



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:52 AM UTC

PDB ID : 8HG5 / pdb_00008hg5
EMDB ID : EMD-34735
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 : 2.90 Å (reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

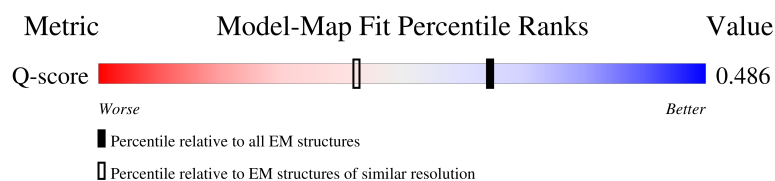
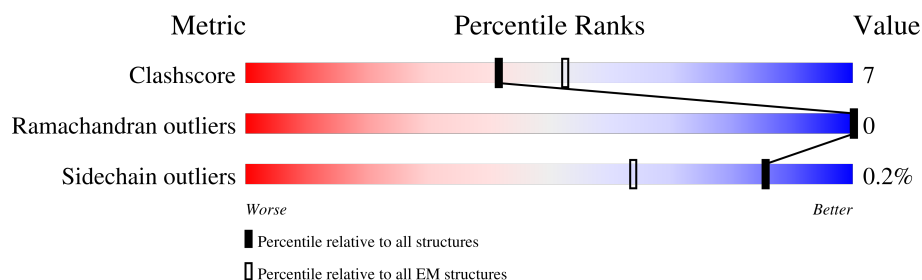
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	P	233	26% 78% 8% 14%
1	R	233	24% 70% 16% 14%
2	Q	226	19% 84% 16%

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
3	CLA	P	301	X	-	-	-
3	CLA	P	302	X	-	-	-
3	CLA	P	303	X	-	-	-
3	CLA	P	309	X	-	-	-
3	CLA	P	310	X	-	-	-
3	CLA	P	311	X	-	-	-
3	CLA	P	312	X	-	-	-
3	CLA	Q	302	X	-	-	-
3	CLA	Q	303	X	-	-	-
3	CLA	Q	304	X	-	-	-
3	CLA	Q	309	X	-	-	-
3	CLA	Q	310	X	-	-	-
3	CLA	Q	311	X	-	-	-
3	CLA	Q	312	X	-	-	-
3	CLA	Q	313	X	-	-	-
3	CLA	R	305	X	-	-	-
3	CLA	R	306	X	-	-	-
3	CLA	R	307	X	-	-	-
3	CLA	R	313	X	-	-	-
3	CLA	R	314	X	-	-	-
3	CLA	R	315	X	-	-	-
3	CLA	R	316	X	-	-	-
4	CHL	P	304	X	-	-	-
4	CHL	P	305	X	-	-	-
4	CHL	P	306	X	-	-	-
4	CHL	P	307	X	-	-	-
4	CHL	P	314	X	-	-	-
4	CHL	Q	305	X	-	-	-
4	CHL	Q	306	X	-	-	-
4	CHL	Q	307	X	-	-	-
4	CHL	Q	314	X	-	-	-
4	CHL	R	302	X	-	-	-
4	CHL	R	308	X	-	-	-
4	CHL	R	309	X	-	-	-
4	CHL	R	310	X	-	-	-
4	CHL	R	311	X	-	-	-
4	CHL	R	318	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7794 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
1	P	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
1	R	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		

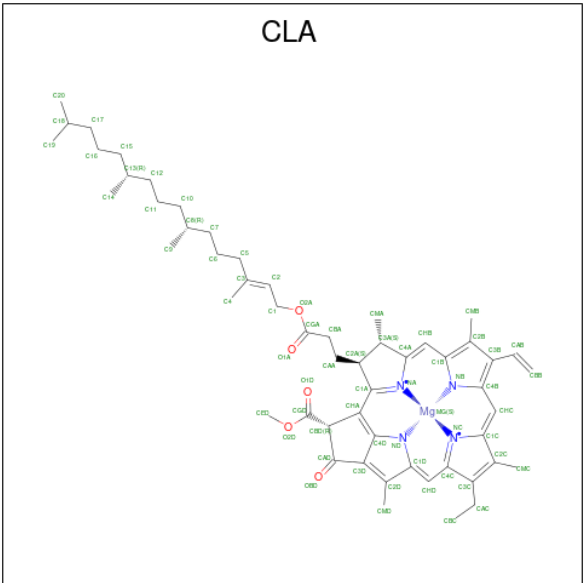
- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Q	226	Total	C	N	O	P	S	0	0
			1706	1100	285	313	1	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	28	ACE	-	acetylation	UNP A0A090LYE8

- Molecule 3 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



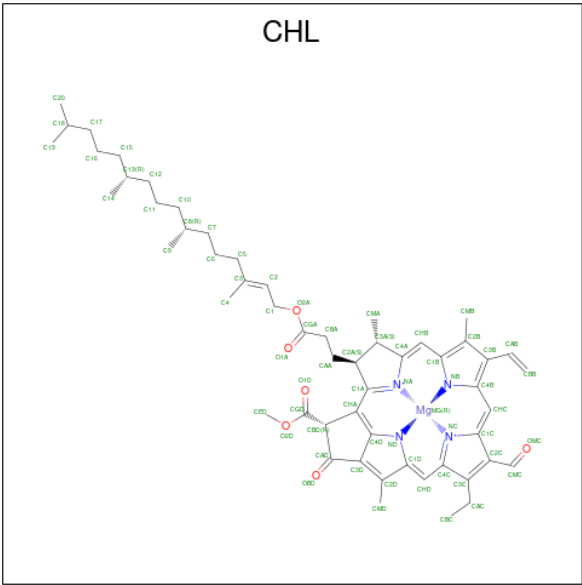
Mol	Chain	Residues	Atoms					AltConf
3	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	P	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
3	Q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
3	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
3	Q	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
3	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

- Molecule 4 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
4	P	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	P	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	P	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
4	P	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
4	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	Q	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	Q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
4	Q	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
4	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

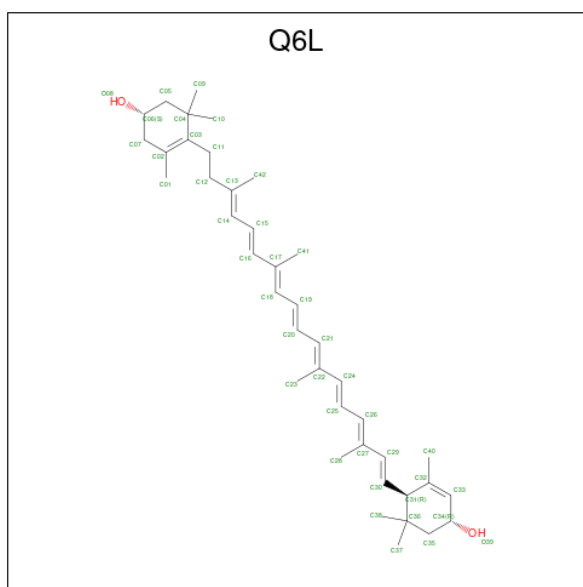
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Mol	Chain	Residues	Atoms					AltConf
4	R	1	Total 47	C 36	Mg 1	N 4	O 6	0
4	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
4	R	1	Total 52	C 41	Mg 1	N 4	O 6	0
4	R	1	Total 44	C 35	Mg 1	N 4	O 4	0
4	R	1	Total 45	C 35	Mg 1	N 4	O 5	0

- ## KC2

Mol	Chain	Residues	Atoms					AltConf
5	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	R	1	Total 45	C 35	Mg 1	N 4	O 5	0

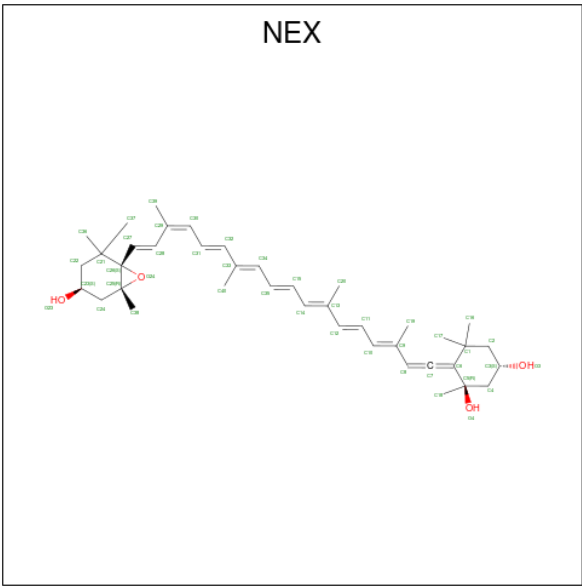
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- WORLD WIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms			AltConf
6	P	1	Total	C	O	0
			42	40	2	
6	P	1	Total	C	O	0
			42	40	2	
6	P	1	Total	C	O	0
			42	40	2	
6	P	1	Total	C	O	0
			42	40	2	
6	Q	1	Total	C	O	0
			42	40	2	
6	Q	1	Total	C	O	0
			42	40	2	
6	Q	1	Total	C	O	0
			42	40	2	
6	R	1	Total	C	O	0
			42	40	2	
6	R	1	Total	C	O	0
			42	40	2	
6	R	1	Total	C	O	0
			42	40	2	
6	R	1	Total	C	O	0
			42	40	2	

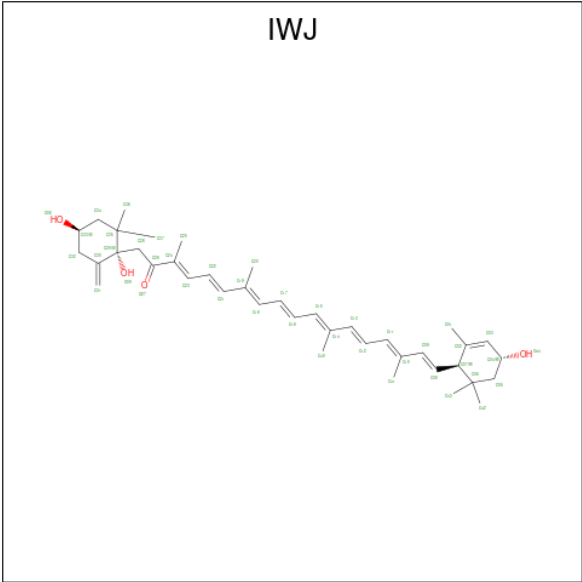
- Molecule 7 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,

3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
7	P	1	Total	C	O	0
			44	40	4	
7	Q	1	Total	C	O	0
			44	40	4	
7	R	1	Total	C	O	0
			44	40	4	

- Molecule 8 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-octaen-2-one (CCD ID: IWJ) (formula: C₄₀H₅₆O₄).

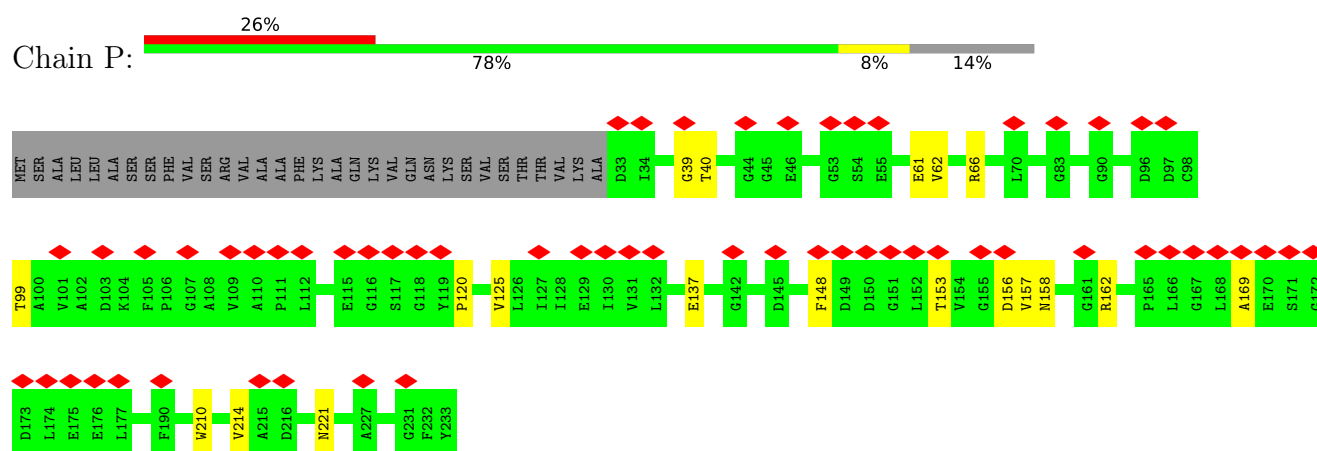


Mol	Chain	Residues	Atoms			AltConf
8	P	1	Total	C	O	0
			44	40	4	
8	P	1	Total	C	O	0
			44	40	4	
8	Q	1	Total	C	O	0
			44	40	4	
8	Q	1	Total	C	O	0
			44	40	4	
8	R	1	Total	C	O	0
			44	40	4	
8	R	1	Total	C	O	0
			44	40	4	

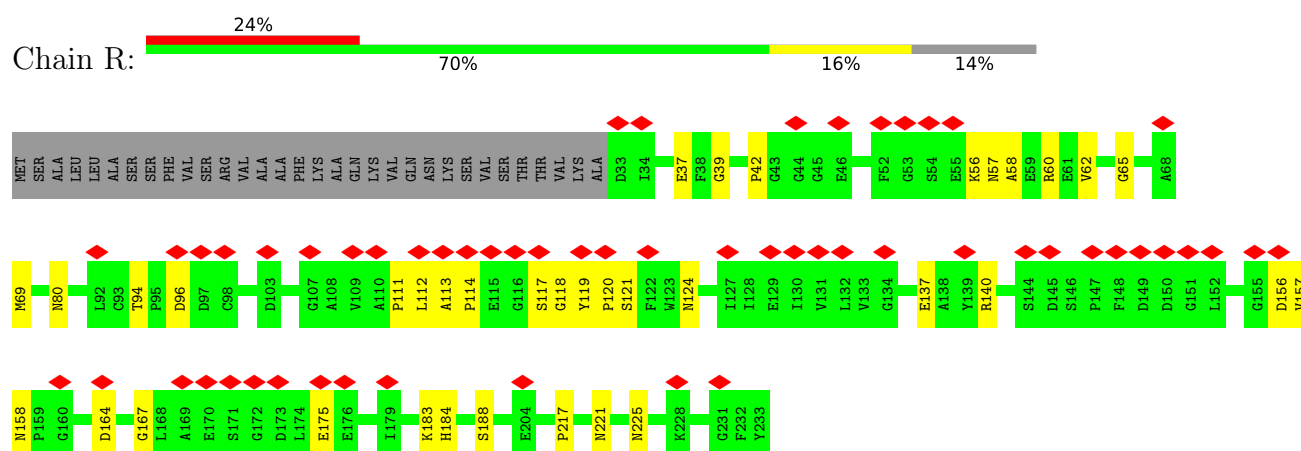
3 Residue-property plots

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

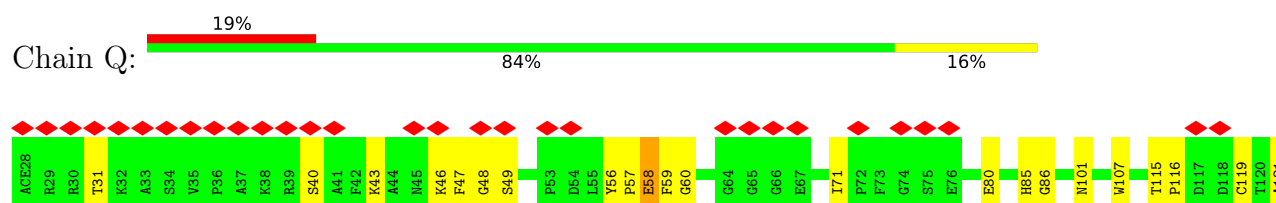
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



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



- Molecule 2: 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	0.113	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0274	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	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: NEX, IWJ, CLA, Q6L, CHL, KC2, TPO, ACE

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	P	0.46	0/1553	0.69	0/2122
1	R	0.47	0/1553	0.77	2/2122 (0.1%)
2	Q	0.50	1/1746 (0.1%)	0.72	1/2379 (0.0%)
All	All	0.48	1/4852 (0.0%)	0.73	3/6623 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	80	GLU	CD-OE1	-5.16	1.15	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	111	PRO	CA-N-CD	-8.52	100.07	112.00
1	R	175	GLU	CG-CD-OE2	5.56	131.19	118.40
2	Q	80	GLU	CB-CG-CD	5.31	121.63	112.60

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	P	1507	0	1429	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1507	0	1429	40	0
2	Q	1706	0	1649	30	0
3	P	467	0	454	5	0
3	Q	403	0	338	7	0
3	R	467	0	454	5	0
4	P	233	0	163	1	0
4	Q	185	0	130	1	0
4	R	284	0	200	9	0
5	P	45	0	0	1	0
5	Q	45	0	0	0	0
5	R	45	0	0	2	0
6	P	168	0	0	1	0
6	Q	126	0	0	1	0
6	R	210	0	0	0	0
7	P	44	0	56	1	0
7	Q	44	0	56	0	0
7	R	44	0	56	0	0
8	P	88	0	0	2	0
8	Q	88	0	0	1	0
8	R	88	0	0	1	0
All	All	7794	0	6414	94	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 (94) 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)
2:Q:209:MET:HE1	3:Q:302:CLA:HAB	1.18	1.12
2:Q:209:MET:CE	3:Q:302:CLA:HAB	1.81	1.10
1:P:66:ARG:HH22	1:P:158:ASN:HB3	1.23	1.01
1:R:114:PRO:HB2	1:R:117:SER:HB3	1.56	0.87
1:R:114:PRO:HG3	4:R:308:CHL:C3B	2.12	0.80
2:Q:121:ALA:O	2:Q:125:LYS:NZ	2.11	0.78
2:Q:209:MET:HE1	3:Q:302:CLA:CAB	2.07	0.77
1:R:114:PRO:HG2	1:R:119:TYR:HD1	1.51	0.76
1:R:94:THR:OG1	1:R:96:ASP:OD1	2.03	0.76
2:Q:85:HIS:HB3	2:Q:209:MET:HE3	1.68	0.75
1:P:66:ARG:NH2	1:P:158:ASN:HB3	2.01	0.74
1:R:65:GLY:O	1:R:69:MET:HG3	1.89	0.72
1:R:80:ASN:ND2	8:R:322:IWJ:O44	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:66:ARG:HH22	1:P:158:ASN:CB	2.07	0.64
1:R:137:GLU:OE1	5:R:312:KC2:NB	2.30	0.64
1:R:62:VAL:HG11	1:R:157:VAL:HG11	1.81	0.63
2:Q:177:VAL:HG23	2:Q:178:THR:HG23	1.79	0.63
1:R:69:MET:HE3	1:R:184:HIS:HB3	1.80	0.62
1:R:113:ALA:HB1	1:R:118:GLY:HA2	1.81	0.62
8:P:320:IWJ:O27	8:P:320:IWJ:O39	2.17	0.62
2:Q:58:GLU:OE1	2:Q:203:LYS:NZ	2.34	0.61
1:R:69:MET:HG2	1:R:188:SER:OG	2.01	0.61
1:R:56:LYS:HB3	1:R:60:ARG:NH1	2.16	0.60
1:R:39:GLY:HA3	3:R:305:CLA:HMD1	1.83	0.59
2:Q:209:MET:HE2	3:Q:302:CLA:HAB	1.82	0.59
1:R:114:PRO:HD2	1:R:119:TYR:H	1.69	0.58
1:R:164:ASP:OD1	1:R:167:GLY:N	2.36	0.58
1:P:39:GLY:HA3	3:P:301:CLA:HMD1	1.87	0.56
1:R:112:LEU:HD21	4:R:308:CHL:CHD	2.36	0.56
1:P:158:ASN:HB2	3:P:309:CLA:CGD	2.36	0.56
2:Q:60:GLY:HA3	3:Q:302:CLA:HMD1	1.87	0.55
2:Q:40:SER:HB3	2:Q:43:LYS:HB2	1.88	0.55
2:Q:57:PRO:HG2	2:Q:58:GLU:OE2	2.06	0.55
2:Q:85:HIS:HB3	2:Q:209:MET:CE	2.37	0.55
2:Q:49:SER:HB3	2:Q:193:ASP:HB3	1.90	0.54
1:R:37:GLU:OE1	1:R:183:LYS:NZ	2.42	0.53
1:R:42:PRO:HA	3:R:305:CLA:HED3	1.90	0.53
1:R:114:PRO:CD	1:R:119:TYR:H	2.22	0.53
2:Q:101:ASN:ND2	8:Q:319:IWJ:O44	2.41	0.53
1:P:61:GLU:OE1	3:P:301:CLA:C4A	2.56	0.52
1:P:137:GLU:OE1	5:P:308:KC2:C4A	2.55	0.52
2:Q:123:ALA:HB1	2:Q:134:ALA:H	1.75	0.52
1:R:62:VAL:CG1	1:R:157:VAL:HG11	2.40	0.52
1:R:120:PRO:HG3	4:R:308:CHL:C4C	2.39	0.52
1:R:69:MET:CG	1:R:188:SER:OG	2.58	0.52
2:Q:245:ASN:ND2	3:Q:312:CLA:OBD	2.42	0.51
2:Q:46:LYS:HD2	2:Q:191:ALA:O	2.11	0.51
1:P:66:ARG:NH1	1:P:157:VAL:HG12	2.25	0.51
1:R:156:ASP:OD1	1:R:158:ASN:N	2.41	0.50
1:R:114:PRO:HG2	1:R:119:TYR:CD1	2.40	0.50
8:P:318:IWJ:O39	8:P:318:IWJ:O27	2.29	0.50
1:R:114:PRO:HG3	4:R:308:CHL:C2B	2.41	0.50
1:P:153:THR:O	1:P:156:ASP:HB3	2.11	0.50
2:Q:71:ILE:HG22	3:Q:302:CLA:HBA2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:210:TRP:CZ3	1:P:214:VAL:HG21	2.48	0.49
1:R:140:ARG:HG3	4:R:311:CHL:C1D	2.43	0.49
1:R:69:MET:HG2	1:R:188:SER:CB	2.43	0.48
2:Q:48:GLY:N	2:Q:192:GLY:HA2	2.28	0.48
1:R:140:ARG:HG3	4:R:311:CHL:CHD	2.44	0.48
1:R:58:ALA:HA	3:R:305:CLA:HMA1	1.95	0.47
1:R:121:SER:H	1:R:124:ASN:HB2	1.80	0.47
1:P:148:PHE:HB3	1:P:162:ARG:NH1	2.30	0.46
7:P:317:NEX:H193	7:P:317:NEX:H162	1.96	0.46
1:R:56:LYS:NZ	5:R:312:KC2:O2A	2.47	0.46
3:P:301:CLA:HMC1	6:P:316:Q6L:C15	2.46	0.46
2:Q:56:TYR:HE1	2:Q:59:PHE:O	1.98	0.46
2:Q:47:PHE:CE2	2:Q:191:ALA:HB3	2.52	0.45
1:P:66:ARG:HH12	1:P:157:VAL:HG12	1.81	0.45
2:Q:49:SER:HB3	2:Q:193:ASP:CB	2.47	0.45
1:R:57:ASN:OD1	3:R:306:CLA:HED3	2.17	0.45
1:P:62:VAL:CG1	1:P:157:VAL:HG11	2.47	0.44
1:P:153:THR:HG23	1:P:156:ASP:CB	2.47	0.44
2:Q:119:CYS:O	2:Q:122:VAL:HG12	2.17	0.44
1:R:120:PRO:HG3	4:R:308:CHL:C3C	2.47	0.44
2:Q:48:GLY:CA	2:Q:192:GLY:HA2	2.47	0.44
1:P:125:VAL:HG11	4:P:305:CHL:HMD2	2.00	0.43
1:P:99:THR:HG22	1:P:120:PRO:HG2	2.01	0.43
2:Q:86:GLY:HA3	2:Q:205:SER:HB3	2.00	0.43
1:P:210:TRP:CH2	1:P:214:VAL:HG11	2.54	0.42
2:Q:131:ALA:HB1	4:Q:305:CHL:HMA3	2.01	0.42
2:Q:134:ALA:HA	2:Q:140:TYR:HA	2.01	0.42
1:R:58:ALA:O	1:R:62:VAL:HG23	2.19	0.42
1:P:169:ALA:HB2	3:P:309:CLA:HAA2	2.01	0.42
1:R:225:ASN:ND2	3:R:316:CLA:OBD	2.51	0.42
1:R:120:PRO:HG3	4:R:308:CHL:C1C	2.50	0.42
1:R:217:PRO:O	1:R:221:ASN:ND2	2.53	0.41
2:Q:107:TRP:O	6:Q:318:Q6L:O08	2.38	0.41
1:R:114:PRO:HG3	4:R:308:CHL:CAB	2.51	0.41
1:P:39:GLY:C	1:P:40:THR:HG23	2.45	0.41
2:Q:115:THR:CG2	2:Q:116:PRO:HD2	2.51	0.41
1:R:65:GLY:O	1:R:69:MET:CG	2.65	0.41
1:R:96:ASP:OD1	1:R:96:ASP:N	2.54	0.41
1:P:221:ASN:OD1	1:P:221:ASN:N	2.53	0.41
2:Q:43:LYS:C	2:Q:43:LYS:HD3	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	199/233 (85%)	191 (96%)	8 (4%)	0	100	100
1	R	199/233 (85%)	185 (93%)	14 (7%)	0	100	100
2	Q	223/226 (99%)	212 (95%)	11 (5%)	0	100	100
All	All	621/692 (90%)	588 (95%)	33 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	153/179 (86%)	153 (100%)	0	100	100
1	R	153/179 (86%)	153 (100%)	0	100	100
2	Q	167/167 (100%)	166 (99%)	1 (1%)	78	93
All	All	473/525 (90%)	472 (100%)	1 (0%)	85	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Q	58	GLU

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

Mol	Chain	Res	Type
1	P	211	GLN
2	Q	229	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TPO	Q	31	2	8,10,11	1.75	1 (12%)	10,14,16	1.21	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	Q	31	2	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	31	TPO	P-O1P	3.60	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	31	TPO	P-OG1-CB	-2.57	116.33	123.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	31	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

63 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	$\# Z > 2$
5	KC2	R	312	1	49,53,53	2.16	14 (28%)	60,89,89	2.18	19 (31%)
6	Q6L	R	319	-	42,43,43	1.93	8 (19%)	51,60,60	1.68	6 (11%)
6	Q6L	Q	318	-	42,43,43	1.91	7 (16%)	51,60,60	1.86	12 (23%)
8	IWJ	R	322	-	43,45,45	1.52	4 (9%)	47,65,65	1.19	4 (8%)
6	Q6L	Q	317	-	42,43,43	1.81	6 (14%)	51,60,60	1.63	7 (13%)
3	CLA	P	313	-	52,56,73	1.33	6 (11%)	61,92,113	1.24	6 (9%)
6	Q6L	P	321	-	42,43,43	1.92	8 (19%)	51,60,60	1.58	7 (13%)
6	Q6L	Q	316	-	42,43,43	1.85	6 (14%)	51,60,60	1.76	9 (17%)
3	CLA	R	313	1	68,72,73	1.20	7 (10%)	80,111,113	1.31	10 (12%)
4	CHL	R	309	-	44,58,74	2.82	13 (29%)	37,94,114	2.16	15 (40%)
3	CLA	Q	303	-	47,52,73	1.39	6 (12%)	55,87,113	1.22	4 (7%)
4	CHL	Q	307	-	38,52,74	3.01	10 (26%)	31,87,114	1.96	12 (38%)
4	CHL	R	308	1	40,54,74	2.89	11 (27%)	34,90,114	1.83	13 (38%)
8	IWJ	R	303	-	43,45,45	1.55	5 (11%)	47,65,65	1.40	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	Q6L	R	304	-	42,43,43	1.94	8 (19%)	51,60,60	1.68	7 (13%)
5	KC2	P	308	1	49,53,53	2.13	15 (30%)	60,89,89	2.40	17 (28%)
3	CLA	Q	302	2	69,73,73	1.21	8 (11%)	82,113,113	1.54	6 (7%)
3	CLA	R	314	1	64,68,73	1.24	6 (9%)	76,107,113	1.43	9 (11%)
8	IWJ	Q	301	-	43,45,45	1.58	6 (13%)	47,65,65	1.50	9 (19%)
4	CHL	R	311	-	38,52,74	3.12	14 (36%)	31,87,114	1.86	7 (22%)
4	CHL	P	314	1	38,53,74	3.02	10 (26%)	31,88,114	1.81	10 (32%)
6	Q6L	R	323	-	42,43,43	1.93	7 (16%)	51,60,60	1.94	10 (19%)
3	CLA	P	303	-	54,58,73	1.31	5 (9%)	64,95,113	1.31	9 (14%)
4	CHL	R	318	1	38,53,74	3.02	9 (23%)	31,88,114	1.85	10 (32%)
3	CLA	R	305	1	69,73,73	1.20	5 (7%)	82,113,113	1.37	8 (9%)
4	CHL	P	305	-	40,54,74	3.09	12 (30%)	34,90,114	1.97	11 (32%)
4	CHL	P	306	-	46,60,74	2.68	14 (30%)	40,97,114	1.77	15 (37%)
4	CHL	R	310	-	46,60,74	2.73	13 (28%)	40,97,114	1.93	14 (35%)
3	CLA	P	312	1	59,63,73	1.26	5 (8%)	70,101,113	1.34	8 (11%)
4	CHL	Q	314	2	38,53,74	3.04	10 (26%)	31,88,114	2.12	13 (41%)
7	NEX	R	321	-	40,46,46	1.43	8 (20%)	50,70,70	2.42	17 (34%)
3	CLA	P	311	-	64,68,73	1.18	4 (6%)	76,107,113	1.39	12 (15%)
8	IWJ	P	318	-	43,45,45	1.49	5 (11%)	47,65,65	1.27	4 (8%)
3	CLA	R	315	-	64,68,73	1.26	7 (10%)	76,107,113	1.37	8 (10%)
4	CHL	Q	306	2	44,58,74	3.00	16 (36%)	37,94,114	1.79	5 (13%)
4	CHL	P	307	-	38,52,74	3.26	11 (28%)	31,87,114	1.99	10 (32%)
6	Q6L	P	319	-	42,43,43	1.91	7 (16%)	51,60,60	1.76	9 (17%)
3	CLA	P	309	1	68,72,73	1.12	7 (10%)	80,111,113	1.47	11 (13%)
3	CLA	P	301	1	69,73,73	1.16	8 (11%)	82,113,113	1.36	10 (12%)
4	CHL	Q	305	2	40,54,74	3.01	8 (20%)	34,90,114	2.07	12 (35%)
4	CHL	R	302	-	41,55,74	2.87	12 (29%)	35,91,114	1.95	12 (34%)
8	IWJ	Q	319	-	43,45,45	1.44	4 (9%)	47,65,65	1.67	9 (19%)
3	CLA	Q	312	2	57,61,73	1.24	5 (8%)	67,98,113	1.37	7 (10%)
4	CHL	P	304	1	40,54,74	3.03	10 (25%)	34,90,114	2.19	16 (47%)
5	KC2	Q	308	2	49,53,53	2.20	13 (26%)	60,89,89	2.26	13 (21%)
3	CLA	Q	304	-	54,58,73	1.35	9 (16%)	64,95,113	1.52	12 (18%)
3	CLA	R	306	-	69,73,73	1.15	7 (10%)	82,113,113	1.14	3 (3%)
7	NEX	P	317	-	40,46,46	1.33	8 (20%)	50,70,70	2.45	16 (32%)
3	CLA	R	307	-	54,58,73	1.32	7 (12%)	64,95,113	1.26	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	IWJ	P	320	-	43,45,45	1.61	6 (13%)	47,65,65	1.70	7 (14%)
3	CLA	Q	311	-	50,54,73	1.33	7 (14%)	59,90,113	1.45	6 (10%)
3	CLA	R	316	1	59,63,73	1.27	6 (10%)	70,101,113	1.54	9 (12%)
6	Q6L	P	315	-	42,43,43	1.96	8 (19%)	51,60,60	1.63	7 (13%)
6	Q6L	R	320	-	42,43,43	1.92	7 (16%)	51,60,60	1.74	10 (19%)
3	CLA	Q	309	2	59,63,73	1.22	5 (8%)	70,101,113	1.25	8 (11%)
3	CLA	P	310	1	64,68,73	1.22	6 (9%)	76,107,113	1.28	8 (10%)
3	CLA	R	317	-	52,56,73	1.32	6 (11%)	61,92,113	1.36	8 (13%)
6	Q6L	R	301	-	42,43,43	1.91	7 (16%)	51,60,60	2.04	8 (15%)
7	NEX	Q	315	-	40,46,46	1.42	9 (22%)	50,70,70	2.32	18 (36%)
3	CLA	Q	313	-	52,56,73	1.32	7 (13%)	61,92,113	1.41	8 (13%)
3	CLA	Q	310	2	46,50,73	1.41	7 (15%)	53,85,113	1.18	4 (7%)
6	Q6L	P	316	-	42,43,43	1.96	9 (21%)	51,60,60	1.77	9 (17%)
3	CLA	P	302	-	69,73,73	1.14	7 (10%)	82,113,113	1.34	10 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	KC2	R	312	1	-	7/15/71/71	-
6	Q6L	R	319	-	-	10/29/67/67	0/2/2/2
6	Q6L	Q	318	-	-	5/29/67/67	0/2/2/2
8	IWJ	R	322	-	-	7/33/76/76	1/2/2/2
6	Q6L	Q	317	-	-	6/29/67/67	0/2/2/2
3	CLA	P	313	-	-	6/19/95/115	-
6	Q6L	P	321	-	-	7/29/67/67	0/2/2/2
6	Q6L	Q	316	-	-	7/29/67/67	0/2/2/2
3	CLA	R	313	1	1/1/14/20	16/38/114/115	-
4	CHL	R	309	-	3/3/16/26	6/20/118/137	-
3	CLA	Q	303	-	1/1/10/20	0/14/90/115	-
4	CHL	Q	307	-	3/3/15/26	2/13/111/137	-
4	CHL	R	308	1	3/3/16/26	3/15/113/137	-
8	IWJ	R	303	-	-	4/33/76/76	0/2/2/2
6	Q6L	R	304	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	KC2	P	308	1	-	8/15/71/71	-
3	CLA	Q	302	2	1/1/15/20	11/39/115/115	-
3	CLA	R	314	1	1/1/14/20	12/33/109/115	-
8	IWJ	Q	301	-	-	4/33/76/76	0/2/2/2
4	CHL	R	311	-	3/3/15/26	2/13/111/137	-
4	CHL	P	314	1	3/3/15/26	4/14/112/137	-
6	Q6L	R	323	-	-	9/29/67/67	0/2/2/2
3	CLA	P	303	-	1/1/12/20	9/21/97/115	-
4	CHL	R	318	1	3/3/15/26	3/14/112/137	-
3	CLA	R	305	1	1/1/15/20	11/39/115/115	-
4	CHL	P	305	-	3/3/16/26	4/15/113/137	-
4	CHL	P	306	-	3/3/17/26	8/23/121/137	-
4	CHL	R	310	-	3/3/17/26	8/23/121/137	-
3	CLA	P	312	1	1/1/13/20	10/27/103/115	-
4	CHL	Q	314	2	3/3/15/26	5/14/112/137	-
7	NEX	R	321	-	-	3/27/83/83	0/3/3/3
3	CLA	P	311	-	1/1/14/20	9/33/109/115	-
8	IWJ	P	318	-	-	2/33/76/76	0/2/2/2
3	CLA	R	315	-	1/1/14/20	10/33/109/115	-
4	CHL	Q	306	2	3/3/16/26	6/20/118/137	-
4	CHL	P	307	-	3/3/15/26	2/13/111/137	-
6	Q6L	P	319	-	-	6/29/67/67	0/2/2/2
3	CLA	P	309	1	1/1/14/20	15/38/114/115	-
3	CLA	P	301	1	1/1/15/20	10/39/115/115	-
4	CHL	Q	305	2	3/3/16/26	8/15/113/137	-
4	CHL	R	302	-	3/3/16/26	7/17/115/137	-
8	IWJ	Q	319	-	-	11/33/76/76	0/2/2/2
3	CLA	Q	312	2	1/1/12/20	10/25/101/115	-
4	CHL	P	304	1	3/3/16/26	5/15/113/137	-
5	KC2	Q	308	2	-	6/15/71/71	-
3	CLA	Q	304	-	1/1/12/20	7/21/97/115	-
3	CLA	R	306	-	1/1/15/20	13/39/115/115	-
7	NEX	P	317	-	-	2/27/83/83	0/3/3/3
3	CLA	R	307	-	1/1/12/20	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	IWJ	P	320	-	-	3/33/76/76	0/2/2/2
3	CLA	Q	311	-	1/1/11/20	11/17/93/115	-
3	CLA	R	316	1	1/1/13/20	9/27/103/115	-
6	Q6L	P	315	-	-	6/29/67/67	0/2/2/2
6	Q6L	R	320	-	-	0/29/67/67	0/2/2/2
3	CLA	Q	309	2	1/1/13/20	7/27/103/115	-
3	CLA	P	310	1	1/1/14/20	8/33/109/115	-
3	CLA	R	317	-	-	5/19/95/115	-
6	Q6L	R	301	-	-	10/29/67/67	0/2/2/2
7	NEX	Q	315	-	-	3/27/83/83	0/3/3/3
3	CLA	Q	313	-	1/1/11/20	4/19/95/115	-
3	CLA	Q	310	2	1/1/10/20	3/12/88/115	-
6	Q6L	P	316	-	-	2/29/67/67	0/2/2/2
3	CLA	P	302	-	1/1/15/20	15/39/115/115	-

