



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:46 AM UTC

PDB ID : 6YP7 / pdb_00006yp7
EMDB ID : EMD-10865
Title : PSII-LHCII C2S2 supercomplex from *Pisum sativum* grown in high light conditions
Authors : Grinzato, A.; Albanese, P.; Zanotti, G.; Pagliano, C.
Deposited on : 2020-04-15
Resolution : 3.80 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

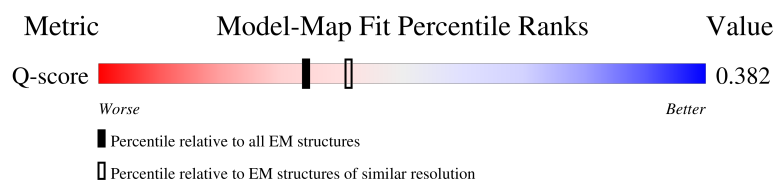
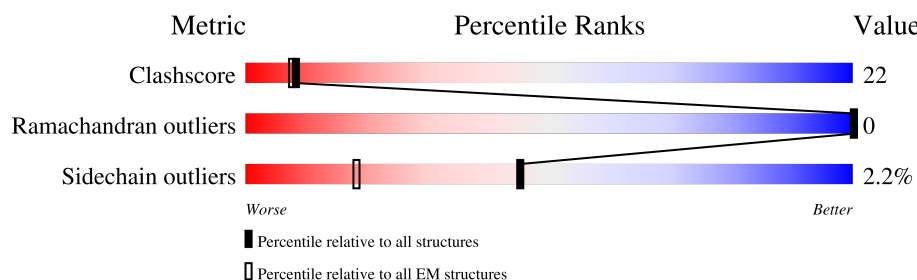
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	G	219	33% 66% 32%
1	N	219	25% 65% 33%
1	Y	219	13% 64% 35%
1	g	219	34% 65% 33%

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Mol	Chain	Length	Quality of chain
1	n	219	
1	y	219	
2	A	334	
2	a	334	
3	B	503	
3	b	503	
4	C	450	
4	c	450	
5	D	341	
5	d	341	
6	E	75	
6	e	75	
7	F	30	
7	f	30	
8	H	60	
8	h	60	
9	I	34	
9	i	34	
10	J	35	
10	j	35	
11	K	37	
11	k	37	
12	L	37	
12	l	37	
13	M	33	

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Mol	Chain	Length	Quality of chain
13	m	33	
14	O	248	
14	o	248	
15	T	32	
15	t	32	
16	W	54	
16	w	54	
17	X	39	
17	x	39	
18	Z	62	
18	z	62	
19	R	222	
19	r	222	
20	S	218	
20	s	218	

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
21	CHL	G	601	X	-	X	-
21	CHL	G	605	X	-	-	-
21	CHL	G	606	X	-	X	-
21	CHL	G	607	X	-	X	-
21	CHL	G	608	X	-	X	-
21	CHL	G	609	X	-	X	-
21	CHL	N	601	X	-	X	-
21	CHL	N	605	X	-	X	-
21	CHL	N	606	X	-	X	-
21	CHL	N	607	X	-	X	-
21	CHL	N	608	X	-	X	-
21	CHL	R	305	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	R	306	X	-	X	-
21	CHL	R	307	X	-	-	-
21	CHL	S	301	X	-	X	-
21	CHL	S	302	X	-	-	-
21	CHL	S	306	X	-	-	-
21	CHL	S	307	X	-	X	-
21	CHL	Y	601	X	-	X	-
21	CHL	Y	605	X	-	X	-
21	CHL	Y	606	X	-	X	-
21	CHL	Y	607	X	-	X	-
21	CHL	Y	608	X	-	X	-
21	CHL	g	601	X	-	X	-
21	CHL	g	605	X	-	-	-
21	CHL	g	606	X	-	X	-
21	CHL	g	607	X	-	X	-
21	CHL	g	608	X	-	X	-
21	CHL	g	609	X	-	X	-
21	CHL	n	601	X	-	X	-
21	CHL	n	605	X	-	X	-
21	CHL	n	606	X	-	-	-
21	CHL	n	607	X	-	X	-
21	CHL	n	608	X	-	X	-
21	CHL	r	301	X	-	X	-
21	CHL	r	306	X	-	X	-
21	CHL	r	307	X	-	X	-
21	CHL	r	308	X	-	-	-
21	CHL	s	301	X	-	X	-
21	CHL	s	302	X	-	-	-
21	CHL	s	306	X	-	-	-
21	CHL	s	307	X	-	X	-
21	CHL	y	601	X	-	X	-
21	CHL	y	605	X	-	X	-
21	CHL	y	606	X	-	X	-
21	CHL	y	607	X	-	-	-
21	CHL	y	608	X	-	X	-
21	CHL	y	609	X	-	X	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	407	X	-	-	-
22	CLA	A	409	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	B	618	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	X	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	C	515	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	G	602	X	-	-	-
22	CLA	G	603	X	-	-	-
22	CLA	G	604	X	-	-	-
22	CLA	G	610	X	-	-	-
22	CLA	G	611	X	-	-	-
22	CLA	G	612	X	-	-	-
22	CLA	G	613	X	-	-	-
22	CLA	G	614	X	-	-	-
22	CLA	N	602	X	-	-	-
22	CLA	N	603	X	-	-	-
22	CLA	N	604	X	-	-	-
22	CLA	N	609	X	-	-	-
22	CLA	N	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	N	611	X	-	-	-
22	CLA	N	612	X	-	-	-
22	CLA	N	613	X	-	-	-
22	CLA	R	302	X	-	-	-
22	CLA	R	303	X	-	-	-
22	CLA	R	304	X	-	-	-
22	CLA	R	308	X	-	-	-
22	CLA	R	309	X	-	-	-
22	CLA	R	310	X	-	-	-
22	CLA	R	311	X	-	-	-
22	CLA	S	303	X	-	-	-
22	CLA	S	304	X	-	-	-
22	CLA	S	305	X	-	-	-
22	CLA	S	309	X	-	-	-
22	CLA	S	310	X	-	-	-
22	CLA	S	311	X	-	-	-
22	CLA	S	312	X	-	-	-
22	CLA	S	313	X	-	-	-
22	CLA	W	101	X	-	-	-
22	CLA	Y	602	X	-	-	-
22	CLA	Y	603	X	-	-	-
22	CLA	Y	604	X	-	-	-
22	CLA	Y	609	X	-	-	-
22	CLA	Y	610	X	-	-	-
22	CLA	Y	611	X	-	X	-
22	CLA	Y	612	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	X	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	g	602	X	-	-	-
22	CLA	g	603	X	-	-	-
22	CLA	g	604	X	-	-	-
22	CLA	g	610	X	-	-	-
22	CLA	g	611	X	-	-	-
22	CLA	g	612	X	-	-	-
22	CLA	g	613	X	-	-	-
22	CLA	g	614	X	-	-	-
22	CLA	n	602	X	-	-	-
22	CLA	n	603	X	-	-	-
22	CLA	n	604	X	-	-	-
22	CLA	n	609	X	-	-	-
22	CLA	n	610	X	-	-	-
22	CLA	n	611	X	-	-	-
22	CLA	n	612	X	-	-	-
22	CLA	n	613	X	-	-	-
22	CLA	r	303	X	-	-	-
22	CLA	r	304	X	-	-	-
22	CLA	r	305	X	-	-	-
22	CLA	r	309	X	-	-	-
22	CLA	r	310	X	-	-	-
22	CLA	r	311	X	-	-	-
22	CLA	r	312	X	-	-	-
22	CLA	s	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	s	304	X	-	-	-
22	CLA	s	305	X	-	-	-
22	CLA	s	309	X	-	-	-
22	CLA	s	310	X	-	-	-
22	CLA	s	311	X	-	-	-
22	CLA	s	312	X	-	-	-
22	CLA	s	313	X	-	-	-
22	CLA	w	101	X	-	-	-
22	CLA	x	101	X	-	-	-
22	CLA	y	602	X	-	-	-
22	CLA	y	603	X	-	-	-
22	CLA	y	604	X	-	-	-
22	CLA	y	610	X	-	-	-
22	CLA	y	611	X	-	-	-
22	CLA	y	612	X	-	X	-
22	CLA	y	613	X	-	-	-
24	XAT	G	617	X	-	-	-
24	XAT	N	616	X	-	-	-
24	XAT	R	313	X	-	-	-
24	XAT	Y	615	X	-	-	-
24	XAT	g	617	X	-	-	-
24	XAT	n	615	X	-	-	-
24	XAT	r	314	X	-	-	-
24	XAT	y	615	X	-	-	-
25	NEX	N	617	X	-	-	-
25	NEX	Y	616	X	-	-	-
25	NEX	g	618	X	-	-	-
25	NEX	n	616	X	-	-	-
25	NEX	r	315	X	-	-	-
25	NEX	y	616	X	-	-	-
25	NEX	y	618	X	-	-	-
33	SQD	D	402	X	-	-	-
33	SQD	d	402	X	-	-	-
34	BCT	D	403	-	X	X	-
34	BCT	a	412	-	X	X	-
36	LMG	B	623	-	-	X	-
36	LMG	b	620	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 71784 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 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	n	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	G	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	N	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	Y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		

- Molecule 2 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		
2	A	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		

- Molecule 3 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		
3	B	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		
4	C	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		
5	D	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	75	Total	C	N	O	0	0
			612	400	100	112		
6	E	75	Total	C	N	O	0	0
			612	400	100	112		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
7	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	26	PHE	SER	conflict	UNP P62096
F	26	PHE	SER	conflict	UNP P62096

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	60	Total	C	N	O	S	0	0
			452	296	72	81	3		
8	H	60	Total	C	N	O	S	0	0
			452	296	72	81	3		

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	34	Total	C	N	O	S	0	0
			278	191	43	43	1		
9	I	34	Total	C	N	O	S	0	0
			278	191	43	43	1		

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	35	Total	C	N	O	0	0
			256	174	39	43		
10	J	35	Total	C	N	O	0	0
			256	174	39	43		

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	37	Total	C	N	O	S	0	0
			306	215	44	46	1		
11	K	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	l	37	Total	C	N	O	0	0
			311	205	49	57		
12	L	37	Total	C	N	O	0	0
			311	205	49	57		

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	33	Total	C	N	O	S	0	0
			256	176	36	43	1		
13	M	33	Total	C	N	O	S	0	0
			256	176	36	43	1		

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		
14	O	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	t	32	Total	C	N	O	S	0	0
			261	182	37	41	1		
15	T	32	Total	C	N	O	S	0	0
			261	182	37	41	1		

- Molecule 16 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	w	54	Total	C	N	O	S	0	0
			419	275	61	82	1		
16	W	54	Total	C	N	O	S	0	0
			419	275	61	82	1		

- Molecule 17 is a protein called Ultraviolet-B-repressible protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	x	39	Total	C	N	O	0	0
			276	180	46	50		
17	X	39	Total	C	N	O	0	0
			276	180	46	50		

- Molecule 18 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		
18	Z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		

- Molecule 19 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	222	Total	C	N	O	S	0	0
			1732	1133	281	314	4		

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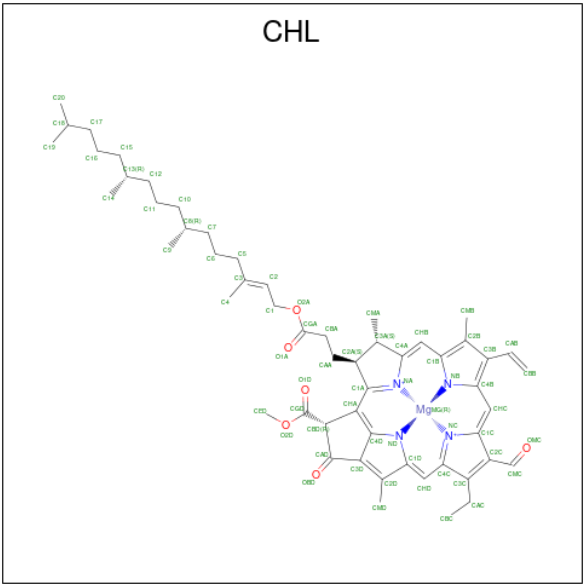
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Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	222	Total	C	N	O	S	0	0
			1732	1133	281	314	4		

- Molecule 20 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	s	218	Total	C	N	O	S	0	0
			1688	1105	271	308	4		
20	S	218	Total	C	N	O	S	0	0
			1688	1105	271	308	4		

- Molecule 21 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



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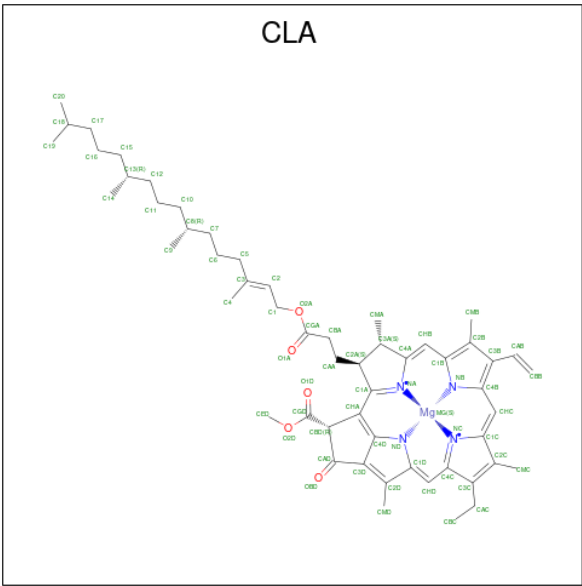
Mol	Chain	Residues	Atoms					AltConf
21	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	y	1	Total 48	C 37	Mg 1	N 4	O 6	0
21	y	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	G	1	Total 61	C 50	Mg 1	N 4	O 6	0
21	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	N	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	r	1	Total 48	C 37	Mg 1	N 4	O 6	0
21	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	r	1	Total 56	C 45	Mg 1	N 4	O 6	0
21	r	1	Total 61	C 50	Mg 1	N 4	O 6	0
21	s	1	Total 48	C 37	Mg 1	N 4	O 6	0
21	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	S	1	Total 48	C 37	Mg 1	N 4	O 6	0
21	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	R	1	Total 56	C 45	Mg 1	N 4	O 6	0
21	R	1	Total 61	C 50	Mg 1	N 4	O 6	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
22	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	n	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	y	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	G	1	Total 64	C 54	Mg 1	N 4	O 5	0
22	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	G	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	N	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	N	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Y	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	w	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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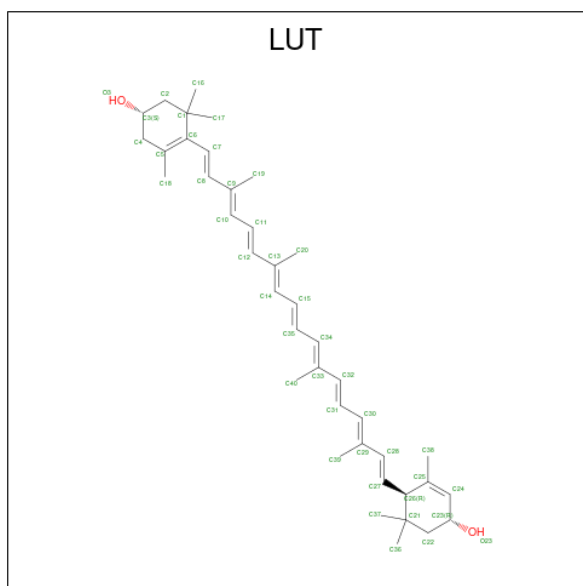
Mol	Chain	Residues	Atoms					AltConf
22	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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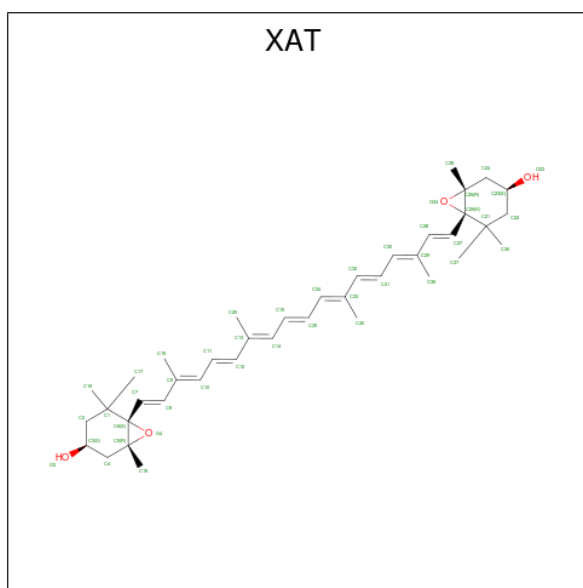
Mol	Chain	Residues	Atoms					AltConf
22	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



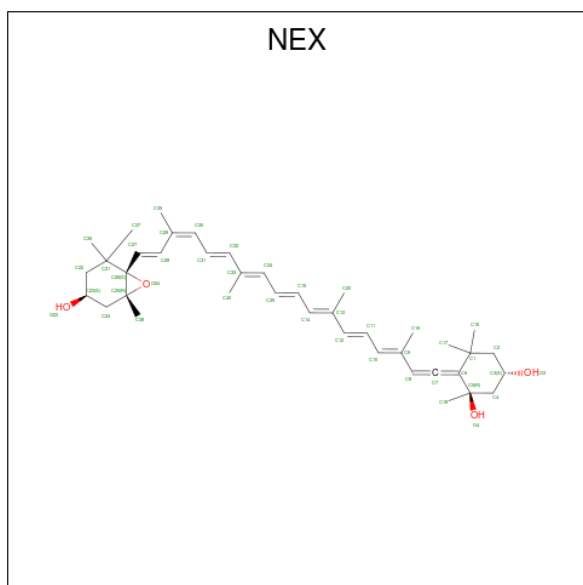
Mol	Chain	Residues	Atoms			AltConf
23	g	1	Total	C	O	0
			42	40	2	
23	g	1	Total	C	O	0
			42	40	2	
23	n	1	Total	C	O	0
			42	40	2	
23	y	1	Total	C	O	0
			42	40	2	
23	G	1	Total	C	O	0
			42	40	2	
23	G	1	Total	C	O	0
			42	40	2	
23	N	1	Total	C	O	0
			42	40	2	
23	N	1	Total	C	O	0
			42	40	2	
23	Y	1	Total	C	O	0
			42	40	2	
23	Y	1	Total	C	O	0
			42	40	2	
23	r	1	Total	C	O	0
			42	40	2	
23	R	1	Total	C	O	0
			42	40	2	

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
24	g	1	Total	C	O	0
			44	40	4	
24	n	1	Total	C	O	0
			44	40	4	
24	y	1	Total	C	O	0
			44	40	4	
24	G	1	Total	C	O	0
			44	40	4	
24	N	1	Total	C	O	0
			44	40	4	
24	Y	1	Total	C	O	0
			44	40	4	
24	r	1	Total	C	O	0
			44	40	4	
24	R	1	Total	C	O	0
			44	40	4	

- Molecule 25 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



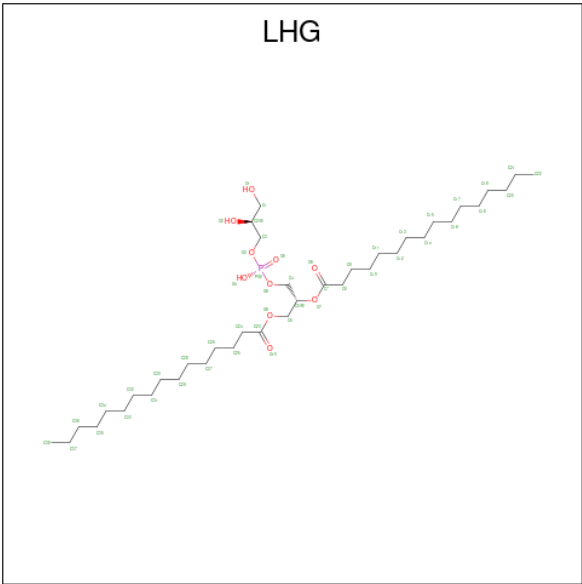
Mol	Chain	Residues	Atoms			AltConf
25	g	1	Total	C	O	0
			44	40	4	
25	n	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
25	y	1	Total	C	O	0
			44	40	4	
25	y	1	Total	C	O	0
			44	40	4	
25	N	1	Total	C	O	0
			44	40	4	
25	Y	1	Total	C	O	0
			44	40	4	
25	r	1	Total	C	O	0
			44	40	4	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



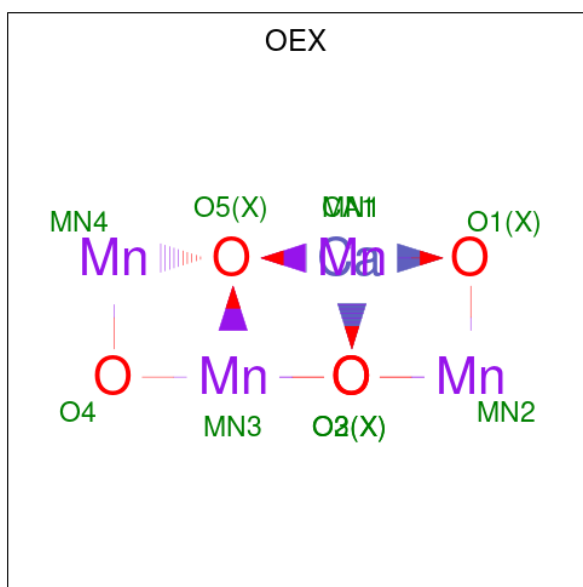
Mol	Chain	Residues	Atoms				AltConf
26	g	1	Total	C	O	P	0
			49	38	10	1	
26	n	1	Total	C	O	P	0
			49	38	10	1	
26	y	1	Total	C	O	P	0
			49	38	10	1	
26	G	1	Total	C	O	P	0
			49	38	10	1	
26	N	1	Total	C	O	P	0
			49	38	10	1	
26	Y	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	b	1	Total	C	O	P	0
			49	38	10	1	
26	c	1	Total	C	O	P	0
			49	38	10	1	
26	c	1	Total	C	O	P	0
			49	38	10	1	
26	c	1	Total	C	O	P	0
			49	38	10	1	
26	d	1	Total	C	O	P	0
			46	35	10	1	
26	d	1	Total	C	O	P	0
			49	38	10	1	
26	d	1	Total	C	O	P	0
			43	32	10	1	
26	l	1	Total	C	O	P	0
			49	38	10	1	
26	B	1	Total	C	O	P	0
			49	38	10	1	
26	C	1	Total	C	O	P	0
			49	38	10	1	
26	C	1	Total	C	O	P	0
			49	38	10	1	
26	C	1	Total	C	O	P	0
			49	38	10	1	
26	D	1	Total	C	O	P	0
			46	35	10	1	
26	D	1	Total	C	O	P	0
			49	38	10	1	
26	D	1	Total	C	O	P	0
			43	32	10	1	
26	L	1	Total	C	O	P	0
			49	38	10	1	
26	r	1	Total	C	O	P	0
			47	36	10	1	
26	s	1	Total	C	O	P	0
			49	38	10	1	
26	S	1	Total	C	O	P	0
			49	38	10	1	
26	R	1	Total	C	O	P	0
			47	36	10	1	

- Molecule 27 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
27	a	1	Total	Ca	Mn	O	0
			10	1	4	5	
27	A	1	Total	Ca	Mn	O	0
			10	1	4	5	

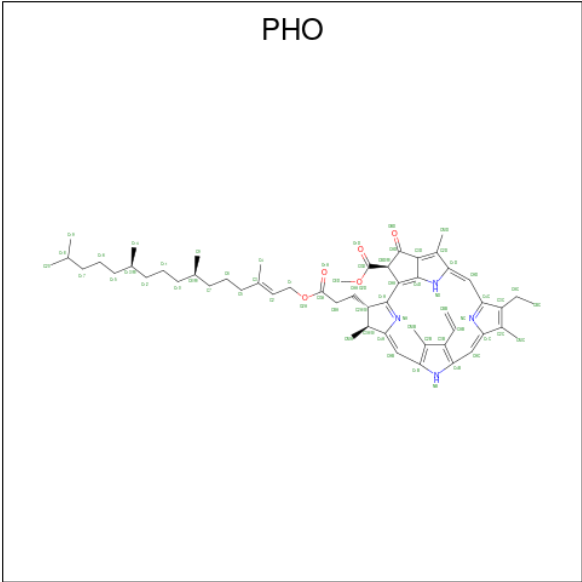
- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
28	a	1	Total	Fe	0
			1	1	
28	A	1	Total	Fe	0
			1	1	

- Molecule 29 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

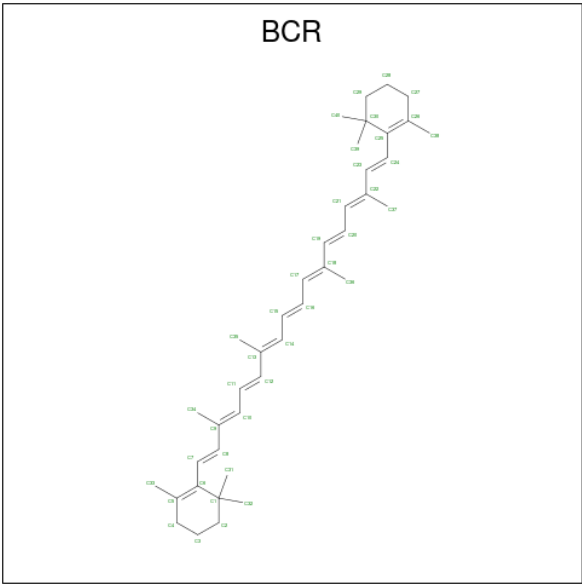
Mol	Chain	Residues	Atoms		AltConf
29	a	1	Total	Cl	0
			1	1	
29	c	1	Total	Cl	0
			1	1	
29	A	1	Total	Cl	0
			1	1	
29	C	1	Total	Cl	0
			1	1	

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



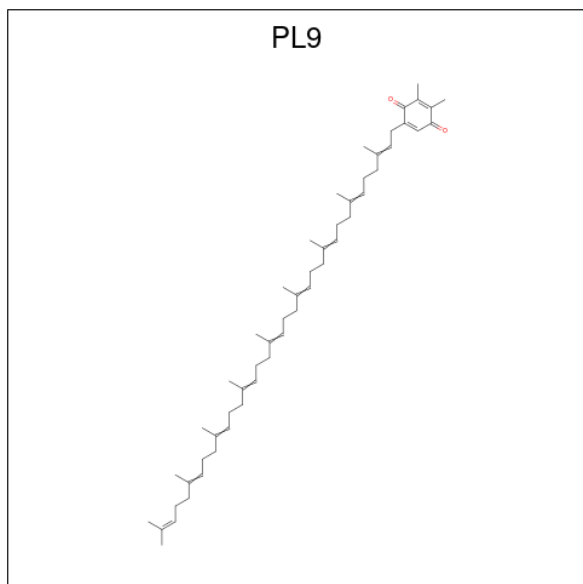
Mol	Chain	Residues	Atoms				AltConf
30	a	1	Total	C	N	O	0
			64	55	4	5	
30	d	1	Total	C	N	O	0
			64	55	4	5	
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



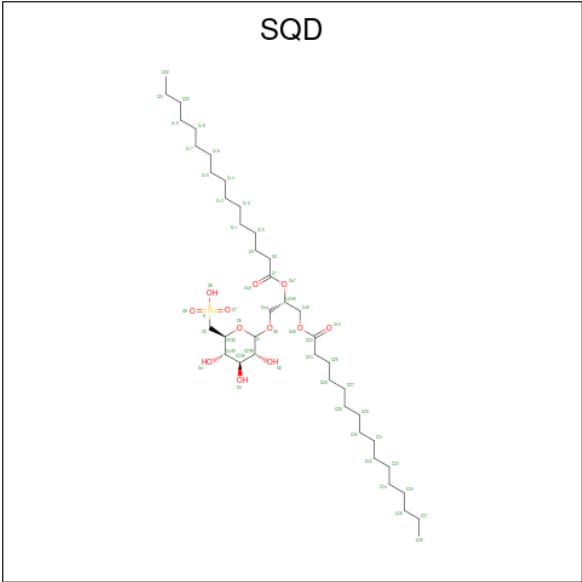
Mol	Chain	Residues	Atoms	AltConf
31	a	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	h	1	Total C 40 40	0
31	k	1	Total C 40 40	0
31	k	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	H	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	T	1	Total C 40 40	0

- Molecule 32 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



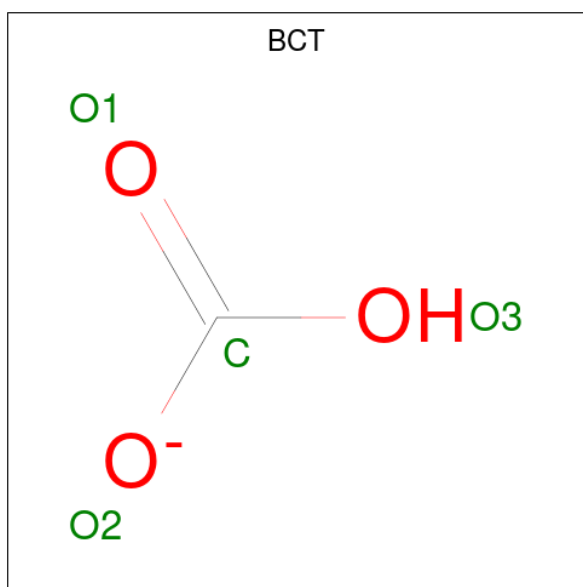
Mol	Chain	Residues	Atoms			AltConf
32	a	1	Total	C	O	0
			13	11	2	
32	d	1	Total	C	O	0
			55	53	2	
32	A	1	Total	C	O	0
			13	11	2	
32	D	1	Total	C	O	0
			55	53	2	

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



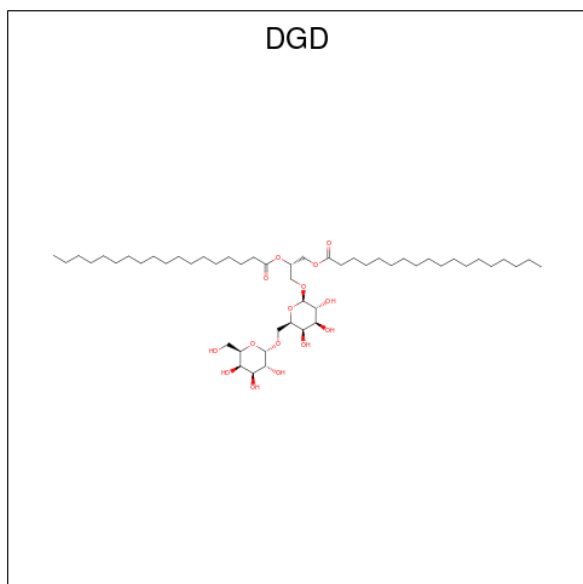
Mol	Chain	Residues	Atoms				AltConf
33	a	1	Total	C	O	S	0
			54	41	12	1	
33	d	1	Total	C	O	S	0
			50	37	12	1	
33	l	1	Total	C	O	S	0
			42	29	12	1	
33	l	1	Total	C	O	S	0
			54	41	12	1	
33	A	1	Total	C	O	S	0
			54	41	12	1	
33	D	1	Total	C	O	S	0
			50	37	12	1	
33	L	1	Total	C	O	S	0
			54	41	12	1	
33	L	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
34	a	1	Total	C	O	0
			4	1	3	
34	D	1	Total	C	O	0
			4	1	3	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



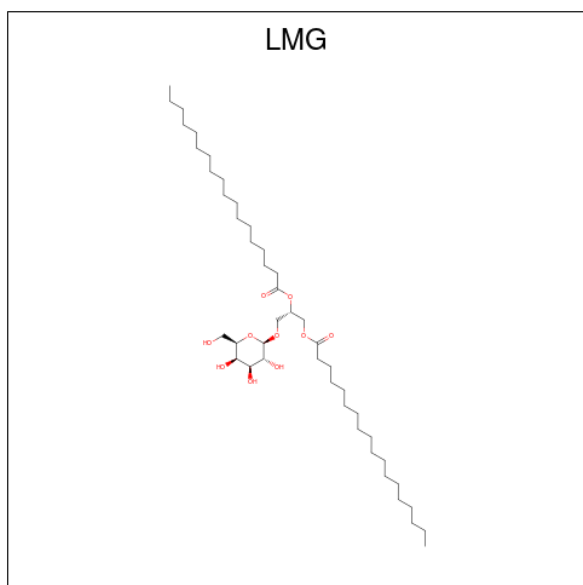
Mol	Chain	Residues	Atoms			AltConf
35	a	1	Total	C	O	0
			59	44	15	

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Mol	Chain	Residues	Atoms			AltConf
35	c	1	Total	C	O	0
			55	40	15	
35	c	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			60	45	15	
35	h	1	Total	C	O	0
			62	47	15	
35	A	1	Total	C	O	0
			59	44	15	
35	C	1	Total	C	O	0
			55	40	15	
35	C	1	Total	C	O	0
			62	47	15	
35	H	1	Total	C	O	0
			62	47	15	
35	J	1	Total	C	O	0
			60	45	15	

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



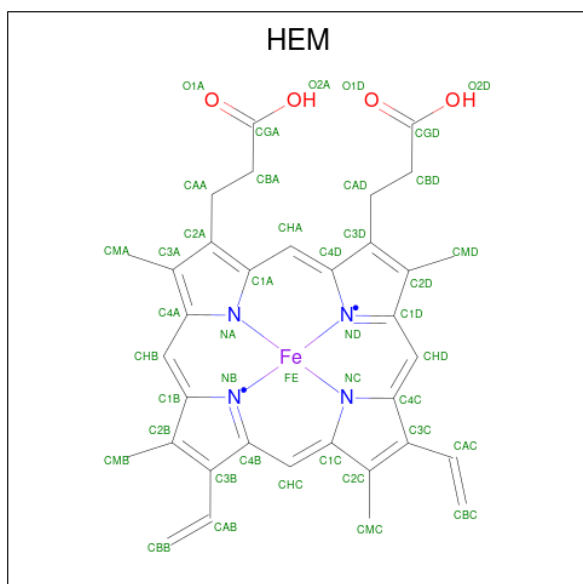
Mol	Chain	Residues	Atoms			AltConf
36	b	1	Total	C	O	0
			55	45	10	
36	c	1	Total	C	O	0
			51	41	10	

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Mol	Chain	Residues	Atoms			AltConf
36	d	1	Total 46	C 36	O 10	0
36	k	1	Total 51	C 41	O 10	0
36	w	1	Total 48	C 38	O 10	0
36	B	1	Total 40	C 30	O 10	0
36	B	1	Total 55	C 45	O 10	0
36	C	1	Total 48	C 38	O 10	0
36	C	1	Total 51	C 41	O 10	0
36	D	1	Total 46	C 36	O 10	0
36	I	1	Total 40	C 30	O 10	0
36	K	1	Total 51	C 41	O 10	0
36	M	1	Total 51	C 41	O 10	0
36	T	1	Total 51	C 41	O 10	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

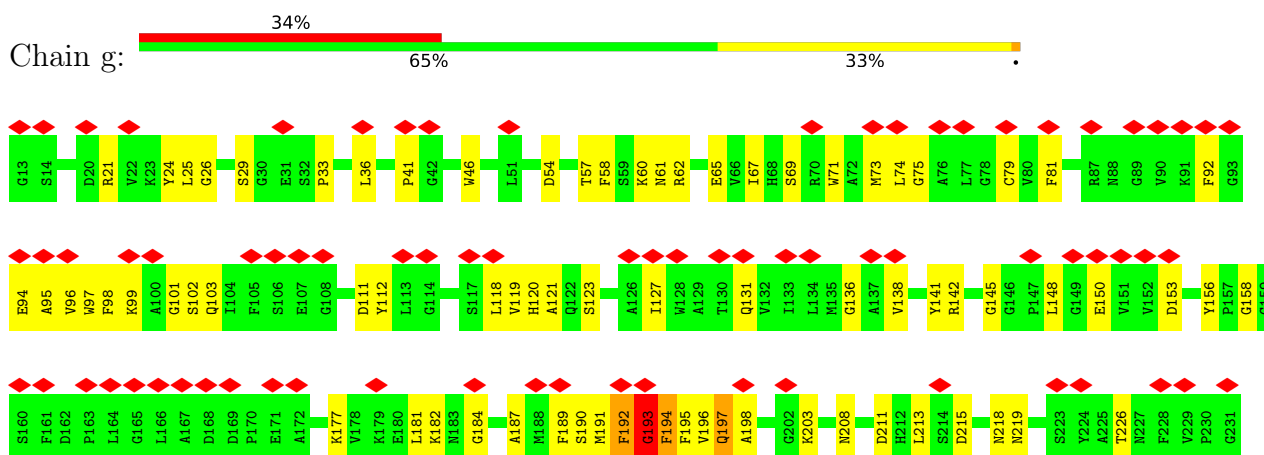


Mol	Chain	Residues	Atoms					AltConf
37	f	1	Total 43	C 34	Fe 1	N 4	O 4	0
37	F	1	Total 43	C 34	Fe 1	N 4	O 4	0

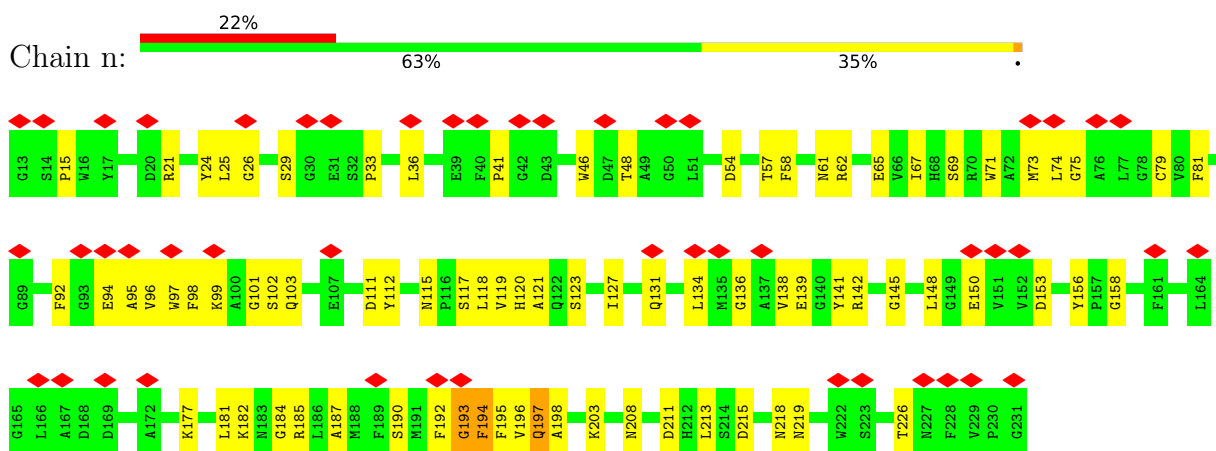
3 Residue-property plots

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.

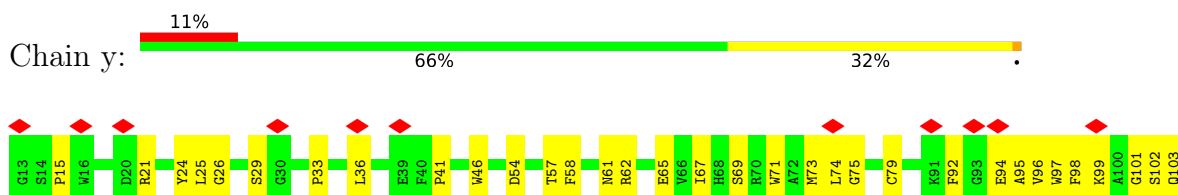
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

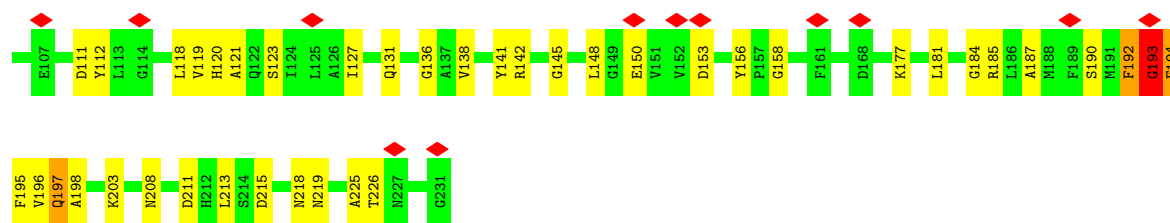


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

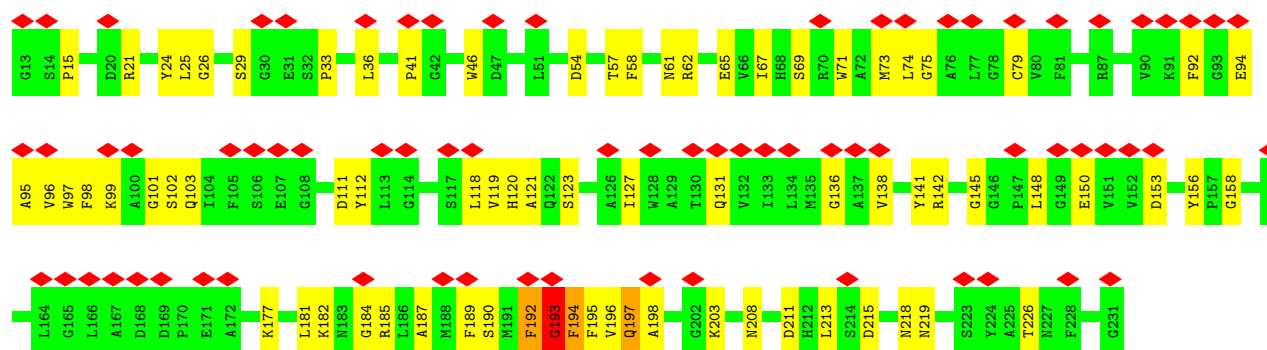


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

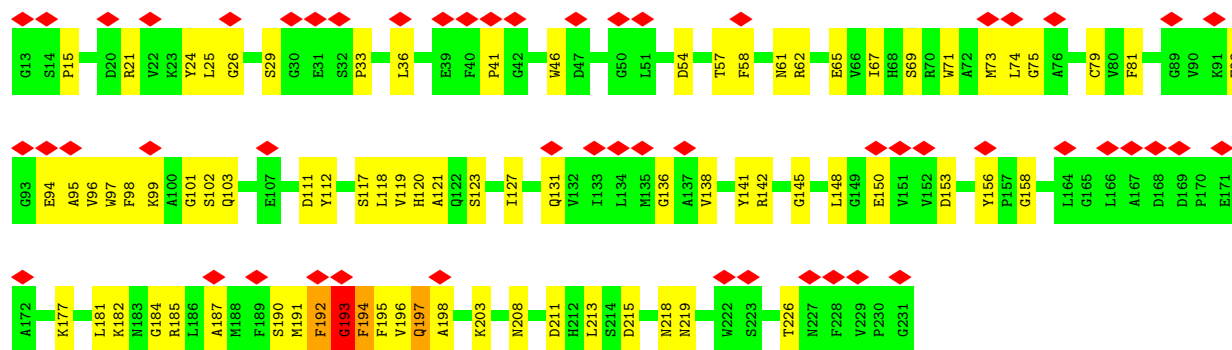




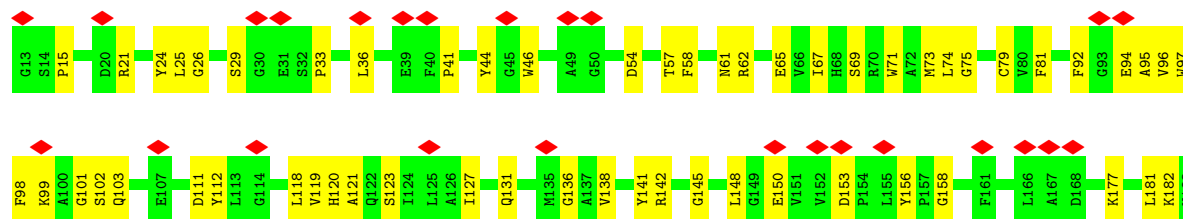
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

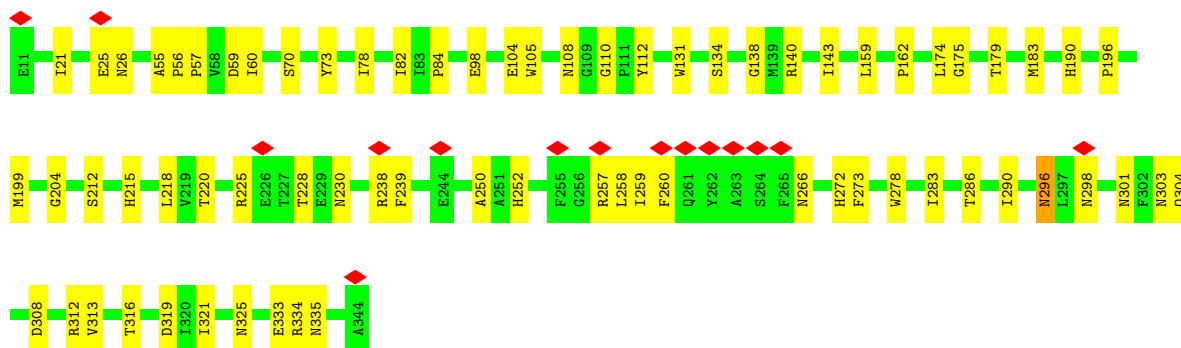
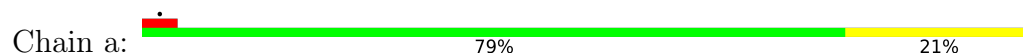


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

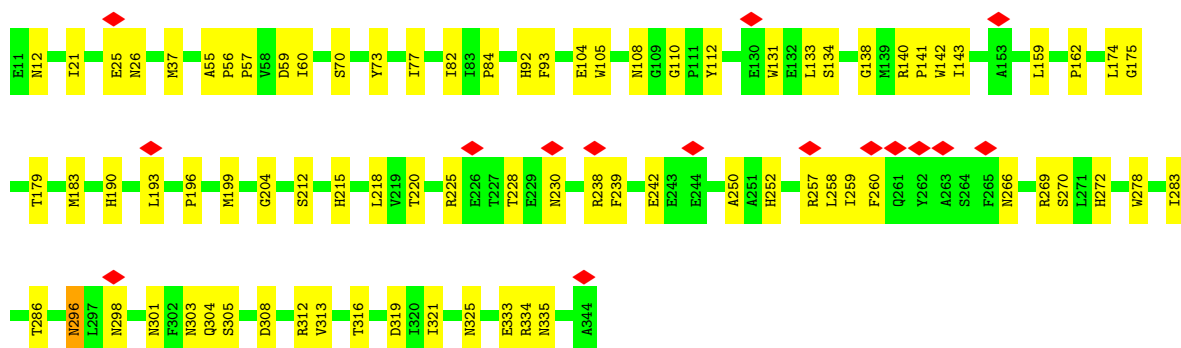
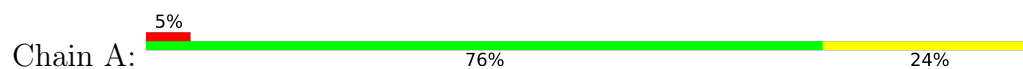




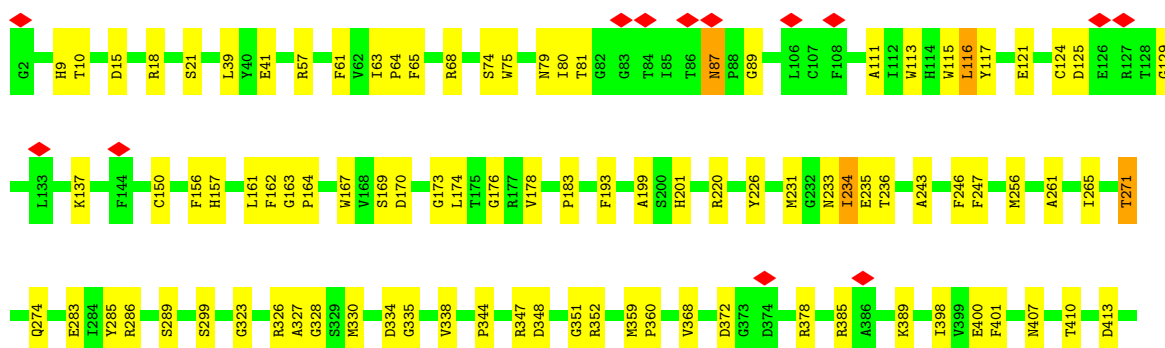
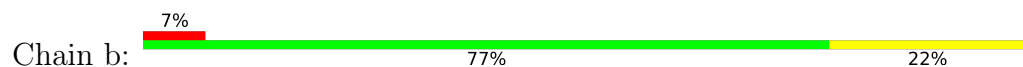
• Molecule 2: Photosystem II protein D1

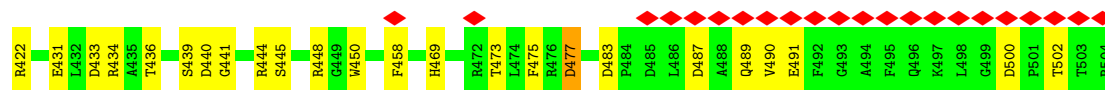


• Molecule 2: Photosystem II protein D1

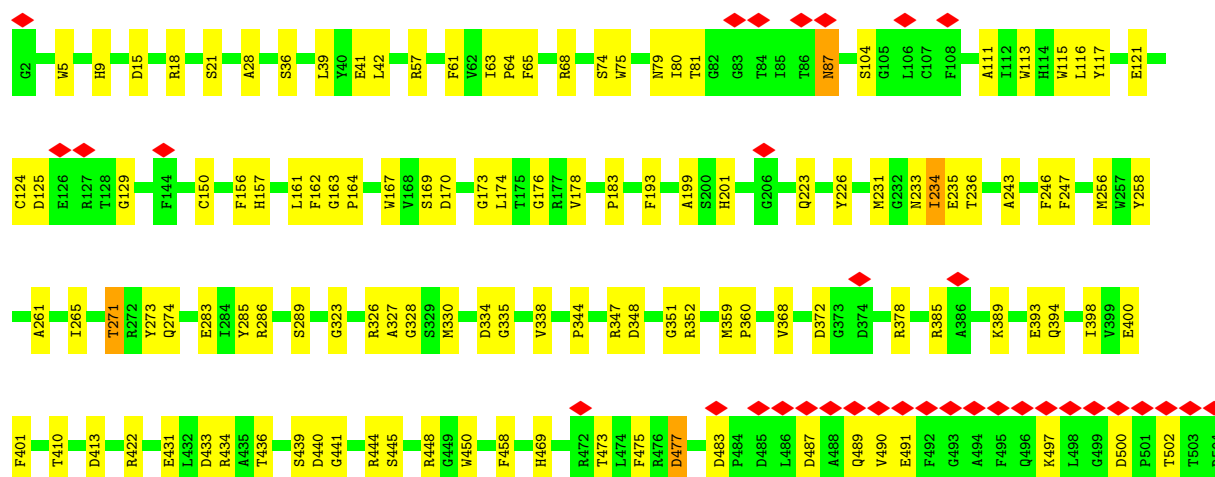
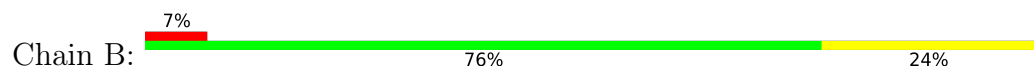


• Molecule 3: Photosystem II CP47 reaction center protein

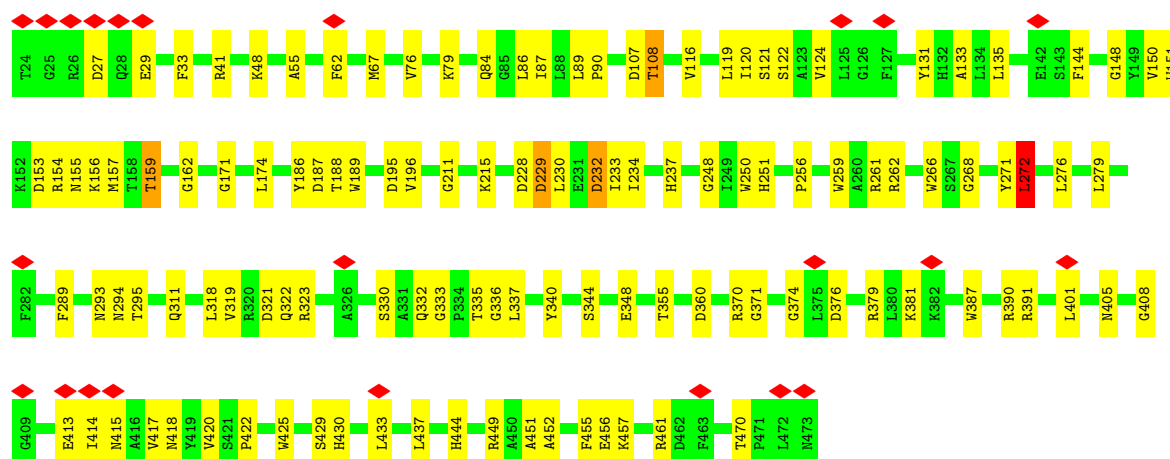




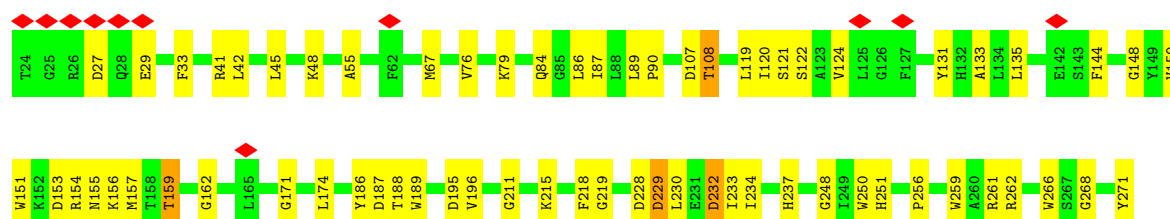
• Molecule 3: Photosystem II CP47 reaction center protein

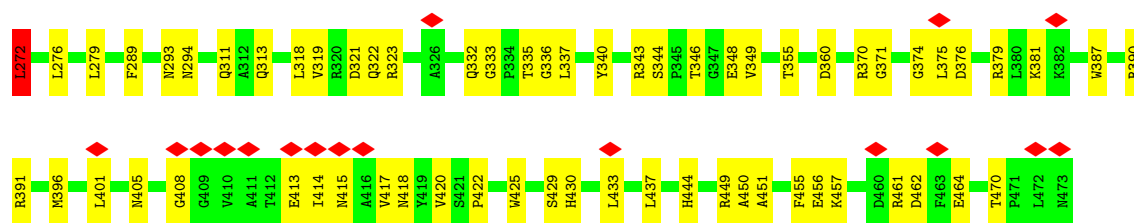


• Molecule 4: Photosystem II CP43 reaction center protein

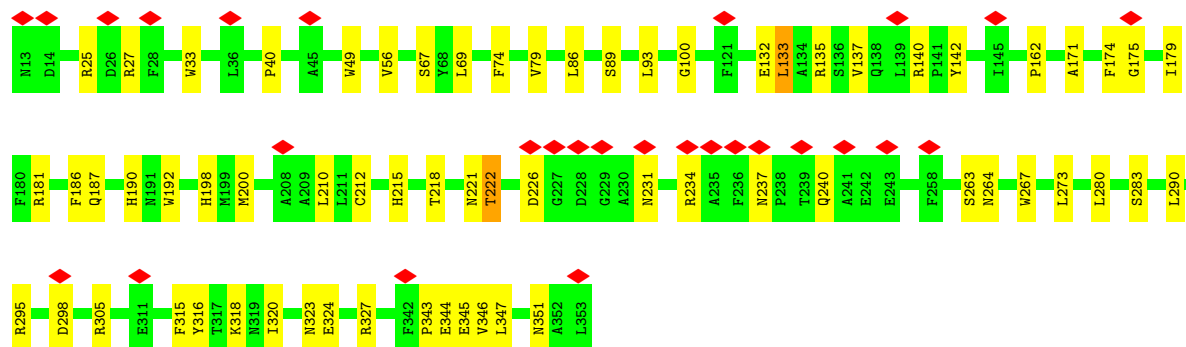
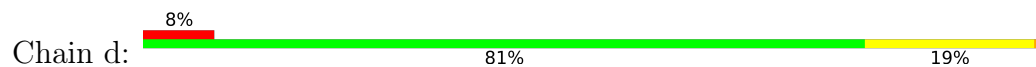


• Molecule 4: Photosystem II CP43 reaction center protein

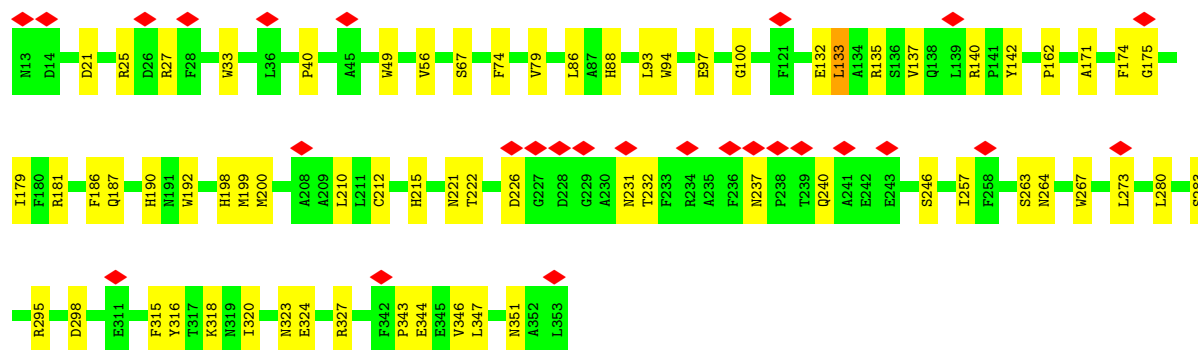
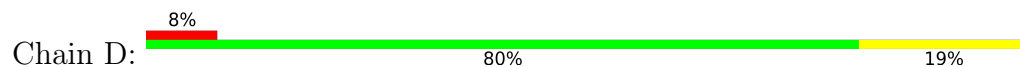




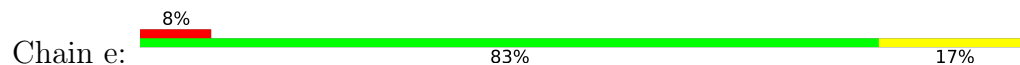
• Molecule 5: Photosystem II D2 protein



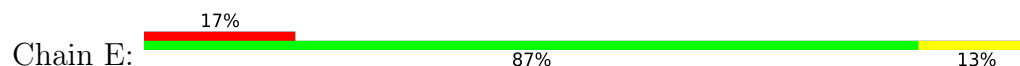
• Molecule 5: Photosystem II D2 protein

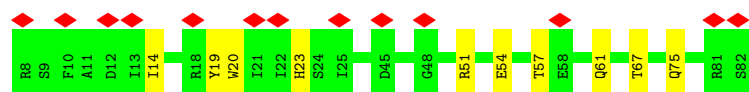


• Molecule 6: Cytochrome b559 subunit alpha

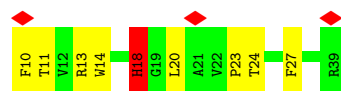


• Molecule 6: Cytochrome b559 subunit alpha

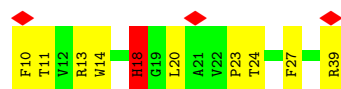




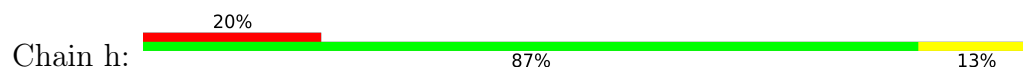
- Molecule 7: Cytochrome b559 subunit beta



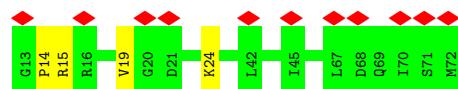
- Molecule 7: Cytochrome b559 subunit beta



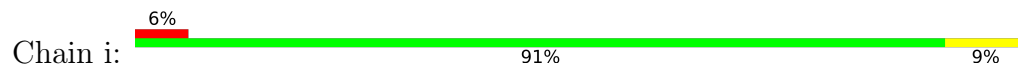
- Molecule 8: Photosystem II reaction center protein H



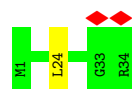
- Molecule 8: Photosystem II reaction center protein H



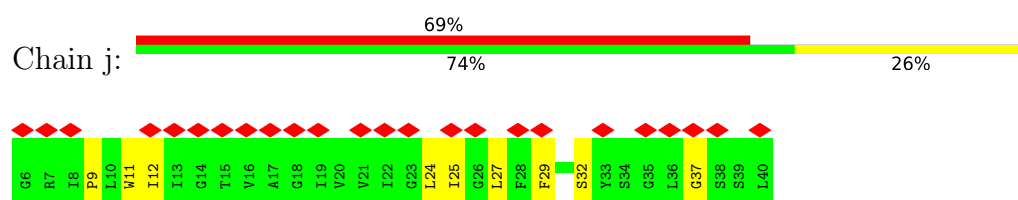
- Molecule 9: Photosystem II reaction center protein I



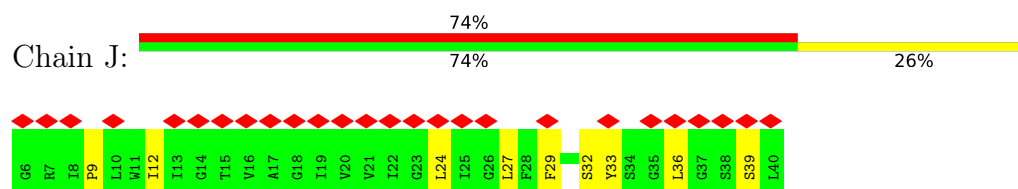
- Molecule 9: Photosystem II reaction center protein I



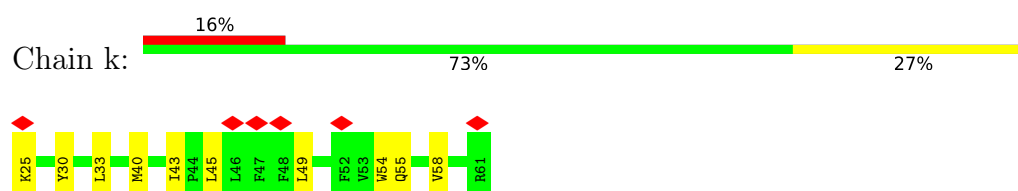
- Molecule 10: Photosystem II reaction center protein J



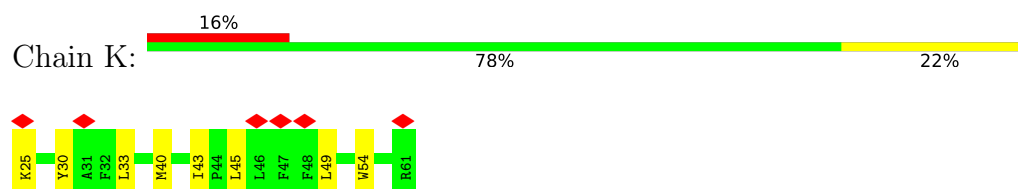
- Molecule 10: Photosystem II reaction center protein J



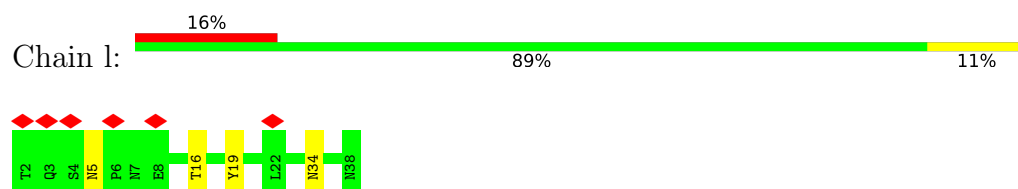
- Molecule 11: Photosystem II reaction center protein K



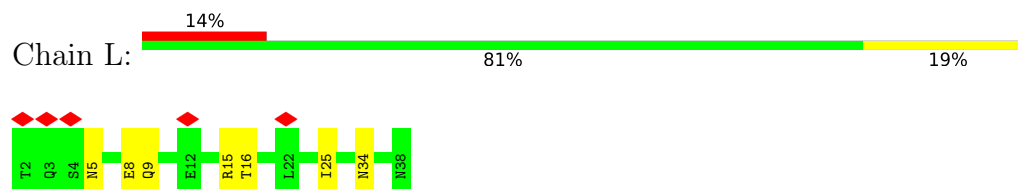
- Molecule 11: Photosystem II reaction center protein K



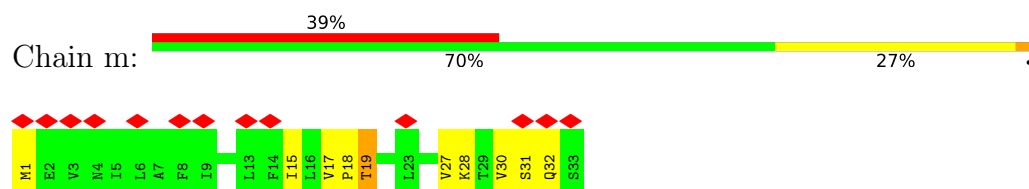
- Molecule 12: Photosystem II reaction center protein L



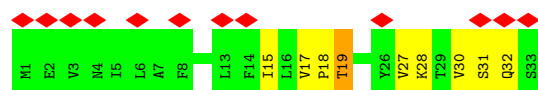
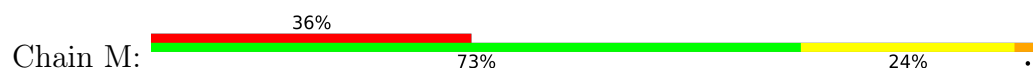
- Molecule 12: Photosystem II reaction center protein L



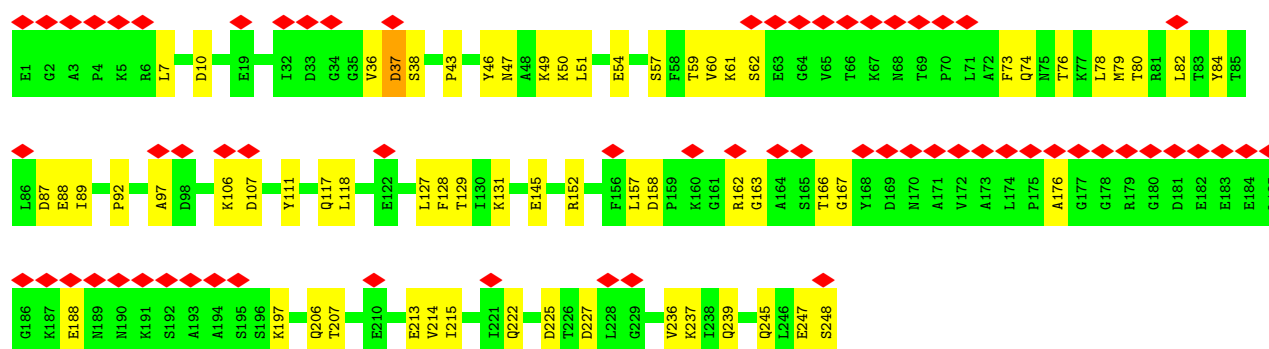
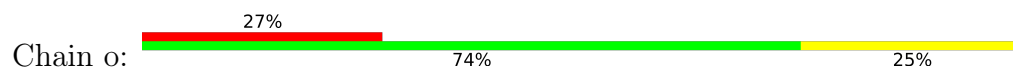
- Molecule 13: Photosystem II reaction center protein M



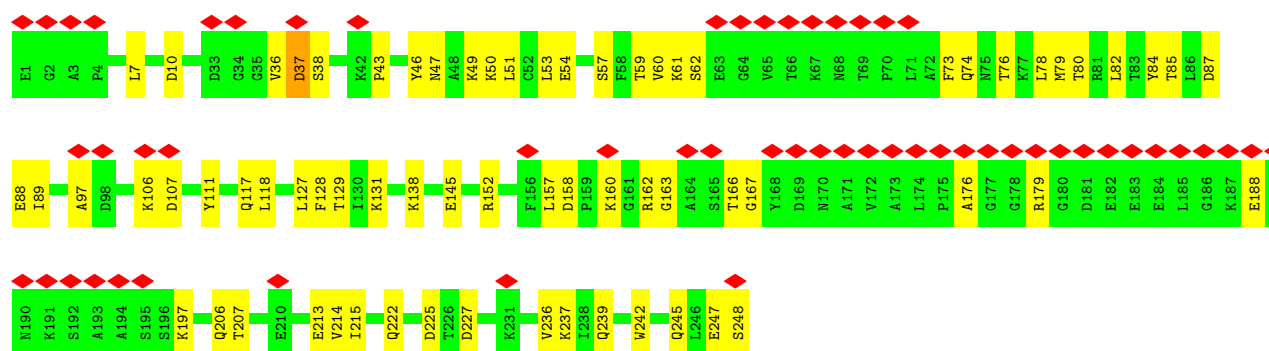
- Molecule 13: Photosystem II reaction center protein M



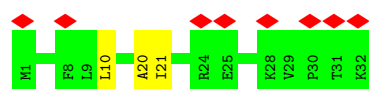
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic



- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic



- Molecule 15: Photosystem II reaction center protein T

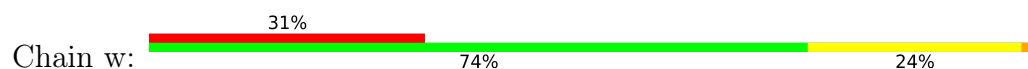


- Molecule 15: Photosystem II reaction center protein T

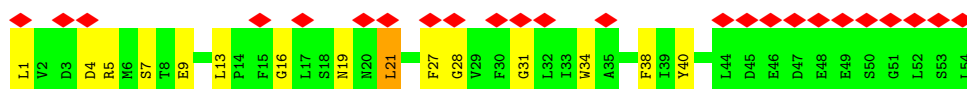




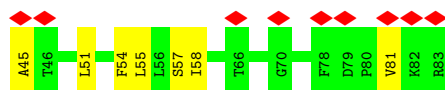
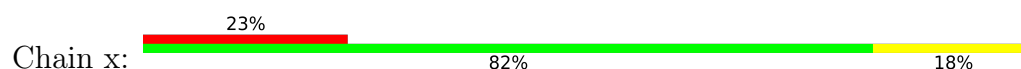
- Molecule 16: Photosystem II reaction center protein W



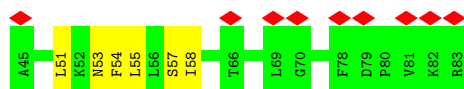
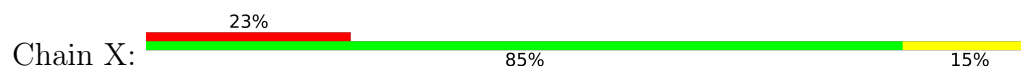
- Molecule 16: Photosystem II reaction center protein W



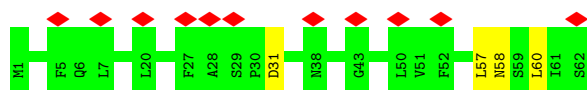
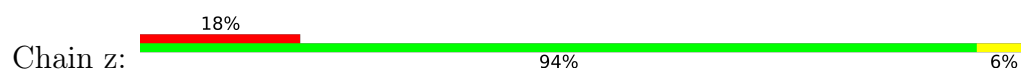
- Molecule 17: Ultraviolet-B-repressible protein



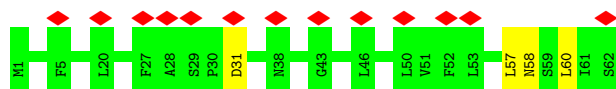
- Molecule 17: Ultraviolet-B-repressible protein



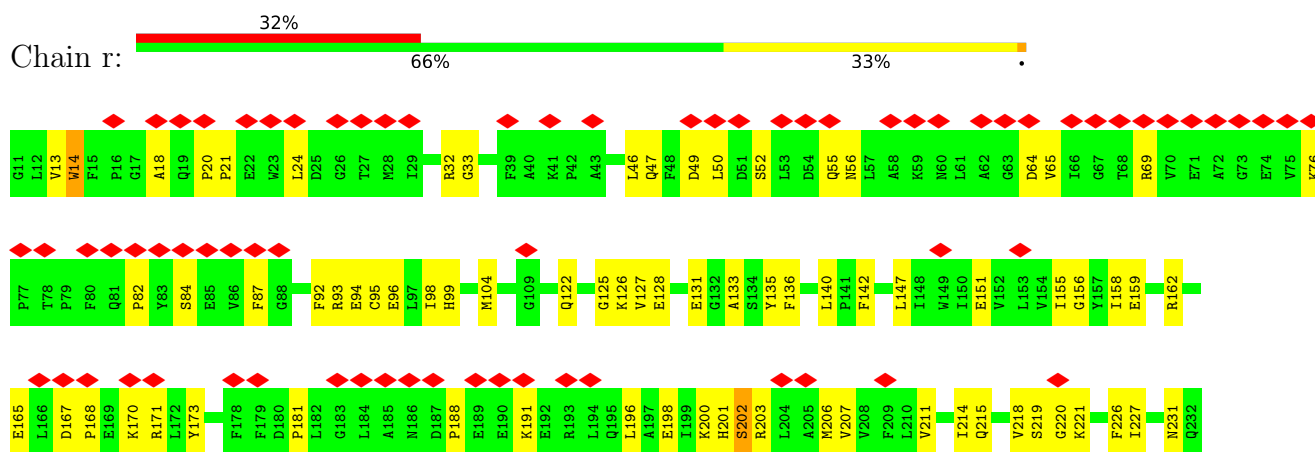
- Molecule 18: Photosystem II reaction center protein Z



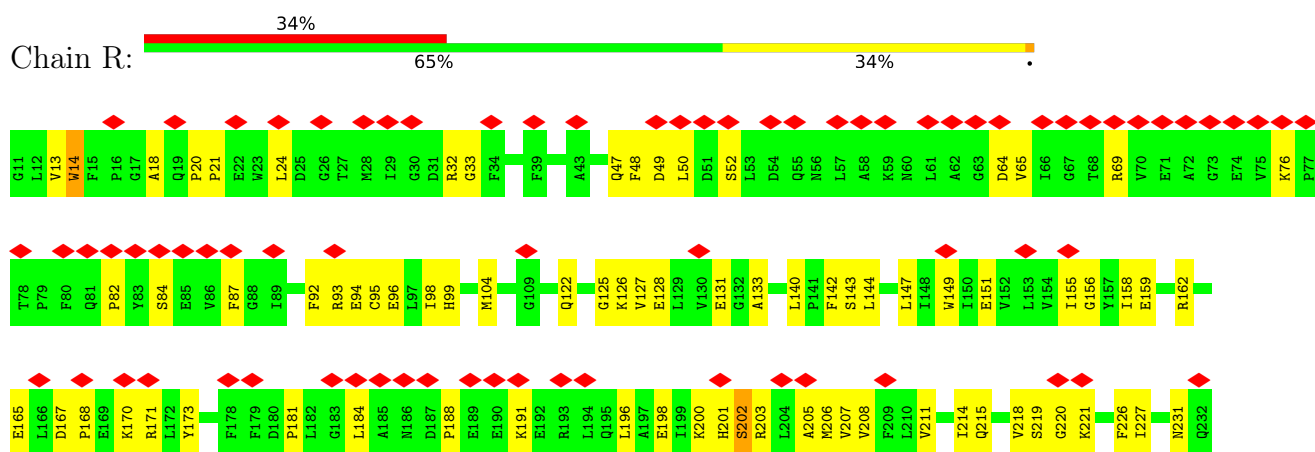
- Molecule 18: Photosystem II reaction center protein Z



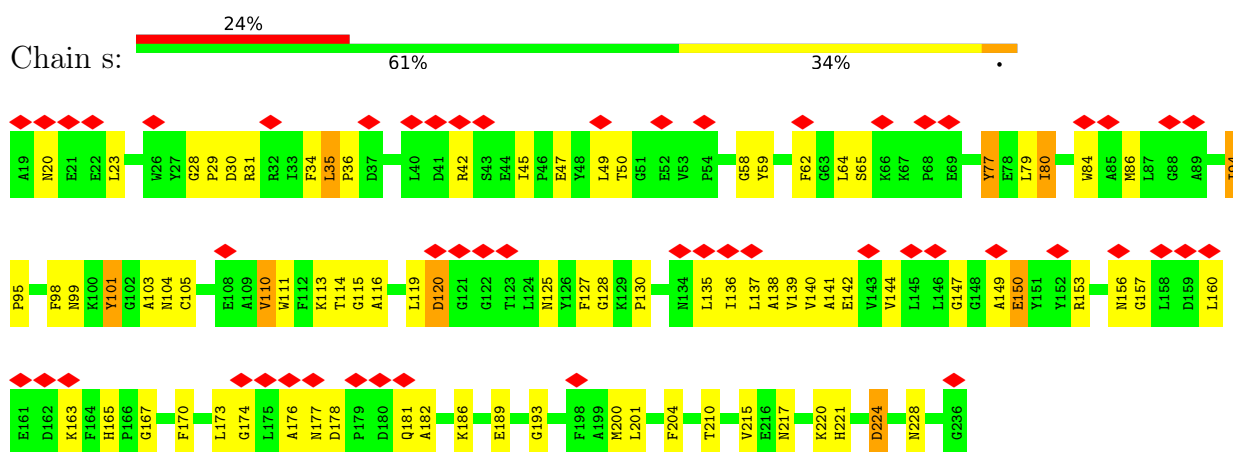
- Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4.3



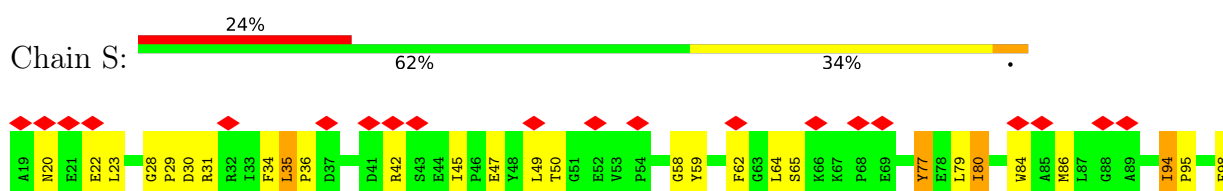
• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4.3

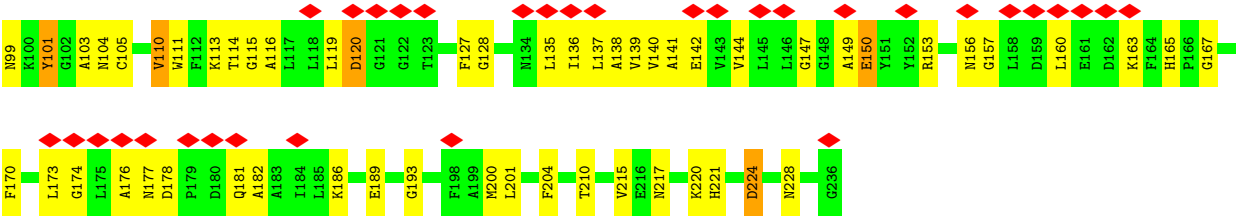


• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26



• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	27942	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 ($e^-/\text{\AA}^2$)	40, 40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k), GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.923	Depositor
Minimum map value	-0.630	Depositor
Average map value	0.055	Depositor
Map value standard deviation	0.166	Depositor
Recommended contour level	0.85	Depositor
Map size ($\text{\AA}$)	374.0, 374.0, 374.0	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, LHG, OEX, LMG, CLA, BCT, NEX, PL9, BCR, CHL, XAT, FE2, CL, LUT, PHO, SQD, HEM

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	G	0.22	0/1720	0.47	3/2342 (0.1%)
1	N	0.22	0/1720	0.47	3/2342 (0.1%)
1	Y	0.22	0/1720	0.47	3/2342 (0.1%)
1	g	0.22	0/1720	0.47	3/2342 (0.1%)
1	n	0.22	0/1720	0.47	3/2342 (0.1%)
1	y	0.22	0/1720	0.47	3/2342 (0.1%)
2	A	0.22	0/2697	0.39	0/3677
2	a	0.22	0/2697	0.39	0/3677
3	B	0.21	0/4081	0.36	0/5556
3	b	0.21	0/4081	0.36	0/5556
4	C	0.88	1/3614 (0.0%)	0.40	2/4922 (0.0%)
4	c	0.88	1/3614 (0.0%)	0.40	2/4922 (0.0%)
5	D	0.21	0/2804	0.36	0/3823
5	d	0.21	0/2804	0.36	0/3823
6	E	0.17	0/630	0.34	0/857
6	e	0.17	0/630	0.34	0/857
7	F	0.66	1/248 (0.4%)	0.58	0/335
7	f	0.66	1/248 (0.4%)	0.58	0/335
8	H	0.19	0/461	0.37	0/626
8	h	0.19	0/461	0.36	0/626
9	I	0.25	0/286	0.39	0/386
9	i	0.24	0/286	0.39	0/386
10	J	0.13	0/262	0.34	0/354
10	j	0.14	0/262	0.34	0/354
11	K	0.21	0/318	0.46	0/434
11	k	0.21	0/318	0.46	0/434
12	L	0.21	0/319	0.37	0/434
12	l	0.21	0/319	0.37	0/434
13	M	0.20	0/260	0.37	0/355
13	m	0.20	0/260	0.37	0/355
14	O	0.17	0/1906	0.33	0/2575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	o	0.17	0/1906	0.33	0/2575
15	T	0.25	0/269	0.35	0/365
15	t	0.25	0/269	0.35	0/365
16	W	0.25	0/429	0.38	0/581
16	w	0.25	0/429	0.38	0/581
17	X	0.18	0/279	0.35	0/380
17	x	0.19	0/279	0.35	0/380
18	Z	0.17	0/474	0.26	0/648
18	z	0.17	0/474	0.27	0/648
19	R	0.17	0/1780	0.34	0/2417
19	r	0.17	0/1780	0.34	0/2417
20	S	0.20	0/1737	0.41	0/2361
20	s	0.20	0/1737	0.41	0/2361
All	All	0.37	4/56028 (0.0%)	0.39	22/76224 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	2
1	N	0	2
1	Y	0	2
1	g	0	2
1	n	0	2
1	y	0	2
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	272	LEU	CG-CD1	50.99	3.20	1.52
4	C	272	LEU	CG-CD1	50.99	3.20	1.52
7	F	18	HIS	CB-CG	9.20	1.63	1.50
7	f	18	HIS	CB-CG	9.17	1.62	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	194	PHE	N-CA-C	8.26	121.89	111.24
1	Y	194	PHE	N-CA-C	8.25	121.88	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	194	PHE	N-CA-C	8.24	121.87	111.24
1	G	194	PHE	N-CA-C	8.24	121.87	111.24
1	y	194	PHE	N-CA-C	8.22	121.85	111.24
1	N	194	PHE	N-CA-C	8.21	121.83	111.24
1	N	193	GLY	CA-C-N	7.41	132.88	120.88
1	N	193	GLY	C-N-CA	7.41	132.88	120.88
1	n	193	GLY	CA-C-N	7.40	132.87	120.88
1	n	193	GLY	C-N-CA	7.40	132.87	120.88
1	Y	193	GLY	CA-C-N	7.40	132.87	120.88
1	Y	193	GLY	C-N-CA	7.40	132.87	120.88
4	c	272	LEU	CB-CG-CD1	7.40	132.89	110.70
1	y	193	GLY	CA-C-N	7.39	132.85	120.88
1	y	193	GLY	C-N-CA	7.39	132.85	120.88
4	C	272	LEU	CB-CG-CD1	7.39	132.87	110.70
1	G	193	GLY	CA-C-N	7.39	132.85	120.88
1	G	193	GLY	C-N-CA	7.39	132.85	120.88
1	g	193	GLY	CA-C-N	7.38	132.84	120.88
1	g	193	GLY	C-N-CA	7.38	132.84	120.88
4	C	272	LEU	CD1-CG-CD2	5.43	122.76	110.80
4	c	272	LEU	CD1-CG-CD2	5.42	122.71	110.80

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	193	GLY	Mainchain
1	G	197	GLN	Sidechain
1	N	193	GLY	Mainchain
1	N	197	GLN	Sidechain
1	Y	193	GLY	Mainchain
1	Y	197	GLN	Sidechain
1	g	193	GLY	Mainchain
1	g	197	GLN	Sidechain
1	n	193	GLY	Mainchain
1	n	197	GLN	Sidechain
1	y	193	GLY	Mainchain
1	y	197	GLN	Sidechain

5.2 Too-close contacts ⓘ

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	G	1668	0	1596	144	0
1	N	1668	0	1596	150	0
1	Y	1668	0	1596	149	0
1	g	1668	0	1596	146	0
1	n	1668	0	1596	146	0
1	y	1668	0	1596	148	0
2	A	2616	0	2522	70	0
2	a	2616	0	2522	60	0
3	B	3948	0	3818	97	0
3	b	3948	0	3818	93	0
4	C	3497	0	3422	107	0
4	c	3497	0	3422	105	0
5	D	2712	0	2604	52	0
5	d	2712	0	2604	47	0
6	E	612	0	595	7	0
6	e	612	0	595	8	0
7	F	241	0	246	24	0
7	f	241	0	246	23	0
8	H	452	0	473	4	0
8	h	452	0	473	11	0
9	I	278	0	291	1	0
9	i	278	0	291	3	0
10	J	256	0	269	7	0
10	j	256	0	269	6	0
11	K	306	0	313	4	0
11	k	306	0	313	8	0
12	L	311	0	298	10	0
12	l	311	0	298	6	0
13	M	256	0	284	7	0
13	m	256	0	284	8	0
14	O	1870	0	1851	47	0
14	o	1870	0	1851	44	0
15	T	261	0	280	2	0
15	t	261	0	280	3	0
16	W	419	0	402	19	0
16	w	419	0	402	13	0
17	X	276	0	301	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	x	276	0	301	5	0
18	Z	464	0	493	3	0
18	z	464	0	493	2	0
19	R	1732	0	1697	67	0
19	r	1732	0	1697	71	0
20	S	1688	0	1649	118	0
20	s	1688	0	1650	120	0
21	G	355	0	335	168	0
21	N	314	0	317	147	0
21	R	183	0	173	76	0
21	S	186	0	124	104	0
21	Y	314	0	317	145	0
21	g	355	0	335	145	0
21	n	314	0	317	142	0
21	r	231	0	206	83	0
21	s	186	0	124	107	0
21	y	362	0	350	154	0
22	A	240	0	242	10	0
22	B	1040	0	1152	40	0
22	C	845	0	935	64	0
22	D	130	0	144	5	0
22	G	477	0	471	55	0
22	N	473	0	462	59	0
22	R	400	0	373	29	0
22	S	471	0	389	34	0
22	W	60	0	59	16	0
22	Y	413	0	403	66	0
22	a	240	0	242	12	0
22	b	975	0	1080	37	0
22	c	845	0	935	67	0
22	d	130	0	144	7	0
22	g	477	0	471	54	0
22	n	473	0	462	54	0
22	r	400	0	373	23	0
22	s	471	0	389	30	0
22	w	60	0	58	5	0
22	x	65	0	72	2	0
22	y	413	0	403	50	0
23	G	84	0	112	21	0
23	N	84	0	112	28	0
23	R	42	0	55	2	0
23	Y	84	0	112	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	g	84	0	112	24	0
23	n	42	0	56	12	0
23	r	42	0	55	2	0
23	y	42	0	56	11	0
24	G	44	0	55	1	0
24	N	44	0	55	2	0
24	R	44	0	55	5	0
24	Y	44	0	55	2	0
24	g	44	0	55	0	0
24	n	44	0	55	2	0
24	r	44	0	55	5	0
24	y	44	0	55	2	0
25	N	44	0	56	9	0
25	Y	44	0	56	9	0
25	g	44	0	56	8	0
25	n	44	0	56	12	0
25	r	44	0	56	8	0
25	y	88	0	112	16	0
26	B	49	0	74	1	0
26	C	147	0	220	14	0
26	D	138	0	195	9	0
26	G	49	0	74	13	0
26	L	49	0	74	2	0
26	N	49	0	74	9	0
26	R	47	0	66	5	0
26	S	49	0	74	6	0
26	Y	49	0	74	10	0
26	b	49	0	74	1	0
26	c	147	0	220	8	0
26	d	138	0	195	12	0
26	g	49	0	74	6	0
26	l	49	0	74	0	0
26	n	49	0	74	10	0
26	r	47	0	66	3	0
26	s	49	0	74	7	0
26	y	49	0	74	9	0
27	A	10	0	0	0	0
27	a	10	0	0	0	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	1	0	0	1	0
29	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	a	1	0	0	1	0
29	c	1	0	0	0	0
30	A	64	0	74	4	0
30	D	64	0	74	6	0
30	a	64	0	74	5	0
30	d	64	0	74	6	0
31	A	40	0	56	2	0
31	B	160	0	224	8	0
31	C	80	0	112	8	0
31	D	40	0	56	4	0
31	H	40	0	56	3	0
31	K	80	0	112	5	0
31	T	40	0	56	2	0
31	a	40	0	56	1	0
31	b	120	0	168	8	0
31	c	80	0	112	7	0
31	d	40	0	56	4	0
31	h	40	0	56	5	0
31	k	80	0	112	5	0
32	A	13	0	7	2	0
32	D	55	0	80	3	0
32	a	13	0	7	2	0
32	d	55	0	80	3	0
33	A	54	0	78	4	0
33	D	50	0	66	3	0
33	L	96	0	125	9	0
33	a	54	0	78	4	0
33	d	50	0	66	3	0
33	l	96	0	125	7	0
34	D	4	0	0	4	0
34	a	4	0	0	4	0
35	A	59	0	76	7	0
35	C	117	0	150	10	0
35	H	62	0	82	8	0
35	J	60	0	78	6	0
35	a	59	0	76	7	0
35	c	177	0	228	14	0
35	h	62	0	82	4	0
36	B	95	0	134	58	0
36	C	99	0	138	5	0
36	D	46	0	62	2	0
36	I	40	0	50	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	K	51	0	72	1	0
36	M	51	0	72	5	0
36	T	51	0	72	5	0
36	b	55	0	86	36	0
36	c	51	0	72	3	0
36	d	46	0	62	4	0
36	k	51	0	72	1	0
36	w	48	0	66	3	0
37	F	43	0	30	17	0
37	f	43	0	30	20	0
All	All	71784	0	72432	3133	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 22.

