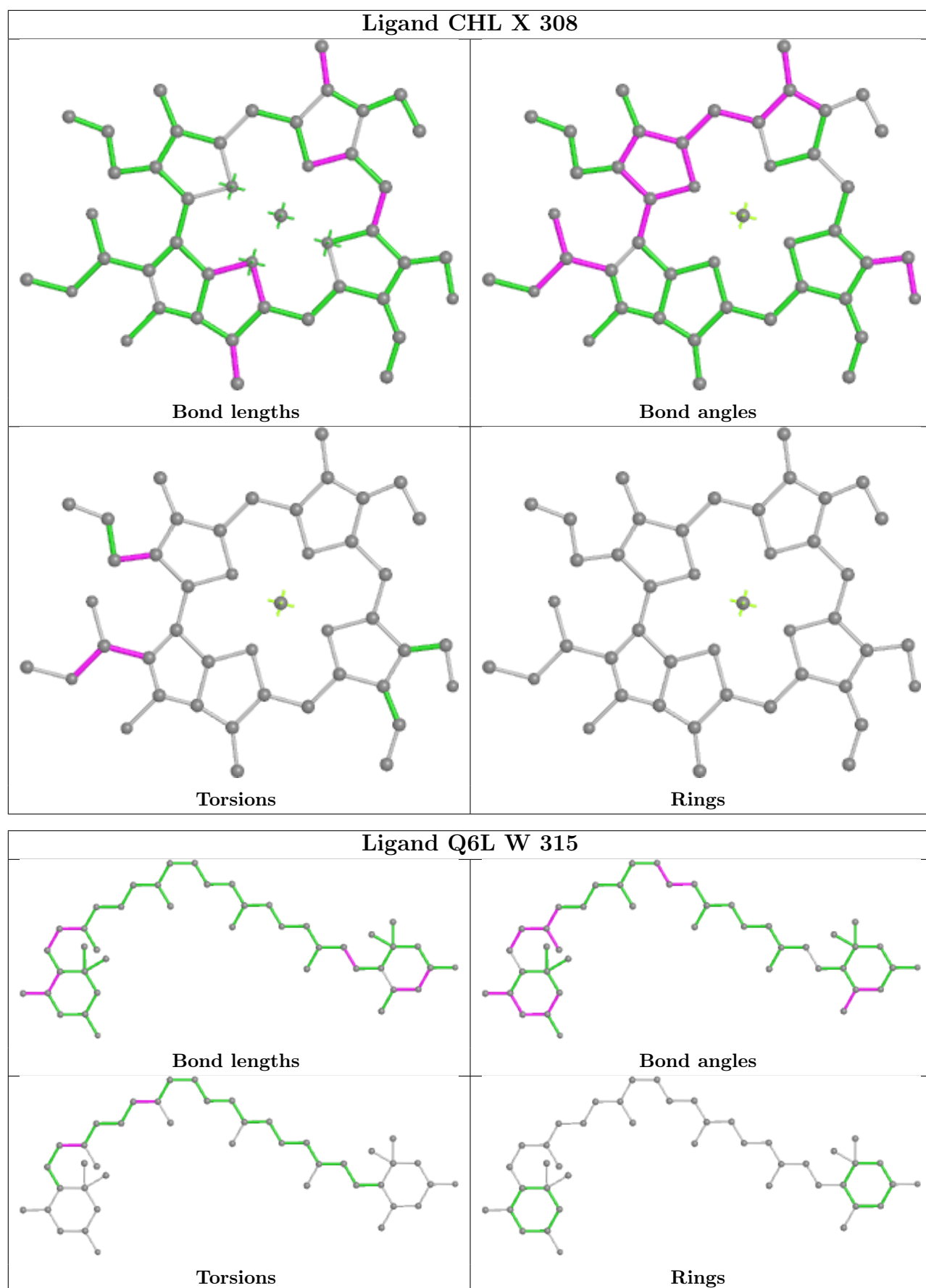
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

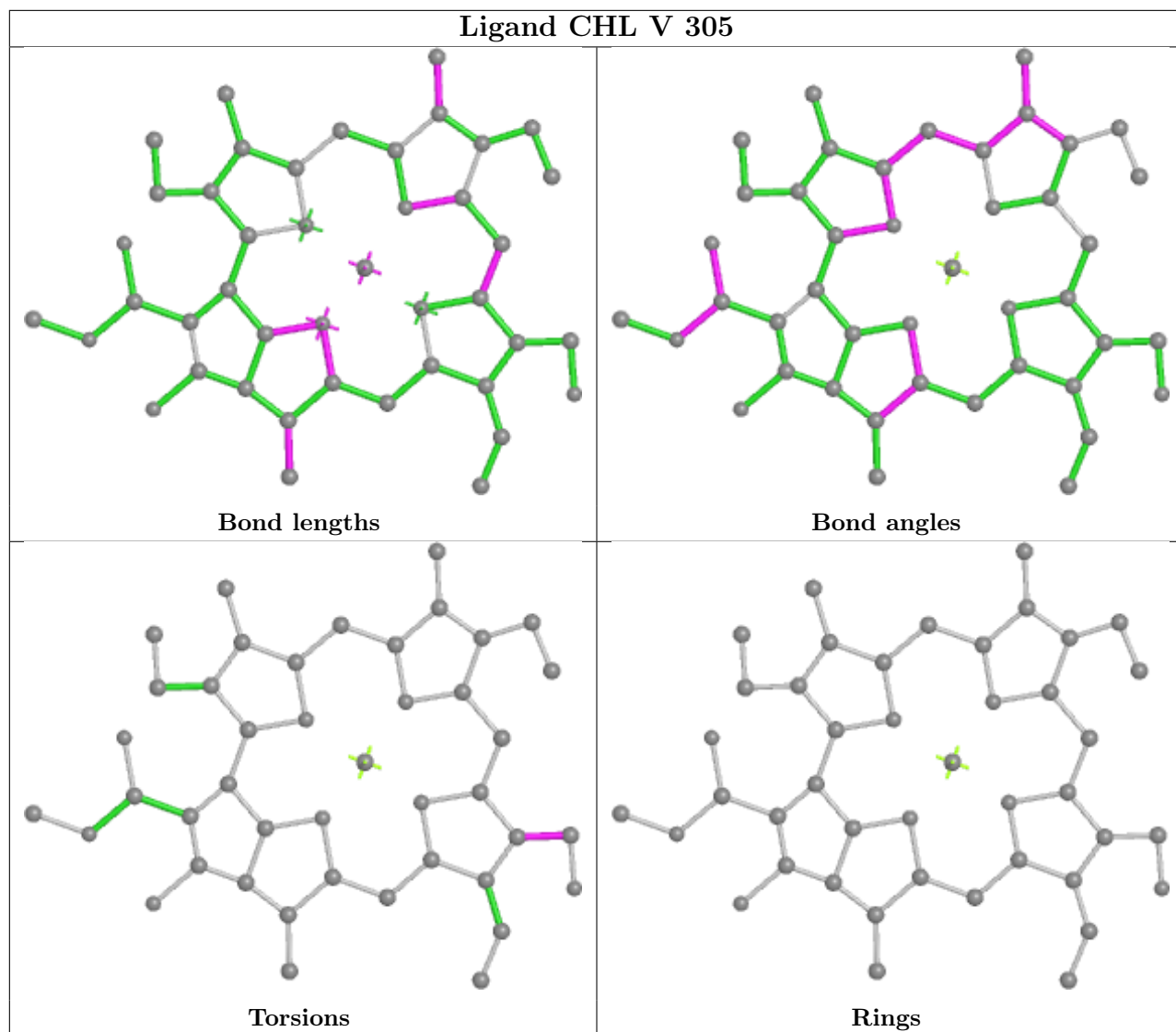
equivalents in the CSD to analyse the geometry.