All (511) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	307	CHL	C3B-C4B	11.68	1.52	1.41
4	P	304	CHL	C3B-C4B	11.21	1.52	1.41
4	Q	306	CHL	C3B-C4B	11.02	1.52	1.41
4	R	318	CHL	C3B-C4B	10.59	1.51	1.41
4	Q	314	CHL	C3B-C4B	10.48	1.51	1.41
4	R	311	CHL	C3B-C4B	10.45	1.51	1.41
4	P	305	CHL	C3B-C4B	10.43	1.51	1.41
4	Q	305	CHL	C3B-C4B	10.34	1.51	1.41
4	R	309	CHL	C3B-C4B	10.25	1.51	1.41
4	P	314	CHL	C3B-C4B	10.15	1.51	1.41
4	P	305	CHL	C1B-C2B	10.00	1.50	1.39
4	R	302	CHL	C3B-C4B	9.89	1.51	1.41
4	Q	307	CHL	C3B-C4B	9.88	1.51	1.41
4	R	308	CHL	C3B-C4B	9.84	1.51	1.41
4	R	311	CHL	C1B-C2B	9.66	1.50	1.39
4	Q	305	CHL	C1B-C2B	9.59	1.50	1.39
4	R	309	CHL	C1B-C2B	9.58	1.50	1.39
4	P	307	CHL	C1B-C2B	9.58	1.50	1.39
4	Q	307	CHL	C1B-C2B	9.56	1.50	1.39
4	R	310	CHL	C3B-C4B	9.41	1.50	1.41
4	Q	306	CHL	C1B-C2B	9.20	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	306	CHL	C1B-C2B	9.20	1.50	1.39
4	R	302	CHL	C1B-C2B	9.15	1.50	1.39
4	Q	314	CHL	C1B-C2B	9.12	1.49	1.39
6	P	321	Q6L	C29-C30	9.05	1.52	1.32
4	R	310	CHL	C1B-C2B	9.03	1.49	1.39
4	P	314	CHL	C1B-C2B	9.00	1.49	1.39
6	P	316	Q6L	C29-C30	8.94	1.52	1.32
4	R	318	CHL	C1B-C2B	8.93	1.49	1.39
6	R	304	Q6L	C29-C30	8.91	1.52	1.32
6	R	301	Q6L	C29-C30	8.89	1.52	1.32
6	R	319	Q6L	C29-C30	8.88	1.52	1.32
6	P	319	Q6L	C29-C30	8.86	1.52	1.32
6	P	315	Q6L	C29-C30	8.85	1.52	1.32
6	R	323	Q6L	C29-C30	8.85	1.52	1.32
6	R	320	Q6L	C29-C30	8.83	1.52	1.32
4	R	308	CHL	C1B-C2B	8.81	1.49	1.39
6	Q	316	Q6L	C29-C30	8.68	1.51	1.32
6	Q	318	Q6L	C29-C30	8.64	1.51	1.32
4	P	304	CHL	C1B-C2B	8.56	1.49	1.39
6	Q	317	Q6L	C29-C30	8.46	1.51	1.32
4	P	306	CHL	C3B-C4B	8.44	1.49	1.41
5	Q	308	KC2	C2A-C3A	8.32	1.54	1.37
5	R	312	KC2	C2A-C3A	8.28	1.54	1.37
4	Q	314	CHL	C1D-C2D	7.89	1.48	1.39
4	P	307	CHL	C1D-C2D	7.89	1.48	1.39
5	P	308	KC2	C2A-C3A	7.86	1.53	1.37
4	Q	305	CHL	C1D-C2D	7.78	1.48	1.39
4	P	306	CHL	C1D-C2D	7.69	1.48	1.39
4	P	314	CHL	C1D-C2D	7.61	1.48	1.39
4	R	310	CHL	C1D-C2D	7.58	1.48	1.39
4	R	308	CHL	C1D-C2D	7.54	1.48	1.39
4	R	302	CHL	C1D-C2D	7.53	1.48	1.39
4	Q	307	CHL	C1D-C2D	7.45	1.48	1.39
4	R	318	CHL	C1D-C2D	7.43	1.48	1.39
4	P	305	CHL	C1D-C2D	7.42	1.48	1.39
4	P	304	CHL	C1D-C2D	7.37	1.47	1.39
8	P	320	IWJ	C29-C30	-7.35	1.45	1.53
4	R	309	CHL	C1D-C2D	6.91	1.47	1.39
8	P	318	IWJ	C29-C30	-6.86	1.46	1.53
8	R	303	IWJ	C29-C30	-6.85	1.46	1.53
8	Q	301	IWJ	C29-C30	-6.80	1.46	1.53
8	R	322	IWJ	C29-C30	-6.76	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	308	KC2	CBA-CAA	6.41	1.52	1.33
4	Q	306	CHL	C1D-C2D	6.37	1.46	1.39
8	Q	319	IWJ	C29-C30	-6.30	1.46	1.53
5	P	308	KC2	CBA-CAA	6.08	1.51	1.33
4	R	311	CHL	C1D-C2D	6.08	1.46	1.39
5	R	312	KC2	CBA-CAA	6.07	1.51	1.33
6	R	301	Q6L	C12-C11	-5.14	1.34	1.51
6	R	323	Q6L	C12-C11	-5.08	1.34	1.51
4	Q	306	CHL	CMD-C2D	-5.06	1.41	1.51
6	P	315	Q6L	C12-C11	-5.06	1.34	1.51
4	R	311	CHL	C2C-C3C	5.06	1.41	1.36
6	Q	316	Q6L	C12-C11	-4.99	1.34	1.51
6	R	319	Q6L	C12-C11	-4.92	1.34	1.51
6	P	321	Q6L	C12-C11	-4.91	1.34	1.51
6	Q	318	Q6L	C12-C11	-4.91	1.34	1.51
6	Q	317	Q6L	C12-C11	-4.87	1.35	1.51
6	R	304	Q6L	C12-C11	-4.85	1.35	1.51
6	R	320	Q6L	C12-C11	-4.82	1.35	1.51
6	P	316	Q6L	C12-C11	-4.78	1.35	1.51
6	P	319	Q6L	C12-C11	-4.77	1.35	1.51
4	R	318	CHL	C2C-C3C	4.60	1.40	1.36
4	Q	305	CHL	C3D-C4D	4.57	1.48	1.41
4	P	305	CHL	C3D-C4D	4.47	1.48	1.41
4	R	308	CHL	C3D-C4D	4.46	1.48	1.41
4	P	304	CHL	C3D-C4D	4.44	1.48	1.41
4	P	307	CHL	C3D-C4D	4.43	1.48	1.41
4	P	314	CHL	C3D-C4D	4.35	1.48	1.41
4	P	314	CHL	C2C-C3C	4.30	1.40	1.36
4	R	310	CHL	C2C-C3C	4.30	1.40	1.36
4	Q	307	CHL	C3D-C4D	4.27	1.48	1.41
4	P	306	CHL	C3D-C4D	4.24	1.48	1.41
4	R	311	CHL	CMD-C2D	-4.21	1.43	1.51
4	R	310	CHL	C3D-C4D	4.20	1.47	1.41
4	P	305	CHL	C2C-C3C	4.17	1.40	1.36
4	Q	305	CHL	C2C-C3C	4.15	1.40	1.36
7	R	321	NEX	C7-C6	-4.12	1.25	1.30
5	R	312	KC2	C4A-C3A	4.12	1.52	1.44
4	Q	306	CHL	C2C-C3C	4.10	1.40	1.36
4	R	318	CHL	C3D-C4D	4.08	1.47	1.41
4	P	307	CHL	C2C-C3C	4.07	1.40	1.36
4	Q	314	CHL	C3D-C4D	4.06	1.47	1.41
4	R	302	CHL	C3D-C4D	4.05	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	308	KC2	MG-ND	-4.05	1.97	2.05
5	P	308	KC2	C4A-C3A	3.91	1.52	1.44
4	P	306	CHL	C2C-C3C	3.90	1.40	1.36
4	P	304	CHL	C2C-C3C	3.89	1.40	1.36
4	P	304	CHL	C3A-C2A	3.84	1.58	1.54
4	Q	307	CHL	C2C-C3C	3.83	1.40	1.36
4	Q	314	CHL	C2C-C3C	3.81	1.40	1.36
7	R	321	NEX	C7-C8	-3.81	1.25	1.31
4	Q	306	CHL	C1A-CHA	-3.79	1.35	1.40
4	R	308	CHL	C2C-C3C	3.77	1.40	1.36
4	R	311	CHL	C3D-C4D	3.73	1.47	1.41
8	Q	301	IWJ	C09-C10	3.71	1.53	1.46
3	R	313	CLA	C1D-ND	3.71	1.42	1.37
3	P	310	CLA	C1D-ND	3.71	1.42	1.37
4	R	309	CHL	C3D-C4D	3.70	1.47	1.41
7	Q	315	NEX	C7-C6	-3.62	1.26	1.30
4	R	309	CHL	C2C-C3C	3.59	1.39	1.36
3	Q	310	CLA	C4B-NB	3.57	1.42	1.37
3	R	314	CLA	C1D-ND	3.55	1.42	1.37
5	Q	308	KC2	C4A-C3A	3.55	1.51	1.44
4	R	311	CHL	C1A-CHA	-3.51	1.36	1.40
4	R	310	CHL	CMD-C2D	-3.49	1.44	1.51
3	R	305	CLA	C1D-ND	3.46	1.42	1.37
3	P	302	CLA	C1D-ND	3.45	1.42	1.37
3	P	303	CLA	C1D-ND	3.45	1.42	1.37
3	P	313	CLA	C1D-ND	3.45	1.42	1.37
4	P	307	CHL	C1A-CHA	-3.43	1.36	1.40
8	R	303	IWJ	C09-C10	3.40	1.53	1.46
8	R	322	IWJ	C09-C10	3.38	1.53	1.46
7	Q	315	NEX	C7-C8	-3.38	1.26	1.31
3	R	315	CLA	C4B-NB	3.36	1.42	1.37
3	R	316	CLA	C1D-ND	3.35	1.42	1.37
3	R	313	CLA	C4B-NB	3.34	1.42	1.37
3	R	317	CLA	C1D-ND	3.33	1.42	1.37
3	Q	309	CLA	C1D-ND	3.32	1.42	1.37
3	P	311	CLA	C1D-ND	3.30	1.42	1.37
3	Q	303	CLA	C1D-ND	3.28	1.42	1.37
3	P	301	CLA	C1D-ND	3.28	1.42	1.37
3	Q	304	CLA	C1D-ND	3.28	1.42	1.37
3	Q	313	CLA	C1D-ND	3.28	1.42	1.37
3	R	315	CLA	C1D-ND	3.27	1.42	1.37
3	P	312	CLA	C1D-ND	3.26	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	310	CLA	C1D-ND	3.26	1.42	1.37
3	Q	302	CLA	C1D-ND	3.26	1.42	1.37
8	P	320	IWJ	C09-C10	3.24	1.52	1.46
7	P	317	NEX	C7-C6	-3.23	1.26	1.30
8	Q	319	IWJ	C09-C10	3.22	1.52	1.46
8	P	318	IWJ	C09-C10	3.20	1.52	1.46
3	Q	311	CLA	C1D-ND	3.18	1.42	1.37
3	R	316	CLA	C4B-NB	3.18	1.42	1.37
4	R	302	CHL	CAC-C3C	-3.17	1.46	1.51
5	P	308	KC2	C1D-ND	3.15	1.42	1.37
3	R	307	CLA	C1D-ND	3.12	1.42	1.37
3	P	309	CLA	C1D-ND	3.08	1.41	1.37
3	Q	303	CLA	CMD-C2D	-3.07	1.44	1.50
3	R	306	CLA	C1D-ND	3.05	1.41	1.37
3	R	305	CLA	CMA-C3A	-3.05	1.46	1.53
3	P	312	CLA	C4B-NB	3.05	1.41	1.37
3	R	307	CLA	C4B-NB	3.04	1.41	1.37
4	Q	306	CHL	C3D-C2D	-3.04	1.34	1.39
6	P	316	Q6L	C02-C03	3.02	1.38	1.34
4	Q	306	CHL	C3D-C4D	3.00	1.46	1.41
5	Q	308	KC2	C2A-C1A	2.98	1.53	1.44
3	P	313	CLA	C4B-NB	2.96	1.41	1.37
4	P	305	CHL	CBD-CGD	-2.95	1.48	1.52
4	R	309	CHL	C1A-CHA	-2.95	1.36	1.40
3	Q	312	CLA	C1D-ND	2.95	1.41	1.37
3	Q	313	CLA	C4B-NB	2.95	1.41	1.37
3	R	313	CLA	C3B-C4B	2.94	1.51	1.42
3	R	314	CLA	C4B-NB	2.94	1.41	1.37
4	P	314	CHL	C1A-CHA	-2.93	1.36	1.40
3	P	310	CLA	C4B-NB	2.93	1.41	1.37
4	P	306	CHL	CMD-C2D	-2.93	1.45	1.51
6	R	301	Q6L	C12-C13	-2.92	1.45	1.51
4	R	318	CHL	CMD-C2D	-2.91	1.45	1.51
6	P	315	Q6L	C34-C33	2.91	1.54	1.50
8	R	322	IWJ	C04-C03	2.90	1.54	1.50
6	P	315	Q6L	C12-C13	-2.90	1.45	1.51
6	R	323	Q6L	C34-C33	2.90	1.54	1.50
6	Q	318	Q6L	C34-C33	2.90	1.54	1.50
3	P	303	CLA	C4B-NB	2.90	1.41	1.37
3	Q	312	CLA	CMD-C2D	-2.89	1.44	1.50
6	R	319	Q6L	C02-C03	2.89	1.38	1.34
8	Q	319	IWJ	C04-C03	2.88	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	306	CHL	CBD-CGD	-2.88	1.48	1.52
3	P	301	CLA	C3B-C4B	2.87	1.51	1.42
4	R	311	CHL	CMB-C2B	-2.87	1.45	1.51
3	Q	312	CLA	C1B-C2B	2.86	1.49	1.43
4	Q	307	CHL	CMD-C2D	-2.85	1.45	1.51
5	P	308	KC2	C4B-NB	2.85	1.41	1.37
8	P	320	IWJ	C04-C03	2.84	1.54	1.50
7	P	317	NEX	C7-C8	-2.84	1.27	1.31
3	R	316	CLA	C1B-C2B	2.83	1.49	1.43
4	R	318	CHL	C1A-CHA	-2.83	1.36	1.40
4	R	310	CHL	C1A-CHA	-2.82	1.36	1.40
8	R	303	IWJ	C04-C03	2.82	1.54	1.50
8	Q	301	IWJ	C04-C03	2.82	1.54	1.50
3	P	311	CLA	C4B-NB	2.81	1.41	1.37
6	R	323	Q6L	C12-C13	-2.81	1.45	1.51
7	P	317	NEX	C12-C13	2.80	1.52	1.46
3	P	309	CLA	C4B-NB	2.80	1.41	1.37
4	P	306	CHL	CHC-C4B	-2.80	1.35	1.39
3	Q	313	CLA	C1B-C2B	2.80	1.49	1.43
5	R	312	KC2	C3D-C4D	2.79	1.47	1.40
3	R	306	CLA	CMD-C2D	-2.78	1.45	1.50
3	P	311	CLA	C1B-C2B	2.78	1.49	1.43
3	R	313	CLA	C1B-C2B	2.77	1.49	1.43
3	P	302	CLA	C4B-NB	2.77	1.41	1.37
8	Q	301	IWJ	C03-C02	2.77	1.36	1.33
3	Q	302	CLA	C3B-C4B	2.77	1.50	1.42
6	P	319	Q6L	C02-C03	2.77	1.37	1.34
6	R	320	Q6L	C34-C33	2.76	1.54	1.50
4	P	304	CHL	CHC-C1C	2.76	1.44	1.39
6	Q	318	Q6L	C33-C32	2.75	1.36	1.33
5	P	308	KC2	C3D-C4D	2.74	1.47	1.40
3	Q	311	CLA	C4B-NB	2.74	1.41	1.37
4	P	306	CHL	CAC-C3C	-2.73	1.46	1.51
3	R	315	CLA	C1B-C2B	2.73	1.49	1.43
5	R	312	KC2	C2A-C1A	2.72	1.53	1.44
5	Q	308	KC2	C3D-C4D	2.72	1.47	1.40
8	P	318	IWJ	C04-C03	2.72	1.54	1.50
6	Q	316	Q6L	C12-C13	-2.72	1.45	1.51
4	P	305	CHL	CMD-C2D	-2.72	1.46	1.51
4	P	307	CHL	CAC-C3C	-2.72	1.46	1.51
3	R	317	CLA	C4B-NB	2.71	1.41	1.37
3	P	313	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	314	CHL	CMD-C2D	-2.69	1.46	1.51
3	Q	303	CLA	C4B-NB	2.69	1.41	1.37
4	Q	307	CHL	C1A-CHA	-2.69	1.36	1.40
6	R	320	Q6L	C12-C13	-2.69	1.45	1.51
4	Q	307	CHL	CMB-C2B	-2.69	1.46	1.51
6	P	319	Q6L	C33-C32	2.68	1.36	1.33
6	Q	317	Q6L	C02-C03	2.67	1.37	1.34
3	R	317	CLA	C1B-C2B	2.67	1.49	1.43
6	R	304	Q6L	C34-C33	2.67	1.54	1.50
7	Q	315	NEX	C22-C21	-2.66	1.50	1.54
4	Q	306	CHL	CMB-C2B	-2.66	1.46	1.51
8	R	322	IWJ	C03-C02	2.66	1.36	1.33
5	R	312	KC2	C4B-NB	2.66	1.41	1.37
3	P	312	CLA	C1B-C2B	2.66	1.49	1.43
4	R	302	CHL	CMA-C3A	-2.65	1.48	1.53
5	R	312	KC2	MG-ND	-2.65	2.00	2.05
6	R	319	Q6L	C12-C13	-2.64	1.45	1.51
5	R	312	KC2	CMC-C2C	-2.64	1.45	1.50
3	Q	310	CLA	C1B-C2B	2.63	1.49	1.43
3	Q	304	CLA	C4B-NB	2.63	1.41	1.37
6	R	304	Q6L	C02-C03	2.63	1.37	1.34
3	Q	303	CLA	C1B-C2B	2.62	1.49	1.43
3	R	317	CLA	CMC-C2C	-2.62	1.45	1.50
6	P	316	Q6L	C12-C13	-2.62	1.45	1.51
7	Q	315	NEX	C12-C13	2.62	1.51	1.46
3	Q	304	CLA	CMB-C2B	-2.62	1.45	1.50
6	P	316	Q6L	C34-C33	2.61	1.54	1.50
3	R	305	CLA	C3B-C4B	2.61	1.50	1.42
3	R	305	CLA	C4B-NB	2.61	1.41	1.37
8	P	320	IWJ	C03-C02	2.61	1.36	1.33
3	R	305	CLA	C1B-C2B	2.61	1.49	1.43
4	Q	306	CHL	C3D-CAD	-2.60	1.42	1.47
4	P	307	CHL	CMD-C2D	-2.60	1.46	1.51
4	Q	306	CHL	CAC-C3C	-2.60	1.47	1.51
4	P	307	CHL	CMB-C2B	-2.60	1.46	1.51
3	Q	309	CLA	C1B-C2B	2.59	1.49	1.43
8	R	303	IWJ	C03-C02	2.59	1.36	1.33
5	Q	308	KC2	C4B-NB	2.58	1.41	1.37
6	Q	318	Q6L	C02-C03	2.58	1.37	1.34
8	P	320	IWJ	O39-C29	-2.57	1.39	1.43
4	R	309	CHL	C3D-CAD	-2.57	1.42	1.47
6	R	304	Q6L	C12-C13	-2.57	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	309	CLA	C1B-C2B	2.57	1.49	1.43
4	P	307	CHL	CBD-CGD	-2.56	1.49	1.52
4	P	306	CHL	CMB-C2B	-2.55	1.46	1.51
3	Q	302	CLA	CAA-C2A	-2.55	1.49	1.54
4	P	304	CHL	CMD-C2D	-2.55	1.46	1.51
6	R	301	Q6L	C33-C32	2.54	1.36	1.33
6	R	320	Q6L	C02-C03	2.54	1.37	1.34
3	Q	311	CLA	C1B-C2B	2.54	1.49	1.43
6	Q	317	Q6L	C12-C13	-2.54	1.46	1.51
3	R	307	CLA	C1B-C2B	2.54	1.49	1.43
4	R	310	CHL	CBD-CGD	-2.54	1.49	1.52
6	P	321	Q6L	C12-C13	-2.53	1.46	1.51
4	P	306	CHL	CBD-CGD	-2.53	1.49	1.52
7	Q	315	NEX	C38-C25	2.53	1.55	1.51
3	R	317	CLA	CHC-C1C	2.53	1.43	1.38
8	Q	319	IWJ	C03-C02	2.52	1.36	1.33
3	P	310	CLA	C1B-C2B	2.52	1.49	1.43
5	Q	308	KC2	CMC-C2C	-2.52	1.45	1.50
3	R	306	CLA	C1B-C2B	2.52	1.49	1.43
4	R	309	CHL	OBD-CAD	-2.51	1.19	1.22
5	P	308	KC2	C2A-C1A	2.51	1.52	1.44
3	Q	312	CLA	C3B-C4B	2.50	1.50	1.42
5	Q	308	KC2	C1D-ND	2.50	1.41	1.37
3	R	317	CLA	C3B-C4B	2.50	1.50	1.42
4	R	311	CHL	CMC-C2C	2.50	1.50	1.44
3	Q	312	CLA	C4B-NB	2.49	1.41	1.37
4	Q	306	CHL	CMA-C3A	-2.49	1.49	1.53
3	R	314	CLA	C1B-C2B	2.49	1.49	1.43
5	P	308	KC2	CMC-C2C	-2.49	1.45	1.50
6	P	315	Q6L	C02-C03	2.48	1.37	1.34
6	Q	318	Q6L	C12-C13	-2.48	1.46	1.51
6	R	301	Q6L	C34-C33	2.48	1.53	1.50
5	Q	308	KC2	C1B-C2B	2.48	1.50	1.45
5	Q	308	KC2	O2A-CGA	2.48	1.36	1.30
4	Q	305	CHL	CMD-C2D	-2.47	1.46	1.51
3	Q	309	CLA	C3B-C4B	2.47	1.49	1.42
3	P	301	CLA	C1B-C2B	2.47	1.48	1.43
5	P	308	KC2	CMB-C2B	-2.46	1.45	1.50
6	R	304	Q6L	C33-C32	2.46	1.36	1.33
4	Q	305	CHL	CHC-C4B	-2.46	1.35	1.39
4	R	308	CHL	CMD-C2D	-2.46	1.46	1.51
4	R	309	CHL	CMD-C2D	-2.45	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	311	CHL	MG-NB	-2.45	2.00	2.05
3	R	315	CLA	C3B-C4B	2.45	1.49	1.42
6	P	319	Q6L	C01-C02	2.45	1.54	1.50
3	P	303	CLA	C1B-C2B	2.44	1.48	1.43
6	R	319	Q6L	C34-C33	2.43	1.53	1.50
4	P	305	CHL	C1A-CHA	-2.43	1.37	1.40
6	R	319	Q6L	C01-C02	2.43	1.54	1.50
5	R	312	KC2	C1D-ND	2.42	1.41	1.37
6	P	316	Q6L	C33-C32	2.42	1.36	1.33
4	P	304	CHL	CHB-C4A	-2.42	1.35	1.38
6	R	323	Q6L	C01-C02	2.42	1.54	1.50
6	Q	316	Q6L	C02-C03	2.41	1.37	1.34
3	P	309	CLA	C3B-C4B	2.41	1.49	1.42
6	P	321	Q6L	C01-C02	2.41	1.54	1.50
6	R	304	Q6L	C01-C02	2.41	1.54	1.50
6	P	315	Q6L	C01-C02	2.40	1.54	1.50
4	R	302	CHL	CHC-C4B	-2.40	1.35	1.39
3	R	316	CLA	C3B-C4B	2.40	1.49	1.42
5	P	308	KC2	O2A-CGA	2.39	1.36	1.30
5	R	312	KC2	CMB-C2B	-2.39	1.45	1.50
3	Q	313	CLA	C3B-C4B	2.39	1.49	1.42
3	Q	304	CLA	MG-NB	-2.38	2.01	2.05
5	R	312	KC2	CMD-C2D	-2.38	1.45	1.50
6	Q	316	Q6L	C34-C33	2.38	1.53	1.50
3	Q	309	CLA	C4B-NB	2.38	1.41	1.37
7	R	321	NEX	C28-C29	2.38	1.51	1.46
3	P	311	CLA	C3B-C4B	2.37	1.49	1.42
6	P	316	Q6L	C04-C03	2.37	1.56	1.53
4	P	305	CHL	CAC-C3C	-2.37	1.47	1.51
5	R	312	KC2	MG-NB	-2.37	2.01	2.05
5	Q	308	KC2	CMD-C2D	-2.37	1.45	1.50
4	Q	314	CHL	C1A-CHA	-2.36	1.37	1.40
3	P	303	CLA	C3B-C4B	2.36	1.49	1.42
4	R	302	CHL	CMB-C2B	-2.36	1.46	1.51
4	R	308	CHL	CBD-CGD	-2.36	1.49	1.52
4	R	311	CHL	CBD-CGD	-2.35	1.49	1.52
4	Q	314	CHL	CMD-C2D	-2.35	1.46	1.51
3	R	306	CLA	C4B-NB	2.34	1.40	1.37
5	R	312	KC2	O2A-CGA	2.34	1.36	1.30
3	P	302	CLA	C1B-C2B	2.33	1.48	1.43
6	P	319	Q6L	C34-C33	2.33	1.53	1.50
3	Q	311	CLA	CMD-C2D	-2.33	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	310	CHL	CMB-C2B	-2.33	1.47	1.51
3	R	307	CLA	C3B-C4B	2.33	1.49	1.42
7	R	321	NEX	C32-C33	2.33	1.50	1.46
3	P	301	CLA	CHC-C1C	2.33	1.43	1.38
3	P	303	CLA	CHC-C1C	2.32	1.43	1.38
3	P	312	CLA	C3B-C4B	2.32	1.49	1.42
3	R	315	CLA	CHC-C1C	2.32	1.43	1.38
4	P	314	CHL	CMB-C2B	-2.32	1.47	1.51
6	P	316	Q6L	C01-C02	2.32	1.54	1.50
6	P	319	Q6L	C12-C13	-2.31	1.46	1.51
7	R	321	NEX	C12-C13	2.31	1.50	1.46
4	R	309	CHL	CAC-C3C	-2.30	1.47	1.51
4	Q	307	CHL	CBD-CGD	-2.30	1.49	1.52
7	P	317	NEX	C28-C29	2.30	1.50	1.46
5	P	308	KC2	CMD-C2D	-2.29	1.46	1.50
6	P	321	Q6L	C02-C03	2.29	1.37	1.34
7	R	321	NEX	O24-C25	-2.29	1.43	1.46
4	Q	306	CHL	MG-ND	-2.29	2.01	2.05
4	P	306	CHL	CMC-C2C	2.28	1.49	1.44
3	R	306	CLA	C3B-C4B	2.28	1.49	1.42
4	P	307	CHL	CMC-C2C	2.28	1.49	1.44
3	R	316	CLA	CMB-C2B	-2.27	1.46	1.50
3	Q	311	CLA	C3B-C4B	2.27	1.49	1.42
4	R	310	CHL	CHC-C4B	-2.27	1.36	1.39
6	P	321	Q6L	C33-C32	2.27	1.35	1.33
8	P	318	IWJ	C26-C24	-2.27	1.45	1.49
3	Q	303	CLA	CMB-C2B	-2.26	1.46	1.50
3	R	307	CLA	CMB-C2B	-2.26	1.46	1.50
3	P	312	CLA	CHC-C1C	2.26	1.43	1.38
7	P	317	NEX	C32-C33	2.26	1.50	1.46
4	R	310	CHL	CMC-C2C	2.26	1.49	1.44
4	Q	314	CHL	CMB-C2B	-2.26	1.47	1.51
4	P	305	CHL	CMB-C2B	-2.25	1.47	1.51
3	P	310	CLA	C3B-C4B	2.25	1.49	1.42
3	Q	302	CLA	C1B-C2B	2.24	1.48	1.43
3	P	302	CLA	C3B-C4B	2.24	1.49	1.42
7	Q	315	NEX	C32-C33	2.24	1.50	1.46
3	R	307	CLA	CMD-C2D	-2.24	1.46	1.50
4	R	302	CHL	CMD-C2D	-2.24	1.47	1.51
4	R	308	CHL	CHC-C4B	-2.24	1.36	1.39
4	R	302	CHL	CBD-CGD	-2.24	1.49	1.52
3	P	313	CLA	C3B-C4B	2.23	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	318	Q6L	C01-C02	2.22	1.54	1.50
6	Q	317	Q6L	C01-C02	2.22	1.54	1.50
3	R	307	CLA	CHC-C1C	2.22	1.42	1.38
6	P	321	Q6L	C34-C33	2.22	1.53	1.50
6	P	315	Q6L	C33-C32	2.22	1.35	1.33
3	Q	310	CLA	CMD-C2D	-2.22	1.46	1.50
6	R	323	Q6L	C33-C32	2.22	1.35	1.33
3	Q	313	CLA	CMD-C2D	-2.21	1.46	1.50
3	P	310	CLA	CHC-C1C	2.20	1.42	1.38
3	Q	302	CLA	CMA-C3A	-2.20	1.48	1.53
6	R	320	Q6L	C33-C32	2.20	1.35	1.33
6	R	319	Q6L	C33-C32	2.20	1.35	1.33
3	P	301	CLA	C4B-NB	2.20	1.40	1.37
6	R	301	Q6L	C02-C03	2.20	1.37	1.34
3	Q	304	CLA	C1B-C2B	2.20	1.48	1.43
3	Q	304	CLA	C3B-C4B	2.20	1.49	1.42
4	P	306	CHL	MG-NB	-2.19	2.01	2.05
3	Q	310	CLA	C3B-C4B	2.19	1.49	1.42
4	R	318	CHL	CMB-C2B	-2.19	1.47	1.51
3	P	302	CLA	CHC-C1C	2.18	1.42	1.38
3	R	315	CLA	CMB-C2B	-2.18	1.46	1.50
7	R	321	NEX	C22-C21	-2.18	1.51	1.54
3	P	313	CLA	CMB-C2B	-2.17	1.46	1.50
7	P	317	NEX	C35-C15	-2.17	1.30	1.36
4	Q	307	CHL	CHC-C4B	-2.17	1.36	1.39
7	P	317	NEX	C22-C21	-2.17	1.51	1.54
3	R	315	CLA	CMD-C2D	-2.17	1.46	1.50
6	Q	316	Q6L	C01-C02	2.17	1.54	1.50
6	P	315	Q6L	C11-C03	-2.17	1.48	1.51
3	R	306	CLA	CMB-C2B	-2.16	1.46	1.50
4	R	302	CHL	C3D-CAD	-2.16	1.43	1.47
3	Q	310	CLA	CMB-C2B	-2.16	1.46	1.50
3	Q	310	CLA	CHC-C1C	2.16	1.42	1.38
4	P	304	CHL	MG-ND	-2.15	2.01	2.05
6	R	320	Q6L	C01-C02	2.15	1.54	1.50
4	R	308	CHL	MG-ND	-2.15	2.01	2.05
4	Q	314	CHL	CHC-C4B	-2.14	1.36	1.39
3	Q	302	CLA	CHC-C4B	-2.14	1.34	1.39
3	R	314	CLA	C3B-C4B	2.14	1.49	1.42
3	Q	313	CLA	CMC-C2C	-2.14	1.46	1.50
4	P	306	CHL	C1A-CHA	-2.13	1.37	1.40
6	P	321	Q6L	C29-C27	2.13	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	309	CLA	CHC-C1C	2.13	1.42	1.38
6	Q	317	Q6L	C34-C33	2.13	1.53	1.50
3	Q	304	CLA	MG-ND	-2.13	2.01	2.05
5	P	308	KC2	MG-ND	-2.13	2.01	2.05
4	R	309	CHL	CMB-C2B	-2.12	1.47	1.51
6	P	316	Q6L	C29-C27	2.12	1.50	1.46
7	Q	315	NEX	O24-C25	-2.12	1.43	1.46
3	R	306	CLA	CMC-C2C	-2.11	1.46	1.50
3	P	301	CLA	CMD-C2D	-2.11	1.46	1.50
7	P	317	NEX	O24-C25	-2.10	1.43	1.46
6	R	304	Q6L	C04-C03	2.10	1.56	1.53
3	P	313	CLA	CHC-C1C	2.10	1.42	1.38
4	R	309	CHL	CHD-C1D	-2.10	1.36	1.39
3	Q	302	CLA	CMD-C2D	-2.09	1.46	1.50
4	R	311	CHL	CHC-C1C	2.09	1.43	1.39
3	R	314	CLA	CMB-C2B	-2.09	1.46	1.50
4	Q	305	CHL	C1A-CHA	-2.09	1.37	1.40
4	R	310	CHL	MG-ND	-2.09	2.01	2.05
4	P	305	CHL	CMC-C2C	2.09	1.49	1.44
4	P	305	CHL	CMA-C3A	-2.09	1.49	1.53
4	P	314	CHL	CMC-C2C	2.09	1.49	1.44
4	Q	306	CHL	MG-NB	-2.09	2.01	2.05
7	R	321	NEX	C35-C15	-2.09	1.30	1.36
5	Q	308	KC2	CMB-C2B	-2.09	1.46	1.50
3	R	313	CLA	CAA-C2A	-2.09	1.50	1.54
3	R	314	CLA	CHC-C1C	2.09	1.42	1.38
3	Q	311	CLA	CMB-C2B	-2.09	1.46	1.50
5	P	308	KC2	CHB-C1B	2.09	1.42	1.38
6	R	323	Q6L	C02-C03	2.09	1.37	1.34
7	Q	315	NEX	C1-C6	-2.08	1.51	1.54
7	Q	315	NEX	C35-C15	-2.08	1.30	1.36
4	R	311	CHL	CHB-C1B	2.08	1.43	1.39
8	Q	301	IWJ	O39-C29	-2.08	1.39	1.43
4	R	318	CHL	CMC-C2C	2.08	1.49	1.44
6	R	301	Q6L	C01-C02	2.08	1.54	1.50
3	P	302	CLA	CMD-C2D	-2.08	1.46	1.50
3	P	302	CLA	CMB-C2B	-2.07	1.46	1.50
8	P	320	IWJ	C26-C24	-2.07	1.45	1.49
3	Q	302	CLA	CHC-C1C	2.06	1.42	1.38
4	R	308	CHL	CMC-C2C	2.06	1.49	1.44
5	R	312	KC2	C1B-C2B	2.06	1.49	1.45
4	Q	306	CHL	CMC-C2C	2.06	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	308	KC2	C1B-C2B	2.05	1.49	1.45
3	R	313	CLA	CHC-C1C	2.05	1.42	1.38
4	R	310	CHL	MG-NB	-2.05	2.01	2.05
4	P	314	CHL	CBD-CGD	-2.05	1.49	1.52
3	P	301	CLA	CMB-C2B	-2.05	1.46	1.50
3	P	309	CLA	CMB-C2B	-2.04	1.46	1.50
8	R	303	IWJ	O39-C29	-2.04	1.39	1.43
4	R	308	CHL	CAC-C3C	-2.04	1.48	1.51
8	P	318	IWJ	C32-C30	2.04	1.55	1.51
6	R	319	Q6L	C04-C03	2.04	1.56	1.53
3	Q	303	CLA	C3B-C4B	2.03	1.48	1.42
5	P	308	KC2	MG-NB	-2.03	2.01	2.05
3	Q	304	CLA	CHC-C1C	2.02	1.42	1.38
4	R	309	CHL	CMC-C2C	2.02	1.49	1.44
4	Q	314	CHL	C3A-C2A	2.02	1.56	1.54
3	Q	309	CLA	CHC-C1C	2.02	1.42	1.38
3	P	310	CLA	CMB-C2B	-2.02	1.46	1.50
3	P	309	CLA	CMD-C2D	-2.02	1.46	1.50
3	R	316	CLA	CHC-C1C	2.01	1.42	1.38
4	R	311	CHL	CAC-C3C	-2.01	1.48	1.51
3	R	313	CLA	MG-NA	2.01	2.11	2.06
4	P	306	CHL	C3B-C2B	-2.01	1.37	1.40
4	R	302	CHL	C1A-C2A	2.01	1.55	1.51
3	Q	304	CLA	C1A-CHA	-2.00	1.34	1.43
3	Q	313	CLA	CHC-C1C	2.00	1.42	1.38
3	Q	311	CLA	CHC-C4B	-2.00	1.34	1.39
3	P	301	CLA	CMA-C3A	-2.00	1.49	1.53
8	Q	301	IWJ	C09-C08	2.00	1.36	1.32