All (3133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:121:ALA:CB	21:y:605:CHL:CB	1.79	1.57
1:y:102:SER:CB	21:y:607:CHL:HED3	1.35	1.56
20:S:101:TYR:CE1	21:S:301:CHL:CMA	1.87	1.54
1:y:102:SER:HB3	21:y:607:CHL:CED	1.34	1.53
1:g:102:SER:HB3	21:g:607:CHL:CED	1.34	1.53
1:Y:121:ALA:CB	21:r:301:CHL:CB	1.84	1.53
1:n:121:ALA:CB	21:s:301:CHL:CB	1.87	1.53
1:G:121:ALA:CB	21:G:605:CHL:CB	1.86	1.53
1:g:102:SER:CB	21:g:607:CHL:HED3	1.36	1.53
1:N:102:SER:HB3	21:N:606:CHL:CED	1.37	1.52
1:N:121:ALA:CB	21:S:301:CHL:CB	1.84	1.52
1:Y:102:SER:CB	21:Y:606:CHL:HED3	1.40	1.51
1:Y:102:SER:HB3	21:Y:606:CHL:CED	1.36	1.51
1:g:121:ALA:CB	21:g:605:CHL:CB	1.86	1.51
20:s:116:ALA:HA	21:s:307:CHL:CMD	1.36	1.51
20:S:101:TYR:CD1	21:S:301:CHL:HMA2	1.46	1.51
1:y:121:ALA:CB	21:y:605:CHL:HBC2	1.38	1.50
1:G:102:SER:CB	21:G:607:CHL:HED3	1.41	1.49
1:G:102:SER:HB3	21:G:607:CHL:CED	1.37	1.49
20:S:116:ALA:HA	21:S:307:CHL:CMD	1.38	1.49
1:n:102:SER:HB3	21:n:606:CHL:CED	1.42	1.48
20:s:101:TYR:CE1	21:s:301:CHL:H2A	1.47	1.48
1:N:102:SER:CB	21:N:606:CHL:HED3	1.41	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:101:TYR:HE1	21:S:301:CHL:C2A	1.26	1.45
21:N:601:CHL:CHD	26:N:618:LHG:HC82	1.48	1.43
21:G:601:CHL:CHD	26:G:618:LHG:HC82	1.46	1.43
1:N:121:ALA:CB	21:S:301:CHL:HBC2	1.42	1.42
1:n:102:SER:CB	21:n:606:CHL:HED3	1.49	1.40
20:s:101:TYR:CE1	21:s:301:CHL:CMA	2.04	1.39
16:W:38:PHE:CE2	22:W:101:CLA:H42	1.57	1.39
20:S:101:TYR:CE1	21:S:301:CHL:H2A	1.29	1.37
36:b:620:LMG:H252	21:r:307:CHL:C4C	1.53	1.37
1:y:121:ALA:HB1	21:y:605:CHL:CBC	1.45	1.36
1:Y:121:ALA:CB	21:r:301:CHL:HBC2	1.42	1.36
36:b:620:LMG:H211	21:r:307:CHL:C4A	0.89	1.36
36:B:623:LMG:H261	21:R:305:CHL:C2C	1.55	1.34
36:B:623:LMG:H221	21:R:306:CHL:NC	1.41	1.34
4:c:272:LEU:HG	22:c:510:CLA:ND	1.43	1.33
1:G:121:ALA:HB1	21:G:605:CHL:CBC	1.49	1.33
20:S:101:TYR:CD1	21:S:301:CHL:CMA	2.06	1.33
1:n:121:ALA:CB	21:s:301:CHL:HBC2	1.47	1.32
36:B:623:LMG:H232	21:R:306:CHL:C1D	1.59	1.31
1:g:121:ALA:CB	21:g:605:CHL:HBC2	1.44	1.31
1:N:121:ALA:HB1	21:S:301:CHL:CBC	1.48	1.30
20:s:115:GLY:O	21:s:307:CHL:C2D	1.77	1.30
1:G:121:ALA:CB	21:G:605:CHL:HBC2	1.45	1.30
36:B:623:LMG:H232	21:R:306:CHL:CHD	1.61	1.29
4:C:272:LEU:HG	22:C:511:CLA:ND	1.44	1.29
1:g:121:ALA:HB1	21:g:605:CHL:CBC	1.50	1.28
1:n:121:ALA:HB1	21:s:301:CHL:CBC	1.50	1.28
36:b:620:LMG:H212	21:r:307:CHL:C1A	1.21	1.27
20:s:101:TYR:OH	21:s:301:CHL:C1A	1.82	1.26
1:Y:121:ALA:HB1	21:r:301:CHL:CBC	1.49	1.26
20:S:115:GLY:O	21:S:307:CHL:C2D	1.82	1.24
20:s:101:TYR:CD1	21:s:301:CHL:HMA2	1.71	1.23
1:g:71:TRP:CD1	21:g:609:CHL:HMD3	1.74	1.23
1:Y:71:TRP:CD1	21:Y:608:CHL:HMD3	1.74	1.23
1:G:121:ALA:CB	21:G:605:CHL:HBC3	1.59	1.22
1:N:71:TRP:CD1	21:N:608:CHL:HMD3	1.75	1.22
20:s:101:TYR:CE1	21:s:301:CHL:C2A	2.22	1.22
20:s:101:TYR:OH	21:s:301:CHL:CHA	1.87	1.21
1:y:71:TRP:CD1	21:y:609:CHL:HMD3	1.74	1.20
1:N:121:ALA:CB	21:S:301:CHL:HBC3	1.59	1.20
20:S:101:TYR:CZ	21:S:301:CHL:HMA3	1.77	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:121:ALA:CB	21:g:605:CHL:HBC3	1.60	1.18
36:B:623:LMG:H261	21:R:305:CHL:CMC	1.73	1.18
1:n:121:ALA:CB	21:s:301:CHL:HBC3	1.58	1.17
36:b:620:LMG:H212	21:r:307:CHL:CHA	1.73	1.17
1:y:121:ALA:HB2	21:y:605:CHL:CBC	1.59	1.16
36:b:620:LMG:H211	21:r:307:CHL:CHB	1.75	1.16
20:S:101:TYR:CE1	21:S:301:CHL:HMA3	1.63	1.16
20:S:101:TYR:CE1	21:S:301:CHL:C3A	2.29	1.15
20:s:101:TYR:CZ	21:s:301:CHL:HMA3	1.80	1.14
1:Y:121:ALA:CB	21:r:301:CHL:HBC3	1.60	1.14
36:b:620:LMG:H261	21:r:306:CHL:CMC	1.76	1.14
20:s:101:TYR:CE1	21:s:301:CHL:HMA3	1.81	1.14
1:y:121:ALA:CB	21:y:605:CHL:HBC3	1.55	1.14
1:N:121:ALA:HB2	21:S:301:CHL:CBC	1.63	1.13
20:s:101:TYR:HE1	21:s:301:CHL:C2A	1.58	1.12
20:s:116:ALA:CA	21:s:307:CHL:HMD2	1.80	1.11
20:S:116:ALA:CA	21:S:307:CHL:HMD2	1.80	1.11
36:B:623:LMG:C23	21:R:306:CHL:ND	2.15	1.10
20:s:101:TYR:CE1	21:s:301:CHL:HMA2	1.78	1.10
19:r:136:PHE:HB3	21:r:301:CHL:C1	1.81	1.09
21:N:601:CHL:HHO	26:N:618:LHG:HC82	1.15	1.09
20:s:142:GLU:HG3	21:s:306:CHL:HMA3	1.34	1.09
20:S:142:GLU:HG3	21:S:306:CHL:HMA3	1.34	1.09
20:S:101:TYR:CE1	21:S:301:CHL:C2A	1.96	1.08
1:G:121:ALA:HB2	21:G:605:CHL:CBC	1.64	1.07
20:s:116:ALA:CA	21:s:307:CHL:CMD	2.33	1.05
4:c:272:LEU:CD1	22:c:510:CLA:NC	2.20	1.05
1:Y:142:ARG:HG3	21:Y:607:CHL:CHD	1.87	1.05
20:S:116:ALA:CA	21:S:307:CHL:CMD	2.35	1.05
1:G:142:ARG:HG3	21:G:608:CHL:CHD	1.87	1.04
1:y:142:ARG:HG3	21:y:608:CHL:CHD	1.87	1.04
1:N:142:ARG:HG3	21:N:607:CHL:CHD	1.87	1.04
36:B:623:LMG:H252	21:R:306:CHL:C4C	1.87	1.04
4:C:272:LEU:CD1	22:C:511:CLA:NC	2.20	1.04
1:N:142:ARG:HG3	21:N:607:CHL:C1D	1.88	1.04
1:g:142:ARG:HG3	21:g:608:CHL:C1D	1.88	1.03
1:g:142:ARG:HG3	21:g:608:CHL:CHD	1.87	1.03
1:n:142:ARG:HG3	21:n:607:CHL:CHD	1.87	1.03
1:y:142:ARG:HG3	21:y:608:CHL:C1D	1.88	1.03
1:G:142:ARG:HG3	21:G:608:CHL:C1D	1.88	1.03
21:G:601:CHL:H62	21:Y:608:CHL:H92	1.36	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:142:ARG:HG3	21:Y:607:CHL:C1D	1.88	1.03
21:G:601:CHL:HHD	26:G:618:LHG:C8	1.87	1.02
1:n:142:ARG:HG3	21:n:607:CHL:C1D	1.88	1.02
1:Y:121:ALA:HB2	21:r:301:CHL:CBC	1.63	1.02
1:y:101:GLY:C	21:y:607:CHL:O1D	2.03	1.02
20:s:101:TYR:OH	21:s:301:CHL:O1D	1.78	1.01
36:b:620:LMG:H232	21:r:307:CHL:C1D	1.50	1.01
36:B:623:LMG:C20	21:R:306:CHL:NB	2.22	1.01
20:s:115:GLY:O	21:s:307:CHL:C1D	2.07	1.01
21:G:601:CHL:CHD	26:G:618:LHG:C8	2.36	1.01
21:Y:605:CHL:HAA1	25:Y:616:NEX:H31	1.43	1.01
16:W:38:PHE:CZ	22:W:101:CLA:H42	1.95	1.01
21:s:302:CHL:C1D	26:s:314:LHG:HC82	1.91	1.01
1:g:101:GLY:C	21:g:607:CHL:O1D	2.03	1.01
1:n:121:ALA:HB2	21:s:301:CHL:CBC	1.65	1.01
1:G:101:GLY:C	21:G:607:CHL:O1D	2.04	1.01
36:b:620:LMG:H261	21:r:306:CHL:C2C	1.89	1.00
21:S:302:CHL:C1D	26:S:314:LHG:HC82	1.91	1.00
1:g:121:ALA:HB2	21:g:605:CHL:CBC	1.64	1.00
1:Y:101:GLY:C	21:Y:606:CHL:O1D	2.04	1.00
1:N:141:TYR:O	21:N:607:CHL:HBC2	1.62	1.00
1:N:101:GLY:C	21:N:606:CHL:O1D	2.04	1.00
1:n:101:GLY:C	21:n:606:CHL:O1D	2.05	0.99
1:y:141:TYR:O	21:y:608:CHL:HBC2	1.62	0.99
20:s:141:ALA:HB3	21:s:306:CHL:HED2	1.44	0.99
20:S:119:LEU:HD11	21:S:307:CHL:CMD	1.92	0.99
1:n:141:TYR:O	21:n:607:CHL:HBC2	1.62	0.99
1:G:141:TYR:O	21:G:608:CHL:HBC2	1.62	0.98
1:g:141:TYR:O	21:g:608:CHL:HBC2	1.62	0.98
20:s:101:TYR:OH	21:s:301:CHL:CGD	2.09	0.98
21:N:601:CHL:HHD	26:N:618:LHG:C8	1.93	0.98
1:Y:141:TYR:O	21:Y:607:CHL:HBC2	1.62	0.98
20:S:115:GLY:O	21:S:307:CHL:C1D	2.10	0.98
21:G:601:CHL:HHD	26:G:618:LHG:HC82	1.00	0.98
20:s:119:LEU:HD11	21:s:307:CHL:CMD	1.94	0.98
1:g:136:GLY:HA2	21:g:609:CHL:HBB1	1.46	0.97
20:s:116:ALA:HA	21:s:307:CHL:HMD2	0.99	0.97
36:B:623:LMG:C23	21:R:306:CHL:C1D	2.42	0.97
1:n:71:TRP:CD1	21:n:608:CHL:HMD2	1.99	0.97
36:b:620:LMG:C23	21:r:307:CHL:C1D	2.35	0.97
20:s:101:TYR:CD1	21:s:301:CHL:CMA	2.38	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:601:CHL:CHD	26:g:619:LHG:HC82	1.95	0.97
20:s:116:ALA:HA	21:s:307:CHL:HMD3	1.44	0.97
20:S:116:ALA:HA	21:S:307:CHL:HMD2	0.97	0.97
1:G:71:TRP:CD1	21:G:609:CHL:HMD2	1.99	0.96
36:b:620:LMG:H232	21:r:307:CHL:CHD	1.66	0.96
16:W:38:PHE:CE2	22:W:101:CLA:C4	2.48	0.96
36:B:623:LMG:C22	21:R:306:CHL:NC	2.27	0.96
20:s:101:TYR:CZ	21:s:301:CHL:O1D	2.18	0.96
20:S:101:TYR:CZ	21:S:301:CHL:O1D	2.18	0.95
1:G:136:GLY:HA2	21:G:609:CHL:HBB1	1.46	0.95
36:B:623:LMG:C22	21:R:306:CHL:ND	2.27	0.95
1:g:102:SER:N	21:g:607:CHL:O1D	1.99	0.95
1:n:136:GLY:HA2	21:n:608:CHL:HBB1	1.46	0.95
1:N:136:GLY:HA2	21:N:608:CHL:HBB1	1.46	0.95
21:y:605:CHL:CBC	21:y:606:CHL:HMD1	1.96	0.95
36:b:620:LMG:C25	21:r:307:CHL:C4C	2.45	0.95
21:Y:605:CHL:HMD1	21:r:301:CHL:CBC	1.97	0.94
1:Y:102:SER:N	21:Y:606:CHL:O1D	2.00	0.94
22:B:611:CLA:H2	22:B:612:CLA:HBB2	1.49	0.94
22:b:608:CLA:H2	22:b:609:CLA:HBB2	1.49	0.94
20:S:141:ALA:HB3	21:S:306:CHL:HED2	1.49	0.94
1:G:102:SER:N	21:G:607:CHL:O1D	2.00	0.94
1:g:101:GLY:CA	21:g:607:CHL:O1D	2.16	0.94
21:n:605:CHL:HMD1	21:s:301:CHL:CBC	1.97	0.94
1:y:102:SER:N	21:y:607:CHL:O1D	1.99	0.94
1:N:101:GLY:CA	21:N:606:CHL:O1D	2.16	0.94
1:Y:136:GLY:HA2	21:Y:608:CHL:HBB1	1.45	0.94
1:n:101:GLY:CA	21:n:606:CHL:O1D	2.16	0.94
1:y:101:GLY:CA	21:y:607:CHL:O1D	2.16	0.94
1:y:136:GLY:HA2	21:y:609:CHL:HBB1	1.46	0.93
1:N:102:SER:N	21:N:606:CHL:O1D	2.00	0.93
1:Y:101:GLY:CA	21:Y:606:CHL:O1D	2.16	0.93
21:N:605:CHL:HMD1	21:S:301:CHL:CBC	1.97	0.93
1:n:67:ILE:HG22	21:n:608:CHL:HMD2	1.48	0.93
1:n:102:SER:N	21:n:606:CHL:O1D	2.01	0.93
4:c:272:LEU:CG	22:c:510:CLA:ND	2.31	0.93
1:G:101:GLY:CA	21:G:607:CHL:O1D	2.16	0.93
1:G:121:ALA:HB2	21:G:605:CHL:HBC3	0.93	0.93
4:C:272:LEU:CG	22:C:511:CLA:ND	2.31	0.93
21:g:605:CHL:CBC	21:g:606:CHL:HMD1	1.98	0.92
21:G:605:CHL:CBC	21:G:606:CHL:HMD1	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:116:ALA:HA	21:S:307:CHL:HMD3	1.49	0.92
1:n:121:ALA:HB2	21:s:301:CHL:HBC3	0.93	0.92
1:N:121:ALA:HB2	21:S:301:CHL:HBC3	0.92	0.92
16:W:38:PHE:CD2	22:W:101:CLA:H42	2.04	0.92
21:G:601:CHL:H2	21:Y:608:CHL:CGA	1.98	0.92
21:N:606:CHL:HMA3	23:N:615:LUT:H172	1.49	0.92
36:B:623:LMG:H232	21:R:306:CHL:ND	1.78	0.92
1:g:121:ALA:HB2	21:g:605:CHL:HBC3	0.93	0.92
1:G:67:ILE:HG22	21:G:609:CHL:HMD2	1.48	0.92
19:r:136:PHE:HB3	21:r:301:CHL:H11	1.48	0.92
21:g:601:CHL:C1D	26:g:619:LHG:HC82	1.99	0.92
21:G:601:CHL:H62	21:Y:608:CHL:C9	2.00	0.92
1:Y:121:ALA:HB2	21:r:301:CHL:HBC3	0.93	0.91
19:r:136:PHE:HB3	21:r:301:CHL:H12	1.50	0.91
1:n:142:ARG:O	21:n:607:CHL:HBC3	1.71	0.91
1:Y:142:ARG:O	21:Y:607:CHL:HBC3	1.71	0.91
1:G:142:ARG:O	21:G:608:CHL:HBC3	1.71	0.91
21:N:605:CHL:HMD1	21:S:301:CHL:HBC3	1.53	0.91
1:g:142:ARG:O	21:g:608:CHL:HBC3	1.71	0.91
1:y:142:ARG:O	21:y:608:CHL:HBC3	1.71	0.90
36:b:620:LMG:H252	21:r:307:CHL:CHD	2.02	0.90
1:N:142:ARG:O	21:N:607:CHL:HBC3	1.71	0.90
36:B:623:LMG:C26	21:R:305:CHL:CMC	2.49	0.90
21:y:605:CHL:HBC3	21:y:606:CHL:HMD1	1.54	0.90
21:N:601:CHL:CHD	26:N:618:LHG:C8	2.44	0.90
20:S:101:TYR:CE1	21:S:301:CHL:HMA2	1.75	0.90
21:n:605:CHL:HMD1	21:s:301:CHL:HBC3	1.53	0.89
4:C:272:LEU:CG	22:C:511:CLA:NC	2.36	0.89
21:Y:605:CHL:HMD1	21:r:301:CHL:HBC3	1.52	0.89
4:c:272:LEU:CG	22:c:510:CLA:NC	2.36	0.89
21:Y:606:CHL:HMA3	23:Y:614:LUT:H172	1.53	0.88
36:B:623:LMG:H142	21:R:306:CHL:HBA1	1.54	0.88
19:r:135:TYR:O	21:r:301:CHL:H12	1.74	0.88
21:g:605:CHL:HBC3	21:g:606:CHL:HMD1	1.54	0.88
21:G:607:CHL:HBC2	21:G:607:CHL:HHH	1.56	0.88
20:s:101:TYR:CE1	21:s:301:CHL:C3A	2.57	0.88
1:y:121:ALA:HB2	21:y:605:CHL:HBC3	0.88	0.88
21:G:607:CHL:HMA3	23:G:616:LUT:H172	1.55	0.88
21:y:605:CHL:HMA2	21:y:605:CHL:H12	1.55	0.88
20:S:119:LEU:HD11	21:S:307:CHL:HMD3	1.56	0.88
21:g:607:CHL:HBC2	21:g:607:CHL:HHH	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:606:CHL:HHD	21:n:606:CHL:HBC2	1.56	0.87
21:y:607:CHL:HHD	21:y:607:CHL:HBC2	1.56	0.87
20:s:101:TYR:CZ	21:s:301:CHL:H2A	2.09	0.87
19:R:162:ARG:HG3	21:R:307:CHL:HHD	1.55	0.87
21:N:606:CHL:HHD	21:N:606:CHL:HBC2	1.56	0.87
20:s:119:LEU:HD11	21:s:307:CHL:HMD3	1.54	0.87
19:r:162:ARG:HG3	21:r:308:CHL:HHD	1.56	0.86
5:D:88:HIS:HD1	35:H:102:DGD:HO2D	1.23	0.86
20:s:101:TYR:HE1	21:s:301:CHL:H2A	0.75	0.86
19:R:122:GLN:O	21:R:306:CHL:HMA3	1.76	0.86
1:n:101:GLY:HA3	21:n:606:CHL:O1D	1.76	0.86
21:Y:606:CHL:HHD	21:Y:606:CHL:HBC2	1.56	0.86
20:s:101:TYR:CZ	21:s:301:CHL:CGD	2.59	0.85
36:B:623:LMG:C27	21:R:305:CHL:OMC	2.25	0.85
1:n:102:SER:HB3	21:n:606:CHL:HED3	0.87	0.85
20:s:115:GLY:C	21:s:307:CHL:C2D	2.49	0.85
21:G:605:CHL:HBC3	21:G:606:CHL:HMD1	1.55	0.85
1:N:101:GLY:HA3	21:N:606:CHL:O1D	1.76	0.85
1:g:102:SER:HB2	21:g:607:CHL:HED3	1.55	0.85
1:Y:101:GLY:HA3	21:Y:606:CHL:O1D	1.77	0.85
1:y:102:SER:HB2	21:y:607:CHL:HED3	1.55	0.84
36:b:620:LMG:C25	21:r:307:CHL:CHD	2.55	0.84
21:G:601:CHL:H202	21:Y:606:CHL:CMB	2.07	0.84
36:B:623:LMG:C22	21:R:306:CHL:NB	2.39	0.84
36:b:620:LMG:H212	21:r:307:CHL:C4D	1.97	0.84
36:B:623:LMG:H201	21:R:306:CHL:NB	1.93	0.84
26:C:521:LHG:H202	16:W:31:GLY:HA3	1.56	0.84
19:r:122:GLN:O	21:r:307:CHL:HMA3	1.76	0.84
20:s:101:TYR:CZ	21:s:301:CHL:C2A	2.59	0.84
1:g:101:GLY:HA3	21:g:607:CHL:O1D	1.77	0.83
1:N:71:TRP:CE2	21:N:608:CHL:HHD	2.14	0.83
1:g:71:TRP:CE2	21:g:609:CHL:HHD	2.14	0.83
20:s:115:GLY:O	21:s:307:CHL:CMD	2.25	0.83
20:S:101:TYR:CZ	21:S:301:CHL:CGD	2.61	0.83
1:G:101:GLY:HA3	21:G:607:CHL:O1D	1.76	0.83
4:C:272:LEU:CD1	22:C:511:CLA:C4C	2.56	0.83
21:y:601:CHL:C1D	26:y:617:LHG:HC82	2.08	0.83
4:c:272:LEU:CD1	22:c:510:CLA:C4C	2.56	0.83
1:G:71:TRP:CE2	21:G:609:CHL:HHD	2.14	0.82
20:S:101:TYR:OH	21:S:301:CHL:O1D	1.97	0.82
1:Y:71:TRP:CE2	21:Y:608:CHL:HHD	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:138:ALA:HA	21:S:306:CHL:HED1	1.60	0.82
1:n:71:TRP:CE2	21:n:608:CHL:HHD	2.14	0.82
1:y:101:GLY:HA3	21:y:607:CHL:O1D	1.77	0.82
21:y:605:CHL:HBC1	21:y:606:CHL:CMD	2.10	0.82
1:y:71:TRP:CE2	21:y:609:CHL:HHD	2.14	0.82
1:N:102:SER:HB2	21:N:606:CHL:HED3	1.57	0.82
21:Y:605:CHL:CAA	25:Y:616:NEX:H31	2.09	0.82
22:Y:604:CLA:HMB1	23:Y:613:LUT:H12	1.61	0.82
36:B:623:LMG:H261	21:R:305:CHL:C1C	2.09	0.82
20:s:138:ALA:HA	21:s:306:CHL:HED1	1.60	0.82
20:S:101:TYR:CD1	21:S:301:CHL:HMA3	1.95	0.82
20:S:119:LEU:CD1	21:S:307:CHL:CMD	2.58	0.82
1:Y:102:SER:HB2	21:Y:606:CHL:HED3	1.57	0.81
4:C:272:LEU:CD1	22:C:511:CLA:C1D	2.59	0.81
1:G:102:SER:HB2	21:G:607:CHL:HED3	1.57	0.81
22:G:603:CLA:H71	22:Y:603:CLA:H122	1.62	0.81
4:c:272:LEU:CD1	22:c:510:CLA:C1D	2.59	0.81
20:s:116:ALA:HA	21:s:307:CHL:C2D	2.09	0.81
20:S:115:GLY:C	21:S:307:CHL:C2D	2.53	0.81
21:y:605:CHL:CBC	21:y:606:CHL:CMD	2.58	0.81
20:s:119:LEU:CD1	21:s:307:CHL:CMD	2.58	0.81
1:Y:71:TRP:CZ2	21:Y:608:CHL:HHD	2.16	0.81
1:g:67:ILE:HG22	21:g:609:CHL:HMD1	1.62	0.80
1:N:67:ILE:HG22	21:N:608:CHL:HMD1	1.62	0.80
1:n:71:TRP:CZ2	21:n:608:CHL:HHD	2.17	0.80
36:B:623:LMG:C23	21:R:306:CHL:CHD	2.55	0.80
1:Y:67:ILE:HG22	21:Y:608:CHL:HMD1	1.63	0.80
1:g:71:TRP:CZ2	21:g:609:CHL:HHD	2.17	0.80
1:n:71:TRP:CD1	21:n:608:CHL:CMD	2.64	0.80
21:n:605:CHL:CMD	21:s:301:CHL:CBC	2.60	0.80
1:G:71:TRP:CZ2	21:G:609:CHL:HHD	2.17	0.80
7:f:18:HIS:CD2	37:f:101:HEM:NA	2.50	0.80
19:r:128:GLU:HG3	21:r:306:CHL:HAC1	1.64	0.79
1:y:71:TRP:CZ2	21:y:609:CHL:HHD	2.17	0.79
36:B:623:LMG:H273	21:R:305:CHL:OMC	1.81	0.79
21:g:601:CHL:CHD	26:g:619:LHG:C8	2.61	0.79
1:G:71:TRP:CD1	21:G:609:CHL:CMD	2.64	0.79
21:G:601:CHL:H202	21:Y:606:CHL:HMB2	1.64	0.79
1:N:71:TRP:CZ2	21:N:608:CHL:HHD	2.17	0.79
21:Y:605:CHL:CMD	21:r:301:CHL:CBC	2.60	0.79
7:F:18:HIS:CD2	37:F:101:HEM:NA	2.50	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:115:GLY:O	21:S:307:CHL:CMD	2.30	0.79
21:N:605:CHL:CMD	21:S:301:CHL:CBC	2.60	0.79
1:n:102:SER:HB2	21:n:606:CHL:HED3	1.61	0.79
1:y:67:ILE:HG22	21:y:609:CHL:HMD1	1.62	0.79
20:S:116:ALA:HA	21:S:307:CHL:C2D	2.12	0.79
19:R:128:GLU:HG3	21:R:305:CHL:HAC1	1.64	0.79
1:N:142:ARG:O	21:N:607:CHL:CBC	2.31	0.79
21:s:306:CHL:HAA2	21:s:306:CHL:O1D	1.83	0.79
1:Y:142:ARG:O	21:Y:607:CHL:CBC	2.31	0.78
1:G:131:GLN:HE22	21:G:607:CHL:CMC	1.97	0.78
1:G:142:ARG:O	21:G:608:CHL:CBC	2.31	0.78
1:N:131:GLN:HE22	21:N:606:CHL:CMC	1.97	0.78
21:N:605:CHL:CMD	21:S:301:CHL:HBC1	2.13	0.78
20:S:101:TYR:CE2	21:S:301:CHL:HMA3	2.18	0.78
1:Y:131:GLN:HE22	21:Y:606:CHL:CMC	1.97	0.78
1:n:142:ARG:O	21:n:607:CHL:CBC	2.32	0.78
1:g:131:GLN:HE22	21:g:607:CHL:CMC	1.97	0.78
1:g:142:ARG:O	21:g:608:CHL:CBC	2.31	0.77
1:Y:71:TRP:CD1	21:Y:608:CHL:CMD	2.64	0.77
1:g:71:TRP:CD1	21:g:609:CHL:CMD	2.64	0.77
7:f:18:HIS:CD2	37:f:101:HEM:C4A	2.73	0.77
36:B:623:LMG:H252	21:R:306:CHL:CHD	2.14	0.77
26:D:408:LHG:H111	26:L:103:LHG:H102	1.66	0.77
1:n:138:VAL:HG11	21:n:607:CHL:HMB3	1.66	0.77
1:y:131:GLN:HE22	21:y:607:CHL:CMC	1.97	0.77
1:y:142:ARG:O	21:y:608:CHL:CBC	2.32	0.77
1:G:102:SER:HB3	21:G:607:CHL:HED3	0.77	0.77
1:n:131:GLN:HE22	21:n:606:CHL:CMC	1.97	0.77
21:n:605:CHL:CMD	21:s:301:CHL:HBC1	2.13	0.77
21:s:302:CHL:CHD	26:s:314:LHG:HC82	2.14	0.77
23:N:614:LUT:H8	23:N:615:LUT:H41	1.65	0.77
1:Y:138:VAL:HG11	21:Y:607:CHL:HMB3	1.66	0.77
21:Y:605:CHL:CMD	21:r:301:CHL:HBC1	2.13	0.77
7:F:18:HIS:CD2	37:F:101:HEM:C4A	2.73	0.77
36:b:620:LMG:C26	21:r:306:CHL:CMC	2.62	0.77
20:s:105:CYS:HA	20:s:127:PHE:HA	1.67	0.77
21:g:605:CHL:CBC	21:g:606:CHL:CMD	2.62	0.77
21:G:605:CHL:CBC	21:G:606:CHL:CMD	2.63	0.77
1:N:71:TRP:CD1	21:N:608:CHL:CMD	2.64	0.76
20:S:105:CYS:HA	20:S:127:PHE:HA	1.67	0.76
1:n:25:LEU:O	21:n:601:CHL:HBB1	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:302:CHL:CHD	26:S:314:LHG:HC82	2.14	0.76
21:G:601:CHL:C1D	26:G:618:LHG:HC82	2.14	0.76
16:W:38:PHE:CD2	22:W:101:CLA:C4	2.68	0.76
21:G:609:CHL:C9	21:N:601:CHL:H62	2.15	0.76
21:S:306:CHL:HAA2	21:S:306:CHL:O1D	1.84	0.76
1:G:138:VAL:HG11	21:G:608:CHL:HMB3	1.66	0.76
21:G:605:CHL:HBC1	21:G:606:CHL:CMD	2.16	0.76
1:G:25:LEU:O	21:G:601:CHL:HBB1	1.86	0.76
1:g:138:VAL:HG11	21:g:608:CHL:HMB3	1.66	0.75
1:N:138:VAL:HG11	21:N:607:CHL:HMB3	1.66	0.75
21:G:608:CHL:HBA2	21:G:608:CHL:HBD	1.69	0.75
21:g:605:CHL:HBC1	21:g:606:CHL:CMD	2.15	0.75
1:Y:25:LEU:O	21:Y:601:CHL:HBB1	1.86	0.75
36:B:623:LMG:H231	19:R:125:GLY:HA3	1.68	0.75
21:y:608:CHL:HBA2	21:y:608:CHL:HBD	1.69	0.75
21:G:601:CHL:C6	21:Y:608:CHL:H92	2.14	0.75
36:b:620:LMG:H252	21:r:307:CHL:C3C	2.17	0.75
26:N:618:LHG:H122	26:N:618:LHG:H262	1.68	0.75
36:B:623:LMG:H201	21:R:306:CHL:NC	2.02	0.75
21:n:607:CHL:HBA2	21:n:607:CHL:HBD	1.69	0.75
21:N:607:CHL:HBA2	21:N:607:CHL:HBD	1.69	0.75
21:Y:607:CHL:HBA2	21:Y:607:CHL:HBD	1.69	0.75
7:f:18:HIS:CG	37:f:101:HEM:NC	2.55	0.75
21:g:608:CHL:HBA2	21:g:608:CHL:HBD	1.69	0.74
1:y:25:LEU:O	21:y:601:CHL:HBB1	1.86	0.74
1:y:138:VAL:HG11	21:y:608:CHL:HMB3	1.66	0.74
1:N:25:LEU:O	21:N:601:CHL:HBB1	1.86	0.74
4:c:272:LEU:HD13	22:c:510:CLA:C4C	2.17	0.74
21:G:609:CHL:HBC3	21:G:609:CHL:HMC	1.69	0.74
19:r:128:GLU:HB2	21:r:306:CHL:HBC1	1.69	0.74
1:g:25:LEU:O	21:g:601:CHL:HBB1	1.86	0.74
19:R:128:GLU:HB2	21:R:305:CHL:HBC1	1.69	0.74
22:R:303:CLA:HAB	24:R:313:XAT:H35	1.68	0.74
4:C:272:LEU:HD13	22:C:511:CLA:C4C	2.17	0.74
1:g:182:LYS:NZ	26:g:619:LHG:O4	2.19	0.74
1:G:71:TRP:HD1	21:G:609:CHL:HMD2	1.53	0.74
21:N:606:CHL:CMA	23:N:615:LUT:H172	2.16	0.74
1:Y:102:SER:HB3	21:Y:606:CHL:HED3	0.75	0.74
20:s:101:TYR:CZ	21:s:301:CHL:CMA	2.53	0.74
21:N:606:CHL:HMA3	23:N:615:LUT:C17	2.16	0.73
21:g:607:CHL:HMA3	23:g:616:LUT:H172	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:71:TRP:HD1	21:n:608:CHL:HMD2	1.53	0.73
1:n:97:TRP:HB2	23:n:614:LUT:H22	1.70	0.73
21:n:608:CHL:HBC3	21:n:608:CHL:HMC	1.69	0.73
7:F:18:HIS:CG	37:F:101:HEM:NC	2.55	0.73
21:y:609:CHL:HBC3	21:y:609:CHL:HMC	1.69	0.73
1:y:97:TRP:HB2	23:y:614:LUT:H22	1.70	0.73
1:Y:97:TRP:HB2	23:Y:613:LUT:H22	1.70	0.73
21:g:609:CHL:HBC3	21:g:609:CHL:HMC	1.69	0.73
21:N:608:CHL:HBC3	21:N:608:CHL:HMC	1.69	0.73
23:G:615:LUT:H182	23:G:616:LUT:H192	1.69	0.73
21:n:605:CHL:H3A	25:n:616:NEX:H31	1.69	0.73
1:N:102:SER:HB3	21:N:606:CHL:HED3	0.77	0.73
1:N:97:TRP:HB2	23:N:614:LUT:H22	1.70	0.72
23:N:614:LUT:H203	23:N:615:LUT:H8	1.70	0.72
21:Y:608:CHL:HBC3	21:Y:608:CHL:HMC	1.70	0.72
1:g:97:TRP:HB2	23:g:615:LUT:H22	1.70	0.72
22:r:304:CLA:HAB	24:r:314:XAT:H35	1.68	0.72
20:S:101:TYR:CE2	21:S:301:CHL:O1D	2.42	0.72
21:n:601:CHL:C1D	26:n:617:LHG:HC82	2.19	0.72
21:G:609:CHL:H111	21:N:601:CHL:C10	2.19	0.72
1:G:97:TRP:HB2	23:G:615:LUT:H22	1.70	0.72
1:y:211:ASP:O	1:y:219:ASN:ND2	2.23	0.72
20:S:101:TYR:OH	21:S:301:CHL:CGD	2.28	0.72
23:g:615:LUT:H7	23:g:616:LUT:H21	1.71	0.72
1:n:211:ASP:O	1:n:219:ASN:ND2	2.23	0.72
22:Y:602:CLA:H122	23:Y:614:LUT:H393	1.70	0.72
22:a:404:CLA:H122	30:a:407:PHO:H3A	1.71	0.72
5:D:324:GLU:HG2	5:D:327:ARG:HH22	1.54	0.72
19:r:76:LYS:HE3	19:r:84:SER:HB2	1.71	0.72
1:y:71:TRP:CD1	21:y:609:CHL:CMD	2.64	0.72
1:G:211:ASP:O	1:G:219:ASN:ND2	2.23	0.72
22:s:305:CLA:HBA1	21:s:306:CHL:C2D	2.19	0.72
20:S:101:TYR:CZ	21:S:301:CHL:CMA	2.50	0.72
21:g:606:CHL:H3A	25:g:618:NEX:H31	1.72	0.72
4:C:272:LEU:HG	22:C:511:CLA:C1D	2.19	0.72
14:O:206:GLN:HB2	14:O:215:ILE:HD11	1.72	0.72
1:G:24:TYR:CD2	21:G:601:CHL:HAA2	2.25	0.71
3:b:385:ARG:NH1	14:o:167:GLY:O	2.23	0.71
1:n:197:GLN:HG3	22:n:612:CLA:NA	2.05	0.71
1:Y:24:TYR:CD2	21:Y:601:CHL:HAA2	2.25	0.71
2:A:333:GLU:N	29:A:404:CL:CL	2.60	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:211:ASP:O	1:Y:219:ASN:ND2	2.23	0.71
4:c:272:LEU:HG	22:c:510:CLA:C1D	2.19	0.71
22:A:405:CLA:H122	30:A:408:PHO:H3A	1.72	0.71
1:n:24:TYR:CD2	21:n:601:CHL:HAA2	2.25	0.71
2:A:140:ARG:NH2	26:D:410:LHG:O5	2.23	0.71
1:y:24:TYR:CD2	21:y:601:CHL:HAA2	2.25	0.71
1:y:197:GLN:HG3	22:y:612:CLA:NA	2.05	0.71
5:d:324:GLU:HG2	5:d:327:ARG:HH22	1.54	0.71
20:s:119:LEU:HD11	21:s:307:CHL:HMD1	1.73	0.71
22:S:305:CLA:HBA1	21:S:306:CHL:C2D	2.20	0.71
19:R:76:LYS:HE3	19:R:84:SER:HB2	1.71	0.71
1:G:197:GLN:HG3	22:G:613:CLA:NA	2.05	0.71
14:o:206:GLN:HB2	14:o:215:ILE:HD11	1.72	0.71
1:g:24:TYR:CD2	21:g:601:CHL:HAA2	2.25	0.71
21:G:607:CHL:HMA3	23:G:616:LUT:C17	2.20	0.71
21:G:607:CHL:CMB	21:N:601:CHL:H202	2.20	0.71
20:s:101:TYR:OH	21:s:301:CHL:C2A	2.38	0.71
1:N:211:ASP:O	1:N:219:ASN:ND2	2.23	0.71
23:N:615:LUT:H8	23:N:615:LUT:H182	1.71	0.71
1:g:197:GLN:HG3	22:g:613:CLA:NA	2.05	0.70
1:g:211:ASP:O	1:g:219:ASN:ND2	2.23	0.70
1:G:131:GLN:HE22	21:G:607:CHL:HMC	1.56	0.70
1:N:24:TYR:CD2	21:N:601:CHL:HAA2	2.25	0.70
1:N:142:ARG:HA	21:N:607:CHL:C4C	2.21	0.70
4:c:272:LEU:CG	22:c:510:CLA:C4C	2.69	0.70
36:b:620:LMG:C23	21:r:307:CHL:CHD	2.58	0.70
1:g:142:ARG:HA	21:g:608:CHL:C4C	2.21	0.70
2:a:301:ASN:O	4:c:405:ASN:ND2	2.24	0.70
23:G:615:LUT:H7	23:G:616:LUT:H21	1.72	0.70
1:Y:131:GLN:HE22	21:Y:606:CHL:HMC	1.57	0.70
31:D:406:BCR:H16C	7:F:27:PHE:HD2	1.54	0.70
1:n:102:SER:HB3	21:n:606:CHL:O2D	1.92	0.70
1:Y:71:TRP:NE1	21:Y:608:CHL:HMD3	2.05	0.70
5:d:89:SER:OG	6:e:69:ARG:NH2	2.25	0.70
3:B:323:GLY:H	3:B:326:ARG:HD2	1.56	0.70
1:g:71:TRP:NE1	21:g:609:CHL:HMD3	2.05	0.70
1:G:142:ARG:HA	21:G:608:CHL:C4C	2.21	0.70
21:G:609:CHL:H92	21:N:601:CHL:H62	1.74	0.70
26:D:409:LHG:HC12	12:L:16:THR:HG21	1.73	0.70
20:S:119:LEU:HD11	21:S:307:CHL:HMD1	1.70	0.70
1:y:142:ARG:HA	21:y:608:CHL:C4C	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:131:GLN:HE22	21:N:606:CHL:HMC	1.56	0.70
26:s:314:LHG:H301	26:s:314:LHG:HC92	1.74	0.70
1:y:71:TRP:NE1	21:y:609:CHL:HMD3	2.06	0.70
1:N:197:GLN:HG3	22:N:612:CLA:NA	2.05	0.70
6:E:19:TYR:O	6:E:23:HIS:ND1	2.24	0.70
1:n:25:LEU:HB2	1:n:29:SER:HA	1.73	0.70
1:n:142:ARG:HA	21:n:607:CHL:C4C	2.22	0.70
1:Y:25:LEU:HB2	1:Y:29:SER:HA	1.73	0.70
1:Y:142:ARG:HA	21:Y:607:CHL:C4C	2.21	0.70
6:e:19:TYR:O	6:e:23:HIS:ND1	2.24	0.70
21:S:302:CHL:HBC3	21:S:302:CHL:OMC	1.91	0.70
21:g:605:CHL:HBC1	21:g:606:CHL:HMD1	1.74	0.70
1:y:25:LEU:HB2	1:y:29:SER:HA	1.73	0.70
1:G:25:LEU:HB2	1:G:29:SER:HA	1.73	0.70
1:Y:142:ARG:CG	21:Y:607:CHL:CHD	2.70	0.70
20:s:101:TYR:CE2	21:s:301:CHL:HMA3	2.27	0.70
4:c:272:LEU:CG	22:c:510:CLA:C1D	2.70	0.69
4:C:272:LEU:CG	22:C:511:CLA:C4C	2.69	0.69
6:e:57:THR:O	6:e:61:GLN:NE2	2.25	0.69
20:s:141:ALA:CB	21:s:306:CHL:HED2	2.21	0.69
21:s:302:CHL:HBC3	21:s:302:CHL:OMC	1.92	0.69
20:S:34:PHE:CD2	21:S:302:CHL:HAA2	2.28	0.69
1:Y:197:GLN:HG3	22:Y:611:CLA:NA	2.05	0.69
14:O:49:LYS:HG2	14:O:50:LYS:HG2	1.75	0.69
3:b:400:GLU:OE1	3:b:410:THR:OG1	2.10	0.69
4:C:272:LEU:CG	22:C:511:CLA:C1D	2.70	0.69
20:s:34:PHE:CD2	21:s:302:CHL:HAA2	2.27	0.69
21:G:609:CHL:H111	21:N:601:CHL:C11	2.22	0.69
21:N:605:CHL:HMD1	21:S:301:CHL:HBC1	1.74	0.69
2:a:333:GLU:N	29:a:403:CL:CL	2.60	0.69
4:C:422:PRO:HA	4:C:425:TRP:HD1	1.58	0.69
1:n:131:GLN:HE22	21:n:606:CHL:HMC	1.57	0.69
1:y:131:GLN:HE22	21:y:607:CHL:HMC	1.57	0.69
1:G:142:ARG:HG3	21:G:608:CHL:HHD	1.74	0.69
1:Y:136:GLY:HA2	21:Y:608:CHL:CBB	2.22	0.69
3:B:273:TYR:CG	35:H:102:DGD:HD61	2.27	0.69
4:C:272:LEU:CD1	22:C:511:CLA:CHD	2.70	0.69
19:r:95:CYS:O	19:r:99:HIS:ND1	2.25	0.69
20:S:141:ALA:CB	21:S:306:CHL:HED2	2.22	0.69
1:N:142:ARG:CG	21:N:607:CHL:CHD	2.70	0.69
3:b:121:GLU:HG2	8:h:14:PRO:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:s:101:TYR:OH	21:s:301:CHL:CBD	2.40	0.69
20:s:110:VAL:HB	20:s:113:LYS:HB2	1.74	0.69
19:R:95:CYS:O	19:R:99:HIS:ND1	2.25	0.69
1:n:131:GLN:OE1	21:n:605:CHL:C1B	2.41	0.69
1:y:131:GLN:OE1	21:y:606:CHL:C1B	2.41	0.69
3:b:323:GLY:H	3:b:326:ARG:HD2	1.56	0.69
20:s:34:PHE:CE2	21:s:302:CHL:HAA2	2.28	0.69
20:S:98:PHE:CZ	21:S:301:CHL:HED1	2.28	0.68
1:g:131:GLN:HE22	21:g:607:CHL:HMC	1.56	0.68
1:g:71:TRP:CZ2	21:g:609:CHL:CHD	2.76	0.68
1:G:102:SER:HB3	21:G:607:CHL:O2D	1.93	0.68
21:G:607:CHL:CMA	23:G:616:LUT:H172	2.23	0.68
26:N:618:LHG:H291	26:N:618:LHG:H171	1.75	0.68
1:Y:71:TRP:CZ2	21:Y:608:CHL:CHD	2.76	0.68
1:y:142:ARG:HG3	21:y:608:CHL:HHH	1.74	0.68
1:y:142:ARG:HA	21:y:608:CHL:CBC	2.24	0.68
1:N:131:GLN:OE1	21:N:605:CHL:C1B	2.42	0.68
21:Y:606:CHL:HMA3	23:Y:614:LUT:C17	2.22	0.68
2:a:56:PRO:HA	2:a:73:TYR:HE2	1.59	0.68
2:A:82:ILE:HB	2:A:174:LEU:HB2	1.75	0.68
1:g:25:LEU:HB2	1:g:29:SER:HA	1.73	0.68
23:g:615:LUT:H182	23:g:616:LUT:H192	1.74	0.68
26:S:314:LHG:H301	26:S:314:LHG:HC92	1.74	0.68
1:g:142:ARG:HA	21:g:608:CHL:CBC	2.24	0.68
1:G:131:GLN:OE1	21:G:606:CHL:C1B	2.42	0.68
1:N:25:LEU:HB2	1:N:29:SER:HA	1.73	0.68
4:c:272:LEU:CD1	22:c:510:CLA:CHD	2.70	0.68
21:n:605:CHL:HMA2	25:n:616:NEX:H32	1.74	0.68
1:y:102:SER:HB3	21:y:607:CHL:HED3	0.68	0.68
1:N:142:ARG:HA	21:N:607:CHL:CBC	2.24	0.68
7:F:18:HIS:HD2	37:F:101:HEM:C1A	2.12	0.68
22:s:305:CLA:HED2	22:s:305:CLA:H2A	1.76	0.68
20:S:34:PHE:CE2	21:S:302:CHL:HAA2	2.28	0.68
21:y:605:CHL:HBC1	21:y:606:CHL:HMD1	1.71	0.68
1:N:71:TRP:NE1	21:N:608:CHL:HMD3	2.06	0.68
2:a:82:ILE:HB	2:a:174:LEU:HB2	1.75	0.68
36:B:623:LMG:H221	21:R:306:CHL:NB	2.09	0.68
20:S:110:VAL:HB	20:S:113:LYS:HB2	1.74	0.68
1:n:142:ARG:HG3	21:n:607:CHL:HHH	1.74	0.68
1:G:142:ARG:CG	21:G:608:CHL:CHD	2.70	0.68
1:N:71:TRP:CZ2	21:N:608:CHL:CHD	2.77	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:142:ARG:C	21:N:607:CHL:CBC	2.67	0.68
6:E:57:THR:O	6:E:61:GLN:NE2	2.25	0.68
1:g:131:GLN:OE1	21:g:606:CHL:C1B	2.42	0.68
1:n:71:TRP:CZ2	21:n:608:CHL:CHD	2.76	0.68
1:G:142:ARG:HA	21:G:608:CHL:CBC	2.24	0.68
1:y:142:ARG:CG	21:y:608:CHL:CHD	2.70	0.67
1:Y:142:ARG:C	21:Y:607:CHL:CBC	2.67	0.67
4:c:229:ASP:N	4:c:229:ASP:OD1	2.28	0.67
1:g:102:SER:HB3	21:g:607:CHL:HED3	0.70	0.67
1:g:102:SER:CB	21:g:607:CHL:CED	2.24	0.67
1:n:142:ARG:HA	21:n:607:CHL:CBC	2.24	0.67
1:y:142:ARG:C	21:y:608:CHL:CBC	2.67	0.67
1:G:142:ARG:C	21:G:608:CHL:CBC	2.67	0.67
1:Y:142:ARG:HA	21:Y:607:CHL:CBC	2.24	0.67
3:B:400:GLU:OE1	3:B:410:THR:OG1	2.10	0.67
1:y:136:GLY:HA2	21:y:609:CHL:CBB	2.24	0.67
22:N:602:CLA:H122	23:N:615:LUT:H393	1.77	0.67
3:B:156:PHE:HB3	3:B:162:PHE:HB3	1.77	0.67
19:R:173:TYR:HB3	22:R:309:CLA:HED2	1.76	0.67
3:b:220:ARG:NE	8:h:32:LYS:O	2.22	0.67
4:c:422:PRO:HA	4:c:425:TRP:HD1	1.57	0.67
7:f:18:HIS:HD2	37:f:101:HEM:C1A	2.12	0.67
1:G:71:TRP:CZ2	21:G:609:CHL:CHD	2.76	0.67
1:N:136:GLY:HA2	21:N:608:CHL:CBB	2.24	0.67
4:C:229:ASP:N	4:C:229:ASP:OD1	2.28	0.67
1:Y:131:GLN:OE1	21:Y:605:CHL:C1B	2.42	0.67
1:g:142:ARG:C	21:g:608:CHL:CBC	2.67	0.67
1:n:142:ARG:C	21:n:607:CHL:CBC	2.68	0.67
1:n:182:LYS:NZ	26:n:617:LHG:O4	2.28	0.67
1:y:71:TRP:CZ2	21:y:609:CHL:CHD	2.77	0.67
1:Y:142:ARG:HG3	21:Y:607:CHL:HHH	1.74	0.67
21:y:606:CHL:H3A	25:y:616:NEX:H31	1.77	0.67
23:Y:613:LUT:H182	23:Y:614:LUT:H192	1.76	0.67
14:o:49:LYS:HG2	14:o:50:LYS:HG2	1.75	0.67
1:n:142:ARG:CG	21:n:607:CHL:CHD	2.70	0.66
21:y:601:CHL:CHD	26:y:617:LHG:C8	2.73	0.66
1:N:142:ARG:HG3	21:N:607:CHL:HHH	1.74	0.66
25:y:616:NEX:H371	25:y:616:NEX:H28	1.75	0.66
22:G:602:CLA:H122	23:G:616:LUT:H393	1.76	0.66
3:b:156:PHE:HB3	3:b:162:PHE:HB3	1.77	0.66
21:N:608:CHL:CGA	21:Y:601:CHL:H2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:605:CHL:CMD	21:r:301:CHL:HBC3	2.25	0.66
19:r:173:TYR:HB3	22:r:310:CLA:HED2	1.76	0.66
22:S:305:CLA:HED2	22:S:305:CLA:H2A	1.75	0.66
21:n:605:CHL:CMD	21:s:301:CHL:HBC3	2.24	0.66
36:b:620:LMG:C27	21:r:306:CHL:OMC	2.44	0.66
26:c:521:LHG:O1	26:c:522:LHG:O5	2.14	0.66
19:R:155:ILE:HD12	19:R:158:ILE:HD11	1.77	0.66
1:G:136:GLY:HA2	21:G:609:CHL:CBB	2.24	0.66
1:Y:79:CYS:SG	23:Y:614:LUT:O3	2.48	0.66
4:c:272:LEU:HD13	22:c:510:CLA:NC	2.11	0.66
22:y:612:CLA:HBD	22:y:612:CLA:HAA1	1.77	0.66
21:G:601:CHL:C1D	26:G:618:LHG:H102	2.26	0.66
1:N:102:SER:HB3	21:N:606:CHL:O2D	1.93	0.66
1:y:142:ARG:CG	21:y:608:CHL:C1D	2.72	0.66
1:G:203:LYS:HB2	1:G:208:ASN:HD21	1.61	0.66
21:n:605:CHL:HBA2	21:n:605:CHL:CHA	2.26	0.66
21:Y:605:CHL:HBA2	21:Y:605:CHL:CHA	2.26	0.66
22:n:612:CLA:HAA1	22:n:612:CLA:HBD	1.77	0.65
1:y:119:VAL:HG13	21:y:605:CHL:HHH	1.78	0.65
22:G:613:CLA:HBD	22:G:613:CLA:HAA1	1.77	0.65
1:N:203:LYS:HB2	1:N:208:ASN:HD21	1.61	0.65
2:A:56:PRO:HA	2:A:73:TYR:HE2	1.59	0.65
20:S:101:TYR:HE1	21:S:301:CHL:H2A	0.53	0.65
1:n:203:LYS:HB2	1:n:208:ASN:HD21	1.61	0.65
21:y:605:CHL:HBC3	21:y:606:CHL:CMD	2.25	0.65
2:A:301:ASN:O	4:C:405:ASN:ND2	2.29	0.65
3:B:283:GLU:OE2	3:B:286:ARG:NH2	2.29	0.65
36:B:623:LMG:C26	21:R:305:CHL:C2C	2.52	0.65
19:r:155:ILE:HD12	19:r:158:ILE:HD11	1.77	0.65
1:y:101:GLY:HA2	21:y:606:CHL:HBC1	1.79	0.65
21:N:605:CHL:HBA2	21:N:605:CHL:CHA	2.26	0.65
1:Y:101:GLY:HA2	21:Y:605:CHL:HBC1	1.79	0.65
3:b:477:ASP:N	3:b:477:ASP:OD1	2.26	0.65
1:g:203:LYS:HB2	1:g:208:ASN:HD21	1.61	0.65
1:n:142:ARG:HA	21:n:607:CHL:CHD	2.26	0.65
1:y:142:ARG:HA	21:y:608:CHL:CHD	2.26	0.65
1:G:24:TYR:HD2	21:G:601:CHL:HAA2	1.61	0.65
1:n:101:GLY:HA2	21:n:605:CHL:HBC1	1.78	0.65
1:G:197:GLN:HE21	22:G:613:CLA:H2A	1.62	0.65
1:Y:203:LYS:HB2	1:Y:208:ASN:HD21	1.61	0.65
23:Y:613:LUT:H7	23:Y:614:LUT:H21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:67:ILE:HG22	21:y:609:CHL:CMD	2.27	0.65
2:a:215:HIS:NE2	34:a:412:BCT:O1	2.30	0.65
3:b:235:GLU:OE2	3:b:469:HIS:ND1	2.29	0.65
1:g:67:ILE:HG22	21:g:609:CHL:CMD	2.27	0.65
1:g:142:ARG:CG	21:g:608:CHL:CHD	2.70	0.65
1:G:142:ARG:HA	21:G:608:CHL:CHD	2.26	0.65
1:G:142:ARG:CG	21:G:608:CHL:C1D	2.72	0.65
1:N:101:GLY:HA2	21:N:605:CHL:HBC1	1.79	0.65
1:N:142:ARG:HA	21:N:607:CHL:CHD	2.26	0.65
22:N:612:CLA:HBD	22:N:612:CLA:HAA1	1.77	0.65
1:Y:142:ARG:HA	21:Y:607:CHL:CHD	2.26	0.65
22:Y:611:CLA:HBD	22:Y:611:CLA:HAA1	1.77	0.65
7:f:11:THR:HB	7:f:14:TRP:HB3	1.77	0.65
36:B:623:LMG:H232	21:R:306:CHL:C4C	2.26	0.65
1:y:24:TYR:HD2	21:y:601:CHL:HAA2	1.61	0.65
1:y:102:SER:HB3	21:y:607:CHL:O2D	1.95	0.65
1:N:67:ILE:HG22	21:N:608:CHL:CMD	2.27	0.65
4:c:461:ARG:NH1	5:d:226:ASP:OD2	2.28	0.65
14:o:36:VAL:HG12	14:o:38:SER:H	1.61	0.65
14:O:47:ASN:HB2	14:O:247:GLU:HB2	1.79	0.65
21:g:606:CHL:HMA2	25:g:618:NEX:H32	1.77	0.65
1:y:203:LYS:HB2	1:y:208:ASN:HD21	1.61	0.65
21:Y:601:CHL:CHD	26:Y:617:LHG:HC82	2.26	0.65
20:s:220:LYS:O	20:s:228:ASN:ND2	2.30	0.65
21:g:606:CHL:HBA2	21:g:606:CHL:CHA	2.26	0.65
1:n:24:TYR:HD2	21:n:601:CHL:HAA2	1.61	0.65
1:n:121:ALA:HB1	21:s:301:CHL:HBC2	0.71	0.65
1:y:197:GLN:HE21	22:y:612:CLA:H2A	1.62	0.65
26:C:521:LHG:O1	26:C:522:LHG:O5	2.14	0.65
1:g:136:GLY:HA2	21:g:609:CHL:CBB	2.24	0.64
22:Y:611:CLA:H102	24:Y:615:XAT:H14	1.79	0.64
36:B:623:LMG:H202	21:R:306:CHL:NB	2.13	0.64
6:E:23:HIS:CE1	7:F:18:HIS:HE2	2.15	0.64
36:I:101:LMG:HC5	36:I:101:LMG:H322	1.78	0.64
14:O:36:VAL:HG12	14:O:38:SER:H	1.62	0.64
20:S:220:LYS:O	20:S:228:ASN:ND2	2.30	0.64
1:g:142:ARG:HA	21:g:608:CHL:CHD	2.26	0.64
22:g:613:CLA:HBD	22:g:613:CLA:HAA1	1.77	0.64
1:Y:102:SER:HB3	21:Y:606:CHL:O2D	1.94	0.64
1:g:197:GLN:HE21	22:g:613:CLA:H2A	1.62	0.64
20:S:101:TYR:CG	21:S:301:CHL:CMA	2.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:24:TYR:HD2	21:Y:601:CHL:HAA2	1.61	0.64
1:Y:197:GLN:HE21	22:Y:611:CLA:H2A	1.62	0.64
21:Y:606:CHL:CMA	23:Y:614:LUT:H172	2.26	0.64
4:c:418:ASN:HD21	35:c:518:DGD:HD62	1.62	0.64
12:L:15:ARG:NH2	15:T:25:GLU:OE1	2.30	0.64
1:n:136:GLY:HA2	21:n:608:CHL:CBB	2.24	0.64
21:Y:605:CHL:HAA1	25:Y:616:NEX:C31	2.26	0.64
5:d:267:TRP:CD1	26:d:408:LHG:HO1	2.15	0.64
1:n:119:VAL:HG13	21:s:301:CHL:HHD	1.79	0.64
1:n:197:GLN:HE21	22:n:612:CLA:H2A	1.62	0.64
36:B:601:LMG:H322	36:B:601:LMG:HC5	1.79	0.64
5:D:267:TRP:CD1	26:D:409:LHG:HO1	2.16	0.64
7:F:11:THR:HB	7:F:14:TRP:HB3	1.77	0.64
1:g:142:ARG:HG3	21:g:608:CHL:HHD	1.74	0.64
1:G:119:VAL:HG13	21:G:605:CHL:HHD	1.80	0.64
21:g:609:CHL:H111	21:n:601:CHL:H121	1.79	0.64
21:y:606:CHL:HBA2	21:y:606:CHL:CHA	2.26	0.64
21:Y:605:CHL:HMD1	21:r:301:CHL:HBC1	1.73	0.64
20:s:28:GLY:O	20:s:31:ARG:NH1	2.30	0.64
20:s:101:TYR:CE2	21:s:301:CHL:O1D	2.51	0.64
1:G:101:GLY:HA2	21:G:606:CHL:HBC1	1.79	0.64
1:N:119:VAL:HG13	21:S:301:CHL:HHD	1.80	0.64
1:N:197:GLN:HE21	22:N:612:CLA:H2A	1.62	0.64
3:b:15:ASP:OD2	12:l:5:ASN:ND2	2.31	0.64
26:C:521:LHG:H211	16:W:28:GLY:HA2	1.80	0.64
21:g:605:CHL:HBC3	21:g:606:CHL:CMD	2.27	0.63
1:N:182:LYS:NZ	26:N:618:LHG:O4	2.30	0.63
1:Y:67:ILE:HG22	21:Y:608:CHL:CMD	2.27	0.63
1:Y:119:VAL:HG13	21:r:301:CHL:HHD	1.80	0.63
3:b:283:GLU:OE2	3:b:286:ARG:NH2	2.29	0.63
4:c:148:GLY:O	4:c:156:LYS:NZ	2.31	0.63
4:C:272:LEU:HD12	22:C:511:CLA:C1D	2.27	0.63
4:C:418:ASN:HD21	35:C:519:DGD:HD62	1.62	0.63
20:S:28:GLY:O	20:S:31:ARG:NH1	2.30	0.63
21:G:601:CHL:H71	22:Y:603:CLA:C2D	2.27	0.63
1:N:142:ARG:C	21:N:607:CHL:HBC3	2.24	0.63
36:B:623:LMG:H111	21:R:306:CHL:HBA1	1.79	0.63
1:g:101:GLY:HA2	21:g:606:CHL:HBC1	1.79	0.63
1:g:119:VAL:HG13	21:g:605:CHL:HHD	1.81	0.63
21:G:606:CHL:HBA2	21:G:606:CHL:CHA	2.26	0.63
1:n:102:SER:CB	21:n:606:CHL:CED	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:603:CLA:H62	22:Y:603:CLA:H101	1.81	0.63
21:N:605:CHL:CMD	21:S:301:CHL:HBC3	2.25	0.63
14:o:47:ASN:HB2	14:o:247:GLU:HB2	1.79	0.63
4:C:148:GLY:O	4:C:156:LYS:NZ	2.31	0.63
22:R:311:CLA:HED2	22:R:311:CLA:H2A	1.81	0.63
1:g:102:SER:HB3	21:g:607:CHL:O2D	1.95	0.63
1:g:142:ARG:CG	21:g:608:CHL:C1D	2.72	0.63
21:y:601:CHL:HMD1	26:y:617:LHG:H251	1.79	0.63
1:g:136:GLY:CA	21:g:609:CHL:HBB1	2.25	0.63
1:n:26:GLY:CA	21:n:601:CHL:OMC	2.47	0.63
14:o:62:SER:OG	14:o:74:GLN:NE2	2.31	0.63
36:B:623:LMG:H242	21:R:305:CHL:CMC	2.29	0.63
19:r:221:LYS:HE2	19:r:226:PHE:HZ	1.63	0.63
22:r:312:CLA:HED2	22:r:312:CLA:H2A	1.81	0.63
20:s:29:PRO:O	20:s:42:ARG:NH2	2.32	0.63
1:N:142:ARG:CG	21:N:607:CHL:C1D	2.72	0.63
33:d:402:SQD:H45	26:d:409:LHG:H152	1.80	0.63
2:A:305:SER:HA	10:J:39:SER:HB3	1.79	0.63
1:g:24:TYR:HD2	21:g:601:CHL:HAA2	1.61	0.63
23:g:615:LUT:H8	23:g:616:LUT:H41	1.80	0.63
1:y:142:ARG:C	21:y:608:CHL:HBC3	2.24	0.63
4:c:387:TRP:HA	4:c:390:ARG:HD3	1.81	0.63
5:d:231:ASN:ND2	33:d:402:SQD:O8	2.32	0.63
36:B:623:LMG:H242	21:R:305:CHL:HMC	1.81	0.63
14:O:62:SER:OG	14:O:74:GLN:NE2	2.31	0.63
1:g:142:ARG:C	21:g:608:CHL:HBC3	2.24	0.63
1:Y:26:GLY:CA	21:Y:601:CHL:OMC	2.47	0.63
3:B:477:ASP:OD1	3:B:477:ASP:N	2.26	0.63
20:s:119:LEU:CD1	21:s:307:CHL:HMD3	2.27	0.63
1:g:26:GLY:CA	21:g:601:CHL:OMC	2.47	0.62
1:g:153:ASP:OD1	1:g:156:TYR:N	2.32	0.62
1:y:26:GLY:CA	21:y:601:CHL:OMC	2.47	0.62
21:G:609:CHL:H111	21:N:601:CHL:H101	1.80	0.62
1:N:96:VAL:HB	1:N:99:LYS:HB2	1.81	0.62
1:N:153:ASP:OD1	1:N:156:TYR:N	2.32	0.62
1:Y:136:GLY:CA	21:Y:608:CHL:HBB1	2.24	0.62
1:Y:153:ASP:OD1	1:Y:156:TYR:N	2.32	0.62
36:B:623:LMG:C25	21:R:306:CHL:CHD	2.76	0.62
22:S:305:CLA:H11	21:S:306:CHL:CAD	2.29	0.62
21:S:306:CHL:HBB2	21:S:307:CHL:HBB1	1.81	0.62
1:y:96:VAL:HB	1:y:99:LYS:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:142:ARG:C	21:Y:607:CHL:HBC3	2.24	0.62
4:c:272:LEU:HD12	22:c:510:CLA:C1D	2.28	0.62
4:c:333:GLY:N	4:c:337:LEU:O	2.27	0.62
1:G:26:GLY:CA	21:G:601:CHL:OMC	2.47	0.62
1:N:24:TYR:HD2	21:N:601:CHL:HAA2	1.61	0.62
2:a:228:THR:OG1	2:a:230:ASN:OD1	2.17	0.62
1:n:153:ASP:OD1	1:n:156:TYR:N	2.32	0.62
4:c:259:TRP:HA	4:c:262:ARG:HG2	1.81	0.62
4:C:259:TRP:HA	4:C:262:ARG:HG2	1.81	0.62
1:G:136:GLY:CA	21:G:609:CHL:HBB1	2.25	0.62
1:G:142:ARG:C	21:G:608:CHL:HBC3	2.24	0.62
3:B:235:GLU:OE2	3:B:469:HIS:ND1	2.29	0.62
1:n:67:ILE:HG22	21:n:608:CHL:CMD	2.27	0.62
1:N:26:GLY:CA	21:N:601:CHL:OMC	2.47	0.62
22:b:606:CLA:H2	36:T:101:LMG:H222	1.82	0.62
4:c:371:GLY:N	4:c:374:GLY:O	2.28	0.62
2:A:228:THR:OG1	2:A:230:ASN:OD1	2.17	0.62
1:g:96:VAL:HB	1:g:99:LYS:HB2	1.82	0.62
1:n:142:ARG:C	21:n:607:CHL:HBC3	2.24	0.62
1:Y:121:ALA:HB1	21:r:301:CHL:HBC2	0.66	0.62
22:B:606:CLA:H142	22:B:612:CLA:H92	1.82	0.62
22:s:305:CLA:H11	21:s:306:CHL:CAD	2.28	0.62
1:y:123:SER:N	21:y:605:CHL:OMC	2.28	0.62
1:G:153:ASP:OD1	1:G:156:TYR:N	2.32	0.62
1:N:136:GLY:CA	21:N:608:CHL:HBB1	2.25	0.62
36:b:620:LMG:H142	21:r:307:CHL:HBA1	1.81	0.62
35:h:102:DGD:O5D	35:h:102:DGD:O4D	2.16	0.62
2:A:321:ILE:O	2:A:325:ASN:ND2	2.33	0.62
20:S:29:PRO:O	20:S:42:ARG:NH2	2.32	0.62
19:R:221:LYS:HE2	19:R:226:PHE:HZ	1.63	0.62
1:g:121:ALA:HB1	21:g:605:CHL:HBC2	0.68	0.62
1:y:153:ASP:OD1	1:y:156:TYR:N	2.32	0.62
1:G:96:VAL:HB	1:G:99:LYS:HB2	1.82	0.62
1:Y:96:VAL:HB	1:Y:99:LYS:HB2	1.82	0.62
21:n:607:CHL:HBA2	21:n:607:CHL:CBD	2.30	0.62
21:G:608:CHL:HBA2	21:G:608:CHL:CBD	2.30	0.62
4:C:405:ASN:HA	35:J:101:DGD:HB21	1.82	0.62
18:Z:57:LEU:HD23	18:Z:60:LEU:HD12	1.82	0.62
21:g:607:CHL:CMA	23:g:616:LUT:H172	2.30	0.61
1:n:96:VAL:HB	1:n:99:LYS:HB2	1.82	0.61
1:G:25:LEU:O	21:G:601:CHL:CBB	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:308:ASP:OD1	2:a:312:ARG:N	2.31	0.61
36:B:623:LMG:C24	21:R:305:CHL:CMC	2.78	0.61
1:y:69:SER:HB3	1:y:184:GLY:HA3	1.82	0.61
2:a:303:ASN:O	4:c:415:ASN:ND2	2.33	0.61
21:g:608:CHL:HBA2	21:g:608:CHL:CBD	2.30	0.61
8:h:31:GLY:O	19:r:47:GLN:NE2	2.33	0.61
4:C:232:ASP:OD1	4:C:232:ASP:N	2.30	0.61
22:g:604:CLA:NB	25:g:618:NEX:H242	2.15	0.61
1:n:69:SER:HB3	1:n:184:GLY:HA3	1.82	0.61
21:Y:607:CHL:HBA2	21:Y:607:CHL:CBD	2.30	0.61
36:b:620:LMG:H261	21:r:306:CHL:OMC	1.98	0.61
4:C:333:GLY:N	4:C:337:LEU:O	2.27	0.61
21:s:306:CHL:HMC	21:s:307:CHL:C4C	2.30	0.61
1:Y:69:SER:HB3	1:Y:184:GLY:HA3	1.82	0.61
4:c:154:ARG:NH2	16:w:49:GLU:OE1	2.33	0.61
4:c:335:THR:O	14:o:152:ARG:NH2	2.33	0.61
1:y:25:LEU:O	21:y:601:CHL:CBB	2.48	0.61
26:G:618:LHG:O1	26:G:618:LHG:O3	2.18	0.61
21:N:607:CHL:HBA2	21:N:607:CHL:CBD	2.30	0.61
1:G:69:SER:HB3	1:G:184:GLY:HA3	1.82	0.61
3:b:125:ASP:O	3:b:129:GLY:N	2.32	0.61
2:A:334:ARG:O	5:D:351:ASN:ND2	2.34	0.61
4:C:387:TRP:HA	4:C:390:ARG:HD3	1.81	0.61
20:S:59:TYR:CE1	21:S:302:CHL:HBA1	2.36	0.61
1:g:69:SER:HB3	1:g:184:GLY:HA3	1.82	0.61
1:n:136:GLY:CA	21:n:608:CHL:HBB1	2.25	0.61
1:N:69:SER:HB3	1:N:184:GLY:HA3	1.82	0.61
4:c:232:ASP:OD1	4:c:232:ASP:N	2.30	0.61
20:S:101:TYR:CG	21:S:301:CHL:HMA3	2.34	0.61
21:y:601:CHL:CHD	26:y:617:LHG:HC81	2.31	0.61
21:y:608:CHL:HBA2	21:y:608:CHL:CBD	2.30	0.61
1:Y:142:ARG:CG	21:Y:607:CHL:C1D	2.72	0.61
26:d:408:LHG:O3	26:d:408:LHG:O1	2.17	0.61
33:D:402:SQD:H45	26:D:410:LHG:H152	1.83	0.61
20:s:115:GLY:O	21:s:307:CHL:HMD2	1.99	0.61
21:n:607:CHL:H92	20:s:173:LEU:HD11	1.82	0.61
2:a:321:ILE:O	2:a:325:ASN:ND2	2.33	0.61
21:s:306:CHL:HBB2	21:s:307:CHL:HBB1	1.82	0.61
1:g:138:VAL:CG1	21:g:608:CHL:CMB	2.79	0.60
21:g:607:CHL:CMB	21:n:601:CHL:H202	2.32	0.60
1:n:25:LEU:O	21:n:601:CHL:CBB	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:102:SER:CB	21:N:606:CHL:CED	2.27	0.60
18:z:57:LEU:HD23	18:z:60:LEU:HD12	1.82	0.60
2:A:257:ARG:HH12	3:B:490:VAL:C	2.10	0.60
3:B:475:PHE:HE1	5:D:135:ARG:HD2	1.65	0.60
20:s:111:TRP:HZ2	22:s:305:CLA:HMB2	1.66	0.60
22:S:310:CLA:H3A	22:S:310:CLA:O2A	2.01	0.60
1:n:138:VAL:CG1	21:n:607:CHL:CMB	2.79	0.60
1:n:142:ARG:CG	21:n:607:CHL:C1D	2.72	0.60
1:G:138:VAL:CG1	21:G:608:CHL:CMB	2.79	0.60
1:N:138:VAL:CG1	21:N:607:CHL:CMB	2.79	0.60
1:Y:138:VAL:HG11	21:Y:607:CHL:CMB	2.32	0.60
22:b:603:CLA:H142	22:b:609:CLA:H92	1.82	0.60
4:c:279:LEU:HB3	4:c:437:LEU:HD23	1.83	0.60
3:B:125:ASP:O	3:B:129:GLY:N	2.32	0.60
7:F:18:HIS:HD2	37:F:101:HEM:NA	2.00	0.60
20:S:111:TRP:HZ2	22:S:305:CLA:HMB2	1.66	0.60
1:Y:138:VAL:CG1	21:Y:607:CHL:CMB	2.79	0.60
35:c:518:DGD:HAF1	10:j:25:ILE:HG21	1.83	0.60
20:s:59:TYR:CE1	21:s:302:CHL:HBA1	2.36	0.60
19:R:144:LEU:HD12	26:R:301:LHG:H251	1.82	0.60
19:R:151:GLU:CD	21:R:305:CHL:HMB1	2.27	0.60
1:G:67:ILE:HG22	21:G:609:CHL:CMD	2.27	0.60
21:G:601:CHL:H52	21:Y:608:CHL:O1A	2.01	0.60
34:a:412:BCT:O1	5:d:215:HIS:NE2	2.26	0.60
14:o:128:PHE:HA	14:o:222:GLN:HE22	1.66	0.60
12:L:9:GLN:O	33:L:102:SQD:O3	2.19	0.60
1:N:25:LEU:O	21:N:601:CHL:CBB	2.48	0.60
1:Y:225:ALA:HA	24:Y:615:XAT:H42	1.83	0.60
22:B:609:CLA:H2	36:M:101:LMG:H222	1.82	0.60
20:S:115:GLY:O	21:S:307:CHL:HMD2	2.02	0.60
21:n:607:CHL:HBC3	21:n:607:CHL:HHB	1.84	0.60
1:G:121:ALA:HB1	21:G:605:CHL:HBC2	0.68	0.60
1:N:121:ALA:HB1	21:S:301:CHL:HBC2	0.66	0.60
13:m:15:ILE:O	13:m:19:THR:OG1	2.19	0.60
20:S:210:THR:HG21	20:S:217:ASN:HD21	1.67	0.60
1:g:197:GLN:HE22	22:g:613:CLA:CGD	2.15	0.60
1:y:138:VAL:CG1	21:y:608:CHL:CMB	2.79	0.60
1:Y:197:GLN:HE22	22:Y:611:CLA:CGD	2.15	0.60
2:A:131:TRP:HZ2	4:C:449:ARG:HD2	1.67	0.60
19:R:14:TRP:H	19:R:14:TRP:CD1	2.18	0.60
1:g:25:LEU:O	21:g:601:CHL:CBB	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:197:GLN:HE22	22:N:612:CLA:CGD	2.15	0.60
1:Y:25:LEU:O	21:Y:601:CHL:CBB	2.49	0.60
21:Y:605:CHL:H3A	25:Y:616:NEX:H31	1.82	0.60
7:f:18:HIS:HA	37:f:101:HEM:NC	2.17	0.60
2:A:303:ASN:O	4:C:415:ASN:ND2	2.35	0.60
19:r:14:TRP:CD1	19:r:14:TRP:H	2.18	0.60
22:s:310:CLA:H3A	22:s:310:CLA:O2A	2.00	0.60
4:C:48:LYS:NZ	4:C:133:ALA:O	2.35	0.60
1:G:79:CYS:SG	23:G:616:LUT:O3	2.59	0.59
1:n:138:VAL:HG11	21:n:607:CHL:CMB	2.32	0.59
1:y:197:GLN:HE22	22:y:612:CLA:CGD	2.15	0.59
21:y:605:CHL:HMA2	21:y:605:CHL:C1	2.29	0.59
21:G:608:CHL:HBC3	21:G:608:CHL:HHH	1.83	0.59
4:c:405:ASN:HA	35:c:519:DGD:HB21	1.82	0.59
1:n:197:GLN:HE22	22:n:612:CLA:CGD	2.15	0.59
1:y:136:GLY:CA	21:y:609:CHL:HBB1	2.26	0.59
1:N:138:VAL:HG11	21:N:607:CHL:CMB	2.32	0.59
23:N:614:LUT:H7	23:N:615:LUT:H21	1.83	0.59
20:s:101:TYR:HH	21:s:301:CHL:CHA	2.11	0.59
21:g:608:CHL:HBC3	21:g:608:CHL:HHH	1.83	0.59
1:y:101:GLY:HA2	21:y:606:CHL:CBC	2.33	0.59
1:G:197:GLN:HE22	22:G:613:CLA:CGD	2.15	0.59
1:Y:101:GLY:HA2	21:Y:605:CHL:CBC	2.33	0.59
13:M:15:ILE:O	13:M:19:THR:OG1	2.19	0.59
14:O:128:PHE:HA	14:O:222:GLN:HE22	1.66	0.59
1:y:138:VAL:HG11	21:y:608:CHL:CMB	2.32	0.59
2:A:308:ASP:OD1	2:A:312:ARG:N	2.31	0.59
3:B:440:ASP:O	14:O:179:ARG:NH1	2.35	0.59
14:O:158:ASP:OD1	14:O:162:ARG:N	2.35	0.59
20:s:157:GLY:H	20:s:160:LEU:HD11	1.67	0.59
20:S:157:GLY:H	20:S:160:LEU:HD11	1.67	0.59
1:n:208:ASN:HB2	22:n:612:CLA:HMA3	1.84	0.59
33:A:412:SQD:H142	33:A:412:SQD:H281	1.84	0.59
1:y:119:VAL:HG13	21:y:605:CHL:CHD	2.32	0.59
21:y:608:CHL:HBC3	21:y:608:CHL:HHH	1.83	0.59
1:G:138:VAL:HG11	21:G:608:CHL:CMB	2.32	0.59
21:N:607:CHL:HBC3	21:N:607:CHL:HHH	1.84	0.59
33:a:411:SQD:H142	33:a:411:SQD:H281	1.84	0.59
3:b:327:ALA:O	3:b:444:ARG:NE	2.33	0.59
1:g:142:ARG:HA	21:g:608:CHL:HBC3	1.84	0.59
1:n:101:GLY:HA2	21:n:605:CHL:CBC	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:605:CHL:HAA1	25:n:616:NEX:C31	2.32	0.59
1:N:142:ARG:HA	21:N:607:CHL:HBC3	1.84	0.59
1:Y:208:ASN:HB2	22:Y:611:CLA:HMA3	1.84	0.59
2:a:238:ARG:NH2	2:a:239:PHE:O	2.36	0.59
4:C:76:VAL:O	4:C:84:GLN:NE2	2.31	0.59
4:C:279:LEU:HB3	4:C:437:LEU:HD23	1.83	0.59
26:D:409:LHG:O3	26:D:409:LHG:O1	2.17	0.59
21:r:306:CHL:CAA	25:r:315:NEX:C38	2.81	0.59
1:y:208:ASN:HB2	22:y:612:CLA:HMA3	1.84	0.59
19:r:151:GLU:CD	21:r:306:CHL:HMB1	2.27	0.59
20:S:34:PHE:HE2	21:S:302:CHL:CAA	2.16	0.59
21:Y:607:CHL:HBC3	21:Y:607:CHL:HHH	1.83	0.59
2:A:104:GLU:OE2	2:A:108:ASN:ND2	2.32	0.59
20:s:210:THR:HG21	20:s:217:ASN:HD21	1.67	0.59
1:N:197:GLN:NE2	22:N:612:CLA:H2A	2.18	0.58
35:a:413:DGD:O5E	35:a:413:DGD:O4E	2.20	0.58
4:c:76:VAL:O	4:c:84:GLN:NE2	2.31	0.58
14:o:158:ASP:OD1	14:o:162:ARG:N	2.35	0.58
31:D:406:BCR:H16C	7:F:27:PHE:CD2	2.37	0.58
1:N:101:GLY:HA2	21:N:605:CHL:CBC	2.33	0.58
7:f:18:HIS:HB2	37:f:101:HEM:NA	2.18	0.58
3:B:41:GLU:OE2	3:B:61:PHE:N	2.34	0.58
21:s:306:CHL:HAA2	21:s:306:CHL:CGD	2.33	0.58
21:S:306:CHL:HMC	21:S:307:CHL:C4C	2.34	0.58
1:g:197:GLN:NE2	22:g:613:CLA:H2A	2.19	0.58
21:g:601:CHL:H2	21:y:609:CHL:CGA	2.33	0.58
21:y:606:CHL:HMA2	25:y:616:NEX:H32	1.84	0.58
1:G:142:ARG:HA	21:G:608:CHL:HBC3	1.84	0.58
1:N:191:MET:HG3	23:N:615:LUT:H202	1.85	0.58
1:Y:197:GLN:NE2	22:Y:611:CLA:H2A	2.18	0.58
2:a:140:ARG:NH2	26:d:409:LHG:O5	2.36	0.58
4:c:418:ASN:ND2	35:c:518:DGD:O4D	2.36	0.58
1:g:21:ARG:NH2	1:g:36:LEU:O	2.37	0.58
22:G:603:CLA:H122	22:N:603:CLA:H71	1.86	0.58
7:F:18:HIS:HB2	37:F:101:HEM:NA	2.18	0.58
22:s:310:CLA:H3A	22:s:310:CLA:CGA	2.34	0.58
25:y:618:NEX:C38	21:R:305:CHL:CAA	2.81	0.58
21:N:601:CHL:HHH	26:N:618:LHG:C7	2.34	0.58
2:A:257:ARG:NH2	3:B:491:GLU:O	2.36	0.58
22:B:612:CLA:H93	22:B:617:CLA:HAA1	1.85	0.58
22:B:616:CLA:H62	33:L:102:SQD:H292	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:18:HIS:HA	37:F:101:HEM:NC	2.17	0.58
1:g:138:VAL:HG11	21:g:608:CHL:CMB	2.32	0.58
1:G:101:GLY:HA2	21:G:606:CHL:CBC	2.33	0.58
1:G:197:GLN:NE2	22:G:613:CLA:H2A	2.18	0.58
4:c:79:LYS:HB3	4:c:84:GLN:HE21	1.68	0.58
19:r:126:LYS:HD3	21:r:307:CHL:CED	2.33	0.58
19:R:126:LYS:HD3	21:R:306:CHL:CED	2.33	0.58
1:g:65:GLU:O	1:g:69:SER:OG	2.20	0.58
1:y:142:ARG:HA	21:y:608:CHL:HBC3	1.84	0.58
1:G:197:GLN:NE2	22:G:613:CLA:C2A	2.59	0.58
1:N:208:ASN:HB2	22:N:612:CLA:HMA3	1.84	0.58
1:g:101:GLY:HA2	21:g:606:CHL:CBC	2.33	0.58
1:G:208:ASN:HB2	22:G:613:CLA:HMA3	1.84	0.58
1:N:21:ARG:NH2	1:N:36:LEU:O	2.37	0.58
2:a:196:PRO:HA	2:a:199:MET:HE3	1.86	0.58
2:a:334:ARG:O	5:d:351:ASN:ND2	2.36	0.58
36:b:620:LMG:H252	21:r:307:CHL:NC	2.13	0.58
14:o:46:TYR:HD1	14:o:248:SER:HA	1.69	0.58
3:B:124:CYS:SG	8:H:14:PRO:HG2	2.43	0.58
4:C:33:PHE:O	4:C:41:ARG:NH2	2.37	0.58
20:s:34:PHE:HE2	21:s:302:CHL:CAA	2.16	0.58
1:Y:21:ARG:NH2	1:Y:36:LEU:O	2.37	0.58
4:c:33:PHE:O	4:c:41:ARG:NH2	2.37	0.58
4:C:272:LEU:HD13	22:C:511:CLA:NC	2.11	0.58
19:r:165:GLU:O	19:r:171:ARG:NH2	2.33	0.58
19:r:221:LYS:HB2	19:r:226:PHE:HZ	1.69	0.58
1:y:21:ARG:NH2	1:y:36:LEU:O	2.37	0.58
1:Y:102:SER:CB	21:Y:606:CHL:CED	2.26	0.58
22:b:609:CLA:H93	22:b:614:CLA:HAA1	1.85	0.58
4:C:418:ASN:ND2	35:C:519:DGD:O4D	2.36	0.58
20:S:34:PHE:CE2	21:S:302:CHL:CAA	2.87	0.58
1:g:208:ASN:HB2	22:g:613:CLA:HMA3	1.84	0.57
1:n:142:ARG:HA	21:n:607:CHL:HBC3	1.84	0.57
1:n:197:GLN:NE2	22:n:612:CLA:H2A	2.18	0.57
1:Y:102:SER:N	21:Y:606:CHL:CGD	2.68	0.57
37:f:101:HEM:HBC2	37:f:101:HEM:HHD	1.86	0.57
3:B:233:ASN:HD22	3:B:473:THR:HG23	1.69	0.57
4:C:311:GLN:OE1	4:C:355:THR:OG1	2.22	0.57
21:N:605:CHL:H3A	25:N:617:NEX:H30	1.86	0.57
1:g:102:SER:N	21:g:607:CHL:CGD	2.68	0.57
1:n:102:SER:N	21:n:606:CHL:CGD	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:ARG:NH2	1:G:36:LEU:O	2.37	0.57
35:a:413:DGD:HD5	3:B:75:TRP:HB3	1.87	0.57
4:c:370:ARG:O	4:c:379:ARG:NH2	2.37	0.57
2:A:238:ARG:NH2	2:A:239:PHE:O	2.36	0.57
4:C:370:ARG:O	4:C:379:ARG:NH2	2.37	0.57
20:s:34:PHE:CE2	21:s:302:CHL:CAA	2.87	0.57
1:n:21:ARG:NH2	1:n:36:LEU:O	2.37	0.57
36:b:620:LMG:C23	21:r:307:CHL:C4C	2.81	0.57
2:A:196:PRO:HA	2:A:199:MET:HE3	1.86	0.57
2:A:252:HIS:NE2	2:A:266:ASN:OD1	2.38	0.57
7:F:39:ARG:HB3	10:J:36:LEU:HD21	1.86	0.57
19:R:93:ARG:NH2	22:R:302:CLA:O1D	2.37	0.57
22:b:613:CLA:H62	33:l:101:SQD:H292	1.86	0.57
3:B:327:ALA:O	3:B:444:ARG:NE	2.33	0.57
19:r:93:ARG:NH2	22:r:303:CLA:O1D	2.37	0.57
21:G:601:CHL:H72	22:Y:603:CLA:C3D	2.33	0.57
21:G:605:CHL:HBC3	21:G:606:CHL:CMD	2.27	0.57
2:a:25:GLU:OE1	2:a:25:GLU:N	2.38	0.57
3:b:75:TRP:HB3	35:A:401:DGD:HD5	1.87	0.57
3:b:169:SER:HA	3:b:176:GLY:HA2	1.87	0.57
4:C:343:ARG:NH2	14:O:85:THR:O	2.37	0.57
20:S:98:PHE:CE1	21:S:301:CHL:HED1	2.38	0.57
19:R:162:ARG:HG3	21:R:307:CHL:CHD	2.33	0.57
19:R:221:LYS:HB2	19:R:226:PHE:HZ	1.69	0.57
1:n:119:VAL:HG13	21:s:301:CHL:CHD	2.34	0.57
21:n:607:CHL:HBA2	21:n:607:CHL:CHA	2.35	0.57
1:Y:119:VAL:HG13	21:r:301:CHL:CHD	2.34	0.57
1:Y:142:ARG:HA	21:Y:607:CHL:HBC3	1.84	0.57
3:b:413:ASP:N	3:b:413:ASP:OD1	2.33	0.57
2:A:175:GLY:O	2:A:179:THR:OG1	2.22	0.57
37:F:101:HEM:HBC2	37:F:101:HEM:HHD	1.86	0.57
21:S:306:CHL:HAA2	21:S:306:CHL:CGD	2.33	0.57
1:g:119:VAL:HG13	21:g:605:CHL:CHD	2.35	0.57
22:y:604:CLA:H42	25:y:616:NEX:H23	1.87	0.57
1:G:111:ASP:OD1	1:G:120:HIS:ND1	2.37	0.57
1:N:119:VAL:HG13	21:S:301:CHL:CHD	2.34	0.57
14:O:46:TYR:HD1	14:O:248:SER:HA	1.69	0.57
1:g:111:ASP:OD1	1:g:120:HIS:ND1	2.37	0.57
4:C:79:LYS:HB3	4:C:84:GLN:HE21	1.68	0.57
21:Y:607:CHL:HBA2	21:Y:607:CHL:CHA	2.35	0.57
4:c:311:GLN:OE1	4:c:355:THR:OG1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:25:GLU:OE1	2:A:25:GLU:N	2.38	0.57
3:B:169:SER:HA	3:B:176:GLY:HA2	1.87	0.57
36:B:623:LMG:O2	19:R:126:LYS:NZ	2.38	0.57
5:D:280:LEU:HD22	30:D:401:PHO:HBC3	1.87	0.57
22:n:604:CLA:H42	25:n:616:NEX:H23	1.87	0.56
22:S:310:CLA:H3A	22:S:310:CLA:CGA	2.34	0.56
1:G:65:GLU:O	1:G:69:SER:OG	2.20	0.56
1:G:119:VAL:HG13	21:G:605:CHL:CHD	2.35	0.56
2:a:252:HIS:NE2	2:a:266:ASN:OD1	2.38	0.56
2:a:321:ILE:HG22	2:a:325:ASN:HD21	1.70	0.56
3:B:413:ASP:N	3:B:413:ASP:OD1	2.33	0.56
26:C:522:LHG:O3	26:C:522:LHG:O1	2.18	0.56
1:g:79:CYS:HG	23:g:616:LUT:HO3	1.46	0.56
21:g:601:CHL:H62	21:y:609:CHL:H92	1.86	0.56
1:y:65:GLU:O	1:y:69:SER:OG	2.20	0.56
1:y:102:SER:CB	21:y:607:CHL:CED	2.24	0.56
21:G:601:CHL:H8	21:Y:608:CHL:H111	1.86	0.56
21:G:605:CHL:HBC1	21:G:606:CHL:HMD1	1.75	0.56
1:N:79:CYS:SG	23:N:615:LUT:O3	2.59	0.56
1:N:102:SER:N	21:N:606:CHL:CGD	2.67	0.56
1:Y:46:TRP:HZ2	21:Y:601:CHL:H11	1.70	0.56
33:a:411:SQD:HO4	33:a:411:SQD:HO8	1.54	0.56
33:a:411:SQD:H252	33:a:411:SQD:H122	1.87	0.56
2:A:335:ASN:HA	5:D:351:ASN:HD22	1.68	0.56
19:r:96:GLU:OE2	19:r:203:ARG:NE	2.35	0.56
21:n:601:CHL:CHD	26:n:617:LHG:C8	2.83	0.56
21:y:605:CHL:HBC1	21:y:606:CHL:HMD3	1.87	0.56
2:a:218:LEU:HD12	32:a:410:PL9:HC72	1.88	0.56
14:o:188:GLU:OE1	14:o:188:GLU:N	2.38	0.56
5:D:215:HIS:NE2	34:D:403:BCT:O1	2.26	0.56
1:n:111:ASP:OD1	1:n:120:HIS:ND1	2.37	0.56
1:G:46:TRP:HZ2	21:G:601:CHL:H11	1.70	0.56
21:G:609:CHL:H92	21:N:601:CHL:C6	2.36	0.56
1:N:46:TRP:HZ2	21:N:601:CHL:H11	1.70	0.56
2:a:104:GLU:OE2	2:a:108:ASN:ND2	2.32	0.56
2:a:250:ALA:HA	3:b:490:VAL:HG21	1.86	0.56
3:b:233:ASN:HD22	3:b:473:THR:HG23	1.69	0.56
3:b:274:GLN:OE1	3:b:274:GLN:N	2.39	0.56
22:c:509:CLA:H43	22:c:512:CLA:HAC1	1.87	0.56
1:g:46:TRP:HZ2	21:g:601:CHL:H11	1.70	0.56
1:y:46:TRP:HZ2	21:y:601:CHL:H11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:y:618:NEX:C38	21:R:305:CHL:HAA1	2.36	0.56
3:b:220:ARG:HH21	8:h:32:LYS:H	1.51	0.56
21:g:601:CHL:H62	21:y:609:CHL:C9	2.35	0.56
21:g:601:CHL:HBC3	21:g:601:CHL:CMC	2.36	0.56
21:y:601:CHL:CMC	21:y:601:CHL:HBC3	2.36	0.56
1:G:103:GLN:NE2	22:G:604:CLA:O1D	2.36	0.56
21:G:608:CHL:HBA2	21:G:608:CHL:CHA	2.35	0.56
21:N:607:CHL:HBA2	21:N:607:CHL:CHA	2.35	0.56
21:Y:601:CHL:C2D	26:Y:617:LHG:H102	2.35	0.56
22:Y:610:CLA:H43	22:W:101:CLA:HMD2	1.88	0.56
1:y:138:VAL:CG1	21:y:608:CHL:HMB3	2.36	0.56
21:y:601:CHL:CHD	26:y:617:LHG:HC82	2.36	0.56
21:G:606:CHL:HBA2	21:G:606:CHL:HBD	1.88	0.56
1:Y:123:SER:N	21:r:301:CHL:OMC	2.30	0.56
5:d:263:SER:N	26:d:408:LHG:O5	2.39	0.56
3:B:247:PHE:HE1	22:B:604:CLA:H143	1.71	0.56
5:D:94:TRP:HB2	17:X:53:ASN:HB3	1.88	0.56
21:S:302:CHL:HBC1	26:S:314:LHG:HC11	1.88	0.56
1:G:26:GLY:HA2	21:G:601:CHL:OMC	2.06	0.56
1:G:123:SER:N	21:G:605:CHL:OMC	2.31	0.56
4:c:322:GLN:HE22	4:c:381:LYS:HA	1.71	0.56
14:O:188:GLU:OE1	14:O:188:GLU:N	2.38	0.56
19:r:128:GLU:HG3	21:r:306:CHL:CAC	2.36	0.56
1:g:196:VAL:H	22:g:613:CLA:C2C	2.19	0.56
22:n:610:CLA:H43	22:n:611:CLA:HMD2	1.88	0.56
1:y:121:ALA:HB1	21:y:605:CHL:HBC2	0.63	0.56
1:Y:79:CYS:SG	23:Y:613:LUT:H11	2.46	0.56
21:Y:605:CHL:HBA2	21:Y:605:CHL:HBD	1.88	0.56
4:c:272:LEU:CG	22:c:510:CLA:CHD	2.83	0.56
33:A:412:SQD:H252	33:A:412:SQD:H122	1.87	0.56
22:C:510:CLA:H43	22:C:513:CLA:HAC1	1.87	0.56
1:G:79:CYS:SG	23:G:615:LUT:H11	2.47	0.55
1:G:102:SER:N	21:G:607:CHL:CGD	2.67	0.55
2:a:175:GLY:O	2:a:179:THR:OG1	2.22	0.55
5:d:140:ARG:NH2	5:d:142:TYR:OH	2.38	0.55
5:D:140:ARG:NH2	5:D:142:TYR:OH	2.38	0.55
14:O:51:LEU:HB3	14:O:89:ILE:HB	1.88	0.55
21:r:306:CHL:HAA1	25:r:315:NEX:C38	2.36	0.55
1:g:123:SER:N	21:g:605:CHL:OMC	2.31	0.55
1:g:142:ARG:CA	21:g:608:CHL:CBC	2.84	0.55
21:n:601:CHL:HBC3	21:n:601:CHL:CMC	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:196:VAL:H	22:y:612:CLA:C2C	2.19	0.55
1:G:196:VAL:H	22:G:613:CLA:C2C	2.19	0.55
21:G:601:CHL:HBC3	21:G:601:CHL:CMC	2.36	0.55
1:N:111:ASP:OD1	1:N:120:HIS:ND1	2.37	0.55
22:b:606:CLA:HAC2	31:T:102:BCR:H272	1.89	0.55
14:o:51:LEU:HB3	14:o:89:ILE:HB	1.88	0.55
19:r:162:ARG:HG3	21:r:308:CHL:CHD	2.33	0.55
1:g:79:CYS:SG	23:g:615:LUT:H11	2.47	0.55
1:N:79:CYS:SG	23:N:614:LUT:H11	2.47	0.55
36:b:620:LMG:C21	21:r:307:CHL:CHB	2.57	0.55
3:B:500:ASP:OD2	3:B:502:THR:OG1	2.23	0.55
36:B:623:LMG:H252	21:R:306:CHL:C3C	2.36	0.55
4:C:322:GLN:HE22	4:C:381:LYS:HA	1.71	0.55
26:C:520:LHG:H272	22:S:311:CLA:H102	1.89	0.55
5:D:263:SER:N	26:D:409:LHG:O5	2.39	0.55
1:g:26:GLY:HA2	21:g:601:CHL:OMC	2.06	0.55
1:n:26:GLY:HA2	21:n:601:CHL:OMC	2.06	0.55
1:n:79:CYS:SG	23:n:614:LUT:H11	2.47	0.55
1:n:196:VAL:H	22:n:612:CLA:C2C	2.19	0.55
1:y:142:ARG:CA	21:y:608:CHL:CBC	2.84	0.55
21:y:608:CHL:HBA2	21:y:608:CHL:CHA	2.35	0.55
1:N:196:VAL:H	22:N:612:CLA:C2C	2.19	0.55
1:Y:196:VAL:H	22:Y:611:CLA:C2C	2.19	0.55
3:b:500:ASP:OD2	3:b:502:THR:OG1	2.23	0.55
4:c:48:LYS:NZ	4:c:133:ALA:O	2.35	0.55
3:B:157:HIS:HA	3:B:163:GLY:HA3	1.89	0.55
3:B:233:ASN:OD1	3:B:234:ILE:N	2.39	0.55
10:J:32:SER:O	35:J:101:DGD:O2D	2.24	0.55
21:r:306:CHL:OMC	24:r:314:XAT:H163	2.07	0.55
1:n:46:TRP:HZ2	21:n:601:CHL:H11	1.70	0.55
22:n:604:CLA:NB	25:n:616:NEX:H242	2.22	0.55
21:y:606:CHL:HBA2	21:y:606:CHL:HBD	1.88	0.55
21:N:601:CHL:CMC	21:N:601:CHL:HBC3	2.36	0.55
3:b:445:SER:OG	3:b:450:TRP:NE1	2.39	0.55
2:A:218:LEU:HD12	32:A:411:PL9:HC72	1.88	0.55
3:B:274:GLN:OE1	3:B:274:GLN:N	2.39	0.55
21:R:305:CHL:OMC	24:R:313:XAT:H163	2.07	0.55
1:N:197:GLN:NE2	22:N:612:CLA:C2A	2.59	0.55
21:Y:601:CHL:CMC	21:Y:601:CHL:HBC3	2.36	0.55
3:b:87:ASN:N	3:b:87:ASN:OD1	2.39	0.55
4:c:186:TYR:HA	4:c:196:VAL:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:r:159:GLU:OE1	19:r:162:ARG:NH2	2.32	0.55
22:r:311:CLA:HED2	23:r:313:LUT:H12	1.89	0.55
22:R:310:CLA:HED2	23:R:312:LUT:H12	1.89	0.55
22:n:604:CLA:HMB2	23:n:614:LUT:H12	1.89	0.55
21:n:605:CHL:HBA2	21:n:605:CHL:HBD	1.88	0.55
1:y:102:SER:N	21:y:607:CHL:CGD	2.68	0.55
22:G:604:CLA:HMB2	23:G:615:LUT:H12	1.89	0.55
1:N:142:ARG:CA	21:N:607:CHL:CBC	2.84	0.55
20:S:101:TYR:CD2	21:S:301:CHL:HMA3	2.42	0.55
19:R:128:GLU:HG3	21:R:305:CHL:CAC	2.36	0.55
1:y:197:GLN:NE2	22:y:612:CLA:H2A	2.18	0.55
1:y:225:ALA:HA	24:y:615:XAT:H42	1.88	0.55
21:y:601:CHL:C1D	26:y:617:LHG:C8	2.83	0.55
1:G:102:SER:CB	21:G:607:CHL:CED	2.26	0.55
1:G:142:ARG:CA	21:G:608:CHL:CBC	2.84	0.55
3:b:157:HIS:HA	3:b:163:GLY:HA3	1.89	0.55
3:b:233:ASN:OD1	3:b:234:ILE:N	2.39	0.55
4:C:272:LEU:CG	22:C:511:CLA:CHD	2.83	0.55
35:H:102:DGD:O5D	35:H:102:DGD:O4D	2.15	0.55
31:K:101:BCR:HC7	31:K:102:BCR:H353	1.89	0.55
14:O:78:LEU:HD11	14:O:80:THR:HG22	1.89	0.55
20:s:115:GLY:C	21:s:307:CHL:C3D	2.79	0.55
19:R:159:GLU:OE1	19:R:162:ARG:NH2	2.32	0.55
19:R:221:LYS:HB2	19:R:226:PHE:CZ	2.42	0.55
21:g:608:CHL:HBA2	21:g:608:CHL:CHA	2.35	0.55
1:n:142:ARG:CA	21:n:607:CHL:CBC	2.84	0.55
21:n:608:CHL:CGA	21:y:601:CHL:H2	2.36	0.55
22:y:604:CLA:HMB2	23:y:614:LUT:H12	1.89	0.55
21:G:601:CHL:H102	22:Y:603:CLA:C1D	2.37	0.55
1:N:65:GLU:O	1:N:69:SER:OG	2.20	0.55
1:Y:26:GLY:HA2	21:Y:601:CHL:OMC	2.07	0.55
1:Y:142:ARG:CA	21:Y:607:CHL:CBC	2.84	0.55
4:c:272:LEU:HD12	22:c:510:CLA:ND	2.04	0.55
7:f:18:HIS:CD2	37:f:101:HEM:C1A	2.95	0.55
3:B:87:ASN:N	3:B:87:ASN:OD1	2.39	0.55
4:C:461:ARG:NH1	5:D:226:ASP:OD2	2.34	0.55
20:S:119:LEU:CD1	21:S:307:CHL:HMD3	2.31	0.55
22:N:604:CLA:HMB2	23:N:614:LUT:H12	1.89	0.55
2:A:272:HIS:NE2	34:D:403:BCT:O1	2.32	0.55
1:N:26:GLY:HA2	21:N:601:CHL:OMC	2.06	0.54
3:B:445:SER:OG	3:B:450:TRP:NE1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:371:GLY:N	4:C:374:GLY:O	2.28	0.54
22:Y:603:CLA:HBC3	23:Y:614:LUT:H12	1.90	0.54
2:A:321:ILE:HG22	2:A:325:ASN:HD21	1.70	0.54
21:s:302:CHL:HBC1	26:s:314:LHG:HC11	1.88	0.54
21:s:306:CHL:HAA2	21:s:306:CHL:CBD	2.37	0.54
1:g:138:VAL:CG1	21:g:608:CHL:HMB3	2.36	0.54
21:n:608:CHL:CHC	21:n:608:CHL:C2	2.86	0.54
21:y:609:CHL:CHC	21:y:609:CHL:C2	2.86	0.54
1:G:94:GLU:HB2	1:G:103:GLN:HB3	1.90	0.54
1:G:136:GLY:CA	21:G:609:CHL:CBB	2.85	0.54
21:G:609:CHL:H111	21:N:601:CHL:C12	2.37	0.54
31:b:616:BCR:H383	33:L:101:SQD:H141	1.89	0.54
16:w:4:ASP:OD1	16:w:5:ARG:N	2.40	0.54
3:B:440:ASP:OD1	3:B:441:GLY:N	2.41	0.54
36:B:623:LMG:C26	21:R:305:CHL:C1C	2.84	0.54
4:C:344:SER:OG	4:C:348:GLU:OE1	2.23	0.54
31:D:406:BCR:H14C	7:F:27:PHE:CE2	2.42	0.54
19:r:221:LYS:HB2	19:r:226:PHE:CZ	2.42	0.54
1:g:136:GLY:CA	21:g:609:CHL:CBB	2.85	0.54
1:g:197:GLN:OE1	22:g:613:CLA:C3D	2.55	0.54
21:g:606:CHL:HBA2	21:g:606:CHL:HBD	1.88	0.54
1:y:94:GLU:HB2	1:y:103:GLN:HB3	1.90	0.54
1:N:197:GLN:NE2	22:N:612:CLA:CGD	2.71	0.54
21:N:608:CHL:C2	21:N:608:CHL:CHC	2.86	0.54
1:Y:94:GLU:HB2	1:Y:103:GLN:HB3	1.90	0.54
4:c:344:SER:OG	4:c:348:GLU:OE1	2.23	0.54
16:W:4:ASP:OD1	16:W:5:ARG:N	2.40	0.54
1:g:94:GLU:HB2	1:g:103:GLN:HB3	1.90	0.54
22:g:604:CLA:HMB2	23:g:615:LUT:H12	1.89	0.54
1:n:74:LEU:HD13	23:n:614:LUT:H402	1.89	0.54
1:y:26:GLY:HA2	21:y:601:CHL:OMC	2.06	0.54
21:G:601:CHL:H152	22:Y:603:CLA:HMC2	1.89	0.54
1:N:73:MET:HE3	22:N:609:CLA:HMC3	1.90	0.54
22:N:610:CLA:H43	22:N:611:CLA:HMD2	1.88	0.54
22:Y:604:CLA:NB	25:Y:616:NEX:H242	2.22	0.54
2:a:225:ARG:HH12	3:b:483:ASP:HA	1.73	0.54
22:C:503:CLA:C1D	22:C:505:CLA:H51	2.38	0.54
22:g:604:CLA:HMA1	21:g:606:CHL:HMC	1.90	0.54
1:y:79:CYS:SG	23:y:614:LUT:H11	2.47	0.54
1:y:119:VAL:CG1	21:y:605:CHL:HHH	2.37	0.54
21:G:609:CHL:CHC	21:G:609:CHL:C2	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:609:CHL:CHC	21:g:609:CHL:C2	2.86	0.54
22:g:611:CLA:H43	22:g:612:CLA:HMD2	1.88	0.54
1:y:74:LEU:HD13	23:y:614:LUT:H402	1.89	0.54
22:G:604:CLA:HMA1	21:G:606:CHL:HMC	1.90	0.54
21:G:609:CHL:H111	21:N:601:CHL:H121	1.90	0.54
1:N:94:GLU:HB2	1:N:103:GLN:HB3	1.90	0.54
21:N:605:CHL:HBA2	21:N:605:CHL:HBD	1.88	0.54
2:a:257:ARG:NH2	3:b:491:GLU:O	2.40	0.54
33:l:103:SQD:O49	33:L:102:SQD:O2	2.24	0.54
22:s:305:CLA:CBA	21:s:306:CHL:C1D	2.86	0.54
1:y:103:GLN:NE2	22:y:604:CLA:O1D	2.36	0.54
1:G:189:PHE:HE2	26:G:618:LHG:H302	1.73	0.54
22:N:604:CLA:HMA1	21:N:605:CHL:HMC	1.90	0.54
2:A:138:GLY:HA2	4:C:455:PHE:CZ	2.42	0.54
4:C:186:TYR:HA	4:C:196:VAL:HA	1.89	0.54
35:H:102:DGD:O6D	35:H:102:DGD:O3D	2.24	0.54
21:S:306:CHL:HAA2	21:S:306:CHL:CBD	2.37	0.54
21:G:607:CHL:HMB1	21:N:601:CHL:H202	1.90	0.54
1:N:74:LEU:HD13	23:N:614:LUT:H402	1.89	0.54
25:N:617:NEX:H8	25:N:617:NEX:H171	1.89	0.54
4:c:321:ASP:OD2	4:c:340:TYR:OH	2.21	0.54
22:c:505:CLA:H42	35:c:518:DGD:HA21	1.89	0.54
5:d:283:SER:HB2	22:d:403:CLA:HED1	1.90	0.54
7:f:14:TRP:HE1	37:f:101:HEM:HHB	1.73	0.54
14:o:78:LEU:HD11	14:o:80:THR:HG22	1.89	0.54
4:C:408:GLY:N	4:C:417:VAL:O	2.38	0.54
26:D:410:LHG:O3	26:D:410:LHG:O1	2.22	0.54
1:n:94:GLU:HB2	1:n:103:GLN:HB3	1.90	0.54
1:n:123:SER:N	21:s:301:CHL:OMC	2.30	0.54
1:N:123:SER:N	21:S:301:CHL:OMC	2.29	0.54
1:N:197:GLN:OE1	22:N:612:CLA:C3D	2.55	0.54
1:Y:111:ASP:OD1	1:Y:120:HIS:ND1	2.37	0.54
3:b:385:ARG:NH2	14:o:163:GLY:O	2.41	0.54
3:b:434:ARG:NH2	3:b:439:SER:O	2.41	0.54
36:B:623:LMG:C26	21:R:305:CHL:OMC	2.55	0.54
21:g:606:CHL:H12	25:g:618:NEX:H403	1.90	0.53
1:n:138:VAL:CG1	21:n:607:CHL:HMB3	2.36	0.53
22:y:604:CLA:HMA1	21:y:606:CHL:HMC	1.90	0.53
1:G:158:GLY:N	22:G:610:CLA:OBD	2.38	0.53
1:Y:33:PRO:HD2	1:Y:36:LEU:HD12	1.90	0.53
1:Y:197:GLN:NE2	22:Y:611:CLA:CGD	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:247:PHE:HE1	22:b:601:CLA:H143	1.71	0.53
3:b:334:ASP:OD1	3:b:335:GLY:N	2.41	0.53
22:S:305:CLA:CBA	21:S:306:CHL:C1D	2.86	0.53
1:n:73:MET:HE3	22:n:609:CLA:HMC3	1.90	0.53
22:n:604:CLA:HMA1	21:n:605:CHL:HMC	1.90	0.53
1:y:33:PRO:HD2	1:y:36:LEU:HD12	1.90	0.53
1:y:197:GLN:NE2	22:y:612:CLA:CGD	2.71	0.53
22:N:603:CLA:C2D	21:Y:601:CHL:H71	2.38	0.53
1:Y:74:LEU:HD13	23:Y:613:LUT:H402	1.89	0.53
19:r:104:MET:HE1	19:r:201:HIS:HD2	1.73	0.53
1:y:197:GLN:NE2	22:y:612:CLA:C2A	2.59	0.53
23:G:615:LUT:H8	23:G:616:LUT:H41	1.89	0.53
1:N:33:PRO:HD2	1:N:36:LEU:HD12	1.90	0.53
1:N:191:MET:HG3	23:N:615:LUT:C20	2.38	0.53
22:Y:604:CLA:HMA1	21:Y:605:CHL:HMC	1.90	0.53
22:b:601:CLA:H102	8:h:58:LEU:HD22	1.90	0.53
31:k:101:BCR:HC7	31:k:102:BCR:H353	1.89	0.53
3:B:434:ARG:NH2	3:B:439:SER:O	2.41	0.53
14:O:43:PRO:HB3	14:O:97:ALA:HA	1.90	0.53
21:r:306:CHL:HAA2	25:r:315:NEX:C38	2.39	0.53
1:g:74:LEU:HD13	23:g:615:LUT:H402	1.89	0.53
25:n:616:NEX:H371	25:n:616:NEX:H28	1.90	0.53
1:G:74:LEU:HD13	23:G:615:LUT:H402	1.89	0.53
21:G:601:CHL:H2	21:Y:608:CHL:CBA	2.38	0.53
1:Y:73:MET:HE3	22:Y:609:CLA:HMC3	1.90	0.53
36:b:620:LMG:C26	21:r:306:CHL:OMC	2.56	0.53
22:C:506:CLA:H42	35:C:519:DGD:HA21	1.89	0.53
20:s:101:TYR:CZ	21:s:301:CHL:C1A	2.80	0.53
1:y:73:MET:HE3	22:y:610:CLA:HMC3	1.90	0.53
22:G:611:CLA:H43	22:G:612:CLA:HMD2	1.88	0.53
1:Y:158:GLY:N	22:Y:609:CLA:OBD	2.38	0.53
36:b:620:LMG:H111	21:r:307:CHL:HBA1	1.91	0.53
22:c:502:CLA:H2A	22:c:502:CLA:HED3	1.90	0.53
7:F:14:TRP:HE1	37:F:101:HEM:HHB	1.73	0.53
1:g:73:MET:HE3	22:g:610:CLA:HMC3	1.90	0.53
1:y:111:ASP:OD1	1:y:120:HIS:ND1	2.37	0.53
25:y:618:NEX:C38	21:R:305:CHL:HAA2	2.39	0.53
21:G:601:CHL:H71	22:Y:603:CLA:HMD2	1.90	0.53
22:Y:604:CLA:HMA2	21:Y:605:CHL:C2C	2.39	0.53
3:b:193:PHE:HA	3:b:261:ALA:HB2	1.90	0.53
20:s:104:ASN:O	20:s:128:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:33:PRO:HD2	1:n:36:LEU:HD12	1.90	0.53
1:G:197:GLN:OE1	22:G:613:CLA:C3D	2.55	0.53
22:c:507:CLA:H2	22:c:508:CLA:H202	1.91	0.53
3:B:487:ASP:HB2	3:B:489:GLN:HG3	1.90	0.53
5:D:283:SER:HB2	22:D:404:CLA:HED1	1.90	0.53
1:N:117:SER:HB3	20:S:103:ALA:HB2	1.90	0.53
21:Y:605:CHL:C3A	25:Y:616:NEX:H31	2.39	0.53
22:C:503:CLA:H2A	22:C:503:CLA:HED3	1.90	0.53
20:S:94:ILE:HG13	20:S:95:PRO:HD3	1.90	0.53
1:g:33:PRO:HD2	1:g:36:LEU:HD12	1.90	0.53
22:y:604:CLA:NB	25:y:616:NEX:H242	2.24	0.53
33:l:103:SQD:H141	31:B:619:BCR:H383	1.89	0.53
3:B:334:ASP:OD1	3:B:335:GLY:N	2.41	0.53
22:s:305:CLA:HBA1	21:s:306:CHL:C1D	2.39	0.53
20:S:221:HIS:HA	20:S:228:ASN:HB2	1.91	0.53
21:y:606:CHL:HBA2	21:y:606:CHL:CBD	2.39	0.53
35:a:413:DGD:HA32	36:B:601:LMG:H302	1.91	0.53
3:b:440:ASP:OD1	3:b:441:GLY:N	2.41	0.53
3:B:193:PHE:HA	3:B:261:ALA:HB2	1.90	0.53
14:O:49:LYS:HB3	14:O:245:GLN:HB2	1.91	0.53
21:n:601:CHL:CHD	26:n:617:LHG:HC82	2.38	0.52
22:n:604:CLA:HMA2	21:n:605:CHL:C2C	2.39	0.52
21:N:605:CHL:HBA2	21:N:605:CHL:CBD	2.39	0.52
1:Y:193:GLY:HA2	26:Y:617:LHG:H383	1.90	0.52
23:Y:613:LUT:H203	23:Y:614:LUT:H8	1.90	0.52
22:c:502:CLA:C1D	22:c:504:CLA:H51	2.38	0.52
1:n:197:GLN:NE2	22:n:612:CLA:CGD	2.71	0.52
1:y:136:GLY:CA	21:y:609:CHL:CBB	2.86	0.52
1:N:103:GLN:NE2	22:N:604:CLA:O1D	2.36	0.52
1:Y:65:GLU:O	1:Y:69:SER:OG	2.20	0.52
4:c:155:ASN:O	4:c:159:THR:OG1	2.26	0.52
26:c:522:LHG:O3	26:c:522:LHG:O1	2.18	0.52
4:C:154:ARG:HB3	4:C:256:PRO:HG2	1.92	0.52
22:C:508:CLA:H2	22:C:509:CLA:H202	1.91	0.52
22:S:305:CLA:HBA1	21:S:306:CHL:C1D	2.40	0.52
1:N:119:VAL:CG1	21:S:301:CHL:HHH	2.40	0.52
3:b:74:SER:OG	3:b:75:TRP:N	2.42	0.52
7:F:18:HIS:CG	37:F:101:HEM:C1C	2.94	0.52
7:F:18:HIS:CG	37:F:101:HEM:C4A	2.97	0.52
20:s:94:ILE:HG13	20:s:95:PRO:HD3	1.90	0.52
20:S:104:ASN:O	20:S:128:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:226:PHE:HB3	22:R:311:CLA:HED1	1.91	0.52
22:y:604:CLA:HMA2	21:y:606:CHL:C2C	2.39	0.52
4:c:86:LEU:HD13	4:c:89:LEU:HD12	1.92	0.52
4:c:250:TRP:HD1	4:c:251:HIS:CD2	2.28	0.52
4:C:119:LEU:O	4:C:122:SER:OG	2.28	0.52
4:C:272:LEU:HD12	22:C:511:CLA:ND	2.04	0.52
4:C:464:GLU:OE2	5:D:246:SER:OG	2.25	0.52
14:O:213:GLU:HG2	14:O:245:GLN:HG2	1.92	0.52
19:r:181:PRO:HD2	23:r:313:LUT:H23	1.91	0.52
20:S:115:GLY:C	21:S:307:CHL:C3D	2.83	0.52
1:y:158:GLY:N	22:y:610:CLA:OBD	2.38	0.52
3:B:487:ASP:OD2	3:B:489:GLN:NE2	2.42	0.52
36:I:101:LMG:H341	36:I:101:LMG:HC3	1.92	0.52
1:n:119:VAL:CG1	21:s:301:CHL:HHD	2.40	0.52
1:G:197:GLN:NE2	22:G:613:CLA:CGD	2.71	0.52
22:G:604:CLA:HMA2	21:G:606:CHL:C2C	2.39	0.52
21:G:607:CHL:HBC2	21:G:607:CHL:CHD	2.36	0.52
22:N:604:CLA:HMA2	21:N:605:CHL:C2C	2.39	0.52
3:b:41:GLU:OE2	3:b:61:PHE:N	2.34	0.52
4:c:55:ALA:HB1	31:k:102:BCR:H373	1.92	0.52
4:c:154:ARG:HB3	4:c:256:PRO:HG2	1.92	0.52
5:d:200:MET:HG2	32:d:406:PL9:H322	1.91	0.52
14:o:213:GLU:HG2	14:o:245:GLN:HG2	1.91	0.52
3:B:74:SER:OG	3:B:75:TRP:N	2.42	0.52
21:g:601:CHL:H202	21:y:607:CHL:CMB	2.40	0.52
21:g:606:CHL:HBA2	21:g:606:CHL:CBD	2.40	0.52
21:y:607:CHL:HBC2	21:y:607:CHL:CHD	2.36	0.52
1:G:73:MET:HE3	22:G:610:CLA:HMC3	1.90	0.52
3:b:487:ASP:HB2	3:b:489:GLN:HG3	1.90	0.52
6:e:67:THR:H	6:e:75:GLN:HE22	1.58	0.52
14:o:43:PRO:HB3	14:o:97:ALA:HA	1.90	0.52
14:o:49:LYS:HB3	14:o:245:GLN:HB2	1.91	0.52
22:w:101:CLA:H12	22:w:101:CLA:CGD	2.40	0.52
2:A:84:PRO:HA	2:A:112:TYR:CG	2.44	0.52
6:E:67:THR:H	6:E:75:GLN:HE22	1.58	0.52
36:M:101:LMG:H171	36:M:101:LMG:H421	1.92	0.52
20:s:221:HIS:HA	20:s:228:ASN:HB2	1.91	0.52
19:R:96:GLU:OE2	19:R:203:ARG:NE	2.35	0.52
1:n:136:GLY:CA	21:n:608:CHL:CBB	2.86	0.52
21:n:607:CHL:CMB	25:n:616:NEX:H35	2.39	0.52
14:o:166:THR:OG1	14:o:167:GLY:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:214:ILE:HG21	22:R:311:CLA:HAC2	1.91	0.52
1:G:33:PRO:HD2	1:G:36:LEU:HD12	1.90	0.52
21:G:606:CHL:HBA2	21:G:606:CHL:CBD	2.39	0.52
1:Y:119:VAL:CG1	21:r:301:CHL:HHD	2.40	0.52
2:a:84:PRO:HA	2:a:112:TYR:CG	2.44	0.52
2:a:212:SER:HB2	5:d:212:CYS:HB2	1.90	0.52
2:a:303:ASN:HB2	4:c:414:ILE:HA	1.91	0.52
5:d:79:VAL:HB	5:d:174:PHE:HB2	1.91	0.52
10:j:29:PHE:O	10:j:32:SER:OG	2.25	0.52
22:W:101:CLA:CGD	22:W:101:CLA:H12	2.40	0.52
19:R:198:GLU:O	19:R:202:SER:HB3	2.10	0.52
21:n:605:CHL:HBA2	21:n:605:CHL:CBD	2.39	0.52
1:Y:197:GLN:OE1	22:Y:611:CLA:C3D	2.55	0.52
36:b:620:LMG:H402	22:x:101:CLA:H2	1.92	0.52
4:c:408:GLY:N	4:c:417:VAL:O	2.38	0.52
22:B:603:CLA:H2	36:B:623:LMG:H402	1.92	0.52
26:C:520:LHG:HC82	22:S:310:CLA:H42	1.90	0.52
36:T:101:LMG:H171	36:T:101:LMG:H421	1.92	0.52
26:r:302:LHG:O8	26:r:302:LHG:O2	2.21	0.52
20:s:101:TYR:HH	21:s:301:CHL:CGD	2.05	0.52
20:S:62:PHE:HB2	22:S:303:CLA:H102	1.91	0.52
21:g:607:CHL:HMA3	23:g:616:LUT:C17	2.38	0.51
1:y:142:ARG:HG3	21:y:608:CHL:C2D	2.40	0.51
1:G:94:GLU:N	1:G:103:GLN:OE1	2.44	0.51
22:a:405:CLA:O1A	22:a:405:CLA:H3A	2.10	0.51
36:b:620:LMG:H231	19:r:125:GLY:HA3	1.92	0.51
3:B:124:CYS:O	8:H:24:LYS:NZ	2.40	0.51
4:C:86:LEU:HD13	4:C:89:LEU:HD12	1.92	0.51
21:G:601:CHL:C7	22:Y:603:CLA:C2D	2.88	0.51
1:N:142:ARG:HG3	21:N:607:CHL:C2D	2.40	0.51
20:s:62:PHE:HB2	22:s:303:CLA:H102	1.91	0.51
22:g:604:CLA:HMA2	21:g:606:CHL:C2C	2.39	0.51
1:y:197:GLN:OE1	22:y:612:CLA:C3D	2.55	0.51
26:G:618:LHG:H111	26:G:618:LHG:H252	1.93	0.51
20:s:36:PRO:HG3	21:s:302:CHL:CBB	2.40	0.51
1:N:94:GLU:N	1:N:103:GLN:OE1	2.44	0.51
25:N:617:NEX:H371	25:N:617:NEX:H28	1.92	0.51
1:Y:94:GLU:N	1:Y:103:GLN:OE1	2.44	0.51
35:c:518:DGD:HA81	35:c:519:DGD:HB71	1.93	0.51
35:A:401:DGD:O5E	35:A:401:DGD:O4E	2.20	0.51
19:R:104:MET:HE1	19:R:201:HIS:HD2	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:606:CHL:HBC2	21:n:606:CHL:CHD	2.36	0.51
1:G:75:GLY:HA2	22:G:604:CLA:HBB2	1.93	0.51
1:N:75:GLY:HA2	22:N:604:CLA:HBB2	1.93	0.51
21:N:605:CHL:HMD3	21:S:301:CHL:HBC1	1.93	0.51
22:N:611:CLA:CGD	22:N:611:CLA:H12	2.40	0.51
4:c:452:ALA:HA	16:w:54:LEU:HB2	1.92	0.51
36:B:623:LMG:C21	21:R:306:CHL:C4D	2.60	0.51
1:n:75:GLY:HA2	22:n:604:CLA:HBB2	1.93	0.51
22:n:611:CLA:H12	22:n:611:CLA:CGD	2.40	0.51
22:G:612:CLA:CGD	22:G:612:CLA:H12	2.40	0.51
1:Y:136:GLY:CA	21:Y:608:CHL:CBB	2.84	0.51
21:Y:605:CHL:HMD3	21:r:301:CHL:HBC1	1.93	0.51
22:A:406:CLA:O1A	22:A:406:CLA:H3A	2.10	0.51
5:D:200:MET:HG2	32:D:407:PL9:H322	1.91	0.51
14:O:166:THR:OG1	14:O:167:GLY:N	2.41	0.51
19:r:226:PHE:HB3	22:r:312:CLA:HED1	1.91	0.51
1:n:65:GLU:O	1:n:69:SER:OG	2.20	0.51
1:n:196:VAL:HG23	22:n:612:CLA:CMC	2.35	0.51
1:y:73:MET:HG3	1:y:184:GLY:HA2	1.93	0.51
22:y:611:CLA:C1D	22:w:101:CLA:HMD2	2.41	0.51
22:y:612:CLA:H162	22:y:613:CLA:C3D	2.41	0.51
1:Y:71:TRP:HD1	21:Y:608:CHL:HMD3	1.63	0.51
1:Y:75:GLY:HA2	22:Y:604:CLA:HBB2	1.93	0.51
19:r:214:ILE:HG21	22:r:312:CLA:HAC2	1.92	0.51
20:S:36:PRO:HG3	21:S:302:CHL:CBB	2.40	0.51
19:R:181:PRO:HD2	23:R:312:LUT:H23	1.91	0.51
1:g:75:GLY:HA2	22:g:604:CLA:HBB2	1.93	0.51
1:n:73:MET:HG3	1:n:184:GLY:HA2	1.93	0.51
1:y:75:GLY:HA2	22:y:604:CLA:HBB2	1.93	0.51
1:G:73:MET:HG3	1:G:184:GLY:HA2	1.93	0.51
1:N:73:MET:HG3	1:N:184:GLY:HA2	1.93	0.51
1:Y:73:MET:HG3	1:Y:184:GLY:HA2	1.93	0.51
19:r:198:GLU:O	19:r:202:SER:HB3	2.10	0.51
19:R:165:GLU:O	19:R:171:ARG:NH2	2.33	0.51
1:g:94:GLU:N	1:g:103:GLN:OE1	2.44	0.51
1:n:142:ARG:HG3	21:n:607:CHL:C2D	2.40	0.51
1:y:79:CYS:HB2	23:y:614:LUT:H193	1.93	0.51
1:G:79:CYS:HB2	23:G:615:LUT:H193	1.93	0.51
1:N:158:GLY:N	22:N:609:CLA:OBD	2.38	0.51
1:Y:103:GLN:NE2	22:Y:604:CLA:O1D	2.36	0.51
6:e:51:ARG:NH1	6:e:54:GLU:OE2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:190:HIS:ND1	2:A:298:ASN:OD1	2.41	0.51
4:C:250:TRP:HD1	4:C:251:HIS:CD2	2.28	0.51
5:D:162:PRO:HG3	5:D:171:ALA:HB2	1.93	0.51
1:g:215:ASP:O	1:g:219:ASN:ND2	2.44	0.51
22:g:612:CLA:CGD	22:g:612:CLA:H12	2.40	0.51
22:n:611:CLA:HMA1	22:n:611:CLA:H2	1.93	0.51
24:n:615:XAT:H402	26:n:617:LHG:H142	1.93	0.51
1:N:79:CYS:HB2	23:N:614:LUT:H193	1.93	0.51
1:N:215:ASP:O	1:N:219:ASN:ND2	2.44	0.51
1:Y:196:VAL:HG23	22:Y:611:CLA:CMC	2.35	0.51
21:Y:605:CHL:HBA2	21:Y:605:CHL:CBD	2.39	0.51
22:c:506:CLA:H71	22:c:506:CLA:HBB1	1.93	0.51
3:B:21:SER:OG	3:B:111:ALA:O	2.26	0.51
3:B:157:HIS:ND1	3:B:164:PRO:HD2	2.26	0.51
22:C:505:CLA:H171	22:C:512:CLA:HBB2	1.93	0.51
22:C:507:CLA:H71	22:C:507:CLA:HBB1	1.93	0.51
19:R:133:ALA:O	19:R:140:LEU:N	2.44	0.51
1:g:73:MET:HG3	1:g:184:GLY:HA2	1.93	0.50
1:y:215:ASP:O	1:y:219:ASN:ND2	2.44	0.50
1:G:119:VAL:CG1	21:G:605:CHL:HHH	2.41	0.50
1:G:142:ARG:HG3	21:G:608:CHL:C2D	2.40	0.50
7:f:18:HIS:CG	37:f:101:HEM:C4A	2.97	0.50
36:B:623:LMG:H191	21:R:306:CHL:CHA	2.41	0.50
36:C:502:LMG:HC4	16:W:9:GLU:HA	1.94	0.50
14:O:54:GLU:OE2	16:W:1:LEU:N	2.42	0.50
1:n:65:GLU:OE2	1:n:185:ARG:NE	2.36	0.50
22:n:604:CLA:HMA2	21:n:605:CHL:C3C	2.41	0.50
22:y:604:CLA:HMA2	21:y:606:CHL:C3C	2.41	0.50
22:N:604:CLA:NB	25:N:617:NEX:H242	2.25	0.50
2:a:190:HIS:ND1	2:a:298:ASN:OD1	2.41	0.50
3:b:458:PHE:HB3	22:b:603:CLA:HBC2	1.94	0.50
36:b:620:LMG:H251	21:r:307:CHL:CHD	2.39	0.50
22:c:503:CLA:H2	22:c:504:CLA:C4D	2.41	0.50
26:c:521:LHG:H111	16:w:34:TRP:CZ2	2.46	0.50
20:s:163:LYS:HE3	22:s:308:CLA:O1D	2.11	0.50
1:n:94:GLU:N	1:n:103:GLN:OE1	2.44	0.50
1:n:103:GLN:NE2	22:n:604:CLA:O1D	2.36	0.50
1:G:138:VAL:CG1	21:G:608:CHL:HMB3	2.36	0.50
22:G:604:CLA:HMA2	21:G:606:CHL:C3C	2.41	0.50
5:d:162:PRO:HG3	5:d:171:ALA:HB2	1.93	0.50
4:C:55:ALA:HB1	31:K:102:BCR:H373	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:r:306:CHL:O1A	25:r:315:NEX:C30	2.60	0.50
1:g:79:CYS:HB2	23:g:615:LUT:H193	1.93	0.50
1:g:103:GLN:NE2	22:g:604:CLA:O1D	2.36	0.50
1:n:79:CYS:HB2	23:n:614:LUT:H193	1.93	0.50
1:y:94:GLU:N	1:y:103:GLN:OE1	2.44	0.50
1:Y:79:CYS:HB2	23:Y:613:LUT:H193	1.93	0.50
3:b:157:HIS:ND1	3:b:164:PRO:HD2	2.26	0.50
22:b:602:CLA:C1D	22:b:604:CLA:H51	2.42	0.50
36:B:601:LMG:HC3	36:B:601:LMG:H341	1.92	0.50
22:C:504:CLA:H2	22:C:505:CLA:C4D	2.41	0.50
16:W:13:LEU:HB2	16:W:16:GLY:HA2	1.94	0.50
21:r:307:CHL:H12	21:r:307:CHL:HMA2	1.93	0.50
20:S:142:GLU:CG	21:S:306:CHL:HMA3	2.25	0.50
1:g:196:VAL:HB	22:g:613:CLA:C4C	2.42	0.50
1:n:197:GLN:OE1	22:n:612:CLA:C3D	2.55	0.50
1:G:156:TYR:CZ	1:G:177:LYS:HE2	2.47	0.50
1:N:65:GLU:OE2	1:N:185:ARG:NE	2.36	0.50
1:Y:138:VAL:CG1	21:Y:607:CHL:HMB3	2.36	0.50
1:Y:215:ASP:O	1:Y:219:ASN:ND2	2.44	0.50
21:Y:605:CHL:H3A	25:Y:616:NEX:C31	2.41	0.50
2:a:78:ILE:HG12	12:l:34:ASN:HD22	1.75	0.50
22:c:512:CLA:HBC2	11:k:55:GLN:HG3	1.93	0.50
5:D:74:PHE:HB2	36:D:411:LMG:H122	1.94	0.50
5:D:79:VAL:HB	5:D:174:PHE:HB2	1.91	0.50
19:r:64:ASP:OD1	19:r:65:VAL:N	2.40	0.50
1:n:197:GLN:NE2	22:n:612:CLA:C2A	2.59	0.50
1:y:54:ASP:OD2	1:y:57:THR:N	2.33	0.50
1:G:215:ASP:O	1:G:219:ASN:ND2	2.44	0.50
1:N:196:VAL:HB	22:N:612:CLA:C4C	2.42	0.50
4:c:119:LEU:O	4:c:122:SER:OG	2.28	0.50
4:c:330:SER:HA	14:o:111:TYR:HE1	1.76	0.50
5:d:74:PHE:HB2	36:d:410:LMG:H122	1.94	0.50
35:C:519:DGD:HA81	35:J:101:DGD:HB71	1.93	0.50
1:N:136:GLY:CA	21:N:608:CHL:CBB	2.86	0.50
1:N:142:ARG:C	21:N:607:CHL:HBC2	2.37	0.50
22:N:604:CLA:HMA2	21:N:605:CHL:C3C	2.41	0.50
23:N:614:LUT:H182	23:N:615:LUT:H192	1.93	0.50
1:Y:156:TYR:CZ	1:Y:177:LYS:HE2	2.47	0.50
1:Y:182:LYS:NZ	26:Y:617:LHG:O4	2.44	0.50
2:a:303:ASN:ND2	4:c:413:GLU:O	2.45	0.50
14:o:59:THR:HB	14:o:73:PHE:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:273:TYR:CD1	35:H:102:DGD:HD61	2.46	0.50
19:r:196:LEU:HG	19:r:200:LYS:HD2	1.93	0.50
1:g:156:TYR:CZ	1:g:177:LYS:HE2	2.47	0.50
22:g:604:CLA:HMA2	21:g:606:CHL:C3C	2.41	0.50
1:y:156:TYR:CZ	1:y:177:LYS:HE2	2.47	0.50
1:y:196:VAL:HG23	22:y:612:CLA:CMC	2.34	0.50
21:N:607:CHL:H92	20:S:173:LEU:HD11	1.93	0.50
22:c:504:CLA:H171	22:c:511:CLA:HBB2	1.93	0.50
30:d:401:PHO:H2	22:d:403:CLA:H13	1.92	0.50
5:D:49:TRP:NE1	30:D:401:PHO:H162	2.26	0.50
1:g:158:GLY:N	22:g:610:CLA:OBD	2.38	0.50
1:g:197:GLN:NE2	22:g:613:CLA:CGD	2.71	0.50
1:y:196:VAL:HB	22:y:612:CLA:C4C	2.41	0.50
1:Y:142:ARG:HG3	21:Y:607:CHL:C2D	2.40	0.50
19:r:133:ALA:O	19:r:140:LEU:N	2.44	0.50
20:S:163:LYS:HE3	22:S:308:CLA:O1D	2.11	0.50
1:g:142:ARG:C	21:g:608:CHL:HBC2	2.37	0.49
1:n:156:TYR:CZ	1:n:177:LYS:HE2	2.47	0.49
1:y:142:ARG:CA	21:y:608:CHL:HBC3	2.43	0.49
22:y:611:CLA:H71	22:w:101:CLA:C4D	2.42	0.49
25:y:618:NEX:C30	21:R:305:CHL:O1A	2.60	0.49
22:G:602:CLA:HAB	23:G:616:LUT:H30	1.94	0.49
22:G:603:CLA:OBD	21:G:609:CHL:O1A	2.30	0.49
22:G:611:CLA:H71	22:G:612:CLA:C4D	2.42	0.49
21:Y:606:CHL:HBC2	21:Y:606:CHL:CHD	2.36	0.49
3:b:285:TYR:O	3:b:289:SER:OG	2.25	0.49
3:b:344:PRO:HB3	3:b:401:PHE:HE1	1.77	0.49
4:c:187:ASP:OD1	4:c:188:THR:N	2.45	0.49
36:B:623:LMG:C23	21:R:306:CHL:C4C	2.90	0.49
26:C:520:LHG:H271	22:S:310:CLA:H93	1.93	0.49
20:S:59:TYR:CE1	21:S:302:CHL:CBA	2.95	0.49
1:g:119:VAL:CG1	21:g:605:CHL:HHH	2.41	0.49
1:n:215:ASP:O	1:n:219:ASN:ND2	2.44	0.49
1:G:54:ASP:OD2	1:G:57:THR:N	2.33	0.49
1:G:142:ARG:CA	21:G:608:CHL:HBC3	2.43	0.49
22:G:612:CLA:H2	22:G:612:CLA:HMA1	1.93	0.49
1:N:156:TYR:CZ	1:N:177:LYS:HE2	2.47	0.49
21:N:607:CHL:CMB	25:N:617:NEX:H35	2.42	0.49
22:c:514:CLA:H42	22:c:514:CLA:C1D	2.42	0.49
14:o:87:ASP:OD1	14:o:88:GLU:N	2.45	0.49
3:B:161:LEU:O	26:R:301:LHG:O1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:17:VAL:HB	13:M:18:PRO:HD3	1.95	0.49
19:r:207:VAL:O	19:r:211:VAL:HG23	2.13	0.49
20:s:59:TYR:CD1	21:s:302:CHL:HBA1	2.47	0.49
22:g:612:CLA:H2	22:g:612:CLA:HMA1	1.93	0.49
1:G:196:VAL:HB	22:G:613:CLA:C4C	2.42	0.49
1:N:142:ARG:CA	21:N:607:CHL:HBC3	2.42	0.49
22:Y:604:CLA:HMA2	21:Y:605:CHL:C3C	2.41	0.49
2:A:215:HIS:NE2	34:D:403:BCT:O1	2.43	0.49
3:B:344:PRO:HB3	3:B:401:PHE:HE1	1.77	0.49
4:C:344:SER:OG	4:C:348:GLU:N	2.44	0.49
5:D:33:TRP:N	5:D:132:GLU:OE2	2.42	0.49
7:F:18:HIS:CE1	37:F:101:HEM:C1C	2.98	0.49
20:s:77:TYR:OH	22:s:304:CLA:H3A	2.13	0.49
20:s:116:ALA:C	21:s:307:CHL:HMD2	2.37	0.49
21:R:306:CHL:H12	21:R:306:CHL:HMA2	1.93	0.49
23:g:615:LUT:H203	23:g:616:LUT:H8	1.93	0.49
1:y:142:ARG:C	21:y:608:CHL:HBC2	2.37	0.49
21:N:606:CHL:HBC2	21:N:606:CHL:CHD	2.36	0.49
21:Y:601:CHL:HHD	26:Y:617:LHG:HC82	1.95	0.49
22:C:515:CLA:H42	22:C:515:CLA:C1D	2.42	0.49
10:J:29:PHE:O	10:J:32:SER:OG	2.25	0.49
20:s:59:TYR:CE1	21:s:302:CHL:CBA	2.95	0.49
19:R:104:MET:HE1	19:R:201:HIS:CD2	2.47	0.49
19:R:196:LEU:HG	19:R:200:LYS:HD2	1.93	0.49
1:G:142:ARG:CA	21:G:608:CHL:HBC2	2.43	0.49
22:Y:603:CLA:OBD	21:Y:608:CHL:O1A	2.30	0.49
2:a:59:ASP:OD1	2:a:60:ILE:N	2.45	0.49
2:a:335:ASN:HA	5:d:351:ASN:HD22	1.78	0.49
35:a:413:DGD:HG2	36:B:601:LMG:H361	1.93	0.49
35:a:413:DGD:HA62	36:B:601:LMG:H291	1.94	0.49
5:D:315:PHE:HA	5:D:318:LYS:HD3	1.94	0.49
14:O:207:THR:HG22	14:O:214:VAL:HG22	1.94	0.49
19:r:215:GLN:OE1	19:r:219:SER:OG	2.22	0.49
19:R:165:GLU:HG2	19:R:170:LYS:HB2	1.94	0.49
21:g:601:CHL:HHD	26:g:619:LHG:C8	2.41	0.49
1:Y:142:ARG:C	21:Y:607:CHL:HBC2	2.37	0.49
23:Y:613:LUT:H8	23:Y:614:LUT:H41	1.95	0.49
3:b:150:CYS:HB2	22:b:602:CLA:HMC1	1.95	0.49
3:b:487:ASP:OD2	3:b:489:GLN:NE2	2.42	0.49
36:B:623:LMG:H191	21:R:306:CHL:C1A	2.43	0.49
4:C:187:ASP:OD1	4:C:188:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:51:ARG:NH1	6:E:54:GLU:OE2	2.38	0.49
1:n:142:ARG:CA	21:n:607:CHL:HBC3	2.42	0.49
1:n:196:VAL:HB	22:n:612:CLA:C4C	2.42	0.49
22:n:610:CLA:H71	22:n:611:CLA:C4D	2.42	0.49
1:y:142:ARG:CA	21:y:608:CHL:HBC2	2.43	0.49
21:y:601:CHL:C2D	26:y:617:LHG:HC82	2.41	0.49
1:G:142:ARG:C	21:G:608:CHL:HBC2	2.37	0.49
3:b:173:GLY:HA3	3:b:265:ILE:HD11	1.95	0.49
3:b:368:VAL:HG21	3:b:422:ARG:HG2	1.95	0.49
3:b:475:PHE:HE1	5:d:135:ARG:HD2	1.77	0.49
36:c:523:LMG:H122	36:c:523:LMG:H371	1.95	0.49
33:l:101:SQD:O2	33:L:101:SQD:O49	2.24	0.49
2:A:59:ASP:OD1	2:A:60:ILE:N	2.45	0.49
3:B:368:VAL:HG21	3:B:422:ARG:HG2	1.95	0.49
4:C:155:ASN:O	4:C:159:THR:OG1	2.26	0.49
22:C:514:CLA:H202	22:S:313:CLA:HAA1	1.94	0.49
5:D:49:TRP:CD1	30:D:401:PHO:H13	2.48	0.49
7:F:18:HIS:CG	37:F:101:HEM:NA	2.81	0.49
19:r:104:MET:HE1	19:r:201:HIS:CD2	2.47	0.49
26:R:301:LHG:O8	26:R:301:LHG:O2	2.21	0.49
1:g:142:ARG:CA	21:g:608:CHL:HBC3	2.43	0.49
1:y:197:GLN:HE21	22:y:612:CLA:C2A	2.11	0.49
22:N:610:CLA:H71	22:N:611:CLA:C4D	2.42	0.49
1:Y:142:ARG:CA	21:Y:607:CHL:HBC3	2.42	0.49
4:c:62:PHE:HZ	11:k:43:ILE:HD12	1.78	0.49
10:j:9:PRO:HD2	10:j:12:ILE:HD11	1.94	0.49
2:A:143:ILE:HG12	5:D:221:ASN:HD22	1.78	0.49
22:B:605:CLA:C1D	22:B:607:CLA:H51	2.42	0.49
19:r:151:GLU:HB2	21:r:306:CHL:HHB	1.94	0.49
19:R:64:ASP:OD1	19:R:65:VAL:N	2.40	0.49
21:n:605:CHL:CAA	25:n:616:NEX:H31	2.42	0.49
22:Y:604:CLA:C4B	25:Y:616:NEX:H242	2.43	0.49
33:l:103:SQD:O47	33:L:102:SQD:O4	2.30	0.49
13:m:17:VAL:HB	13:m:18:PRO:HD3	1.95	0.49
2:A:301:ASN:HB3	4:C:405:ASN:HD21	1.78	0.49
35:A:401:DGD:HG2	36:I:101:LMG:H361	1.95	0.49
33:A:412:SQD:S	33:A:412:SQD:O4	2.62	0.49
3:B:285:TYR:O	3:B:289:SER:OG	2.25	0.49
3:B:458:PHE:HB3	22:B:606:CLA:HBC2	1.94	0.49
22:W:101:CLA:H2	22:W:101:CLA:H62	1.54	0.49
20:S:59:TYR:CD1	21:S:302:CHL:HBA1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:77:TYR:OH	22:S:304:CLA:H3A	2.12	0.49
21:n:601:CHL:C2D	26:n:617:LHG:HC82	2.42	0.49
22:Y:610:CLA:H71	22:W:101:CLA:C4D	2.42	0.49
26:c:520:LHG:H272	22:s:311:CLA:H102	1.94	0.49
7:f:18:HIS:CG	37:f:101:HEM:C1C	2.94	0.49
4:C:124:VAL:HB	31:C:516:BCR:H362	1.95	0.49
19:R:207:VAL:O	19:R:211:VAL:HG23	2.13	0.49
1:g:142:ARG:HG3	21:g:608:CHL:C2D	2.40	0.48
1:n:142:ARG:C	21:n:607:CHL:HBC2	2.37	0.48
1:n:142:ARG:CA	21:n:607:CHL:HBC2	2.43	0.48
1:G:196:VAL:HG23	22:G:613:CLA:CMC	2.34	0.48
1:N:71:TRP:HD1	21:N:608:CHL:HMD3	1.63	0.48
1:Y:196:VAL:HB	22:Y:611:CLA:C4C	2.42	0.48
35:h:102:DGD:O6D	35:h:102:DGD:O3D	2.24	0.48
14:o:82:LEU:HA	14:o:84:TYR:CE1	2.48	0.48
3:B:173:GLY:HA3	3:B:265:ILE:HD11	1.95	0.48
22:r:304:CLA:O2A	22:r:304:CLA:H2A	2.13	0.48
22:g:603:CLA:OBD	21:g:609:CHL:O1A	2.30	0.48
21:y:605:CHL:CBC	21:y:606:CHL:HMD3	2.40	0.48
21:y:606:CHL:H12	25:y:616:NEX:H403	1.95	0.48
1:Y:142:ARG:CA	21:Y:607:CHL:HBC2	2.43	0.48
22:a:408:CLA:H11	9:i:9:TYR:CE1	2.48	0.48
4:c:261:ARG:HA	4:c:266:TRP:HZ2	1.78	0.48
26:c:520:LHG:H271	22:s:310:CLA:H93	1.95	0.48
31:k:101:BCR:H403	31:k:101:BCR:H371	1.95	0.48
13:m:31:SER:HB2	13:M:32:GLN:NE2	2.27	0.48
14:o:157:LEU:HD21	14:o:166:THR:HG23	1.95	0.48
14:O:59:THR:HB	14:O:73:PHE:HB3	1.94	0.48
14:O:82:LEU:HA	14:O:84:TYR:CE1	2.48	0.48
14:O:87:ASP:OD1	14:O:88:GLU:N	2.45	0.48
21:R:307:CHL:HAB	21:R:307:CHL:H62	1.95	0.48
1:N:54:ASP:OD2	1:N:57:THR:N	2.33	0.48
1:Y:24:TYR:CE2	21:Y:601:CHL:HAA2	2.48	0.48
7:f:18:HIS:CG	37:f:101:HEM:NA	2.81	0.48
33:l:103:SQD:H251	33:l:103:SQD:H92	1.95	0.48
16:w:19:ASN:HD21	16:w:21:LEU:HB3	1.79	0.48
19:R:184:LEU:HD12	22:R:309:CLA:H2	1.88	0.48
1:g:54:ASP:OD2	1:g:57:THR:N	2.33	0.48
1:g:61:ASN:HB3	22:g:602:CLA:HHB	1.95	0.48
22:g:610:CLA:H143	22:g:612:CLA:H3A	1.95	0.48
1:n:24:TYR:CE2	21:n:601:CHL:HAA2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:61:ASN:HB3	22:y:602:CLA:HHB	1.96	0.48
1:G:61:ASN:HB3	22:G:602:CLA:HHB	1.95	0.48
22:G:610:CLA:H143	22:G:612:CLA:H3A	1.96	0.48
1:Y:195:PHE:N	22:Y:611:CLA:CMC	2.77	0.48
3:b:124:CYS:SG	3:b:129:GLY:HA2	2.54	0.48
6:e:22:ILE:HD13	37:f:101:HEM:HMA3	1.95	0.48
3:B:150:CYS:HB2	22:B:605:CLA:HMC1	1.95	0.48
22:B:610:CLA:H193	22:D:405:CLA:H12	1.94	0.48
31:K:101:BCR:H403	31:K:101:BCR:H371	1.95	0.48
20:S:20:ASN:HA	20:S:23:LEU:HB2	1.95	0.48
19:R:151:GLU:HB2	21:R:305:CHL:HHB	1.94	0.48
22:y:610:CLA:H143	22:w:101:CLA:H3A	1.95	0.48
1:N:138:VAL:HG11	25:N:617:NEX:H35	1.96	0.48
22:N:603:CLA:OBD	21:N:608:CHL:O1A	2.31	0.48
21:Y:606:CHL:HBA2	21:Y:606:CHL:H3A	1.49	0.48
3:b:137:LYS:HZ1	8:h:29:GLU:HB2	1.79	0.48
3:b:167:TRP:HA	3:b:178:VAL:HA	1.95	0.48
5:d:315:PHE:HA	5:d:318:LYS:HD3	1.94	0.48
12:l:19:TYR:CE2	15:t:20:ALA:HA	2.49	0.48
16:w:13:LEU:HB2	16:w:16:GLY:HA2	1.94	0.48
3:B:113:TRP:CE2	3:B:117:TYR:HD2	2.32	0.48
4:C:171:GLY:HA2	4:C:174:LEU:HD12	1.95	0.48
36:C:523:LMG:H122	36:C:523:LMG:H371	1.95	0.48
19:r:165:GLU:HG2	19:r:170:LYS:HB2	1.94	0.48
19:R:47:GLN:HE21	19:R:69:ARG:HD2	1.78	0.48
22:R:303:CLA:O2A	22:R:303:CLA:H2A	2.13	0.48
1:g:195:PHE:N	22:g:613:CLA:CMC	2.77	0.48
22:g:611:CLA:H71	22:g:612:CLA:C4D	2.42	0.48
21:n:605:CHL:CMA	25:n:616:NEX:H32	2.43	0.48
1:G:102:SER:CA	21:G:607:CHL:HED3	2.34	0.48
1:N:195:PHE:N	22:N:612:CLA:CMC	2.77	0.48
22:b:601:CLA:H41	35:h:102:DGD:HB52	1.94	0.48
4:c:124:VAL:HB	31:c:515:BCR:H362	1.95	0.48
5:d:234:ARG:HG3	33:d:402:SQD:H61	1.96	0.48
33:l:101:SQD:O4	33:L:101:SQD:O47	2.30	0.48
3:B:28:ALA:O	3:B:104:SER:OG	2.28	0.48
3:B:68:ARG:HD2	22:B:605:CLA:HED1	1.95	0.48
22:S:313:CLA:H3A	22:S:313:CLA:HBA2	1.40	0.48
21:g:606:CHL:HAA1	25:g:618:NEX:C31	2.44	0.48
22:g:613:CLA:H3A	22:g:613:CLA:HBA2	1.36	0.48
1:N:61:ASN:HB3	22:N:602:CLA:HHB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:605:CHL:HMD3	21:r:301:CHL:CBC	2.44	0.48
2:a:183:MET:HB3	22:a:404:CLA:HBC2	1.95	0.48
4:c:171:GLY:HA2	4:c:174:LEU:HD12	1.95	0.48
2:A:212:SER:HB2	5:D:212:CYS:HB2	1.96	0.48
14:O:157:LEU:HD21	14:O:166:THR:HG23	1.95	0.48
20:s:20:ASN:HA	20:s:23:LEU:HB2	1.95	0.48
20:s:101:TYR:CD1	21:s:301:CHL:HMA3	2.27	0.48
22:s:305:CLA:HBA2	21:s:306:CHL:C1D	2.44	0.48
1:g:197:GLN:OE1	22:g:613:CLA:CAD	2.60	0.48
1:N:142:ARG:CA	21:N:607:CHL:HBC2	2.43	0.48
2:a:230:ASN:HD22	19:r:56:ASN:HD22	1.60	0.48
3:b:183:PRO:HB3	3:b:199:ALA:HB3	1.96	0.48
26:d:408:LHG:HC62	12:l:16:THR:HG23	1.96	0.48
36:B:623:LMG:H111	21:R:306:CHL:CBA	2.44	0.48
5:D:190:HIS:HA	5:D:295:ARG:HD3	1.95	0.48
7:F:18:HIS:CD2	37:F:101:HEM:C1A	2.95	0.48
1:g:142:ARG:CA	21:g:608:CHL:HBC2	2.43	0.48
21:n:605:CHL:H12	25:n:616:NEX:H403	1.96	0.48
21:n:608:CHL:H193	21:n:608:CHL:H162	1.64	0.48
1:y:121:ALA:HB3	21:y:605:CHL:CBC	2.21	0.48
21:Y:607:CHL:H62	21:Y:607:CHL:H41	1.49	0.48
36:d:410:LMG:O9	36:d:410:LMG:O2	2.29	0.48
14:o:207:THR:HG22	14:o:214:VAL:HG22	1.94	0.48
2:A:183:MET:HB3	22:A:405:CLA:HBC2	1.95	0.48
3:B:36:SER:HB2	31:B:602:BCR:H382	1.95	0.48
20:S:119:LEU:CD1	21:S:307:CHL:HMD1	2.37	0.48
22:S:305:CLA:HBA2	21:S:306:CHL:C1D	2.44	0.48
1:g:60:LYS:NZ	1:n:48:THR:O	2.34	0.48
22:N:602:CLA:HAB	23:N:615:LUT:H30	1.95	0.48
22:Y:609:CLA:H143	22:W:101:CLA:H3A	1.95	0.48
36:b:620:LMG:H273	21:r:306:CHL:OMC	2.13	0.48
3:B:167:TRP:HA	3:B:178:VAL:HA	1.95	0.48
10:J:9:PRO:HD2	10:J:12:ILE:HD11	1.94	0.48
19:R:218:VAL:HG21	22:R:311:CLA:HMD1	1.96	0.48
1:n:195:PHE:N	22:n:612:CLA:CMC	2.77	0.47
22:n:603:CLA:OBD	21:n:608:CHL:O1A	2.31	0.47
22:n:609:CLA:H143	22:n:611:CLA:H3A	1.96	0.47
1:y:215:ASP:OD2	1:y:218:ASN:ND2	2.47	0.47
22:y:603:CLA:OBD	21:y:609:CHL:O1A	2.32	0.47
1:G:215:ASP:OD2	1:G:218:ASN:ND2	2.47	0.47
1:N:196:VAL:HG23	22:N:612:CLA:CMC	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:197:GLN:OE1	22:N:612:CLA:CAD	2.60	0.47
22:N:609:CLA:H143	22:N:611:CLA:H3A	1.95	0.47
3:B:124:CYS:SG	3:B:129:GLY:HA2	2.54	0.47
4:C:261:ARG:HA	4:C:266:TRP:HZ2	1.78	0.47
31:D:406:BCR:H372	36:D:411:LMG:H302	1.96	0.47
19:r:218:VAL:HG21	22:r:312:CLA:HMD1	1.96	0.47
20:s:116:ALA:CA	21:s:307:CHL:C3D	2.92	0.47
21:R:305:CHL:H142	21:R:305:CHL:H111	1.68	0.47
22:g:602:CLA:H122	23:g:616:LUT:H393	1.96	0.47
22:g:612:CLA:H2	22:g:612:CLA:H62	1.54	0.47
21:G:601:CHL:ND	26:G:618:LHG:H102	2.29	0.47
1:N:71:TRP:CE2	21:N:608:CHL:CHD	2.94	0.47
3:b:161:LEU:O	26:r:302:LHG:O1	2.31	0.47
4:c:344:SER:OG	4:c:348:GLU:N	2.44	0.47
14:o:49:LYS:HB2	14:o:247:GLU:HG3	1.95	0.47
36:B:623:LMG:H221	21:R:306:CHL:C1C	2.33	0.47
33:L:101:SQD:H251	33:L:101:SQD:H92	1.95	0.47
36:M:101:LMG:H342	36:M:101:LMG:H141	1.97	0.47
21:r:308:CHL:HAB	21:r:308:CHL:H62	1.95	0.47
22:r:311:CLA:HED2	22:r:311:CLA:H2A	1.97	0.47
20:S:42:ARG:HD2	20:S:45:ILE:HD11	1.96	0.47
22:g:603:CLA:H91	22:n:602:CLA:H172	1.96	0.47
21:n:601:CHL:O1D	26:n:617:LHG:C12	2.62	0.47
1:y:195:PHE:N	22:y:612:CLA:CMC	2.77	0.47
1:Y:197:GLN:OE1	22:Y:611:CLA:CAD	2.60	0.47
2:a:26:ASN:HB3	33:a:411:SQD:H82	1.97	0.47
35:a:413:DGD:HA71	26:B:622:LHG:HC31	1.96	0.47
5:d:190:HIS:HA	5:d:295:ARG:HD3	1.95	0.47
5:d:280:LEU:HD22	30:d:401:PHO:HBC3	1.97	0.47
3:B:5:TRP:NE1	26:L:103:LHG:O9	2.40	0.47
4:C:107:ASP:OD1	4:C:108:THR:N	2.48	0.47
4:C:268:GLY:HA2	4:C:271:TYR:CD2	2.49	0.47
16:W:19:ASN:HD21	16:W:21:LEU:HB3	1.79	0.47
19:R:149:TRP:CZ2	26:R:301:LHG:H191	2.49	0.47
1:g:196:VAL:HG23	22:g:613:CLA:CMC	2.35	0.47
1:G:182:LYS:NZ	26:G:618:LHG:O4	2.47	0.47
1:G:195:PHE:N	22:G:613:CLA:CMC	2.77	0.47
21:G:601:CHL:H102	22:Y:603:CLA:CHD	2.45	0.47
21:G:609:CHL:H122	21:N:601:CHL:H121	1.96	0.47
22:a:408:CLA:H61	22:a:408:CLA:H2	1.63	0.47
3:b:68:ARG:HD2	22:b:602:CLA:HED1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:401:PHO:H143	22:d:403:CLA:H171	1.95	0.47
7:f:18:HIS:CE1	37:f:101:HEM:C1C	2.98	0.47
5:D:93:LEU:O	5:D:100:GLY:N	2.47	0.47
22:r:311:CLA:H2	22:r:311:CLA:O1D	2.14	0.47
20:s:174:GLY:HA2	20:s:177:ASN:OD1	2.14	0.47
22:R:310:CLA:O1D	22:R:310:CLA:H2	2.14	0.47
22:c:513:CLA:H202	22:s:313:CLA:HAA1	1.97	0.47
5:d:33:TRP:N	5:d:132:GLU:OE2	2.42	0.47
22:C:515:CLA:C1C	31:C:516:BCR:H383	2.44	0.47
20:S:116:ALA:CA	21:S:307:CHL:C2D	2.85	0.47
1:g:24:TYR:CE2	21:g:601:CHL:HAA2	2.48	0.47
21:g:601:CHL:C10	21:y:609:CHL:H111	2.44	0.47
1:G:24:TYR:CE2	21:G:601:CHL:HAA2	2.48	0.47
1:G:71:TRP:CE2	21:G:609:CHL:CHD	2.94	0.47
3:b:113:TRP:CE2	3:b:117:TYR:HD2	2.32	0.47
4:c:107:ASP:OD1	4:c:108:THR:N	2.48	0.47
22:c:505:CLA:NB	35:c:518:DGD:HB92	2.29	0.47
3:B:18:ARG:NH1	12:L:5:ASN:HD22	2.11	0.47
3:B:334:ASP:HA	14:O:176:ALA:HB1	1.97	0.47
22:B:613:CLA:HBB1	22:B:615:CLA:H3A	1.96	0.47
22:B:616:CLA:H92	22:B:616:CLA:H61	1.71	0.47
4:C:318:LEU:HD12	4:C:340:TYR:HB3	1.96	0.47
36:M:101:LMG:H141	36:M:101:LMG:H362	1.96	0.47
14:O:57:SER:HB3	14:O:239:GLN:HB2	1.96	0.47
19:r:47:GLN:HE21	19:r:69:ARG:HD2	1.78	0.47
20:S:94:ILE:HG21	22:S:305:CLA:HAC2	1.95	0.47
19:R:188:PRO:HA	19:R:191:LYS:HE2	1.97	0.47
22:R:309:CLA:HBA2	22:R:309:CLA:H3A	1.33	0.47
1:n:61:ASN:HB3	22:n:602:CLA:HHB	1.96	0.47
1:n:215:ASP:OD2	1:n:218:ASN:ND2	2.47	0.47
1:y:24:TYR:CE2	21:y:601:CHL:HAA2	2.48	0.47
1:y:197:GLN:OE1	22:y:612:CLA:CAD	2.60	0.47
1:N:193:GLY:HA2	26:N:618:LHG:H221	1.97	0.47
1:Y:61:ASN:HB3	22:Y:602:CLA:HHB	1.96	0.47
4:c:268:GLY:HA2	4:c:271:TYR:CD2	2.49	0.47
22:c:514:CLA:C1C	31:c:515:BCR:H383	2.44	0.47
5:d:264:ASN:ND2	5:d:267:TRP:H	2.13	0.47
31:d:405:BCR:H372	36:d:410:LMG:H302	1.96	0.47
32:d:406:PL9:H151	32:d:406:PL9:H171	1.61	0.47
2:A:105:TRP:CE2	2:A:110:GLY:HA3	2.50	0.47
3:B:183:PRO:HB3	3:B:199:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:258:TYR:CE1	35:H:102:DGD:HG31	2.49	0.47
4:C:321:ASP:OD2	4:C:340:TYR:OH	2.21	0.47
4:C:430:HIS:HA	4:C:433:LEU:HD12	1.97	0.47
22:C:512:CLA:H162	22:C:512:CLA:H122	1.56	0.47
32:D:407:PL9:H513	15:T:10:LEU:HD13	1.96	0.47
12:L:8:GLU:HB3	33:L:102:SQD:H4	1.97	0.47
20:s:119:LEU:CD1	21:s:307:CHL:HMD1	2.36	0.47
20:S:174:GLY:HA2	20:S:177:ASN:OD1	2.14	0.47
22:n:612:CLA:HBA2	22:n:612:CLA:H3A	1.36	0.47
1:N:24:TYR:CE2	21:N:601:CHL:HAA2	2.48	0.47
1:N:215:ASP:OD2	1:N:218:ASN:ND2	2.47	0.47
21:Y:608:CHL:C2	21:Y:608:CHL:CHC	2.93	0.47
26:b:619:LHG:HC31	35:A:401:DGD:HA71	1.96	0.47
22:c:509:CLA:H3A	22:c:509:CLA:HBA2	1.35	0.47
3:B:497:LYS:NZ	5:D:21:ASP:HA	2.30	0.47
11:K:30:TYR:HB3	11:K:33:LEU:HD12	1.97	0.47
20:S:101:TYR:CZ	21:S:301:CHL:C3A	2.80	0.47
22:b:601:CLA:H91	22:b:601:CLA:H112	1.73	0.47
4:c:430:HIS:HA	4:c:433:LEU:HD12	1.97	0.47
26:c:520:LHG:HC5	22:s:310:CLA:H42	1.45	0.47
22:d:404:CLA:H61	22:d:404:CLA:H41	1.61	0.47
2:A:303:ASN:HB2	4:C:414:ILE:HA	1.97	0.47
22:B:614:CLA:H13	22:B:614:CLA:H171	1.71	0.47
22:B:617:CLA:H72	22:B:618:CLA:HBB1	1.96	0.47
22:C:506:CLA:NB	35:C:519:DGD:HB92	2.29	0.47
5:D:187:GLN:NE2	5:D:323:ASN:OD1	2.47	0.47
5:D:316:TYR:O	5:D:320:ILE:HG12	2.15	0.47
20:s:116:ALA:CA	21:s:307:CHL:C2D	2.83	0.47
21:G:608:CHL:H62	21:G:608:CHL:H41	1.49	0.47
1:Y:215:ASP:OD2	1:Y:218:ASN:ND2	2.47	0.47
4:c:187:ASP:N	4:c:195:ASP:O	2.49	0.47
31:c:515:BCR:HC21	18:z:58:ASN:HD22	1.79	0.47
8:h:32:LYS:HB2	19:r:69:ARG:NH2	2.30	0.47
5:D:264:ASN:ND2	5:D:267:TRP:H	2.13	0.47
14:O:49:LYS:HB2	14:O:247:GLU:HG3	1.95	0.47
20:s:201:LEU:HA	20:s:204:PHE:CD2	2.50	0.47
1:g:197:GLN:NE2	22:g:613:CLA:C2A	2.59	0.46
23:N:614:LUT:H8	23:N:615:LUT:C4	2.43	0.46
21:Y:608:CHL:HBC3	21:Y:608:CHL:CMC	2.42	0.46
31:d:405:BCR:H14C	7:f:27:PHE:CE2	2.51	0.46
14:o:57:SER:HB3	14:o:239:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:162:GLY:HA2	4:C:248:GLY:HA2	1.96	0.46
19:r:140:LEU:HB3	19:r:142:PHE:HD1	1.80	0.46
19:r:156:GLY:HA2	22:r:309:CLA:HAB	1.97	0.46
21:r:308:CHL:H8	21:r:308:CHL:H122	1.35	0.46
22:r:310:CLA:H62	22:r:310:CLA:H41	1.67	0.46
20:S:30:ASP:HA	20:S:42:ARG:HH22	1.81	0.46
21:n:608:CHL:HBC3	21:n:608:CHL:CMC	2.41	0.46
21:G:606:CHL:O1A	21:G:606:CHL:H42	2.16	0.46
22:b:614:CLA:H72	22:b:615:CLA:HBB1	1.96	0.46
5:d:93:LEU:O	5:d:100:GLY:N	2.47	0.46
8:h:35:PRO:HB3	19:r:46:LEU:HD11	1.97	0.46
4:C:187:ASP:N	4:C:195:ASP:O	2.49	0.46
36:T:101:LMG:H342	36:T:101:LMG:H141	1.97	0.46
16:W:38:PHE:CE2	22:W:101:CLA:C3	2.98	0.46
20:s:94:ILE:HG21	22:s:305:CLA:HAC2	1.95	0.46
22:R:308:CLA:H3A	22:R:308:CLA:HBA1	1.46	0.46
21:g:605:CHL:HBC1	21:g:606:CHL:HMD3	1.96	0.46
1:n:54:ASP:OD2	1:n:57:THR:N	2.33	0.46
1:n:197:GLN:OE1	22:n:612:CLA:CAD	2.60	0.46
1:y:187:ALA:O	1:y:190:SER:OG	2.31	0.46
21:Y:601:CHL:H141	21:Y:601:CHL:H161	1.55	0.46
2:a:159:LEU:C	2:a:162:PRO:HD2	2.40	0.46
22:b:610:CLA:HBB1	22:b:612:CLA:H3A	1.96	0.46
4:c:162:GLY:HA2	4:c:248:GLY:HA2	1.96	0.46
4:c:228:ASP:N	4:c:228:ASP:OD1	2.48	0.46
7:f:18:HIS:HD2	37:f:101:HEM:NA	2.00	0.46
13:m:27:VAL:HA	13:m:30:VAL:HG22	1.97	0.46
21:n:601:CHL:CHD	26:n:617:LHG:HC81	2.45	0.46
1:G:197:GLN:OE1	22:G:613:CLA:CAD	2.60	0.46
1:Y:187:ALA:O	1:Y:190:SER:OG	2.31	0.46
21:Y:605:CHL:H42	21:Y:605:CHL:O1A	2.16	0.46
2:a:105:TRP:CE2	2:a:110:GLY:HA3	2.50	0.46
2:a:143:ILE:HG12	5:d:221:ASN:HD22	1.80	0.46
3:b:348:ASP:OD1	3:b:352:ARG:N	2.48	0.46
4:c:62:PHE:CZ	11:k:43:ILE:HD12	2.50	0.46
5:d:237:ASN:HB3	5:d:240:GLN:HB3	1.97	0.46
22:B:608:CLA:O1A	22:B:608:CLA:H3A	2.16	0.46
22:r:309:CLA:HBA1	22:r:309:CLA:H3A	1.46	0.46
20:s:30:ASP:HA	20:s:42:ARG:HH22	1.80	0.46
20:S:35:LEU:HG	20:S:36:PRO:HD2	1.98	0.46
1:g:215:ASP:OD2	1:g:218:ASN:ND2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:y:606:CHL:H42	21:y:606:CHL:O1A	2.16	0.46
21:y:606:CHL:HAA1	25:y:616:NEX:C31	2.45	0.46
21:G:607:CHL:H192	21:G:607:CHL:H162	1.82	0.46
22:G:612:CLA:H2	22:G:612:CLA:H62	1.54	0.46
4:c:151:TRP:CZ2	22:c:510:CLA:HBC2	2.51	0.46
4:c:318:LEU:HD12	4:c:340:TYR:HB3	1.96	0.46
22:c:505:CLA:H43	35:c:519:DGD:HB32	1.98	0.46
26:c:522:LHG:H322	26:c:522:LHG:H291	1.68	0.46
5:d:316:TYR:O	5:d:320:ILE:HG12	2.15	0.46
17:x:51:LEU:O	17:x:55:LEU:HG	2.16	0.46
2:A:26:ASN:HB3	33:A:412:SQD:H82	1.97	0.46
22:C:511:CLA:HED2	22:C:511:CLA:H2A	1.98	0.46
20:s:35:LEU:HG	20:s:36:PRO:HD2	1.98	0.46
20:s:42:ARG:HD2	20:s:45:ILE:HD11	1.96	0.46
22:g:603:CLA:C2D	21:n:601:CHL:H71	2.46	0.46
21:n:606:CHL:H2	21:n:606:CHL:H62	1.72	0.46
21:n:607:CHL:CHA	21:n:607:CHL:CBA	2.94	0.46
1:G:71:TRP:NE1	21:G:609:CHL:CMD	2.78	0.46
21:G:601:CHL:C5	21:Y:608:CHL:O1A	2.63	0.46
1:Y:71:TRP:NE1	21:Y:608:CHL:CMD	2.78	0.46
1:Y:197:GLN:NE2	22:Y:611:CLA:C2A	2.59	0.46
21:Y:607:CHL:H51	21:Y:607:CHL:H8	1.36	0.46
2:a:131:TRP:HZ2	4:c:449:ARG:HD2	1.80	0.46
4:c:87:ILE:C	4:c:90:PRO:HD2	2.41	0.46
31:d:405:BCR:H16C	7:f:27:PHE:HD2	1.79	0.46
7:f:10:PHE:HB3	7:f:14:TRP:HZ3	1.81	0.46
3:B:497:LYS:HA	5:D:25:ARG:HA	1.98	0.46
10:J:33:TYR:CZ	35:J:101:DGD:HG32	2.51	0.46
36:T:101:LMG:H141	36:T:101:LMG:H362	1.96	0.46
20:s:98:PHE:CZ	21:s:301:CHL:HED1	2.50	0.46
19:R:227:ILE:O	19:R:231:ASN:ND2	2.49	0.46
1:y:71:TRP:CE2	21:y:609:CHL:CHD	2.94	0.46
1:N:71:TRP:NE1	21:N:608:CHL:CMD	2.78	0.46
25:N:617:NEX:H191	25:N:617:NEX:H11	1.73	0.46
21:Y:607:CHL:CHA	21:Y:607:CHL:CBA	2.94	0.46
9:i:6:LEU:HD22	16:w:22:LEU:HD13	1.96	0.46
2:A:296:ASN:HD22	4:C:401:LEU:HG	1.81	0.46
20:s:224:ASP:O	20:s:228:ASN:N	2.49	0.46
20:S:116:ALA:C	21:S:307:CHL:HMD2	2.40	0.46
22:S:305:CLA:HBA2	22:S:305:CLA:H3A	1.41	0.46
1:g:191:MET:HG3	23:g:616:LUT:H202	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:142:ARG:CB	21:n:607:CHL:CHD	2.94	0.46
1:n:187:ALA:O	1:n:190:SER:OG	2.31	0.46
22:G:602:CLA:H3A	22:G:602:CLA:HBA2	1.33	0.46
1:Y:142:ARG:CB	21:Y:607:CHL:CHD	2.94	0.46
22:a:405:CLA:H141	22:a:405:CLA:H162	1.66	0.46
37:f:101:HEM:CHC	37:f:101:HEM:HBB2	2.46	0.46
3:B:348:ASP:OD1	3:B:352:ARG:N	2.48	0.46
36:B:623:LMG:C23	21:R:306:CHL:NC	2.79	0.46
5:D:237:ASN:HB3	5:D:240:GLN:HB3	1.98	0.46
20:S:64:LEU:HD11	22:S:303:CLA:H111	1.98	0.46
20:S:224:ASP:O	20:S:228:ASN:N	2.49	0.46
22:R:310:CLA:HED2	22:R:310:CLA:H2A	1.97	0.46
1:g:71:TRP:HD1	21:g:609:CHL:HMD3	1.63	0.46
21:g:609:CHL:O1A	21:n:601:CHL:C5	2.64	0.46
21:G:601:CHL:H61	21:G:601:CHL:H41	1.76	0.46
1:Y:65:GLU:OE2	1:Y:185:ARG:NE	2.36	0.46
22:Y:610:CLA:C4C	26:Y:617:LHG:HC5	2.46	0.46
4:c:211:GLY:O	4:c:215:LYS:HG3	2.16	0.46
22:c:509:CLA:H62	22:c:509:CLA:H41	1.76	0.46
17:x:54:PHE:O	17:x:58:ILE:HG12	2.16	0.46
3:B:243:ALA:HA	3:B:246:PHE:CE2	2.51	0.46
22:C:506:CLA:H43	35:J:101:DGD:HB32	1.98	0.46
19:r:13:VAL:HB	19:r:18:ALA:HB3	1.98	0.46
20:S:86:MET:HG3	20:S:193:GLY:HA2	1.98	0.46
20:S:201:LEU:HA	20:S:204:PHE:CD2	2.51	0.46
21:n:605:CHL:H42	21:n:605:CHL:O1A	2.16	0.46
1:y:65:GLU:OE2	1:y:185:ARG:NE	2.36	0.46
21:G:601:CHL:H2	21:Y:608:CHL:HBA1	1.98	0.46
21:G:605:CHL:HBC1	21:G:606:CHL:HMD3	1.96	0.46
21:G:609:CHL:HBC3	21:G:609:CHL:CMC	2.41	0.46
22:G:613:CLA:H3A	22:G:613:CLA:HBA2	1.36	0.46
21:N:605:CHL:H42	21:N:605:CHL:O1A	2.16	0.46
22:d:403:CLA:H62	22:d:403:CLA:H41	1.70	0.46
36:B:623:LMG:H112	36:B:623:LMG:HC2	1.99	0.46
35:C:519:DGD:HB22	36:K:103:LMG:H391	1.98	0.46
7:F:10:PHE:HB3	7:F:14:TRP:HZ3	1.81	0.46
17:X:51:LEU:O	17:X:55:LEU:HG	2.16	0.46
22:r:304:CLA:C2D	22:r:309:CLA:H62	2.46	0.46
19:R:156:GLY:HA2	22:R:308:CLA:HAB	1.97	0.46
25:g:618:NEX:H28	25:g:618:NEX:H371	1.97	0.45
1:G:187:ALA:O	1:G:190:SER:OG	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:67:ILE:CG2	21:N:608:CHL:HMD1	2.41	0.45
3:b:10:THR:O	19:r:55:GLN:NE2	2.49	0.45
36:b:620:LMG:H222	21:r:307:CHL:CHB	2.45	0.45
22:c:510:CLA:H2A	22:c:510:CLA:HED2	1.98	0.45
22:B:605:CLA:H61	22:B:605:CLA:H41	1.78	0.45
19:r:76:LYS:HB2	19:r:82:PRO:HA	1.99	0.45
19:r:126:LYS:HD3	21:r:307:CHL:HED3	1.98	0.45
19:R:140:LEU:HB3	19:R:142:PHE:HD1	1.80	0.45
1:n:71:TRP:NE1	21:n:608:CHL:CMD	2.78	0.45
22:N:603:CLA:H93	22:N:603:CLA:H112	1.77	0.45
21:N:607:CHL:CHA	21:N:607:CHL:CBA	2.94	0.45
3:b:21:SER:OG	3:b:111:ALA:O	2.26	0.45
3:b:243:ALA:HA	3:b:246:PHE:CE2	2.51	0.45
22:b:605:CLA:O1A	22:b:605:CLA:H3A	2.16	0.45
4:c:27:ASP:OD1	4:c:29:GLU:HG2	2.16	0.45
2:A:77:ILE:H	12:L:34:ASN:HD21	1.63	0.45
22:B:610:CLA:H3A	22:B:610:CLA:HBA2	1.69	0.45
4:C:151:TRP:CZ2	22:C:511:CLA:HBC2	2.51	0.45
22:C:514:CLA:H152	22:S:313:CLA:H92	1.65	0.45
20:s:99:ASN:ND2	20:s:105:CYS:HB3	2.32	0.45
20:S:99:ASN:ND2	20:S:105:CYS:HB3	2.32	0.45
22:S:311:CLA:H52	22:S:311:CLA:H8	1.44	0.45
1:g:26:GLY:O	1:g:29:SER:OG	2.32	0.45
1:g:142:ARG:CB	21:g:608:CHL:CHD	2.94	0.45
22:n:612:CLA:H2	22:n:612:CLA:H61	1.62	0.45
1:G:25:LEU:HA	21:G:601:CHL:CHC	2.47	0.45
1:G:142:ARG:CB	21:G:608:CHL:CHD	2.94	0.45
1:N:142:ARG:CB	21:N:607:CHL:CHD	2.94	0.45
21:N:605:CHL:HMD3	21:S:301:CHL:CBC	2.43	0.45
21:N:608:CHL:H141	21:N:608:CHL:H161	1.66	0.45
30:a:407:PHO:H11	26:d:408:LHG:H362	1.99	0.45
3:b:170:ASP:HB3	3:b:174:LEU:H	1.81	0.45
31:b:618:BCR:H20C	31:b:618:BCR:H361	1.78	0.45
5:d:69:LEU:HD11	6:e:44:TYR:CE1	2.51	0.45
2:A:77:ILE:HB	12:L:34:ASN:HD21	1.82	0.45
19:r:188:PRO:HA	19:r:191:LYS:HE2	1.97	0.45
22:R:304:CLA:H11	22:R:304:CLA:HBA2	1.61	0.45
21:g:606:CHL:O1A	21:g:606:CHL:H42	2.16	0.45
21:g:607:CHL:HBC2	21:g:607:CHL:CHD	2.36	0.45
21:n:607:CHL:H62	21:n:607:CHL:H41	1.49	0.45
1:N:24:TYR:CD1	1:N:46:TRP:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:252:HIS:ND1	32:a:410:PL9:O2	2.50	0.45
11:k:45:LEU:O	11:k:49:LEU:HG	2.17	0.45
2:A:159:LEU:C	2:A:162:PRO:HD2	2.40	0.45
2:A:252:HIS:ND1	32:A:411:PL9:O2	2.50	0.45
3:B:170:ASP:HB3	3:B:174:LEU:H	1.81	0.45
5:D:133:LEU:O	5:D:137:VAL:HG23	2.16	0.45
5:D:231:ASN:ND2	33:D:402:SQD:O8	2.48	0.45
14:O:138:LYS:HE2	14:O:138:LYS:HB2	1.67	0.45
19:R:76:LYS:HB2	19:R:82:PRO:HA	1.99	0.45
21:g:608:CHL:CHA	21:g:608:CHL:CBA	2.94	0.45
1:n:24:TYR:CD1	1:n:46:TRP:HB2	2.52	0.45
1:y:24:TYR:CD1	1:y:46:TRP:HB2	2.52	0.45
1:y:25:LEU:HA	21:y:601:CHL:CHC	2.47	0.45
22:y:604:CLA:HAB	23:y:614:LUT:C34	2.47	0.45
1:N:25:LEU:HA	21:N:601:CHL:CHC	2.47	0.45
21:Y:607:CHL:O2D	21:Y:607:CHL:H2A	2.17	0.45
3:b:65:PHE:CE2	22:b:603:CLA:H2A	2.52	0.45
4:c:322:GLN:NE2	4:c:381:LYS:HA	2.32	0.45
14:o:76:THR:HG22	14:o:118:LEU:HD23	1.99	0.45
2:A:12:ASN:HD21	16:W:40:TYR:HD1	1.64	0.45
3:B:385:ARG:NH1	14:O:167:GLY:O	2.49	0.45
13:M:27:VAL:HA	13:M:30:VAL:HG22	1.97	0.45
20:s:149:ALA:HA	20:s:153:ARG:HG3	1.98	0.45
21:s:302:CHL:O2D	21:s:302:CHL:H2A	2.17	0.45
22:s:311:CLA:H52	22:s:311:CLA:H8	1.44	0.45
19:R:13:VAL:HB	19:R:18:ALA:HB3	1.98	0.45
1:g:24:TYR:CD1	1:g:46:TRP:HB2	2.52	0.45
21:n:607:CHL:O2D	21:n:607:CHL:H2A	2.17	0.45
24:n:615:XAT:H35	24:n:615:XAT:H401	1.74	0.45
21:N:607:CHL:HMB1	25:N:617:NEX:H14	1.98	0.45
36:b:620:LMG:H112	36:b:620:LMG:HC2	1.99	0.45
30:d:401:PHO:H3A	30:d:401:PHO:HBA1	1.59	0.45
26:d:408:LHG:O10	12:l:16:THR:HG23	2.17	0.45
11:k:30:TYR:HB3	11:k:33:LEU:HD12	1.97	0.45
2:A:269:ARG:NH2	5:D:232:THR:O	2.47	0.45
2:A:272:HIS:HE2	34:D:403:BCT:C	2.29	0.45
11:K:45:LEU:O	11:K:49:LEU:HG	2.17	0.45
20:s:210:THR:HG21	20:s:217:ASN:ND2	2.32	0.45
20:S:80:ILE:HD11	20:S:84:TRP:CE2	2.52	0.45
20:S:98:PHE:CZ	21:S:301:CHL:CED	2.98	0.45
19:R:126:LYS:HD3	21:R:306:CHL:HED3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:301:LHG:H121	26:R:301:LHG:HC91	1.71	0.45
22:R:303:CLA:HAB	24:R:313:XAT:C35	2.44	0.45
21:g:607:CHL:H3A	21:g:607:CHL:HBA2	1.49	0.45
1:y:127:ILE:HD11	21:y:605:CHL:CBC	2.46	0.45
22:y:612:CLA:H102	24:y:615:XAT:H14	1.97	0.45
22:y:613:CLA:HBA2	22:y:613:CLA:H3A	1.67	0.45
22:G:604:CLA:HAB	23:G:615:LUT:C34	2.47	0.45
22:N:612:CLA:HBA2	22:N:612:CLA:H3A	1.36	0.45
1:Y:24:TYR:CD1	1:Y:46:TRP:HB2	2.52	0.45
22:a:405:CLA:H142	22:a:405:CLA:H112	1.85	0.45
4:c:261:ARG:NH1	16:w:48:GLU:O	2.50	0.45
22:c:502:CLA:H142	22:c:502:CLA:H111	1.75	0.45
35:c:518:DGD:HB22	36:k:103:LMG:H391	1.97	0.45
2:A:303:ASN:ND2	4:C:413:GLU:O	2.49	0.45
36:B:623:LMG:H191	21:R:306:CHL:C4D	2.47	0.45
4:C:87:ILE:C	4:C:90:PRO:HD2	2.41	0.45
32:D:407:PL9:H171	32:D:407:PL9:H151	1.61	0.45
37:F:101:HEM:CHC	37:F:101:HEM:HBB2	2.46	0.45
19:r:227:ILE:O	19:r:231:ASN:ND2	2.49	0.45
19:R:155:ILE:HA	19:R:158:ILE:HG12	1.98	0.45
1:n:142:ARG:CA	21:n:607:CHL:CHD	2.95	0.45
1:y:142:ARG:CB	21:y:608:CHL:CHD	2.94	0.45
21:y:607:CHL:H2	21:y:607:CHL:H62	1.72	0.45
21:N:607:CHL:O2D	21:N:607:CHL:H2A	2.17	0.45
5:d:133:LEU:O	5:d:137:VAL:HG23	2.16	0.45
13:m:31:SER:HB2	13:M:32:GLN:HE21	1.81	0.45
3:B:167:TRP:HE1	3:B:169:SER:HB3	1.82	0.45
4:C:131:TYR:CD1	4:C:135:LEU:HB3	2.52	0.45
20:s:86:MET:HG3	20:s:193:GLY:HA2	1.98	0.45
21:R:307:CHL:H8	21:R:307:CHL:H122	1.36	0.45
1:g:25:LEU:HA	21:g:601:CHL:CHC	2.47	0.45
22:g:603:CLA:H71	22:y:603:CLA:H122	1.99	0.45
1:n:127:ILE:HD11	21:s:301:CHL:CBC	2.47	0.45
22:a:406:CLA:H3A	22:a:406:CLA:HBA2	1.36	0.45
22:a:408:CLA:H122	36:w:102:LMG:H161	1.99	0.45
4:c:319:VAL:O	4:c:323:ARG:HG3	2.17	0.45
4:C:27:ASP:OD1	4:C:29:GLU:HG2	2.17	0.45
5:D:344:GLU:HA	5:D:347:LEU:HG	1.99	0.45
22:D:405:CLA:H61	22:D:405:CLA:H41	1.61	0.45
7:F:13:ARG:NE	37:F:101:HEM:O2D	2.50	0.45
31:H:101:BCR:H361	31:H:101:BCR:H20C	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:302:CHL:O2D	21:S:302:CHL:H2A	2.17	0.45
1:n:112:TYR:O	1:n:118:LEU:HD12	2.18	0.45
21:y:608:CHL:CHA	21:y:608:CHL:CBA	2.94	0.45
21:y:608:CHL:O2D	21:y:608:CHL:H2A	2.17	0.45
21:G:601:CHL:H71	22:Y:603:CLA:CMD	2.46	0.45
21:G:608:CHL:O2D	21:G:608:CHL:H2A	2.17	0.45
22:G:613:CLA:H61	22:G:613:CLA:H2	1.62	0.45
1:N:26:GLY:O	1:N:29:SER:OG	2.32	0.45
21:N:607:CHL:HMB3	25:N:617:NEX:H403	1.98	0.45
4:c:268:GLY:C	22:c:510:CLA:HAC2	2.42	0.45
22:c:513:CLA:H152	22:s:313:CLA:H92	1.54	0.45
3:B:80:ILE:HG23	3:B:81:THR:HG23	1.99	0.45
31:K:102:BCR:H20C	31:K:102:BCR:H361	1.85	0.45
20:s:64:LEU:HD11	22:s:303:CLA:H111	1.98	0.45
22:S:309:CLA:H52	22:S:309:CLA:H8	1.72	0.45
1:g:25:LEU:C	21:g:601:CHL:HBB1	2.42	0.44
1:n:158:GLY:N	22:n:609:CLA:OBD	2.38	0.44
21:n:601:CHL:O1D	26:n:617:LHG:H121	2.17	0.44
21:n:605:CHL:HMD3	21:s:301:CHL:HBC1	1.93	0.44
1:G:189:PHE:CD2	26:G:618:LHG:H281	2.52	0.44
3:b:167:TRP:HE1	3:b:169:SER:HB3	1.82	0.44
5:d:187:GLN:NE2	5:d:323:ASN:OD1	2.47	0.44
5:d:344:GLU:HA	5:d:347:LEU:HG	1.99	0.44
17:X:54:PHE:O	17:X:58:ILE:HG12	2.16	0.44
19:r:155:ILE:HA	19:r:158:ILE:HG12	1.98	0.44
1:g:112:TYR:O	1:g:118:LEU:HD12	2.17	0.44
22:g:604:CLA:HAB	23:g:615:LUT:C34	2.47	0.44
21:g:609:CHL:CGA	21:n:601:CHL:H2	2.47	0.44
21:n:608:CHL:H91	21:n:608:CHL:H112	1.69	0.44
21:N:601:CHL:HMB2	24:N:616:XAT:H393	2.00	0.44
23:N:615:LUT:H173	23:N:615:LUT:H7	1.74	0.44
3:b:80:ILE:HG23	3:b:81:THR:HG23	1.99	0.44
22:b:601:CLA:H162	22:b:601:CLA:H202	1.73	0.44
14:o:54:GLU:OE2	16:w:1:LEU:N	2.50	0.44
14:o:59:THR:OG1	14:o:237:LYS:HB3	2.17	0.44
2:A:258:LEU:HG	2:A:259:ILE:HG12	1.99	0.44
3:B:15:ASP:OD2	12:L:5:ASN:ND2	2.47	0.44
4:C:211:GLY:O	4:C:215:LYS:HG3	2.16	0.44
4:C:293:ASN:OD1	4:C:294:ASN:N	2.51	0.44
22:C:511:CLA:HBA1	22:C:511:CLA:H3A	1.41	0.44
22:C:513:CLA:H151	11:K:54:TRP:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:520:LHG:H312	26:C:520:LHG:H282	1.87	0.44
20:s:47:GLU:H	20:s:47:GLU:CD	2.25	0.44
20:s:178:ASP:HB3	20:s:181:GLN:HB2	1.99	0.44
20:S:136:ILE:HG23	20:S:137:LEU:HD12	1.99	0.44
21:S:302:CHL:C2D	26:S:314:LHG:HC82	2.47	0.44
22:n:604:CLA:HAB	23:n:614:LUT:C34	2.47	0.44
22:N:604:CLA:HAB	23:N:614:LUT:C34	2.47	0.44
5:d:25:ARG:NH1	17:x:81:VAL:HA	2.32	0.44
3:B:65:PHE:CE2	22:B:606:CLA:H2A	2.52	0.44
3:B:347:ARG:HB2	3:B:398:ILE:HD11	1.99	0.44
4:C:228:ASP:N	4:C:228:ASP:OD1	2.48	0.44
19:r:206:MET:HG2	24:r:314:XAT:H402	1.99	0.44
20:s:80:ILE:HD11	20:s:84:TRP:CE2	2.52	0.44
20:s:140:VAL:O	20:s:144:VAL:HG12	2.17	0.44
20:S:22:GLU:H	20:S:22:GLU:CD	2.24	0.44
20:S:140:VAL:O	20:S:144:VAL:HG12	2.17	0.44
22:R:303:CLA:C2D	22:R:308:CLA:H62	2.46	0.44
22:R:308:CLA:HBA2	22:R:308:CLA:H12	1.60	0.44
1:n:25:LEU:HA	21:n:601:CHL:CHC	2.47	0.44
1:n:71:TRP:NE1	21:n:608:CHL:HMD2	2.30	0.44
21:n:601:CHL:H161	21:n:601:CHL:H141	1.55	0.44
1:y:142:ARG:CA	21:y:608:CHL:CHD	2.95	0.44
1:G:24:TYR:CD1	1:G:46:TRP:HB2	2.52	0.44
1:N:112:TYR:O	1:N:118:LEU:HD12	2.18	0.44
21:Y:608:CHL:H193	21:Y:608:CHL:H162	1.69	0.44
2:a:272:HIS:NE2	34:a:412:BCT:O1	2.37	0.44
2:a:273:PHE:CZ	26:d:409:LHG:H102	2.53	0.44
3:b:116:LEU:HD13	3:b:116:LEU:HA	1.87	0.44
4:c:131:TYR:CD1	4:c:135:LEU:HB3	2.52	0.44
4:c:293:ASN:OD1	4:c:294:ASN:N	2.51	0.44
22:c:512:CLA:H151	11:k:54:TRP:CD1	2.52	0.44
14:o:61:LYS:HA	14:o:73:PHE:HA	1.99	0.44
2:A:283:ILE:HG13	30:A:408:PHO:HBC3	1.98	0.44
20:s:101:TYR:CZ	21:s:301:CHL:C3A	2.95	0.44
20:S:77:TYR:HE1	22:S:303:CLA:HMB2	1.82	0.44
21:g:608:CHL:O2D	21:g:608:CHL:H2A	2.17	0.44
21:n:608:CHL:H141	21:n:608:CHL:H161	1.73	0.44
1:y:71:TRP:NE1	21:y:609:CHL:CMD	2.78	0.44
1:y:138:VAL:HG12	21:y:608:CHL:HMB1	2.00	0.44
21:y:607:CHL:H192	21:y:607:CHL:H162	1.82	0.44
1:N:97:TRP:CE3	1:N:98:PHE:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:138:VAL:CG1	21:N:607:CHL:HMB3	2.36	0.44
1:Y:142:ARG:HA	21:Y:607:CHL:C3C	2.48	0.44
1:Y:213:LEU:HD21	22:Y:612:CLA:HMC2	2.00	0.44
3:b:89:GLY:HA2	36:I:101:LMG:H111	1.99	0.44
3:b:389:LYS:N	5:d:345:GLU:OE2	2.50	0.44
22:c:510:CLA:HBA1	22:c:510:CLA:H3A	1.41	0.44
26:d:409:LHG:H241	26:d:409:LHG:H272	1.62	0.44
22:A:409:CLA:H122	36:C:502:LMG:H161	1.99	0.44
26:r:302:LHG:HC91	26:r:302:LHG:H121	1.71	0.44
20:s:147:GLY:HA2	20:s:150:GLU:HG3	2.00	0.44
19:R:87:PHE:HA	19:R:92:PHE:CZ	2.52	0.44
1:g:97:TRP:CE3	1:g:98:PHE:HB3	2.53	0.44
1:g:213:LEU:HD21	22:g:614:CLA:HMC2	2.00	0.44
1:n:97:TRP:CE3	1:n:98:PHE:HB3	2.53	0.44
23:n:614:LUT:H202	23:n:614:LUT:H15	1.73	0.44
1:y:97:TRP:CE3	1:y:98:PHE:HB3	2.53	0.44
1:G:112:TYR:O	1:G:118:LEU:HD12	2.18	0.44
21:G:601:CHL:H141	21:G:601:CHL:H161	1.55	0.44
1:N:25:LEU:C	21:N:601:CHL:HBB1	2.42	0.44
1:N:102:SER:CA	21:N:606:CHL:HED3	2.34	0.44
22:N:603:CLA:HBC3	23:N:615:LUT:H12	1.98	0.44
1:Y:92:PHE:HB2	1:Y:95:ALA:HB2	2.00	0.44
1:Y:188:MET:HB3	23:Y:614:LUT:H34	1.99	0.44
22:b:613:CLA:H61	22:b:613:CLA:H92	1.71	0.44
22:c:510:CLA:H143	22:c:510:CLA:HAA1	1.99	0.44
22:c:512:CLA:H102	22:c:512:CLA:H62	1.77	0.44
4:C:346:THR:OG1	4:C:348:GLU:OE1	2.26	0.44
22:C:503:CLA:H141	22:C:503:CLA:H162	1.73	0.44
22:C:504:CLA:HBA2	22:C:505:CLA:H191	1.99	0.44
14:O:76:THR:HG22	14:O:118:LEU:HD23	1.99	0.44
20:S:47:GLU:H	20:S:47:GLU:CD	2.25	0.44
1:y:112:TYR:O	1:y:118:LEU:HD12	2.18	0.44
21:G:608:CHL:CHA	21:G:608:CHL:CBA	2.94	0.44
1:Y:54:ASP:OD2	1:Y:57:THR:N	2.33	0.44
1:Y:97:TRP:CE3	1:Y:98:PHE:HB3	2.53	0.44
22:Y:604:CLA:HAB	23:Y:613:LUT:C34	2.47	0.44
22:b:603:CLA:C4D	22:b:611:CLA:H161	2.48	0.44
10:j:24:LEU:O	10:j:27:LEU:HG	2.17	0.44
22:B:617:CLA:H2	22:B:617:CLA:H61	1.64	0.44
22:C:512:CLA:CAD	22:C:513:CLA:HBB2	2.48	0.44
26:C:520:LHG:H141	26:C:520:LHG:H111	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:314:LHG:H241	26:s:314:LHG:H272	1.69	0.44
20:S:210:THR:HG21	20:S:217:ASN:ND2	2.32	0.44
26:S:314:LHG:H331	26:S:314:LHG:H112	2.00	0.44
19:R:127:VAL:O	19:R:131:GLU:HG2	2.18	0.44
1:g:142:ARG:HA	21:g:608:CHL:C3C	2.48	0.44
1:y:181:LEU:HD23	1:y:181:LEU:HA	1.88	0.44
1:G:92:PHE:HB2	1:G:95:ALA:HB2	2.00	0.44
22:G:604:CLA:CMA	21:G:606:CHL:HMC	2.48	0.44
22:N:604:CLA:CMA	21:N:605:CHL:HMC	2.48	0.44
2:a:272:HIS:HE2	34:a:412:BCT:C	2.31	0.44
2:a:316:THR:N	2:a:319:ASP:OD2	2.47	0.44
3:b:347:ARG:HB2	3:b:398:ILE:HD11	1.99	0.44
2:A:204:GLY:HA2	2:A:278:TRP:HE1	1.82	0.44
19:r:87:PHE:HA	19:r:92:PHE:CZ	2.52	0.44
21:n:605:CHL:HMD1	21:s:301:CHL:HBC1	1.74	0.44
21:y:609:CHL:H91	21:y:609:CHL:H112	1.73	0.44
21:N:606:CHL:CMA	23:N:615:LUT:C17	2.86	0.44
22:c:508:CLA:H162	22:c:508:CLA:H141	1.62	0.44
14:o:46:TYR:CD1	14:o:248:SER:HA	2.51	0.44
2:A:335:ASN:HA	5:D:351:ASN:ND2	2.33	0.44
36:B:623:LMG:H273	36:B:623:LMG:H241	1.63	0.44
4:C:268:GLY:C	22:C:511:CLA:HAC2	2.42	0.44
4:C:319:VAL:O	4:C:323:ARG:HG3	2.17	0.44
10:J:24:LEU:O	10:J:27:LEU:HG	2.17	0.44
31:K:102:BCR:H371	31:K:102:BCR:H24C	1.78	0.44
20:s:77:TYR:HE1	22:s:303:CLA:HMB2	1.82	0.44
1:g:187:ALA:O	1:g:190:SER:OG	2.31	0.43
1:n:213:LEU:HD21	22:n:613:CLA:HMC2	2.00	0.43
21:n:608:CHL:H92	21:y:601:CHL:H62	2.00	0.43
1:y:92:PHE:HB2	1:y:95:ALA:HB2	2.00	0.43
22:y:612:CLA:HBA2	22:y:612:CLA:H3A	1.36	0.43
1:N:138:VAL:HG12	21:N:607:CHL:HMB1	2.00	0.43
1:Y:112:TYR:O	1:Y:118:LEU:HD12	2.18	0.43
2:a:204:GLY:HA2	2:a:278:TRP:HE1	1.83	0.43
30:a:407:PHO:NC	5:d:210:LEU:HD12	2.33	0.43
3:b:433:ASP:OD2	3:b:436:THR:OG1	2.31	0.43
22:c:503:CLA:HBA2	22:c:504:CLA:H191	1.99	0.43
22:c:505:CLA:C1D	35:c:518:DGD:HB61	2.48	0.43
22:c:511:CLA:CAD	22:c:512:CLA:HBB2	2.48	0.43
2:A:316:THR:N	2:A:319:ASP:OD2	2.47	0.43
22:A:406:CLA:H141	22:A:406:CLA:H162	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:607:CLA:H93	22:B:607:CLA:H111	1.71	0.43
22:C:506:CLA:C1D	35:C:519:DGD:HB61	2.48	0.43
22:C:510:CLA:H3A	22:C:510:CLA:HBA2	1.35	0.43
22:C:511:CLA:H143	22:C:511:CLA:HAA1	1.99	0.43
26:C:520:LHG:HC5	22:S:310:CLA:H42	1.41	0.43
20:s:59:TYR:HE1	21:s:302:CHL:CGA	2.31	0.43
20:s:200:MET:HG3	20:s:204:PHE:CZ	2.53	0.43
20:S:178:ASP:HB3	20:S:181:GLN:HB2	1.99	0.43
1:g:97:TRP:CH2	1:g:198:ALA:HB1	2.53	0.43
1:y:102:SER:CA	21:y:607:CHL:HED3	2.31	0.43
21:y:601:CHL:HHD	26:y:617:LHG:O7	2.18	0.43
1:G:138:VAL:HG12	21:G:608:CHL:HMB1	2.00	0.43
1:G:142:ARG:HA	21:G:608:CHL:C3C	2.48	0.43
1:G:142:ARG:CA	21:G:608:CHL:CHD	2.95	0.43
1:Y:97:TRP:CH2	1:Y:198:ALA:HB1	2.53	0.43
2:a:257:ARG:HH12	3:b:490:VAL:C	2.26	0.43
2:a:304:GLN:HG2	2:a:313:VAL:HG11	2.01	0.43
22:c:502:CLA:CHB	22:c:502:CLA:H2	2.49	0.43
14:O:59:THR:OG1	14:O:237:LYS:HB3	2.17	0.43
21:r:306:CHL:HAA1	25:r:315:NEX:H381	2.00	0.43
22:r:309:CLA:H12	22:r:309:CLA:HBA2	1.61	0.43
22:s:303:CLA:CHA	22:s:303:CLA:HBA1	2.48	0.43
19:R:151:GLU:CD	21:R:305:CHL:CMB	2.90	0.43
21:R:305:CHL:H122	21:R:305:CHL:H8	1.57	0.43
21:g:609:CHL:HBC3	21:g:609:CHL:CMC	2.41	0.43
1:G:192:PHE:O	1:G:193:GLY:C	2.61	0.43
1:N:142:ARG:HA	21:N:607:CHL:C3C	2.48	0.43
21:N:606:CHL:H192	21:N:606:CHL:H162	1.82	0.43
3:b:39:LEU:HD23	3:b:39:LEU:HA	1.86	0.43
3:b:201:HIS:HE1	22:b:602:CLA:HBB1	1.83	0.43
4:c:272:LEU:O	4:c:276:LEU:HG	2.18	0.43
22:c:506:CLA:HBA2	22:c:506:CLA:H3A	1.69	0.43
30:d:401:PHO:HED2	30:d:401:PHO:H2A	2.01	0.43
32:d:406:PL9:H513	15:t:10:LEU:HD13	2.00	0.43
5:D:181:ARG:HE	5:D:181:ARG:HB3	1.61	0.43
14:O:61:LYS:HA	14:O:73:PHE:HA	1.99	0.43
17:X:54:PHE:O	17:X:57:SER:OG	2.26	0.43
19:r:127:VAL:O	19:r:131:GLU:HG2	2.18	0.43
20:s:136:ILE:HG23	20:s:137:LEU:HD12	2.00	0.43
19:R:206:MET:HG2	24:R:313:XAT:H402	1.99	0.43
21:g:607:CHL:H192	21:g:607:CHL:H162	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:148:LEU:O	21:y:608:CHL:CMC	2.67	0.43
1:y:197:GLN:HG2	22:y:612:CLA:ND	2.34	0.43
1:G:65:GLU:OE2	1:G:185:ARG:NE	2.36	0.43
1:N:97:TRP:CH2	1:N:198:ALA:HB1	2.53	0.43
2:a:283:ILE:HG13	30:a:407:PHO:HBC3	1.98	0.43
3:b:271:THR:OG1	3:b:274:GLN:OE1	2.19	0.43
3:b:330:MET:HA	3:b:444:ARG:HB2	2.01	0.43
31:b:616:BCR:H15C	31:b:616:BCR:H351	1.85	0.43
22:c:511:CLA:H162	22:c:511:CLA:H122	1.56	0.43
5:d:218:THR:O	5:d:222:THR:OG1	2.29	0.43
7:f:18:HIS:HA	37:f:101:HEM:C1C	2.54	0.43
13:m:28:LYS:O	13:m:32:GLN:HG2	2.19	0.43
36:w:102:LMG:H141	36:w:102:LMG:H112	1.85	0.43
2:A:131:TRP:O	2:A:134:SER:OG	2.28	0.43
22:A:407:CLA:H2A	22:A:407:CLA:CED	2.48	0.43
3:B:201:HIS:HE1	22:B:605:CLA:HBB1	1.83	0.43
36:B:623:LMG:H201	21:R:306:CHL:C4B	2.45	0.43
4:C:272:LEU:O	4:C:276:LEU:HG	2.18	0.43
13:M:28:LYS:O	13:M:32:GLN:HG2	2.19	0.43
22:r:305:CLA:H12	21:r:306:CHL:C3D	2.48	0.43
20:S:59:TYR:HE1	21:S:302:CHL:CGA	2.31	0.43
20:S:116:ALA:CA	21:S:307:CHL:C3D	2.96	0.43
20:S:149:ALA:HA	20:S:153:ARG:HG3	1.98	0.43
1:g:92:PHE:HB2	1:g:95:ALA:HB2	2.00	0.43
1:g:138:VAL:HG12	21:g:608:CHL:HMB1	2.00	0.43
1:g:197:GLN:HG2	22:g:613:CLA:ND	2.34	0.43
22:g:604:CLA:HAB	23:g:615:LUT:C35	2.49	0.43
22:y:602:CLA:HBA2	22:y:602:CLA:H3A	1.33	0.43
1:N:142:ARG:CA	21:N:607:CHL:CHD	2.95	0.43
21:N:601:CHL:H61	21:N:601:CHL:H41	1.76	0.43
2:a:296:ASN:HD22	4:c:401:LEU:HG	1.83	0.43
36:b:620:LMG:C21	21:r:307:CHL:C1A	1.84	0.43
22:c:510:CLA:HBD	22:c:510:CLA:H121	2.00	0.43
5:d:192:TRP:CZ2	5:d:198:HIS:HB2	2.54	0.43
22:A:409:CLA:H61	22:A:409:CLA:H2	1.63	0.43
22:B:604:CLA:HBA1	22:B:604:CLA:H3A	1.60	0.43
4:C:120:ILE:HG21	31:C:516:BCR:H12C	2.01	0.43
4:C:418:ASN:HB2	35:J:101:DGD:HE61	2.01	0.43
14:O:46:TYR:CD1	14:O:248:SER:HA	2.51	0.43
20:S:101:TYR:HD1	21:S:301:CHL:HMA2	1.52	0.43
20:S:110:VAL:O	20:S:114:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:g:604:CLA:CMA	21:g:606:CHL:HMC	2.48	0.43
1:n:127:ILE:HD11	21:s:301:CHL:HBC2	2.01	0.43
1:n:134:LEU:HD22	25:n:616:NEX:H15	1.99	0.43
1:y:25:LEU:C	21:y:601:CHL:HBB1	2.42	0.43
1:G:97:TRP:CE3	1:G:98:PHE:HB3	2.53	0.43
1:N:197:GLN:HG2	22:N:612:CLA:ND	2.34	0.43
1:Y:25:LEU:HA	21:Y:601:CHL:CHC	2.48	0.43
1:Y:127:ILE:HD11	21:r:301:CHL:CBC	2.48	0.43
26:Y:617:LHG:H142	26:Y:617:LHG:H111	1.82	0.43
2:a:258:LEU:HG	2:a:259:ILE:HG12	1.99	0.43
3:b:164:PRO:HG3	22:b:605:CLA:O1D	2.19	0.43
22:B:618:CLA:H11	22:B:618:CLA:H51	1.79	0.43
5:D:86:LEU:HD12	5:D:86:LEU:H	1.84	0.43
20:S:98:PHE:O	20:S:103:ALA:HB3	2.19	0.43
21:g:605:CHL:CBC	21:g:606:CHL:HMD3	2.46	0.43
22:g:613:CLA:H141	22:g:613:CLA:H161	1.75	0.43
1:y:97:TRP:CH2	1:y:198:ALA:HB1	2.53	0.43
22:y:612:CLA:H61	22:y:612:CLA:H2	1.62	0.43
1:G:97:TRP:CH2	1:G:198:ALA:HB1	2.53	0.43
22:G:604:CLA:HAB	23:G:615:LUT:C35	2.49	0.43
1:N:127:ILE:HD11	21:S:301:CHL:CBC	2.48	0.43
22:N:604:CLA:HAB	23:N:614:LUT:C35	2.49	0.43
21:N:607:CHL:H41	21:N:607:CHL:H62	1.49	0.43
1:Y:44:TYR:OH	26:Y:617:LHG:O5	2.24	0.43
1:Y:148:LEU:O	21:Y:607:CHL:CMC	2.67	0.43
22:Y:602:CLA:H3A	22:Y:602:CLA:HBA2	1.33	0.43
22:Y:604:CLA:CMA	21:Y:605:CHL:HMC	2.48	0.43
22:Y:611:CLA:H141	22:Y:611:CLA:H161	1.76	0.43
2:a:225:ARG:NH1	3:b:483:ASP:HA	2.33	0.43
22:b:603:CLA:H141	22:b:603:CLA:H162	1.81	0.43
31:b:618:BCR:H15C	31:b:618:BCR:H351	1.89	0.43
5:d:86:LEU:HD12	5:d:86:LEU:H	1.84	0.43
14:o:129:THR:OG1	14:o:131:LYS:HG3	2.19	0.43
3:B:330:MET:HA	3:B:444:ARG:HB2	2.01	0.43
3:B:385:ARG:NH2	14:O:163:GLY:O	2.51	0.43
4:C:230:LEU:O	4:C:234:ILE:HG12	2.18	0.43
22:C:505:CLA:H2A	22:C:505:CLA:O1D	2.19	0.43
22:C:509:CLA:H162	22:C:509:CLA:H141	1.62	0.43
22:C:515:CLA:H143	22:C:515:CLA:H111	1.88	0.43
30:D:401:PHO:HED2	30:D:401:PHO:H2A	2.01	0.43
6:E:14:ILE:O	6:E:20:TRP:NE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:129:THR:OG1	14:O:131:LYS:HG3	2.19	0.43
16:W:34:TRP:CH2	22:W:101:CLA:H52	2.53	0.43
19:r:96:GLU:HB2	22:r:303:CLA:C2B	2.48	0.43
22:r:305:CLA:H12	21:r:306:CHL:C4D	2.49	0.43
19:R:96:GLU:HB2	22:R:302:CLA:C2B	2.48	0.43
1:g:67:ILE:CG2	21:g:609:CHL:HMD1	2.41	0.43
1:g:142:ARG:HA	21:g:608:CHL:HBC2	2.01	0.43
1:g:148:LEU:O	21:g:608:CHL:CMC	2.67	0.43
1:g:191:MET:HG3	23:g:616:LUT:C20	2.49	0.43
23:g:615:LUT:H203	23:g:616:LUT:C8	2.49	0.43
1:n:97:TRP:CH2	1:n:198:ALA:HB1	2.53	0.43
1:n:148:LEU:O	21:n:607:CHL:CMC	2.67	0.43
21:n:605:CHL:HAA1	25:n:616:NEX:H31	1.98	0.43
1:y:213:LEU:HD21	22:y:613:CLA:HMC2	2.00	0.43
22:y:604:CLA:CMA	21:y:606:CHL:HMC	2.48	0.43
1:G:213:LEU:HD21	22:G:614:CLA:HMC2	2.00	0.43
1:N:192:PHE:O	1:N:193:GLY:C	2.61	0.43
21:N:608:CHL:O1A	21:Y:601:CHL:H2	2.17	0.43
21:N:608:CHL:H92	21:Y:601:CHL:H62	2.01	0.43
22:Y:602:CLA:H152	22:Y:602:CLA:H112	1.75	0.43
22:Y:612:CLA:HBA2	22:Y:612:CLA:H3A	1.67	0.43
3:b:271:THR:HG1	3:b:274:GLN:CD	2.20	0.43
4:c:429:SER:O	4:c:433:LEU:HG	2.18	0.43
26:d:409:LHG:O3	26:d:409:LHG:O1	2.22	0.43
6:e:14:ILE:O	6:e:20:TRP:NE1	2.52	0.43
2:A:37:MET:HE2	2:A:37:MET:HB3	1.92	0.43
31:B:621:BCR:H361	31:B:621:BCR:H20C	1.78	0.43
36:B:623:LMG:H201	21:R:306:CHL:C1C	2.49	0.43
19:r:13:VAL:HA	19:r:32:ARG:O	2.19	0.43
22:s:310:CLA:H92	22:s:310:CLA:H62	1.78	0.43
22:g:602:CLA:H112	22:g:602:CLA:H152	1.75	0.43
1:n:138:VAL:HG12	21:n:607:CHL:HMB1	2.00	0.43
1:y:142:ARG:HA	21:y:608:CHL:C3C	2.48	0.43
1:G:127:ILE:HD11	21:G:605:CHL:CBC	2.49	0.43
21:N:606:CHL:H71	1:Y:228:PHE:O	2.19	0.43
22:N:609:CLA:H192	22:N:611:CLA:H111	2.01	0.43
1:Y:25:LEU:C	21:Y:601:CHL:HBB1	2.43	0.43
1:Y:197:GLN:HG2	22:Y:611:CLA:ND	2.34	0.43
22:Y:603:CLA:HMD3	21:Y:608:CHL:O2A	2.19	0.43
2:a:21:ILE:HD13	2:a:21:ILE:HA	1.90	0.43
22:a:406:CLA:CED	22:a:406:CLA:H2A	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:328:GLY:HA3	36:T:101:LMG:H352	2.00	0.43
31:b:616:BCR:H342	31:T:102:BCR:H402	2.00	0.43
31:b:618:BCR:H371	31:b:618:BCR:H24C	1.81	0.43
22:c:513:CLA:H192	22:s:313:CLA:H91	2.01	0.43
2:A:304:GLN:HG2	2:A:313:VAL:HG11	2.01	0.43
35:A:401:DGD:HB51	35:A:401:DGD:HB22	1.78	0.43
3:B:328:GLY:HA3	36:M:101:LMG:H352	2.00	0.43
22:B:606:CLA:C4D	22:B:614:CLA:H161	2.48	0.43
20:S:147:GLY:HA2	20:S:150:GLU:HG3	2.00	0.43
20:S:167:GLY:HA2	20:S:170:PHE:HB2	2.01	0.43
1:n:142:ARG:HA	21:n:607:CHL:C3C	2.48	0.43
22:n:603:CLA:HMD3	21:n:608:CHL:O2A	2.19	0.43
22:n:604:CLA:HAB	23:n:614:LUT:C35	2.49	0.43
1:y:192:PHE:O	1:y:193:GLY:C	2.61	0.43
1:G:197:GLN:HG2	22:G:613:CLA:ND	2.34	0.43
1:N:213:LEU:HD21	22:N:613:CLA:HMC3	2.01	0.43
22:N:613:CLA:H3A	22:N:613:CLA:HBA2	1.67	0.43
22:b:607:CLA:HBA2	22:b:607:CLA:H3A	1.69	0.43
22:c:506:CLA:H92	22:c:506:CLA:H62	1.84	0.43
17:x:54:PHE:O	17:x:57:SER:OG	2.26	0.43
3:B:223:GLN:HG3	19:R:48:PHE:HZ	1.84	0.43
22:C:503:CLA:CHB	22:C:503:CLA:H2	2.49	0.43
5:D:40:PRO:HB2	22:D:405:CLA:HBB1	2.01	0.43
22:s:313:CLA:HBA2	22:s:313:CLA:H3A	1.40	0.43
20:S:120:ASP:N	20:S:120:ASP:OD1	2.51	0.43
1:n:26:GLY:O	1:n:29:SER:OG	2.32	0.42
1:n:92:PHE:HB2	1:n:95:ALA:HB2	2.00	0.42
22:n:604:CLA:HMA2	21:n:605:CHL:CMC	2.50	0.42
25:y:618:NEX:H381	21:R:305:CHL:HAA1	2.00	0.42
25:y:618:NEX:H35	25:y:618:NEX:H401	1.78	0.42
1:Y:138:VAL:HG12	21:Y:607:CHL:HMB1	2.00	0.42
31:a:409:BCR:H15C	31:a:409:BCR:H351	1.83	0.42
13:m:32:GLN:NE2	13:M:31:SER:HB2	2.34	0.42
30:A:408:PHO:H143	30:A:408:PHO:H161	1.82	0.42
3:B:121:GLU:N	8:H:15:ARG:O	2.49	0.42
4:C:322:GLN:NE2	4:C:381:LYS:HA	2.32	0.42
22:C:514:CLA:H122	22:S:313:CLA:H72	1.30	0.42
20:s:156:ASN:OD1	20:s:156:ASN:N	2.52	0.42
26:s:314:LHG:H331	26:s:314:LHG:H112	2.00	0.42
20:S:149:ALA:O	20:S:153:ARG:HB2	2.19	0.42
20:S:200:MET:HG3	20:S:204:PHE:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:220:GLY:C	19:R:221:LYS:HD3	2.44	0.42
22:y:604:CLA:HAB	23:y:614:LUT:C35	2.49	0.42
21:y:608:CHL:H51	21:y:608:CHL:H8	1.36	0.42
1:N:148:LEU:O	21:N:607:CHL:CMC	2.67	0.42
22:N:603:CLA:H191	22:Y:603:CLA:HBB1	2.00	0.42
22:N:604:CLA:HMA2	21:N:605:CHL:CMC	2.50	0.42
22:Y:604:CLA:HMA2	21:Y:605:CHL:CMC	2.49	0.42
3:b:9:HIS:HE1	22:b:612:CLA:HED3	1.84	0.42
3:b:338:VAL:HB	3:b:431:GLU:HB3	2.01	0.42
4:c:230:LEU:O	4:c:234:ILE:HG12	2.19	0.42
14:o:37:ASP:HA	14:o:206:GLN:HG2	2.01	0.42
22:A:406:CLA:O2D	5:D:199:MET:HB3	2.19	0.42
36:B:623:LMG:C25	21:R:306:CHL:C4C	2.78	0.42
4:C:429:SER:O	4:C:433:LEU:HG	2.18	0.42
4:C:451:ALA:HA	4:C:456:GLU:CD	2.45	0.42
22:C:510:CLA:H62	22:C:510:CLA:H41	1.76	0.42
22:C:511:CLA:H121	22:C:511:CLA:HBD	2.00	0.42
22:C:512:CLA:O2D	22:C:512:CLA:H2A	2.19	0.42
26:C:521:LHG:H181	16:W:31:GLY:HA3	2.01	0.42
5:D:192:TRP:CZ2	5:D:198:HIS:HB2	2.54	0.42
19:r:136:PHE:HD2	21:r:301:CHL:C2	2.33	0.42
20:s:165:HIS:ND1	22:s:309:CLA:O1D	2.52	0.42
20:s:167:GLY:HA2	20:s:170:PHE:HB2	2.01	0.42
20:S:34:PHE:CE2	21:S:302:CHL:CBA	3.02	0.42
19:R:215:GLN:OE1	19:R:219:SER:OG	2.22	0.42
22:R:304:CLA:H12	21:R:305:CHL:C3D	2.48	0.42
1:g:127:ILE:HD11	21:g:605:CHL:CBC	2.49	0.42
22:g:604:CLA:HMA2	21:g:606:CHL:CMC	2.50	0.42
23:N:614:LUT:H15	23:N:614:LUT:H202	1.73	0.42
22:Y:604:CLA:HAB	23:Y:613:LUT:C35	2.49	0.42
3:b:157:HIS:CE1	3:b:164:PRO:HD2	2.54	0.42
4:c:233:ILE:O	4:c:237:HIS:ND1	2.47	0.42
4:c:456:GLU:OE1	4:c:456:GLU:N	2.40	0.42
22:c:504:CLA:H2A	22:c:504:CLA:O1D	2.19	0.42
31:k:102:BCR:H20C	31:k:102:BCR:H361	1.85	0.42
30:A:408:PHO:NC	5:D:210:LEU:HD12	2.35	0.42
3:B:63:ILE:N	3:B:64:PRO:HD2	2.35	0.42
22:B:605:CLA:HHC	22:B:607:CLA:H202	2.02	0.42
4:C:233:ILE:O	4:C:237:HIS:ND1	2.47	0.42
22:C:513:CLA:H62	22:C:513:CLA:H102	1.77	0.42
31:C:517:BCR:H11C	31:C:517:BCR:H341	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:18:HIS:HA	37:F:101:HEM:C1C	2.54	0.42
19:r:151:GLU:CD	21:r:306:CHL:CMB	2.90	0.42
20:s:110:VAL:O	20:s:114:THR:HG23	2.18	0.42
21:s:307:CHL:H2A	21:s:307:CHL:O2D	2.19	0.42
20:S:176:ALA:HB2	22:S:309:CLA:HAA2	2.02	0.42
19:R:24:LEU:HB3	19:R:33:GLY:HA2	2.02	0.42
1:g:192:PHE:O	1:g:193:GLY:C	2.61	0.42
1:N:92:PHE:HB2	1:N:95:ALA:HB2	2.00	0.42
22:Y:609:CLA:H101	23:Y:613:LUT:H383	2.01	0.42
25:Y:616:NEX:H393	25:Y:616:NEX:H27	1.88	0.42
3:b:193:PHE:HE2	8:h:72:MET:HE1	1.84	0.42
3:b:226:TYR:CE1	3:b:231:MET:HB2	2.55	0.42
4:c:153:ASP:O	4:c:157:MET:HG2	2.19	0.42
31:d:405:BCR:H14C	7:f:27:PHE:CD2	2.54	0.42
31:h:101:BCR:H15C	31:h:101:BCR:H351	1.84	0.42
14:o:37:ASP:N	14:o:37:ASP:OD1	2.51	0.42
2:A:250:ALA:HA	3:B:490:VAL:HG21	2.01	0.42
3:B:9:HIS:HE1	22:B:615:CLA:HED3	1.84	0.42
3:B:57:ARG:HH22	3:B:334:ASP:CG	2.28	0.42
36:B:623:LMG:H222	21:R:306:CHL:NB	2.29	0.42
4:C:376:ASP:OD2	4:C:379:ARG:HG3	2.19	0.42
35:H:102:DGD:HBW1	35:H:102:DGD:HBN2	1.84	0.42
14:O:37:ASP:N	14:O:37:ASP:OD1	2.52	0.42
20:s:176:ALA:HB2	22:s:309:CLA:HAA2	2.02	0.42
19:R:49:ASP:OD1	19:R:50:LEU:N	2.44	0.42
22:R:304:CLA:H12	21:R:305:CHL:C4D	2.49	0.42
22:R:311:CLA:H8	22:R:311:CLA:H122	1.86	0.42
22:n:609:CLA:H101	23:n:614:LUT:H383	2.01	0.42
21:y:601:CHL:H61	21:y:601:CHL:H41	1.76	0.42
23:y:614:LUT:H15	23:y:614:LUT:H202	1.73	0.42
1:G:58:PHE:O	1:G:62:ARG:HG3	2.20	0.42
1:G:148:LEU:O	21:G:608:CHL:CMC	2.67	0.42
21:G:605:CHL:CBC	21:G:606:CHL:HMD3	2.46	0.42
21:N:608:CHL:HBC3	21:N:608:CHL:CMC	2.41	0.42
21:Y:606:CHL:H62	21:Y:606:CHL:H2	1.72	0.42
22:Y:611:CLA:H3A	22:Y:611:CLA:HBA2	1.36	0.42
2:a:57:PRO:HD3	2:a:73:TYR:CE2	2.55	0.42
2:a:131:TRP:O	2:a:134:SER:OG	2.28	0.42
3:b:121:GLU:O	8:h:24:LYS:NZ	2.51	0.42
5:d:175:GLY:O	5:d:179:ILE:HG12	2.20	0.42
2:A:270:SER:OG	33:D:402:SQD:O2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:39:LEU:HD23	3:B:39:LEU:HA	1.86	0.42
22:B:618:CLA:HMD1	8:H:19:VAL:HB	2.01	0.42
26:C:522:LHG:H322	26:C:522:LHG:H291	1.68	0.42
20:s:34:PHE:CE2	21:s:302:CHL:CBA	3.02	0.42
20:s:150:GLU:HB3	22:s:308:CLA:C4B	2.50	0.42
21:S:307:CHL:H2A	21:S:307:CHL:O2D	2.20	0.42
1:g:102:SER:CA	21:g:607:CHL:HED3	2.31	0.42
22:g:613:CLA:H2	22:g:613:CLA:H61	1.62	0.42
23:g:615:LUT:C33	25:g:618:NEX:H27	2.50	0.42
21:n:606:CHL:H192	21:n:606:CHL:H162	1.81	0.42
1:G:25:LEU:C	21:G:601:CHL:HBB1	2.42	0.42
21:G:601:CHL:H101	21:Y:608:CHL:H102	2.02	0.42
21:Y:607:CHL:H193	21:Y:607:CHL:H162	1.77	0.42
23:Y:613:LUT:H203	23:Y:614:LUT:C8	2.49	0.42
3:b:63:ILE:N	3:b:64:PRO:HD2	2.35	0.42
4:c:418:ASN:HB2	35:c:519:DGD:HE61	2.01	0.42
36:d:410:LMG:O3	10:j:37:GLY:HA3	2.20	0.42
22:w:101:CLA:H62	22:w:101:CLA:H2	1.54	0.42
3:B:223:GLN:HG3	19:R:48:PHE:CZ	2.55	0.42
22:B:606:CLA:H162	22:B:606:CLA:H141	1.81	0.42
22:C:514:CLA:H18	22:S:313:CLA:C4D	2.50	0.42
31:H:101:BCR:H24C	31:H:101:BCR:H371	1.83	0.42
19:r:24:LEU:HB3	19:r:33:GLY:HA2	2.02	0.42
19:r:159:GLU:HG3	22:r:309:CLA:C4B	2.50	0.42
19:r:168:PRO:HA	19:r:171:ARG:HB2	2.01	0.42
20:S:36:PRO:HG3	21:S:302:CHL:HBB2	2.01	0.42
20:S:150:GLU:HB3	22:S:308:CLA:C4B	2.50	0.42
19:R:159:GLU:HG3	22:R:308:CLA:C4B	2.50	0.42
21:g:606:CHL:HBD	21:g:606:CHL:CGA	2.50	0.42
22:y:604:CLA:HMA2	21:y:606:CHL:CMC	2.49	0.42
25:y:618:NEX:H382	21:R:305:CHL:CAA	2.49	0.42
1:G:145:GLY:HA3	1:G:150:GLU:OE1	2.20	0.42
22:G:604:CLA:HMA2	21:G:606:CHL:CMC	2.50	0.42
21:N:607:CHL:H8	21:N:607:CHL:H51	1.36	0.42
22:N:611:CLA:H62	22:N:611:CLA:H2	1.54	0.42
1:Y:182:LYS:HE3	26:Y:617:LHG:HC42	2.01	0.42
22:Y:609:CLA:CHA	22:Y:609:CLA:HBA1	2.49	0.42
22:a:404:CLA:HBA1	22:a:404:CLA:H3A	1.79	0.42
22:b:614:CLA:H61	22:b:614:CLA:H2	1.64	0.42
22:c:511:CLA:O2D	22:c:511:CLA:H2A	2.19	0.42
35:A:401:DGD:HA31	36:I:101:LMG:O9	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:226:TYR:CE1	3:B:231:MET:HB2	2.55	0.42
36:B:623:LMG:H201	21:R:306:CHL:CHC	2.49	0.42
4:C:332:GLN:HE21	4:C:336:GLY:HA2	1.84	0.42
5:D:175:GLY:O	5:D:179:ILE:HG12	2.19	0.42
9:I:24:LEU:HD23	9:I:24:LEU:HA	1.90	0.42
22:s:310:CLA:H11	22:s:310:CLA:H51	1.92	0.42
20:S:49:LEU:HD22	20:S:58:GLY:HA2	2.02	0.42
1:n:25:LEU:C	21:n:601:CHL:HBB1	2.42	0.42
1:n:145:GLY:HA3	1:n:150:GLU:OE1	2.20	0.42
21:n:605:CHL:HMD3	21:s:301:CHL:CBC	2.43	0.42
1:y:58:PHE:O	1:y:62:ARG:HG3	2.20	0.42
21:N:606:CHL:HBA2	21:N:606:CHL:H3A	1.49	0.42
24:N:616:XAT:H15	24:N:616:XAT:H201	1.82	0.42
1:Y:145:GLY:HA3	1:Y:150:GLU:OE1	2.20	0.42
2:a:303:ASN:HB3	4:c:414:ILE:HG22	2.00	0.42
3:b:441:GLY:HA2	14:o:176:ALA:HB3	2.01	0.42
36:b:620:LMG:H231	21:r:307:CHL:C4D	2.49	0.42
4:c:144:PHE:CZ	22:c:514:CLA:HAA1	2.55	0.42
4:c:332:GLN:HE21	4:c:336:GLY:HA2	1.84	0.42
5:d:290:LEU:HD23	5:d:290:LEU:HA	1.78	0.42
11:k:40:MET:O	11:k:43:ILE:HG13	2.19	0.42
14:o:106:LYS:HD3	14:o:106:LYS:HA	1.77	0.42
22:B:616:CLA:H8	31:B:619:BCR:H362	2.02	0.42
31:B:619:BCR:H20C	31:B:619:BCR:H361	1.86	0.42
31:B:620:BCR:H11C	31:B:620:BCR:H341	1.93	0.42
36:B:623:LMG:H251	21:R:305:CHL:HBC2	2.01	0.42
22:C:507:CLA:H62	22:C:507:CLA:H92	1.84	0.42
22:C:510:CLA:H61	22:C:510:CLA:H92	1.76	0.42
11:K:40:MET:O	11:K:43:ILE:HG13	2.19	0.42
20:s:95:PRO:O	20:s:99:ASN:ND2	2.44	0.42
20:s:149:ALA:O	20:s:153:ARG:HB2	2.19	0.42
20:S:165:HIS:ND1	22:S:309:CLA:O1D	2.52	0.42
19:R:13:VAL:HA	19:R:32:ARG:O	2.19	0.42
22:R:308:CLA:H91	22:R:308:CLA:H112	1.82	0.42
22:g:610:CLA:CHA	22:g:610:CLA:HBA1	2.49	0.42
22:N:613:CLA:H3A	22:N:613:CLA:CGA	2.48	0.42
1:Y:71:TRP:CE2	21:Y:608:CHL:CHD	2.94	0.42
1:Y:102:SER:CA	21:Y:606:CHL:HED3	2.33	0.42
22:Y:604:CLA:CMA	21:Y:605:CHL:CMC	2.98	0.42
22:b:602:CLA:HHC	22:b:604:CLA:H202	2.02	0.42
4:c:451:ALA:HA	4:c:456:GLU:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:102:DGD:HB81	35:h:102:DGD:HBE2	1.94	0.42
2:A:21:ILE:HD13	2:A:21:ILE:HA	1.90	0.42
3:B:256:MET:SD	3:B:448:ARG:HG3	2.60	0.42
3:B:338:VAL:HB	3:B:431:GLU:HB3	2.01	0.42
22:C:515:CLA:H192	22:C:515:CLA:H162	1.84	0.42
31:H:101:BCR:H15C	31:H:101:BCR:H351	1.84	0.42
20:s:98:PHE:O	20:s:103:ALA:HB3	2.19	0.42
20:S:165:HIS:HE1	20:S:189:GLU:OE2	2.03	0.42
21:g:601:CHL:H101	21:y:609:CHL:H111	2.01	0.42
22:n:604:CLA:CMA	21:n:605:CHL:CMC	2.98	0.42
22:n:604:CLA:CMA	21:n:605:CHL:HMC	2.48	0.42
1:y:25:LEU:C	21:y:601:CHL:HHC	2.45	0.42
22:y:610:CLA:CHA	22:y:610:CLA:HBA1	2.50	0.42
21:G:609:CHL:C11	21:N:601:CHL:H121	2.50	0.42
1:N:58:PHE:O	1:N:62:ARG:HG3	2.20	0.42
22:a:404:CLA:H142	22:a:404:CLA:H112	1.80	0.42
4:c:120:ILE:HG21	31:c:515:BCR:H12C	2.01	0.42
31:h:101:BCR:H24C	31:h:101:BCR:H371	1.83	0.42
14:o:89:ILE:HG23	14:o:107:ASP:O	2.20	0.42
14:o:145:GLU:HB3	14:o:197:LYS:HE2	2.02	0.42
3:B:157:HIS:CE1	3:B:164:PRO:HD2	2.54	0.42
22:B:614:CLA:H8	22:B:614:CLA:H122	1.86	0.42
22:C:507:CLA:H3A	22:C:507:CLA:HBA2	1.69	0.42
19:r:220:GLY:C	19:r:221:LYS:HD3	2.44	0.42
25:r:315:NEX:H401	25:r:315:NEX:H35	1.78	0.42
20:s:49:LEU:HD22	20:s:58:GLY:HA2	2.02	0.42
20:s:120:ASP:OD1	20:s:120:ASP:N	2.51	0.42
20:S:95:PRO:O	20:S:99:ASN:ND2	2.44	0.42
22:S:310:CLA:H92	22:S:310:CLA:H62	1.78	0.42
21:g:609:CHL:H111	21:n:601:CHL:C12	2.46	0.41
1:y:145:GLY:HA3	1:y:150:GLU:OE1	2.20	0.41
21:y:609:CHL:HBC3	21:y:609:CHL:CMC	2.41	0.41
1:Y:119:VAL:HG13	21:r:301:CHL:C1D	2.50	0.41
30:a:407:PHO:H143	30:a:407:PHO:H161	1.82	0.41
36:b:620:LMG:H261	21:r:306:CHL:C1C	2.47	0.41
22:c:503:CLA:HBB1	22:c:511:CLA:HMC2	2.02	0.41
22:B:604:CLA:H162	22:B:604:CLA:H202	1.74	0.41
4:C:153:ASP:O	4:C:157:MET:HG2	2.19	0.41
14:O:111:TYR:HB2	14:O:127:LEU:HD11	2.02	0.41
22:R:303:CLA:C1C	22:R:308:CLA:H111	2.50	0.41
1:g:58:PHE:O	1:g:62:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:145:GLY:HA3	1:g:150:GLU:OE1	2.20	0.41
22:g:603:CLA:H93	22:g:603:CLA:H112	1.77	0.41
1:n:41:PRO:HB2	1:n:181:LEU:HD12	2.02	0.41
1:n:197:GLN:HG2	22:n:612:CLA:ND	2.34	0.41
1:y:41:PRO:HB2	1:y:181:LEU:HD12	2.02	0.41
26:y:617:LHG:H102	26:y:617:LHG:H262	2.02	0.41
1:G:71:TRP:CD1	21:G:609:CHL:HMD1	2.54	0.41
21:G:606:CHL:HBD	21:G:606:CHL:CGA	2.50	0.41
1:N:25:LEU:C	21:N:601:CHL:HHC	2.45	0.41
1:N:142:ARG:HA	21:N:607:CHL:HBC2	2.01	0.41
21:N:605:CHL:HBD	21:N:605:CHL:CGA	2.50	0.41
1:Y:142:ARG:CA	21:Y:607:CHL:CHD	2.95	0.41
4:c:376:ASP:HB3	4:c:379:ARG:HB2	2.02	0.41
4:c:376:ASP:OD2	4:c:379:ARG:HG3	2.19	0.41
31:c:515:BCR:H20C	31:c:515:BCR:H361	1.92	0.41
2:A:57:PRO:HD3	2:A:73:TYR:CE2	2.55	0.41
2:A:303:ASN:HB3	4:C:414:ILE:HG22	2.03	0.41
31:A:410:BCR:H351	31:A:410:BCR:H15C	1.83	0.41
3:B:18:ARG:HD3	3:B:115:TRP:CZ3	2.55	0.41
3:B:164:PRO:HG3	22:B:608:CLA:O1D	2.19	0.41
3:B:271:THR:OG1	3:B:274:GLN:OE1	2.19	0.41
22:B:607:CLA:H41	22:B:607:CLA:H62	1.83	0.41
4:C:144:PHE:CZ	22:C:515:CLA:HAA1	2.55	0.41
4:C:360:ASP:O	35:C:518:DGD:O2E	2.34	0.41
12:L:25:ILE:HD13	12:L:25:ILE:HA	1.88	0.41
14:O:145:GLU:HB3	14:O:197:LYS:HE2	2.02	0.41
16:W:38:PHE:CE1	22:W:101:CLA:H42	2.48	0.41
20:S:156:ASN:OD1	20:S:156:ASN:N	2.52	0.41
1:G:25:LEU:C	21:G:601:CHL:HHC	2.45	0.41
21:G:609:CHL:CGA	21:N:601:CHL:H2	2.50	0.41
2:a:56:PRO:HA	2:a:73:TYR:CE2	2.47	0.41
3:b:372:ASP:HB3	3:b:378:ARG:HG3	2.02	0.41
22:b:607:CLA:H193	22:d:404:CLA:H12	2.02	0.41
4:c:387:TRP:O	4:c:391:ARG:HG2	2.20	0.41
4:c:420:VAL:N	35:c:518:DGD:O3E	2.48	0.41
22:c:502:CLA:H161	22:c:502:CLA:H192	1.86	0.41
5:d:56:VAL:O	5:d:67:SER:HB3	2.20	0.41
31:h:101:BCR:H361	31:h:101:BCR:H20C	1.74	0.41
2:A:204:GLY:HA2	2:A:278:TRP:NE1	2.36	0.41
35:A:401:DGD:HA32	36:I:101:LMG:H302	2.01	0.41
4:C:420:VAL:N	35:C:519:DGD:O3E	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:298:ASP:OD1	5:D:298:ASP:N	2.51	0.41
6:E:51:ARG:H	6:E:54:GLU:HB2	1.86	0.41
16:W:38:PHE:CE2	22:W:101:CLA:H11	2.55	0.41
25:r:315:NEX:H161	25:r:315:NEX:C9	2.51	0.41
20:s:36:PRO:HG3	21:s:302:CHL:HBB2	2.01	0.41
1:g:142:ARG:CA	21:g:608:CHL:CHD	2.95	0.41
22:g:603:CLA:H162	22:g:603:CLA:H141	1.86	0.41
1:y:119:VAL:HG13	21:y:605:CHL:C1D	2.50	0.41
22:y:604:CLA:CMA	21:y:606:CHL:CMC	2.98	0.41
21:y:605:CHL:HMA2	21:y:605:CHL:C2	2.50	0.41
22:G:603:CLA:HMD3	21:G:609:CHL:O2A	2.21	0.41
22:G:614:CLA:HBA2	22:G:614:CLA:H3A	1.67	0.41
21:Y:605:CHL:HBD	21:Y:605:CHL:CGA	2.50	0.41
3:b:79:ASN:OD1	3:b:80:ILE:N	2.53	0.41
3:b:299:SER:HB3	3:b:407:ASN:HD21	1.86	0.41
22:b:611:CLA:H13	22:b:611:CLA:H171	1.72	0.41
22:b:613:CLA:H8	31:b:616:BCR:H362	2.02	0.41
10:j:11:TRP:H	10:j:11:TRP:CD1	2.38	0.41
14:o:215:ILE:H	14:o:215:ILE:HG13	1.78	0.41
2:A:133:LEU:HD23	5:D:257:ILE:HG12	2.03	0.41
2:A:193:LEU:HD23	2:A:193:LEU:HA	1.89	0.41
3:B:433:ASP:OD2	3:B:436:THR:OG1	2.31	0.41
4:C:335:THR:O	14:O:152:ARG:NH2	2.54	0.41
4:C:387:TRP:O	4:C:391:ARG:HG2	2.20	0.41
30:D:401:PHO:H2	22:D:404:CLA:H13	2.02	0.41
14:O:37:ASP:HA	14:O:206:GLN:HG2	2.02	0.41
20:S:182:ALA:O	20:S:186:LYS:HG3	2.21	0.41
22:R:309:CLA:H93	22:R:309:CLA:H111	1.85	0.41
1:g:189:PHE:CE2	26:g:619:LHG:H291	2.56	0.41
22:g:604:CLA:CMA	21:g:606:CHL:CMC	2.98	0.41
22:n:602:CLA:H3A	22:n:602:CLA:HBA2	1.33	0.41
22:n:602:CLA:H112	22:n:602:CLA:H152	1.75	0.41
21:y:606:CHL:HBD	21:y:606:CHL:CGA	2.51	0.41
21:y:608:CHL:H41	21:y:608:CHL:H62	1.49	0.41
1:G:41:PRO:HB2	1:G:181:LEU:HD12	2.02	0.41
22:G:610:CLA:CHA	22:G:610:CLA:HBA1	2.49	0.41
1:N:41:PRO:HB2	1:N:181:LEU:HD12	2.02	0.41
22:N:609:CLA:H101	23:N:614:LUT:H362	2.03	0.41
1:Y:41:PRO:HB2	1:Y:181:LEU:HD12	2.02	0.41
23:Y:613:LUT:H7	23:Y:613:LUT:H21	1.92	0.41
31:c:515:BCR:H15C	31:c:515:BCR:H351	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:14:TRP:HE1	37:f:101:HEM:CHB	2.34	0.41
14:o:111:TYR:HB2	14:o:127:LEU:HD11	2.02	0.41
16:w:16:GLY:HA2	36:w:102:LMG:O5	2.20	0.41
31:A:410:BCR:H371	31:A:410:BCR:H24C	1.78	0.41
4:C:67:MET:HE1	22:C:506:CLA:C1D	2.51	0.41
14:O:89:ILE:HG23	14:O:107:ASP:O	2.20	0.41
18:Z:57:LEU:HA	18:Z:60:LEU:HB2	2.02	0.41
1:g:41:PRO:HB2	1:g:181:LEU:HD12	2.02	0.41
1:n:25:LEU:C	21:n:601:CHL:HHC	2.45	0.41
1:y:131:GLN:OE1	21:y:606:CHL:CHB	2.69	0.41
22:y:603:CLA:HMD3	21:y:609:CHL:O2A	2.19	0.41
22:G:614:CLA:H3A	22:G:614:CLA:CGA	2.48	0.41
21:N:608:CHL:H91	21:N:608:CHL:H112	1.69	0.41
22:Y:609:CLA:H101	23:Y:613:LUT:H362	2.03	0.41
2:a:138:GLY:HA2	4:c:455:PHE:CZ	2.55	0.41
3:b:256:MET:SD	3:b:448:ARG:HG3	2.60	0.41
5:d:49:TRP:NE1	30:d:401:PHO:H162	2.36	0.41
3:B:372:ASP:HB3	3:B:378:ARG:HG3	2.01	0.41
31:B:619:BCR:H15C	31:B:619:BCR:H351	1.85	0.41
14:O:225:ASP:CG	14:O:227:ASP:H	2.29	0.41
20:S:116:ALA:CA	21:S:307:CHL:HMD3	2.33	0.41
22:R:308:CLA:HED3	22:R:308:CLA:HBD	1.85	0.41
1:n:58:PHE:O	1:n:62:ARG:HG3	2.20	0.41
22:n:609:CLA:CHA	22:n:609:CLA:HBA1	2.49	0.41
22:G:610:CLA:H43	22:G:610:CLA:H172	2.03	0.41
1:N:145:GLY:HA3	1:N:150:GLU:OE1	2.20	0.41
22:N:602:CLA:H3A	22:N:602:CLA:HBA2	1.33	0.41
22:N:603:CLA:HMD3	21:N:608:CHL:O2A	2.20	0.41
22:N:604:CLA:CMA	21:N:605:CHL:CMC	2.98	0.41
22:N:609:CLA:H101	23:N:614:LUT:H383	2.01	0.41
22:N:609:CLA:CHA	22:N:609:CLA:HBA1	2.50	0.41
2:a:78:ILE:HG12	12:l:34:ASN:ND2	2.35	0.41
3:b:18:ARG:HD3	3:b:115:TRP:CZ3	2.55	0.41
31:b:617:BCR:H15C	31:b:617:BCR:H351	1.86	0.41
4:c:449:ARG:HE	22:c:506:CLA:HED1	1.85	0.41
5:d:40:PRO:HB2	22:d:404:CLA:HBB1	2.01	0.41
5:d:298:ASP:N	5:d:298:ASP:OD1	2.51	0.41
4:C:376:ASP:HB3	4:C:379:ARG:HB2	2.02	0.41
30:D:401:PHO:HBA1	30:D:401:PHO:H3A	1.59	0.41
35:H:102:DGD:HB81	35:H:102:DGD:HBE2	1.94	0.41
14:O:215:ILE:H	14:O:215:ILE:HG13	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:r:306:CHL:CAA	25:r:315:NEX:H382	2.49	0.41
20:s:165:HIS:HE1	20:s:189:GLU:OE2	2.03	0.41
19:R:147:LEU:HD22	21:R:305:CHL:O1D	2.21	0.41
24:R:313:XAT:H391	24:R:313:XAT:H31	1.75	0.41
22:g:603:CLA:OBD	21:n:601:CHL:H52	2.21	0.41
21:g:609:CHL:O1A	21:n:601:CHL:H52	2.20	0.41
1:n:71:TRP:CE2	21:n:608:CHL:CHD	2.94	0.41
1:y:138:VAL:HG12	21:y:608:CHL:CMB	2.51	0.41
1:G:15:PRO:O	1:G:21:ARG:HA	2.21	0.41
22:G:604:CLA:CMA	21:G:606:CHL:CMC	2.98	0.41
22:G:610:CLA:H101	23:G:615:LUT:H383	2.01	0.41
1:Y:58:PHE:O	1:Y:62:ARG:HG3	2.20	0.41
22:b:603:CLA:H11	22:b:611:CLA:H151	2.03	0.41
22:b:608:CLA:C3B	31:h:101:BCR:H323	2.51	0.41
4:c:360:ASP:O	35:c:517:DGD:O2E	2.34	0.41
22:c:514:CLA:H62	22:c:514:CLA:H2	1.92	0.41
2:A:77:ILE:N	12:L:34:ASN:HD21	2.19	0.41
3:B:79:ASN:OD1	3:B:80:ILE:N	2.53	0.41
3:B:326:ARG:NE	5:D:298:ASP:OD2	2.53	0.41
22:C:515:CLA:CHC	31:C:516:BCR:H383	2.51	0.41
22:r:310:CLA:H3A	22:r:310:CLA:HBA2	1.33	0.41
20:s:135:LEU:O	20:s:139:VAL:HG23	2.21	0.41
21:s:302:CHL:C2D	26:s:314:LHG:HC82	2.47	0.41
21:s:306:CHL:HAA2	21:s:306:CHL:HBD	2.02	0.41
21:S:306:CHL:HAA2	21:S:306:CHL:HBD	2.02	0.41
21:g:601:CHL:H61	21:g:601:CHL:H41	1.76	0.41
22:g:610:CLA:H101	23:g:615:LUT:H383	2.01	0.41
22:g:610:CLA:H101	23:g:615:LUT:H362	2.03	0.41
1:n:15:PRO:O	1:n:21:ARG:HA	2.21	0.41
1:y:26:GLY:O	1:y:29:SER:OG	2.32	0.41
1:y:67:ILE:CG2	21:y:609:CHL:HMD1	2.41	0.41
21:y:601:CHL:H141	21:y:601:CHL:H161	1.55	0.41
22:y:610:CLA:H101	23:y:614:LUT:H362	2.03	0.41
23:N:614:LUT:H8	23:N:614:LUT:H11	1.77	0.41
1:Y:182:LYS:NZ	22:Y:610:CLA:O1D	2.49	0.41
21:Y:601:CHL:C1D	26:Y:617:LHG:H102	2.50	0.41
2:a:204:GLY:HA2	2:a:278:TRP:NE1	2.36	0.41
3:b:220:ARG:NH2	8:h:32:LYS:H	2.17	0.41
22:b:608:CLA:C4C	31:h:101:BCR:H332	2.51	0.41
22:b:612:CLA:H2A	22:b:612:CLA:O1D	2.21	0.41
22:c:502:CLA:H141	22:c:502:CLA:H162	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:513:CLA:H122	22:s:313:CLA:H72	1.21	0.41
36:c:523:LMG:H321	36:c:523:LMG:C10	2.51	0.41
5:d:181:ARG:HE	5:d:181:ARG:HB3	1.61	0.41
37:f:101:HEM:HBC2	37:f:101:HEM:CHD	2.51	0.41
11:k:55:GLN:HA	11:k:58:VAL:HG22	2.03	0.41
31:k:102:BCR:H371	31:k:102:BCR:H24C	1.78	0.41
2:A:55:ALA:H	2:A:70:SER:HB3	1.86	0.41
2:A:296:ASN:ND2	4:C:401:LEU:HG	2.35	0.41
3:B:42:LEU:HA	3:B:42:LEU:HD23	1.86	0.41
3:B:359:MET:HG2	3:B:360:PRO:O	2.21	0.41
22:B:603:CLA:H92	22:B:603:CLA:H61	1.90	0.41
26:C:520:LHG:H142	22:S:310:CLA:HMB1	2.02	0.41
26:C:521:LHG:H212	16:W:27:PHE:CE2	2.56	0.41
36:C:523:LMG:H322	36:C:523:LMG:HC61	2.02	0.41
36:C:523:LMG:H321	36:C:523:LMG:C10	2.51	0.41
5:D:343:PRO:O	5:D:346:VAL:HG22	2.21	0.41
7:F:20:LEU:O	7:F:23:PRO:HD2	2.21	0.41
14:O:53:LEU:HG	14:O:242:TRP:HB3	2.03	0.41
14:O:106:LYS:HA	14:O:106:LYS:HD3	1.77	0.41
19:r:133:ALA:HB1	21:r:306:CHL:CMD	2.50	0.41
19:r:221:LYS:HE2	19:r:226:PHE:CZ	2.51	0.41
22:r:304:CLA:C1C	22:r:309:CLA:H111	2.50	0.41
24:r:314:XAT:H31	24:r:314:XAT:H391	1.75	0.41
20:s:34:PHE:CE2	21:s:302:CHL:HBA1	2.55	0.41
20:s:182:ALA:O	20:s:186:LYS:HG3	2.21	0.41
20:S:135:LEU:O	20:S:139:VAL:HG23	2.21	0.41
19:R:205:ALA:HA	19:R:208:VAL:HG12	2.03	0.41
22:R:309:CLA:H41	22:R:309:CLA:H62	1.67	0.41
1:g:25:LEU:C	21:g:601:CHL:HHC	2.45	0.41
1:n:131:GLN:OE1	21:n:605:CHL:CHB	2.68	0.41
22:n:609:CLA:H101	23:n:614:LUT:H362	2.03	0.41
25:y:618:NEX:H161	25:y:618:NEX:C9	2.51	0.41
22:G:610:CLA:H101	23:G:615:LUT:H362	2.03	0.41
22:Y:611:CLA:H202	22:Y:612:CLA:C3	2.51	0.41
2:a:55:ALA:H	2:a:70:SER:HB3	1.86	0.41
35:a:413:DGD:HB22	35:a:413:DGD:HB51	1.78	0.41
3:b:57:ARG:HH22	3:b:334:ASP:CG	2.28	0.41
36:b:620:LMG:H273	36:b:620:LMG:H241	1.63	0.41
22:c:506:CLA:CMD	22:c:508:CLA:HAB	2.51	0.41
22:c:514:CLA:H62	22:c:514:CLA:H92	1.93	0.41
36:c:523:LMG:H322	36:c:523:LMG:HC61	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:13:ARG:NE	37:f:101:HEM:O2D	2.50	0.41
14:o:60:VAL:HG22	14:o:236:VAL:HG22	2.03	0.41
3:B:393:GLU:H	3:B:393:GLU:CD	2.29	0.41
22:C:504:CLA:HBB1	22:C:512:CLA:HMC2	2.02	0.41
31:C:517:BCR:H20C	31:C:517:BCR:H361	1.87	0.41
5:D:97:GLU:N	5:D:97:GLU:OE1	2.54	0.41
7:F:20:LEU:HA	7:F:20:LEU:HD23	1.87	0.41
22:W:101:CLA:H2A	22:W:101:CLA:C1	2.51	0.41
19:r:20:PRO:HA	19:r:21:PRO:HD3	1.96	0.41
19:r:94:GLU:O	19:r:98:ILE:HG12	2.21	0.41
20:s:34:PHE:HD2	21:s:302:CHL:HAA2	1.80	0.41
19:R:20:PRO:HA	19:R:21:PRO:HD3	1.96	0.41
22:g:612:CLA:H2A	22:g:612:CLA:C1	2.51	0.40
21:n:608:CHL:C9	21:y:601:CHL:H62	2.51	0.40
22:n:611:CLA:H2A	22:n:611:CLA:C1	2.52	0.40
1:y:127:ILE:HD11	21:y:605:CHL:HBC2	2.03	0.40
25:y:618:NEX:H12	21:R:305:CHL:H152	2.03	0.40
22:N:603:CLA:OBD	21:Y:601:CHL:H52	2.21	0.40
22:N:612:CLA:H61	22:N:612:CLA:H2	1.62	0.40
1:Y:97:TRP:HB2	23:Y:613:LUT:H173	2.03	0.40
23:Y:614:LUT:H8	23:Y:614:LUT:H182	2.02	0.40
3:b:450:TRP:CH2	22:b:606:CLA:H12	2.56	0.40
22:c:514:CLA:CHC	31:c:515:BCR:H383	2.51	0.40
26:c:520:LHG:H312	26:c:520:LHG:H282	1.87	0.40
7:f:10:PHE:HB3	7:f:14:TRP:CZ3	2.56	0.40
14:o:225:ASP:CG	14:o:227:ASP:H	2.29	0.40
17:x:45:ALA:HB2	22:x:101:CLA:H101	2.03	0.40
2:A:92:HIS:HD1	4:C:219:GLY:C	2.27	0.40
2:A:93:PHE:HB2	4:C:218:PHE:CD2	2.56	0.40
3:B:348:ASP:OD1	3:B:351:GLY:N	2.55	0.40
22:C:515:CLA:H11	22:C:515:CLA:C4D	2.51	0.40
5:D:56:VAL:O	5:D:67:SER:HB3	2.20	0.40
22:W:101:CLA:H2	22:W:101:CLA:HMA3	2.03	0.40
22:r:304:CLA:HAB	24:r:314:XAT:C35	2.44	0.40
21:g:609:CHL:CHC	21:g:609:CHL:C3	2.99	0.40
1:n:139:GLU:OE1	1:n:142:ARG:NE	2.46	0.40
21:n:605:CHL:HBD	21:n:605:CHL:CGA	2.51	0.40
1:y:97:TRP:HB2	23:y:614:LUT:H173	2.03	0.40
1:y:131:GLN:CD	21:y:606:CHL:C1B	2.94	0.40
1:y:196:VAL:HB	22:y:612:CLA:CHD	2.51	0.40
22:y:602:CLA:H152	22:y:602:CLA:H112	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:ILE:HG21	21:G:609:CHL:C3D	2.52	0.40
1:G:196:VAL:HB	22:G:613:CLA:CHD	2.51	0.40
21:G:601:CHL:H121	21:Y:608:CHL:H122	2.02	0.40
22:G:604:CLA:CMB	23:G:615:LUT:H12	2.51	0.40
21:G:609:CHL:H112	21:G:609:CHL:H91	1.68	0.40
23:G:616:LUT:H31	23:G:616:LUT:H391	1.88	0.40
24:G:617:XAT:H182	21:Y:606:CHL:C4D	2.52	0.40
1:N:15:PRO:O	1:N:21:ARG:HA	2.21	0.40
1:N:181:LEU:HD23	1:N:181:LEU:HA	1.88	0.40
22:N:603:CLA:C3D	21:Y:601:CHL:H72	2.52	0.40
1:Y:81:PHE:CD2	22:Y:604:CLA:HAC2	2.56	0.40
2:a:290:ILE:HD13	2:a:290:ILE:HA	1.95	0.40
4:c:67:MET:HE1	22:c:505:CLA:C1D	2.51	0.40
4:c:187:ASP:OD1	4:c:189:TRP:N	2.47	0.40
22:c:514:CLA:C4D	22:c:514:CLA:H11	2.51	0.40
7:f:20:LEU:O	7:f:23:PRO:HD2	2.21	0.40
9:i:21:PHE:CZ	16:w:34:TRP:HB2	2.56	0.40
14:o:92:PRO:HD2	14:o:106:LYS:HZ3	1.86	0.40
2:A:242:GLU:OE1	2:A:242:GLU:N	2.55	0.40
22:A:405:CLA:H3A	22:A:405:CLA:HBA1	1.79	0.40
3:B:389:LYS:HA	3:B:394:GLN:HE22	1.87	0.40
4:C:449:ARG:HE	22:C:507:CLA:HED1	1.85	0.40
22:C:514:CLA:H141	22:C:514:CLA:H161	1.86	0.40
22:C:515:CLA:H92	22:C:515:CLA:H62	1.93	0.40
19:r:49:ASP:OD1	19:r:50:LEU:N	2.44	0.40
19:r:104:MET:HE2	19:r:104:MET:HB2	1.93	0.40
19:R:133:ALA:HB1	21:R:305:CHL:CMD	2.50	0.40
19:R:168:PRO:HA	19:R:171:ARG:HB2	2.01	0.40
1:g:81:PHE:CD2	22:g:604:CLA:HAC2	2.56	0.40
1:g:97:TRP:HB2	23:g:615:LUT:H173	2.03	0.40
21:g:606:CHL:H3A	25:g:618:NEX:C31	2.48	0.40
22:n:603:CLA:C2D	21:y:601:CHL:H71	2.51	0.40
22:n:611:CLA:H2	22:n:611:CLA:H62	1.54	0.40
1:y:15:PRO:O	1:y:21:ARG:HA	2.21	0.40
22:y:610:CLA:H101	23:y:614:LUT:H383	2.01	0.40
21:G:609:CHL:CHC	21:G:609:CHL:C3	2.99	0.40
1:N:81:PHE:CD2	22:N:604:CLA:HAC2	2.57	0.40
1:N:131:GLN:CD	21:N:605:CHL:C1B	2.94	0.40
1:N:187:ALA:O	1:N:190:SER:OG	2.31	0.40
21:N:608:CHL:CHC	21:N:608:CHL:C3	3.00	0.40
22:N:611:CLA:H2	22:N:611:CLA:HMA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:15:PRO:O	1:Y:21:ARG:HA	2.21	0.40
1:Y:25:LEU:C	21:Y:601:CHL:HHC	2.46	0.40
1:Y:194:PHE:N	22:Y:611:CLA:CBB	2.85	0.40
2:a:98:GLU:OE2	16:w:8:THR:OG1	2.39	0.40
3:b:271:THR:H	3:b:274:GLN:NE2	2.20	0.40
3:b:359:MET:HG2	3:b:360:PRO:O	2.21	0.40
4:c:261:ARG:HA	4:c:266:TRP:CZ2	2.55	0.40
4:c:456:GLU:OE2	4:c:457:LYS:NZ	2.55	0.40
26:d:408:LHG:H322	15:t:21:ILE:HD11	2.03	0.40
22:A:407:CLA:H3A	22:A:407:CLA:HBA2	1.36	0.40
3:B:150:CYS:HB2	22:B:605:CLA:CMC	2.51	0.40
3:B:450:TRP:CH2	22:B:609:CLA:H12	2.56	0.40
4:C:42:LEU:HD23	4:C:45:LEU:HD12	2.03	0.40
4:C:187:ASP:OD1	4:C:189:TRP:N	2.47	0.40
4:C:261:ARG:HA	4:C:266:TRP:CZ2	2.55	0.40
5:D:25:ARG:HD2	5:D:27:ARG:NH2	2.37	0.40
26:D:410:LHG:H241	26:D:410:LHG:H272	1.62	0.40
14:O:160:LYS:HD3	14:O:160:LYS:HA	1.96	0.40
22:S:311:CLA:H3A	22:S:311:CLA:HBA1	1.75	0.40
1:g:131:GLN:CD	21:g:606:CHL:C1B	2.94	0.40
1:n:67:ILE:HG21	21:n:608:CHL:C3D	2.52	0.40
1:n:81:PHE:CD2	22:n:604:CLA:HAC2	2.56	0.40
1:n:115:ASN:HD21	1:n:117:SER:HB2	1.87	0.40
1:n:138:VAL:HG12	21:n:607:CHL:CMB	2.51	0.40
1:n:196:VAL:HB	22:n:612:CLA:CHD	2.51	0.40
22:n:604:CLA:HMA2	21:n:605:CHL:HAC2	2.04	0.40
22:n:604:CLA:CMB	23:n:614:LUT:H12	2.51	0.40
21:n:608:CHL:CHC	21:n:608:CHL:C3	3.00	0.40
1:G:182:LYS:CE	26:G:618:LHG:HC41	2.52	0.40
22:G:603:CLA:H141	22:G:603:CLA:H162	1.86	0.40
1:N:127:ILE:HD11	21:S:301:CHL:HBC2	2.04	0.40
22:N:611:CLA:H2A	22:N:611:CLA:C1	2.51	0.40
1:Y:131:GLN:OE1	21:Y:605:CHL:CHB	2.69	0.40
3:b:201:HIS:HB2	22:b:601:CLA:C1B	2.52	0.40
3:b:348:ASP:OD1	3:b:351:GLY:N	2.55	0.40
4:c:116:VAL:O	4:c:120:ILE:HG12	2.22	0.40
22:c:502:CLA:H92	22:c:502:CLA:H62	1.73	0.40
5:d:305:ARG:HH11	13:m:1:MET:HE2	1.85	0.40
14:o:79:MET:HE3	14:o:117:GLN:HB3	2.03	0.40
4:C:349:VAL:HB	4:C:375:LEU:H	1.87	0.40
4:C:396:MET:HE3	4:C:396:MET:HB2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:506:CLA:CAD	35:C:519:DGD:HB21	2.52	0.40
14:O:60:VAL:HG22	14:O:236:VAL:HG22	2.03	0.40
19:r:147:LEU:HD22	21:r:306:CHL:O1D	2.21	0.40
20:s:30:ASP:HA	20:s:42:ARG:HH12	1.87	0.40
20:s:125:ASN:HA	20:s:130:PRO:HA	2.04	0.40
20:S:30:ASP:HA	20:S:42:ARG:HH12	1.87	0.40
19:R:94:GLU:O	19:R:98:ILE:HG12	2.21	0.40
1:g:67:ILE:HG21	21:g:609:CHL:C3D	2.52	0.40
1:g:79:CYS:SG	23:g:616:LUT:O3	2.65	0.40
23:n:614:LUT:H21	23:n:614:LUT:H7	1.92	0.40
26:n:617:LHG:H371	26:n:617:LHG:H341	1.64	0.40
1:G:131:GLN:OE1	21:G:606:CHL:CHB	2.69	0.40
23:G:615:LUT:H203	23:G:616:LUT:H8	2.04	0.40
22:Y:602:CLA:HAB	23:Y:614:LUT:H30	2.03	0.40
22:Y:611:CLA:H2	22:Y:611:CLA:H61	1.62	0.40
36:b:620:LMG:C22	21:r:307:CHL:CHB	2.99	0.40
4:c:154:ARG:HH22	16:w:49:GLU:CD	2.29	0.40
4:c:293:ASN:OD1	4:c:295:THR:N	2.49	0.40
22:c:505:CLA:CAD	35:c:518:DGD:HB21	2.52	0.40
22:c:508:CLA:H111	22:c:508:CLA:H91	1.79	0.40
5:d:25:ARG:HD2	5:d:27:ARG:NH2	2.37	0.40
5:d:343:PRO:O	5:d:346:VAL:HG22	2.21	0.40
2:A:141:PRO:HG3	4:C:450:ALA:HB2	2.03	0.40
2:A:142:TRP:C	5:D:221:ASN:HD21	2.30	0.40
2:A:225:ARG:HH12	3:B:483:ASP:HA	1.87	0.40
31:B:602:BCR:H11C	31:B:620:BCR:H382	2.04	0.40
22:B:606:CLA:H11	22:B:614:CLA:H151	2.03	0.40
22:B:615:CLA:O1D	22:B:615:CLA:H2A	2.21	0.40
4:C:313:GLN:HA	4:C:396:MET:SD	2.62	0.40
4:C:456:GLU:OE2	4:C:457:LYS:NZ	2.55	0.40
31:C:516:BCR:H351	31:C:516:BCR:H15C	1.84	0.40
31:C:516:BCR:HC21	18:Z:58:ASN:HD22	1.85	0.40
14:O:79:MET:HE3	14:O:117:GLN:HB3	2.03	0.40
22:S:310:CLA:H61	22:S:310:CLA:H41	1.83	0.40
19:R:143:SER:O	19:R:147:LEU:HG	2.22	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	G	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	N	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	Y	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	g	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	n	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	y	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
2	A	332/334 (99%)	320 (96%)	12 (4%)	0	100	100
2	a	332/334 (99%)	320 (96%)	12 (4%)	0	100	100
3	B	501/503 (100%)	485 (97%)	16 (3%)	0	100	100
3	b	501/503 (100%)	485 (97%)	16 (3%)	0	100	100
4	C	448/450 (100%)	428 (96%)	20 (4%)	0	100	100
4	c	448/450 (100%)	428 (96%)	20 (4%)	0	100	100
5	D	339/341 (99%)	326 (96%)	13 (4%)	0	100	100
5	d	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
6	E	73/75 (97%)	73 (100%)	0	0	100	100
6	e	73/75 (97%)	73 (100%)	0	0	100	100
7	F	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
7	f	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
8	H	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
8	h	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	32 (100%)	0	0	100	100
10	J	33/35 (94%)	33 (100%)	0	0	100	100
10	j	33/35 (94%)	33 (100%)	0	0	100	100
11	K	35/37 (95%)	32 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	k	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
12	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
13	M	31/33 (94%)	31 (100%)	0	0	100	100
13	m	31/33 (94%)	31 (100%)	0	0	100	100
14	O	246/248 (99%)	230 (94%)	16 (6%)	0	100	100
14	o	246/248 (99%)	230 (94%)	16 (6%)	0	100	100
15	T	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
15	t	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
16	W	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
16	w	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
17	X	37/39 (95%)	37 (100%)	0	0	100	100
17	x	37/39 (95%)	37 (100%)	0	0	100	100
18	Z	60/62 (97%)	60 (100%)	0	0	100	100
18	z	60/62 (97%)	60 (100%)	0	0	100	100
19	R	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
19	r	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
20	S	216/218 (99%)	198 (92%)	18 (8%)	0	100	100
20	s	216/218 (99%)	198 (92%)	18 (8%)	0	100	100
All	All	6914/7002 (99%)	6583 (95%)	331 (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	G	171/171 (100%)	168 (98%)	3 (2%)	51	67
1	N	171/171 (100%)	168 (98%)	3 (2%)	51	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	171/171 (100%)	168 (98%)	3 (2%)	51	67
1	g	171/171 (100%)	168 (98%)	3 (2%)	51	67
1	n	171/171 (100%)	168 (98%)	3 (2%)	51	67
1	y	171/171 (100%)	168 (98%)	3 (2%)	51	67
2	A	270/270 (100%)	266 (98%)	4 (2%)	57	69
2	a	270/270 (100%)	266 (98%)	4 (2%)	57	69
3	B	400/400 (100%)	394 (98%)	6 (2%)	57	69
3	b	400/400 (100%)	394 (98%)	6 (2%)	57	69
4	C	352/352 (100%)	341 (97%)	11 (3%)	35	57
4	c	352/352 (100%)	342 (97%)	10 (3%)	38	58
5	D	275/275 (100%)	271 (98%)	4 (2%)	57	69
5	d	275/275 (100%)	271 (98%)	4 (2%)	57	69
6	E	67/67 (100%)	67 (100%)	0	100	100
6	e	67/67 (100%)	67 (100%)	0	100	100
7	F	25/25 (100%)	23 (92%)	2 (8%)	11	36
7	f	25/25 (100%)	23 (92%)	2 (8%)	11	36
8	H	49/49 (100%)	49 (100%)	0	100	100
8	h	49/49 (100%)	49 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	J	26/26 (100%)	26 (100%)	0	100	100
10	j	26/26 (100%)	26 (100%)	0	100	100
11	K	32/32 (100%)	31 (97%)	1 (3%)	35	57
11	k	32/32 (100%)	31 (97%)	1 (3%)	35	57
12	L	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	29/29 (100%)	28 (97%)	1 (3%)	32	55
13	m	29/29 (100%)	28 (97%)	1 (3%)	32	55
14	O	204/204 (100%)	201 (98%)	3 (2%)	57	69
14	o	204/204 (100%)	201 (98%)	3 (2%)	57	69
15	T	29/29 (100%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	t	29/29 (100%)	29 (100%)	0	100	100
16	W	44/44 (100%)	42 (96%)	2 (4%)	24	48
16	w	44/44 (100%)	42 (96%)	2 (4%)	24	48
17	X	32/32 (100%)	32 (100%)	0	100	100
17	x	32/32 (100%)	32 (100%)	0	100	100
18	Z	54/54 (100%)	53 (98%)	1 (2%)	50	66
18	z	54/54 (100%)	53 (98%)	1 (2%)	50	66
19	R	175/175 (100%)	171 (98%)	4 (2%)	44	63
19	r	175/175 (100%)	171 (98%)	4 (2%)	44	63
20	S	169/169 (100%)	156 (92%)	13 (8%)	12	37
20	s	169/169 (100%)	156 (92%)	13 (8%)	12	37
All	All	5622/5622 (100%)	5501 (98%)	121 (2%)	45	63