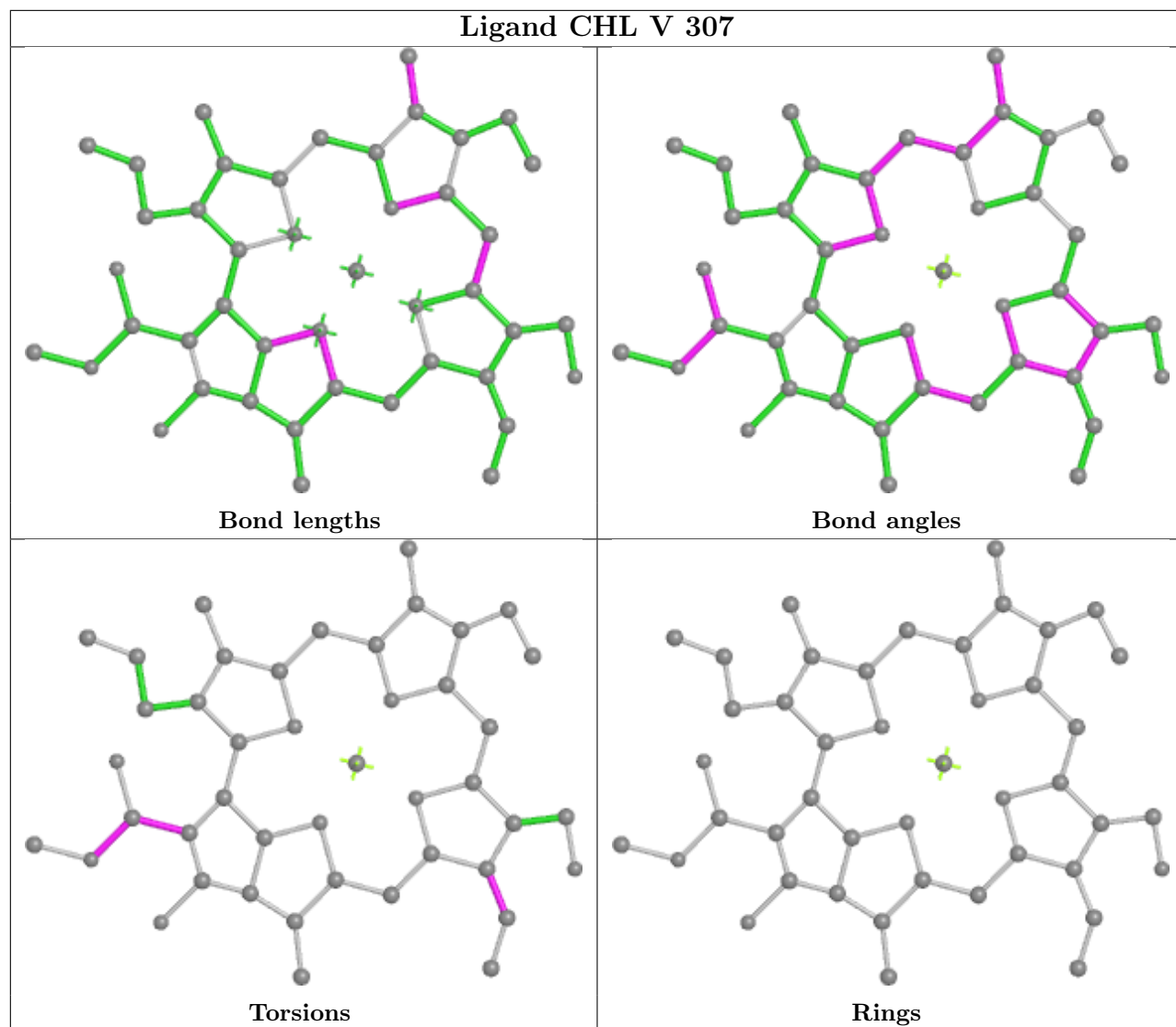


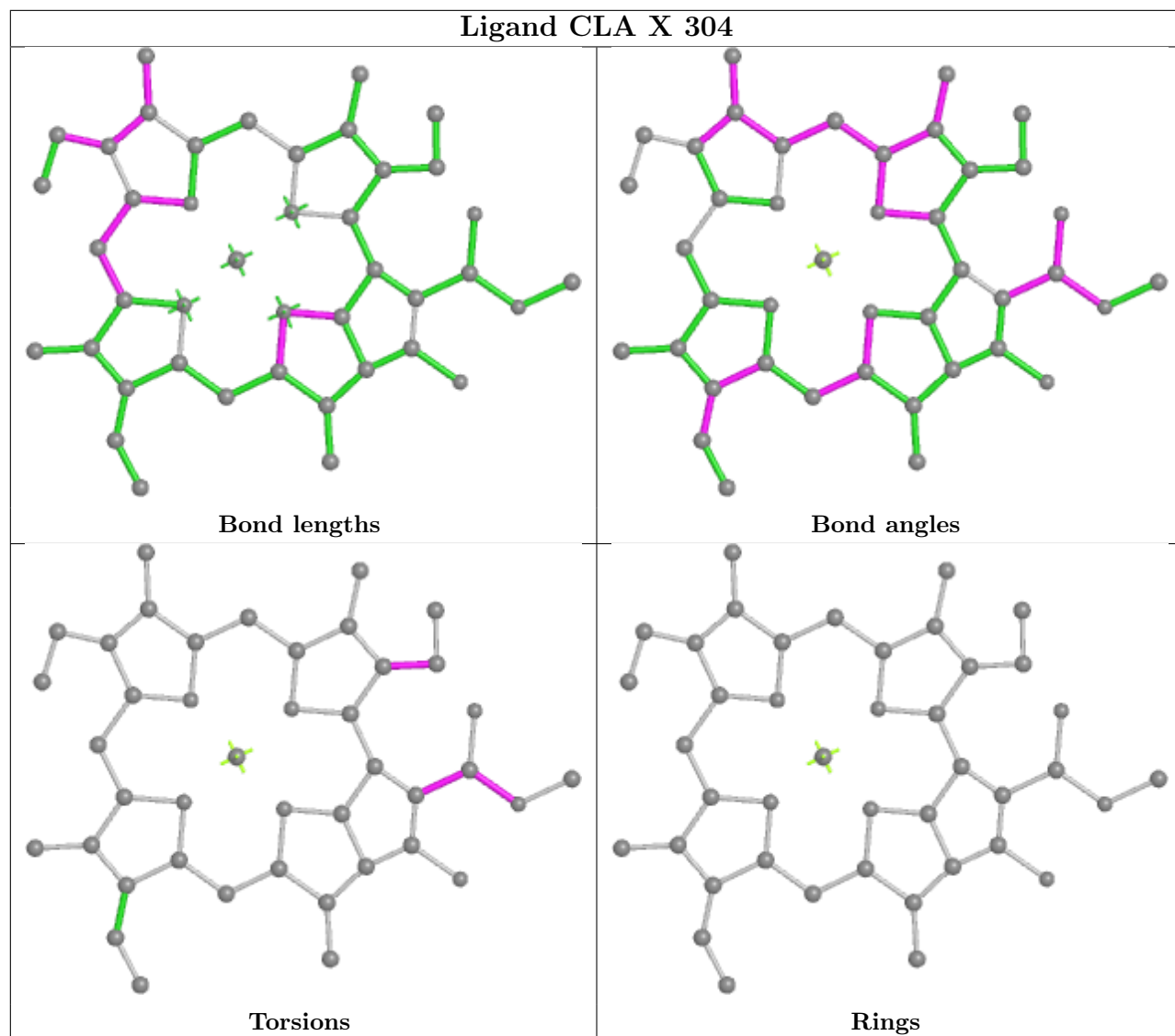


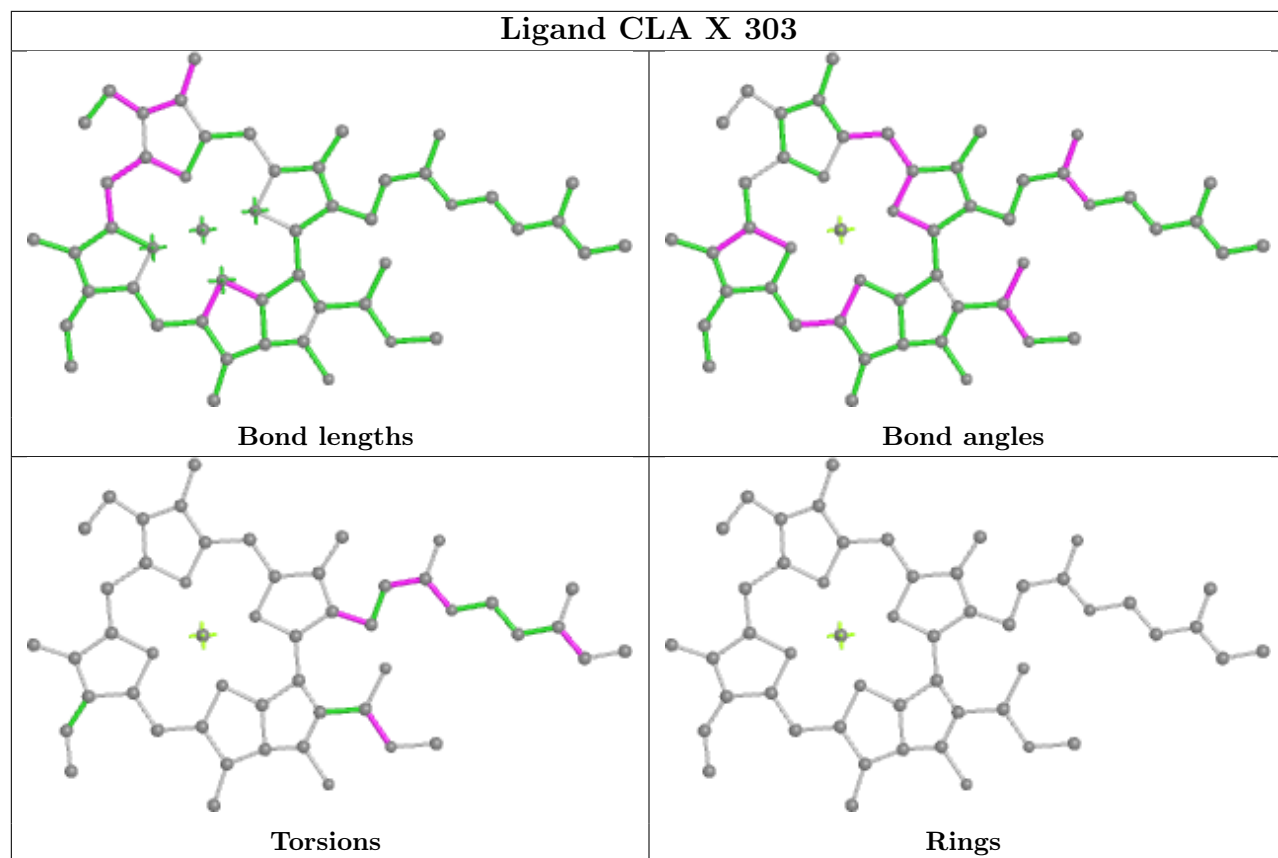


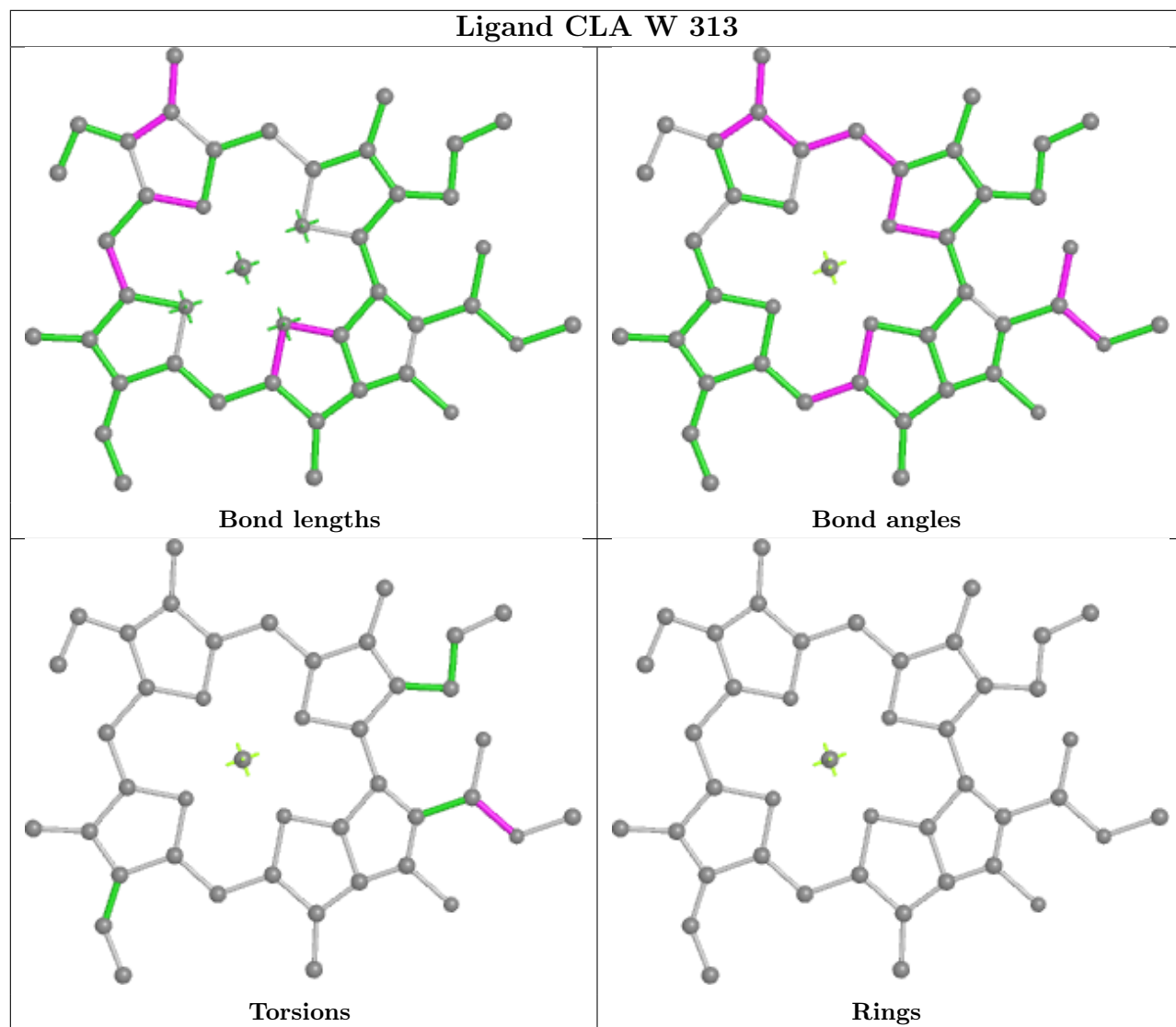


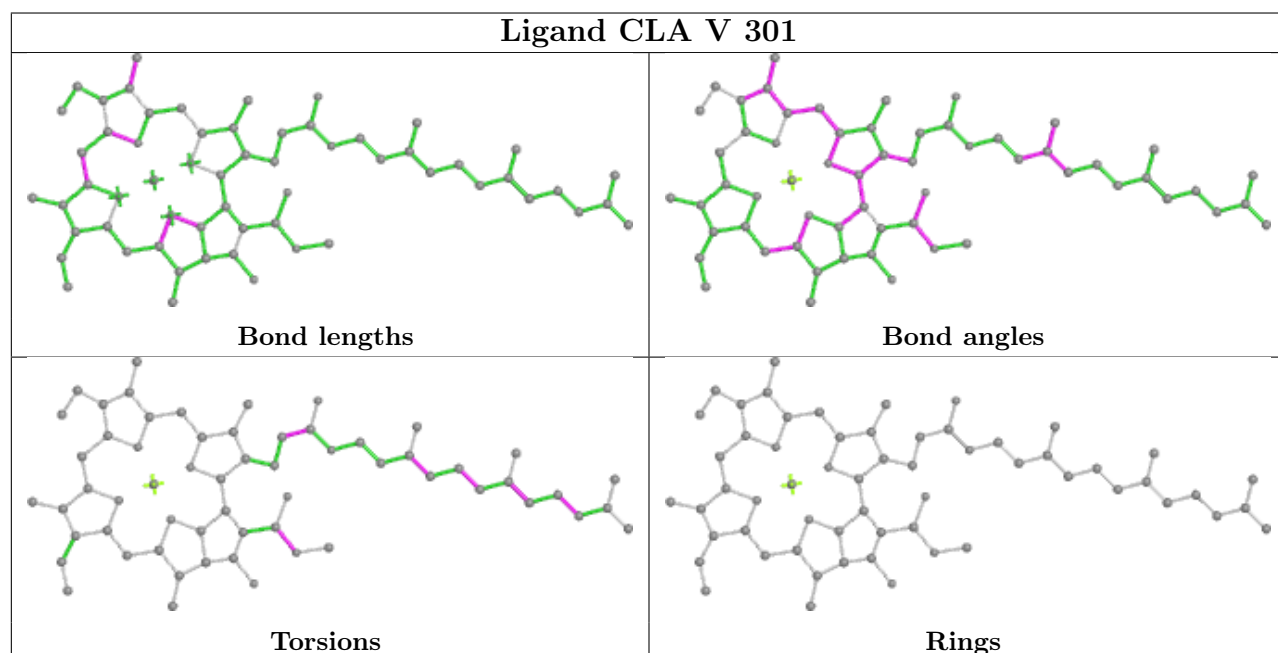
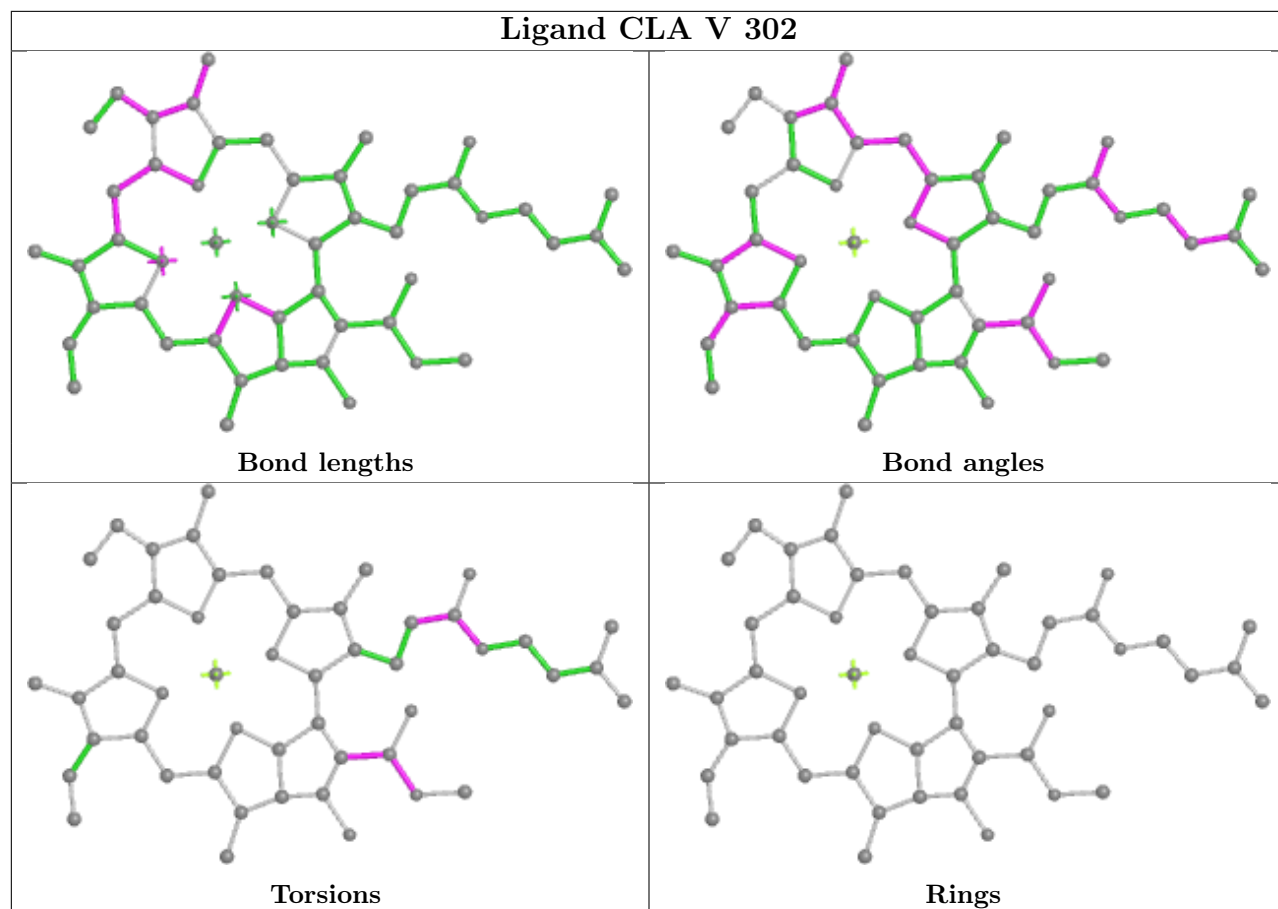


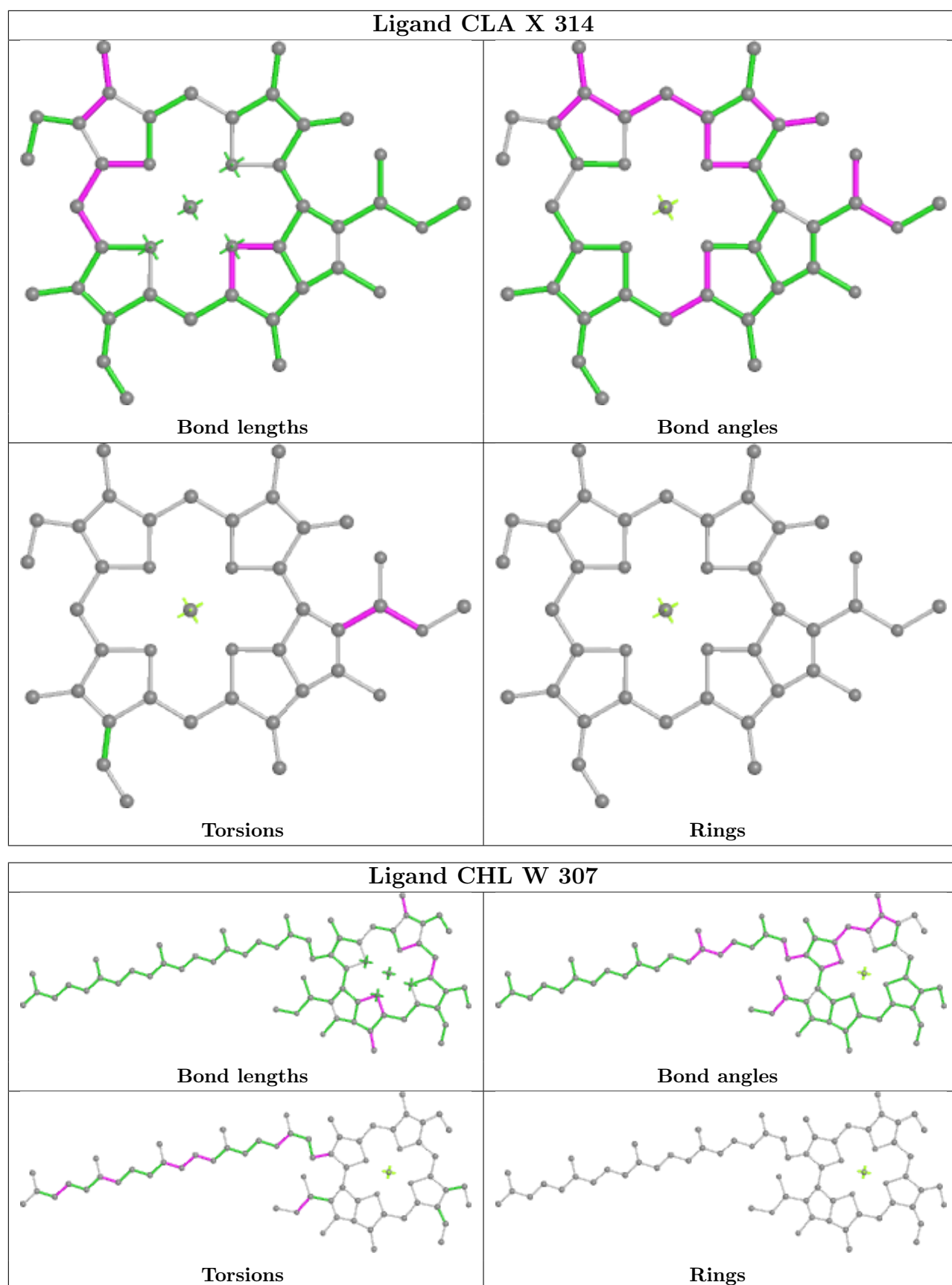


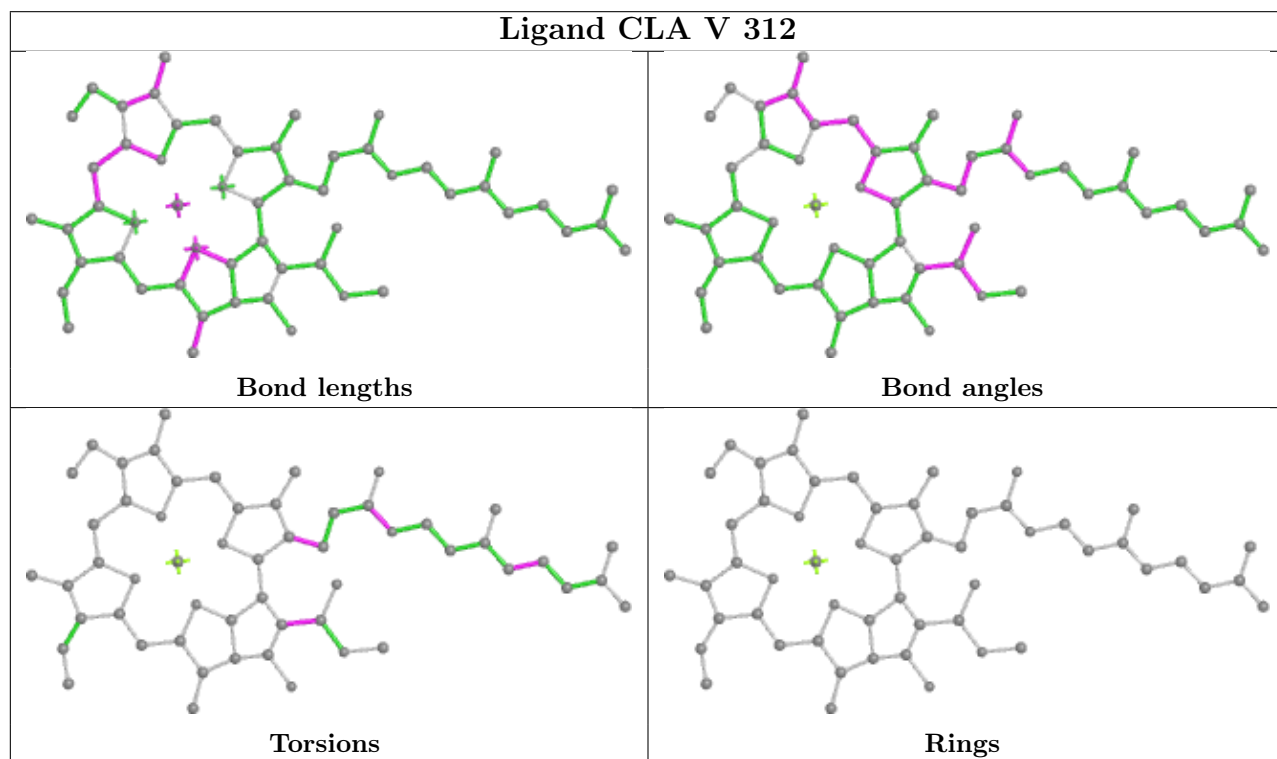
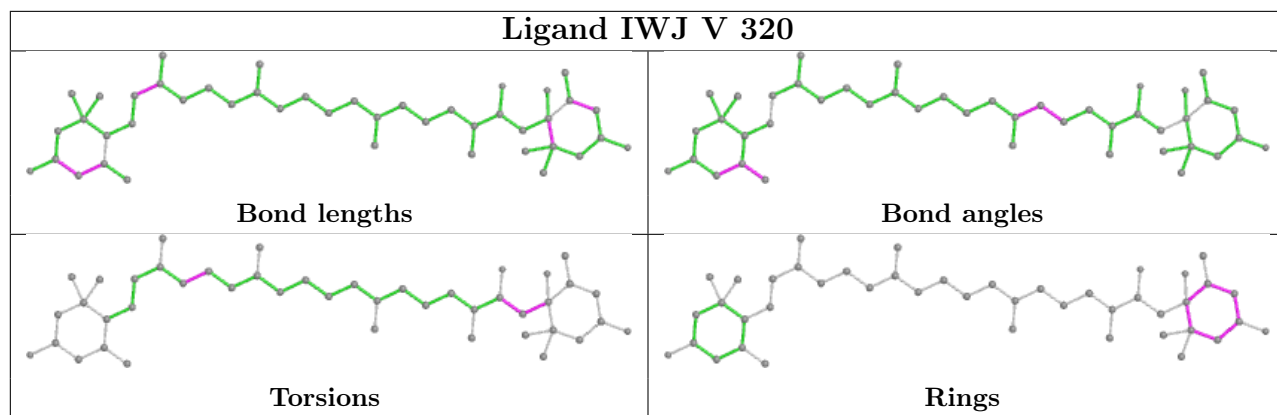


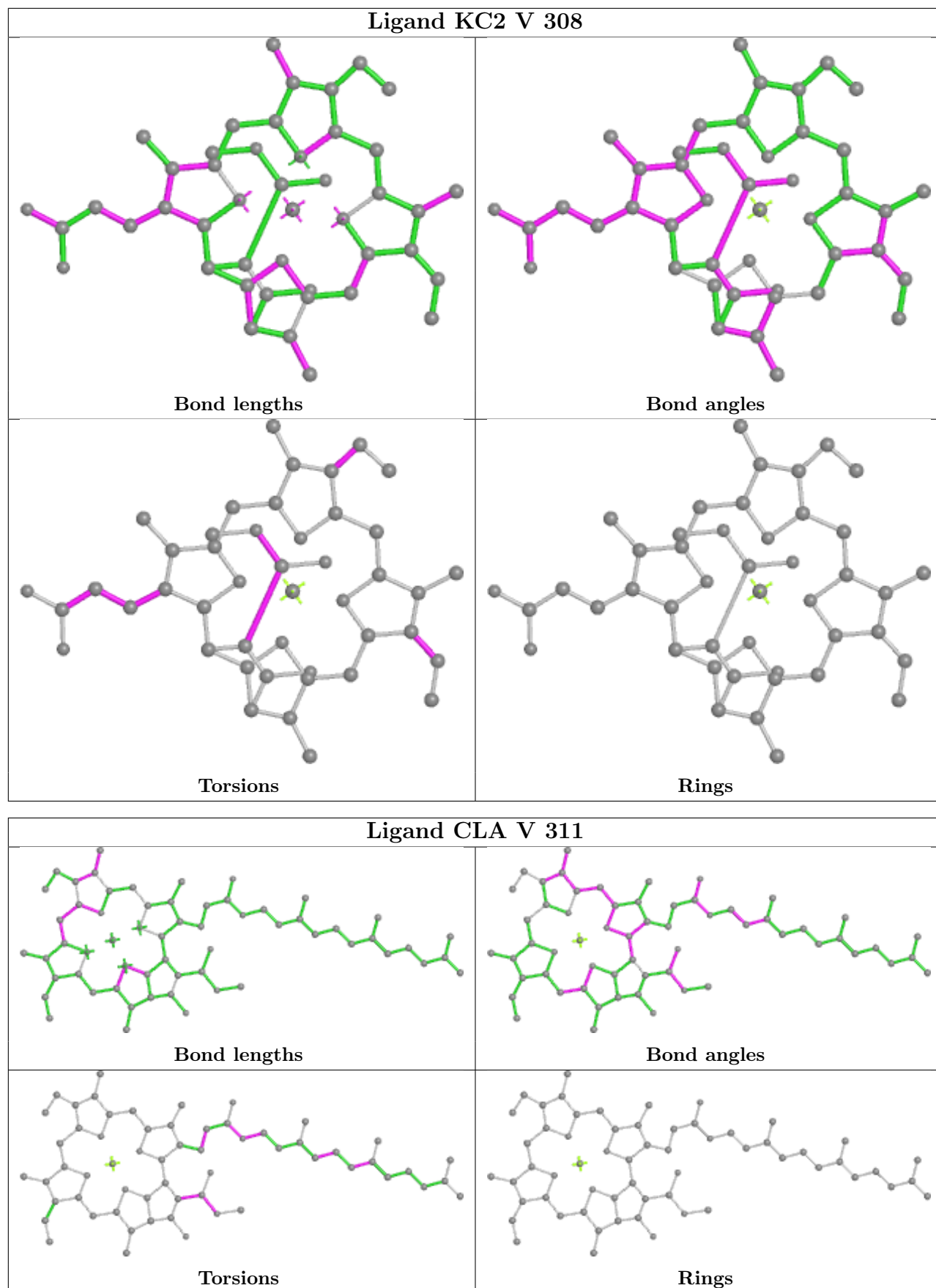


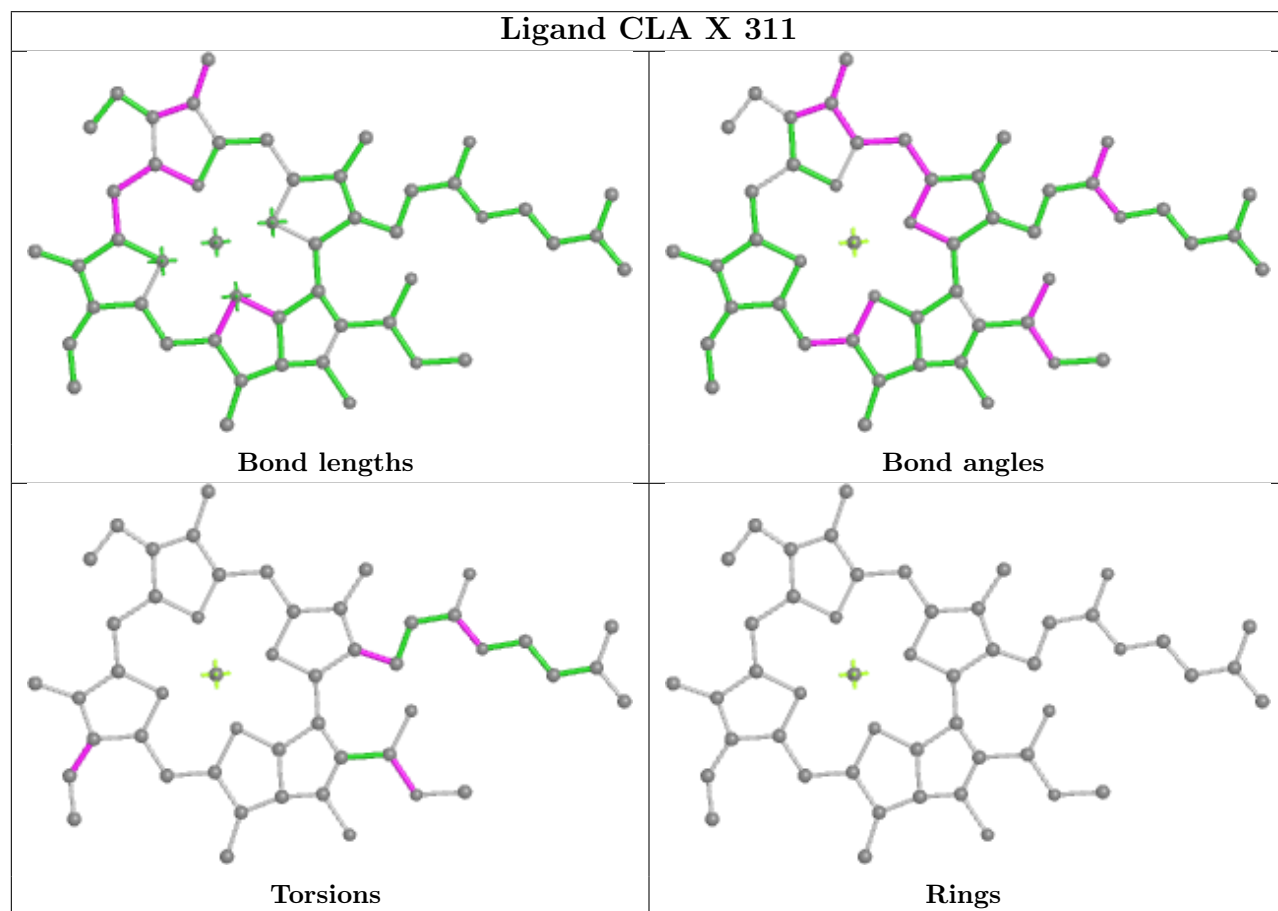
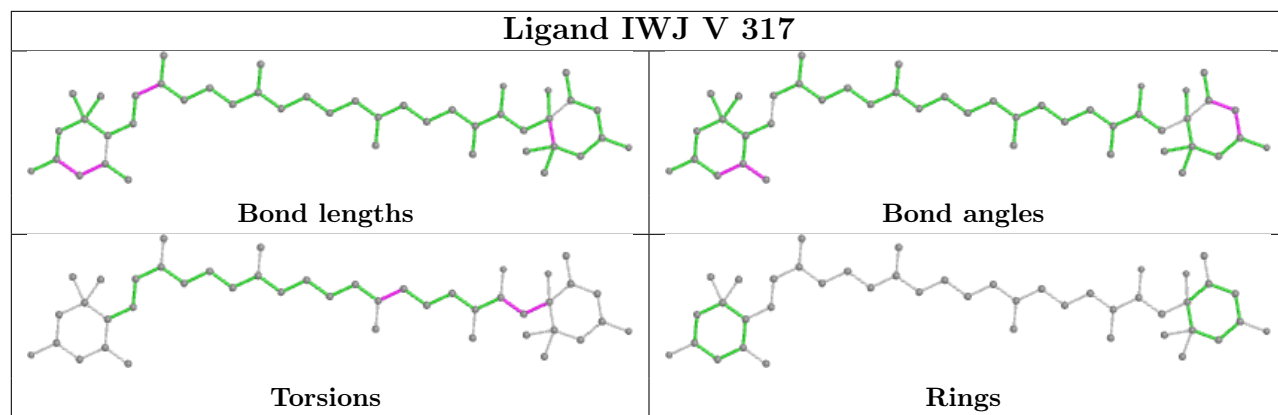