All (606) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	321	NEX	O24-C25-C24	10.63	123.46	113.49
5	P	308	KC2	CMA-C3A-C2A	-8.83	107.06	128.43
5	P	308	KC2	C1A-NA-C4A	8.71	110.65	106.68
7	Q	315	NEX	O24-C25-C24	8.53	121.48	113.49
5	R	312	KC2	C1A-NA-C4A	8.37	110.50	106.68
7	P	317	NEX	O24-C25-C24	8.16	121.14	113.49
3	Q	302	CLA	C4A-NA-C1A	7.99	110.32	106.68
6	R	323	Q6L	C11-C12-C13	7.23	133.09	112.86
5	P	308	KC2	CMA-C3A-C4A	-7.21	113.77	125.03
6	R	301	Q6L	C11-C12-C13	7.15	132.87	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	308	KC2	CMA-C3A-C4A	-7.11	113.92	125.03
5	Q	308	KC2	C1A-NA-C4A	7.07	109.90	106.68
7	P	317	NEX	C16-C1-C6	7.05	116.78	110.47
6	Q	316	Q6L	C11-C12-C13	6.70	131.59	112.86
6	R	301	Q6L	C11-C03-C04	-6.69	112.89	116.81
6	P	321	Q6L	C11-C12-C13	6.63	131.41	112.86
5	Q	308	KC2	C2A-C3A-C4A	-6.60	101.45	106.41
6	R	320	Q6L	C12-C11-C03	6.48	126.56	113.64
6	P	316	Q6L	C12-C11-C03	6.47	126.53	113.64
8	Q	319	IWJ	C35-C29-C30	6.43	115.37	108.78
5	R	312	KC2	CMA-C3A-C2A	-6.40	112.93	128.43
8	P	320	IWJ	C32-C30-C29	-6.40	107.38	113.96
6	R	323	Q6L	C05-C04-C03	6.36	119.02	110.61
3	R	316	CLA	C4A-NA-C1A	6.34	109.57	106.68
6	R	319	Q6L	C11-C12-C13	6.27	130.41	112.86
3	Q	311	CLA	C4A-NA-C1A	6.24	109.52	106.68
6	P	319	Q6L	C11-C12-C13	6.16	130.11	112.86
6	Q	317	Q6L	C12-C11-C03	6.06	125.72	113.64
6	R	301	Q6L	C05-C04-C03	6.02	118.58	110.61
6	Q	318	Q6L	C11-C12-C13	5.93	129.45	112.86
4	R	309	CHL	C1B-CHB-C4A	5.89	125.11	121.32
6	R	304	Q6L	C11-C12-C13	5.83	129.18	112.86
6	P	319	Q6L	C12-C11-C03	5.64	124.89	113.64
6	Q	317	Q6L	C11-C12-C13	5.58	128.48	112.86
6	R	304	Q6L	C12-C11-C03	5.52	124.64	113.64
6	Q	318	Q6L	C12-C11-C03	5.47	124.55	113.64
6	P	315	Q6L	C11-C12-C13	5.47	128.15	112.86
4	R	311	CHL	C1B-CHB-C4A	5.44	124.82	121.32
3	R	315	CLA	C4A-NA-C1A	5.34	109.12	106.68
3	R	316	CLA	C4-C3-C5	5.34	124.50	115.23
5	R	312	KC2	CMA-C3A-C4A	-5.31	116.74	125.03
3	Q	312	CLA	C4A-NA-C1A	5.27	109.08	106.68
3	Q	313	CLA	C4A-NA-C1A	5.25	109.08	106.68
7	Q	315	NEX	C26-C27-C28	-5.04	115.33	125.99
3	P	312	CLA	C4A-NA-C1A	5.03	108.97	106.68
5	Q	308	KC2	CMA-C3A-C2A	-5.01	116.31	128.43
3	P	309	CLA	C4A-NA-C1A	5.00	108.96	106.68
4	Q	306	CHL	C1B-CHB-C4A	4.98	124.53	121.32
3	P	301	CLA	C4A-NA-C1A	4.93	108.93	106.68
3	Q	304	CLA	C4D-C3D-CAD	-4.93	102.75	108.11
4	R	310	CHL	C4-C3-C5	4.91	121.91	116.13
3	P	311	CLA	C4A-NA-C1A	4.90	108.92	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	301	IWJ	C35-C29-C30	4.86	113.76	108.78
6	R	319	Q6L	C12-C11-C03	4.85	123.32	113.64
7	R	321	NEX	C26-C27-C28	-4.82	115.81	125.99
3	R	317	CLA	C4A-NA-C1A	4.79	108.87	106.68
5	Q	308	KC2	CHB-C4A-C3A	-4.78	117.48	125.03
6	P	315	Q6L	C12-C11-C03	4.78	123.18	113.64
3	R	305	CLA	C4A-NA-C1A	4.64	108.80	106.68
4	Q	305	CHL	O2D-CGD-CBD	4.60	116.00	110.95
6	Q	318	Q6L	C05-C04-C03	4.55	116.63	110.61
3	Q	302	CLA	O2A-CGA-O1A	-4.55	112.25	123.63
8	P	320	IWJ	C35-C29-C30	4.53	113.42	108.78
7	P	317	NEX	C26-C27-C28	-4.53	116.42	125.99
6	P	315	Q6L	C11-C03-C04	-4.49	114.18	116.81
5	R	312	KC2	C1A-C2A-C3A	-4.47	103.17	107.28
7	Q	315	NEX	C28-C29-C30	4.47	126.04	119.01
4	P	305	CHL	CED-O2D-CGD	4.47	126.05	115.92
6	P	316	Q6L	C40-C32-C33	-4.40	112.95	123.36
7	P	317	NEX	C28-C29-C30	4.39	125.92	119.01
6	R	304	Q6L	C05-C04-C03	4.38	116.40	110.61
6	P	321	Q6L	C12-C11-C03	4.37	122.36	113.64
3	P	302	CLA	C4A-NA-C1A	4.37	108.67	106.68
4	P	304	CHL	C4D-CHA-CBD	-4.37	104.56	108.97
7	P	317	NEX	O24-C25-C38	4.33	119.89	115.05
8	R	322	IWJ	C32-C30-C29	-4.31	109.53	113.96
8	R	303	IWJ	C32-C30-C29	-4.30	109.54	113.96
6	P	316	Q6L	C11-C12-C13	4.27	124.81	112.86
3	P	301	CLA	C4-C3-C5	4.24	122.59	115.23
6	P	315	Q6L	C05-C04-C03	4.24	116.21	110.61
3	R	307	CLA	C4A-NA-C1A	4.21	108.60	106.68
6	R	320	Q6L	C11-C12-C13	4.21	124.64	112.86
3	R	314	CLA	C4A-NA-C1A	4.21	108.60	106.68
4	Q	314	CHL	O2D-CGD-CBD	4.20	115.57	110.95
7	Q	315	NEX	C16-C1-C6	4.14	114.18	110.47
4	Q	314	CHL	C1B-CHB-C4A	4.13	123.98	121.32
6	P	319	Q6L	C40-C32-C33	-4.13	113.58	123.36
6	R	304	Q6L	C40-C32-C33	-4.12	113.61	123.36
4	Q	305	CHL	C1B-CHB-C4A	4.12	123.97	121.32
4	P	307	CHL	CMB-C2B-C3B	4.11	132.90	124.68
7	R	321	NEX	C28-C29-C30	4.11	125.47	119.01
3	Q	302	CLA	CHB-C4A-NA	4.10	130.32	124.40
3	R	315	CLA	O2D-CGD-O1D	-4.10	115.86	123.85
4	P	304	CHL	O2D-CGD-CBD	4.10	115.45	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	317	NEX	C38-C25-C26	-4.09	115.56	122.30
4	P	307	CHL	C1B-CHB-C4A	4.09	123.95	121.32
6	Q	316	Q6L	C11-C03-C04	-4.06	114.43	116.81
6	P	316	Q6L	C05-C04-C03	4.06	115.99	110.61
3	R	314	CLA	O2D-CGD-O1D	-4.05	115.96	123.85
4	P	304	CHL	CMB-C2B-C3B	4.04	132.76	124.68
6	Q	316	Q6L	C12-C11-C03	4.02	121.66	113.64
5	Q	308	KC2	CBA-CAA-C2A	-4.01	109.36	125.45
3	R	306	CLA	C4A-NA-C1A	3.98	108.50	106.68
4	Q	307	CHL	C1B-CHB-C4A	3.98	123.88	121.32
8	R	303	IWJ	C01-C02-C03	-3.94	114.03	123.36
4	Q	305	CHL	C1C-CHC-C4B	3.92	130.09	116.07
3	Q	310	CLA	O2D-CGD-O1D	-3.91	116.23	123.85
6	R	320	Q6L	C05-C04-C03	3.91	115.79	110.61
4	Q	306	CHL	C1C-CHC-C4B	3.90	130.01	116.07
4	Q	306	CHL	CMB-C2B-C3B	3.87	132.41	124.68
4	Q	305	CHL	CMB-C2B-C3B	3.87	132.41	124.68
8	Q	301	IWJ	C32-C30-C29	-3.86	109.99	113.96
6	P	321	Q6L	C40-C32-C33	-3.84	114.28	123.36
4	R	310	CHL	C1C-CHC-C4B	3.83	129.77	116.07
7	Q	315	NEX	C19-C9-C10	3.82	129.01	122.82
4	P	314	CHL	C1B-CHB-C4A	3.82	123.78	121.32
5	P	308	KC2	C1A-C2A-C3A	-3.81	103.77	107.28
6	Q	318	Q6L	C11-C03-C04	-3.81	114.58	116.81
4	P	307	CHL	C1C-CHC-C4B	3.79	129.65	116.07
8	P	318	IWJ	C32-C30-C29	-3.79	110.06	113.96
4	R	308	CHL	C1C-CHC-C4B	3.77	129.58	116.07
8	Q	301	IWJ	C01-C02-C03	-3.77	114.44	123.36
3	Q	311	CLA	CHB-C4A-NA	3.76	129.83	124.40
6	R	323	Q6L	C11-C03-C04	-3.76	114.61	116.81
4	R	311	CHL	C1C-CHC-C4B	3.76	129.52	116.07
8	P	320	IWJ	C01-C02-C03	-3.76	114.47	123.36
4	R	302	CHL	O2D-CGD-CBD	3.75	115.07	110.95
3	P	309	CLA	O2D-CGD-CBD	3.74	117.77	111.23
4	R	302	CHL	C1C-CHC-C4B	3.73	129.41	116.07
4	R	318	CHL	C1C-CHC-C4B	3.73	129.41	116.07
6	R	301	Q6L	C40-C32-C33	-3.73	114.54	123.36
3	P	309	CLA	O2D-CGD-O1D	-3.71	116.62	123.85
7	R	321	NEX	C19-C9-C10	3.71	128.83	122.82
4	Q	307	CHL	O2D-CGD-CBD	3.71	115.02	110.95
4	R	318	CHL	O2D-CGD-O1D	-3.70	116.64	123.85
4	P	305	CHL	C1C-CHC-C4B	3.66	129.16	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	308	CHL	C4D-CHA-CBD	-3.66	105.28	108.97
3	P	302	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
4	R	311	CHL	CHA-C1A-C2A	-3.63	124.80	133.31
3	R	305	CLA	C1D-ND-C4D	-3.62	103.77	106.31
6	R	319	Q6L	C05-C04-C03	3.62	115.40	110.61
4	Q	314	CHL	C1C-CHC-C4B	3.61	129.00	116.07
4	R	302	CHL	C1B-CHB-C4A	3.61	123.64	121.32
6	R	320	Q6L	C40-C32-C33	-3.60	114.85	123.36
3	Q	304	CLA	CMB-C2B-C1B	-3.60	119.94	125.42
8	Q	319	IWJ	C01-C02-C03	-3.58	114.89	123.36
3	P	310	CLA	C4A-NA-C1A	3.57	108.31	106.68
8	Q	319	IWJ	C28-C29-C35	-3.56	105.96	111.97
4	P	306	CHL	C1C-CHC-C4B	3.56	128.82	116.07
4	R	302	CHL	C4D-CHA-CBD	-3.55	105.38	108.97
4	P	314	CHL	C1C-CHC-C4B	3.55	128.75	116.07
4	P	307	CHL	O2D-CGD-CBD	3.54	114.83	110.95
4	R	309	CHL	C1C-CHC-C4B	3.53	128.72	116.07
4	R	309	CHL	O2D-CGD-CBD	3.53	114.83	110.95
8	R	322	IWJ	C01-C02-C03	-3.53	115.00	123.36
4	P	305	CHL	C4D-CHA-CBD	-3.49	105.45	108.97
6	R	301	Q6L	C12-C11-C03	3.49	120.60	113.64
6	R	319	Q6L	C40-C32-C33	-3.48	115.13	123.36
3	Q	313	CLA	C1-O2A-CGA	3.47	125.06	116.65
4	R	318	CHL	O2D-CGD-CBD	3.46	114.75	110.95
4	Q	314	CHL	OBD-CAD-CBD	-3.42	120.80	125.82
3	P	309	CLA	CHB-C4A-NA	3.42	129.33	124.40
4	Q	305	CHL	O2D-CGD-O1D	-3.38	117.26	123.85
4	R	309	CHL	CHA-C1A-C2A	-3.38	125.37	133.31
4	Q	307	CHL	C1C-CHC-C4B	3.37	128.14	116.07
8	P	318	IWJ	C01-C02-C03	-3.37	115.38	123.36
3	Q	312	CLA	C4-C3-C5	3.36	121.06	115.23
6	Q	317	Q6L	C40-C32-C33	-3.35	115.42	123.36
4	Q	307	CHL	OMC-CMC-C2C	-3.35	119.30	125.12
4	Q	306	CHL	CHA-C1A-C2A	-3.35	125.44	133.31
6	P	319	Q6L	C20-C21-C22	3.35	131.98	127.28
6	R	323	Q6L	C40-C32-C33	-3.35	115.44	123.36
5	P	308	KC2	CBA-CAA-C2A	-3.34	112.03	125.45
6	R	319	Q6L	C11-C03-C04	-3.34	114.86	116.81
3	P	303	CLA	C4A-NA-C1A	3.33	108.20	106.68
4	P	306	CHL	C1B-CHB-C4A	3.33	123.47	121.32
4	P	304	CHL	C1C-CHC-C4B	3.33	127.99	116.07
4	P	304	CHL	CBC-CAC-C3C	-3.33	108.11	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	311	CLA	C4-C3-C2	-3.33	115.08	123.63
5	P	308	KC2	O2D-CGD-O1D	-3.33	117.37	123.85
4	P	307	CHL	CHA-C1A-C2A	-3.32	125.51	133.31
3	P	313	CLA	C4A-NA-C1A	3.29	108.18	106.68
3	P	309	CLA	C4-C3-C5	3.28	120.93	115.23
3	Q	304	CLA	CHD-C1D-ND	-3.28	120.18	124.80
3	P	310	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
4	Q	314	CHL	O2D-CGD-O1D	-3.27	117.49	123.85
8	P	318	IWJ	C35-C29-C30	3.26	112.13	108.78
6	Q	316	Q6L	C40-C32-C33	-3.26	115.65	123.36
4	R	318	CHL	CHA-C1A-C2A	-3.25	125.68	133.31
6	P	319	Q6L	C11-C03-C04	-3.24	114.91	116.81
6	Q	318	Q6L	C40-C32-C33	-3.24	115.69	123.36
4	P	304	CHL	C3D-C4D-CHA	3.24	113.46	108.54
7	Q	315	NEX	O24-C25-C38	3.23	118.66	115.05
6	R	323	Q6L	C12-C11-C03	3.23	120.07	113.64
4	P	305	CHL	CHA-C1A-C2A	-3.22	125.74	133.31
3	Q	309	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
7	Q	315	NEX	C11-C10-C9	-3.22	122.77	127.28
4	R	309	CHL	O2D-CGD-O1D	-3.21	117.60	123.85
4	R	309	CHL	CMB-C2B-C3B	3.20	131.08	124.68
4	R	309	CHL	CBC-CAC-C3C	3.19	117.45	112.87
3	R	313	CLA	O2D-CGD-CBD	3.19	116.81	111.23
5	Q	308	KC2	O2D-CGD-O1D	-3.19	117.63	123.85
3	Q	303	CLA	C4A-NA-C1A	3.19	108.14	106.68
6	R	301	Q6L	C42-C13-C12	3.18	120.75	115.23
4	R	310	CHL	C1B-CHB-C4A	3.18	123.37	121.32
4	Q	307	CHL	CHA-C1A-C2A	-3.18	125.85	133.31
3	Q	304	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
3	Q	313	CLA	O2A-CGA-O1A	-3.16	115.72	123.63
3	R	305	CLA	CBA-CAA-C2A	3.16	123.19	113.79
7	P	317	NEX	C39-C29-C30	-3.15	117.71	122.82
5	R	312	KC2	CBA-CAA-C2A	-3.14	112.83	125.45
3	P	301	CLA	CHB-C4A-NA	3.13	128.92	124.40
6	R	323	Q6L	C35-C34-C33	3.12	115.82	111.18
5	P	308	KC2	CHB-C4A-NA	3.11	129.06	124.23
7	R	321	NEX	C39-C29-C30	-3.11	117.78	122.82
5	R	312	KC2	O2D-CGD-O1D	-3.10	117.81	123.85
4	R	308	CHL	C3D-C4D-CHA	3.10	113.25	108.54
3	Q	309	CLA	C1-C2-C3	-3.09	121.14	126.20
4	Q	307	CHL	CMB-C2B-C3B	3.08	130.84	124.68
8	R	303	IWJ	C35-C29-C30	3.08	111.94	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	305	CHL	C4D-CHA-CBD	-3.07	105.87	108.97
3	P	303	CLA	CHB-C4A-NA	3.06	128.81	124.40
4	P	306	CHL	O2D-CGD-CBD	3.06	114.30	110.95
4	P	305	CHL	CMB-C2B-C3B	3.05	130.78	124.68
3	R	314	CLA	O2D-CGD-CBD	3.05	116.55	111.23
3	Q	309	CLA	C4A-NA-C1A	3.04	108.07	106.68
7	P	317	NEX	C11-C10-C9	-3.03	123.03	127.28
7	P	317	NEX	C40-C33-C32	3.03	122.72	118.09
3	P	302	CLA	CHB-C4A-NA	3.03	128.77	124.40
3	R	305	CLA	CHB-C4A-NA	3.02	128.76	124.40
3	P	311	CLA	O2A-CGA-O1A	-3.02	116.07	123.63
3	R	313	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
3	R	314	CLA	CHB-C4A-NA	3.00	128.73	124.40
4	Q	305	CHL	CHA-C1A-C2A	-3.00	126.27	133.31
7	Q	315	NEX	C12-C13-C14	-3.00	114.30	119.01
6	P	315	Q6L	C40-C32-C33	-2.99	116.27	123.36
5	Q	308	KC2	CHB-C4A-NA	2.99	128.87	124.23
4	P	305	CHL	CBC-CAC-C3C	-2.99	108.60	112.87
3	P	310	CLA	O2A-CGA-O1A	-2.99	116.16	123.63
3	R	306	CLA	CHB-C4A-NA	2.97	128.69	124.40
3	R	316	CLA	CBA-CAA-C2A	2.97	122.64	113.79
7	P	317	NEX	C20-C13-C12	2.97	122.63	118.09
4	P	307	CHL	C3C-C4C-NC	-2.97	107.40	114.65
4	R	302	CHL	C3D-C4D-CHA	2.96	113.05	108.54
7	R	321	NEX	C16-C1-C6	2.96	113.12	110.47
6	Q	316	Q6L	C42-C13-C12	2.96	120.36	115.23
7	R	321	NEX	C38-C25-C26	-2.95	117.45	122.30
6	R	323	Q6L	C42-C13-C12	2.95	120.34	115.23
4	R	302	CHL	C3C-C4C-NC	-2.94	107.45	114.65
4	R	310	CHL	CHA-C1A-C2A	-2.94	126.40	133.31
3	R	317	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
8	Q	319	IWJ	C32-C30-C29	-2.93	110.94	113.96
4	Q	314	CHL	C4D-CHA-CBD	-2.93	106.01	108.97
4	R	302	CHL	O2D-CGD-O1D	-2.93	118.14	123.85
6	P	316	Q6L	C15-C14-C13	-2.92	123.58	127.69
3	Q	303	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
4	R	311	CHL	CMB-C2B-C3B	2.92	130.51	124.68
4	Q	307	CHL	C4D-CHA-CBD	-2.91	106.03	108.97
7	Q	315	NEX	C15-C35-C34	-2.91	117.56	123.52
3	Q	309	CLA	CHB-C4A-NA	2.90	128.58	124.40
6	Q	316	Q6L	C31-C30-C29	-2.90	120.07	124.58
5	R	312	KC2	CMD-C2D-C1D	-2.90	121.01	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	308	KC2	CAA-C2A-C1A	-2.89	111.96	124.64
4	R	308	CHL	CMB-C2B-C3B	2.89	130.45	124.68
3	Q	309	CLA	O2D-CGD-CBD	2.87	116.25	111.23
6	R	320	Q6L	C15-C14-C13	-2.87	123.66	127.69
4	R	310	CHL	C4D-ND-C1D	2.86	107.39	105.22
3	P	311	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
3	R	313	CLA	O2A-CGA-O1A	-2.86	116.47	123.63
4	Q	314	CHL	C3D-C4D-CHA	2.86	112.89	108.54
3	Q	309	CLA	CBA-CAA-C2A	2.86	122.30	113.79
3	R	305	CLA	CAA-CBA-CGA	2.86	121.32	113.21
5	Q	308	KC2	O2A-CGA-O1A	-2.85	116.89	122.70
8	R	322	IWJ	C35-C29-C30	2.85	111.70	108.78
4	P	314	CHL	CHA-C1A-C2A	-2.84	126.63	133.31
3	P	302	CLA	O2D-CGD-CBD	2.84	116.20	111.23
7	R	321	NEX	C40-C33-C32	2.83	122.42	118.09
7	R	321	NEX	C11-C10-C9	-2.83	123.30	127.28
4	P	314	CHL	C4C-CHD-C1D	2.82	126.17	116.07
4	P	306	CHL	C3C-C4C-NC	-2.82	107.75	114.65
3	P	301	CLA	CMC-C2C-C1C	2.81	129.43	125.03
4	Q	306	CHL	C3C-C4C-NC	-2.80	107.80	114.65
4	P	306	CHL	C4D-CHA-CBD	-2.80	106.14	108.97
3	P	302	CLA	C3B-C4B-NB	-2.80	108.03	110.53
6	Q	316	Q6L	C05-C04-C03	2.79	114.31	110.61
3	R	316	CLA	CHB-C4A-NA	2.78	128.42	124.40
3	P	302	CLA	C4-C3-C5	2.78	120.06	115.23
6	P	321	Q6L	C19-C18-C17	-2.78	123.38	127.28
4	R	318	CHL	CMB-C2B-C3B	2.78	130.24	124.68
3	P	310	CLA	CHB-C4A-NA	2.77	128.40	124.40
4	R	310	CHL	C4D-CHA-CBD	-2.77	106.17	108.97
3	R	305	CLA	O2D-CGD-O1D	-2.77	118.47	123.85
3	R	315	CLA	O2D-CGD-CBD	2.76	116.06	111.23
3	R	315	CLA	O2A-CGA-O1A	-2.76	116.71	123.63
4	Q	307	CHL	O2D-CGD-O1D	-2.76	118.48	123.85
3	P	313	CLA	CAA-C2A-C3A	-2.75	105.57	113.00
3	Q	302	CLA	C2B-C1B-NB	2.75	113.17	110.33
5	R	312	KC2	CAA-C2A-C1A	-2.74	112.62	124.64
3	Q	304	CLA	CBA-CAA-C2A	2.74	121.94	113.79
4	P	304	CHL	O2D-CGD-O1D	-2.72	118.55	123.85
4	P	314	CHL	O2D-CGD-O1D	-2.72	118.55	123.85
3	R	307	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
3	R	313	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
7	P	317	NEX	C12-C13-C14	-2.70	114.76	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	316	Q6L	C01-C02-C07	-2.70	109.45	114.42
4	R	310	CHL	CMD-C2D-C3D	2.70	130.08	124.68
4	R	309	CHL	O2A-CGA-O1A	-2.70	116.87	123.63
4	R	308	CHL	C1B-CHB-C4A	2.70	123.06	121.32
4	P	306	CHL	CHA-C1A-C2A	-2.70	126.97	133.31
4	P	305	CHL	CMD-C2D-C3D	2.70	130.08	124.68
4	P	306	CHL	O2D-CGD-O1D	-2.70	118.60	123.85
4	P	305	CHL	C3D-C4D-CHA	2.69	112.63	108.54
3	Q	312	CLA	CHB-C4A-NA	2.69	128.28	124.40
5	R	312	KC2	O1A-CGA-CBA	2.69	129.29	121.06
3	R	316	CLA	C5-C3-C2	-2.69	115.14	121.17
6	Q	317	Q6L	C23-C22-C21	2.68	127.16	122.82
6	P	319	Q6L	C05-C04-C03	2.68	114.16	110.61
3	R	307	CLA	CHB-C4A-NA	2.68	128.27	124.40
3	Q	310	CLA	C4A-NA-C1A	2.68	107.90	106.68
8	Q	319	IWJ	O27-C26-C28	-2.67	116.29	121.76
7	R	321	NEX	C20-C13-C12	2.67	122.17	118.09
8	P	320	IWJ	C25-C24-C26	2.66	120.32	116.00
7	Q	315	NEX	C39-C29-C30	-2.66	118.50	122.82
4	P	314	CHL	O2D-CGD-CBD	2.66	113.87	110.95
3	R	317	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
4	Q	314	CHL	CHA-C1A-C2A	-2.65	127.08	133.31
3	P	313	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
4	P	307	CHL	O2D-CGD-O1D	-2.65	118.70	123.85
4	R	309	CHL	C3D-C4D-CHA	2.65	112.56	108.54
6	R	320	Q6L	C35-C34-C33	2.64	115.11	111.18
3	R	316	CLA	CMB-C2B-C1B	-2.63	121.41	125.42
4	R	310	CHL	CMB-C2B-C3B	2.63	129.94	124.68
4	R	318	CHL	C1B-CHB-C4A	2.63	123.01	121.32
4	P	305	CHL	C3C-C4C-NC	-2.62	108.24	114.65
3	R	305	CLA	CMC-C2C-C1C	2.62	129.13	125.03
4	R	309	CHL	CMD-C2D-C3D	2.62	129.92	124.68
5	R	312	KC2	C3C-C2C-C1C	2.62	108.38	106.41
3	R	314	CLA	C1-C2-C3	-2.62	121.91	126.20
4	P	314	CHL	CMB-C2B-C3B	2.61	129.91	124.68
3	Q	304	CLA	CGD-CBD-CAD	-2.61	102.39	110.85
3	R	317	CLA	CHB-C4A-NA	2.60	128.16	124.40
3	Q	312	CLA	CBA-CAA-C2A	2.60	121.54	113.79
8	P	320	IWJ	C23-C22-C21	-2.60	115.67	123.20
3	P	312	CLA	CHB-C4A-NA	2.60	128.15	124.40
4	Q	314	CHL	CMB-C2B-C3B	2.59	129.87	124.68
3	R	314	CLA	C1-O2A-CGA	2.59	122.92	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	311	CLA	C4-C3-C5	2.59	119.72	115.23
4	R	308	CHL	CMD-C2D-C3D	2.59	129.85	124.68
6	P	316	Q6L	C10-C04-C03	2.58	113.81	109.78
3	R	314	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
4	P	306	CHL	C4-C3-C5	2.58	119.17	116.13
3	R	313	CLA	C1D-ND-C4D	-2.58	104.50	106.31
5	P	308	KC2	CHB-C4A-C3A	-2.58	120.96	125.03
3	R	316	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
4	R	309	CHL	C4D-CHA-CBD	-2.57	106.37	108.97
3	Q	313	CLA	CHB-C4A-NA	2.57	128.11	124.40
3	Q	304	CLA	CMB-C2B-C3B	2.57	132.59	126.55
5	R	312	KC2	CAA-CBA-CGA	-2.56	114.01	127.05
4	P	304	CHL	CBA-CAA-C2A	2.56	121.32	113.78
3	P	311	CLA	CHB-C4A-NA	2.56	128.09	124.40
4	R	318	CHL	O1D-CGD-CBD	2.55	128.60	124.72
3	R	315	CLA	CHB-C4A-NA	2.55	128.08	124.40
4	P	304	CHL	C4D-ND-C1D	2.54	107.15	105.22
6	P	319	Q6L	C23-C22-C21	2.54	126.94	122.82
4	R	311	CHL	C3C-C4C-NC	-2.54	108.43	114.65
5	P	308	KC2	CAA-CBA-CGA	-2.54	114.11	127.05
3	R	307	CLA	CHD-C1D-ND	-2.54	121.22	124.80
6	Q	318	Q6L	C01-C02-C07	-2.54	109.75	114.42
3	Q	313	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
3	R	305	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
7	R	321	NEX	C15-C35-C34	-2.54	118.33	123.52
7	Q	315	NEX	C15-C14-C13	-2.53	123.73	127.28
3	P	312	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
8	P	320	IWJ	C21-C19-C18	-2.52	115.04	119.01
3	P	312	CLA	O2A-C1-C2	2.52	117.81	108.11
3	R	307	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
5	P	308	KC2	O2A-CGA-O1A	-2.52	117.58	122.70
4	P	304	CHL	CMD-C2D-C3D	2.52	129.71	124.68
7	R	321	NEX	C12-C13-C14	-2.51	115.05	119.01
6	R	320	Q6L	C19-C20-C21	-2.51	118.38	123.52
3	P	312	CLA	CHD-C1D-ND	-2.51	121.27	124.80
3	Q	303	CLA	C2D-C1D-ND	-2.50	107.65	110.13
3	R	313	CLA	CMB-C2B-C3B	2.50	132.42	126.55
4	P	314	CHL	C4D-CHA-CBD	-2.49	106.45	108.97
3	P	309	CLA	CHD-C1D-ND	-2.49	121.30	124.80
3	P	303	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
3	P	303	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
7	P	317	NEX	C15-C35-C34	-2.48	118.44	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	317	NEX	C31-C30-C29	-2.47	123.81	127.28
3	Q	312	CLA	C3B-C4B-NB	-2.47	108.33	110.53
3	P	309	CLA	CBA-CAA-C2A	2.47	121.13	113.79
6	P	321	Q6L	C05-C04-C03	2.46	113.87	110.61
4	R	302	CHL	CMB-C2B-C3B	2.46	129.61	124.68
5	R	312	KC2	C2A-C3A-C4A	-2.46	104.56	106.41
5	R	312	KC2	C4C-C3C-C2C	-2.46	105.02	107.28
3	Q	312	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
5	Q	308	KC2	C3A-C4A-NA	2.45	113.49	110.45
4	R	308	CHL	C4D-ND-C1D	2.45	107.08	105.22
8	Q	319	IWJ	C25-C24-C26	2.45	119.98	116.00
4	R	310	CHL	C3C-C4C-NC	-2.45	108.66	114.65
3	P	309	CLA	CAA-C2A-C3A	2.45	119.62	113.00
6	R	304	Q6L	C19-C18-C17	-2.45	123.84	127.28
5	R	312	KC2	CMD-C2D-C3D	2.45	133.40	125.67
7	P	317	NEX	C32-C33-C34	-2.44	115.17	119.01
4	R	308	CHL	CHA-C1A-C2A	-2.43	127.59	133.31
4	Q	307	CHL	C3D-C4D-CHA	2.43	112.24	108.54
3	P	312	CLA	O2D-CGD-CBD	2.43	115.48	111.23
3	P	303	CLA	CMB-C2B-C3B	2.43	132.26	126.55
4	P	314	CHL	C3D-C4D-CHA	2.43	112.23	108.54
3	Q	313	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
7	R	321	NEX	O24-C25-C38	2.42	117.75	115.05
3	P	303	CLA	CHD-C1D-ND	-2.41	121.40	124.80
3	P	311	CLA	CAC-C3C-C4C	2.41	127.93	124.79
7	Q	315	NEX	C20-C13-C12	2.41	121.77	118.09
4	R	310	CHL	O1D-CGD-CBD	2.40	128.37	124.72
4	Q	305	CHL	C3C-C4C-NC	-2.40	108.78	114.65
7	Q	315	NEX	C38-C25-C26	-2.40	118.35	122.30
6	P	319	Q6L	C19-C20-C21	-2.40	118.61	123.52
3	P	302	CLA	C14-C13-C15	2.40	119.83	111.27
6	R	323	Q6L	C10-C04-C03	-2.40	106.05	109.78
6	P	316	Q6L	C19-C20-C21	-2.40	118.62	123.52
3	P	302	CLA	C11-C12-C13	2.39	123.91	115.97
4	R	311	CHL	C4C-CHD-C1D	2.39	124.61	116.07
4	Q	305	CHL	C3D-C4D-CHA	2.39	112.17	108.54
8	Q	319	IWJ	C16-C17-C18	-2.37	118.67	123.52
7	Q	315	NEX	C24-C23-C22	-2.37	106.36	110.79
3	P	301	CLA	C6-C5-C3	2.36	119.23	113.47
3	P	313	CLA	CBA-CAA-C2A	2.35	120.80	113.79
4	R	302	CHL	C1C-C2C-CMC	2.35	131.04	126.80
3	P	309	CLA	C1-C2-C3	-2.35	122.34	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	305	CHL	C4C-CHD-C1D	2.35	124.47	116.07
6	Q	317	Q6L	C06-C07-C02	2.35	118.02	112.18
3	R	317	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
4	Q	314	CHL	C4D-ND-C1D	2.34	106.99	105.22
4	P	304	CHL	CMA-C3A-C4A	2.33	119.64	114.61
3	Q	312	CLA	CAC-C3C-C4C	2.33	127.82	124.79
4	P	306	CHL	C4C-CHD-C1D	2.33	124.39	116.07
4	R	302	CHL	CHA-C1A-C2A	-2.33	127.85	133.31
6	R	320	Q6L	C24-C22-C21	-2.32	115.35	119.01
5	R	312	KC2	O2A-CGA-O1A	-2.32	117.98	122.70
3	R	313	CLA	CAA-C2A-C1A	-2.32	104.37	111.97
8	Q	301	IWJ	C12-C11-C10	2.32	130.53	127.28
4	R	310	CHL	C4C-CHD-C1D	2.32	124.36	116.07
7	Q	315	NEX	C31-C30-C29	-2.32	124.03	127.28
7	Q	315	NEX	C32-C33-C34	-2.32	115.36	119.01
4	R	309	CHL	OBD-CAD-CBD	-2.31	122.43	125.82
3	Q	304	CLA	O2D-CGD-CBD	2.31	115.28	111.23
7	R	321	NEX	C38-C25-C24	-2.31	111.64	114.24
4	R	318	CHL	C3D-C4D-CHA	2.30	112.04	108.54
3	Q	313	CLA	O2A-CGA-CBA	2.30	118.83	111.83
3	R	317	CLA	CMB-C2B-C3B	2.30	131.95	126.55
5	P	308	KC2	CAC-C3C-C2C	-2.29	120.97	128.43
4	P	306	CHL	C3D-C4D-CHA	2.29	112.03	108.54
5	R	312	KC2	CAC-C3C-C2C	-2.29	120.98	128.43
4	P	306	CHL	CMB-C2B-C3B	2.29	129.26	124.68
3	Q	302	CLA	O2A-CGA-CBA	2.29	118.81	111.83
3	Q	304	CLA	C3B-C4B-NB	-2.29	108.49	110.53
4	P	314	CHL	CMD-C2D-C3D	2.28	129.24	124.68
7	P	317	NEX	C35-C15-C14	-2.28	118.86	123.52
3	P	309	CLA	C11-C12-C13	-2.27	108.41	115.97
3	Q	310	CLA	O1D-CGD-CBD	2.27	129.00	124.52
4	R	310	CHL	O2D-CGD-O1D	-2.27	119.42	123.85
4	R	318	CHL	C4D-CHA-CBD	-2.26	106.69	108.97
4	R	310	CHL	O2A-CGA-O1A	-2.26	117.97	123.63
3	P	303	CLA	CBA-CAA-C2A	2.26	120.52	113.79
6	P	321	Q6L	C01-C02-C03	2.26	127.27	124.45
6	P	316	Q6L	C24-C22-C21	-2.26	115.46	119.01
4	Q	305	CHL	CMD-C2D-C3D	2.26	129.19	124.68
7	R	321	NEX	C31-C30-C29	-2.25	124.12	127.28
5	Q	308	KC2	CAA-CBA-CGA	-2.25	115.62	127.05
3	P	310	CLA	C11-C10-C8	2.25	123.43	115.97
4	R	310	CHL	C3D-C4D-CHA	2.25	111.95	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	301	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
3	P	302	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
3	R	314	CLA	CMA-C3A-C4A	2.24	117.80	111.77
3	P	309	CLA	C6-C5-C3	2.24	118.93	113.47
5	P	308	KC2	C3C-C2C-C1C	2.24	108.09	106.41
4	P	304	CHL	CED-O2D-CGD	2.24	120.99	115.92
3	P	313	CLA	CHD-C1D-ND	-2.24	121.66	124.80
3	P	313	CLA	CHB-C4A-NA	2.23	127.62	124.40
3	P	311	CLA	CBA-CAA-C2A	2.23	120.44	113.79
3	P	301	CLA	CAC-C3C-C4C	2.23	127.69	124.79
3	R	317	CLA	CHD-C1D-ND	-2.23	121.67	124.80
8	R	303	IWJ	C21-C19-C18	-2.22	115.51	119.01
3	Q	304	CLA	CHA-C1A-NA	-2.22	121.37	126.39
3	P	301	CLA	C5-C3-C2	-2.21	116.20	121.17
3	P	310	CLA	C1-C2-C3	-2.21	122.57	126.20
4	P	307	CHL	C4D-CHA-CBD	-2.21	106.74	108.97
4	P	304	CHL	C3C-C4C-NC	-2.20	109.27	114.65
5	P	308	KC2	O1A-CGA-CBA	2.20	127.81	121.06
6	R	319	Q6L	C01-C02-C07	-2.20	110.38	114.42
4	P	304	CHL	CHA-C1A-C2A	-2.19	128.16	133.31
3	P	303	CLA	C1-C2-C3	-2.19	123.22	126.76
8	Q	301	IWJ	C21-C19-C18	-2.19	115.56	119.01
4	R	309	CHL	C3C-C4C-NC	-2.18	109.31	114.65
3	R	307	CLA	CMB-C2B-C3B	2.18	131.69	126.55
3	Q	311	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
8	Q	301	IWJ	C36-C35-C34	-2.18	105.14	108.97
4	P	306	CHL	C4D-ND-C1D	2.18	106.87	105.22
3	R	314	CLA	CHA-C1A-NA	-2.17	121.47	126.39
3	R	316	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
4	Q	314	CHL	C1A-CHA-C4D	2.17	122.61	118.98
3	Q	303	CLA	CHB-C4A-NA	2.17	127.53	124.40
5	Q	308	KC2	CAC-C3C-C2C	-2.16	121.40	128.43
4	Q	307	CHL	CMD-C2D-C3D	2.16	129.00	124.68
7	R	321	NEX	C35-C15-C14	-2.16	119.11	123.52
8	Q	301	IWJ	C33-C32-C30	2.15	115.51	112.06
5	R	312	KC2	CAC-C3C-C4C	2.15	133.89	124.39
3	P	310	CLA	CHD-C1D-ND	-2.15	121.78	124.80
4	R	308	CHL	C4C-CHD-C1D	2.14	123.73	116.07
4	Q	307	CHL	C3C-C4C-NC	-2.14	109.42	114.65
8	Q	301	IWJ	C25-C24-C26	2.14	119.47	116.00
3	Q	302	CLA	C1D-ND-C4D	-2.14	104.81	106.31
4	P	306	CHL	CMD-C2D-C3D	2.14	128.96	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	301	Q6L	C14-C15-C16	-2.14	117.01	123.20
5	R	312	KC2	O1D-CGD-CBD	2.13	128.72	124.52
6	Q	318	Q6L	C25-C26-C27	-2.12	124.30	127.28
4	P	307	CHL	C3D-C4D-CHA	2.12	111.76	108.54
3	Q	311	CLA	C2A-C1A-CHA	2.12	127.55	123.87
4	R	311	CHL	O2D-CGD-O1D	-2.12	119.73	123.85
5	Q	308	KC2	O1A-CGA-CBA	2.12	127.55	121.06
4	R	309	CHL	C4C-CHD-C1D	2.12	123.64	116.07
3	Q	311	CLA	CHD-C1D-ND	-2.12	121.82	124.80
4	R	308	CHL	O2A-CGA-O1A	-2.12	117.89	123.33
3	R	313	CLA	CHD-C1D-ND	-2.11	121.83	124.80
4	Q	307	CHL	C4C-CHD-C1D	2.11	123.61	116.07
8	R	303	IWJ	C36-C35-C34	-2.11	105.27	108.97
6	Q	317	Q6L	C10-C04-C03	2.10	113.06	109.78
8	Q	319	IWJ	C21-C19-C18	-2.10	115.70	119.01
6	P	315	Q6L	C01-C02-C07	-2.10	110.56	114.42
4	P	306	CHL	CAA-C2A-C3A	2.10	118.68	113.00
3	R	315	CLA	C5-C3-C2	2.10	125.88	121.17
6	R	320	Q6L	C11-C03-C04	-2.09	115.59	116.81
6	Q	318	Q6L	C38-C36-C35	-2.09	105.50	109.41
6	P	315	Q6L	C19-C20-C21	-2.09	119.24	123.52
5	P	308	KC2	CAC-C3C-C4C	2.09	133.62	124.39
3	Q	304	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
4	P	304	CHL	OMC-CMC-C2C	-2.08	121.50	125.12
4	R	318	CHL	C3C-C4C-NC	-2.08	109.56	114.65
5	R	312	KC2	CHB-C4A-NA	2.08	127.46	124.23
3	R	315	CLA	CAC-C3C-C4C	2.08	127.50	124.79
3	R	315	CLA	CBA-CAA-C2A	2.08	119.98	113.79
3	P	311	CLA	CMC-C2C-C1C	2.08	128.28	125.03
3	P	310	CLA	CHA-C1A-NA	-2.08	121.68	126.39
8	P	318	IWJ	C33-C32-C30	2.08	115.39	112.06
8	R	322	IWJ	C36-C35-C34	-2.08	105.32	108.97
3	P	312	CLA	CBA-CAA-C2A	2.08	119.97	113.79
7	R	321	NEX	C15-C14-C13	-2.08	124.37	127.28
6	R	323	Q6L	C14-C15-C16	-2.08	117.19	123.20
4	Q	314	CHL	CMD-C2D-C3D	2.07	128.83	124.68
6	P	319	Q6L	C01-C02-C07	-2.07	110.61	114.42
3	Q	309	CLA	CHD-C1D-ND	-2.07	121.89	124.80
4	R	302	CHL	CMD-C2D-C3D	2.07	128.81	124.68
6	Q	317	Q6L	C23-C22-C24	-2.06	114.94	118.09
6	P	321	Q6L	C19-C20-C21	-2.06	119.30	123.52
3	Q	304	CLA	CHB-C1B-NB	2.06	127.14	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	315	NEX	C40-C33-C32	2.06	121.23	118.09
4	P	305	CHL	O1A-CGA-CBA	2.05	129.60	123.09
6	R	301	Q6L	C19-C20-C21	-2.05	119.32	123.52
6	Q	316	Q6L	C14-C15-C16	-2.05	117.26	123.20
6	Q	318	Q6L	C16-C17-C18	-2.05	115.79	119.01
5	P	308	KC2	C4C-C3C-C2C	-2.05	105.40	107.28
6	R	323	Q6L	C19-C20-C21	-2.05	119.33	123.52
6	Q	318	Q6L	C42-C13-C12	2.04	118.77	115.23
6	R	320	Q6L	C26-C25-C24	-2.04	117.29	123.20
6	R	304	Q6L	C01-C02-C07	-2.04	110.67	114.42
4	Q	305	CHL	O2A-CGA-O1A	-2.04	118.08	123.33
3	P	312	CLA	CAA-CBA-CGA	-2.04	107.42	113.21
7	Q	315	NEX	C35-C15-C14	-2.04	119.35	123.52
3	R	316	CLA	C1-O2A-CGA	-2.04	111.71	116.65
5	P	308	KC2	O1D-CGD-CBD	2.04	128.53	124.52
4	P	305	CHL	C1A-CHA-C4D	2.04	122.38	118.98
4	R	302	CHL	C4C-CHD-C1D	2.03	123.35	116.07
3	P	311	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
4	P	304	CHL	O1A-CGA-CBA	2.03	129.54	123.09
3	Q	313	CLA	CMB-C2B-C3B	2.03	131.33	126.55
3	P	302	CLA	CHD-C1D-ND	-2.03	121.95	124.80
3	R	306	CLA	CHD-C1D-ND	-2.03	121.95	124.80
4	P	306	CHL	C1C-C2C-CMC	2.03	130.46	126.80
3	R	313	CLA	CAA-C2A-C3A	2.03	118.48	113.00
4	P	307	CHL	CMD-C2D-C3D	2.03	128.73	124.68
8	P	320	IWJ	C36-C35-C34	-2.03	105.41	108.97
3	P	301	CLA	C1D-ND-C4D	-2.03	104.89	106.31
3	Q	310	CLA	O2D-CGD-CBD	2.02	114.77	111.23
3	R	313	CLA	CMC-C2C-C1C	2.02	128.20	125.03
7	P	317	NEX	C36-C21-C22	-2.02	105.42	108.97
4	R	308	CHL	OMC-CMC-C2C	-2.02	121.61	125.12
6	Q	318	Q6L	C35-C34-C33	2.02	114.18	111.18
6	Q	318	Q6L	C20-C19-C18	-2.02	119.39	123.52
3	R	317	CLA	CAC-C3C-C4C	2.02	127.42	124.79
4	Q	314	CHL	C3C-C4C-NC	-2.02	109.72	114.65
3	Q	311	CLA	CMC-C2C-C1C	2.02	128.18	125.03
8	Q	319	IWJ	C36-C35-C34	-2.01	105.43	108.97
6	Q	316	Q6L	C16-C17-C18	-2.01	115.84	119.01
6	R	304	Q6L	C19-C20-C21	-2.01	119.40	123.52
4	R	308	CHL	O2D-CGD-O1D	-2.01	119.93	123.85
8	R	303	IWJ	C25-C24-C26	2.01	119.26	116.00
4	R	309	CHL	C1C-C2C-CMC	2.01	130.42	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	309	CLA	C3B-C4B-NB	-2.01	108.74	110.53
3	P	303	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
3	P	301	CLA	C9-C8-C10	-2.00	104.13	111.27
8	R	303	IWJ	C23-C22-C21	-2.00	117.40	123.20
3	P	311	CLA	CMB-C2B-C3B	2.00	131.26	126.55
3	P	311	CLA	CHA-C1A-NA	-2.00	121.86	126.39
4	R	308	CHL	C3C-C4C-NC	-2.00	109.76	114.65
8	Q	301	IWJ	C23-C22-C21	-2.00	117.40	123.20

All (67) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	P	301	CLA	ND
3	P	302	CLA	ND
3	P	303	CLA	ND
3	P	309	CLA	ND
3	P	310	CLA	ND
3	P	311	CLA	ND
3	P	312	CLA	ND
3	Q	302	CLA	ND
3	Q	303	CLA	ND
3	Q	304	CLA	ND
3	Q	309	CLA	ND
3	Q	310	CLA	ND
3	Q	311	CLA	ND
3	Q	312	CLA	ND
3	Q	313	CLA	ND
3	R	305	CLA	ND
3	R	306	CLA	ND
3	R	307	CLA	ND
3	R	313	CLA	ND
3	R	314	CLA	ND
3	R	315	CLA	ND
3	R	316	CLA	ND
4	P	304	CHL	NA
4	P	304	CHL	ND
4	P	304	CHL	NC
4	P	305	CHL	NA
4	P	305	CHL	ND
4	P	305	CHL	NC
4	P	306	CHL	NA
4	P	306	CHL	ND

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Mol	Chain	Res	Type	Atom
4	P	306	CHL	NC
4	P	307	CHL	NA
4	P	307	CHL	ND
4	P	307	CHL	NC
4	P	314	CHL	NA
4	P	314	CHL	ND
4	P	314	CHL	NC
4	Q	305	CHL	NA
4	Q	305	CHL	ND
4	Q	305	CHL	NC
4	Q	306	CHL	NA
4	Q	306	CHL	ND
4	Q	306	CHL	NC
4	Q	307	CHL	NA
4	Q	307	CHL	ND
4	Q	307	CHL	NC
4	Q	314	CHL	NA
4	Q	314	CHL	ND
4	Q	314	CHL	NC
4	R	302	CHL	NA
4	R	302	CHL	ND
4	R	302	CHL	NC
4	R	308	CHL	NA
4	R	308	CHL	ND
4	R	308	CHL	NC
4	R	309	CHL	NA
4	R	309	CHL	ND
4	R	309	CHL	NC
4	R	310	CHL	NA
4	R	310	CHL	ND
4	R	310	CHL	NC
4	R	311	CHL	NA
4	R	311	CHL	ND
4	R	311	CHL	NC
4	R	318	CHL	NA
4	R	318	CHL	ND
4	R	318	CHL	NC

All (421) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	301	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	P	302	CLA	CAD-CBD-CGD-O1D
3	P	302	CLA	CAD-CBD-CGD-O2D
3	P	303	CLA	C1A-C2A-CAA-CBA
3	P	303	CLA	C3A-C2A-CAA-CBA
3	P	303	CLA	CBD-CGD-O2D-CED
3	P	309	CLA	C3A-C2A-CAA-CBA
3	Q	304	CLA	C1A-C2A-CAA-CBA
3	Q	309	CLA	C1A-C2A-CAA-CBA
3	Q	310	CLA	C1A-C2A-CAA-CBA
3	Q	311	CLA	CBA-CGA-O2A-C1
3	R	305	CLA	C1A-C2A-CAA-CBA
3	R	307	CLA	CHA-CBD-CGD-O2D
3	R	313	CLA	C1A-C2A-CAA-CBA
3	R	313	CLA	C3A-C2A-CAA-CBA
3	R	314	CLA	C3A-C2A-CAA-CBA
3	R	315	CLA	CAD-CBD-CGD-O1D
3	R	315	CLA	CAD-CBD-CGD-O2D
3	R	316	CLA	C1A-C2A-CAA-CBA
3	R	316	CLA	C3A-C2A-CAA-CBA
3	R	317	CLA	O1A-CGA-O2A-C1
4	P	304	CHL	C3A-C2A-CAA-CBA
4	P	304	CHL	C1C-C2C-CMC-OMC
4	P	304	CHL	C3C-C2C-CMC-OMC
4	P	304	CHL	CBD-CGD-O2D-CED
4	P	305	CHL	C1A-C2A-CAA-CBA
4	P	307	CHL	C1A-C2A-CAA-CBA
4	P	314	CHL	C1A-C2A-CAA-CBA
4	Q	305	CHL	C1A-C2A-CAA-CBA
4	Q	314	CHL	CAA-CBA-CGA-O1A
4	R	302	CHL	CBA-CGA-O2A-C1
4	R	309	CHL	CBD-CGD-O2D-CED
4	R	310	CHL	C2-C3-C5-C6
4	R	310	CHL	C4-C3-C5-C6
4	R	311	CHL	CBD-CGD-O2D-CED
4	R	318	CHL	CBD-CGD-O2D-CED
5	P	308	KC2	C1A-C2A-CAA-CBA
5	P	308	KC2	C2A-CAA-CBA-CGA
5	Q	308	KC2	C1A-C2A-CAA-CBA
5	Q	308	KC2	C3A-C2A-CAA-CBA
5	Q	308	KC2	C2A-CAA-CBA-CGA
5	R	312	KC2	C1A-C2A-CAA-CBA
5	R	312	KC2	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
6	P	315	Q6L	C26-C27-C29-C30
6	P	315	Q6L	C15-C16-C17-C18
6	P	319	Q6L	C29-C30-C31-C32
6	P	321	Q6L	C29-C30-C31-C32
6	Q	316	Q6L	C11-C12-C13-C14
6	Q	316	Q6L	C11-C12-C13-C42
6	Q	316	Q6L	C28-C27-C29-C30
6	Q	316	Q6L	C26-C27-C29-C30
6	Q	316	Q6L	C29-C30-C31-C32
6	Q	316	Q6L	C27-C29-C30-C31
6	Q	317	Q6L	C26-C27-C29-C30
6	R	301	Q6L	C21-C22-C24-C25
6	R	301	Q6L	C23-C22-C24-C25
6	R	301	Q6L	C28-C27-C29-C30
6	R	301	Q6L	C26-C27-C29-C30
6	R	301	Q6L	C29-C30-C31-C32
6	R	301	Q6L	C27-C29-C30-C31
6	R	304	Q6L	C29-C30-C31-C32
6	R	319	Q6L	C11-C12-C13-C14
6	R	319	Q6L	C11-C12-C13-C42
6	R	319	Q6L	C21-C22-C24-C25
6	R	319	Q6L	C29-C30-C31-C36
6	R	319	Q6L	C29-C30-C31-C32
6	R	323	Q6L	C28-C27-C29-C30
6	R	323	Q6L	C29-C30-C31-C32
6	R	323	Q6L	C27-C29-C30-C31
7	Q	315	NEX	O24-C26-C27-C28
8	P	318	IWJ	C18-C19-C21-C22
8	P	318	IWJ	C20-C19-C21-C22
8	P	320	IWJ	C26-C28-C29-C30
8	P	320	IWJ	C26-C28-C29-O39
8	Q	301	IWJ	C26-C28-C29-C30
8	Q	301	IWJ	C26-C28-C29-O39
8	Q	319	IWJ	C18-C19-C21-C22
8	Q	319	IWJ	O27-C26-C28-C29
8	Q	319	IWJ	C26-C28-C29-C30
8	Q	319	IWJ	C26-C28-C29-O39
8	R	303	IWJ	C26-C28-C29-C30
8	R	303	IWJ	C26-C28-C29-C35
8	R	303	IWJ	C26-C28-C29-O39
8	R	322	IWJ	C18-C19-C21-C22
8	R	322	IWJ	O27-C26-C28-C29

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Mol	Chain	Res	Type	Atoms
8	R	322	IWJ	C26-C28-C29-C30
8	R	322	IWJ	C26-C28-C29-C35
8	R	322	IWJ	C26-C28-C29-O39
4	P	304	CHL	O1D-CGD-O2D-CED
3	P	311	CLA	CBD-CGD-O2D-CED
3	Q	312	CLA	CBD-CGD-O2D-CED
3	R	306	CLA	CBD-CGD-O2D-CED
3	Q	313	CLA	O1A-CGA-O2A-C1
3	R	314	CLA	O1A-CGA-O2A-C1
3	Q	311	CLA	O1A-CGA-O2A-C1
3	Q	313	CLA	CBA-CGA-O2A-C1
3	R	317	CLA	CBA-CGA-O2A-C1
3	P	302	CLA	O1A-CGA-O2A-C1
3	P	311	CLA	O1A-CGA-O2A-C1
3	Q	302	CLA	O1A-CGA-O2A-C1
3	R	305	CLA	O1A-CGA-O2A-C1
3	R	315	CLA	O1A-CGA-O2A-C1
4	P	306	CHL	O1A-CGA-O2A-C1
4	R	310	CHL	O1A-CGA-O2A-C1
4	R	302	CHL	O1A-CGA-O2A-C1
3	P	303	CLA	O1D-CGD-O2D-CED
3	R	306	CLA	O1D-CGD-O2D-CED
4	R	309	CHL	O1D-CGD-O2D-CED
4	R	311	CHL	O1D-CGD-O2D-CED
4	R	318	CHL	O1D-CGD-O2D-CED
3	R	316	CLA	CBD-CGD-O2D-CED
3	R	315	CLA	C3-C5-C6-C7
3	P	302	CLA	CBA-CGA-O2A-C1
3	Q	302	CLA	CBA-CGA-O2A-C1
3	R	305	CLA	CBA-CGA-O2A-C1
3	R	314	CLA	CBA-CGA-O2A-C1
3	R	316	CLA	CBA-CGA-O2A-C1
4	P	306	CHL	CBA-CGA-O2A-C1
3	Q	309	CLA	CBD-CGD-O2D-CED
4	Q	305	CHL	CBD-CGD-O2D-CED
5	P	308	KC2	CBD-CGD-O2D-CED
3	P	311	CLA	O1D-CGD-O2D-CED
3	P	301	CLA	C4-C3-C5-C6
3	R	316	CLA	C4-C3-C5-C6
6	P	319	Q6L	C11-C12-C13-C42
6	R	301	Q6L	C11-C12-C13-C42
6	R	323	Q6L	C11-C12-C13-C42