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	g	192	PHE
1	g	194	PHE
1	g	226	THR
1	n	192	PHE
1	n	194	PHE
1	n	226	THR
1	y	192	PHE
1	y	194	PHE
1	y	226	THR
1	G	192	PHE
1	G	194	PHE
1	G	226	THR
1	N	192	PHE
1	N	194	PHE
1	N	226	THR
1	Y	192	PHE
1	Y	194	PHE
1	Y	226	THR
2	a	220	THR
2	a	260	PHE
2	a	286	THR
2	a	296	ASN

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Mol	Chain	Res	Type
3	b	87	ASN
3	b	116	LEU
3	b	234	ILE
3	b	236	THR
3	b	271	THR
3	b	477	ASP
4	c	108	THR
4	c	121	SER
4	c	150	VAL
4	c	159	THR
4	c	229	ASP
4	c	232	ASP
4	c	272	LEU
4	c	289	PHE
4	c	444	HIS
4	c	470	THR
5	d	133	LEU
5	d	186	PHE
5	d	222	THR
5	d	273	LEU
7	f	18	HIS
7	f	24	THR
11	k	25	LYS
13	m	19	THR
14	o	7	LEU
14	o	10	ASP
14	o	37	ASP
16	w	7	SER
16	w	21	LEU
18	z	31	ASP
2	A	220	THR
2	A	260	PHE
2	A	286	THR
2	A	296	ASN
3	B	87	ASN
3	B	116	LEU
3	B	234	ILE
3	B	236	THR
3	B	271	THR
3	B	477	ASP
4	C	108	THR
4	C	121	SER

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Mol	Chain	Res	Type
4	C	150	VAL
4	C	159	THR
4	C	229	ASP
4	C	232	ASP
4	C	272	LEU
4	C	289	PHE
4	C	444	HIS
4	C	462	ASP
4	C	470	THR
5	D	133	LEU
5	D	186	PHE
5	D	222	THR
5	D	273	LEU
7	F	18	HIS
7	F	24	THR
11	K	25	LYS
13	M	19	THR
14	O	7	LEU
14	O	10	ASP
14	O	37	ASP
16	W	7	SER
16	W	21	LEU
18	Z	31	ASP
19	r	14	TRP
19	r	52	SER
19	r	167	ASP
19	r	202	SER
20	s	35	LEU
20	s	50	THR
20	s	65	SER
20	s	77	TYR
20	s	79	LEU
20	s	80	ILE
20	s	94	ILE
20	s	101	TYR
20	s	110	VAL
20	s	120	ASP
20	s	150	GLU
20	s	215	VAL
20	s	224	ASP
20	S	35	LEU
20	S	50	THR

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Mol	Chain	Res	Type
20	S	65	SER
20	S	77	TYR
20	S	79	LEU
20	S	80	ILE
20	S	94	ILE
20	S	101	TYR
20	S	110	VAL
20	S	120	ASP
20	S	150	GLU
20	S	215	VAL
20	S	224	ASP
19	R	14	TRP
19	R	52	SER
19	R	167	ASP
19	R	202	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	g	131	GLN
1	g	197	GLN
1	g	208	ASN
1	g	218	ASN
1	g	219	ASN
1	n	122	GLN
1	n	131	GLN
1	n	208	ASN
1	n	218	ASN
1	n	219	ASN
1	y	131	GLN
1	y	208	ASN
1	y	218	ASN
1	y	219	ASN
1	G	131	GLN
1	G	208	ASN
1	G	218	ASN
1	G	219	ASN
1	N	131	GLN
1	N	208	ASN
1	N	218	ASN
1	N	219	ASN
1	Y	122	GLN

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Mol	Chain	Res	Type
1	Y	131	GLN
1	Y	208	ASN
1	Y	218	ASN
1	Y	219	ASN
2	a	187	GLN
2	a	303	ASN
2	a	325	ASN
3	b	9	HIS
3	b	157	HIS
3	b	216	HIS
3	b	317	ASN
3	b	343	HIS
3	b	466	HIS
4	c	322	GLN
4	c	385	GLN
4	c	415	ASN
4	c	418	ASN
5	d	62	HIS
5	d	84	ASN
5	d	143	ASN
5	d	221	ASN
5	d	351	ASN
6	e	75	GLN
12	l	34	ASN
14	o	74	GLN
14	o	222	GLN
18	z	58	ASN
2	A	187	GLN
2	A	303	ASN
2	A	325	ASN
3	B	9	HIS
3	B	157	HIS
3	B	317	ASN
3	B	343	HIS
3	B	466	HIS
3	B	496	GLN
4	C	322	GLN
4	C	332	GLN
4	C	373	ASN
4	C	415	ASN
4	C	418	ASN
5	D	62	HIS