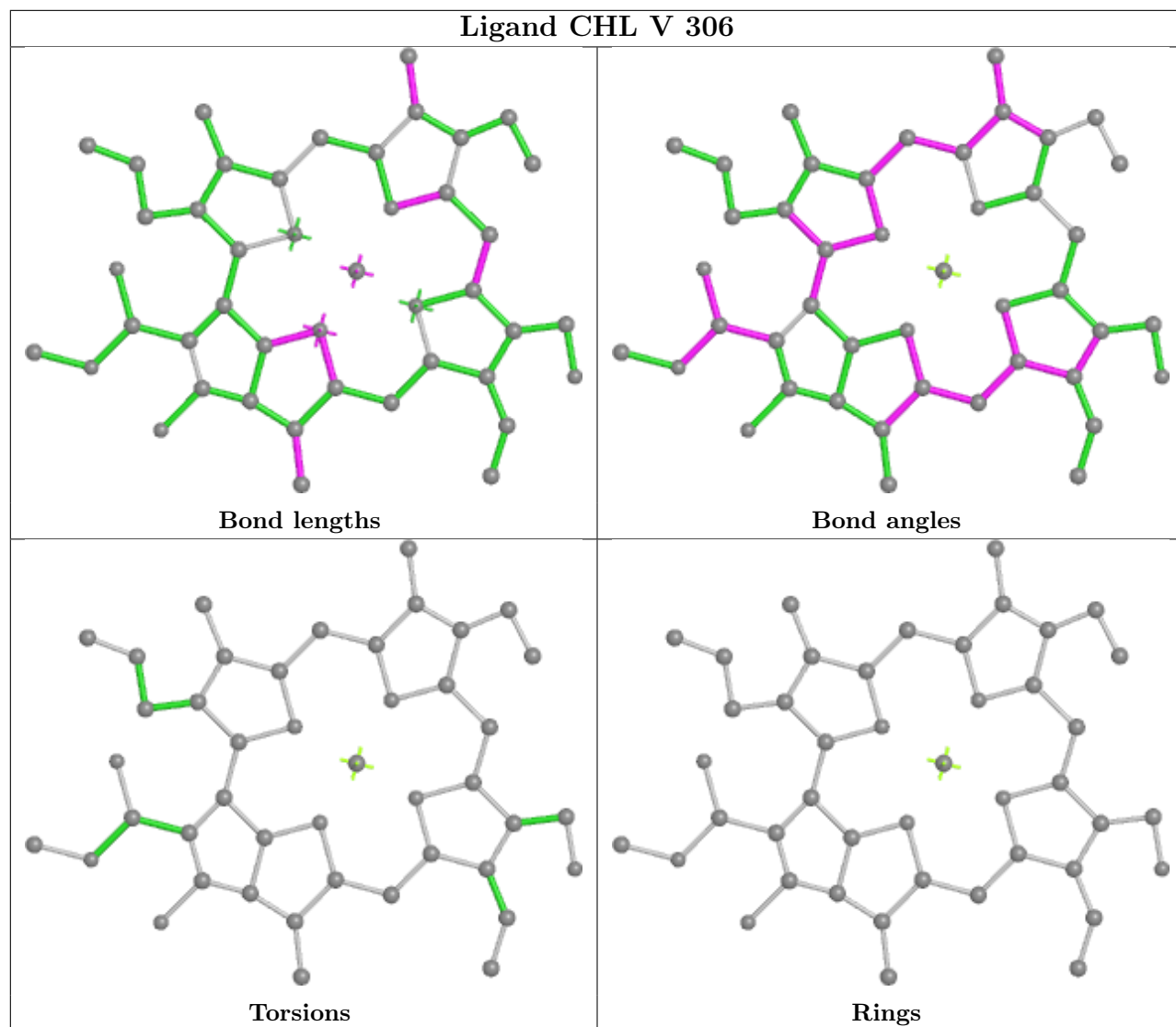


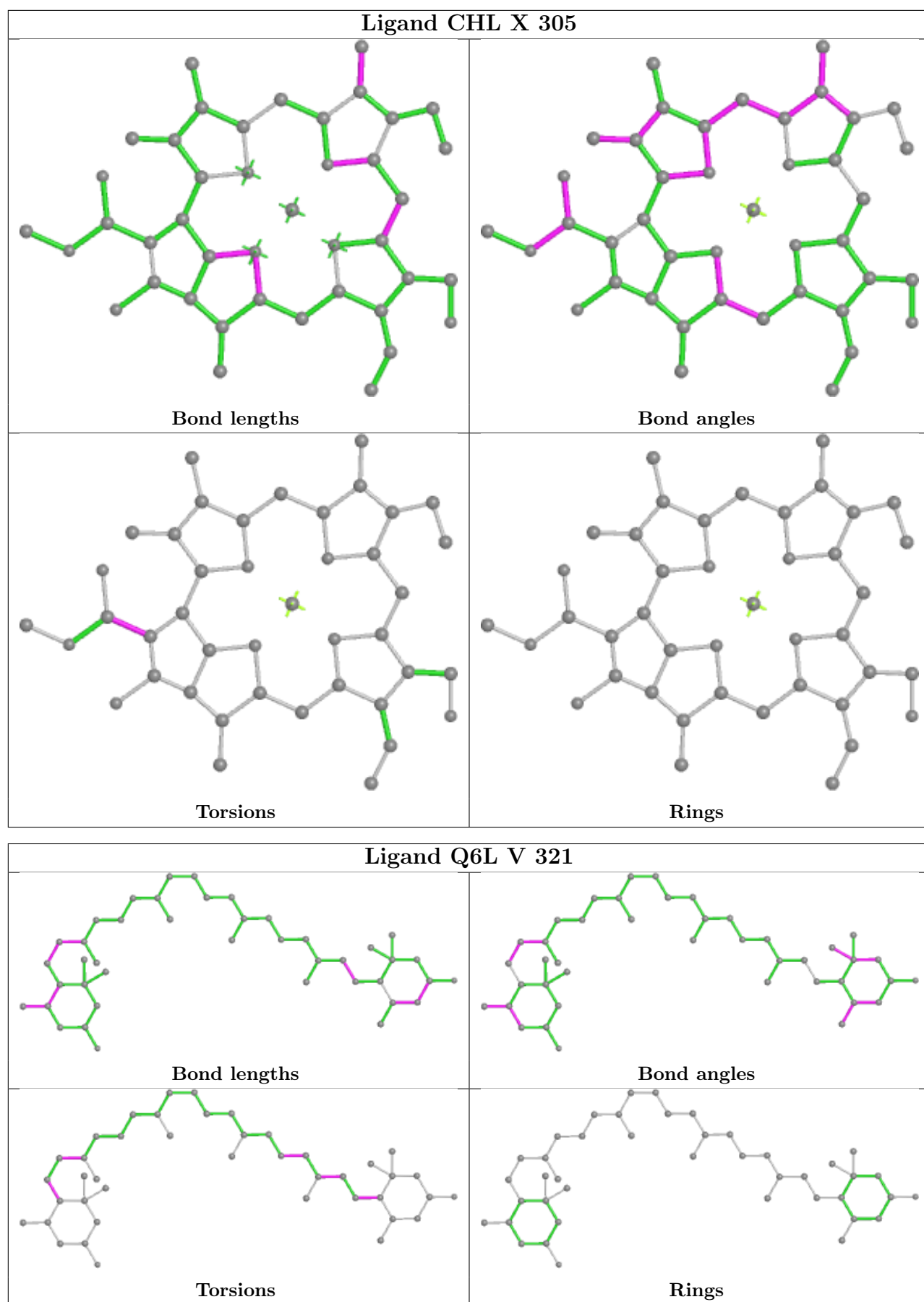


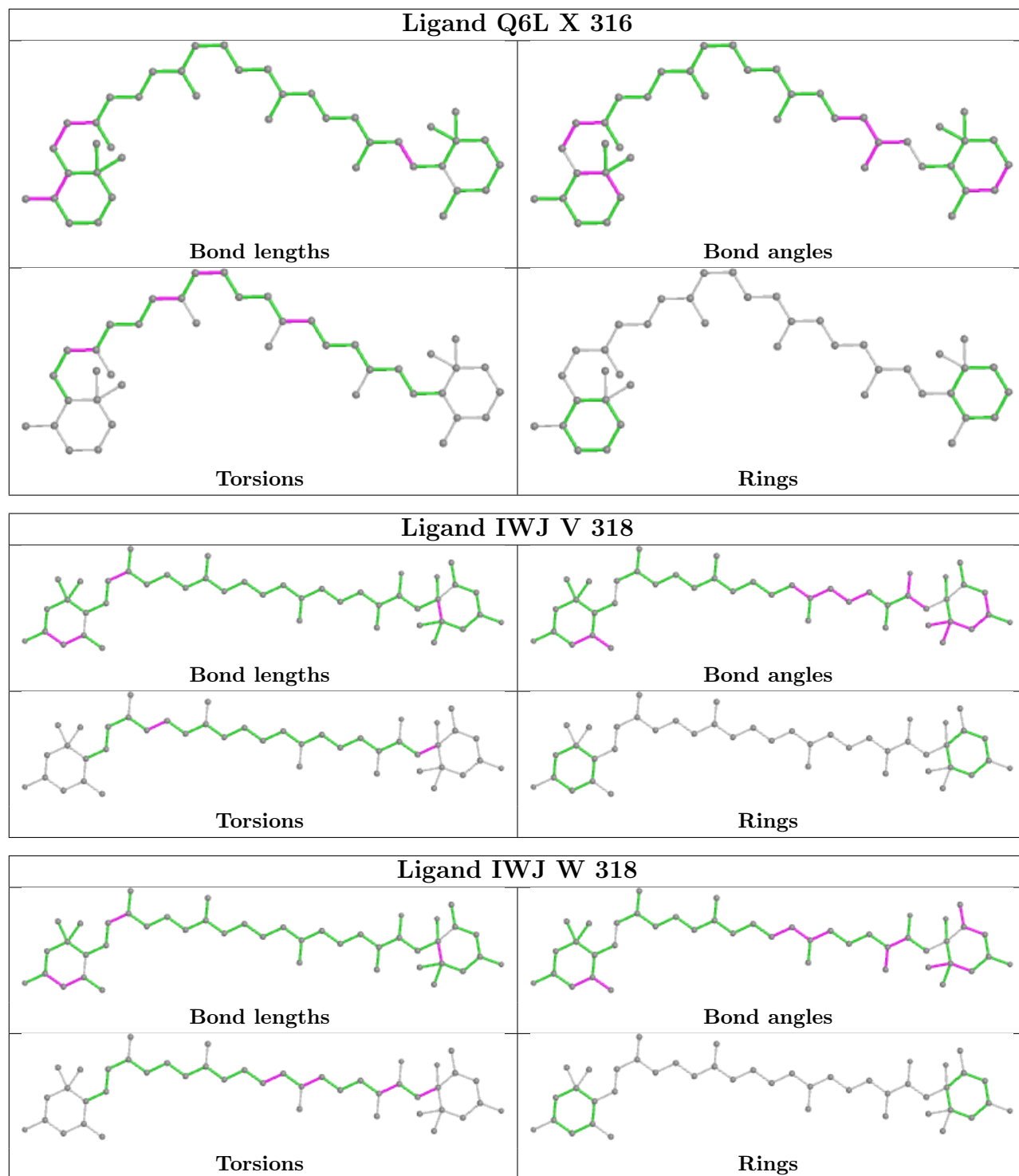


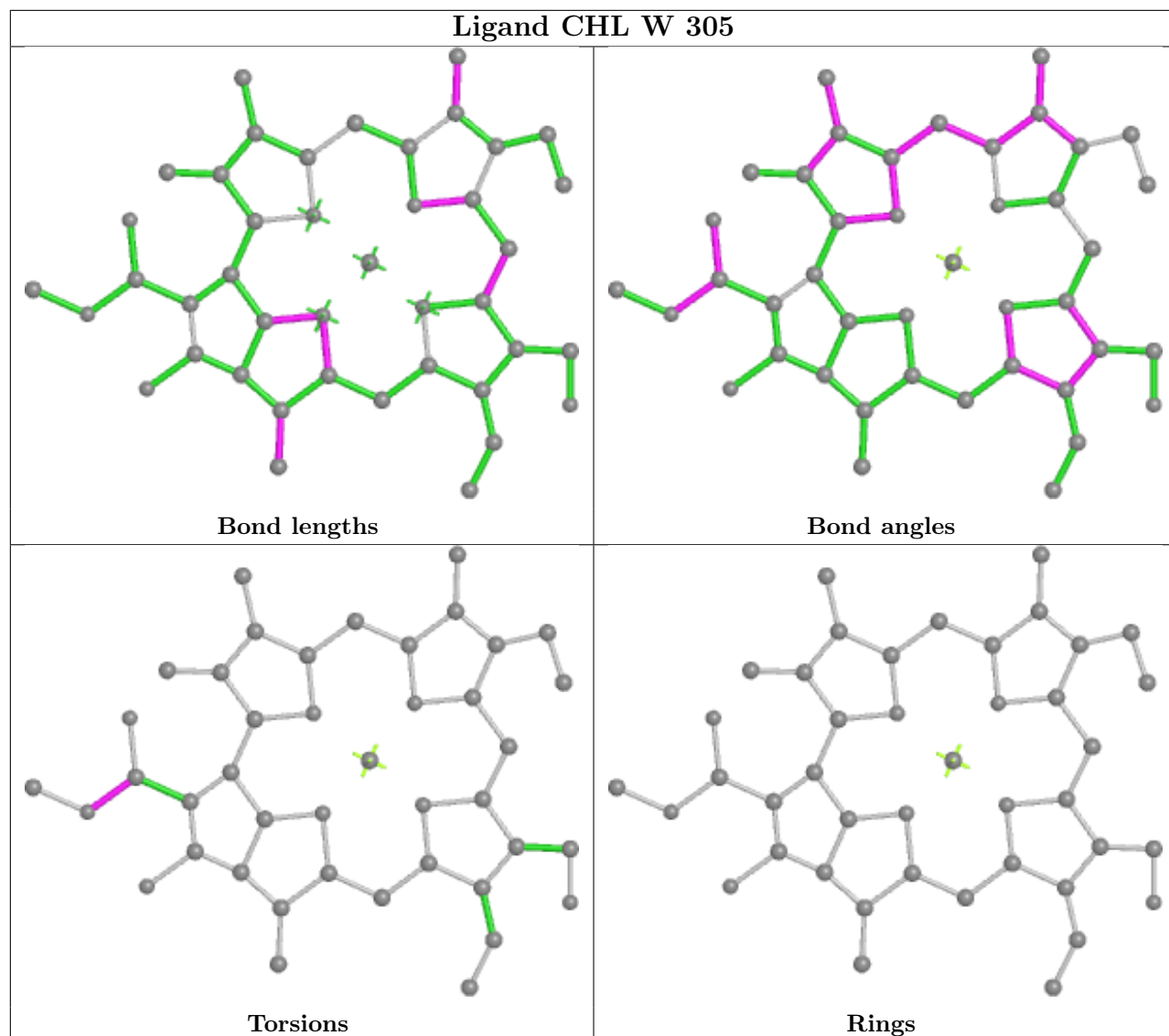


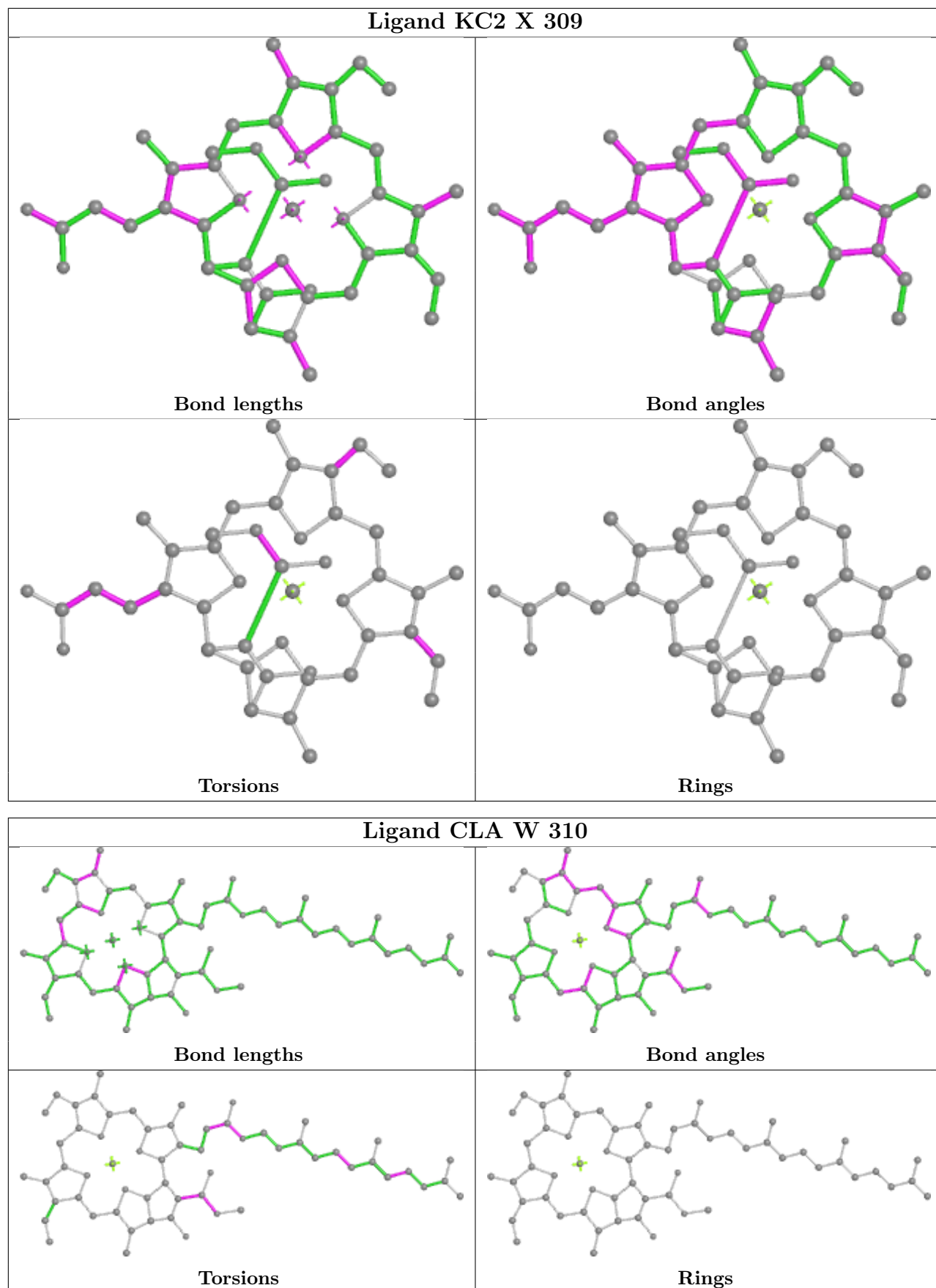


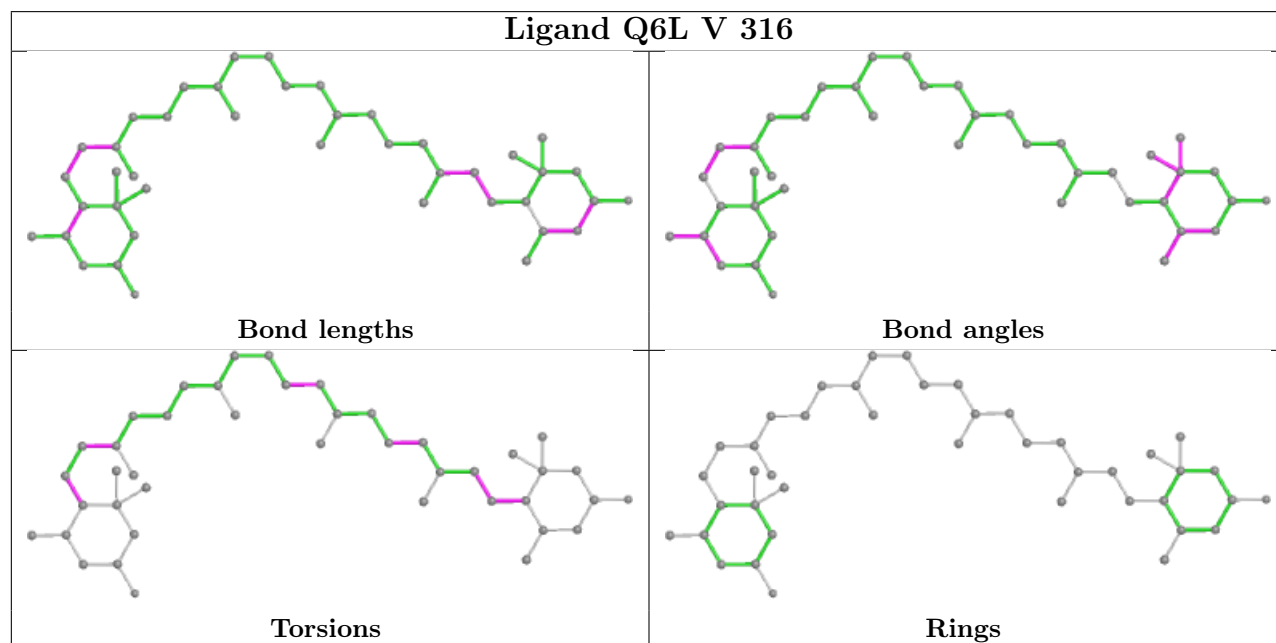
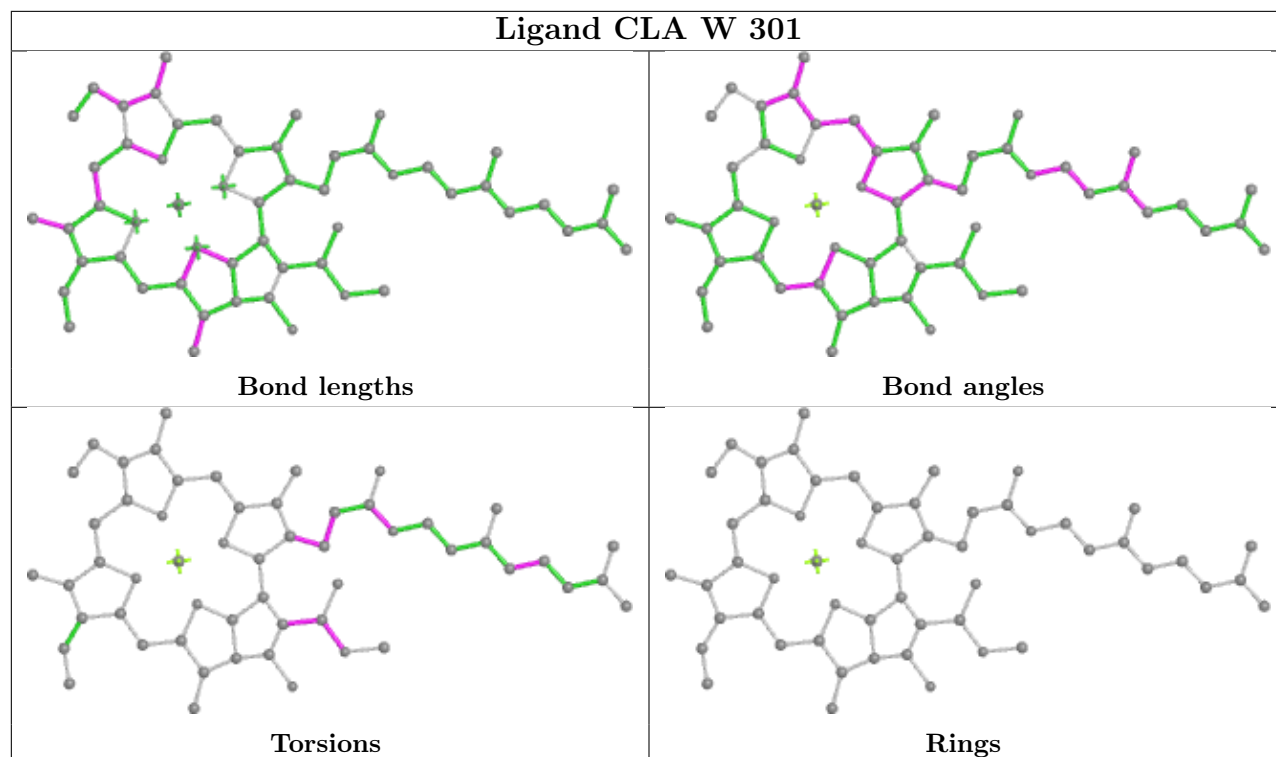