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Mol	Chain	Res	Type	Atoms
3	P	301	CLA	C2-C3-C5-C6
6	P	319	Q6L	C11-C12-C13-C14
3	P	311	CLA	CBA-CGA-O2A-C1
3	Q	312	CLA	CBA-CGA-O2A-C1
3	R	315	CLA	CBA-CGA-O2A-C1
4	R	310	CHL	CBA-CGA-O2A-C1
6	P	321	Q6L	C13-C14-C15-C16
6	R	323	Q6L	C24-C25-C26-C27
3	Q	312	CLA	O1A-CGA-O2A-C1
3	Q	302	CLA	C3-C5-C6-C7
3	P	309	CLA	CBD-CGD-O2D-CED
3	Q	302	CLA	CBD-CGD-O2D-CED
3	Q	312	CLA	O1D-CGD-O2D-CED
6	Q	318	Q6L	C11-C12-C13-C42
3	R	316	CLA	C2-C3-C5-C6
6	Q	318	Q6L	C11-C12-C13-C14
6	R	301	Q6L	C11-C12-C13-C14
6	R	323	Q6L	C11-C12-C13-C14
3	R	316	CLA	O1A-CGA-O2A-C1
4	Q	306	CHL	C2A-CAA-CBA-CGA
3	Q	304	CLA	CBD-CGD-O2D-CED
3	R	307	CLA	CBD-CGD-O2D-CED
4	P	306	CHL	CBD-CGD-O2D-CED
5	R	312	KC2	CAA-CBA-CGA-O1A
6	P	319	Q6L	C13-C14-C15-C16
3	P	301	CLA	CBA-CGA-O2A-C1
3	R	316	CLA	O1D-CGD-O2D-CED
4	Q	305	CHL	O1D-CGD-O2D-CED
3	Q	312	CLA	C2-C3-C5-C6
3	P	310	CLA	C11-C10-C8-C9
3	R	315	CLA	C11-C10-C8-C9
6	P	315	Q6L	C28-C27-C29-C30
6	P	315	Q6L	C15-C16-C17-C41
6	P	321	Q6L	C28-C27-C29-C30
6	Q	317	Q6L	C28-C27-C29-C30
6	Q	318	Q6L	C28-C27-C29-C30
6	R	304	Q6L	C28-C27-C29-C30
6	R	319	Q6L	C23-C22-C24-C25
6	R	323	Q6L	C23-C22-C24-C25
8	Q	319	IWJ	C20-C19-C21-C22
8	R	322	IWJ	C20-C19-C21-C22
6	P	319	Q6L	C26-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
6	P	321	Q6L	C26-C27-C29-C30
6	Q	318	Q6L	C26-C27-C29-C30
6	R	304	Q6L	C26-C27-C29-C30
6	R	323	Q6L	C26-C27-C29-C30
3	Q	312	CLA	C2A-CAA-CBA-CGA
5	R	312	KC2	CAA-CBA-CGA-O2A
5	P	308	KC2	O1D-CGD-O2D-CED
3	Q	309	CLA	O1D-CGD-O2D-CED
4	P	314	CHL	CBD-CGD-O2D-CED
3	Q	302	CLA	O1D-CGD-O2D-CED
3	R	305	CLA	C13-C15-C16-C17
3	P	301	CLA	C10-C11-C12-C13
3	R	306	CLA	C10-C11-C12-C13
3	P	301	CLA	O1A-CGA-O2A-C1
3	R	306	CLA	C15-C16-C17-C18
3	P	310	CLA	CBA-CGA-O2A-C1
3	R	314	CLA	C3-C5-C6-C7
3	P	309	CLA	O1D-CGD-O2D-CED
4	Q	306	CHL	CBA-CGA-O2A-C1
4	R	309	CHL	CBA-CGA-O2A-C1
3	P	310	CLA	C8-C10-C11-C12
3	P	311	CLA	C8-C10-C11-C12
3	R	314	CLA	C5-C6-C7-C8
3	P	309	CLA	C13-C15-C16-C17
3	R	313	CLA	C8-C10-C11-C12
3	Q	304	CLA	O1D-CGD-O2D-CED
6	P	315	Q6L	C11-C12-C13-C42
3	R	314	CLA	CBD-CGD-O2D-CED
6	P	319	Q6L	C28-C27-C29-C30
6	R	319	Q6L	C28-C27-C29-C30
6	R	319	Q6L	C26-C27-C29-C30
6	R	323	Q6L	C21-C22-C24-C25
3	P	310	CLA	O1A-CGA-O2A-C1
4	R	309	CHL	O1A-CGA-O2A-C1
4	P	306	CHL	C2-C1-O2A-CGA
3	Q	304	CLA	CBA-CGA-O2A-C1
3	P	313	CLA	C4B-C3B-CAB-CBB
3	Q	310	CLA	C4B-C3B-CAB-CBB
3	R	305	CLA	C4B-C3B-CAB-CBB
3	R	315	CLA	C4B-C3B-CAB-CBB
3	Q	309	CLA	C6-C7-C8-C10
3	R	306	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
3	Q	304	CLA	C3A-C2A-CAA-CBA
3	Q	309	CLA	C3A-C2A-CAA-CBA
3	Q	311	CLA	C3A-C2A-CAA-CBA
3	R	305	CLA	C3A-C2A-CAA-CBA
4	P	305	CHL	C3A-C2A-CAA-CBA
4	P	314	CHL	C3A-C2A-CAA-CBA
4	Q	305	CHL	C3A-C2A-CAA-CBA
4	R	302	CHL	C3A-C2A-CAA-CBA
3	R	307	CLA	O1D-CGD-O2D-CED
4	P	306	CHL	O1D-CGD-O2D-CED
3	Q	309	CLA	C6-C7-C8-C9
3	P	313	CLA	CBA-CGA-O2A-C1
3	Q	311	CLA	C2B-C3B-CAB-CBB
3	R	315	CLA	C2B-C3B-CAB-CBB
3	P	312	CLA	CBA-CGA-O2A-C1
3	Q	312	CLA	C4-C3-C5-C6
6	P	315	Q6L	C11-C12-C13-C14
3	R	313	CLA	CBA-CGA-O2A-C1
3	R	306	CLA	C3-C5-C6-C7
3	P	311	CLA	C5-C6-C7-C8
4	Q	306	CHL	O1A-CGA-O2A-C1
6	R	319	Q6L	C15-C16-C17-C41
3	Q	304	CLA	O1A-CGA-O2A-C1
3	R	313	CLA	O1A-CGA-O2A-C1
5	P	308	KC2	C4C-C3C-CAC-CBC
5	Q	308	KC2	C4C-C3C-CAC-CBC
3	Q	302	CLA	C10-C11-C12-C13
3	R	306	CLA	C8-C10-C11-C12
3	P	312	CLA	O1A-CGA-O2A-C1
3	Q	313	CLA	C2-C1-O2A-CGA
3	R	315	CLA	C2A-CAA-CBA-CGA
3	P	313	CLA	O1A-CGA-O2A-C1
3	P	301	CLA	C1A-C2A-CAA-CBA
3	P	309	CLA	C1A-C2A-CAA-CBA
3	Q	311	CLA	C1A-C2A-CAA-CBA
3	R	306	CLA	C1A-C2A-CAA-CBA
3	R	314	CLA	C1A-C2A-CAA-CBA
3	R	314	CLA	O1D-CGD-O2D-CED
3	R	305	CLA	C11-C12-C13-C15
3	P	312	CLA	C2A-CAA-CBA-CGA
3	R	313	CLA	C2A-CAA-CBA-CGA
3	P	309	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
4	P	314	CHL	O1D-CGD-O2D-CED
3	P	311	CLA	C11-C12-C13-C14
4	Q	305	CHL	CHA-CBD-CGD-O1D
4	R	302	CHL	CHA-CBD-CGD-O1D
4	R	302	CHL	CHA-CBD-CGD-O2D
6	P	321	Q6L	C11-C12-C13-C14
3	P	309	CLA	O1A-CGA-O2A-C1
3	P	313	CLA	O2A-C1-C2-C3
4	R	302	CHL	C3C-C2C-CMC-OMC
3	P	303	CLA	CBA-CGA-O2A-C1
6	R	304	Q6L	C11-C12-C13-C14
3	R	305	CLA	CBD-CGD-O2D-CED
3	P	302	CLA	C2-C1-O2A-CGA
4	Q	307	CHL	C1C-C2C-CMC-OMC
3	P	312	CLA	C3-C5-C6-C7
3	P	311	CLA	C11-C12-C13-C15
3	Q	302	CLA	C6-C7-C8-C9
3	R	305	CLA	C11-C12-C13-C14
3	R	306	CLA	C11-C12-C13-C14
3	Q	302	CLA	C4B-C3B-CAB-CBB
3	Q	311	CLA	C4B-C3B-CAB-CBB
3	R	314	CLA	C4B-C3B-CAB-CBB
3	P	310	CLA	C11-C10-C8-C7
3	P	309	CLA	C15-C16-C17-C18
6	R	304	Q6L	C11-C12-C13-C42
6	Q	317	Q6L	C11-C12-C13-C14
3	R	317	CLA	O2A-C1-C2-C3
3	P	311	CLA	C2A-CAA-CBA-CGA
8	Q	319	IWJ	C25-C24-C26-O27
4	R	302	CHL	C1A-C2A-CAA-CBA
6	P	321	Q6L	C11-C12-C13-C42
6	Q	317	Q6L	C11-C12-C13-C42
8	Q	319	IWJ	C23-C24-C26-O27
3	Q	310	CLA	C2B-C3B-CAB-CBB
4	Q	306	CHL	O2A-C1-C2-C3
3	Q	311	CLA	C2A-CAA-CBA-CGA
3	P	312	CLA	O1D-CGD-O2D-CED
3	R	313	CLA	C12-C13-C15-C16
3	R	314	CLA	C6-C7-C8-C10
3	P	303	CLA	O1A-CGA-O2A-C1
6	Q	316	Q6L	C02-C03-C11-C12
5	R	312	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	R	316	CLA	C5-C6-C7-C8
3	R	315	CLA	C10-C11-C12-C13
4	R	310	CHL	C4C-C3C-CAC-CBC
3	P	302	CLA	C4B-C3B-CAB-CBB
3	R	306	CLA	C4B-C3B-CAB-CBB
8	Q	301	IWJ	O27-C26-C28-C29
8	R	303	IWJ	O27-C26-C28-C29
3	R	305	CLA	O1D-CGD-O2D-CED
6	R	319	Q6L	C15-C16-C17-C18
3	Q	304	CLA	C2A-CAA-CBA-CGA
3	P	312	CLA	CBD-CGD-O2D-CED
3	P	309	CLA	C6-C7-C8-C10
3	P	309	CLA	C11-C12-C13-C15
3	R	313	CLA	C14-C13-C15-C16
3	R	314	CLA	C6-C7-C8-C9
4	R	308	CHL	CAD-CBD-CGD-O2D
3	Q	311	CLA	CHA-CBD-CGD-O1D
3	Q	311	CLA	CHA-CBD-CGD-O2D
3	R	307	CLA	CHA-CBD-CGD-O1D
4	P	306	CHL	CHA-CBD-CGD-O1D
4	P	306	CHL	CHA-CBD-CGD-O2D
4	Q	305	CHL	CHA-CBD-CGD-O2D
4	Q	306	CHL	CHA-CBD-CGD-O1D
4	Q	306	CHL	CHA-CBD-CGD-O2D
4	Q	314	CHL	CHA-CBD-CGD-O1D
4	Q	314	CHL	CHA-CBD-CGD-O2D
4	R	308	CHL	CAD-CBD-CGD-O1D
4	R	310	CHL	CHA-CBD-CGD-O1D
4	R	310	CHL	CHA-CBD-CGD-O2D
6	Q	317	Q6L	C04-C03-C11-C12
6	Q	317	Q6L	C24-C25-C26-C27
6	Q	318	Q6L	C24-C25-C26-C27
8	P	320	IWJ	C26-C28-C29-C35
8	Q	301	IWJ	C26-C28-C29-C35
8	Q	319	IWJ	C23-C24-C26-C28
3	P	302	CLA	C2B-C3B-CAB-CBB
3	P	313	CLA	C2B-C3B-CAB-CBB
3	R	305	CLA	C2B-C3B-CAB-CBB
3	R	306	CLA	C2B-C3B-CAB-CBB
3	P	310	CLA	CAA-CBA-CGA-O2A
8	Q	319	IWJ	C08-C09-C10-C41
8	Q	319	IWJ	C25-C24-C26-C28

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Mol	Chain	Res	Type	Atoms
4	Q	307	CHL	C3C-C2C-CMC-OMC
6	R	301	Q6L	C17-C18-C19-C20
3	R	313	CLA	C4-C3-C5-C6
4	R	309	CHL	O2A-C1-C2-C3
8	Q	319	IWJ	C08-C09-C10-C11
3	R	306	CLA	C5-C6-C7-C8
3	P	309	CLA	C11-C12-C13-C14
3	P	301	CLA	C4B-C3B-CAB-CBB
3	P	302	CLA	C13-C15-C16-C17
3	Q	313	CLA	O2A-C1-C2-C3
3	P	301	CLA	C8-C10-C11-C12
3	P	302	CLA	C11-C12-C13-C15
3	P	312	CLA	C3A-C2A-CAA-CBA
3	P	313	CLA	C3A-C2A-CAA-CBA
3	Q	312	CLA	C3A-C2A-CAA-CBA
4	Q	314	CHL	C3A-C2A-CAA-CBA
7	P	317	NEX	C39-C29-C30-C31
7	Q	315	NEX	C39-C29-C30-C31
7	R	321	NEX	C39-C29-C30-C31
4	R	310	CHL	C2-C1-O2A-CGA
6	P	316	Q6L	C24-C25-C26-C27
6	P	321	Q6L	C24-C25-C26-C27
3	P	302	CLA	C11-C12-C13-C14
4	R	318	CHL	C1A-C2A-CAA-CBA
3	P	312	CLA	C1A-C2A-CAA-CBA
3	Q	312	CLA	C1A-C2A-CAA-CBA
7	P	317	NEX	C28-C29-C30-C31
7	Q	315	NEX	C28-C29-C30-C31
7	R	321	NEX	C28-C29-C30-C31
3	Q	302	CLA	C6-C7-C8-C10
3	Q	312	CLA	C5-C6-C7-C8
3	R	317	CLA	C2A-CAA-CBA-CGA
5	Q	308	KC2	O1D-CGD-O2D-CED
4	P	305	CHL	CAA-CBA-CGA-O2A
3	Q	302	CLA	C2A-CAA-CBA-CGA
3	P	302	CLA	C5-C6-C7-C8
3	P	309	CLA	C4B-C3B-CAB-CBB
3	R	313	CLA	C6-C7-C8-C10
4	Q	305	CHL	CAA-CBA-CGA-O2A
5	P	308	KC2	CAA-CBA-CGA-O2A
3	P	309	CLA	C6-C7-C8-C9
4	P	305	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
4	Q	314	CHL	C3C-C2C-CMC-OMC
4	Q	305	CHL	CAA-CBA-CGA-O1A
3	P	302	CLA	C8-C10-C11-C12
6	R	301	Q6L	C02-C03-C11-C12
7	R	321	NEX	O24-C26-C27-C28
5	R	312	KC2	C4B-C3B-CAB-CBB
5	P	308	KC2	CAA-CBA-CGA-O1A
3	P	302	CLA	CAA-CBA-CGA-O2A
8	R	322	IWJ	C14-C15-C16-C17
3	R	306	CLA	C12-C13-C15-C16
3	P	301	CLA	C2B-C3B-CAB-CBB
3	P	309	CLA	C2B-C3B-CAB-CBB
3	P	310	CLA	C2B-C3B-CAB-CBB
3	Q	302	CLA	C2B-C3B-CAB-CBB
3	R	314	CLA	C2B-C3B-CAB-CBB
3	R	313	CLA	C15-C16-C17-C18
4	R	308	CHL	C1C-C2C-CMC-OMC
3	P	303	CLA	C2A-CAA-CBA-CGA
3	P	303	CLA	CAA-CBA-CGA-O2A
3	Q	311	CLA	CAA-CBA-CGA-O2A
3	R	313	CLA	CAA-CBA-CGA-O2A
5	Q	308	KC2	CBD-CGD-O2D-CED
3	Q	309	CLA	C5-C6-C7-C8
3	P	310	CLA	C4B-C3B-CAB-CBB
3	P	309	CLA	C4-C3-C5-C6
3	R	313	CLA	C2-C3-C5-C6
3	P	312	CLA	CAA-CBA-CGA-O2A
4	P	306	CHL	C2-C3-C5-C6
3	R	317	CLA	C2-C1-O2A-CGA
3	R	313	CLA	C16-C17-C18-C19
3	P	302	CLA	C10-C11-C12-C13
4	P	307	CHL	C3A-C2A-CAA-CBA
3	P	312	CLA	CAA-CBA-CGA-O1A
3	P	303	CLA	CAA-CBA-CGA-O1A
3	R	313	CLA	C6-C7-C8-C9
3	Q	311	CLA	CAA-CBA-CGA-O1A
5	P	308	KC2	C3A-C2A-CAA-CBA
6	P	316	Q6L	C29-C30-C31-C36
3	P	302	CLA	CAA-CBA-CGA-O1A
3	R	313	CLA	CAA-CBA-CGA-O1A
5	R	312	KC2	C2B-C3B-CAB-CBB
4	R	309	CHL	C2-C1-O2A-CGA

All (1) ring outliers are listed below:

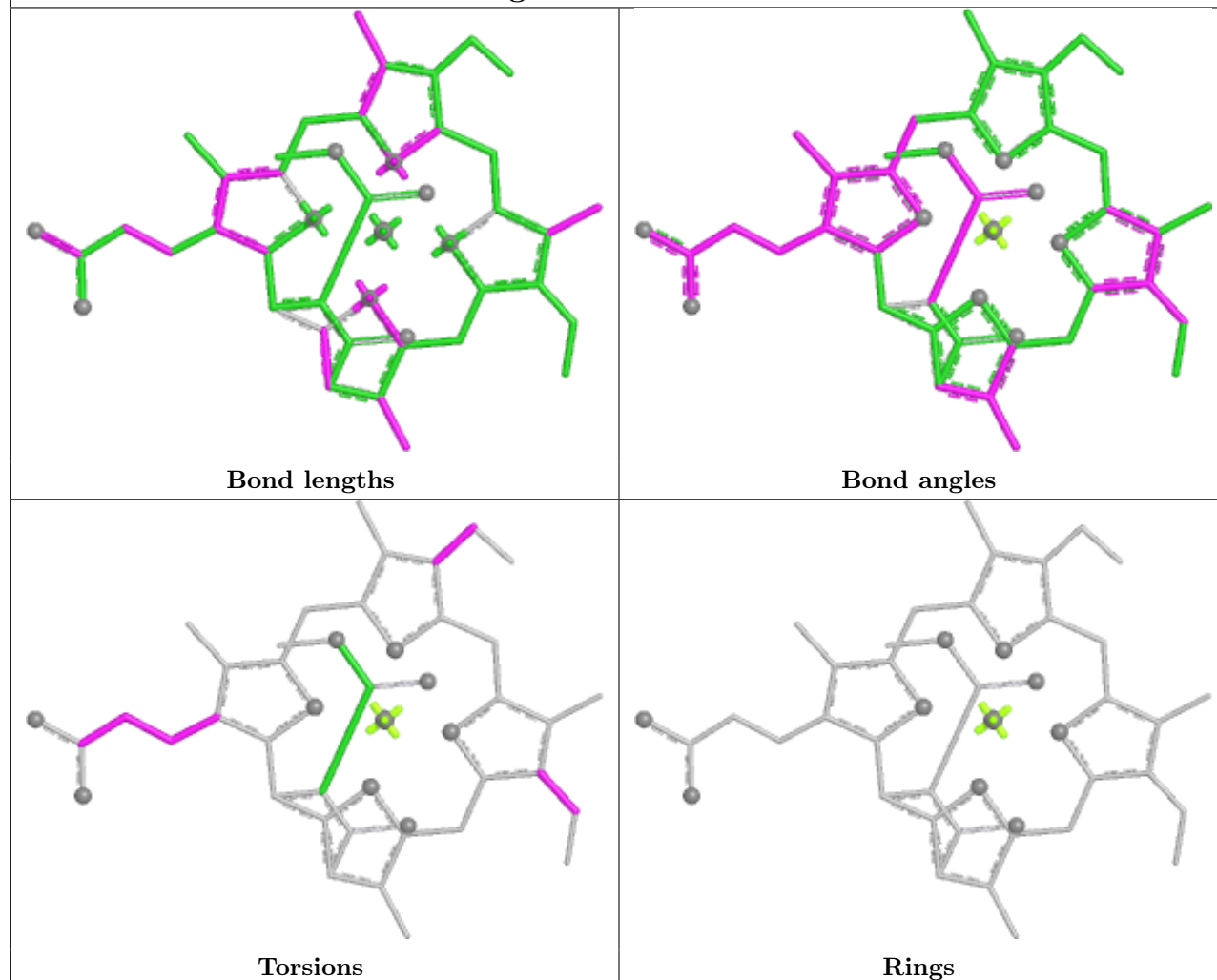
Mol	Chain	Res	Type	Atoms
8	R	322	IWJ	C29-C30-C32-C33-C34-C35

20 monomers are involved in 37 short contacts:

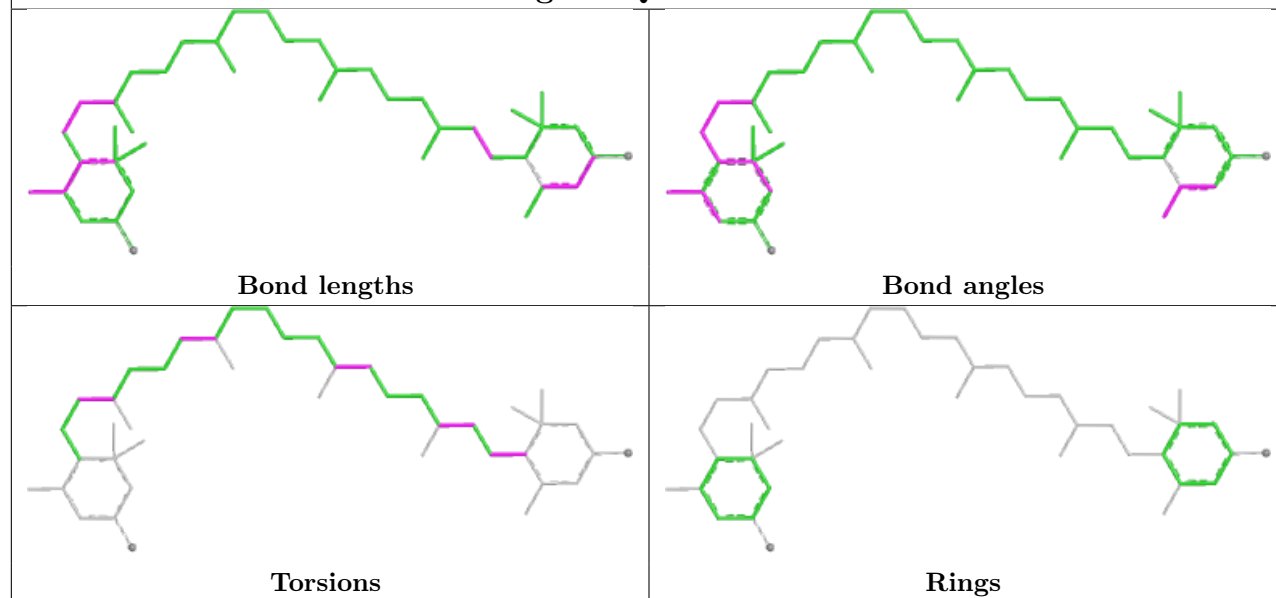
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	312	KC2	2	0
6	Q	318	Q6L	1	0
8	R	322	IWJ	1	0
4	R	308	CHL	7	0
5	P	308	KC2	1	0
3	Q	302	CLA	6	0
4	R	311	CHL	2	0
3	R	305	CLA	3	0
4	P	305	CHL	1	0
8	P	318	IWJ	1	0
3	P	309	CLA	2	0
3	P	301	CLA	3	0
4	Q	305	CHL	1	0
8	Q	319	IWJ	1	0
3	Q	312	CLA	1	0
3	R	306	CLA	1	0
7	P	317	NEX	1	0
8	P	320	IWJ	1	0
3	R	316	CLA	1	0
6	P	316	Q6L	1	0

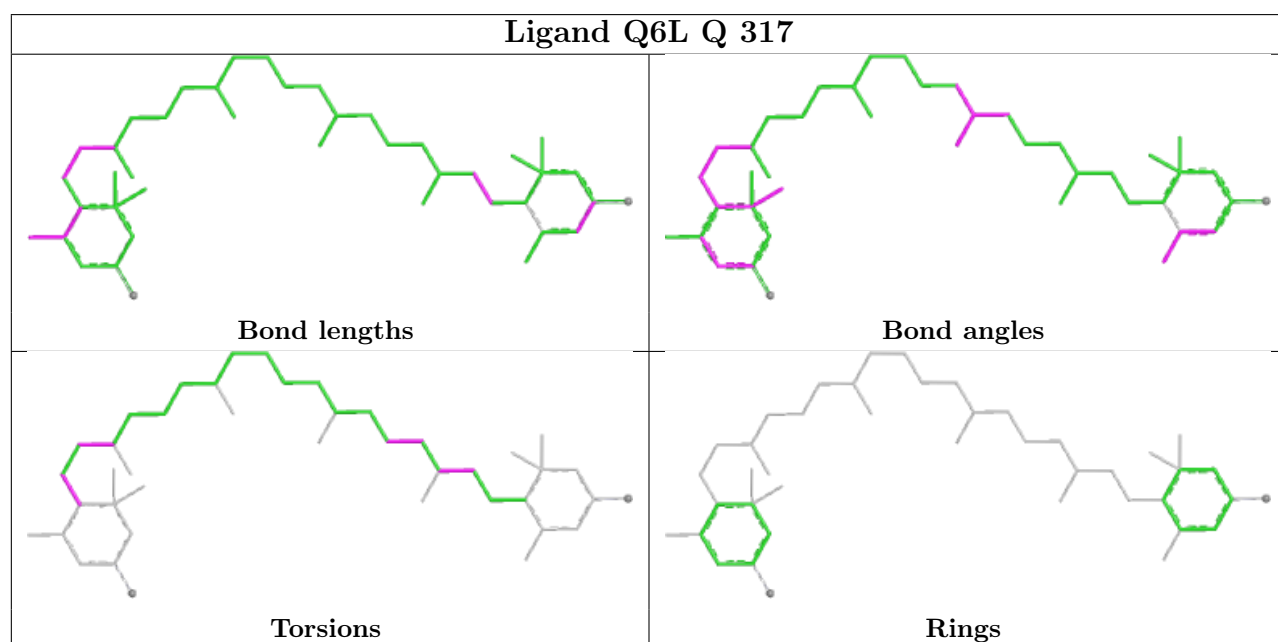
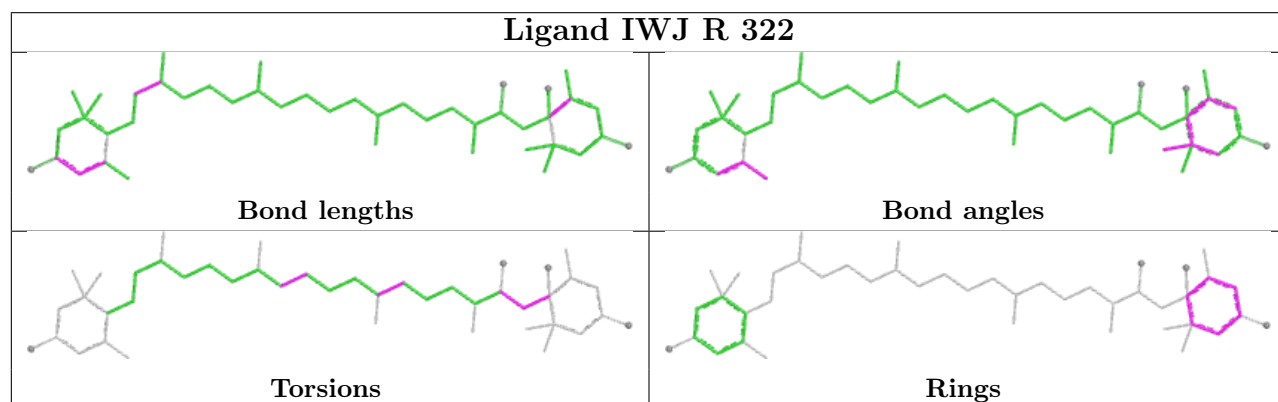
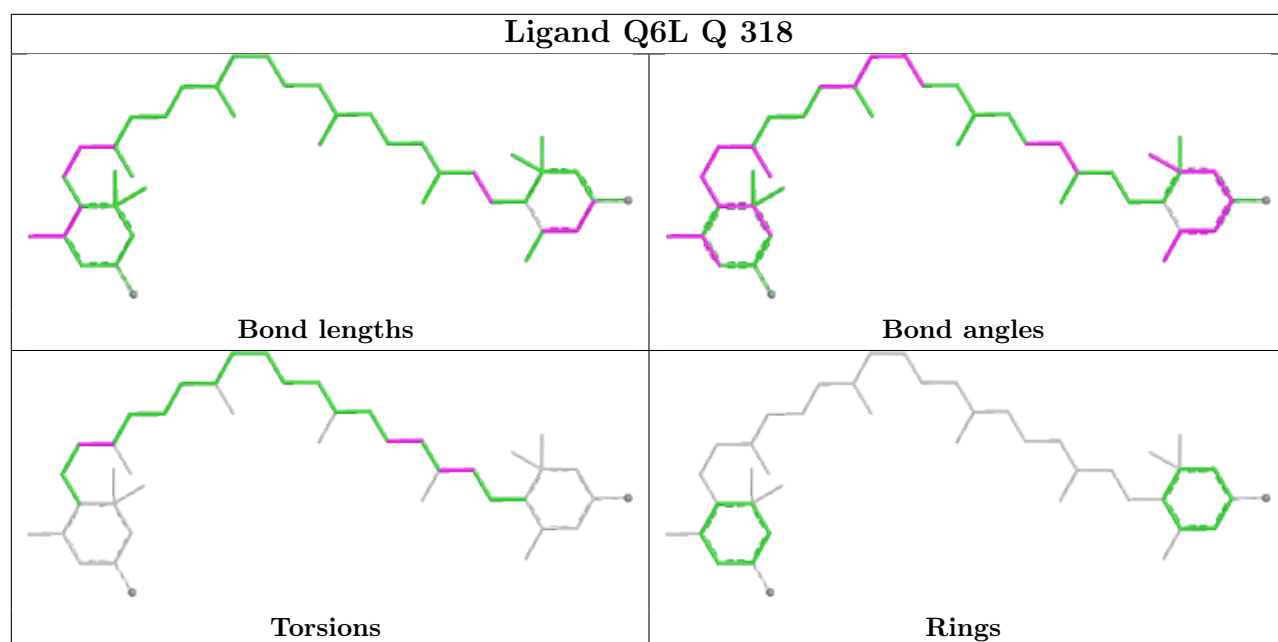
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand KC2 R 312