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Mol	Chain	Res	Type
5	D	84	ASN
5	D	143	ASN
5	D	221	ASN
5	D	351	ASN
6	E	75	GLN
12	L	9	GLN
12	L	34	ASN
13	M	4	ASN
14	O	74	GLN
14	O	222	GLN
18	Z	58	ASN
19	r	19	GLN
19	r	47	GLN
19	r	56	ASN
19	r	231	ASN
19	r	232	GLN
20	s	81	HIS
20	S	81	HIS
19	R	19	GLN
19	R	47	GLN
19	R	231	ASN
19	R	232	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 325 ligands modelled in this entry, 6 are monoatomic - leaving 319 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	509	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	6 (7%)
25	NEX	Y	616	22	40,46,46	4.83	17 (42%)	50,70,70	9.76	28 (56%)
22	CLA	b	610	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
25	NEX	y	616	22	40,46,46	4.84	16 (40%)	50,70,70	9.98	27 (54%)
22	CLA	b	603	-	69,73,73	1.14	9 (13%)	82,113,113	1.27	5 (6%)
21	CHL	n	608	-	60,74,74	3.62	18 (30%)	58,114,114	1.98	13 (22%)
21	CHL	R	305	-	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
22	CLA	r	303	-	64,68,73	1.21	9 (14%)	76,107,113	1.30	5 (6%)
21	CHL	y	609	-	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
26	LHG	n	617	22	48,48,48	0.65	1 (2%)	51,54,54	1.31	7 (13%)
22	CLA	g	611	-	64,68,73	1.20	9 (14%)	76,107,113	1.29	5 (6%)
22	CLA	c	507	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
22	CLA	G	614	-	52,56,73	1.32	9 (17%)	61,92,113	1.35	5 (8%)
22	CLA	C	512	-	69,73,73	1.16	10 (14%)	82,113,113	1.26	6 (7%)
23	LUT	Y	613	-	42,43,43	4.65	18 (42%)	51,60,60	5.32	26 (50%)
22	CLA	n	612	1	64,68,73	1.66	11 (17%)	76,107,113	1.86	17 (22%)
22	CLA	B	614	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	4 (4%)
22	CLA	y	610	-	64,68,73	1.21	9 (14%)	76,107,113	1.32	5 (6%)
36	LMG	d	410	-	46,46,55	0.81	3 (6%)	54,54,63	1.39	6 (11%)
22	CLA	y	603	-	69,73,73	1.15	10 (14%)	82,113,113	1.23	6 (7%)
32	PL9	a	410	-	13,13,55	1.44	2 (15%)	17,17,69	1.79	4 (23%)
22	CLA	N	602	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
22	CLA	N	610	-	64,68,73	1.19	9 (14%)	76,107,113	1.28	5 (6%)
31	BCR	C	517	-	41,41,41	1.24	2 (4%)	56,56,56	1.30	7 (12%)
25	NEX	y	618	-	40,46,46	5.03	17 (42%)	50,70,70	8.52	27 (54%)
22	CLA	y	613	-	52,56,73	1.32	9 (17%)	61,92,113	1.34	5 (8%)
23	LUT	G	616	-	42,43,43	4.83	19 (45%)	51,60,60	4.79	24 (47%)
22	CLA	G	612	-	64,68,73	1.23	8 (12%)	76,107,113	1.28	4 (5%)
21	CHL	S	301	-	42,56,74	4.31	18 (42%)	36,92,114	2.30	11 (30%)
21	CHL	y	607	-	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	604	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	5 (6%)
22	CLA	c	509	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)
22	CLA	n	613	-	52,56,73	1.33	9 (17%)	61,92,113	1.35	5 (8%)
22	CLA	A	405	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
31	BCR	B	621	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	3 (5%)
27	OEX	A	402	4,2	0,15,15	-	-	-	-	-
22	CLA	g	613	1	69,73,73	1.61	12 (17%)	82,113,113	1.81	17 (20%)
22	CLA	b	604	-	69,73,73	1.15	10 (14%)	82,113,113	1.25	4 (4%)
22	CLA	B	611	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)
31	BCR	A	410	-	41,41,41	1.25	3 (7%)	56,56,56	1.27	7 (12%)
22	CLA	B	606	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
22	CLA	S	304	-	49,53,73	1.38	9 (18%)	58,89,113	1.34	4 (6%)
22	CLA	Y	612	-	52,56,73	1.32	9 (17%)	61,92,113	1.34	5 (8%)
22	CLA	b	605	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
21	CHL	G	608	-	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
31	BCR	k	102	-	41,41,41	1.21	3 (7%)	56,56,56	1.26	7 (12%)
22	CLA	y	604	25	54,58,73	1.29	7 (12%)	64,95,113	1.45	6 (9%)
31	BCR	b	616	-	41,41,41	1.25	2 (4%)	56,56,56	1.25	7 (12%)
26	LHG	N	618	-	48,48,48	0.64	2 (4%)	51,54,54	1.25	7 (13%)
31	BCR	B	620	-	41,41,41	1.21	2 (4%)	56,56,56	1.27	6 (10%)
21	CHL	r	308	-	55,69,74	3.77	18 (32%)	52,108,114	2.07	13 (25%)
22	CLA	C	513	4	69,73,73	1.16	9 (13%)	82,113,113	1.30	8 (9%)
26	LHG	c	520	22	48,48,48	0.81	4 (8%)	51,54,54	1.32	7 (13%)
22	CLA	C	507	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
22	CLA	w	101	-	64,68,73	1.22	9 (14%)	76,107,113	1.27	4 (5%)
24	XAT	g	617	-	41,47,47	3.64	23 (56%)	54,74,74	11.18	32 (59%)
22	CLA	y	612	1	69,73,73	1.60	11 (15%)	82,113,113	1.80	17 (20%)
22	CLA	B	607	-	69,73,73	1.15	10 (14%)	82,113,113	1.26	4 (4%)
31	BCR	b	618	-	41,41,41	1.17	2 (4%)	56,56,56	1.25	3 (5%)
22	CLA	B	613	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
21	CHL	y	605	-	42,56,74	4.31	18 (42%)	36,92,114	2.29	11 (30%)
22	CLA	N	609	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	5 (6%)
22	CLA	W	101	-	64,68,73	1.22	8 (12%)	76,107,113	1.27	4 (5%)
22	CLA	B	603	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
22	CLA	b	613	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	d	403	-	69,73,73	1.15	10 (14%)	82,113,113	1.25	6 (7%)
22	CLA	n	603	-	69,73,73	1.16	10 (14%)	82,113,113	1.25	6 (7%)
21	CHL	y	608	-	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
22	CLA	g	614	-	52,56,73	1.32	9 (17%)	61,92,113	1.35	5 (8%)
21	CHL	N	605	-	44,58,74	4.22	18 (40%)	37,94,114	2.27	11 (29%)
22	CLA	B	617	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
22	CLA	R	310	23	53,57,73	1.35	7 (13%)	61,93,113	1.32	4 (6%)
22	CLA	c	514	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
26	LHG	c	521	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	7 (13%)
22	CLA	b	606	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	6 (7%)
22	CLA	r	312	-	64,68,73	1.21	9 (14%)	76,107,113	1.30	4 (5%)
22	CLA	S	303	20	65,69,73	1.19	8 (12%)	77,108,113	1.28	6 (7%)
26	LHG	C	521	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	7 (13%)
21	CHL	R	307	-	55,69,74	3.77	18 (32%)	52,108,114	2.08	13 (25%)
22	CLA	C	503	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	4 (4%)
22	CLA	N	603	-	69,73,73	1.16	10 (14%)	82,113,113	1.25	6 (7%)
35	DGD	H	102	-	63,63,67	0.95	3 (4%)	77,77,81	1.48	14 (18%)
32	PL9	A	411	-	13,13,55	1.46	2 (15%)	17,17,69	1.77	4 (23%)
22	CLA	C	504	-	69,73,73	1.15	10 (14%)	82,113,113	1.29	6 (7%)
22	CLA	n	602	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	6 (7%)
21	CHL	R	306	-	50,64,74	3.95	18 (36%)	46,102,114	2.18	13 (28%)
21	CHL	s	302	-	40,54,74	4.42	18 (45%)	34,90,114	2.33	10 (29%)
21	CHL	n	601	1	60,74,74	3.60	18 (30%)	58,114,114	1.98	13 (22%)
21	CHL	N	606	-	60,74,74	3.62	18 (30%)	58,114,114	1.98	13 (22%)
26	LHG	d	409	-	42,42,48	0.69	1 (2%)	45,48,54	1.28	5 (11%)
22	CLA	c	513	22	69,73,73	1.16	10 (14%)	82,113,113	1.21	4 (4%)
32	PL9	d	406	-	55,55,55	1.31	4 (7%)	68,69,69	1.51	12 (17%)
36	LMG	D	411	-	46,46,55	0.81	3 (6%)	54,54,63	1.39	6 (11%)
22	CLA	B	605	-	69,73,73	1.14	9 (13%)	82,113,113	1.29	6 (7%)
36	LMG	B	601	-	40,40,55	0.84	1 (2%)	48,48,63	1.31	5 (10%)
26	LHG	Y	617	22	48,48,48	0.67	1 (2%)	51,54,54	1.28	7 (13%)
21	CHL	G	606	-	44,58,74	4.22	18 (40%)	37,94,114	2.28	11 (29%)
21	CHL	Y	606	-	60,74,74	3.61	18 (30%)	58,114,114	1.97	13 (22%)
33	SQD	L	102	-	40,42,54	1.08	3 (7%)	50,53,65	1.54	10 (20%)
25	NEX	n	616	22	40,46,46	4.86	17 (42%)	50,70,70	10.00	26 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	n	604	25	54,58,73	1.29	6 (11%)	64,95,113	1.45	6 (9%)
21	CHL	Y	605	-	44,58,74	4.21	18 (40%)	37,94,114	2.27	11 (29%)
22	CLA	Y	611	1	69,73,73	1.60	11 (15%)	82,113,113	1.80	17 (20%)
22	CLA	b	614	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
23	LUT	g	616	-	42,43,43	4.84	19 (45%)	51,60,60	4.79	24 (47%)
32	PL9	D	407	-	55,55,55	1.32	5 (9%)	68,69,69	1.51	12 (17%)
26	LHG	d	408	-	48,48,48	0.65	1 (2%)	51,54,54	1.31	6 (11%)
22	CLA	Y	602	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
22	CLA	N	613	-	52,56,73	1.32	9 (17%)	61,92,113	1.34	5 (8%)
22	CLA	C	508	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
26	LHG	S	314	22	48,48,48	0.63	1 (2%)	51,54,54	1.29	6 (11%)
23	LUT	Y	614	-	42,43,43	4.79	20 (47%)	51,60,60	4.75	23 (45%)
22	CLA	g	612	-	64,68,73	1.22	8 (12%)	76,107,113	1.28	4 (5%)
33	SQD	d	402	-	48,50,54	1.01	3 (6%)	58,61,65	1.49	10 (17%)
22	CLA	R	309	19	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
22	CLA	C	506	-	69,73,73	1.15	8 (11%)	82,113,113	1.34	5 (6%)
22	CLA	s	313	22	59,63,73	1.24	9 (15%)	70,101,113	1.36	5 (7%)
31	BCR	c	516	-	41,41,41	1.26	3 (7%)	56,56,56	1.29	7 (12%)
31	BCR	c	515	-	41,41,41	1.26	3 (7%)	56,56,56	1.26	6 (10%)
27	OEX	a	401	4,2	0,15,15	-	-	-	-	-
36	LMG	k	103	-	51,51,55	0.73	0	59,59,63	1.34	6 (10%)
22	CLA	C	514	22	69,73,73	1.15	10 (14%)	82,113,113	1.21	4 (4%)
22	CLA	B	616	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
21	CHL	Y	607	-	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
22	CLA	C	505	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	7 (8%)
26	LHG	c	522	-	48,48,48	0.61	1 (2%)	51,54,54	1.31	8 (15%)
22	CLA	g	610	-	68,72,73	1.18	9 (13%)	80,111,113	1.32	5 (6%)
23	LUT	G	615	-	42,43,43	4.66	18 (42%)	51,60,60	5.32	26 (50%)
26	LHG	G	618	-	48,48,48	0.66	1 (2%)	51,54,54	1.30	7 (13%)
21	CHL	n	607	-	60,74,74	3.62	18 (30%)	58,114,114	1.98	13 (22%)
21	CHL	g	609	-	55,69,74	3.78	18 (32%)	52,108,114	2.07	13 (25%)
21	CHL	r	306	-	60,74,74	3.60	18 (30%)	58,114,114	1.98	13 (22%)
22	CLA	C	515	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	6 (7%)
35	DGD	J	101	-	61,61,67	0.98	5 (8%)	75,75,81	1.52	11 (14%)
22	CLA	s	310	26	59,63,73	1.25	9 (15%)	70,101,113	1.32	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	C	522	-	48,48,48	0.61	1 (2%)	51,54,54	1.31	8 (15%)
22	CLA	c	508	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	5 (6%)
36	LMG	C	502	-	48,48,55	0.79	2 (4%)	56,56,63	1.42	8 (14%)
22	CLA	G	611	-	64,68,73	1.20	9 (14%)	76,107,113	1.29	5 (6%)
22	CLA	b	611	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	4 (4%)
26	LHG	b	619	-	48,48,48	0.62	2 (4%)	51,54,54	1.28	6 (11%)
30	PHO	D	401	-	58,69,69	2.12	11 (18%)	55,99,99	1.50	7 (12%)
22	CLA	y	602	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
37	HEM	f	101	-	50,50,50	7.20	11 (22%)	67,82,82	3.51	31 (46%)
22	CLA	b	612	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	4 (4%)
22	CLA	c	511	-	69,73,73	1.16	10 (14%)	82,113,113	1.26	6 (7%)
35	DGD	C	518	-	56,56,67	1.00	4 (7%)	70,70,81	1.55	12 (17%)
21	CHL	S	306	20	40,54,74	4.42	18 (45%)	34,90,114	2.33	10 (29%)
26	LHG	D	410	-	42,42,48	0.69	1 (2%)	45,48,54	1.28	5 (11%)
22	CLA	C	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)
30	PHO	A	408	-	58,69,69	2.10	12 (20%)	55,99,99	1.43	6 (10%)
26	LHG	r	302	-	46,46,48	0.65	2 (4%)	49,52,54	1.30	7 (14%)
36	LMG	C	523	-	51,51,55	0.73	1 (1%)	59,59,63	1.38	8 (13%)
22	CLA	R	308	-	62,66,73	1.23	9 (14%)	73,104,113	1.32	5 (6%)
24	XAT	R	313	-	41,47,47	3.57	22 (53%)	54,74,74	11.15	27 (50%)
22	CLA	a	406	-	54,58,73	1.30	9 (16%)	64,95,113	1.38	6 (9%)
31	BCR	k	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
21	CHL	s	301	-	42,56,74	4.31	18 (42%)	36,92,114	2.30	11 (30%)
22	CLA	D	404	-	69,73,73	1.15	10 (14%)	82,113,113	1.25	6 (7%)
26	LHG	s	314	22	48,48,48	0.63	1 (2%)	51,54,54	1.29	6 (11%)
22	CLA	S	308	-	49,53,73	1.37	7 (14%)	58,89,113	1.33	3 (5%)
22	CLA	b	601	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	5 (6%)
22	CLA	g	604	25	54,58,73	1.29	7 (12%)	64,95,113	1.44	6 (9%)
22	CLA	c	510	-	69,73,73	3.21	14 (20%)	82,113,113	2.26	20 (24%)
22	CLA	c	512	4	69,73,73	1.15	9 (13%)	82,113,113	1.30	7 (8%)
22	CLA	r	310	19	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
21	CHL	G	609	-	55,69,74	3.77	18 (32%)	52,108,114	2.07	13 (25%)
21	CHL	G	601	1	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
22	CLA	c	505	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	5 (6%)
36	LMG	K	103	-	51,51,55	0.72	0	59,59,63	1.34	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CHL	n	605	-	44,58,74	4.22	18 (40%)	37,94,114	2.28	11 (29%)
22	CLA	b	615	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
22	CLA	A	407	-	54,58,73	1.30	9 (16%)	64,95,113	1.38	6 (9%)
22	CLA	S	313	22	59,63,73	1.25	9 (15%)	70,101,113	1.35	5 (7%)
31	BCR	B	619	-	41,41,41	1.25	2 (4%)	56,56,56	1.25	7 (12%)
22	CLA	S	305	-	54,58,73	1.30	9 (16%)	64,95,113	1.44	6 (9%)
33	SQD	l	101	-	40,42,54	1.09	3 (7%)	50,53,65	1.54	10 (20%)
36	LMG	I	101	-	40,40,55	0.84	0	48,48,63	1.31	5 (10%)
22	CLA	x	101	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
22	CLA	B	612	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
22	CLA	s	311	22	60,64,73	1.24	9 (15%)	71,102,113	1.28	6 (8%)
22	CLA	R	304	-	52,56,73	1.32	8 (15%)	61,92,113	1.38	5 (8%)
24	XAT	Y	615	-	41,47,47	3.67	23 (56%)	54,74,74	11.16	31 (57%)
21	CHL	Y	601	1	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
23	LUT	R	312	22	42,43,43	4.71	19 (45%)	51,60,60	5.05	29 (56%)
21	CHL	r	301	-	42,56,74	4.32	18 (42%)	36,92,114	2.30	11 (30%)
21	CHL	y	601	1	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
33	SQD	L	101	-	52,54,54	0.97	4 (7%)	62,65,65	1.54	11 (17%)
22	CLA	G	602	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
35	DGD	h	102	-	63,63,67	0.95	3 (4%)	77,77,81	1.48	14 (18%)
35	DGD	c	518	-	63,63,67	0.93	4 (6%)	77,77,81	1.46	10 (12%)
22	CLA	Y	609	-	64,68,73	1.20	9 (14%)	76,107,113	1.32	5 (6%)
26	LHG	C	520	22	48,48,48	0.81	4 (8%)	51,54,54	1.32	7 (13%)
22	CLA	C	511	-	69,73,73	3.21	14 (20%)	82,113,113	2.26	19 (23%)
36	LMG	c	523	-	51,51,55	0.72	1 (1%)	59,59,63	1.39	8 (13%)
22	CLA	G	610	-	68,72,73	1.17	8 (11%)	80,111,113	1.33	6 (7%)
22	CLA	G	603	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
21	CHL	s	306	20	40,54,74	4.42	18 (45%)	34,90,114	2.33	10 (29%)
21	CHL	g	601	1	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
31	BCR	K	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
22	CLA	S	311	22	60,64,73	1.25	9 (15%)	71,102,113	1.29	6 (8%)
21	CHL	N	607	-	60,74,74	3.62	18 (30%)	58,114,114	1.98	13 (22%)
31	BCR	h	101	-	41,41,41	1.20	2 (4%)	56,56,56	1.31	6 (10%)
22	CLA	g	603	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
22	CLA	y	611	-	64,68,73	1.20	9 (14%)	76,107,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CHL	n	606	-	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
22	CLA	r	305	-	52,56,73	1.33	7 (13%)	61,92,113	1.38	5 (8%)
22	CLA	d	404	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
22	CLA	S	310	26	59,63,73	1.25	9 (15%)	70,101,113	1.32	5 (7%)
22	CLA	R	303	-	64,68,73	1.21	9 (14%)	76,107,113	1.31	5 (6%)
31	BCR	H	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.30	6 (10%)
22	CLA	r	309	-	62,66,73	1.23	9 (14%)	73,104,113	1.31	5 (6%)
22	CLA	a	404	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
23	LUT	y	614	-	42,43,43	4.66	18 (42%)	51,60,60	5.32	26 (50%)
22	CLA	n	611	-	64,68,73	1.23	8 (12%)	76,107,113	1.27	4 (5%)
21	CHL	g	606	-	44,58,74	4.22	18 (40%)	37,94,114	2.28	11 (29%)
22	CLA	Y	610	26	64,68,73	1.20	9 (14%)	76,107,113	1.28	5 (6%)
22	CLA	s	308	-	49,53,73	1.37	8 (16%)	58,89,113	1.34	3 (5%)
26	LHG	y	617	-	48,48,48	0.66	1 (2%)	51,54,54	1.31	7 (13%)
25	NEX	N	617	22	40,46,46	4.99	17 (42%)	50,70,70	9.45	27 (54%)
22	CLA	Y	603	-	69,73,73	1.16	10 (14%)	82,113,113	1.24	6 (7%)
21	CHL	y	606	-	44,58,74	4.22	18 (40%)	37,94,114	2.28	11 (29%)
22	CLA	A	406	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	4 (4%)
36	LMG	T	101	-	51,51,55	0.74	1 (1%)	59,59,63	1.36	6 (10%)
22	CLA	B	610	-	69,73,73	1.14	9 (13%)	82,113,113	1.29	8 (9%)
35	DGD	a	413	-	60,60,67	0.88	2 (3%)	74,74,81	1.44	11 (14%)
22	CLA	s	312	20	53,57,73	1.31	8 (15%)	61,93,113	1.36	5 (8%)
22	CLA	N	604	25	54,58,73	1.29	6 (11%)	64,95,113	1.46	6 (9%)
26	LHG	L	103	-	48,48,48	0.65	1 (2%)	51,54,54	1.31	7 (13%)
21	CHL	s	307	-	40,54,74	4.42	18 (45%)	34,90,114	2.33	10 (29%)
33	SQD	D	402	-	48,50,54	1.01	5 (10%)	58,61,65	1.50	10 (17%)
22	CLA	c	502	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	5 (6%)
22	CLA	N	612	1	64,68,73	1.67	11 (17%)	76,107,113	1.86	17 (22%)
31	BCR	B	602	-	41,41,41	1.17	2 (4%)	56,56,56	1.24	6 (10%)
22	CLA	B	615	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	4 (4%)
35	DGD	c	517	-	56,56,67	1.00	4 (7%)	70,70,81	1.55	12 (17%)
22	CLA	G	604	-	54,58,73	1.29	6 (11%)	64,95,113	1.44	6 (9%)
22	CLA	B	608	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
24	XAT	r	314	-	41,47,47	3.57	22 (53%)	54,74,74	11.15	27 (50%)
23	LUT	g	615	-	42,43,43	4.65	18 (42%)	51,60,60	5.32	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	608	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
36	LMG	B	623	-	55,55,55	0.89	3 (5%)	63,63,63	1.36	8 (12%)
31	BCR	b	617	-	41,41,41	1.21	2 (4%)	56,56,56	1.27	6 (10%)
21	CHL	g	607	-	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
33	SQD	a	411	-	52,54,54	0.97	3 (5%)	62,65,65	1.54	12 (19%)
30	PHO	a	407	-	58,69,69	2.09	12 (20%)	55,99,99	1.42	6 (10%)
21	CHL	S	307	-	40,54,74	4.43	18 (45%)	34,90,114	2.33	10 (29%)
22	CLA	g	602	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
22	CLA	c	503	-	69,73,73	1.15	10 (14%)	82,113,113	1.29	6 (7%)
23	LUT	N	614	-	42,43,43	4.66	18 (42%)	51,60,60	5.32	26 (50%)
35	DGD	c	519	-	61,61,67	0.98	5 (8%)	75,75,81	1.52	11 (14%)
31	BCR	d	405	-	41,41,41	1.23	3 (7%)	56,56,56	1.26	7 (12%)
22	CLA	s	304	-	49,53,73	1.38	9 (18%)	58,89,113	1.34	4 (6%)
22	CLA	R	302	-	64,68,73	1.20	9 (14%)	76,107,113	1.30	5 (6%)
23	LUT	r	313	22	42,43,43	4.70	19 (45%)	51,60,60	5.04	29 (56%)
33	SQD	A	412	-	52,54,54	0.97	3 (5%)	62,65,65	1.54	12 (19%)
21	CHL	S	302	-	40,54,74	4.43	18 (45%)	34,90,114	2.33	10 (29%)
22	CLA	c	504	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	7 (8%)
22	CLA	Y	604	25	54,58,73	1.29	7 (12%)	64,95,113	1.45	6 (9%)
22	CLA	B	618	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
24	XAT	G	617	-	41,47,47	3.63	22 (53%)	54,74,74	11.18	32 (59%)
22	CLA	D	405	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
21	CHL	G	605	-	40,54,74	4.42	18 (45%)	34,90,114	2.32	10 (29%)
23	LUT	N	615	-	42,43,43	4.84	20 (47%)	51,60,60	4.51	28 (54%)
22	CLA	B	609	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	5 (6%)
22	CLA	S	309	20,22	59,63,73	1.25	8 (13%)	70,101,113	1.38	6 (8%)
22	CLA	n	609	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	5 (6%)
22	CLA	s	305	-	54,58,73	1.30	9 (16%)	64,95,113	1.43	6 (9%)
22	CLA	c	506	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	5 (6%)
34	BCT	a	412	-	3,3,3	3.21	1 (33%)	2,3,3	2.84	2 (100%)
22	CLA	r	304	-	64,68,73	1.21	9 (14%)	76,107,113	1.31	5 (6%)
25	NEX	g	618	22	40,46,46	4.81	16 (40%)	50,70,70	9.98	27 (54%)
26	LHG	B	622	-	48,48,48	0.62	2 (4%)	51,54,54	1.28	6 (11%)
22	CLA	r	311	23	53,57,73	1.35	7 (13%)	61,93,113	1.32	4 (6%)
21	CHL	N	601	1	60,74,74	3.61	18 (30%)	58,114,114	1.99	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	R	301	-	46,46,48	0.65	2 (4%)	49,52,54	1.30	7 (14%)
22	CLA	b	607	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	8 (9%)
26	LHG	l	102	-	48,48,48	0.65	1 (2%)	51,54,54	1.31	7 (13%)
22	CLA	G	613	1	69,73,73	1.60	11 (15%)	82,113,113	1.80	17 (20%)
34	BCT	D	403	-	3,3,3	3.20	1 (33%)	2,3,3	2.83	2 (100%)
31	BCR	T	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	6 (10%)
26	LHG	D	409	-	48,48,48	0.65	1 (2%)	51,54,54	1.31	6 (11%)
36	LMG	w	102	-	48,48,55	0.79	2 (4%)	56,56,63	1.42	8 (14%)
36	LMG	M	101	-	51,51,55	0.75	1 (1%)	59,59,63	1.36	6 (10%)
24	XAT	N	616	-	41,47,47	3.59	22 (53%)	54,74,74	11.35	32 (59%)
31	BCR	C	516	-	41,41,41	1.26	2 (4%)	56,56,56	1.28	7 (12%)
33	SQD	l	103	-	52,54,54	0.97	3 (5%)	62,65,65	1.54	11 (17%)
26	LHG	g	619	-	48,48,48	0.63	1 (2%)	51,54,54	1.33	8 (15%)
22	CLA	A	409	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	6 (7%)
21	CHL	N	608	-	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
30	PHO	d	401	-	58,69,69	2.12	11 (18%)	55,99,99	1.50	7 (12%)
23	LUT	n	614	-	42,43,43	4.66	19 (45%)	51,60,60	5.32	26 (50%)
22	CLA	s	303	20	65,69,73	1.19	8 (12%)	77,108,113	1.28	7 (9%)
22	CLA	a	408	-	64,68,73	1.21	8 (12%)	76,107,113	1.33	6 (7%)
21	CHL	G	607	-	60,74,74	3.61	18 (30%)	58,114,114	1.99	13 (22%)
26	LHG	D	408	-	45,45,48	0.66	1 (2%)	48,51,54	1.26	4 (8%)
35	DGD	A	401	-	60,60,67	0.88	2 (3%)	74,74,81	1.44	11 (14%)
22	CLA	n	610	26	64,68,73	1.20	9 (14%)	76,107,113	1.28	5 (6%)
21	CHL	g	605	-	40,54,74	4.42	18 (45%)	34,90,114	2.33	10 (29%)
21	CHL	Y	608	-	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
22	CLA	b	609	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	6 (7%)
22	CLA	s	309	20,22	59,63,73	1.25	8 (13%)	70,101,113	1.38	6 (8%)
37	HEM	F	101	-	50,50,50	7.20	12 (24%)	67,82,82	3.51	31 (46%)
24	XAT	y	615	-	41,47,47	3.65	23 (56%)	54,74,74	11.15	31 (57%)
21	CHL	r	307	-	50,64,74	3.95	18 (36%)	46,102,114	2.18	13 (28%)
22	CLA	R	311	-	64,68,73	1.20	8 (12%)	76,107,113	1.28	4 (5%)
22	CLA	N	611	-	64,68,73	1.23	8 (12%)	76,107,113	1.28	4 (5%)
35	DGD	C	519	-	63,63,67	0.93	4 (6%)	77,77,81	1.46	10 (12%)
22	CLA	a	405	-	69,73,73	1.15	10 (14%)	82,113,113	1.25	4 (4%)
25	NEX	r	315	-	40,46,46	5.01	17 (42%)	50,70,70	8.52	28 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	d	407	-	45,45,48	0.66	1 (2%)	48,51,54	1.26	5 (10%)
21	CHL	g	608	-	60,74,74	3.61	18 (30%)	58,114,114	1.98	13 (22%)
22	CLA	b	602	-	69,73,73	1.14	9 (13%)	82,113,113	1.30	6 (7%)
31	BCR	D	406	-	41,41,41	1.22	3 (7%)	56,56,56	1.25	7 (12%)
36	LMG	b	620	-	55,55,55	0.88	3 (5%)	63,63,63	1.36	9 (14%)
24	XAT	n	615	-	41,47,47	3.61	21 (51%)	54,74,74	11.31	32 (59%)
31	BCR	a	409	-	41,41,41	1.25	3 (7%)	56,56,56	1.27	7 (12%)
31	BCR	K	102	-	41,41,41	1.21	3 (7%)	56,56,56	1.27	7 (12%)
22	CLA	S	312	20	53,57,73	1.31	7 (13%)	61,93,113	1.35	5 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	509	-	1/1/15/20	14/39/115/115	-
25	NEX	Y	616	22	2/2/12/25	16/27/83/83	0/3/3/3
22	CLA	b	610	-	1/1/15/20	12/39/115/115	-
25	NEX	y	616	22	2/2/12/25	15/27/83/83	0/3/3/3
22	CLA	b	603	-	1/1/15/20	10/39/115/115	-
21	CHL	n	608	-	4/4/20/26	15/39/137/137	-
21	CHL	R	305	-	4/4/20/26	18/39/137/137	-
22	CLA	r	303	-	1/1/14/20	10/33/109/115	-
21	CHL	y	609	-	4/4/20/26	14/39/137/137	-
26	LHG	n	617	22	-	25/53/53/53	-
22	CLA	g	611	-	1/1/14/20	10/33/109/115	-
22	CLA	c	507	-	1/1/15/20	11/39/115/115	-
22	CLA	G	614	-	1/1/11/20	11/19/95/115	-
22	CLA	C	512	-	1/1/15/20	14/39/115/115	-
23	LUT	Y	613	-	-	17/29/67/67	0/2/2/2
22	CLA	n	612	1	1/1/14/20	15/33/109/115	-
22	CLA	B	614	-	1/1/15/20	17/39/115/115	-
22	CLA	y	610	-	1/1/14/20	16/33/109/115	-
36	LMG	d	410	-	-	11/41/61/70	0/1/1/1
22	CLA	y	603	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PL9	a	410	-	-	3/5/18/73	0/1/1/1
22	CLA	N	602	-	1/1/15/20	14/39/115/115	-
22	CLA	N	610	-	1/1/14/20	11/33/109/115	-
31	BCR	C	517	-	-	6/29/63/63	0/2/2/2
25	NEX	y	618	-	2/2/12/25	15/27/83/83	0/3/3/3
22	CLA	y	613	-	1/1/11/20	11/19/95/115	-
23	LUT	G	616	-	-	16/29/67/67	0/2/2/2
22	CLA	G	612	-	1/1/14/20	13/33/109/115	-
21	CHL	S	301	-	3/3/16/26	11/18/116/137	-
21	CHL	y	607	-	4/4/20/26	20/39/137/137	-
22	CLA	B	604	-	1/1/15/20	17/39/115/115	-
22	CLA	c	509	-	1/1/15/20	15/39/115/115	-
22	CLA	n	613	-	1/1/11/20	11/19/95/115	-
22	CLA	A	405	-	1/1/15/20	3/39/115/115	-
31	BCR	B	621	-	-	1/29/63/63	0/2/2/2
22	CLA	g	613	1	1/1/15/20	17/39/115/115	-
22	CLA	b	604	-	1/1/15/20	16/39/115/115	-
22	CLA	B	611	-	1/1/15/20	9/39/115/115	-
31	BCR	A	410	-	-	5/29/63/63	0/2/2/2
22	CLA	B	606	-	1/1/15/20	10/39/115/115	-
22	CLA	S	304	-	1/1/11/20	8/15/91/115	-
22	CLA	Y	612	-	1/1/11/20	11/19/95/115	-
22	CLA	b	605	-	1/1/15/20	9/39/115/115	-
21	CHL	G	608	-	4/4/20/26	22/39/137/137	-
31	BCR	k	102	-	-	5/29/63/63	0/2/2/2
22	CLA	y	604	25	1/1/12/20	7/21/97/115	-
31	BCR	b	616	-	-	5/29/63/63	0/2/2/2
26	LHG	N	618	-	-	29/53/53/53	-
31	BCR	B	620	-	-	5/29/63/63	0/2/2/2
21	CHL	r	308	-	4/4/19/26	19/33/131/137	-
22	CLA	C	513	4	1/1/15/20	11/39/115/115	-
26	LHG	c	520	22	-	29/53/53/53	-
22	CLA	C	507	-	1/1/15/20	16/39/115/115	-
22	CLA	w	101	-	1/1/14/20	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	XAT	g	617	-	2/2/12/26	17/31/93/93	0/4/4/4
22	CLA	y	612	1	1/1/15/20	19/39/115/115	-
22	CLA	B	607	-	1/1/15/20	16/39/115/115	-
31	BCR	b	618	-	-	1/29/63/63	0/2/2/2
22	CLA	B	613	-	1/1/15/20	12/39/115/115	-
21	CHL	y	605	-	3/3/16/26	12/18/116/137	-
22	CLA	N	609	-	1/1/15/20	16/39/115/115	-
22	CLA	W	101	-	1/1/14/20	13/33/109/115	-
22	CLA	B	603	-	1/1/15/20	15/39/115/115	-
22	CLA	b	613	-	1/1/15/20	11/39/115/115	-
22	CLA	d	403	-	1/1/15/20	14/39/115/115	-
22	CLA	n	603	-	1/1/15/20	17/39/115/115	-
21	CHL	y	608	-	4/4/20/26	22/39/137/137	-
22	CLA	g	614	-	1/1/11/20	11/19/95/115	-
21	CHL	N	605	-	3/3/16/26	12/20/118/137	-
22	CLA	B	617	-	1/1/15/20	18/39/115/115	-
22	CLA	R	310	23	1/1/11/20	13/20/96/115	-
22	CLA	c	514	-	1/1/15/20	15/39/115/115	-
26	LHG	c	521	-	-	21/53/53/53	-
22	CLA	b	606	-	1/1/15/20	7/39/115/115	-
22	CLA	r	312	-	1/1/14/20	14/33/109/115	-
22	CLA	S	303	20	1/1/14/20	14/35/111/115	-
26	LHG	C	521	-	-	21/53/53/53	-
21	CHL	R	307	-	4/4/19/26	19/33/131/137	-
22	CLA	C	503	-	1/1/15/20	17/39/115/115	-
22	CLA	N	603	-	1/1/15/20	17/39/115/115	-
35	DGD	H	102	-	-	20/51/91/95	0/2/2/2
32	PL9	A	411	-	-	3/5/18/73	0/1/1/1
22	CLA	C	504	-	1/1/15/20	13/39/115/115	-
22	CLA	n	602	-	1/1/15/20	14/39/115/115	-
21	CHL	R	306	-	4/4/18/26	15/27/125/137	-
21	CHL	s	302	-	3/3/16/26	8/15/113/137	-
21	CHL	n	601	1	4/4/20/26	23/39/137/137	-
21	CHL	N	606	-	4/4/20/26	20/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	d	409	-	-	18/47/47/53	-
22	CLA	c	513	22	1/1/15/20	18/39/115/115	-
32	PL9	d	406	-	-	17/53/73/73	0/1/1/1
36	LMG	D	411	-	-	11/41/61/70	0/1/1/1
22	CLA	B	605	-	1/1/15/20	11/39/115/115	-
36	LMG	B	601	-	-	18/35/55/70	0/1/1/1
26	LHG	Y	617	22	-	28/53/53/53	-
21	CHL	G	606	-	3/3/16/26	12/20/118/137	-
21	CHL	Y	606	-	4/4/20/26	20/39/137/137	-
33	SQD	L	102	-	-	13/37/57/69	0/1/1/1
25	NEX	n	616	22	2/2/12/25	16/27/83/83	0/3/3/3
22	CLA	n	604	25	1/1/12/20	7/21/97/115	-
21	CHL	Y	605	-	3/3/16/26	12/20/118/137	-
22	CLA	Y	611	1	1/1/15/20	17/39/115/115	-
22	CLA	b	614	-	1/1/15/20	18/39/115/115	-
23	LUT	g	616	-	-	15/29/67/67	0/2/2/2
32	PL9	D	407	-	-	17/53/73/73	0/1/1/1
26	LHG	d	408	-	-	18/53/53/53	-
22	CLA	Y	602	-	1/1/15/20	14/39/115/115	-
22	CLA	N	613	-	1/1/11/20	11/19/95/115	-
22	CLA	C	508	-	1/1/15/20	11/39/115/115	-
26	LHG	S	314	22	-	29/53/53/53	-
23	LUT	Y	614	-	-	14/29/67/67	0/2/2/2
22	CLA	g	612	-	1/1/14/20	13/33/109/115	-
33	SQD	d	402	-	1/1/9/9	18/45/65/69	0/1/1/1
22	CLA	R	309	19	1/1/15/20	15/39/115/115	-
22	CLA	C	506	-	1/1/15/20	7/39/115/115	-
22	CLA	s	313	22	1/1/13/20	11/27/103/115	-
31	BCR	c	516	-	-	6/29/63/63	0/2/2/2
31	BCR	c	515	-	-	6/29/63/63	0/2/2/2
36	LMG	k	103	-	-	26/46/66/70	0/1/1/1
22	CLA	C	514	22	1/1/15/20	18/39/115/115	-
22	CLA	B	616	-	1/1/15/20	11/39/115/115	-
21	CHL	Y	607	-	4/4/20/26	22/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	505	-	1/1/15/20	12/39/115/115	-
26	LHG	c	522	-	-	22/53/53/53	-
22	CLA	g	610	-	1/1/14/20	16/38/114/115	-
23	LUT	G	615	-	-	17/29/67/67	0/2/2/2
26	LHG	G	618	-	-	28/53/53/53	-
21	CHL	n	607	-	4/4/20/26	22/39/137/137	-
21	CHL	g	609	-	4/4/19/26	10/33/131/137	-
21	CHL	r	306	-	4/4/20/26	18/39/137/137	-
22	CLA	C	515	-	1/1/15/20	15/39/115/115	-
35	DGD	J	101	-	-	17/49/89/95	0/2/2/2
22	CLA	s	310	26	1/1/13/20	14/27/103/115	-
26	LHG	C	522	-	-	22/53/53/53	-
22	CLA	c	508	-	1/1/15/20	13/39/115/115	-
36	LMG	C	502	-	-	16/43/63/70	0/1/1/1
22	CLA	G	611	-	1/1/14/20	10/33/109/115	-
22	CLA	b	611	-	1/1/15/20	17/39/115/115	-
26	LHG	b	619	-	-	27/53/53/53	-
30	PHO	D	401	-	-	15/37/103/103	0/5/6/6
22	CLA	y	602	-	1/1/15/20	14/39/115/115	-
37	HEM	f	101	-	-	5/14/54/54	-
22	CLA	b	612	-	1/1/15/20	7/39/115/115	-
22	CLA	c	511	-	1/1/15/20	14/39/115/115	-
35	DGD	C	518	-	-	18/44/84/95	0/2/2/2
21	CHL	S	306	20	3/3/16/26	9/15/113/137	-
26	LHG	D	410	-	-	18/47/47/53	-
22	CLA	C	510	-	1/1/15/20	15/39/115/115	-
30	PHO	A	408	-	-	12/37/103/103	0/5/6/6
26	LHG	r	302	-	-	24/51/51/53	-
36	LMG	C	523	-	-	20/46/66/70	0/1/1/1
22	CLA	R	308	-	1/1/13/20	11/31/107/115	-
24	XAT	R	313	-	1/1/12/26	14/31/93/93	0/4/4/4
22	CLA	a	406	-	1/1/12/20	8/21/97/115	-
31	BCR	k	101	-	-	16/29/63/63	0/2/2/2
21	CHL	s	301	-	3/3/16/26	12/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	D	404	-	1/1/15/20	15/39/115/115	-
26	LHG	s	314	22	-	29/53/53/53	-
22	CLA	S	308	-	-	9/15/91/115	-
22	CLA	b	601	-	1/1/15/20	17/39/115/115	-
22	CLA	g	604	25	1/1/12/20	7/21/97/115	-
22	CLA	c	510	-	1/1/15/20	10/39/115/115	-
22	CLA	c	512	4	1/1/15/20	11/39/115/115	-
22	CLA	r	310	19	1/1/15/20	15/39/115/115	-
21	CHL	G	609	-	4/4/19/26	10/33/131/137	-
21	CHL	G	601	1	4/4/20/26	23/39/137/137	-
22	CLA	c	505	-	1/1/15/20	7/39/115/115	-
36	LMG	K	103	-	-	26/46/66/70	0/1/1/1
21	CHL	n	605	-	3/3/16/26	12/20/118/137	-
22	CLA	b	615	-	1/1/15/20	12/39/115/115	-
22	CLA	A	407	-	1/1/12/20	8/21/97/115	-
22	CLA	S	313	22	1/1/13/20	11/27/103/115	-
31	BCR	B	619	-	-	5/29/63/63	0/2/2/2
22	CLA	S	305	-	1/1/12/20	10/21/97/115	-
33	SQD	l	101	-	-	13/37/57/69	0/1/1/1
36	LMG	I	101	-	-	18/35/55/70	0/1/1/1
22	CLA	x	101	-	1/1/15/20	15/39/115/115	-
22	CLA	B	612	-	1/1/15/20	9/39/115/115	-
22	CLA	s	311	22	1/1/13/20	10/29/105/115	-
22	CLA	R	304	-	1/1/11/20	8/19/95/115	-
24	XAT	Y	615	-	2/2/12/26	18/31/93/93	0/4/4/4
21	CHL	Y	601	1	4/4/20/26	23/39/137/137	-
23	LUT	R	312	22	-	18/29/67/67	0/2/2/2
21	CHL	r	301	-	3/3/16/26	8/18/116/137	-
21	CHL	y	601	1	4/4/20/26	23/39/137/137	-
33	SQD	L	101	-	-	18/49/69/69	0/1/1/1
22	CLA	G	602	-	1/1/15/20	14/39/115/115	-
35	DGD	h	102	-	-	20/51/91/95	0/2/2/2
35	DGD	c	518	-	-	26/51/91/95	0/2/2/2
22	CLA	Y	609	-	1/1/14/20	16/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	C	520	22	-	29/53/53/53	-
22	CLA	C	511	-	1/1/15/20	10/39/115/115	-
36	LMG	c	523	-	-	20/46/66/70	0/1/1/1
22	CLA	G	610	-	1/1/14/20	19/38/114/115	-
22	CLA	G	603	-	1/1/15/20	17/39/115/115	-
21	CHL	s	306	20	3/3/16/26	9/15/113/137	-
21	CHL	g	601	1	4/4/20/26	23/39/137/137	-
31	BCR	K	101	-	-	16/29/63/63	0/2/2/2
22	CLA	S	311	22	1/1/13/20	10/29/105/115	-
21	CHL	N	607	-	4/4/20/26	22/39/137/137	-
31	BCR	h	101	-	-	7/29/63/63	0/2/2/2
22	CLA	g	603	-	1/1/15/20	17/39/115/115	-
22	CLA	y	611	-	1/1/14/20	11/33/109/115	-
21	CHL	n	606	-	4/4/20/26	20/39/137/137	-
22	CLA	r	305	-	1/1/11/20	8/19/95/115	-
22	CLA	d	404	-	1/1/15/20	14/39/115/115	-
22	CLA	S	310	26	1/1/13/20	14/27/103/115	-
22	CLA	R	303	-	1/1/14/20	11/33/109/115	-
31	BCR	H	101	-	-	7/29/63/63	0/2/2/2
22	CLA	r	309	-	1/1/13/20	11/31/107/115	-
22	CLA	a	404	-	1/1/15/20	3/39/115/115	-
23	LUT	y	614	-	-	17/29/67/67	0/2/2/2
22	CLA	n	611	-	1/1/14/20	13/33/109/115	-
21	CHL	g	606	-	3/3/16/26	12/20/118/137	-
22	CLA	Y	610	26	1/1/14/20	10/33/109/115	-
22	CLA	s	308	-	-	9/15/91/115	-
26	LHG	y	617	-	-	22/53/53/53	-
25	NEX	N	617	22	2/2/12/25	15/27/83/83	0/3/3/3
22	CLA	Y	603	-	1/1/15/20	17/39/115/115	-
21	CHL	y	606	-	3/3/16/26	12/20/118/137	-
22	CLA	A	406	-	1/1/15/20	15/39/115/115	-
36	LMG	T	101	-	-	23/46/66/70	0/1/1/1
22	CLA	B	610	-	1/1/15/20	12/39/115/115	-
35	DGD	a	413	-	-	21/48/88/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	s	312	20	1/1/11/20	9/20/96/115	-
22	CLA	N	604	25	1/1/12/20	7/21/97/115	-
26	LHG	L	103	-	-	18/53/53/53	-
21	CHL	s	307	-	3/3/16/26	9/15/113/137	-
33	SQD	D	402	-	1/1/9/9	18/45/65/69	0/1/1/1
22	CLA	c	502	-	1/1/15/20	17/39/115/115	-
22	CLA	N	612	1	1/1/14/20	15/33/109/115	-
31	BCR	B	602	-	-	19/29/63/63	0/2/2/2
22	CLA	B	615	-	1/1/15/20	7/39/115/115	-
35	DGD	c	517	-	-	18/44/84/95	0/2/2/2
22	CLA	G	604	-	1/1/12/20	7/21/97/115	-
22	CLA	B	608	-	1/1/15/20	9/39/115/115	-
24	XAT	r	314	-	1/1/12/26	14/31/93/93	0/4/4/4
23	LUT	g	615	-	-	17/29/67/67	0/2/2/2
22	CLA	b	608	-	1/1/15/20	9/39/115/115	-
36	LMG	B	623	-	-	21/50/70/70	0/1/1/1
31	BCR	b	617	-	-	5/29/63/63	0/2/2/2
21	CHL	g	607	-	4/4/20/26	20/39/137/137	-
33	SQD	a	411	-	-	23/49/69/69	0/1/1/1
30	PHO	a	407	-	-	12/37/103/103	0/5/6/6
21	CHL	S	307	-	3/3/16/26	10/15/113/137	-
22	CLA	g	602	-	1/1/15/20	14/39/115/115	-
22	CLA	c	503	-	1/1/15/20	13/39/115/115	-
23	LUT	N	614	-	-	17/29/67/67	0/2/2/2
35	DGD	c	519	-	-	16/49/89/95	0/2/2/2
31	BCR	d	405	-	-	8/29/63/63	0/2/2/2
22	CLA	s	304	-	1/1/11/20	8/15/91/115	-
22	CLA	R	302	-	1/1/14/20	10/33/109/115	-
23	LUT	r	313	22	-	18/29/67/67	0/2/2/2
33	SQD	A	412	-	-	23/49/69/69	0/1/1/1
21	CHL	S	302	-	3/3/16/26	8/15/113/137	-
22	CLA	c	504	-	1/1/15/20	12/39/115/115	-
22	CLA	Y	604	25	1/1/12/20	7/21/97/115	-
22	CLA	B	618	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	XAT	G	617	-	3/3/12/26	17/31/93/93	0/4/4/4
22	CLA	D	405	-	1/1/15/20	14/39/115/115	-
21	CHL	G	605	-	3/3/16/26	11/15/113/137	-
23	LUT	N	615	-	-	14/29/67/67	0/2/2/2
22	CLA	B	609	-	1/1/15/20	7/39/115/115	-
22	CLA	S	309	20,22	1/1/13/20	9/27/103/115	-
22	CLA	n	609	-	1/1/15/20	17/39/115/115	-
22	CLA	s	305	-	1/1/12/20	10/21/97/115	-
22	CLA	c	506	-	1/1/15/20	15/39/115/115	-
22	CLA	r	304	-	1/1/14/20	11/33/109/115	-
25	NEX	g	618	22	2/2/12/25	15/27/83/83	0/3/3/3
26	LHG	B	622	-	-	27/53/53/53	-
22	CLA	r	311	23	1/1/11/20	13/20/96/115	-
21	CHL	N	601	1	4/4/20/26	22/39/137/137	-
26	LHG	R	301	-	-	24/51/51/53	-
22	CLA	b	607	-	1/1/15/20	12/39/115/115	-
26	LHG	l	102	-	-	18/53/53/53	-
22	CLA	G	613	1	1/1/15/20	19/39/115/115	-
31	BCR	T	102	-	-	19/29/63/63	0/2/2/2
26	LHG	D	409	-	-	19/53/53/53	-
36	LMG	w	102	-	-	16/43/63/70	0/1/1/1
36	LMG	M	101	-	-	23/46/66/70	0/1/1/1
24	XAT	N	616	-	2/2/12/26	17/31/93/93	0/4/4/4
31	BCR	C	516	-	-	6/29/63/63	0/2/2/2
33	SQD	l	103	-	-	18/49/69/69	0/1/1/1
26	LHG	g	619	-	-	23/53/53/53	-
22	CLA	A	409	-	1/1/14/20	1/33/109/115	-
21	CHL	N	608	-	4/4/20/26	15/39/137/137	-
30	PHO	d	401	-	-	15/37/103/103	0/5/6/6
23	LUT	n	614	-	-	17/29/67/67	0/2/2/2
22	CLA	s	303	20	1/1/14/20	14/35/111/115	-
22	CLA	a	408	-	1/1/14/20	2/33/109/115	-
21	CHL	G	607	-	4/4/20/26	20/39/137/137	-
26	LHG	D	408	-	-	24/50/50/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	A	401	-	-	21/48/88/95	0/2/2/2
22	CLA	n	610	26	1/1/14/20	11/33/109/115	-
21	CHL	g	605	-	3/3/16/26	11/15/113/137	-
21	CHL	Y	608	-	4/4/20/26	12/39/137/137	-
22	CLA	b	609	-	1/1/15/20	9/39/115/115	-
22	CLA	s	309	20,22	1/1/13/20	9/27/103/115	-
37	HEM	F	101	-	-	5/14/54/54	-
24	XAT	y	615	-	2/2/12/26	18/31/93/93	0/4/4/4
21	CHL	r	307	-	4/4/18/26	15/27/125/137	-
22	CLA	R	311	-	1/1/14/20	14/33/109/115	-
22	CLA	N	611	-	1/1/14/20	13/33/109/115	-
35	DGD	C	519	-	-	26/51/91/95	0/2/2/2
22	CLA	a	405	-	1/1/15/20	15/39/115/115	-
25	NEX	r	315	-	2/2/12/25	15/27/83/83	0/3/3/3
26	LHG	d	407	-	-	23/50/50/53	-
21	CHL	g	608	-	4/4/20/26	22/39/137/137	-
22	CLA	b	602	-	1/1/15/20	11/39/115/115	-
31	BCR	D	406	-	-	8/29/63/63	0/2/2/2
36	LMG	b	620	-	-	21/50/70/70	0/1/1/1
24	XAT	n	615	-	2/2/12/26	16/31/93/93	0/4/4/4
31	BCR	a	409	-	-	5/29/63/63	0/2/2/2
31	BCR	K	102	-	-	6/29/63/63	0/2/2/2
22	CLA	S	312	20	1/1/11/20	9/20/96/115	-