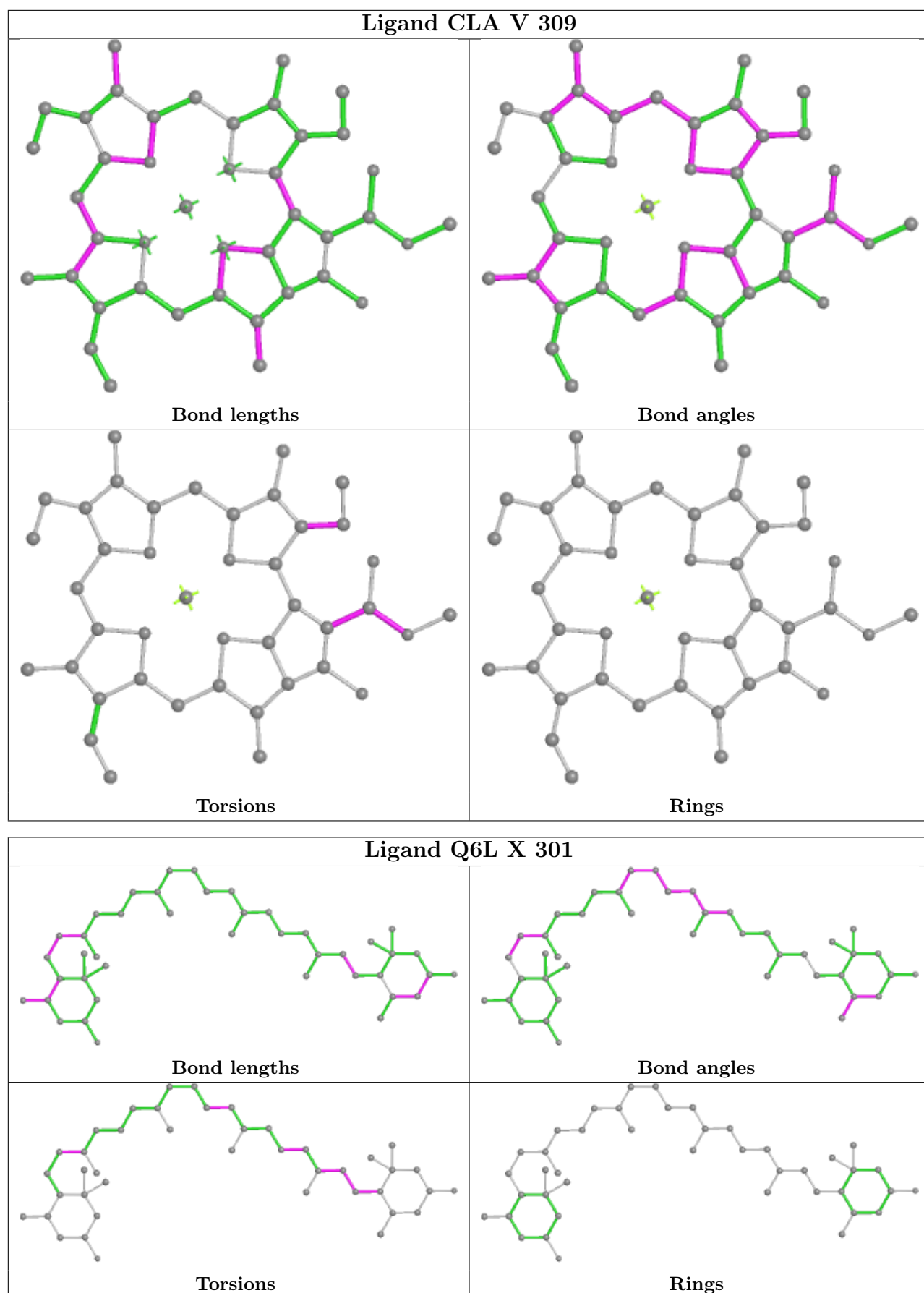


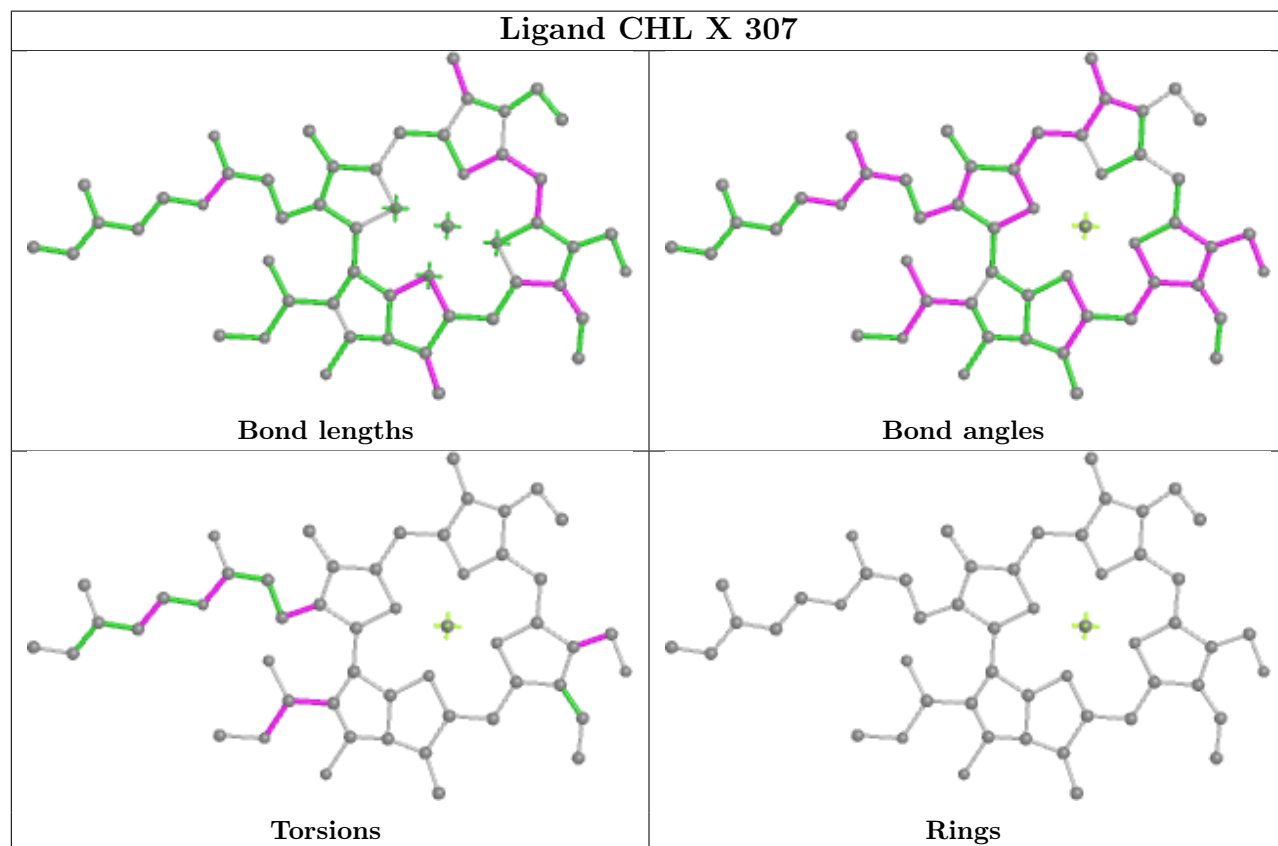
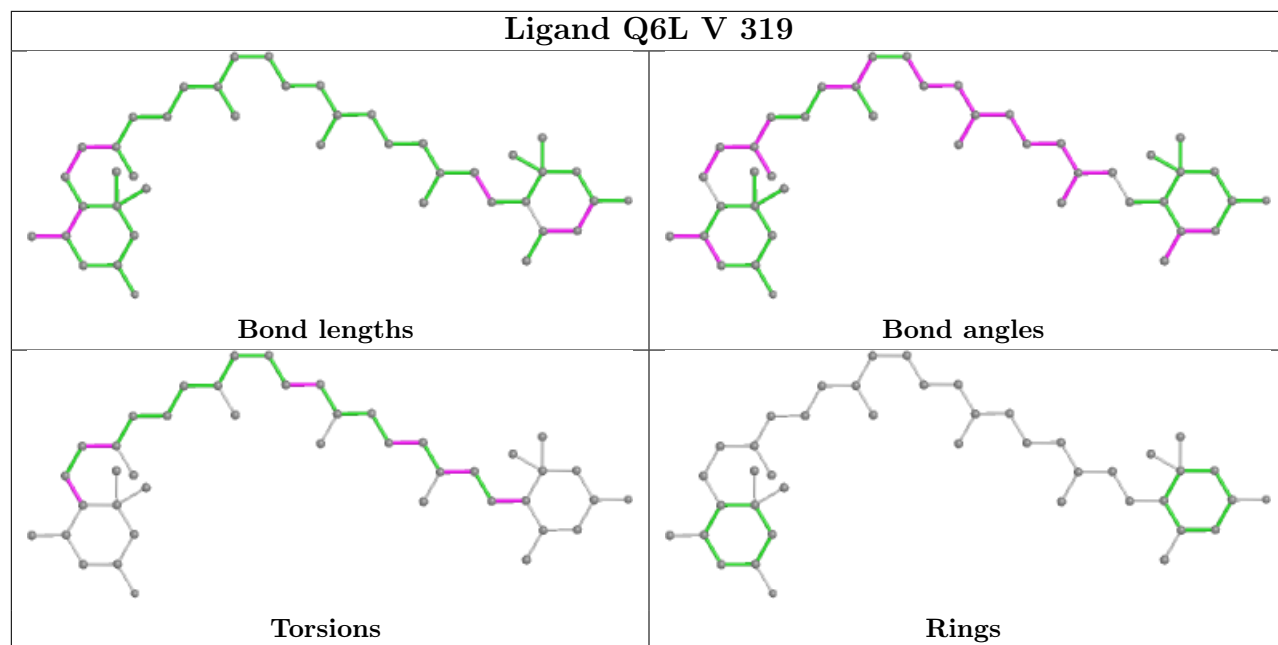


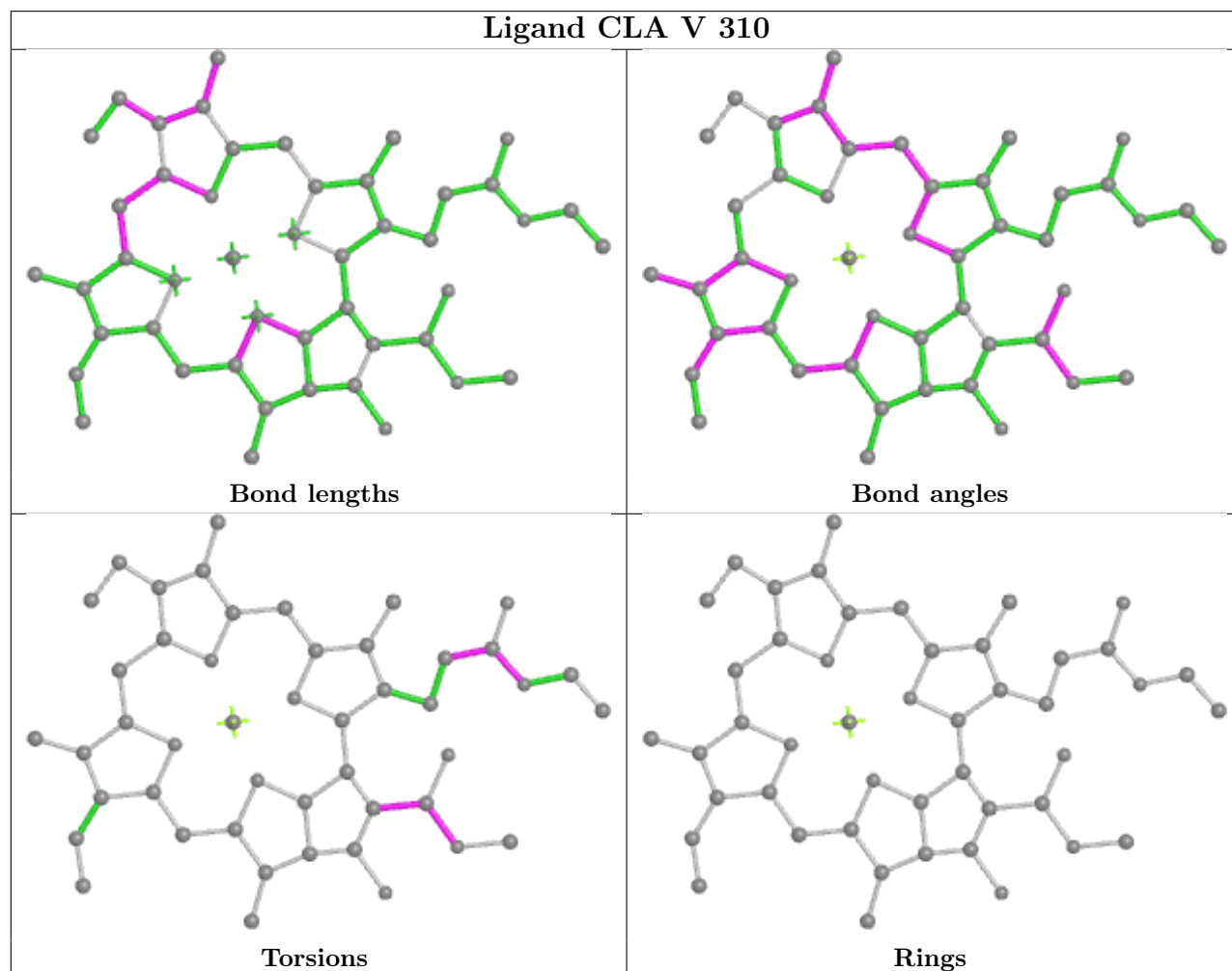
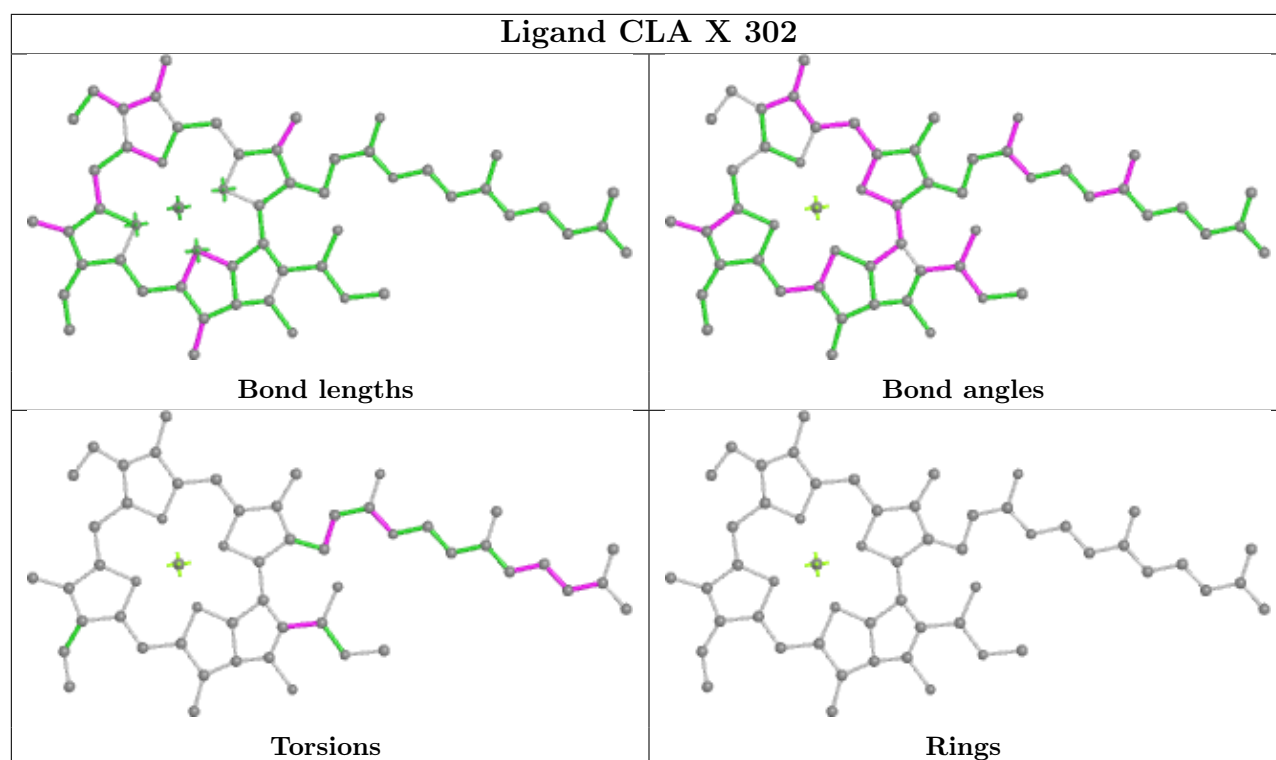