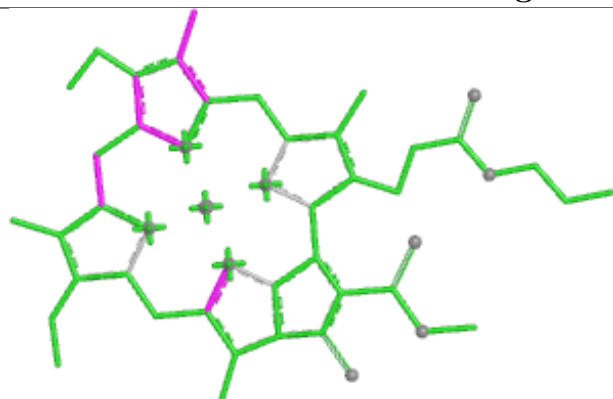


Ligand Q6L R 319

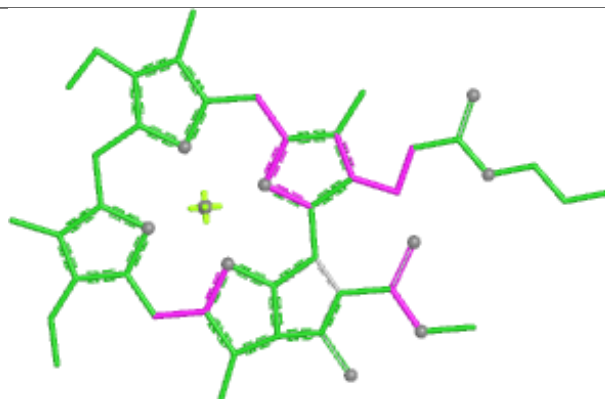




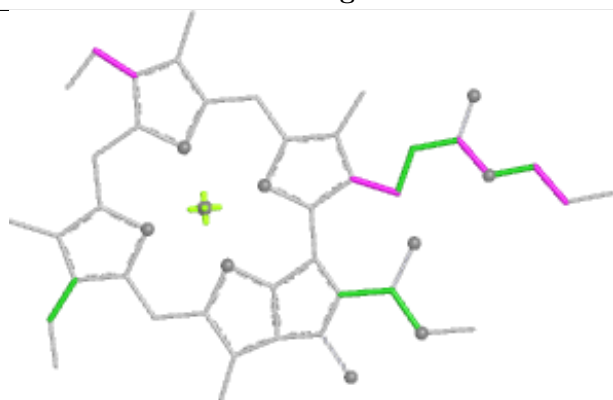
Ligand CLA P 313



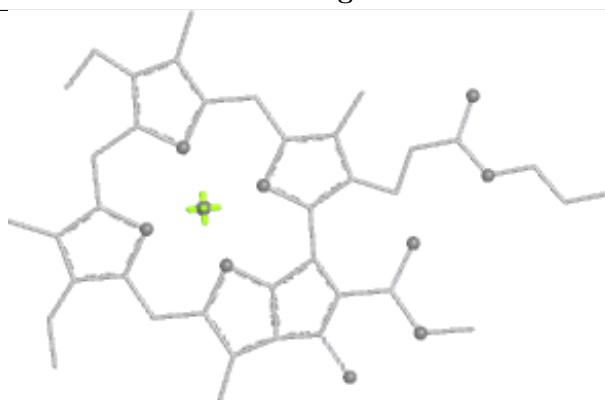
Bond lengths



Bond angles

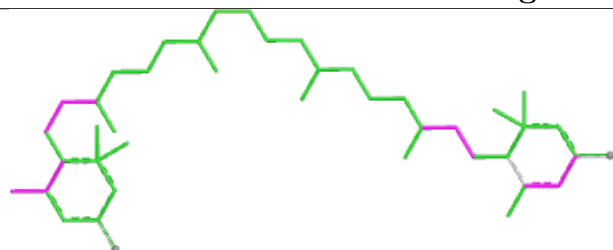


Torsions

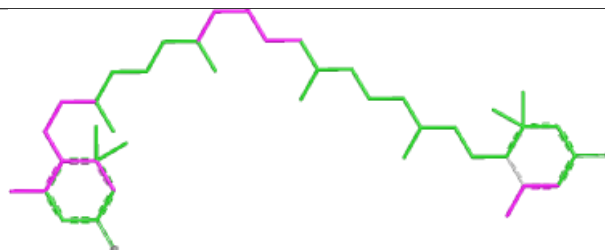


Rings

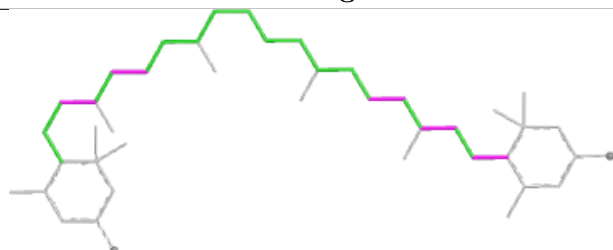
Ligand Q6L P 321



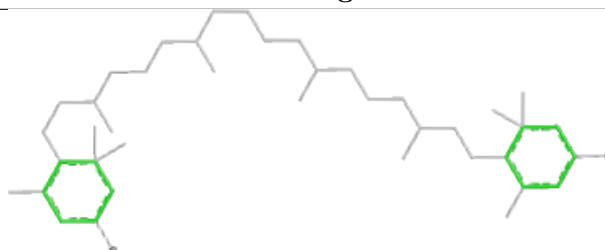
Bond lengths



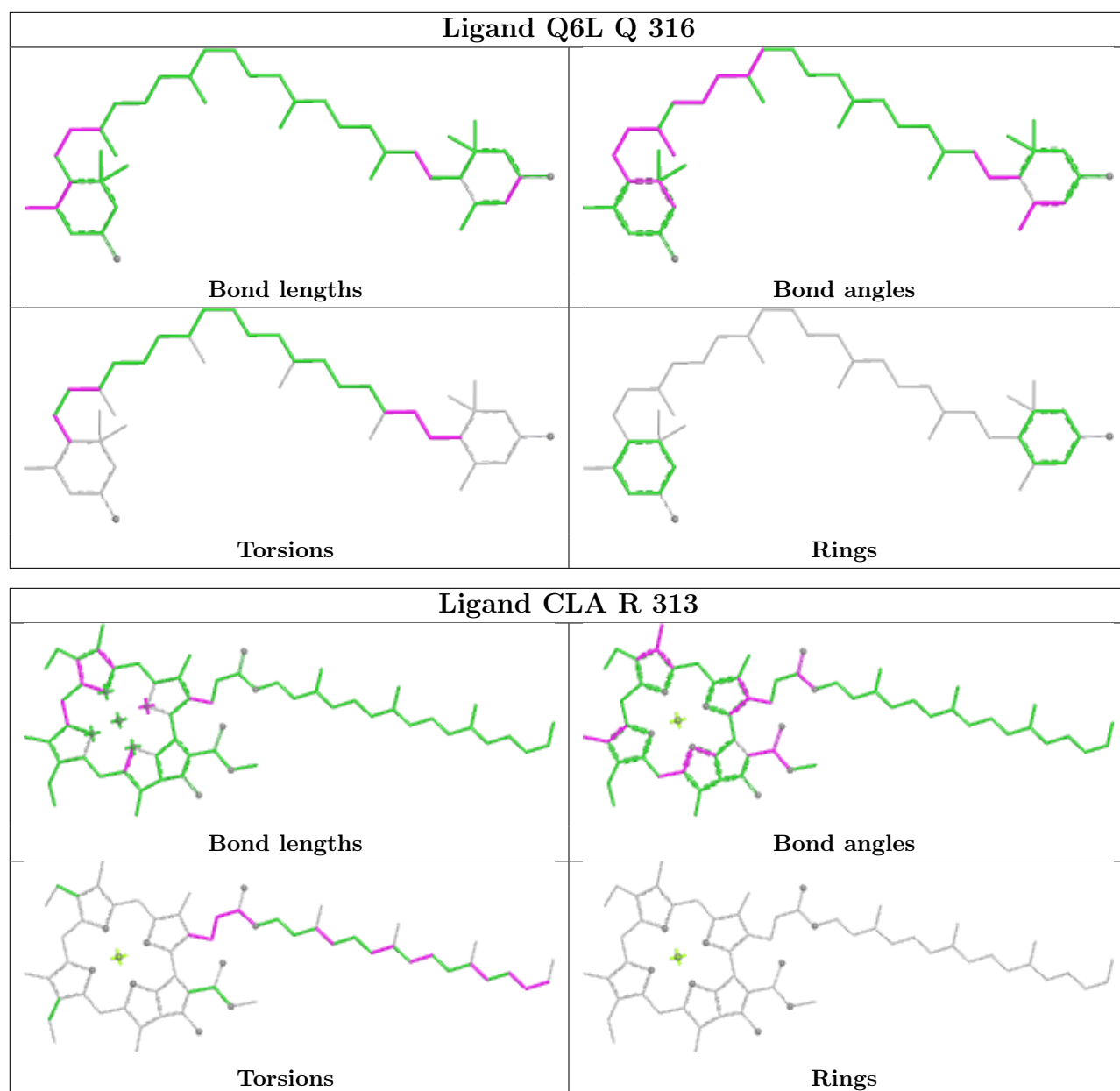
Bond angles

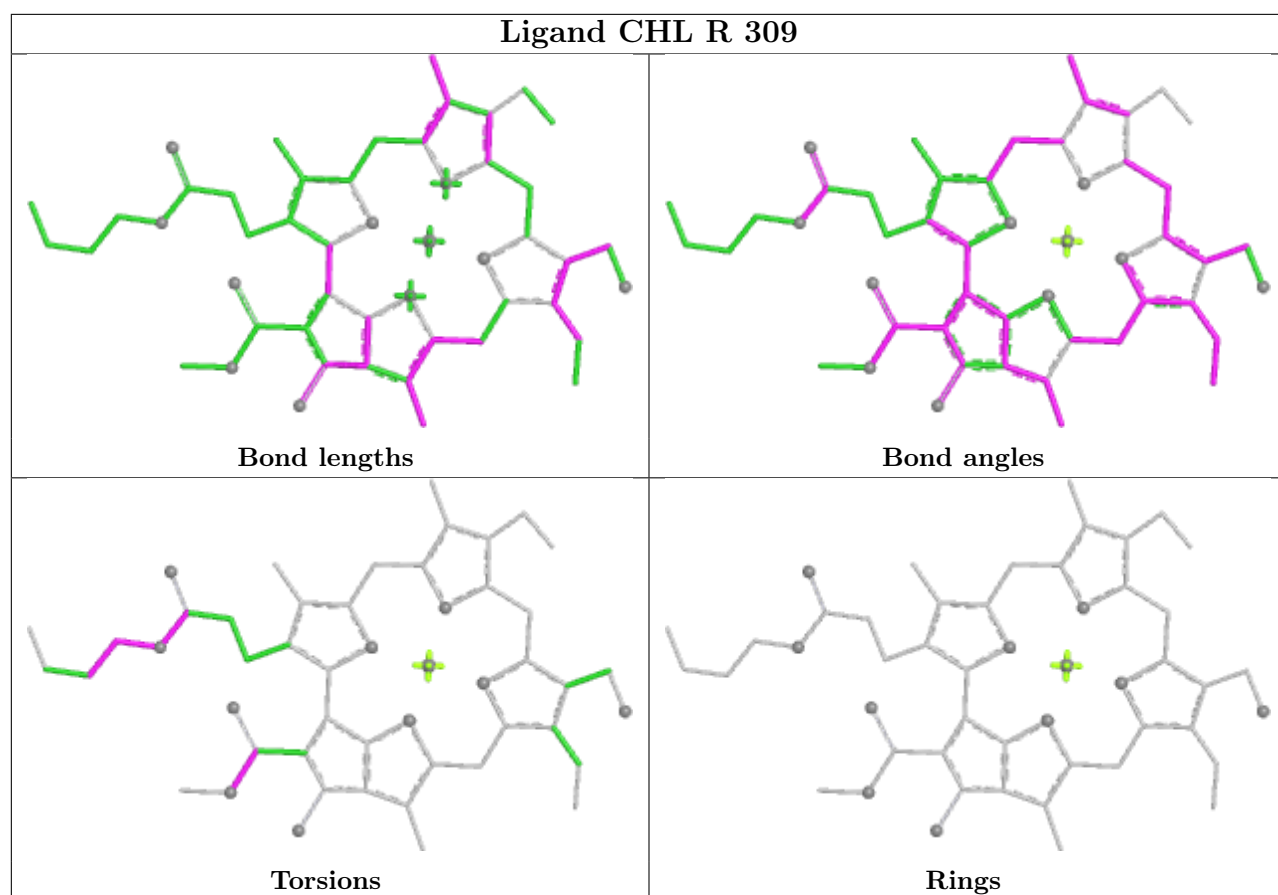


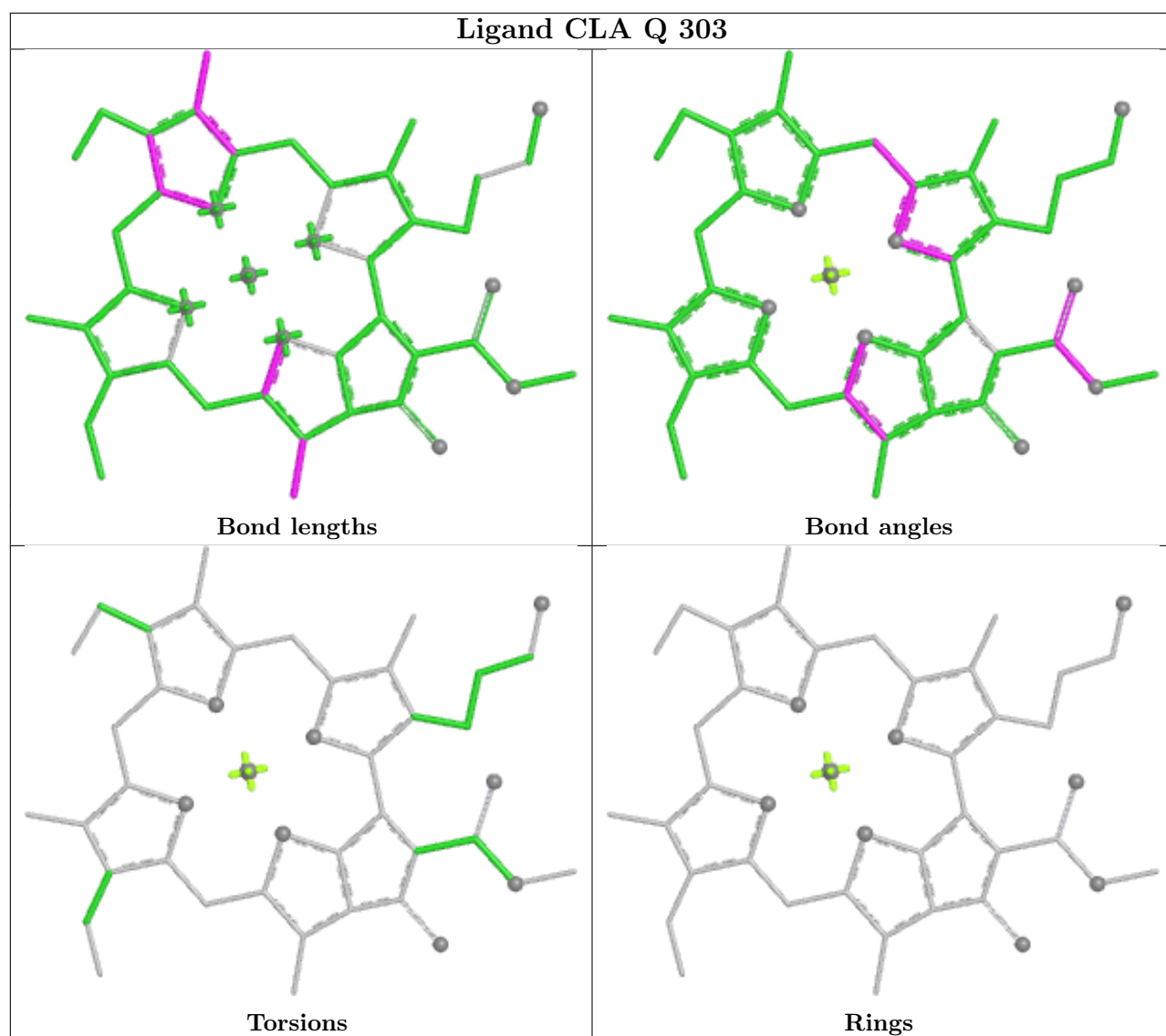
Torsions

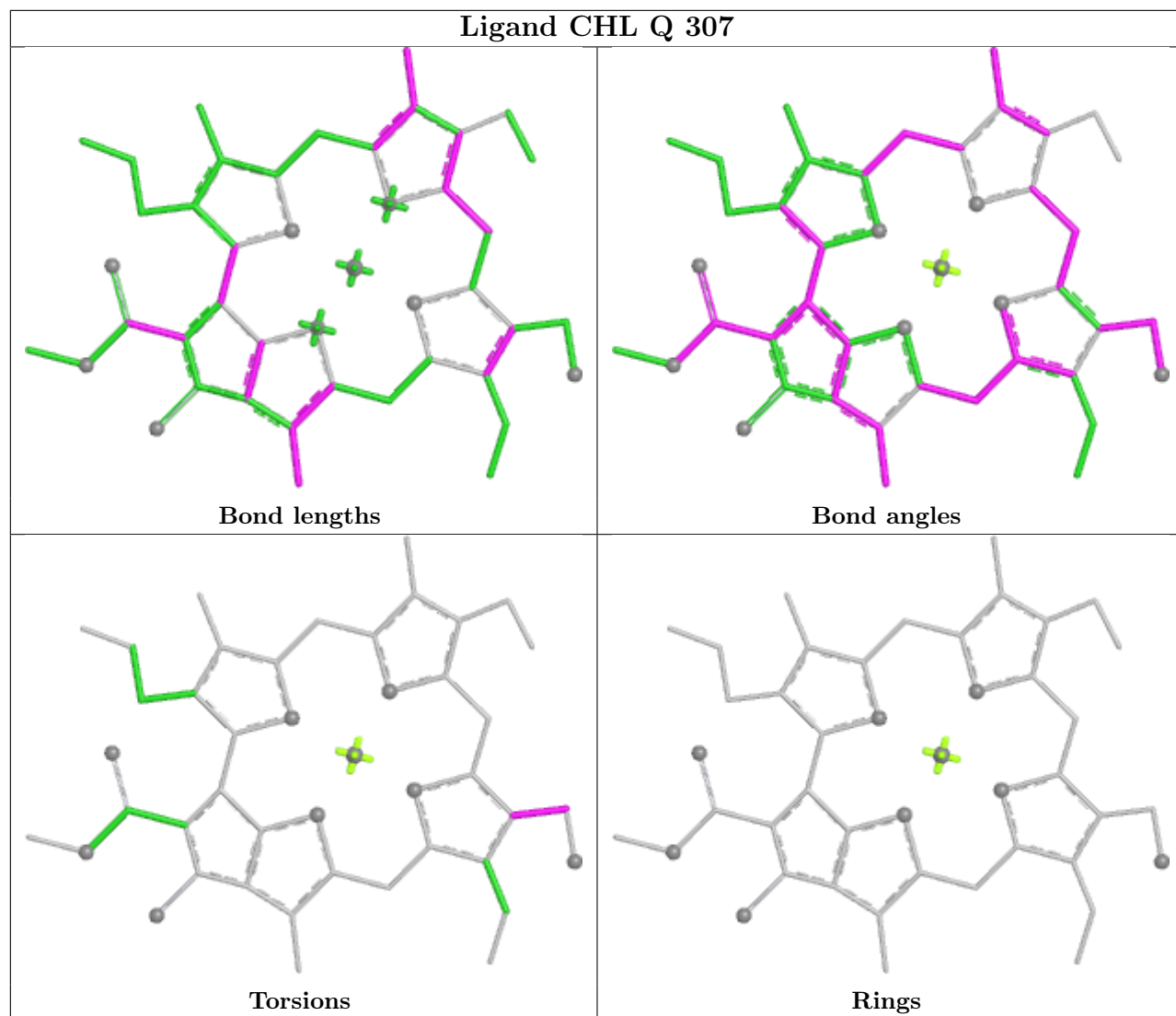


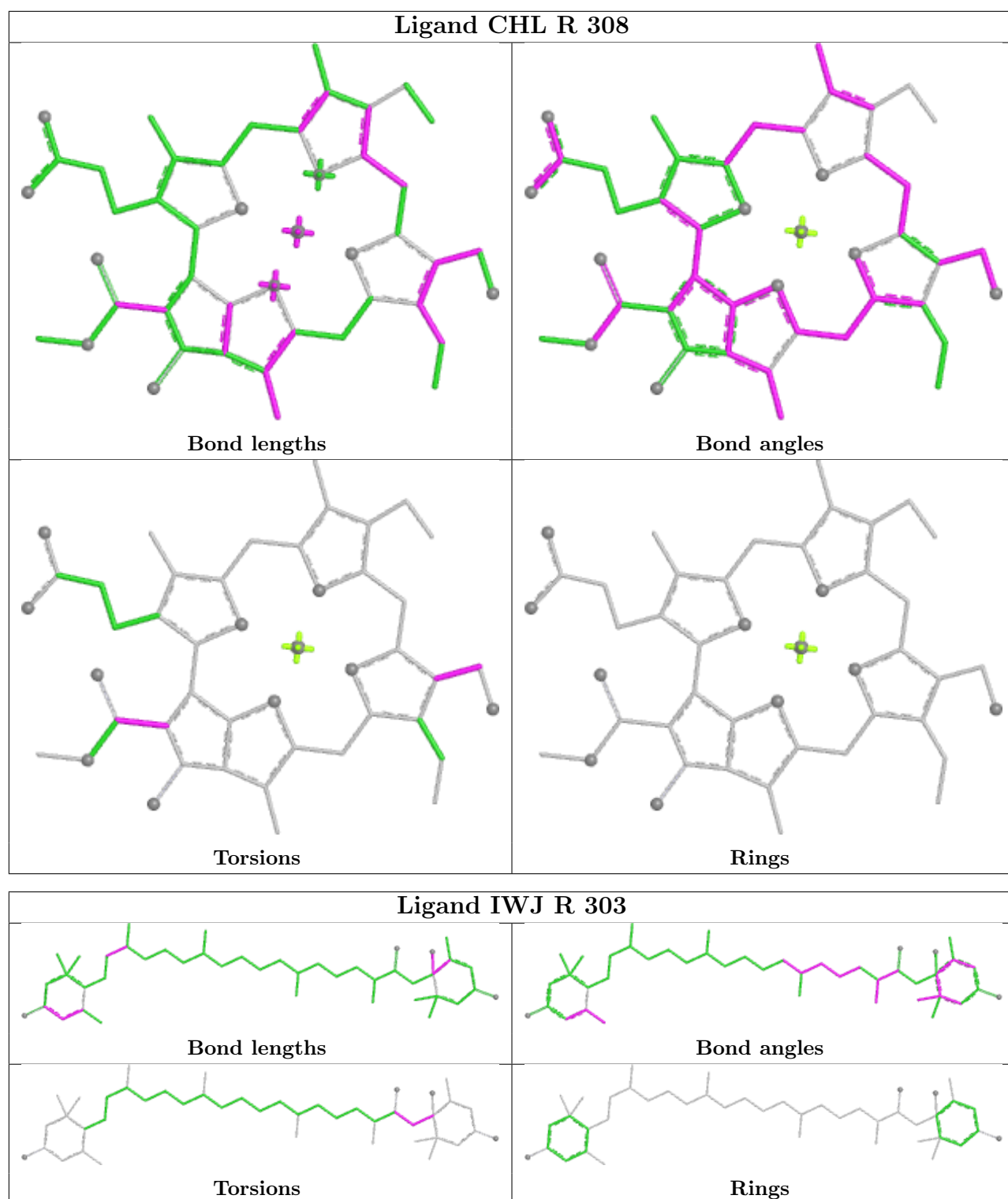
Rings

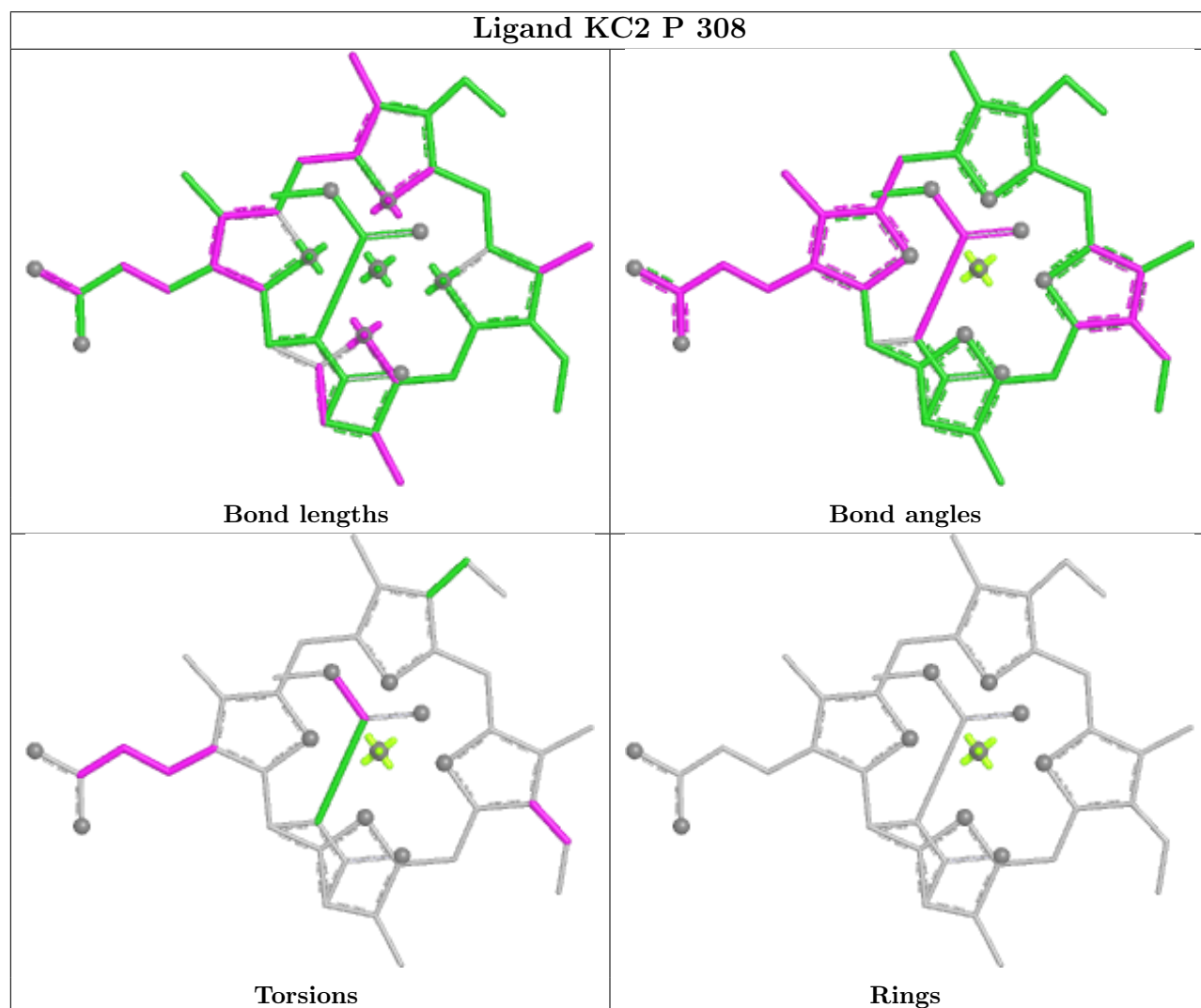
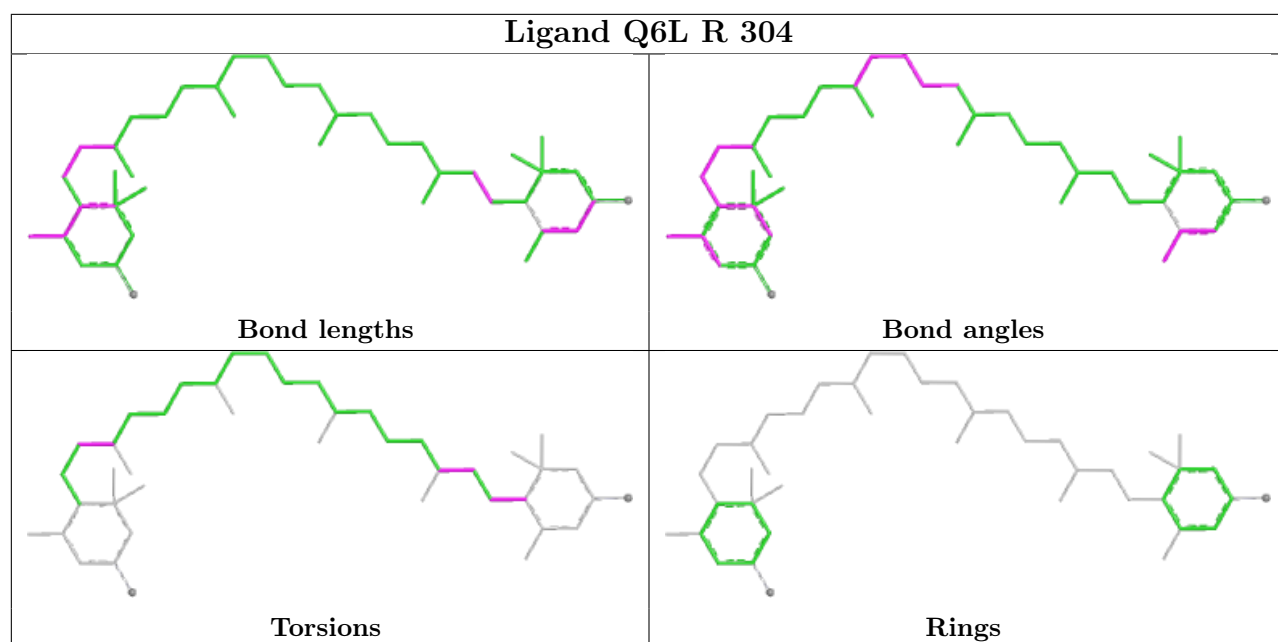


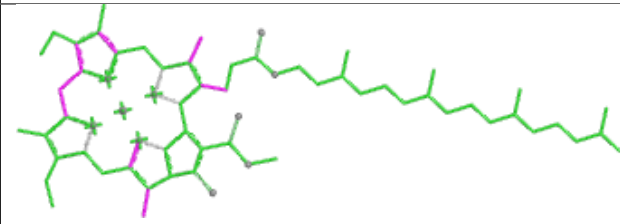
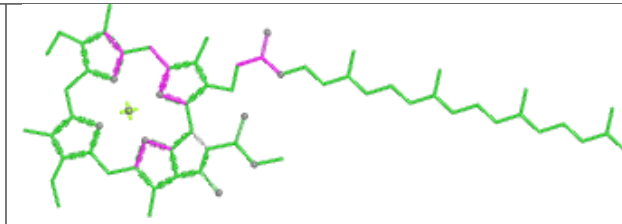
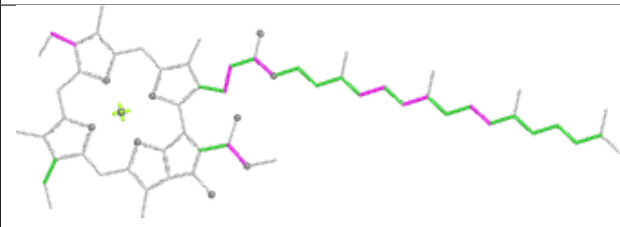
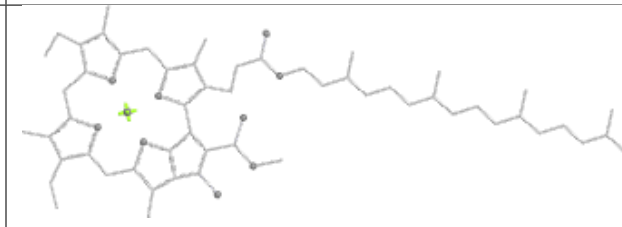


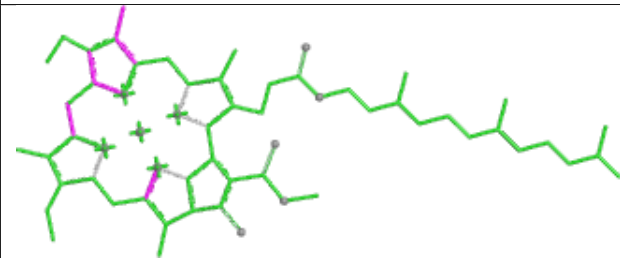
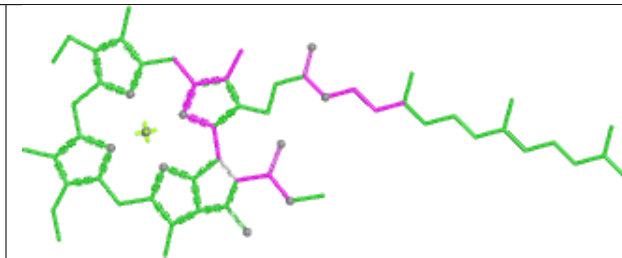
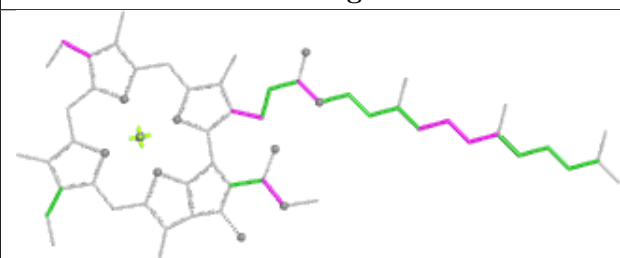
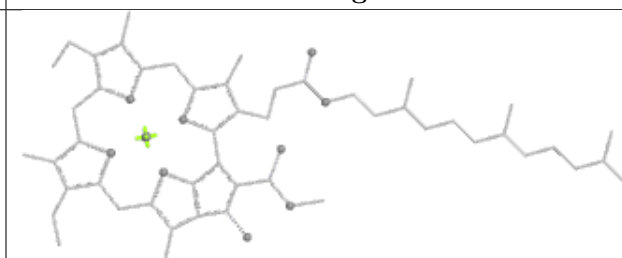


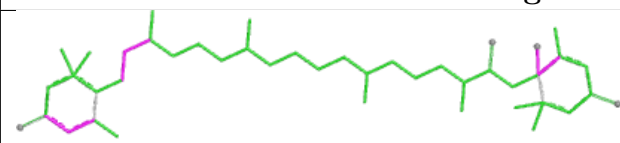
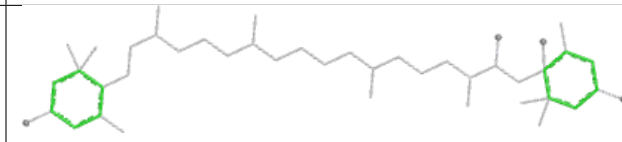




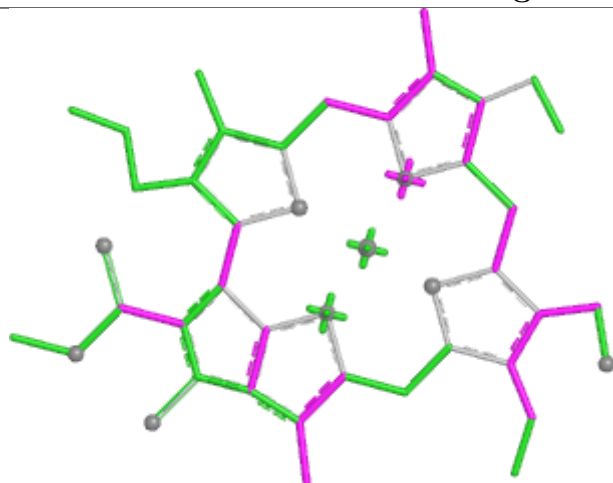


Ligand CLA Q 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

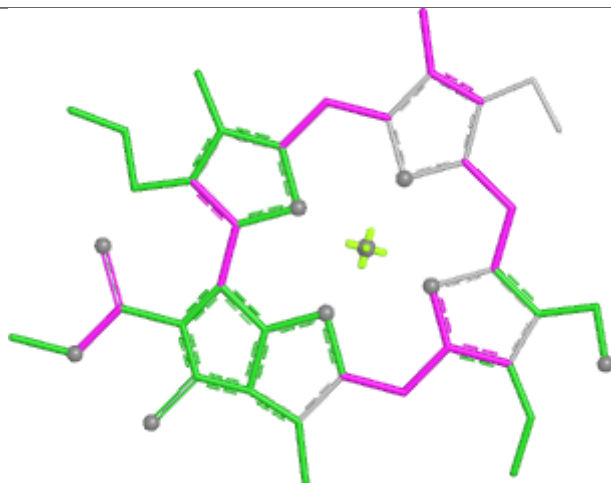
Ligand CLA R 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand IWJ Q 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

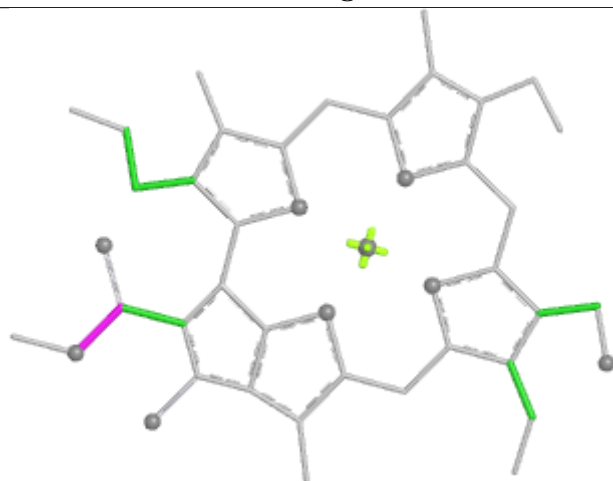
Ligand CHL R 311



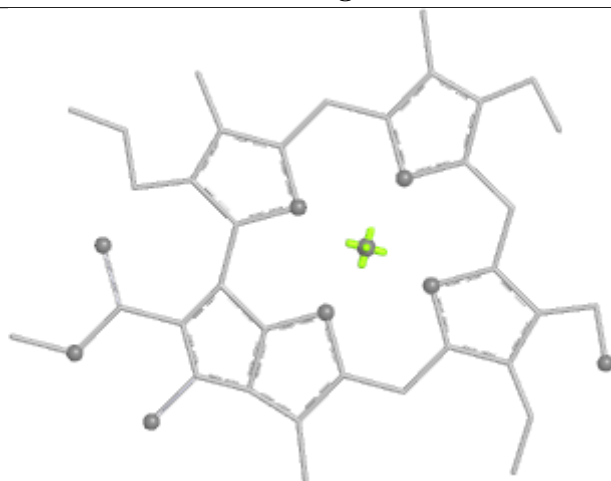
Bond lengths



Bond angles

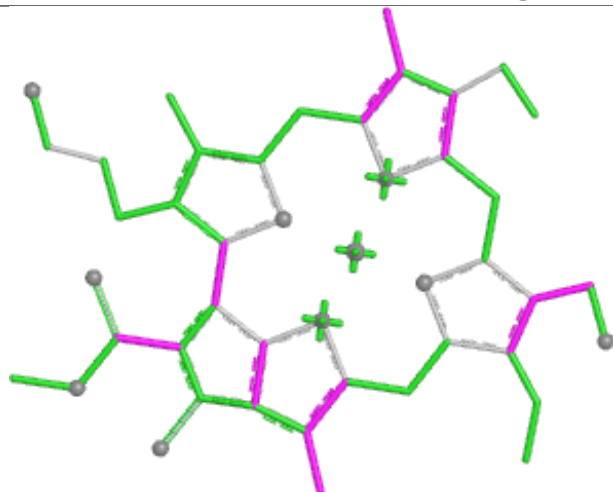


Torsions

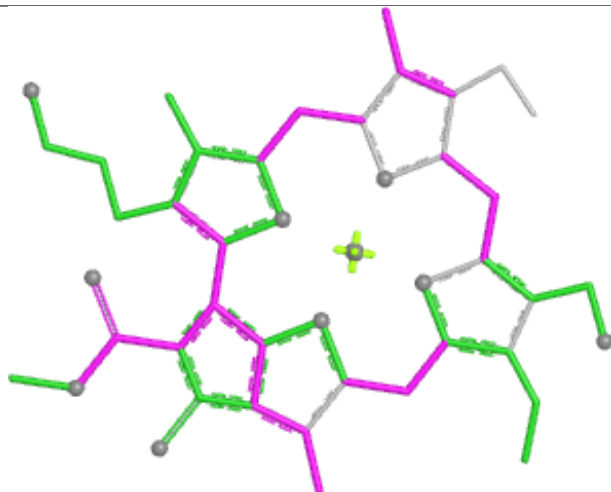


Rings

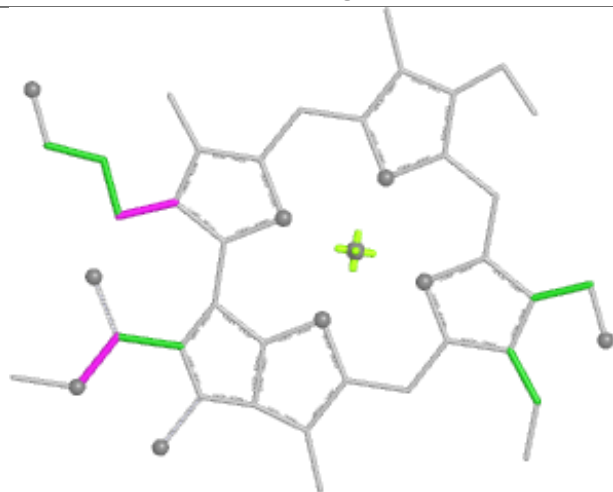
Ligand CHL P 314



Bond lengths



Bond angles

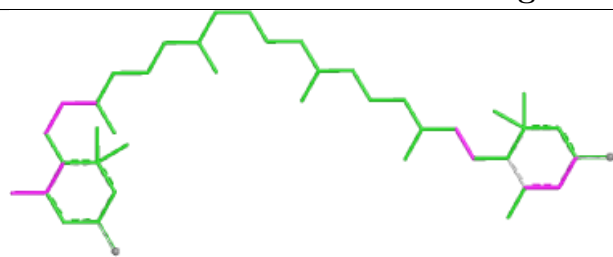


Torsions

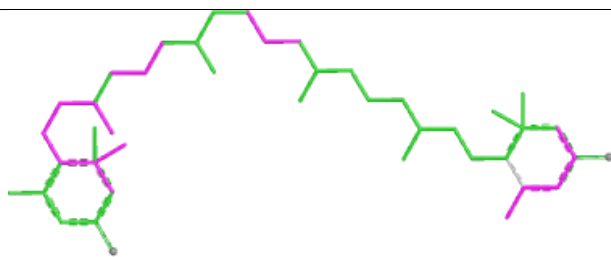


Rings

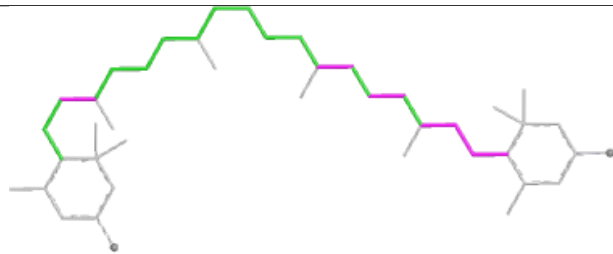
Ligand Q6L R 323



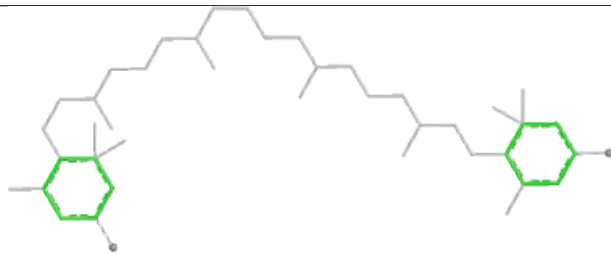
Bond lengths



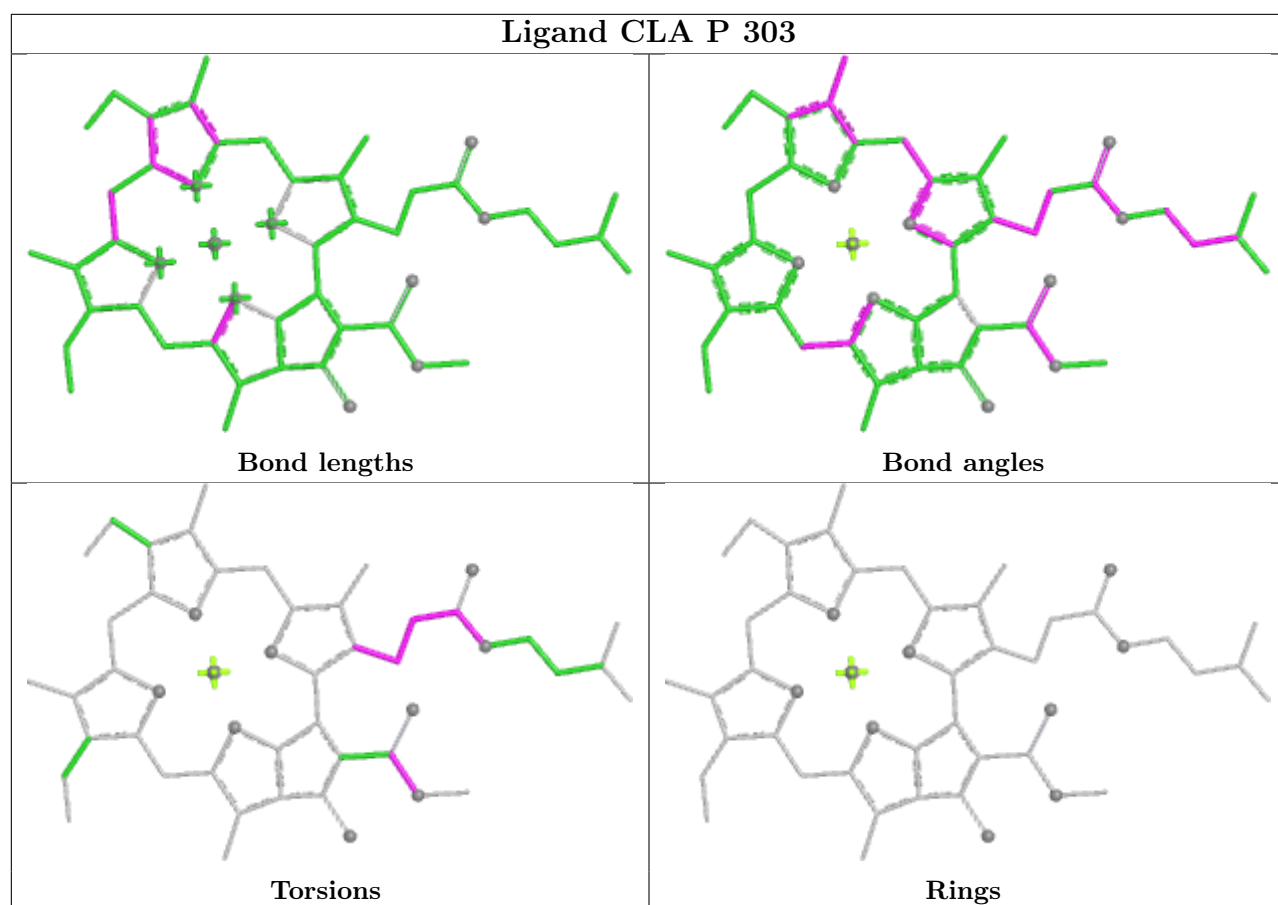
Bond angles



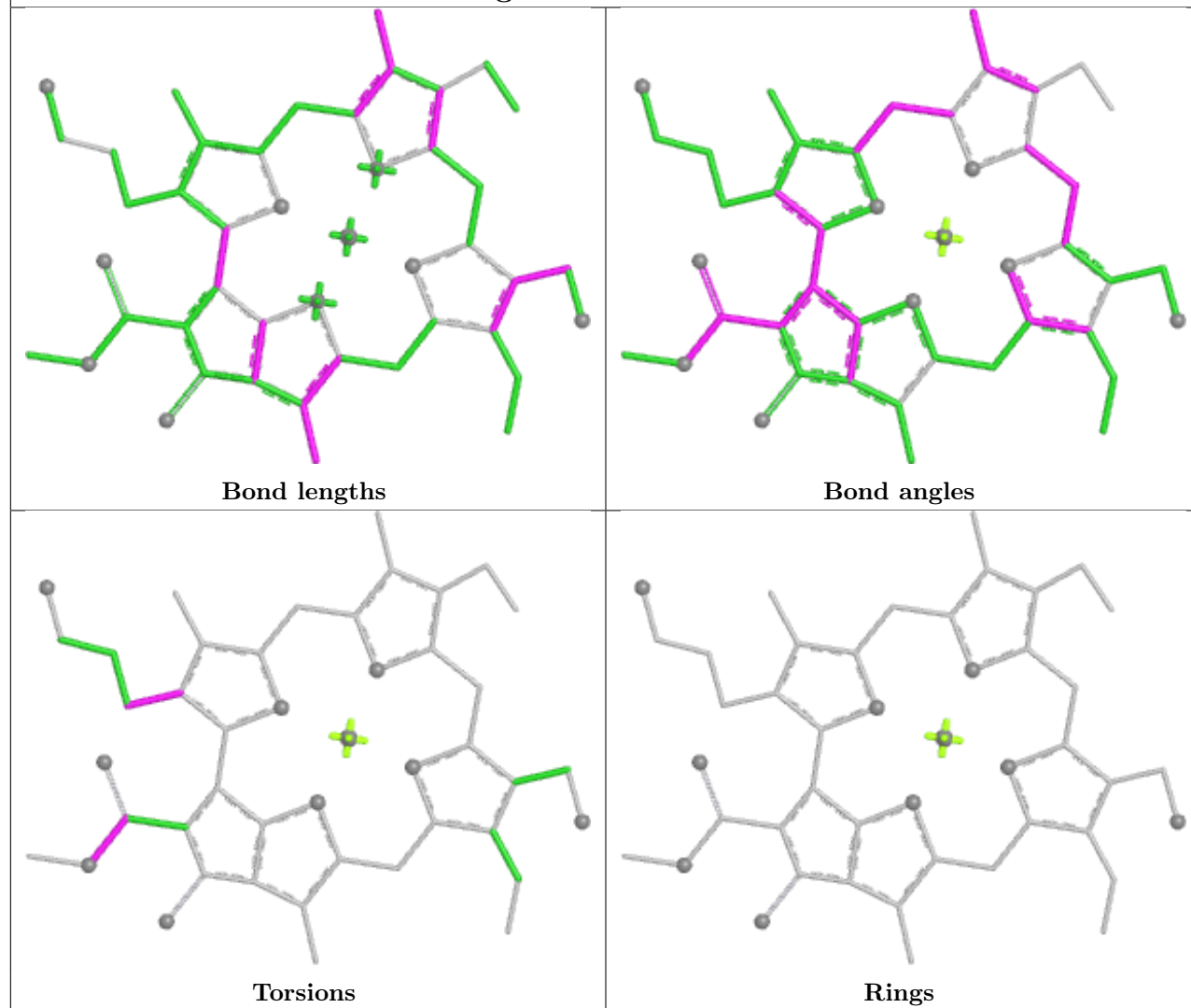
Torsions



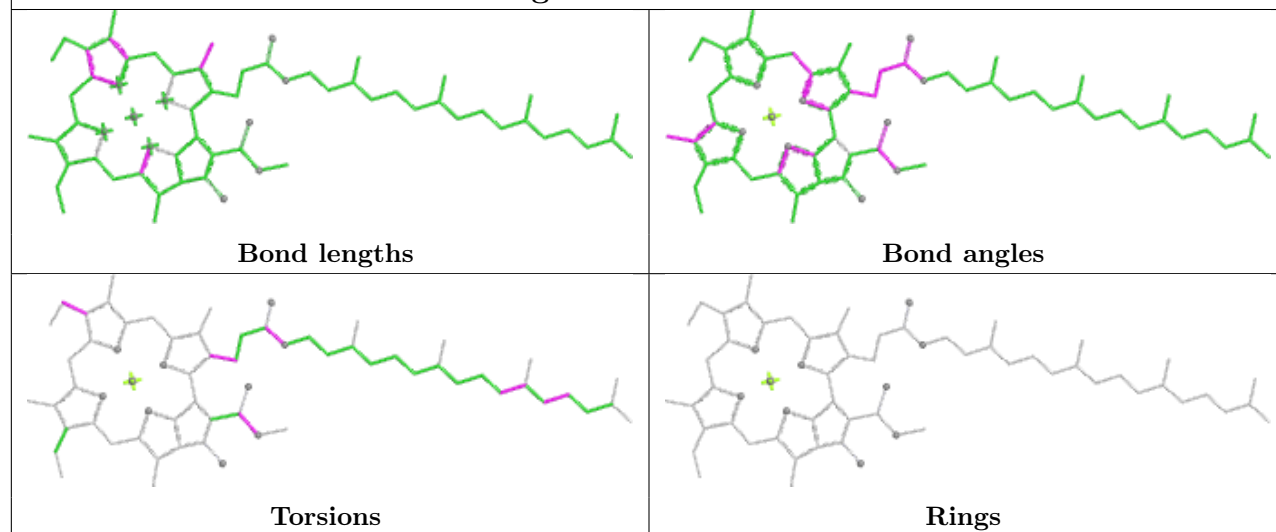
Rings



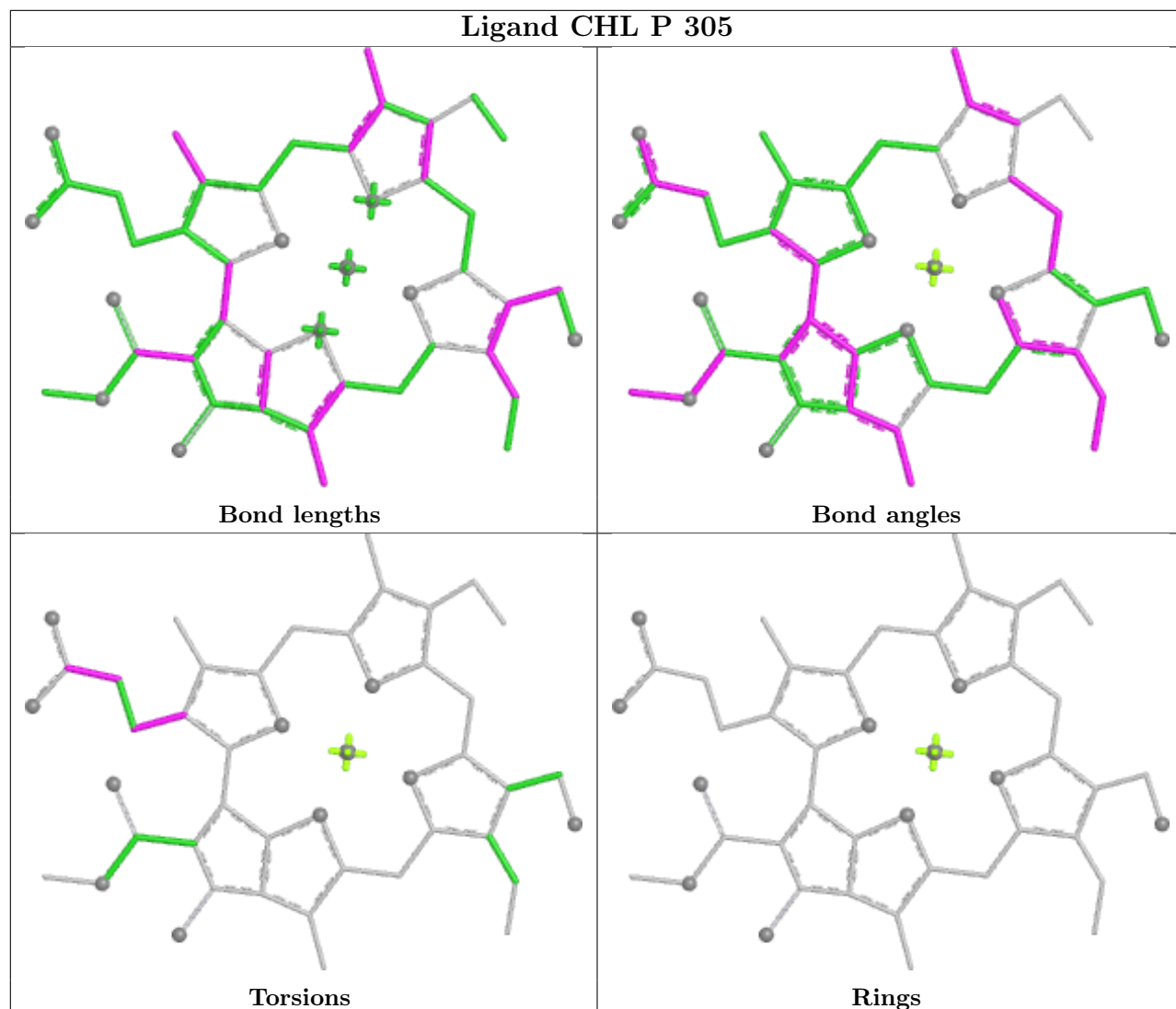
Ligand CHL R 318

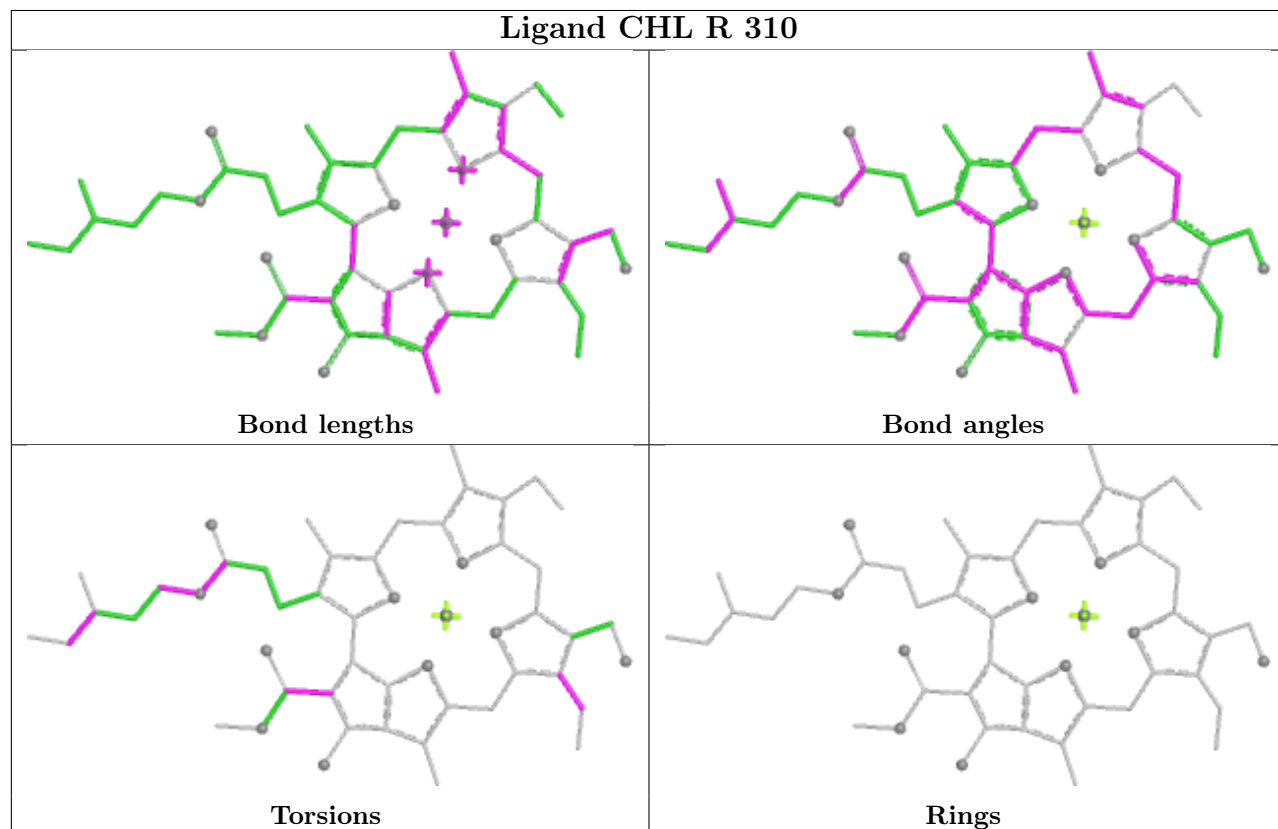
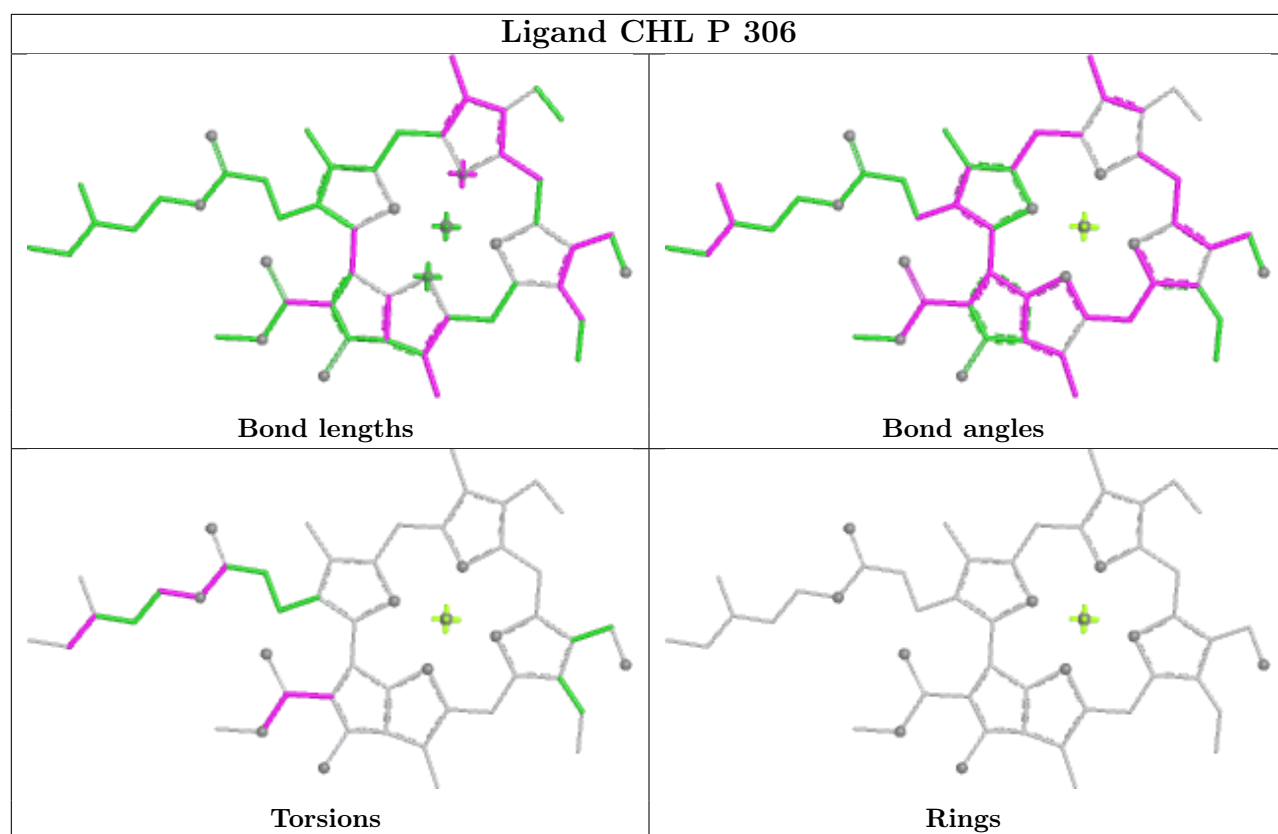