All (2975) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	f	101	HEM	FE-NB	41.17	3.21	1.94
37	F	101	HEM	FE-NB	41.15	3.21	1.94
25	y	618	NEX	C7-C6	22.94	1.57	1.30
25	r	315	NEX	C7-C6	22.84	1.57	1.30
25	N	617	NEX	C7-C6	22.54	1.56	1.30
25	y	616	NEX	C7-C6	21.38	1.55	1.30
25	n	616	NEX	C7-C6	21.35	1.55	1.30
25	Y	616	NEX	C7-C6	21.27	1.55	1.30
25	g	618	NEX	C7-C6	21.23	1.55	1.30
37	F	101	HEM	FE-NA	21.02	2.64	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	f	101	HEM	FE-NA	21.01	2.64	1.95
23	N	615	LUT	C24-C25	18.14	1.54	1.33
23	N	614	LUT	C24-C25	18.12	1.54	1.33
23	n	614	LUT	C24-C25	18.11	1.54	1.33
23	G	615	LUT	C24-C25	18.10	1.54	1.33
23	Y	613	LUT	C24-C25	18.10	1.54	1.33
23	g	615	LUT	C24-C25	18.09	1.54	1.33
23	y	614	LUT	C24-C25	18.08	1.54	1.33
23	g	616	LUT	C24-C25	18.04	1.54	1.33
23	r	313	LUT	C24-C25	17.91	1.54	1.33
23	R	312	LUT	C24-C25	17.91	1.54	1.33
23	G	616	LUT	C24-C25	17.89	1.54	1.33
23	Y	614	LUT	C24-C25	17.64	1.54	1.33
22	c	510	CLA	C1D-ND	15.50	1.58	1.37
22	C	511	CLA	C1D-ND	15.47	1.58	1.37
37	f	101	HEM	FE-NC	14.79	2.44	1.95
37	F	101	HEM	FE-NC	14.77	2.43	1.95
23	G	616	LUT	C5-C6	12.22	1.55	1.34
23	R	312	LUT	C5-C6	12.19	1.55	1.34
23	g	616	LUT	C5-C6	12.19	1.54	1.34
23	r	313	LUT	C5-C6	12.13	1.54	1.34
23	Y	614	LUT	C5-C6	12.05	1.54	1.34
21	y	606	CHL	C2C-C3C	11.74	1.47	1.36
21	N	601	CHL	C2C-C3C	11.73	1.47	1.36
21	g	607	CHL	C2C-C3C	11.73	1.47	1.36
21	g	608	CHL	C2C-C3C	11.72	1.47	1.36
21	N	606	CHL	C2C-C3C	11.71	1.47	1.36
21	s	302	CHL	C2C-C3C	11.70	1.47	1.36
21	N	607	CHL	C2C-C3C	11.70	1.47	1.36
21	y	607	CHL	C2C-C3C	11.69	1.47	1.36
21	G	608	CHL	C2C-C3C	11.69	1.47	1.36
21	S	307	CHL	C2C-C3C	11.69	1.47	1.36
21	Y	607	CHL	C2C-C3C	11.69	1.47	1.36
21	S	301	CHL	C2C-C3C	11.69	1.47	1.36
21	N	605	CHL	C2C-C3C	11.69	1.47	1.36
21	n	606	CHL	C2C-C3C	11.68	1.47	1.36
21	S	302	CHL	C2C-C3C	11.68	1.47	1.36
21	r	307	CHL	C2C-C3C	11.68	1.47	1.36
21	Y	606	CHL	C2C-C3C	11.67	1.47	1.36
21	y	605	CHL	C2C-C3C	11.67	1.47	1.36
21	g	601	CHL	C2C-C3C	11.67	1.47	1.36
21	r	301	CHL	C2C-C3C	11.67	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	N	615	LUT	C5-C6	11.66	1.54	1.34
21	y	608	CHL	C2C-C3C	11.66	1.47	1.36
21	g	605	CHL	C2C-C3C	11.66	1.47	1.36
21	S	306	CHL	C2C-C3C	11.66	1.47	1.36
21	R	307	CHL	C2C-C3C	11.66	1.47	1.36
21	R	305	CHL	C2C-C3C	11.66	1.47	1.36
21	n	607	CHL	C2C-C3C	11.65	1.47	1.36
21	g	606	CHL	C2C-C3C	11.65	1.47	1.36
21	G	606	CHL	C2C-C3C	11.65	1.47	1.36
21	Y	608	CHL	C2C-C3C	11.65	1.47	1.36
21	s	306	CHL	C2C-C3C	11.65	1.47	1.36
21	y	601	CHL	C2C-C3C	11.65	1.47	1.36
21	r	306	CHL	C2C-C3C	11.64	1.47	1.36
21	G	607	CHL	C2C-C3C	11.64	1.47	1.36
21	y	609	CHL	C2C-C3C	11.64	1.47	1.36
21	n	601	CHL	C2C-C3C	11.63	1.47	1.36
21	G	605	CHL	C2C-C3C	11.63	1.47	1.36
21	s	307	CHL	C2C-C3C	11.63	1.47	1.36
21	N	608	CHL	C2C-C3C	11.62	1.47	1.36
21	n	608	CHL	C2C-C3C	11.62	1.47	1.36
21	G	601	CHL	C2C-C3C	11.62	1.47	1.36
21	g	609	CHL	C2C-C3C	11.61	1.47	1.36
21	s	301	CHL	C2C-C3C	11.61	1.47	1.36
21	n	605	CHL	C2C-C3C	11.61	1.47	1.36
21	Y	601	CHL	C2C-C3C	11.59	1.47	1.36
21	R	306	CHL	C2C-C3C	11.59	1.47	1.36
21	G	609	CHL	C2C-C3C	11.59	1.47	1.36
21	r	308	CHL	C2C-C3C	11.58	1.47	1.36
21	Y	605	CHL	C2C-C3C	11.58	1.47	1.36
22	c	510	CLA	MG-NC	11.29	2.33	2.06
22	C	511	CLA	MG-NC	11.27	2.33	2.06
23	y	614	LUT	C5-C6	11.16	1.53	1.34
23	N	614	LUT	C5-C6	11.13	1.53	1.34
23	G	615	LUT	C5-C6	11.10	1.53	1.34
23	n	614	LUT	C5-C6	11.09	1.53	1.34
23	g	615	LUT	C5-C6	11.09	1.53	1.34
23	Y	613	LUT	C5-C6	11.07	1.53	1.34
21	r	301	CHL	C1D-C2D	10.84	1.51	1.39
21	n	608	CHL	C1D-C2D	10.84	1.51	1.39
21	Y	607	CHL	C1D-C2D	10.83	1.51	1.39
21	n	606	CHL	C1D-C2D	10.82	1.51	1.39
21	G	606	CHL	C1D-C2D	10.82	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	n	605	CHL	C1D-C2D	10.81	1.51	1.39
21	Y	601	CHL	C1D-C2D	10.81	1.51	1.39
21	N	607	CHL	C1D-C2D	10.80	1.51	1.39
21	y	601	CHL	C1D-C2D	10.79	1.51	1.39
21	S	302	CHL	C1D-C2D	10.79	1.51	1.39
21	Y	608	CHL	C1D-C2D	10.79	1.51	1.39
21	G	601	CHL	C1D-C2D	10.79	1.51	1.39
21	r	306	CHL	C1D-C2D	10.78	1.51	1.39
21	y	609	CHL	C1D-C2D	10.78	1.51	1.39
21	N	606	CHL	C1D-C2D	10.78	1.51	1.39
21	n	607	CHL	C1D-C2D	10.78	1.51	1.39
21	y	605	CHL	C1D-C2D	10.77	1.51	1.39
21	G	609	CHL	C1D-C2D	10.77	1.51	1.39
21	s	302	CHL	C1D-C2D	10.77	1.51	1.39
21	N	601	CHL	C1D-C2D	10.77	1.51	1.39
21	y	608	CHL	C1D-C2D	10.77	1.51	1.39
21	s	301	CHL	C1D-C2D	10.76	1.51	1.39
21	N	605	CHL	C1D-C2D	10.76	1.51	1.39
21	y	607	CHL	C1D-C2D	10.76	1.51	1.39
21	S	306	CHL	C1D-C2D	10.76	1.51	1.39
21	g	606	CHL	C1D-C2D	10.76	1.51	1.39
21	g	609	CHL	C1D-C2D	10.76	1.51	1.39
21	S	307	CHL	C1D-C2D	10.76	1.51	1.39
21	s	306	CHL	C1D-C2D	10.75	1.51	1.39
21	g	608	CHL	C1D-C2D	10.75	1.51	1.39
21	Y	605	CHL	C1D-C2D	10.75	1.51	1.39
21	r	307	CHL	C1D-C2D	10.75	1.51	1.39
21	s	307	CHL	C1D-C2D	10.75	1.51	1.39
21	g	605	CHL	C1D-C2D	10.75	1.51	1.39
21	n	601	CHL	C1D-C2D	10.74	1.51	1.39
21	S	301	CHL	C1D-C2D	10.74	1.51	1.39
21	g	607	CHL	C1D-C2D	10.74	1.51	1.39
21	y	606	CHL	C1D-C2D	10.74	1.51	1.39
21	R	306	CHL	C1D-C2D	10.74	1.51	1.39
21	Y	606	CHL	C1D-C2D	10.73	1.51	1.39
21	R	307	CHL	C1D-C2D	10.73	1.51	1.39
21	G	607	CHL	C1D-C2D	10.73	1.51	1.39
21	R	305	CHL	C1D-C2D	10.73	1.51	1.39
21	g	601	CHL	C1D-C2D	10.73	1.51	1.39
21	r	308	CHL	C1D-C2D	10.73	1.51	1.39
21	G	608	CHL	C1D-C2D	10.73	1.51	1.39
21	N	608	CHL	C1D-C2D	10.73	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	605	CHL	C1D-C2D	10.71	1.51	1.39
30	D	401	PHO	C1B-C2B	9.47	1.49	1.39
30	d	401	PHO	C1B-C2B	9.44	1.49	1.39
22	C	511	CLA	CHD-C1D	9.42	1.56	1.38
22	c	510	CLA	CHD-C1D	9.40	1.56	1.38
30	A	408	PHO	C1B-C2B	9.22	1.49	1.39
30	a	407	PHO	C1B-C2B	9.21	1.49	1.39
22	C	511	CLA	MG-ND	9.19	2.24	2.05
22	c	510	CLA	MG-ND	9.17	2.24	2.05
23	g	616	LUT	C14-C13	9.07	1.56	1.35
23	N	615	LUT	C14-C13	9.03	1.56	1.35
23	G	616	LUT	C14-C13	9.02	1.56	1.35
23	Y	614	LUT	C14-C13	8.85	1.56	1.35
22	c	510	CLA	CHD-C4C	8.85	1.59	1.39
23	R	312	LUT	C14-C13	8.82	1.56	1.35
21	G	607	CHL	C1B-C2B	8.81	1.49	1.39
22	C	511	CLA	CHD-C4C	8.80	1.59	1.39
23	Y	614	LUT	C10-C9	8.80	1.56	1.35
21	y	608	CHL	C1B-C2B	8.79	1.49	1.39
21	r	308	CHL	C1B-C2B	8.79	1.49	1.39
21	S	302	CHL	C1B-C2B	8.79	1.49	1.39
21	g	606	CHL	C1B-C2B	8.79	1.49	1.39
23	r	313	LUT	C14-C13	8.78	1.56	1.35
21	y	601	CHL	C1B-C2B	8.78	1.49	1.39
21	N	601	CHL	C1B-C2B	8.76	1.49	1.39
21	s	307	CHL	C1B-C2B	8.76	1.49	1.39
21	n	606	CHL	C1B-C2B	8.76	1.49	1.39
21	N	608	CHL	C1B-C2B	8.76	1.49	1.39
21	n	605	CHL	C1B-C2B	8.75	1.49	1.39
21	y	606	CHL	C1B-C2B	8.75	1.49	1.39
21	S	307	CHL	C1B-C2B	8.75	1.49	1.39
21	G	609	CHL	C1B-C2B	8.75	1.49	1.39
21	g	605	CHL	C1B-C2B	8.74	1.49	1.39
21	s	301	CHL	C1B-C2B	8.74	1.49	1.39
21	G	608	CHL	C1B-C2B	8.74	1.49	1.39
21	N	605	CHL	C1B-C2B	8.74	1.49	1.39
21	N	607	CHL	C1B-C2B	8.74	1.49	1.39
21	r	301	CHL	C1B-C2B	8.74	1.49	1.39
21	R	307	CHL	C1B-C2B	8.73	1.49	1.39
21	n	608	CHL	C1B-C2B	8.73	1.49	1.39
21	S	301	CHL	C1B-C2B	8.72	1.49	1.39
21	R	306	CHL	C1B-C2B	8.72	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	g	608	CHL	C1B-C2B	8.72	1.49	1.39
21	R	305	CHL	C1B-C2B	8.72	1.49	1.39
21	s	306	CHL	C1B-C2B	8.72	1.49	1.39
21	Y	601	CHL	C1B-C2B	8.72	1.49	1.39
21	S	306	CHL	C1B-C2B	8.72	1.49	1.39
21	n	607	CHL	C1B-C2B	8.71	1.49	1.39
23	G	616	LUT	C10-C9	8.71	1.55	1.35
21	r	306	CHL	C1B-C2B	8.71	1.49	1.39
21	g	609	CHL	C1B-C2B	8.71	1.49	1.39
21	G	601	CHL	C1B-C2B	8.70	1.49	1.39
21	Y	607	CHL	C1B-C2B	8.70	1.49	1.39
23	G	616	LUT	C34-C33	8.70	1.55	1.35
37	F	101	HEM	FE-ND	-8.70	1.68	1.94
23	g	616	LUT	C10-C9	8.70	1.55	1.35
37	f	101	HEM	FE-ND	-8.70	1.68	1.94
21	n	601	CHL	C1B-C2B	8.70	1.49	1.39
21	y	609	CHL	C1B-C2B	8.69	1.49	1.39
21	G	605	CHL	C1B-C2B	8.69	1.49	1.39
23	g	616	LUT	C34-C33	8.69	1.55	1.35
21	y	605	CHL	C1B-C2B	8.68	1.49	1.39
21	g	607	CHL	C1B-C2B	8.68	1.49	1.39
21	r	307	CHL	C1B-C2B	8.68	1.49	1.39
21	Y	605	CHL	C1B-C2B	8.67	1.49	1.39
21	Y	606	CHL	C1B-C2B	8.67	1.49	1.39
21	g	601	CHL	C1B-C2B	8.67	1.49	1.39
21	G	606	CHL	C1B-C2B	8.67	1.49	1.39
21	y	607	CHL	C1B-C2B	8.66	1.49	1.39
23	N	615	LUT	C10-C9	8.66	1.55	1.35
23	y	614	LUT	C10-C9	8.66	1.55	1.35
21	s	302	CHL	C1B-C2B	8.66	1.49	1.39
21	Y	608	CHL	C1B-C2B	8.66	1.49	1.39
21	N	606	CHL	C1B-C2B	8.64	1.49	1.39
23	g	615	LUT	C10-C9	8.64	1.55	1.35
23	N	615	LUT	C34-C33	8.63	1.55	1.35
23	G	615	LUT	C10-C9	8.63	1.55	1.35
23	Y	613	LUT	C10-C9	8.62	1.55	1.35
23	Y	614	LUT	C34-C33	8.62	1.55	1.35
23	y	614	LUT	C14-C13	8.62	1.55	1.35
23	Y	613	LUT	C14-C13	8.61	1.55	1.35
23	N	614	LUT	C10-C9	8.61	1.55	1.35
23	g	615	LUT	C14-C13	8.61	1.55	1.35
23	n	614	LUT	C10-C9	8.61	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	n	614	LUT	C14-C13	8.60	1.55	1.35
23	N	614	LUT	C14-C13	8.60	1.55	1.35
23	G	615	LUT	C14-C13	8.60	1.55	1.35
23	N	615	LUT	C30-C29	8.57	1.55	1.35
24	Y	615	XAT	C30-C29	8.49	1.55	1.35
24	Y	615	XAT	C34-C33	8.47	1.55	1.35
24	y	615	XAT	C30-C29	8.46	1.55	1.35
24	y	615	XAT	C34-C33	8.41	1.55	1.35
24	Y	615	XAT	C14-C13	8.41	1.55	1.35
24	y	615	XAT	C14-C13	8.41	1.55	1.35
24	r	314	XAT	C30-C29	8.40	1.55	1.35
24	N	616	XAT	C30-C29	8.39	1.55	1.35
23	R	312	LUT	C34-C33	8.38	1.55	1.35
24	r	314	XAT	C10-C9	8.36	1.55	1.35
23	R	312	LUT	C10-C9	8.36	1.55	1.35
23	r	313	LUT	C34-C33	8.35	1.55	1.35
24	G	617	XAT	C30-C29	8.35	1.55	1.35
24	g	617	XAT	C30-C29	8.35	1.55	1.35
24	Y	615	XAT	C10-C9	8.35	1.55	1.35
24	R	313	XAT	C30-C29	8.35	1.55	1.35
25	y	616	NEX	C10-C9	8.34	1.55	1.35
23	g	616	LUT	C30-C29	8.34	1.55	1.35
23	Y	614	LUT	C30-C29	8.34	1.55	1.35
24	n	615	XAT	C30-C29	8.33	1.55	1.35
23	r	313	LUT	C10-C9	8.33	1.55	1.35
24	r	314	XAT	C34-C33	8.33	1.55	1.35
24	g	617	XAT	C34-C33	8.33	1.55	1.35
24	R	313	XAT	C10-C9	8.33	1.55	1.35
24	G	617	XAT	C34-C33	8.33	1.55	1.35
24	G	617	XAT	C10-C9	8.32	1.55	1.35
24	R	313	XAT	C34-C33	8.32	1.55	1.35
24	g	617	XAT	C10-C9	8.32	1.55	1.35
24	G	617	XAT	C14-C13	8.31	1.55	1.35
23	g	615	LUT	C34-C33	8.31	1.55	1.35
24	n	615	XAT	C34-C33	8.31	1.55	1.35
23	G	616	LUT	C30-C29	8.31	1.55	1.35
23	n	614	LUT	C34-C33	8.30	1.55	1.35
23	G	615	LUT	C34-C33	8.30	1.55	1.35
23	N	614	LUT	C34-C33	8.29	1.55	1.35
23	y	614	LUT	C34-C33	8.29	1.55	1.35
25	y	616	NEX	C14-C13	8.28	1.54	1.35
24	R	313	XAT	C14-C13	8.27	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	617	NEX	C10-C9	8.27	1.54	1.35
24	y	615	XAT	C10-C9	8.27	1.54	1.35
24	n	615	XAT	C10-C9	8.26	1.54	1.35
25	n	616	NEX	C14-C13	8.26	1.54	1.35
23	Y	613	LUT	C34-C33	8.26	1.54	1.35
30	d	401	PHO	C3B-C4B	8.26	1.49	1.41
25	Y	616	NEX	C10-C9	8.26	1.54	1.35
24	N	616	XAT	C34-C33	8.26	1.54	1.35
24	n	615	XAT	C14-C13	8.25	1.54	1.35
24	g	617	XAT	C14-C13	8.25	1.54	1.35
24	N	616	XAT	C10-C9	8.24	1.54	1.35
24	r	314	XAT	C14-C13	8.24	1.54	1.35
25	n	616	NEX	C10-C9	8.23	1.54	1.35
25	N	617	NEX	C34-C33	8.23	1.54	1.35
25	Y	616	NEX	C34-C33	8.23	1.54	1.35
30	D	401	PHO	C3B-C4B	8.21	1.49	1.41
23	y	614	LUT	C30-C29	8.21	1.54	1.35
25	N	617	NEX	C14-C13	8.20	1.54	1.35
25	g	618	NEX	C10-C9	8.20	1.54	1.35
25	y	616	NEX	C34-C33	8.20	1.54	1.35
23	n	614	LUT	C30-C29	8.19	1.54	1.35
23	G	615	LUT	C30-C29	8.19	1.54	1.35
25	Y	616	NEX	C14-C13	8.19	1.54	1.35
25	y	618	NEX	C10-C9	8.18	1.54	1.35
23	g	615	LUT	C30-C29	8.18	1.54	1.35
25	n	616	NEX	C30-C29	8.17	1.54	1.35
25	n	616	NEX	C34-C33	8.16	1.54	1.35
24	N	616	XAT	C14-C13	8.16	1.54	1.35
23	N	614	LUT	C30-C29	8.15	1.54	1.35
23	Y	613	LUT	C30-C29	8.15	1.54	1.35
25	N	617	NEX	C30-C29	8.15	1.54	1.35
25	r	315	NEX	C10-C9	8.14	1.54	1.35
25	y	618	NEX	C14-C13	8.13	1.54	1.35
25	r	315	NEX	C14-C13	8.13	1.54	1.35
30	A	408	PHO	C3B-C4B	8.12	1.49	1.41
25	g	618	NEX	C14-C13	8.12	1.54	1.35
25	r	315	NEX	C34-C33	8.12	1.54	1.35
25	y	616	NEX	C30-C29	8.11	1.54	1.35
25	y	618	NEX	C34-C33	8.09	1.54	1.35
30	a	407	PHO	C3B-C4B	8.06	1.49	1.41
25	g	618	NEX	C34-C33	8.04	1.54	1.35
25	g	618	NEX	C30-C29	8.03	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	618	NEX	C30-C29	8.01	1.54	1.35
23	R	312	LUT	C30-C29	7.98	1.54	1.35
25	r	315	NEX	C30-C29	7.98	1.54	1.35
23	r	313	LUT	C30-C29	7.97	1.54	1.35
25	Y	616	NEX	C30-C29	7.96	1.54	1.35
21	G	609	CHL	C3B-C4B	7.76	1.48	1.41
21	G	605	CHL	C1A-CHA	7.75	1.48	1.40
21	N	607	CHL	C1A-CHA	7.75	1.48	1.40
21	n	605	CHL	C3B-C4B	7.75	1.48	1.41
21	g	609	CHL	C1A-CHA	7.75	1.48	1.40
21	g	609	CHL	C3B-C4B	7.74	1.48	1.41
21	G	608	CHL	C1A-CHA	7.74	1.48	1.40
21	s	306	CHL	C1A-CHA	7.74	1.48	1.40
21	g	605	CHL	C3B-C4B	7.74	1.48	1.41
21	G	607	CHL	C1A-CHA	7.74	1.48	1.40
21	r	308	CHL	C3B-C4B	7.74	1.48	1.41
21	n	608	CHL	C1A-CHA	7.73	1.48	1.40
21	r	307	CHL	C1A-CHA	7.73	1.48	1.40
21	y	607	CHL	C3B-C4B	7.73	1.48	1.41
21	y	608	CHL	C3B-C4B	7.73	1.48	1.41
21	G	601	CHL	C3B-C4B	7.73	1.48	1.41
21	y	606	CHL	C3B-C4B	7.72	1.48	1.41
21	Y	601	CHL	C1A-CHA	7.72	1.48	1.40
21	R	305	CHL	C1A-CHA	7.72	1.48	1.40
21	n	607	CHL	C3B-C4B	7.72	1.48	1.41
21	Y	606	CHL	C1A-CHA	7.72	1.48	1.40
21	y	608	CHL	C1A-CHA	7.72	1.48	1.40
21	n	608	CHL	C3B-C4B	7.72	1.48	1.41
21	G	605	CHL	C3B-C4B	7.72	1.48	1.41
21	S	302	CHL	C3B-C4B	7.72	1.48	1.41
21	y	606	CHL	C1A-CHA	7.72	1.48	1.40
21	g	601	CHL	C1A-CHA	7.72	1.48	1.40
21	g	606	CHL	C3B-C4B	7.71	1.48	1.41
21	G	606	CHL	C3B-C4B	7.71	1.48	1.41
21	N	606	CHL	C1A-CHA	7.71	1.48	1.40
21	R	307	CHL	C3B-C4B	7.71	1.48	1.41
21	N	608	CHL	C1A-CHA	7.71	1.48	1.40
21	S	306	CHL	C1A-CHA	7.71	1.48	1.40
21	N	605	CHL	C3B-C4B	7.71	1.48	1.41
21	n	606	CHL	C1A-CHA	7.71	1.48	1.40
21	S	307	CHL	C1A-CHA	7.71	1.48	1.40
21	Y	606	CHL	C3B-C4B	7.71	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	r	308	CHL	C1A-CHA	7.71	1.48	1.40
21	R	307	CHL	C1A-CHA	7.70	1.48	1.40
21	y	605	CHL	C3B-C4B	7.70	1.48	1.41
21	r	301	CHL	C3B-C4B	7.70	1.48	1.41
21	y	601	CHL	C1A-CHA	7.70	1.48	1.40
21	r	306	CHL	C3B-C4B	7.70	1.48	1.41
21	N	605	CHL	C1A-CHA	7.70	1.48	1.40
21	Y	607	CHL	C1A-CHA	7.70	1.48	1.40
21	G	601	CHL	C1A-CHA	7.70	1.48	1.40
21	g	607	CHL	C3B-C4B	7.70	1.48	1.41
21	s	302	CHL	C1A-CHA	7.70	1.48	1.40
21	y	609	CHL	C3B-C4B	7.69	1.48	1.41
21	R	306	CHL	C1A-CHA	7.69	1.48	1.40
21	s	307	CHL	C1A-CHA	7.69	1.48	1.40
21	N	606	CHL	C3B-C4B	7.69	1.48	1.41
21	n	601	CHL	C1A-CHA	7.69	1.48	1.40
21	G	609	CHL	C1A-CHA	7.68	1.48	1.40
21	R	305	CHL	C3B-C4B	7.68	1.48	1.41
21	g	607	CHL	C1A-CHA	7.68	1.48	1.40
21	S	307	CHL	C3B-C4B	7.68	1.48	1.41
21	n	605	CHL	C1A-CHA	7.68	1.48	1.40
21	N	608	CHL	C3B-C4B	7.68	1.48	1.41
21	s	307	CHL	C3B-C4B	7.68	1.48	1.41
21	S	301	CHL	C1A-CHA	7.68	1.48	1.40
21	g	608	CHL	C3B-C4B	7.68	1.48	1.41
21	Y	605	CHL	C3B-C4B	7.68	1.48	1.41
21	r	307	CHL	C3B-C4B	7.68	1.48	1.41
21	G	606	CHL	C1A-CHA	7.67	1.48	1.40
21	g	605	CHL	C1A-CHA	7.67	1.48	1.40
21	Y	608	CHL	C1A-CHA	7.67	1.48	1.40
21	N	607	CHL	C3B-C4B	7.67	1.48	1.41
21	s	306	CHL	C3B-C4B	7.67	1.48	1.41
21	S	302	CHL	C1A-CHA	7.67	1.48	1.40
21	S	306	CHL	C3B-C4B	7.67	1.48	1.41
21	Y	605	CHL	C1A-CHA	7.67	1.48	1.40
21	n	607	CHL	C1A-CHA	7.66	1.48	1.40
21	y	609	CHL	C1A-CHA	7.66	1.48	1.40
21	n	606	CHL	C3B-C4B	7.66	1.48	1.41
21	s	301	CHL	C1A-CHA	7.66	1.48	1.40
21	y	605	CHL	C1A-CHA	7.66	1.48	1.40
21	r	301	CHL	C1A-CHA	7.65	1.48	1.40
21	Y	608	CHL	C3B-C4B	7.65	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	601	CHL	C1A-CHA	7.65	1.48	1.40
21	g	601	CHL	C3B-C4B	7.64	1.48	1.41
21	Y	607	CHL	C3B-C4B	7.64	1.48	1.41
21	s	301	CHL	C3B-C4B	7.64	1.48	1.41
21	n	601	CHL	C3B-C4B	7.63	1.48	1.41
21	s	302	CHL	C3B-C4B	7.63	1.48	1.41
21	G	608	CHL	C3B-C4B	7.63	1.48	1.41
21	G	607	CHL	C3B-C4B	7.63	1.48	1.41
21	g	606	CHL	C1A-CHA	7.63	1.48	1.40
21	g	608	CHL	C1A-CHA	7.62	1.48	1.40
21	r	306	CHL	C1A-CHA	7.62	1.48	1.40
21	y	607	CHL	C1A-CHA	7.62	1.48	1.40
21	S	301	CHL	C3B-C4B	7.61	1.48	1.41
21	R	306	CHL	C3B-C4B	7.59	1.48	1.41
21	y	601	CHL	C3B-C4B	7.59	1.48	1.41
21	N	601	CHL	C3B-C4B	7.58	1.48	1.41
21	Y	601	CHL	C3B-C4B	7.57	1.48	1.41
22	y	612	CLA	CHC-C1C	7.15	1.52	1.38
22	g	613	CLA	CHC-C1C	7.14	1.52	1.38
22	n	612	CLA	CHC-C1C	7.13	1.52	1.38
22	N	612	CLA	CHC-C1C	7.13	1.52	1.38
22	G	613	CLA	CHC-C1C	7.12	1.52	1.38
22	Y	611	CLA	CHC-C1C	7.11	1.52	1.38
25	n	616	NEX	C24-C25	6.24	1.60	1.52
25	g	618	NEX	C24-C25	6.20	1.60	1.52
25	y	618	NEX	C24-C25	6.11	1.60	1.52
25	r	315	NEX	C24-C25	6.07	1.60	1.52
25	Y	616	NEX	C24-C25	6.03	1.60	1.52
25	N	617	NEX	C24-C25	6.02	1.60	1.52
21	N	606	CHL	C3B-C2B	5.83	1.48	1.40
21	y	606	CHL	C3B-C2B	5.83	1.48	1.40
25	y	616	NEX	C24-C25	5.83	1.60	1.52
21	g	605	CHL	C3B-C2B	5.82	1.48	1.40
21	S	307	CHL	C3B-C2B	5.82	1.48	1.40
21	Y	608	CHL	C3B-C2B	5.81	1.48	1.40
21	Y	607	CHL	C3B-C2B	5.81	1.48	1.40
21	s	301	CHL	C3B-C2B	5.81	1.48	1.40
21	G	601	CHL	C3B-C2B	5.81	1.48	1.40
21	Y	601	CHL	C3B-C2B	5.81	1.48	1.40
21	N	601	CHL	C3B-C2B	5.80	1.48	1.40
21	g	609	CHL	C3B-C2B	5.80	1.48	1.40
21	s	302	CHL	C3B-C2B	5.80	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	605	CHL	C3B-C2B	5.80	1.48	1.40
21	S	301	CHL	C3B-C2B	5.80	1.48	1.40
21	g	601	CHL	C3B-C2B	5.80	1.48	1.40
21	N	607	CHL	C3B-C2B	5.79	1.48	1.40
21	y	609	CHL	C3B-C2B	5.79	1.48	1.40
21	G	608	CHL	C3B-C2B	5.79	1.48	1.40
21	s	307	CHL	C3B-C2B	5.79	1.48	1.40
21	G	605	CHL	C3B-C2B	5.79	1.48	1.40
21	Y	606	CHL	C3B-C2B	5.79	1.48	1.40
21	n	608	CHL	C3B-C2B	5.79	1.48	1.40
21	R	307	CHL	C3B-C2B	5.78	1.48	1.40
21	R	306	CHL	C3B-C2B	5.78	1.48	1.40
21	y	608	CHL	C3B-C2B	5.78	1.48	1.40
21	n	605	CHL	C3B-C2B	5.78	1.48	1.40
21	n	607	CHL	C3B-C2B	5.77	1.48	1.40
21	y	601	CHL	C3B-C2B	5.77	1.48	1.40
21	N	605	CHL	C3B-C2B	5.77	1.48	1.40
21	r	307	CHL	C3B-C2B	5.77	1.48	1.40
21	s	306	CHL	C3B-C2B	5.77	1.48	1.40
21	g	608	CHL	C3B-C2B	5.76	1.48	1.40
21	n	606	CHL	C3B-C2B	5.76	1.48	1.40
21	r	301	CHL	C3B-C2B	5.76	1.48	1.40
21	y	607	CHL	C3B-C2B	5.76	1.48	1.40
21	S	302	CHL	C3B-C2B	5.76	1.48	1.40
21	g	606	CHL	C3B-C2B	5.76	1.48	1.40
21	g	607	CHL	C3B-C2B	5.76	1.48	1.40
21	G	606	CHL	C3B-C2B	5.76	1.48	1.40
21	N	608	CHL	C3B-C2B	5.75	1.48	1.40
21	r	308	CHL	C3B-C2B	5.74	1.48	1.40
21	y	605	CHL	C3B-C2B	5.74	1.48	1.40
21	n	601	CHL	C3B-C2B	5.74	1.48	1.40
21	G	607	CHL	C3B-C2B	5.74	1.48	1.40
21	R	305	CHL	C3B-C2B	5.74	1.48	1.40
21	G	609	CHL	C3B-C2B	5.74	1.48	1.40
21	r	306	CHL	C3B-C2B	5.72	1.48	1.40
24	g	617	XAT	C24-C25	5.71	1.60	1.52
21	S	306	CHL	C3B-C2B	5.70	1.48	1.40
37	f	101	HEM	C4B-NB	5.59	1.49	1.38
24	R	313	XAT	C24-C25	5.59	1.60	1.52
37	F	101	HEM	C4B-NB	5.55	1.49	1.38
21	g	608	CHL	CHC-C4B	5.52	1.48	1.39
21	g	606	CHL	CHC-C4B	5.50	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	g	607	CHL	CHD-C1D	5.50	1.48	1.39
24	Y	615	XAT	C24-C25	5.50	1.59	1.52
21	Y	608	CHL	CHC-C4B	5.49	1.48	1.39
21	G	607	CHL	CHC-C4B	5.49	1.48	1.39
24	r	314	XAT	C24-C25	5.49	1.59	1.52
21	g	601	CHL	CHC-C4B	5.49	1.48	1.39
24	y	615	XAT	C24-C25	5.49	1.59	1.52
21	Y	601	CHL	CHC-C4B	5.48	1.48	1.39
21	n	607	CHL	CHC-C4B	5.48	1.48	1.39
21	S	306	CHL	CHC-C4B	5.48	1.48	1.39
21	g	609	CHL	CHC-C4B	5.48	1.48	1.39
21	G	605	CHL	CHC-C4B	5.48	1.48	1.39
21	s	306	CHL	CHC-C4B	5.48	1.48	1.39
21	R	307	CHL	CHC-C4B	5.48	1.48	1.39
21	y	607	CHL	CHC-C4B	5.48	1.48	1.39
21	g	601	CHL	CHD-C1D	5.48	1.48	1.39
21	S	302	CHL	CHC-C4B	5.48	1.48	1.39
21	r	301	CHL	CHC-C4B	5.47	1.48	1.39
21	r	307	CHL	CHC-C4B	5.47	1.48	1.39
21	s	301	CHL	CHD-C1D	5.47	1.48	1.39
21	n	607	CHL	CHD-C1D	5.47	1.48	1.39
21	n	608	CHL	CHC-C4B	5.47	1.48	1.39
21	y	601	CHL	CHC-C4B	5.47	1.48	1.39
37	f	101	HEM	CHC-C4B	5.47	1.51	1.39
21	g	606	CHL	CHD-C1D	5.47	1.48	1.39
21	G	601	CHL	CHC-C4B	5.47	1.48	1.39
21	n	606	CHL	CHC-C4B	5.47	1.48	1.39
21	N	605	CHL	CHC-C4B	5.47	1.48	1.39
21	N	606	CHL	CHC-C4B	5.47	1.48	1.39
21	s	302	CHL	CHC-C4B	5.47	1.48	1.39
21	y	605	CHL	CHC-C4B	5.46	1.48	1.39
21	n	605	CHL	CHC-C4B	5.46	1.48	1.39
21	y	606	CHL	CHC-C4B	5.46	1.48	1.39
21	N	608	CHL	CHD-C1D	5.46	1.48	1.39
21	s	302	CHL	CHD-C1D	5.46	1.48	1.39
21	S	301	CHL	CHC-C4B	5.46	1.48	1.39
21	n	601	CHL	CHC-C4B	5.46	1.48	1.39
21	N	608	CHL	CHC-C4B	5.46	1.48	1.39
21	Y	605	CHL	CHC-C4B	5.46	1.48	1.39
21	s	307	CHL	CHC-C4B	5.46	1.48	1.39
21	N	601	CHL	CHC-C4B	5.46	1.48	1.39
21	s	301	CHL	CHC-C4B	5.46	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	r	307	CHL	CHD-C1D	5.46	1.48	1.39
21	g	605	CHL	CHC-C4B	5.46	1.48	1.39
21	G	606	CHL	CHC-C4B	5.46	1.48	1.39
21	s	306	CHL	CHD-C1D	5.46	1.48	1.39
37	F	101	HEM	CHC-C4B	5.46	1.51	1.39
21	Y	606	CHL	CHC-C4B	5.46	1.48	1.39
21	S	302	CHL	CHD-C1D	5.46	1.48	1.39
21	R	307	CHL	CHD-C1D	5.46	1.48	1.39
21	y	608	CHL	CHD-C1D	5.45	1.48	1.39
21	G	601	CHL	CHD-C1D	5.45	1.48	1.39
21	Y	605	CHL	CHD-C1D	5.45	1.48	1.39
21	G	608	CHL	CHD-C1D	5.45	1.48	1.39
21	G	605	CHL	CHD-C1D	5.45	1.48	1.39
21	G	608	CHL	CHC-C4B	5.45	1.48	1.39
21	s	307	CHL	CHD-C1D	5.45	1.48	1.39
21	y	606	CHL	CHD-C1D	5.45	1.48	1.39
21	R	306	CHL	CHC-C4B	5.45	1.48	1.39
21	g	609	CHL	CHD-C1D	5.45	1.48	1.39
21	R	305	CHL	CHC-C4B	5.45	1.48	1.39
21	Y	608	CHL	CHD-C1D	5.44	1.48	1.39
21	g	605	CHL	CHD-C1D	5.44	1.48	1.39
21	g	607	CHL	CHC-C4B	5.44	1.48	1.39
21	S	306	CHL	CHD-C1D	5.44	1.48	1.39
21	G	609	CHL	CHC-C4B	5.44	1.48	1.39
21	Y	606	CHL	CHD-C1D	5.44	1.48	1.39
21	Y	607	CHL	CHC-C4B	5.43	1.48	1.39
21	n	608	CHL	CHD-C1D	5.43	1.48	1.39
21	n	605	CHL	CHD-C1D	5.43	1.48	1.39
21	S	301	CHL	CHD-C1D	5.43	1.48	1.39
21	N	605	CHL	CHD-C1D	5.43	1.48	1.39
21	r	308	CHL	CHC-C4B	5.43	1.48	1.39
21	R	306	CHL	CHD-C1D	5.43	1.48	1.39
21	y	601	CHL	CHD-C1D	5.43	1.48	1.39
21	N	607	CHL	CHC-C4B	5.43	1.48	1.39
21	r	308	CHL	CHD-C1D	5.43	1.48	1.39
21	y	607	CHL	CHD-C1D	5.43	1.48	1.39
21	y	608	CHL	CHC-C4B	5.43	1.48	1.39
21	y	609	CHL	CHC-C4B	5.43	1.48	1.39
21	G	606	CHL	CHD-C1D	5.43	1.48	1.39
21	r	306	CHL	CHC-C4B	5.43	1.48	1.39
21	n	601	CHL	CHD-C1D	5.43	1.48	1.39
21	G	609	CHL	CHD-C1D	5.42	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	R	305	CHL	CHD-C1D	5.42	1.48	1.39
21	r	306	CHL	CHD-C1D	5.42	1.48	1.39
21	S	307	CHL	CHD-C1D	5.42	1.48	1.39
21	G	607	CHL	CHD-C1D	5.42	1.48	1.39
21	g	608	CHL	CHD-C1D	5.41	1.48	1.39
21	N	606	CHL	CHD-C1D	5.41	1.48	1.39
21	N	601	CHL	CHD-C1D	5.40	1.48	1.39
21	S	307	CHL	CHC-C4B	5.40	1.48	1.39
21	n	606	CHL	CHD-C1D	5.40	1.48	1.39
21	Y	601	CHL	CHD-C1D	5.40	1.48	1.39
21	y	609	CHL	CHD-C1D	5.39	1.48	1.39
21	N	607	CHL	CHD-C1D	5.38	1.48	1.39
21	r	301	CHL	CHD-C1D	5.38	1.48	1.39
21	y	605	CHL	CHD-C1D	5.38	1.48	1.39
21	Y	607	CHL	CHD-C1D	5.36	1.48	1.39
21	n	606	CHL	CHD-C4C	5.34	1.49	1.39
21	n	605	CHL	CHD-C4C	5.33	1.49	1.39
21	G	605	CHL	CHD-C4C	5.33	1.49	1.39
21	S	307	CHL	CHD-C4C	5.33	1.49	1.39
21	r	306	CHL	CHD-C4C	5.33	1.49	1.39
21	y	606	CHL	CHD-C4C	5.32	1.49	1.39
21	N	607	CHL	CHD-C4C	5.32	1.49	1.39
21	r	301	CHL	CHD-C4C	5.32	1.49	1.39
21	Y	607	CHL	CHD-C4C	5.32	1.49	1.39
21	R	305	CHL	CHD-C4C	5.32	1.49	1.39
21	s	307	CHL	CHD-C4C	5.32	1.49	1.39
21	G	601	CHL	CHD-C4C	5.32	1.49	1.39
21	S	301	CHL	CHB-C1B	5.32	1.48	1.39
21	g	608	CHL	CHD-C4C	5.32	1.49	1.39
21	g	607	CHL	CHB-C1B	5.31	1.48	1.39
21	r	308	CHL	CHD-C4C	5.31	1.49	1.39
21	R	306	CHL	CHD-C4C	5.31	1.49	1.39
21	G	609	CHL	CHD-C4C	5.31	1.49	1.39
21	n	601	CHL	CHD-C4C	5.31	1.49	1.39
21	g	601	CHL	CHB-C1B	5.31	1.48	1.39
21	Y	601	CHL	CHD-C4C	5.31	1.49	1.39
21	G	606	CHL	CHB-C1B	5.31	1.48	1.39
21	n	607	CHL	CHD-C4C	5.31	1.49	1.39
21	y	607	CHL	CHD-C4C	5.31	1.49	1.39
21	N	607	CHL	CHB-C1B	5.31	1.48	1.39
21	g	605	CHL	CHD-C4C	5.31	1.49	1.39
21	y	605	CHL	CHD-C4C	5.31	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	601	CHL	CHD-C4C	5.31	1.49	1.39
21	n	608	CHL	CHB-C1B	5.30	1.48	1.39
21	n	608	CHL	CHD-C4C	5.30	1.49	1.39
21	n	607	CHL	CHB-C1B	5.30	1.48	1.39
21	r	301	CHL	CHB-C1B	5.30	1.48	1.39
21	s	302	CHL	C3D-C4D	-5.30	1.33	1.41
21	s	307	CHL	CHB-C1B	5.30	1.48	1.39
21	R	307	CHL	C3D-C4D	-5.30	1.33	1.41
21	N	608	CHL	CHD-C4C	5.30	1.49	1.39
21	s	302	CHL	CHB-C1B	5.30	1.48	1.39
21	r	307	CHL	CHD-C4C	5.30	1.49	1.39
21	g	606	CHL	CHD-C4C	5.29	1.49	1.39
21	N	607	CHL	C3D-C4D	-5.29	1.33	1.41
21	Y	608	CHL	CHD-C4C	5.29	1.49	1.39
21	s	306	CHL	CHD-C4C	5.29	1.49	1.39
21	G	605	CHL	CHB-C1B	5.29	1.48	1.39
21	y	609	CHL	CHD-C4C	5.29	1.49	1.39
21	y	601	CHL	CHB-C1B	5.29	1.48	1.39
21	G	609	CHL	CHB-C1B	5.29	1.48	1.39
21	R	307	CHL	CHB-C1B	5.29	1.48	1.39
21	g	609	CHL	CHD-C4C	5.29	1.49	1.39
21	y	605	CHL	CHB-C1B	5.29	1.48	1.39
21	G	606	CHL	C3D-C4D	-5.29	1.33	1.41
21	N	606	CHL	C3D-C4D	-5.29	1.33	1.41
21	r	307	CHL	C3D-C4D	-5.29	1.33	1.41
21	s	302	CHL	CHD-C4C	5.29	1.49	1.39
21	G	606	CHL	CHD-C4C	5.29	1.49	1.39
21	N	606	CHL	CHD-C4C	5.29	1.49	1.39
21	N	606	CHL	CHB-C1B	5.29	1.48	1.39
21	S	306	CHL	CHB-C1B	5.29	1.48	1.39
21	N	605	CHL	CHD-C4C	5.28	1.49	1.39
21	S	302	CHL	CHD-C4C	5.28	1.49	1.39
21	R	307	CHL	CHD-C4C	5.28	1.49	1.39
21	g	608	CHL	CHB-C1B	5.28	1.48	1.39
21	y	607	CHL	CHB-C1B	5.28	1.48	1.39
21	y	601	CHL	CHD-C4C	5.28	1.49	1.39
21	G	607	CHL	CHB-C1B	5.28	1.48	1.39
21	G	607	CHL	CHD-C4C	5.28	1.49	1.39
21	g	601	CHL	CHD-C4C	5.28	1.49	1.39
21	S	306	CHL	CHD-C4C	5.28	1.49	1.39
21	Y	605	CHL	CHB-C1B	5.28	1.48	1.39
21	n	601	CHL	CHB-C1B	5.28	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	R	305	CHL	CHB-C1B	5.28	1.48	1.39
21	N	601	CHL	CHB-C1B	5.28	1.48	1.39
21	r	306	CHL	CHB-C1B	5.28	1.48	1.39
21	G	609	CHL	C3D-C4D	-5.28	1.33	1.41
21	Y	608	CHL	C3D-C4D	-5.27	1.33	1.41
21	y	606	CHL	CHB-C1B	5.27	1.48	1.39
21	G	608	CHL	CHD-C4C	5.27	1.49	1.39
21	y	609	CHL	CHB-C1B	5.27	1.48	1.39
21	G	608	CHL	CHB-C1B	5.27	1.48	1.39
21	y	608	CHL	CHD-C4C	5.27	1.49	1.39
21	g	607	CHL	CHD-C4C	5.27	1.49	1.39
21	n	607	CHL	C3D-C4D	-5.27	1.33	1.41
21	s	301	CHL	CHB-C1B	5.27	1.48	1.39
21	g	605	CHL	C3D-C4D	-5.27	1.33	1.41
21	s	306	CHL	C3D-C4D	-5.27	1.33	1.41
21	Y	601	CHL	CHB-C1B	5.27	1.48	1.39
21	g	606	CHL	CHB-C1B	5.27	1.48	1.39
21	Y	606	CHL	CHD-C4C	5.27	1.49	1.39
21	S	307	CHL	CHB-C1B	5.27	1.48	1.39
21	r	308	CHL	CHB-C1B	5.27	1.48	1.39
21	S	302	CHL	CHB-C1B	5.27	1.48	1.39
21	s	301	CHL	CHD-C4C	5.27	1.49	1.39
21	R	306	CHL	CHB-C1B	5.26	1.48	1.39
21	Y	605	CHL	CHD-C4C	5.26	1.49	1.39
21	y	609	CHL	C3D-C4D	-5.26	1.33	1.41
21	Y	606	CHL	C3D-C4D	-5.26	1.33	1.41
21	s	307	CHL	C3D-C4D	-5.26	1.33	1.41
21	Y	606	CHL	CHB-C1B	5.26	1.48	1.39
21	s	306	CHL	CHB-C1B	5.26	1.48	1.39
21	G	601	CHL	CHB-C1B	5.26	1.48	1.39
21	y	608	CHL	CHB-C1B	5.26	1.48	1.39
21	r	307	CHL	CHB-C1B	5.26	1.48	1.39
21	g	609	CHL	CHB-C1B	5.26	1.48	1.39
21	N	605	CHL	C3D-C4D	-5.26	1.33	1.41
21	Y	608	CHL	CHB-C1B	5.26	1.48	1.39
21	R	306	CHL	C3D-C4D	-5.26	1.33	1.41
21	S	301	CHL	CHD-C4C	5.26	1.49	1.39
21	y	606	CHL	C3D-C4D	-5.25	1.33	1.41
21	Y	601	CHL	C3D-C4D	-5.25	1.33	1.41
21	y	605	CHL	C3D-C4D	-5.25	1.33	1.41
34	a	412	BCT	O1-C	5.25	1.43	1.25
21	S	306	CHL	C3D-C4D	-5.25	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	605	CHL	CHB-C1B	5.25	1.48	1.39
21	G	607	CHL	C3D-C4D	-5.25	1.33	1.41
21	G	605	CHL	C3D-C4D	-5.24	1.33	1.41
21	S	307	CHL	C3D-C4D	-5.24	1.33	1.41
21	g	605	CHL	CHB-C1B	5.24	1.48	1.39
21	Y	607	CHL	CHB-C1B	5.24	1.48	1.39
21	N	601	CHL	C3D-C4D	-5.24	1.33	1.41
21	s	301	CHL	C3D-C4D	-5.24	1.33	1.41
21	S	301	CHL	C3D-C4D	-5.24	1.33	1.41
21	N	608	CHL	C3D-C4D	-5.24	1.33	1.41
21	n	605	CHL	CHB-C1B	5.24	1.48	1.39
21	y	608	CHL	C3D-C4D	-5.24	1.33	1.41
21	S	302	CHL	C3D-C4D	-5.24	1.33	1.41
21	G	608	CHL	C3D-C4D	-5.23	1.33	1.41
21	Y	607	CHL	C3D-C4D	-5.23	1.33	1.41
21	N	608	CHL	CHB-C1B	5.23	1.48	1.39
21	g	609	CHL	C3D-C4D	-5.23	1.33	1.41
21	G	601	CHL	C3D-C4D	-5.23	1.33	1.41
21	g	608	CHL	C3D-C4D	-5.23	1.33	1.41
21	r	306	CHL	C3D-C4D	-5.22	1.33	1.41
21	g	606	CHL	C3D-C4D	-5.22	1.33	1.41
21	r	301	CHL	C3D-C4D	-5.22	1.33	1.41
21	y	607	CHL	C3D-C4D	-5.22	1.33	1.41
34	D	403	BCT	O1-C	5.22	1.43	1.25
21	Y	605	CHL	C3D-C4D	-5.22	1.33	1.41
21	n	606	CHL	CHB-C1B	5.22	1.48	1.39
21	n	605	CHL	C3D-C4D	-5.21	1.33	1.41
21	n	606	CHL	C3D-C4D	-5.21	1.33	1.41
21	y	601	CHL	C3D-C4D	-5.21	1.33	1.41
21	r	308	CHL	C3D-C4D	-5.21	1.33	1.41
21	g	601	CHL	C3D-C4D	-5.21	1.33	1.41
21	n	608	CHL	C3D-C4D	-5.21	1.33	1.41
21	n	601	CHL	C3D-C4D	-5.21	1.33	1.41
21	R	305	CHL	C3D-C4D	-5.19	1.33	1.41
22	N	612	CLA	C1C-C2C	5.18	1.55	1.44
24	n	615	XAT	C24-C25	5.17	1.59	1.52
21	G	601	CHL	O2D-CGD	5.17	1.45	1.33
22	g	613	CLA	C1C-C2C	5.17	1.55	1.44
21	G	607	CHL	O2D-CGD	5.17	1.45	1.33
21	N	606	CHL	O2D-CGD	5.17	1.45	1.33
21	g	605	CHL	O2D-CGD	5.17	1.45	1.33
21	g	607	CHL	C3D-C4D	-5.17	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	g	609	CHL	O2D-CGD	5.16	1.45	1.33
21	n	607	CHL	O2D-CGD	5.16	1.45	1.33
21	g	608	CHL	O2D-CGD	5.16	1.45	1.33
21	G	605	CHL	O2D-CGD	5.16	1.45	1.33
21	N	606	CHL	C3D-C2D	5.16	1.48	1.39
22	y	612	CLA	C1C-C2C	5.16	1.55	1.44
21	y	609	CHL	O2D-CGD	5.15	1.45	1.33
21	Y	607	CHL	O2D-CGD	5.15	1.45	1.33
21	R	307	CHL	O2D-CGD	5.15	1.45	1.33
21	S	301	CHL	O2D-CGD	5.15	1.45	1.33
21	G	608	CHL	O2D-CGD	5.15	1.45	1.33
21	S	307	CHL	O2D-CGD	5.15	1.45	1.33
21	Y	605	CHL	O2D-CGD	5.15	1.45	1.33
21	s	302	CHL	O2D-CGD	5.15	1.45	1.33
21	y	605	CHL	O2D-CGD	5.15	1.45	1.33
21	N	605	CHL	O2D-CGD	5.15	1.45	1.33
24	G	617	XAT	C24-C25	5.15	1.59	1.52
22	G	613	CLA	C1C-C2C	5.14	1.55	1.44
21	R	306	CHL	C3D-C2D	5.14	1.48	1.39
21	y	607	CHL	O2D-CGD	5.14	1.45	1.33
21	Y	606	CHL	O2D-CGD	5.14	1.45	1.33
21	s	301	CHL	O2D-CGD	5.14	1.45	1.33
21	N	601	CHL	O2D-CGD	5.14	1.45	1.33
21	r	307	CHL	O2D-CGD	5.14	1.45	1.33
21	r	301	CHL	O2D-CGD	5.14	1.45	1.33
21	g	601	CHL	C3D-C2D	5.14	1.48	1.39
21	y	609	CHL	C3D-C2D	5.14	1.48	1.39
21	R	305	CHL	O2D-CGD	5.14	1.45	1.33
21	g	609	CHL	C3D-C2D	5.13	1.48	1.39
21	s	307	CHL	O2D-CGD	5.13	1.45	1.33
21	Y	601	CHL	O2D-CGD	5.13	1.45	1.33
21	r	308	CHL	O2D-CGD	5.13	1.45	1.33
21	s	306	CHL	O2D-CGD	5.13	1.45	1.33
21	y	606	CHL	O2D-CGD	5.13	1.45	1.33
21	g	607	CHL	O2D-CGD	5.13	1.45	1.33
22	n	612	CLA	C1C-C2C	5.13	1.54	1.44
21	N	605	CHL	C3D-C2D	5.13	1.48	1.39
21	n	608	CHL	O2D-CGD	5.13	1.45	1.33
21	r	306	CHL	O2D-CGD	5.13	1.45	1.33
21	n	606	CHL	O2D-CGD	5.13	1.45	1.33
21	G	609	CHL	O2D-CGD	5.13	1.45	1.33
21	R	306	CHL	O2D-CGD	5.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	s	301	CHL	OBD-CAD	5.13	1.29	1.22
22	Y	611	CLA	C1C-C2C	5.12	1.54	1.44
21	g	609	CHL	OBD-CAD	5.12	1.29	1.22
21	G	601	CHL	OBD-CAD	5.12	1.29	1.22
21	n	601	CHL	O2D-CGD	5.12	1.45	1.33
21	y	608	CHL	O2D-CGD	5.12	1.45	1.33
21	g	607	CHL	C3D-C2D	5.12	1.48	1.39
21	n	605	CHL	OBD-CAD	5.12	1.29	1.22
21	S	306	CHL	O2D-CGD	5.12	1.45	1.33
21	y	601	CHL	O2D-CGD	5.12	1.45	1.33
21	G	601	CHL	C3D-C2D	5.12	1.48	1.39
21	g	606	CHL	O2D-CGD	5.12	1.45	1.33
21	G	605	CHL	C3D-C2D	5.12	1.48	1.39
21	g	601	CHL	O2D-CGD	5.12	1.45	1.33
21	n	605	CHL	O2D-CGD	5.11	1.45	1.33
21	Y	608	CHL	O2D-CGD	5.11	1.45	1.33
21	G	606	CHL	O2D-CGD	5.11	1.45	1.33
21	S	302	CHL	O2D-CGD	5.11	1.45	1.33
21	R	307	CHL	C3D-C2D	5.11	1.48	1.39
21	s	302	CHL	C3D-C2D	5.11	1.48	1.39
21	N	608	CHL	O2D-CGD	5.11	1.45	1.33
21	G	606	CHL	C3D-C2D	5.11	1.48	1.39
21	s	307	CHL	C3D-C2D	5.11	1.48	1.39
21	y	609	CHL	OBD-CAD	5.11	1.29	1.22
21	n	605	CHL	C3D-C2D	5.11	1.48	1.39
21	y	601	CHL	C3D-C2D	5.11	1.48	1.39
21	G	609	CHL	C3D-C2D	5.11	1.48	1.39
21	N	607	CHL	O2D-CGD	5.11	1.45	1.33
21	r	308	CHL	C3D-C2D	5.11	1.48	1.39
21	G	609	CHL	OBD-CAD	5.11	1.29	1.22
21	y	607	CHL	C3D-C2D	5.10	1.48	1.39
21	y	608	CHL	C3D-C2D	5.10	1.48	1.39
24	N	616	XAT	C24-C25	5.10	1.59	1.52
21	n	608	CHL	C3D-C2D	5.10	1.48	1.39
21	n	606	CHL	OBD-CAD	5.10	1.29	1.22
21	r	301	CHL	C3D-C2D	5.10	1.48	1.39
21	G	606	CHL	OBD-CAD	5.10	1.29	1.22
21	S	301	CHL	C3D-C2D	5.10	1.48	1.39
21	N	601	CHL	C3D-C2D	5.10	1.48	1.39
21	n	601	CHL	OBD-CAD	5.10	1.29	1.22
21	g	608	CHL	C3D-C2D	5.10	1.48	1.39
21	g	606	CHL	C3D-C2D	5.10	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	g	607	CHL	OBD-CAD	5.09	1.29	1.22
21	S	301	CHL	OBD-CAD	5.09	1.29	1.22
21	s	307	CHL	OBD-CAD	5.09	1.29	1.22
21	Y	608	CHL	C3D-C2D	5.09	1.48	1.39
21	y	605	CHL	C3D-C2D	5.09	1.48	1.39
21	S	306	CHL	C3D-C2D	5.09	1.48	1.39
21	N	607	CHL	C3D-C2D	5.09	1.48	1.39
21	s	301	CHL	C3D-C2D	5.09	1.48	1.39
21	n	606	CHL	C3D-C2D	5.09	1.48	1.39
21	Y	605	CHL	C3D-C2D	5.09	1.48	1.39
21	n	607	CHL	OBD-CAD	5.09	1.29	1.22
21	G	608	CHL	C3D-C2D	5.09	1.48	1.39
21	R	305	CHL	C3D-C2D	5.09	1.48	1.39
21	N	607	CHL	OBD-CAD	5.09	1.29	1.22
21	y	607	CHL	OBD-CAD	5.09	1.29	1.22
21	n	607	CHL	C3D-C2D	5.08	1.48	1.39
21	Y	605	CHL	OBD-CAD	5.08	1.29	1.22
21	r	308	CHL	OBD-CAD	5.08	1.29	1.22
21	r	306	CHL	C3D-C2D	5.08	1.48	1.39
21	S	307	CHL	C3D-C2D	5.08	1.48	1.39
21	g	606	CHL	OBD-CAD	5.08	1.29	1.22
21	s	306	CHL	OBD-CAD	5.08	1.29	1.22
21	g	605	CHL	C3D-C2D	5.08	1.48	1.39
21	n	601	CHL	C3D-C2D	5.08	1.48	1.39
21	S	302	CHL	C3D-C2D	5.08	1.48	1.39
21	y	605	CHL	OBD-CAD	5.08	1.29	1.22
21	s	306	CHL	C3D-C2D	5.07	1.48	1.39
21	Y	601	CHL	C3D-C2D	5.07	1.48	1.39
21	G	605	CHL	OBD-CAD	5.07	1.29	1.22
21	G	607	CHL	C3D-C2D	5.07	1.48	1.39
21	y	601	CHL	OBD-CAD	5.07	1.29	1.22
21	N	608	CHL	OBD-CAD	5.07	1.29	1.22
21	S	302	CHL	OBD-CAD	5.07	1.29	1.22
21	R	306	CHL	OBD-CAD	5.07	1.28	1.22
21	Y	601	CHL	OBD-CAD	5.07	1.28	1.22
21	R	307	CHL	OBD-CAD	5.07	1.28	1.22
21	y	606	CHL	C3D-C2D	5.07	1.48	1.39
21	R	305	CHL	OBD-CAD	5.07	1.28	1.22
21	n	608	CHL	OBD-CAD	5.07	1.28	1.22
21	S	306	CHL	OBD-CAD	5.06	1.28	1.22
21	G	608	CHL	OBD-CAD	5.06	1.28	1.22
21	N	606	CHL	OBD-CAD	5.06	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	606	CHL	C3D-C2D	5.05	1.48	1.39
21	N	601	CHL	OBD-CAD	5.05	1.28	1.22
21	y	606	CHL	OBD-CAD	5.05	1.28	1.22
21	N	608	CHL	C3D-C2D	5.05	1.48	1.39
21	y	608	CHL	OBD-CAD	5.05	1.28	1.22
21	S	307	CHL	OBD-CAD	5.05	1.28	1.22
21	G	607	CHL	OBD-CAD	5.05	1.28	1.22
21	r	307	CHL	C3D-C2D	5.05	1.48	1.39
21	Y	608	CHL	OBD-CAD	5.04	1.28	1.22
21	g	601	CHL	OBD-CAD	5.04	1.28	1.22
21	s	302	CHL	OBD-CAD	5.04	1.28	1.22
21	Y	607	CHL	C3D-C2D	5.04	1.48	1.39
21	g	605	CHL	OBD-CAD	5.04	1.28	1.22
21	Y	606	CHL	OBD-CAD	5.04	1.28	1.22
21	r	301	CHL	OBD-CAD	5.02	1.28	1.22
21	r	307	CHL	OBD-CAD	5.02	1.28	1.22
21	g	608	CHL	OBD-CAD	5.02	1.28	1.22
21	N	605	CHL	OBD-CAD	5.02	1.28	1.22
21	r	306	CHL	OBD-CAD	5.01	1.28	1.22
21	R	306	CHL	CHC-C1C	5.01	1.49	1.39
21	Y	607	CHL	OBD-CAD	5.00	1.28	1.22
21	Y	601	CHL	CHC-C1C	4.99	1.49	1.39
21	S	306	CHL	CHC-C1C	4.99	1.49	1.39
21	n	601	CHL	CHC-C1C	4.99	1.49	1.39
21	r	306	CHL	CHC-C1C	4.99	1.49	1.39
21	S	307	CHL	CHC-C1C	4.99	1.49	1.39
21	Y	605	CHL	CHC-C1C	4.98	1.48	1.39
21	r	308	CHL	CHC-C1C	4.98	1.48	1.39
21	n	608	CHL	CHC-C1C	4.97	1.48	1.39
21	n	607	CHL	CHC-C1C	4.97	1.48	1.39
21	G	608	CHL	CHC-C1C	4.97	1.48	1.39
21	y	609	CHL	CHC-C1C	4.97	1.48	1.39
21	G	605	CHL	CHC-C1C	4.97	1.48	1.39
21	R	307	CHL	CHC-C1C	4.97	1.48	1.39
21	N	601	CHL	CHC-C1C	4.97	1.48	1.39
21	g	601	CHL	CHC-C1C	4.97	1.48	1.39
21	S	301	CHL	CHC-C1C	4.96	1.48	1.39
21	r	301	CHL	CHC-C1C	4.96	1.48	1.39
21	R	305	CHL	CHC-C1C	4.96	1.48	1.39
21	N	607	CHL	CHC-C1C	4.96	1.48	1.39
21	g	606	CHL	CHC-C1C	4.96	1.48	1.39
21	g	608	CHL	CHC-C1C	4.96	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	606	CHL	CHC-C1C	4.96	1.48	1.39
21	s	307	CHL	CHC-C1C	4.96	1.48	1.39
21	g	607	CHL	CHC-C1C	4.96	1.48	1.39
21	r	307	CHL	CHC-C1C	4.96	1.48	1.39
21	G	606	CHL	CHC-C1C	4.95	1.48	1.39
21	G	609	CHL	CHC-C1C	4.95	1.48	1.39
21	y	608	CHL	CHC-C1C	4.95	1.48	1.39
21	y	601	CHL	CHC-C1C	4.95	1.48	1.39
21	Y	607	CHL	CHC-C1C	4.95	1.48	1.39
21	N	608	CHL	CHC-C1C	4.95	1.48	1.39
21	y	605	CHL	CHC-C1C	4.95	1.48	1.39
21	y	606	CHL	CHC-C1C	4.95	1.48	1.39
21	Y	606	CHL	CHC-C1C	4.95	1.48	1.39
21	G	607	CHL	CHC-C1C	4.95	1.48	1.39
21	Y	608	CHL	CHC-C1C	4.95	1.48	1.39
21	s	306	CHL	CHC-C1C	4.94	1.48	1.39
21	s	302	CHL	CHC-C1C	4.94	1.48	1.39
21	g	609	CHL	CHC-C1C	4.94	1.48	1.39
21	S	302	CHL	CHC-C1C	4.94	1.48	1.39
21	n	605	CHL	CHC-C1C	4.93	1.48	1.39
21	n	606	CHL	CHC-C1C	4.93	1.48	1.39
21	g	605	CHL	CHC-C1C	4.93	1.48	1.39
21	s	301	CHL	CHC-C1C	4.93	1.48	1.39
21	y	607	CHL	CHC-C1C	4.93	1.48	1.39
23	N	615	LUT	C26-C27	4.92	1.57	1.50
21	G	601	CHL	CHC-C1C	4.92	1.48	1.39
21	N	605	CHL	CHC-C1C	4.90	1.48	1.39
23	N	615	LUT	C28-C29	4.77	1.56	1.46
23	Y	614	LUT	C26-C27	4.71	1.57	1.50
23	Y	614	LUT	C28-C29	4.62	1.55	1.46
23	R	312	LUT	C12-C13	4.58	1.55	1.46
21	G	605	CHL	O2A-CGA	4.58	1.45	1.30
21	g	605	CHL	O2A-CGA	4.57	1.45	1.30
21	s	302	CHL	O2A-CGA	4.55	1.45	1.30
21	S	306	CHL	O2A-CGA	4.55	1.45	1.30
23	G	616	LUT	C28-C29	4.55	1.55	1.46
21	S	307	CHL	O2A-CGA	4.54	1.45	1.30
23	r	313	LUT	C12-C13	4.54	1.55	1.46
21	s	307	CHL	O2A-CGA	4.54	1.45	1.30
21	s	306	CHL	O2A-CGA	4.52	1.45	1.30
21	S	302	CHL	O2A-CGA	4.52	1.45	1.30
24	N	616	XAT	C4-C5	4.48	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	615	XAT	C4-C5	4.48	1.58	1.52
23	g	616	LUT	C28-C29	4.47	1.55	1.46
23	g	616	LUT	C26-C27	4.41	1.56	1.50
23	g	616	LUT	C12-C13	4.41	1.55	1.46
24	y	615	XAT	C15-C14	4.38	1.56	1.43
25	Y	616	NEX	C28-C29	4.38	1.55	1.46
24	Y	615	XAT	C15-C14	4.37	1.56	1.43
23	Y	614	LUT	C12-C13	4.37	1.55	1.46
24	Y	615	XAT	C31-C30	4.35	1.56	1.43
23	G	616	LUT	C12-C13	4.35	1.55	1.46
24	y	615	XAT	C31-C30	4.34	1.56	1.43
25	Y	616	NEX	C26-C27	4.34	1.58	1.50
24	Y	615	XAT	C35-C34	4.33	1.56	1.43
37	f	101	HEM	CHC-C1C	4.33	1.46	1.38
24	G	617	XAT	C15-C14	4.33	1.56	1.43
23	G	616	LUT	C26-C27	4.32	1.56	1.50
21	N	605	CHL	O2A-CGA	4.32	1.45	1.33
21	R	306	CHL	O2A-CGA	4.31	1.45	1.33
21	n	605	CHL	O2A-CGA	4.31	1.45	1.33
21	Y	606	CHL	O2A-CGA	4.31	1.45	1.33
21	g	601	CHL	O2A-CGA	4.31	1.45	1.33
21	r	308	CHL	O2A-CGA	4.30	1.45	1.33
21	y	609	CHL	O2A-CGA	4.30	1.45	1.33
21	R	307	CHL	O2A-CGA	4.30	1.45	1.33
21	N	608	CHL	O2A-CGA	4.30	1.45	1.33
24	g	617	XAT	C15-C14	4.30	1.56	1.43
21	Y	607	CHL	O2A-CGA	4.30	1.45	1.33
21	g	607	CHL	O2A-CGA	4.30	1.45	1.33
21	y	605	CHL	O2A-CGA	4.30	1.45	1.33
21	Y	601	CHL	O2A-CGA	4.30	1.45	1.33
23	N	615	LUT	C12-C13	4.30	1.55	1.46
21	G	606	CHL	O2A-CGA	4.30	1.45	1.33
21	g	606	CHL	O2A-CGA	4.29	1.45	1.33
21	n	606	CHL	O2A-CGA	4.29	1.45	1.33
21	G	601	CHL	O2A-CGA	4.29	1.45	1.33
21	n	608	CHL	O2A-CGA	4.29	1.45	1.33
21	r	307	CHL	O2A-CGA	4.29	1.45	1.33
24	G	617	XAT	C35-C34	4.29	1.56	1.43
21	r	306	CHL	O2A-CGA	4.29	1.45	1.33
21	r	301	CHL	O2A-CGA	4.29	1.45	1.33
21	S	301	CHL	O2A-CGA	4.29	1.45	1.33
21	y	606	CHL	O2A-CGA	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	607	CHL	O2A-CGA	4.29	1.45	1.33
21	Y	605	CHL	O2A-CGA	4.29	1.45	1.33
21	g	608	CHL	O2A-CGA	4.29	1.45	1.33
24	Y	615	XAT	C11-C10	4.29	1.56	1.43
37	F	101	HEM	CHC-C1C	4.28	1.46	1.38
21	n	607	CHL	O2A-CGA	4.28	1.45	1.33
21	g	609	CHL	O2A-CGA	4.28	1.45	1.33
21	y	607	CHL	O2A-CGA	4.28	1.45	1.33
21	G	609	CHL	O2A-CGA	4.28	1.45	1.33
21	Y	608	CHL	O2A-CGA	4.28	1.45	1.33
21	y	601	CHL	O2A-CGA	4.28	1.45	1.33
21	s	301	CHL	O2A-CGA	4.27	1.45	1.33
24	y	615	XAT	C35-C34	4.27	1.56	1.43
25	y	616	NEX	C11-C10	4.27	1.56	1.43
21	N	606	CHL	O2A-CGA	4.27	1.45	1.33
21	G	608	CHL	O2A-CGA	4.27	1.45	1.33
24	y	615	XAT	C11-C10	4.27	1.56	1.43
23	N	614	LUT	C28-C29	4.27	1.55	1.46
24	G	617	XAT	C11-C10	4.27	1.56	1.43
21	G	607	CHL	O2A-CGA	4.27	1.45	1.33
21	y	608	CHL	O2A-CGA	4.27	1.45	1.33
21	n	601	CHL	O2A-CGA	4.27	1.45	1.33
25	N	617	NEX	C11-C10	4.27	1.56	1.43
23	Y	613	LUT	C28-C29	4.27	1.55	1.46
24	G	617	XAT	C31-C30	4.27	1.56	1.43
21	R	305	CHL	O2A-CGA	4.26	1.45	1.33
23	r	313	LUT	C28-C29	4.26	1.55	1.46
24	R	313	XAT	C11-C10	4.26	1.56	1.43
21	N	601	CHL	O2A-CGA	4.26	1.45	1.33
24	g	617	XAT	C11-C10	4.26	1.56	1.43
25	r	315	NEX	C28-C29	4.26	1.55	1.46
23	G	615	LUT	C28-C29	4.25	1.55	1.46
25	Y	616	NEX	C11-C10	4.25	1.56	1.43
25	N	617	NEX	C26-C27	4.25	1.57	1.50
24	n	615	XAT	C15-C14	4.25	1.56	1.43
25	g	618	NEX	C26-C27	4.25	1.57	1.50
23	g	616	LUT	C15-C14	4.25	1.56	1.43
24	g	617	XAT	C31-C30	4.24	1.56	1.43
24	r	314	XAT	C11-C10	4.24	1.56	1.43
25	N	617	NEX	C28-C29	4.24	1.55	1.46
25	n	616	NEX	C11-C10	4.24	1.56	1.43
24	g	617	XAT	C35-C34	4.24	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	615	XAT	C31-C30	4.24	1.56	1.43
23	G	616	LUT	C15-C14	4.24	1.56	1.43
23	n	614	LUT	C28-C29	4.23	1.55	1.46
25	y	618	NEX	C28-C29	4.23	1.55	1.46
23	g	615	LUT	C28-C29	4.23	1.55	1.46
23	y	614	LUT	C28-C29	4.23	1.55	1.46
23	R	312	LUT	C28-C29	4.23	1.55	1.46
24	R	313	XAT	C31-C30	4.22	1.56	1.43
25	r	315	NEX	C26-C27	4.22	1.57	1.50
24	N	616	XAT	C15-C14	4.22	1.56	1.43
24	r	314	XAT	C31-C30	4.22	1.56	1.43
24	n	615	XAT	C11-C10	4.22	1.56	1.43
25	y	618	NEX	C11-C10	4.21	1.56	1.43
24	N	616	XAT	C31-C30	4.21	1.56	1.43
23	n	614	LUT	C12-C13	4.21	1.55	1.46
23	N	615	LUT	C8-C9	4.20	1.55	1.46
25	n	616	NEX	C26-C27	4.20	1.57	1.50
25	r	315	NEX	C11-C10	4.20	1.56	1.43
24	N	616	XAT	C11-C10	4.20	1.56	1.43
25	N	617	NEX	C15-C14	4.20	1.56	1.43
25	n	616	NEX	C28-C29	4.19	1.54	1.46
24	n	615	XAT	C35-C34	4.19	1.56	1.43
23	Y	613	LUT	C12-C13	4.19	1.54	1.46
25	n	616	NEX	C15-C14	4.19	1.56	1.43
23	G	615	LUT	C12-C13	4.19	1.54	1.46
25	N	617	NEX	C35-C34	4.19	1.56	1.43
23	N	614	LUT	C12-C13	4.19	1.54	1.46
25	g	618	NEX	C11-C10	4.18	1.56	1.43
25	y	616	NEX	C35-C34	4.18	1.56	1.43
23	Y	614	LUT	C8-C9	4.18	1.54	1.46
24	g	617	XAT	C4-C5	4.18	1.58	1.52
31	c	515	BCR	C1-C6	-4.18	1.48	1.53
25	y	616	NEX	C15-C14	4.17	1.56	1.43
25	g	618	NEX	C28-C29	4.17	1.54	1.46
31	C	516	BCR	C1-C6	-4.17	1.48	1.53
23	g	615	LUT	C12-C13	4.17	1.54	1.46
25	Y	616	NEX	C35-C34	4.17	1.56	1.43
23	y	614	LUT	C12-C13	4.17	1.54	1.46
25	y	618	NEX	C26-C27	4.16	1.57	1.50
23	N	615	LUT	C15-C14	4.16	1.56	1.43
24	r	314	XAT	C15-C14	4.16	1.56	1.43
25	n	616	NEX	C35-C34	4.15	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	313	XAT	C15-C14	4.15	1.56	1.43
23	Y	614	LUT	C15-C14	4.14	1.56	1.43
24	G	617	XAT	C4-C5	4.14	1.58	1.52
23	g	616	LUT	C8-C9	4.13	1.54	1.46
25	y	618	NEX	C35-C34	4.13	1.56	1.43
25	Y	616	NEX	C15-C14	4.13	1.56	1.43
25	g	618	NEX	C35-C34	4.12	1.56	1.43
25	r	315	NEX	C35-C34	4.12	1.56	1.43
25	g	618	NEX	C15-C14	4.12	1.55	1.43
24	R	313	XAT	C35-C34	4.10	1.55	1.43
31	c	516	BCR	C1-C6	-4.10	1.48	1.53
24	N	616	XAT	C35-C34	4.10	1.55	1.43
25	r	315	NEX	C15-C14	4.10	1.55	1.43
24	r	314	XAT	C35-C34	4.09	1.55	1.43
32	d	406	PL9	C3-C4	-4.09	1.43	1.49
25	y	618	NEX	C15-C14	4.08	1.55	1.43
25	y	616	NEX	C28-C29	4.08	1.54	1.46
23	G	616	LUT	C8-C9	4.07	1.54	1.46
31	C	517	BCR	C1-C6	-4.07	1.48	1.53
31	a	409	BCR	C1-C6	-4.07	1.48	1.53
25	N	617	NEX	C31-C30	4.06	1.55	1.43
32	D	407	PL9	C3-C4	-4.06	1.43	1.49
25	r	315	NEX	C31-C30	4.06	1.55	1.43
25	y	618	NEX	C31-C30	4.05	1.55	1.43
25	n	616	NEX	C31-C30	4.05	1.55	1.43
31	K	102	BCR	C1-C6	-4.05	1.48	1.53
31	k	102	BCR	C1-C6	-4.03	1.48	1.53
25	g	618	NEX	C31-C30	4.01	1.55	1.43
25	y	616	NEX	C26-C27	4.01	1.57	1.50
31	H	101	BCR	C1-C6	-4.01	1.48	1.53
23	G	616	LUT	C35-C34	4.00	1.55	1.43
31	C	516	BCR	C30-C25	-4.00	1.48	1.53
31	b	616	BCR	C1-C6	-4.00	1.48	1.53
31	b	616	BCR	C30-C25	-4.00	1.48	1.53
31	A	410	BCR	C1-C6	-4.00	1.48	1.53
25	y	616	NEX	C31-C30	4.00	1.55	1.43
23	G	616	LUT	C7-C6	4.00	1.58	1.45
24	Y	615	XAT	C26-C27	4.00	1.57	1.50
24	y	615	XAT	C32-C33	4.00	1.54	1.46
23	g	616	LUT	C7-C6	3.99	1.58	1.45
24	N	616	XAT	C26-C27	3.99	1.57	1.50
24	y	615	XAT	C4-C5	3.98	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	515	BCR	C30-C25	-3.98	1.48	1.53
24	Y	615	XAT	C32-C33	3.98	1.54	1.46
23	g	616	LUT	C35-C34	3.97	1.55	1.43
31	B	619	BCR	C30-C25	-3.97	1.48	1.53
31	B	619	BCR	C1-C6	-3.97	1.48	1.53
23	y	614	LUT	C15-C14	3.96	1.55	1.43
24	N	616	XAT	C28-C29	3.95	1.54	1.46
23	n	614	LUT	C15-C14	3.95	1.55	1.43
23	Y	614	LUT	C7-C6	3.95	1.58	1.45
23	N	614	LUT	C15-C14	3.95	1.55	1.43
23	r	313	LUT	C15-C14	3.94	1.55	1.43
31	D	406	BCR	C1-C6	-3.94	1.48	1.53
23	G	615	LUT	C15-C14	3.93	1.55	1.43
24	y	615	XAT	C26-C27	3.93	1.57	1.50
23	Y	614	LUT	C35-C34	3.93	1.55	1.43
23	g	615	LUT	C15-C14	3.93	1.55	1.43
24	Y	615	XAT	C4-C5	3.92	1.57	1.52
23	Y	613	LUT	C15-C14	3.92	1.55	1.43
24	Y	615	XAT	C8-C9	3.92	1.54	1.46
24	Y	615	XAT	C12-C13	3.92	1.54	1.46
31	h	101	BCR	C1-C6	-3.92	1.48	1.53
24	G	617	XAT	C32-C33	3.92	1.54	1.46
23	r	313	LUT	C26-C27	3.91	1.56	1.50
24	r	314	XAT	C4-C5	3.91	1.57	1.52
24	n	615	XAT	C32-C33	3.91	1.54	1.46
31	b	617	BCR	C1-C6	-3.91	1.48	1.53
31	d	405	BCR	C1-C6	-3.91	1.48	1.53
23	R	312	LUT	C15-C14	3.91	1.55	1.43
25	Y	616	NEX	C31-C30	3.91	1.55	1.43
24	R	313	XAT	C4-C5	3.90	1.57	1.52
24	g	617	XAT	C26-C27	3.90	1.57	1.50
24	Y	615	XAT	C28-C29	3.90	1.54	1.46
24	Y	615	XAT	C6-C7	3.90	1.57	1.50
31	c	516	BCR	C30-C25	-3.90	1.48	1.53
24	G	617	XAT	C28-C29	3.90	1.54	1.46
23	N	615	LUT	C35-C34	3.90	1.55	1.43
24	y	615	XAT	C28-C29	3.90	1.54	1.46
25	n	616	NEX	C32-C33	3.89	1.54	1.46
24	n	615	XAT	C26-C27	3.89	1.57	1.50
24	y	615	XAT	C12-C13	3.89	1.54	1.46
31	K	101	BCR	C1-C6	-3.89	1.48	1.53
23	R	312	LUT	C26-C27	3.89	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	517	BCR	C30-C25	-3.88	1.48	1.53
24	g	617	XAT	C6-C7	3.88	1.57	1.50
24	G	617	XAT	C26-C27	3.88	1.57	1.50
24	G	617	XAT	C8-C9	3.88	1.54	1.46
24	R	313	XAT	C28-C29	3.88	1.54	1.46
24	g	617	XAT	C32-C33	3.87	1.54	1.46
23	Y	613	LUT	C26-C27	3.87	1.56	1.50
25	y	616	NEX	C32-C33	3.87	1.54	1.46
24	g	617	XAT	C28-C29	3.87	1.54	1.46
31	B	620	BCR	C1-C6	-3.87	1.48	1.53
24	r	314	XAT	C28-C29	3.86	1.54	1.46
24	g	617	XAT	C8-C9	3.86	1.54	1.46
24	n	615	XAT	C28-C29	3.85	1.54	1.46
24	y	615	XAT	C8-C9	3.85	1.54	1.46
24	N	616	XAT	C32-C33	3.85	1.54	1.46
24	G	617	XAT	C12-C13	3.84	1.54	1.46
31	k	101	BCR	C1-C6	-3.84	1.48	1.53
23	G	615	LUT	C26-C27	3.84	1.56	1.50
23	n	614	LUT	C26-C27	3.84	1.56	1.50
24	R	313	XAT	C26-C27	3.83	1.57	1.50
24	y	615	XAT	C6-C7	3.83	1.57	1.50
24	r	314	XAT	C26-C27	3.83	1.57	1.50
30	d	401	PHO	C1D-C2D	3.83	1.43	1.39
24	G	617	XAT	C6-C7	3.82	1.57	1.50
23	g	615	LUT	C26-C27	3.82	1.56	1.50
24	R	313	XAT	C32-C33	3.82	1.54	1.46
24	N	616	XAT	C6-C7	3.82	1.57	1.50
31	A	410	BCR	C30-C25	-3.81	1.48	1.53
24	r	314	XAT	C32-C33	3.81	1.54	1.46
24	g	617	XAT	C12-C13	3.80	1.54	1.46
23	y	614	LUT	C26-C27	3.80	1.56	1.50
25	y	618	NEX	C32-C33	3.80	1.54	1.46
23	N	614	LUT	C26-C27	3.79	1.55	1.50
31	a	409	BCR	C30-C25	-3.78	1.48	1.53
31	d	405	BCR	C30-C25	-3.78	1.48	1.53
25	r	315	NEX	C32-C33	3.78	1.54	1.46
30	D	401	PHO	C1D-C2D	3.78	1.43	1.39
23	N	615	LUT	C7-C6	3.78	1.58	1.45
24	n	615	XAT	C6-C7	3.77	1.57	1.50
24	N	616	XAT	C12-C13	3.77	1.54	1.46
25	g	618	NEX	C32-C33	3.77	1.54	1.46
21	G	608	CHL	CHB-C4A	-3.76	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	617	NEX	C12-C13	3.76	1.54	1.46
24	n	615	XAT	C12-C13	3.76	1.54	1.46
24	r	314	XAT	C12-C13	3.76	1.54	1.46
22	Y	611	CLA	C3B-C4B	3.76	1.53	1.42
21	s	307	CHL	CHB-C4A	-3.75	1.34	1.38
25	n	616	NEX	C12-C13	3.75	1.54	1.46
21	g	601	CHL	CHB-C4A	-3.75	1.34	1.38
23	N	614	LUT	C35-C34	3.75	1.54	1.43
21	G	601	CHL	CHB-C4A	-3.75	1.34	1.38
23	n	614	LUT	C35-C34	3.75	1.54	1.43
23	y	614	LUT	C35-C34	3.74	1.54	1.43
22	n	612	CLA	C3B-C4B	3.74	1.53	1.42
25	Y	616	NEX	C12-C13	3.74	1.54	1.46
21	g	609	CHL	CHB-C4A	-3.74	1.34	1.38
25	y	616	NEX	C12-C13	3.74	1.54	1.46
30	A	408	PHO	C1D-C2D	3.74	1.43	1.39
21	y	601	CHL	CHB-C4A	-3.74	1.34	1.38
23	R	312	LUT	C35-C34	3.74	1.54	1.43
21	N	601	CHL	CHB-C4A	-3.73	1.34	1.38
23	g	615	LUT	C35-C34	3.73	1.54	1.43
23	G	615	LUT	C35-C34	3.73	1.54	1.43
22	G	613	CLA	C3B-C4B	3.73	1.53	1.42
30	a	407	PHO	C1D-C2D	3.73	1.43	1.39
22	N	612	CLA	C3B-C4B	3.73	1.53	1.42
24	n	615	XAT	C8-C9	3.73	1.53	1.46
22	y	612	CLA	C3B-C4B	3.73	1.53	1.42
24	R	313	XAT	C12-C13	3.73	1.53	1.46
21	n	608	CHL	CHB-C4A	-3.72	1.34	1.38
21	r	301	CHL	CHB-C4A	-3.72	1.34	1.38
31	D	406	BCR	C30-C25	-3.72	1.49	1.53
24	N	616	XAT	C8-C9	3.72	1.53	1.46
22	g	613	CLA	C3B-C4B	3.72	1.53	1.42
21	N	607	CHL	CHB-C4A	-3.72	1.34	1.38
21	r	308	CHL	CHB-C4A	-3.72	1.34	1.38
21	S	301	CHL	CHB-C4A	-3.71	1.34	1.38
21	S	302	CHL	CHB-C4A	-3.71	1.34	1.38
23	Y	613	LUT	C35-C34	3.71	1.54	1.43
25	y	618	NEX	C7-C8	3.71	1.37	1.31
21	S	306	CHL	CHB-C4A	-3.71	1.34	1.38
21	y	608	CHL	CHB-C4A	-3.71	1.34	1.38
21	Y	601	CHL	CHB-C4A	-3.70	1.34	1.38
21	s	301	CHL	CHB-C4A	-3.70	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	g	606	CHL	CHB-C4A	-3.70	1.34	1.38
21	G	606	CHL	CHB-C4A	-3.70	1.34	1.38
21	S	307	CHL	CHB-C4A	-3.70	1.34	1.38
21	y	605	CHL	CHB-C4A	-3.70	1.34	1.38
23	r	313	LUT	C35-C34	3.70	1.54	1.43
21	G	605	CHL	CHB-C4A	-3.70	1.34	1.38
21	r	307	CHL	CHB-C4A	-3.70	1.34	1.38
21	n	607	CHL	CHB-C4A	-3.70	1.34	1.38
23	N	615	LUT	C31-C30	3.70	1.54	1.43
21	y	607	CHL	CHB-C4A	-3.70	1.34	1.38
21	y	606	CHL	CHB-C4A	-3.70	1.34	1.38
21	N	608	CHL	CHB-C4A	-3.70	1.34	1.38
25	r	315	NEX	C7-C8	3.69	1.37	1.31
31	T	102	BCR	C1-C6	-3.69	1.49	1.53
21	N	606	CHL	CHB-C4A	-3.69	1.34	1.38
25	N	617	NEX	C32-C33	3.69	1.53	1.46
24	r	314	XAT	C8-C9	3.69	1.53	1.46
21	Y	607	CHL	CHB-C4A	-3.69	1.34	1.38
21	G	607	CHL	CHB-C4A	-3.69	1.34	1.38
21	R	306	CHL	CHB-C4A	-3.69	1.34	1.38
21	R	305	CHL	CHB-C4A	-3.69	1.34	1.38
21	Y	606	CHL	CHB-C4A	-3.68	1.34	1.38
24	R	313	XAT	C8-C9	3.68	1.53	1.46
22	C	511	CLA	C4B-NB	3.68	1.42	1.37
21	y	609	CHL	CHB-C4A	-3.68	1.34	1.38
21	n	606	CHL	CHB-C4A	-3.68	1.34	1.38
21	G	609	CHL	CHB-C4A	-3.67	1.34	1.38
21	N	605	CHL	CHB-C4A	-3.67	1.34	1.38
21	r	306	CHL	CHB-C4A	-3.67	1.34	1.38
21	Y	608	CHL	CHB-C4A	-3.67	1.34	1.38
21	g	607	CHL	CHB-C4A	-3.66	1.34	1.38
21	g	608	CHL	CHB-C4A	-3.66	1.34	1.38
31	B	602	BCR	C1-C6	-3.66	1.49	1.53
21	R	307	CHL	CHB-C4A	-3.66	1.34	1.38
22	c	510	CLA	C4B-NB	3.66	1.42	1.37
25	Y	616	NEX	C32-C33	3.66	1.53	1.46
21	s	302	CHL	CHB-C4A	-3.66	1.34	1.38
25	r	315	NEX	C12-C13	3.65	1.53	1.46
21	g	605	CHL	CHB-C4A	-3.65	1.34	1.38
21	Y	605	CHL	CHB-C4A	-3.65	1.34	1.38
21	n	605	CHL	CHB-C4A	-3.65	1.34	1.38
21	n	601	CHL	CHB-C4A	-3.64	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	s	306	CHL	CHB-C4A	-3.64	1.34	1.38
31	b	618	BCR	C1-C6	-3.64	1.49	1.53
25	y	618	NEX	C12-C13	3.64	1.53	1.46
23	g	616	LUT	C11-C10	3.63	1.54	1.43
31	B	620	BCR	C30-C25	-3.63	1.49	1.53
22	r	311	CLA	C1D-ND	3.63	1.42	1.37
31	b	617	BCR	C30-C25	-3.62	1.49	1.53
25	g	618	NEX	C12-C13	3.61	1.53	1.46
24	R	313	XAT	C6-C7	3.61	1.56	1.50
23	Y	614	LUT	C11-C10	3.61	1.54	1.43
23	G	616	LUT	C31-C30	3.61	1.54	1.43
23	G	616	LUT	C11-C10	3.61	1.54	1.43
24	r	314	XAT	C6-C7	3.60	1.56	1.50
23	g	616	LUT	C31-C30	3.59	1.54	1.43
32	D	407	PL9	C7-C3	-3.58	1.46	1.51
23	Y	614	LUT	C31-C30	3.55	1.54	1.43
23	Y	613	LUT	C8-C9	3.55	1.53	1.46
30	d	401	PHO	C4D-CHA	3.54	1.44	1.39
23	G	615	LUT	C8-C9	3.54	1.53	1.46
23	N	614	LUT	C8-C9	3.53	1.53	1.46
23	y	614	LUT	C8-C9	3.53	1.53	1.46
22	R	310	CLA	C1D-ND	3.53	1.42	1.37
22	S	308	CLA	C1D-ND	3.53	1.42	1.37
23	n	614	LUT	C8-C9	3.52	1.53	1.46
30	D	401	PHO	C4D-CHA	3.51	1.44	1.39
23	g	615	LUT	C8-C9	3.51	1.53	1.46
31	B	621	BCR	C1-C6	-3.51	1.49	1.53
31	K	101	BCR	C30-C25	-3.50	1.49	1.53
32	A	411	PL9	C3-C4	-3.49	1.44	1.49
31	B	602	BCR	C30-C25	-3.49	1.49	1.53
22	s	308	CLA	C1D-ND	3.49	1.42	1.37
32	a	410	PL9	C3-C4	-3.47	1.44	1.49
23	r	313	LUT	C8-C9	3.46	1.53	1.46
23	g	615	LUT	C31-C30	3.46	1.53	1.43
23	R	312	LUT	C8-C9	3.46	1.53	1.46
32	d	406	PL9	C7-C3	-3.46	1.46	1.51
23	Y	613	LUT	C31-C30	3.45	1.53	1.43
23	N	614	LUT	C31-C30	3.45	1.53	1.43
31	k	101	BCR	C30-C25	-3.44	1.49	1.53
31	T	102	BCR	C30-C25	-3.44	1.49	1.53
31	H	101	BCR	C30-C25	-3.43	1.49	1.53
23	R	312	LUT	C11-C10	3.43	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	309	CLA	C1D-ND	3.43	1.42	1.37
23	n	614	LUT	C31-C30	3.43	1.53	1.43
31	k	102	BCR	C30-C25	-3.42	1.49	1.53
23	G	615	LUT	C31-C30	3.42	1.53	1.43
30	A	408	PHO	C4D-CHA	3.42	1.44	1.39
23	r	313	LUT	C7-C6	3.42	1.56	1.45
22	C	513	CLA	C1D-ND	3.42	1.42	1.37
23	y	614	LUT	C31-C30	3.41	1.53	1.43
31	K	102	BCR	C30-C25	-3.41	1.49	1.53
23	R	312	LUT	C7-C6	3.41	1.56	1.45
23	r	313	LUT	C11-C10	3.41	1.53	1.43
22	n	611	CLA	C1D-ND	3.40	1.42	1.37
22	N	609	CLA	C1D-ND	3.39	1.42	1.37
22	s	309	CLA	C1D-ND	3.39	1.42	1.37
23	N	615	LUT	C32-C33	3.38	1.53	1.46
30	a	407	PHO	C4D-CHA	3.38	1.44	1.39
22	S	309	CLA	C1D-ND	3.38	1.42	1.37
23	N	615	LUT	C11-C10	3.38	1.53	1.43
23	R	312	LUT	C31-C30	3.38	1.53	1.43
22	r	311	CLA	C1B-C2B	3.38	1.51	1.43
31	B	621	BCR	C30-C25	-3.38	1.49	1.53
22	G	612	CLA	C1D-ND	3.37	1.42	1.37
22	r	303	CLA	C1D-ND	3.37	1.42	1.37
22	c	512	CLA	C1D-ND	3.37	1.42	1.37
23	g	615	LUT	C7-C6	3.36	1.56	1.45
22	R	310	CLA	C1B-C2B	3.36	1.51	1.43
22	R	302	CLA	C1D-ND	3.36	1.42	1.37
23	G	615	LUT	C7-C6	3.36	1.56	1.45
22	g	610	CLA	C1D-ND	3.36	1.42	1.37
22	y	611	CLA	C1D-ND	3.36	1.42	1.37
22	r	310	CLA	C1D-ND	3.36	1.42	1.37
22	N	611	CLA	C1D-ND	3.36	1.42	1.37
22	Y	612	CLA	C1D-ND	3.36	1.42	1.37
22	W	101	CLA	C1D-ND	3.36	1.42	1.37
22	N	613	CLA	C1D-ND	3.35	1.42	1.37
22	Y	602	CLA	C1D-ND	3.35	1.42	1.37
22	Y	609	CLA	C1D-ND	3.35	1.42	1.37
31	h	101	BCR	C30-C25	-3.35	1.49	1.53
22	R	308	CLA	C1D-ND	3.35	1.42	1.37
22	R	309	CLA	C1D-ND	3.35	1.42	1.37
31	b	618	BCR	C30-C25	-3.35	1.49	1.53
23	G	616	LUT	C32-C33	3.35	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	r	313	LUT	C31-C30	3.34	1.53	1.43
23	N	614	LUT	C7-C6	3.34	1.56	1.45
22	S	303	CLA	C1D-ND	3.34	1.42	1.37
23	G	615	LUT	C11-C10	3.34	1.53	1.43
23	g	616	LUT	C32-C33	3.34	1.53	1.46
23	Y	613	LUT	C7-C6	3.34	1.56	1.45
22	G	610	CLA	C1D-ND	3.34	1.42	1.37
22	n	609	CLA	C1D-ND	3.33	1.42	1.37
22	y	613	CLA	C1D-ND	3.33	1.42	1.37
22	G	614	CLA	C1D-ND	3.33	1.42	1.37
23	n	614	LUT	C7-C6	3.33	1.56	1.45
23	g	615	LUT	C11-C10	3.33	1.53	1.43
22	n	613	CLA	C1D-ND	3.33	1.42	1.37
22	w	101	CLA	C1D-ND	3.33	1.42	1.37
23	y	614	LUT	C7-C6	3.33	1.56	1.45
22	y	610	CLA	C1D-ND	3.32	1.42	1.37
23	n	614	LUT	C11-C10	3.32	1.53	1.43
22	S	313	CLA	C1D-ND	3.32	1.42	1.37
23	Y	613	LUT	C11-C10	3.32	1.53	1.43
22	r	312	CLA	C1D-ND	3.32	1.42	1.37
23	N	614	LUT	C11-C10	3.31	1.53	1.43
22	S	305	CLA	C1D-ND	3.31	1.42	1.37
22	y	602	CLA	C1D-ND	3.31	1.42	1.37
22	s	303	CLA	C1D-ND	3.31	1.42	1.37
22	S	304	CLA	C1D-ND	3.30	1.42	1.37
22	Y	610	CLA	C1D-ND	3.30	1.42	1.37
22	g	614	CLA	C1D-ND	3.30	1.42	1.37
22	n	610	CLA	C1D-ND	3.30	1.42	1.37
23	y	614	LUT	C11-C10	3.30	1.53	1.43
22	g	611	CLA	C1D-ND	3.30	1.42	1.37
22	g	602	CLA	C1D-ND	3.29	1.42	1.37
22	s	313	CLA	C1D-ND	3.29	1.42	1.37
22	N	602	CLA	C1D-ND	3.29	1.42	1.37
25	N	617	NEX	C7-C8	3.29	1.37	1.31
22	C	515	CLA	C1D-ND	3.29	1.42	1.37
22	g	612	CLA	C1D-ND	3.29	1.42	1.37
22	G	604	CLA	C1D-ND	3.29	1.42	1.37
22	R	303	CLA	C1D-ND	3.28	1.42	1.37
22	N	610	CLA	C1D-ND	3.28	1.42	1.37
22	s	310	CLA	C1D-ND	3.28	1.42	1.37
22	s	304	CLA	C1D-ND	3.28	1.42	1.37
22	c	507	CLA	C1D-ND	3.28	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	611	CLA	C1D-ND	3.27	1.42	1.37
22	c	514	CLA	C1D-ND	3.27	1.42	1.37
22	S	310	CLA	C1D-ND	3.27	1.42	1.37
22	s	312	CLA	C1D-ND	3.27	1.42	1.37
22	R	311	CLA	C1D-ND	3.26	1.42	1.37
22	B	612	CLA	C1D-ND	3.26	1.42	1.37
22	C	508	CLA	C1D-ND	3.26	1.42	1.37
37	f	101	HEM	CHB-C1B	3.25	1.45	1.38
22	S	311	CLA	C1D-ND	3.25	1.42	1.37
37	F	101	HEM	CHB-C1B	3.25	1.45	1.38
22	N	604	CLA	C1D-ND	3.24	1.42	1.37
22	s	305	CLA	C1D-ND	3.24	1.42	1.37
22	G	602	CLA	C1D-ND	3.24	1.42	1.37
23	Y	614	LUT	C32-C33	3.24	1.52	1.46
22	n	602	CLA	C1D-ND	3.24	1.42	1.37
22	C	512	CLA	C1D-ND	3.23	1.42	1.37
22	S	312	CLA	C1D-ND	3.22	1.42	1.37
22	C	509	CLA	C1D-ND	3.22	1.42	1.37
22	r	304	CLA	C1D-ND	3.22	1.42	1.37
22	A	409	CLA	C1D-ND	3.22	1.42	1.37
22	b	613	CLA	C1D-ND	3.22	1.42	1.37
22	b	606	CLA	C1D-ND	3.21	1.42	1.37
22	b	607	CLA	C1D-ND	3.21	1.42	1.37
22	A	407	CLA	C1D-ND	3.21	1.42	1.37
22	C	507	CLA	C1D-ND	3.21	1.42	1.37
22	n	604	CLA	C1D-ND	3.20	1.42	1.37
22	c	511	CLA	C1D-ND	3.20	1.42	1.37
22	c	508	CLA	C1D-ND	3.20	1.42	1.37
22	s	311	CLA	C1D-ND	3.20	1.42	1.37
22	B	609	CLA	C1D-ND	3.20	1.42	1.37
22	x	101	CLA	C1D-ND	3.19	1.42	1.37
22	y	604	CLA	C1D-ND	3.19	1.42	1.37
22	a	404	CLA	C1D-ND	3.19	1.42	1.37
22	c	506	CLA	C1D-ND	3.19	1.42	1.37
22	B	616	CLA	C1D-ND	3.18	1.42	1.37
22	b	609	CLA	C1D-ND	3.18	1.42	1.37
22	D	405	CLA	C1D-ND	3.18	1.42	1.37
22	a	406	CLA	C1D-ND	3.18	1.42	1.37
22	g	604	CLA	C1D-ND	3.17	1.42	1.37
22	s	308	CLA	C4B-NB	3.17	1.42	1.37
22	B	603	CLA	C1D-ND	3.17	1.42	1.37
22	b	601	CLA	C1D-ND	3.17	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	305	CLA	C1D-ND	3.17	1.42	1.37
22	b	608	CLA	C1D-ND	3.17	1.42	1.37
33	l	103	SQD	O48-C23	3.17	1.42	1.33
33	D	402	SQD	O48-C23	3.16	1.42	1.33
22	c	505	CLA	C1D-ND	3.16	1.42	1.37
33	L	101	SQD	O48-C23	3.16	1.42	1.33
22	b	611	CLA	C1D-ND	3.15	1.42	1.37
23	G	615	LUT	C32-C33	3.15	1.52	1.46
22	a	408	CLA	C1D-ND	3.15	1.42	1.37
22	B	617	CLA	C1D-ND	3.15	1.42	1.37
22	Y	604	CLA	C1D-ND	3.15	1.42	1.37
22	b	604	CLA	C1D-ND	3.15	1.42	1.37
22	B	610	CLA	C1D-ND	3.14	1.42	1.37
33	d	402	SQD	O48-C23	3.14	1.42	1.33
22	c	502	CLA	C1D-ND	3.14	1.42	1.37
22	B	604	CLA	C1D-ND	3.14	1.42	1.37
22	C	505	CLA	C1D-ND	3.14	1.42	1.37
22	B	607	CLA	C1D-ND	3.13	1.42	1.37
22	N	611	CLA	C4B-NB	3.13	1.42	1.37
22	b	614	CLA	C1D-ND	3.13	1.42	1.37
22	c	509	CLA	C1D-ND	3.13	1.42	1.37
22	d	404	CLA	C1D-ND	3.13	1.42	1.37
22	w	101	CLA	C4B-NB	3.13	1.42	1.37
22	b	610	CLA	C1D-ND	3.13	1.42	1.37
22	B	614	CLA	C1D-ND	3.13	1.42	1.37
22	S	308	CLA	C4B-NB	3.13	1.42	1.37
22	G	612	CLA	C4B-NB	3.13	1.42	1.37
22	a	405	CLA	C1D-ND	3.13	1.42	1.37
22	B	605	CLA	C1D-ND	3.13	1.42	1.37
22	B	606	CLA	C1D-ND	3.12	1.42	1.37
22	C	514	CLA	C1D-ND	3.12	1.42	1.37
23	Y	613	LUT	C32-C33	3.12	1.52	1.46
32	d	406	PL9	C6-C1	-3.12	1.43	1.48
22	S	304	CLA	C4B-NB	3.12	1.42	1.37
22	s	304	CLA	C4B-NB	3.12	1.42	1.37
22	B	615	CLA	C1D-ND	3.12	1.42	1.37
23	N	614	LUT	C32-C33	3.12	1.52	1.46
23	y	614	LUT	C32-C33	3.11	1.52	1.46
22	B	618	CLA	C1D-ND	3.11	1.42	1.37
22	B	613	CLA	C1D-ND	3.11	1.41	1.37
22	n	611	CLA	C4B-NB	3.11	1.41	1.37
22	b	602	CLA	C1D-ND	3.11	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	C1D-ND	3.11	1.41	1.37
23	g	615	LUT	C32-C33	3.11	1.52	1.46
22	b	615	CLA	C1D-ND	3.11	1.41	1.37
22	R	310	CLA	C4B-NB	3.10	1.41	1.37
25	n	616	NEX	C7-C8	3.10	1.36	1.31
22	g	603	CLA	C1D-ND	3.10	1.41	1.37
22	c	513	CLA	C1D-ND	3.10	1.41	1.37
25	y	616	NEX	C7-C8	3.10	1.36	1.31
22	c	504	CLA	C1D-ND	3.10	1.41	1.37
23	n	614	LUT	C32-C33	3.10	1.52	1.46
22	C	503	CLA	C1D-ND	3.10	1.41	1.37
22	A	406	CLA	C1D-ND	3.10	1.41	1.37
32	D	407	PL9	C6-C1	-3.09	1.43	1.48
22	b	612	CLA	C1D-ND	3.09	1.41	1.37
22	b	603	CLA	C1D-ND	3.09	1.41	1.37
22	C	506	CLA	C1D-ND	3.09	1.41	1.37
22	B	608	CLA	C1D-ND	3.09	1.41	1.37
22	Y	603	CLA	C1D-ND	3.08	1.41	1.37
22	s	303	CLA	C4B-NB	3.08	1.41	1.37
22	W	101	CLA	C4B-NB	3.08	1.41	1.37
22	B	611	CLA	C1D-ND	3.07	1.41	1.37
22	b	605	CLA	C1D-ND	3.07	1.41	1.37
22	C	510	CLA	C1D-ND	3.07	1.41	1.37
33	L	102	SQD	O48-C23	3.07	1.42	1.33
22	n	603	CLA	C1D-ND	3.06	1.41	1.37
22	R	304	CLA	C1D-ND	3.06	1.41	1.37
33	l	101	SQD	O48-C23	3.06	1.42	1.33
22	C	504	CLA	C1D-ND	3.06	1.41	1.37
33	a	411	SQD	O48-C23	3.06	1.42	1.33
33	A	412	SQD	O48-C23	3.06	1.42	1.33
22	g	610	CLA	C4B-NB	3.06	1.41	1.37
25	Y	616	NEX	C7-C8	3.06	1.36	1.31
22	G	610	CLA	C4B-NB	3.05	1.41	1.37
22	N	609	CLA	C4B-NB	3.05	1.41	1.37
22	N	603	CLA	C1D-ND	3.05	1.41	1.37
22	r	311	CLA	C4B-NB	3.05	1.41	1.37
22	g	612	CLA	C4B-NB	3.04	1.41	1.37
22	D	404	CLA	C1D-ND	3.04	1.41	1.37
32	A	411	PL9	C7-C3	-3.04	1.47	1.51
22	S	303	CLA	C4B-NB	3.04	1.41	1.37
22	c	503	CLA	C1D-ND	3.03	1.41	1.37
22	G	603	CLA	C1D-ND	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	309	CLA	C4B-NB	3.01	1.41	1.37
22	d	403	CLA	C1D-ND	3.01	1.41	1.37
22	x	101	CLA	C4B-NB	3.01	1.41	1.37
22	y	610	CLA	C4B-NB	3.00	1.41	1.37
22	y	603	CLA	C1D-ND	2.99	1.41	1.37
32	a	410	PL9	C7-C3	-2.99	1.47	1.51
22	s	312	CLA	C4B-NB	2.98	1.41	1.37
22	Y	609	CLA	C4B-NB	2.98	1.41	1.37
22	B	603	CLA	C4B-NB	2.98	1.41	1.37
35	J	101	DGD	O2G-C2G	-2.97	1.39	1.46
35	c	519	DGD	O2G-C2G	-2.96	1.39	1.46
22	r	310	CLA	C4B-NB	2.95	1.41	1.37
22	S	312	CLA	C4B-NB	2.95	1.41	1.37
23	r	313	LUT	C32-C33	2.95	1.52	1.46
22	n	609	CLA	C4B-NB	2.95	1.41	1.37
22	r	312	CLA	C4B-NB	2.95	1.41	1.37
22	N	612	CLA	C1D-ND	2.93	1.41	1.37
25	g	618	NEX	C7-C8	2.93	1.36	1.31
22	R	311	CLA	C4B-NB	2.92	1.41	1.37
22	y	612	CLA	C1D-ND	2.92	1.41	1.37
22	n	612	CLA	C1D-ND	2.91	1.41	1.37
22	B	611	CLA	C4B-NB	2.91	1.41	1.37
23	R	312	LUT	C32-C33	2.91	1.52	1.46
24	n	615	XAT	C2-C1	-2.91	1.50	1.54
22	S	311	CLA	C4B-NB	2.91	1.41	1.37
22	Y	611	CLA	C1D-ND	2.90	1.41	1.37
22	g	613	CLA	C1D-ND	2.90	1.41	1.37
24	G	617	XAT	C2-C1	-2.90	1.50	1.54
22	s	305	CLA	C4B-NB	2.89	1.41	1.37
24	g	617	XAT	C2-C1	-2.89	1.50	1.54
22	g	614	CLA	C4B-NB	2.88	1.41	1.37
35	C	518	DGD	O2G-C2G	-2.88	1.39	1.46
33	l	103	SQD	O47-C7	2.88	1.42	1.34
22	r	304	CLA	C4B-NB	2.88	1.41	1.37
35	c	517	DGD	O2G-C2G	-2.88	1.39	1.46
37	F	101	HEM	CAB-C3B	2.87	1.55	1.47
22	d	404	CLA	C4B-NB	2.87	1.41	1.37
33	L	101	SQD	O47-C7	2.87	1.42	1.34
22	y	613	CLA	C4B-NB	2.86	1.41	1.37
22	G	611	CLA	C4B-NB	2.86	1.41	1.37
33	D	402	SQD	O47-C7	2.86	1.42	1.34
33	A	412	SQD	O47-C7	2.85	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	617	LHG	O7-C5	-2.85	1.39	1.46
22	a	406	CLA	C4B-NB	2.85	1.41	1.37
22	R	308	CLA	C4B-NB	2.85	1.41	1.37
22	n	613	CLA	C4B-NB	2.85	1.41	1.37
22	G	613	CLA	C1D-ND	2.85	1.41	1.37
22	D	405	CLA	C4B-NB	2.85	1.41	1.37
30	a	407	PHO	CMC-C2C	-2.85	1.46	1.50
33	d	402	SQD	O47-C7	2.85	1.42	1.34
30	A	408	PHO	CMC-C2C	-2.85	1.46	1.50
22	b	608	CLA	C4B-NB	2.85	1.41	1.37
22	N	613	CLA	C4B-NB	2.84	1.41	1.37
22	s	311	CLA	C4B-NB	2.84	1.41	1.37
22	Y	610	CLA	C4B-NB	2.84	1.41	1.37
22	R	302	CLA	C4B-NB	2.84	1.41	1.37
22	R	303	CLA	C4B-NB	2.83	1.41	1.37
22	N	603	CLA	C4B-NB	2.83	1.41	1.37
22	r	303	CLA	C4B-NB	2.83	1.41	1.37
22	g	611	CLA	C4B-NB	2.83	1.41	1.37
37	f	101	HEM	CAB-C3B	2.83	1.54	1.47
22	c	511	CLA	C4B-NB	2.83	1.41	1.37
22	n	610	CLA	C4B-NB	2.82	1.41	1.37
33	a	411	SQD	O47-C7	2.82	1.42	1.34
36	b	620	LMG	C21-C20	2.82	1.65	1.51
22	Y	612	CLA	C4B-NB	2.82	1.41	1.37
24	y	615	XAT	C2-C1	-2.81	1.50	1.54
22	A	407	CLA	C4B-NB	2.81	1.41	1.37
22	W	101	CLA	C1B-C2B	2.81	1.49	1.43
37	F	101	HEM	CAC-C3C	2.81	1.54	1.47
36	B	623	LMG	C21-C20	2.81	1.65	1.51
22	g	603	CLA	C4B-NB	2.81	1.41	1.37
22	y	602	CLA	C4B-NB	2.81	1.41	1.37
22	S	305	CLA	C4B-NB	2.81	1.41	1.37
24	r	314	XAT	C2-C1	-2.80	1.50	1.54
22	y	611	CLA	C4B-NB	2.80	1.41	1.37
22	N	612	CLA	C4B-NB	2.80	1.41	1.37
37	f	101	HEM	CAC-C3C	2.80	1.54	1.47
22	N	611	CLA	C1B-C2B	2.80	1.49	1.43
22	Y	602	CLA	C4B-NB	2.80	1.41	1.37
35	c	518	DGD	O2G-C2G	-2.80	1.40	1.46
22	G	602	CLA	C4B-NB	2.80	1.41	1.37
22	C	512	CLA	C4B-NB	2.80	1.41	1.37
22	r	309	CLA	C4B-NB	2.80	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	603	CLA	C4B-NB	2.80	1.41	1.37
22	S	309	CLA	C4B-NB	2.79	1.41	1.37
22	N	602	CLA	C4B-NB	2.79	1.41	1.37
22	d	403	CLA	C4B-NB	2.79	1.41	1.37
30	D	401	PHO	CMC-C2C	-2.79	1.46	1.50
30	d	401	PHO	CMC-C2C	-2.79	1.46	1.50
22	n	603	CLA	C4B-NB	2.79	1.41	1.37
22	y	603	CLA	C4B-NB	2.79	1.41	1.37
22	n	612	CLA	C4B-NB	2.79	1.41	1.37
24	Y	615	XAT	C2-C1	-2.79	1.50	1.54
22	G	614	CLA	C4B-NB	2.78	1.41	1.37
22	C	506	CLA	C4B-NB	2.78	1.41	1.37
22	Y	603	CLA	C4B-NB	2.78	1.41	1.37
22	s	309	CLA	C4B-NB	2.78	1.41	1.37
22	c	506	CLA	C4B-NB	2.77	1.41	1.37
22	g	612	CLA	C1B-C2B	2.77	1.49	1.43
22	w	101	CLA	C1B-C2B	2.77	1.49	1.43
22	N	610	CLA	C4B-NB	2.77	1.41	1.37
22	n	611	CLA	C1B-C2B	2.77	1.49	1.43
22	r	305	CLA	C4B-NB	2.77	1.41	1.37
22	y	612	CLA	C4B-NB	2.77	1.41	1.37
22	C	507	CLA	C4B-NB	2.77	1.41	1.37
35	C	519	DGD	O2G-C2G	-2.77	1.40	1.46
22	B	618	CLA	C4B-NB	2.77	1.41	1.37
22	g	613	CLA	C4B-NB	2.76	1.41	1.37
22	B	615	CLA	C4B-NB	2.76	1.41	1.37
23	N	615	LUT	C8-C7	2.76	1.41	1.33
22	b	612	CLA	C4B-NB	2.76	1.41	1.37
22	S	313	CLA	C4B-NB	2.76	1.41	1.37
22	Y	611	CLA	C4B-NB	2.76	1.41	1.37
22	G	612	CLA	C1B-C2B	2.76	1.49	1.43
22	G	613	CLA	C4B-NB	2.75	1.41	1.37
33	l	101	SQD	O47-C7	2.75	1.42	1.34
25	r	315	NEX	C38-C25	2.75	1.55	1.51
22	b	610	CLA	C4B-NB	2.75	1.41	1.37
22	C	515	CLA	C4B-NB	2.75	1.41	1.37
22	a	404	CLA	C4B-NB	2.74	1.41	1.37
22	B	613	CLA	C4B-NB	2.74	1.41	1.37
22	D	404	CLA	C4B-NB	2.74	1.41	1.37
22	n	602	CLA	C4B-NB	2.74	1.41	1.37
32	D	407	PL9	C53-C6	-2.74	1.45	1.50
33	L	102	SQD	O47-C7	2.74	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	C4B-NB	2.74	1.41	1.37
22	R	304	CLA	C1B-C2B	2.73	1.49	1.43
35	h	102	DGD	O2G-C2G	-2.73	1.40	1.46
24	N	616	XAT	C2-C1	-2.73	1.50	1.54
22	g	602	CLA	C4B-NB	2.73	1.41	1.37
22	B	617	CLA	C4B-NB	2.73	1.41	1.37
22	s	313	CLA	C4B-NB	2.73	1.41	1.37
24	R	313	XAT	C2-C1	-2.72	1.50	1.54
22	B	608	CLA	C4B-NB	2.72	1.41	1.37
22	c	505	CLA	C4B-NB	2.72	1.41	1.37
26	y	617	LHG	O7-C5	-2.72	1.40	1.46
22	c	514	CLA	C4B-NB	2.72	1.41	1.37
22	R	304	CLA	C4B-NB	2.72	1.41	1.37
30	a	407	PHO	CAC-C3C	-2.71	1.46	1.51
32	d	406	PL9	C53-C6	-2.71	1.45	1.50
21	g	606	CHL	C3A-C2A	-2.71	1.52	1.54
22	B	607	CLA	C4B-NB	2.71	1.41	1.37
22	C	510	CLA	C4B-NB	2.71	1.41	1.37
30	A	408	PHO	CAC-C3C	-2.71	1.46	1.51
22	b	605	CLA	C4B-NB	2.71	1.41	1.37
22	b	614	CLA	C4B-NB	2.71	1.41	1.37
35	H	102	DGD	O2G-C2G	-2.71	1.40	1.46
22	c	507	CLA	C4B-NB	2.70	1.41	1.37
22	b	606	CLA	C4B-NB	2.70	1.41	1.37
22	r	305	CLA	C1B-C2B	2.70	1.49	1.43
22	b	611	CLA	C4B-NB	2.70	1.41	1.37
21	N	606	CHL	C3A-C2A	-2.70	1.52	1.54
26	d	408	LHG	O7-C5	-2.69	1.40	1.46
22	A	405	CLA	C4B-NB	2.69	1.41	1.37
22	B	609	CLA	C4B-NB	2.69	1.41	1.37
26	n	617	LHG	O7-C5	-2.69	1.40	1.46
22	C	513	CLA	C4B-NB	2.69	1.41	1.37
21	n	605	CHL	C3A-C2A	-2.69	1.52	1.54
22	C	503	CLA	C4B-NB	2.69	1.41	1.37
21	g	601	CHL	C3A-C2A	-2.69	1.52	1.54
26	D	409	LHG	O7-C5	-2.69	1.40	1.46
25	y	618	NEX	C38-C25	2.69	1.55	1.51
21	R	305	CHL	C3A-C2A	-2.69	1.52	1.54
22	B	616	CLA	C4B-NB	2.68	1.41	1.37
21	N	605	CHL	C3A-C2A	-2.68	1.52	1.54
22	B	614	CLA	C4B-NB	2.68	1.41	1.37
22	b	603	CLA	C4B-NB	2.68	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	407	PHO	CMD-C2D	-2.68	1.46	1.51
22	B	606	CLA	C4B-NB	2.68	1.41	1.37
22	b	613	CLA	C4B-NB	2.68	1.41	1.37
21	S	307	CHL	C3A-C2A	-2.68	1.52	1.54
21	N	601	CHL	C3A-C2A	-2.68	1.52	1.54
21	r	307	CHL	C3A-C2A	-2.67	1.52	1.54
21	s	302	CHL	C3A-C2A	-2.67	1.52	1.54
22	S	310	CLA	C4B-NB	2.67	1.41	1.37
25	Y	616	NEX	C38-C25	2.67	1.55	1.51
22	C	515	CLA	C1B-C2B	2.66	1.49	1.43
21	S	306	CHL	C3A-C2A	-2.66	1.52	1.54
26	l	102	LHG	O7-C5	-2.66	1.40	1.46
21	N	608	CHL	C3A-C2A	-2.66	1.52	1.54
21	r	301	CHL	C3A-C2A	-2.66	1.52	1.54
21	N	607	CHL	C3A-C2A	-2.66	1.52	1.54
22	a	408	CLA	C4B-NB	2.66	1.41	1.37
26	G	618	LHG	O7-C5	-2.66	1.40	1.46
21	Y	607	CHL	C3A-C2A	-2.65	1.52	1.54
21	g	605	CHL	C3A-C2A	-2.65	1.52	1.54
22	b	615	CLA	C4B-NB	2.65	1.41	1.37
22	b	607	CLA	C4B-NB	2.65	1.41	1.37
21	g	607	CHL	C3A-C2A	-2.65	1.52	1.54
36	w	102	LMG	O7-C8	-2.65	1.40	1.46
21	S	301	CHL	C3A-C2A	-2.65	1.52	1.54
21	y	607	CHL	C3A-C2A	-2.65	1.52	1.54
22	S	305	CLA	C1B-C2B	2.65	1.49	1.43
22	r	303	CLA	C1B-C2B	2.64	1.49	1.43
30	A	408	PHO	CMD-C2D	-2.64	1.46	1.51
22	c	513	CLA	C4B-NB	2.64	1.41	1.37
22	C	508	CLA	C4B-NB	2.64	1.41	1.37
22	S	312	CLA	C1B-C2B	2.64	1.49	1.43
36	C	502	LMG	O7-C8	-2.64	1.40	1.46
22	c	514	CLA	C1B-C2B	2.63	1.49	1.43
26	L	103	LHG	O7-C5	-2.63	1.40	1.46
22	N	609	CLA	C1B-C2B	2.63	1.49	1.43
22	R	302	CLA	C1B-C2B	2.63	1.49	1.43
22	b	604	CLA	C4B-NB	2.63	1.41	1.37
35	h	102	DGD	O5D-C6D	-2.63	1.39	1.43
21	S	302	CHL	C3A-C2A	-2.63	1.52	1.54
21	G	607	CHL	C3A-C2A	-2.63	1.52	1.54
22	B	608	CLA	C1B-C2B	2.62	1.49	1.43
21	r	308	CHL	C3A-C2A	-2.62	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	508	CLA	C4B-NB	2.62	1.41	1.37
21	y	601	CHL	C3A-C2A	-2.62	1.52	1.54
22	s	312	CLA	C1B-C2B	2.62	1.49	1.43
21	s	307	CHL	C3A-C2A	-2.62	1.52	1.54
22	y	610	CLA	C1B-C2B	2.62	1.49	1.43
30	a	407	PHO	CMB-C2B	-2.62	1.46	1.51
21	s	301	CHL	C3A-C2A	-2.62	1.52	1.54
35	c	517	DGD	O1G-C1G	-2.62	1.39	1.45
21	n	607	CHL	C3A-C2A	-2.62	1.52	1.54
22	s	305	CLA	C1B-C2B	2.62	1.49	1.43
22	c	505	CLA	C1B-C2B	2.61	1.49	1.43
22	Y	602	CLA	C1B-C2B	2.61	1.49	1.43
22	Y	604	CLA	C1B-C2B	2.61	1.49	1.43
22	r	309	CLA	C1B-C2B	2.61	1.49	1.43
26	d	409	LHG	O7-C5	-2.61	1.40	1.46
21	G	601	CHL	C3A-C2A	-2.61	1.52	1.54
21	Y	605	CHL	C3A-C2A	-2.61	1.52	1.54
22	c	512	CLA	C4B-NB	2.61	1.41	1.37
35	c	519	DGD	O1G-C1G	-2.61	1.39	1.45
22	R	308	CLA	C1B-C2B	2.61	1.49	1.43
22	n	613	CLA	C1B-C2B	2.61	1.49	1.43
21	R	307	CHL	C3A-C2A	-2.61	1.52	1.54
22	n	609	CLA	C1B-C2B	2.61	1.49	1.43
22	b	609	CLA	C4B-NB	2.61	1.41	1.37
22	s	304	CLA	C1B-C2B	2.61	1.49	1.43
23	G	616	LUT	C8-C7	2.60	1.40	1.33
21	y	608	CHL	C3A-C2A	-2.60	1.52	1.54
21	n	601	CHL	C3A-C2A	-2.60	1.52	1.54
22	b	601	CLA	C4B-NB	2.60	1.41	1.37
22	B	612	CLA	C4B-NB	2.60	1.41	1.37
22	g	610	CLA	C1B-C2B	2.60	1.49	1.43
22	G	610	CLA	C1B-C2B	2.60	1.49	1.43
22	B	616	CLA	C1B-C2B	2.60	1.49	1.43
35	J	101	DGD	O1G-C1G	-2.60	1.39	1.45
22	C	504	CLA	C4B-NB	2.60	1.41	1.37
26	D	410	LHG	O7-C5	-2.60	1.40	1.46
21	g	609	CHL	C3A-C2A	-2.60	1.52	1.54
22	r	312	CLA	C1B-C2B	2.60	1.49	1.43
22	C	511	CLA	CMD-C2D	-2.60	1.45	1.50
22	Y	609	CLA	C1B-C2B	2.60	1.49	1.43
22	S	304	CLA	C1B-C2B	2.60	1.49	1.43
35	H	102	DGD	O5D-C6D	-2.60	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	r	306	CHL	C3A-C2A	-2.60	1.52	1.54
21	n	606	CHL	C3A-C2A	-2.60	1.52	1.54
21	y	609	CHL	C3A-C2A	-2.60	1.52	1.54
21	y	606	CHL	C3A-C2A	-2.60	1.52	1.54
23	Y	614	LUT	C8-C7	2.60	1.40	1.33
30	d	401	PHO	CMD-C2D	-2.59	1.46	1.51
22	b	605	CLA	C1B-C2B	2.59	1.49	1.43
22	d	404	CLA	C1B-C2B	2.59	1.49	1.43
22	A	406	CLA	C4B-NB	2.59	1.41	1.37
21	s	306	CHL	C3A-C2A	-2.59	1.52	1.54
22	C	506	CLA	C1B-C2B	2.59	1.49	1.43
21	G	606	CHL	C3A-C2A	-2.59	1.52	1.54
22	B	604	CLA	C4B-NB	2.59	1.41	1.37
22	g	614	CLA	C1B-C2B	2.59	1.49	1.43
22	R	311	CLA	C1B-C2B	2.59	1.49	1.43
35	C	518	DGD	O1G-C1G	-2.59	1.39	1.45
22	b	615	CLA	C1B-C2B	2.59	1.49	1.43
26	D	408	LHG	O7-C5	-2.59	1.40	1.46
22	A	409	CLA	C4B-NB	2.58	1.41	1.37
22	C	509	CLA	C4B-NB	2.58	1.41	1.37
22	A	406	CLA	C1B-C2B	2.58	1.49	1.43
22	y	602	CLA	C1B-C2B	2.58	1.49	1.43
22	s	310	CLA	C4B-NB	2.58	1.41	1.37
26	d	407	LHG	O7-C5	-2.58	1.40	1.46
22	N	602	CLA	C1B-C2B	2.58	1.49	1.43
22	B	603	CLA	C1B-C2B	2.58	1.49	1.43
22	b	606	CLA	C1B-C2B	2.58	1.49	1.43
22	r	310	CLA	C1B-C2B	2.58	1.49	1.43
22	y	613	CLA	C1B-C2B	2.58	1.49	1.43
22	g	602	CLA	C1B-C2B	2.58	1.49	1.43
22	c	507	CLA	C1B-C2B	2.58	1.49	1.43
21	y	605	CHL	C3A-C2A	-2.58	1.52	1.54
23	g	616	LUT	C8-C7	2.58	1.40	1.33
22	g	604	CLA	C1B-C2B	2.58	1.49	1.43
22	Y	612	CLA	C1B-C2B	2.58	1.49	1.43
22	B	610	CLA	C4B-NB	2.57	1.41	1.37
22	c	510	CLA	CMD-C2D	-2.57	1.45	1.50
22	B	609	CLA	C1B-C2B	2.57	1.49	1.43
22	N	613	CLA	C1B-C2B	2.57	1.49	1.43
22	S	309	CLA	C1B-C2B	2.57	1.49	1.43
22	B	618	CLA	C1B-C2B	2.57	1.49	1.43
21	Y	601	CHL	C3A-C2A	-2.57	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	n	602	CLA	C1B-C2B	2.57	1.49	1.43
22	y	604	CLA	C1B-C2B	2.57	1.49	1.43
22	N	604	CLA	C1B-C2B	2.57	1.49	1.43
22	C	507	CLA	C1B-C2B	2.57	1.49	1.43
22	D	405	CLA	C1B-C2B	2.57	1.49	1.43
22	c	502	CLA	C4B-NB	2.57	1.41	1.37
22	C	514	CLA	C4B-NB	2.57	1.41	1.37
22	C	504	CLA	C1B-C2B	2.57	1.49	1.43
22	G	604	CLA	C1B-C2B	2.56	1.49	1.43
21	G	609	CHL	C3A-C2A	-2.56	1.52	1.54
30	d	401	PHO	CAC-C3C	-2.56	1.47	1.51
22	G	602	CLA	C1B-C2B	2.56	1.49	1.43
22	a	405	CLA	C4B-NB	2.56	1.41	1.37
30	D	401	PHO	CMD-C2D	-2.56	1.46	1.51
22	n	604	CLA	C1B-C2B	2.56	1.49	1.43
21	G	608	CHL	C3A-C2A	-2.56	1.52	1.54
22	G	614	CLA	C1B-C2B	2.56	1.49	1.43
22	s	309	CLA	C1B-C2B	2.56	1.49	1.43
21	G	605	CHL	C3A-C2A	-2.55	1.52	1.54
22	b	604	CLA	C1B-C2B	2.55	1.49	1.43
22	c	506	CLA	C1B-C2B	2.55	1.49	1.43
22	R	309	CLA	C1B-C2B	2.55	1.49	1.43
22	b	601	CLA	C1B-C2B	2.55	1.49	1.43
22	s	308	CLA	C1B-C2B	2.55	1.49	1.43
22	S	313	CLA	C1B-C2B	2.55	1.49	1.43
22	C	514	CLA	C1B-C2B	2.55	1.49	1.43
22	C	513	CLA	C1B-C2B	2.55	1.49	1.43
22	R	303	CLA	C1B-C2B	2.55	1.49	1.43
21	Y	608	CHL	C3A-C2A	-2.55	1.52	1.54
21	g	608	CHL	C3A-C2A	-2.55	1.52	1.54
22	r	304	CLA	C1B-C2B	2.55	1.49	1.43
22	S	310	CLA	C1B-C2B	2.55	1.49	1.43
22	Y	610	CLA	C1B-C2B	2.55	1.49	1.43
22	c	504	CLA	C4B-NB	2.54	1.41	1.37
26	c	521	LHG	O7-C5	-2.54	1.40	1.46
35	c	518	DGD	O1G-C1G	-2.54	1.39	1.45
22	b	613	CLA	C1B-C2B	2.54	1.49	1.43
22	B	607	CLA	C1B-C2B	2.54	1.49	1.43
22	c	503	CLA	C1B-C2B	2.54	1.49	1.43
22	G	611	CLA	C1B-C2B	2.54	1.49	1.43
22	x	101	CLA	C1B-C2B	2.54	1.49	1.43
22	a	405	CLA	C1B-C2B	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	408	PHO	CMB-C2B	-2.54	1.46	1.51
22	N	610	CLA	C1B-C2B	2.54	1.49	1.43
22	B	606	CLA	C1B-C2B	2.54	1.49	1.43
22	B	611	CLA	C1B-C2B	2.54	1.49	1.43
22	c	503	CLA	C4B-NB	2.54	1.41	1.37
22	C	508	CLA	C1B-C2B	2.54	1.49	1.43
22	s	310	CLA	C1B-C2B	2.54	1.49	1.43
23	r	313	LUT	C4-C5	2.53	1.55	1.51
22	A	405	CLA	C1B-C2B	2.53	1.49	1.43
22	S	308	CLA	C1B-C2B	2.53	1.49	1.43
22	n	610	CLA	C1B-C2B	2.53	1.49	1.43
22	A	409	CLA	C1B-C2B	2.53	1.49	1.43
22	c	513	CLA	C1B-C2B	2.53	1.49	1.43
22	b	614	CLA	C1B-C2B	2.52	1.49	1.43
35	H	102	DGD	O1G-C1G	-2.52	1.39	1.45
22	c	512	CLA	C1B-C2B	2.52	1.49	1.43
21	R	306	CHL	C3A-C2A	-2.52	1.52	1.54
22	S	311	CLA	C1B-C2B	2.52	1.49	1.43
22	s	313	CLA	C1B-C2B	2.52	1.49	1.43
35	C	519	DGD	O1G-C1G	-2.52	1.39	1.45
22	a	406	CLA	C1B-C2B	2.52	1.49	1.43
24	G	617	XAT	O24-C25	2.52	1.49	1.46
22	B	605	CLA	C4B-NB	2.52	1.41	1.37
22	b	607	CLA	C1B-C2B	2.52	1.49	1.43
22	B	604	CLA	C1B-C2B	2.52	1.49	1.43
26	C	521	LHG	O7-C5	-2.51	1.40	1.46
22	C	505	CLA	C4B-NB	2.51	1.41	1.37
21	n	608	CHL	C3A-C2A	-2.51	1.52	1.54
22	b	603	CLA	C1B-C2B	2.51	1.49	1.43
22	c	504	CLA	C1B-C2B	2.51	1.49	1.43
22	C	510	CLA	CMB-C2B	-2.51	1.45	1.50
30	D	401	PHO	CAC-C3C	-2.51	1.47	1.51
24	n	615	XAT	O24-C25	2.51	1.49	1.46
22	C	511	CLA	C3C-C2C	2.51	1.42	1.36
22	B	618	CLA	MG-NB	-2.51	2.00	2.05
21	Y	606	CHL	C3A-C2A	-2.51	1.52	1.54
22	a	408	CLA	C1B-C2B	2.51	1.49	1.43
22	c	513	CLA	MG-NB	-2.51	2.00	2.05
22	g	611	CLA	C1B-C2B	2.51	1.49	1.43
22	B	613	CLA	C1B-C2B	2.51	1.49	1.43
22	B	610	CLA	C1B-C2B	2.51	1.49	1.43
22	y	611	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	C1B-C2B	2.51	1.49	1.43
22	C	509	CLA	C1B-C2B	2.50	1.49	1.43
22	b	602	CLA	C4B-NB	2.50	1.41	1.37
22	C	505	CLA	C1B-C2B	2.50	1.49	1.43
23	R	312	LUT	C4-C5	2.50	1.54	1.51
35	a	413	DGD	O2G-C2G	-2.50	1.40	1.46
22	b	609	CLA	C1B-C2B	2.50	1.49	1.43
22	b	602	CLA	C1B-C2B	2.50	1.49	1.43
22	n	603	CLA	C1B-C2B	2.50	1.49	1.43
22	C	510	CLA	MG-NB	-2.50	2.00	2.05
22	a	404	CLA	C1B-C2B	2.50	1.49	1.43
22	c	510	CLA	C3C-C2C	2.50	1.42	1.36
35	A	401	DGD	O2G-C2G	-2.49	1.40	1.46
22	c	508	CLA	C1B-C2B	2.49	1.49	1.43
30	D	401	PHO	CMB-C2B	-2.49	1.46	1.51
22	C	512	CLA	C1B-C2B	2.49	1.49	1.43
24	g	617	XAT	O24-C25	2.49	1.49	1.46
22	a	408	CLA	MG-NB	-2.49	2.00	2.05
22	A	407	CLA	C1B-C2B	2.49	1.49	1.43
22	B	617	CLA	MG-NB	-2.49	2.00	2.05
22	N	603	CLA	C1B-C2B	2.49	1.49	1.43
22	b	608	CLA	C1B-C2B	2.49	1.49	1.43
22	C	511	CLA	CHC-C1C	2.49	1.43	1.38
35	h	102	DGD	O1G-C1G	-2.49	1.39	1.45
22	B	617	CLA	C1B-C2B	2.48	1.49	1.43
22	s	311	CLA	C1B-C2B	2.48	1.49	1.43
22	N	604	CLA	MG-NB	-2.48	2.00	2.05
22	C	504	CLA	MG-NB	-2.48	2.00	2.05
22	C	514	CLA	MG-NB	-2.48	2.00	2.05
22	c	509	CLA	MG-NB	-2.48	2.00	2.05
22	b	610	CLA	C1B-C2B	2.48	1.48	1.43
22	G	603	CLA	C1B-C2B	2.48	1.48	1.43
22	b	602	CLA	MG-NB	-2.48	2.00	2.05
22	c	511	CLA	C1B-C2B	2.48	1.48	1.43
22	B	605	CLA	MG-NB	-2.48	2.00	2.05
22	B	614	CLA	C1B-C2B	2.47	1.48	1.43
22	N	603	CLA	MG-NB	-2.47	2.00	2.05
22	B	606	CLA	MG-NB	-2.47	2.00	2.05
22	b	604	CLA	MG-NB	-2.47	2.00	2.05
22	b	611	CLA	C1B-C2B	2.47	1.48	1.43
22	d	403	CLA	C1B-C2B	2.47	1.48	1.43
22	g	603	CLA	C1B-C2B	2.47	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	401	PHO	CMB-C2B	-2.47	1.46	1.51
22	C	503	CLA	C1B-C2B	2.47	1.48	1.43
22	c	503	CLA	MG-NB	-2.46	2.00	2.05
22	b	607	CLA	MG-NB	-2.46	2.00	2.05
25	y	616	NEX	C38-C25	2.46	1.55	1.51
22	g	603	CLA	MG-NB	-2.46	2.00	2.05
22	B	610	CLA	MG-NB	-2.46	2.00	2.05
22	Y	604	CLA	MG-NB	-2.46	2.00	2.05
22	D	404	CLA	C1B-C2B	2.46	1.48	1.43
22	b	615	CLA	MG-NB	-2.46	2.00	2.05
22	B	605	CLA	C1B-C2B	2.46	1.48	1.43
22	G	604	CLA	MG-NB	-2.45	2.00	2.05
22	c	509	CLA	CMB-C2B	-2.45	1.45	1.50
22	Y	603	CLA	C1B-C2B	2.45	1.48	1.43
22	B	607	CLA	MG-NB	-2.45	2.00	2.05
22	b	614	CLA	MG-NB	-2.45	2.00	2.05
22	c	510	CLA	CHC-C1C	2.45	1.43	1.38
22	y	603	CLA	C1B-C2B	2.45	1.48	1.43
22	s	303	CLA	C1B-C2B	2.45	1.48	1.43
22	y	604	CLA	C4B-NB	2.45	1.41	1.37
22	c	508	CLA	MG-NB	-2.45	2.00	2.05
24	G	617	XAT	C18-C5	2.45	1.55	1.51
22	C	509	CLA	MG-NB	-2.45	2.00	2.05
22	A	409	CLA	MG-NB	-2.44	2.00	2.05
23	n	614	LUT	C8-C7	2.44	1.40	1.33
22	S	303	CLA	C1B-C2B	2.44	1.48	1.43
22	N	604	CLA	C4B-NB	2.44	1.41	1.37
22	c	507	CLA	MG-NB	-2.44	2.00	2.05
23	y	614	LUT	C8-C7	2.44	1.40	1.33
22	G	613	CLA	C3D-C4D	2.44	1.49	1.44
22	G	603	CLA	MG-NB	-2.44	2.00	2.05
22	g	613	CLA	C3D-C4D	2.44	1.49	1.44
22	y	604	CLA	MG-NB	-2.44	2.01	2.05
22	C	511	CLA	C1B-C2B	2.44	1.48	1.43
22	C	512	CLA	MG-NB	-2.44	2.01	2.05
22	B	612	CLA	MG-NB	-2.43	2.01	2.05
22	b	609	CLA	MG-NB	-2.43	2.01	2.05
22	c	514	CLA	MG-NB	-2.43	2.01	2.05
22	c	502	CLA	C1B-C2B	2.43	1.48	1.43
22	y	612	CLA	C3D-C4D	2.43	1.49	1.44
22	B	615	CLA	C1B-C2B	2.43	1.48	1.43
22	Y	604	CLA	C4B-NB	2.43	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	515	CLA	MG-NB	-2.43	2.01	2.05
22	n	604	CLA	C4B-NB	2.43	1.41	1.37
22	A	406	CLA	MG-NB	-2.43	2.01	2.05
22	c	511	CLA	MG-NB	-2.43	2.01	2.05
22	b	605	CLA	MG-NB	-2.42	2.01	2.05
22	G	604	CLA	C4B-NB	2.42	1.41	1.37
22	b	603	CLA	MG-NB	-2.42	2.01	2.05
22	C	510	CLA	C1B-C2B	2.42	1.48	1.43
23	N	614	LUT	C8-C7	2.42	1.40	1.33
22	n	604	CLA	MG-NB	-2.42	2.01	2.05
22	g	604	CLA	C4B-NB	2.42	1.41	1.37
22	Y	603	CLA	MG-NB	-2.42	2.01	2.05
22	B	615	CLA	MG-NB	-2.42	2.01	2.05
22	Y	611	CLA	C3D-C4D	2.42	1.49	1.44
22	N	612	CLA	C3D-C4D	2.42	1.49	1.44
23	Y	613	LUT	C8-C7	2.42	1.40	1.33
22	b	606	CLA	MG-NB	-2.42	2.01	2.05
22	n	603	CLA	MG-NB	-2.42	2.01	2.05
22	n	612	CLA	C3D-C4D	2.42	1.49	1.44
22	c	502	CLA	MG-NB	-2.41	2.01	2.05
22	B	608	CLA	MG-NB	-2.41	2.01	2.05
23	g	615	LUT	C8-C7	2.41	1.40	1.33
22	b	612	CLA	MG-NB	-2.41	2.01	2.05
22	y	603	CLA	MG-NB	-2.41	2.01	2.05
22	a	405	CLA	MG-NB	-2.41	2.01	2.05
24	g	617	XAT	C18-C5	2.41	1.55	1.51
23	G	615	LUT	C8-C7	2.41	1.40	1.33
22	N	612	CLA	CMC-C2C	-2.41	1.45	1.50
22	b	610	CLA	MG-NB	-2.41	2.01	2.05
22	c	504	CLA	MG-NB	-2.41	2.01	2.05
22	G	613	CLA	CMC-C2C	-2.41	1.45	1.50
22	d	403	CLA	MG-NB	-2.41	2.01	2.05
22	C	511	CLA	C3B-C4B	2.41	1.49	1.42
23	N	614	LUT	C4-C5	2.41	1.54	1.51
22	g	604	CLA	MG-NB	-2.41	2.01	2.05
22	s	311	CLA	MG-NB	-2.41	2.01	2.05
22	r	304	CLA	MG-NB	-2.40	2.01	2.05
22	c	509	CLA	C1B-C2B	2.40	1.48	1.43
22	C	508	CLA	MG-NB	-2.39	2.01	2.05
23	g	615	LUT	C4-C5	2.39	1.54	1.51
22	y	612	CLA	CMC-C2C	-2.39	1.45	1.50
22	B	614	CLA	MG-NB	-2.39	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	314	LHG	O7-C5	-2.39	1.41	1.46
22	b	611	CLA	MG-NB	-2.39	2.01	2.05
22	s	310	CLA	MG-NB	-2.39	2.01	2.05
22	g	613	CLA	CMC-C2C	-2.39	1.45	1.50
22	c	510	CLA	C3B-C4B	2.39	1.49	1.42
22	C	503	CLA	MG-NB	-2.39	2.01	2.05
22	r	305	CLA	MG-NB	-2.39	2.01	2.05
24	y	615	XAT	C18-C5	2.39	1.55	1.51
22	b	612	CLA	C1B-C2B	2.38	1.48	1.43
22	B	609	CLA	MG-NB	-2.38	2.01	2.05
26	c	520	LHG	O8-C6	2.38	1.50	1.45
26	R	301	LHG	O7-C5	-2.38	1.41	1.46
22	n	612	CLA	CMC-C2C	-2.38	1.45	1.50
22	C	507	CLA	MG-NB	-2.38	2.01	2.05
26	S	314	LHG	O7-C5	-2.38	1.41	1.46
22	B	613	CLA	MG-NB	-2.38	2.01	2.05
26	r	302	LHG	O7-C5	-2.38	1.41	1.46
22	C	513	CLA	MG-NB	-2.38	2.01	2.05
22	C	505	CLA	MG-NB	-2.38	2.01	2.05
24	G	617	XAT	C38-C25	2.38	1.55	1.51
22	c	510	CLA	C1B-C2B	2.37	1.48	1.43
22	R	303	CLA	MG-NB	-2.37	2.01	2.05
22	S	311	CLA	MG-NB	-2.37	2.01	2.05
22	B	611	CLA	MG-NB	-2.37	2.01	2.05
22	c	512	CLA	MG-NB	-2.37	2.01	2.05
22	b	608	CLA	MG-NB	-2.37	2.01	2.05
22	D	405	CLA	MG-NB	-2.37	2.01	2.05
26	C	520	LHG	C6-C5	2.37	1.58	1.50
26	C	520	LHG	O8-C6	2.37	1.50	1.45
22	Y	611	CLA	CMC-C2C	-2.37	1.45	1.50
22	G	611	CLA	MG-NB	-2.36	2.01	2.05
36	B	623	LMG	C22-C21	2.36	1.63	1.51
22	s	311	CLA	C3B-C4B	2.36	1.49	1.42
22	R	304	CLA	MG-NB	-2.36	2.01	2.05
36	b	620	LMG	C22-C21	2.36	1.63	1.51
24	y	615	XAT	O24-C25	2.36	1.49	1.46
22	D	404	CLA	MG-NB	-2.36	2.01	2.05
24	g	617	XAT	C38-C25	2.36	1.55	1.51
22	N	610	CLA	MG-NB	-2.36	2.01	2.05
23	g	616	LUT	C23-C24	2.35	1.53	1.50
22	S	313	CLA	MG-NB	-2.35	2.01	2.05
26	C	520	LHG	O8-C23	2.35	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	n	614	LUT	C4-C5	2.35	1.54	1.51
22	B	603	CLA	MG-NB	-2.35	2.01	2.05
22	g	611	CLA	MG-NB	-2.35	2.01	2.05
22	R	304	CLA	CMB-C2B	-2.35	1.46	1.50
26	c	520	LHG	C6-C5	2.34	1.58	1.50
23	Y	613	LUT	C4-C5	2.34	1.54	1.51
24	Y	615	XAT	O24-C25	2.34	1.49	1.46
24	n	615	XAT	C18-C5	2.34	1.55	1.51
26	c	520	LHG	O8-C23	2.34	1.40	1.33
26	c	522	LHG	O7-C5	-2.34	1.41	1.46
22	S	310	CLA	MG-NB	-2.34	2.01	2.05
22	B	604	CLA	MG-NB	-2.34	2.01	2.05
22	A	405	CLA	MG-NB	-2.34	2.01	2.05
22	c	505	CLA	MG-NB	-2.34	2.01	2.05
26	C	522	LHG	O7-C5	-2.34	1.41	1.46
23	y	614	LUT	C4-C5	2.34	1.54	1.51
22	y	611	CLA	MG-NB	-2.34	2.01	2.05
22	R	311	CLA	C3B-C4B	2.33	1.49	1.42
22	b	613	CLA	MG-NB	-2.33	2.01	2.05
22	r	312	CLA	C3B-C4B	2.33	1.49	1.42
22	s	304	CLA	C3B-C4B	2.33	1.49	1.42
24	Y	615	XAT	C18-C5	2.33	1.55	1.51
22	C	506	CLA	MG-NB	-2.33	2.01	2.05
22	s	313	CLA	MG-NB	-2.33	2.01	2.05
24	y	615	XAT	C38-C25	2.33	1.55	1.51
22	Y	610	CLA	MG-NB	-2.33	2.01	2.05
23	G	615	LUT	C4-C5	2.33	1.54	1.51
22	a	406	CLA	MG-NB	-2.32	2.01	2.05
22	S	304	CLA	C3B-C4B	2.32	1.49	1.42
22	c	506	CLA	MG-NB	-2.32	2.01	2.05
22	b	601	CLA	MG-NB	-2.32	2.01	2.05
22	a	404	CLA	MG-NB	-2.32	2.01	2.05
24	N	616	XAT	C38-C25	2.32	1.55	1.51
22	d	404	CLA	MG-NB	-2.32	2.01	2.05
23	N	615	LUT	C23-C24	2.32	1.53	1.50
22	r	305	CLA	CMB-C2B	-2.32	1.46	1.50
22	n	610	CLA	MG-NB	-2.32	2.01	2.05
22	C	511	CLA	MG-NB	-2.32	2.01	2.05
22	g	603	CLA	CMD-C2D	-2.32	1.46	1.50
24	n	615	XAT	C38-C25	2.32	1.55	1.51
22	D	404	CLA	CMD-C2D	-2.31	1.46	1.50
22	Y	602	CLA	MG-NB	-2.31	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	311	CLA	C3B-C4B	2.31	1.49	1.42
26	g	619	LHG	O7-C5	-2.31	1.41	1.46
22	A	407	CLA	MG-NB	-2.31	2.01	2.05
22	R	302	CLA	MG-NB	-2.31	2.01	2.05
22	s	304	CLA	CMD-C2D	-2.31	1.46	1.50
22	n	602	CLA	MG-NB	-2.31	2.01	2.05
22	y	602	CLA	MG-NB	-2.31	2.01	2.05
22	c	510	CLA	MG-NB	-2.31	2.01	2.05
24	N	616	XAT	C18-C5	2.31	1.55	1.51
22	R	308	CLA	MG-NB	-2.31	2.01	2.05
22	y	610	CLA	C3B-C4B	2.31	1.49	1.42
22	n	613	CLA	C3B-C4B	2.30	1.49	1.42
22	r	310	CLA	C3B-C4B	2.30	1.49	1.42
36	C	523	LMG	O7-C8	-2.30	1.41	1.46
35	A	401	DGD	O1G-C1G	-2.30	1.40	1.45
22	G	614	CLA	C3B-C4B	2.30	1.49	1.42
22	g	614	CLA	C3B-C4B	2.30	1.49	1.42
22	a	406	CLA	C3B-C4B	2.30	1.49	1.42
22	s	303	CLA	C3B-C4B	2.30	1.49	1.42
22	S	312	CLA	MG-NB	-2.30	2.01	2.05
36	M	101	LMG	O7-C8	-2.30	1.41	1.46
22	b	612	CLA	C3B-C4B	2.30	1.49	1.42
25	n	616	NEX	C38-C25	2.30	1.55	1.51
22	n	609	CLA	C3B-C4B	2.29	1.49	1.42
24	Y	615	XAT	C38-C25	2.29	1.55	1.51
22	B	616	CLA	MG-NB	-2.29	2.01	2.05
36	c	523	LMG	O7-C8	-2.29	1.41	1.46
22	g	610	CLA	C3B-C4B	2.29	1.49	1.42
22	N	602	CLA	MG-NB	-2.29	2.01	2.05
30	A	408	PHO	C3B-C2B	-2.29	1.37	1.40
22	B	613	CLA	CMD-C2D	-2.29	1.46	1.50
22	Y	609	CLA	C3B-C4B	2.29	1.49	1.42
22	C	507	CLA	CMD-C2D	-2.29	1.46	1.50
22	R	303	CLA	CMD-C2D	-2.29	1.46	1.50
22	G	610	CLA	C3B-C4B	2.29	1.49	1.42
22	G	603	CLA	CMD-C2D	-2.29	1.46	1.50
22	N	612	CLA	C4D-CHA	2.29	1.46	1.38
22	Y	612	CLA	C3B-C4B	2.29	1.49	1.42
22	A	407	CLA	C3B-C4B	2.29	1.49	1.42
22	B	611	CLA	CMD-C2D	-2.29	1.46	1.50
25	g	618	NEX	C38-C25	2.29	1.55	1.51
22	y	604	CLA	CMB-C2B	-2.29	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	303	CLA	C3B-C4B	2.29	1.49	1.42
22	G	602	CLA	MG-NB	-2.28	2.01	2.05
22	N	604	CLA	CMB-C2B	-2.28	1.46	1.50
24	N	616	XAT	O24-C25	2.28	1.49	1.46
22	c	506	CLA	CMD-C2D	-2.28	1.46	1.50
22	r	309	CLA	MG-NB	-2.28	2.01	2.05
22	Y	611	CLA	C4D-CHA	2.28	1.46	1.38
22	x	101	CLA	MG-NB	-2.28	2.01	2.05
22	a	404	CLA	C3B-C4B	2.28	1.49	1.42
22	N	609	CLA	C3B-C4B	2.28	1.49	1.42
22	n	603	CLA	CMD-C2D	-2.28	1.46	1.50
35	a	413	DGD	O1G-C1G	-2.28	1.40	1.45
22	R	311	CLA	MG-NB	-2.28	2.01	2.05
22	A	405	CLA	C3B-C4B	2.28	1.49	1.42
22	R	309	CLA	C3B-C4B	2.28	1.49	1.42
22	g	604	CLA	CMB-C2B	-2.28	1.46	1.50
22	g	613	CLA	C2A-C1A	2.28	1.57	1.52
22	Y	612	CLA	MG-NB	-2.27	2.01	2.05
22	s	305	CLA	MG-NB	-2.27	2.01	2.05
22	r	303	CLA	C3B-C4B	2.27	1.49	1.42
22	y	603	CLA	CMD-C2D	-2.27	1.46	1.50
22	d	403	CLA	CMD-C2D	-2.27	1.46	1.50
22	B	608	CLA	CMD-C2D	-2.27	1.46	1.50
22	D	404	CLA	C3B-C4B	2.27	1.49	1.42
22	s	312	CLA	MG-NB	-2.27	2.01	2.05
22	Y	604	CLA	CMB-C2B	-2.27	1.46	1.50
36	D	411	LMG	O7-C8	-2.27	1.41	1.46
22	G	613	CLA	C4D-CHA	2.27	1.46	1.38
22	r	312	CLA	MG-NB	-2.27	2.01	2.05
22	S	309	CLA	MG-NB	-2.27	2.01	2.05
22	N	603	CLA	CMD-C2D	-2.27	1.46	1.50
22	A	409	CLA	CMD-C2D	-2.27	1.46	1.50
22	N	613	CLA	C3B-C4B	2.27	1.49	1.42
22	n	604	CLA	CMB-C2B	-2.27	1.46	1.50
23	N	615	LUT	C28-C27	2.26	1.37	1.32
22	y	613	CLA	C3B-C4B	2.26	1.49	1.42
22	N	613	CLA	MG-NB	-2.26	2.01	2.05
22	Y	603	CLA	CMD-C2D	-2.26	1.46	1.50
22	S	304	CLA	CMD-C2D	-2.26	1.46	1.50
22	n	613	CLA	MG-NB	-2.26	2.01	2.05
22	y	612	CLA	C4D-CHA	2.26	1.46	1.38
36	B	623	LMG	O7-C8	-2.26	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	C3B-C4B	2.26	1.49	1.42
22	B	615	CLA	C3B-C4B	2.26	1.49	1.42
22	G	604	CLA	CMB-C2B	-2.26	1.46	1.50
22	B	604	CLA	CMD-C2D	-2.25	1.46	1.50
22	b	608	CLA	CMD-C2D	-2.25	1.46	1.50
30	d	401	PHO	C3D-C4D	2.25	1.44	1.41
22	r	303	CLA	MG-NB	-2.25	2.01	2.05
36	T	101	LMG	O7-C8	-2.25	1.41	1.46
24	R	313	XAT	C8-C7	2.25	1.37	1.32
22	S	309	CLA	C3B-C4B	2.25	1.49	1.42
22	s	310	CLA	C3B-C4B	2.25	1.49	1.42
22	n	612	CLA	C4D-CHA	2.25	1.46	1.38
22	R	309	CLA	CHC-C1C	2.25	1.43	1.38
22	y	612	CLA	C2A-C1A	2.25	1.57	1.52
22	C	503	CLA	CMB-C2B	-2.25	1.46	1.50
22	s	303	CLA	MG-NB	-2.25	2.01	2.05
23	G	616	LUT	C4-C5	2.25	1.54	1.51
22	g	613	CLA	C4D-CHA	2.25	1.46	1.38
22	c	504	CLA	CMD-C2D	-2.25	1.46	1.50
22	b	605	CLA	CMD-C2D	-2.25	1.46	1.50
22	s	309	CLA	C3B-C4B	2.24	1.49	1.42
22	B	609	CLA	CMD-C2D	-2.24	1.46	1.50
22	n	612	CLA	C2A-C1A	2.24	1.57	1.52
22	B	610	CLA	C3B-C4B	2.24	1.49	1.42
22	Y	610	CLA	C3B-C4B	2.24	1.49	1.42
22	g	602	CLA	MG-NB	-2.24	2.01	2.05
22	S	310	CLA	C3B-C4B	2.24	1.49	1.42
24	r	314	XAT	O24-C25	2.24	1.49	1.46
30	A	408	PHO	C4D-ND	-2.24	1.35	1.38
22	d	404	CLA	C3B-C4B	2.24	1.49	1.42
30	D	401	PHO	C3D-C4D	2.24	1.44	1.41
22	y	602	CLA	C3B-C4B	2.24	1.49	1.42
22	y	613	CLA	MG-NB	-2.24	2.01	2.05
22	y	611	CLA	C3B-C4B	2.24	1.49	1.42
22	A	407	CLA	CMB-C2B	-2.23	1.46	1.50
22	b	611	CLA	CMD-C2D	-2.23	1.46	1.50
22	s	309	CLA	MG-NB	-2.23	2.01	2.05
22	c	511	CLA	C3B-C4B	2.23	1.49	1.42
26	b	619	LHG	O7-C5	-2.23	1.41	1.46
22	N	612	CLA	C2A-C1A	2.23	1.57	1.52
22	N	610	CLA	C3B-C4B	2.23	1.49	1.42
22	r	304	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	610	CLA	CMB-C2B	-2.23	1.46	1.50
22	C	504	CLA	CMD-C2D	-2.23	1.46	1.50
36	d	410	LMG	O7-C8	-2.23	1.41	1.46
22	A	406	CLA	CMD-C2D	-2.23	1.46	1.50
22	a	408	CLA	CMD-C2D	-2.23	1.46	1.50
22	S	305	CLA	MG-NB	-2.23	2.01	2.05
22	C	508	CLA	CMD-C2D	-2.23	1.46	1.50
22	B	616	CLA	CMD-C2D	-2.23	1.46	1.50
22	R	302	CLA	C3B-C4B	2.23	1.49	1.42
22	c	505	CLA	CMD-C2D	-2.23	1.46	1.50
22	G	602	CLA	C3B-C4B	2.23	1.49	1.42
22	b	604	CLA	CMD-C2D	-2.23	1.46	1.50
22	G	614	CLA	MG-NB	-2.23	2.01	2.05
22	g	602	CLA	C3B-C4B	2.23	1.49	1.42
22	N	602	CLA	C3B-C4B	2.23	1.49	1.42
22	Y	603	CLA	C3B-C4B	2.23	1.49	1.42
22	R	308	CLA	C3B-C4B	2.23	1.49	1.42
22	x	101	CLA	CMD-C2D	-2.23	1.46	1.50
22	b	614	CLA	CMD-C2D	-2.22	1.46	1.50
22	r	309	CLA	C3B-C4B	2.22	1.49	1.42
22	n	603	CLA	C3B-C4B	2.22	1.49	1.42
22	D	405	CLA	C3B-C4B	2.22	1.49	1.42
23	R	312	LUT	C8-C7	2.22	1.39	1.33
22	a	405	CLA	CMD-C2D	-2.22	1.46	1.50
22	a	406	CLA	CMB-C2B	-2.22	1.46	1.50
22	b	610	CLA	CMD-C2D	-2.22	1.46	1.50
22	A	405	CLA	CMB-C2B	-2.22	1.46	1.50
22	W	101	CLA	C3B-C4B	2.22	1.49	1.42
22	b	606	CLA	CMD-C2D	-2.22	1.46	1.50
22	N	611	CLA	C3B-C4B	2.22	1.49	1.42
23	Y	614	LUT	C23-C24	2.22	1.53	1.50
22	b	613	CLA	CMD-C2D	-2.22	1.46	1.50
22	c	502	CLA	CMB-C2B	-2.22	1.46	1.50
22	C	505	CLA	CMD-C2D	-2.22	1.46	1.50
22	y	610	CLA	MG-NB	-2.22	2.01	2.05
22	C	512	CLA	C3B-C4B	2.22	1.49	1.42
22	c	503	CLA	CMD-C2D	-2.22	1.46	1.50
30	a	407	PHO	C3B-C2B	-2.22	1.37	1.40
22	c	507	CLA	CMD-C2D	-2.22	1.46	1.50
22	G	611	CLA	C3B-C4B	2.22	1.49	1.42
22	g	614	CLA	MG-NB	-2.22	2.01	2.05
22	B	613	CLA	CMC-C2C	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	g	611	CLA	C3B-C4B	2.22	1.49	1.42
22	S	308	CLA	MG-NB	-2.22	2.01	2.05
22	B	611	CLA	C3B-C4B	2.22	1.49	1.42
22	g	610	CLA	MG-NB	-2.21	2.01	2.05
22	B	606	CLA	CMD-C2D	-2.21	1.46	1.50
22	Y	611	CLA	C2A-C1A	2.21	1.57	1.52
22	b	608	CLA	C3B-C4B	2.21	1.49	1.42
22	c	511	CLA	CMB-C2B	-2.21	1.46	1.50
22	n	610	CLA	C3B-C4B	2.21	1.49	1.42
22	S	311	CLA	CHC-C1C	2.21	1.42	1.38
22	b	607	CLA	C3B-C4B	2.21	1.49	1.42
22	b	610	CLA	CMC-C2C	-2.21	1.46	1.50
22	B	617	CLA	CMD-C2D	-2.21	1.46	1.50
23	r	313	LUT	C8-C7	2.21	1.39	1.33
22	b	612	CLA	CMD-C2D	-2.21	1.46	1.50
22	c	508	CLA	CMB-C2B	-2.21	1.46	1.50
22	S	309	CLA	CHC-C1C	2.21	1.42	1.38
22	B	603	CLA	CMD-C2D	-2.21	1.46	1.50
22	s	313	CLA	CMD-C2D	-2.21	1.46	1.50
22	S	312	CLA	CMD-C2D	-2.21	1.46	1.50
22	s	308	CLA	MG-NB	-2.21	2.01	2.05
22	B	613	CLA	CMB-C2B	-2.21	1.46	1.50
22	S	308	CLA	C3B-C4B	2.21	1.49	1.42
24	R	313	XAT	O24-C25	2.21	1.49	1.46
36	b	620	LMG	O7-C8	-2.21	1.41	1.46
22	r	303	CLA	CHC-C1C	2.21	1.42	1.38
22	b	601	CLA	CMD-C2D	-2.21	1.46	1.50
26	B	622	LHG	O7-C5	-2.21	1.41	1.46
22	Y	602	CLA	C3B-C4B	2.21	1.49	1.42
22	S	303	CLA	MG-NB	-2.21	2.01	2.05
22	C	509	CLA	CMB-C2B	-2.21	1.46	1.50
22	y	603	CLA	C3B-C4B	2.21	1.49	1.42
22	a	404	CLA	CMB-C2B	-2.21	1.46	1.50
22	C	512	CLA	CMB-C2B	-2.21	1.46	1.50
22	G	612	CLA	C3B-C4B	2.21	1.49	1.42
22	g	603	CLA	C3B-C4B	2.20	1.49	1.42
22	G	613	CLA	C2A-C1A	2.20	1.57	1.52
22	w	101	CLA	C3B-C4B	2.20	1.49	1.42
22	N	611	CLA	MG-NB	-2.20	2.01	2.05
22	c	513	CLA	CMD-C2D	-2.20	1.46	1.50
22	s	311	CLA	CHC-C1C	2.20	1.42	1.38
22	r	310	CLA	CHC-C1C	2.20	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	616	LUT	C23-C24	2.20	1.53	1.50
22	G	612	CLA	MG-NB	-2.20	2.01	2.05
22	x	101	CLA	C3B-C4B	2.20	1.49	1.42
22	N	603	CLA	C3B-C4B	2.20	1.49	1.42
22	C	507	CLA	C3B-C4B	2.20	1.49	1.42
22	g	612	CLA	C3B-C4B	2.20	1.49	1.42
22	G	603	CLA	C3B-C4B	2.20	1.49	1.42
24	r	314	XAT	C8-C7	2.20	1.37	1.32
22	D	405	CLA	CMD-C2D	-2.20	1.46	1.50
22	B	603	CLA	C3B-C4B	2.20	1.49	1.42
22	G	602	CLA	CHC-C1C	2.20	1.42	1.38
22	B	614	CLA	CMB-C2B	-2.20	1.46	1.50
22	B	618	CLA	CMB-C2B	-2.20	1.46	1.50
22	G	610	CLA	MG-NB	-2.20	2.01	2.05
22	w	101	CLA	MG-NB	-2.19	2.01	2.05
22	c	511	CLA	CMD-C2D	-2.19	1.46	1.50
22	c	514	CLA	CMD-C2D	-2.19	1.46	1.50
22	n	603	CLA	CMB-C2B	-2.19	1.46	1.50
22	d	404	CLA	CMD-C2D	-2.19	1.46	1.50
22	b	611	CLA	CMB-C2B	-2.19	1.46	1.50
22	g	603	CLA	CMB-C2B	-2.19	1.46	1.50
22	B	610	CLA	CMD-C2D	-2.19	1.46	1.50
22	B	615	CLA	CMD-C2D	-2.19	1.46	1.50
22	B	618	CLA	CMD-C2D	-2.19	1.46	1.50
22	C	514	CLA	CMD-C2D	-2.19	1.46	1.50
22	b	607	CLA	CMD-C2D	-2.19	1.46	1.50
22	D	405	CLA	CMB-C2B	-2.19	1.46	1.50
22	g	614	CLA	CHC-C1C	2.19	1.42	1.38
22	Y	602	CLA	CHC-C1C	2.19	1.42	1.38
22	B	617	CLA	C3B-C4B	2.19	1.49	1.42
22	n	602	CLA	C3B-C4B	2.19	1.49	1.42
22	b	613	CLA	CMB-C2B	-2.19	1.46	1.50
22	C	503	CLA	CMD-C2D	-2.19	1.46	1.50
22	y	603	CLA	CMB-C2B	-2.19	1.46	1.50
22	c	509	CLA	CMD-C2D	-2.19	1.46	1.50
22	b	601	CLA	CHC-C1C	2.19	1.42	1.38
22	S	313	CLA	CMD-C2D	-2.19	1.46	1.50
22	c	506	CLA	C3B-C4B	2.19	1.49	1.42
22	B	615	CLA	CMB-C2B	-2.18	1.46	1.50
22	s	308	CLA	C3B-C4B	2.18	1.49	1.42
22	a	404	CLA	CMD-C2D	-2.18	1.46	1.50
22	c	502	CLA	C3B-C4B	2.18	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	309	CLA	CHC-C1C	2.18	1.42	1.38
22	d	404	CLA	CMB-C2B	-2.18	1.46	1.50
22	R	303	CLA	CMB-C2B	-2.18	1.46	1.50
22	c	502	CLA	CMD-C2D	-2.18	1.46	1.50
22	a	406	CLA	CMC-C2C	-2.18	1.46	1.50
30	a	407	PHO	C4D-ND	-2.18	1.35	1.38
22	Y	603	CLA	CMB-C2B	-2.18	1.46	1.50
22	G	603	CLA	CMB-C2B	-2.18	1.46	1.50
22	A	405	CLA	CMC-C2C	-2.18	1.46	1.50
22	C	515	CLA	CMD-C2D	-2.18	1.46	1.50
22	n	602	CLA	CHC-C1C	2.18	1.42	1.38
22	R	303	CLA	C3B-C4B	2.18	1.49	1.42
35	c	517	DGD	O6D-C5D	-2.18	1.39	1.44
22	r	304	CLA	C3B-C4B	2.18	1.49	1.42
22	b	605	CLA	CMB-C2B	-2.17	1.46	1.50
22	d	403	CLA	CMB-C2B	-2.17	1.46	1.50
36	d	410	LMG	O1-C7	-2.17	1.40	1.43
22	C	506	CLA	CMD-C2D	-2.17	1.46	1.50
22	s	310	CLA	CHC-C1C	2.17	1.42	1.38
22	S	303	CLA	CHC-C1C	2.17	1.42	1.38
22	W	101	CLA	MG-NB	-2.17	2.01	2.05
22	C	503	CLA	C3B-C4B	2.17	1.49	1.42
22	B	607	CLA	CMD-C2D	-2.17	1.46	1.50
22	R	302	CLA	CHC-C1C	2.17	1.42	1.38
22	n	611	CLA	C3B-C4B	2.17	1.49	1.42
22	A	407	CLA	CMC-C2C	-2.17	1.46	1.50
22	B	614	CLA	CMD-C2D	-2.17	1.46	1.50
22	A	405	CLA	CMD-C2D	-2.17	1.46	1.50
22	B	616	CLA	CMB-C2B	-2.17	1.46	1.50
22	n	604	CLA	CMD-C2D	-2.17	1.46	1.50
22	b	615	CLA	CMD-C2D	-2.17	1.46	1.50
22	B	607	CLA	CMC-C2C	-2.17	1.46	1.50
22	n	609	CLA	MG-NB	-2.17	2.01	2.05
22	b	614	CLA	C3B-C4B	2.17	1.49	1.42
22	c	508	CLA	CMD-C2D	-2.17	1.46	1.50
22	C	512	CLA	CMD-C2D	-2.17	1.46	1.50
22	r	304	CLA	CMB-C2B	-2.17	1.46	1.50
22	A	407	CLA	CHC-C1C	2.17	1.42	1.38
22	y	602	CLA	CHC-C1C	2.17	1.42	1.38
22	b	612	CLA	CMB-C2B	-2.17	1.46	1.50
22	B	608	CLA	CMB-C2B	-2.17	1.46	1.50
22	b	609	CLA	C3B-C4B	2.17	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	406	CLA	CMD-C2D	-2.17	1.46	1.50
22	b	615	CLA	CMB-C2B	-2.17	1.46	1.50
22	N	603	CLA	CMB-C2B	-2.16	1.46	1.50
22	c	510	CLA	C1D-C2D	2.16	1.49	1.45
22	C	511	CLA	C1D-C2D	2.16	1.49	1.45
22	a	405	CLA	CMB-C2B	-2.16	1.46	1.50
22	b	603	CLA	CMD-C2D	-2.16	1.46	1.50
22	C	508	CLA	C3B-C4B	2.16	1.49	1.42
22	Y	604	CLA	CMD-C2D	-2.16	1.46	1.50
22	b	601	CLA	CMC-C2C	-2.16	1.46	1.50
22	A	406	CLA	CMB-C2B	-2.16	1.46	1.50
22	Y	612	CLA	CHC-C1C	2.16	1.42	1.38
22	n	613	CLA	CHC-C1C	2.16	1.42	1.38
22	N	609	CLA	MG-NB	-2.16	2.01	2.05
26	N	618	LHG	P-O6	2.16	1.67	1.59
22	c	507	CLA	C3B-C4B	2.16	1.49	1.42
22	n	611	CLA	MG-NB	-2.16	2.01	2.05
23	Y	614	LUT	C4-C5	2.16	1.54	1.51
22	S	305	CLA	CMD-C2D	-2.15	1.46	1.50
22	s	304	CLA	CHC-C1C	2.15	1.42	1.38
22	a	408	CLA	CMB-C2B	-2.15	1.46	1.50
22	D	404	CLA	CMB-C2B	-2.15	1.46	1.50
35	C	518	DGD	O6D-C5D	-2.15	1.39	1.44
37	f	101	HEM	C4A-NA	2.15	1.43	1.39
22	B	603	CLA	CMB-C2B	-2.15	1.46	1.50
22	B	612	CLA	C3B-C4B	2.15	1.49	1.42
22	g	613	CLA	CMD-C2D	-2.15	1.46	1.50
22	N	602	CLA	CHC-C1C	2.15	1.42	1.38
22	y	613	CLA	CHC-C1C	2.15	1.42	1.38
22	c	512	CLA	C3B-C4B	2.15	1.49	1.42
22	S	313	CLA	C3B-C4B	2.15	1.49	1.42
23	g	616	LUT	C4-C5	2.15	1.54	1.51
22	A	407	CLA	CMD-C2D	-2.15	1.46	1.50
22	s	305	CLA	C3B-C4B	2.15	1.49	1.42
22	g	612	CLA	MG-NB	-2.15	2.01	2.05
22	Y	609	CLA	MG-NB	-2.15	2.01	2.05
37	F	101	HEM	C4A-NA	2.15	1.43	1.39
22	A	409	CLA	C3B-C4B	2.15	1.49	1.42
22	Y	609	CLA	CMD-C2D	-2.15	1.46	1.50
22	b	604	CLA	CMB-C2B	-2.15	1.46	1.50
22	C	513	CLA	C3B-C4B	2.15	1.49	1.42
22	A	409	CLA	CMB-C2B	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	309	CLA	CMD-C2D	-2.15	1.46	1.50
22	s	312	CLA	CMD-C2D	-2.15	1.46	1.50
22	B	616	CLA	C3B-C4B	2.15	1.49	1.42
22	c	506	CLA	CMB-C2B	-2.15	1.46	1.50
22	S	310	CLA	CMD-C2D	-2.15	1.46	1.50
22	B	614	CLA	C3B-C4B	2.15	1.49	1.42
22	c	513	CLA	CMB-C2B	-2.15	1.46	1.50
24	n	615	XAT	C8-C7	2.15	1.37	1.32
22	g	604	CLA	CMD-C2D	-2.15	1.46	1.50
22	S	303	CLA	CMB-C2B	-2.15	1.46	1.50
22	s	303	CLA	CHC-C1C	2.15	1.42	1.38
22	g	602	CLA	CHC-C1C	2.15	1.42	1.38
22	b	607	CLA	CHC-C1C	2.15	1.42	1.38
22	S	312	CLA	CMB-C2B	-2.15	1.46	1.50
22	B	605	CLA	CHC-C1C	2.15	1.42	1.38
30	A	408	PHO	C3D-C4D	2.15	1.44	1.41
22	w	101	CLA	CMD-C2D	-2.15	1.46	1.50
22	s	312	CLA	C3B-C4B	2.14	1.49	1.42
22	W	101	CLA	CMD-C2D	-2.14	1.46	1.50
22	b	613	CLA	C3B-C4B	2.14	1.49	1.42
22	S	313	CLA	CMB-C2B	-2.14	1.46	1.50
24	Y	615	XAT	C8-C7	2.14	1.37	1.32
25	N	617	NEX	C38-C25	2.14	1.55	1.51
24	N	616	XAT	C28-C27	2.14	1.37	1.32
22	G	612	CLA	CMD-C2D	-2.14	1.46	1.50
22	b	604	CLA	CMC-C2C	-2.14	1.46	1.50
22	R	311	CLA	CMD-C2D	-2.14	1.46	1.50
22	N	613	CLA	CHC-C1C	2.14	1.42	1.38
22	B	617	CLA	CHC-C1C	2.14	1.42	1.38
22	B	607	CLA	CMB-C2B	-2.14	1.46	1.50
22	s	303	CLA	CMD-C2D	-2.14	1.46	1.50
22	g	611	CLA	CMD-C2D	-2.14	1.46	1.50
22	D	404	CLA	CMC-C2C	-2.14	1.46	1.50
22	B	604	CLA	CHC-C1C	2.14	1.42	1.38
22	B	609	CLA	CMC-C2C	-2.14	1.46	1.50
22	R	308	CLA	CHC-C1C	2.14	1.42	1.38
22	s	313	CLA	C3B-C4B	2.14	1.49	1.42
22	G	604	CLA	CMD-C2D	-2.14	1.46	1.50
22	B	604	CLA	CMC-C2C	-2.14	1.46	1.50
22	S	310	CLA	CHC-C1C	2.14	1.42	1.38
22	S	304	CLA	MG-NB	-2.14	2.01	2.05
22	a	408	CLA	C3B-C4B	2.14	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	CMD-C2D	-2.14	1.46	1.50
22	a	406	CLA	CHC-C1C	2.14	1.42	1.38
22	b	611	CLA	C3B-C4B	2.14	1.49	1.42
22	S	312	CLA	C3B-C4B	2.14	1.49	1.42
36	D	411	LMG	O1-C7	-2.14	1.40	1.43
22	B	617	CLA	CMB-C2B	-2.13	1.46	1.50
22	R	304	CLA	CMD-C2D	-2.13	1.46	1.50
22	R	310	CLA	C3B-C4B	2.13	1.49	1.42
22	Y	610	CLA	CMD-C2D	-2.13	1.46	1.50
22	s	309	CLA	CMB-C2B	-2.13	1.46	1.50
24	r	314	XAT	C18-C5	2.13	1.55	1.51
22	a	404	CLA	CMC-C2C	-2.13	1.46	1.50
22	s	310	CLA	CMD-C2D	-2.13	1.46	1.50
22	N	612	CLA	CMD-C2D	-2.13	1.46	1.50
22	C	514	CLA	CMB-C2B	-2.13	1.46	1.50
22	r	309	CLA	CHC-C1C	2.13	1.42	1.38
22	r	310	CLA	CMD-C2D	-2.13	1.46	1.50
22	r	311	CLA	C3B-C4B	2.13	1.48	1.42
22	S	304	CLA	CHC-C1C	2.13	1.42	1.38
22	C	515	CLA	C3B-C4B	2.13	1.48	1.42
22	y	610	CLA	CHC-C1C	2.13	1.42	1.38
22	y	612	CLA	CMD-C2D	-2.13	1.46	1.50
22	B	605	CLA	CMB-C2B	-2.13	1.46	1.50
22	b	603	CLA	C3B-C4B	2.13	1.48	1.42
22	g	610	CLA	CMB-C2B	-2.13	1.46	1.50
22	c	505	CLA	C3B-C4B	2.13	1.48	1.42
22	n	611	CLA	CMB-C2B	-2.13	1.46	1.50
22	x	101	CLA	CMB-C2B	-2.13	1.46	1.50
22	r	312	CLA	CMD-C2D	-2.13	1.46	1.50
22	r	309	CLA	CMB-C2B	-2.13	1.46	1.50
22	d	403	CLA	CHC-C1C	2.13	1.42	1.38
22	c	514	CLA	C3B-C4B	2.13	1.48	1.42
22	b	602	CLA	CMD-C2D	-2.13	1.46	1.50
22	B	606	CLA	CMB-C2B	-2.13	1.46	1.50
22	s	313	CLA	CMB-C2B	-2.13	1.46	1.50
22	Y	609	CLA	CMB-C2B	-2.12	1.46	1.50
22	Y	612	CLA	CMB-C2B	-2.12	1.46	1.50
22	B	604	CLA	CMB-C2B	-2.12	1.46	1.50
22	B	605	CLA	CMD-C2D	-2.12	1.46	1.50
22	R	309	CLA	CMD-C2D	-2.12	1.46	1.50
22	R	309	CLA	MG-NB	-2.12	2.01	2.05
25	y	618	NEX	C4-C3	2.12	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	611	CLA	CMD-C2D	-2.12	1.46	1.50
22	Y	602	CLA	CMD-C2D	-2.12	1.46	1.50
22	b	609	CLA	CHC-C1C	2.12	1.42	1.38
22	g	603	CLA	CHC-C1C	2.12	1.42	1.38
22	B	616	CLA	CMC-C2C	-2.12	1.46	1.50
22	Y	602	CLA	CMB-C2B	-2.12	1.46	1.50
22	d	403	CLA	CMC-C2C	-2.12	1.46	1.50
22	B	608	CLA	C3B-C4B	2.12	1.48	1.42
22	C	505	CLA	C3B-C4B	2.12	1.48	1.42
22	n	612	CLA	CMD-C2D	-2.12	1.46	1.50
22	G	610	CLA	CMD-C2D	-2.12	1.46	1.50
22	R	308	CLA	CMB-C2B	-2.12	1.46	1.50
22	N	602	CLA	CMD-C2D	-2.12	1.46	1.50
22	B	612	CLA	CMB-C2B	-2.12	1.46	1.50
22	c	505	CLA	CMB-C2B	-2.12	1.46	1.50
22	S	305	CLA	CMB-C2B	-2.12	1.46	1.50
35	C	519	DGD	O6D-C5D	-2.12	1.39	1.44
36	C	502	LMG	O8-C9	-2.12	1.40	1.45
22	G	614	CLA	CHC-C1C	2.12	1.42	1.38
22	g	612	CLA	CMD-C2D	-2.12	1.46	1.50
22	r	305	CLA	CMD-C2D	-2.12	1.46	1.50
35	c	518	DGD	O6D-C5D	-2.12	1.39	1.44
35	c	517	DGD	O5D-C6D	-2.12	1.40	1.43
22	b	602	CLA	CMB-C2B	-2.12	1.46	1.50
22	B	604	CLA	C3B-C4B	2.12	1.48	1.42
22	s	303	CLA	CMB-C2B	-2.12	1.46	1.50
22	S	305	CLA	C3B-C4B	2.12	1.48	1.42
22	g	613	CLA	C1B-C2B	2.12	1.48	1.43
22	y	610	CLA	CMB-C2B	-2.12	1.46	1.50
36	w	102	LMG	O8-C9	-2.12	1.40	1.45
22	G	610	CLA	CMB-C2B	-2.12	1.46	1.50
22	b	603	CLA	CMB-C2B	-2.12	1.46	1.50
22	N	609	CLA	CMB-C2B	-2.12	1.46	1.50
22	W	101	CLA	CMB-C2B	-2.12	1.46	1.50
22	b	601	CLA	C3B-C4B	2.12	1.48	1.42
22	y	611	CLA	CMD-C2D	-2.12	1.46	1.50
22	N	609	CLA	CMD-C2D	-2.12	1.46	1.50
22	B	605	CLA	CMC-C2C	-2.12	1.46	1.50
22	b	615	CLA	C3B-C4B	2.12	1.48	1.42
24	r	314	XAT	C38-C25	2.12	1.55	1.51
22	C	509	CLA	C3B-C4B	2.12	1.48	1.42
22	G	612	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	g	602	CLA	CMB-C2B	-2.11	1.46	1.50
22	n	609	CLA	CMD-C2D	-2.11	1.46	1.50
22	n	610	CLA	CMD-C2D	-2.11	1.46	1.50
22	y	604	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	614	CLA	CMC-C2C	-2.11	1.46	1.50
22	C	507	CLA	CMB-C2B	-2.11	1.46	1.50
22	S	303	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	606	CLA	C3B-C4B	2.11	1.48	1.42
22	r	310	CLA	MG-NB	-2.11	2.01	2.05
22	n	609	CLA	CMB-C2B	-2.11	1.46	1.50
22	N	611	CLA	CMB-C2B	-2.11	1.46	1.50
22	g	610	CLA	CHC-C1C	2.11	1.42	1.38
22	C	509	CLA	CMD-C2D	-2.11	1.46	1.50
24	g	617	XAT	C8-C7	2.11	1.37	1.32
22	C	504	CLA	CMB-C2B	-2.11	1.46	1.50
22	c	504	CLA	C3B-C4B	2.11	1.48	1.42
22	b	614	CLA	CHC-C1C	2.11	1.42	1.38
22	N	613	CLA	CMB-C2B	-2.11	1.46	1.50
22	b	611	CLA	CMC-C2C	-2.11	1.46	1.50
22	N	604	CLA	CMD-C2D	-2.11	1.46	1.50
22	n	603	CLA	CHC-C1C	2.11	1.42	1.38
22	G	610	CLA	CHC-C1C	2.11	1.42	1.38
22	N	609	CLA	CHC-C1C	2.11	1.42	1.38
22	C	504	CLA	C3B-C4B	2.11	1.48	1.42
22	G	602	CLA	CMB-C2B	-2.11	1.46	1.50
22	G	602	CLA	CMD-C2D	-2.11	1.46	1.50
22	b	601	CLA	CMB-C2B	-2.11	1.46	1.50
33	d	402	SQD	O2-C2	-2.11	1.37	1.43
22	r	310	CLA	CMB-C2B	-2.11	1.46	1.50
22	S	310	CLA	CMC-C2C	-2.11	1.46	1.50
22	b	602	CLA	CHC-C1C	2.11	1.42	1.38
22	c	512	CLA	CHC-C1C	2.11	1.42	1.38
22	C	514	CLA	CMC-C2C	-2.11	1.46	1.50
22	B	611	CLA	CHC-C1C	2.11	1.42	1.38
23	R	312	LUT	C23-C24	2.11	1.53	1.50
22	G	613	CLA	CMD-C2D	-2.11	1.46	1.50
22	s	304	CLA	MG-NB	-2.11	2.01	2.05
26	N	618	LHG	O7-C5	-2.11	1.41	1.46
22	s	305	CLA	CMD-C2D	-2.11	1.46	1.50
22	s	311	CLA	CMD-C2D	-2.11	1.46	1.50
22	n	613	CLA	CMD-C2D	-2.11	1.46	1.50
22	b	605	CLA	C3B-C4B	2.11	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	g	610	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	611	CLA	CMB-C2B	-2.11	1.46	1.50
22	G	611	CLA	CMD-C2D	-2.11	1.46	1.50
22	Y	611	CLA	CMD-C2D	-2.11	1.46	1.50
22	C	515	CLA	CMB-C2B	-2.11	1.46	1.50
22	b	610	CLA	C3B-C4B	2.11	1.48	1.42
22	c	508	CLA	C3B-C4B	2.10	1.48	1.42
22	R	308	CLA	CMD-C2D	-2.10	1.46	1.50
24	y	615	XAT	C28-C27	2.10	1.37	1.32
22	N	612	CLA	C1B-C2B	2.10	1.48	1.43
22	c	507	CLA	CMC-C2C	-2.10	1.46	1.50
22	B	613	CLA	C3B-C4B	2.10	1.48	1.42
22	N	602	CLA	CMB-C2B	-2.10	1.46	1.50
22	b	607	CLA	CMC-C2C	-2.10	1.46	1.50
22	y	602	CLA	CMD-C2D	-2.10	1.46	1.50
22	R	303	CLA	CHC-C1C	2.10	1.42	1.38
24	Y	615	XAT	C28-C27	2.10	1.37	1.32
26	c	520	LHG	P-O6	2.10	1.67	1.59
22	c	514	CLA	CMB-C2B	-2.10	1.46	1.50
22	N	610	CLA	CMD-C2D	-2.10	1.46	1.50
22	C	506	CLA	C3B-C4B	2.10	1.48	1.42
22	n	611	CLA	CMD-C2D	-2.10	1.46	1.50
22	b	614	CLA	CMB-C2B	-2.10	1.46	1.50
22	B	618	CLA	C3B-C4B	2.10	1.48	1.42
22	n	602	CLA	CMB-C2B	-2.10	1.46	1.50
22	D	404	CLA	CHC-C1C	2.10	1.42	1.38
22	s	308	CLA	CMD-C2D	-2.10	1.46	1.50
22	B	614	CLA	CHC-C1C	2.10	1.42	1.38
22	b	606	CLA	CMB-C2B	-2.10	1.46	1.50
22	b	607	CLA	CMB-C2B	-2.10	1.46	1.50
22	S	309	CLA	CMB-C2B	-2.10	1.46	1.50
22	b	606	CLA	CMC-C2C	-2.10	1.46	1.50
24	y	615	XAT	C8-C7	2.10	1.37	1.32
22	C	508	CLA	CHC-C1C	2.10	1.42	1.38
24	R	313	XAT	C38-C25	2.10	1.54	1.51
22	r	303	CLA	CMB-C2B	-2.10	1.46	1.50
22	b	613	CLA	CHC-C1C	2.10	1.42	1.38
22	C	513	CLA	CHC-C1C	2.10	1.42	1.38
22	n	602	CLA	CMD-C2D	-2.09	1.46	1.50
22	B	612	CLA	CMC-C2C	-2.09	1.46	1.50
22	Y	609	CLA	CHC-C1C	2.09	1.42	1.38
22	c	504	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	602	CLA	C3B-C4B	2.09	1.48	1.42
35	C	518	DGD	O5D-C6D	-2.09	1.40	1.43
22	G	611	CLA	CMB-C2B	-2.09	1.46	1.50
22	c	511	CLA	CHC-C1C	2.09	1.42	1.38
22	B	609	CLA	C3B-C4B	2.09	1.48	1.42
22	a	408	CLA	CMC-C2C	-2.09	1.46	1.50
22	s	304	CLA	CMB-C2B	-2.09	1.46	1.50
22	b	608	CLA	CHC-C1C	2.09	1.42	1.38
36	D	411	LMG	O8-C9	-2.09	1.40	1.45
22	b	609	CLA	CMD-C2D	-2.09	1.46	1.50
22	y	612	CLA	C1B-C2B	2.09	1.48	1.43
22	c	503	CLA	C3B-C4B	2.09	1.48	1.42
22	c	506	CLA	CMC-C2C	-2.09	1.46	1.50
22	C	508	CLA	CMC-C2C	-2.09	1.46	1.50
22	c	505	CLA	CMC-C2C	-2.09	1.46	1.50
22	w	101	CLA	CMB-C2B	-2.09	1.46	1.50
22	s	310	CLA	CMC-C2C	-2.09	1.46	1.50
22	y	603	CLA	CHC-C1C	2.09	1.42	1.38
26	C	520	LHG	P-O6	2.09	1.67	1.59
22	n	610	CLA	CMB-C2B	-2.09	1.46	1.50
22	N	610	CLA	CHC-C1C	2.09	1.42	1.38
22	d	404	CLA	CHC-C1C	2.09	1.42	1.38
22	c	503	CLA	CMC-C2C	-2.09	1.46	1.50
22	C	506	CLA	CMB-C2B	-2.09	1.46	1.50
22	c	503	CLA	CHC-C1C	2.09	1.42	1.38
22	S	311	CLA	CMD-C2D	-2.09	1.46	1.50
22	C	503	CLA	CMC-C2C	-2.09	1.46	1.50
22	B	605	CLA	C3B-C4B	2.09	1.48	1.42
22	b	609	CLA	CMB-C2B	-2.09	1.46	1.50
24	G	617	XAT	O4-C5	-2.09	1.43	1.46
22	g	611	CLA	CMB-C2B	-2.09	1.46	1.50
22	y	602	CLA	CMB-C2B	-2.09	1.46	1.50
22	Y	610	CLA	CMB-C2B	-2.09	1.46	1.50
22	b	602	CLA	CMC-C2C	-2.09	1.46	1.50
22	R	310	CLA	CMD-C2D	-2.09	1.46	1.50
33	L	102	SQD	O2-C2	-2.09	1.37	1.43
22	B	612	CLA	CMD-C2D	-2.09	1.46	1.50
22	s	305	CLA	CMB-C2B	-2.09	1.46	1.50
22	B	603	CLA	CMC-C2C	-2.08	1.46	1.50
22	S	311	CLA	CMB-C2B	-2.08	1.46	1.50
22	R	309	CLA	CMB-C2B	-2.08	1.46	1.50
33	D	402	SQD	O2-C2	-2.08	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	515	CLA	CHC-C1C	2.08	1.42	1.38
36	d	410	LMG	O8-C9	-2.08	1.40	1.45
22	y	610	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	610	CLA	CMC-C2C	-2.08	1.46	1.50
22	Y	603	CLA	CHC-C1C	2.08	1.42	1.38
22	S	313	CLA	CHC-C1C	2.08	1.42	1.38
22	n	609	CLA	CHC-C1C	2.08	1.42	1.38
22	B	610	CLA	CHC-C1C	2.08	1.42	1.38
22	C	512	CLA	CHC-C1C	2.08	1.42	1.38
22	c	513	CLA	C3B-C4B	2.08	1.48	1.42
22	C	510	CLA	C3B-C4B	2.08	1.48	1.42
22	C	504	CLA	CHC-C1C	2.08	1.42	1.38
22	c	502	CLA	CMC-C2C	-2.08	1.46	1.50
22	C	515	CLA	CMC-C2C	-2.08	1.46	1.50
22	Y	611	CLA	C1B-C2B	2.08	1.48	1.43
24	G	617	XAT	C8-C7	2.08	1.37	1.32
22	g	612	CLA	CMB-C2B	-2.08	1.46	1.50
22	y	613	CLA	CMB-C2B	-2.08	1.46	1.50
22	c	514	CLA	CMC-C2C	-2.08	1.46	1.50
22	B	607	CLA	CHC-C1C	2.08	1.42	1.38
22	Y	610	CLA	CHC-C1C	2.08	1.42	1.38
22	b	610	CLA	CHC-C1C	2.08	1.42	1.38
25	Y	616	NEX	C28-C27	2.08	1.37	1.32
22	c	502	CLA	CHC-C1C	2.08	1.42	1.38
22	n	613	CLA	CMB-C2B	-2.08	1.46	1.50
22	s	312	CLA	CMB-C2B	-2.08	1.46	1.50
22	C	503	CLA	CHC-C1C	2.08	1.42	1.38
22	c	507	CLA	CMB-C2B	-2.08	1.46	1.50
22	s	311	CLA	CMB-C2B	-2.08	1.46	1.50
22	b	606	CLA	C3B-C4B	2.08	1.48	1.42
22	r	311	CLA	CHC-C1C	2.08	1.42	1.38
22	R	311	CLA	CMB-C2B	-2.08	1.46	1.50
25	r	315	NEX	C4-C3	2.08	1.55	1.52
22	y	611	CLA	CMB-C2B	-2.08	1.46	1.50
22	n	610	CLA	CHC-C1C	2.07	1.42	1.38
22	C	514	CLA	C3B-C4B	2.07	1.48	1.42
22	G	614	CLA	CMB-C2B	-2.07	1.46	1.50
22	N	603	CLA	CHC-C1C	2.07	1.42	1.38
30	a	407	PHO	C3D-C4D	2.07	1.44	1.41
22	b	614	CLA	CMC-C2C	-2.07	1.46	1.50
22	R	310	CLA	CHC-C1C	2.07	1.42	1.38
22	B	617	CLA	CMC-C2C	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	CMC-C2C	-2.07	1.46	1.50
22	B	612	CLA	CHC-C1C	2.07	1.42	1.38
22	g	611	CLA	CHC-C1C	2.07	1.42	1.38
22	B	611	CLA	CMC-C2C	-2.07	1.46	1.50
22	C	512	CLA	CMC-C2C	-2.07	1.46	1.50
22	C	513	CLA	CMC-C2C	-2.07	1.46	1.50
22	R	302	CLA	CMB-C2B	-2.07	1.46	1.50
22	b	604	CLA	CHC-C1C	2.07	1.42	1.38
31	H	101	BCR	C33-C5	-2.07	1.47	1.50
22	N	610	CLA	CMB-C2B	-2.07	1.46	1.50
22	a	405	CLA	CMC-C2C	-2.07	1.46	1.50
22	c	503	CLA	CMB-C2B	-2.07	1.46	1.50
23	r	313	LUT	C23-C24	2.07	1.53	1.50
22	a	405	CLA	C3B-C4B	2.07	1.48	1.42
22	g	611	CLA	CMC-C2C	-2.07	1.46	1.50
22	r	311	CLA	CMD-C2D	-2.07	1.46	1.50
22	G	603	CLA	CHC-C1C	2.07	1.42	1.38
22	c	507	CLA	CHC-C1C	2.07	1.42	1.38
22	c	512	CLA	CMC-C2C	-2.07	1.46	1.50
22	c	513	CLA	CMC-C2C	-2.07	1.46	1.50
22	c	504	CLA	CHC-C1C	2.07	1.42	1.38
22	c	513	CLA	CHC-C1C	2.07	1.42	1.38
22	g	602	CLA	CMD-C2D	-2.07	1.46	1.50
22	S	308	CLA	CMD-C2D	-2.07	1.46	1.50
22	w	101	CLA	CHC-C1C	2.07	1.42	1.38
22	c	513	CLA	MG-ND	-2.07	2.01	2.05
22	D	404	CLA	MG-ND	-2.07	2.01	2.05
22	b	608	CLA	CMB-C2B	-2.07	1.46	1.50
22	x	101	CLA	CMC-C2C	-2.07	1.46	1.50
23	Y	614	LUT	C28-C27	2.07	1.37	1.32
22	G	611	CLA	CMC-C2C	-2.07	1.46	1.50
22	B	609	CLA	CMB-C2B	-2.07	1.46	1.50
30	A	408	PHO	CBD-CGD	-2.07	1.49	1.52
22	b	611	CLA	CHC-C1C	2.07	1.42	1.38
22	C	513	CLA	CMD-C2D	-2.07	1.46	1.50
22	S	304	CLA	CMB-C2B	-2.07	1.46	1.50
22	A	406	CLA	C3B-C4B	2.07	1.48	1.42
22	G	611	CLA	CHC-C1C	2.06	1.42	1.38
22	c	514	CLA	CHC-C1C	2.06	1.42	1.38
22	n	612	CLA	C1B-C2B	2.06	1.48	1.43
22	d	403	CLA	MG-ND	-2.06	2.01	2.05
22	g	614	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	CMD-C2D	-2.06	1.46	1.50
24	N	616	XAT	C8-C7	2.06	1.37	1.32
22	c	509	CLA	CMC-C2C	-2.06	1.46	1.50
22	B	610	CLA	CMB-C2B	-2.06	1.46	1.50
22	y	610	CLA	CMC-C2C	-2.06	1.46	1.50
22	c	508	CLA	CMC-C2C	-2.06	1.46	1.50
33	l	101	SQD	O2-C2	-2.06	1.37	1.43
22	C	509	CLA	CMC-C2C	-2.06	1.46	1.50
22	G	613	CLA	C1B-C2B	2.06	1.48	1.43
22	g	612	CLA	CHC-C1C	2.06	1.42	1.38
22	b	613	CLA	CMC-C2C	-2.06	1.46	1.50
22	c	509	CLA	C3B-C4B	2.06	1.48	1.42
22	G	612	CLA	CHC-C1C	2.06	1.42	1.38
22	B	618	CLA	CHC-C1C	2.06	1.42	1.38
22	r	304	CLA	CHC-C1C	2.06	1.42	1.38
22	s	313	CLA	CHC-C1C	2.06	1.42	1.38
22	Y	612	CLA	CMC-C2C	-2.06	1.46	1.50
22	A	409	CLA	CMC-C2C	-2.06	1.46	1.50
22	n	611	CLA	CHC-C1C	2.06	1.42	1.38
22	b	615	CLA	CHC-C1C	2.06	1.42	1.38
35	J	101	DGD	O6D-C5D	-2.06	1.39	1.44
31	d	405	BCR	C33-C5	-2.06	1.47	1.50
35	c	518	DGD	O5D-C6D	-2.06	1.40	1.43
22	N	611	CLA	CHC-C1C	2.06	1.42	1.38
22	y	611	CLA	CMC-C2C	-2.06	1.46	1.50
22	B	616	CLA	CHC-C1C	2.06	1.42	1.38
22	b	603	CLA	CMC-C2C	-2.06	1.46	1.50
22	g	614	CLA	CMD-C2D	-2.06	1.46	1.50
22	b	604	CLA	C3B-C4B	2.06	1.48	1.42
22	C	505	CLA	CMB-C2B	-2.06	1.46	1.50
35	J	101	DGD	C4E-C5E	2.06	1.57	1.53
22	C	513	CLA	CMB-C2B	-2.05	1.46	1.50
22	G	614	CLA	CMD-C2D	-2.05	1.46	1.50
22	S	308	CLA	CMB-C2B	-2.05	1.46	1.50
22	r	303	CLA	CMD-C2D	-2.05	1.46	1.50
22	C	507	CLA	CMC-C2C	-2.05	1.46	1.50
35	c	519	DGD	C4E-C3E	2.05	1.57	1.52
22	C	508	CLA	CMB-C2B	-2.05	1.46	1.50
22	C	507	CLA	CHC-C1C	2.05	1.42	1.38
22	r	312	CLA	CMB-C2B	-2.05	1.46	1.50
22	C	504	CLA	CMC-C2C	-2.05	1.46	1.50
22	A	406	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	312	CLA	CMC-C2C	-2.05	1.46	1.50
22	s	309	CLA	CMD-C2D	-2.05	1.46	1.50
22	C	514	CLA	MG-ND	-2.05	2.01	2.05
22	r	311	CLA	MG-NB	-2.05	2.01	2.05
22	s	308	CLA	CMB-C2B	-2.05	1.46	1.50
22	s	308	CLA	CHC-C1C	2.05	1.42	1.38
24	R	313	XAT	C18-C5	2.05	1.54	1.51
22	S	313	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	607	CLA	MG-ND	-2.05	2.01	2.05
22	B	608	CLA	CHC-C1C	2.05	1.42	1.38
22	B	615	CLA	CHC-C1C	2.05	1.42	1.38
22	N	613	CLA	CMC-C2C	-2.05	1.46	1.50
22	b	609	CLA	CMC-C2C	-2.05	1.46	1.50
22	D	405	CLA	CMC-C2C	-2.05	1.46	1.50
22	b	603	CLA	CHC-C1C	2.05	1.42	1.38
22	c	509	CLA	CHC-C1C	2.05	1.42	1.38
30	D	401	PHO	C4D-ND	-2.05	1.35	1.38
22	b	605	CLA	CHC-C1C	2.04	1.42	1.38
24	R	313	XAT	C28-C27	2.04	1.37	1.32
22	g	614	CLA	CMC-C2C	-2.04	1.46	1.50
32	D	407	PL9	C31-C29	-2.04	1.47	1.51
22	y	611	CLA	CHC-C1C	2.04	1.42	1.38
26	r	302	LHG	P-O6	2.04	1.67	1.59
22	B	603	CLA	CHC-C1C	2.04	1.42	1.38
22	W	101	CLA	CHC-C1C	2.04	1.42	1.38
22	B	615	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	608	CLA	CMC-C2C	-2.04	1.46	1.50
33	A	412	SQD	O2-C2	-2.04	1.37	1.43
22	N	613	CLA	CMD-C2D	-2.04	1.46	1.50
22	c	504	CLA	CMB-C2B	-2.04	1.46	1.50
22	y	613	CLA	CMD-C2D	-2.04	1.46	1.50
22	r	304	CLA	CMC-C2C	-2.04	1.46	1.50
22	R	302	CLA	CMD-C2D	-2.04	1.46	1.50
22	D	405	CLA	CHC-C1C	2.04	1.42	1.38
22	C	510	CLA	CMC-C2C	-2.04	1.46	1.50
22	S	305	CLA	CMC-C2C	-2.04	1.46	1.50
22	c	510	CLA	CMB-C2B	-2.04	1.46	1.50
22	b	612	CLA	CHC-C1C	2.04	1.42	1.38
22	C	514	CLA	CHC-C1C	2.04	1.42	1.38
33	l	103	SQD	O2-C2	-2.04	1.37	1.43
22	b	608	CLA	CMC-C2C	-2.04	1.46	1.50
22	s	310	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	303	CLA	CMC-C2C	-2.04	1.46	1.50
22	r	303	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	607	CLA	C3B-C4B	2.04	1.48	1.42
22	c	511	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	606	CLA	CMC-C2C	-2.04	1.46	1.50
22	A	405	CLA	CHC-C1C	2.04	1.42	1.38
22	C	510	CLA	CHC-C1C	2.04	1.42	1.38
30	d	401	PHO	C4D-ND	-2.04	1.35	1.38
22	d	404	CLA	CMC-C2C	-2.04	1.46	1.50
24	r	314	XAT	C28-C27	2.04	1.37	1.32
31	k	102	BCR	C33-C5	-2.03	1.47	1.50
22	r	305	CLA	CMC-C2C	-2.03	1.46	1.50
35	c	519	DGD	C4E-C5E	2.03	1.57	1.53
22	g	610	CLA	CMC-C2C	-2.03	1.46	1.50
22	B	606	CLA	CHC-C1C	2.03	1.42	1.38
22	C	505	CLA	CMC-C2C	-2.03	1.46	1.50
22	B	613	CLA	CHC-C1C	2.03	1.42	1.38
24	y	615	XAT	O4-C5	-2.03	1.43	1.46
25	n	616	NEX	C28-C27	2.03	1.37	1.32
22	x	101	CLA	CHC-C1C	2.03	1.42	1.38
37	F	101	HEM	C3B-C4B	2.03	1.48	1.44
35	J	101	DGD	C4E-C3E	2.03	1.57	1.52
22	b	615	CLA	CMC-C2C	-2.03	1.46	1.50
22	C	504	CLA	MG-ND	-2.03	2.01	2.05
22	n	610	CLA	CMC-C2C	-2.03	1.46	1.50
31	A	410	BCR	C38-C26	-2.03	1.47	1.50
22	y	603	CLA	CMC-C2C	-2.03	1.46	1.50
24	Y	615	XAT	O4-C5	-2.03	1.43	1.46
22	Y	612	CLA	CMD-C2D	-2.03	1.46	1.50
30	a	407	PHO	CBD-CGD	-2.03	1.49	1.52
35	c	519	DGD	O6D-C5D	-2.03	1.39	1.44
22	b	604	CLA	MG-ND	-2.03	2.01	2.05
22	R	302	CLA	CMC-C2C	-2.03	1.46	1.50
26	R	301	LHG	P-O6	2.03	1.67	1.59
31	c	515	BCR	C38-C26	-2.03	1.47	1.50
30	d	401	PHO	C3B-C2B	-2.03	1.37	1.40
22	y	613	CLA	CMC-C2C	-2.03	1.46	1.50
22	b	605	CLA	CMC-C2C	-2.03	1.46	1.50
22	S	304	CLA	CMC-C2C	-2.03	1.46	1.50
22	Y	610	CLA	CMC-C2C	-2.03	1.46	1.50
23	N	615	LUT	C31-C32	2.03	1.40	1.34
22	R	310	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	304	CLA	CMC-C2C	-2.02	1.46	1.50
24	g	617	XAT	O4-C5	-2.02	1.43	1.46
22	N	603	CLA	CMC-C2C	-2.02	1.46	1.50
22	r	312	CLA	CHC-C1C	2.02	1.42	1.38
31	c	516	BCR	C33-C5	-2.02	1.47	1.50
22	N	610	CLA	CMC-C2C	-2.02	1.46	1.50
22	c	512	CLA	CMB-C2B	-2.02	1.46	1.50
26	B	622	LHG	P-O6	2.02	1.67	1.59
22	g	603	CLA	CMC-C2C	-2.02	1.46	1.50
22	R	304	CLA	C3B-C4B	2.02	1.48	1.42
22	s	313	CLA	CMC-C2C	-2.02	1.46	1.50
22	B	618	CLA	CMC-C2C	-2.02	1.46	1.50
22	R	311	CLA	CMC-C2C	-2.02	1.46	1.50
22	a	404	CLA	CHC-C1C	2.02	1.42	1.38
22	C	511	CLA	CMB-C2B	-2.02	1.46	1.50
36	B	601	LMG	O7-C8	-2.02	1.41	1.46
35	C	519	DGD	O5D-C6D	-2.02	1.40	1.43
22	N	609	CLA	CMC-C2C	-2.02	1.46	1.50
22	b	612	CLA	CMC-C2C	-2.02	1.46	1.50
22	n	603	CLA	MG-ND	-2.02	2.01	2.05
22	S	310	CLA	CMB-C2B	-2.02	1.46	1.50
23	n	614	LUT	C23-C24	2.02	1.53	1.50
22	y	603	CLA	MG-ND	-2.02	2.01	2.05
22	R	308	CLA	CMC-C2C	-2.02	1.46	1.50
22	C	512	CLA	MG-ND	-2.02	2.01	2.05
22	g	604	CLA	CMC-C2C	-2.01	1.46	1.50
33	L	101	SQD	O4-C4	-2.01	1.38	1.43
22	S	309	CLA	CMD-C2D	-2.01	1.46	1.50
30	D	401	PHO	CBD-CGD	-2.01	1.50	1.52
22	n	613	CLA	CMC-C2C	-2.01	1.46	1.50
22	Y	603	CLA	CMC-C2C	-2.01	1.46	1.50
24	g	617	XAT	C28-C27	2.01	1.37	1.32
22	a	405	CLA	MG-ND	-2.01	2.01	2.05
22	g	613	CLA	CMB-C2B	-2.01	1.46	1.50
22	s	311	CLA	CMC-C2C	-2.01	1.46	1.50
33	D	402	SQD	O47-C45	-2.01	1.41	1.46
31	a	409	BCR	C38-C26	-2.01	1.47	1.50
33	a	411	SQD	O2-C2	-2.01	1.38	1.43
22	Y	609	CLA	CMC-C2C	-2.01	1.46	1.50
22	c	503	CLA	MG-ND	-2.01	2.01	2.05
22	s	312	CLA	CMC-C2C	-2.01	1.46	1.50
22	Y	602	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	304	CLA	CMC-C2C	-2.01	1.46	1.50
33	L	101	SQD	O3-C3	-2.01	1.38	1.43
22	c	511	CLA	MG-ND	-2.01	2.01	2.05
22	Y	604	CLA	CMC-C2C	-2.01	1.46	1.50
22	Y	603	CLA	MG-ND	-2.01	2.01	2.05
26	b	619	LHG	P-O6	2.01	1.67	1.59
22	n	603	CLA	CMC-C2C	-2.01	1.46	1.50
22	G	603	CLA	CMC-C2C	-2.01	1.46	1.50
22	r	309	CLA	CMC-C2C	-2.01	1.46	1.50
22	w	101	CLA	CMC-C2C	-2.01	1.46	1.50
22	s	305	CLA	CHC-C1C	2.01	1.42	1.38
31	K	102	BCR	C33-C5	-2.00	1.47	1.50
31	D	406	BCR	C33-C5	-2.00	1.47	1.50
22	G	614	CLA	CMC-C2C	-2.00	1.46	1.50
22	c	506	CLA	CHC-C1C	2.00	1.42	1.38
22	g	602	CLA	CMC-C2C	-2.00	1.46	1.50
22	a	405	CLA	CHC-C1C	2.00	1.42	1.38
25	N	617	NEX	C28-C27	2.00	1.37	1.32
22	S	311	CLA	CMC-C2C	-2.00	1.46	1.50
22	A	409	CLA	CHC-C1C	2.00	1.42	1.38
22	S	305	CLA	CHC-C1C	2.00	1.42	1.38
22	y	604	CLA	CMC-C2C	-2.00	1.46	1.50
33	D	402	SQD	O3-C3	-2.00	1.38	1.43
22	s	305	CLA	CMC-C2C	-2.00	1.46	1.50
22	N	603	CLA	MG-ND	-2.00	2.01	2.05