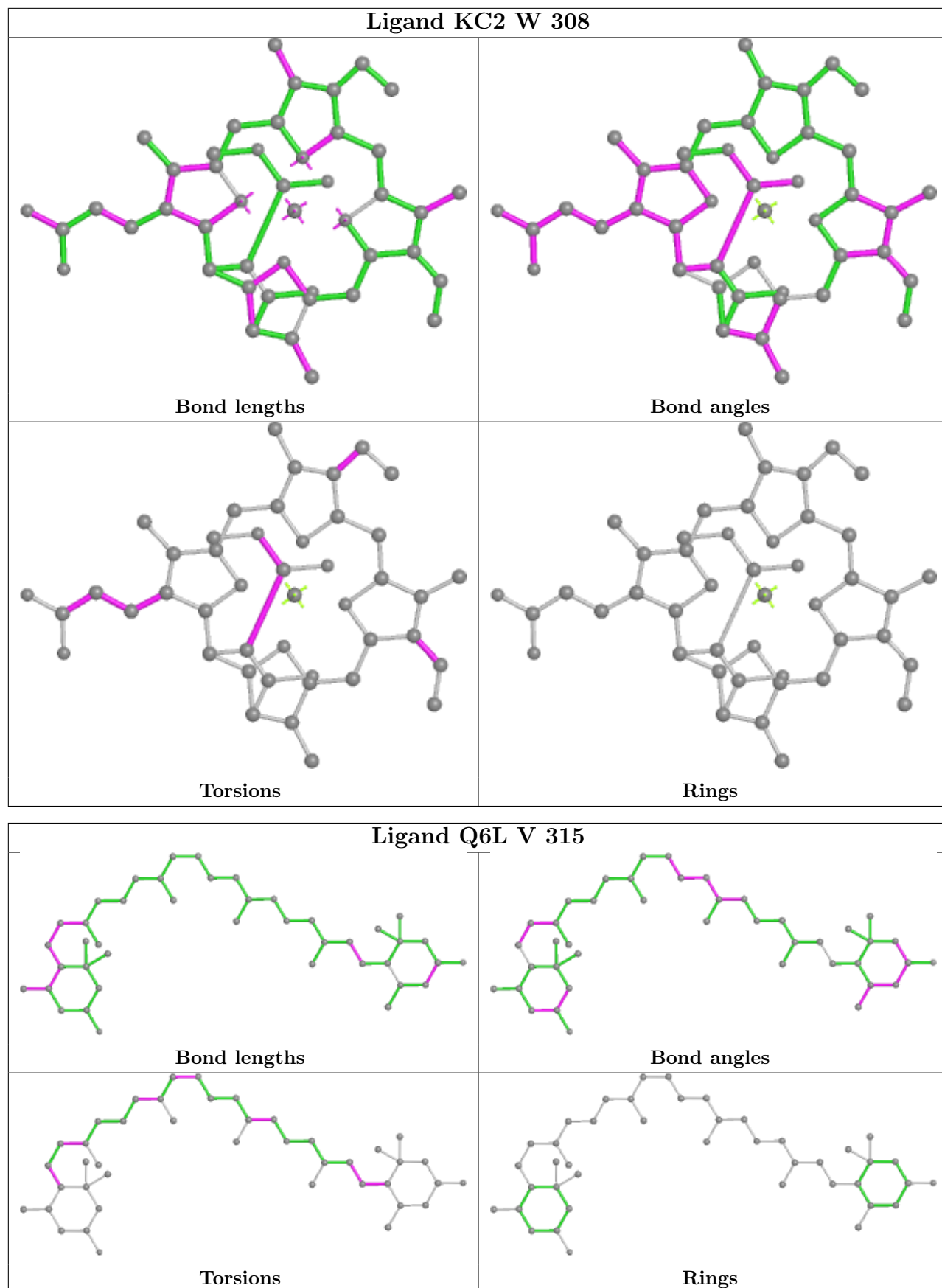


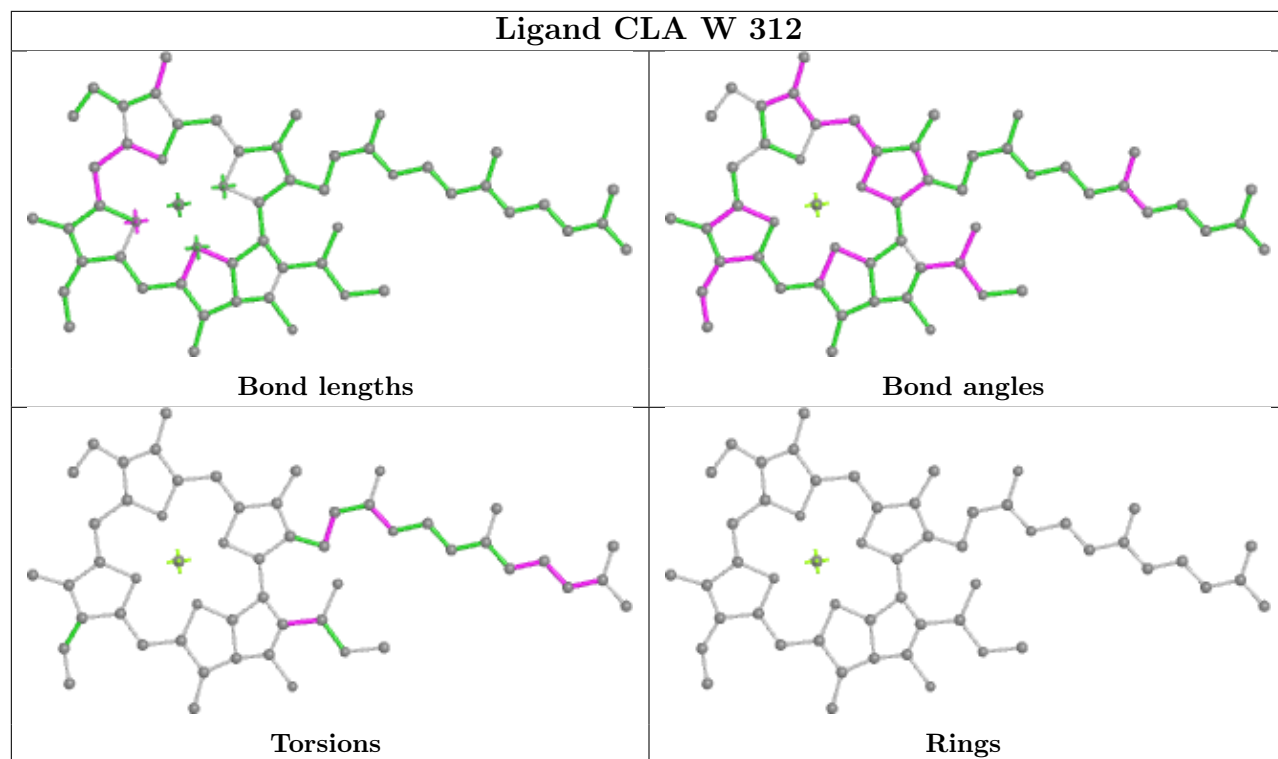


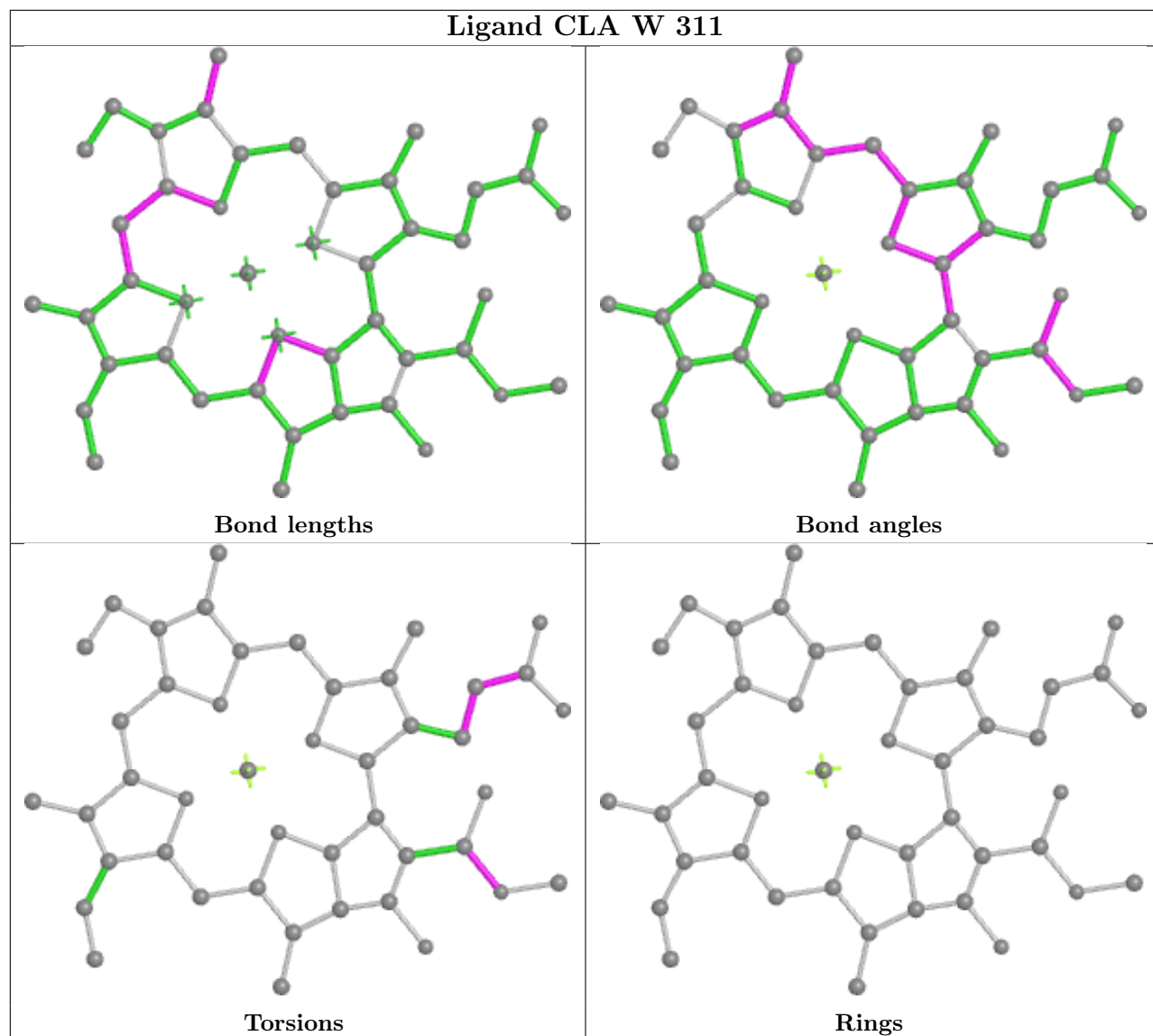


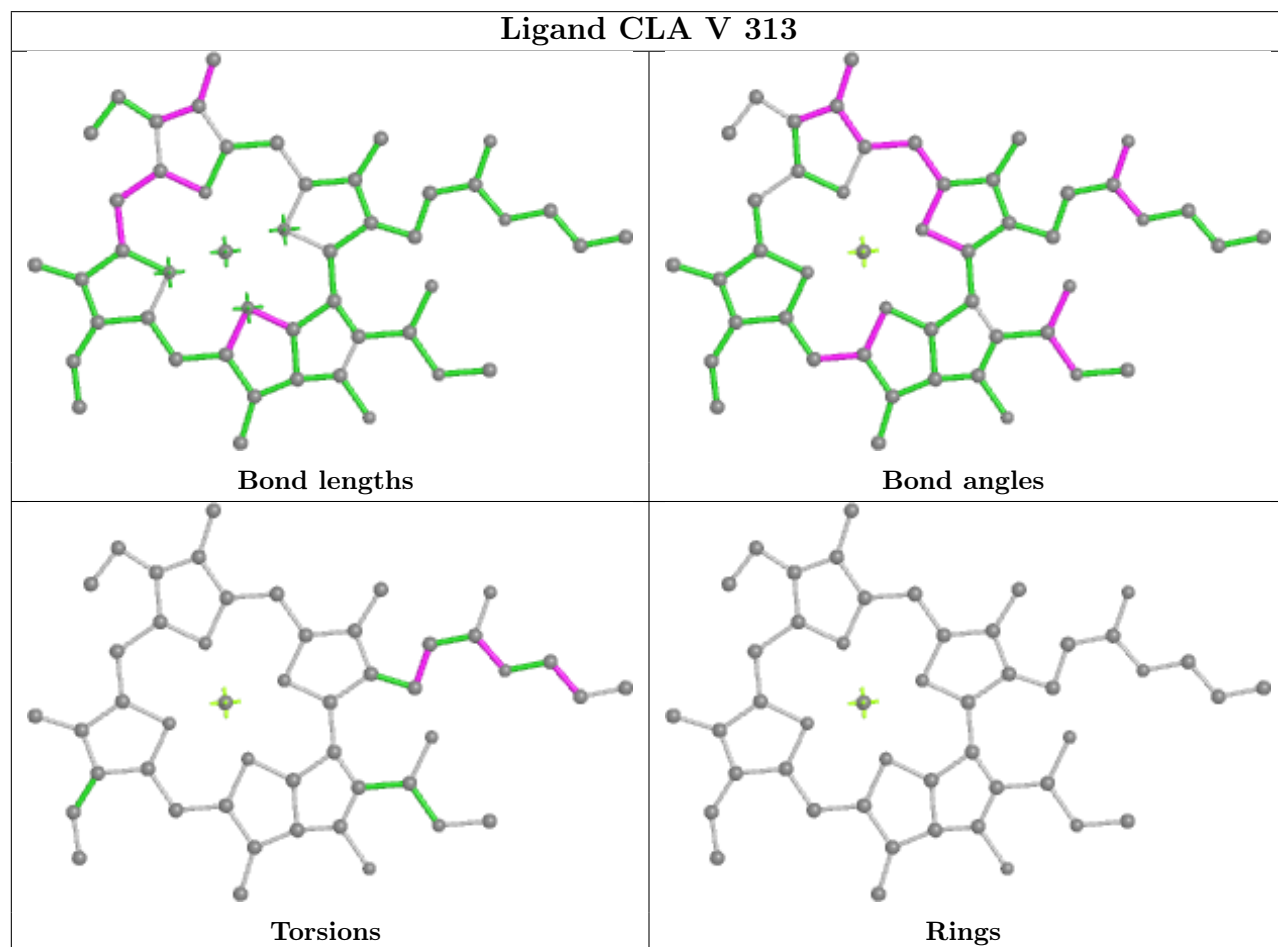
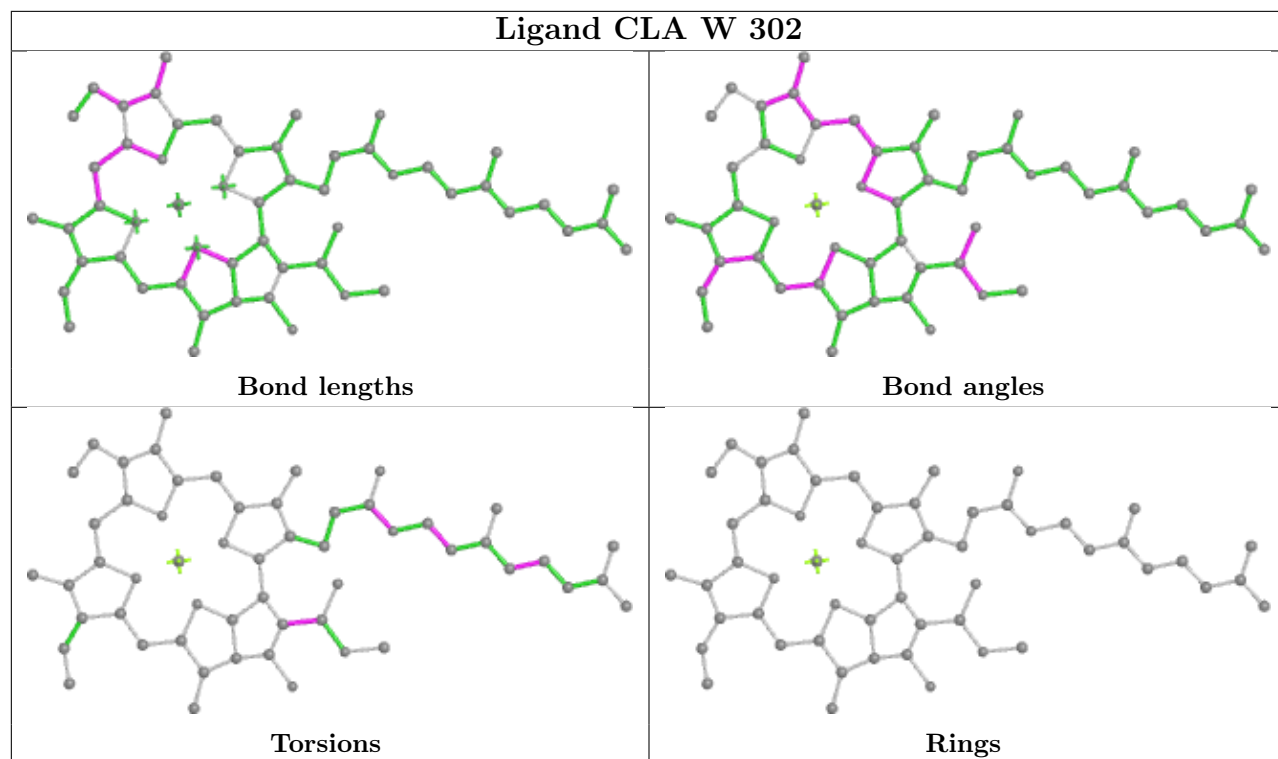