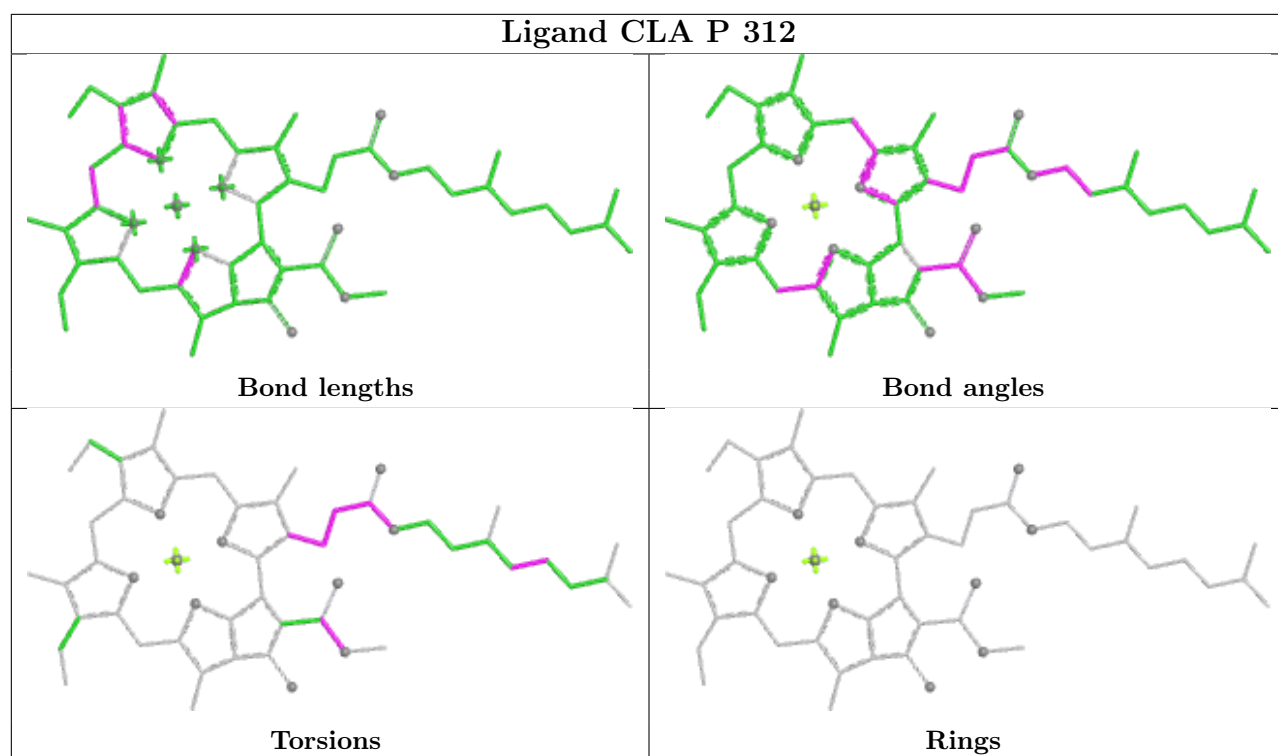
Ligand CLA R 305

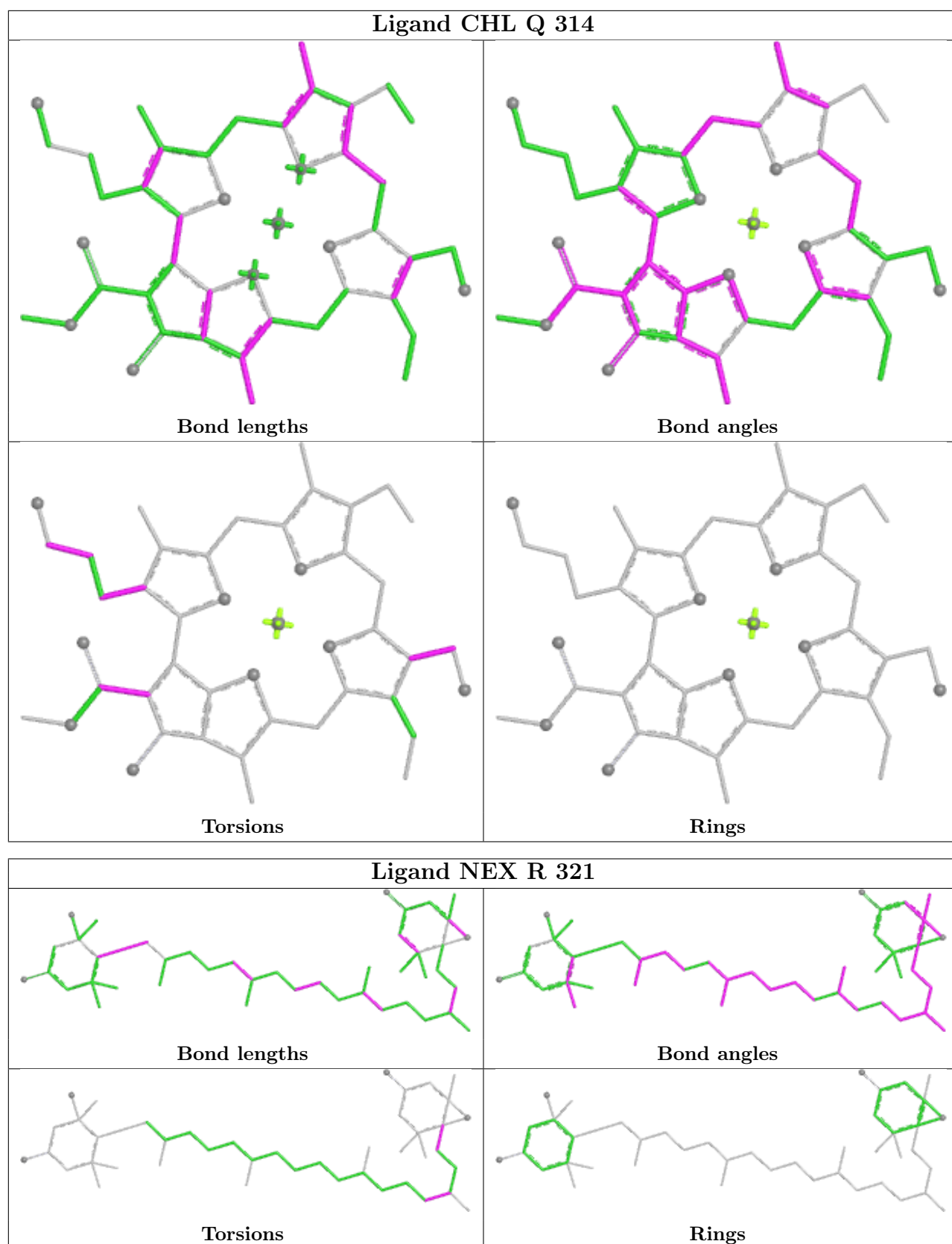


Ligand CHL P 305

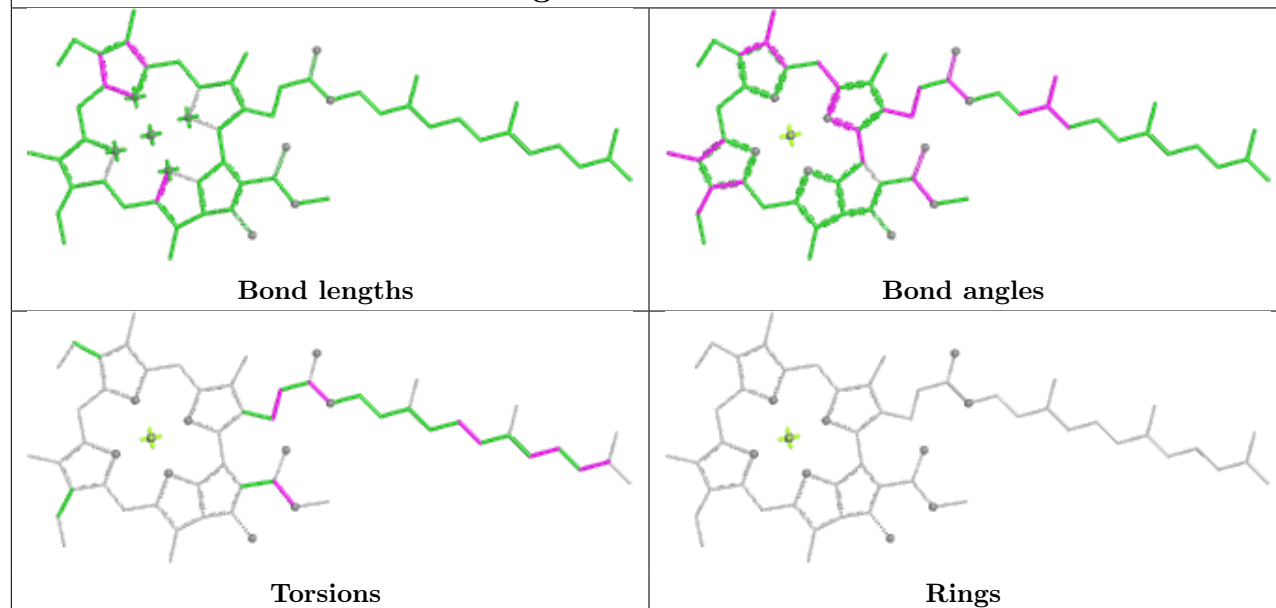




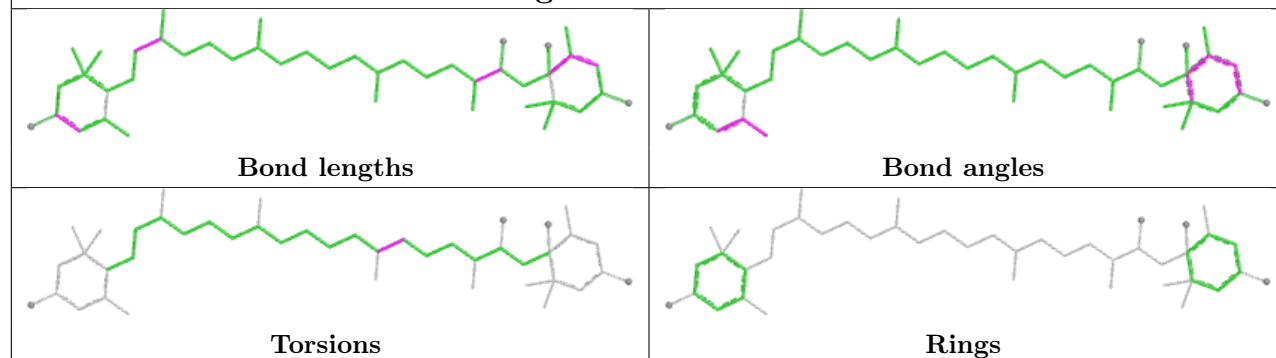




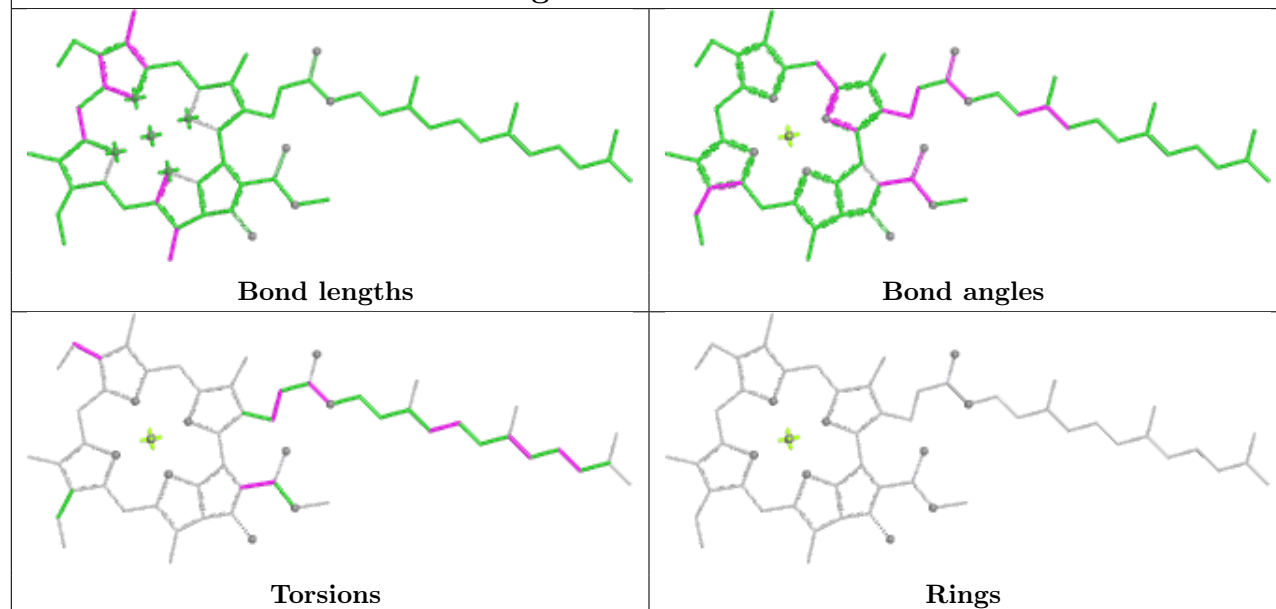
Ligand CLA P 311

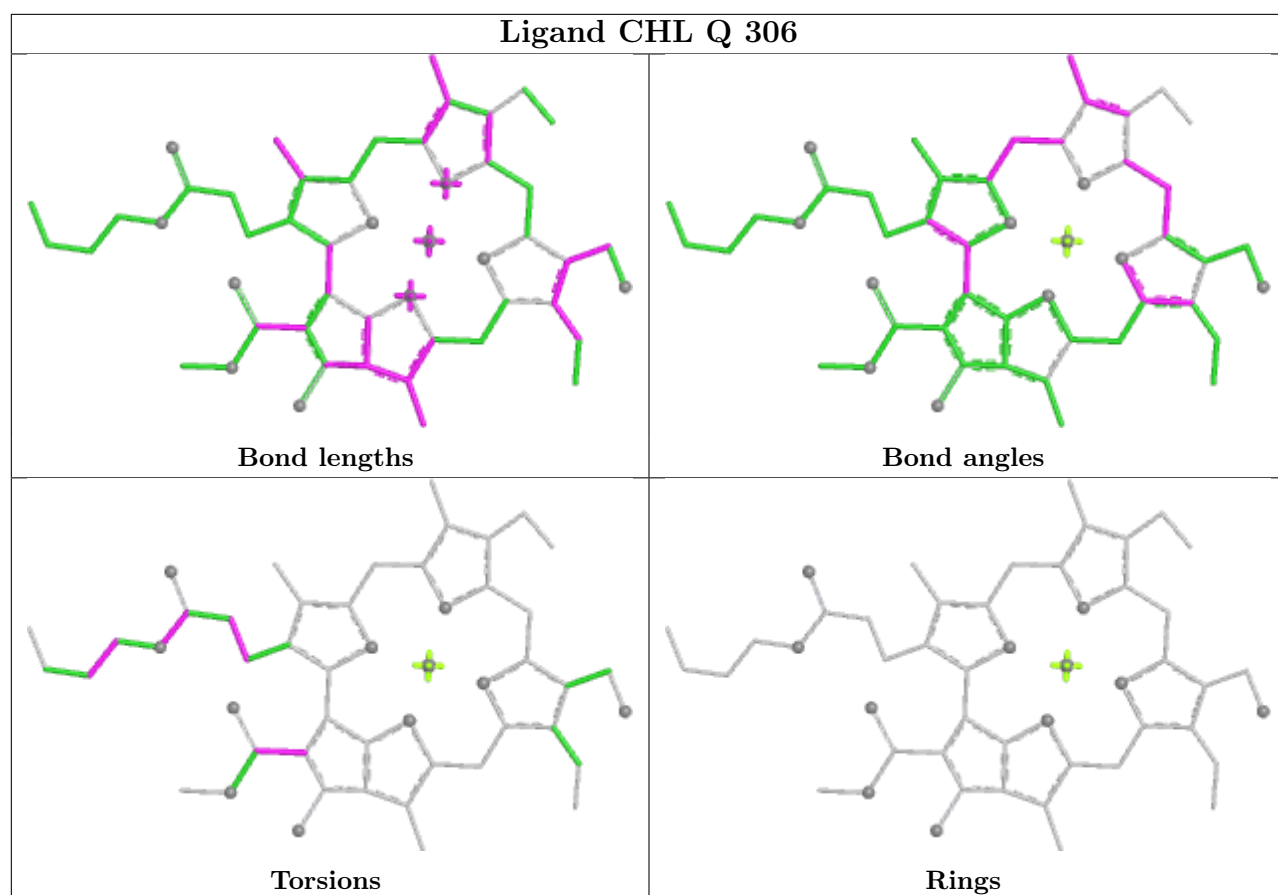


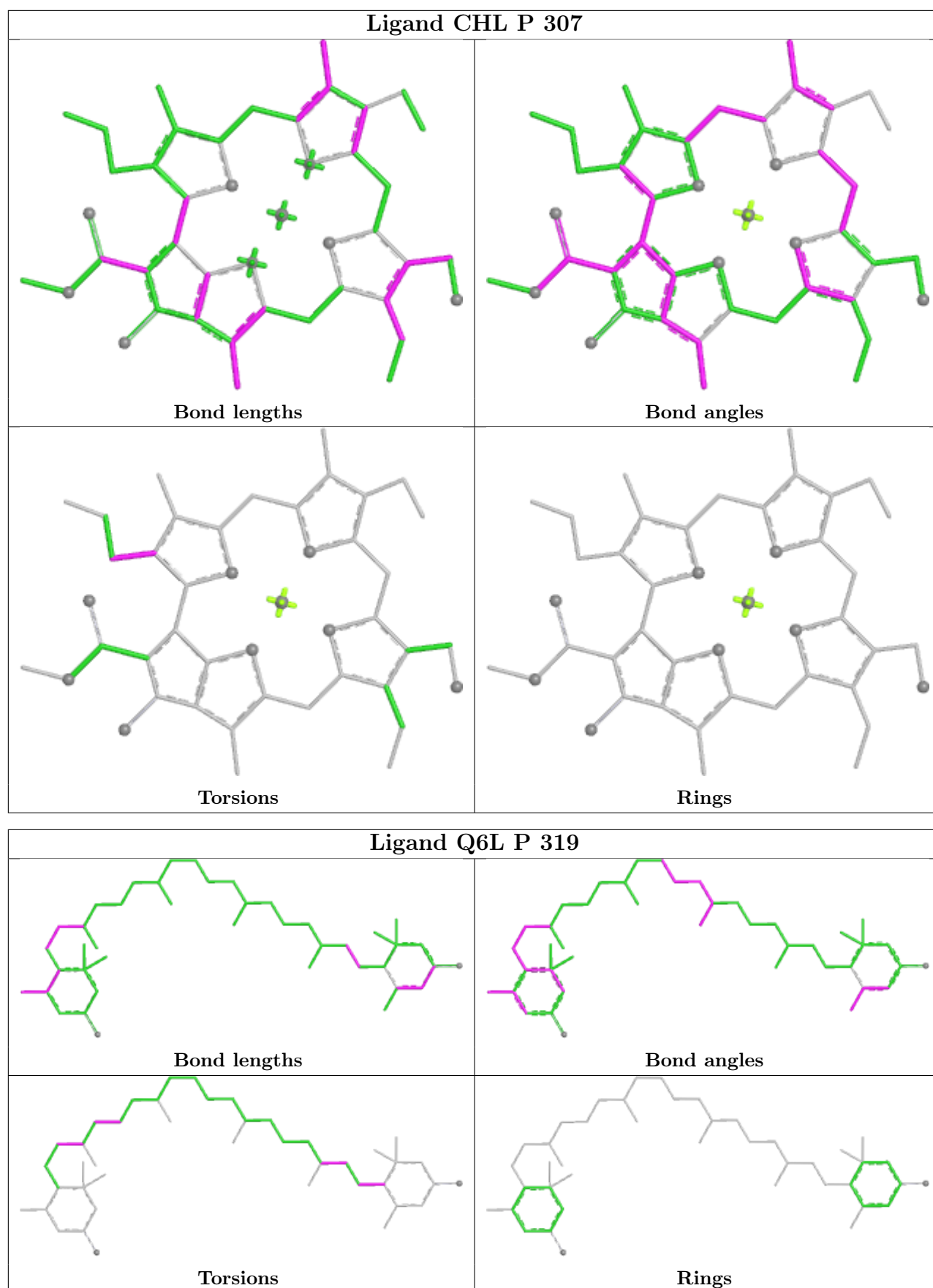
Ligand IWJ P 318

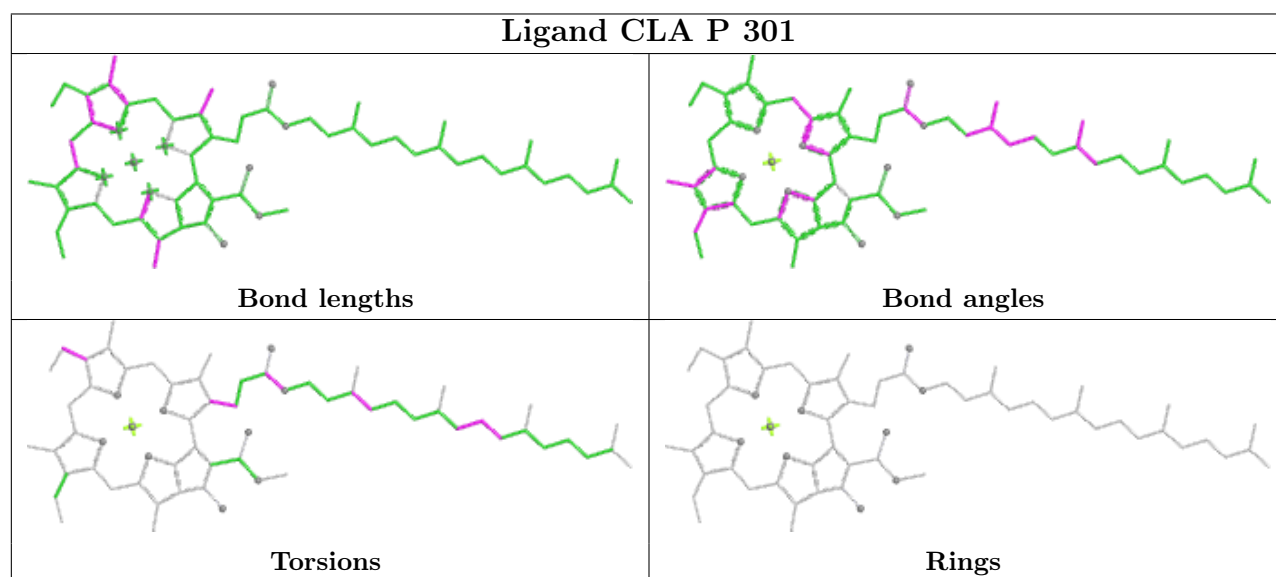
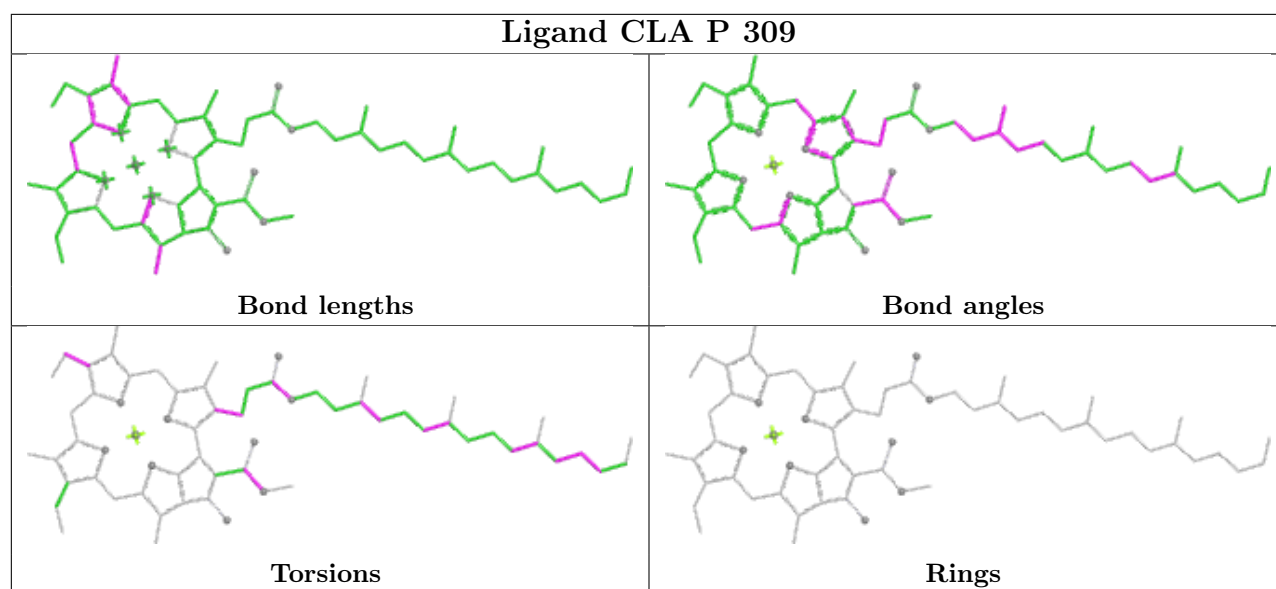