All (2953) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	617	XAT	O24-C25-C24	-62.78	54.66	113.49
24	N	616	XAT	O24-C25-C24	-62.64	54.78	113.49
24	R	313	XAT	O24-C25-C24	-62.35	55.06	113.49
24	r	314	XAT	O24-C25-C24	-62.32	55.08	113.49
24	g	617	XAT	O24-C25-C24	-62.20	55.19	113.49
24	n	615	XAT	O24-C25-C24	-61.90	55.48	113.49
24	y	615	XAT	O24-C25-C24	-61.90	55.48	113.49
24	Y	615	XAT	O24-C25-C24	-61.87	55.50	113.49
25	n	616	NEX	C8-C7-C6	-48.98	119.86	177.66
25	g	618	NEX	C8-C7-C6	-48.86	120.01	177.66
25	Y	616	NEX	C8-C7-C6	-48.06	120.95	177.66
25	y	616	NEX	C8-C7-C6	-48.01	121.01	177.66
25	N	617	NEX	O24-C25-C24	-41.57	74.53	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	617	NEX	C8-C7-C6	-41.53	128.66	177.66
25	y	616	NEX	O24-C25-C24	-40.97	75.09	113.49
24	n	615	XAT	O4-C5-C4	40.63	151.57	113.49
25	n	616	NEX	O24-C25-C24	-40.15	75.86	113.49
24	N	616	XAT	O4-C5-C4	39.58	150.59	113.49
25	g	618	NEX	O24-C25-C24	-39.42	76.54	113.49
24	r	314	XAT	O4-C5-C4	39.20	150.23	113.49
24	R	313	XAT	O4-C5-C4	39.17	150.20	113.49
24	g	617	XAT	O4-C5-C4	38.71	149.78	113.49
24	Y	615	XAT	O4-C5-C4	38.32	149.41	113.49
24	y	615	XAT	O4-C5-C4	38.21	149.30	113.49
25	Y	616	NEX	O24-C25-C24	-38.03	77.85	113.49
24	G	617	XAT	O4-C5-C4	37.94	149.05	113.49
25	y	618	NEX	C8-C7-C6	-35.91	135.29	177.66
25	r	315	NEX	C8-C7-C6	-35.88	135.33	177.66
25	y	618	NEX	O24-C25-C24	-35.02	80.67	113.49
25	r	315	NEX	O24-C25-C24	-35.02	80.67	113.49
37	F	101	HEM	C3B-C4B-NB	-14.78	98.85	109.47
37	f	101	HEM	C3B-C4B-NB	-14.78	98.86	109.47
24	N	616	XAT	C31-C30-C29	-12.96	109.10	127.28
23	R	312	LUT	C18-C5-C6	-12.60	110.74	124.48
23	r	313	LUT	C18-C5-C6	-12.56	110.77	124.48
23	Y	613	LUT	C18-C5-C6	-12.37	110.98	124.48
23	n	614	LUT	C18-C5-C6	-12.37	110.99	124.48
23	y	614	LUT	C18-C5-C6	-12.37	110.99	124.48
23	G	615	LUT	C18-C5-C6	-12.36	111.00	124.48
23	N	614	LUT	C18-C5-C6	-12.36	111.00	124.48
23	g	615	LUT	C18-C5-C6	-12.36	111.00	124.48
24	Y	615	XAT	C11-C10-C9	-12.20	110.17	127.28
24	G	617	XAT	C31-C30-C29	-11.80	110.73	127.28
24	g	617	XAT	C31-C30-C29	-11.67	110.92	127.28
23	y	614	LUT	C1-C6-C5	-11.64	106.73	122.64
23	N	614	LUT	C1-C6-C5	-11.64	106.73	122.64
23	g	615	LUT	C1-C6-C5	-11.63	106.74	122.64
23	Y	613	LUT	C1-C6-C5	-11.63	106.74	122.64
23	G	615	LUT	C1-C6-C5	-11.63	106.74	122.64
23	n	614	LUT	C1-C6-C5	-11.62	106.76	122.64
24	y	615	XAT	C11-C10-C9	-11.60	111.01	127.28
23	n	614	LUT	C35-C34-C33	-11.59	111.02	127.28
24	n	615	XAT	C31-C30-C29	-11.59	111.02	127.28
23	g	615	LUT	C35-C34-C33	-11.59	111.02	127.28
23	G	615	LUT	C35-C34-C33	-11.59	111.03	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	y	614	LUT	C35-C34-C33	-11.57	111.05	127.28
23	N	614	LUT	C35-C34-C33	-11.57	111.05	127.28
23	Y	613	LUT	C35-C34-C33	-11.56	111.07	127.28
23	Y	614	LUT	C18-C5-C6	-11.36	112.09	124.48
24	n	615	XAT	C35-C34-C33	-11.35	111.36	127.28
24	Y	615	XAT	C31-C30-C29	-11.21	111.55	127.28
24	y	615	XAT	C31-C30-C29	-11.12	111.68	127.28
24	N	616	XAT	C35-C34-C33	-11.10	111.71	127.28
23	R	312	LUT	C15-C14-C13	-11.00	111.85	127.28
23	r	313	LUT	C15-C14-C13	-10.97	111.89	127.28
23	G	616	LUT	C18-C5-C6	-10.94	112.55	124.48
23	g	616	LUT	C18-C5-C6	-10.90	112.59	124.48
24	r	314	XAT	C35-C34-C33	-10.82	112.10	127.28
25	N	617	NEX	C31-C30-C29	-10.81	112.12	127.28
24	R	313	XAT	C35-C34-C33	-10.80	112.12	127.28
23	r	313	LUT	C31-C30-C29	-10.76	112.19	127.28
23	R	312	LUT	C31-C30-C29	-10.75	112.20	127.28
25	g	618	NEX	C15-C14-C13	-10.69	112.28	127.28
23	G	615	LUT	C31-C30-C29	-10.68	112.29	127.28
23	N	614	LUT	C31-C30-C29	-10.68	112.30	127.28
23	y	614	LUT	C31-C30-C29	-10.68	112.30	127.28
23	n	614	LUT	C31-C30-C29	-10.67	112.31	127.28
23	g	615	LUT	C31-C30-C29	-10.67	112.32	127.28
24	N	616	XAT	C11-C10-C9	-10.66	112.32	127.28
23	Y	613	LUT	C31-C30-C29	-10.66	112.33	127.28
24	g	617	XAT	C35-C34-C33	-10.58	112.44	127.28
23	g	615	LUT	C11-C10-C9	-10.54	112.49	127.28
23	Y	613	LUT	C11-C10-C9	-10.54	112.50	127.28
23	G	615	LUT	C11-C10-C9	-10.54	112.50	127.28
25	Y	616	NEX	C15-C14-C13	-10.53	112.50	127.28
23	n	614	LUT	C11-C10-C9	-10.53	112.51	127.28
23	y	614	LUT	C11-C10-C9	-10.52	112.52	127.28
25	N	617	NEX	C11-C10-C9	-10.52	112.52	127.28
24	r	314	XAT	C15-C14-C13	-10.52	112.53	127.28
23	N	614	LUT	C11-C10-C9	-10.51	112.53	127.28
24	R	313	XAT	C15-C14-C13	-10.49	112.57	127.28
23	R	312	LUT	C11-C10-C9	-10.43	112.65	127.28
25	g	618	NEX	C35-C34-C33	-10.40	112.69	127.28
23	R	312	LUT	C35-C34-C33	-10.37	112.73	127.28
23	r	313	LUT	C11-C10-C9	-10.37	112.74	127.28
24	n	615	XAT	C11-C10-C9	-10.36	112.75	127.28
23	r	313	LUT	C35-C34-C33	-10.34	112.77	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	617	XAT	C11-C10-C9	-10.28	112.86	127.28
24	G	617	XAT	C35-C34-C33	-10.23	112.93	127.28
25	r	315	NEX	C15-C14-C13	-10.18	113.00	127.28
25	y	618	NEX	C15-C14-C13	-10.16	113.03	127.28
24	Y	615	XAT	C35-C34-C33	-10.15	113.05	127.28
23	y	614	LUT	C15-C14-C13	-10.14	113.05	127.28
23	n	614	LUT	C15-C14-C13	-10.14	113.06	127.28
24	R	313	XAT	C31-C30-C29	-10.14	113.06	127.28
24	r	314	XAT	C31-C30-C29	-10.14	113.06	127.28
23	g	615	LUT	C15-C14-C13	-10.13	113.07	127.28
23	G	615	LUT	C15-C14-C13	-10.12	113.08	127.28
23	Y	613	LUT	C15-C14-C13	-10.11	113.09	127.28
23	N	614	LUT	C15-C14-C13	-10.10	113.12	127.28
24	y	615	XAT	C35-C34-C33	-10.07	113.16	127.28
23	Y	613	LUT	C20-C13-C14	-9.94	106.71	122.82
23	y	614	LUT	C20-C13-C14	-9.93	106.73	122.82
23	N	614	LUT	C20-C13-C14	-9.93	106.73	122.82
23	g	615	LUT	C20-C13-C14	-9.92	106.74	122.82
23	n	614	LUT	C20-C13-C14	-9.90	106.77	122.82
23	G	615	LUT	C20-C13-C14	-9.90	106.78	122.82
25	y	616	NEX	C15-C14-C13	-9.79	113.55	127.28
25	y	618	NEX	C11-C10-C9	-9.78	113.56	127.28
24	G	617	XAT	C11-C10-C9	-9.76	113.58	127.28
25	r	315	NEX	C11-C10-C9	-9.76	113.59	127.28
24	N	616	XAT	C15-C14-C13	-9.73	113.63	127.28
25	n	616	NEX	C15-C14-C13	-9.71	113.65	127.28
25	g	618	NEX	C31-C30-C29	-9.70	113.67	127.28
24	N	616	XAT	C18-C5-C4	-9.70	103.35	114.24
24	n	615	XAT	C18-C5-C4	-9.68	103.36	114.24
25	r	315	NEX	C35-C34-C33	-9.66	113.73	127.28
23	N	615	LUT	C1-C6-C5	-9.65	109.45	122.64
25	y	618	NEX	C35-C34-C33	-9.64	113.76	127.28
23	g	616	LUT	C15-C14-C13	-9.62	113.79	127.28
24	G	617	XAT	C15-C14-C13	-9.60	113.81	127.28
23	Y	614	LUT	C35-C34-C33	-9.55	113.89	127.28
24	g	617	XAT	C15-C14-C13	-9.52	113.92	127.28
25	r	315	NEX	C31-C30-C29	-9.52	113.93	127.28
25	y	618	NEX	C31-C30-C29	-9.51	113.93	127.28
25	N	617	NEX	C15-C14-C13	-9.50	113.95	127.28
22	c	510	CLA	C2D-C1D-ND	-9.49	100.74	110.13
25	r	315	NEX	O24-C25-C38	-9.48	104.46	115.05
24	r	314	XAT	C18-C5-C4	-9.47	103.60	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	615	XAT	C15-C14-C13	-9.47	113.99	127.28
22	C	511	CLA	C2D-C1D-ND	-9.46	100.76	110.13
24	R	313	XAT	C18-C5-C4	-9.46	103.61	114.24
24	G	617	XAT	C18-C5-C4	-9.45	103.62	114.24
23	Y	614	LUT	C15-C14-C13	-9.45	114.03	127.28
25	y	618	NEX	O24-C25-C38	-9.44	104.50	115.05
23	G	616	LUT	C35-C34-C33	-9.44	114.04	127.28
24	g	617	XAT	C18-C5-C4	-9.44	103.64	114.24
24	n	615	XAT	C15-C14-C13	-9.43	114.05	127.28
25	Y	616	NEX	C31-C30-C29	-9.41	114.09	127.28
24	y	615	XAT	C18-C5-C4	-9.40	103.68	114.24
23	G	616	LUT	C11-C10-C9	-9.35	114.17	127.28
23	g	616	LUT	C31-C30-C29	-9.33	114.20	127.28
25	y	616	NEX	C35-C34-C33	-9.31	114.22	127.28
25	n	616	NEX	C35-C34-C33	-9.31	114.22	127.28
25	Y	616	NEX	C11-C10-C9	-9.29	114.24	127.28
23	G	616	LUT	C19-C9-C10	-9.29	107.77	122.82
25	n	616	NEX	C31-C30-C29	-9.28	114.26	127.28
24	Y	615	XAT	C18-C5-C4	-9.21	103.89	114.24
23	N	615	LUT	C15-C14-C13	-9.21	114.36	127.28
23	g	616	LUT	C35-C34-C33	-9.21	114.36	127.28
37	f	101	HEM	C1B-NB-C4B	9.19	116.09	105.21
37	F	101	HEM	C1B-NB-C4B	9.19	116.09	105.21
23	G	616	LUT	C15-C14-C13	-9.18	114.40	127.28
25	n	616	NEX	C40-C33-C34	-9.15	108.00	122.82
23	N	615	LUT	C18-C5-C6	-9.14	114.51	124.48
25	n	616	NEX	C11-C10-C9	-9.14	114.46	127.28
24	Y	615	XAT	C15-C14-C13	-9.12	114.48	127.28
25	y	616	NEX	C31-C30-C29	-9.11	114.51	127.28
24	n	615	XAT	O4-C5-C18	-9.07	104.91	115.05
23	G	616	LUT	C31-C30-C29	-9.07	114.56	127.28
23	N	615	LUT	C35-C34-C33	-9.06	114.57	127.28
23	Y	614	LUT	C19-C9-C10	-9.06	108.14	122.82
25	g	618	NEX	C11-C10-C9	-9.05	114.58	127.28
25	Y	616	NEX	C39-C29-C30	-9.05	108.16	122.82
23	g	616	LUT	C19-C9-C10	-9.05	108.16	122.82
23	Y	614	LUT	C1-C6-C5	-9.03	110.30	122.64
25	g	618	NEX	C40-C33-C34	-8.95	108.31	122.82
23	g	616	LUT	C11-C10-C9	-8.82	114.91	127.28
25	y	616	NEX	C11-C10-C9	-8.80	114.93	127.28
24	r	314	XAT	C20-C13-C14	-8.80	108.55	122.82
24	R	313	XAT	C20-C13-C14	-8.80	108.56	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	614	LUT	C11-C10-C9	-8.79	114.96	127.28
24	Y	615	XAT	C19-C9-C10	-8.74	108.65	122.82
24	N	616	XAT	C18-C5-C6	-8.68	108.01	122.30
24	y	615	XAT	C19-C9-C10	-8.65	108.81	122.82
24	N	616	XAT	C39-C29-C30	-8.63	108.83	122.82
25	y	616	NEX	C40-C33-C34	-8.63	108.84	122.82
25	y	618	NEX	C39-C29-C30	-8.60	108.89	122.82
24	y	615	XAT	C18-C5-C6	-8.59	108.17	122.30
23	g	616	LUT	C1-C6-C5	-8.58	110.92	122.64
25	r	315	NEX	C39-C29-C30	-8.57	108.94	122.82
24	G	617	XAT	C18-C5-C6	-8.53	108.27	122.30
23	G	616	LUT	C1-C6-C5	-8.52	111.00	122.64
24	n	615	XAT	C40-C33-C34	-8.47	109.09	122.82
25	Y	616	NEX	C20-C13-C14	-8.45	109.13	122.82
23	R	312	LUT	C19-C9-C10	-8.44	109.14	122.82
24	r	314	XAT	C11-C10-C9	-8.44	115.44	127.28
24	R	313	XAT	C11-C10-C9	-8.43	115.45	127.28
21	s	307	CHL	O2D-CGD-CBD	8.43	120.21	110.95
24	G	617	XAT	C39-C29-C30	-8.43	109.16	122.82
24	n	615	XAT	C39-C29-C30	-8.43	109.16	122.82
23	r	313	LUT	C19-C9-C10	-8.43	109.16	122.82
21	R	306	CHL	O2D-CGD-CBD	8.42	120.20	110.95
21	G	608	CHL	O2D-CGD-CBD	8.42	120.20	110.95
21	G	601	CHL	O2D-CGD-CBD	8.42	120.20	110.95
21	y	606	CHL	O2D-CGD-CBD	8.42	120.20	110.95
21	n	605	CHL	O2D-CGD-CBD	8.42	120.19	110.95
21	G	606	CHL	O2D-CGD-CBD	8.42	120.19	110.95
21	S	302	CHL	O2D-CGD-CBD	8.42	120.19	110.95
21	Y	601	CHL	O2D-CGD-CBD	8.41	120.19	110.95
21	g	601	CHL	O2D-CGD-CBD	8.41	120.19	110.95
21	N	601	CHL	O2D-CGD-CBD	8.41	120.19	110.95
21	y	608	CHL	O2D-CGD-CBD	8.41	120.18	110.95
21	s	302	CHL	O2D-CGD-CBD	8.41	120.18	110.95
21	n	606	CHL	O2D-CGD-CBD	8.40	120.18	110.95
21	R	307	CHL	O2D-CGD-CBD	8.40	120.18	110.95
21	s	306	CHL	O2D-CGD-CBD	8.40	120.18	110.95
21	s	301	CHL	O2D-CGD-CBD	8.40	120.17	110.95
25	Y	616	NEX	C35-C34-C33	-8.40	115.50	127.28
21	Y	607	CHL	O2D-CGD-CBD	8.39	120.17	110.95
21	g	609	CHL	O2D-CGD-CBD	8.39	120.17	110.95
23	R	312	LUT	C39-C29-C30	-8.39	109.22	122.82
21	n	607	CHL	O2D-CGD-CBD	8.39	120.16	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	606	CHL	O2D-CGD-CBD	8.39	120.16	110.95
21	Y	606	CHL	O2D-CGD-CBD	8.39	120.16	110.95
21	Y	608	CHL	O2D-CGD-CBD	8.39	120.16	110.95
21	S	307	CHL	O2D-CGD-CBD	8.39	120.16	110.95
21	G	607	CHL	O2D-CGD-CBD	8.38	120.16	110.95
21	y	601	CHL	O2D-CGD-CBD	8.38	120.16	110.95
21	r	301	CHL	O2D-CGD-CBD	8.38	120.16	110.95
21	n	601	CHL	O2D-CGD-CBD	8.38	120.15	110.95
21	r	307	CHL	O2D-CGD-CBD	8.38	120.15	110.95
23	r	313	LUT	C39-C29-C30	-8.37	109.25	122.82
21	y	609	CHL	O2D-CGD-CBD	8.37	120.15	110.95
21	g	606	CHL	O2D-CGD-CBD	8.37	120.15	110.95
24	g	617	XAT	C39-C29-C30	-8.37	109.25	122.82
21	g	605	CHL	O2D-CGD-CBD	8.37	120.15	110.95
21	n	608	CHL	O2D-CGD-CBD	8.37	120.15	110.95
21	N	608	CHL	O2D-CGD-CBD	8.37	120.15	110.95
21	Y	605	CHL	O2D-CGD-CBD	8.37	120.15	110.95
21	r	306	CHL	O2D-CGD-CBD	8.37	120.15	110.95
21	g	607	CHL	O2D-CGD-CBD	8.37	120.14	110.95
21	r	308	CHL	O2D-CGD-CBD	8.37	120.14	110.95
21	G	609	CHL	O2D-CGD-CBD	8.37	120.14	110.95
21	S	306	CHL	O2D-CGD-CBD	8.37	120.14	110.95
21	N	605	CHL	O2D-CGD-CBD	8.37	120.14	110.95
21	R	305	CHL	O2D-CGD-CBD	8.37	120.14	110.95
21	N	607	CHL	O2D-CGD-CBD	8.37	120.14	110.95
21	S	301	CHL	O2D-CGD-CBD	8.37	120.14	110.95
21	G	605	CHL	O2D-CGD-CBD	8.36	120.14	110.95
24	Y	615	XAT	C40-C33-C34	-8.36	109.27	122.82
21	y	607	CHL	O2D-CGD-CBD	8.36	120.13	110.95
25	n	616	NEX	C20-C13-C14	-8.35	109.28	122.82
24	g	617	XAT	C40-C33-C34	-8.35	109.29	122.82
24	r	314	XAT	O4-C5-C18	-8.35	105.72	115.05
21	g	608	CHL	O2D-CGD-CBD	8.34	120.11	110.95
24	y	615	XAT	C39-C29-C30	-8.34	109.31	122.82
24	R	313	XAT	O4-C5-C18	-8.33	105.74	115.05
23	y	614	LUT	C40-C33-C34	-8.33	109.33	122.82
21	y	605	CHL	O2D-CGD-CBD	8.32	120.09	110.95
23	N	614	LUT	C40-C33-C34	-8.32	109.33	122.82
25	r	315	NEX	C40-C33-C34	-8.32	109.34	122.82
23	g	615	LUT	C40-C33-C34	-8.32	109.34	122.82
24	r	314	XAT	C39-C29-C30	-8.31	109.34	122.82
23	n	614	LUT	C40-C33-C34	-8.31	109.35	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	615	XAT	C39-C29-C30	-8.30	109.36	122.82
24	R	313	XAT	C40-C33-C34	-8.30	109.36	122.82
25	g	618	NEX	C20-C13-C14	-8.30	109.37	122.82
24	R	313	XAT	C39-C29-C30	-8.28	109.40	122.82
23	G	615	LUT	C40-C33-C34	-8.28	109.40	122.82
24	g	617	XAT	C18-C5-C6	-8.28	108.67	122.30
23	Y	613	LUT	C40-C33-C34	-8.28	109.40	122.82
24	y	615	XAT	C40-C33-C34	-8.27	109.41	122.82
24	r	314	XAT	C40-C33-C34	-8.27	109.41	122.82
25	N	617	NEX	C20-C13-C14	-8.27	109.42	122.82
25	y	618	NEX	C40-C33-C34	-8.27	109.42	122.82
24	G	617	XAT	C40-C33-C34	-8.24	109.46	122.82
24	N	616	XAT	O4-C5-C18	-8.21	105.88	115.05
25	y	618	NEX	C19-C9-C10	-8.20	109.53	122.82
24	g	617	XAT	C19-C9-C10	-8.20	109.53	122.82
25	r	315	NEX	C19-C9-C10	-8.20	109.53	122.82
25	y	616	NEX	C20-C13-C14	-8.20	109.53	122.82
25	g	618	NEX	C39-C29-C30	-8.19	109.54	122.82
23	R	312	LUT	C40-C33-C34	-8.19	109.55	122.82
24	y	615	XAT	C20-C13-C14	-8.19	109.55	122.82
25	N	617	NEX	C19-C9-C10	-8.18	109.56	122.82
24	Y	615	XAT	C20-C13-C14	-8.18	109.56	122.82
25	N	617	NEX	C35-C34-C33	-8.18	115.81	127.28
23	N	615	LUT	C19-C9-C10	-8.17	109.58	122.82
24	N	616	XAT	C19-C9-C10	-8.17	109.58	122.82
24	n	615	XAT	C18-C5-C6	-8.17	108.86	122.30
25	y	618	NEX	C20-C13-C14	-8.17	109.58	122.82
25	r	315	NEX	C20-C13-C14	-8.17	109.58	122.82
23	r	313	LUT	C40-C33-C34	-8.16	109.60	122.82
23	N	615	LUT	C20-C13-C14	-8.16	109.60	122.82
23	Y	614	LUT	C20-C13-C14	-8.15	109.61	122.82
24	N	616	XAT	C40-C33-C34	-8.15	109.62	122.82
24	g	617	XAT	C20-C13-C14	-8.12	109.66	122.82
24	N	616	XAT	C20-C13-C14	-8.12	109.66	122.82
24	n	615	XAT	C19-C9-C10	-8.09	109.70	122.82
24	n	615	XAT	C20-C13-C14	-8.08	109.72	122.82
24	Y	615	XAT	C18-C5-C6	-8.06	109.03	122.30
24	G	617	XAT	C20-C13-C14	-8.05	109.77	122.82
23	g	616	LUT	C39-C29-C30	-8.02	109.83	122.82
25	N	617	NEX	C40-C33-C34	-8.00	109.86	122.82
23	g	615	LUT	C19-C9-C10	-7.94	109.95	122.82
24	G	617	XAT	C19-C9-C10	-7.93	109.97	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	r	314	XAT	C18-C5-C6	-7.92	109.26	122.30
23	G	615	LUT	C19-C9-C10	-7.91	109.99	122.82
23	N	614	LUT	C19-C9-C10	-7.91	110.00	122.82
23	y	614	LUT	C19-C9-C10	-7.91	110.00	122.82
23	Y	613	LUT	C19-C9-C10	-7.91	110.00	122.82
23	n	614	LUT	C19-C9-C10	-7.91	110.01	122.82
23	G	616	LUT	C39-C29-C30	-7.90	110.01	122.82
23	g	615	LUT	C39-C29-C30	-7.90	110.02	122.82
23	G	615	LUT	C39-C29-C30	-7.90	110.02	122.82
23	Y	613	LUT	C39-C29-C30	-7.90	110.02	122.82
24	r	314	XAT	C19-C9-C10	-7.89	110.03	122.82
24	R	313	XAT	C18-C5-C6	-7.88	109.33	122.30
23	y	614	LUT	C39-C29-C30	-7.88	110.05	122.82
23	n	614	LUT	C39-C29-C30	-7.88	110.06	122.82
24	R	313	XAT	C19-C9-C10	-7.87	110.07	122.82
24	y	615	XAT	O4-C6-C7	-7.86	94.35	116.88
24	Y	615	XAT	O4-C6-C7	-7.86	94.35	116.88
23	N	614	LUT	C39-C29-C30	-7.85	110.09	122.82
25	N	617	NEX	C39-C29-C30	-7.85	110.10	122.82
25	n	616	NEX	C19-C9-C10	-7.84	110.11	122.82
25	Y	616	NEX	C40-C33-C34	-7.84	110.11	122.82
25	n	616	NEX	C39-C29-C30	-7.84	110.12	122.82
24	Y	615	XAT	O4-C5-C18	-7.82	106.31	115.05
23	Y	614	LUT	C39-C29-C30	-7.81	110.16	122.82
24	g	617	XAT	O4-C5-C18	-7.79	106.34	115.05
37	f	101	HEM	C4D-ND-C1D	7.79	114.43	105.21
23	Y	614	LUT	C40-C33-C34	-7.75	110.26	122.82
37	F	101	HEM	C4D-ND-C1D	7.75	114.38	105.21
23	G	616	LUT	C20-C13-C14	-7.74	110.28	122.82
23	g	616	LUT	C40-C33-C34	-7.73	110.30	122.82
25	y	616	NEX	C19-C9-C10	-7.69	110.36	122.82
23	g	616	LUT	C20-C13-C14	-7.66	110.41	122.82
25	y	618	NEX	C16-C1-C6	7.66	117.32	110.47
24	G	617	XAT	O4-C6-C7	-7.66	94.95	116.88
25	r	315	NEX	C16-C1-C6	7.66	117.32	110.47
25	Y	616	NEX	C19-C9-C10	-7.65	110.43	122.82
23	Y	614	LUT	C31-C30-C29	-7.63	116.57	127.28
23	G	616	LUT	C40-C33-C34	-7.61	110.48	122.82
25	g	618	NEX	C19-C9-C10	-7.55	110.58	122.82
24	y	615	XAT	O4-C5-C18	-7.49	106.67	115.05
25	y	616	NEX	C39-C29-C30	-7.47	110.72	122.82
24	g	617	XAT	O4-C6-C7	-7.47	95.49	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	615	XAT	C7-C8-C9	-7.45	113.96	125.53
23	N	615	LUT	C38-C25-C24	-7.42	105.79	123.36
23	N	615	LUT	C40-C33-C34	-7.41	110.81	122.82
23	R	312	LUT	C20-C13-C14	-7.37	110.87	122.82
23	r	313	LUT	C20-C13-C14	-7.37	110.88	122.82
37	f	101	HEM	C3B-C2B-C1B	7.32	111.91	106.41
23	N	615	LUT	C39-C29-C30	-7.31	110.98	122.82
37	F	101	HEM	C3B-C2B-C1B	7.30	111.89	106.41
24	N	616	XAT	O4-C6-C7	-7.28	96.04	116.88
22	g	613	CLA	C4A-NA-C1A	7.27	110.00	106.68
25	y	616	NEX	O24-C25-C38	-7.26	106.94	115.05
37	f	101	HEM	C2B-C1B-NB	-7.24	101.52	109.84
22	c	510	CLA	C4A-NA-C1A	7.23	109.98	106.68
37	F	101	HEM	C2B-C1B-NB	-7.22	101.55	109.84
22	Y	611	CLA	C4A-NA-C1A	7.21	109.97	106.68
22	y	612	CLA	C4A-NA-C1A	7.21	109.97	106.68
22	G	613	CLA	C4A-NA-C1A	7.21	109.97	106.68
23	G	616	LUT	C38-C25-C24	-7.20	106.31	123.36
22	N	612	CLA	C4A-NA-C1A	7.17	109.95	106.68
24	G	617	XAT	O4-C5-C18	-7.17	107.04	115.05
22	n	612	CLA	C4A-NA-C1A	7.15	109.94	106.68
22	c	514	CLA	C4A-NA-C1A	7.10	109.92	106.68
23	g	616	LUT	C38-C25-C24	-7.09	106.57	123.36
22	C	511	CLA	C4A-NA-C1A	7.06	109.90	106.68
24	y	615	XAT	C7-C8-C9	-7.06	114.58	125.53
22	g	610	CLA	C4A-NA-C1A	7.05	109.90	106.68
22	C	515	CLA	C4A-NA-C1A	7.03	109.89	106.68
25	Y	616	NEX	O24-C25-C38	-7.02	107.20	115.05
22	n	609	CLA	C4A-NA-C1A	7.01	109.88	106.68
22	G	610	CLA	C4A-NA-C1A	7.01	109.88	106.68
22	N	609	CLA	C4A-NA-C1A	7.00	109.87	106.68
23	N	615	LUT	C31-C30-C29	-6.92	117.58	127.28
23	Y	614	LUT	C38-C25-C24	-6.90	107.03	123.36
24	r	314	XAT	C38-C25-C26	-6.90	110.94	122.30
22	y	610	CLA	C4A-NA-C1A	6.90	109.83	106.68
22	N	604	CLA	C4A-NA-C1A	6.90	109.83	106.68
22	Y	609	CLA	C4A-NA-C1A	6.90	109.83	106.68
24	R	313	XAT	C38-C25-C26	-6.88	110.97	122.30
22	c	505	CLA	C4A-NA-C1A	6.88	109.82	106.68
22	N	611	CLA	C4A-NA-C1A	6.86	109.81	106.68
22	Y	604	CLA	C4A-NA-C1A	6.86	109.81	106.68
22	S	305	CLA	C4A-NA-C1A	6.86	109.81	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	510	CLA	C3C-C4C-NC	-6.80	101.72	110.43
22	n	604	CLA	C4A-NA-C1A	6.80	109.78	106.68
22	y	604	CLA	C4A-NA-C1A	6.80	109.78	106.68
24	y	615	XAT	C19-C9-C8	-6.80	107.70	118.09
22	G	612	CLA	C4A-NA-C1A	6.79	109.78	106.68
23	g	616	LUT	C20-C13-C12	-6.79	107.72	118.09
22	s	305	CLA	C4A-NA-C1A	6.79	109.78	106.68
22	C	511	CLA	C3C-C4C-NC	-6.78	101.74	110.43
24	Y	615	XAT	C19-C9-C8	-6.78	107.73	118.09
22	G	604	CLA	C4A-NA-C1A	6.75	109.76	106.68
22	g	612	CLA	C4A-NA-C1A	6.73	109.75	106.68
24	n	615	XAT	O4-C6-C7	-6.73	97.59	116.88
22	C	506	CLA	C4A-NA-C1A	6.73	109.75	106.68
22	g	604	CLA	C4A-NA-C1A	6.72	109.75	106.68
22	s	313	CLA	C4A-NA-C1A	6.72	109.75	106.68
22	c	507	CLA	C4A-NA-C1A	6.72	109.74	106.68
22	r	312	CLA	C4A-NA-C1A	6.71	109.74	106.68
22	w	101	CLA	C4A-NA-C1A	6.70	109.74	106.68
22	C	508	CLA	C4A-NA-C1A	6.70	109.73	106.68
23	N	615	LUT	C11-C10-C9	-6.69	117.89	127.28
22	b	611	CLA	C4A-NA-C1A	6.69	109.73	106.68
22	n	611	CLA	C4A-NA-C1A	6.68	109.73	106.68
22	b	606	CLA	C4A-NA-C1A	6.68	109.73	106.68
22	W	101	CLA	C4A-NA-C1A	6.68	109.73	106.68
22	d	404	CLA	C4A-NA-C1A	6.67	109.72	106.68
22	S	313	CLA	C4A-NA-C1A	6.66	109.72	106.68
22	D	405	CLA	C4A-NA-C1A	6.66	109.72	106.68
25	g	618	NEX	O24-C25-C38	-6.65	107.61	115.05
22	R	303	CLA	C4A-NA-C1A	6.65	109.71	106.68
22	r	304	CLA	C4A-NA-C1A	6.64	109.71	106.68
22	A	406	CLA	C4A-NA-C1A	6.63	109.71	106.68
22	B	614	CLA	C4A-NA-C1A	6.63	109.70	106.68
23	G	616	LUT	C20-C13-C12	-6.62	107.97	118.09
22	y	602	CLA	C4A-NA-C1A	6.62	109.70	106.68
22	R	302	CLA	C4A-NA-C1A	6.62	109.70	106.68
22	B	611	CLA	C4A-NA-C1A	6.62	109.70	106.68
22	G	602	CLA	C4A-NA-C1A	6.60	109.69	106.68
22	B	609	CLA	C4A-NA-C1A	6.60	109.69	106.68
22	r	310	CLA	C4A-NA-C1A	6.58	109.68	106.68
22	g	602	CLA	C4A-NA-C1A	6.57	109.68	106.68
22	r	303	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	N	602	CLA	C4A-NA-C1A	6.55	109.67	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	409	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	b	608	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	c	506	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	B	608	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	n	602	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	R	311	CLA	C4A-NA-C1A	6.53	109.66	106.68
22	b	605	CLA	C4A-NA-C1A	6.52	109.66	106.68
22	R	304	CLA	C4A-NA-C1A	6.52	109.65	106.68
22	R	308	CLA	C4A-NA-C1A	6.52	109.65	106.68
22	s	312	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	a	405	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	B	604	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	b	601	CLA	C4A-NA-C1A	6.50	109.64	106.68
23	G	616	LUT	C40-C33-C32	-6.50	108.16	118.09
23	R	312	LUT	C38-C25-C24	-6.50	107.98	123.36
22	Y	602	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	B	606	CLA	C4A-NA-C1A	6.49	109.64	106.68
23	y	614	LUT	C8-C9-C10	-6.49	108.79	119.01
22	x	101	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	r	305	CLA	C4A-NA-C1A	6.48	109.64	106.68
22	r	309	CLA	C4A-NA-C1A	6.48	109.63	106.68
23	r	313	LUT	C38-C25-C24	-6.48	108.03	123.36
22	b	610	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	R	309	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	B	613	CLA	C4A-NA-C1A	6.46	109.63	106.68
23	N	614	LUT	C8-C9-C10	-6.46	108.85	119.01
23	G	615	LUT	C8-C9-C10	-6.46	108.86	119.01
22	b	613	CLA	C4A-NA-C1A	6.45	109.62	106.68
22	b	602	CLA	C4A-NA-C1A	6.44	109.62	106.68
22	b	615	CLA	C4A-NA-C1A	6.44	109.62	106.68
23	Y	613	LUT	C8-C9-C10	-6.44	108.88	119.01
22	a	408	CLA	C4A-NA-C1A	6.44	109.62	106.68
23	g	615	LUT	C8-C9-C10	-6.44	108.89	119.01
22	d	403	CLA	C4A-NA-C1A	6.44	109.61	106.68
22	S	312	CLA	C4A-NA-C1A	6.44	109.61	106.68
23	n	614	LUT	C8-C9-C10	-6.44	108.89	119.01
24	R	313	XAT	C8-C9-C10	-6.44	108.89	119.01
22	B	607	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	C	507	CLA	C4A-NA-C1A	6.43	109.61	106.68
23	g	616	LUT	C40-C33-C32	-6.43	108.27	118.09
22	C	509	CLA	C4A-NA-C1A	6.42	109.61	106.68
24	g	617	XAT	C38-C25-C26	-6.42	111.74	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	C4A-NA-C1A	6.41	109.60	106.68
23	Y	614	LUT	C40-C33-C32	-6.41	108.30	118.09
24	r	314	XAT	C8-C9-C10	-6.41	108.93	119.01
22	B	618	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	C	505	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	D	404	CLA	C4A-NA-C1A	6.40	109.60	106.68
24	Y	615	XAT	C20-C13-C12	-6.39	108.32	118.09
22	B	616	CLA	C4A-NA-C1A	6.39	109.60	106.68
25	Y	616	NEX	C32-C33-C34	-6.39	108.96	119.01
22	B	605	CLA	C4A-NA-C1A	6.39	109.59	106.68
22	a	406	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	c	502	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	A	407	CLA	C4A-NA-C1A	6.36	109.58	106.68
24	N	616	XAT	C19-C9-C8	-6.36	108.37	118.09
24	Y	615	XAT	C40-C33-C32	-6.36	108.38	118.09
22	b	607	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	c	508	CLA	C4A-NA-C1A	6.35	109.58	106.68
24	N	616	XAT	C38-C25-C26	-6.35	111.86	122.30
30	d	401	PHO	C4D-CHA-CBD	-6.34	105.41	108.45
22	B	603	CLA	C4A-NA-C1A	6.34	109.57	106.68
23	G	615	LUT	C38-C25-C24	-6.34	108.36	123.36
23	n	614	LUT	C38-C25-C24	-6.34	108.36	123.36
22	c	504	CLA	C4A-NA-C1A	6.34	109.57	106.68
22	C	511	CLA	C1D-ND-C4D	6.34	110.76	106.31
24	Y	615	XAT	C39-C29-C28	-6.33	108.41	118.09
23	Y	613	LUT	C38-C25-C24	-6.33	108.37	123.36
22	G	614	CLA	C4A-NA-C1A	6.33	109.57	106.68
22	C	504	CLA	C4A-NA-C1A	6.33	109.56	106.68
23	Y	614	LUT	C20-C13-C12	-6.32	108.43	118.09
22	B	612	CLA	C4A-NA-C1A	6.32	109.56	106.68
23	y	614	LUT	C38-C25-C24	-6.32	108.39	123.36
23	g	615	LUT	C38-C25-C24	-6.32	108.39	123.36
22	C	510	CLA	C4A-NA-C1A	6.32	109.56	106.68
23	N	614	LUT	C38-C25-C24	-6.32	108.40	123.36
22	c	510	CLA	C1D-ND-C4D	6.31	110.74	106.31
22	c	503	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	S	309	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	b	604	CLA	C4A-NA-C1A	6.30	109.55	106.68
30	D	401	PHO	C4D-CHA-CBD	-6.30	105.43	108.45
22	B	610	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	c	509	CLA	C4A-NA-C1A	6.29	109.55	106.68
24	y	615	XAT	C39-C29-C28	-6.29	108.48	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4A-NA-C1A	6.29	109.55	106.68
22	A	405	CLA	C4A-NA-C1A	6.29	109.55	106.68
22	s	309	CLA	C4A-NA-C1A	6.28	109.55	106.68
22	R	310	CLA	C4A-NA-C1A	6.28	109.54	106.68
22	Y	612	CLA	C4A-NA-C1A	6.27	109.54	106.68
22	B	615	CLA	C4A-NA-C1A	6.27	109.54	106.68
24	y	615	XAT	C38-C25-C26	-6.27	111.98	122.30
22	g	614	CLA	C4A-NA-C1A	6.27	109.54	106.68
25	n	616	NEX	O24-C25-C38	-6.26	108.05	115.05
22	G	611	CLA	C4A-NA-C1A	6.26	109.54	106.68
22	n	613	CLA	C4A-NA-C1A	6.26	109.53	106.68
22	b	609	CLA	C4A-NA-C1A	6.25	109.53	106.68
24	g	617	XAT	C39-C29-C28	-6.23	108.57	118.09
22	N	613	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	a	404	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	g	611	CLA	C4A-NA-C1A	6.22	109.52	106.68
24	n	615	XAT	C19-C9-C8	-6.21	108.60	118.09
23	Y	614	LUT	C28-C29-C30	-6.21	109.24	119.01
22	y	611	CLA	C4A-NA-C1A	6.21	109.51	106.68
22	r	311	CLA	C4A-NA-C1A	6.21	109.51	106.68
24	y	615	XAT	C40-C33-C32	-6.19	108.62	118.09
22	n	610	CLA	C4A-NA-C1A	6.19	109.50	106.68
22	y	613	CLA	C4A-NA-C1A	6.19	109.50	106.68
24	G	617	XAT	C39-C29-C28	-6.17	108.67	118.09
22	b	612	CLA	C4A-NA-C1A	6.16	109.49	106.68
22	N	610	CLA	C4A-NA-C1A	6.16	109.49	106.68
24	Y	615	XAT	C38-C25-C26	-6.16	112.17	122.30
25	N	617	NEX	C32-C33-C34	-6.16	109.32	119.01
25	Y	616	NEX	C2-C1-C6	6.15	115.19	109.21
22	Y	610	CLA	C4A-NA-C1A	6.15	109.48	106.68
22	C	513	CLA	C4A-NA-C1A	6.14	109.48	106.68
24	y	615	XAT	C20-C13-C12	-6.14	108.71	118.09
25	n	616	NEX	C32-C33-C34	-6.11	109.40	119.01
22	c	512	CLA	C4A-NA-C1A	6.10	109.46	106.68
22	C	512	CLA	C4A-NA-C1A	6.09	109.46	106.68
22	n	603	CLA	C4A-NA-C1A	6.08	109.45	106.68
22	s	303	CLA	C4A-NA-C1A	6.08	109.45	106.68
22	c	511	CLA	C4A-NA-C1A	6.07	109.45	106.68
24	N	616	XAT	C27-C28-C29	-6.06	116.12	125.53
22	b	614	CLA	C4A-NA-C1A	6.06	109.44	106.68
23	r	313	LUT	C40-C33-C32	-6.05	108.84	118.09
24	G	617	XAT	C38-C25-C26	-6.05	112.34	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	617	CLA	C4A-NA-C1A	6.05	109.44	106.68
22	g	603	CLA	C4A-NA-C1A	6.05	109.44	106.68
22	N	603	CLA	C4A-NA-C1A	6.04	109.43	106.68
23	R	312	LUT	C40-C33-C32	-6.03	108.87	118.09
23	R	312	LUT	C28-C29-C30	-6.03	109.52	119.01
22	c	513	CLA	C4A-NA-C1A	6.03	109.43	106.68
22	S	304	CLA	C4A-NA-C1A	6.03	109.43	106.68
22	Y	603	CLA	C4A-NA-C1A	6.02	109.43	106.68
22	G	603	CLA	C4A-NA-C1A	6.02	109.42	106.68
22	S	303	CLA	C4A-NA-C1A	6.02	109.42	106.68
23	r	313	LUT	C28-C29-C30	-6.01	109.55	119.01
23	r	313	LUT	C19-C9-C8	-6.00	108.92	118.09
23	R	312	LUT	C19-C9-C8	-5.99	108.93	118.09
24	n	615	XAT	C39-C29-C28	-5.99	108.94	118.09
22	g	613	CLA	CMC-C2C-C1C	5.99	134.39	125.03
22	s	310	CLA	C4A-NA-C1A	5.98	109.41	106.68
22	n	612	CLA	CMC-C2C-C1C	5.98	134.38	125.03
22	y	612	CLA	CMC-C2C-C1C	5.98	134.37	125.03
22	N	612	CLA	CMC-C2C-C1C	5.97	134.37	125.03
22	G	613	CLA	CMC-C2C-C1C	5.97	134.37	125.03
22	S	310	CLA	C4A-NA-C1A	5.97	109.40	106.68
24	g	617	XAT	C19-C9-C8	-5.97	108.97	118.09
22	C	514	CLA	C4A-NA-C1A	5.96	109.40	106.68
22	s	304	CLA	C4A-NA-C1A	5.96	109.40	106.68
25	r	315	NEX	C40-C33-C32	-5.95	109.00	118.09
23	N	615	LUT	C20-C13-C12	-5.95	109.00	118.09
22	Y	611	CLA	CMC-C2C-C1C	5.94	134.32	125.03
24	r	314	XAT	C20-C13-C12	-5.94	109.01	118.09
25	y	616	NEX	C2-C1-C6	5.94	114.99	109.21
24	G	617	XAT	C40-C33-C32	-5.94	109.02	118.09
22	C	511	CLA	CHD-C4C-C3C	5.93	133.42	124.77
25	N	617	NEX	C20-C13-C12	-5.93	109.04	118.09
25	y	618	NEX	C40-C33-C32	-5.92	109.04	118.09
24	n	615	XAT	C40-C33-C32	-5.92	109.04	118.09
22	s	308	CLA	C4A-NA-C1A	5.91	109.38	106.68
22	c	510	CLA	CHD-C4C-C3C	5.91	133.39	124.77
22	y	603	CLA	C4A-NA-C1A	5.90	109.37	106.68
22	S	311	CLA	C4A-NA-C1A	5.90	109.37	106.68
24	n	615	XAT	C38-C25-C26	-5.90	112.59	122.30
24	R	313	XAT	C20-C13-C12	-5.89	109.10	118.09
37	F	101	HEM	C3D-C4D-ND	-5.88	103.72	110.17
37	f	101	HEM	C3D-C4D-ND	-5.88	103.72	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	408	PHO	C4D-CHA-CBD	-5.87	105.64	108.45
24	R	313	XAT	C39-C29-C28	-5.87	109.12	118.09
24	g	617	XAT	C40-C33-C32	-5.86	109.13	118.09
25	Y	616	NEX	C40-C33-C32	-5.84	109.17	118.09
37	f	101	HEM	C2D-C1D-ND	-5.83	103.16	109.90
37	F	101	HEM	C2D-C1D-ND	-5.83	103.17	109.90
30	a	407	PHO	C4D-CHA-CBD	-5.83	105.66	108.45
24	G	617	XAT	C19-C9-C8	-5.83	109.19	118.09
24	r	314	XAT	C39-C29-C28	-5.82	109.20	118.09
24	N	616	XAT	C20-C13-C12	-5.81	109.21	118.09
24	R	313	XAT	C19-C9-C8	-5.79	109.24	118.09
23	g	615	LUT	C12-C13-C14	-5.78	109.91	119.01
23	N	614	LUT	C12-C13-C14	-5.78	109.92	119.01
23	G	615	LUT	C12-C13-C14	-5.77	109.93	119.01
23	n	614	LUT	C12-C13-C14	-5.77	109.93	119.01
24	r	314	XAT	C19-C9-C8	-5.77	109.27	118.09
23	y	614	LUT	C12-C13-C14	-5.77	109.93	119.01
22	s	311	CLA	C4A-NA-C1A	5.77	109.31	106.68
24	n	615	XAT	C20-C13-C12	-5.76	109.28	118.09
23	Y	613	LUT	C12-C13-C14	-5.76	109.95	119.01
25	g	618	NEX	C32-C33-C34	-5.76	109.95	119.01
22	S	308	CLA	C4A-NA-C1A	5.75	109.30	106.68
23	G	615	LUT	C39-C29-C28	-5.75	109.30	118.09
23	g	616	LUT	C7-C8-C9	-5.75	117.72	126.23
23	g	615	LUT	C39-C29-C28	-5.75	109.30	118.09
23	Y	613	LUT	C39-C29-C28	-5.75	109.31	118.09
23	N	614	LUT	C39-C29-C28	-5.74	109.31	118.09
25	Y	616	NEX	C20-C13-C12	-5.74	109.32	118.09
23	n	614	LUT	C39-C29-C28	-5.73	109.33	118.09
23	y	614	LUT	C39-C29-C28	-5.73	109.34	118.09
24	g	617	XAT	C20-C13-C12	-5.73	109.34	118.09
25	g	618	NEX	C2-C1-C6	5.72	114.77	109.21
25	r	315	NEX	C39-C29-C28	-5.71	109.36	118.09
25	y	618	NEX	C39-C29-C28	-5.71	109.37	118.09
25	y	616	NEX	C32-C33-C34	-5.71	110.03	119.01
25	Y	616	NEX	C39-C29-C28	-5.70	109.38	118.09
25	n	616	NEX	C20-C13-C12	-5.70	109.38	118.09
25	y	618	NEX	C20-C13-C12	-5.67	109.43	118.09
24	R	313	XAT	C40-C33-C32	-5.66	109.45	118.09
25	N	617	NEX	C40-C33-C32	-5.65	109.45	118.09
25	g	618	NEX	C20-C13-C12	-5.65	109.45	118.09
23	r	313	LUT	C32-C33-C34	-5.65	110.12	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	R	312	LUT	C32-C33-C34	-5.65	110.13	119.01
24	N	616	XAT	C12-C13-C14	-5.64	110.14	119.01
24	r	314	XAT	C40-C33-C32	-5.64	109.48	118.09
25	r	315	NEX	C20-C13-C12	-5.64	109.48	118.09
25	y	616	NEX	C20-C13-C12	-5.63	109.49	118.09
25	r	315	NEX	C12-C13-C14	-5.63	110.16	119.01
24	G	617	XAT	C20-C13-C12	-5.61	109.52	118.09
24	n	615	XAT	C27-C28-C29	-5.61	116.83	125.53
23	G	616	LUT	C7-C8-C9	-5.60	117.95	126.23
24	n	615	XAT	C12-C13-C14	-5.60	110.20	119.01
25	y	616	NEX	C28-C29-C30	-5.59	110.21	119.01
23	G	615	LUT	C28-C29-C30	-5.59	110.22	119.01
23	Y	613	LUT	C28-C29-C30	-5.59	110.22	119.01
23	N	614	LUT	C20-C13-C12	-5.59	109.55	118.09
23	y	614	LUT	C28-C29-C30	-5.59	110.22	119.01
23	N	614	LUT	C28-C29-C30	-5.59	110.22	119.01
23	n	614	LUT	C28-C29-C30	-5.59	110.22	119.01
25	y	618	NEX	C12-C13-C14	-5.59	110.22	119.01
23	g	615	LUT	C28-C29-C30	-5.58	110.23	119.01
23	N	615	LUT	C32-C33-C34	-5.58	110.23	119.01
25	n	616	NEX	C2-C1-C6	5.58	114.63	109.21
23	N	615	LUT	C39-C29-C28	-5.58	109.57	118.09
23	y	614	LUT	C20-C13-C12	-5.57	109.58	118.09
23	Y	613	LUT	C20-C13-C12	-5.57	109.58	118.09
23	n	614	LUT	C20-C13-C12	-5.57	109.58	118.09
24	G	617	XAT	C27-C28-C29	-5.57	116.89	125.53
23	G	615	LUT	C20-C13-C12	-5.56	109.59	118.09
23	g	616	LUT	C28-C29-C30	-5.56	110.26	119.01
23	g	615	LUT	C20-C13-C12	-5.56	109.60	118.09
24	N	616	XAT	C40-C33-C32	-5.53	109.64	118.09
23	g	616	LUT	C39-C29-C28	-5.53	109.64	118.09
25	N	617	NEX	C39-C29-C28	-5.53	109.64	118.09
23	G	616	LUT	C28-C29-C30	-5.53	110.31	119.01
25	g	618	NEX	C39-C29-C28	-5.46	109.74	118.09
24	g	617	XAT	C12-C13-C14	-5.46	110.42	119.01
25	y	616	NEX	C39-C29-C28	-5.45	109.76	118.09
25	n	616	NEX	C39-C29-C28	-5.44	109.78	118.09
23	G	616	LUT	C39-C29-C28	-5.43	109.79	118.09
25	g	618	NEX	C28-C29-C30	-5.43	110.47	119.01
23	Y	613	LUT	C40-C33-C32	-5.42	109.80	118.09
23	N	615	LUT	C40-C33-C32	-5.42	109.81	118.09
24	G	617	XAT	O24-C25-C38	-5.41	109.00	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	g	615	LUT	C40-C33-C32	-5.41	109.83	118.09
23	N	614	LUT	C40-C33-C32	-5.40	109.83	118.09
23	G	615	LUT	C40-C33-C32	-5.40	109.84	118.09
25	y	616	NEX	C40-C33-C32	-5.40	109.85	118.09
23	y	614	LUT	C40-C33-C32	-5.39	109.85	118.09
23	n	614	LUT	C40-C33-C32	-5.37	109.88	118.09
23	r	313	LUT	C39-C29-C28	-5.36	109.89	118.09
23	R	312	LUT	C39-C29-C28	-5.33	109.94	118.09
23	r	313	LUT	C7-C6-C5	-5.31	109.33	121.56
23	R	312	LUT	C7-C6-C5	-5.29	109.36	121.56
23	N	615	LUT	C28-C29-C30	-5.28	110.70	119.01
24	n	615	XAT	O24-C25-C38	-5.23	109.20	115.05
25	y	618	NEX	C32-C33-C34	-5.22	110.79	119.01
22	Y	611	CLA	CHC-C1C-NC	-5.21	116.46	124.31
25	r	315	NEX	C32-C33-C34	-5.21	110.81	119.01
22	y	612	CLA	CHC-C1C-NC	-5.21	116.47	124.31
23	N	614	LUT	C32-C33-C34	-5.20	110.82	119.01
22	G	613	CLA	CHC-C1C-NC	-5.20	116.47	124.31
25	g	618	NEX	C40-C33-C32	-5.20	110.14	118.09
24	Y	615	XAT	C27-C28-C29	-5.20	117.47	125.53
23	g	615	LUT	C32-C33-C34	-5.19	110.84	119.01
23	G	615	LUT	C32-C33-C34	-5.19	110.84	119.01
22	n	612	CLA	CHC-C1C-NC	-5.19	116.50	124.31
22	g	613	CLA	CHC-C1C-NC	-5.19	116.50	124.31
23	y	614	LUT	C32-C33-C34	-5.18	110.86	119.01
23	n	614	LUT	C32-C33-C34	-5.18	110.86	119.01
22	N	612	CLA	CHC-C1C-NC	-5.17	116.53	124.31
23	R	312	LUT	C8-C9-C10	-5.16	110.89	119.01
23	Y	613	LUT	C32-C33-C34	-5.16	110.89	119.01
25	y	616	NEX	C12-C13-C14	-5.15	110.90	119.01
23	r	313	LUT	C8-C9-C10	-5.15	110.91	119.01
24	g	617	XAT	C27-C28-C29	-5.15	117.55	125.53
25	n	616	NEX	C12-C13-C14	-5.14	110.92	119.01
24	g	617	XAT	C7-C8-C9	-5.13	117.56	125.53
24	N	616	XAT	C39-C29-C28	-5.13	110.26	118.09
24	n	615	XAT	C8-C9-C10	-5.12	110.96	119.01
24	N	616	XAT	C7-C8-C9	-5.11	117.61	125.53
25	N	617	NEX	O24-C25-C38	-5.11	109.34	115.05
24	G	617	XAT	C7-C8-C9	-5.10	117.62	125.53
23	g	616	LUT	C19-C9-C8	-5.10	110.30	118.09
23	y	614	LUT	C4-C5-C6	-5.07	110.34	120.76
25	g	618	NEX	C12-C13-C14	-5.07	111.04	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	617	NEX	C28-C29-C30	-5.06	111.04	119.01
24	y	615	XAT	C27-C28-C29	-5.06	117.68	125.53
23	N	614	LUT	C4-C5-C6	-5.05	110.38	120.76
23	g	615	LUT	C4-C5-C6	-5.05	110.39	120.76
25	N	617	NEX	C12-C13-C14	-5.05	111.07	119.01
23	n	614	LUT	C4-C5-C6	-5.04	110.39	120.76
23	Y	613	LUT	C4-C5-C6	-5.04	110.40	120.76
23	G	615	LUT	C4-C5-C6	-5.03	110.43	120.76
23	R	312	LUT	C1-C6-C5	-5.02	115.77	122.64
23	Y	614	LUT	C39-C29-C28	-5.01	110.44	118.09
23	r	313	LUT	C1-C6-C5	-4.98	115.83	122.64
24	G	617	XAT	C12-C13-C14	-4.98	111.18	119.01
25	Y	616	NEX	C12-C13-C14	-4.96	111.21	119.01
25	n	616	NEX	C40-C33-C32	-4.96	110.52	118.09
23	G	616	LUT	C19-C9-C8	-4.93	110.56	118.09
25	n	616	NEX	C28-C29-C30	-4.93	111.26	119.01
25	N	617	NEX	C5-C6-C1	-4.93	114.81	119.70
23	Y	614	LUT	C12-C13-C14	-4.93	111.26	119.01
24	y	615	XAT	O24-C25-C38	-4.91	109.56	115.05
37	f	101	HEM	C4C-NC-C1C	4.91	113.82	105.82
24	Y	615	XAT	O24-C25-C38	-4.90	109.57	115.05
25	N	617	NEX	C19-C9-C8	-4.90	108.06	118.94
37	F	101	HEM	C4C-NC-C1C	4.90	113.81	105.82
24	r	314	XAT	C32-C33-C34	-4.89	111.32	119.01
25	r	315	NEX	C28-C29-C30	-4.88	111.33	119.01
25	y	618	NEX	C28-C29-C30	-4.88	111.33	119.01
24	R	313	XAT	C12-C13-C14	-4.88	111.34	119.01
24	R	313	XAT	C32-C33-C34	-4.87	111.34	119.01
21	G	609	CHL	C1B-CHB-C4A	-4.87	118.19	121.32
24	r	314	XAT	C12-C13-C14	-4.87	111.35	119.01
21	g	605	CHL	C1B-CHB-C4A	-4.87	118.19	121.32
22	c	510	CLA	CHD-C1D-C2D	4.87	135.61	125.49
25	N	617	NEX	C37-C21-C26	4.87	123.19	110.05
22	C	511	CLA	CHD-C1D-C2D	4.86	135.60	125.49
25	y	616	NEX	C37-C21-C26	4.86	123.16	110.05
23	Y	614	LUT	C7-C8-C9	-4.86	119.05	126.23
32	D	407	PL9	C7-C3-C4	4.86	120.91	116.91
21	R	307	CHL	C1B-CHB-C4A	-4.85	118.20	121.32
32	d	406	PL9	C7-C3-C4	4.84	120.90	116.91
21	r	307	CHL	C1B-CHB-C4A	-4.83	118.21	121.32
24	r	314	XAT	C28-C29-C30	-4.83	111.41	119.01
24	R	313	XAT	C28-C29-C30	-4.83	111.41	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	617	XAT	O24-C25-C38	-4.83	109.65	115.05
24	N	616	XAT	C8-C9-C10	-4.83	111.42	119.01
23	g	616	LUT	C32-C33-C34	-4.82	111.43	119.01
21	g	606	CHL	C1B-CHB-C4A	-4.81	118.23	121.32
21	g	607	CHL	C1B-CHB-C4A	-4.81	118.23	121.32
21	G	607	CHL	C1B-CHB-C4A	-4.81	118.23	121.32
21	s	306	CHL	C1B-CHB-C4A	-4.81	118.23	121.32
23	Y	614	LUT	C19-C9-C8	-4.80	110.75	118.09
21	G	601	CHL	C1B-CHB-C4A	-4.80	118.24	121.32
21	N	601	CHL	C1B-CHB-C4A	-4.80	118.24	121.32
21	g	608	CHL	C1B-CHB-C4A	-4.79	118.24	121.32
21	n	601	CHL	C1B-CHB-C4A	-4.79	118.24	121.32
35	C	518	DGD	O3G-C3G-C2G	-4.79	99.17	110.82
24	R	313	XAT	O24-C25-C38	-4.79	109.70	115.05
21	Y	601	CHL	C1B-CHB-C4A	-4.79	118.24	121.32
21	S	301	CHL	C1B-CHB-C4A	-4.79	118.24	121.32
21	S	306	CHL	C1B-CHB-C4A	-4.78	118.25	121.32
21	Y	605	CHL	C1B-CHB-C4A	-4.77	118.25	121.32
21	S	302	CHL	C1B-CHB-C4A	-4.77	118.25	121.32
21	N	608	CHL	C1B-CHB-C4A	-4.77	118.25	121.32
21	r	306	CHL	C1B-CHB-C4A	-4.77	118.25	121.32
21	s	307	CHL	C1B-CHB-C4A	-4.77	118.25	121.32
21	N	607	CHL	C1B-CHB-C4A	-4.77	118.25	121.32
21	n	608	CHL	C1B-CHB-C4A	-4.77	118.25	121.32
21	r	308	CHL	C1B-CHB-C4A	-4.77	118.25	121.32
35	c	517	DGD	O3G-C3G-C2G	-4.77	99.22	110.82
21	N	605	CHL	C1B-CHB-C4A	-4.77	118.26	121.32
21	n	605	CHL	C1B-CHB-C4A	-4.77	118.26	121.32
21	R	306	CHL	C1B-CHB-C4A	-4.76	118.26	121.32
21	n	607	CHL	C1B-CHB-C4A	-4.76	118.26	121.32
21	Y	607	CHL	C1B-CHB-C4A	-4.76	118.26	121.32
21	y	607	CHL	C1B-CHB-C4A	-4.76	118.26	121.32
21	G	608	CHL	C1B-CHB-C4A	-4.76	118.26	121.32
24	r	314	XAT	O24-C25-C38	-4.75	109.74	115.05
23	N	615	LUT	C8-C9-C10	-4.75	111.54	119.01
21	y	605	CHL	C1B-CHB-C4A	-4.75	118.27	121.32
21	y	601	CHL	C1B-CHB-C4A	-4.75	118.27	121.32
21	s	302	CHL	C1B-CHB-C4A	-4.75	118.27	121.32
21	y	606	CHL	C1B-CHB-C4A	-4.74	118.27	121.32
21	R	305	CHL	C1B-CHB-C4A	-4.74	118.27	121.32
21	g	609	CHL	C1B-CHB-C4A	-4.73	118.28	121.32
21	G	606	CHL	C1B-CHB-C4A	-4.73	118.28	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	613	LUT	C19-C9-C8	-4.73	110.86	118.09
21	S	307	CHL	C1B-CHB-C4A	-4.73	118.28	121.32
21	y	608	CHL	C1B-CHB-C4A	-4.73	118.28	121.32
21	s	301	CHL	C1B-CHB-C4A	-4.73	118.28	121.32
21	Y	608	CHL	C1B-CHB-C4A	-4.72	118.28	121.32
23	Y	614	LUT	C32-C33-C34	-4.72	111.58	119.01
23	n	614	LUT	C19-C9-C8	-4.72	110.88	118.09
21	g	601	CHL	C1B-CHB-C4A	-4.72	118.29	121.32
21	r	301	CHL	C1B-CHB-C4A	-4.71	118.29	121.32
23	G	615	LUT	C19-C9-C8	-4.71	110.89	118.09
21	y	609	CHL	C1B-CHB-C4A	-4.71	118.30	121.32
21	G	605	CHL	C1B-CHB-C4A	-4.70	118.30	121.32
21	n	606	CHL	C1B-CHB-C4A	-4.69	118.30	121.32
21	N	606	CHL	C1B-CHB-C4A	-4.69	118.31	121.32
21	Y	606	CHL	C1B-CHB-C4A	-4.68	118.31	121.32
24	y	615	XAT	C12-C13-C14	-4.68	111.64	119.01
23	g	615	LUT	C19-C9-C8	-4.67	110.95	118.09
23	y	614	LUT	C19-C9-C8	-4.67	110.95	118.09
23	N	614	LUT	C19-C9-C8	-4.67	110.96	118.09
37	F	101	HEM	C4B-C3B-C2B	4.67	111.57	107.28
37	f	101	HEM	C4B-C3B-C2B	4.66	111.57	107.28
23	r	313	LUT	C12-C13-C14	-4.66	111.67	119.01
23	R	312	LUT	C12-C13-C14	-4.65	111.69	119.01
24	G	617	XAT	C8-C9-C10	-4.64	111.71	119.01
24	N	616	XAT	O24-C25-C38	-4.63	109.87	115.05
23	G	616	LUT	C32-C33-C34	-4.58	111.81	119.01
24	n	615	XAT	C7-C8-C9	-4.57	118.44	125.53
23	N	615	LUT	C12-C13-C14	-4.57	111.83	119.01
23	G	616	LUT	C12-C13-C14	-4.55	111.85	119.01
35	c	519	DGD	O3G-C3G-C2G	-4.53	99.79	110.82
35	J	101	DGD	O3G-C3G-C2G	-4.52	99.83	110.82
25	n	616	NEX	C37-C21-C26	4.51	122.23	110.05
23	N	615	LUT	C4-C5-C6	-4.50	111.51	120.76
25	Y	616	NEX	C19-C9-C8	-4.49	108.98	118.94
26	d	407	LHG	O4-P-O5	4.48	133.27	112.44
26	D	408	LHG	O4-P-O5	4.47	133.25	112.44
26	G	618	LHG	O4-P-O5	4.47	133.24	112.44
26	g	619	LHG	O4-P-O5	4.47	133.23	112.44
24	g	617	XAT	C8-C9-C10	-4.46	111.99	119.01
26	D	409	LHG	O4-P-O5	4.46	133.21	112.44
26	S	314	LHG	O4-P-O5	4.46	133.19	112.44
26	d	408	LHG	O4-P-O5	4.46	133.19	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	522	LHG	O4-P-O5	4.45	133.16	112.44
26	c	522	LHG	O4-P-O5	4.45	133.14	112.44
26	s	314	LHG	O4-P-O5	4.44	133.12	112.44
26	y	617	LHG	O4-P-O5	4.44	133.11	112.44
26	c	520	LHG	O4-P-O5	4.44	133.11	112.44
35	c	518	DGD	O3G-C3G-C2G	-4.43	100.04	110.82
24	N	616	XAT	C32-C33-C34	-4.43	112.04	119.01
35	C	519	DGD	O3G-C3G-C2G	-4.43	100.05	110.82
26	C	520	LHG	O4-P-O5	4.42	133.02	112.44
26	n	617	LHG	O4-P-O5	4.42	133.02	112.44
26	L	103	LHG	O4-P-O5	4.42	133.01	112.44
26	d	409	LHG	O4-P-O5	4.42	133.01	112.44
26	D	410	LHG	O4-P-O5	4.42	133.01	112.44
26	l	102	LHG	O4-P-O5	4.42	133.00	112.44
25	y	616	NEX	C19-C9-C8	-4.42	109.13	118.94
26	b	619	LHG	O4-P-O5	4.41	132.98	112.44
26	B	622	LHG	O4-P-O5	4.41	132.96	112.44
26	c	521	LHG	O4-P-O5	4.41	132.95	112.44
35	A	401	DGD	O3G-C3G-C2G	-4.40	100.11	110.82
26	C	521	LHG	O4-P-O5	4.40	132.91	112.44
26	Y	617	LHG	O4-P-O5	4.39	132.89	112.44
35	a	413	DGD	O3G-C3G-C2G	-4.39	100.15	110.82
25	g	618	NEX	C19-C9-C8	-4.38	109.21	118.94
26	R	301	LHG	O4-P-O5	4.37	132.79	112.44
26	r	302	LHG	O4-P-O5	4.37	132.79	112.44
26	N	618	LHG	O4-P-O5	4.36	132.74	112.44
24	Y	615	XAT	C12-C13-C14	-4.35	112.16	119.01
25	r	315	NEX	C19-C9-C8	-4.35	109.28	118.94
25	y	618	NEX	C19-C9-C8	-4.33	109.32	118.94
23	R	312	LUT	C21-C26-C27	-4.28	107.90	112.83
24	g	617	XAT	C32-C33-C34	-4.27	112.29	119.01
23	r	313	LUT	C21-C26-C27	-4.26	107.93	112.83
35	h	102	DGD	O3G-C3G-C2G	-4.23	100.54	110.82
24	G	617	XAT	C32-C33-C34	-4.21	112.38	119.01
35	H	102	DGD	O3G-C3G-C2G	-4.21	100.58	110.82
25	n	616	NEX	C19-C9-C8	-4.20	109.61	118.94
23	N	614	LUT	C7-C6-C5	-4.19	111.89	121.56
24	R	313	XAT	C6-C7-C8	-4.19	117.13	125.99
23	y	614	LUT	C7-C6-C5	-4.19	111.91	121.56
23	Y	613	LUT	C7-C6-C5	-4.18	111.92	121.56
23	G	615	LUT	C7-C6-C5	-4.18	111.93	121.56
23	g	615	LUT	C7-C6-C5	-4.18	111.94	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	r	314	XAT	C6-C7-C8	-4.17	117.17	125.99
23	n	614	LUT	C7-C6-C5	-4.17	111.94	121.56
25	g	618	NEX	C37-C21-C26	4.17	121.31	110.05
23	N	615	LUT	C19-C9-C8	-4.16	111.73	118.09
24	n	615	XAT	C32-C33-C34	-4.14	112.50	119.01
25	N	617	NEX	C2-C1-C6	4.12	113.22	109.21
23	G	615	LUT	C21-C26-C27	-4.09	108.12	112.83
25	n	616	NEX	C17-C1-C6	-4.09	106.81	110.47
23	Y	613	LUT	C21-C26-C27	-4.09	108.13	112.83
24	G	617	XAT	C38-C25-C24	-4.08	109.66	114.24
23	y	614	LUT	C21-C26-C27	-4.08	108.13	112.83
23	N	614	LUT	C21-C26-C27	-4.07	108.14	112.83
23	n	614	LUT	C21-C26-C27	-4.06	108.16	112.83
23	g	615	LUT	C21-C26-C27	-4.05	108.17	112.83
37	f	101	HEM	CHC-C4B-C3B	4.05	133.16	125.07
37	F	101	HEM	CHC-C4B-C3B	4.04	133.14	125.07
25	r	315	NEX	C5-C6-C1	-4.04	115.69	119.70
37	F	101	HEM	CHD-C4C-C3C	4.02	131.99	125.21
23	R	312	LUT	C20-C13-C12	-4.00	111.98	118.09
37	f	101	HEM	CHD-C4C-C3C	4.00	131.95	125.21
23	r	313	LUT	C20-C13-C12	-3.98	112.01	118.09
24	y	615	XAT	C32-C33-C34	-3.98	112.75	119.01
25	y	618	NEX	C5-C6-C1	-3.97	115.75	119.70
33	l	103	SQD	O9-S-O7	-3.97	100.91	113.82
33	D	402	SQD	O9-S-O7	-3.96	100.94	113.82
33	L	101	SQD	O9-S-O7	-3.96	100.94	113.82
33	A	412	SQD	O9-S-O7	-3.96	100.95	113.82
33	d	402	SQD	O9-S-O7	-3.96	100.95	113.82
33	a	411	SQD	O9-S-O7	-3.96	100.95	113.82
21	Y	601	CHL	CHA-C1A-C2A	-3.92	124.10	133.31
21	r	308	CHL	CHA-C1A-C2A	-3.92	124.10	133.31
21	G	605	CHL	CHA-C1A-C2A	-3.92	124.10	133.31
21	Y	608	CHL	CHA-C1A-C2A	-3.92	124.11	133.31
21	G	606	CHL	CHA-C1A-C2A	-3.92	124.11	133.31
21	y	609	CHL	CHA-C1A-C2A	-3.91	124.11	133.31
21	n	608	CHL	CHA-C1A-C2A	-3.91	124.12	133.31
21	g	608	CHL	CHA-C1A-C2A	-3.91	124.12	133.31
32	d	406	PL9	C7-C3-C2	-3.91	118.78	123.39
21	S	302	CHL	CHA-C1A-C2A	-3.91	124.12	133.31
24	y	615	XAT	C38-C25-C24	-3.91	109.85	114.24
21	y	608	CHL	CHA-C1A-C2A	-3.91	124.13	133.31
21	G	607	CHL	CHA-C1A-C2A	-3.91	124.13	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	g	605	CHL	CHA-C1A-C2A	-3.91	124.13	133.31
21	y	605	CHL	CHA-C1A-C2A	-3.91	124.13	133.31
21	g	607	CHL	CHA-C1A-C2A	-3.91	124.13	133.31
21	R	307	CHL	CHA-C1A-C2A	-3.91	124.14	133.31
21	G	608	CHL	CHA-C1A-C2A	-3.90	124.14	133.31
21	s	302	CHL	CHA-C1A-C2A	-3.90	124.14	133.31
21	S	307	CHL	CHA-C1A-C2A	-3.90	124.14	133.31
32	D	407	PL9	C7-C3-C2	-3.90	118.79	123.39
21	G	609	CHL	CHA-C1A-C2A	-3.90	124.14	133.31
21	Y	606	CHL	CHA-C1A-C2A	-3.90	124.14	133.31
21	N	601	CHL	CHA-C1A-C2A	-3.90	124.15	133.31
21	S	301	CHL	CHA-C1A-C2A	-3.90	124.15	133.31
21	s	306	CHL	CHA-C1A-C2A	-3.90	124.15	133.31
21	R	306	CHL	CHA-C1A-C2A	-3.90	124.15	133.31
21	r	307	CHL	CHA-C1A-C2A	-3.90	124.16	133.31
21	g	601	CHL	CHA-C1A-C2A	-3.90	124.16	133.31
21	n	606	CHL	CHA-C1A-C2A	-3.90	124.16	133.31
21	r	301	CHL	CHA-C1A-C2A	-3.90	124.16	133.31
33	L	102	SQD	O9-S-O7	-3.90	101.15	113.82
21	R	305	CHL	CHA-C1A-C2A	-3.90	124.16	133.31
21	N	607	CHL	CHA-C1A-C2A	-3.90	124.16	133.31
21	y	606	CHL	CHA-C1A-C2A	-3.89	124.16	133.31
21	N	605	CHL	CHA-C1A-C2A	-3.89	124.16	133.31
21	g	609	CHL	CHA-C1A-C2A	-3.89	124.17	133.31
21	y	607	CHL	CHA-C1A-C2A	-3.89	124.17	133.31
21	G	601	CHL	CHA-C1A-C2A	-3.89	124.17	133.31
21	s	307	CHL	CHA-C1A-C2A	-3.89	124.17	133.31
21	N	608	CHL	CHA-C1A-C2A	-3.89	124.17	133.31
21	s	301	CHL	CHA-C1A-C2A	-3.89	124.17	133.31
21	N	606	CHL	CHA-C1A-C2A	-3.89	124.17	133.31
21	Y	607	CHL	CHA-C1A-C2A	-3.89	124.17	133.31
21	y	601	CHL	CHA-C1A-C2A	-3.89	124.17	133.31
21	S	306	CHL	CHA-C1A-C2A	-3.89	124.18	133.31
21	n	607	CHL	CHA-C1A-C2A	-3.89	124.18	133.31
21	Y	605	CHL	CHA-C1A-C2A	-3.89	124.18	133.31
21	r	306	CHL	CHA-C1A-C2A	-3.89	124.18	133.31
33	l	101	SQD	O9-S-O7	-3.89	101.19	113.82
23	g	616	LUT	C4-C5-C6	-3.88	112.78	120.76
21	g	606	CHL	CHA-C1A-C2A	-3.88	124.19	133.31
21	n	601	CHL	CHA-C1A-C2A	-3.88	124.19	133.31
33	l	103	SQD	O47-C7-C8	3.88	119.87	111.48
21	n	605	CHL	CHA-C1A-C2A	-3.88	124.20	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	410	PL9	C7-C3-C2	-3.87	118.83	123.39
33	L	101	SQD	O47-C7-C8	3.85	119.82	111.48
24	Y	615	XAT	C38-C25-C24	-3.84	109.93	114.24
25	Y	616	NEX	C17-C1-C6	-3.83	107.04	110.47
25	Y	616	NEX	C37-C21-C26	3.83	120.38	110.05
32	A	411	PL9	C7-C3-C2	-3.83	118.88	123.39
23	G	616	LUT	C4-C5-C6	-3.82	112.91	120.76
25	r	315	NEX	C37-C21-C26	3.82	120.35	110.05
25	g	618	NEX	C17-C1-C6	-3.81	107.06	110.47
25	y	618	NEX	C37-C21-C26	3.80	120.29	110.05
24	r	314	XAT	C27-C28-C29	-3.80	119.64	125.53
25	y	616	NEX	C17-C1-C6	-3.79	107.08	110.47
24	N	616	XAT	C28-C29-C30	-3.78	113.06	119.01
24	R	313	XAT	C27-C28-C29	-3.78	119.67	125.53
24	n	615	XAT	C28-C29-C30	-3.77	113.08	119.01
23	g	616	LUT	C12-C13-C14	-3.76	113.09	119.01
37	F	101	HEM	C4C-C3C-C2C	3.76	110.07	106.81
25	Y	616	NEX	C28-C29-C30	-3.76	113.10	119.01
24	g	617	XAT	C38-C25-C24	-3.75	110.03	114.24
25	Y	616	NEX	C27-C28-C29	-3.75	119.71	125.53
23	Y	614	LUT	C4-C5-C6	-3.74	113.07	120.76
35	J	101	DGD	O6D-C1D-O3G	-3.73	101.23	110.04
35	c	519	DGD	O6D-C1D-O3G	-3.73	101.24	110.04
37	f	101	HEM	C3A-C4A-NA	-3.69	104.22	110.14
37	f	101	HEM	C4C-C3C-C2C	3.69	110.01	106.81
37	F	101	HEM	C3A-C4A-NA	-3.68	104.24	110.14
37	F	101	HEM	C2A-C1A-NA	-3.68	106.07	110.15
37	f	101	HEM	C2A-C1A-NA	-3.68	106.07	110.15
35	c	517	DGD	O6D-C1D-O3G	-3.67	101.36	110.04
24	n	615	XAT	C38-C25-C24	-3.67	110.12	114.24
25	r	315	NEX	C27-C28-C29	-3.67	119.84	125.53
24	N	616	XAT	C38-C25-C24	-3.67	110.12	114.24
35	C	518	DGD	O6D-C1D-O3G	-3.66	101.39	110.04
25	y	618	NEX	C27-C28-C29	-3.65	119.87	125.53
23	n	614	LUT	C1-C6-C7	-3.64	105.79	115.65
33	L	102	SQD	O47-C7-C8	3.63	119.33	111.48
23	G	615	LUT	C1-C6-C7	-3.63	105.81	115.65
23	g	615	LUT	C1-C6-C7	-3.62	105.83	115.65
23	Y	613	LUT	C1-C6-C7	-3.62	105.84	115.65
23	N	614	LUT	C1-C6-C7	-3.62	105.84	115.65
23	y	614	LUT	C1-C6-C7	-3.61	105.86	115.65
33	l	101	SQD	O47-C7-C8	3.61	119.29	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	615	XAT	C28-C29-C30	-3.61	113.34	119.01
22	C	511	CLA	C3B-C4B-NB	-3.61	107.31	110.53
24	g	617	XAT	C28-C29-C30	-3.60	113.34	119.01
33	a	411	SQD	O47-C7-C8	3.59	119.24	111.48
24	Y	615	XAT	C32-C33-C34	-3.58	113.38	119.01
33	D	402	SQD	O47-C7-C8	3.57	119.21	111.48
22	c	510	CLA	C3B-C4B-NB	-3.57	107.34	110.53
33	d	402	SQD	O47-C7-C8	3.57	119.20	111.48
24	R	313	XAT	C38-C25-C24	-3.56	110.24	114.24
33	A	412	SQD	O47-C7-C8	3.56	119.19	111.48
33	D	402	SQD	O9-S-C6	3.55	112.06	106.76
33	d	402	SQD	O9-S-C6	3.55	112.05	106.76
30	D	401	PHO	C2B-C1B-NB	-3.54	106.87	109.43
37	F	101	HEM	C2C-C1C-NC	-3.54	103.09	109.64
25	N	617	NEX	O24-C26-C27	-3.54	106.75	116.88
30	d	401	PHO	C2B-C1B-NB	-3.53	106.88	109.43
37	f	101	HEM	C2C-C1C-NC	-3.53	103.11	109.64
35	a	413	DGD	O6D-C1D-O3G	-3.52	101.72	110.04
21	y	601	CHL	C1-C2-C3	-3.51	120.44	126.20
21	R	305	CHL	C1-C2-C3	-3.51	120.45	126.20
33	A	412	SQD	C1-O5-C5	3.51	120.57	113.72
35	A	401	DGD	O6D-C1D-O3G	-3.50	101.76	110.04
21	N	607	CHL	C1-C2-C3	-3.50	120.46	126.20
24	r	314	XAT	C38-C25-C24	-3.50	110.31	114.24
21	Y	601	CHL	C1-C2-C3	-3.50	120.46	126.20
21	r	307	CHL	C1-C2-C3	-3.50	120.46	126.20
21	r	308	CHL	C1-C2-C3	-3.49	120.47	126.20
21	G	609	CHL	C1-C2-C3	-3.49	120.47	126.20
36	w	102	LMG	O6-C1-O1	-3.49	101.79	110.04
33	a	411	SQD	C1-O5-C5	3.49	120.53	113.72
21	g	609	CHL	C1-C2-C3	-3.49	120.48	126.20
21	n	601	CHL	C1-C2-C3	-3.49	120.49	126.20
21	G	607	CHL	C1-C2-C3	-3.48	120.49	126.20
21	g	601	CHL	C1-C2-C3	-3.48	120.49	126.20
21	r	306	CHL	C1-C2-C3	-3.48	120.49	126.20
21	n	608	CHL	C1-C2-C3	-3.48	120.49	126.20
21	y	608	CHL	C1-C2-C3	-3.48	120.50	126.20
36	C	502	LMG	O6-C1-O1	-3.48	101.83	110.04
21	N	608	CHL	C1-C2-C3	-3.48	120.50	126.20
21	Y	607	CHL	C1-C2-C3	-3.48	120.50	126.20
21	Y	606	CHL	C1-C2-C3	-3.48	120.50	126.20
21	N	601	CHL	C1-C2-C3	-3.47	120.50	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	617	XAT	C28-C29-C30	-3.47	113.55	119.01
21	g	607	CHL	C1-C2-C3	-3.47	120.51	126.20
37	f	101	HEM	CHB-C1B-C2B	3.47	136.81	126.95
21	R	307	CHL	C1-C2-C3	-3.47	120.51	126.20
21	y	609	CHL	C1-C2-C3	-3.47	120.52	126.20
21	n	607	CHL	C1-C2-C3	-3.46	120.52	126.20
21	g	608	CHL	C1-C2-C3	-3.46	120.52	126.20
21	N	606	CHL	C1-C2-C3	-3.46	120.53	126.20
21	R	306	CHL	C1-C2-C3	-3.46	120.53	126.20
21	Y	608	CHL	C1-C2-C3	-3.46	120.53	126.20
30	D	401	PHO	O1D-CGD-CBD	3.46	129.96	124.72
24	Y	615	XAT	C28-C29-C30	-3.45	113.58	119.01
37	F	101	HEM	CHB-C1B-C2B	3.45	136.75	126.95
21	n	606	CHL	C1-C2-C3	-3.44	120.56	126.20
21	y	607	CHL	C1-C2-C3	-3.44	120.56	126.20
22	S	309	CLA	C1-C2-C3	-3.44	120.56	126.20
21	G	601	CHL	C1-C2-C3	-3.44	120.56	126.20
21	G	608	CHL	C1-C2-C3	-3.44	120.56	126.20
22	s	309	CLA	C1-C2-C3	-3.44	120.56	126.20
30	d	401	PHO	O1D-CGD-CBD	3.42	129.91	124.72
33	L	101	SQD	C44-O6-C1	3.41	121.12	113.80
35	c	518	DGD	O6D-C1D-O3G	-3.41	102.00	110.04
25	y	616	NEX	C5-C6-C1	-3.40	116.32	119.70
33	A	412	SQD	C44-O6-C1	3.40	121.09	113.80
33	a	411	SQD	C44-O6-C1	3.39	121.06	113.80
30	A	408	PHO	C2B-C1B-NB	-3.38	106.98	109.43
35	C	519	DGD	O6D-C1D-O3G	-3.38	102.05	110.04
33	l	103	SQD	C44-O6-C1	3.38	121.04	113.80
30	a	407	PHO	C2B-C1B-NB	-3.36	107.00	109.43
35	h	102	DGD	O6D-C1D-O3G	-3.36	102.11	110.04
35	H	102	DGD	O6D-C1D-O3G	-3.34	102.14	110.04
33	L	101	SQD	C1-O5-C5	3.33	120.23	113.72
24	N	616	XAT	C31-C32-C33	-3.33	117.22	126.36
23	Y	613	LUT	C27-C28-C29	-3.33	119.15	126.32
37	F	101	HEM	CHB-C4A-NA	3.33	129.90	123.86
22	g	613	CLA	C4D-CHA-C1A	-3.33	117.28	121.24
22	Y	611	CLA	C4D-CHA-C1A	-3.33	117.28	121.24
37	f	101	HEM	CHB-C4A-NA	3.32	129.88	123.86
23	R	312	LUT	C7-C8-C9	-3.31	121.33	126.23
34	a	412	BCT	O2-C-O1	-3.31	111.21	119.68
33	l	103	SQD	C1-O5-C5	3.31	120.18	113.72
22	G	613	CLA	C4D-CHA-C1A	-3.31	117.30	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	612	CLA	C4D-CHA-C1A	-3.31	117.30	121.24
23	G	615	LUT	C27-C28-C29	-3.31	119.21	126.32
23	n	614	LUT	C27-C28-C29	-3.31	119.22	126.32
30	A	408	PHO	O1D-CGD-CBD	3.30	129.74	124.72
37	F	101	HEM	CHC-C4B-NB	3.30	127.98	124.42
22	N	612	CLA	C4D-CHA-C1A	-3.30	117.31	121.24
23	r	313	LUT	C7-C8-C9	-3.30	121.35	126.23
23	N	614	LUT	C27-C28-C29	-3.30	119.22	126.32
34	D	403	BCT	O2-C-O1	-3.30	111.23	119.68
23	g	615	LUT	C27-C28-C29	-3.30	119.23	126.32
23	y	614	LUT	C27-C28-C29	-3.29	119.25	126.32
33	A	412	SQD	O7-S-C6	3.29	111.66	106.76
37	f	101	HEM	CHC-C4B-NB	3.28	127.96	124.42
33	a	411	SQD	O7-S-C6	3.28	111.66	106.76
33	D	402	SQD	C1-O5-C5	3.28	120.13	113.72
22	n	612	CLA	C4D-CHA-C1A	-3.28	117.34	121.24
33	l	101	SQD	O9-S-C6	3.27	111.64	106.76
30	a	407	PHO	O1D-CGD-CBD	3.26	129.67	124.72
33	d	402	SQD	C1-O5-C5	3.26	120.08	113.72
25	N	617	NEX	C16-C1-C6	3.25	113.38	110.47
33	L	102	SQD	O9-S-C6	3.23	111.58	106.76
25	y	616	NEX	C27-C28-C29	-3.21	120.55	125.53
23	r	313	LUT	C4-C5-C6	-3.20	114.17	120.76
22	C	510	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
25	r	315	NEX	C17-C1-C6	-3.19	107.62	110.47
23	R	312	LUT	C4-C5-C6	-3.18	114.22	120.76
22	c	509	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
23	R	312	LUT	C18-C5-C4	-3.17	108.59	114.42
23	r	313	LUT	C18-C5-C4	-3.17	108.59	114.42
25	y	618	NEX	C17-C1-C6	-3.16	107.64	110.47
25	n	616	NEX	C5-C6-C1	-3.16	116.56	119.70
33	L	102	SQD	O7-S-C6	3.16	111.47	106.76
33	l	101	SQD	O7-S-C6	3.16	111.47	106.76
23	Y	614	LUT	C8-C9-C10	-3.15	114.06	119.01
22	y	612	CLA	C3B-C4B-NB	-3.14	107.73	110.53
22	G	613	CLA	C3A-C2A-C1A	3.13	106.03	101.34
22	G	613	CLA	C3B-C4B-NB	-3.13	107.73	110.53
22	B	615	CLA	C3B-C4B-NB	-3.13	107.74	110.53
37	F	101	HEM	CHD-C1D-C2D	3.12	129.95	125.03
22	g	613	CLA	C3B-C4B-NB	-3.12	107.75	110.53
22	Y	611	CLA	C3B-C4B-NB	-3.11	107.75	110.53
22	b	614	CLA	C3B-C4B-NB	-3.11	107.76	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	611	CLA	C3A-C2A-C1A	3.10	105.98	101.34
22	n	612	CLA	C3A-C2A-C1A	3.10	105.98	101.34
22	g	613	CLA	C3A-C2A-C1A	3.09	105.97	101.34
22	s	311	CLA	C3B-C4B-NB	-3.09	107.77	110.53
33	l	103	SQD	O7-S-C6	3.09	111.37	106.76
22	b	612	CLA	C3B-C4B-NB	-3.09	107.77	110.53
33	L	101	SQD	O7-S-C6	3.09	111.37	106.76
22	y	612	CLA	C3A-C2A-C1A	3.09	105.97	101.34
37	f	101	HEM	CHD-C1D-C2D	3.09	129.90	125.03
22	N	612	CLA	C3B-C4B-NB	-3.09	107.77	110.53
22	B	617	CLA	C3B-C4B-NB	-3.08	107.78	110.53
22	n	612	CLA	C3B-C4B-NB	-3.08	107.78	110.53
25	n	616	NEX	O24-C26-C27	-3.08	108.06	116.88
22	c	510	CLA	C4D-C3D-CAD	-3.08	104.76	108.11
22	a	404	CLA	C3B-C4B-NB	-3.07	107.78	110.53
22	S	311	CLA	C3B-C4B-NB	-3.07	107.79	110.53
33	l	103	SQD	O5-C5-C4	3.07	115.23	109.70
23	g	616	LUT	C26-C27-C28	-3.07	119.80	124.58
22	a	406	CLA	C3B-C4B-NB	-3.07	107.79	110.53
22	N	612	CLA	C3A-C2A-C1A	3.06	105.92	101.34
25	Y	616	NEX	C5-C6-C1	-3.06	116.66	119.70
22	C	511	CLA	C4D-C3D-CAD	-3.06	104.79	108.11
33	L	101	SQD	O5-C5-C4	3.05	115.20	109.70
25	g	618	NEX	O24-C26-C27	-3.05	108.13	116.88
32	a	410	PL9	O2-C1-C2	-3.04	117.09	121.43
33	l	103	SQD	O9-S-C6	3.04	111.30	106.76
33	L	101	SQD	O9-S-C6	3.03	111.28	106.76
22	d	403	CLA	C3B-C4B-NB	-3.03	107.83	110.53
22	A	407	CLA	C3B-C4B-NB	-3.03	107.83	110.53
22	s	309	CLA	C3B-C4B-NB	-3.02	107.83	110.53
23	Y	614	LUT	C26-C27-C28	-3.02	119.88	124.58
24	Y	615	XAT	C31-C32-C33	-3.02	118.08	126.36
33	D	402	SQD	O7-S-C6	3.02	111.26	106.76
33	d	402	SQD	O7-S-C6	3.01	111.25	106.76
22	A	405	CLA	C3B-C4B-NB	-3.01	107.84	110.53
22	y	612	CLA	C1C-C2C-C3C	-3.00	103.83	106.98
32	A	411	PL9	O2-C1-C2	-3.00	117.16	121.43
22	g	613	CLA	C1C-C2C-C3C	-2.99	103.83	106.98
22	g	613	CLA	CHB-C4A-NA	2.99	128.72	124.40
22	B	605	CLA	C3B-C4B-NB	-2.99	107.86	110.53
25	g	618	NEX	C27-C28-C29	-2.99	120.89	125.53
22	D	404	CLA	O2D-CGD-O1D	-2.99	118.03	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	612	CLA	CHB-C4A-NA	2.99	128.71	124.40
22	S	309	CLA	C3B-C4B-NB	-2.99	107.86	110.53
23	G	616	LUT	C8-C9-C10	-2.98	114.31	119.01
33	a	411	SQD	O5-C1-C2	2.98	116.50	110.37
33	A	412	SQD	O5-C1-C2	2.98	116.50	110.37
22	C	512	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
22	n	612	CLA	CHB-C4A-NA	2.98	128.70	124.40
21	Y	605	CHL	OMC-CMC-C2C	-2.98	119.94	125.12
22	N	612	CLA	CHB-C4A-NA	2.98	128.70	124.40
21	G	607	CHL	OMC-CMC-C2C	-2.98	119.94	125.12
22	C	504	CLA	C3B-C4B-NB	-2.98	107.87	110.53
22	D	404	CLA	C3B-C4B-NB	-2.98	107.87	110.53
21	R	306	CHL	OMC-CMC-C2C	-2.98	119.95	125.12
31	c	516	BCR	C15-C14-C13	-2.98	123.10	127.28
22	N	612	CLA	C1C-C2C-C3C	-2.98	103.85	106.98
21	n	601	CHL	OMC-CMC-C2C	-2.98	119.95	125.12
24	y	615	XAT	C8-C9-C10	-2.97	114.33	119.01
22	Y	611	CLA	CHB-C4A-NA	2.97	128.69	124.40
22	G	613	CLA	C1C-C2C-C3C	-2.97	103.85	106.98
21	s	307	CHL	OMC-CMC-C2C	-2.97	119.96	125.12
22	n	612	CLA	C1C-C2C-C3C	-2.97	103.86	106.98
21	r	307	CHL	OMC-CMC-C2C	-2.97	119.97	125.12
36	C	502	LMG	O1-C1-C2	-2.97	103.77	108.27
21	R	305	CHL	OMC-CMC-C2C	-2.97	119.97	125.12
31	C	517	BCR	C7-C8-C9	-2.97	121.85	126.23
21	N	607	CHL	OMC-CMC-C2C	-2.97	119.97	125.12
31	C	517	BCR	C11-C10-C9	-2.97	123.12	127.28
25	y	616	NEX	C24-C23-C22	2.97	116.34	110.79
21	g	609	CHL	OMC-CMC-C2C	-2.97	119.97	125.12
21	y	607	CHL	OMC-CMC-C2C	-2.96	119.97	125.12
21	y	608	CHL	OMC-CMC-C2C	-2.96	119.97	125.12
22	c	503	CLA	C3B-C4B-NB	-2.96	107.88	110.53
21	g	608	CHL	OMC-CMC-C2C	-2.96	119.97	125.12
22	C	514	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	R	308	CLA	C3B-C4B-NB	-2.96	107.89	110.53
21	r	301	CHL	OMC-CMC-C2C	-2.96	119.97	125.12
22	d	403	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
22	G	613	CLA	CHB-C4A-NA	2.96	128.68	124.40
22	C	509	CLA	C3B-C4B-NB	-2.96	107.89	110.53
21	N	601	CHL	OMC-CMC-C2C	-2.96	119.98	125.12
31	H	101	BCR	C24-C23-C22	-2.96	121.86	126.23
22	Y	611	CLA	O2D-CGD-O1D	-2.96	118.09	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	609	CHL	OMC-CMC-C2C	-2.96	119.98	125.12
21	N	606	CHL	OMC-CMC-C2C	-2.96	119.98	125.12
21	S	306	CHL	OMC-CMC-C2C	-2.96	119.98	125.12
21	y	605	CHL	OMC-CMC-C2C	-2.96	119.98	125.12
21	r	308	CHL	OMC-CMC-C2C	-2.96	119.98	125.12
21	S	301	CHL	OMC-CMC-C2C	-2.96	119.98	125.12
22	b	602	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	c	508	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	c	513	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	B	612	CLA	C3B-C4B-NB	-2.96	107.89	110.53
31	C	517	BCR	C15-C14-C13	-2.95	123.13	127.28
21	S	302	CHL	OMC-CMC-C2C	-2.95	119.99	125.12
21	S	307	CHL	OMC-CMC-C2C	-2.95	119.99	125.12
22	C	503	CLA	C3B-C4B-NB	-2.95	107.89	110.53
21	g	606	CHL	OMC-CMC-C2C	-2.95	119.99	125.12
21	n	605	CHL	OMC-CMC-C2C	-2.95	119.99	125.12
21	n	606	CHL	OMC-CMC-C2C	-2.95	119.99	125.12
21	N	608	CHL	OMC-CMC-C2C	-2.95	119.99	125.12
22	C	515	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
21	g	607	CHL	OMC-CMC-C2C	-2.95	119.99	125.12
21	R	307	CHL	OMC-CMC-C2C	-2.95	119.99	125.12
22	n	604	CLA	C3B-C4B-NB	-2.95	107.89	110.53
21	y	601	CHL	OMC-CMC-C2C	-2.95	120.00	125.12
21	s	306	CHL	OMC-CMC-C2C	-2.95	120.00	125.12
22	Y	603	CLA	C3B-C4B-NB	-2.95	107.90	110.53
36	w	102	LMG	O1-C1-C2	-2.95	103.79	108.27
21	g	601	CHL	OMC-CMC-C2C	-2.95	120.00	125.12
32	D	407	PL9	C40-C39-C41	2.95	120.35	115.23
22	G	613	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
21	G	608	CHL	OMC-CMC-C2C	-2.95	120.00	125.12
21	N	605	CHL	OMC-CMC-C2C	-2.95	120.00	125.12
21	y	606	CHL	OMC-CMC-C2C	-2.95	120.00	125.12
22	c	511	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
21	Y	607	CHL	OMC-CMC-C2C	-2.94	120.01	125.12
21	n	607	CHL	OMC-CMC-C2C	-2.94	120.01	125.12
22	N	612	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	b	609	CLA	C3B-C4B-NB	-2.94	107.90	110.53
21	G	605	CHL	OMC-CMC-C2C	-2.94	120.01	125.12
22	Y	611	CLA	C1C-C2C-C3C	-2.94	103.89	106.98
21	y	609	CHL	OMC-CMC-C2C	-2.94	120.01	125.12
31	h	101	BCR	C24-C23-C22	-2.94	121.89	126.23
21	r	306	CHL	OMC-CMC-C2C	-2.94	120.02	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	620	LMG	O6-C1-O1	-2.94	103.11	110.04
22	y	612	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
22	c	504	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
22	g	603	CLA	C3B-C4B-NB	-2.93	107.91	110.53
32	d	406	PL9	C40-C39-C41	2.93	120.32	115.23
22	c	514	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
31	c	516	BCR	C7-C8-C9	-2.93	121.89	126.23
21	Y	601	CHL	OMC-CMC-C2C	-2.93	120.03	125.12
24	n	615	XAT	C31-C32-C33	-2.93	118.32	126.36
36	B	623	LMG	O6-C1-O1	-2.93	103.12	110.04
21	s	302	CHL	OMC-CMC-C2C	-2.93	120.03	125.12
22	A	405	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
23	g	616	LUT	C8-C9-C10	-2.93	114.40	119.01
22	r	303	CLA	C3B-C4B-NB	-2.93	107.92	110.53
21	G	601	CHL	OMC-CMC-C2C	-2.93	120.04	125.12
22	g	604	CLA	C3B-C4B-NB	-2.93	107.92	110.53
22	a	404	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
22	n	612	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
21	n	608	CHL	OMC-CMC-C2C	-2.92	120.05	125.12
21	Y	608	CHL	OMC-CMC-C2C	-2.92	120.05	125.12
22	C	513	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
25	n	616	NEX	C27-C28-C29	-2.92	121.00	125.53
21	g	605	CHL	OMC-CMC-C2C	-2.92	120.05	125.12
22	g	613	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	G	617	XAT	C31-C32-C33	-2.92	118.36	126.36
22	C	511	CLA	CHC-C4B-NB	2.92	128.43	124.05
22	r	309	CLA	C3B-C4B-NB	-2.92	107.93	110.53
31	B	620	BCR	C15-C14-C13	-2.92	123.19	127.28
21	Y	606	CHL	OMC-CMC-C2C	-2.92	120.06	125.12
22	G	604	CLA	C3B-C4B-NB	-2.91	107.93	110.53
22	C	512	CLA	C3B-C4B-NB	-2.91	107.93	110.53
21	s	301	CHL	OMC-CMC-C2C	-2.91	120.06	125.12
22	d	404	CLA	C3B-C4B-NB	-2.91	107.93	110.53
21	G	606	CHL	OMC-CMC-C2C	-2.91	120.06	125.12
24	g	617	XAT	C31-C32-C33	-2.91	118.38	126.36
31	b	617	BCR	C15-C14-C13	-2.91	123.20	127.28
35	J	101	DGD	C3D-C4D-C5D	-2.91	104.95	110.23
37	F	101	HEM	C4A-NA-C1A	2.91	110.56	105.82
32	D	407	PL9	C22-C23-C24	-2.91	120.97	127.62
22	G	602	CLA	C3B-C4B-NB	-2.91	107.94	110.53
37	f	101	HEM	C4A-NA-C1A	2.91	110.56	105.82
22	c	512	CLA	O2D-CGD-O1D	-2.91	118.19	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	516	BCR	C15-C16-C17	-2.90	117.58	123.52
22	b	615	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	c	511	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	b	611	CLA	C3B-C4B-NB	-2.90	107.94	110.53
31	c	516	BCR	C11-C10-C9	-2.90	123.21	127.28
31	C	516	BCR	C24-C23-C22	-2.90	121.95	126.23
22	y	603	CLA	C3B-C4B-NB	-2.90	107.94	110.53
31	k	102	BCR	C15-C16-C17	-2.90	117.59	123.52
22	n	603	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	N	603	CLA	C3B-C4B-NB	-2.90	107.94	110.53
31	K	102	BCR	C15-C16-C17	-2.90	117.59	123.52
31	c	515	BCR	C24-C23-C22	-2.90	121.95	126.23
22	y	604	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	c	502	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	B	618	CLA	C3B-C4B-NB	-2.89	107.95	110.53
35	c	519	DGD	O6E-C5E-C4E	2.89	114.91	109.70
26	l	102	LHG	O8-C23-C24	2.89	120.65	111.83
26	L	103	LHG	O8-C23-C24	2.89	120.64	111.83
22	b	609	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
36	D	411	LMG	O6-C1-O1	-2.89	103.22	110.04
22	C	505	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
35	c	519	DGD	C3D-C4D-C5D	-2.89	105.00	110.23
22	D	405	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	B	612	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	B	607	CLA	C3B-C4B-NB	-2.88	107.96	110.53
37	f	101	HEM	C4A-C3A-C2A	2.88	110.11	106.82
22	B	614	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	g	602	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	s	303	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
32	d	406	PL9	C22-C23-C24	-2.88	121.04	127.62
35	J	101	DGD	O6E-C5E-C4E	2.88	114.88	109.70
22	Y	604	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	y	602	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	N	604	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	N	602	CLA	C3B-C4B-NB	-2.87	107.97	110.53
31	c	515	BCR	C15-C16-C17	-2.87	117.65	123.52
25	y	618	NEX	C38-C25-C24	2.87	117.46	114.24
22	Y	609	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	c	510	CLA	CHC-C4B-NB	2.86	128.35	124.05
22	b	604	CLA	C3B-C4B-NB	-2.86	107.97	110.53
22	C	509	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
22	N	609	CLA	C3B-C4B-NB	-2.86	107.97	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	d	410	LMG	O6-C1-O1	-2.86	103.28	110.04
22	c	508	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
22	r	310	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	b	615	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
22	G	603	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	B	611	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
22	n	613	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
22	b	613	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
31	B	621	BCR	C24-C23-C22	-2.85	122.01	126.23
22	g	610	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	b	601	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	B	615	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
22	B	608	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	S	303	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	r	315	NEX	C38-C25-C24	2.85	117.44	114.24
22	B	618	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	b	608	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
22	Y	602	CLA	C3B-C4B-NB	-2.85	107.99	110.53
22	B	616	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
31	C	516	BCR	C27-C26-C25	2.84	126.55	122.70
31	B	619	BCR	C33-C5-C6	-2.84	121.38	124.48
22	B	611	CLA	C3B-C4B-NB	-2.84	107.99	110.53
31	b	618	BCR	C24-C23-C22	-2.84	122.03	126.23
31	a	409	BCR	C27-C26-C25	2.84	126.55	122.70
37	F	101	HEM	C4A-C3A-C2A	2.84	110.07	106.82
22	C	506	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
36	C	523	LMG	O6-C1-O1	-2.84	103.33	110.04
22	y	613	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
31	b	616	BCR	C33-C5-C6	-2.84	121.39	124.48
31	b	616	BCR	C27-C26-C25	2.84	126.53	122.70
22	y	611	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	Y	610	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	C	515	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	R	309	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	b	603	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
22	G	610	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	b	608	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	c	505	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
26	S	314	LHG	O8-C23-C24	2.83	120.47	111.83
22	Y	609	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
22	g	611	CLA	C3B-C4B-NB	-2.83	108.01	110.53
33	A	412	SQD	O9-S-C6	2.83	110.98	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	607	CLA	C3B-C4B-NB	-2.83	108.01	110.53
22	g	614	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
22	G	614	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
33	a	411	SQD	O9-S-C6	2.83	110.97	106.76
22	s	309	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
22	n	610	CLA	C3B-C4B-NB	-2.82	108.01	110.53
22	c	514	CLA	C3B-C4B-NB	-2.82	108.01	110.53
22	b	612	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
31	B	620	BCR	C15-C16-C17	-2.82	117.75	123.52
22	N	609	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	r	304	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	R	303	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
23	G	616	LUT	C26-C27-C28	-2.82	120.19	124.58
22	Y	612	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	N	613	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
36	c	523	LMG	O6-C1-O1	-2.82	103.39	110.04
26	R	301	LHG	O8-C23-C24	2.82	120.42	111.83
31	b	617	BCR	C15-C16-C17	-2.82	117.76	123.52
31	D	406	BCR	C24-C23-C22	-2.82	122.07	126.23
22	n	602	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	C	507	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
35	H	102	DGD	CDB-CCB-CBB	-2.81	100.15	114.37
26	s	314	LHG	O8-C23-C24	2.81	120.41	111.83
22	B	610	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	B	606	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
22	G	610	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
22	g	610	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
22	C	510	CLA	C3B-C4B-NB	-2.81	108.02	110.53
35	h	102	DGD	CDB-CCB-CBB	-2.81	100.16	114.37
31	A	410	BCR	C27-C26-C25	2.81	126.50	122.70
22	y	610	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
26	r	302	LHG	O8-C23-C24	2.81	120.40	111.83
22	b	605	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	B	604	CLA	C3B-C4B-NB	-2.81	108.02	110.53
31	C	516	BCR	C33-C5-C6	-2.81	121.42	124.48
22	b	603	CLA	C3B-C4B-NB	-2.80	108.03	110.53
24	y	615	XAT	C31-C32-C33	-2.80	118.67	126.36
26	C	521	LHG	O8-C23-C24	2.80	120.38	111.83
22	n	609	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
31	B	619	BCR	C27-C26-C25	2.80	126.49	122.70
22	y	610	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	R	302	CLA	C3B-C4B-NB	-2.80	108.03	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	405	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	c	509	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	c	506	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
35	c	518	DGD	CDB-CCB-CBB	-2.79	100.24	114.37
22	B	608	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
31	c	515	BCR	C27-C26-C25	2.79	126.48	122.70
22	S	309	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
22	n	609	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	B	610	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	A	407	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	G	611	CLA	C3B-C4B-NB	-2.79	108.04	110.53
31	k	101	BCR	C24-C23-C22	-2.78	122.12	126.23
35	C	519	DGD	CDB-CCB-CBB	-2.78	100.30	114.37
21	R	307	CHL	C4-C3-C5	2.78	120.06	115.23
22	b	607	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
26	c	521	LHG	O8-C23-C24	2.78	120.31	111.83
21	n	608	CHL	C4-C3-C5	2.78	120.05	115.23
23	R	312	LUT	C27-C28-C29	-2.77	120.36	126.32
22	s	310	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
31	d	405	BCR	C24-C23-C22	-2.77	122.14	126.23
22	B	606	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	c	507	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
31	D	406	BCR	C33-C5-C6	-2.77	121.46	124.48
26	d	409	LHG	O8-C23-C24	2.77	120.28	111.83
21	Y	601	CHL	C4-C3-C5	2.77	120.03	115.23
22	A	406	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	C	513	CLA	C3B-C4B-NB	-2.77	108.06	110.53
31	C	517	BCR	C27-C26-C25	2.77	126.44	122.70
22	g	611	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
22	c	507	CLA	C3B-C4B-NB	-2.77	108.06	110.53
31	d	405	BCR	C33-C5-C6	-2.76	121.47	124.48
22	S	304	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
22	B	616	CLA	C3B-C4B-NB	-2.76	108.06	110.53
21	Y	607	CHL	C4-C3-C5	2.76	120.02	115.23
21	R	305	CHL	C4-C3-C5	2.76	120.02	115.23
37	f	101	HEM	C3C-C2C-C1C	2.76	109.66	107.05
22	a	406	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
31	K	101	BCR	C24-C23-C22	-2.76	122.15	126.23
21	N	601	CHL	C4-C3-C5	2.76	120.02	115.23
22	s	313	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
21	G	607	CHL	C4-C3-C5	2.76	120.02	115.23
31	c	515	BCR	C33-C5-C6	-2.76	121.47	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	610	CLA	C3B-C4B-NB	-2.76	108.07	110.53
22	b	605	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
22	B	613	CLA	C3B-C4B-NB	-2.76	108.07	110.53
33	L	102	SQD	O5-C5-C4	2.76	114.67	109.70
21	g	609	CHL	C4-C3-C5	2.76	120.01	115.23
21	N	607	CHL	C4-C3-C5	2.76	120.01	115.23
26	D	410	LHG	O8-C23-C24	2.76	120.24	111.83
21	r	308	CHL	C4-C3-C5	2.76	120.01	115.23
21	n	601	CHL	C4-C3-C5	2.75	120.01	115.23
22	s	304	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
21	G	609	CHL	C4-C3-C5	2.75	120.01	115.23
23	r	313	LUT	C27-C28-C29	-2.75	120.40	126.32
22	S	313	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
22	G	611	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
22	C	508	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
21	g	607	CHL	C4-C3-C5	2.75	120.00	115.23
21	N	606	CHL	O2A-CGA-CBA	2.75	120.22	111.83
22	Y	610	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
22	n	610	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
21	G	608	CHL	C4-C3-C5	2.75	120.00	115.23
22	C	508	CLA	C3B-C4B-NB	-2.75	108.08	110.53
21	y	607	CHL	C4-C3-C5	2.75	120.00	115.23
22	r	311	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
21	R	306	CHL	C4-C3-C5	2.75	119.99	115.23
21	g	601	CHL	O2A-CGA-CBA	2.74	120.20	111.83
25	g	618	NEX	C5-C6-C1	-2.74	116.97	119.70
21	y	601	CHL	C4-C3-C5	2.74	119.99	115.23
22	N	610	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
22	R	311	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
26	D	409	LHG	O8-C23-C24	2.74	120.20	111.83
22	R	309	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
21	r	308	CHL	O2A-CGA-CBA	2.74	120.20	111.83
21	y	606	CHL	O2A-CGA-CBA	2.74	120.19	111.83
21	N	607	CHL	O2A-CGA-CBA	2.74	120.19	111.83
21	g	609	CHL	O2A-CGA-CBA	2.74	120.19	111.83
22	C	507	CLA	C3B-C4B-NB	-2.74	108.08	110.53
21	y	601	CHL	O2A-CGA-CBA	2.74	120.19	111.83
22	R	310	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
21	n	607	CHL	C4-C3-C5	2.74	119.98	115.23
32	d	406	PL9	C27-C28-C29	-2.74	121.35	127.62
21	N	601	CHL	O2A-CGA-CBA	2.74	120.19	111.83
21	y	608	CHL	O2A-CGA-CBA	2.74	120.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	408	LHG	O8-C23-C24	2.74	120.19	111.83
21	N	608	CHL	O2A-CGA-CBA	2.74	120.18	111.83
21	G	608	CHL	O2A-CGA-CBA	2.74	120.18	111.83
21	r	307	CHL	C4-C3-C5	2.74	119.98	115.23
21	n	607	CHL	O2A-CGA-CBA	2.74	120.18	111.83
21	n	608	CHL	O2A-CGA-CBA	2.74	120.18	111.83
21	y	607	CHL	O2A-CGA-CBA	2.74	120.18	111.83
21	G	601	CHL	C4-C3-C5	2.74	119.98	115.23
21	Y	608	CHL	C4-C3-C5	2.74	119.98	115.23
21	G	601	CHL	O2A-CGA-CBA	2.74	120.18	111.83
22	c	506	CLA	C3B-C4B-NB	-2.74	108.09	110.53
22	c	512	CLA	C3B-C4B-NB	-2.74	108.09	110.53
21	y	609	CHL	O2A-CGA-CBA	2.74	120.17	111.83
21	n	601	CHL	O2A-CGA-CBA	2.73	120.17	111.83
31	c	516	BCR	C15-C16-C17	-2.73	117.92	123.52
21	R	307	CHL	O2A-CGA-CBA	2.73	120.17	111.83
21	G	606	CHL	O2A-CGA-CBA	2.73	120.17	111.83
21	g	601	CHL	C4-C3-C5	2.73	119.97	115.23
21	r	301	CHL	O2A-CGA-CBA	2.73	120.17	111.83
21	Y	607	CHL	O2A-CGA-CBA	2.73	120.17	111.83
21	Y	608	CHL	O2A-CGA-CBA	2.73	120.17	111.83
22	C	506	CLA	C1-C2-C3	-2.73	121.72	126.20
37	F	101	HEM	C3C-C2C-C1C	2.73	109.63	107.05
21	r	307	CHL	O2A-CGA-CBA	2.73	120.17	111.83
21	g	608	CHL	C4-C3-C5	2.73	119.97	115.23
21	G	609	CHL	O2A-CGA-CBA	2.73	120.16	111.83
33	l	101	SQD	O5-C5-C4	2.73	114.62	109.70
21	R	305	CHL	O2A-CGA-CBA	2.73	120.16	111.83
21	R	306	CHL	O2A-CGA-CBA	2.73	120.16	111.83
21	n	606	CHL	O2A-CGA-CBA	2.73	120.16	111.83
21	g	608	CHL	O2A-CGA-CBA	2.73	120.16	111.83
21	G	607	CHL	O2A-CGA-CBA	2.73	120.15	111.83
21	n	606	CHL	C4-C3-C5	2.73	119.96	115.23
22	x	101	CLA	C3B-C4B-NB	-2.73	108.09	110.53
22	b	606	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
26	Y	617	LHG	O8-C23-C24	2.73	120.15	111.83
21	y	605	CHL	O2A-CGA-CBA	2.73	120.15	111.83
22	r	310	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
21	Y	601	CHL	O2A-CGA-CBA	2.73	120.15	111.83
21	S	301	CHL	O2A-CGA-CBA	2.73	120.15	111.83
31	c	516	BCR	C27-C26-C25	2.73	126.39	122.70
22	S	310	CLA	O2D-CGD-O1D	-2.73	118.54	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	r	306	CHL	O2A-CGA-CBA	2.73	120.15	111.83
21	y	608	CHL	C4-C3-C5	2.72	119.96	115.23
21	r	306	CHL	C4-C3-C5	2.72	119.96	115.23
22	b	610	CLA	C3B-C4B-NB	-2.72	108.10	110.53
21	n	605	CHL	O2A-CGA-CBA	2.72	120.14	111.83
22	c	505	CLA	C1-C2-C3	-2.72	121.73	126.20
32	D	407	PL9	C27-C28-C29	-2.72	121.39	127.62
21	N	606	CHL	C4-C3-C5	2.72	119.96	115.23
21	N	608	CHL	C4-C3-C5	2.72	119.96	115.23
22	B	609	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
21	g	607	CHL	O2A-CGA-CBA	2.72	120.14	111.83
21	s	301	CHL	O2A-CGA-CBA	2.72	120.14	111.83
35	a	413	DGD	CDB-CCB-CBB	-2.72	100.61	114.37
22	b	613	CLA	C3B-C4B-NB	-2.72	108.10	110.53
22	B	603	CLA	C3B-C4B-NB	-2.72	108.10	110.53
35	A	401	DGD	CDB-CCB-CBB	-2.72	100.62	114.37
21	N	605	CHL	O2A-CGA-CBA	2.72	120.13	111.83
22	r	312	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
21	g	606	CHL	O2A-CGA-CBA	2.72	120.12	111.83
21	Y	605	CHL	O2A-CGA-CBA	2.72	120.11	111.83
21	y	608	CHL	O1D-CGD-CBD	-2.72	120.61	124.72
22	y	611	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
31	d	405	BCR	C27-C26-C25	2.71	126.37	122.70
21	Y	606	CHL	O2A-CGA-CBA	2.71	120.11	111.83
21	y	609	CHL	C4-C3-C5	2.71	119.94	115.23
22	g	614	CLA	C3B-C4B-NB	-2.71	108.11	110.53
21	Y	606	CHL	C4-C3-C5	2.71	119.93	115.23
24	n	615	XAT	O24-C26-C27	2.71	124.64	116.88
35	c	517	DGD	CDB-CCB-CBB	-2.71	100.68	114.37
22	B	605	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
22	b	614	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
22	d	404	CLA	CHB-C4A-NA	2.70	128.30	124.40
22	n	613	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	r	305	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
22	N	603	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
22	A	409	CLA	C3B-C4B-NB	-2.70	108.12	110.53
21	G	606	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
21	s	302	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
26	y	617	LHG	C11-C10-C9	-2.70	100.74	114.37
22	b	602	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
21	s	307	CHL	O1D-CGD-CBD	-2.70	120.64	124.72
35	C	518	DGD	CDB-CCB-CBB	-2.69	100.75	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	n	603	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
22	c	502	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
21	y	601	CHL	O1D-CGD-CBD	-2.69	120.64	124.72
21	y	606	CHL	O1D-CGD-CBD	-2.69	120.64	124.72
22	r	303	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
22	R	302	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
21	s	306	CHL	O1D-CGD-CBD	-2.69	120.64	124.72
31	C	517	BCR	C15-C16-C17	-2.69	118.01	123.52
22	S	310	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	G	602	CLA	CHB-C4A-NA	2.69	128.28	124.40
22	S	305	CLA	C1-C2-C3	-2.69	122.41	126.76
21	n	608	CHL	O1D-CGD-CBD	-2.69	120.64	124.72
30	D	401	PHO	O2D-CGD-O1D	-2.69	118.61	123.85
21	y	609	CHL	O1D-CGD-CBD	-2.69	120.65	124.72
21	N	607	CHL	O1D-CGD-CBD	-2.69	120.65	124.72
26	y	617	LHG	O8-C23-C24	2.69	120.03	111.83
22	R	304	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
32	a	410	PL9	C7-C3-C4	2.69	120.85	117.88
21	g	601	CHL	O1D-CGD-CBD	-2.69	120.65	124.72
21	S	301	CHL	O1D-CGD-CBD	-2.69	120.65	124.72
22	g	602	CLA	CHB-C4A-NA	2.69	128.28	124.40
21	r	306	CHL	O1D-CGD-CBD	-2.68	120.65	124.72
21	S	307	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
21	S	306	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
32	d	406	PL9	C7-C8-C9	-2.68	122.21	126.83
22	g	603	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
22	B	617	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
22	C	503	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
21	G	605	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
21	R	306	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
22	a	405	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
21	n	605	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
21	Y	607	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
21	G	608	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
22	y	603	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
21	y	607	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
21	S	302	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
22	A	409	CLA	C1-C2-C3	-2.68	121.81	126.20
21	Y	601	CHL	O1D-CGD-CBD	-2.68	120.67	124.72
22	g	610	CLA	CHB-C4A-NA	2.68	128.26	124.40
31	a	409	BCR	C15-C14-C13	-2.68	123.53	127.28
22	s	313	CLA	C3B-C4B-NB	-2.68	108.14	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	303	CLA	C3B-C4B-NB	-2.68	108.14	110.53
31	D	406	BCR	C27-C26-C25	2.67	126.32	122.70
22	D	405	CLA	CHB-C4A-NA	2.67	128.26	124.40
21	g	607	CHL	O1D-CGD-CBD	-2.67	120.67	124.72
31	A	410	BCR	C15-C14-C13	-2.67	123.53	127.28
21	s	301	CHL	O1D-CGD-CBD	-2.67	120.67	124.72
22	S	305	CLA	CHB-C4A-NA	2.67	128.26	124.40
22	y	613	CLA	C3B-C4B-NB	-2.67	108.14	110.53
22	N	609	CLA	CHB-C4A-NA	2.67	128.25	124.40
21	g	609	CHL	O1D-CGD-CBD	-2.67	120.67	124.72
21	G	601	CHL	O1D-CGD-CBD	-2.67	120.67	124.72
22	s	305	CLA	C1-C2-C3	-2.67	122.44	126.76
21	Y	608	CHL	O1D-CGD-CBD	-2.67	120.67	124.72
21	R	307	CHL	O1D-CGD-CBD	-2.67	120.67	124.72
35	C	519	DGD	C3G-C2G-C1G	-2.67	105.56	111.78
22	N	604	CLA	CHB-C4A-NA	2.67	128.25	124.40
22	r	309	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
22	a	408	CLA	C3B-C4B-NB	-2.67	108.15	110.53
22	S	313	CLA	C3B-C4B-NB	-2.67	108.15	110.53
21	n	606	CHL	O1D-CGD-CBD	-2.67	120.68	124.72
21	N	601	CHL	O1D-CGD-CBD	-2.67	120.68	124.72
21	g	606	CHL	O1D-CGD-CBD	-2.67	120.68	124.72
21	N	608	CHL	O1D-CGD-CBD	-2.67	120.68	124.72
22	Y	602	CLA	CHB-C4A-NA	2.67	128.25	124.40
21	N	606	CHL	O1D-CGD-CBD	-2.67	120.68	124.72
22	r	312	CLA	C3B-C4B-NB	-2.66	108.15	110.53
22	G	603	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
21	G	607	CHL	O1D-CGD-CBD	-2.66	120.68	124.72
35	c	518	DGD	C3G-C2G-C1G	-2.66	105.57	111.78
21	r	301	CHL	O1D-CGD-CBD	-2.66	120.68	124.72
21	r	308	CHL	O1D-CGD-CBD	-2.66	120.68	124.72
31	K	102	BCR	C24-C23-C22	-2.66	122.30	126.23
24	G	617	XAT	O24-C26-C27	2.66	124.50	116.88
22	A	406	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
22	B	614	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
22	s	310	CLA	C3B-C4B-NB	-2.66	108.15	110.53
22	n	602	CLA	CHB-C4A-NA	2.66	128.24	124.40
22	n	609	CLA	CHB-C4A-NA	2.66	128.24	124.40
22	b	611	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
22	r	304	CLA	C3B-C4B-NB	-2.66	108.16	110.53
22	y	602	CLA	CHB-C4A-NA	2.66	128.24	124.40
35	c	519	DGD	O5D-C6D-C5D	-2.66	103.42	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	s	312	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
21	G	609	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
22	Y	603	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
22	c	503	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
21	N	605	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
21	Y	606	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
22	S	305	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
21	n	607	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
21	r	307	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
22	R	308	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
22	r	312	CLA	CHB-C4A-NA	2.66	128.23	124.40
33	D	402	SQD	O5-C5-C4	2.65	114.48	109.70
22	B	604	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
22	Y	604	CLA	CHB-C4A-NA	2.65	128.23	124.40
33	d	402	SQD	O5-C5-C4	2.65	114.48	109.70
22	s	305	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
30	d	401	PHO	O2D-CGD-O1D	-2.65	118.68	123.85
22	B	613	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
32	A	411	PL9	C7-C3-C4	2.65	120.81	117.88
26	G	618	LHG	O8-C23-C24	2.65	119.92	111.83
21	y	605	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
32	D	407	PL9	C7-C8-C9	-2.65	122.26	126.83
21	n	601	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
22	G	614	CLA	C3B-C4B-NB	-2.65	108.16	110.53
21	R	305	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
21	Y	605	CHL	O1D-CGD-CBD	-2.65	120.71	124.72
23	N	615	LUT	C3-C4-C5	-2.65	105.58	112.18
31	k	102	BCR	C24-C23-C22	-2.65	122.32	126.23
35	J	101	DGD	O5D-C6D-C5D	-2.65	103.46	109.42
23	r	313	LUT	C26-C27-C28	-2.64	120.46	124.58
22	b	610	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
22	y	610	CLA	CHB-C4A-NA	2.64	128.22	124.40
22	N	602	CLA	CHB-C4A-NA	2.64	128.22	124.40
26	g	619	LHG	O8-C23-C24	2.64	119.89	111.83
23	R	312	LUT	C26-C27-C28	-2.64	120.47	124.58
21	g	608	CHL	O1D-CGD-CBD	-2.64	120.72	124.72
22	Y	609	CLA	CHB-C4A-NA	2.64	128.21	124.40
22	a	408	CLA	C1-C2-C3	-2.64	121.87	126.20
26	g	619	LHG	C11-C10-C9	-2.64	101.03	114.37
22	G	610	CLA	CHB-C4A-NA	2.64	128.21	124.40
35	C	518	DGD	C3G-C2G-C1G	-2.64	105.64	111.78
22	n	604	CLA	O2D-CGD-O1D	-2.64	118.72	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	s	305	CLA	CHB-C4A-NA	2.64	128.21	124.40
22	R	311	CLA	C3B-C4B-NB	-2.64	108.18	110.53
22	N	604	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
30	d	401	PHO	CMB-C2B-C3B	2.63	129.95	124.68
21	g	605	CHL	O1D-CGD-CBD	-2.63	120.73	124.72
22	S	312	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
30	D	401	PHO	CMB-C2B-C3B	2.63	129.94	124.68
22	x	101	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
22	a	408	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
36	M	101	LMG	O6-C1-O1	-2.63	103.83	110.04
35	c	517	DGD	C3G-C2G-C1G	-2.63	105.66	111.78
36	C	502	LMG	O3-C3-C2	-2.63	104.19	110.38
22	y	604	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
35	c	519	DGD	C3G-C2G-C1G	-2.63	105.66	111.78
31	b	618	BCR	C27-C26-C25	2.62	126.25	122.70
36	T	101	LMG	O6-C1-O1	-2.62	103.84	110.04
22	G	604	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
22	B	603	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
22	b	601	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
22	C	504	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
22	Y	604	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
22	Y	602	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
31	K	102	BCR	C33-C5-C6	-2.62	121.63	124.48
22	y	602	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
22	G	602	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
22	g	604	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
22	A	409	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
22	g	613	CLA	CHB-C1B-C2B	-2.62	119.83	127.43
22	y	604	CLA	CHB-C4A-NA	2.62	128.18	124.40
35	J	101	DGD	C3G-C2G-C1G	-2.62	105.69	111.78
22	b	604	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
31	B	621	BCR	C27-C26-C25	2.61	126.24	122.70
22	n	602	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
22	n	604	CLA	CHB-C4A-NA	2.61	128.17	124.40
31	A	410	BCR	C33-C5-C6	-2.61	121.63	124.48
22	G	604	CLA	CHB-C4A-NA	2.61	128.17	124.40
26	n	617	LHG	O8-C23-C24	2.61	119.80	111.83
22	y	612	CLA	CHB-C1B-C2B	-2.61	119.85	127.43
22	R	309	CLA	CHB-C4A-NA	2.61	128.16	124.40
22	d	404	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
35	C	518	DGD	O3G-C1D-C2D	-2.61	104.31	108.27
22	Y	612	CLA	C3B-C4B-NB	-2.61	108.20	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	502	CLA	CHB-C4A-NA	2.61	128.16	124.40
22	N	613	CLA	C3B-C4B-NB	-2.61	108.20	110.53
22	n	612	CLA	CHB-C1B-C2B	-2.60	119.87	127.43
22	c	510	CLA	C3D-C2D-C1D	2.60	109.38	105.83
31	C	517	BCR	C33-C5-C6	-2.60	121.64	124.48
22	g	604	CLA	CHB-C4A-NA	2.60	128.16	124.40
24	Y	615	XAT	C11-C12-C13	-2.60	119.23	126.36
31	c	516	BCR	C33-C5-C6	-2.60	121.65	124.48
22	R	311	CLA	CHB-C4A-NA	2.60	128.15	124.40
22	N	612	CLA	CHB-C1B-C2B	-2.60	119.89	127.43
22	D	405	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
36	w	102	LMG	O3-C3-C2	-2.59	104.27	110.38
31	k	102	BCR	C33-C5-C6	-2.59	121.66	124.48
22	c	505	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	B	607	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
22	g	602	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
22	Y	611	CLA	CHB-C1B-C2B	-2.59	119.92	127.43
35	c	517	DGD	O3G-C1D-C2D	-2.59	104.34	108.27
22	C	506	CLA	C3B-C4B-NB	-2.59	108.22	110.53
23	N	614	LUT	C31-C32-C33	-2.59	119.27	126.36
30	A	408	PHO	O2D-CGD-O1D	-2.59	118.82	123.85
31	b	616	BCR	C11-C10-C9	-2.58	123.65	127.28
22	A	409	CLA	CHB-C4A-NA	2.58	128.13	124.40
22	C	503	CLA	CHB-C4A-NA	2.58	128.13	124.40
22	G	613	CLA	CHB-C1B-C2B	-2.58	119.93	127.43
23	G	615	LUT	C31-C32-C33	-2.58	119.28	126.36
22	b	611	CLA	CHB-C4A-NA	2.58	128.13	124.40
23	R	312	LUT	C8-C7-C6	-2.58	120.10	127.00
31	a	409	BCR	C33-C5-C6	-2.58	121.67	124.48
22	C	506	CLA	CHB-C4A-NA	2.58	128.12	124.40
31	a	409	BCR	C11-C10-C9	-2.58	123.66	127.28
22	B	609	CLA	C3B-C4B-NB	-2.58	108.23	110.53
26	b	619	LHG	O8-C23-C24	2.58	119.69	111.83
23	n	614	LUT	C31-C32-C33	-2.58	119.30	126.36
23	g	615	LUT	C31-C32-C33	-2.57	119.30	126.36
30	A	408	PHO	CMB-C2B-C3B	2.57	129.82	124.68
26	n	617	LHG	C11-C10-C9	-2.57	101.36	114.37
22	r	310	CLA	CHB-C4A-NA	2.57	128.11	124.40
22	C	511	CLA	C3D-C2D-C1D	2.57	109.34	105.83
22	b	606	CLA	CHB-C4A-NA	2.57	128.11	124.40
30	a	407	PHO	CMB-C2B-C3B	2.57	129.82	124.68
24	N	616	XAT	O24-C26-C27	2.57	124.24	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	CHB-C4A-NA	2.57	128.11	124.40
22	B	614	CLA	CHB-C4A-NA	2.57	128.11	124.40
22	N	602	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
31	B	602	BCR	C15-C16-C17	-2.57	118.26	123.52
22	c	505	CLA	C3B-C4B-NB	-2.57	108.24	110.53
22	C	508	CLA	CHB-C4A-NA	2.57	128.11	124.40
31	b	617	BCR	C27-C26-C25	2.57	126.17	122.70
22	G	612	CLA	C3B-C4B-NB	-2.57	108.24	110.53
22	W	101	CLA	C3B-C4B-NB	-2.57	108.24	110.53
33	L	102	SQD	C4-C3-C2	2.57	115.34	110.83
23	r	313	LUT	C8-C7-C6	-2.57	120.14	127.00
23	y	614	LUT	C31-C32-C33	-2.57	119.33	126.36
31	B	619	BCR	C11-C10-C9	-2.57	123.68	127.28
31	T	102	BCR	C15-C14-C13	-2.56	123.68	127.28
22	N	611	CLA	C3B-C4B-NB	-2.56	108.24	110.53
35	C	518	DGD	O5D-C6D-C5D	-2.56	103.64	109.42
31	B	602	BCR	C15-C14-C13	-2.56	123.68	127.28
22	c	503	CLA	C1-C2-C3	-2.56	122.00	126.20
22	b	606	CLA	C3B-C4B-NB	-2.56	108.24	110.53
22	n	611	CLA	C3B-C4B-NB	-2.56	108.25	110.53
22	r	309	CLA	CHB-C4A-NA	2.56	128.09	124.40
26	B	622	LHG	O8-C23-C24	2.56	119.63	111.83
35	c	517	DGD	O5D-C6D-C5D	-2.56	103.66	109.42
31	B	602	BCR	C27-C26-C25	2.56	126.16	122.70
26	D	408	LHG	O8-C23-C24	2.56	119.63	111.83
23	Y	613	LUT	C31-C32-C33	-2.56	119.36	126.36
31	a	409	BCR	C24-C23-C22	-2.55	122.46	126.23
30	a	407	PHO	O2D-CGD-O1D	-2.55	118.88	123.85
26	d	407	LHG	O8-C23-C24	2.55	119.62	111.83
22	c	508	CLA	CHB-C4A-NA	2.55	128.08	124.40
22	c	513	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
22	R	308	CLA	CHB-C4A-NA	2.55	128.08	124.40
33	l	101	SQD	C4-C3-C2	2.55	115.30	110.83
31	A	410	BCR	C11-C10-C9	-2.55	123.71	127.28
22	C	509	CLA	CHB-C4A-NA	2.54	128.07	124.40
31	T	102	BCR	C33-C5-C6	-2.54	121.71	124.48
31	T	102	BCR	C15-C16-C17	-2.54	118.32	123.52
31	B	620	BCR	C27-C26-C25	2.54	126.14	122.70
31	B	602	BCR	C24-C23-C22	-2.54	122.48	126.23
31	T	102	BCR	C27-C26-C25	2.54	126.14	122.70
26	D	409	LHG	C11-C10-C9	-2.54	101.53	114.37
31	h	101	BCR	C33-C5-C6	-2.54	121.71	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	g	612	CLA	C3B-C4B-NB	-2.54	108.27	110.53
26	L	103	LHG	C11-C10-C9	-2.54	101.55	114.37
22	C	504	CLA	C1-C2-C3	-2.54	122.04	126.20
26	d	408	LHG	C11-C10-C9	-2.54	101.55	114.37
22	a	408	CLA	CHB-C4A-NA	2.54	128.06	124.40
22	c	513	CLA	CHB-C4A-NA	2.53	128.06	124.40
22	w	101	CLA	C3B-C4B-NB	-2.53	108.27	110.53
21	N	607	CHL	CMB-C2B-C3B	2.53	129.74	124.68
31	k	101	BCR	C33-C5-C6	-2.53	121.72	124.48
21	y	601	CHL	CMB-C2B-C3B	2.53	129.74	124.68
21	G	607	CHL	CMB-C2B-C3B	2.53	129.74	124.68
21	S	306	CHL	CMB-C2B-C3B	2.53	129.74	124.68
22	C	514	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
21	N	601	CHL	CMB-C2B-C3B	2.53	129.74	124.68
21	S	307	CHL	CMB-C2B-C3B	2.53	129.74	124.68
26	l	102	LHG	C11-C10-C9	-2.53	101.59	114.37
21	s	301	CHL	CMB-C2B-C3B	2.53	129.73	124.68
22	c	504	CLA	C3B-C4B-NB	-2.53	108.27	110.53
21	S	301	CHL	CMB-C2B-C3B	2.53	129.73	124.68
31	T	102	BCR	C24-C23-C22	-2.53	122.50	126.23
31	K	101	BCR	C33-C5-C6	-2.53	121.73	124.48
22	B	606	CLA	CHB-C4A-NA	2.53	128.05	124.40
31	k	102	BCR	C15-C14-C13	-2.53	123.73	127.28
37	F	101	HEM	CHA-C4D-C3D	2.53	129.88	125.23
22	C	514	CLA	CHB-C4A-NA	2.53	128.04	124.40
21	r	308	CHL	CMB-C2B-C3B	2.53	129.73	124.68
21	n	601	CHL	CMB-C2B-C3B	2.53	129.73	124.68
22	r	304	CLA	CHB-C4A-NA	2.53	128.04	124.40
21	R	305	CHL	CMB-C2B-C3B	2.52	129.73	124.68
22	c	514	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	s	311	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
22	S	310	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	S	311	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
21	y	608	CHL	CMB-C2B-C3B	2.52	129.72	124.68
21	r	301	CHL	CMB-C2B-C3B	2.52	129.72	124.68
22	R	303	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	C	515	CLA	CHB-C4A-NA	2.52	128.04	124.40
31	A	410	BCR	C24-C23-C22	-2.52	122.51	126.23
31	K	102	BCR	C27-C26-C25	2.52	126.11	122.70
21	n	607	CHL	CMB-C2B-C3B	2.52	129.72	124.68
21	s	306	CHL	CMB-C2B-C3B	2.52	129.72	124.68
30	d	401	PHO	C1-C2-C3	-2.52	122.07	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	609	CLA	CHB-C4A-NA	2.52	128.04	124.40
21	G	608	CHL	CMB-C2B-C3B	2.52	129.72	124.68
22	s	310	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	R	304	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
31	K	102	BCR	C15-C14-C13	-2.52	123.75	127.28
21	r	306	CHL	CMB-C2B-C3B	2.52	129.72	124.68
21	y	605	CHL	CMB-C2B-C3B	2.52	129.71	124.68
21	g	601	CHL	CMB-C2B-C3B	2.52	129.71	124.68
21	S	302	CHL	CMB-C2B-C3B	2.52	129.71	124.68
21	n	605	CHL	CMB-C2B-C3B	2.52	129.71	124.68
22	A	406	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	S	313	CLA	CHB-C4A-NA	2.52	128.03	124.40
21	g	608	CHL	CMB-C2B-C3B	2.52	129.71	124.68
21	s	307	CHL	CMB-C2B-C3B	2.52	129.71	124.68
21	N	605	CHL	CMB-C2B-C3B	2.51	129.71	124.68
21	N	608	CHL	CMB-C2B-C3B	2.51	129.71	124.68
26	c	520	LHG	O8-C23-C24	2.51	119.50	111.83
36	k	103	LMG	O6-C1-O1	-2.51	104.10	110.04
31	h	101	BCR	C27-C26-C25	2.51	126.10	122.70
21	y	606	CHL	CMB-C2B-C3B	2.51	129.70	124.68
21	Y	607	CHL	CMB-C2B-C3B	2.51	129.70	124.68
21	R	307	CHL	CMB-C2B-C3B	2.51	129.70	124.68
22	r	303	CLA	CHB-C4A-NA	2.51	128.02	124.40
21	R	306	CHL	CMB-C2B-C3B	2.51	129.70	124.68
37	f	101	HEM	CHA-C4D-C3D	2.51	129.85	125.23
22	R	310	CLA	CAA-C2A-C3A	-2.51	106.22	113.00
21	G	605	CHL	CMB-C2B-C3B	2.51	129.69	124.68
35	C	519	DGD	O5D-C6D-C5D	-2.51	103.77	109.42
21	g	606	CHL	CMB-C2B-C3B	2.51	129.69	124.68
21	G	609	CHL	CMB-C2B-C3B	2.51	129.69	124.68
25	Y	616	NEX	C36-C21-C22	-2.51	104.56	108.97
36	K	103	LMG	O6-C1-O1	-2.51	104.12	110.04
22	C	505	CLA	CHB-C4A-NA	2.51	128.02	124.40
21	Y	601	CHL	CMB-C2B-C3B	2.51	129.69	124.68
21	s	302	CHL	CMB-C2B-C3B	2.51	129.69	124.68
22	s	313	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	R	302	CLA	CHB-C4A-NA	2.50	128.01	124.40
21	g	605	CHL	CMB-C2B-C3B	2.50	129.69	124.68
21	Y	608	CHL	CMB-C2B-C3B	2.50	129.69	124.68
21	n	606	CHL	CMB-C2B-C3B	2.50	129.69	124.68
31	K	101	BCR	C27-C26-C25	2.50	126.09	122.70
26	C	520	LHG	O8-C23-C24	2.50	119.46	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	CHB-C4A-NA	2.50	128.01	124.40
31	k	102	BCR	C27-C26-C25	2.50	126.08	122.70
22	b	608	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	R	304	CLA	C3B-C4B-NB	-2.50	108.30	110.53
21	N	606	CHL	CMB-C2B-C3B	2.50	129.68	124.68
21	n	608	CHL	CMB-C2B-C3B	2.50	129.68	124.68
21	Y	606	CHL	CMB-C2B-C3B	2.50	129.67	124.68
31	B	602	BCR	C33-C5-C6	-2.50	121.76	124.48
21	g	607	CHL	CMB-C2B-C3B	2.50	129.67	124.68
22	a	405	CLA	CHB-C4A-NA	2.50	128.00	124.40
21	g	609	CHL	CMB-C2B-C3B	2.50	129.67	124.68
24	y	615	XAT	C11-C12-C13	-2.49	119.52	126.36
22	n	612	CLA	C2A-C1A-CHA	2.49	128.20	123.87
31	C	516	BCR	C15-C14-C13	-2.49	123.78	127.28
21	y	607	CHL	CMB-C2B-C3B	2.49	129.67	124.68
31	b	617	BCR	C11-C10-C9	-2.49	123.78	127.28
22	C	504	CLA	CHB-C4A-NA	2.49	128.00	124.40
21	G	606	CHL	CMB-C2B-C3B	2.49	129.66	124.68
21	y	609	CHL	CMB-C2B-C3B	2.49	129.66	124.68
31	B	620	BCR	C11-C10-C9	-2.49	123.78	127.28
25	r	315	NEX	C36-C21-C22	-2.49	104.59	108.97
24	Y	615	XAT	C8-C9-C10	-2.49	115.09	119.01
22	r	305	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
22	G	613	CLA	C2A-C1A-CHA	2.49	128.19	123.87
22	C	505	CLA	C3B-C4B-NB	-2.49	108.31	110.53
22	g	613	CLA	C2A-C1A-CHA	2.49	128.19	123.87
31	c	515	BCR	C15-C14-C13	-2.49	123.79	127.28
22	r	311	CLA	CAA-C2A-C3A	-2.49	106.28	113.00
22	B	611	CLA	CHB-C4A-NA	2.49	127.99	124.40
35	c	518	DGD	O5D-C6D-C5D	-2.49	103.81	109.42
21	G	601	CHL	CMB-C2B-C3B	2.49	129.65	124.68
22	b	613	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	s	303	CLA	CHB-C4A-NA	2.49	127.99	124.40
30	D	401	PHO	C1-C2-C3	-2.49	122.12	126.20
22	b	607	CLA	CHB-C4A-NA	2.49	127.99	124.40
21	Y	605	CHL	CMB-C2B-C3B	2.49	129.65	124.68
22	c	503	CLA	CHB-C4A-NA	2.48	127.98	124.40
26	n	617	LHG	C20-C19-C18	-2.48	101.81	114.37
36	c	523	LMG	O1-C7-C8	-2.48	104.78	110.82
22	B	616	CLA	CHB-C4A-NA	2.48	127.98	124.40
21	r	307	CHL	CMB-C2B-C3B	2.48	129.64	124.68
36	C	523	LMG	O1-C7-C8	-2.48	104.78	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	619	LHG	C11-C10-C9	-2.48	101.83	114.37
22	Y	611	CLA	C2A-C1A-CHA	2.48	128.17	123.87
26	c	520	LHG	C11-C10-C9	-2.48	101.84	114.37
31	b	616	BCR	C24-C23-C22	-2.48	122.57	126.23
22	B	607	CLA	CHB-C4A-NA	2.48	127.97	124.40
33	L	101	SQD	O8-S-C6	2.48	110.75	105.97
26	C	520	LHG	C11-C10-C9	-2.48	101.85	114.37
24	G	617	XAT	C11-C12-C13	-2.48	119.58	126.36
31	k	101	BCR	C27-C26-C25	2.48	126.05	122.70
23	N	615	LUT	C7-C8-C9	-2.48	122.57	126.23
26	B	622	LHG	C11-C10-C9	-2.48	101.86	114.37
25	y	618	NEX	C36-C21-C22	-2.47	104.62	108.97
22	S	308	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
22	s	303	CLA	C3B-C4B-NB	-2.47	108.32	110.53
22	c	504	CLA	CHB-C4A-NA	2.47	127.97	124.40
23	N	615	LUT	C10-C11-C12	-2.47	116.04	123.20
22	b	601	CLA	C1-C2-C3	-2.47	122.15	126.20
31	B	619	BCR	C24-C23-C22	-2.47	122.58	126.23
22	S	303	CLA	CHB-C4A-NA	2.47	127.96	124.40
31	H	101	BCR	C33-C5-C6	-2.47	121.79	124.48
26	D	410	LHG	C11-C10-C9	-2.47	101.89	114.37
33	l	103	SQD	O8-S-C6	2.47	110.74	105.97
22	s	308	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
22	y	612	CLA	C2A-C1A-CHA	2.47	128.15	123.87
37	F	101	HEM	C1D-C2D-C3D	2.46	109.57	106.98
22	N	612	CLA	C2A-C1A-CHA	2.46	128.14	123.87
25	g	618	NEX	C11-C12-C13	-2.46	119.61	126.36
22	b	602	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	y	616	NEX	O24-C26-C27	-2.46	109.82	116.88
22	r	305	CLA	C3B-C4B-NB	-2.46	108.33	110.53
31	H	101	BCR	C27-C26-C25	2.46	126.03	122.70
22	G	611	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	b	605	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	d	409	LHG	C11-C10-C9	-2.46	101.93	114.37
26	d	408	LHG	C20-C19-C18	-2.46	101.93	114.37
22	B	610	CLA	CHB-C4A-NA	2.46	127.95	124.40
31	b	618	BCR	C33-C5-C6	-2.46	121.80	124.48
36	C	523	LMG	C38-C37-C36	-2.46	101.94	114.37
26	g	619	LHG	C5-O7-C7	-2.46	111.92	117.80
31	B	621	BCR	C33-C5-C6	-2.45	121.81	124.48
22	B	608	CLA	CHB-C4A-NA	2.45	127.94	124.40
33	d	402	SQD	O48-C23-C24	2.45	119.31	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	s	305	CLA	C3B-C4B-NB	-2.45	108.34	110.53
25	N	617	NEX	C27-C28-C29	-2.45	121.73	125.53
36	b	620	LMG	O1-C7-C8	-2.45	104.86	110.82
22	G	610	CLA	C16-C15-C13	-2.45	107.83	115.97
36	c	523	LMG	C38-C37-C36	-2.45	101.99	114.37
26	D	409	LHG	C20-C19-C18	-2.45	102.00	114.37
22	c	509	CLA	CHB-C4A-NA	2.45	127.93	124.40
26	c	520	LHG	O8-C6-C5	-2.45	101.35	108.40
26	G	618	LHG	C20-C19-C18	-2.45	102.01	114.37
22	B	604	CLA	C1-C2-C3	-2.45	122.19	126.20
22	r	303	CLA	C1-C2-C3	-2.45	122.19	126.20
22	C	515	CLA	C1-C2-C3	-2.44	122.19	126.20
36	B	623	LMG	O1-C7-C8	-2.44	104.88	110.82
33	D	402	SQD	O48-C23-C24	2.44	119.28	111.83
22	c	514	CLA	C1-C2-C3	-2.44	122.20	126.20
22	B	610	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
22	B	605	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	R	302	CLA	C1-C2-C3	-2.44	122.20	126.20
36	K	103	LMG	C40-C39-C38	-2.44	102.04	114.37
26	y	617	LHG	C5-O7-C7	-2.44	111.96	117.80
26	C	520	LHG	O8-C6-C5	-2.44	101.37	108.40
22	S	303	CLA	C3B-C4B-NB	-2.44	108.35	110.53
22	S	305	CLA	C3B-C4B-NB	-2.44	108.35	110.53
22	b	607	CLA	CMB-C2B-C1B	-2.44	121.71	125.42
22	C	510	CLA	CHB-C4A-NA	2.44	127.92	124.40
37	f	101	HEM	C1D-C2D-C3D	2.44	109.54	106.98
36	c	523	LMG	C40-C39-C38	-2.44	102.06	114.37
36	k	103	LMG	C40-C39-C38	-2.43	102.06	114.37
36	c	523	LMG	O1-C1-C2	-2.43	104.58	108.27
31	T	102	BCR	C11-C10-C9	-2.43	123.87	127.28
26	N	618	LHG	C5-O7-C7	-2.43	111.98	117.80
36	k	103	LMG	C38-C37-C36	-2.43	102.08	114.37
36	D	411	LMG	O2-C2-C1	-2.43	104.28	110.08
22	b	615	CLA	CHB-C4A-NA	2.43	127.91	124.40
36	C	502	LMG	O2-C2-C1	-2.43	104.29	110.08
36	C	502	LMG	O7-C10-O9	-2.43	118.03	123.70
22	b	604	CLA	CHB-C4A-NA	2.43	127.90	124.40
36	w	102	LMG	O2-C2-C1	-2.43	104.29	110.08
22	B	618	CLA	CHB-C4A-NA	2.43	127.90	124.40
21	g	605	CHL	O2D-CGD-O1D	-2.43	119.12	123.85
36	C	523	LMG	C40-C39-C38	-2.43	102.10	114.37
22	B	604	CLA	CHB-C4A-NA	2.43	127.90	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	601	CHL	O2D-CGD-O1D	-2.43	119.13	123.85
36	b	620	LMG	O3-C3-C2	-2.42	104.66	110.38
22	Y	610	CLA	CHB-C4A-NA	2.42	127.90	124.40
36	d	410	LMG	O2-C2-C1	-2.42	104.30	110.08
22	y	611	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	c	510	CLA	CHB-C4A-NA	2.42	127.90	124.40
26	r	302	LHG	C20-C19-C18	-2.42	102.12	114.37
26	G	618	LHG	C11-C10-C9	-2.42	102.12	114.37
23	Y	613	LUT	C26-C27-C28	-2.42	120.81	124.58
22	C	507	CLA	CHB-C4A-NA	2.42	127.89	124.40
21	N	601	CHL	O2D-CGD-O1D	-2.42	119.13	123.85
36	K	103	LMG	C38-C37-C36	-2.42	102.13	114.37
31	B	602	BCR	C11-C10-C9	-2.42	123.88	127.28
21	G	608	CHL	O2D-CGD-O1D	-2.42	119.14	123.85
32	d	406	PL9	O1-C4-C3	-2.42	118.18	120.73
22	c	506	CLA	CHB-C4A-NA	2.42	127.89	124.40
22	x	101	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	y	615	XAT	O4-C5-C6	2.42	60.85	58.93
21	R	306	CHL	O2D-CGD-O1D	-2.42	119.14	123.85
24	g	617	XAT	O4-C5-C6	2.42	60.85	58.93
22	g	611	CLA	CHB-C4A-NA	2.42	127.89	124.40
26	s	314	LHG	C11-C10-C9	-2.42	102.14	114.37
21	n	606	CHL	O2D-CGD-O1D	-2.42	119.14	123.85
25	N	617	NEX	C36-C21-C26	-2.42	103.52	110.05
26	N	618	LHG	O8-C23-C24	2.42	119.20	111.83
21	n	605	CHL	O2D-CGD-O1D	-2.42	119.14	123.85
21	n	607	CHL	O2D-CGD-O1D	-2.42	119.14	123.85
21	S	302	CHL	O2D-CGD-O1D	-2.42	119.14	123.85
21	R	307	CHL	O2D-CGD-O1D	-2.42	119.14	123.85
21	N	607	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
21	n	601	CHL	O2D-CGD-O1D	-2.42	119.15	123.85
21	Y	601	CHL	O2D-CGD-O1D	-2.42	119.15	123.85
21	Y	606	CHL	O2D-CGD-O1D	-2.42	119.15	123.85
21	Y	605	CHL	O2D-CGD-O1D	-2.41	119.15	123.85
21	G	605	CHL	CBC-CAC-C3C	-2.41	109.42	112.87
22	A	405	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	A	407	CLA	CHB-C4A-NA	2.41	127.88	124.40
32	D	407	PL9	O1-C4-C3	-2.41	118.19	120.73
36	B	601	LMG	C40-C39-C38	-2.41	102.17	114.37
36	I	101	LMG	C40-C39-C38	-2.41	102.17	114.37
26	S	314	LHG	C11-C10-C9	-2.41	102.18	114.37
21	g	601	CHL	CBC-CAC-C3C	-2.41	109.42	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	s	301	CHL	O2D-CGD-O1D	-2.41	119.15	123.85
26	R	301	LHG	C20-C19-C18	-2.41	102.18	114.37
21	s	307	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
21	R	305	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
21	r	307	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
23	R	312	LUT	C31-C32-C33	-2.41	119.76	126.36
22	r	305	CLA	CHB-C4A-NA	2.41	127.88	124.40
32	D	407	PL9	O2-C1-C6	2.41	124.31	120.48
26	S	314	LHG	C20-C19-C18	-2.41	102.19	114.37
21	G	607	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
21	N	606	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
23	N	615	LUT	C26-C27-C28	-2.41	120.83	124.58
21	g	609	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
31	B	620	BCR	C33-C5-C6	-2.41	121.86	124.48
21	g	601	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
21	r	301	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
22	b	601	CLA	CHB-C4A-NA	2.41	127.87	124.40
22	C	513	CLA	CHB-C4A-NA	2.41	127.87	124.40
36	w	102	LMG	O7-C10-O9	-2.41	118.08	123.70
23	N	614	LUT	C26-C27-C28	-2.41	120.83	124.58
21	r	306	CHL	CBC-CAC-C3C	-2.41	109.43	112.87
36	C	523	LMG	O1-C1-C2	-2.41	104.62	108.27
22	a	406	CLA	CHB-C4A-NA	2.41	127.87	124.40
21	g	608	CHL	CBC-CAC-C3C	-2.41	109.43	112.87
22	a	404	CLA	C1-C2-C3	-2.41	122.25	126.20
21	y	606	CHL	O2D-CGD-O1D	-2.41	119.17	123.85
21	Y	608	CHL	O2D-CGD-O1D	-2.41	119.17	123.85
21	s	301	CHL	CBC-CAC-C3C	-2.41	109.43	112.87
21	G	609	CHL	O2D-CGD-O1D	-2.41	119.17	123.85
21	N	605	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
21	g	608	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
21	Y	607	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
26	s	314	LHG	C20-C19-C18	-2.40	102.22	114.37
26	Y	617	LHG	C11-C10-C9	-2.40	102.22	114.37
31	A	410	BCR	C7-C8-C9	-2.40	122.68	126.23
26	r	302	LHG	C11-C10-C9	-2.40	102.22	114.37
22	A	405	CLA	C1-C2-C3	-2.40	122.26	126.20
26	c	522	LHG	C11-C10-C9	-2.40	102.23	114.37
23	G	615	LUT	C26-C27-C28	-2.40	120.84	124.58
21	N	608	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
21	r	308	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
21	r	308	CHL	CBC-CAC-C3C	-2.40	109.44	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	511	CLA	CHB-C4A-NA	2.40	127.86	124.40
21	g	606	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
21	G	606	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
21	y	609	CHL	CBC-CAC-C3C	-2.40	109.44	112.87
36	C	502	LMG	C40-C39-C38	-2.40	102.24	114.37
26	C	522	LHG	C5-O7-C7	-2.40	112.05	117.80
21	Y	608	CHL	CBC-CAC-C3C	-2.40	109.44	112.87
22	b	610	CLA	CHB-C4A-NA	2.40	127.86	124.40
36	B	623	LMG	C40-C39-C38	-2.40	102.24	114.37
23	n	614	LUT	C26-C27-C28	-2.40	120.84	124.58
26	R	301	LHG	C11-C10-C9	-2.40	102.24	114.37
31	A	410	BCR	C15-C16-C17	-2.40	118.61	123.52
21	G	601	CHL	CBC-CAC-C3C	-2.40	109.44	112.87
36	B	623	LMG	O3-C3-C2	-2.40	104.72	110.38
22	R	304	CLA	CHB-C4A-NA	2.40	127.86	124.40
31	a	409	BCR	C15-C16-C17	-2.40	118.61	123.52
32	d	406	PL9	O2-C1-C6	2.40	124.30	120.48
21	n	601	CHL	CBC-CAC-C3C	-2.40	109.44	112.87
31	H	101	BCR	C11-C10-C9	-2.40	123.92	127.28
36	D	411	LMG	O3-C3-C2	-2.40	104.72	110.38
21	s	306	CHL	O2D-CGD-O1D	-2.40	119.18	123.85
22	g	603	CLA	CHB-C4A-NA	2.40	127.86	124.40
21	s	302	CHL	O2D-CGD-O1D	-2.40	119.18	123.85
21	R	307	CHL	CBC-CAC-C3C	-2.40	109.44	112.87
26	C	522	LHG	C11-C10-C9	-2.40	102.26	114.37
36	w	102	LMG	C40-C39-C38	-2.40	102.26	114.37
21	g	607	CHL	O2D-CGD-O1D	-2.40	119.19	123.85
21	S	307	CHL	O2D-CGD-O1D	-2.40	119.19	123.85
22	Y	603	CLA	CHB-C4A-NA	2.40	127.86	124.40
35	a	413	DGD	C3G-C2G-C1G	-2.40	106.20	111.78
26	c	520	LHG	C20-C19-C18	-2.40	102.26	114.37
22	n	603	CLA	CHB-C4A-NA	2.39	127.86	124.40
26	L	103	LHG	C20-C19-C18	-2.39	102.26	114.37
35	A	401	DGD	C3G-C2G-C1G	-2.39	106.20	111.78
21	g	605	CHL	CBC-CAC-C3C	-2.39	109.45	112.87
21	g	607	CHL	CBC-CAC-C3C	-2.39	109.45	112.87
21	n	606	CHL	CBC-CAC-C3C	-2.39	109.45	112.87
21	G	607	CHL	CBC-CAC-C3C	-2.39	109.45	112.87
31	h	101	BCR	C11-C10-C9	-2.39	123.92	127.28
22	b	609	CLA	CHB-C4A-NA	2.39	127.85	124.40
36	b	620	LMG	C40-C39-C38	-2.39	102.27	114.37
24	N	616	XAT	C11-C12-C13	-2.39	119.80	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	l	103	SQD	O6-C1-C2	2.39	111.91	108.27
22	N	603	CLA	CHB-C4A-NA	2.39	127.85	124.40
26	c	522	LHG	C5-O7-C7	-2.39	112.07	117.80
26	l	102	LHG	C20-C19-C18	-2.39	102.28	114.37
22	N	610	CLA	CHB-C4A-NA	2.39	127.85	124.40
24	g	617	XAT	O24-C26-C27	2.39	123.73	116.88
26	C	520	LHG	C20-C19-C18	-2.39	102.29	114.37
21	y	605	CHL	CBC-CAC-C3C	-2.39	109.45	112.87
21	Y	607	CHL	CBC-CAC-C3C	-2.39	109.45	112.87
21	G	609	CHL	CBC-CAC-C3C	-2.39	109.45	112.87
33	L	101	SQD	O48-C23-C24	2.39	119.12	111.83
21	G	608	CHL	CBC-CAC-C3C	-2.39	109.45	112.87
21	r	306	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
21	r	301	CHL	CBC-CAC-C3C	-2.39	109.45	112.87
22	G	604	CLA	C1-C2-C3	-2.39	122.90	126.76
21	G	605	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
21	S	306	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
21	r	307	CHL	CBC-CAC-C3C	-2.39	109.46	112.87
21	y	605	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
21	y	609	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
22	a	404	CLA	CHB-C4A-NA	2.39	127.84	124.40
22	n	610	CLA	CHB-C4A-NA	2.39	127.84	124.40
22	B	612	CLA	CHB-C4A-NA	2.39	127.84	124.40
21	y	607	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
21	Y	606	CHL	CBC-CAC-C3C	-2.38	109.46	112.87
21	y	601	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
36	d	410	LMG	O3-C3-C2	-2.38	104.76	110.38
21	N	601	CHL	CBC-CAC-C3C	-2.38	109.46	112.87
23	r	313	LUT	C31-C32-C33	-2.38	119.83	126.36
21	n	608	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
21	g	609	CHL	CBC-CAC-C3C	-2.38	109.46	112.87
31	H	101	BCR	C15-C14-C13	-2.38	123.94	127.28
22	c	503	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
21	y	608	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
21	S	301	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
21	s	302	CHL	CBC-CAC-C3C	-2.38	109.46	112.87
35	H	102	DGD	O2D-C2D-C1D	-2.38	104.40	110.08
21	S	307	CHL	CBC-CAC-C3C	-2.38	109.46	112.87
22	s	309	CLA	CHB-C4A-NA	2.38	127.84	124.40
21	N	607	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
22	y	603	CLA	CHB-C4A-NA	2.38	127.83	124.40
21	R	305	CHL	CBC-CAC-C3C	-2.38	109.47	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	S	302	CHL	CBC-CAC-C3C	-2.38	109.47	112.87
24	Y	615	XAT	O4-C5-C6	2.38	60.81	58.93
36	d	410	LMG	O1-C1-C2	-2.38	104.66	108.27
31	d	405	BCR	C11-C10-C9	-2.38	123.95	127.28
22	c	511	CLA	CHB-C4A-NA	2.38	127.83	124.40
21	N	605	CHL	CBC-CAC-C3C	-2.38	109.47	112.87
21	n	608	CHL	CBC-CAC-C3C	-2.37	109.47	112.87
21	n	605	CHL	CBC-CAC-C3C	-2.37	109.47	112.87
36	D	411	LMG	O1-C1-C2	-2.37	104.67	108.27
22	c	512	CLA	CHB-C4A-NA	2.37	127.83	124.40
22	B	613	CLA	CHB-C4A-NA	2.37	127.83	124.40
21	Y	601	CHL	CBC-CAC-C3C	-2.37	109.47	112.87
26	B	622	LHG	C20-C19-C18	-2.37	102.37	114.37
21	s	307	CHL	CBC-CAC-C3C	-2.37	109.48	112.87
33	l	103	SQD	O48-C23-C24	2.37	119.07	111.83
22	B	603	CLA	CHB-C4A-NA	2.37	127.82	124.40
26	c	522	LHG	C20-C19-C18	-2.37	102.38	114.37
23	g	615	LUT	C26-C27-C28	-2.37	120.89	124.58
21	R	306	CHL	CBC-CAC-C3C	-2.37	109.48	112.87
22	C	504	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
21	y	607	CHL	CBC-CAC-C3C	-2.37	109.48	112.87
23	y	614	LUT	C26-C27-C28	-2.37	120.89	124.58
22	y	604	CLA	C1-C2-C3	-2.37	122.93	126.76
22	G	614	CLA	CHB-C4A-NA	2.37	127.82	124.40
21	g	606	CHL	CBC-CAC-C3C	-2.37	109.48	112.87
26	b	619	LHG	C20-C19-C18	-2.37	102.41	114.37
21	S	306	CHL	CBC-CAC-C3C	-2.36	109.49	112.87
22	b	606	CLA	C1-C2-C3	-2.36	122.32	126.20
26	C	522	LHG	C20-C19-C18	-2.36	102.42	114.37
21	y	608	CHL	CBC-CAC-C3C	-2.36	109.49	112.87
31	a	409	BCR	C7-C8-C9	-2.36	122.74	126.23
21	Y	605	CHL	CBC-CAC-C3C	-2.36	109.49	112.87
21	G	606	CHL	CBC-CAC-C3C	-2.36	109.49	112.87
36	d	410	LMG	O1-C7-C8	-2.36	105.08	110.82
22	N	604	CLA	C1-C2-C3	-2.36	122.94	126.76
26	d	407	LHG	C11-C10-C9	-2.36	102.44	114.37
22	S	311	CLA	CHB-C4A-NA	2.36	127.80	124.40
36	D	411	LMG	O1-C7-C8	-2.36	105.08	110.82
21	y	601	CHL	CBC-CAC-C3C	-2.36	109.50	112.87
22	B	615	CLA	CHB-C4A-NA	2.36	127.80	124.40
31	b	617	BCR	C33-C5-C6	-2.36	121.91	124.48
36	M	101	LMG	C38-C37-C36	-2.36	102.45	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	n	612	CLA	C2B-C1B-NB	2.36	112.77	110.33
26	c	521	LHG	C11-C10-C9	-2.36	102.46	114.37
21	y	606	CHL	CBC-CAC-C3C	-2.36	109.50	112.87
35	h	102	DGD	O2D-C2D-C1D	-2.36	104.46	110.08
25	N	617	NEX	C11-C12-C13	-2.36	119.90	126.36
31	h	101	BCR	C15-C14-C13	-2.36	123.97	127.28
22	b	614	CLA	CHB-C4A-NA	2.35	127.80	124.40
21	n	607	CHL	CBC-CAC-C3C	-2.35	109.50	112.87
36	T	101	LMG	C38-C37-C36	-2.35	102.47	114.37
25	Y	616	NEX	C36-C21-C26	-2.35	103.69	110.05
37	F	101	HEM	C4A-CHB-C1B	-2.35	120.71	126.25
22	n	604	CLA	C1-C2-C3	-2.35	122.95	126.76
21	N	606	CHL	CBC-CAC-C3C	-2.35	109.50	112.87
22	B	609	CLA	C1-C2-C3	-2.35	122.34	126.20
22	G	603	CLA	CHB-C4A-NA	2.35	127.80	124.40
22	S	309	CLA	CHB-C4A-NA	2.35	127.80	124.40
22	g	614	CLA	CHB-C4A-NA	2.35	127.79	124.40
36	B	601	LMG	C38-C37-C36	-2.35	102.49	114.37
26	D	408	LHG	C11-C10-C9	-2.35	102.49	114.37
26	G	618	LHG	C5-O7-C7	-2.35	112.18	117.80
33	L	101	SQD	O6-C1-C2	2.35	111.84	108.27
21	N	608	CHL	CBC-CAC-C3C	-2.35	109.51	112.87
22	N	603	CLA	C1-C2-C3	-2.35	122.35	126.20
22	n	613	CLA	CHB-C4A-NA	2.35	127.78	124.40
31	D	406	BCR	C11-C10-C9	-2.35	123.99	127.28
22	C	512	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	b	612	CLA	CHB-C4A-NA	2.34	127.78	124.40
36	B	623	LMG	C38-C37-C36	-2.34	102.53	114.37
21	S	301	CHL	CBC-CAC-C3C	-2.34	109.52	112.87
36	b	620	LMG	C38-C37-C36	-2.34	102.53	114.37
22	b	605	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
37	f	101	HEM	C4A-CHB-C1B	-2.34	120.74	126.25
26	C	521	LHG	C11-C10-C9	-2.34	102.54	114.37
22	B	617	CLA	CHB-C4A-NA	2.34	127.78	124.40
26	g	619	LHG	C20-C19-C18	-2.34	102.55	114.37
36	I	101	LMG	C38-C37-C36	-2.34	102.55	114.37
22	N	612	CLA	C2B-C1B-NB	2.34	112.75	110.33
22	Y	612	CLA	CHB-C4A-NA	2.34	127.77	124.40
35	h	102	DGD	C3G-C2G-C1G	-2.34	106.33	111.78
22	Y	611	CLA	C2B-C1B-NB	2.34	112.75	110.33
21	s	306	CHL	CBC-CAC-C3C	-2.34	109.53	112.87
32	a	410	PL9	C2-C3-C4	2.34	120.32	118.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	611	CLA	CHB-C4A-NA	2.34	127.77	124.40
22	g	604	CLA	C1-C2-C3	-2.33	122.98	126.76
22	B	606	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
23	R	312	LUT	C1-C6-C7	-2.33	109.32	115.65
22	B	608	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
37	f	101	HEM	CHD-C1D-ND	2.33	126.93	124.42
22	N	613	CLA	CHB-C4A-NA	2.33	127.76	124.40
23	r	313	LUT	C1-C6-C7	-2.33	109.34	115.65
24	g	617	XAT	C11-C12-C13	-2.33	119.98	126.36
22	g	613	CLA	C2B-C1B-NB	2.33	112.74	110.33
26	y	617	LHG	C20-C19-C18	-2.33	102.61	114.37
22	g	612	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
22	g	612	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	r	314	XAT	C31-C32-C33	-2.32	119.99	126.36
26	C	522	LHG	O8-C23-C24	2.32	118.92	111.83
22	Y	604	CLA	C1-C2-C3	-2.32	123.00	126.76
22	G	612	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
21	y	608	CHL	C1C-CHC-C4B	2.32	124.37	116.07
25	N	617	NEX	C38-C25-C26	-2.32	118.48	122.30
36	C	502	LMG	C38-C37-C36	-2.32	102.64	114.37
24	R	313	XAT	C31-C32-C33	-2.32	120.00	126.36
33	A	412	SQD	O8-S-C6	2.32	110.45	105.97
22	G	612	CLA	CHB-C4A-NA	2.32	127.75	124.40
26	r	302	LHG	C5-O7-C7	-2.32	112.25	117.80
21	G	608	CHL	C1C-CHC-C4B	2.32	124.36	116.07
21	Y	607	CHL	C1C-CHC-C4B	2.32	124.36	116.07
21	N	605	CHL	C1C-CHC-C4B	2.32	124.36	116.07
36	w	102	LMG	C38-C37-C36	-2.32	102.65	114.37
32	A	411	PL9	C2-C3-C4	2.32	120.31	118.66
21	g	607	CHL	C1C-CHC-C4B	2.32	124.36	116.07
21	n	606	CHL	C1C-CHC-C4B	2.32	124.36	116.07
21	G	601	CHL	C1C-CHC-C4B	2.32	124.36	116.07
21	s	306	CHL	C1C-CHC-C4B	2.32	124.35	116.07
22	w	101	CLA	CHB-C4A-NA	2.32	127.74	124.40
22	s	311	CLA	CHB-C4A-NA	2.32	127.74	124.40
21	y	601	CHL	C1C-CHC-C4B	2.31	124.35	116.07
22	b	603	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
21	s	307	CHL	C1C-CHC-C4B	2.31	124.35	116.07
21	g	605	CHL	C1C-CHC-C4B	2.31	124.35	116.07
21	y	609	CHL	C1C-CHC-C4B	2.31	124.35	116.07
22	y	613	CLA	CHB-C4A-NA	2.31	127.74	124.40
21	G	607	CHL	C1C-CHC-C4B	2.31	124.35	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	306	CHL	C1C-CHC-C4B	2.31	124.35	116.07
21	s	302	CHL	C1C-CHC-C4B	2.31	124.35	116.07
21	G	606	CHL	C1C-CHC-C4B	2.31	124.34	116.07
35	c	517	DGD	O2D-C2D-C1D	-2.31	104.56	110.08
33	a	411	SQD	O8-S-C6	2.31	110.44	105.97
22	W	101	CLA	CHB-C4A-NA	2.31	127.74	124.40
21	r	301	CHL	C1C-CHC-C4B	2.31	124.34	116.07
21	g	606	CHL	C1C-CHC-C4B	2.31	124.34	116.07
21	n	601	CHL	C1C-CHC-C4B	2.31	124.34	116.07
22	D	405	CLA	C1-C2-C3	-2.31	122.41	126.20
21	g	601	CHL	C1C-CHC-C4B	2.31	124.33	116.07
21	s	301	CHL	C1C-CHC-C4B	2.31	124.33	116.07
22	W	101	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
21	n	605	CHL	C1C-CHC-C4B	2.31	124.33	116.07
26	Y	617	LHG	C20-C19-C18	-2.31	102.70	114.37
21	G	605	CHL	C1C-CHC-C4B	2.31	124.33	116.07
21	Y	606	CHL	C1C-CHC-C4B	2.31	124.33	116.07
22	Y	611	CLA	CHC-C1C-C2C	2.31	133.51	126.95
21	y	606	CHL	C1C-CHC-C4B	2.31	124.33	116.07
21	N	608	CHL	C1C-CHC-C4B	2.31	124.33	116.07
21	Y	601	CHL	C1C-CHC-C4B	2.31	124.33	116.07
24	N	616	XAT	O4-C5-C6	2.31	60.76	58.93
26	c	522	LHG	O8-C23-C24	2.31	118.87	111.83
21	Y	605	CHL	C1C-CHC-C4B	2.31	124.32	116.07
22	y	612	CLA	CHC-C1C-C2C	2.31	133.50	126.95
21	r	307	CHL	C1C-CHC-C4B	2.31	124.32	116.07
21	r	308	CHL	C1C-CHC-C4B	2.31	124.32	116.07
21	g	609	CHL	C1C-CHC-C4B	2.30	124.31	116.07
21	n	607	CHL	C1C-CHC-C4B	2.30	124.31	116.07
21	N	607	CHL	C1C-CHC-C4B	2.30	124.31	116.07
22	B	616	CLA	C1-C2-C3	-2.30	122.42	126.20
21	S	307	CHL	C1C-CHC-C4B	2.30	124.31	116.07
24	n	615	XAT	O4-C5-C6	2.30	60.76	58.93
21	N	601	CHL	C1C-CHC-C4B	2.30	124.31	116.07
21	y	605	CHL	C1C-CHC-C4B	2.30	124.31	116.07
35	h	102	DGD	C1D-C2D-C3D	-2.30	105.17	110.01
21	S	302	CHL	C1C-CHC-C4B	2.30	124.31	116.07
35	H	102	DGD	C3G-C2G-C1G	-2.30	106.42	111.78
21	S	301	CHL	C1C-CHC-C4B	2.30	124.31	116.07
22	G	613	CLA	CHC-C1C-C2C	2.30	133.49	126.95
36	c	523	LMG	O3-C3-C2	-2.30	104.95	110.38
22	G	603	CLA	C1-C2-C3	-2.30	122.43	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	606	CHL	C1C-CHC-C4B	2.30	124.30	116.07
21	S	306	CHL	C1C-CHC-C4B	2.30	124.30	116.07
24	Y	615	XAT	O24-C26-C27	2.30	123.47	116.88
36	C	523	LMG	O3-C3-C2	-2.30	104.96	110.38
22	y	612	CLA	C2B-C1B-NB	2.30	112.71	110.33
24	G	617	XAT	O4-C5-C6	2.30	60.75	58.93
24	n	615	XAT	C11-C12-C13	-2.30	120.06	126.36
22	n	611	CLA	CHB-C4A-NA	2.30	127.72	124.40
21	r	306	CHL	C1C-CHC-C4B	2.30	124.29	116.07
21	R	305	CHL	C1C-CHC-C4B	2.30	124.29	116.07
35	C	518	DGD	O2D-C2D-C1D	-2.30	104.60	110.08
22	G	613	CLA	C2B-C1B-NB	2.30	112.71	110.33
21	g	608	CHL	C1C-CHC-C4B	2.30	124.29	116.07
21	G	609	CHL	C1C-CHC-C4B	2.30	124.29	116.07
35	H	102	DGD	C1D-C2D-C3D	-2.30	105.18	110.01
26	R	301	LHG	C5-O7-C7	-2.30	112.30	117.80
22	C	511	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
21	Y	608	CHL	C1C-CHC-C4B	2.30	124.28	116.07
26	D	409	LHG	C18-C17-C16	-2.30	102.76	114.37
21	R	307	CHL	C1C-CHC-C4B	2.30	124.28	116.07
22	d	404	CLA	C1-C2-C3	-2.29	122.44	126.20
22	g	603	CLA	C1-C2-C3	-2.29	122.44	126.20
22	s	303	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
22	S	303	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
22	c	510	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
21	y	607	CHL	C1C-CHC-C4B	2.29	124.27	116.07
22	N	611	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
26	d	408	LHG	C18-C17-C16	-2.29	102.79	114.37
21	n	608	CHL	C1C-CHC-C4B	2.29	124.26	116.07
22	a	406	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
22	n	611	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
22	w	101	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
22	Y	603	CLA	C1-C2-C3	-2.29	122.45	126.20
22	n	612	CLA	CHC-C1C-C2C	2.29	133.45	126.95
22	g	613	CLA	CHC-C1C-C2C	2.29	133.45	126.95
35	A	401	DGD	C4E-C3E-C2E	-2.29	106.81	110.83
37	F	101	HEM	CHD-C1D-ND	2.29	126.88	124.42
22	b	602	CLA	C1-C2-C3	-2.29	122.45	126.20
22	C	512	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
22	N	612	CLA	CHC-C1C-C2C	2.29	133.44	126.95
31	B	619	BCR	C7-C8-C9	-2.28	122.86	126.23
22	y	603	CLA	C1-C2-C3	-2.28	122.45	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	511	CLA	C4D-CHA-C1A	2.28	123.96	121.24
31	H	101	BCR	C20-C21-C22	-2.28	124.08	127.28
31	d	405	BCR	C15-C16-C17	-2.28	118.86	123.52
22	c	511	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
26	l	102	LHG	C18-C17-C16	-2.28	102.86	114.37
35	a	413	DGD	C4E-C3E-C2E	-2.28	106.83	110.83
26	D	409	LHG	C27-C26-C25	-2.28	102.86	114.37
26	d	408	LHG	C27-C26-C25	-2.28	102.87	114.37
22	R	310	CLA	C3B-C4B-NB	-2.27	108.50	110.53
22	A	407	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
32	d	406	PL9	C37-C38-C39	-2.27	122.43	127.62
31	b	616	BCR	C7-C8-C9	-2.27	122.88	126.23
26	L	103	LHG	C18-C17-C16	-2.27	102.89	114.37
22	b	613	CLA	C1-C2-C3	-2.27	122.48	126.20
34	a	412	BCT	O3-C-O1	-2.27	113.88	119.68
26	c	522	LHG	O8-C6-C5	-2.27	101.86	108.40
22	B	605	CLA	C1-C2-C3	-2.27	122.48	126.20
31	C	517	BCR	C24-C23-C22	-2.27	122.88	126.23
33	L	102	SQD	C44-O6-C1	2.27	118.65	113.80
25	g	618	NEX	C36-C21-C22	-2.26	104.99	108.97
33	l	101	SQD	C44-O6-C1	2.26	118.65	113.80
26	N	618	LHG	C20-C19-C18	-2.26	102.93	114.37
25	y	618	NEX	C36-C21-C26	-2.26	103.94	110.05
34	D	403	BCT	O3-C-O1	-2.26	113.89	119.68
33	l	101	SQD	O48-C23-C24	2.26	118.73	111.83
33	L	102	SQD	O48-C23-C24	2.26	118.72	111.83
25	r	315	NEX	C36-C21-C26	-2.26	103.95	110.05
26	C	522	LHG	O8-C6-C5	-2.26	101.89	108.40
22	B	610	CLA	C1-C2-C3	-2.26	122.50	126.20
22	d	403	CLA	CHB-C4A-NA	2.25	127.65	124.40
22	s	312	CLA	CHB-C4A-NA	2.25	127.65	124.40
23	N	615	LUT	C7-C6-C5	-2.25	116.36	121.56
31	h	101	BCR	C20-C21-C22	-2.25	124.12	127.28
22	b	607	CLA	C1-C2-C3	-2.25	122.51	126.20
36	B	601	LMG	O3-C3-C2	-2.25	105.07	110.38
22	n	603	CLA	C1-C2-C3	-2.25	122.51	126.20
36	k	103	LMG	C1-C2-C3	-2.25	105.28	110.01
22	D	404	CLA	CHB-C4A-NA	2.25	127.64	124.40
26	n	617	LHG	C18-C17-C16	-2.25	103.01	114.37
36	K	103	LMG	C1-C2-C3	-2.25	105.28	110.01
22	S	310	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
36	T	101	LMG	C40-C39-C38	-2.24	103.02	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	406	BCR	C15-C16-C17	-2.24	118.93	123.52
22	c	510	CLA	C4D-CHA-C1A	2.24	123.92	121.24
31	c	516	BCR	C24-C23-C22	-2.24	122.92	126.23
25	Y	616	NEX	C11-C12-C13	-2.24	120.21	126.36
32	D	407	PL9	C37-C38-C39	-2.24	122.49	127.62
36	M	101	LMG	C40-C39-C38	-2.24	103.03	114.37
31	B	619	BCR	C15-C14-C13	-2.24	124.14	127.28
36	M	101	LMG	O2-C2-C1	-2.24	104.74	110.08
22	s	304	CLA	C3B-C4B-NB	-2.24	108.53	110.53
35	C	519	DGD	CBB-CAB-C9B	-2.24	103.06	114.37
24	y	615	XAT	O24-C26-C27	2.24	123.28	116.88
36	I	101	LMG	O3-C3-C2	-2.23	105.11	110.38
22	C	513	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
22	S	312	CLA	CHB-C4A-NA	2.23	127.62	124.40
22	g	614	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
26	c	522	LHG	C18-C17-C16	-2.23	103.09	114.37
22	c	512	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
26	C	520	LHG	C18-C17-C16	-2.23	103.10	114.37
36	B	623	LMG	C42-C41-C40	-2.23	103.10	114.37
26	N	618	LHG	C11-C10-C9	-2.23	103.11	114.37
35	c	518	DGD	CBB-CAB-C9B	-2.23	103.11	114.37
36	b	620	LMG	C42-C41-C40	-2.23	103.12	114.37
36	I	101	LMG	O6-C1-O1	-2.23	104.79	110.04
22	B	605	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
22	N	613	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
36	B	601	LMG	O6-C1-O1	-2.22	104.79	110.04
26	c	520	LHG	C18-C17-C16	-2.22	103.14	114.37
22	b	602	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
36	T	101	LMG	O2-C2-C1	-2.22	104.78	110.08
22	n	613	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
31	b	616	BCR	C15-C14-C13	-2.22	124.16	127.28
22	Y	612	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
22	s	310	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
22	C	510	CLA	O2D-CGD-CBD	2.22	115.11	111.23
26	C	522	LHG	C18-C17-C16	-2.22	103.16	114.37
26	r	302	LHG	C18-C17-C16	-2.22	103.16	114.37
35	C	519	DGD	C1D-C2D-C3D	-2.22	105.35	110.01
22	r	311	CLA	C3B-C4B-NB	-2.22	108.55	110.53
35	c	518	DGD	C1D-C2D-C3D	-2.22	105.35	110.01
22	y	613	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
26	R	301	LHG	C18-C17-C16	-2.21	103.19	114.37
35	C	518	DGD	CBB-CAB-C9B	-2.21	103.19	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	M	101	LMG	O3-C3-C2	-2.21	105.17	110.38
26	Y	617	LHG	C27-C26-C25	-2.21	103.20	114.37
35	c	517	DGD	CBB-CAB-C9B	-2.21	103.20	114.37
22	Y	602	CLA	C1-C2-C3	-2.21	122.58	126.20
22	N	602	CLA	C1-C2-C3	-2.20	122.59	126.20
22	G	614	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
35	c	519	DGD	C5B-C4B-C3B	-2.20	103.25	114.37
33	D	402	SQD	O8-S-C6	2.20	110.22	105.97
35	H	102	DGD	CBB-CAB-C9B	-2.20	103.26	114.37
22	s	312	CLA	C3B-C4B-NB	-2.20	108.57	110.53
35	J	101	DGD	C5B-C4B-C3B	-2.20	103.27	114.37
31	K	102	BCR	C7-C8-C9	-2.20	122.99	126.23
36	T	101	LMG	O3-C3-C2	-2.19	105.20	110.38
37	f	101	HEM	CHB-C1B-NB	-2.19	121.65	124.37
22	G	602	CLA	C1-C2-C3	-2.19	122.60	126.20
26	b	619	LHG	C18-C17-C16	-2.19	103.28	114.37
26	R	301	LHG	C27-C26-C25	-2.19	103.28	114.37
22	s	305	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
22	y	602	CLA	C1-C2-C3	-2.19	122.61	126.20
26	r	302	LHG	C27-C26-C25	-2.19	103.30	114.37
26	g	619	LHG	C27-C26-C25	-2.19	103.30	114.37
22	S	304	CLA	C3B-C4B-NB	-2.19	108.58	110.53
22	r	304	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
22	S	311	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
23	N	615	LUT	C16-C1-C6	-2.19	106.81	110.24
26	B	622	LHG	C18-C17-C16	-2.19	103.31	114.37
35	h	102	DGD	CBB-CAB-C9B	-2.19	103.31	114.37
25	y	618	NEX	C31-C32-C33	-2.19	120.37	126.36
25	r	315	NEX	C31-C32-C33	-2.19	120.37	126.36
26	L	103	LHG	C5-O7-C7	-2.19	112.56	117.80
26	G	618	LHG	C18-C17-C16	-2.19	103.32	114.37
22	c	509	CLA	O2D-CGD-CBD	2.19	115.05	111.23
22	S	305	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
22	n	602	CLA	C1-C2-C3	-2.18	122.62	126.20
23	G	616	LUT	C27-C28-C29	-2.18	121.63	126.32
22	N	609	CLA	C1-C2-C3	-2.18	122.62	126.20
26	l	102	LHG	C5-O7-C7	-2.18	112.57	117.80
22	a	406	CLA	C1-C2-C3	-2.18	123.23	126.76
24	N	616	XAT	C35-C15-C14	-2.18	119.06	123.52
22	y	610	CLA	C1-C2-C3	-2.18	122.62	126.20
22	R	303	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
33	d	402	SQD	O8-S-C6	2.18	110.18	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	612	CLA	CHB-C1B-NB	2.18	127.32	124.05
35	J	101	DGD	CAB-C9B-C8B	-2.18	103.36	114.37
22	s	311	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
22	g	613	CLA	CHB-C1B-NB	2.18	127.31	124.05
31	k	102	BCR	C11-C10-C9	-2.17	124.23	127.28
22	g	602	CLA	C1-C2-C3	-2.17	122.64	126.20
31	b	616	BCR	C15-C16-C17	-2.17	119.07	123.52
31	B	619	BCR	C15-C16-C17	-2.17	119.07	123.52
22	x	101	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
31	K	102	BCR	C11-C10-C9	-2.17	124.23	127.28
35	J	101	DGD	CBB-CAB-C9B	-2.17	103.41	114.37
37	F	101	HEM	CHB-C1B-NB	-2.17	121.69	124.37
26	s	314	LHG	C18-C17-C16	-2.17	103.41	114.37
31	k	101	BCR	C11-C10-C9	-2.17	124.24	127.28
26	s	314	LHG	C27-C26-C25	-2.17	103.42	114.37
22	N	610	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
22	C	510	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
26	C	521	LHG	C27-C26-C25	-2.17	103.42	114.37
26	S	314	LHG	C27-C26-C25	-2.16	103.43	114.37
33	D	402	SQD	C44-O6-C1	2.16	118.43	113.80
22	b	607	CLA	CMB-C2B-C3B	2.16	131.64	126.55
22	C	511	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
22	G	610	CLA	C1-C2-C3	-2.16	122.66	126.20
22	Y	610	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
26	S	314	LHG	C18-C17-C16	-2.16	103.44	114.37
35	c	519	DGD	CBB-CAB-C9B	-2.16	103.44	114.37
26	B	622	LHG	C27-C26-C25	-2.16	103.45	114.37
22	A	407	CLA	C1-C2-C3	-2.16	123.27	126.76
26	c	521	LHG	C27-C26-C25	-2.16	103.45	114.37
22	c	509	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
35	c	519	DGD	CAB-C9B-C8B	-2.16	103.46	114.37
22	s	309	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
22	S	309	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
26	y	617	LHG	C27-C26-C25	-2.16	103.47	114.37
22	n	610	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
26	n	617	LHG	C27-C26-C25	-2.16	103.47	114.37
35	c	517	DGD	C5B-C4B-C3B	-2.16	103.47	114.37
35	c	518	DGD	C5B-C4B-C3B	-2.16	103.47	114.37
36	M	101	LMG	C1-C2-C3	-2.15	105.48	110.01
32	D	407	PL9	C32-C33-C34	-2.15	122.69	127.62
22	g	610	CLA	C1-C2-C3	-2.15	122.67	126.20
33	d	402	SQD	C44-O6-C1	2.15	118.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	519	DGD	C5B-C4B-C3B	-2.15	103.49	114.37
26	n	617	LHG	C5-O7-C7	-2.15	112.65	117.80
26	b	619	LHG	C27-C26-C25	-2.15	103.50	114.37
36	T	101	LMG	C1-C2-C3	-2.15	105.49	110.01
35	C	518	DGD	C5B-C4B-C3B	-2.15	103.50	114.37
22	n	609	CLA	C1-C2-C3	-2.15	122.67	126.20
22	G	611	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
22	y	611	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
22	g	611	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
26	C	520	LHG	C27-C26-C25	-2.15	103.52	114.37
33	A	412	SQD	O48-C23-C24	2.15	118.38	111.83
22	s	308	CLA	CED-O2D-CGD	2.14	120.78	115.92
22	S	303	CLA	C1-C2-C3	-2.14	122.68	126.20
35	c	517	DGD	O3E-C3E-C2E	-2.14	105.32	110.38
31	K	101	BCR	C7-C8-C9	-2.14	123.06	126.23
26	Y	617	LHG	C18-C17-C16	-2.14	103.54	114.37
22	c	510	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
22	d	403	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
35	h	102	DGD	O3E-C3E-C2E	-2.14	105.33	110.38
22	D	404	CLA	C1-C2-C3	-2.14	122.69	126.20
22	c	504	CLA	C1-C2-C3	-2.14	122.69	126.20
33	a	411	SQD	O48-C23-C24	2.14	118.36	111.83
26	c	520	LHG	C27-C26-C25	-2.14	103.55	114.37
26	L	103	LHG	C27-C26-C25	-2.14	103.55	114.37
22	B	610	CLA	CMB-C2B-C3B	2.14	131.58	126.55
31	k	102	BCR	C7-C8-C9	-2.14	123.07	126.23
26	d	407	LHG	C27-C26-C25	-2.14	103.56	114.37
35	C	518	DGD	O3E-C3E-C2E	-2.14	105.34	110.38
22	D	404	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
22	d	403	CLA	C1-C2-C3	-2.14	122.69	126.20
26	D	408	LHG	C27-C26-C25	-2.14	103.56	114.37
32	d	406	PL9	C32-C33-C34	-2.14	122.73	127.62
22	Y	609	CLA	C1-C2-C3	-2.14	122.70	126.20
36	b	620	LMG	O2-C2-C1	-2.14	104.99	110.08
22	B	603	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
31	k	101	BCR	C15-C14-C13	-2.13	124.28	127.28
35	C	519	DGD	CAB-C9B-C8B	-2.13	103.58	114.37
22	n	612	CLA	CHB-C1B-NB	2.13	127.25	124.05
22	C	505	CLA	C1-C2-C3	-2.13	122.70	126.20
36	I	101	LMG	O2-C2-C1	-2.13	105.00	110.08
33	a	411	SQD	O48-C23-O10	-2.13	118.30	123.63
26	l	102	LHG	C27-C26-C25	-2.13	103.59	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	413	DGD	C1D-C2D-C3D	-2.13	105.53	110.01
22	G	613	CLA	CHB-C1B-NB	2.13	127.25	124.05
22	S	304	CLA	CHB-C4A-NA	2.13	127.47	124.40
23	N	615	LUT	C1-C6-C7	-2.13	109.88	115.65
37	f	101	HEM	CHC-C1C-NC	2.13	126.77	124.45
22	C	511	CLA	CMC-C2C-C1C	-2.13	121.71	125.03
22	N	612	CLA	CHB-C1B-NB	2.13	127.24	124.05
31	K	101	BCR	C15-C16-C17	-2.13	119.17	123.52
36	c	523	LMG	O2-C2-C1	-2.13	105.01	110.08
26	Y	617	LHG	C5-O7-C7	-2.13	112.71	117.80
26	g	619	LHG	C18-C17-C16	-2.13	103.62	114.37
36	B	601	LMG	O2-C2-C1	-2.13	105.01	110.08
35	H	102	DGD	O3E-C3E-C2E	-2.12	105.37	110.38
26	g	619	LHG	O8-C6-C5	-2.12	102.27	108.40
31	K	101	BCR	C15-C14-C13	-2.12	124.30	127.28
36	B	623	LMG	O2-C2-C1	-2.12	105.02	110.08
33	d	402	SQD	O5-C1-C2	2.12	114.73	110.37
31	K	101	BCR	C11-C10-C9	-2.12	124.30	127.28
35	h	102	DGD	CAB-C9B-C8B	-2.12	103.64	114.37
32	D	407	PL9	O2-C1-C2	-2.12	117.00	121.83
31	k	101	BCR	C15-C16-C17	-2.12	119.18	123.52
33	A	412	SQD	O48-C23-O10	-2.12	118.32	123.63
35	A	401	DGD	C1D-C2D-C3D	-2.12	105.55	110.01
22	d	404	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
35	c	518	DGD	CAB-C9B-C8B	-2.12	103.65	114.37
22	C	511	CLA	C1-C2-C3	-2.12	122.72	126.20
22	b	610	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
26	D	410	LHG	C27-C26-C25	-2.12	103.66	114.37
35	a	413	DGD	CBB-CAB-C9B	-2.12	103.66	114.37
23	N	615	LUT	C15-C35-C34	-2.12	119.19	123.52
23	g	616	LUT	C27-C28-C29	-2.12	121.77	126.32
26	D	410	LHG	C5-O7-C7	-2.12	112.73	117.80
22	c	510	CLA	CMC-C2C-C1C	-2.12	121.72	125.03
26	C	521	LHG	C20-C19-C18	-2.12	103.67	114.37
25	n	616	NEX	C38-C25-C26	-2.12	118.82	122.30
22	c	510	CLA	C1-C2-C3	-2.12	122.73	126.20
22	B	613	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
32	d	406	PL9	O2-C1-C2	-2.11	117.02	121.83
26	G	618	LHG	C27-C26-C25	-2.11	103.68	114.37
35	h	102	DGD	C3D-C4D-C5D	-2.11	106.40	110.23
22	Y	611	CLA	CHB-C1B-NB	2.11	127.22	124.05
31	D	406	BCR	C7-C8-C9	-2.11	123.11	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	523	LMG	O2-C2-C1	-2.11	105.04	110.08
22	c	508	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
22	G	613	CLA	CHD-C4C-C3C	-2.11	121.69	124.77
35	A	401	DGD	CBB-CAB-C9B	-2.11	103.70	114.37
35	H	102	DGD	CAB-C9B-C8B	-2.11	103.70	114.37
35	A	401	DGD	O3E-C3E-C2E	-2.11	105.40	110.38
31	k	101	BCR	C7-C8-C9	-2.11	123.11	126.23
26	d	409	LHG	C27-C26-C25	-2.11	103.70	114.37
22	s	303	CLA	C1-C2-C3	-2.11	122.74	126.20
33	A	412	SQD	C1-C2-C3	2.11	114.45	110.01
26	y	617	LHG	C18-C17-C16	-2.11	103.71	114.37
26	c	521	LHG	C20-C19-C18	-2.11	103.71	114.37
26	C	521	LHG	C5-O7-C7	-2.11	112.75	117.80
33	D	402	SQD	O5-C1-C2	2.11	114.70	110.37
35	H	102	DGD	C3D-C4D-C5D	-2.11	106.41	110.23
23	g	616	LUT	C31-C32-C33	-2.11	120.59	126.36
35	a	413	DGD	CAB-C9B-C8B	-2.11	103.72	114.37
22	S	312	CLA	C3B-C4B-NB	-2.11	108.65	110.53
37	F	101	HEM	CHC-C1C-NC	2.10	126.75	124.45
22	A	409	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
35	c	518	DGD	O2D-C2D-C1D	-2.10	105.06	110.08
32	D	407	PL9	C20-C19-C21	2.10	118.88	115.23
35	a	413	DGD	O3E-C3E-C2E	-2.10	105.42	110.38
32	d	406	PL9	C20-C19-C21	2.10	118.88	115.23
36	b	620	LMG	O7-C10-O9	-2.10	118.79	123.70
22	S	308	CLA	CED-O2D-CGD	2.10	120.68	115.92
22	D	405	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
26	c	521	LHG	C5-O7-C7	-2.10	112.77	117.80
25	g	618	NEX	C36-C21-C26	-2.10	104.38	110.05
36	B	623	LMG	O7-C10-O9	-2.10	118.80	123.70
22	C	512	CLA	O2D-CGD-CBD	2.10	114.90	111.23
22	a	408	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
22	C	513	CLA	C1-C2-C3	-2.10	122.76	126.20
35	A	401	DGD	CAB-C9B-C8B	-2.10	103.77	114.37
26	c	521	LHG	C18-C17-C16	-2.10	103.77	114.37
25	n	616	NEX	C36-C21-C26	-2.10	104.38	110.05
31	d	405	BCR	C7-C8-C9	-2.10	123.13	126.23
35	H	102	DGD	O3D-C3D-C4D	-2.10	105.44	110.38
33	l	101	SQD	O8-S-C6	2.10	110.02	105.97
26	C	521	LHG	C18-C17-C16	-2.10	103.77	114.37
35	h	102	DGD	O3D-C3D-C4D	-2.10	105.44	110.38
22	C	507	CLA	O2A-CGA-O1A	-2.09	118.39	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	g	613	CLA	CHD-C4C-C3C	-2.09	121.72	124.77
22	C	511	CLA	CMB-C2B-C3B	2.09	131.47	126.55
22	Y	611	CLA	CHD-C4C-C3C	-2.09	121.72	124.77
22	s	304	CLA	CHB-C4A-NA	2.09	127.42	124.40
31	D	406	BCR	C15-C14-C13	-2.09	124.35	127.28
22	b	615	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
22	C	509	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
33	L	102	SQD	O8-S-C6	2.09	110.00	105.97
35	C	519	DGD	O2D-C2D-C1D	-2.09	105.10	110.08
22	c	506	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
33	l	103	SQD	O5-C1-C2	2.09	114.66	110.37
31	b	617	BCR	C24-C23-C22	-2.09	123.15	126.23
33	a	411	SQD	C1-C2-C3	2.09	114.40	110.01
23	G	616	LUT	C31-C32-C33	-2.08	120.65	126.36
36	k	103	LMG	O3-C3-C2	-2.08	105.47	110.38
22	N	612	CLA	CHD-C4C-C3C	-2.08	121.74	124.77
37	F	101	HEM	CAA-CBA-CGA	-2.08	108.14	113.67
35	C	518	DGD	CAB-C9B-C8B	-2.08	103.85	114.37
26	c	522	LHG	C27-C26-C25	-2.08	103.85	114.37
36	K	103	LMG	O3-C3-C2	-2.08	105.47	110.38
37	f	101	HEM	CAA-CBA-CGA	-2.08	108.15	113.67
22	r	310	CLA	C1-C2-C3	-2.08	122.79	126.20
37	F	101	HEM	CHC-C1C-C2C	2.08	129.81	125.49
22	c	511	CLA	O2D-CGD-CBD	2.08	114.86	111.23
26	C	522	LHG	C27-C26-C25	-2.08	103.88	114.37
35	c	517	DGD	CAB-C9B-C8B	-2.07	103.88	114.37
22	n	612	CLA	CHD-C4C-C3C	-2.07	121.75	124.77
26	d	409	LHG	C5-O7-C7	-2.07	112.83	117.80
22	c	510	CLA	CMB-C2B-C3B	2.07	131.43	126.55
22	B	618	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
22	c	512	CLA	C1-C2-C3	-2.07	122.81	126.20
22	C	508	CLA	C1-C2-C3	-2.07	122.81	126.20
37	F	101	HEM	C4C-CHD-C1D	2.07	130.41	126.02
30	A	408	PHO	C1-C2-C3	-2.07	122.81	126.20
22	Y	602	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
26	N	618	LHG	C18-C17-C16	-2.07	103.92	114.37
22	B	610	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
22	y	612	CLA	CHD-C4C-C3C	-2.07	121.76	124.77
35	a	413	DGD	O2D-C2D-C1D	-2.07	105.15	110.08
36	K	103	LMG	O2-C2-C1	-2.06	105.16	110.08
22	Y	611	CLA	CAA-CBA-CGA	-2.06	107.35	113.21
31	B	620	BCR	C24-C23-C22	-2.06	123.18	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	405	BCR	C15-C14-C13	-2.06	124.38	127.28
22	b	609	CLA	C1-C2-C3	-2.06	122.82	126.20
22	B	612	CLA	C1-C2-C3	-2.06	122.82	126.20
36	c	523	LMG	O7-C10-O9	-2.06	118.89	123.70
22	c	507	CLA	C1-C2-C3	-2.06	122.82	126.20
35	h	102	DGD	C5B-C4B-C3B	-2.06	103.96	114.37
22	R	309	CLA	C1-C2-C3	-2.06	122.82	126.20
33	L	101	SQD	O5-C1-C2	2.06	114.60	110.37
22	N	612	CLA	CAA-CBA-CGA	-2.06	107.36	113.21
36	k	103	LMG	O2-C2-C1	-2.06	105.17	110.08
35	H	102	DGD	C5B-C4B-C3B	-2.06	103.96	114.37
37	f	101	HEM	CHC-C1C-C2C	2.06	129.77	125.49
22	N	602	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
22	B	611	CLA	O1D-CGD-CBD	2.06	128.58	124.52
22	C	511	CLA	C1C-C2C-C3C	2.06	109.14	106.98
22	R	308	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
35	A	401	DGD	O2D-C2D-C1D	-2.06	105.18	110.08
22	S	311	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
22	g	604	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
25	Y	616	NEX	C24-C23-C22	2.05	114.63	110.79
33	a	411	SQD	O5-C5-C4	2.05	113.39	109.70
22	b	607	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	c	507	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	a	404	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
22	y	602	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
22	r	309	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
26	N	618	LHG	C27-C26-C25	-2.05	104.02	114.37
22	b	608	CLA	O1D-CGD-CBD	2.05	128.55	124.52
22	g	613	CLA	CAA-CBA-CGA	-2.05	107.40	113.21
21	n	606	CHL	CAC-C3C-C4C	2.05	129.29	124.03
22	G	602	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
22	Y	604	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
22	y	612	CLA	CAA-CBA-CGA	-2.05	107.40	113.21
22	G	613	CLA	CAA-CBA-CGA	-2.04	107.41	113.21
22	c	504	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
22	s	313	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
21	y	606	CHL	CAC-C3C-C4C	2.04	129.28	124.03
22	n	612	CLA	CAA-CBA-CGA	-2.04	107.41	113.21
35	h	102	DGD	O5D-C6D-C5D	-2.04	104.82	109.42
30	d	401	PHO	O2A-CGA-O1A	-2.04	118.52	123.63
37	f	101	HEM	C4C-CHD-C1D	2.04	130.36	126.02
22	n	604	CLA	O2A-CGA-O1A	-2.04	118.52	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	C1-C2-C3	-2.04	122.86	126.20
35	H	102	DGD	O5D-C6D-C5D	-2.04	104.82	109.42
21	y	607	CHL	CAC-C3C-C4C	2.04	129.27	124.03
36	C	523	LMG	O7-C10-O9	-2.04	118.94	123.70
21	N	601	CHL	CAC-C3C-C4C	2.04	129.27	124.03
21	g	606	CHL	CAC-C3C-C4C	2.04	129.27	124.03
21	S	307	CHL	CAC-C3C-C4C	2.04	129.27	124.03
22	N	612	CLA	C1-C2-C3	-2.04	122.86	126.20
21	g	605	CHL	CAC-C3C-C4C	2.04	129.27	124.03
21	G	608	CHL	CAC-C3C-C4C	2.04	129.27	124.03
21	N	607	CHL	CAC-C3C-C4C	2.04	129.27	124.03
24	g	617	XAT	C4-C3-C2	2.04	114.60	110.79
22	C	510	CLA	C1-C2-C3	-2.04	122.86	126.20
22	n	612	CLA	C1-C2-C3	-2.04	122.86	126.20
21	y	601	CHL	CAC-C3C-C4C	2.03	129.26	124.03
35	C	518	DGD	O6E-C1E-O5D	-2.03	105.24	110.04
21	S	302	CHL	CAC-C3C-C4C	2.03	129.26	124.03
22	c	512	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
21	G	607	CHL	CAC-C3C-C4C	2.03	129.26	124.03
21	N	608	CHL	CAC-C3C-C4C	2.03	129.26	124.03
21	Y	607	CHL	CAC-C3C-C4C	2.03	129.26	124.03
36	C	502	LMG	C3-C4-C5	-2.03	106.55	110.23
21	r	301	CHL	CAC-C3C-C4C	2.03	129.25	124.03
33	l	101	SQD	O6-C1-C2	2.03	111.36	108.27
33	L	102	SQD	O6-C1-C2	2.03	111.36	108.27
21	r	306	CHL	CAC-C3C-C4C	2.03	129.25	124.03
22	C	505	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
22	N	604	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
23	Y	614	LUT	C1-C6-C7	-2.03	110.14	115.65
35	c	517	DGD	O6E-C1E-O5D	-2.03	105.25	110.04
35	H	102	DGD	C7B-C6B-C5B	-2.03	104.11	114.37
35	c	519	DGD	O2D-C2D-C1D	-2.03	105.24	110.08
22	B	612	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
35	a	413	DGD	C5B-C4B-C3B	-2.03	104.11	114.37
35	h	102	DGD	C7B-C6B-C5B	-2.03	104.11	114.37
21	g	608	CHL	CAC-C3C-C4C	2.03	129.25	124.03
21	Y	606	CHL	CAC-C3C-C4C	2.03	129.25	124.03
21	Y	608	CHL	CAC-C3C-C4C	2.03	129.25	124.03
22	c	510	CLA	C1C-C2C-C3C	2.03	109.11	106.98
22	g	602	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
21	g	607	CHL	CAC-C3C-C4C	2.03	129.24	124.03
21	G	606	CHL	CAC-C3C-C4C	2.03	129.24	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	606	CHL	CAC-C3C-C4C	2.03	129.24	124.03
22	g	613	CLA	C1-C2-C3	-2.03	122.87	126.20
22	S	313	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
21	g	609	CHL	CAC-C3C-C4C	2.03	129.24	124.03
21	n	605	CHL	CAC-C3C-C4C	2.03	129.24	124.03
21	s	306	CHL	CAC-C3C-C4C	2.03	129.24	124.03
22	N	603	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
21	n	607	CHL	CAC-C3C-C4C	2.03	129.24	124.03
22	n	602	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
22	c	514	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
22	G	613	CLA	C1-C2-C3	-2.03	122.88	126.20
33	A	412	SQD	O5-C5-C4	2.02	113.35	109.70
21	y	605	CHL	CAC-C3C-C4C	2.02	129.23	124.03
22	B	617	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
21	y	609	CHL	CAC-C3C-C4C	2.02	129.23	124.03
21	N	605	CHL	CAC-C3C-C4C	2.02	129.23	124.03
22	C	513	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
22	c	502	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	y	616	NEX	C36-C21-C26	-2.02	104.58	110.05
21	y	608	CHL	CAC-C3C-C4C	2.02	129.23	124.03
21	s	301	CHL	CAC-C3C-C4C	2.02	129.23	124.03
35	A	401	DGD	C5B-C4B-C3B	-2.02	104.15	114.37
22	C	511	CLA	O1D-CGD-CBD	2.02	128.51	124.52
21	r	308	CHL	CAC-C3C-C4C	2.02	129.23	124.03
22	G	604	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
21	Y	601	CHL	CAC-C3C-C4C	2.02	129.22	124.03
22	Y	603	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
22	C	508	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
22	C	513	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
21	s	302	CHL	CAC-C3C-C4C	2.02	129.22	124.03
21	R	305	CHL	CAC-C3C-C4C	2.02	129.22	124.03
31	C	516	BCR	C11-C10-C9	-2.02	124.45	127.28
21	S	301	CHL	CAC-C3C-C4C	2.02	129.22	124.03
22	c	504	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
22	r	310	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
21	G	605	CHL	CAC-C3C-C4C	2.02	129.22	124.03
21	n	601	CHL	CAC-C3C-C4C	2.02	129.22	124.03
24	n	615	XAT	C35-C15-C14	-2.02	119.39	123.52
36	D	411	LMG	C1-C2-C3	-2.02	105.77	110.01
21	r	307	CHL	CAC-C3C-C4C	2.02	129.22	124.03
22	b	614	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
30	D	401	PHO	O2A-CGA-O1A	-2.02	118.58	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	612	CLA	C1-C2-C3	-2.02	122.89	126.20
22	y	604	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
22	Y	611	CLA	C1-C2-C3	-2.02	122.89	126.20
22	C	505	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
21	n	608	CHL	CAC-C3C-C4C	2.02	129.21	124.03
24	G	617	XAT	C4-C3-C2	2.02	114.56	110.79
21	G	609	CHL	CAC-C3C-C4C	2.02	129.21	124.03
22	C	515	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
21	S	306	CHL	CAC-C3C-C4C	2.01	129.21	124.03
35	c	519	DGD	O3E-C3E-C2E	-2.01	105.63	110.38
30	a	407	PHO	C1-C2-C3	-2.01	122.90	126.20
36	b	620	LMG	C24-C23-C22	-2.01	104.20	114.37
21	G	601	CHL	CAC-C3C-C4C	2.01	129.20	124.03
22	c	510	CLA	C3A-C2A-C1A	2.01	104.35	101.34
21	R	307	CHL	CAC-C3C-C4C	2.01	129.20	124.03
22	g	603	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
22	s	312	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
22	b	609	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
21	g	601	CHL	CAC-C3C-C4C	2.01	129.19	124.03
22	s	303	CLA	O2D-CGD-CBD	2.01	114.74	111.23
22	A	405	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
22	c	510	CLA	O1D-CGD-CBD	2.01	128.48	124.52
22	C	509	CLA	C1-C2-C3	-2.01	122.91	126.20
22	S	312	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
31	C	516	BCR	C7-C8-C9	-2.01	123.26	126.23
22	n	603	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
35	J	101	DGD	O2D-C2D-C1D	-2.01	105.29	110.08
22	R	309	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
21	R	306	CHL	CAC-C3C-C4C	2.01	129.19	124.03
25	y	616	NEX	C36-C21-C22	-2.01	105.44	108.97
21	s	307	CHL	CAC-C3C-C4C	2.01	129.19	124.03
22	y	603	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
21	Y	605	CHL	CAC-C3C-C4C	2.00	129.18	124.03
26	d	407	LHG	C5-O7-C7	-2.00	113.00	117.80
22	b	606	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
25	r	315	NEX	C11-C12-C13	-2.00	120.87	126.36
36	d	410	LMG	C1-C2-C3	-2.00	105.80	110.01
31	c	515	BCR	C11-C10-C9	-2.00	124.47	127.28
25	Y	616	NEX	O24-C26-C27	-2.00	111.14	116.88
36	w	102	LMG	C3-C4-C5	-2.00	106.60	110.23
22	s	311	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
35	J	101	DGD	O3E-C3E-C2E	-2.00	105.66	110.38