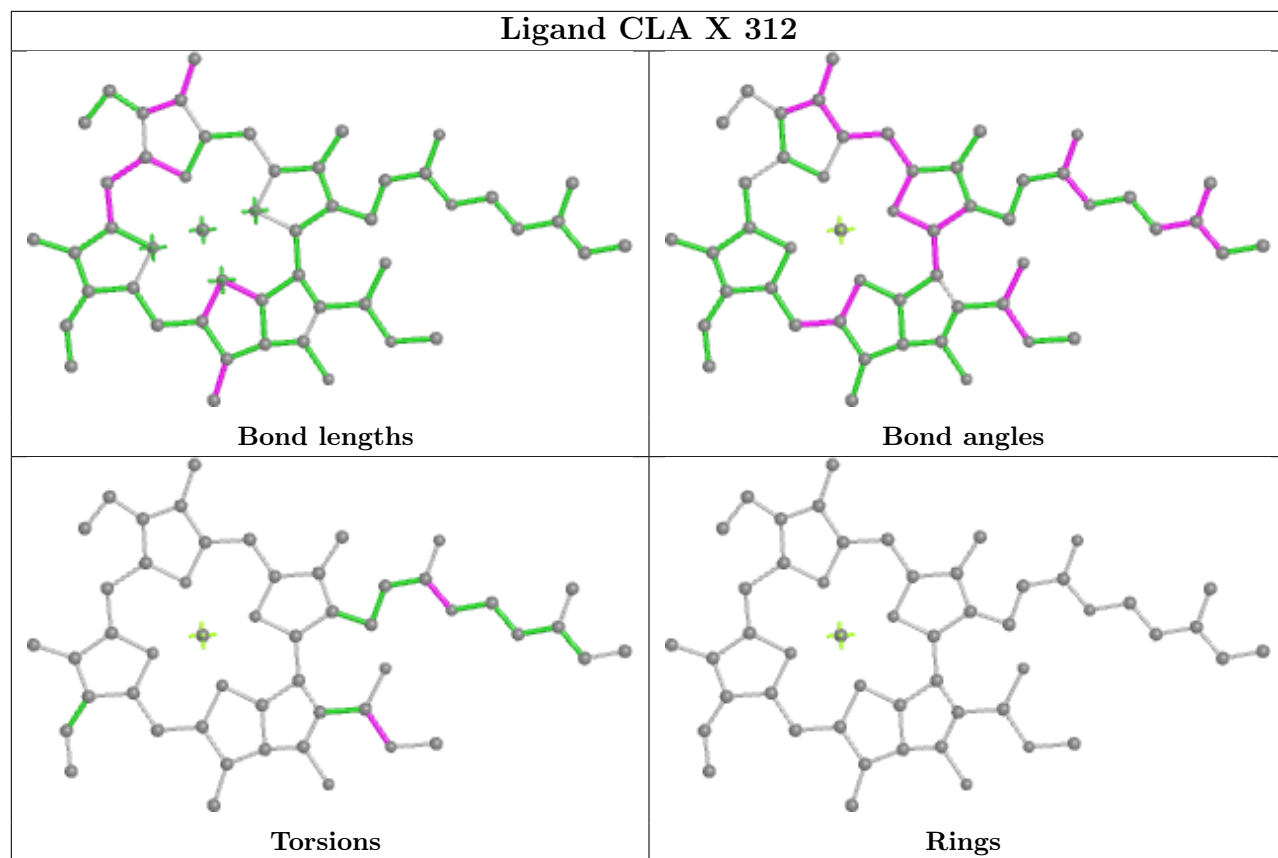


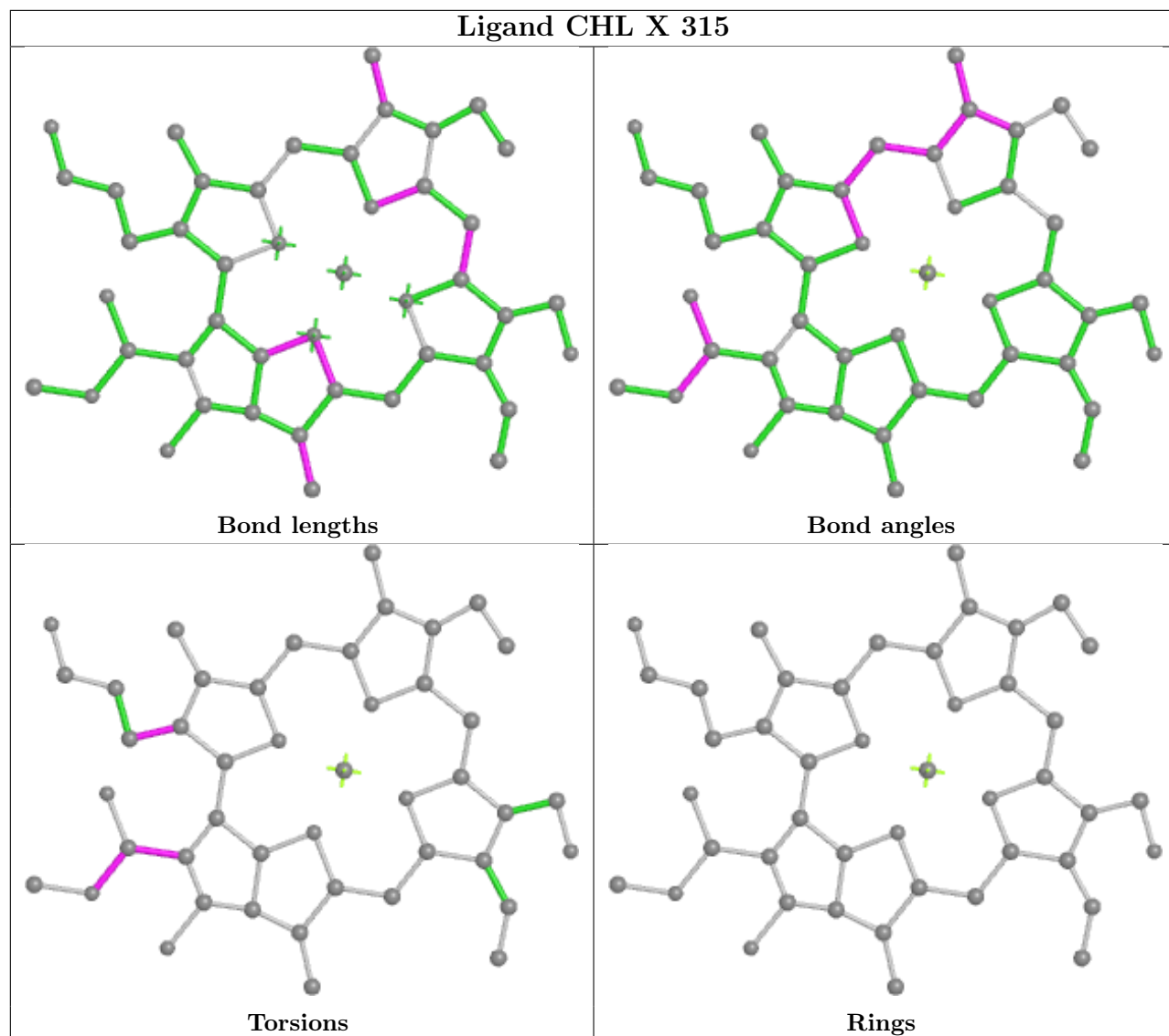


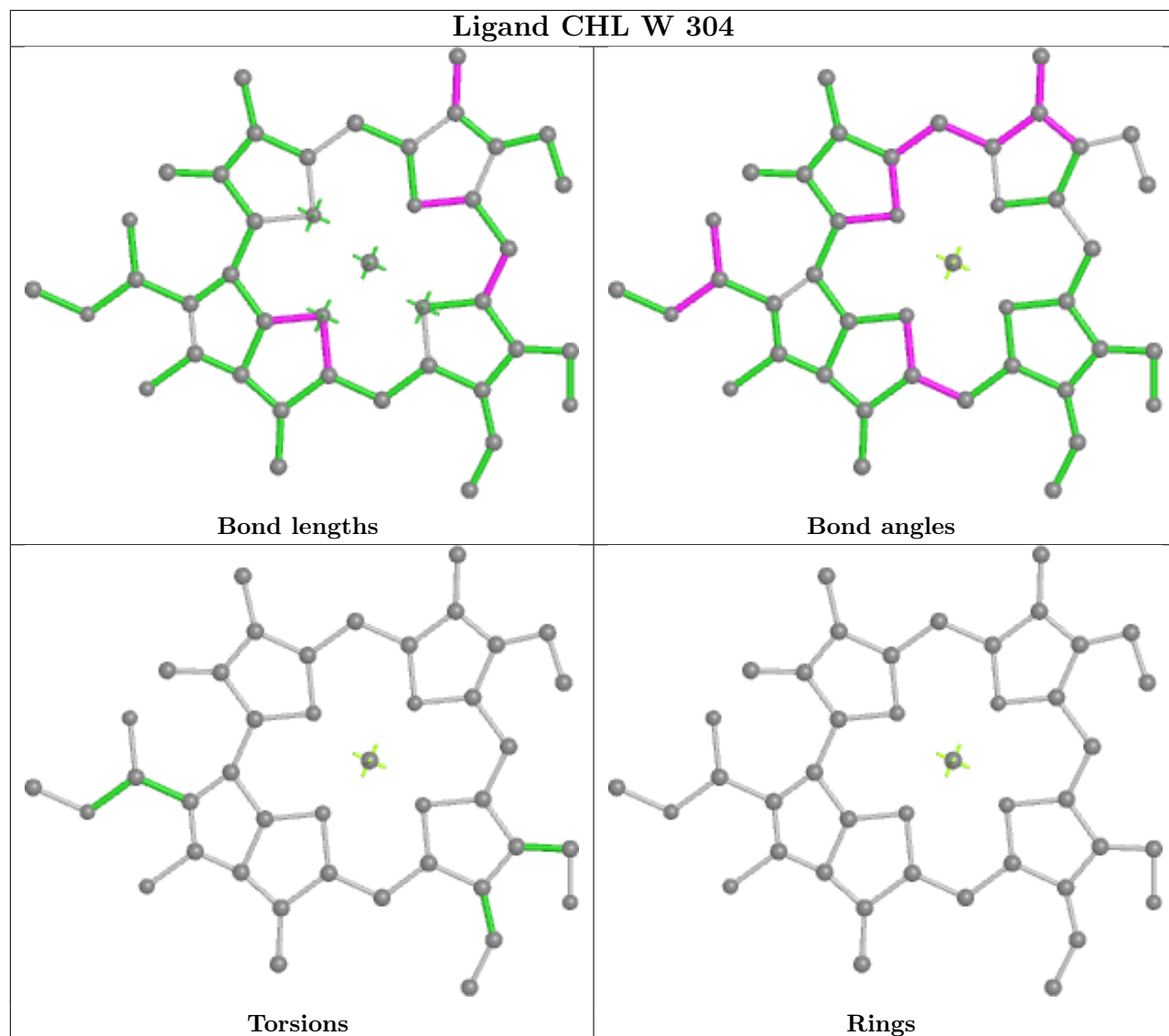


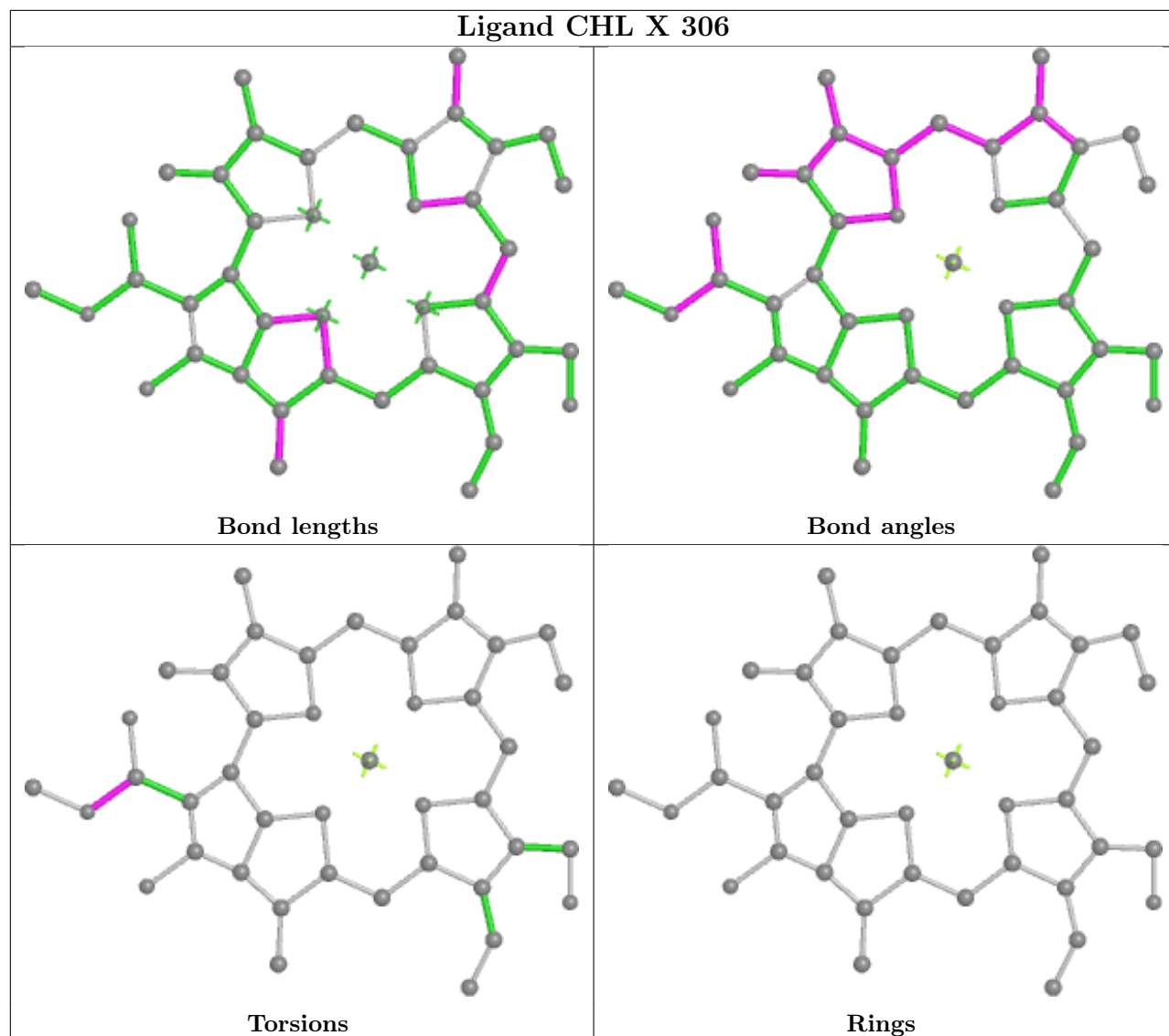


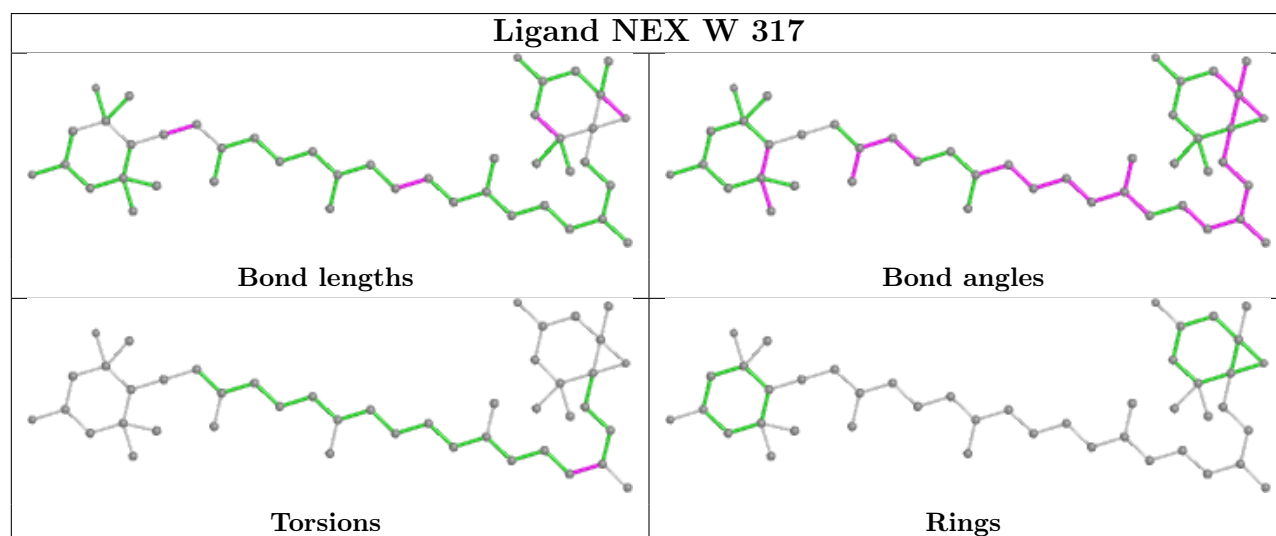
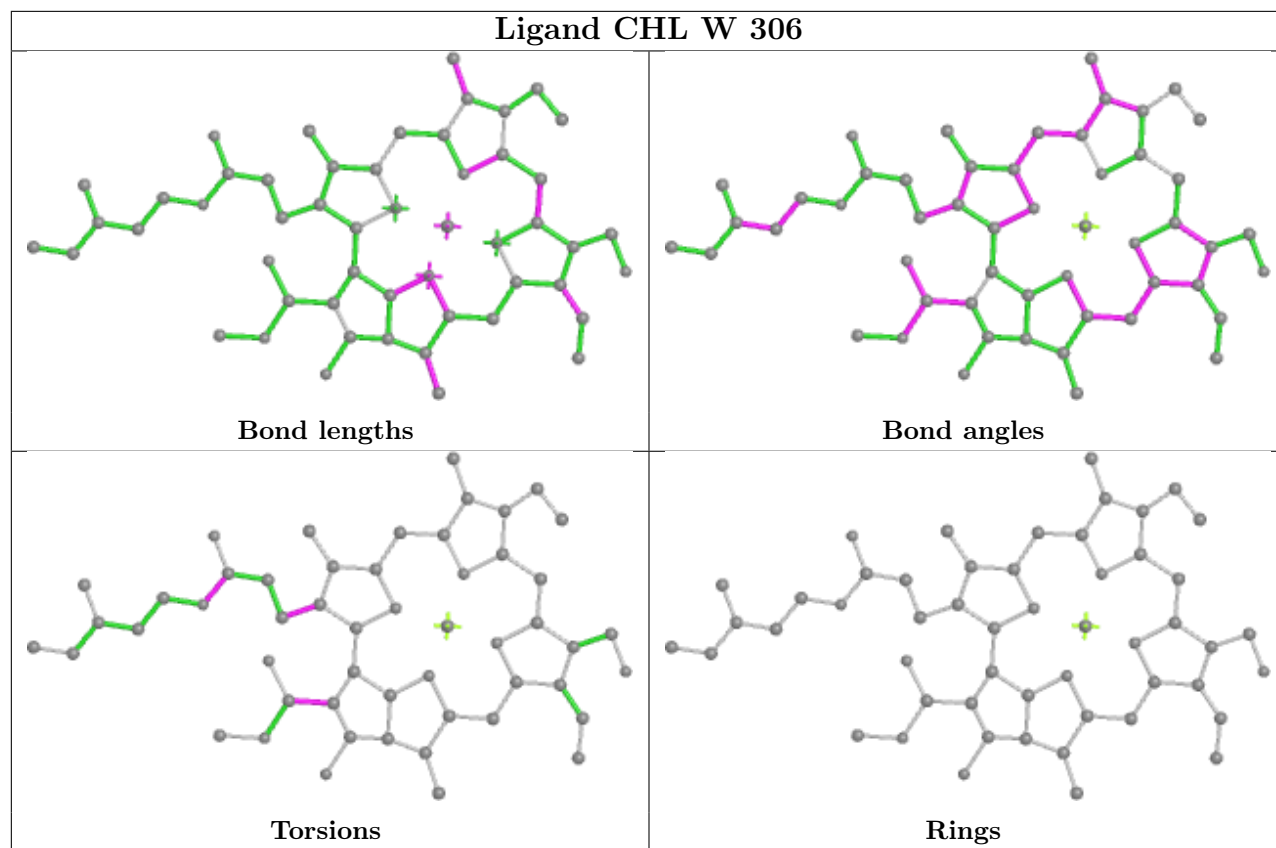


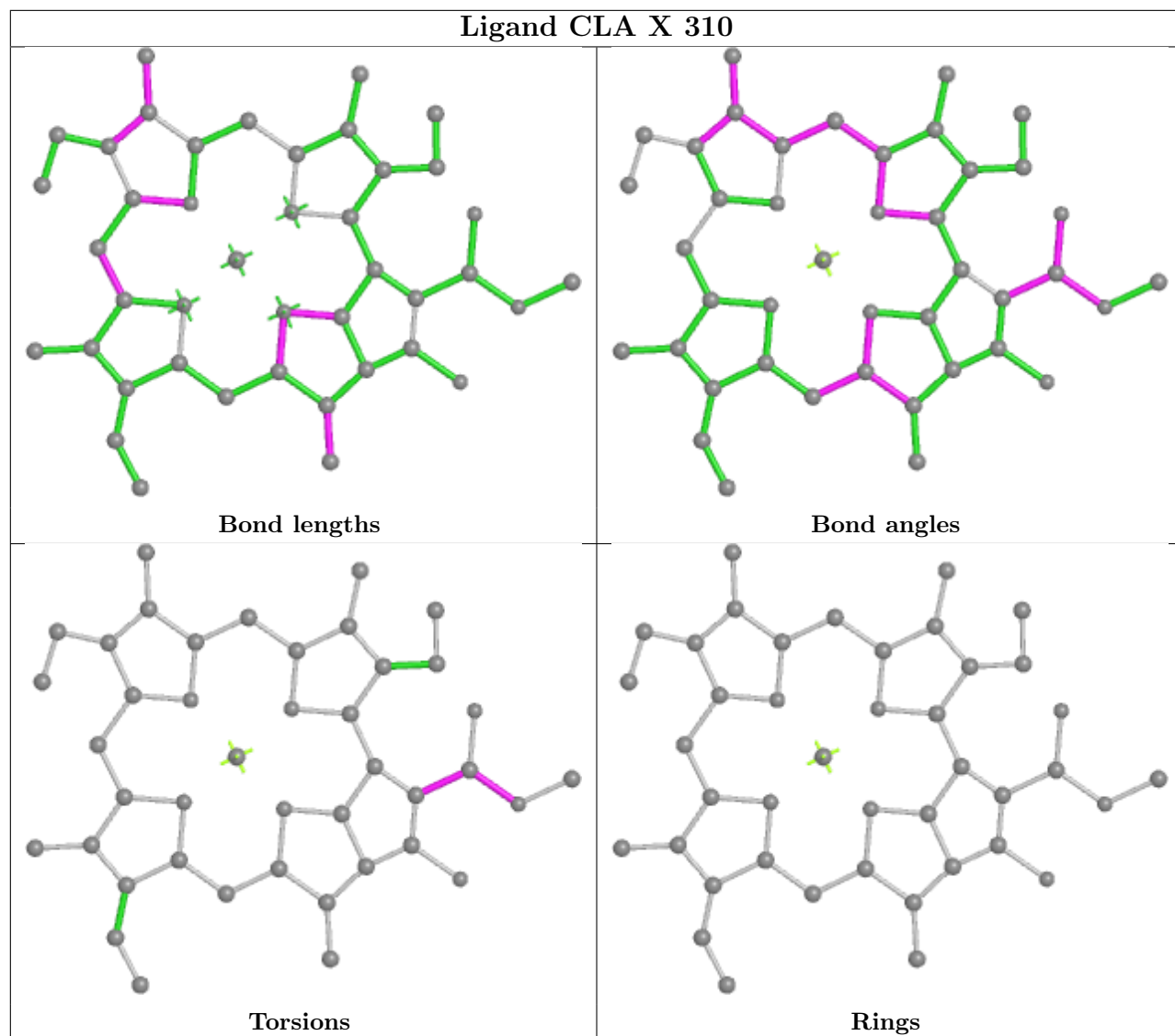


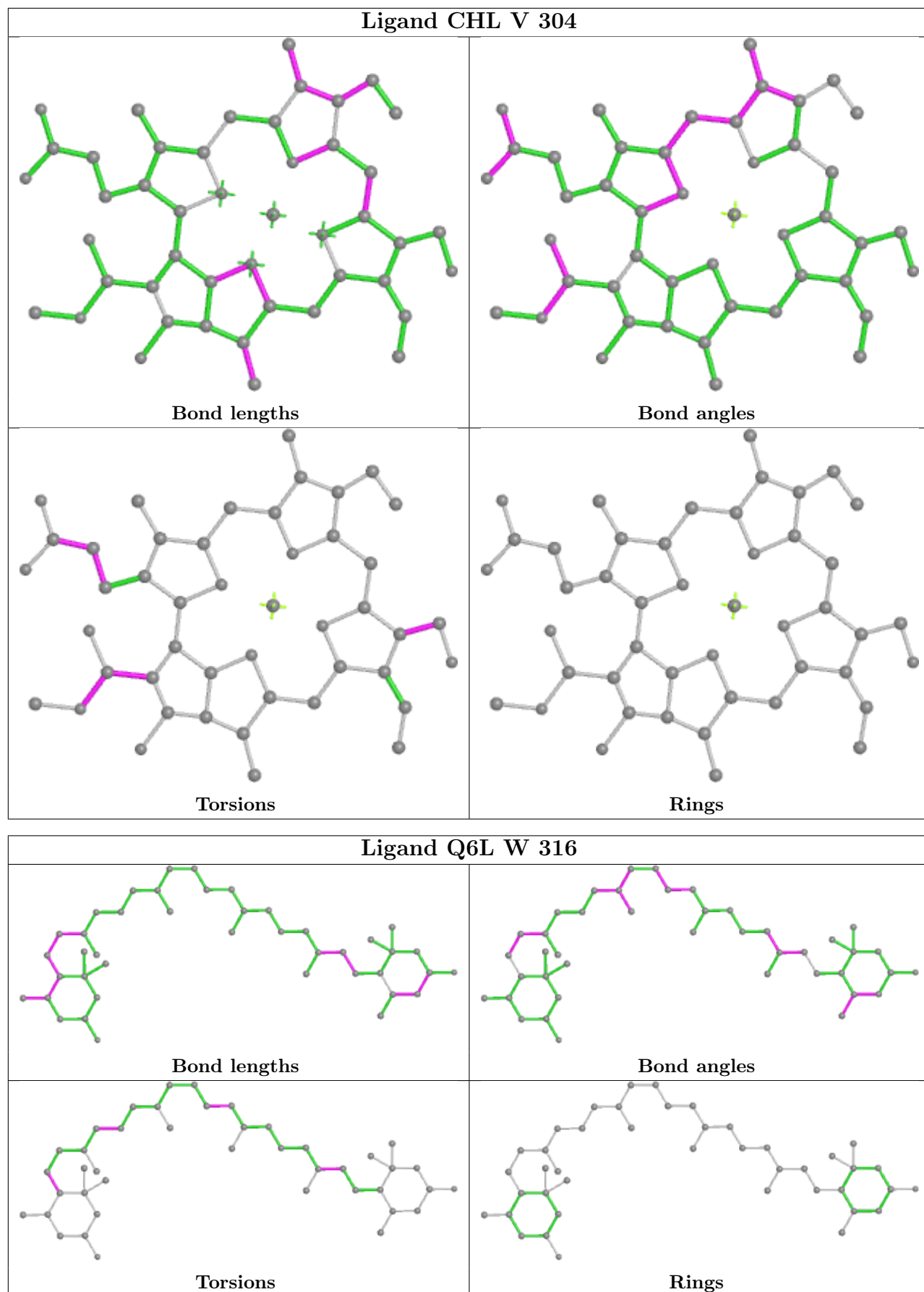


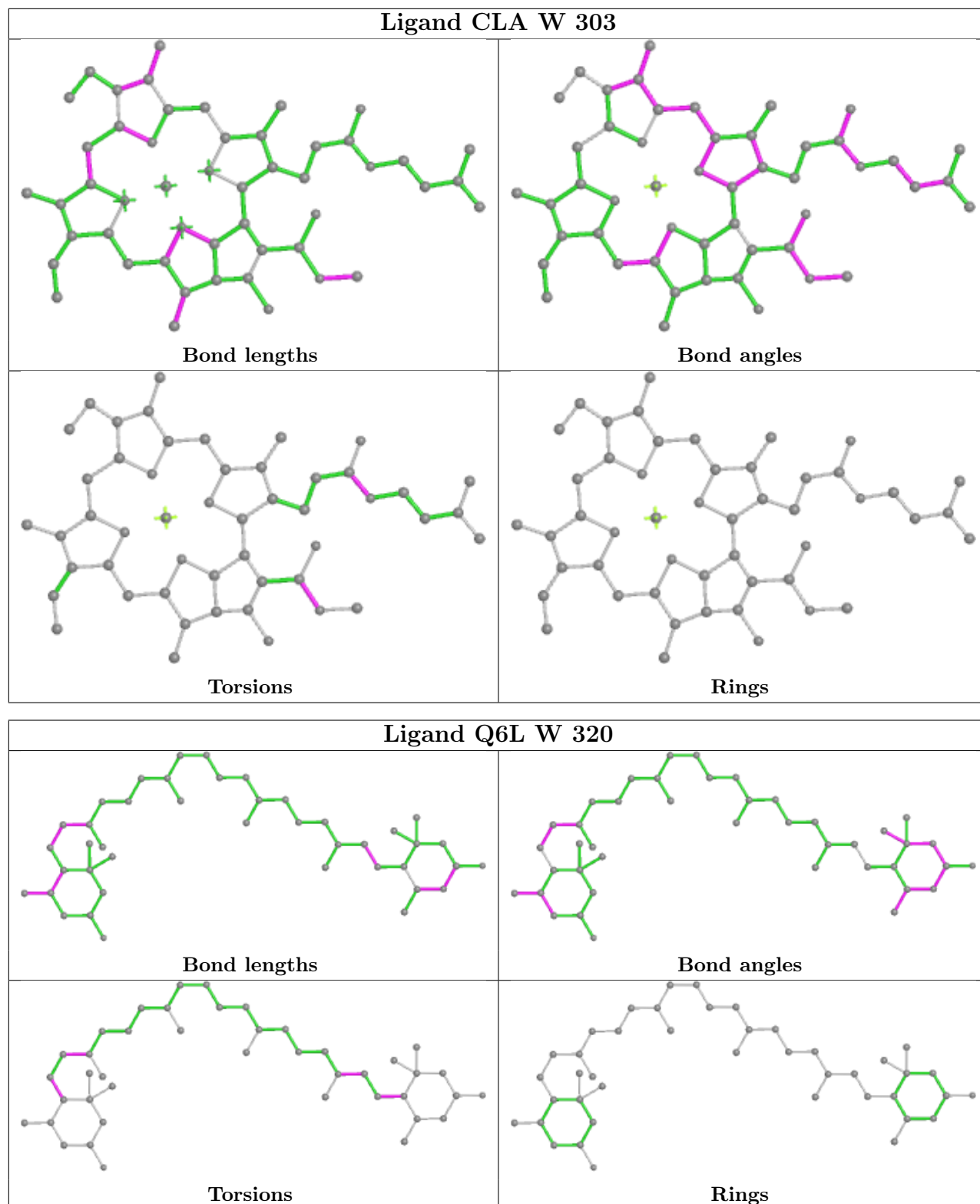


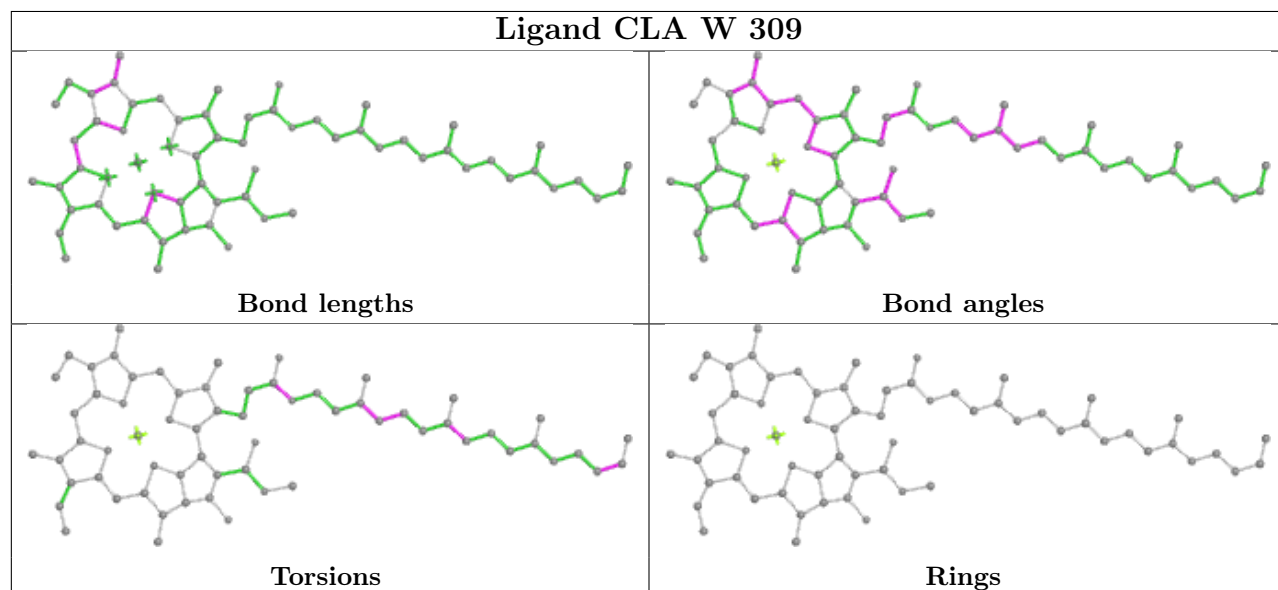
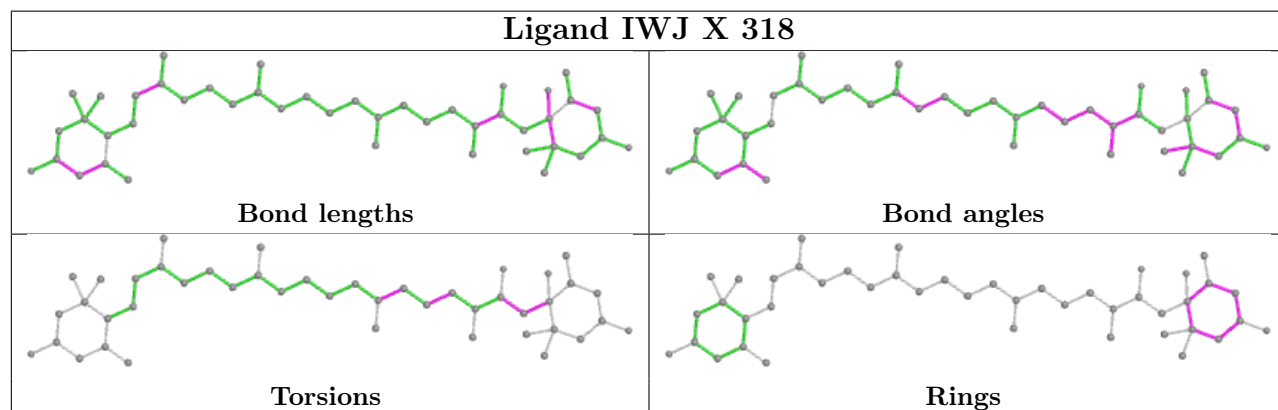
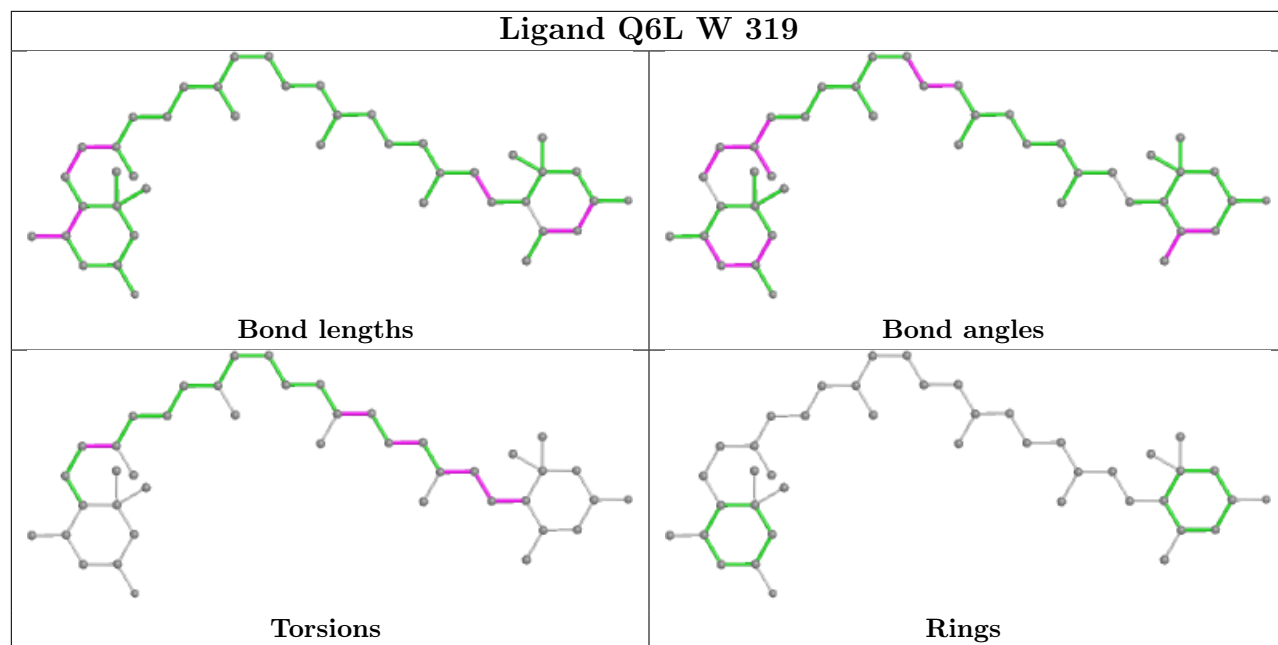