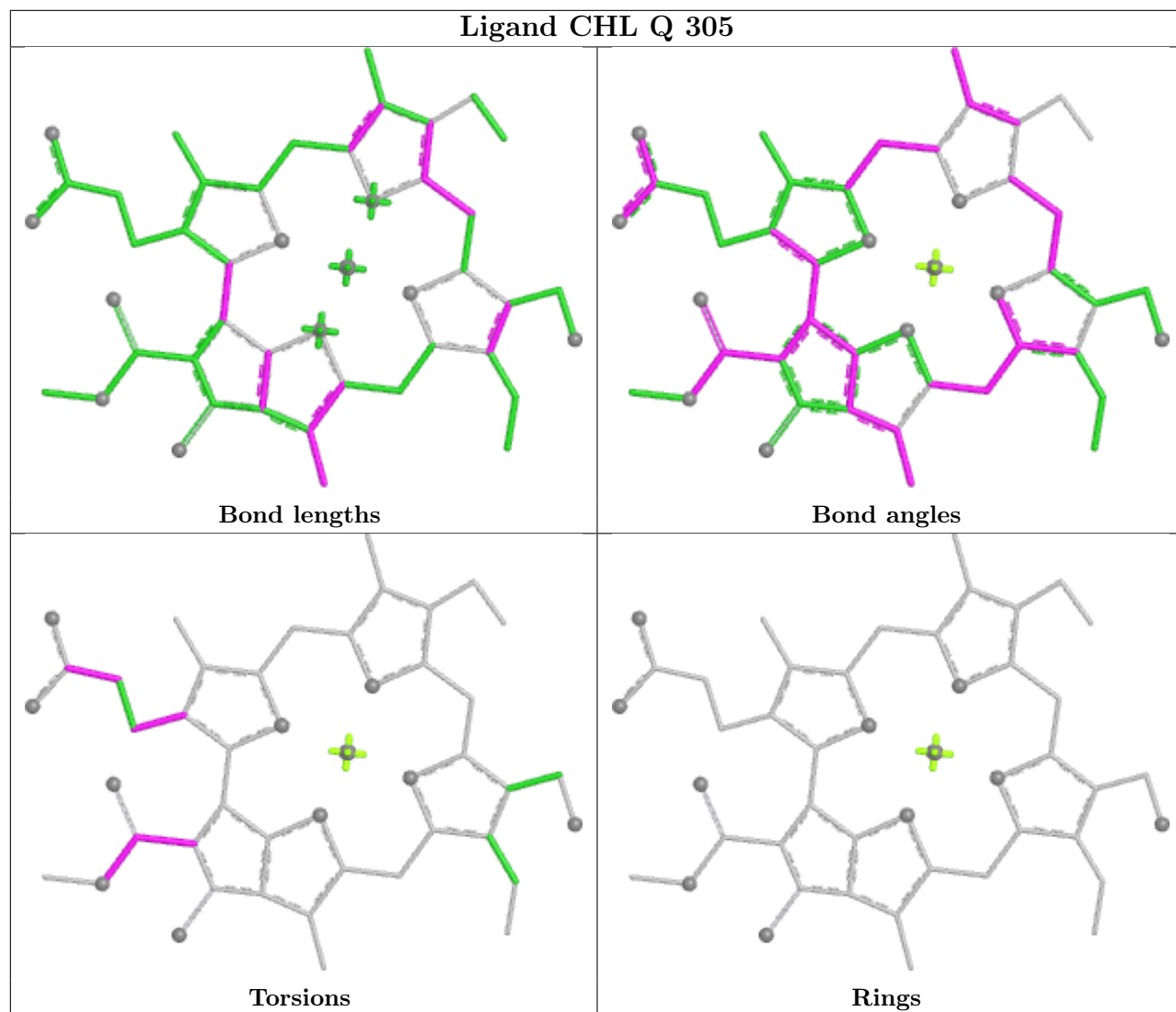
Ligand CLA R 315

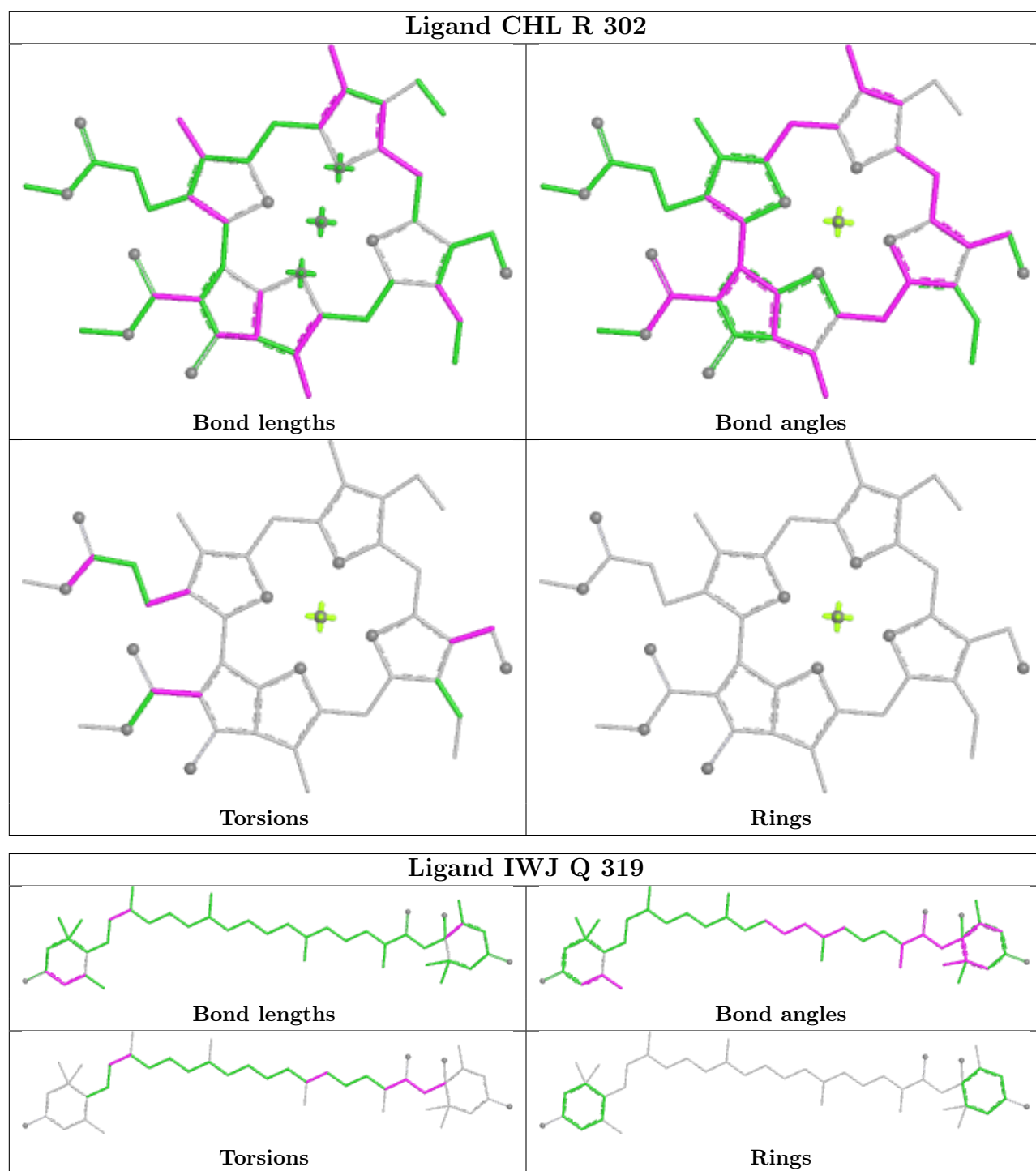


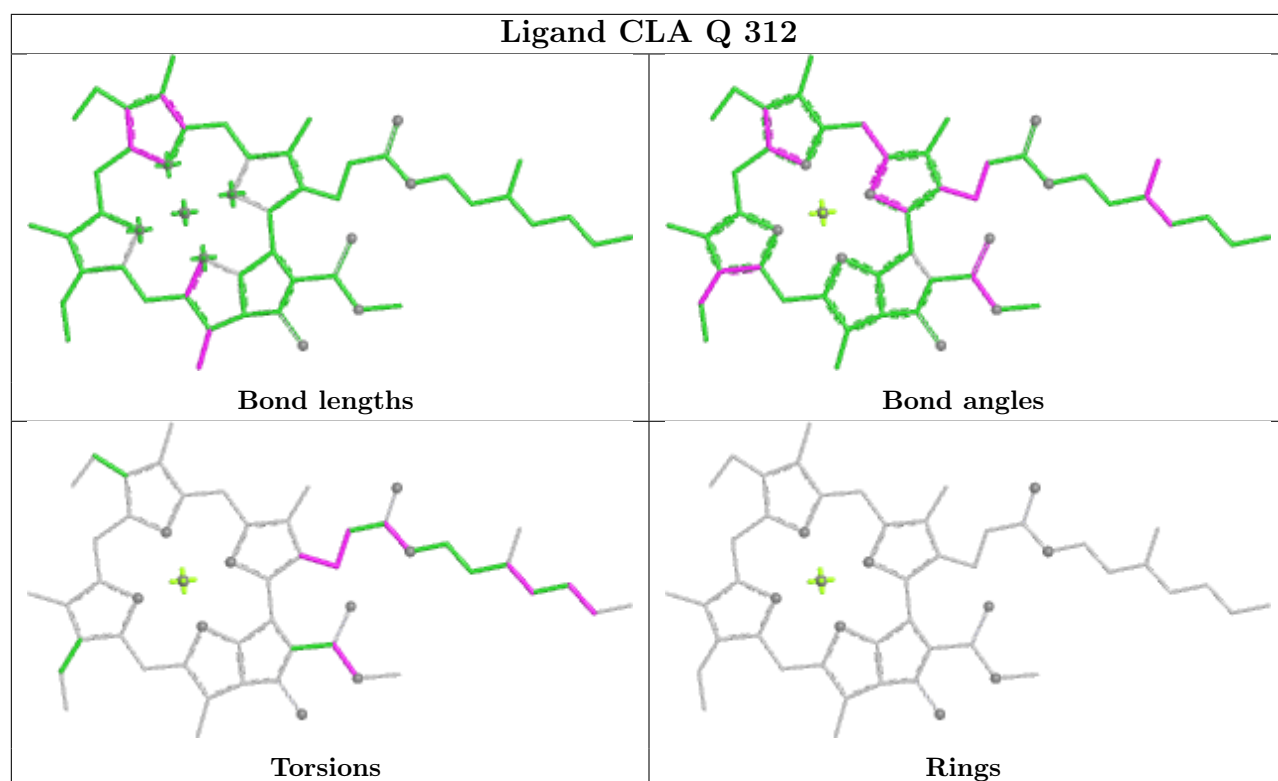




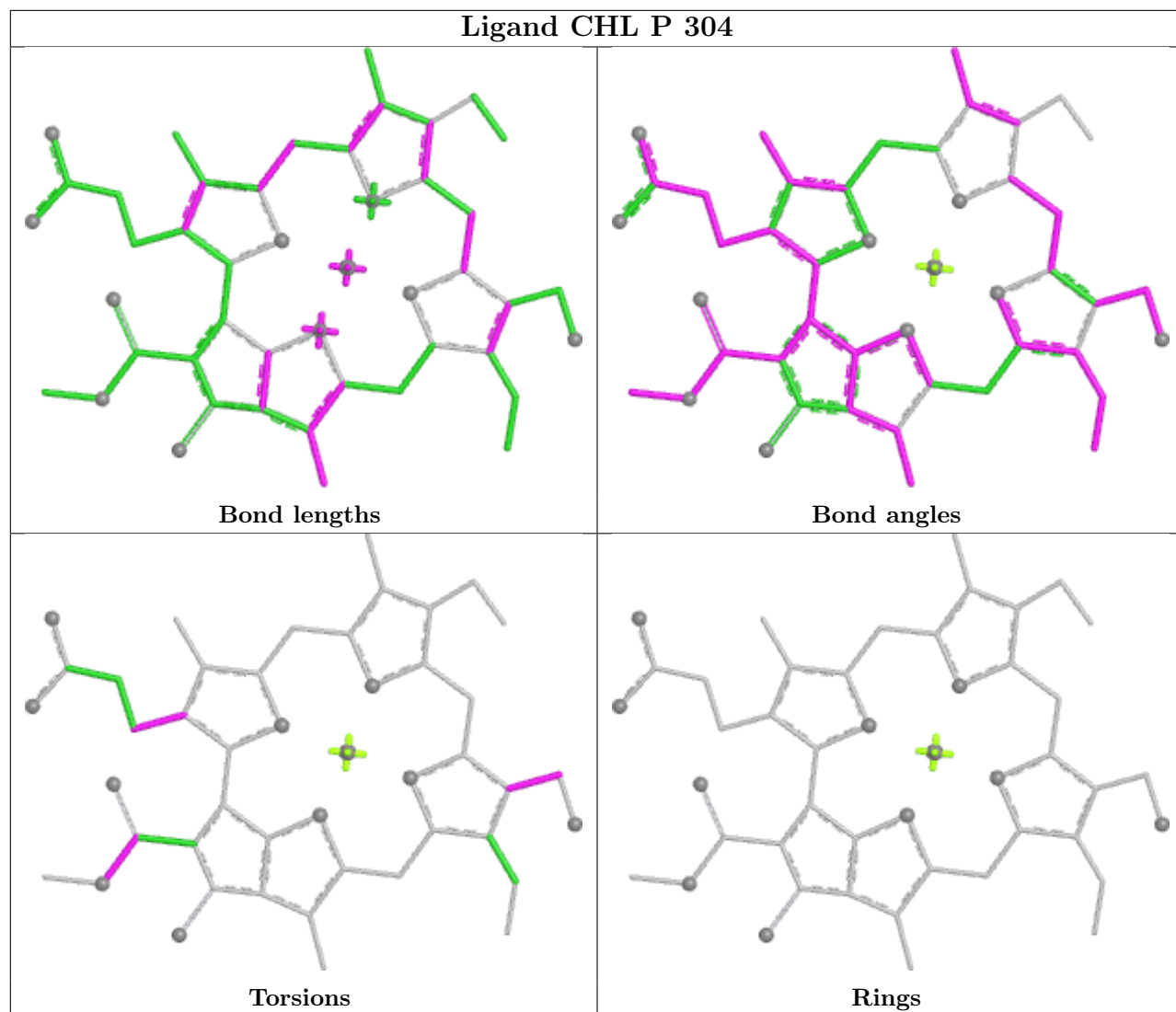




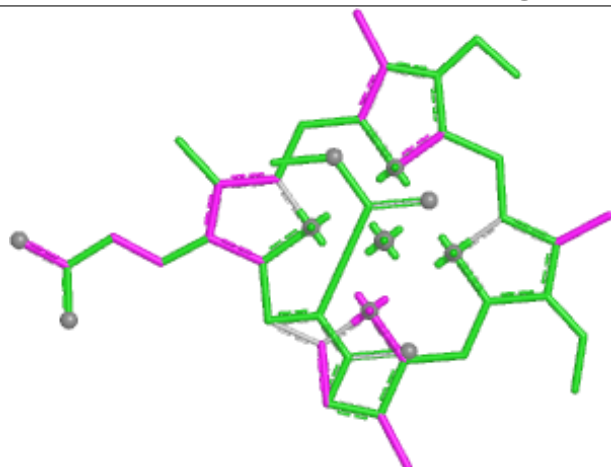




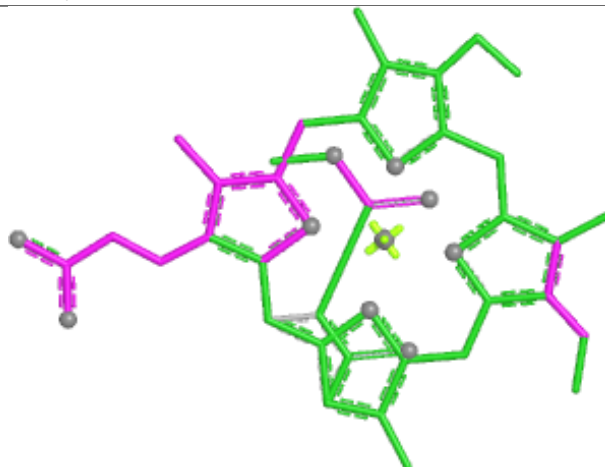
Ligand CHL P 304



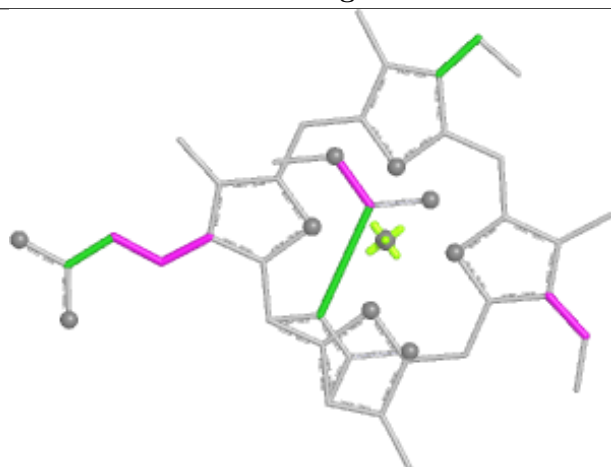
Ligand KC2 Q 308



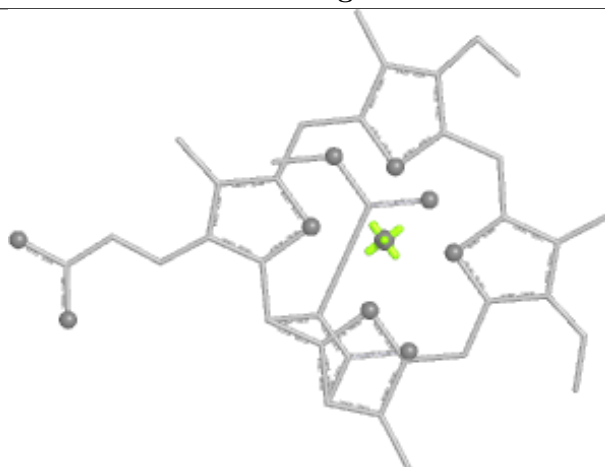
Bond lengths



Bond angles

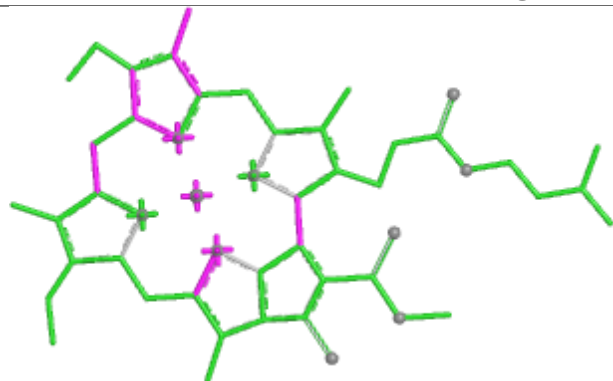


Torsions

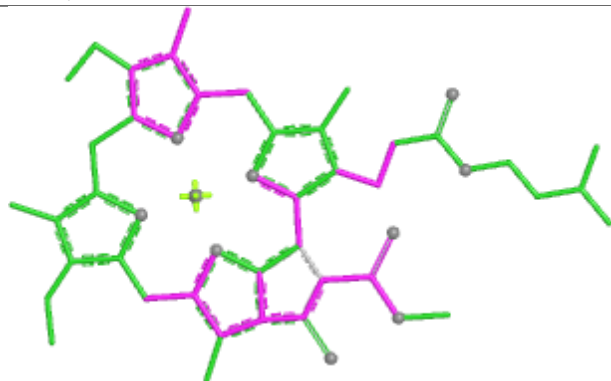


Rings

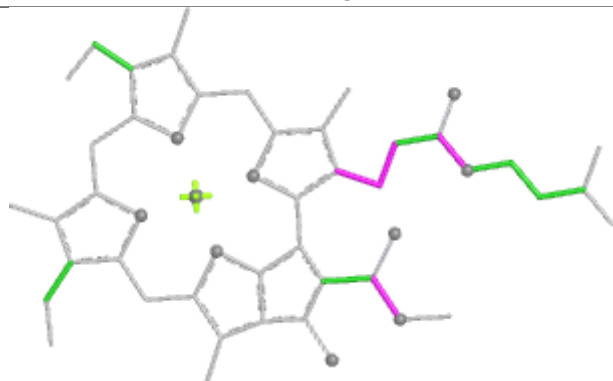
Ligand CLA Q 304



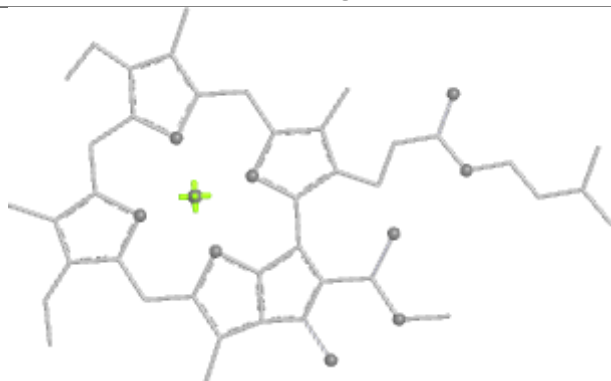
Bond lengths



Bond angles

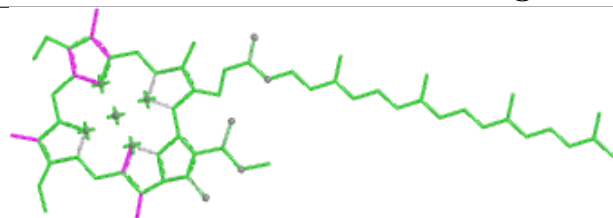


Torsions

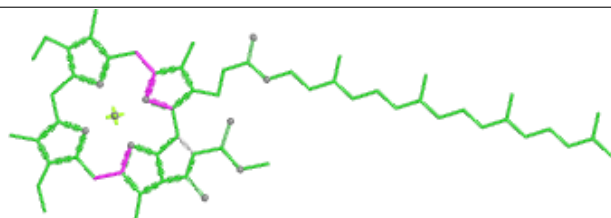


Rings

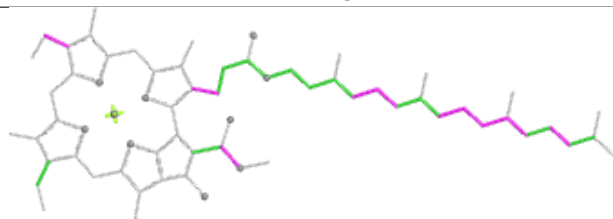
Ligand CLA R 306



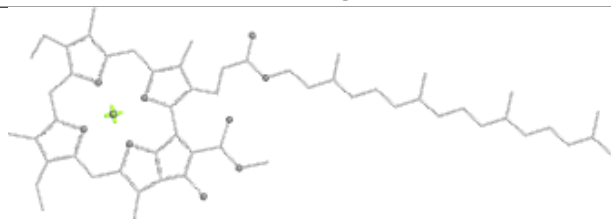
Bond lengths



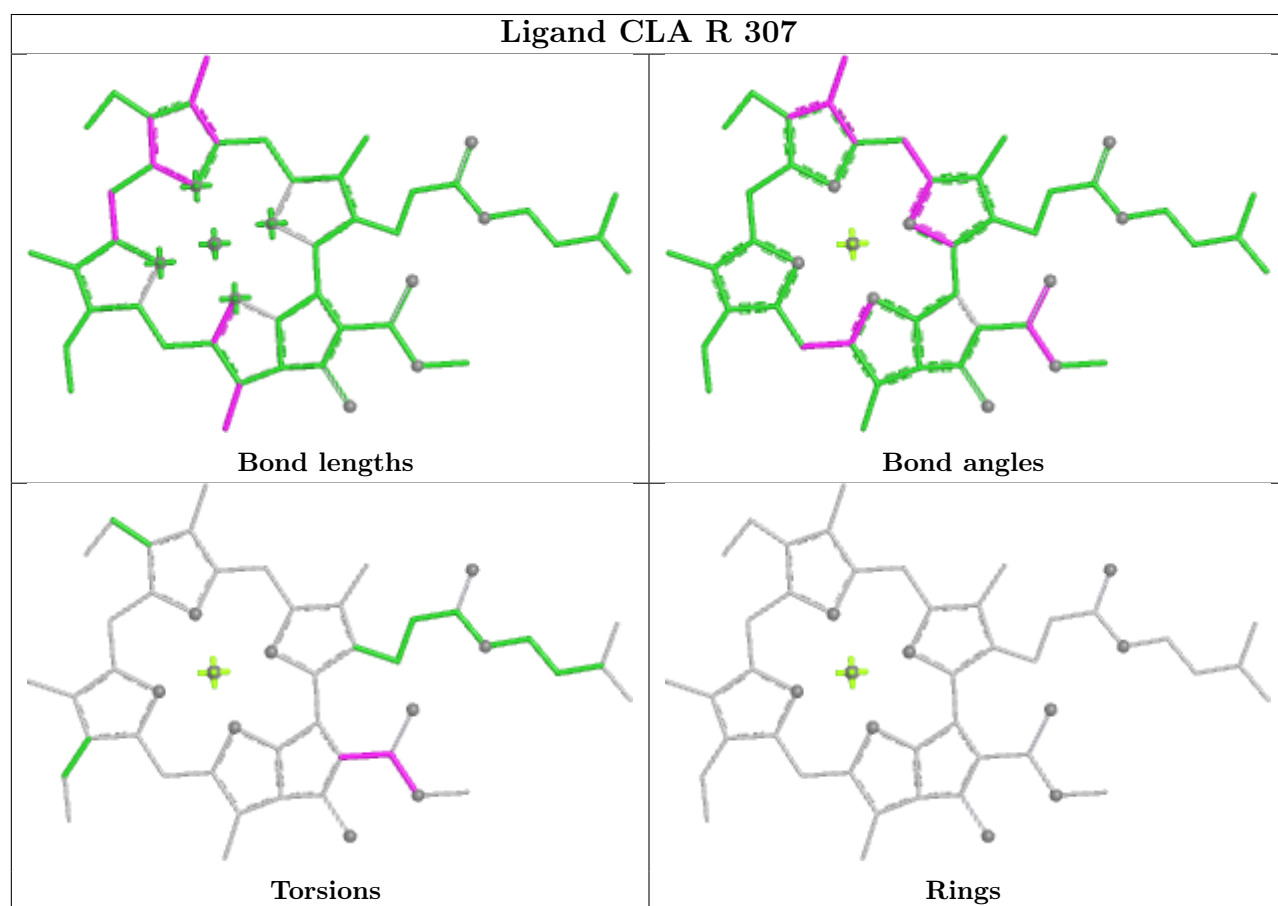
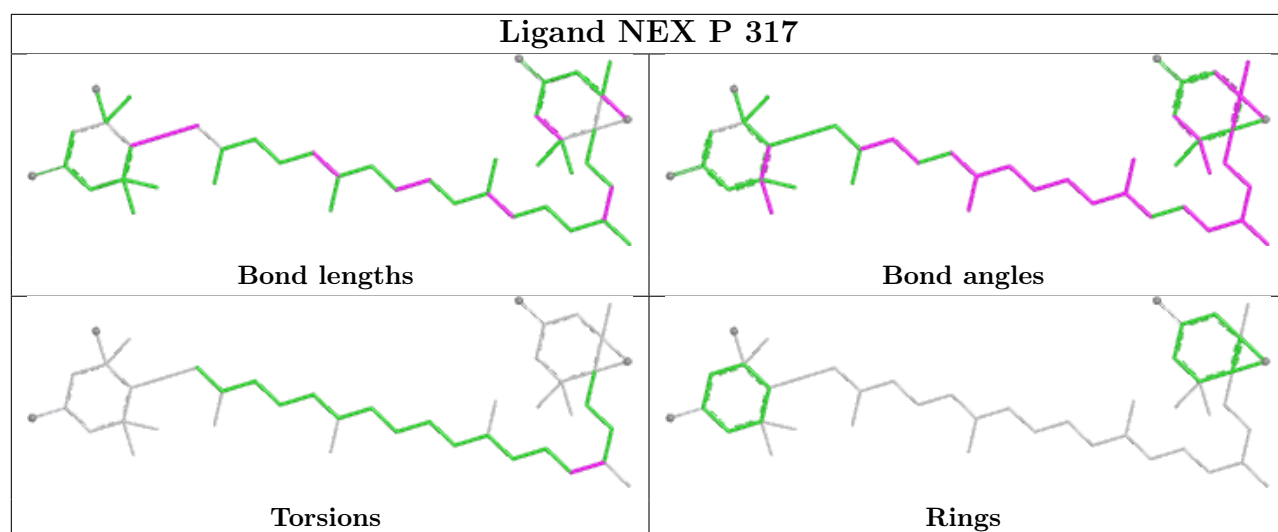
Bond angles



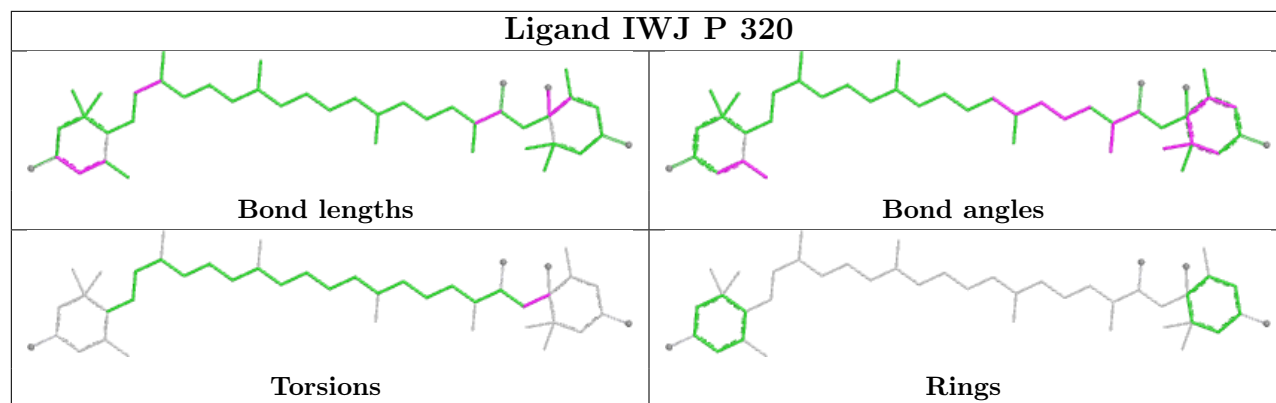
Torsions



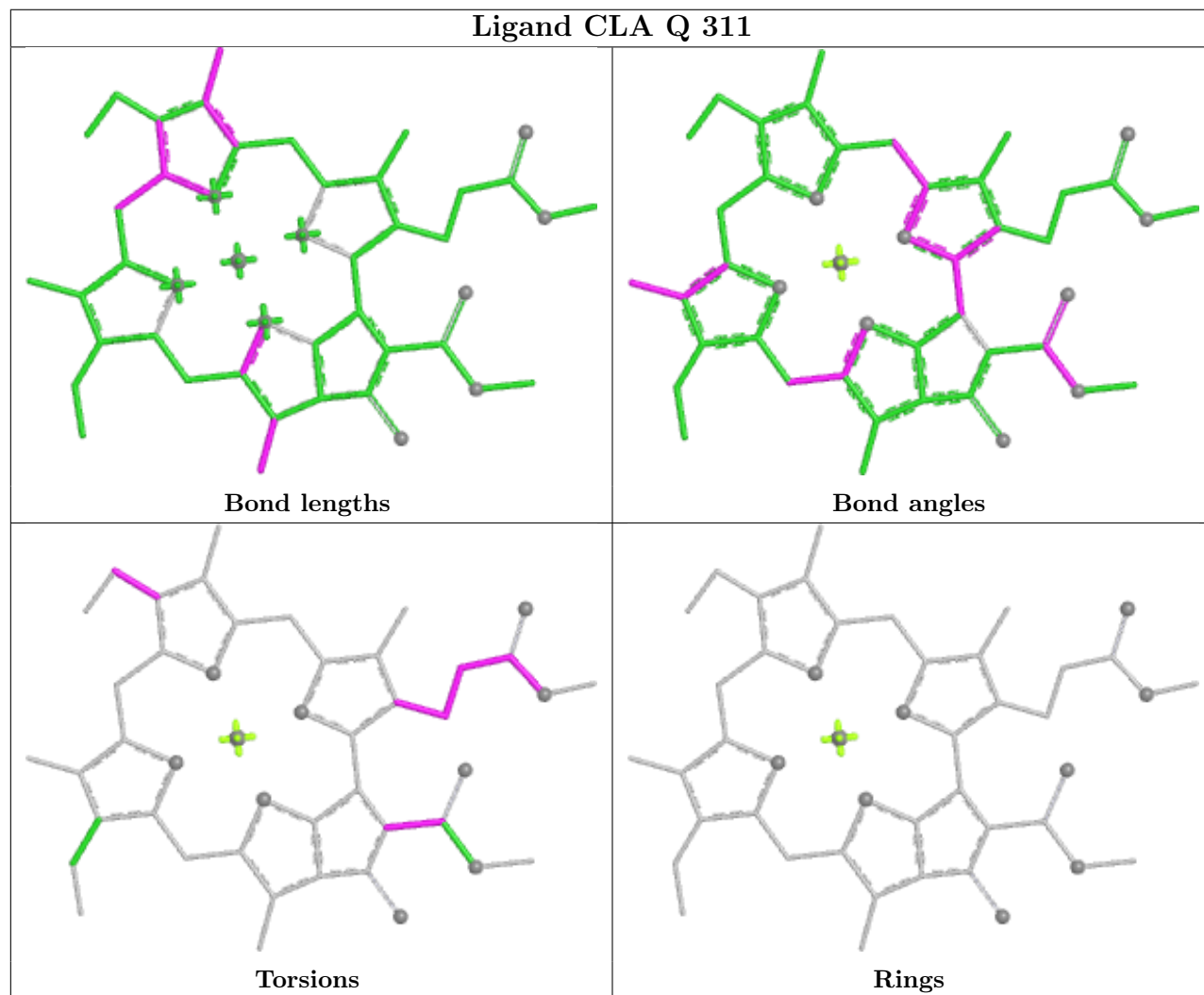
Rings

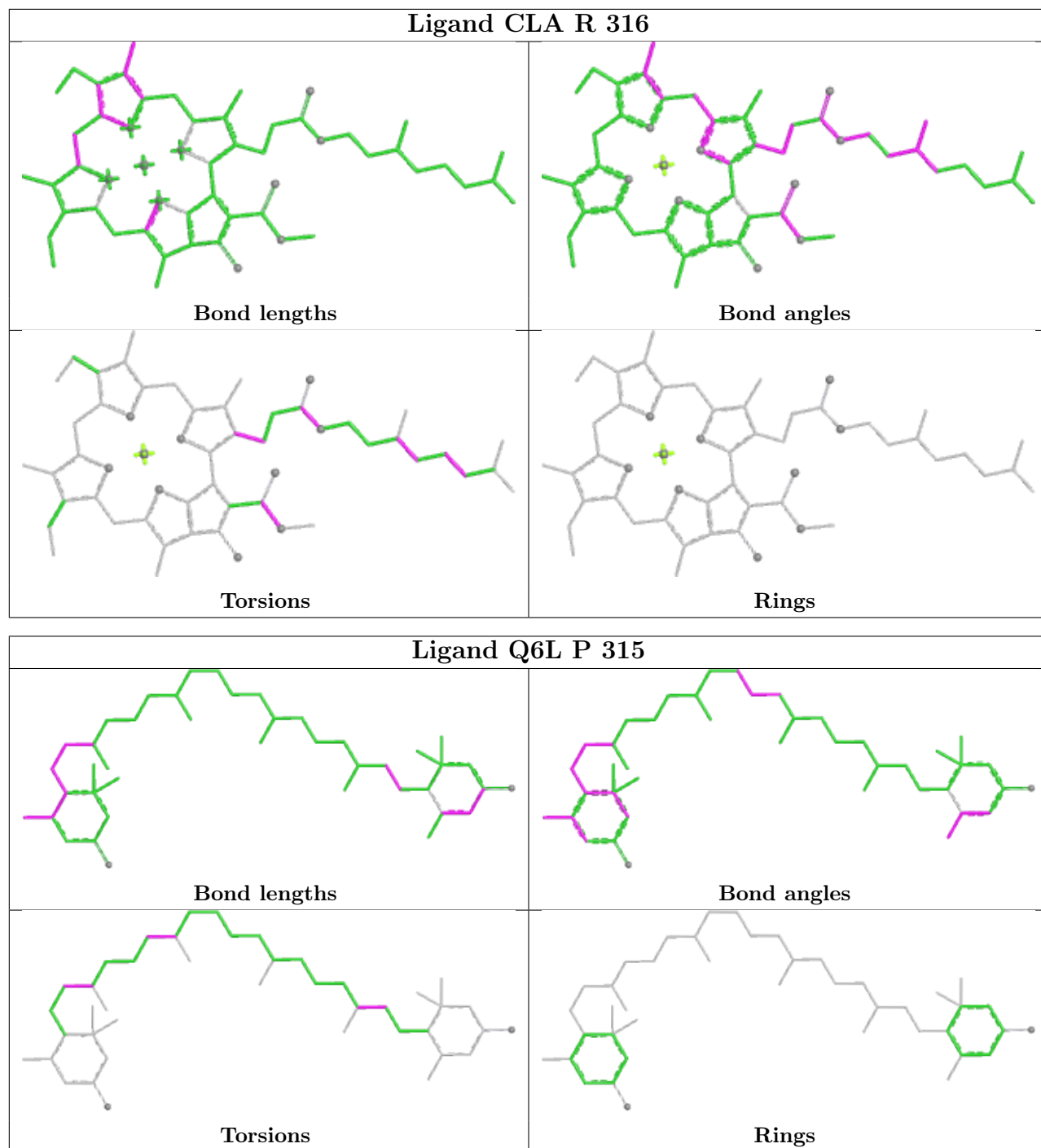


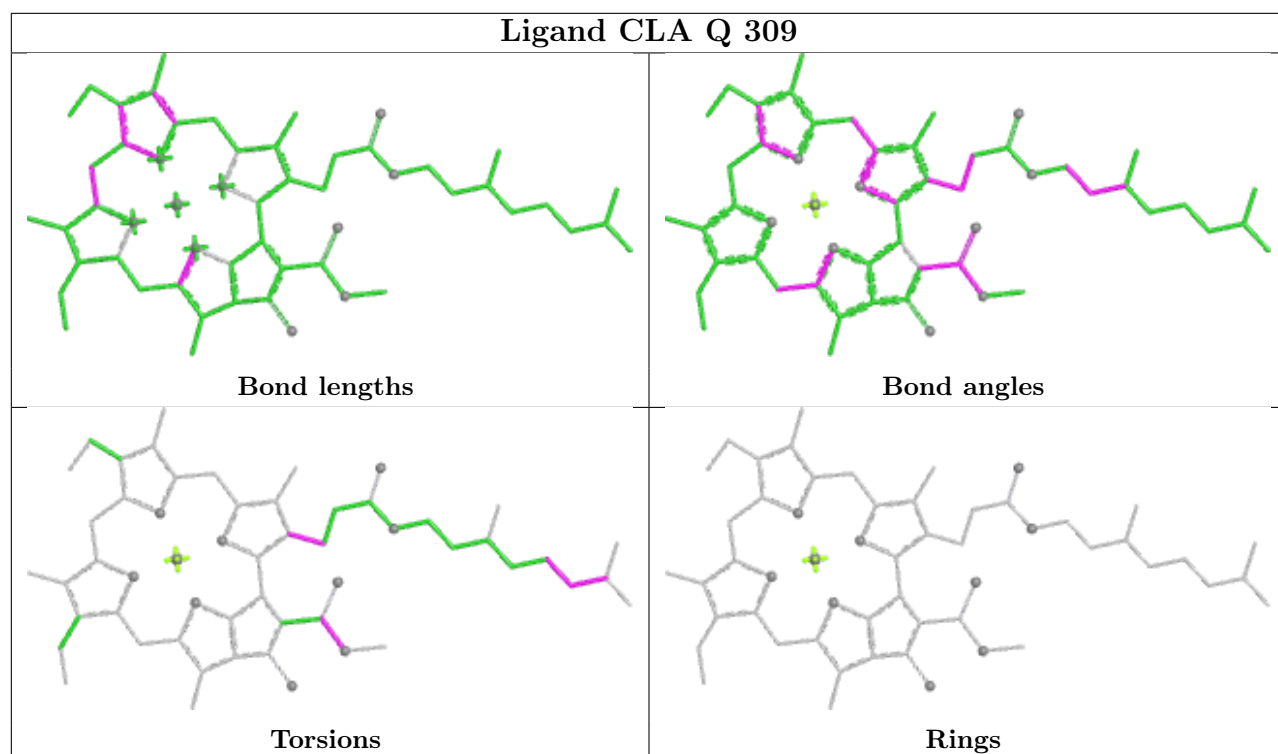
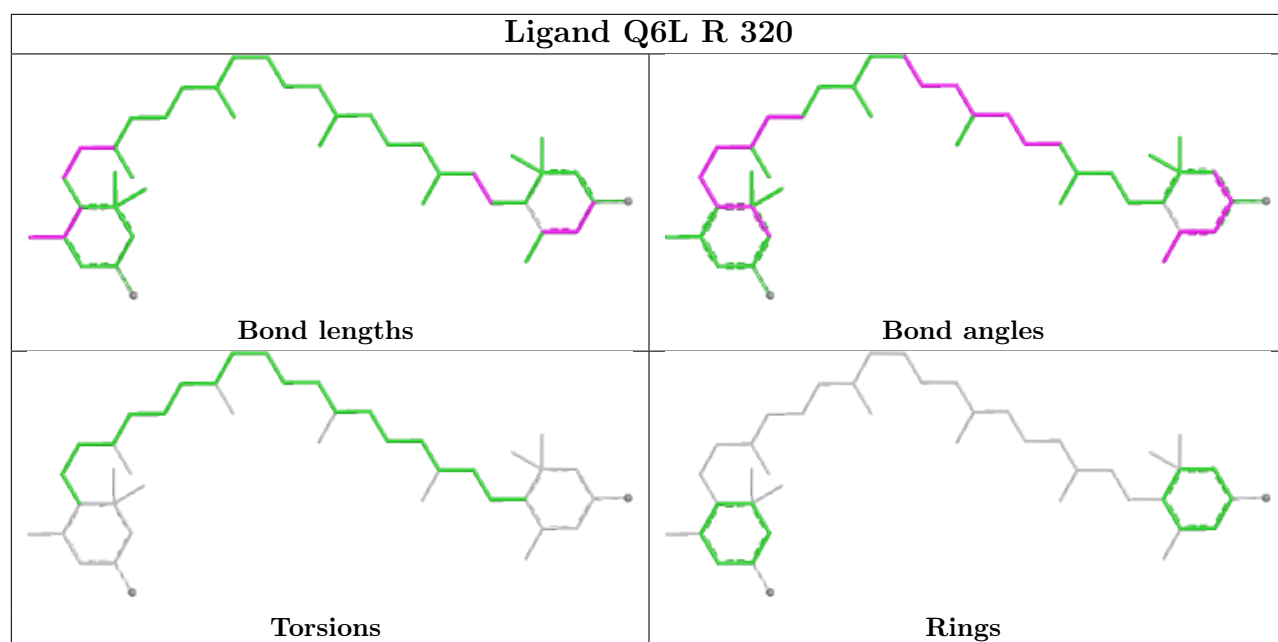
Ligand IWJ P 320



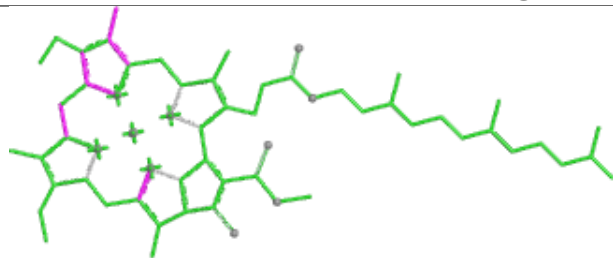
Ligand CLA Q 311



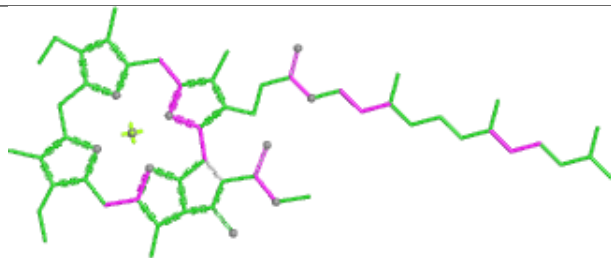




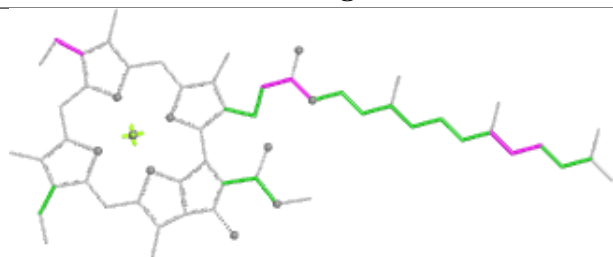
Ligand CLA P 310



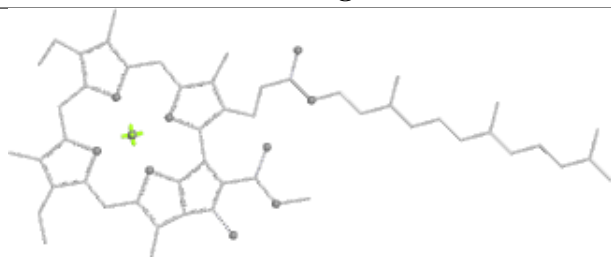
Bond lengths



Bond angles

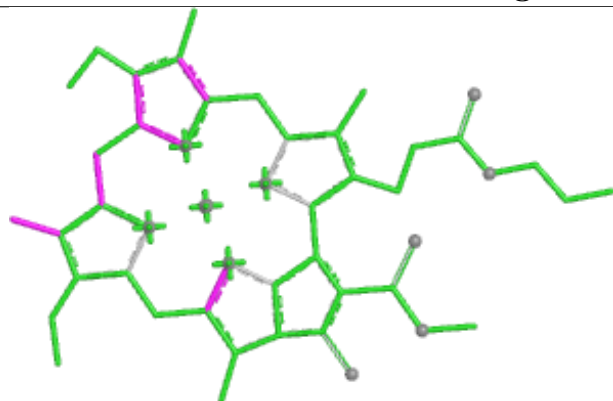


Torsions

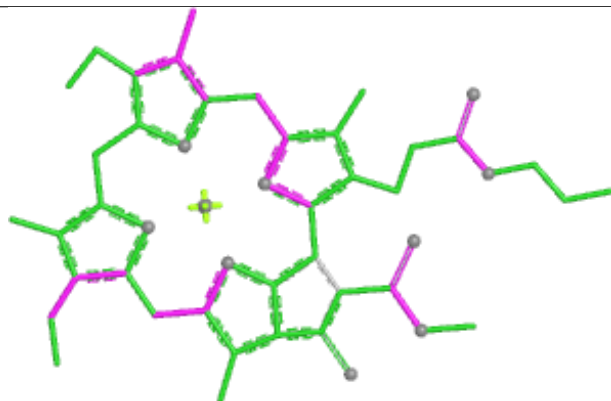


Rings

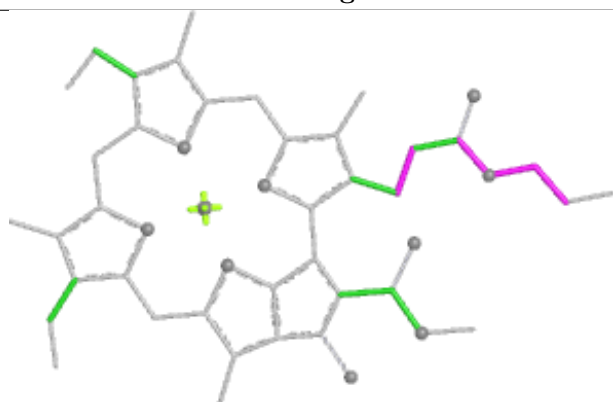
Ligand CLA R 317



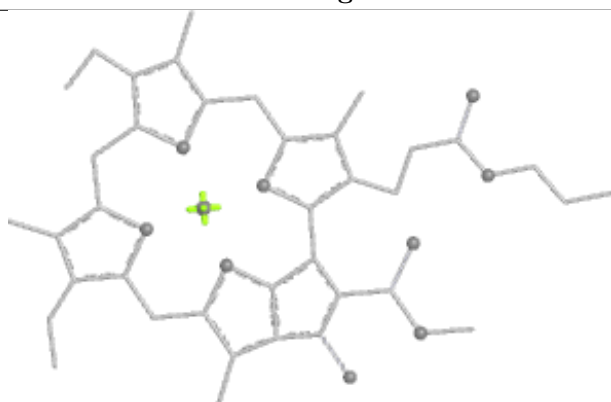
Bond lengths



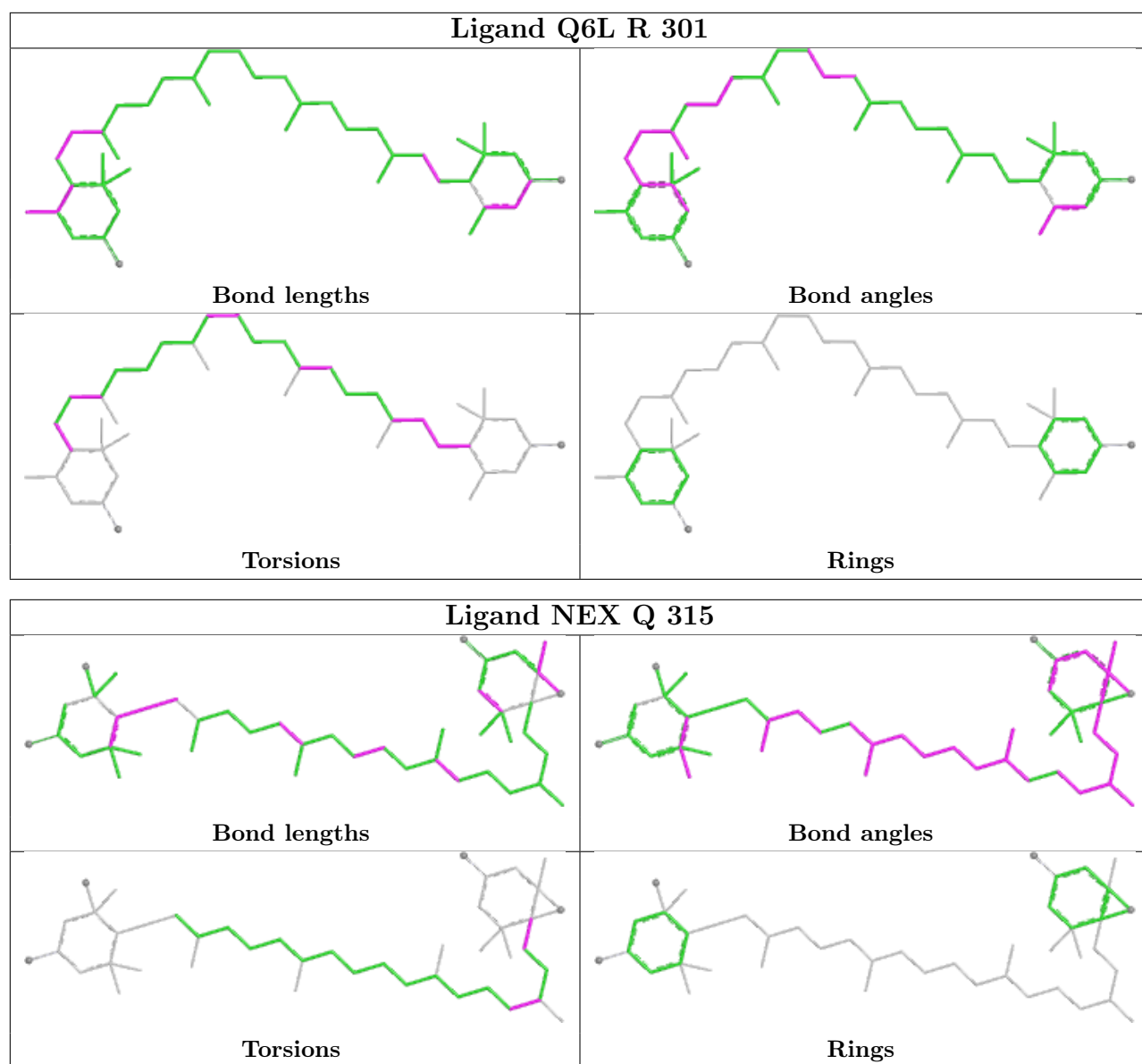
Bond angles

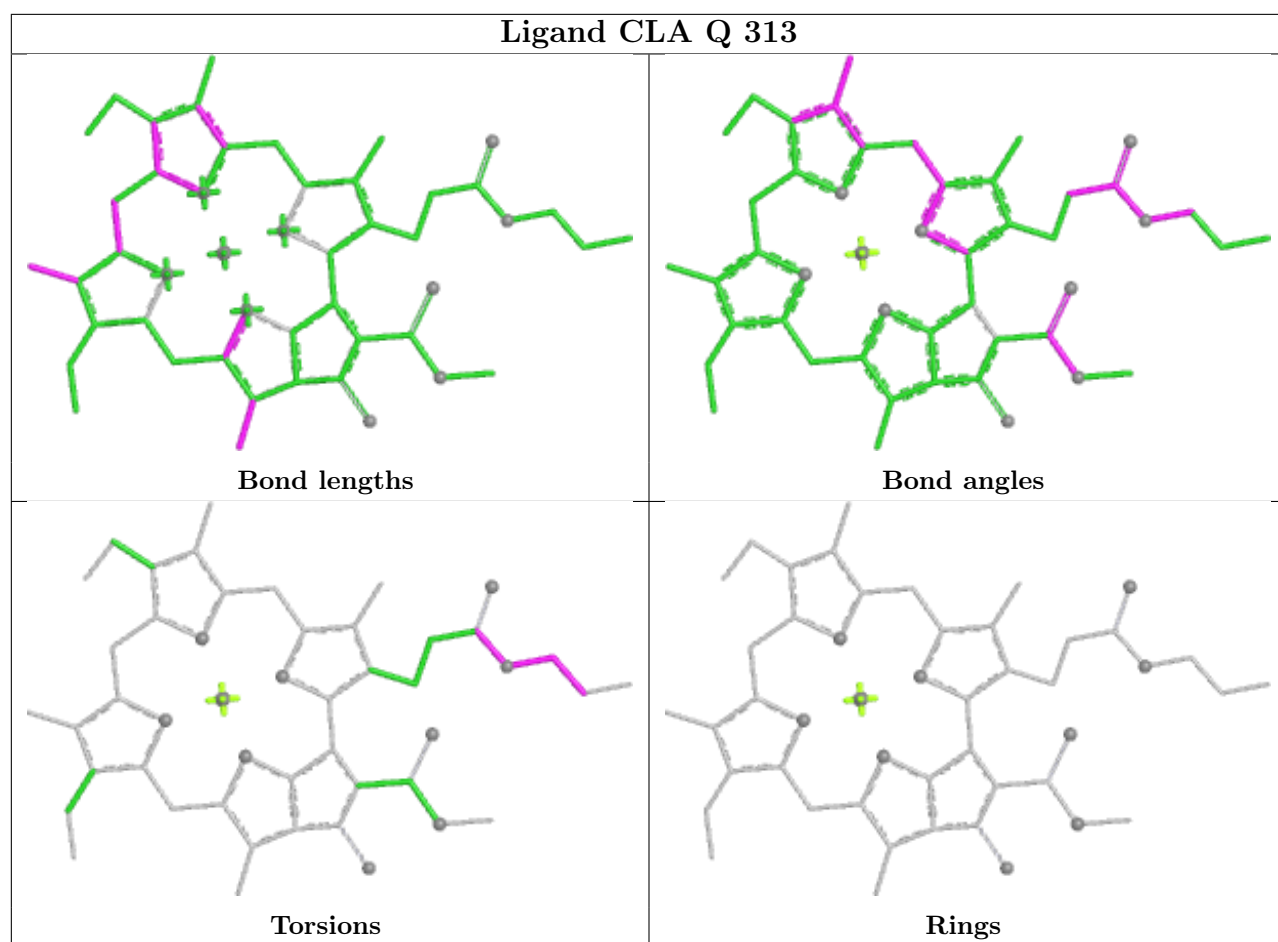


Torsions

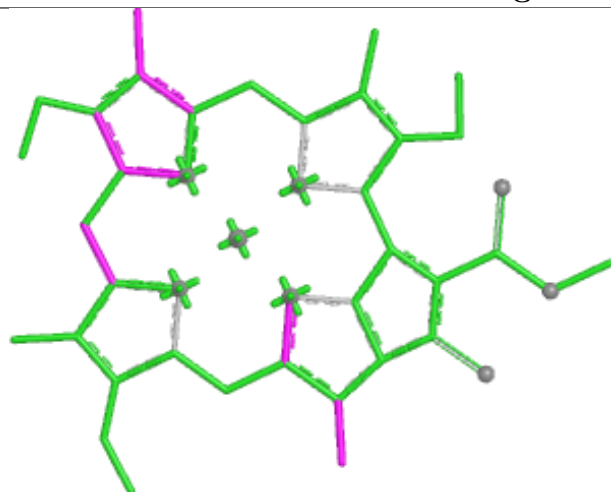


Rings

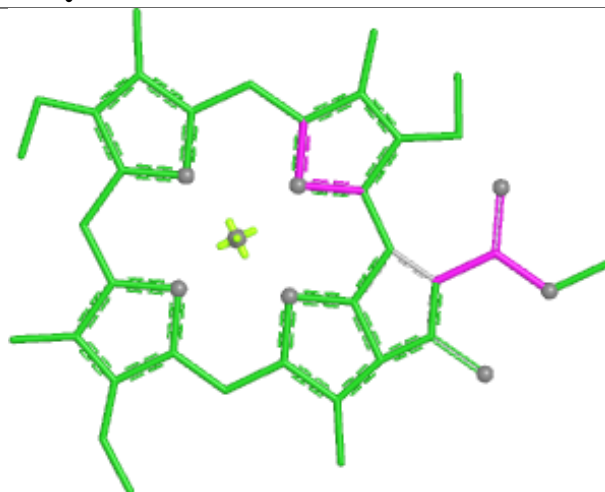




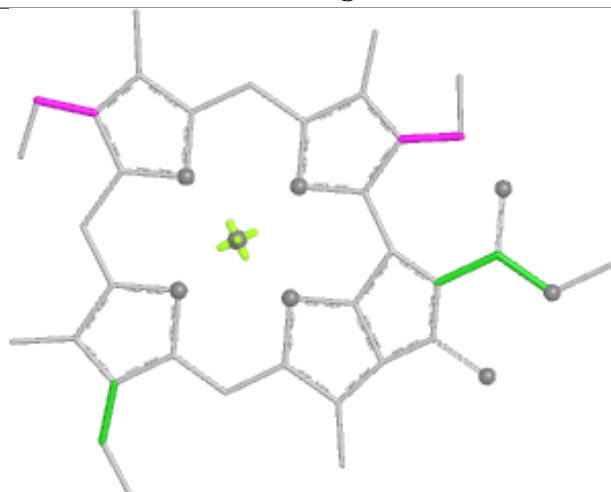
Ligand CLA Q 310



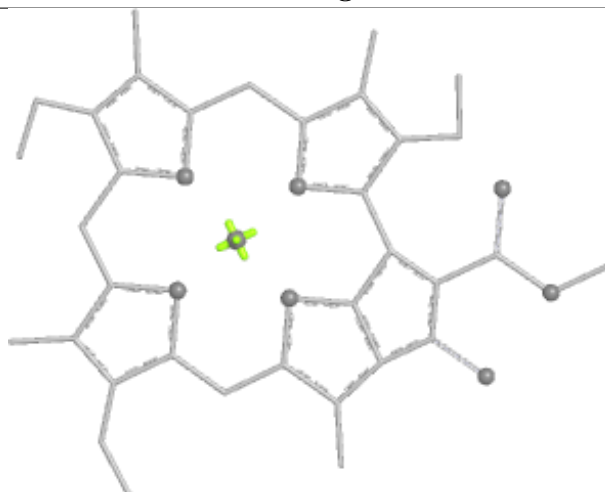
Bond lengths



Bond angles

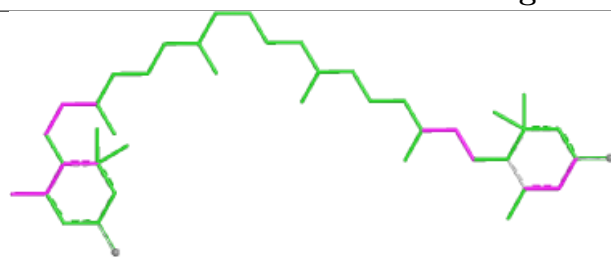


Torsions

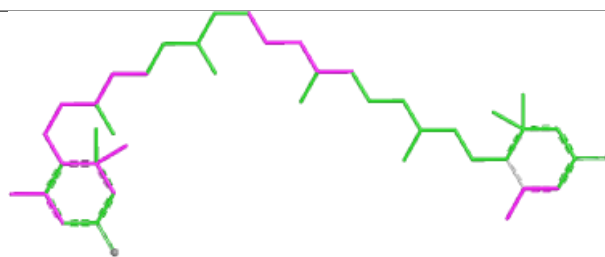


Rings

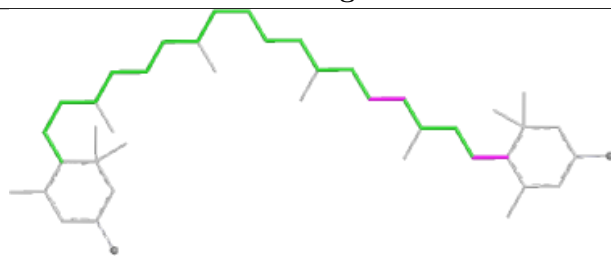
Ligand Q6L P 316



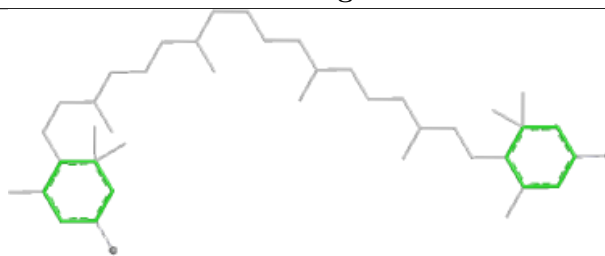
Bond lengths



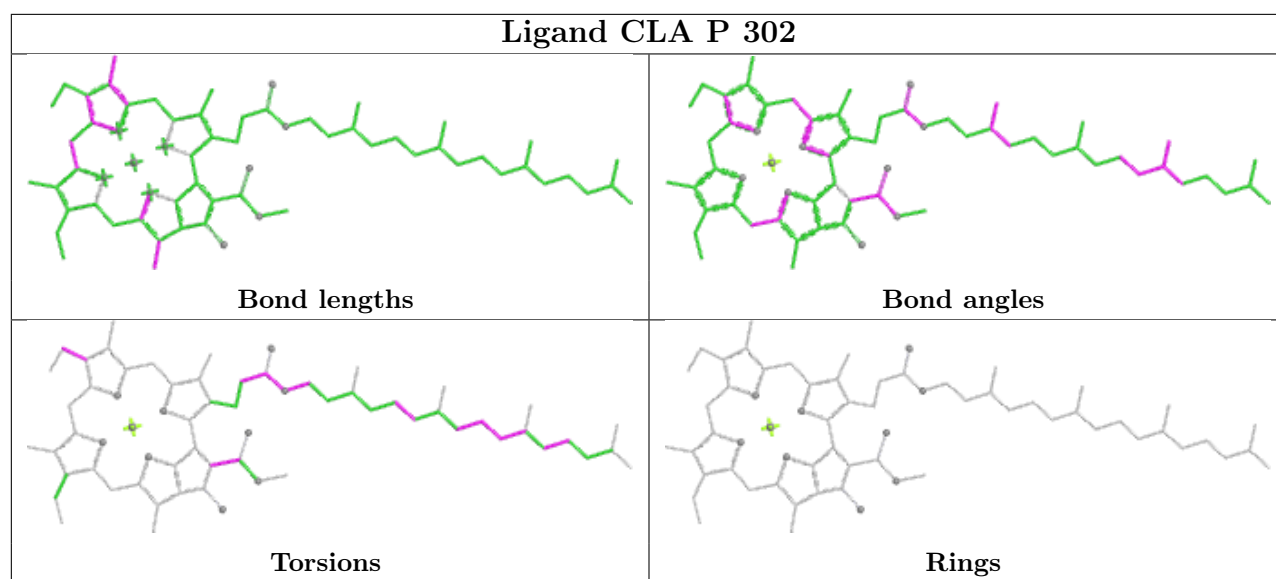
Bond angles



Torsions



Rings



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.