All (353) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	g	601	CHL	ND
21	g	601	CHL	C8
21	g	601	CHL	NC
21	g	601	CHL	NA
21	g	605	CHL	ND
21	g	605	CHL	NC
21	g	605	CHL	NA
21	g	606	CHL	ND
21	g	606	CHL	NC
21	g	606	CHL	NA
21	g	607	CHL	ND
21	g	607	CHL	C8
21	g	607	CHL	NC
21	g	607	CHL	NA
21	g	608	CHL	ND
21	g	608	CHL	C8
21	g	608	CHL	NC
21	g	608	CHL	NA
21	g	609	CHL	ND
21	g	609	CHL	C8
21	g	609	CHL	NC
21	g	609	CHL	NA
21	n	601	CHL	ND
21	n	601	CHL	C8
21	n	601	CHL	NC
21	n	601	CHL	NA
21	n	605	CHL	ND
21	n	605	CHL	NC
21	n	605	CHL	NA
21	n	606	CHL	ND
21	n	606	CHL	C8
21	n	606	CHL	NC
21	n	606	CHL	NA
21	n	607	CHL	ND
21	n	607	CHL	C8
21	n	607	CHL	NC
21	n	607	CHL	NA
21	n	608	CHL	ND
21	n	608	CHL	C8
21	n	608	CHL	NC
21	n	608	CHL	NA
21	y	601	CHL	ND

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Mol	Chain	Res	Type	Atom
21	y	601	CHL	C8
21	y	601	CHL	NC
21	y	601	CHL	NA
21	y	605	CHL	ND
21	y	605	CHL	NC
21	y	605	CHL	NA
21	y	606	CHL	ND
21	y	606	CHL	NC
21	y	606	CHL	NA
21	y	607	CHL	ND
21	y	607	CHL	C8
21	y	607	CHL	NC
21	y	607	CHL	NA
21	y	608	CHL	ND
21	y	608	CHL	C8
21	y	608	CHL	NC
21	y	608	CHL	NA
21	y	609	CHL	ND
21	y	609	CHL	C8
21	y	609	CHL	NC
21	y	609	CHL	NA
21	G	601	CHL	ND
21	G	601	CHL	C8
21	G	601	CHL	NC
21	G	601	CHL	NA
21	G	605	CHL	ND
21	G	605	CHL	NC
21	G	605	CHL	NA
21	G	606	CHL	ND
21	G	606	CHL	NC
21	G	606	CHL	NA
21	G	607	CHL	ND
21	G	607	CHL	C8
21	G	607	CHL	NC
21	G	607	CHL	NA
21	G	608	CHL	ND
21	G	608	CHL	C8
21	G	608	CHL	NC
21	G	608	CHL	NA
21	G	609	CHL	ND
21	G	609	CHL	C8
21	G	609	CHL	NC

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Mol	Chain	Res	Type	Atom
21	G	609	CHL	NA
21	N	601	CHL	ND
21	N	601	CHL	C8
21	N	601	CHL	NC
21	N	601	CHL	NA
21	N	605	CHL	ND
21	N	605	CHL	NC
21	N	605	CHL	NA
21	N	606	CHL	ND
21	N	606	CHL	C8
21	N	606	CHL	NC
21	N	606	CHL	NA
21	N	607	CHL	ND
21	N	607	CHL	C8
21	N	607	CHL	NC
21	N	607	CHL	NA
21	N	608	CHL	ND
21	N	608	CHL	C8
21	N	608	CHL	NC
21	N	608	CHL	NA
21	Y	601	CHL	ND
21	Y	601	CHL	C8
21	Y	601	CHL	NC
21	Y	601	CHL	NA
21	Y	605	CHL	ND
21	Y	605	CHL	NC
21	Y	605	CHL	NA
21	Y	606	CHL	ND
21	Y	606	CHL	C8
21	Y	606	CHL	NC
21	Y	606	CHL	NA
21	Y	607	CHL	ND
21	Y	607	CHL	C8
21	Y	607	CHL	NC
21	Y	607	CHL	NA
21	Y	608	CHL	ND
21	Y	608	CHL	C8
21	Y	608	CHL	NC
21	Y	608	CHL	NA
21	r	301	CHL	ND
21	r	301	CHL	NC
21	r	301	CHL	NA

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Mol	Chain	Res	Type	Atom
21	r	306	CHL	ND
21	r	306	CHL	C8
21	r	306	CHL	NC
21	r	306	CHL	NA
21	r	307	CHL	ND
21	r	307	CHL	C8
21	r	307	CHL	NC
21	r	307	CHL	NA
21	r	308	CHL	ND
21	r	308	CHL	C8
21	r	308	CHL	NC
21	r	308	CHL	NA
21	s	301	CHL	ND
21	s	301	CHL	NC
21	s	301	CHL	NA
21	s	302	CHL	ND
21	s	302	CHL	NC
21	s	302	CHL	NA
21	s	306	CHL	ND
21	s	306	CHL	NC
21	s	306	CHL	NA
21	s	307	CHL	ND
21	s	307	CHL	NC
21	s	307	CHL	NA
21	S	301	CHL	ND
21	S	301	CHL	NC
21	S	301	CHL	NA
21	S	302	CHL	ND
21	S	302	CHL	NC
21	S	302	CHL	NA
21	S	306	CHL	ND
21	S	306	CHL	NC
21	S	306	CHL	NA
21	S	307	CHL	ND
21	S	307	CHL	NC
21	S	307	CHL	NA
21	R	305	CHL	ND
21	R	305	CHL	C8
21	R	305	CHL	NC
21	R	305	CHL	NA
21	R	306	CHL	ND
21	R	306	CHL	C8

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Mol	Chain	Res	Type	Atom
21	R	306	CHL	NC
21	R	306	CHL	NA
21	R	307	CHL	ND
21	R	307	CHL	C8
21	R	307	CHL	NC
21	R	307	CHL	NA
22	g	602	CLA	ND
22	g	603	CLA	ND
22	g	604	CLA	ND
22	g	610	CLA	ND
22	g	611	CLA	ND
22	g	612	CLA	ND
22	g	613	CLA	ND
22	g	614	CLA	ND
22	n	602	CLA	ND
22	n	603	CLA	ND
22	n	604	CLA	ND
22	n	609	CLA	ND
22	n	610	CLA	ND
22	n	611	CLA	ND
22	n	612	CLA	ND
22	n	613	CLA	ND
22	y	602	CLA	ND
22	y	603	CLA	ND
22	y	604	CLA	ND
22	y	610	CLA	ND
22	y	611	CLA	ND
22	y	612	CLA	ND
22	y	613	CLA	ND
22	G	602	CLA	ND
22	G	603	CLA	ND
22	G	604	CLA	ND
22	G	610	CLA	ND
22	G	611	CLA	ND
22	G	612	CLA	ND
22	G	613	CLA	ND
22	G	614	CLA	ND
22	N	602	CLA	ND
22	N	603	CLA	ND
22	N	604	CLA	ND
22	N	609	CLA	ND
22	N	610	CLA	ND

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Mol	Chain	Res	Type	Atom
22	N	611	CLA	ND
22	N	612	CLA	ND
22	N	613	CLA	ND
22	Y	602	CLA	ND
22	Y	603	CLA	ND
22	Y	604	CLA	ND
22	Y	609	CLA	ND
22	Y	610	CLA	ND
22	Y	611	CLA	ND
22	Y	612	CLA	ND
22	a	404	CLA	ND
22	a	405	CLA	ND
22	a	406	CLA	ND
22	a	408	CLA	ND
22	b	601	CLA	ND
22	b	602	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	608	CLA	ND
22	b	609	CLA	ND
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	c	502	CLA	ND
22	c	503	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	c	514	CLA	ND

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Mol	Chain	Res	Type	Atom
22	d	403	CLA	ND
22	d	404	CLA	ND
22	w	101	CLA	ND
22	x	101	CLA	ND
22	A	405	CLA	ND
22	A	406	CLA	ND
22	A	407	CLA	ND
22	A	409	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	608	CLA	ND
22	B	609	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	B	617	CLA	ND
22	B	618	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	508	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	513	CLA	ND
22	C	514	CLA	ND
22	C	515	CLA	ND
22	D	404	CLA	ND
22	D	405	CLA	ND
22	W	101	CLA	ND
22	r	303	CLA	ND
22	r	304	CLA	ND

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Mol	Chain	Res	Type	Atom
22	r	305	CLA	ND
22	r	309	CLA	ND
22	r	310	CLA	ND
22	r	311	CLA	ND
22	r	312	CLA	ND
22	s	303	CLA	ND
22	s	304	CLA	ND
22	s	305	CLA	ND
22	s	309	CLA	ND
22	s	310	CLA	ND
22	s	311	CLA	ND
22	s	312	CLA	ND
22	s	313	CLA	ND
22	S	303	CLA	ND
22	S	304	CLA	ND
22	S	305	CLA	ND
22	S	309	CLA	ND
22	S	310	CLA	ND
22	S	311	CLA	ND
22	S	312	CLA	ND
22	S	313	CLA	ND
22	R	302	CLA	ND
22	R	303	CLA	ND
22	R	304	CLA	ND
22	R	308	CLA	ND
22	R	309	CLA	ND
22	R	310	CLA	ND
22	R	311	CLA	ND
24	g	617	XAT	C6
24	g	617	XAT	C25
24	n	615	XAT	C6
24	n	615	XAT	C25
24	y	615	XAT	C6
24	y	615	XAT	C25
24	G	617	XAT	C6
24	G	617	XAT	C25
24	G	617	XAT	C26
24	N	616	XAT	C6
24	N	616	XAT	C25
24	Y	615	XAT	C6
24	Y	615	XAT	C25
24	r	314	XAT	C25

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Mol	Chain	Res	Type	Atom
24	R	313	XAT	C25
25	g	618	NEX	C26
25	g	618	NEX	C25
25	n	616	NEX	C26
25	n	616	NEX	C25
25	y	616	NEX	C26
25	y	616	NEX	C25
25	y	618	NEX	C26
25	y	618	NEX	C25
25	N	617	NEX	C26
25	N	617	NEX	C25
25	Y	616	NEX	C26
25	Y	616	NEX	C25
25	r	315	NEX	C26
25	r	315	NEX	C25
33	d	402	SQD	C5
33	D	402	SQD	C5

All (4526) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	g	601	CHL	C1C-C2C-CMC-OMC
21	g	601	CHL	C3C-C2C-CMC-OMC
21	g	601	CHL	C4C-C3C-CAC-CBC
21	g	605	CHL	C1C-C2C-CMC-OMC
21	g	605	CHL	C3C-C2C-CMC-OMC
21	g	605	CHL	CBD-CGD-O2D-CED
21	g	605	CHL	O1D-CGD-O2D-CED
21	g	606	CHL	C2-C1-O2A-CGA
21	g	606	CHL	C1C-C2C-CMC-OMC
21	g	606	CHL	C3C-C2C-CMC-OMC
21	g	606	CHL	C4C-C3C-CAC-CBC
21	g	606	CHL	CBD-CGD-O2D-CED
21	g	607	CHL	C1A-C2A-CAA-CBA
21	g	607	CHL	C3A-C2A-CAA-CBA
21	g	607	CHL	C1C-C2C-CMC-OMC
21	g	607	CHL	C3C-C2C-CMC-OMC
21	g	607	CHL	C4C-C3C-CAC-CBC
21	g	607	CHL	CBD-CGD-O2D-CED
21	g	607	CHL	O1D-CGD-O2D-CED
21	g	608	CHL	C1C-C2C-CMC-OMC
21	g	608	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
21	g	609	CHL	CBA-CGA-O2A-C1
21	g	609	CHL	O1A-CGA-O2A-C1
21	g	609	CHL	C4C-C3C-CAC-CBC
21	n	601	CHL	C1C-C2C-CMC-OMC
21	n	601	CHL	C3C-C2C-CMC-OMC
21	n	601	CHL	C4C-C3C-CAC-CBC
21	n	605	CHL	C1C-C2C-CMC-OMC
21	n	605	CHL	C3C-C2C-CMC-OMC
21	n	605	CHL	C4C-C3C-CAC-CBC
21	n	605	CHL	CBD-CGD-O2D-CED
21	n	606	CHL	C1A-C2A-CAA-CBA
21	n	606	CHL	C3A-C2A-CAA-CBA
21	n	606	CHL	C1C-C2C-CMC-OMC
21	n	606	CHL	C3C-C2C-CMC-OMC
21	n	606	CHL	C4C-C3C-CAC-CBC
21	n	606	CHL	CBD-CGD-O2D-CED
21	n	607	CHL	C1C-C2C-CMC-OMC
21	n	607	CHL	C3C-C2C-CMC-OMC
21	n	608	CHL	CBA-CGA-O2A-C1
21	n	608	CHL	O1A-CGA-O2A-C1
21	n	608	CHL	C4C-C3C-CAC-CBC
21	y	601	CHL	C1C-C2C-CMC-OMC
21	y	601	CHL	C3C-C2C-CMC-OMC
21	y	601	CHL	C4C-C3C-CAC-CBC
21	y	605	CHL	CBA-CGA-O2A-C1
21	y	605	CHL	O1A-CGA-O2A-C1
21	y	605	CHL	C1C-C2C-CMC-OMC
21	y	605	CHL	C3C-C2C-CMC-OMC
21	y	605	CHL	CBD-CGD-O2D-CED
21	y	606	CHL	C1C-C2C-CMC-OMC
21	y	606	CHL	C3C-C2C-CMC-OMC
21	y	606	CHL	C4C-C3C-CAC-CBC
21	y	606	CHL	CBD-CGD-O2D-CED
21	y	607	CHL	C1A-C2A-CAA-CBA
21	y	607	CHL	C3A-C2A-CAA-CBA
21	y	607	CHL	C1C-C2C-CMC-OMC
21	y	607	CHL	C3C-C2C-CMC-OMC
21	y	607	CHL	C4C-C3C-CAC-CBC
21	y	607	CHL	CBD-CGD-O2D-CED
21	y	607	CHL	O1D-CGD-O2D-CED
21	y	608	CHL	C1C-C2C-CMC-OMC
21	y	608	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
21	y	609	CHL	CBA-CGA-O2A-C1
21	y	609	CHL	O1A-CGA-O2A-C1
21	y	609	CHL	C4C-C3C-CAC-CBC
21	G	601	CHL	C1C-C2C-CMC-OMC
21	G	601	CHL	C3C-C2C-CMC-OMC
21	G	601	CHL	C4C-C3C-CAC-CBC
21	G	605	CHL	C1C-C2C-CMC-OMC
21	G	605	CHL	C3C-C2C-CMC-OMC
21	G	605	CHL	CBD-CGD-O2D-CED
21	G	605	CHL	O1D-CGD-O2D-CED
21	G	606	CHL	C2-C1-O2A-CGA
21	G	606	CHL	C1C-C2C-CMC-OMC
21	G	606	CHL	C3C-C2C-CMC-OMC
21	G	606	CHL	C4C-C3C-CAC-CBC
21	G	606	CHL	CBD-CGD-O2D-CED
21	G	607	CHL	C1A-C2A-CAA-CBA
21	G	607	CHL	C3A-C2A-CAA-CBA
21	G	607	CHL	C1C-C2C-CMC-OMC
21	G	607	CHL	C3C-C2C-CMC-OMC
21	G	607	CHL	C4C-C3C-CAC-CBC
21	G	607	CHL	CBD-CGD-O2D-CED
21	G	607	CHL	O1D-CGD-O2D-CED
21	G	608	CHL	C1C-C2C-CMC-OMC
21	G	608	CHL	C3C-C2C-CMC-OMC
21	G	609	CHL	CBA-CGA-O2A-C1
21	G	609	CHL	O1A-CGA-O2A-C1
21	G	609	CHL	C4C-C3C-CAC-CBC
21	N	601	CHL	C1C-C2C-CMC-OMC
21	N	601	CHL	C3C-C2C-CMC-OMC
21	N	601	CHL	C4C-C3C-CAC-CBC
21	N	605	CHL	C1C-C2C-CMC-OMC
21	N	605	CHL	C3C-C2C-CMC-OMC
21	N	605	CHL	C4C-C3C-CAC-CBC
21	N	605	CHL	CBD-CGD-O2D-CED
21	N	606	CHL	C1A-C2A-CAA-CBA
21	N	606	CHL	C3A-C2A-CAA-CBA
21	N	606	CHL	C1C-C2C-CMC-OMC
21	N	606	CHL	C3C-C2C-CMC-OMC
21	N	606	CHL	C4C-C3C-CAC-CBC
21	N	606	CHL	CBD-CGD-O2D-CED
21	N	606	CHL	O1D-CGD-O2D-CED
21	N	607	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
21	N	607	CHL	C3C-C2C-CMC-OMC
21	N	608	CHL	CBA-CGA-O2A-C1
21	N	608	CHL	O1A-CGA-O2A-C1
21	N	608	CHL	C4C-C3C-CAC-CBC
21	Y	601	CHL	C1C-C2C-CMC-OMC
21	Y	601	CHL	C3C-C2C-CMC-OMC
21	Y	601	CHL	C4C-C3C-CAC-CBC
21	Y	605	CHL	C2-C1-O2A-CGA
21	Y	605	CHL	C1C-C2C-CMC-OMC
21	Y	605	CHL	C3C-C2C-CMC-OMC
21	Y	605	CHL	C4C-C3C-CAC-CBC
21	Y	605	CHL	CBD-CGD-O2D-CED
21	Y	606	CHL	C1A-C2A-CAA-CBA
21	Y	606	CHL	C3A-C2A-CAA-CBA
21	Y	606	CHL	C1C-C2C-CMC-OMC
21	Y	606	CHL	C3C-C2C-CMC-OMC
21	Y	606	CHL	C4C-C3C-CAC-CBC
21	Y	606	CHL	CBD-CGD-O2D-CED
21	Y	606	CHL	O1D-CGD-O2D-CED
21	Y	607	CHL	C1C-C2C-CMC-OMC
21	Y	607	CHL	C3C-C2C-CMC-OMC
21	Y	608	CHL	CBA-CGA-O2A-C1
21	Y	608	CHL	O1A-CGA-O2A-C1
21	Y	608	CHL	C4C-C3C-CAC-CBC
21	r	301	CHL	C1C-C2C-CMC-OMC
21	r	301	CHL	C3C-C2C-CMC-OMC
21	r	301	CHL	CBD-CGD-O2D-CED
21	r	306	CHL	C1A-C2A-CAA-CBA
21	r	306	CHL	CBD-CGD-O2D-CED
21	r	306	CHL	O1D-CGD-O2D-CED
21	r	307	CHL	C1A-C2A-CAA-CBA
21	r	307	CHL	CBA-CGA-O2A-C1
21	r	307	CHL	O1A-CGA-O2A-C1
21	r	307	CHL	CBD-CGD-O2D-CED
21	r	307	CHL	O1D-CGD-O2D-CED
21	r	308	CHL	C1C-C2C-CMC-OMC
21	r	308	CHL	C3C-C2C-CMC-OMC
21	r	308	CHL	C4C-C3C-CAC-CBC
21	r	308	CHL	CHA-CBD-CGD-O1D
21	r	308	CHL	CHA-CBD-CGD-O2D
21	r	308	CHL	CBD-CGD-O2D-CED
21	r	308	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	s	301	CHL	C3A-C2A-CAA-CBA
21	s	301	CHL	C1C-C2C-CMC-OMC
21	s	301	CHL	C3C-C2C-CMC-OMC
21	s	301	CHL	CBD-CGD-O2D-CED
21	s	301	CHL	O1D-CGD-O2D-CED
21	s	302	CHL	C4C-C3C-CAC-CBC
21	s	306	CHL	C1C-C2C-CMC-OMC
21	s	306	CHL	C3C-C2C-CMC-OMC
21	s	306	CHL	C4C-C3C-CAC-CBC
21	s	307	CHL	C1C-C2C-CMC-OMC
21	s	307	CHL	C3C-C2C-CMC-OMC
21	s	307	CHL	C4C-C3C-CAC-CBC
21	S	301	CHL	C1C-C2C-CMC-OMC
21	S	301	CHL	C3C-C2C-CMC-OMC
21	S	301	CHL	CBD-CGD-O2D-CED
21	S	302	CHL	C4C-C3C-CAC-CBC
21	S	306	CHL	C1C-C2C-CMC-OMC
21	S	306	CHL	C3C-C2C-CMC-OMC
21	S	306	CHL	C4C-C3C-CAC-CBC
21	S	307	CHL	C1A-C2A-CAA-CBA
21	S	307	CHL	C1C-C2C-CMC-OMC
21	S	307	CHL	C3C-C2C-CMC-OMC
21	S	307	CHL	C4C-C3C-CAC-CBC
21	R	305	CHL	C1A-C2A-CAA-CBA
21	R	305	CHL	CBD-CGD-O2D-CED
21	R	305	CHL	O1D-CGD-O2D-CED
21	R	306	CHL	C1A-C2A-CAA-CBA
21	R	306	CHL	CBA-CGA-O2A-C1
21	R	306	CHL	O1A-CGA-O2A-C1
21	R	306	CHL	CBD-CGD-O2D-CED
21	R	306	CHL	O1D-CGD-O2D-CED
21	R	307	CHL	C1C-C2C-CMC-OMC
21	R	307	CHL	C3C-C2C-CMC-OMC
21	R	307	CHL	C4C-C3C-CAC-CBC
21	R	307	CHL	CHA-CBD-CGD-O1D
21	R	307	CHL	CHA-CBD-CGD-O2D
21	R	307	CHL	CBD-CGD-O2D-CED
21	R	307	CHL	O1D-CGD-O2D-CED
22	g	602	CLA	C1A-C2A-CAA-CBA
22	g	602	CLA	C3A-C2A-CAA-CBA
22	g	603	CLA	CHA-CBD-CGD-O1D
22	g	603	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	g	610	CLA	C1A-C2A-CAA-CBA
22	g	613	CLA	C1A-C2A-CAA-CBA
22	g	614	CLA	C1A-C2A-CAA-CBA
22	g	614	CLA	C3A-C2A-CAA-CBA
22	n	602	CLA	C1A-C2A-CAA-CBA
22	n	602	CLA	C3A-C2A-CAA-CBA
22	n	603	CLA	CHA-CBD-CGD-O1D
22	n	603	CLA	CHA-CBD-CGD-O2D
22	n	609	CLA	C1A-C2A-CAA-CBA
22	n	612	CLA	C1A-C2A-CAA-CBA
22	n	613	CLA	C1A-C2A-CAA-CBA
22	n	613	CLA	C3A-C2A-CAA-CBA
22	y	602	CLA	C1A-C2A-CAA-CBA
22	y	602	CLA	C3A-C2A-CAA-CBA
22	y	603	CLA	CHA-CBD-CGD-O1D
22	y	603	CLA	CHA-CBD-CGD-O2D
22	y	610	CLA	C1A-C2A-CAA-CBA
22	y	612	CLA	C1A-C2A-CAA-CBA
22	y	613	CLA	C1A-C2A-CAA-CBA
22	y	613	CLA	C3A-C2A-CAA-CBA
22	G	602	CLA	C1A-C2A-CAA-CBA
22	G	602	CLA	C3A-C2A-CAA-CBA
22	G	603	CLA	CHA-CBD-CGD-O1D
22	G	603	CLA	CHA-CBD-CGD-O2D
22	G	610	CLA	C1A-C2A-CAA-CBA
22	G	613	CLA	C1A-C2A-CAA-CBA
22	G	614	CLA	C1A-C2A-CAA-CBA
22	G	614	CLA	C3A-C2A-CAA-CBA
22	N	602	CLA	C1A-C2A-CAA-CBA
22	N	602	CLA	C3A-C2A-CAA-CBA
22	N	603	CLA	CHA-CBD-CGD-O1D
22	N	603	CLA	CHA-CBD-CGD-O2D
22	N	609	CLA	C1A-C2A-CAA-CBA
22	N	612	CLA	C1A-C2A-CAA-CBA
22	N	613	CLA	C1A-C2A-CAA-CBA
22	N	613	CLA	C3A-C2A-CAA-CBA
22	Y	602	CLA	C1A-C2A-CAA-CBA
22	Y	602	CLA	C3A-C2A-CAA-CBA
22	Y	603	CLA	CHA-CBD-CGD-O1D
22	Y	603	CLA	CHA-CBD-CGD-O2D
22	Y	609	CLA	C1A-C2A-CAA-CBA
22	Y	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	Y	612	CLA	C1A-C2A-CAA-CBA
22	Y	612	CLA	C3A-C2A-CAA-CBA
22	a	406	CLA	C1A-C2A-CAA-CBA
22	a	406	CLA	C3A-C2A-CAA-CBA
22	b	603	CLA	CBD-CGD-O2D-CED
22	b	608	CLA	CHA-CBD-CGD-O1D
22	b	608	CLA	CHA-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O1D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	b	611	CLA	C1A-C2A-CAA-CBA
22	b	611	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	CHA-CBD-CGD-O1D
22	b	611	CLA	CHA-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CBD-CGD-O2D-CED
22	c	504	CLA	C1A-C2A-CAA-CBA
22	c	504	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O2D
22	c	504	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	O1A-CGA-O2A-C1
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	C1A-C2A-CAA-CBA
22	c	509	CLA	C3A-C2A-CAA-CBA
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	C1A-C2A-CAA-CBA
22	c	510	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
22	c	513	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	C14-C13-C15-C16
22	c	514	CLA	C1A-C2A-CAA-CBA
22	c	514	CLA	CAD-CBD-CGD-O1D
22	c	514	CLA	CAD-CBD-CGD-O2D
22	d	403	CLA	CHA-CBD-CGD-O1D
22	d	403	CLA	CHA-CBD-CGD-O2D
22	A	407	CLA	C1A-C2A-CAA-CBA
22	A	407	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	CBD-CGD-O2D-CED
22	B	611	CLA	CHA-CBD-CGD-O1D
22	B	611	CLA	CHA-CBD-CGD-O2D
22	B	612	CLA	CAD-CBD-CGD-O1D
22	B	612	CLA	CAD-CBD-CGD-O2D
22	B	614	CLA	C1A-C2A-CAA-CBA
22	B	614	CLA	C3A-C2A-CAA-CBA
22	B	614	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	C1A-C2A-CAA-CBA
22	C	505	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CBD-CGD-O2D-CED
22	C	506	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	O1A-CGA-O2A-C1
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CBD-CGD-O2D-CED
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	C1A-C2A-CAA-CBA
22	C	510	CLA	C3A-C2A-CAA-CBA
22	C	510	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	C	511	CLA	C1A-C2A-CAA-CBA
22	C	511	CLA	C3A-C2A-CAA-CBA
22	C	513	CLA	C3A-C2A-CAA-CBA
22	C	514	CLA	CBD-CGD-O2D-CED
22	C	514	CLA	C14-C13-C15-C16
22	C	515	CLA	C1A-C2A-CAA-CBA
22	C	515	CLA	CAD-CBD-CGD-O1D
22	C	515	CLA	CAD-CBD-CGD-O2D
22	D	404	CLA	CHA-CBD-CGD-O1D
22	D	404	CLA	CHA-CBD-CGD-O2D
22	r	303	CLA	C2B-C3B-CAB-CBB
22	r	303	CLA	C4B-C3B-CAB-CBB
22	r	304	CLA	CHA-CBD-CGD-O1D
22	r	304	CLA	CHA-CBD-CGD-O2D
22	r	305	CLA	CBA-CGA-O2A-C1
22	r	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	r	309	CLA	C3A-C2A-CAA-CBA
22	r	309	CLA	C4B-C3B-CAB-CBB
22	r	309	CLA	CBD-CGD-O2D-CED
22	r	310	CLA	C3A-C2A-CAA-CBA
22	r	311	CLA	C1A-C2A-CAA-CBA
22	r	311	CLA	C3A-C2A-CAA-CBA
22	r	311	CLA	CHA-CBD-CGD-O1D
22	r	311	CLA	CHA-CBD-CGD-O2D
22	r	311	CLA	CBD-CGD-O2D-CED
22	s	303	CLA	C1A-C2A-CAA-CBA
22	s	305	CLA	C1A-C2A-CAA-CBA
22	s	305	CLA	C3A-C2A-CAA-CBA
22	s	308	CLA	CAD-CBD-CGD-O1D
22	s	308	CLA	CAD-CBD-CGD-O2D
22	s	310	CLA	CAD-CBD-CGD-O1D
22	s	310	CLA	CAD-CBD-CGD-O2D
22	s	310	CLA	CBD-CGD-O2D-CED
22	s	312	CLA	C2B-C3B-CAB-CBB
22	s	312	CLA	C4B-C3B-CAB-CBB
22	s	312	CLA	CBD-CGD-O2D-CED
22	s	313	CLA	C3A-C2A-CAA-CBA
22	S	303	CLA	C1A-C2A-CAA-CBA
22	S	305	CLA	C1A-C2A-CAA-CBA
22	S	305	CLA	C3A-C2A-CAA-CBA
22	S	308	CLA	CAD-CBD-CGD-O1D
22	S	308	CLA	CAD-CBD-CGD-O2D
22	S	310	CLA	CAD-CBD-CGD-O1D
22	S	310	CLA	CAD-CBD-CGD-O2D
22	S	310	CLA	CBD-CGD-O2D-CED
22	S	312	CLA	C2B-C3B-CAB-CBB
22	S	312	CLA	C4B-C3B-CAB-CBB
22	S	312	CLA	CBD-CGD-O2D-CED
22	S	313	CLA	C3A-C2A-CAA-CBA
22	R	302	CLA	C2B-C3B-CAB-CBB
22	R	302	CLA	C4B-C3B-CAB-CBB
22	R	303	CLA	CHA-CBD-CGD-O1D
22	R	303	CLA	CHA-CBD-CGD-O2D
22	R	304	CLA	CBA-CGA-O2A-C1
22	R	308	CLA	C1A-C2A-CAA-CBA
22	R	308	CLA	C3A-C2A-CAA-CBA
22	R	308	CLA	C4B-C3B-CAB-CBB
22	R	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	R	309	CLA	C3A-C2A-CAA-CBA
22	R	310	CLA	C1A-C2A-CAA-CBA
22	R	310	CLA	C3A-C2A-CAA-CBA
22	R	310	CLA	CHA-CBD-CGD-O1D
22	R	310	CLA	CHA-CBD-CGD-O2D
22	R	310	CLA	CBD-CGD-O2D-CED
23	g	615	LUT	C11-C10-C9-C8
23	g	615	LUT	C11-C10-C9-C19
23	g	615	LUT	C11-C12-C13-C20
23	g	615	LUT	C12-C13-C14-C15
23	g	615	LUT	C20-C13-C14-C15
23	g	615	LUT	C27-C28-C29-C39
23	g	615	LUT	C39-C29-C30-C31
23	g	615	LUT	C32-C33-C34-C35
23	g	615	LUT	C40-C33-C34-C35
23	g	616	LUT	C5-C6-C7-C8
23	g	616	LUT	C7-C8-C9-C19
23	g	616	LUT	C11-C10-C9-C8
23	g	616	LUT	C11-C12-C13-C14
23	g	616	LUT	C20-C13-C14-C15
23	g	616	LUT	C39-C29-C30-C31
23	g	616	LUT	C31-C32-C33-C34
23	g	616	LUT	C32-C33-C34-C35
23	g	616	LUT	C40-C33-C34-C35
23	n	614	LUT	C11-C10-C9-C8
23	n	614	LUT	C11-C10-C9-C19
23	n	614	LUT	C11-C12-C13-C20
23	n	614	LUT	C12-C13-C14-C15
23	n	614	LUT	C20-C13-C14-C15
23	n	614	LUT	C27-C28-C29-C39
23	n	614	LUT	C39-C29-C30-C31
23	n	614	LUT	C32-C33-C34-C35
23	n	614	LUT	C40-C33-C34-C35
23	y	614	LUT	C11-C10-C9-C8
23	y	614	LUT	C11-C10-C9-C19
23	y	614	LUT	C11-C12-C13-C20
23	y	614	LUT	C12-C13-C14-C15
23	y	614	LUT	C20-C13-C14-C15
23	y	614	LUT	C27-C28-C29-C39
23	y	614	LUT	C39-C29-C30-C31
23	y	614	LUT	C32-C33-C34-C35
23	y	614	LUT	C40-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	G	615	LUT	C11-C10-C9-C8
23	G	615	LUT	C11-C10-C9-C19
23	G	615	LUT	C11-C12-C13-C20
23	G	615	LUT	C12-C13-C14-C15
23	G	615	LUT	C20-C13-C14-C15
23	G	615	LUT	C27-C28-C29-C39
23	G	615	LUT	C39-C29-C30-C31
23	G	615	LUT	C32-C33-C34-C35
23	G	615	LUT	C40-C33-C34-C35
23	G	616	LUT	C5-C6-C7-C8
23	G	616	LUT	C7-C8-C9-C19
23	G	616	LUT	C11-C10-C9-C8
23	G	616	LUT	C11-C12-C13-C14
23	G	616	LUT	C20-C13-C14-C15
23	G	616	LUT	C39-C29-C30-C31
23	G	616	LUT	C31-C32-C33-C34
23	G	616	LUT	C32-C33-C34-C35
23	G	616	LUT	C40-C33-C34-C35
23	N	614	LUT	C11-C10-C9-C8
23	N	614	LUT	C11-C10-C9-C19
23	N	614	LUT	C11-C12-C13-C20
23	N	614	LUT	C12-C13-C14-C15
23	N	614	LUT	C20-C13-C14-C15
23	N	614	LUT	C27-C28-C29-C39
23	N	614	LUT	C39-C29-C30-C31
23	N	614	LUT	C32-C33-C34-C35
23	N	614	LUT	C40-C33-C34-C35
23	N	615	LUT	C11-C12-C13-C14
23	N	615	LUT	C11-C12-C13-C20
23	N	615	LUT	C20-C13-C14-C15
23	N	615	LUT	C27-C28-C29-C39
23	N	615	LUT	C39-C29-C30-C31
23	N	615	LUT	C31-C32-C33-C40
23	N	615	LUT	C40-C33-C34-C35
23	Y	613	LUT	C11-C10-C9-C8
23	Y	613	LUT	C11-C10-C9-C19
23	Y	613	LUT	C11-C12-C13-C20
23	Y	613	LUT	C12-C13-C14-C15
23	Y	613	LUT	C20-C13-C14-C15
23	Y	613	LUT	C27-C28-C29-C39
23	Y	613	LUT	C39-C29-C30-C31
23	Y	613	LUT	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	Y	613	LUT	C40-C33-C34-C35
23	Y	614	LUT	C5-C6-C7-C8
23	Y	614	LUT	C7-C8-C9-C19
23	Y	614	LUT	C11-C10-C9-C8
23	Y	614	LUT	C11-C12-C13-C14
23	Y	614	LUT	C11-C12-C13-C20
23	Y	614	LUT	C20-C13-C14-C15
23	Y	614	LUT	C39-C29-C30-C31
23	Y	614	LUT	C31-C32-C33-C34
23	Y	614	LUT	C32-C33-C34-C35
23	Y	614	LUT	C40-C33-C34-C35
23	r	313	LUT	C5-C6-C7-C8
23	r	313	LUT	C11-C10-C9-C8
23	r	313	LUT	C11-C10-C9-C19
23	r	313	LUT	C11-C12-C13-C14
23	r	313	LUT	C20-C13-C14-C15
23	r	313	LUT	C28-C29-C30-C31
23	r	313	LUT	C32-C33-C34-C35
23	r	313	LUT	C40-C33-C34-C35
23	R	312	LUT	C5-C6-C7-C8
23	R	312	LUT	C11-C10-C9-C8
23	R	312	LUT	C11-C10-C9-C19
23	R	312	LUT	C11-C12-C13-C14
23	R	312	LUT	C20-C13-C14-C15
23	R	312	LUT	C28-C29-C30-C31
23	R	312	LUT	C32-C33-C34-C35
23	R	312	LUT	C40-C33-C34-C35
24	g	617	XAT	C7-C8-C9-C19
24	g	617	XAT	C11-C10-C9-C19
24	g	617	XAT	C27-C28-C29-C30
24	g	617	XAT	C27-C28-C29-C39
24	g	617	XAT	C28-C29-C30-C31
24	g	617	XAT	C39-C29-C30-C31
24	g	617	XAT	C31-C32-C33-C40
24	n	615	XAT	C7-C8-C9-C19
24	n	615	XAT	C11-C10-C9-C19
24	n	615	XAT	C11-C12-C13-C14
24	n	615	XAT	C11-C12-C13-C20
24	n	615	XAT	C20-C13-C14-C15
24	n	615	XAT	C27-C28-C29-C30
24	n	615	XAT	C27-C28-C29-C39
24	n	615	XAT	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
24	n	615	XAT	C39-C29-C30-C31
24	n	615	XAT	C40-C33-C34-C35
24	y	615	XAT	C11-C10-C9-C19
24	y	615	XAT	C11-C12-C13-C20
24	y	615	XAT	C20-C13-C14-C15
24	y	615	XAT	C27-C28-C29-C30
24	y	615	XAT	C27-C28-C29-C39
24	y	615	XAT	C28-C29-C30-C31
24	y	615	XAT	C39-C29-C30-C31
24	y	615	XAT	C32-C33-C34-C35
24	G	617	XAT	C7-C8-C9-C19
24	G	617	XAT	C11-C10-C9-C19
24	G	617	XAT	C20-C13-C14-C15
24	G	617	XAT	C27-C28-C29-C30
24	G	617	XAT	C27-C28-C29-C39
24	G	617	XAT	C28-C29-C30-C31
24	G	617	XAT	C39-C29-C30-C31
24	G	617	XAT	C32-C33-C34-C35
24	N	616	XAT	C7-C8-C9-C19
24	N	616	XAT	C11-C10-C9-C19
24	N	616	XAT	C11-C12-C13-C14
24	N	616	XAT	C11-C12-C13-C20
24	N	616	XAT	C20-C13-C14-C15
24	N	616	XAT	C27-C28-C29-C30
24	N	616	XAT	C27-C28-C29-C39
24	N	616	XAT	C28-C29-C30-C31
24	N	616	XAT	C39-C29-C30-C31
24	N	616	XAT	C40-C33-C34-C35
24	Y	615	XAT	C11-C10-C9-C19
24	Y	615	XAT	C11-C12-C13-C14
24	Y	615	XAT	C11-C12-C13-C20
24	Y	615	XAT	C27-C28-C29-C30
24	Y	615	XAT	C27-C28-C29-C39
24	Y	615	XAT	C28-C29-C30-C31
24	Y	615	XAT	C39-C29-C30-C31
24	Y	615	XAT	C32-C33-C34-C35
24	r	314	XAT	C7-C8-C9-C10
24	r	314	XAT	C7-C8-C9-C19
24	r	314	XAT	C11-C10-C9-C8
24	r	314	XAT	C12-C13-C14-C15
24	r	314	XAT	C20-C13-C14-C15
24	r	314	XAT	C40-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
24	R	313	XAT	C7-C8-C9-C10
24	R	313	XAT	C7-C8-C9-C19
24	R	313	XAT	C11-C10-C9-C8
24	R	313	XAT	C12-C13-C14-C15
24	R	313	XAT	C20-C13-C14-C15
24	R	313	XAT	C40-C33-C34-C35
25	g	618	NEX	C7-C8-C9-C10
25	g	618	NEX	C11-C10-C9-C8
25	g	618	NEX	C11-C12-C13-C20
25	g	618	NEX	C20-C13-C14-C15
25	g	618	NEX	C21-C26-C27-C28
25	g	618	NEX	C28-C29-C30-C31
25	g	618	NEX	C39-C29-C30-C31
25	g	618	NEX	C31-C32-C33-C40
25	g	618	NEX	C40-C33-C34-C35
25	n	616	NEX	C7-C8-C9-C19
25	n	616	NEX	C11-C10-C9-C19
25	n	616	NEX	C11-C12-C13-C14
25	n	616	NEX	C20-C13-C14-C15
25	n	616	NEX	C21-C26-C27-C28
25	n	616	NEX	C28-C29-C30-C31
25	n	616	NEX	C39-C29-C30-C31
25	n	616	NEX	C40-C33-C34-C35
25	y	616	NEX	C11-C10-C9-C8
25	y	616	NEX	C11-C12-C13-C14
25	y	616	NEX	C20-C13-C14-C15
25	y	616	NEX	C21-C26-C27-C28
25	y	616	NEX	C28-C29-C30-C31
25	y	616	NEX	C39-C29-C30-C31
25	y	616	NEX	C31-C32-C33-C34
25	y	616	NEX	C31-C32-C33-C40
25	y	618	NEX	C11-C10-C9-C8
25	y	618	NEX	C11-C10-C9-C19
25	y	618	NEX	C11-C12-C13-C14
25	y	618	NEX	C20-C13-C14-C15
25	y	618	NEX	C27-C28-C29-C30
25	y	618	NEX	C28-C29-C30-C31
25	y	618	NEX	C39-C29-C30-C31
25	N	617	NEX	C7-C8-C9-C19
25	N	617	NEX	C11-C12-C13-C20
25	N	617	NEX	C20-C13-C14-C15
25	N	617	NEX	C21-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
25	N	617	NEX	C28-C29-C30-C31
25	N	617	NEX	C39-C29-C30-C31
25	N	617	NEX	C31-C32-C33-C34
25	N	617	NEX	C31-C32-C33-C40
25	N	617	NEX	C32-C33-C34-C35
25	Y	616	NEX	C7-C8-C9-C10
25	Y	616	NEX	C11-C10-C9-C8
25	Y	616	NEX	C11-C12-C13-C20
25	Y	616	NEX	C20-C13-C14-C15
25	Y	616	NEX	C27-C28-C29-C30
25	Y	616	NEX	C28-C29-C30-C31
25	Y	616	NEX	C31-C32-C33-C34
25	Y	616	NEX	C31-C32-C33-C40
25	Y	616	NEX	C32-C33-C34-C35
25	r	315	NEX	C11-C10-C9-C8
25	r	315	NEX	C11-C10-C9-C19
25	r	315	NEX	C11-C12-C13-C14
25	r	315	NEX	C20-C13-C14-C15
25	r	315	NEX	C27-C28-C29-C30
25	r	315	NEX	C28-C29-C30-C31
25	r	315	NEX	C39-C29-C30-C31
26	g	619	LHG	O1-C1-C2-C3
26	g	619	LHG	O2-C2-C3-O3
26	g	619	LHG	C3-O3-P-O4
26	g	619	LHG	C3-O3-P-O6
26	n	617	LHG	O1-C1-C2-C3
26	n	617	LHG	C1-C2-C3-O3
26	n	617	LHG	O2-C2-C3-O3
26	n	617	LHG	C3-O3-P-O4
26	n	617	LHG	C3-O3-P-O6
26	y	617	LHG	O2-C2-C3-O3
26	y	617	LHG	C3-O3-P-O5
26	y	617	LHG	C3-O3-P-O6
26	G	618	LHG	O1-C1-C2-O2
26	G	618	LHG	C3-O3-P-O6
26	G	618	LHG	C4-O6-P-O3
26	G	618	LHG	C4-O6-P-O5
26	N	618	LHG	O1-C1-C2-C3
26	N	618	LHG	O2-C2-C3-O3
26	N	618	LHG	C3-O3-P-O4
26	N	618	LHG	C3-O3-P-O6
26	Y	617	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
26	Y	617	LHG	C4-O6-P-O3
26	Y	617	LHG	C4-O6-P-O4
26	Y	617	LHG	O7-C5-C6-O8
26	b	619	LHG	C3-O3-P-O5
26	b	619	LHG	C4-O6-P-O4
26	b	619	LHG	C4-O6-P-O5
26	c	520	LHG	C3-O3-P-O5
26	c	520	LHG	C4-O6-P-O3
26	c	520	LHG	C8-C7-O7-C5
26	c	521	LHG	C3-O3-P-O5
26	c	521	LHG	C3-O3-P-O6
26	c	521	LHG	C4-O6-P-O5
26	c	522	LHG	O1-C1-C2-C3
26	c	522	LHG	C3-O3-P-O4
26	d	407	LHG	C3-O3-P-O5
26	d	407	LHG	C4-O6-P-O3
26	d	407	LHG	C4-O6-P-O4
26	d	408	LHG	O1-C1-C2-C3
26	d	408	LHG	C3-O3-P-O4
26	d	408	LHG	C4-O6-P-O3
26	d	408	LHG	C4-O6-P-O5
26	d	409	LHG	C3-O3-P-O4
26	d	409	LHG	C3-O3-P-O5
26	d	409	LHG	C4-O6-P-O5
26	l	102	LHG	O1-C1-C2-C3
26	l	102	LHG	C3-O3-P-O4
26	B	622	LHG	C3-O3-P-O5
26	B	622	LHG	C4-O6-P-O4
26	B	622	LHG	C4-O6-P-O5
26	C	520	LHG	C3-O3-P-O5
26	C	520	LHG	C4-O6-P-O3
26	C	520	LHG	C8-C7-O7-C5
26	C	521	LHG	C3-O3-P-O5
26	C	521	LHG	C3-O3-P-O6
26	C	521	LHG	C4-O6-P-O5
26	C	522	LHG	O1-C1-C2-C3
26	C	522	LHG	C3-O3-P-O4
26	D	408	LHG	C3-O3-P-O5
26	D	408	LHG	C4-O6-P-O3
26	D	408	LHG	C4-O6-P-O4
26	D	409	LHG	O1-C1-C2-C3
26	D	409	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
26	D	409	LHG	C4-O6-P-O3
26	D	409	LHG	C4-O6-P-O5
26	D	410	LHG	C3-O3-P-O4
26	D	410	LHG	C3-O3-P-O5
26	D	410	LHG	C4-O6-P-O5
26	L	103	LHG	O1-C1-C2-C3
26	L	103	LHG	C3-O3-P-O4
26	r	302	LHG	O1-C1-C2-C3
26	r	302	LHG	C3-O3-P-O4
26	s	314	LHG	C4-O6-P-O5
26	S	314	LHG	C4-O6-P-O5
26	R	301	LHG	O1-C1-C2-C3
26	R	301	LHG	C3-O3-P-O4
30	d	401	PHO	CBD-CGD-O2D-CED
30	D	401	PHO	CBD-CGD-O2D-CED
31	b	617	BCR	C7-C8-C9-C10
31	d	405	BCR	C6-C7-C8-C9
31	h	101	BCR	C6-C7-C8-C9
31	h	101	BCR	C7-C8-C9-C10
31	h	101	BCR	C7-C8-C9-C34
31	k	101	BCR	C18-C19-C20-C21
31	k	101	BCR	C37-C22-C23-C24
31	k	101	BCR	C22-C23-C24-C25
31	B	602	BCR	C9-C10-C11-C12
31	B	602	BCR	C11-C12-C13-C14
31	B	602	BCR	C16-C17-C18-C36
31	B	602	BCR	C21-C22-C23-C24
31	B	620	BCR	C7-C8-C9-C10
31	D	406	BCR	C6-C7-C8-C9
31	H	101	BCR	C6-C7-C8-C9
31	H	101	BCR	C7-C8-C9-C10
31	H	101	BCR	C7-C8-C9-C34
31	K	101	BCR	C18-C19-C20-C21
31	K	101	BCR	C37-C22-C23-C24
31	K	101	BCR	C22-C23-C24-C25
31	T	102	BCR	C9-C10-C11-C12
31	T	102	BCR	C11-C12-C13-C14
31	T	102	BCR	C16-C17-C18-C36
31	T	102	BCR	C21-C22-C23-C24
32	d	406	PL9	C12-C13-C14-C15
32	d	406	PL9	C18-C19-C21-C22
32	d	406	PL9	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	D	407	PL9	C12-C13-C14-C15
32	D	407	PL9	C18-C19-C21-C22
32	D	407	PL9	C27-C28-C29-C30
33	a	411	SQD	O5-C1-O6-C44
33	a	411	SQD	C8-C7-O47-C45
33	a	411	SQD	C5-C6-S-O8
33	a	411	SQD	C5-C6-S-O9
33	d	402	SQD	C5-C6-S-O7
33	d	402	SQD	C5-C6-S-O8
33	l	101	SQD	O49-C7-O47-C45
33	l	101	SQD	C8-C7-O47-C45
33	l	103	SQD	C2-C1-O6-C44
33	l	103	SQD	O5-C1-O6-C44
33	l	103	SQD	O49-C7-O47-C45
33	A	412	SQD	O5-C1-O6-C44
33	A	412	SQD	C8-C7-O47-C45
33	A	412	SQD	C5-C6-S-O8
33	A	412	SQD	C5-C6-S-O9
33	D	402	SQD	C5-C6-S-O7
33	D	402	SQD	C5-C6-S-O8
33	L	101	SQD	C2-C1-O6-C44
33	L	101	SQD	O5-C1-O6-C44
33	L	101	SQD	O49-C7-O47-C45
33	L	102	SQD	O49-C7-O47-C45
33	L	102	SQD	C8-C7-O47-C45
35	c	518	DGD	O1G-C1G-C2G-O2G
35	c	518	DGD	O6E-C1E-O5D-C6D
35	c	519	DGD	C2D-C1D-O3G-C3G
35	c	519	DGD	O6D-C1D-O3G-C3G
35	C	519	DGD	O1G-C1G-C2G-O2G
35	C	519	DGD	O6E-C1E-O5D-C6D
35	J	101	DGD	C2D-C1D-O3G-C3G
35	J	101	DGD	O6D-C1D-O3G-C3G
36	c	523	LMG	O7-C8-C9-O8
36	c	523	LMG	O9-C10-O7-C8
36	c	523	LMG	C11-C10-O7-C8
36	B	601	LMG	O6-C1-O1-C7
36	C	523	LMG	O7-C8-C9-O8
36	C	523	LMG	O9-C10-O7-C8
36	C	523	LMG	C11-C10-O7-C8
36	I	101	LMG	O6-C1-O1-C7
37	f	101	HEM	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	F	101	HEM	C1A-C2A-CAA-CBA
21	n	606	CHL	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
22	b	611	CLA	O1D-CGD-O2D-CED
22	b	615	CLA	O1D-CGD-O2D-CED
22	c	505	CLA	O1D-CGD-O2D-CED
22	c	513	CLA	O1D-CGD-O2D-CED
22	B	611	CLA	O1D-CGD-O2D-CED
22	B	614	CLA	O1D-CGD-O2D-CED
22	B	618	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	O1D-CGD-O2D-CED
22	C	514	CLA	O1D-CGD-O2D-CED
22	r	309	CLA	O1D-CGD-O2D-CED
22	R	308	CLA	O1D-CGD-O2D-CED
21	g	601	CHL	C2C-C3C-CAC-CBC
21	n	601	CHL	C2C-C3C-CAC-CBC
21	y	601	CHL	C2C-C3C-CAC-CBC
21	G	601	CHL	C2C-C3C-CAC-CBC
21	N	601	CHL	C2C-C3C-CAC-CBC
21	Y	601	CHL	C2C-C3C-CAC-CBC
21	g	609	CHL	O1D-CGD-O2D-CED
21	n	608	CHL	O1D-CGD-O2D-CED
21	y	609	CHL	O1D-CGD-O2D-CED
21	G	609	CHL	O1D-CGD-O2D-CED
21	N	608	CHL	O1D-CGD-O2D-CED
21	Y	608	CHL	O1D-CGD-O2D-CED
22	g	604	CLA	O1D-CGD-O2D-CED
22	n	604	CLA	O1D-CGD-O2D-CED
22	y	604	CLA	O1D-CGD-O2D-CED
22	G	604	CLA	O1D-CGD-O2D-CED
22	N	604	CLA	O1D-CGD-O2D-CED
22	Y	604	CLA	O1D-CGD-O2D-CED
22	c	503	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	O1D-CGD-O2D-CED
22	r	303	CLA	O1D-CGD-O2D-CED
22	s	308	CLA	O1D-CGD-O2D-CED
22	S	308	CLA	O1D-CGD-O2D-CED
22	R	302	CLA	O1D-CGD-O2D-CED
21	g	608	CHL	CBD-CGD-O2D-CED
21	g	609	CHL	CBD-CGD-O2D-CED
21	n	607	CHL	CBD-CGD-O2D-CED
21	n	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	y	608	CHL	CBD-CGD-O2D-CED
21	y	609	CHL	CBD-CGD-O2D-CED
21	G	608	CHL	CBD-CGD-O2D-CED
21	G	609	CHL	CBD-CGD-O2D-CED
21	N	607	CHL	CBD-CGD-O2D-CED
21	N	608	CHL	CBD-CGD-O2D-CED
21	Y	607	CHL	CBD-CGD-O2D-CED
21	Y	608	CHL	CBD-CGD-O2D-CED
21	s	307	CHL	CBD-CGD-O2D-CED
21	S	307	CHL	CBD-CGD-O2D-CED
22	g	604	CLA	CBD-CGD-O2D-CED
22	g	610	CLA	CBD-CGD-O2D-CED
22	g	612	CLA	CBD-CGD-O2D-CED
22	g	613	CLA	CBD-CGD-O2D-CED
22	n	604	CLA	CBD-CGD-O2D-CED
22	n	609	CLA	CBD-CGD-O2D-CED
22	n	611	CLA	CBD-CGD-O2D-CED
22	n	612	CLA	CBD-CGD-O2D-CED
22	y	604	CLA	CBD-CGD-O2D-CED
22	y	610	CLA	CBD-CGD-O2D-CED
22	y	612	CLA	CBD-CGD-O2D-CED
22	G	604	CLA	CBD-CGD-O2D-CED
22	G	610	CLA	CBD-CGD-O2D-CED
22	G	612	CLA	CBD-CGD-O2D-CED
22	G	613	CLA	CBD-CGD-O2D-CED
22	N	604	CLA	CBD-CGD-O2D-CED
22	N	609	CLA	CBD-CGD-O2D-CED
22	N	611	CLA	CBD-CGD-O2D-CED
22	N	612	CLA	CBD-CGD-O2D-CED
22	Y	604	CLA	CBD-CGD-O2D-CED
22	Y	609	CLA	CBD-CGD-O2D-CED
22	Y	611	CLA	CBD-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
22	b	604	CLA	CBD-CGD-O2D-CED
22	b	608	CLA	CBD-CGD-O2D-CED
22	b	611	CLA	CBD-CGD-O2D-CED
22	b	612	CLA	CBD-CGD-O2D-CED
22	b	613	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	CBD-CGD-O2D-CED
22	w	101	CLA	CBD-CGD-O2D-CED
22	x	101	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	CBD-CGD-O2D-CED
22	B	604	CLA	CBD-CGD-O2D-CED
22	B	607	CLA	CBD-CGD-O2D-CED
22	B	611	CLA	CBD-CGD-O2D-CED
22	B	614	CLA	CBD-CGD-O2D-CED
22	B	615	CLA	CBD-CGD-O2D-CED
22	B	616	CLA	CBD-CGD-O2D-CED
22	B	618	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
22	W	101	CLA	CBD-CGD-O2D-CED
22	r	303	CLA	CBD-CGD-O2D-CED
22	r	305	CLA	CBD-CGD-O2D-CED
22	s	303	CLA	CBD-CGD-O2D-CED
22	s	305	CLA	CBD-CGD-O2D-CED
22	s	308	CLA	CBD-CGD-O2D-CED
22	S	303	CLA	CBD-CGD-O2D-CED
22	S	305	CLA	CBD-CGD-O2D-CED
22	S	308	CLA	CBD-CGD-O2D-CED
22	R	302	CLA	CBD-CGD-O2D-CED
22	R	304	CLA	CBD-CGD-O2D-CED
30	a	407	PHO	CBD-CGD-O2D-CED
30	A	408	PHO	CBD-CGD-O2D-CED
22	g	602	CLA	O1A-CGA-O2A-C1
22	n	602	CLA	O1A-CGA-O2A-C1
22	y	602	CLA	O1A-CGA-O2A-C1
22	G	602	CLA	O1A-CGA-O2A-C1
22	N	602	CLA	O1A-CGA-O2A-C1
22	Y	602	CLA	O1A-CGA-O2A-C1
22	c	514	CLA	O1A-CGA-O2A-C1
22	C	515	CLA	O1A-CGA-O2A-C1
22	r	305	CLA	O1A-CGA-O2A-C1
22	r	309	CLA	O1A-CGA-O2A-C1
22	R	304	CLA	O1A-CGA-O2A-C1
22	R	308	CLA	O1A-CGA-O2A-C1
21	y	605	CHL	O1D-CGD-O2D-CED
21	r	301	CHL	O1D-CGD-O2D-CED
21	S	301	CHL	O1D-CGD-O2D-CED
21	n	608	CHL	C2C-C3C-CAC-CBC
21	Y	608	CHL	C2C-C3C-CAC-CBC
22	b	601	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	O1D-CGD-O2D-CED
22	r	305	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	R	304	CLA	O1D-CGD-O2D-CED
22	c	514	CLA	CBA-CGA-O2A-C1
22	C	515	CLA	CBA-CGA-O2A-C1
22	r	309	CLA	CBA-CGA-O2A-C1
22	R	308	CLA	CBA-CGA-O2A-C1
33	l	101	SQD	C24-C23-O48-C46
33	L	102	SQD	C24-C23-O48-C46
22	g	611	CLA	CBD-CGD-O2D-CED
22	n	610	CLA	CBD-CGD-O2D-CED
22	y	611	CLA	CBD-CGD-O2D-CED
22	G	611	CLA	CBD-CGD-O2D-CED
22	N	610	CLA	CBD-CGD-O2D-CED
22	Y	610	CLA	CBD-CGD-O2D-CED
21	g	607	CHL	O1A-CGA-O2A-C1
21	n	606	CHL	O1A-CGA-O2A-C1
21	y	607	CHL	O1A-CGA-O2A-C1
21	G	607	CHL	O1A-CGA-O2A-C1
21	N	606	CHL	O1A-CGA-O2A-C1
21	Y	606	CHL	O1A-CGA-O2A-C1
21	r	306	CHL	O1A-CGA-O2A-C1
21	R	305	CHL	O1A-CGA-O2A-C1
22	g	604	CLA	O1A-CGA-O2A-C1
22	g	610	CLA	O1A-CGA-O2A-C1
22	g	611	CLA	O1A-CGA-O2A-C1
22	n	604	CLA	O1A-CGA-O2A-C1
22	n	609	CLA	O1A-CGA-O2A-C1
22	n	610	CLA	O1A-CGA-O2A-C1
22	y	604	CLA	O1A-CGA-O2A-C1
22	y	610	CLA	O1A-CGA-O2A-C1
22	y	611	CLA	O1A-CGA-O2A-C1
22	G	604	CLA	O1A-CGA-O2A-C1
22	G	610	CLA	O1A-CGA-O2A-C1
22	G	611	CLA	O1A-CGA-O2A-C1
22	N	604	CLA	O1A-CGA-O2A-C1
22	N	609	CLA	O1A-CGA-O2A-C1
22	N	610	CLA	O1A-CGA-O2A-C1
22	Y	604	CLA	O1A-CGA-O2A-C1
22	Y	609	CLA	O1A-CGA-O2A-C1
22	Y	610	CLA	O1A-CGA-O2A-C1
22	a	406	CLA	O1A-CGA-O2A-C1
22	c	505	CLA	O1A-CGA-O2A-C1
22	x	101	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	407	CLA	O1A-CGA-O2A-C1
22	B	603	CLA	O1A-CGA-O2A-C1
22	C	506	CLA	O1A-CGA-O2A-C1
26	c	522	LHG	O10-C23-O8-C6
26	C	522	LHG	O10-C23-O8-C6
33	l	101	SQD	O10-C23-O48-C46
33	L	102	SQD	O10-C23-O48-C46
35	a	413	DGD	O1A-C1A-O1G-C1G
35	A	401	DGD	O1A-C1A-O1G-C1G
21	r	308	CHL	C8-C10-C11-C12
21	R	307	CHL	C8-C10-C11-C12
21	g	609	CHL	C2C-C3C-CAC-CBC
21	y	609	CHL	C2C-C3C-CAC-CBC
21	G	609	CHL	C2C-C3C-CAC-CBC
21	N	608	CHL	C2C-C3C-CAC-CBC
22	g	612	CLA	O1D-CGD-O2D-CED
22	n	611	CLA	O1D-CGD-O2D-CED
22	G	612	CLA	O1D-CGD-O2D-CED
22	N	611	CLA	O1D-CGD-O2D-CED
22	b	604	CLA	O1D-CGD-O2D-CED
22	w	101	CLA	O1D-CGD-O2D-CED
22	x	101	CLA	O1D-CGD-O2D-CED
22	B	603	CLA	O1D-CGD-O2D-CED
22	B	607	CLA	O1D-CGD-O2D-CED
22	W	101	CLA	O1D-CGD-O2D-CED
21	g	606	CHL	O1D-CGD-O2D-CED
21	n	605	CHL	O1D-CGD-O2D-CED
21	y	606	CHL	O1D-CGD-O2D-CED
21	G	606	CHL	O1D-CGD-O2D-CED
21	N	605	CHL	O1D-CGD-O2D-CED
21	Y	605	CHL	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	O1D-CGD-O2D-CED
22	s	310	CLA	O1D-CGD-O2D-CED
22	s	312	CLA	O1D-CGD-O2D-CED
22	S	310	CLA	O1D-CGD-O2D-CED
22	S	312	CLA	O1D-CGD-O2D-CED
30	d	401	PHO	O1D-CGD-O2D-CED
30	D	401	PHO	O1D-CGD-O2D-CED
30	a	407	PHO	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	A	408	PHO	O1A-CGA-O2A-C1
26	c	520	LHG	O9-C7-O7-C5
26	C	520	LHG	O9-C7-O7-C5
21	g	608	CHL	C3-C5-C6-C7
21	n	607	CHL	C3-C5-C6-C7
21	y	608	CHL	C3-C5-C6-C7
21	G	608	CHL	C3-C5-C6-C7
21	N	607	CHL	C3-C5-C6-C7
21	Y	607	CHL	C3-C5-C6-C7
22	g	611	CLA	C3-C5-C6-C7
22	g	612	CLA	C3-C5-C6-C7
22	n	610	CLA	C3-C5-C6-C7
22	n	611	CLA	C3-C5-C6-C7
22	y	611	CLA	C3-C5-C6-C7
22	G	611	CLA	C3-C5-C6-C7
22	G	612	CLA	C3-C5-C6-C7
22	N	610	CLA	C3-C5-C6-C7
22	N	611	CLA	C3-C5-C6-C7
22	Y	610	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
22	b	612	CLA	C3-C5-C6-C7
22	b	613	CLA	C3-C5-C6-C7
22	c	502	CLA	C3-C5-C6-C7
22	c	508	CLA	C3-C5-C6-C7
22	w	101	CLA	C3-C5-C6-C7
22	x	101	CLA	C3-C5-C6-C7
22	B	603	CLA	C3-C5-C6-C7
22	B	604	CLA	C3-C5-C6-C7
22	B	615	CLA	C3-C5-C6-C7
22	B	616	CLA	C3-C5-C6-C7
22	C	503	CLA	C3-C5-C6-C7
22	C	509	CLA	C3-C5-C6-C7
22	W	101	CLA	C3-C5-C6-C7
22	r	304	CLA	C3-C5-C6-C7
22	R	303	CLA	C3-C5-C6-C7
30	a	407	PHO	C3-C5-C6-C7
30	d	401	PHO	C3-C5-C6-C7
30	A	408	PHO	C3-C5-C6-C7
30	D	401	PHO	C3-C5-C6-C7
33	l	103	SQD	C45-C46-O48-C23
33	L	101	SQD	C45-C46-O48-C23
21	g	607	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
21	n	606	CHL	C2C-C3C-CAC-CBC
22	b	603	CLA	O1D-CGD-O2D-CED
22	B	606	CLA	O1D-CGD-O2D-CED
21	g	601	CHL	CBA-CGA-O2A-C1
21	n	601	CHL	CBA-CGA-O2A-C1
21	y	601	CHL	CBA-CGA-O2A-C1
21	G	601	CHL	CBA-CGA-O2A-C1
21	N	601	CHL	CBA-CGA-O2A-C1
21	Y	601	CHL	CBA-CGA-O2A-C1
21	r	306	CHL	CBA-CGA-O2A-C1
21	R	305	CHL	CBA-CGA-O2A-C1
22	g	602	CLA	CBA-CGA-O2A-C1
22	g	604	CLA	CBA-CGA-O2A-C1
22	g	610	CLA	CBA-CGA-O2A-C1
22	n	602	CLA	CBA-CGA-O2A-C1
22	n	609	CLA	CBA-CGA-O2A-C1
22	y	602	CLA	CBA-CGA-O2A-C1
22	y	610	CLA	CBA-CGA-O2A-C1
22	G	602	CLA	CBA-CGA-O2A-C1
22	G	604	CLA	CBA-CGA-O2A-C1
22	G	610	CLA	CBA-CGA-O2A-C1
22	N	602	CLA	CBA-CGA-O2A-C1
22	N	604	CLA	CBA-CGA-O2A-C1
22	Y	602	CLA	CBA-CGA-O2A-C1
22	Y	604	CLA	CBA-CGA-O2A-C1
22	Y	609	CLA	CBA-CGA-O2A-C1
22	a	406	CLA	CBA-CGA-O2A-C1
22	b	603	CLA	CBA-CGA-O2A-C1
22	c	507	CLA	CBA-CGA-O2A-C1
22	x	101	CLA	CBA-CGA-O2A-C1
22	A	407	CLA	CBA-CGA-O2A-C1
22	B	603	CLA	CBA-CGA-O2A-C1
22	B	606	CLA	CBA-CGA-O2A-C1
22	C	508	CLA	CBA-CGA-O2A-C1
26	c	522	LHG	C24-C23-O8-C6
26	C	522	LHG	C24-C23-O8-C6
35	a	413	DGD	C2A-C1A-O1G-C1G
35	A	401	DGD	C2A-C1A-O1G-C1G
36	M	101	LMG	C29-C28-O8-C9
36	T	101	LMG	C29-C28-O8-C9
22	a	405	CLA	CBD-CGD-O2D-CED
22	b	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	b	610	CLA	CBD-CGD-O2D-CED
22	c	502	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	CBD-CGD-O2D-CED
22	A	406	CLA	CBD-CGD-O2D-CED
22	B	605	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	CBD-CGD-O2D-CED
22	C	503	CLA	CBD-CGD-O2D-CED
22	C	510	CLA	CBD-CGD-O2D-CED
22	r	312	CLA	CBD-CGD-O2D-CED
22	s	311	CLA	CBD-CGD-O2D-CED
22	S	311	CLA	CBD-CGD-O2D-CED
22	R	311	CLA	CBD-CGD-O2D-CED
33	l	103	SQD	C8-C7-O47-C45
33	L	101	SQD	C8-C7-O47-C45
36	b	620	LMG	C11-C10-O7-C8
36	B	623	LMG	C11-C10-O7-C8
21	N	606	CHL	C2C-C3C-CAC-CBC
21	Y	606	CHL	C2C-C3C-CAC-CBC
22	c	510	CLA	O1D-CGD-O2D-CED
22	r	311	CLA	O1D-CGD-O2D-CED
22	s	303	CLA	O1D-CGD-O2D-CED
22	S	303	CLA	O1D-CGD-O2D-CED
22	R	310	CLA	O1D-CGD-O2D-CED
21	s	301	CHL	C2-C1-O2A-CGA
21	y	607	CHL	C2C-C3C-CAC-CBC
21	G	607	CHL	C2C-C3C-CAC-CBC
21	r	308	CHL	C2C-C3C-CAC-CBC
21	R	307	CHL	C2C-C3C-CAC-CBC
22	g	613	CLA	O1D-CGD-O2D-CED
22	n	612	CLA	O1D-CGD-O2D-CED
22	y	612	CLA	O1D-CGD-O2D-CED
22	G	613	CLA	O1D-CGD-O2D-CED
22	N	612	CLA	O1D-CGD-O2D-CED
22	Y	611	CLA	O1D-CGD-O2D-CED
22	C	511	CLA	O1D-CGD-O2D-CED
21	g	608	CHL	C4-C3-C5-C6
21	n	607	CHL	C4-C3-C5-C6
21	y	608	CHL	C4-C3-C5-C6
21	G	608	CHL	C4-C3-C5-C6
21	N	607	CHL	C4-C3-C5-C6
21	Y	607	CHL	C4-C3-C5-C6
22	d	404	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	D	405	CLA	C4-C3-C5-C6
21	g	608	CHL	C2-C3-C5-C6
21	n	607	CHL	C2-C3-C5-C6
21	y	608	CHL	C2-C3-C5-C6
21	G	608	CHL	C2-C3-C5-C6
21	N	607	CHL	C2-C3-C5-C6
21	Y	607	CHL	C2-C3-C5-C6
22	d	404	CLA	C2-C3-C5-C6
22	D	405	CLA	C2-C3-C5-C6
32	d	406	PL9	C13-C14-C16-C17
32	D	407	PL9	C13-C14-C16-C17
22	g	610	CLA	O1D-CGD-O2D-CED
22	n	609	CLA	O1D-CGD-O2D-CED
22	y	610	CLA	O1D-CGD-O2D-CED
22	G	610	CLA	O1D-CGD-O2D-CED
22	N	609	CLA	O1D-CGD-O2D-CED
22	Y	609	CLA	O1D-CGD-O2D-CED
30	a	407	PHO	O1D-CGD-O2D-CED
30	A	408	PHO	O1D-CGD-O2D-CED
36	k	103	LMG	O6-C5-C6-O5
36	K	103	LMG	O6-C5-C6-O5
22	g	603	CLA	C2A-CAA-CBA-CGA
22	n	603	CLA	C2A-CAA-CBA-CGA
22	y	603	CLA	C2A-CAA-CBA-CGA
22	G	603	CLA	C2A-CAA-CBA-CGA
22	N	603	CLA	C2A-CAA-CBA-CGA
22	Y	603	CLA	C2A-CAA-CBA-CGA
22	b	614	CLA	C2A-CAA-CBA-CGA
22	c	508	CLA	C2A-CAA-CBA-CGA
22	B	617	CLA	C2A-CAA-CBA-CGA
22	C	509	CLA	C2A-CAA-CBA-CGA
22	b	601	CLA	O1A-CGA-O2A-C1
22	B	604	CLA	O1A-CGA-O2A-C1
21	g	607	CHL	CBA-CGA-O2A-C1
21	g	608	CHL	CBA-CGA-O2A-C1
21	n	606	CHL	CBA-CGA-O2A-C1
21	n	607	CHL	CBA-CGA-O2A-C1
21	y	607	CHL	CBA-CGA-O2A-C1
21	G	607	CHL	CBA-CGA-O2A-C1
21	N	606	CHL	CBA-CGA-O2A-C1
21	Y	606	CHL	CBA-CGA-O2A-C1
22	g	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	g	613	CLA	CBA-CGA-O2A-C1
22	n	604	CLA	CBA-CGA-O2A-C1
22	n	610	CLA	CBA-CGA-O2A-C1
22	n	612	CLA	CBA-CGA-O2A-C1
22	y	604	CLA	CBA-CGA-O2A-C1
22	y	611	CLA	CBA-CGA-O2A-C1
22	y	612	CLA	CBA-CGA-O2A-C1
22	G	611	CLA	CBA-CGA-O2A-C1
22	G	613	CLA	CBA-CGA-O2A-C1
22	N	609	CLA	CBA-CGA-O2A-C1
22	N	610	CLA	CBA-CGA-O2A-C1
22	N	612	CLA	CBA-CGA-O2A-C1
22	Y	610	CLA	CBA-CGA-O2A-C1
22	Y	611	CLA	CBA-CGA-O2A-C1
22	b	601	CLA	CBA-CGA-O2A-C1
22	b	606	CLA	CBA-CGA-O2A-C1
22	b	615	CLA	CBA-CGA-O2A-C1
22	c	505	CLA	CBA-CGA-O2A-C1
22	B	604	CLA	CBA-CGA-O2A-C1
22	B	609	CLA	CBA-CGA-O2A-C1
22	B	618	CLA	CBA-CGA-O2A-C1
22	C	506	CLA	CBA-CGA-O2A-C1
22	r	310	CLA	CBA-CGA-O2A-C1
22	s	305	CLA	CBA-CGA-O2A-C1
22	s	311	CLA	CBA-CGA-O2A-C1
22	S	305	CLA	CBA-CGA-O2A-C1
22	R	309	CLA	CBA-CGA-O2A-C1
30	a	407	PHO	CBA-CGA-O2A-C1
30	A	408	PHO	CBA-CGA-O2A-C1
32	d	406	PL9	C12-C13-C14-C16
32	d	406	PL9	C27-C28-C29-C31
32	d	406	PL9	C42-C43-C44-C46
32	D	407	PL9	C12-C13-C14-C16
32	D	407	PL9	C27-C28-C29-C31
32	D	407	PL9	C42-C43-C44-C46
23	r	313	LUT	C9-C10-C11-C12
23	R	312	LUT	C9-C10-C11-C12
24	n	615	XAT	C9-C10-C11-C12
24	N	616	XAT	C9-C10-C11-C12
31	B	602	BCR	C19-C20-C21-C22
31	T	102	BCR	C19-C20-C21-C22
21	r	308	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	R	307	CHL	O1A-CGA-O2A-C1
22	b	606	CLA	O1A-CGA-O2A-C1
22	b	615	CLA	O1A-CGA-O2A-C1
22	B	609	CLA	O1A-CGA-O2A-C1
22	B	618	CLA	O1A-CGA-O2A-C1
22	r	304	CLA	O1A-CGA-O2A-C1
22	r	312	CLA	O1A-CGA-O2A-C1
22	R	303	CLA	O1A-CGA-O2A-C1
22	R	311	CLA	O1A-CGA-O2A-C1
33	l	103	SQD	O10-C23-O48-C46
33	L	101	SQD	O10-C23-O48-C46
33	a	411	SQD	O49-C7-O47-C45
33	A	412	SQD	O49-C7-O47-C45
21	g	608	CHL	O1D-CGD-O2D-CED
21	n	607	CHL	O1D-CGD-O2D-CED
21	y	608	CHL	O1D-CGD-O2D-CED
21	G	608	CHL	O1D-CGD-O2D-CED
21	N	607	CHL	O1D-CGD-O2D-CED
21	Y	607	CHL	O1D-CGD-O2D-CED
21	g	606	CHL	C2C-C3C-CAC-CBC
21	n	605	CHL	C2C-C3C-CAC-CBC
21	y	606	CHL	C2C-C3C-CAC-CBC
21	G	606	CHL	C2C-C3C-CAC-CBC
21	N	605	CHL	C2C-C3C-CAC-CBC
21	Y	605	CHL	C2C-C3C-CAC-CBC
22	a	406	CLA	CBD-CGD-O2D-CED
22	A	407	CLA	CBD-CGD-O2D-CED
26	G	618	LHG	O2-C2-C3-O3
26	Y	617	LHG	O2-C2-C3-O3
21	s	307	CHL	O1D-CGD-O2D-CED
21	S	307	CHL	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
22	B	616	CLA	O1D-CGD-O2D-CED
22	s	305	CLA	O1D-CGD-O2D-CED
22	S	305	CLA	O1D-CGD-O2D-CED
21	y	608	CHL	CBA-CGA-O2A-C1
21	G	608	CHL	CBA-CGA-O2A-C1
21	N	607	CHL	CBA-CGA-O2A-C1
21	Y	607	CHL	CBA-CGA-O2A-C1
22	a	405	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	b	611	CLA	CBA-CGA-O2A-C1
22	c	509	CLA	CBA-CGA-O2A-C1
22	A	406	CLA	CBA-CGA-O2A-C1
22	B	614	CLA	CBA-CGA-O2A-C1
22	C	510	CLA	CBA-CGA-O2A-C1
22	r	312	CLA	CBA-CGA-O2A-C1
22	s	310	CLA	CBA-CGA-O2A-C1
22	S	310	CLA	CBA-CGA-O2A-C1
22	S	311	CLA	CBA-CGA-O2A-C1
22	R	311	CLA	CBA-CGA-O2A-C1
21	g	601	CHL	O1A-CGA-O2A-C1
21	n	601	CHL	O1A-CGA-O2A-C1
21	y	601	CHL	O1A-CGA-O2A-C1
21	G	601	CHL	O1A-CGA-O2A-C1
21	N	601	CHL	O1A-CGA-O2A-C1
21	Y	601	CHL	O1A-CGA-O2A-C1
22	g	613	CLA	O1A-CGA-O2A-C1
22	n	612	CLA	O1A-CGA-O2A-C1
22	y	612	CLA	O1A-CGA-O2A-C1
22	G	613	CLA	O1A-CGA-O2A-C1
22	N	612	CLA	O1A-CGA-O2A-C1
22	Y	611	CLA	O1A-CGA-O2A-C1
22	b	603	CLA	O1A-CGA-O2A-C1
22	B	606	CLA	O1A-CGA-O2A-C1
22	s	305	CLA	O1A-CGA-O2A-C1
22	S	305	CLA	O1A-CGA-O2A-C1
36	k	103	LMG	C4-C5-C6-O5
36	K	103	LMG	C4-C5-C6-O5
22	b	607	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	B	612	CLA	CBD-CGD-O2D-CED
21	S	307	CHL	C2C-C3C-CAC-CBC
21	y	608	CHL	O1A-CGA-O2A-C1
21	G	608	CHL	O1A-CGA-O2A-C1
21	N	607	CHL	O1A-CGA-O2A-C1
21	Y	607	CHL	O1A-CGA-O2A-C1
22	c	511	CLA	C3-C5-C6-C7
22	C	512	CLA	C3-C5-C6-C7
35	c	518	DGD	C4D-C5D-C6D-O5D
35	C	519	DGD	C4D-C5D-C6D-O5D
21	s	302	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	S	302	CHL	CBD-CGD-O2D-CED
22	g	602	CLA	CBD-CGD-O2D-CED
22	n	602	CLA	CBD-CGD-O2D-CED
22	y	602	CLA	CBD-CGD-O2D-CED
22	G	602	CLA	CBD-CGD-O2D-CED
22	N	602	CLA	CBD-CGD-O2D-CED
22	Y	602	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
21	r	308	CHL	CBA-CGA-O2A-C1
21	R	307	CHL	CBA-CGA-O2A-C1
22	r	304	CLA	CBA-CGA-O2A-C1
22	R	303	CLA	CBA-CGA-O2A-C1
26	c	520	LHG	C24-C23-O8-C6
22	c	512	CLA	C4-C3-C5-C6
22	C	513	CLA	C4-C3-C5-C6
22	r	310	CLA	C4-C3-C5-C6
22	s	310	CLA	C4-C3-C5-C6
22	S	310	CLA	C4-C3-C5-C6
22	R	309	CLA	C4-C3-C5-C6
21	g	608	CHL	O1A-CGA-O2A-C1
21	n	607	CHL	O1A-CGA-O2A-C1
22	b	611	CLA	O1A-CGA-O2A-C1
22	c	509	CLA	O1A-CGA-O2A-C1
22	B	614	CLA	O1A-CGA-O2A-C1
22	C	510	CLA	O1A-CGA-O2A-C1
22	r	310	CLA	O1A-CGA-O2A-C1
22	s	310	CLA	O1A-CGA-O2A-C1
22	s	311	CLA	O1A-CGA-O2A-C1
22	S	310	CLA	O1A-CGA-O2A-C1
22	S	311	CLA	O1A-CGA-O2A-C1
22	R	309	CLA	O1A-CGA-O2A-C1
32	d	406	PL9	C9-C11-C12-C13
32	d	406	PL9	C14-C16-C17-C18
32	d	406	PL9	C24-C26-C27-C28
32	d	406	PL9	C39-C41-C42-C43
32	D	407	PL9	C9-C11-C12-C13
32	D	407	PL9	C14-C16-C17-C18
32	D	407	PL9	C24-C26-C27-C28
32	D	407	PL9	C39-C41-C42-C43
21	s	307	CHL	C2C-C3C-CAC-CBC
21	S	302	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	C	513	CLA	CBD-CGD-O2D-CED
21	g	608	CHL	C5-C6-C7-C8
21	n	607	CHL	C5-C6-C7-C8
21	y	608	CHL	C5-C6-C7-C8
21	G	608	CHL	C5-C6-C7-C8
21	N	607	CHL	C5-C6-C7-C8
21	Y	607	CHL	C5-C6-C7-C8
22	a	405	CLA	O1A-CGA-O2A-C1
22	A	406	CLA	O1A-CGA-O2A-C1
36	M	101	LMG	O10-C28-O8-C9
36	T	101	LMG	O10-C28-O8-C9
33	l	101	SQD	O5-C1-O6-C44
33	L	102	SQD	O5-C1-O6-C44
35	a	413	DGD	O6D-C1D-O3G-C3G
35	c	518	DGD	O6D-C1D-O3G-C3G
35	A	401	DGD	O6D-C1D-O3G-C3G
35	C	519	DGD	O6D-C1D-O3G-C3G
36	c	523	LMG	O6-C1-O1-C7
36	w	102	LMG	O6-C1-O1-C7
36	C	502	LMG	O6-C1-O1-C7
36	C	523	LMG	O6-C1-O1-C7
22	s	313	CLA	CBA-CGA-O2A-C1
22	S	313	CLA	CBA-CGA-O2A-C1
26	C	520	LHG	C24-C23-O8-C6
22	c	512	CLA	CBD-CGD-O2D-CED
36	M	101	LMG	O6-C5-C6-O5
36	T	101	LMG	O6-C5-C6-O5
21	s	302	CHL	C2C-C3C-CAC-CBC
36	C	523	LMG	O6-C5-C6-O5
22	g	611	CLA	O1D-CGD-O2D-CED
22	n	610	CLA	O1D-CGD-O2D-CED
22	y	611	CLA	O1D-CGD-O2D-CED
22	G	611	CLA	O1D-CGD-O2D-CED
22	N	610	CLA	O1D-CGD-O2D-CED
22	Y	610	CLA	O1D-CGD-O2D-CED
22	g	614	CLA	CBD-CGD-O2D-CED
22	n	613	CLA	CBD-CGD-O2D-CED
22	y	613	CLA	CBD-CGD-O2D-CED
22	G	614	CLA	CBD-CGD-O2D-CED
22	N	613	CLA	CBD-CGD-O2D-CED
22	Y	612	CLA	CBD-CGD-O2D-CED
32	d	406	PL9	C47-C48-C49-C51