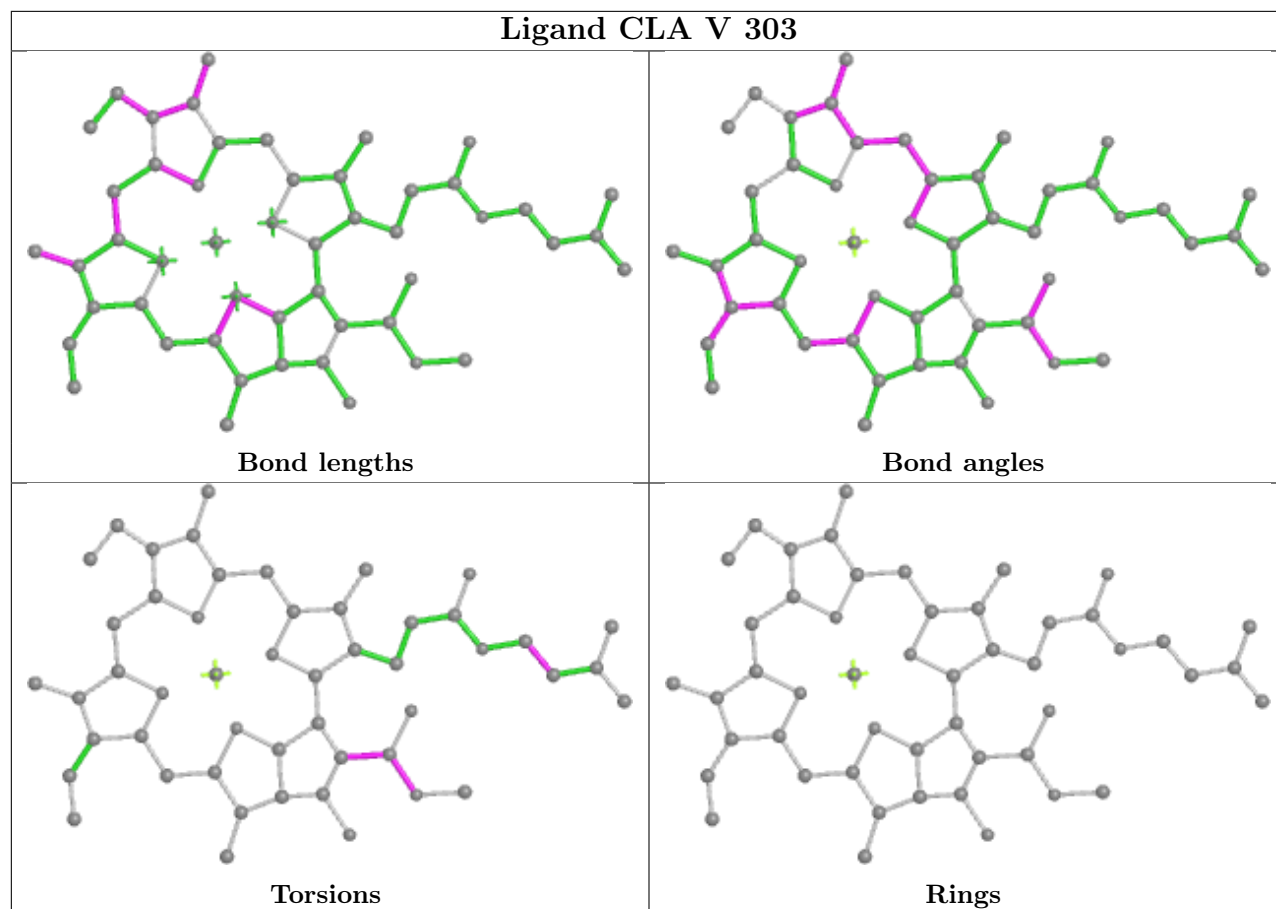












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

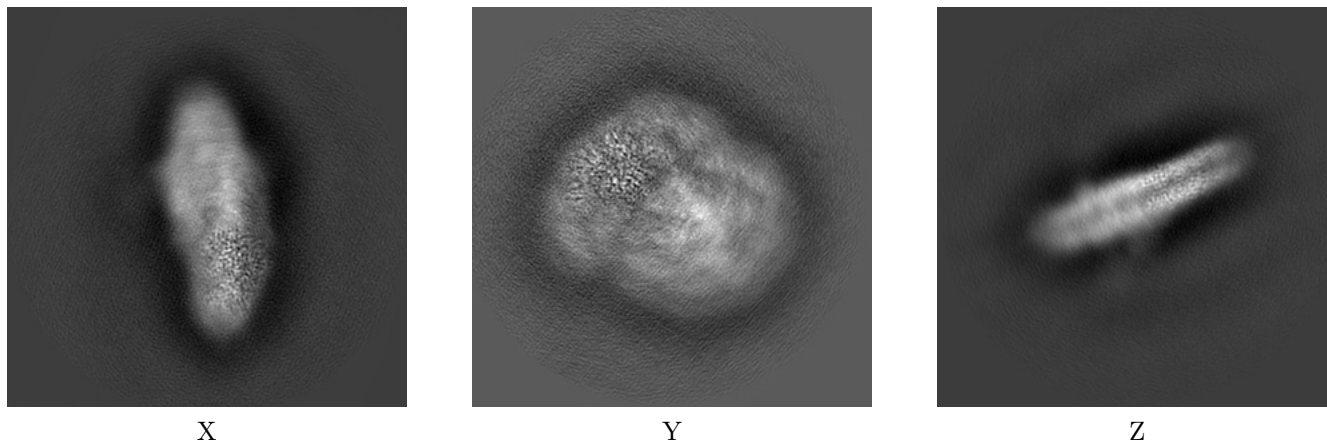
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34736. These allow visual inspection of the internal detail of the map and identification of artifacts.

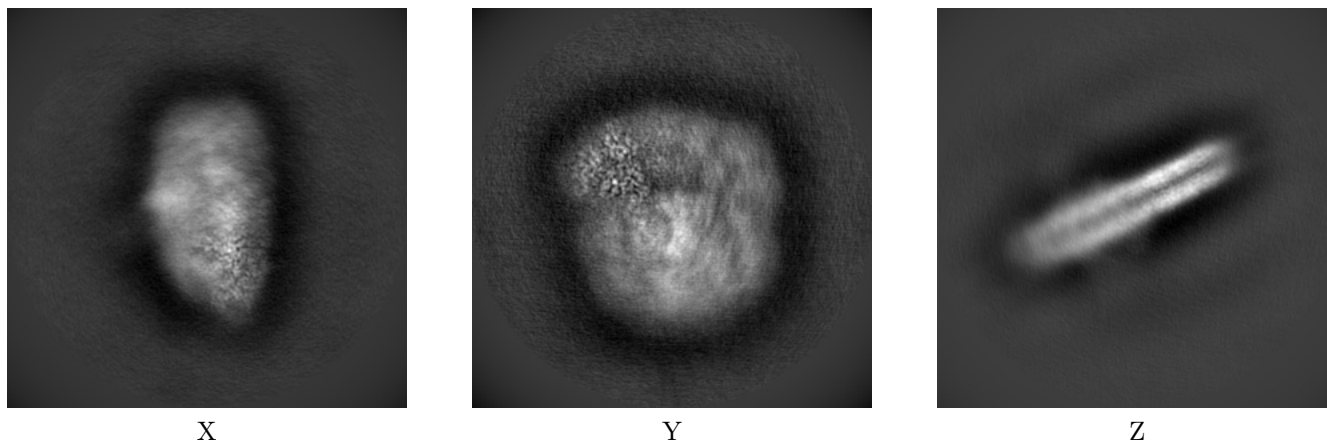
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



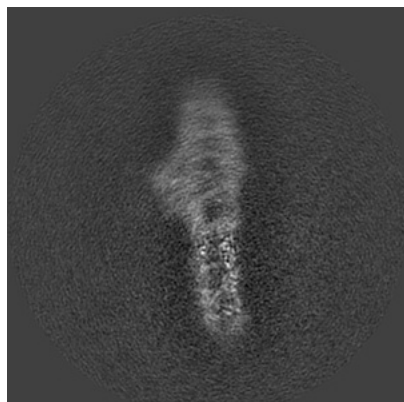
6.1.2 Raw map



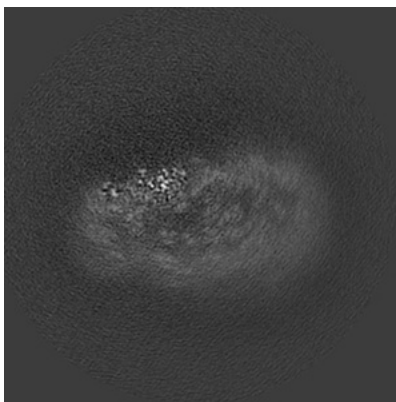
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

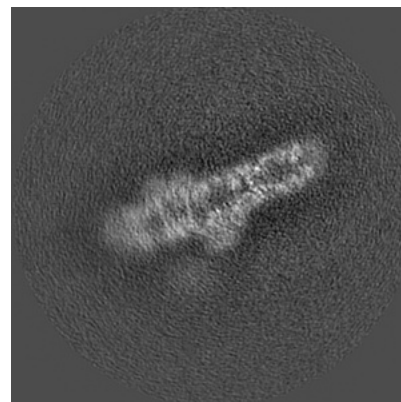
6.2.1 Primary map



X Index: 192

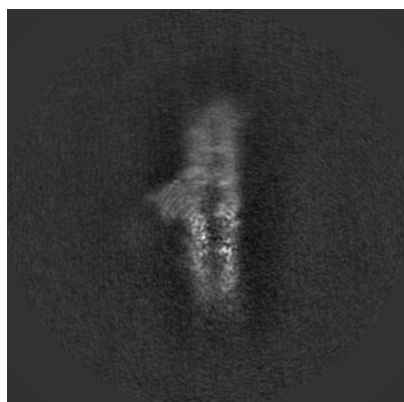


Y Index: 192

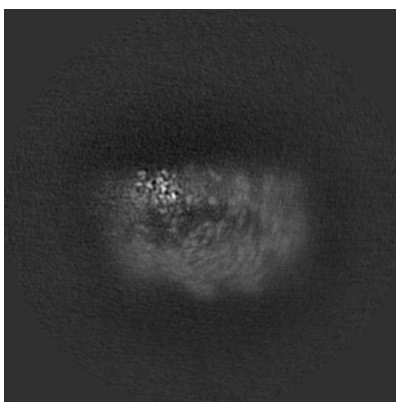


Z Index: 192

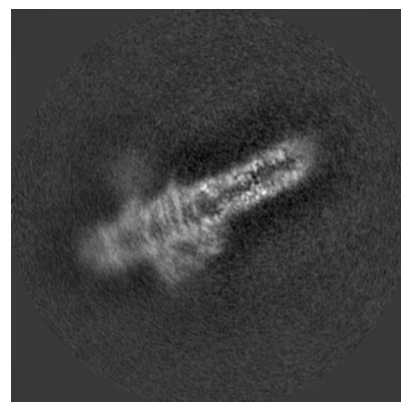
6.2.2 Raw map



X Index: 192



Y Index: 192

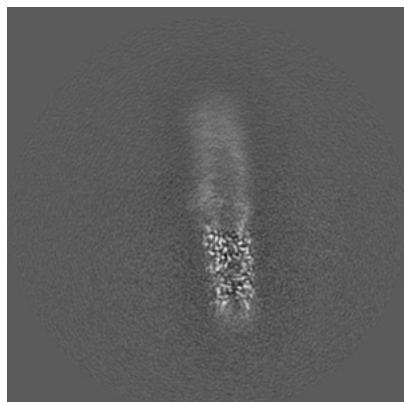


Z Index: 192

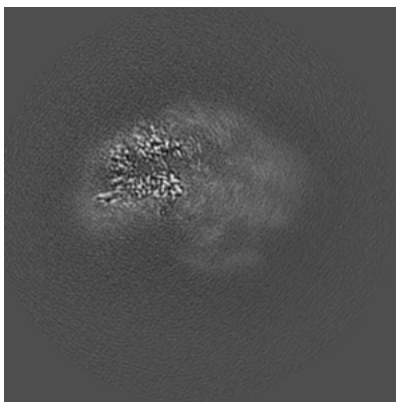
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

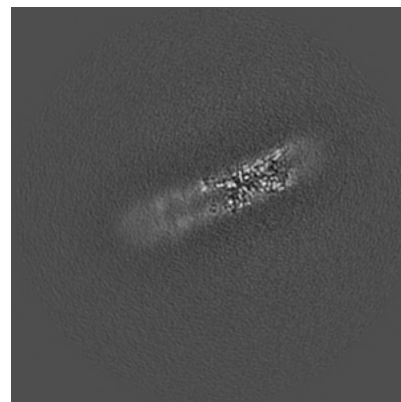
6.3.1 Primary map



X Index: 224

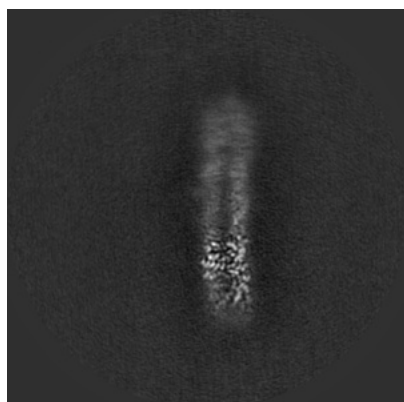


Y Index: 218

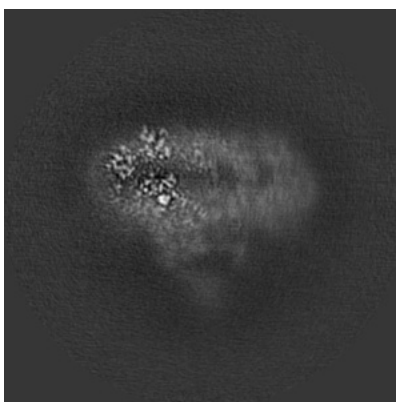


Z Index: 150

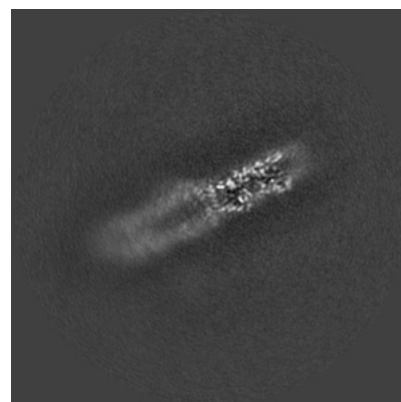
6.3.2 Raw map



X Index: 215



Y Index: 213

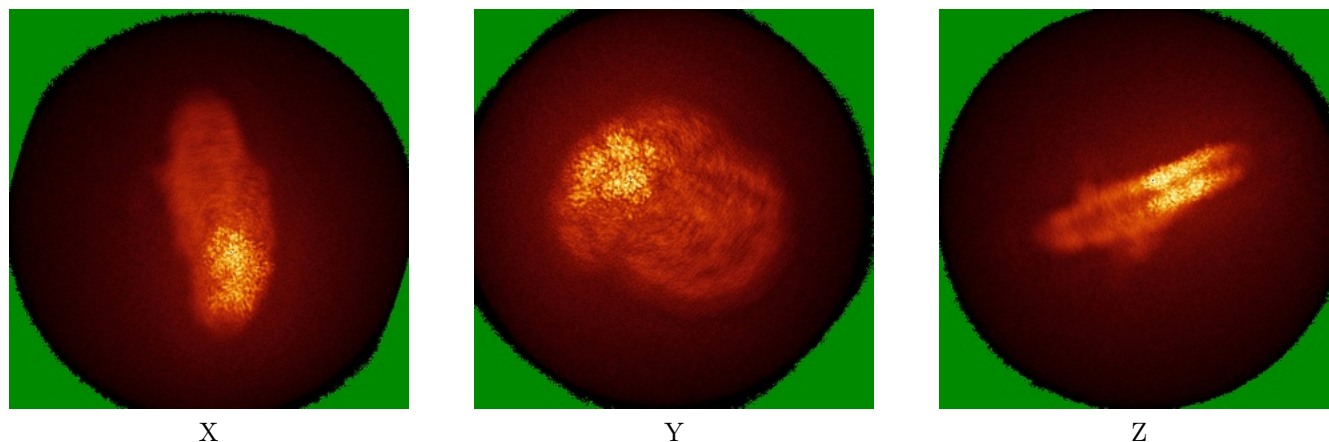


Z Index: 151

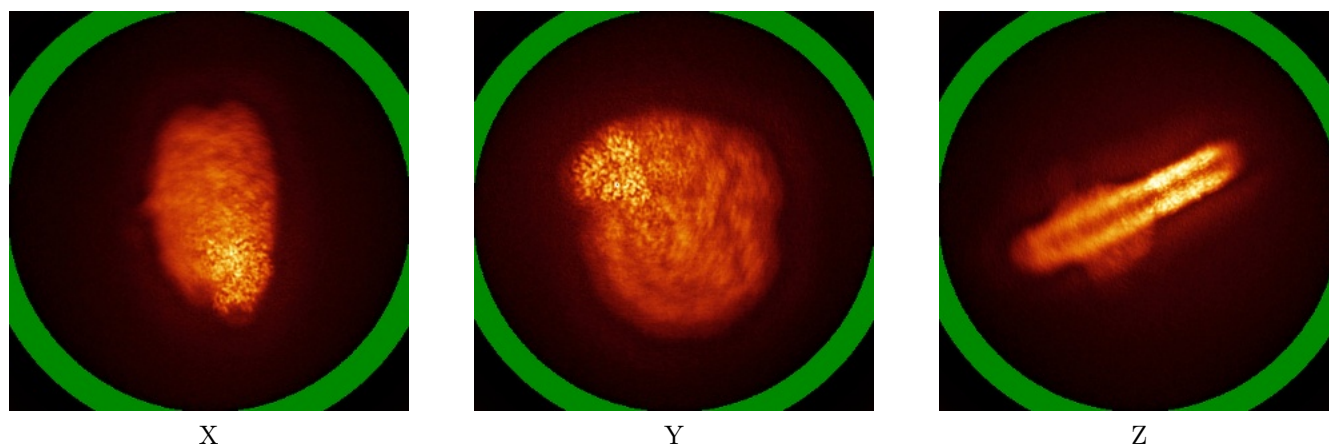
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



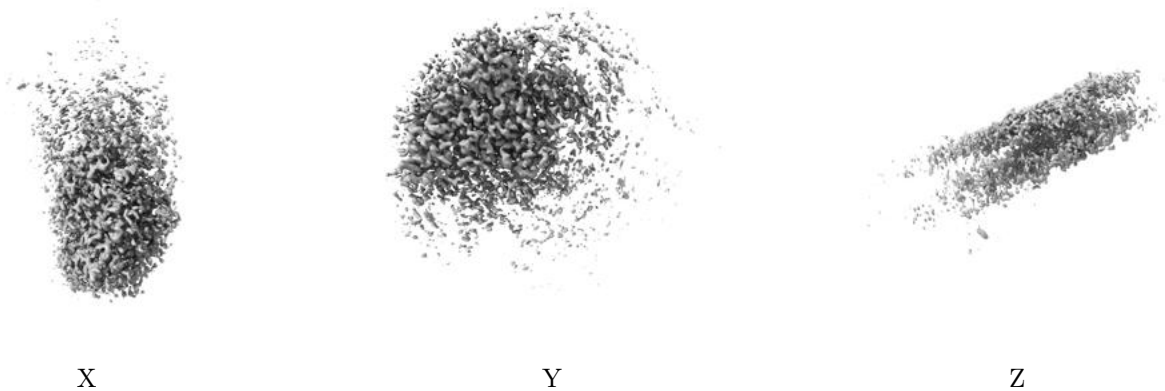
6.4.2 Raw map



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

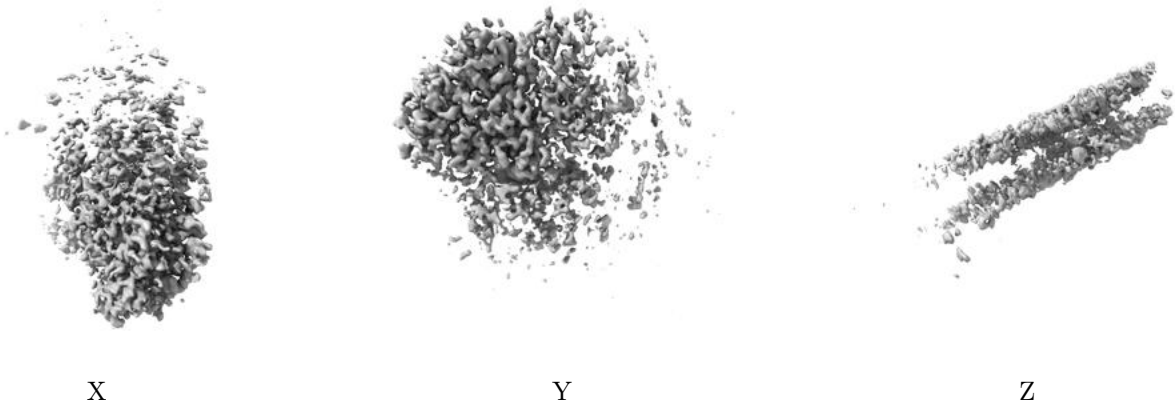
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0154. 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.