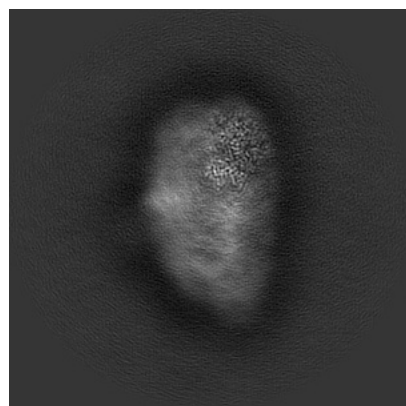
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34735. These allow visual inspection of the internal detail of the map and identification of artifacts.

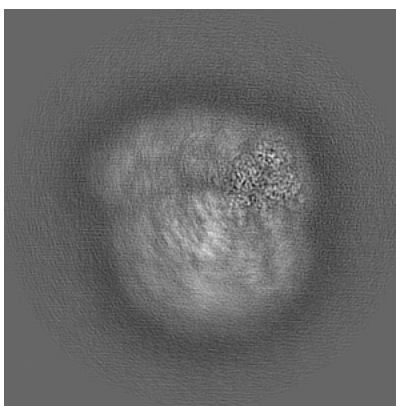
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

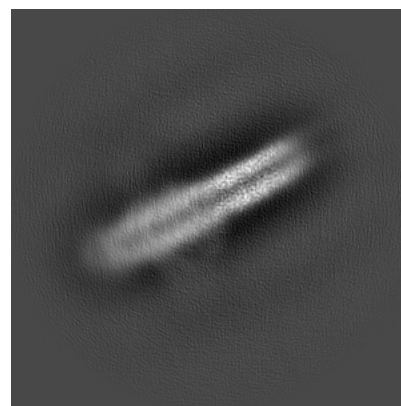
6.1.1 Primary map



X

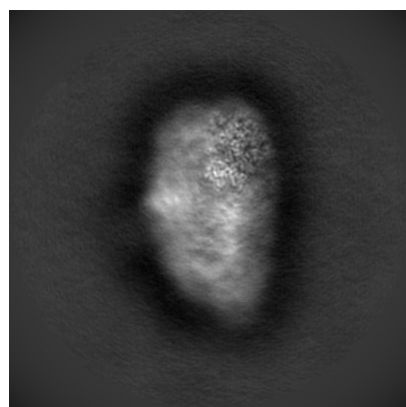


Y

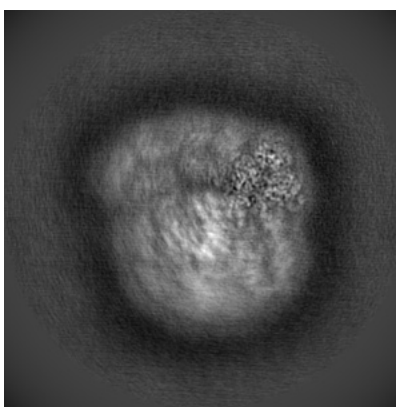


Z

6.1.2 Raw map



X



Y

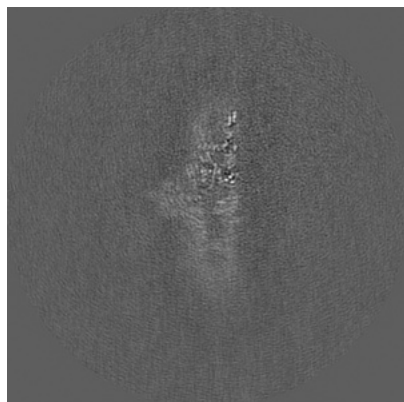


Z

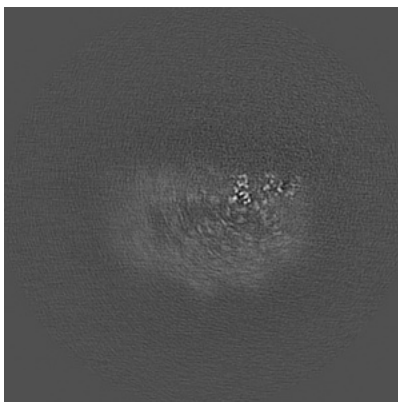
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

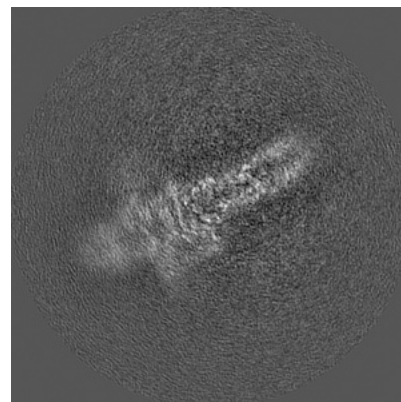
6.2.1 Primary map



X Index: 192

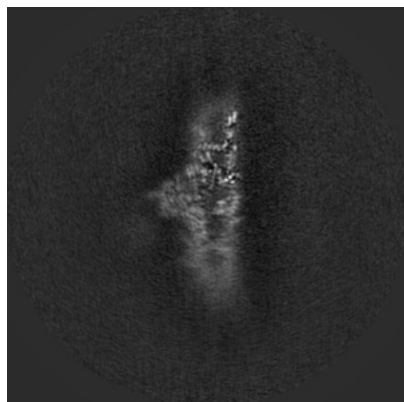


Y Index: 192

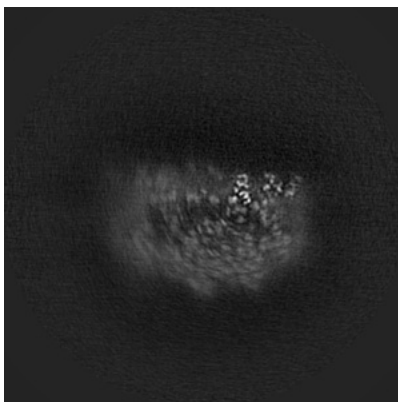


Z Index: 192

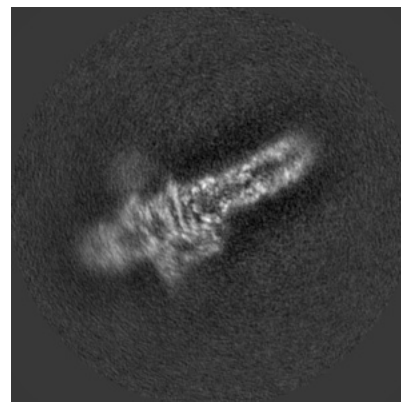
6.2.2 Raw map



X Index: 192



Y Index: 192

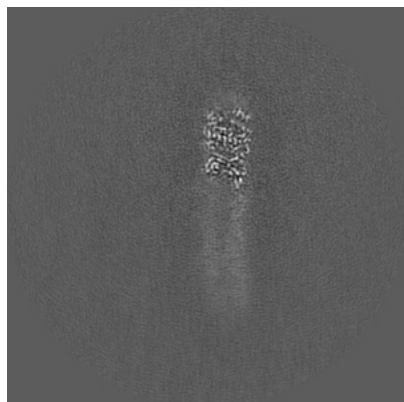


Z Index: 192

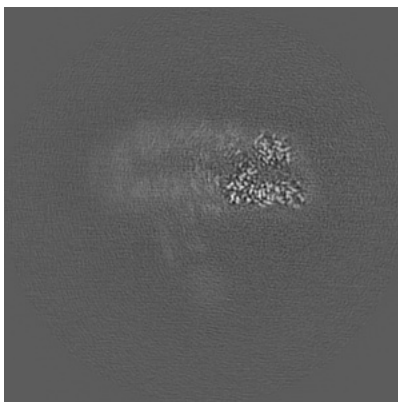
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

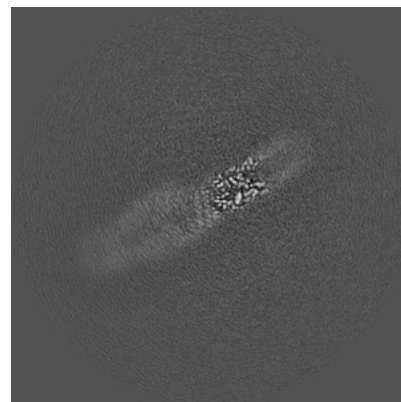
6.3.1 Primary map



X Index: 212

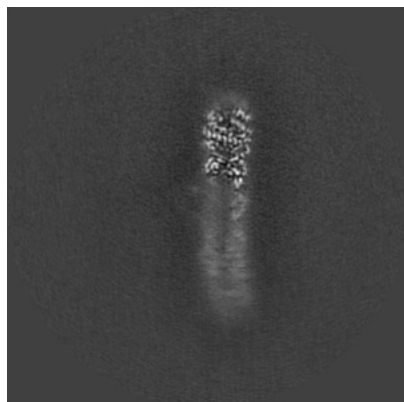


Y Index: 219

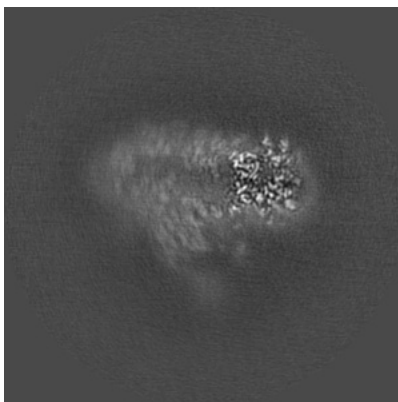


Z Index: 228

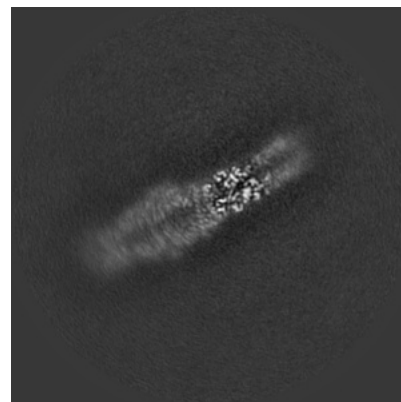
6.3.2 Raw map



X Index: 212



Y Index: 213

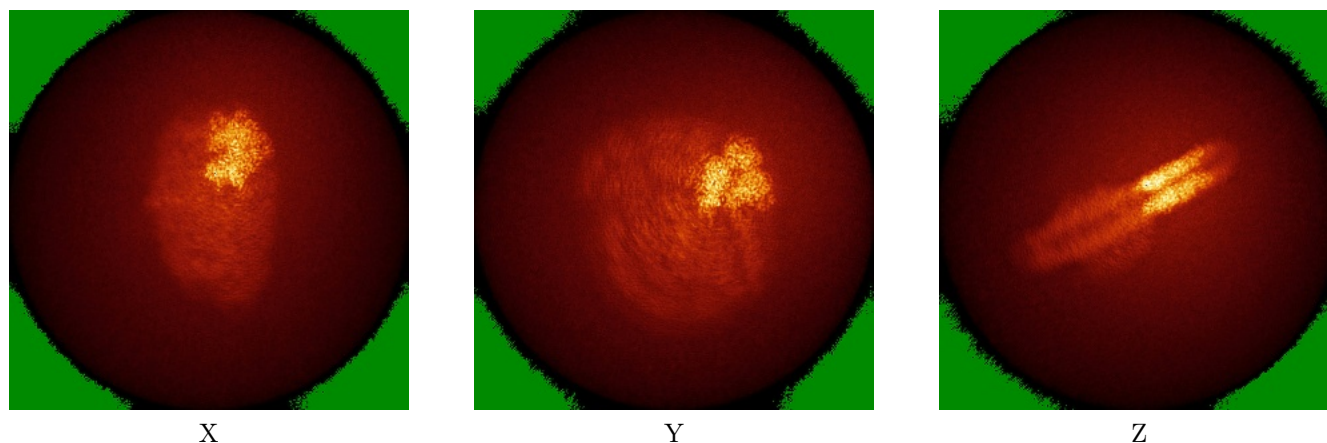


Z Index: 225

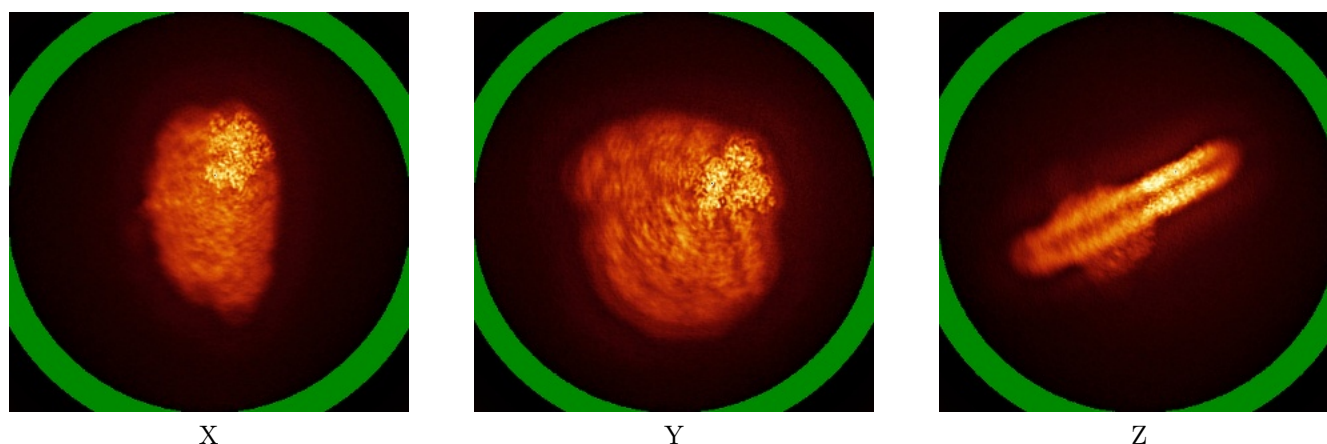
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

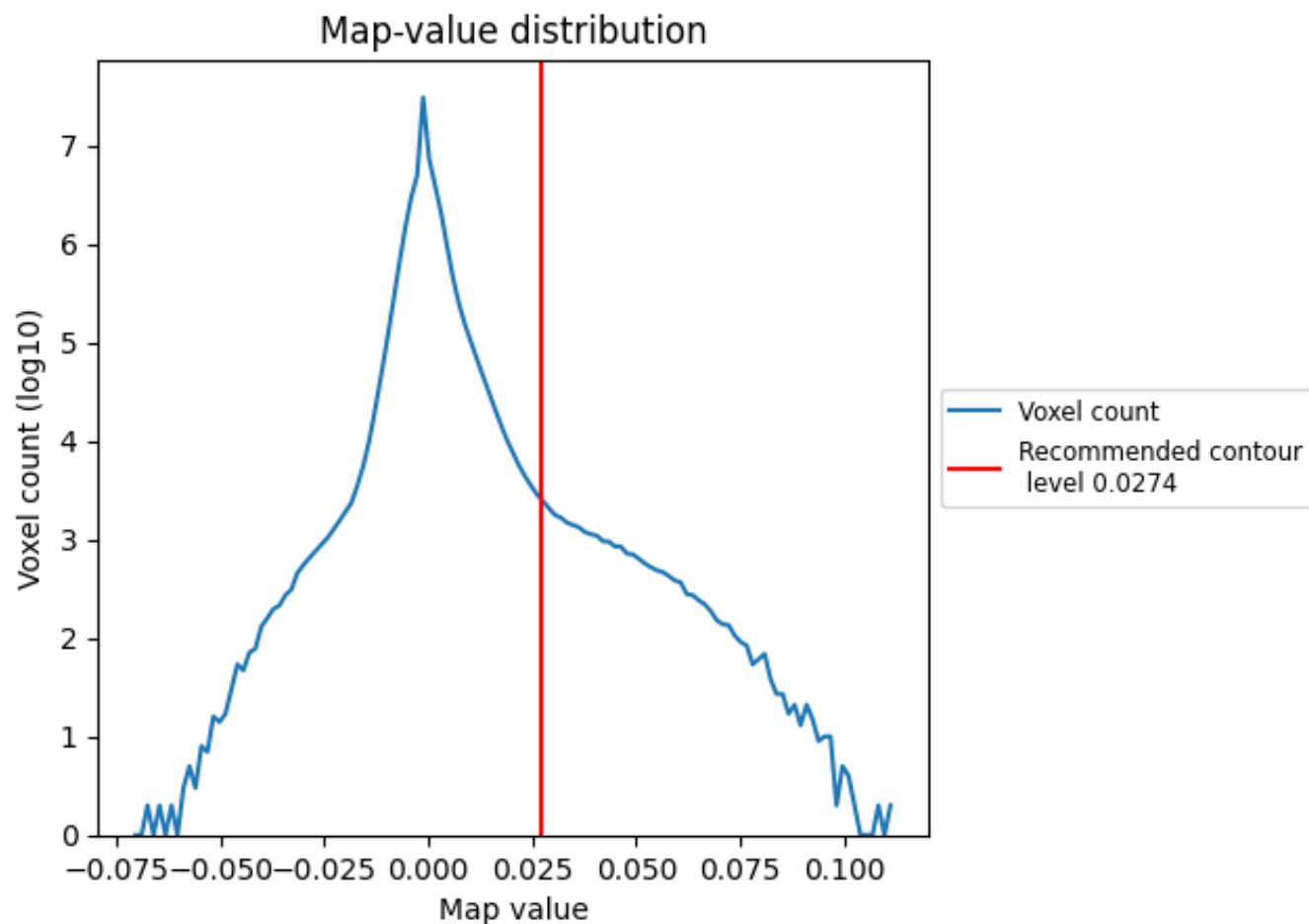
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

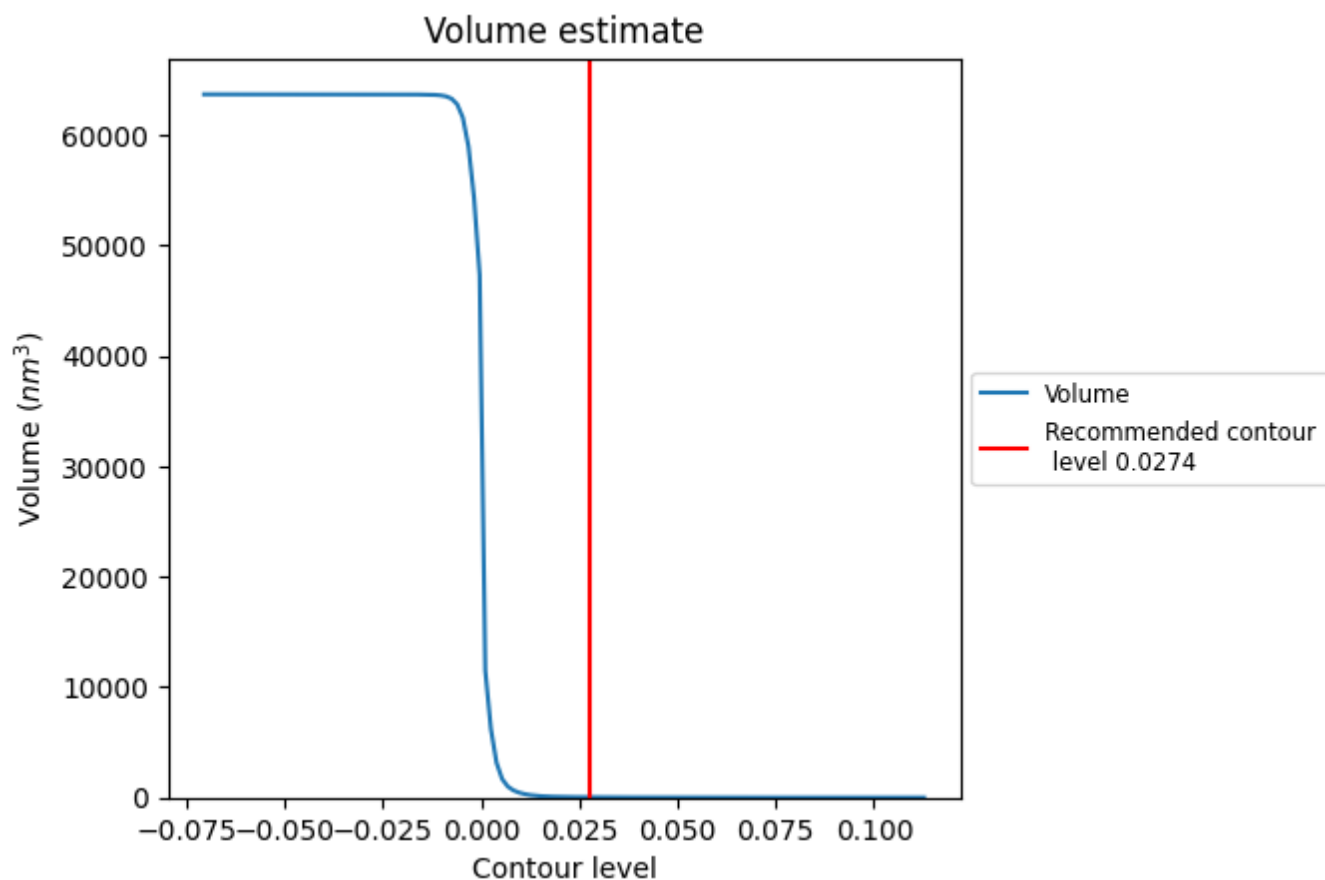
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

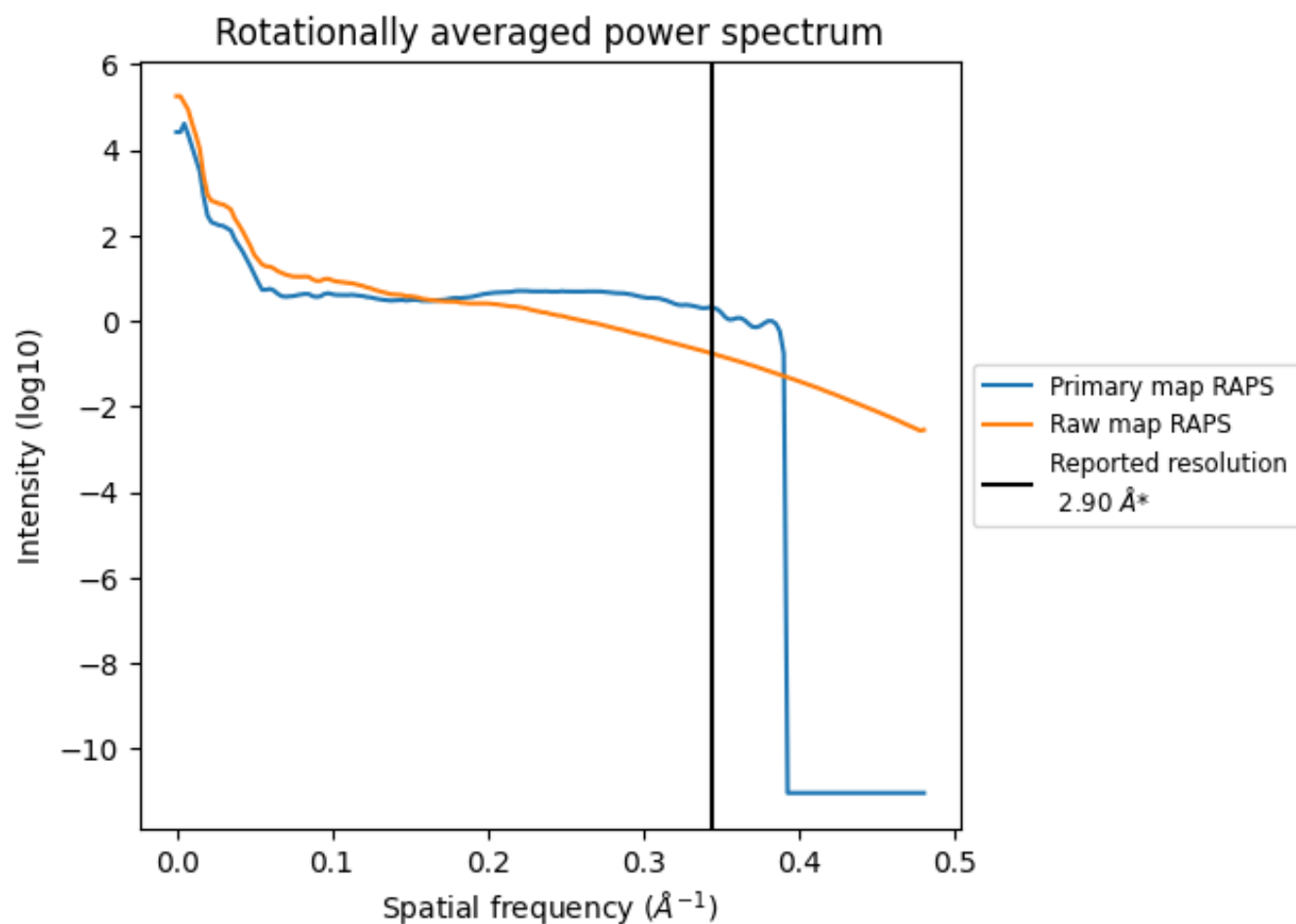
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 31 nm³; this corresponds to an approximate mass of 28 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

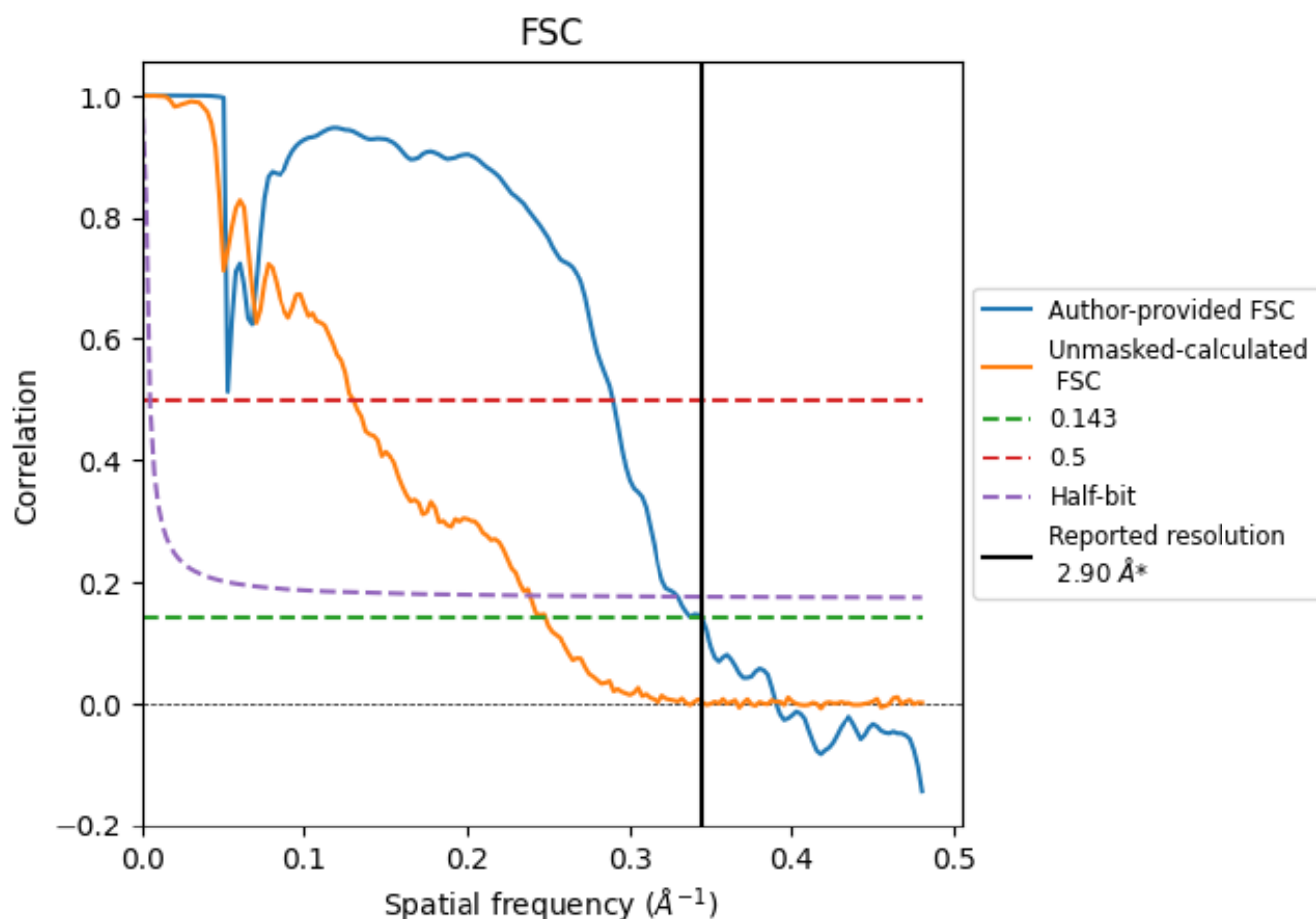


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

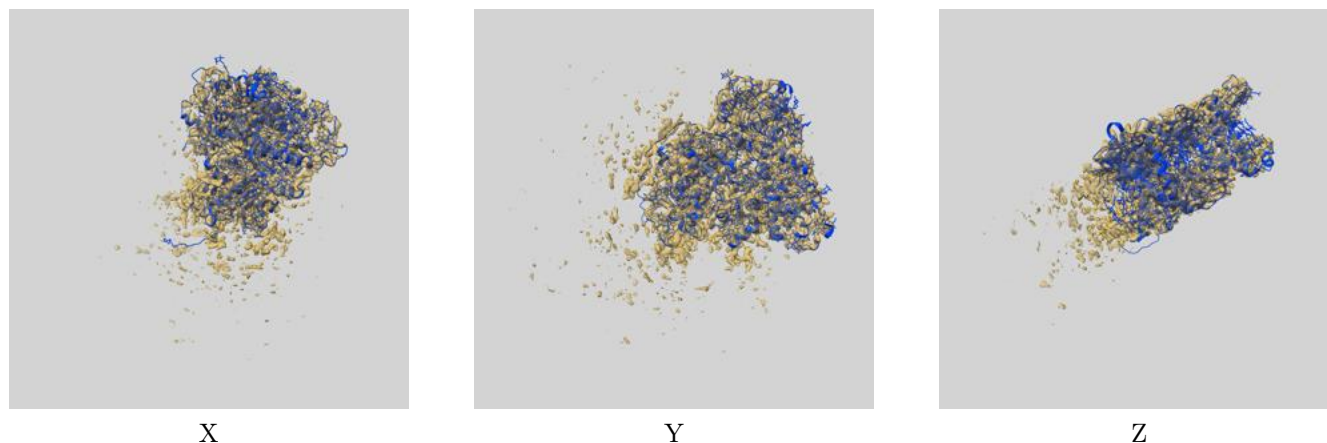
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.96	3.45	3.03
Unmasked-calculated*	4.02	7.69	4.18

*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 4.02 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

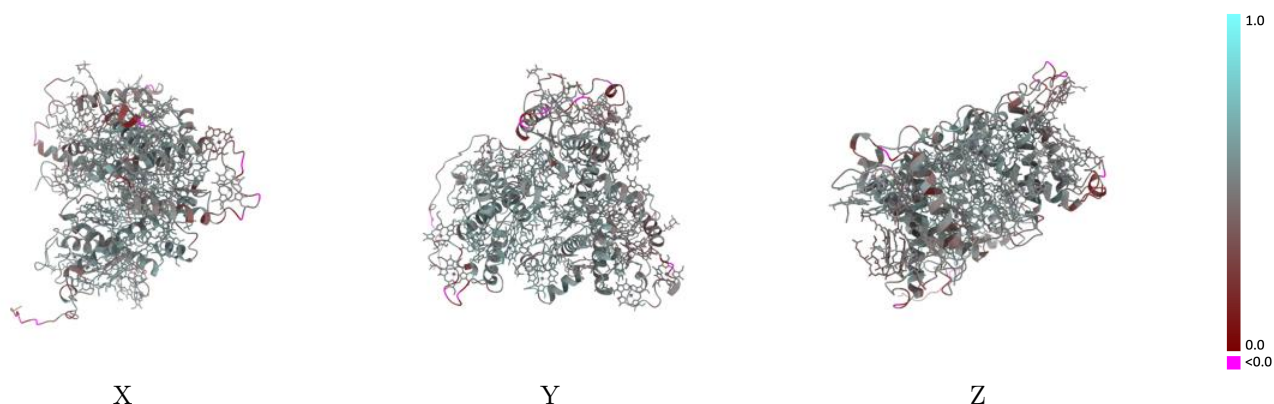
This section contains information regarding the fit between EMDB map EMD-34735 and PDB model 8HG5. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



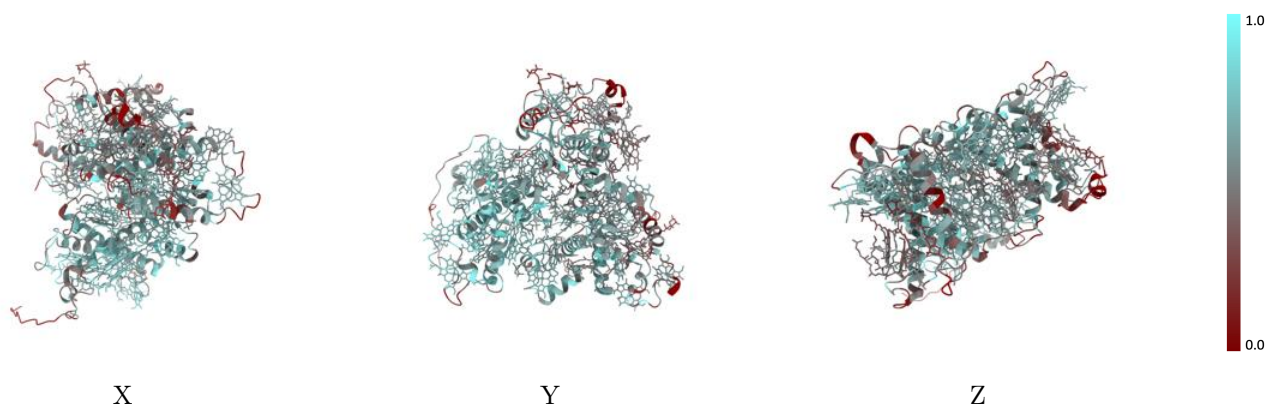
The images above show the 3D surface view of the map at the recommended contour level 0.0274 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



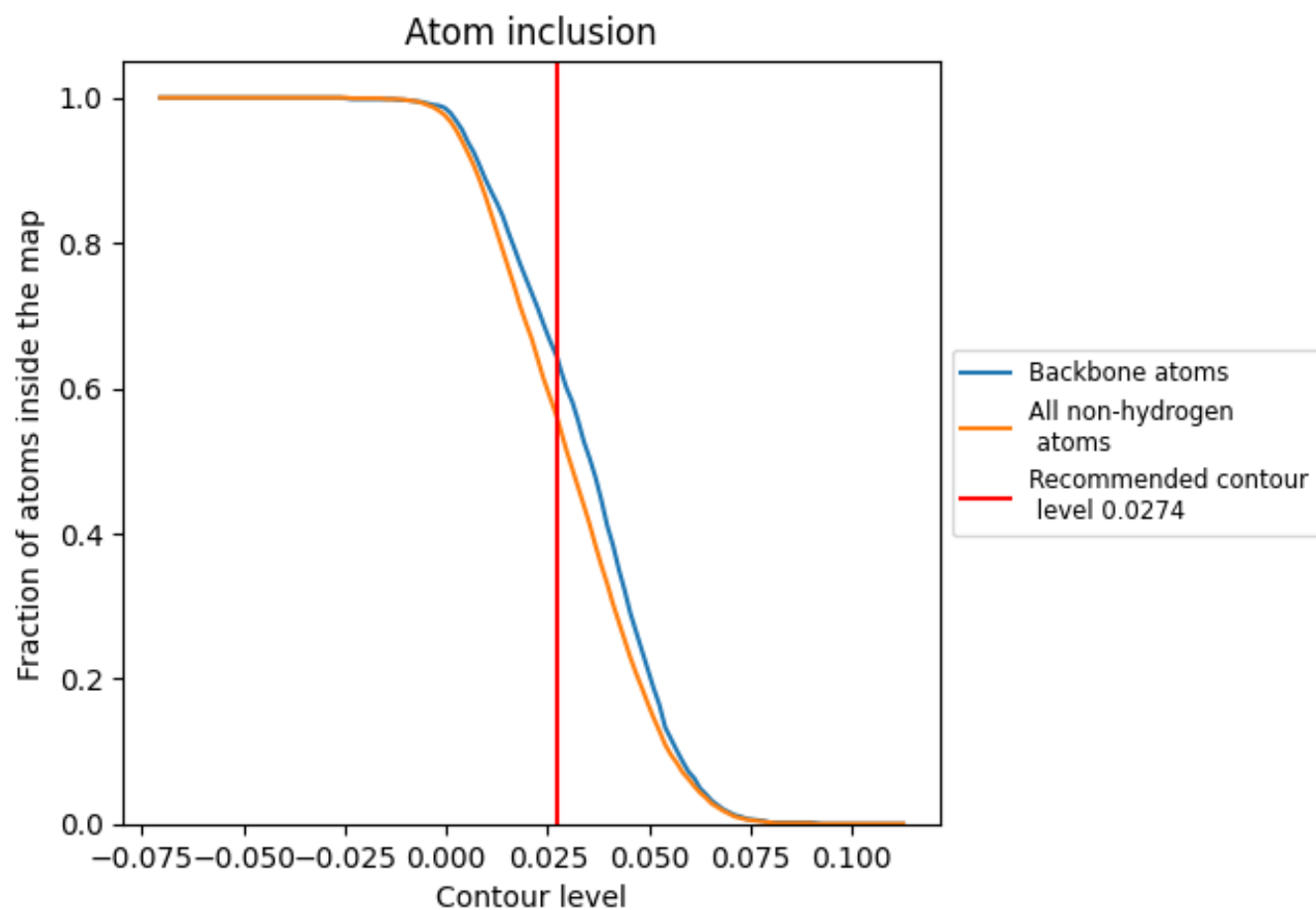
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0274).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0274) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5590	0.4860
P	0.5090	0.4720
Q	0.6270	0.5010
R	0.5400	0.4850