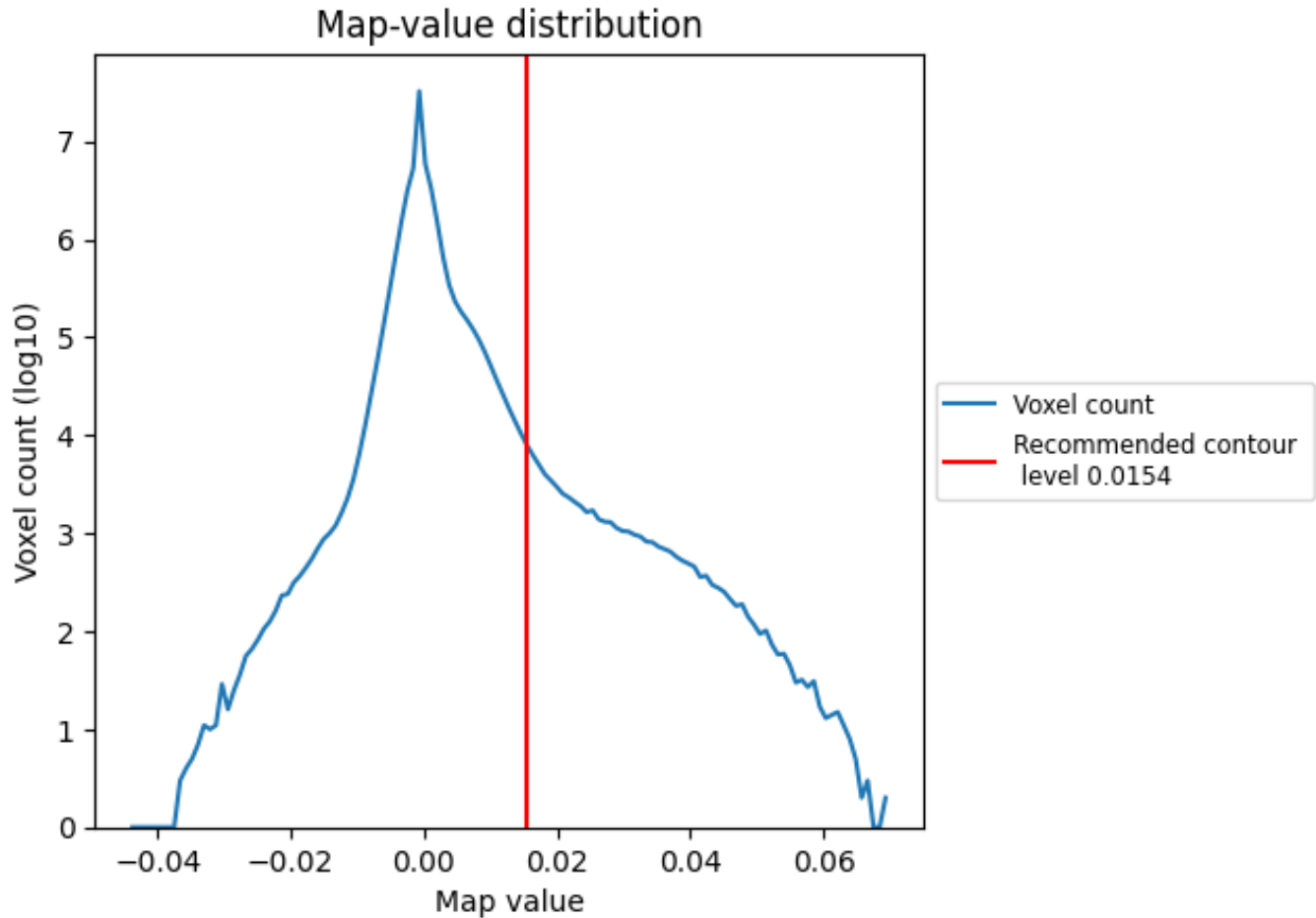
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

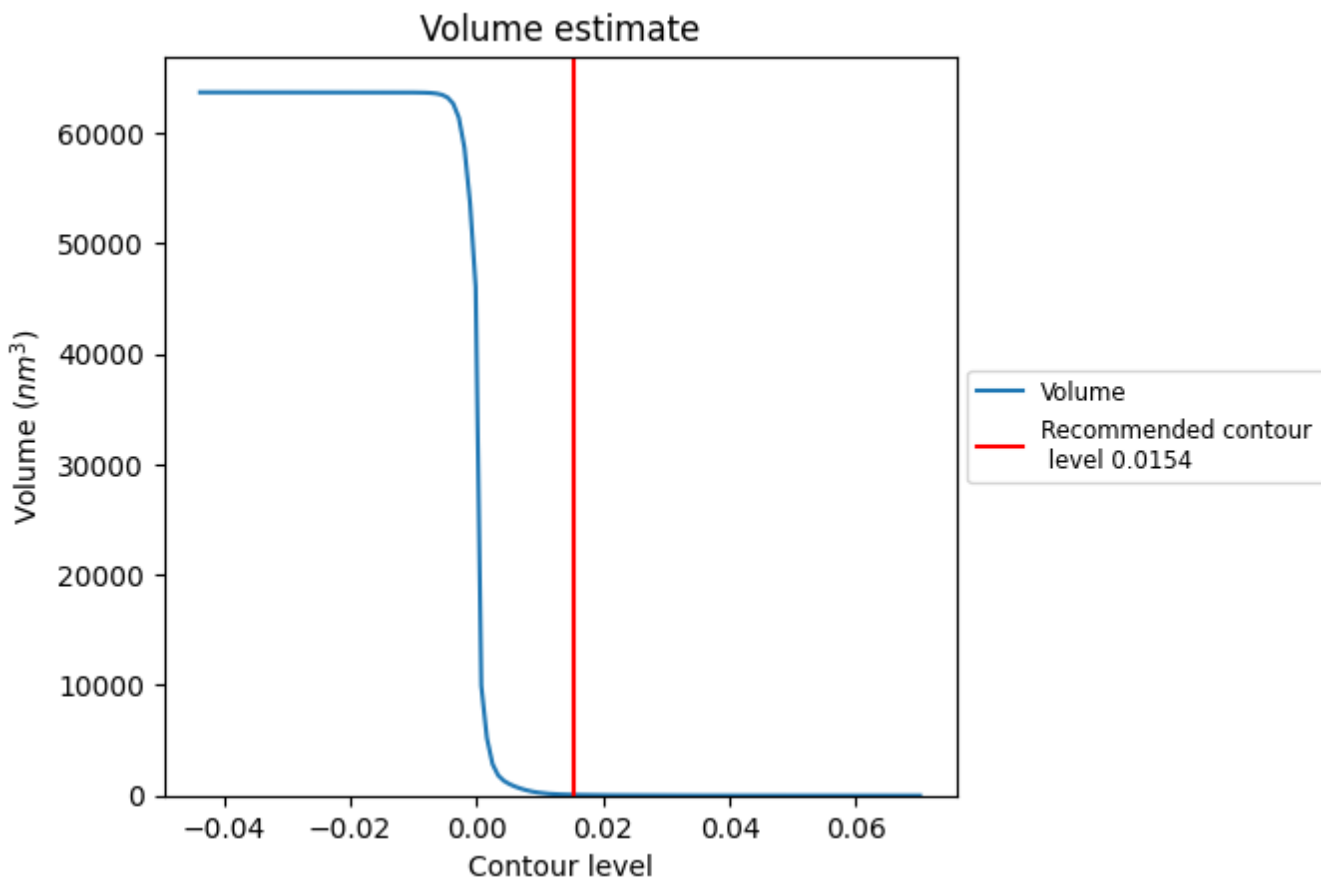
This section contains the results of statistical analysis of the map.

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.

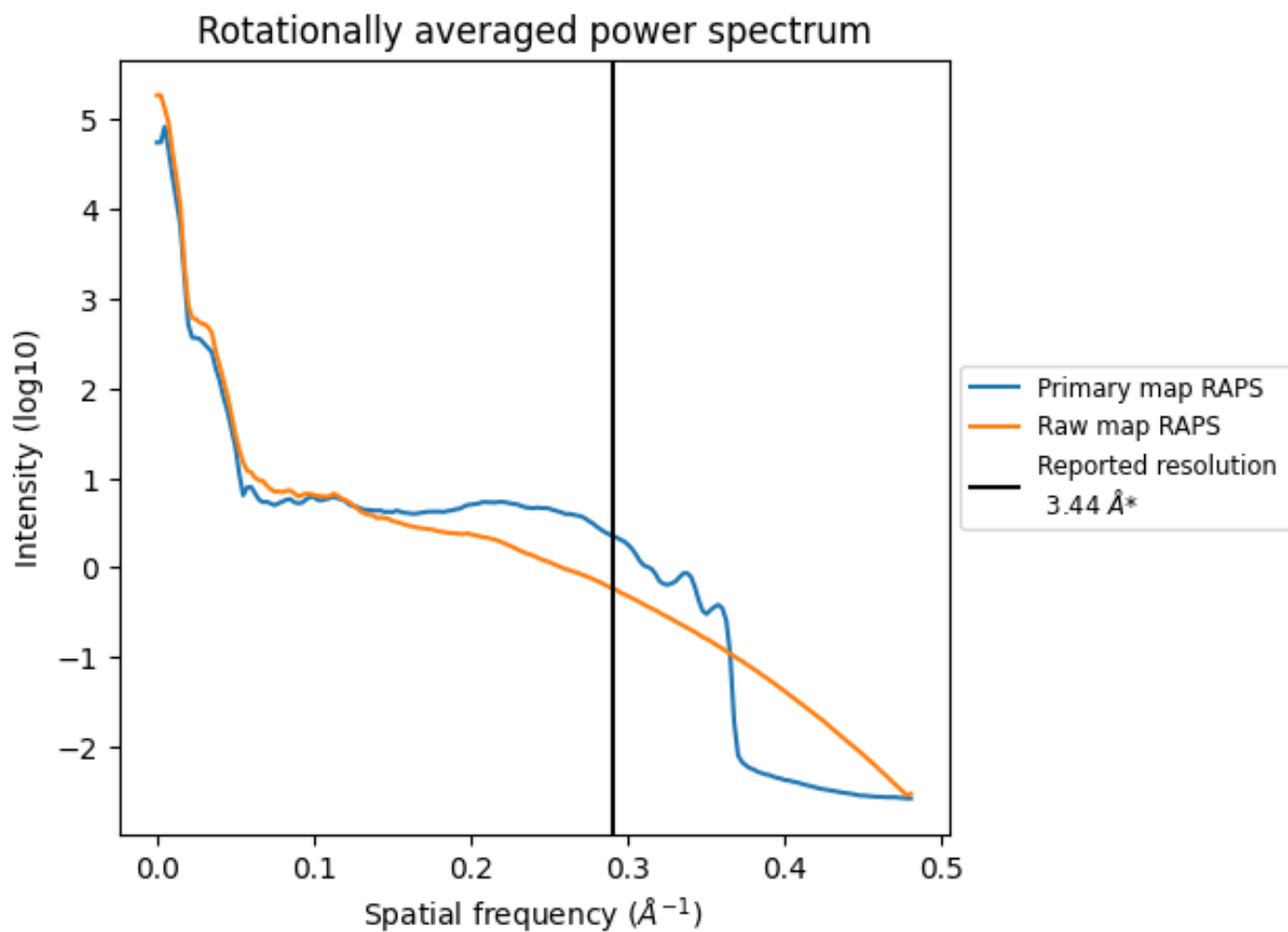
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 68 nm³; this corresponds to an approximate mass of 62 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

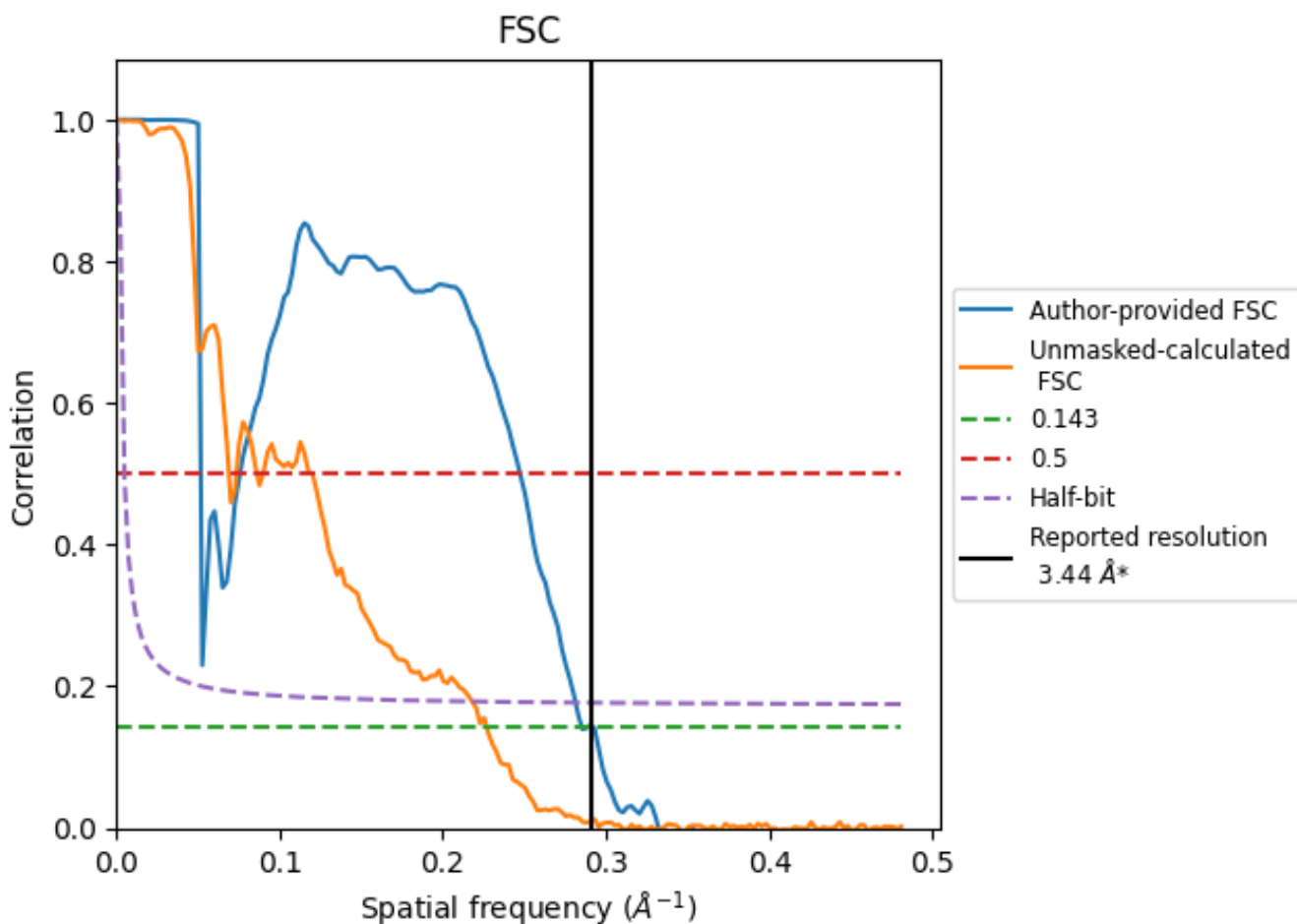


*Reported resolution corresponds to spatial frequency of 0.291 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.291 Å⁻¹

8.2 Resolution estimates [i](#)

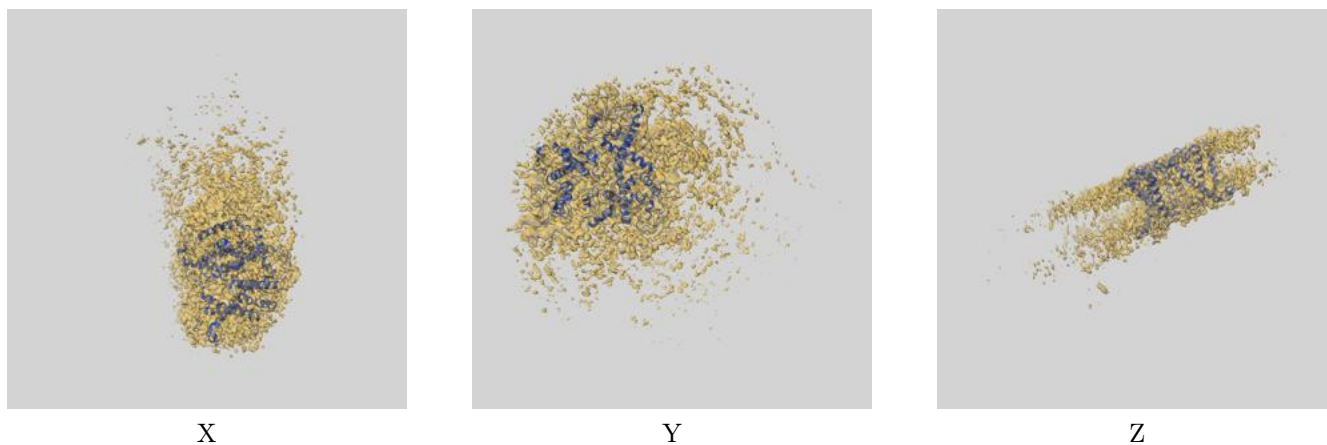
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.51	19.34	3.55
Unmasked-calculated*	4.41	14.51	4.59

*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 4.41 differs from the reported value 3.44 by more than 10 %

9 Map-model fit [i](#)

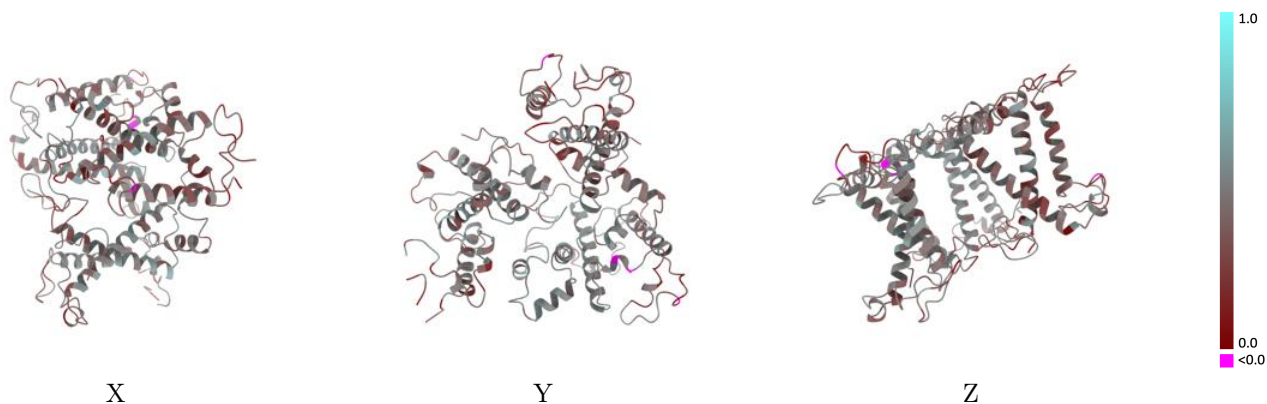
This section contains information regarding the fit between EMDB map EMD-34736 and PDB model 8HG6. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



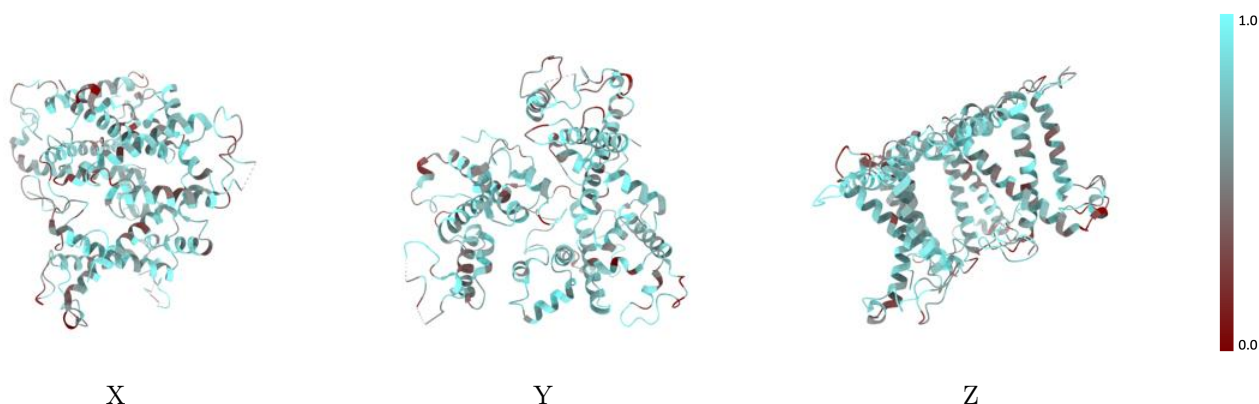
The images above show the 3D surface view of the map at the recommended contour level 0.0154 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



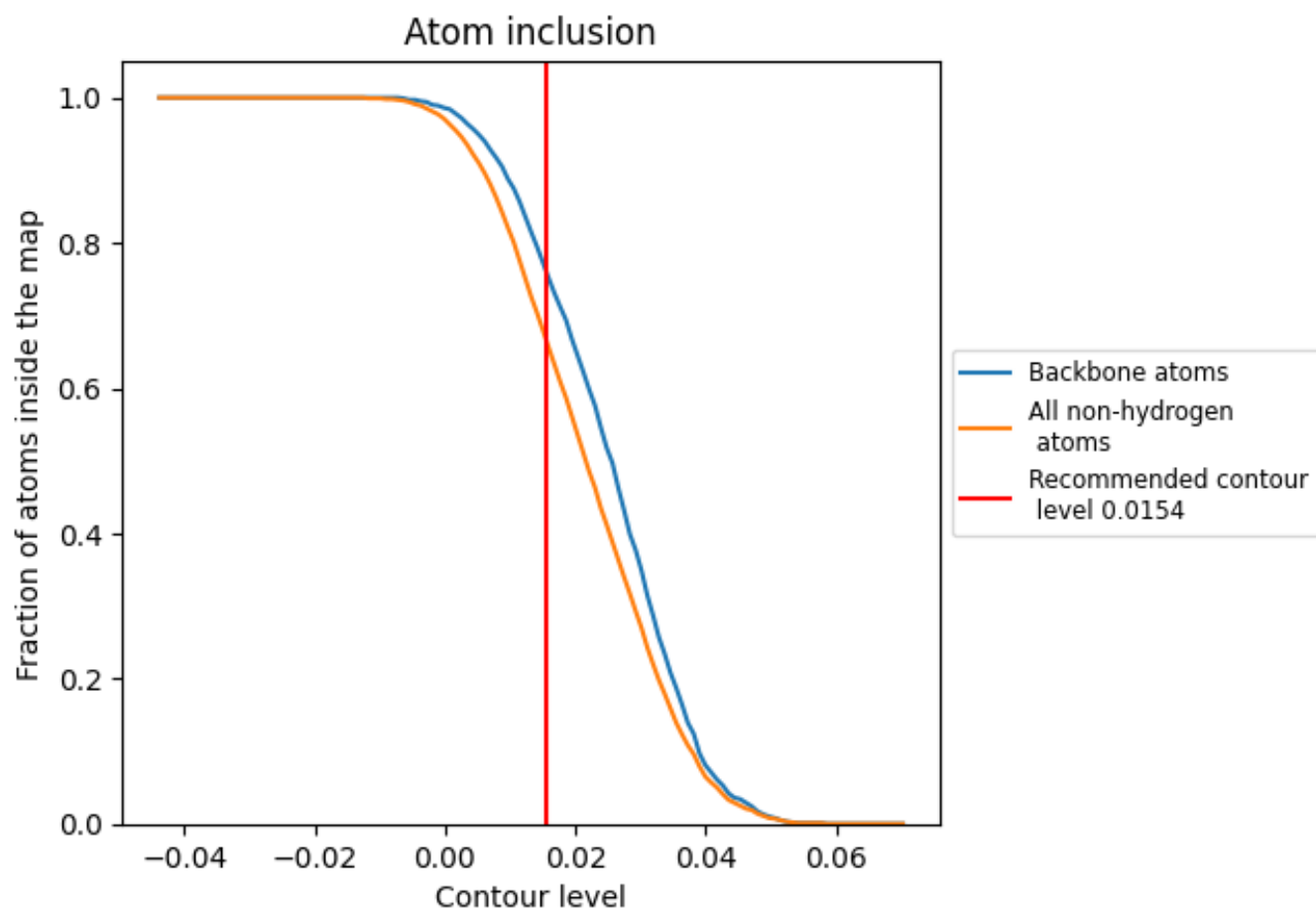
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0154).








9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0154) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6690	 0.4120
V	 0.6500	 0.3850
W	 0.6930	 0.4400
X	 0.6620	 0.4110