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Mol	Chain	Res	Type	Atoms
32	D	407	PL9	C47-C48-C49-C51
36	c	523	LMG	O6-C5-C6-O5
22	s	313	CLA	O1A-CGA-O2A-C1
22	S	313	CLA	O1A-CGA-O2A-C1
26	N	618	LHG	C1-C2-C3-O3
26	Y	617	LHG	C1-C2-C3-O3
21	s	301	CHL	CBA-CGA-O2A-C1
22	b	614	CLA	CBA-CGA-O2A-C1
22	B	617	CLA	CBA-CGA-O2A-C1
22	r	311	CLA	CBA-CGA-O2A-C1
22	R	310	CLA	CBA-CGA-O2A-C1
26	r	302	LHG	C24-C23-O8-C6
26	R	301	LHG	C24-C23-O8-C6
33	a	411	SQD	C24-C23-O48-C46
33	l	103	SQD	C24-C23-O48-C46
33	A	412	SQD	C24-C23-O48-C46
33	L	101	SQD	C24-C23-O48-C46
35	c	518	DGD	O6D-C5D-C6D-O5D
35	C	519	DGD	O6D-C5D-C6D-O5D
26	d	407	LHG	C28-C29-C30-C31
26	D	408	LHG	C28-C29-C30-C31
22	s	311	CLA	O1D-CGD-O2D-CED
22	S	311	CLA	O1D-CGD-O2D-CED
26	b	619	LHG	C28-C29-C30-C31
26	B	622	LHG	C28-C29-C30-C31
21	g	601	CHL	C4-C3-C5-C6
21	n	601	CHL	C4-C3-C5-C6
21	y	601	CHL	C4-C3-C5-C6
21	G	601	CHL	C4-C3-C5-C6
21	N	601	CHL	C4-C3-C5-C6
21	Y	601	CHL	C4-C3-C5-C6
22	s	309	CLA	C4-C3-C5-C6
22	S	309	CLA	C4-C3-C5-C6
21	g	601	CHL	C2-C3-C5-C6
21	n	601	CHL	C2-C3-C5-C6
21	y	601	CHL	C2-C3-C5-C6
21	G	601	CHL	C2-C3-C5-C6
21	N	601	CHL	C2-C3-C5-C6
21	Y	601	CHL	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
22	C	513	CLA	C2-C3-C5-C6
22	r	310	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	g	601	CHL	C14-C13-C15-C16
21	n	601	CHL	C14-C13-C15-C16
21	n	608	CHL	C14-C13-C15-C16
21	y	601	CHL	C14-C13-C15-C16
21	y	609	CHL	C14-C13-C15-C16
21	G	601	CHL	C14-C13-C15-C16
21	N	601	CHL	C14-C13-C15-C16
21	N	608	CHL	C14-C13-C15-C16
21	Y	601	CHL	C14-C13-C15-C16
21	Y	608	CHL	C14-C13-C15-C16
22	g	612	CLA	C6-C7-C8-C9
22	n	611	CLA	C6-C7-C8-C9
22	G	612	CLA	C6-C7-C8-C9
22	N	611	CLA	C6-C7-C8-C9
22	a	405	CLA	C6-C7-C8-C9
22	b	601	CLA	C11-C10-C8-C9
22	c	514	CLA	C11-C10-C8-C9
22	w	101	CLA	C6-C7-C8-C9
22	A	406	CLA	C6-C7-C8-C9
22	B	604	CLA	C11-C10-C8-C9
22	C	515	CLA	C11-C10-C8-C9
22	W	101	CLA	C6-C7-C8-C9
22	a	405	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
22	c	502	CLA	O1D-CGD-O2D-CED
22	A	406	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	O1D-CGD-O2D-CED
22	C	503	CLA	O1D-CGD-O2D-CED
22	r	312	CLA	O1D-CGD-O2D-CED
22	R	311	CLA	O1D-CGD-O2D-CED
33	l	101	SQD	C2-C1-O6-C44
33	L	102	SQD	C2-C1-O6-C44
35	a	413	DGD	C2D-C1D-O3G-C3G
35	c	518	DGD	C2E-C1E-O5D-C6D
35	A	401	DGD	C2D-C1D-O3G-C3G
35	C	519	DGD	C2E-C1E-O5D-C6D
36	c	523	LMG	C2-C1-O1-C7
36	w	102	LMG	C2-C1-O1-C7
36	C	502	LMG	C2-C1-O1-C7
36	C	523	LMG	C2-C1-O1-C7
26	c	520	LHG	C28-C29-C30-C31
26	C	520	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	r	311	CLA	O1A-CGA-O2A-C1
22	R	310	CLA	O1A-CGA-O2A-C1
23	g	615	LUT	C7-C8-C9-C19
23	g	615	LUT	C31-C32-C33-C40
23	g	616	LUT	C31-C32-C33-C40
23	n	614	LUT	C7-C8-C9-C19
23	n	614	LUT	C31-C32-C33-C40
23	y	614	LUT	C7-C8-C9-C19
23	y	614	LUT	C31-C32-C33-C40
23	G	615	LUT	C7-C8-C9-C19
23	G	615	LUT	C31-C32-C33-C40
23	N	614	LUT	C7-C8-C9-C19
23	N	614	LUT	C31-C32-C33-C40
23	N	615	LUT	C7-C8-C9-C19
23	Y	613	LUT	C7-C8-C9-C19
23	Y	613	LUT	C31-C32-C33-C40
23	Y	614	LUT	C27-C28-C29-C39
23	r	313	LUT	C7-C8-C9-C19
23	r	313	LUT	C31-C32-C33-C40
23	R	312	LUT	C7-C8-C9-C19
23	R	312	LUT	C31-C32-C33-C40
24	y	615	XAT	C7-C8-C9-C19
24	y	615	XAT	C31-C32-C33-C40
24	G	617	XAT	C31-C32-C33-C40
24	Y	615	XAT	C7-C8-C9-C19
24	Y	615	XAT	C31-C32-C33-C40
24	r	314	XAT	C31-C32-C33-C40
24	R	313	XAT	C27-C28-C29-C39
24	R	313	XAT	C31-C32-C33-C40
25	g	618	NEX	C27-C28-C29-C39
25	n	616	NEX	C11-C12-C13-C20
25	n	616	NEX	C31-C32-C33-C40
25	y	618	NEX	C31-C32-C33-C40
25	N	617	NEX	C27-C28-C29-C39
25	r	315	NEX	C31-C32-C33-C40
31	b	617	BCR	C7-C8-C9-C34
31	b	617	BCR	C37-C22-C23-C24
31	c	515	BCR	C7-C8-C9-C34
31	d	405	BCR	C7-C8-C9-C34
31	B	602	BCR	C7-C8-C9-C34
31	B	602	BCR	C11-C12-C13-C35
31	B	602	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	B	602	BCR	C37-C22-C23-C24
31	B	620	BCR	C7-C8-C9-C34
31	B	620	BCR	C37-C22-C23-C24
31	C	516	BCR	C7-C8-C9-C34
31	D	406	BCR	C7-C8-C9-C34
31	T	102	BCR	C7-C8-C9-C34
31	T	102	BCR	C11-C12-C13-C35
31	T	102	BCR	C36-C18-C19-C20
31	T	102	BCR	C37-C22-C23-C24
23	g	615	LUT	C11-C12-C13-C14
23	g	615	LUT	C27-C28-C29-C30
23	g	616	LUT	C7-C8-C9-C10
23	n	614	LUT	C11-C12-C13-C14
23	n	614	LUT	C27-C28-C29-C30
23	y	614	LUT	C11-C12-C13-C14
23	y	614	LUT	C27-C28-C29-C30
23	G	615	LUT	C11-C12-C13-C14
23	G	615	LUT	C27-C28-C29-C30
23	G	616	LUT	C7-C8-C9-C10
23	N	614	LUT	C11-C12-C13-C14
23	N	614	LUT	C27-C28-C29-C30
23	Y	613	LUT	C11-C12-C13-C14
23	Y	613	LUT	C27-C28-C29-C30
23	Y	614	LUT	C7-C8-C9-C10
23	r	313	LUT	C27-C28-C29-C30
23	R	312	LUT	C27-C28-C29-C30
31	d	405	BCR	C7-C8-C9-C10
31	k	101	BCR	C21-C22-C23-C24
31	B	602	BCR	C7-C8-C9-C10
31	D	406	BCR	C7-C8-C9-C10
31	K	101	BCR	C21-C22-C23-C24
31	T	102	BCR	C7-C8-C9-C10
26	c	521	LHG	C23-C24-C25-C26
26	d	407	LHG	C23-C24-C25-C26
26	C	521	LHG	C23-C24-C25-C26
26	D	408	LHG	C23-C24-C25-C26
22	b	602	CLA	O1D-CGD-O2D-CED
22	B	605	CLA	O1D-CGD-O2D-CED
21	s	301	CHL	O1A-CGA-O2A-C1
26	G	618	LHG	O6-C4-C5-O7
26	s	314	LHG	O7-C5-C6-O8
26	S	314	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
22	g	603	CLA	CBA-CGA-O2A-C1
22	n	603	CLA	CBA-CGA-O2A-C1
22	y	603	CLA	CBA-CGA-O2A-C1
22	G	603	CLA	CBA-CGA-O2A-C1
22	N	603	CLA	CBA-CGA-O2A-C1
22	Y	603	CLA	CBA-CGA-O2A-C1
36	B	601	LMG	C29-C28-O8-C9
36	I	101	LMG	C29-C28-O8-C9
21	G	607	CHL	C8-C10-C11-C12
21	N	606	CHL	C8-C10-C11-C12
22	g	611	CLA	C5-C6-C7-C8
22	y	611	CLA	C5-C6-C7-C8
22	G	611	CLA	C5-C6-C7-C8
22	Y	610	CLA	C5-C6-C7-C8
21	n	605	CHL	C2-C1-O2A-CGA
21	y	606	CHL	C2-C1-O2A-CGA
21	N	605	CHL	C2-C1-O2A-CGA
21	g	607	CHL	C8-C10-C11-C12
21	n	606	CHL	C8-C10-C11-C12
21	y	607	CHL	C8-C10-C11-C12
21	y	609	CHL	C8-C10-C11-C12
21	Y	606	CHL	C8-C10-C11-C12
22	g	603	CLA	C10-C11-C12-C13
22	g	613	CLA	C8-C10-C11-C12
22	n	603	CLA	C10-C11-C12-C13
22	n	610	CLA	C5-C6-C7-C8
22	n	612	CLA	C8-C10-C11-C12
22	y	603	CLA	C10-C11-C12-C13
22	y	612	CLA	C8-C10-C11-C12
22	G	603	CLA	C10-C11-C12-C13
22	G	613	CLA	C8-C10-C11-C12
22	N	603	CLA	C10-C11-C12-C13
22	N	610	CLA	C5-C6-C7-C8
22	N	612	CLA	C8-C10-C11-C12
22	Y	603	CLA	C10-C11-C12-C13
22	Y	611	CLA	C8-C10-C11-C12
22	r	309	CLA	C5-C6-C7-C8
22	R	308	CLA	C5-C6-C7-C8
35	h	102	DGD	O6E-C5E-C6E-O5E
35	H	102	DGD	O6E-C5E-C6E-O5E
36	B	601	LMG	O6-C5-C6-O5
36	I	101	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
26	g	619	LHG	O1-C1-C2-O2
26	d	408	LHG	O1-C1-C2-O2
26	D	409	LHG	O1-C1-C2-O2
26	r	302	LHG	O1-C1-C2-O2
26	R	301	LHG	O1-C1-C2-O2
26	r	302	LHG	C23-C24-C25-C26
26	R	301	LHG	C23-C24-C25-C26
36	d	410	LMG	C29-C28-O8-C9
26	y	617	LHG	C7-C8-C9-C10
24	g	617	XAT	C9-C10-C11-C12
24	y	615	XAT	C9-C10-C11-C12
24	G	617	XAT	C9-C10-C11-C12
24	Y	615	XAT	C9-C10-C11-C12
25	g	618	NEX	C13-C14-C15-C35
22	c	509	CLA	O1D-CGD-O2D-CED
22	C	510	CLA	O1D-CGD-O2D-CED
22	a	408	CLA	C3-C5-C6-C7
22	A	409	CLA	C3-C5-C6-C7
21	n	608	CHL	C8-C10-C11-C12
21	N	608	CHL	C8-C10-C11-C12
22	G	610	CLA	C13-C15-C16-C17
22	C	514	CLA	C15-C16-C17-C18
26	Y	617	LHG	C7-C8-C9-C10
26	b	619	LHG	C23-C24-C25-C26
26	B	622	LHG	C23-C24-C25-C26
26	r	302	LHG	C7-C8-C9-C10
26	R	301	LHG	C7-C8-C9-C10
35	h	102	DGD	C1B-C2B-C3B-C4B
35	H	102	DGD	C1B-C2B-C3B-C4B
36	D	411	LMG	C29-C28-O8-C9
21	Y	608	CHL	C8-C10-C11-C12
22	g	610	CLA	C8-C10-C11-C12
22	N	609	CLA	C8-C10-C11-C12
22	Y	609	CLA	C8-C10-C11-C12
22	b	601	CLA	C15-C16-C17-C18
22	b	615	CLA	C15-C16-C17-C18
22	c	502	CLA	C13-C15-C16-C17
22	c	513	CLA	C15-C16-C17-C18
22	d	404	CLA	C8-C10-C11-C12
22	d	404	CLA	C13-C15-C16-C17
22	B	604	CLA	C15-C16-C17-C18
22	B	618	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	C	503	CLA	C13-C15-C16-C17
22	D	405	CLA	C8-C10-C11-C12
22	D	405	CLA	C13-C15-C16-C17
37	f	101	HEM	C3D-CAD-CBD-CGD
37	F	101	HEM	C3D-CAD-CBD-CGD
21	g	607	CHL	C2A-CAA-CBA-CGA
21	n	606	CHL	C2A-CAA-CBA-CGA
21	y	607	CHL	C2A-CAA-CBA-CGA
21	G	607	CHL	C2A-CAA-CBA-CGA
21	N	606	CHL	C2A-CAA-CBA-CGA
21	Y	606	CHL	C2A-CAA-CBA-CGA
21	s	302	CHL	C2A-CAA-CBA-CGA
21	S	302	CHL	C2A-CAA-CBA-CGA
22	b	609	CLA	C2A-CAA-CBA-CGA
22	b	611	CLA	C2A-CAA-CBA-CGA
22	c	507	CLA	C2A-CAA-CBA-CGA
22	B	612	CLA	C2A-CAA-CBA-CGA
22	B	614	CLA	C2A-CAA-CBA-CGA
22	C	508	CLA	C2A-CAA-CBA-CGA
26	c	522	LHG	C29-C30-C31-C32
21	r	308	CHL	C10-C11-C12-C13
21	R	307	CHL	C10-C11-C12-C13
22	n	609	CLA	C8-C10-C11-C12
22	y	610	CLA	C8-C10-C11-C12
22	G	610	CLA	C8-C10-C11-C12
22	G	613	CLA	C13-C15-C16-C17
22	b	601	CLA	C8-C10-C11-C12
22	b	614	CLA	C15-C16-C17-C18
22	c	506	CLA	C10-C11-C12-C13
22	B	604	CLA	C8-C10-C11-C12
22	B	617	CLA	C15-C16-C17-C18
22	C	507	CLA	C10-C11-C12-C13
22	s	311	CLA	C5-C6-C7-C8
22	S	311	CLA	C5-C6-C7-C8
26	N	618	LHG	C7-C8-C9-C10
26	c	520	LHG	C7-C8-C9-C10
26	C	520	LHG	C7-C8-C9-C10
26	s	314	LHG	C7-C8-C9-C10
26	s	314	LHG	C23-C24-C25-C26
26	S	314	LHG	C7-C8-C9-C10
26	S	314	LHG	C23-C24-C25-C26
35	c	517	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
35	C	518	DGD	C1B-C2B-C3B-C4B
36	w	102	LMG	C28-C29-C30-C31
36	C	502	LMG	C28-C29-C30-C31
22	b	614	CLA	O1A-CGA-O2A-C1
22	B	617	CLA	O1A-CGA-O2A-C1
21	r	307	CHL	C3-C5-C6-C7
21	R	306	CHL	C3-C5-C6-C7
26	C	522	LHG	C29-C30-C31-C32
22	n	609	CLA	C15-C16-C17-C18
22	b	613	CLA	C5-C6-C7-C8
22	c	505	CLA	C10-C11-C12-C13
22	c	510	CLA	C13-C15-C16-C17
22	B	616	CLA	C5-C6-C7-C8
22	C	506	CLA	C10-C11-C12-C13
22	C	511	CLA	C13-C15-C16-C17
22	r	310	CLA	C10-C11-C12-C13
22	r	310	CLA	C15-C16-C17-C18
22	R	309	CLA	C10-C11-C12-C13
22	R	309	CLA	C15-C16-C17-C18
26	s	314	LHG	O2-C2-C3-O3
26	S	314	LHG	O2-C2-C3-O3
22	d	404	CLA	CBA-CGA-O2A-C1
22	D	405	CLA	CBA-CGA-O2A-C1
21	g	601	CHL	C13-C15-C16-C17
21	n	601	CHL	C13-C15-C16-C17
21	y	601	CHL	C13-C15-C16-C17
21	G	601	CHL	C13-C15-C16-C17
21	N	601	CHL	C13-C15-C16-C17
21	Y	601	CHL	C13-C15-C16-C17
22	b	609	CLA	C10-C11-C12-C13
22	B	612	CLA	C10-C11-C12-C13
36	M	101	LMG	C4-C5-C6-O5
36	T	101	LMG	C4-C5-C6-O5
22	c	503	CLA	C13-C15-C16-C17
22	C	504	CLA	C13-C15-C16-C17
22	R	309	CLA	C2-C3-C5-C6
26	n	617	LHG	C7-C8-C9-C10
26	c	522	LHG	C23-C24-C25-C26
26	d	407	LHG	C7-C8-C9-C10
26	d	409	LHG	C23-C24-C25-C26
26	C	522	LHG	C23-C24-C25-C26
26	D	408	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	D	410	LHG	C23-C24-C25-C26
22	a	406	CLA	O1D-CGD-O2D-CED
22	A	407	CLA	O1D-CGD-O2D-CED
21	g	608	CHL	C8-C10-C11-C12
21	n	607	CHL	C8-C10-C11-C12
21	y	608	CHL	C8-C10-C11-C12
21	G	608	CHL	C8-C10-C11-C12
21	N	607	CHL	C8-C10-C11-C12
21	Y	607	CHL	C8-C10-C11-C12
21	r	306	CHL	C10-C11-C12-C13
21	R	305	CHL	C10-C11-C12-C13
22	b	604	CLA	C10-C11-C12-C13
22	B	607	CLA	C10-C11-C12-C13
22	s	310	CLA	C5-C6-C7-C8
22	S	310	CLA	C5-C6-C7-C8
22	g	614	CLA	O2A-C1-C2-C3
22	n	613	CLA	O2A-C1-C2-C3
22	y	613	CLA	O2A-C1-C2-C3
22	G	614	CLA	O2A-C1-C2-C3
22	N	613	CLA	O2A-C1-C2-C3
22	Y	612	CLA	O2A-C1-C2-C3
22	C	507	CLA	CBD-CGD-O2D-CED
22	S	313	CLA	CBD-CGD-O2D-CED
24	g	617	XAT	C33-C34-C35-C15
25	g	618	NEX	C9-C10-C11-C12
25	Y	616	NEX	C29-C30-C31-C32
31	k	101	BCR	C19-C20-C21-C22
31	K	101	BCR	C19-C20-C21-C22
35	c	518	DGD	O1B-C1B-O2G-C2G
35	C	519	DGD	O1B-C1B-O2G-C2G
26	g	619	LHG	C1-C2-C3-O3
26	y	617	LHG	C1-C2-C3-O3
26	G	618	LHG	C1-C2-C3-O3
26	s	314	LHG	C1-C2-C3-O3
26	S	314	LHG	C1-C2-C3-O3
21	g	605	CHL	C2A-CAA-CBA-CGA
21	G	605	CHL	C2A-CAA-CBA-CGA
21	Y	608	CHL	C2A-CAA-CBA-CGA
21	r	301	CHL	C2A-CAA-CBA-CGA
21	r	307	CHL	C2A-CAA-CBA-CGA
21	R	306	CHL	C2A-CAA-CBA-CGA
22	g	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	n	611	CLA	CBA-CGA-O2A-C1
22	G	612	CLA	CBA-CGA-O2A-C1
22	N	611	CLA	CBA-CGA-O2A-C1
22	w	101	CLA	CBA-CGA-O2A-C1
22	W	101	CLA	CBA-CGA-O2A-C1
26	d	407	LHG	C24-C23-O8-C6
26	D	408	LHG	C24-C23-O8-C6
31	k	101	BCR	C14-C15-C16-C17
31	K	101	BCR	C14-C15-C16-C17
21	g	609	CHL	C8-C10-C11-C12
21	G	609	CHL	C8-C10-C11-C12
22	c	503	CLA	C8-C10-C11-C12
22	c	509	CLA	C5-C6-C7-C8
22	C	504	CLA	C8-C10-C11-C12
22	C	510	CLA	C5-C6-C7-C8
22	c	506	CLA	CBD-CGD-O2D-CED
22	s	313	CLA	CBD-CGD-O2D-CED
22	c	506	CLA	C13-C15-C16-C17
22	C	507	CLA	C13-C15-C16-C17
21	y	609	CHL	C15-C16-C17-C18
22	b	603	CLA	C15-C16-C17-C18
22	B	606	CLA	C15-C16-C17-C18
22	b	607	CLA	O1D-CGD-O2D-CED
22	c	502	CLA	CBA-CGA-O2A-C1
22	C	503	CLA	CBA-CGA-O2A-C1
22	d	403	CLA	C4-C3-C5-C6
22	D	404	CLA	C4-C3-C5-C6
22	Y	602	CLA	O1D-CGD-O2D-CED
26	N	618	LHG	C8-C7-O7-C5
22	g	602	CLA	O1D-CGD-O2D-CED
22	n	602	CLA	O1D-CGD-O2D-CED
22	y	602	CLA	O1D-CGD-O2D-CED
22	G	602	CLA	O1D-CGD-O2D-CED
22	N	602	CLA	O1D-CGD-O2D-CED
22	B	610	CLA	O1D-CGD-O2D-CED
35	a	413	DGD	C2E-C1E-O5D-C6D
35	c	518	DGD	C2D-C1D-O3G-C3G
35	A	401	DGD	C2E-C1E-O5D-C6D
35	C	519	DGD	C2D-C1D-O3G-C3G
26	G	618	LHG	C23-C24-C25-C26
22	B	612	CLA	O1D-CGD-O2D-CED
26	C	520	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
22	b	609	CLA	O1D-CGD-O2D-CED
22	s	303	CLA	CBA-CGA-O2A-C1
22	S	303	CLA	CBA-CGA-O2A-C1
26	N	618	LHG	C24-C23-O8-C6
36	b	620	LMG	O6-C5-C6-O5
36	B	623	LMG	O6-C5-C6-O5
21	r	307	CHL	C6-C7-C8-C10
21	R	306	CHL	C6-C7-C8-C10
22	b	611	CLA	C16-C17-C18-C20
22	c	513	CLA	C16-C17-C18-C20
22	B	614	CLA	C16-C17-C18-C20
22	C	514	CLA	C16-C17-C18-C20
22	g	603	CLA	O1A-CGA-O2A-C1
22	n	603	CLA	O1A-CGA-O2A-C1
22	y	603	CLA	O1A-CGA-O2A-C1
22	G	603	CLA	O1A-CGA-O2A-C1
22	N	603	CLA	O1A-CGA-O2A-C1
22	Y	603	CLA	O1A-CGA-O2A-C1
23	N	615	LUT	C11-C10-C9-C19
23	r	313	LUT	C39-C29-C30-C31
23	R	312	LUT	C39-C29-C30-C31
24	g	617	XAT	C20-C13-C14-C15
24	g	617	XAT	C40-C33-C34-C35
24	y	615	XAT	C40-C33-C34-C35
24	G	617	XAT	C40-C33-C34-C35
24	Y	615	XAT	C20-C13-C14-C15
24	Y	615	XAT	C40-C33-C34-C35
24	r	314	XAT	C11-C10-C9-C19
24	r	314	XAT	C39-C29-C30-C31
24	R	313	XAT	C11-C10-C9-C19
24	R	313	XAT	C39-C29-C30-C31
25	y	616	NEX	C40-C33-C34-C35
25	y	618	NEX	C40-C33-C34-C35
25	N	617	NEX	C11-C10-C9-C19
25	r	315	NEX	C40-C33-C34-C35
31	c	516	BCR	C20-C21-C22-C37
31	B	602	BCR	C11-C10-C9-C34
31	C	517	BCR	C20-C21-C22-C37
31	T	102	BCR	C11-C10-C9-C34
22	s	311	CLA	C3-C5-C6-C7
22	S	311	CLA	C3-C5-C6-C7
22	c	508	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	C8-C10-C11-C12
23	g	616	LUT	C11-C12-C13-C20
23	g	616	LUT	C27-C28-C29-C39
23	G	616	LUT	C11-C12-C13-C20
23	G	616	LUT	C27-C28-C29-C39
23	r	313	LUT	C11-C12-C13-C20
23	R	312	LUT	C11-C12-C13-C20
24	g	617	XAT	C11-C12-C13-C20
24	n	615	XAT	C31-C32-C33-C40
24	G	617	XAT	C11-C12-C13-C20
24	N	616	XAT	C31-C32-C33-C40
24	r	314	XAT	C11-C12-C13-C20
24	r	314	XAT	C27-C28-C29-C39
24	R	313	XAT	C11-C12-C13-C20
25	n	616	NEX	C27-C28-C29-C39
25	y	616	NEX	C27-C28-C29-C39
25	y	618	NEX	C11-C12-C13-C20
25	r	315	NEX	C11-C12-C13-C20
31	k	101	BCR	C11-C12-C13-C35
23	g	615	LUT	C31-C32-C33-C34
23	n	614	LUT	C31-C32-C33-C34
23	y	614	LUT	C31-C32-C33-C34
23	G	615	LUT	C31-C32-C33-C34
23	N	614	LUT	C31-C32-C33-C34
23	Y	613	LUT	C31-C32-C33-C34
24	y	615	XAT	C11-C12-C13-C14
35	a	413	DGD	O6D-C5D-C6D-O5D
22	g	612	CLA	O1A-CGA-O2A-C1
22	n	611	CLA	O1A-CGA-O2A-C1
22	G	612	CLA	O1A-CGA-O2A-C1
22	N	611	CLA	O1A-CGA-O2A-C1
22	w	101	CLA	O1A-CGA-O2A-C1
22	W	101	CLA	O1A-CGA-O2A-C1
26	r	302	LHG	O10-C23-O8-C6
26	R	301	LHG	O10-C23-O8-C6
21	g	609	CHL	C2A-CAA-CBA-CGA
21	n	608	CHL	C2A-CAA-CBA-CGA
21	y	609	CHL	C2A-CAA-CBA-CGA
21	G	609	CHL	C2A-CAA-CBA-CGA
21	N	608	CHL	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	S	308	CLA	C2A-CAA-CBA-CGA
22	c	502	CLA	C5-C6-C7-C8
22	C	503	CLA	C5-C6-C7-C8
26	G	618	LHG	O1-C1-C2-C3
26	c	520	LHG	O1-C1-C2-C3
26	d	407	LHG	O1-C1-C2-C3
26	C	520	LHG	O1-C1-C2-C3
26	D	408	LHG	O1-C1-C2-C3
21	s	302	CHL	O1D-CGD-O2D-CED
21	S	302	CHL	O1D-CGD-O2D-CED
33	a	411	SQD	C46-C45-O47-C7
33	A	412	SQD	C46-C45-O47-C7
24	g	617	XAT	C29-C30-C31-C32
22	d	404	CLA	C16-C17-C18-C19
22	d	404	CLA	C16-C17-C18-C20
22	D	405	CLA	C16-C17-C18-C19
22	D	405	CLA	C16-C17-C18-C20
22	s	309	CLA	C6-C7-C8-C9
22	s	309	CLA	C6-C7-C8-C10
22	S	309	CLA	C6-C7-C8-C9
22	S	309	CLA	C6-C7-C8-C10
22	g	603	CLA	C3-C5-C6-C7
22	n	603	CLA	C3-C5-C6-C7
22	y	603	CLA	C3-C5-C6-C7
22	G	603	CLA	C3-C5-C6-C7
22	N	603	CLA	C3-C5-C6-C7
22	Y	603	CLA	C3-C5-C6-C7
22	a	405	CLA	C3-C5-C6-C7
22	A	406	CLA	C3-C5-C6-C7
22	s	310	CLA	C3-C5-C6-C7
22	S	310	CLA	C3-C5-C6-C7
23	G	616	LUT	C12-C13-C14-C15
23	N	615	LUT	C11-C10-C9-C8
23	N	615	LUT	C28-C29-C30-C31
23	N	615	LUT	C32-C33-C34-C35
23	Y	614	LUT	C28-C29-C30-C31
24	g	617	XAT	C11-C10-C9-C8
24	g	617	XAT	C12-C13-C14-C15
24	g	617	XAT	C32-C33-C34-C35
24	n	615	XAT	C11-C10-C9-C8
24	n	615	XAT	C12-C13-C14-C15
24	y	615	XAT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	G	617	XAT	C11-C10-C9-C8
24	G	617	XAT	C12-C13-C14-C15
24	N	616	XAT	C11-C10-C9-C8
24	N	616	XAT	C12-C13-C14-C15
24	N	616	XAT	C32-C33-C34-C35
24	Y	615	XAT	C12-C13-C14-C15
24	r	314	XAT	C28-C29-C30-C31
24	R	313	XAT	C28-C29-C30-C31
25	n	616	NEX	C11-C10-C9-C8
25	n	616	NEX	C12-C13-C14-C15
25	y	616	NEX	C32-C33-C34-C35
25	y	618	NEX	C32-C33-C34-C35
25	N	617	NEX	C11-C10-C9-C8
25	r	315	NEX	C32-C33-C34-C35
31	k	101	BCR	C16-C17-C18-C19
31	k	101	BCR	C20-C21-C22-C23
31	B	602	BCR	C11-C10-C9-C8
31	K	101	BCR	C16-C17-C18-C19
31	K	101	BCR	C20-C21-C22-C23
31	T	102	BCR	C11-C10-C9-C8
35	a	413	DGD	O6E-C1E-O5D-C6D
35	A	401	DGD	O6E-C1E-O5D-C6D
35	A	401	DGD	O6D-C5D-C6D-O5D
26	s	314	LHG	C8-C7-O7-C5
26	S	314	LHG	C8-C7-O7-C5
22	r	312	CLA	C5-C6-C7-C8
22	R	311	CLA	C5-C6-C7-C8
35	a	413	DGD	C4D-C5D-C6D-O5D
35	A	401	DGD	C4D-C5D-C6D-O5D
22	c	511	CLA	O1D-CGD-O2D-CED
22	C	512	CLA	O1D-CGD-O2D-CED
22	c	513	CLA	CBA-CGA-O2A-C1
26	n	617	LHG	C24-C23-O8-C6
21	R	306	CHL	C5-C6-C7-C8
26	l	102	LHG	C23-C24-C25-C26
26	L	103	LHG	C23-C24-C25-C26
22	c	512	CLA	C3-C5-C6-C7
22	C	513	CLA	C3-C5-C6-C7
21	r	306	CHL	C16-C17-C18-C20
21	r	307	CHL	C6-C7-C8-C9
21	R	305	CHL	C16-C17-C18-C20
21	R	306	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	a	405	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C19
22	A	406	CLA	C16-C17-C18-C20
22	B	614	CLA	C16-C17-C18-C19
22	s	313	CLA	C6-C7-C8-C10
22	S	313	CLA	C6-C7-C8-C10
21	r	307	CHL	C5-C6-C7-C8
22	a	404	CLA	C15-C16-C17-C18
22	A	405	CLA	C15-C16-C17-C18
26	b	619	LHG	C32-C33-C34-C35
26	B	622	LHG	C32-C33-C34-C35
35	h	102	DGD	C5A-C6A-C7A-C8A
36	M	101	LMG	C17-C18-C19-C20
36	T	101	LMG	C17-C18-C19-C20
26	N	618	LHG	C29-C30-C31-C32
26	Y	617	LHG	C32-C33-C34-C35
26	c	520	LHG	C27-C28-C29-C30
26	c	521	LHG	C11-C10-C9-C8
26	d	408	LHG	C27-C28-C29-C30
26	C	520	LHG	C27-C28-C29-C30
26	C	521	LHG	C11-C10-C9-C8
26	D	409	LHG	C27-C28-C29-C30
26	D	410	LHG	C27-C28-C29-C30
26	r	302	LHG	C32-C33-C34-C35
26	R	301	LHG	C32-C33-C34-C35
35	H	102	DGD	C5A-C6A-C7A-C8A
36	c	523	LMG	C11-C12-C13-C14
36	B	601	LMG	C30-C31-C32-C33
36	C	523	LMG	C11-C12-C13-C14
36	I	101	LMG	C30-C31-C32-C33
22	C	512	CLA	C5-C6-C7-C8
26	c	520	LHG	C12-C13-C14-C15
26	d	409	LHG	C27-C28-C29-C30
26	C	520	LHG	C12-C13-C14-C15
26	c	520	LHG	O10-C23-O8-C6
26	C	520	LHG	O10-C23-O8-C6
22	C	514	CLA	CBA-CGA-O2A-C1
26	n	617	LHG	C24-C25-C26-C27
26	N	618	LHG	C15-C16-C17-C18
26	c	521	LHG	C18-C19-C20-C21
26	d	408	LHG	C32-C33-C34-C35
26	C	521	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
26	D	409	LHG	C32-C33-C34-C35
26	D	410	LHG	C10-C11-C12-C13
26	r	302	LHG	C12-C13-C14-C15
26	R	301	LHG	C12-C13-C14-C15
35	c	519	DGD	C6B-C7B-C8B-C9B
35	J	101	DGD	C6B-C7B-C8B-C9B
36	b	620	LMG	C22-C23-C24-C25
36	B	623	LMG	C22-C23-C24-C25
36	b	620	LMG	O9-C10-O7-C8
36	B	623	LMG	O9-C10-O7-C8
26	n	617	LHG	O1-C1-C2-O2
26	N	618	LHG	O1-C1-C2-O2
26	c	522	LHG	O1-C1-C2-O2
26	C	522	LHG	O1-C1-C2-O2
26	g	619	LHG	C26-C27-C28-C29
26	d	409	LHG	C10-C11-C12-C13
22	c	512	CLA	O1D-CGD-O2D-CED
22	C	513	CLA	O1D-CGD-O2D-CED
22	c	511	CLA	C5-C6-C7-C8
22	g	612	CLA	C4B-C3B-CAB-CBB
22	n	611	CLA	C4B-C3B-CAB-CBB
22	G	612	CLA	C4B-C3B-CAB-CBB
22	N	611	CLA	C4B-C3B-CAB-CBB
22	c	502	CLA	C4B-C3B-CAB-CBB
22	c	508	CLA	C4B-C3B-CAB-CBB
22	w	101	CLA	C4B-C3B-CAB-CBB
22	C	503	CLA	C4B-C3B-CAB-CBB
22	C	509	CLA	C4B-C3B-CAB-CBB
22	W	101	CLA	C4B-C3B-CAB-CBB
22	s	309	CLA	C4B-C3B-CAB-CBB
22	S	309	CLA	C4B-C3B-CAB-CBB
36	M	101	LMG	C33-C34-C35-C36
36	T	101	LMG	C33-C34-C35-C36
22	a	405	CLA	C16-C17-C18-C19
22	x	101	CLA	C16-C17-C18-C19
22	A	406	CLA	C16-C17-C18-C19
22	B	603	CLA	C16-C17-C18-C19
22	d	404	CLA	O1A-CGA-O2A-C1
22	D	405	CLA	O1A-CGA-O2A-C1
22	s	308	CLA	C2A-CAA-CBA-CGA
26	r	302	LHG	C27-C28-C29-C30
26	R	301	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
33	a	411	SQD	C26-C27-C28-C29
33	A	412	SQD	C26-C27-C28-C29
35	c	519	DGD	C5B-C6B-C7B-C8B
35	J	101	DGD	C5B-C6B-C7B-C8B
26	c	520	LHG	O2-C2-C3-O3
33	A	412	SQD	C23-C24-C25-C26
22	y	612	CLA	C15-C16-C17-C18
26	n	617	LHG	C30-C31-C32-C33
26	b	619	LHG	C29-C30-C31-C32
26	d	408	LHG	C30-C31-C32-C33
26	B	622	LHG	C29-C30-C31-C32
36	b	620	LMG	C19-C20-C21-C22
36	B	623	LMG	C19-C20-C21-C22
36	M	101	LMG	C30-C31-C32-C33
36	T	101	LMG	C30-C31-C32-C33
21	g	605	CHL	C3A-C2A-CAA-CBA
21	y	605	CHL	C3A-C2A-CAA-CBA
21	G	605	CHL	C3A-C2A-CAA-CBA
21	r	301	CHL	C3A-C2A-CAA-CBA
21	r	306	CHL	C3A-C2A-CAA-CBA
21	r	307	CHL	C3A-C2A-CAA-CBA
21	S	301	CHL	C3A-C2A-CAA-CBA
21	R	305	CHL	C3A-C2A-CAA-CBA
21	R	306	CHL	C3A-C2A-CAA-CBA
22	g	610	CLA	C3A-C2A-CAA-CBA
22	g	613	CLA	C3A-C2A-CAA-CBA
22	n	609	CLA	C3A-C2A-CAA-CBA
22	n	612	CLA	C3A-C2A-CAA-CBA
22	y	610	CLA	C3A-C2A-CAA-CBA
22	y	612	CLA	C3A-C2A-CAA-CBA
22	G	610	CLA	C3A-C2A-CAA-CBA
22	G	613	CLA	C3A-C2A-CAA-CBA
22	N	609	CLA	C3A-C2A-CAA-CBA
22	N	612	CLA	C3A-C2A-CAA-CBA
22	Y	609	CLA	C3A-C2A-CAA-CBA
22	Y	611	CLA	C3A-C2A-CAA-CBA
22	b	614	CLA	C3A-C2A-CAA-CBA
22	c	511	CLA	C3A-C2A-CAA-CBA
22	x	101	CLA	C3A-C2A-CAA-CBA
22	B	603	CLA	C3A-C2A-CAA-CBA
22	B	617	CLA	C3A-C2A-CAA-CBA
22	C	512	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	s	304	CLA	C3A-C2A-CAA-CBA
22	S	304	CLA	C3A-C2A-CAA-CBA
30	a	407	PHO	C3A-C2A-CAA-CBA
30	A	408	PHO	C3A-C2A-CAA-CBA
26	G	618	LHG	C29-C30-C31-C32
26	d	408	LHG	C29-C30-C31-C32
26	l	102	LHG	C25-C26-C27-C28
26	D	409	LHG	C29-C30-C31-C32
26	D	409	LHG	C30-C31-C32-C33
26	L	103	LHG	C25-C26-C27-C28
22	g	603	CLA	C8-C10-C11-C12
22	n	603	CLA	C8-C10-C11-C12
22	y	603	CLA	C8-C10-C11-C12
22	G	603	CLA	C8-C10-C11-C12
22	N	603	CLA	C8-C10-C11-C12
22	Y	603	CLA	C8-C10-C11-C12
30	a	407	PHO	C5-C6-C7-C8
30	A	408	PHO	C5-C6-C7-C8
26	r	302	LHG	C5-C6-O8-C23
26	R	301	LHG	C5-C6-O8-C23
33	a	411	SQD	C23-C24-C25-C26
26	y	617	LHG	C29-C30-C31-C32
35	h	102	DGD	C3B-C4B-C5B-C6B
35	H	102	DGD	C3B-C4B-C5B-C6B
24	y	615	XAT	C33-C34-C35-C15
22	x	101	CLA	C16-C17-C18-C20
22	B	603	CLA	C16-C17-C18-C20
26	c	520	LHG	C32-C33-C34-C35
26	C	520	LHG	C32-C33-C34-C35
26	s	314	LHG	C32-C33-C34-C35
26	S	314	LHG	C32-C33-C34-C35
33	l	103	SQD	C9-C10-C11-C12
33	L	101	SQD	C9-C10-C11-C12
35	h	102	DGD	C4A-C5A-C6A-C7A
36	K	103	LMG	C32-C33-C34-C35
33	D	402	SQD	C12-C13-C14-C15
35	H	102	DGD	C4A-C5A-C6A-C7A
36	k	103	LMG	C32-C33-C34-C35
22	c	503	CLA	CBA-CGA-O2A-C1
22	C	504	CLA	CBA-CGA-O2A-C1
26	G	618	LHG	C24-C23-O8-C6
26	b	619	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	d	408	LHG	C11-C10-C9-C8
26	B	622	LHG	C11-C12-C13-C14
26	D	409	LHG	C11-C10-C9-C8
26	s	314	LHG	C27-C28-C29-C30
33	d	402	SQD	C12-C13-C14-C15
33	l	103	SQD	C27-C28-C29-C30
33	L	101	SQD	C27-C28-C29-C30
36	c	523	LMG	C33-C34-C35-C36
36	C	523	LMG	C33-C34-C35-C36
36	M	101	LMG	C29-C30-C31-C32
36	T	101	LMG	C29-C30-C31-C32
26	g	619	LHG	C28-C29-C30-C31
26	b	619	LHG	C30-C31-C32-C33
26	B	622	LHG	C30-C31-C32-C33
26	S	314	LHG	C27-C28-C29-C30
35	a	413	DGD	C8A-C9A-CAA-CBA
35	h	102	DGD	C5B-C6B-C7B-C8B
35	A	401	DGD	C8A-C9A-CAA-CBA
35	H	102	DGD	C5B-C6B-C7B-C8B
36	b	620	LMG	C34-C35-C36-C37
36	B	623	LMG	C34-C35-C36-C37
36	M	101	LMG	C16-C17-C18-C19
22	c	502	CLA	O1A-CGA-O2A-C1
22	C	503	CLA	O1A-CGA-O2A-C1
22	s	303	CLA	O1A-CGA-O2A-C1
22	S	303	CLA	O1A-CGA-O2A-C1
35	J	101	DGD	C7B-C8B-C9B-CAB
36	T	101	LMG	C16-C17-C18-C19
26	g	619	LHG	C11-C12-C13-C14
26	c	521	LHG	C29-C30-C31-C32
35	c	519	DGD	C7B-C8B-C9B-CAB
26	G	618	LHG	C16-C17-C18-C19
26	C	521	LHG	C29-C30-C31-C32
26	s	314	LHG	C30-C31-C32-C33
26	S	314	LHG	C30-C31-C32-C33
35	a	413	DGD	C2A-C3A-C4A-C5A
35	A	401	DGD	C2A-C3A-C4A-C5A
36	B	623	LMG	C20-C21-C22-C23
22	g	611	CLA	C2B-C3B-CAB-CBB
22	g	612	CLA	C2B-C3B-CAB-CBB
22	n	610	CLA	C2B-C3B-CAB-CBB
22	n	611	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	y	611	CLA	C2B-C3B-CAB-CBB
22	G	611	CLA	C2B-C3B-CAB-CBB
22	G	612	CLA	C2B-C3B-CAB-CBB
22	N	610	CLA	C2B-C3B-CAB-CBB
22	N	611	CLA	C2B-C3B-CAB-CBB
22	Y	610	CLA	C2B-C3B-CAB-CBB
22	c	502	CLA	C2B-C3B-CAB-CBB
22	c	508	CLA	C2B-C3B-CAB-CBB
22	w	101	CLA	C2B-C3B-CAB-CBB
22	C	503	CLA	C2B-C3B-CAB-CBB
22	C	509	CLA	C2B-C3B-CAB-CBB
22	W	101	CLA	C2B-C3B-CAB-CBB
22	r	309	CLA	C2B-C3B-CAB-CBB
22	s	309	CLA	C2B-C3B-CAB-CBB
22	S	309	CLA	C2B-C3B-CAB-CBB
22	R	308	CLA	C2B-C3B-CAB-CBB
23	g	615	LUT	C5-C6-C7-C8
23	n	614	LUT	C5-C6-C7-C8
23	y	614	LUT	C5-C6-C7-C8
23	G	615	LUT	C5-C6-C7-C8
23	N	614	LUT	C5-C6-C7-C8
23	Y	613	LUT	C5-C6-C7-C8
31	d	405	BCR	C1-C6-C7-C8
31	D	406	BCR	C1-C6-C7-C8
26	d	409	LHG	C29-C30-C31-C32
26	D	410	LHG	C29-C30-C31-C32
36	b	620	LMG	C20-C21-C22-C23
33	d	402	SQD	C8-C7-O47-C45
33	D	402	SQD	C8-C7-O47-C45
26	N	618	LHG	C27-C28-C29-C30
26	b	619	LHG	C33-C34-C35-C36
26	l	102	LHG	C12-C13-C14-C15
26	B	622	LHG	C33-C34-C35-C36
35	c	518	DGD	C7A-C8A-C9A-CAA
35	C	519	DGD	C7A-C8A-C9A-CAA
36	M	101	LMG	C34-C35-C36-C37
36	T	101	LMG	C34-C35-C36-C37
26	n	617	LHG	C28-C29-C30-C31
26	L	103	LHG	C12-C13-C14-C15
35	c	519	DGD	C6A-C7A-C8A-C9A
21	Y	601	CHL	C2A-CAA-CBA-CGA
21	s	301	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	S	301	CHL	C2A-CAA-CBA-CGA
22	s	313	CLA	C2A-CAA-CBA-CGA
22	S	313	CLA	C2A-CAA-CBA-CGA
26	C	521	LHG	C27-C28-C29-C30
26	C	522	LHG	C9-C10-C11-C12
35	J	101	DGD	C6A-C7A-C8A-C9A
36	b	620	LMG	C38-C39-C40-C41
36	B	623	LMG	C38-C39-C40-C41
22	c	513	CLA	O1A-CGA-O2A-C1
22	C	514	CLA	O1A-CGA-O2A-C1
26	Y	617	LHG	C27-C28-C29-C30
26	c	521	LHG	C27-C28-C29-C30
26	c	522	LHG	C9-C10-C11-C12
35	c	519	DGD	C2B-C3B-C4B-C5B
35	J	101	DGD	C2B-C3B-C4B-C5B
36	b	620	LMG	C16-C17-C18-C19
36	B	623	LMG	C16-C17-C18-C19
26	N	618	LHG	O9-C7-O7-C5
21	g	607	CHL	C4-C3-C5-C6
21	n	606	CHL	C4-C3-C5-C6
21	y	607	CHL	C4-C3-C5-C6
21	G	607	CHL	C4-C3-C5-C6
21	N	606	CHL	C4-C3-C5-C6
21	Y	606	CHL	C4-C3-C5-C6
22	b	602	CLA	C4-C3-C5-C6
22	B	605	CLA	C4-C3-C5-C6
31	k	102	BCR	C10-C11-C12-C13
31	B	602	BCR	C18-C19-C20-C21
31	K	102	BCR	C10-C11-C12-C13
31	T	102	BCR	C18-C19-C20-C21
22	s	309	CLA	C2-C3-C5-C6
22	S	309	CLA	C2-C3-C5-C6
22	c	513	CLA	C16-C17-C18-C19
22	C	514	CLA	C16-C17-C18-C19
26	g	619	LHG	C29-C30-C31-C32
26	n	617	LHG	C12-C13-C14-C15
36	c	523	LMG	C12-C13-C14-C15
36	C	523	LMG	C12-C13-C14-C15
26	N	618	LHG	C24-C25-C26-C27
26	D	410	LHG	C15-C16-C17-C18
22	d	404	CLA	C10-C11-C12-C13
22	D	405	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	N	618	LHG	C10-C11-C12-C13
26	d	409	LHG	C15-C16-C17-C18
36	T	101	LMG	C32-C33-C34-C35
31	a	409	BCR	C6-C7-C8-C9
31	A	410	BCR	C6-C7-C8-C9
36	M	101	LMG	C32-C33-C34-C35
22	c	508	CLA	C13-C15-C16-C17
22	C	509	CLA	C13-C15-C16-C17
26	g	619	LHG	C30-C31-C32-C33
26	C	522	LHG	C32-C33-C34-C35
22	Y	612	CLA	O1D-CGD-O2D-CED
26	G	618	LHG	C25-C26-C27-C28
26	c	522	LHG	C32-C33-C34-C35
36	d	410	LMG	C15-C16-C17-C18
36	k	103	LMG	C38-C39-C40-C41
36	D	411	LMG	C15-C16-C17-C18
36	K	103	LMG	C38-C39-C40-C41
26	b	619	LHG	C26-C27-C28-C29
26	B	622	LHG	C26-C27-C28-C29
36	c	523	LMG	C14-C15-C16-C17
36	C	523	LMG	C14-C15-C16-C17
21	G	608	CHL	C16-C17-C18-C20
21	N	607	CHL	C16-C17-C18-C20
26	G	618	LHG	C8-C7-O7-C5
35	c	518	DGD	C2B-C1B-O2G-C2G
35	C	519	DGD	C2B-C1B-O2G-C2G
36	M	101	LMG	C28-C29-C30-C31
36	T	101	LMG	C28-C29-C30-C31
30	a	407	PHO	C13-C15-C16-C17
30	A	408	PHO	C13-C15-C16-C17
26	n	617	LHG	C11-C12-C13-C14
26	G	618	LHG	C17-C18-C19-C20
22	n	613	CLA	O1D-CGD-O2D-CED
22	G	614	CLA	O1D-CGD-O2D-CED
31	K	101	BCR	C11-C12-C13-C35
36	k	103	LMG	C28-C29-C30-C31
36	K	103	LMG	C28-C29-C30-C31
26	c	522	LHG	C30-C31-C32-C33
26	C	522	LHG	C30-C31-C32-C33
33	a	411	SQD	C14-C15-C16-C17
33	A	412	SQD	C14-C15-C16-C17
35	a	413	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
36	B	623	LMG	C31-C32-C33-C34
21	g	608	CHL	C2C-C3C-CAC-CBC
21	G	608	CHL	C2C-C3C-CAC-CBC
23	r	313	LUT	C7-C8-C9-C10
23	R	312	LUT	C7-C8-C9-C10
33	l	101	SQD	C12-C13-C14-C15
36	b	620	LMG	C31-C32-C33-C34
36	K	103	LMG	C30-C31-C32-C33
21	r	308	CHL	C2A-CAA-CBA-CGA
21	R	307	CHL	C2A-CAA-CBA-CGA
21	Y	607	CHL	C2C-C3C-CAC-CBC
21	g	608	CHL	C16-C17-C18-C20
21	n	607	CHL	C16-C17-C18-C20
21	y	608	CHL	C16-C17-C18-C20
21	Y	607	CHL	C16-C17-C18-C20
21	r	306	CHL	C16-C17-C18-C19
21	R	305	CHL	C16-C17-C18-C19
22	r	312	CLA	C11-C12-C13-C14
22	r	312	CLA	C11-C12-C13-C15
22	R	311	CLA	C11-C12-C13-C14
22	R	311	CLA	C11-C12-C13-C15
33	L	102	SQD	C12-C13-C14-C15
35	c	517	DGD	C4A-C5A-C6A-C7A
35	A	401	DGD	C4A-C5A-C6A-C7A
36	k	103	LMG	C18-C19-C20-C21
36	k	103	LMG	C30-C31-C32-C33
36	K	103	LMG	C18-C19-C20-C21
21	n	607	CHL	C2C-C3C-CAC-CBC
21	y	608	CHL	C2C-C3C-CAC-CBC
21	N	607	CHL	C2C-C3C-CAC-CBC
26	c	521	LHG	C13-C14-C15-C16
26	c	522	LHG	C13-C14-C15-C16
26	C	521	LHG	C13-C14-C15-C16
26	C	522	LHG	C13-C14-C15-C16
26	s	314	LHG	C24-C25-C26-C27
35	C	518	DGD	C4A-C5A-C6A-C7A
22	g	614	CLA	O1D-CGD-O2D-CED
22	y	613	CLA	O1D-CGD-O2D-CED
22	N	613	CLA	O1D-CGD-O2D-CED
26	S	314	LHG	C24-C25-C26-C27
36	b	620	LMG	C37-C38-C39-C40
36	B	623	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
26	B	622	LHG	C27-C28-C29-C30
26	b	619	LHG	C8-C7-O7-C5
26	B	622	LHG	C8-C7-O7-C5
26	b	619	LHG	C27-C28-C29-C30
22	C	504	CLA	O1A-CGA-O2A-C1
35	c	519	DGD	C4A-C5A-C6A-C7A
36	k	103	LMG	C29-C30-C31-C32
36	K	103	LMG	C29-C30-C31-C32
22	b	610	CLA	C5-C6-C7-C8
22	B	607	CLA	C8-C10-C11-C12
22	B	613	CLA	C5-C6-C7-C8
35	J	101	DGD	C4A-C5A-C6A-C7A
36	b	620	LMG	C15-C16-C17-C18
36	B	623	LMG	C15-C16-C17-C18
26	d	408	LHG	O7-C5-C6-O8
26	D	409	LHG	O7-C5-C6-O8
33	a	411	SQD	C11-C12-C13-C14
33	l	103	SQD	C25-C26-C27-C28
33	A	412	SQD	C11-C12-C13-C14
33	L	101	SQD	C25-C26-C27-C28
22	b	610	CLA	CBA-CGA-O2A-C1
22	B	613	CLA	CBA-CGA-O2A-C1
22	c	503	CLA	O1A-CGA-O2A-C1
26	c	521	LHG	C28-C29-C30-C31
26	C	521	LHG	C28-C29-C30-C31
33	a	411	SQD	C10-C11-C12-C13
33	A	412	SQD	C10-C11-C12-C13
36	c	523	LMG	C19-C20-C21-C22
36	C	523	LMG	C19-C20-C21-C22
21	N	608	CHL	C13-C15-C16-C17
22	b	604	CLA	C8-C10-C11-C12
36	k	103	LMG	C16-C17-C18-C19
36	K	103	LMG	C16-C17-C18-C19
21	g	609	CHL	C11-C12-C13-C15
21	G	609	CHL	C11-C12-C13-C15
21	g	607	CHL	C2-C3-C5-C6
21	n	606	CHL	C2-C3-C5-C6
21	y	607	CHL	C2-C3-C5-C6
21	G	607	CHL	C2-C3-C5-C6
21	N	606	CHL	C2-C3-C5-C6
21	Y	606	CHL	C2-C3-C5-C6
26	s	314	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
26	S	314	LHG	O9-C7-O7-C5
35	c	519	DGD	O1B-C1B-O2G-C2G
35	J	101	DGD	O1B-C1B-O2G-C2G
26	N	618	LHG	C11-C10-C9-C8
26	Y	617	LHG	C15-C16-C17-C18
26	c	520	LHG	C30-C31-C32-C33
26	C	520	LHG	C30-C31-C32-C33
33	L	101	SQD	C14-C15-C16-C17
21	g	601	CHL	C2A-CAA-CBA-CGA
21	n	601	CHL	C2A-CAA-CBA-CGA
21	y	601	CHL	C2A-CAA-CBA-CGA
21	y	605	CHL	C2A-CAA-CBA-CGA
21	G	601	CHL	C2A-CAA-CBA-CGA
21	N	601	CHL	C2A-CAA-CBA-CGA
22	g	614	CLA	C2A-CAA-CBA-CGA
22	n	613	CLA	C2A-CAA-CBA-CGA
22	y	613	CLA	C2A-CAA-CBA-CGA
22	G	614	CLA	C2A-CAA-CBA-CGA
22	N	613	CLA	C2A-CAA-CBA-CGA
22	Y	612	CLA	C2A-CAA-CBA-CGA
22	r	310	CLA	C2A-CAA-CBA-CGA
22	s	310	CLA	C2A-CAA-CBA-CGA
22	S	310	CLA	C2A-CAA-CBA-CGA
22	R	309	CLA	C2A-CAA-CBA-CGA
26	S	314	LHG	C24-C23-O8-C6
26	g	619	LHG	C33-C34-C35-C36
33	l	103	SQD	C14-C15-C16-C17
35	c	517	DGD	C2B-C3B-C4B-C5B
35	C	518	DGD	C2B-C3B-C4B-C5B
36	w	102	LMG	C18-C19-C20-C21
36	C	502	LMG	C18-C19-C20-C21
22	C	509	CLA	C5-C6-C7-C8
35	H	102	DGD	C4B-C5B-C6B-C7B
26	y	617	LHG	C27-C28-C29-C30
26	y	617	LHG	C33-C34-C35-C36
26	s	314	LHG	C15-C16-C17-C18
26	S	314	LHG	C15-C16-C17-C18
35	h	102	DGD	C4B-C5B-C6B-C7B
21	r	306	CHL	C8-C10-C11-C12
21	R	305	CHL	C8-C10-C11-C12
26	c	520	LHG	O1-C1-C2-O2
26	d	407	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
26	l	102	LHG	O1-C1-C2-O2
26	C	520	LHG	O1-C1-C2-O2
26	D	408	LHG	O1-C1-C2-O2
26	L	103	LHG	O1-C1-C2-O2
22	a	405	CLA	C1A-C2A-CAA-CBA
22	b	614	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
22	x	101	CLA	C1A-C2A-CAA-CBA
22	A	406	CLA	C1A-C2A-CAA-CBA
22	B	603	CLA	C1A-C2A-CAA-CBA
22	B	617	CLA	C1A-C2A-CAA-CBA
22	C	507	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C1A-C2A-CAA-CBA
22	r	305	CLA	C1A-C2A-CAA-CBA
22	r	310	CLA	C1A-C2A-CAA-CBA
22	s	304	CLA	C1A-C2A-CAA-CBA
22	s	309	CLA	C1A-C2A-CAA-CBA
22	s	313	CLA	C1A-C2A-CAA-CBA
22	S	304	CLA	C1A-C2A-CAA-CBA
22	S	309	CLA	C1A-C2A-CAA-CBA
22	S	313	CLA	C1A-C2A-CAA-CBA
22	R	304	CLA	C1A-C2A-CAA-CBA
22	R	309	CLA	C1A-C2A-CAA-CBA
26	s	314	LHG	C24-C23-O8-C6
22	c	508	CLA	C5-C6-C7-C8
26	n	617	LHG	C33-C34-C35-C36
26	N	618	LHG	C28-C29-C30-C31
26	L	103	LHG	C32-C33-C34-C35
35	c	517	DGD	C6B-C7B-C8B-C9B
35	C	518	DGD	C6B-C7B-C8B-C9B
26	Y	617	LHG	C17-C18-C19-C20
26	d	409	LHG	C24-C25-C26-C27
26	l	102	LHG	C32-C33-C34-C35
21	g	607	CHL	C3-C5-C6-C7
21	n	606	CHL	C3-C5-C6-C7
21	y	607	CHL	C3-C5-C6-C7
21	G	607	CHL	C3-C5-C6-C7
21	N	606	CHL	C3-C5-C6-C7
21	Y	606	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	G	610	CLA	C12-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C10
22	b	611	CLA	C6-C7-C8-C10
22	b	612	CLA	C11-C10-C8-C7
22	c	504	CLA	C11-C10-C8-C7
22	c	513	CLA	C12-C13-C15-C16
22	B	605	CLA	C6-C7-C8-C10
22	B	614	CLA	C6-C7-C8-C10
22	B	615	CLA	C11-C10-C8-C7
22	C	505	CLA	C11-C10-C8-C7
22	C	514	CLA	C12-C13-C15-C16
26	c	522	LHG	C25-C26-C27-C28
26	C	522	LHG	C25-C26-C27-C28
22	a	405	CLA	C13-C15-C16-C17
22	A	406	CLA	C13-C15-C16-C17
36	D	411	LMG	O6-C5-C6-O5
26	D	410	LHG	C24-C25-C26-C27
35	A	401	DGD	C7B-C8B-C9B-CAB
35	a	413	DGD	C7B-C8B-C9B-CAB
26	d	409	LHG	C7-C8-C9-C10
26	D	410	LHG	C7-C8-C9-C10
22	d	403	CLA	C2-C3-C5-C6
22	D	404	CLA	C2-C3-C5-C6
36	k	103	LMG	C17-C18-C19-C20
36	K	103	LMG	C17-C18-C19-C20
36	d	410	LMG	O6-C5-C6-O5
22	g	610	CLA	C5-C6-C7-C8
22	n	609	CLA	C5-C6-C7-C8
22	G	610	CLA	C5-C6-C7-C8
22	Y	609	CLA	C5-C6-C7-C8
26	c	522	LHG	C8-C7-O7-C5
26	C	522	LHG	C8-C7-O7-C5
22	g	613	CLA	C2A-CAA-CBA-CGA
22	n	612	CLA	C2A-CAA-CBA-CGA
22	y	612	CLA	C2A-CAA-CBA-CGA
22	G	613	CLA	C2A-CAA-CBA-CGA
22	N	612	CLA	C2A-CAA-CBA-CGA
22	Y	611	CLA	C2A-CAA-CBA-CGA
22	b	601	CLA	C2A-CAA-CBA-CGA
22	B	604	CLA	C2A-CAA-CBA-CGA
21	g	608	CHL	C11-C10-C8-C9
21	n	607	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
21	y	608	CHL	C11-C10-C8-C9
21	G	608	CHL	C11-C10-C8-C9
21	N	607	CHL	C11-C10-C8-C9
21	Y	607	CHL	C11-C10-C8-C9
22	g	602	CLA	C14-C13-C15-C16
22	n	602	CLA	C14-C13-C15-C16
22	y	602	CLA	C14-C13-C15-C16
22	G	602	CLA	C14-C13-C15-C16
22	N	602	CLA	C14-C13-C15-C16
22	Y	602	CLA	C14-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C9
22	b	606	CLA	C14-C13-C15-C16
22	b	609	CLA	C6-C7-C8-C9
22	b	612	CLA	C11-C10-C8-C9
22	b	614	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C10-C8-C9
22	B	605	CLA	C6-C7-C8-C9
22	B	609	CLA	C14-C13-C15-C16
22	B	612	CLA	C6-C7-C8-C9
22	B	615	CLA	C11-C10-C8-C9
22	B	617	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C10-C8-C9
26	c	520	LHG	C33-C34-C35-C36
26	C	520	LHG	C33-C34-C35-C36
35	c	518	DGD	C6A-C7A-C8A-C9A
26	Y	617	LHG	C30-C31-C32-C33
33	a	411	SQD	C18-C19-C20-C21
35	H	102	DGD	C8A-C9A-CAA-CBA
22	c	504	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	CBA-CGA-O2A-C1
22	y	610	CLA	C5-C6-C7-C8
22	N	609	CLA	C5-C6-C7-C8
22	c	502	CLA	C15-C16-C17-C18
22	C	503	CLA	C15-C16-C17-C18
33	A	412	SQD	C18-C19-C20-C21
35	h	102	DGD	C8A-C9A-CAA-CBA
35	C	519	DGD	C6A-C7A-C8A-C9A
35	a	413	DGD	O6E-C5E-C6E-O5E
35	A	401	DGD	O6E-C5E-C6E-O5E
33	a	411	SQD	C2-C1-O6-C44
33	A	412	SQD	C2-C1-O6-C44
22	g	613	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	b	608	CLA	C8-C10-C11-C12
22	B	611	CLA	C8-C10-C11-C12
26	y	617	LHG	C28-C29-C30-C31
26	Y	617	LHG	C4-C5-C6-O8
26	b	619	LHG	C4-C5-C6-O8
26	c	522	LHG	C4-C5-C6-O8
26	d	408	LHG	C4-C5-C6-O8
26	B	622	LHG	C4-C5-C6-O8
26	C	522	LHG	C4-C5-C6-O8
26	D	409	LHG	C4-C5-C6-O8
33	l	103	SQD	O6-C44-C45-C46
33	L	101	SQD	O6-C44-C45-C46
36	c	523	LMG	C7-C8-C9-O8
36	B	601	LMG	C7-C8-C9-O8
36	C	523	LMG	C7-C8-C9-O8
36	I	101	LMG	C7-C8-C9-O8
36	B	601	LMG	C4-C5-C6-O5
36	I	101	LMG	C4-C5-C6-O5
36	w	102	LMG	C30-C31-C32-C33
36	C	502	LMG	C30-C31-C32-C33
26	c	520	LHG	C11-C10-C9-C8
26	C	520	LHG	C11-C10-C9-C8
22	g	610	CLA	C15-C16-C17-C18
26	b	619	LHG	C24-C23-O8-C6
26	B	622	LHG	C24-C23-O8-C6
21	g	609	CHL	C11-C12-C13-C14
21	G	609	CHL	C11-C12-C13-C14
26	y	617	LHG	C24-C25-C26-C27
26	d	407	LHG	C27-C28-C29-C30
26	c	520	LHG	C16-C17-C18-C19
26	C	520	LHG	C16-C17-C18-C19
26	D	408	LHG	C27-C28-C29-C30
26	y	617	LHG	C12-C13-C14-C15
26	r	302	LHG	C26-C27-C28-C29
26	R	301	LHG	C26-C27-C28-C29
36	d	410	LMG	C18-C19-C20-C21
36	D	411	LMG	C18-C19-C20-C21
31	k	101	BCR	C16-C17-C18-C36
31	B	602	BCR	C20-C21-C22-C37
31	K	101	BCR	C16-C17-C18-C36
31	T	102	BCR	C20-C21-C22-C37
22	G	613	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C3-C5-C6-C7
22	B	617	CLA	C3-C5-C6-C7
26	n	617	LHG	C23-C24-C25-C26
33	a	411	SQD	O10-C23-O48-C46
33	A	412	SQD	O10-C23-O48-C46
32	d	406	PL9	C20-C19-C21-C22
32	D	407	PL9	C20-C19-C21-C22
22	c	511	CLA	C2-C3-C5-C6
22	C	512	CLA	C2-C3-C5-C6
22	b	614	CLA	C13-C15-C16-C17
22	c	508	CLA	C10-C11-C12-C13
22	C	509	CLA	C10-C11-C12-C13
22	C	515	CLA	C8-C10-C11-C12
22	r	312	CLA	C10-C11-C12-C13
22	R	311	CLA	C10-C11-C12-C13
21	n	608	CHL	C16-C17-C18-C20
26	l	102	LHG	C33-C34-C35-C36
26	L	103	LHG	C33-C34-C35-C36
22	b	610	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	O1A-CGA-O2A-C1
36	I	101	LMG	O10-C28-O8-C9
21	r	306	CHL	C5-C6-C7-C8
21	R	305	CHL	C5-C6-C7-C8
22	Y	611	CLA	C13-C15-C16-C17
22	c	514	CLA	C8-C10-C11-C12
22	B	617	CLA	C13-C15-C16-C17
22	c	503	CLA	C2A-CAA-CBA-CGA
22	C	504	CLA	C2A-CAA-CBA-CGA
35	c	519	DGD	C5A-C6A-C7A-C8A
35	J	101	DGD	C5A-C6A-C7A-C8A
26	n	617	LHG	C11-C10-C9-C8
26	d	409	LHG	C28-C29-C30-C31
33	l	101	SQD	C10-C11-C12-C13
33	L	102	SQD	C10-C11-C12-C13
22	d	403	CLA	CBA-CGA-O2A-C1
22	D	404	CLA	CBA-CGA-O2A-C1
21	r	307	CHL	O2A-C1-C2-C3
21	R	306	CHL	O2A-C1-C2-C3
26	l	102	LHG	C29-C30-C31-C32
26	D	410	LHG	C12-C13-C14-C15
26	D	410	LHG	C28-C29-C30-C31
26	L	103	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
26	d	409	LHG	C12-C13-C14-C15
36	B	601	LMG	C32-C33-C34-C35
36	B	601	LMG	C38-C39-C40-C41
36	I	101	LMG	C32-C33-C34-C35
36	I	101	LMG	C38-C39-C40-C41
24	G	617	XAT	C33-C34-C35-C15
25	N	617	NEX	C29-C30-C31-C32
26	N	618	LHG	C23-C24-C25-C26
22	c	504	CLA	O1A-CGA-O2A-C1
36	B	601	LMG	O10-C28-O8-C9
24	y	615	XAT	C11-C10-C9-C8
25	g	618	NEX	C32-C33-C34-C35
31	d	405	BCR	C12-C13-C14-C15
31	D	406	BCR	C12-C13-C14-C15
26	b	619	LHG	C11-C10-C9-C8
26	y	617	LHG	O6-C4-C5-O7
26	s	314	LHG	O6-C4-C5-O7
26	S	314	LHG	O6-C4-C5-O7
22	c	502	CLA	C10-C11-C12-C13
26	B	622	LHG	C11-C10-C9-C8
21	g	606	CHL	CBA-CGA-O2A-C1
21	Y	605	CHL	CBA-CGA-O2A-C1
22	C	505	CLA	O1A-CGA-O2A-C1
35	a	413	DGD	C9A-CAA-CBA-CCA
36	k	103	LMG	C14-C15-C16-C17
36	K	103	LMG	C14-C15-C16-C17
26	n	617	LHG	C32-C33-C34-C35
26	s	314	LHG	C33-C34-C35-C36
26	S	314	LHG	C33-C34-C35-C36
35	A	401	DGD	C9A-CAA-CBA-CCA
36	D	411	LMG	C4-C5-C6-O5
22	C	503	CLA	C10-C11-C12-C13
22	b	602	CLA	C2-C3-C5-C6
22	B	605	CLA	C2-C3-C5-C6
35	c	517	DGD	C5A-C6A-C7A-C8A
35	C	518	DGD	C5A-C6A-C7A-C8A
36	k	103	LMG	C34-C35-C36-C37
36	K	103	LMG	C34-C35-C36-C37
22	a	404	CLA	C16-C17-C18-C20
22	A	405	CLA	C16-C17-C18-C20
26	c	522	LHG	C27-C28-C29-C30
35	C	518	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
26	n	617	LHG	C19-C20-C21-C22
26	G	618	LHG	C31-C32-C33-C34
26	N	618	LHG	C12-C13-C14-C15
26	C	522	LHG	C27-C28-C29-C30
35	a	413	DGD	C4B-C5B-C6B-C7B
35	c	517	DGD	C5B-C6B-C7B-C8B
35	c	518	DGD	C5A-C6A-C7A-C8A
35	A	401	DGD	C4B-C5B-C6B-C7B
35	C	519	DGD	C5A-C6A-C7A-C8A
26	r	302	LHG	O7-C5-C6-O8
26	R	301	LHG	O7-C5-C6-O8
33	d	402	SQD	O6-C44-C45-O47
33	l	101	SQD	O47-C45-C46-O48
33	D	402	SQD	O6-C44-C45-O47
33	L	102	SQD	O47-C45-C46-O48
35	c	518	DGD	O2G-C2G-C3G-O3G
35	C	519	DGD	O2G-C2G-C3G-O3G
22	S	313	CLA	O1D-CGD-O2D-CED
21	G	606	CHL	CBA-CGA-O2A-C1
21	N	605	CHL	CBA-CGA-O2A-C1
26	c	521	LHG	C32-C33-C34-C35
26	C	521	LHG	C32-C33-C34-C35
22	s	313	CLA	O1D-CGD-O2D-CED
36	d	410	LMG	C4-C5-C6-O5
21	g	606	CHL	CAA-CBA-CGA-O2A
21	n	605	CHL	CAA-CBA-CGA-O2A
21	y	606	CHL	CAA-CBA-CGA-O2A
21	G	606	CHL	CAA-CBA-CGA-O2A
21	N	605	CHL	CAA-CBA-CGA-O2A
21	Y	605	CHL	CAA-CBA-CGA-O2A
26	G	618	LHG	C27-C28-C29-C30
35	h	102	DGD	CCA-CDA-CEA-CFA
26	G	618	LHG	C24-C25-C26-C27
32	d	406	PL9	C44-C46-C47-C48
35	H	102	DGD	CCA-CDA-CEA-CFA
22	b	611	CLA	C5-C6-C7-C8
26	L	103	LHG	C30-C31-C32-C33
36	w	102	LMG	C33-C34-C35-C36
21	n	605	CHL	CBA-CGA-O2A-C1
26	l	102	LHG	C30-C31-C32-C33
36	C	502	LMG	C33-C34-C35-C36
26	c	520	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	C	520	LHG	C9-C10-C11-C12
22	b	608	CLA	C15-C16-C17-C18
22	B	611	CLA	C15-C16-C17-C18
22	B	614	CLA	C5-C6-C7-C8
26	G	618	LHG	C28-C29-C30-C31
26	N	618	LHG	C9-C10-C11-C12
26	d	408	LHG	C19-C20-C21-C22
26	D	409	LHG	C19-C20-C21-C22
21	Y	608	CHL	C15-C16-C17-C18
22	s	311	CLA	C11-C10-C8-C9
22	S	311	CLA	C11-C10-C8-C9
22	b	605	CLA	C16-C17-C18-C20
22	B	608	CLA	C16-C17-C18-C20
22	c	511	CLA	C4-C3-C5-C6
22	C	512	CLA	C4-C3-C5-C6
21	y	606	CHL	CBA-CGA-O2A-C1
21	s	306	CHL	C2C-C3C-CAC-CBC
36	w	102	LMG	C32-C33-C34-C35
36	C	502	LMG	C32-C33-C34-C35
22	n	609	CLA	C14-C13-C15-C16
22	G	610	CLA	C14-C13-C15-C16
22	b	604	CLA	C11-C10-C8-C9
22	c	507	CLA	C6-C7-C8-C9
22	c	510	CLA	C6-C7-C8-C9
22	c	512	CLA	C11-C10-C8-C9
22	B	607	CLA	C11-C10-C8-C9
22	B	610	CLA	C11-C12-C13-C14
22	C	508	CLA	C6-C7-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	b	615	CLA	C13-C15-C16-C17
22	B	618	CLA	C13-C15-C16-C17
22	g	604	CLA	C4B-C3B-CAB-CBB
22	g	611	CLA	C4B-C3B-CAB-CBB
22	g	614	CLA	C4B-C3B-CAB-CBB
22	n	604	CLA	C4B-C3B-CAB-CBB
22	n	610	CLA	C4B-C3B-CAB-CBB
22	n	613	CLA	C4B-C3B-CAB-CBB
22	y	604	CLA	C4B-C3B-CAB-CBB
22	y	611	CLA	C4B-C3B-CAB-CBB
22	y	613	CLA	C4B-C3B-CAB-CBB
22	G	604	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	G	611	CLA	C4B-C3B-CAB-CBB
22	G	614	CLA	C4B-C3B-CAB-CBB
22	N	604	CLA	C4B-C3B-CAB-CBB
22	N	610	CLA	C4B-C3B-CAB-CBB
22	N	613	CLA	C4B-C3B-CAB-CBB
22	Y	604	CLA	C4B-C3B-CAB-CBB
22	Y	610	CLA	C4B-C3B-CAB-CBB
22	Y	612	CLA	C4B-C3B-CAB-CBB
22	b	601	CLA	C4B-C3B-CAB-CBB
22	b	615	CLA	C4B-C3B-CAB-CBB
22	c	509	CLA	C4B-C3B-CAB-CBB
22	d	404	CLA	C4B-C3B-CAB-CBB
22	x	101	CLA	C4B-C3B-CAB-CBB
22	B	603	CLA	C4B-C3B-CAB-CBB
22	B	604	CLA	C4B-C3B-CAB-CBB
22	B	618	CLA	C4B-C3B-CAB-CBB
22	C	510	CLA	C4B-C3B-CAB-CBB
22	D	405	CLA	C4B-C3B-CAB-CBB
22	r	304	CLA	C4B-C3B-CAB-CBB
22	R	303	CLA	C4B-C3B-CAB-CBB
22	g	613	CLA	C15-C16-C17-C18
22	b	608	CLA	C5-C6-C7-C8
22	B	611	CLA	C5-C6-C7-C8
22	c	506	CLA	C16-C17-C18-C19
22	C	507	CLA	C16-C17-C18-C19
26	n	617	LHG	C29-C30-C31-C32
26	D	408	LHG	C32-C33-C34-C35
21	S	307	CHL	C2A-CAA-CBA-CGA
26	N	618	LHG	C25-C26-C27-C28
26	Y	617	LHG	C24-C25-C26-C27
33	d	402	SQD	C14-C15-C16-C17
33	D	402	SQD	C14-C15-C16-C17
36	M	101	LMG	C39-C40-C41-C42
36	T	101	LMG	C39-C40-C41-C42
22	N	609	CLA	C13-C15-C16-C17
26	n	617	LHG	C27-C28-C29-C30
26	d	407	LHG	C32-C33-C34-C35
36	c	523	LMG	C31-C32-C33-C34
36	C	523	LMG	C31-C32-C33-C34
26	G	618	LHG	O6-C4-C5-C6
26	Y	617	LHG	O6-C4-C5-C6
26	c	521	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
26	c	522	LHG	O6-C4-C5-C6
26	C	522	LHG	O6-C4-C5-C6
26	r	302	LHG	O6-C4-C5-C6
26	R	301	LHG	O6-C4-C5-C6
26	y	617	LHG	C14-C15-C16-C17
21	g	608	CHL	C6-C7-C8-C10
21	g	608	CHL	C11-C10-C8-C7
21	n	607	CHL	C6-C7-C8-C10
21	n	607	CHL	C11-C10-C8-C7
21	y	608	CHL	C6-C7-C8-C10
21	y	608	CHL	C11-C10-C8-C7
21	y	609	CHL	C12-C13-C15-C16
21	G	608	CHL	C6-C7-C8-C10
21	G	608	CHL	C11-C10-C8-C7
21	N	607	CHL	C6-C7-C8-C10
21	N	607	CHL	C11-C10-C8-C7
21	Y	607	CHL	C6-C7-C8-C10
21	Y	607	CHL	C11-C10-C8-C7
21	r	306	CHL	C12-C13-C15-C16
21	R	305	CHL	C12-C13-C15-C16
22	g	602	CLA	C11-C10-C8-C7
22	g	602	CLA	C12-C13-C15-C16
22	n	602	CLA	C11-C10-C8-C7
22	n	602	CLA	C12-C13-C15-C16
22	y	602	CLA	C11-C10-C8-C7
22	y	602	CLA	C12-C13-C15-C16
22	y	612	CLA	C12-C13-C15-C16
22	G	602	CLA	C11-C10-C8-C7
22	G	602	CLA	C12-C13-C15-C16
22	N	602	CLA	C11-C10-C8-C7
22	N	602	CLA	C12-C13-C15-C16
22	Y	602	CLA	C11-C10-C8-C7
22	Y	602	CLA	C12-C13-C15-C16
22	b	605	CLA	C12-C13-C15-C16
22	b	606	CLA	C12-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C10
22	b	609	CLA	C6-C7-C8-C10
22	b	614	CLA	C11-C12-C13-C15
22	c	507	CLA	C6-C7-C8-C10
22	c	510	CLA	C6-C7-C8-C10
22	c	512	CLA	C11-C10-C8-C7
22	d	403	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	C12-C13-C15-C16
22	B	609	CLA	C12-C13-C15-C16
22	B	610	CLA	C6-C7-C8-C10
22	B	612	CLA	C6-C7-C8-C10
22	B	617	CLA	C11-C12-C13-C15
22	C	508	CLA	C6-C7-C8-C10
22	C	511	CLA	C6-C7-C8-C10
22	C	513	CLA	C11-C10-C8-C7
22	D	404	CLA	C11-C12-C13-C15
22	r	304	CLA	C6-C7-C8-C10
22	s	303	CLA	C6-C7-C8-C10
22	S	303	CLA	C6-C7-C8-C10
22	R	303	CLA	C6-C7-C8-C10
30	a	407	PHO	C11-C12-C13-C15
30	A	408	PHO	C11-C12-C13-C15
22	g	611	CLA	C8-C10-C11-C12
22	n	610	CLA	C8-C10-C11-C12
22	y	611	CLA	C8-C10-C11-C12
22	N	610	CLA	C8-C10-C11-C12
22	Y	610	CLA	C8-C10-C11-C12
22	x	101	CLA	C8-C10-C11-C12
22	B	603	CLA	C8-C10-C11-C12
22	G	611	CLA	C8-C10-C11-C12
22	a	404	CLA	C16-C17-C18-C19
22	A	405	CLA	C16-C17-C18-C19
21	g	601	CHL	C3A-C2A-CAA-CBA
21	n	601	CHL	C3A-C2A-CAA-CBA
21	y	601	CHL	C3A-C2A-CAA-CBA
21	G	601	CHL	C3A-C2A-CAA-CBA
21	N	601	CHL	C3A-C2A-CAA-CBA
21	Y	601	CHL	C3A-C2A-CAA-CBA
21	s	302	CHL	C3A-C2A-CAA-CBA
21	S	302	CHL	C3A-C2A-CAA-CBA
22	c	504	CLA	C3A-C2A-CAA-CBA
22	c	506	CLA	C3A-C2A-CAA-CBA
22	C	505	CLA	C3A-C2A-CAA-CBA
22	C	507	CLA	C3A-C2A-CAA-CBA
22	s	303	CLA	C4-C3-C5-C6
22	S	303	CLA	C4-C3-C5-C6
21	S	306	CHL	C2C-C3C-CAC-CBC
22	c	506	CLA	O1D-CGD-O2D-CED
22	C	507	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	Y	617	LHG	C25-C26-C27-C28
33	a	411	SQD	C12-C13-C14-C15
33	A	412	SQD	C12-C13-C14-C15
22	c	511	CLA	CBA-CGA-O2A-C1
22	C	512	CLA	CBA-CGA-O2A-C1
26	N	618	LHG	C13-C14-C15-C16
26	n	617	LHG	C35-C36-C37-C38
23	g	615	LUT	C33-C34-C35-C15
23	g	616	LUT	C9-C10-C11-C12
23	n	614	LUT	C33-C34-C35-C15
23	y	614	LUT	C33-C34-C35-C15
23	G	615	LUT	C33-C34-C35-C15
23	N	614	LUT	C33-C34-C35-C15
23	N	615	LUT	C29-C30-C31-C32
23	Y	613	LUT	C33-C34-C35-C15
24	G	617	XAT	C29-C30-C31-C32
25	y	616	NEX	C13-C14-C15-C35
22	c	506	CLA	C16-C17-C18-C20
22	C	507	CLA	C16-C17-C18-C20
21	n	608	CHL	C15-C16-C17-C18
33	a	411	SQD	C9-C10-C11-C12
22	d	403	CLA	O1A-CGA-O2A-C1
22	D	404	CLA	O1A-CGA-O2A-C1
33	A	412	SQD	C9-C10-C11-C12
25	g	618	NEX	C31-C32-C33-C34
31	b	616	BCR	C21-C22-C23-C24
31	B	619	BCR	C21-C22-C23-C24
26	g	619	LHG	C9-C10-C11-C12
35	C	519	DGD	CAA-CBA-CCA-CDA
36	b	620	LMG	C18-C19-C20-C21
36	B	623	LMG	C18-C19-C20-C21
36	K	103	LMG	C10-C11-C12-C13
35	c	518	DGD	CAA-CBA-CCA-CDA
26	c	520	LHG	C1-C2-C3-O3
26	C	520	LHG	C1-C2-C3-O3
35	J	101	DGD	CCA-CDA-CEA-CFA
26	s	314	LHG	C4-C5-C6-O8
26	S	314	LHG	C4-C5-C6-O8
32	D	407	PL9	C44-C46-C47-C48
33	d	402	SQD	O6-C44-C45-C46
33	D	402	SQD	O6-C44-C45-C46
35	c	518	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
35	c	518	DGD	C1G-C2G-C3G-O3G
35	C	519	DGD	O1G-C1G-C2G-C3G
35	C	519	DGD	C1G-C2G-C3G-O3G
36	b	620	LMG	O1-C7-C8-C9
36	k	103	LMG	O1-C7-C8-C9
36	B	623	LMG	O1-C7-C8-C9
36	K	103	LMG	O1-C7-C8-C9
36	M	101	LMG	O1-C7-C8-C9
36	T	101	LMG	O1-C7-C8-C9
26	G	618	LHG	C14-C15-C16-C17
35	c	519	DGD	CCA-CDA-CEA-CFA
22	c	513	CLA	C3-C5-C6-C7
35	c	518	DGD	C4A-C5A-C6A-C7A
35	C	519	DGD	C4A-C5A-C6A-C7A
21	g	605	CHL	C1A-C2A-CAA-CBA
21	y	605	CHL	C1A-C2A-CAA-CBA
21	G	605	CHL	C1A-C2A-CAA-CBA
21	r	301	CHL	C1A-C2A-CAA-CBA
21	s	301	CHL	C1A-C2A-CAA-CBA
21	S	301	CHL	C1A-C2A-CAA-CBA
30	a	407	PHO	C1A-C2A-CAA-CBA
30	A	408	PHO	C1A-C2A-CAA-CBA
36	k	103	LMG	C10-C11-C12-C13
26	d	407	LHG	C30-C31-C32-C33
26	l	102	LHG	C27-C28-C29-C30
26	D	408	LHG	C30-C31-C32-C33
26	L	103	LHG	C27-C28-C29-C30
22	s	303	CLA	C2-C3-C5-C6
22	S	303	CLA	C2-C3-C5-C6
22	C	514	CLA	C3-C5-C6-C7
36	b	620	LMG	C40-C41-C42-C43
36	B	623	LMG	C40-C41-C42-C43
26	n	617	LHG	O6-C4-C5-O7
26	N	618	LHG	O6-C4-C5-O7
26	c	522	LHG	O6-C4-C5-O7
26	C	522	LHG	O6-C4-C5-O7
22	g	603	CLA	C2B-C3B-CAB-CBB
22	g	604	CLA	C2B-C3B-CAB-CBB
22	g	614	CLA	C2B-C3B-CAB-CBB
22	n	603	CLA	C2B-C3B-CAB-CBB
22	n	604	CLA	C2B-C3B-CAB-CBB
22	n	613	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	y	603	CLA	C2B-C3B-CAB-CBB
22	y	604	CLA	C2B-C3B-CAB-CBB
22	y	613	CLA	C2B-C3B-CAB-CBB
22	G	603	CLA	C2B-C3B-CAB-CBB
22	G	604	CLA	C2B-C3B-CAB-CBB
22	G	614	CLA	C2B-C3B-CAB-CBB
22	N	603	CLA	C2B-C3B-CAB-CBB
22	N	604	CLA	C2B-C3B-CAB-CBB
22	N	613	CLA	C2B-C3B-CAB-CBB
22	Y	603	CLA	C2B-C3B-CAB-CBB
22	Y	604	CLA	C2B-C3B-CAB-CBB
22	Y	612	CLA	C2B-C3B-CAB-CBB
22	d	404	CLA	C2B-C3B-CAB-CBB
22	x	101	CLA	C2B-C3B-CAB-CBB
22	B	603	CLA	C2B-C3B-CAB-CBB
22	D	405	CLA	C2B-C3B-CAB-CBB
31	b	616	BCR	C1-C6-C7-C8
31	c	515	BCR	C1-C6-C7-C8
31	k	102	BCR	C1-C6-C7-C8
31	B	602	BCR	C1-C6-C7-C8
31	B	619	BCR	C1-C6-C7-C8
31	C	516	BCR	C1-C6-C7-C8
31	K	102	BCR	C1-C6-C7-C8
31	T	102	BCR	C1-C6-C7-C8
26	Y	617	LHG	C14-C15-C16-C17
26	d	408	LHG	O2-C2-C3-O3
26	D	409	LHG	O2-C2-C3-O3
26	d	409	LHG	C2-C3-O3-P
26	D	410	LHG	C2-C3-O3-P
35	c	518	DGD	C9B-CAB-CBB-CCB
35	C	519	DGD	C9B-CAB-CBB-CCB
22	b	610	CLA	C15-C16-C17-C18
22	B	613	CLA	C15-C16-C17-C18
26	s	314	LHG	C10-C11-C12-C13
26	S	314	LHG	C10-C11-C12-C13
33	L	101	SQD	C17-C18-C19-C20
26	g	619	LHG	C32-C33-C34-C35
21	n	608	CHL	C16-C17-C18-C19
22	b	605	CLA	C16-C17-C18-C19
22	B	608	CLA	C16-C17-C18-C19
33	d	402	SQD	O47-C45-C46-O48
33	D	402	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
36	b	620	LMG	O1-C7-C8-O7
36	w	102	LMG	O1-C7-C8-O7
36	B	623	LMG	O1-C7-C8-O7
36	C	502	LMG	O1-C7-C8-O7
36	M	101	LMG	O1-C7-C8-O7
36	T	101	LMG	O1-C7-C8-O7
33	l	103	SQD	C17-C18-C19-C20
32	a	410	PL9	C4-C3-C7-C8
32	A	411	PL9	C4-C3-C7-C8
26	s	314	LHG	C29-C30-C31-C32
26	S	314	LHG	C29-C30-C31-C32
36	c	523	LMG	C38-C39-C40-C41
36	C	523	LMG	C38-C39-C40-C41
22	c	514	CLA	C4-C3-C5-C6
22	C	515	CLA	C4-C3-C5-C6
26	r	302	LHG	C30-C31-C32-C33
26	R	301	LHG	C30-C31-C32-C33
21	g	608	CHL	C16-C17-C18-C19
21	n	607	CHL	C16-C17-C18-C19
21	y	608	CHL	C16-C17-C18-C19
21	G	608	CHL	C16-C17-C18-C19
21	N	607	CHL	C16-C17-C18-C19
21	Y	607	CHL	C16-C17-C18-C19
22	s	313	CLA	C6-C7-C8-C9
22	S	313	CLA	C6-C7-C8-C9
26	d	407	LHG	C34-C35-C36-C37
26	D	408	LHG	C34-C35-C36-C37
26	r	302	LHG	C24-C25-C26-C27
26	R	301	LHG	C24-C25-C26-C27
26	b	619	LHG	C9-C10-C11-C12
26	B	622	LHG	C9-C10-C11-C12
22	g	603	CLA	C11-C10-C8-C9
22	g	613	CLA	C6-C7-C8-C9
22	n	603	CLA	C11-C10-C8-C9
22	n	612	CLA	C6-C7-C8-C9
22	y	603	CLA	C11-C10-C8-C9
22	y	612	CLA	C6-C7-C8-C9
22	G	603	CLA	C11-C10-C8-C9
22	G	613	CLA	C6-C7-C8-C9
22	N	603	CLA	C11-C10-C8-C9
22	N	612	CLA	C6-C7-C8-C9
22	Y	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	Y	611	CLA	C6-C7-C8-C9
22	b	607	CLA	C6-C7-C8-C9
22	b	607	CLA	C11-C12-C13-C14
22	b	611	CLA	C6-C7-C8-C9
22	B	610	CLA	C6-C7-C8-C9
22	B	614	CLA	C6-C7-C8-C9
30	a	407	PHO	C11-C12-C13-C14
30	A	408	PHO	C11-C12-C13-C14
36	M	101	LMG	C12-C13-C14-C15
36	T	101	LMG	C12-C13-C14-C15
31	b	616	BCR	C6-C7-C8-C9
31	b	616	BCR	C22-C23-C24-C25
31	b	618	BCR	C22-C23-C24-C25
31	B	619	BCR	C6-C7-C8-C9
31	B	619	BCR	C22-C23-C24-C25
31	B	621	BCR	C22-C23-C24-C25
21	g	606	CHL	O1A-CGA-O2A-C1
26	G	618	LHG	C30-C31-C32-C33
26	d	408	LHG	C11-C12-C13-C14
26	D	409	LHG	C11-C12-C13-C14
21	N	608	CHL	C16-C17-C18-C19
26	l	102	LHG	C24-C23-O8-C6
26	L	103	LHG	C24-C23-O8-C6
26	g	619	LHG	C24-C25-C26-C27
22	r	311	CLA	O2A-C1-C2-C3
22	R	310	CLA	O2A-C1-C2-C3
21	Y	605	CHL	O1A-CGA-O2A-C1
26	g	619	LHG	C23-C24-C25-C26
26	Y	617	LHG	C16-C17-C18-C19
26	S	314	LHG	C11-C12-C13-C14
26	s	314	LHG	C11-C12-C13-C14
26	d	409	LHG	C32-C33-C34-C35
26	D	410	LHG	C32-C33-C34-C35
26	s	314	LHG	O1-C1-C2-O2
26	S	314	LHG	O1-C1-C2-O2
35	C	519	DGD	C5B-C6B-C7B-C8B
23	r	313	LUT	C13-C14-C15-C35
23	R	312	LUT	C13-C14-C15-C35
35	c	518	DGD	C5B-C6B-C7B-C8B
36	w	102	LMG	C11-C10-O7-C8
36	C	502	LMG	C11-C10-O7-C8
35	A	401	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
22	c	513	CLA	C5-C6-C7-C8
22	C	514	CLA	C5-C6-C7-C8
26	Y	617	LHG	C11-C10-C9-C8
35	a	413	DGD	C9B-CAB-CBB-CCB
35	c	517	DGD	C7B-C8B-C9B-CAB
35	C	518	DGD	C7B-C8B-C9B-CAB
31	k	101	BCR	C20-C21-C22-C37
31	K	101	BCR	C20-C21-C22-C37
22	N	612	CLA	C3-C5-C6-C7
22	Y	611	CLA	C3-C5-C6-C7
35	h	102	DGD	O2G-C1B-C2B-C3B
35	H	102	DGD	O2G-C1B-C2B-C3B
26	c	520	LHG	C14-C15-C16-C17
26	y	617	LHG	O6-C4-C5-C6
26	C	521	LHG	O6-C4-C5-C6
37	f	101	HEM	C3A-C2A-CAA-CBA
37	F	101	HEM	C3A-C2A-CAA-CBA
26	C	520	LHG	C14-C15-C16-C17
23	Y	614	LUT	C31-C32-C33-C40
26	r	302	LHG	C11-C12-C13-C14
26	R	301	LHG	C11-C12-C13-C14
21	g	607	CHL	C6-C7-C8-C10
21	n	606	CHL	C6-C7-C8-C10
21	y	607	CHL	C6-C7-C8-C10
21	G	607	CHL	C6-C7-C8-C10
21	N	606	CHL	C6-C7-C8-C10
21	Y	606	CHL	C6-C7-C8-C10
22	g	613	CLA	C6-C7-C8-C10
22	n	612	CLA	C6-C7-C8-C10
22	y	612	CLA	C6-C7-C8-C10
22	G	613	CLA	C6-C7-C8-C10
22	N	612	CLA	C6-C7-C8-C10
22	Y	611	CLA	C6-C7-C8-C10
22	b	601	CLA	C11-C10-C8-C7
22	b	612	CLA	C12-C13-C15-C16
22	c	509	CLA	C11-C10-C8-C7
22	B	604	CLA	C11-C10-C8-C7
22	B	615	CLA	C12-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C7
22	r	310	CLA	C6-C7-C8-C10
22	R	309	CLA	C6-C7-C8-C10
36	d	410	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
36	D	411	LMG	C16-C17-C18-C19
22	g	613	CLA	C3-C5-C6-C7
22	n	612	CLA	C3-C5-C6-C7
22	y	612	CLA	C3-C5-C6-C7
22	G	613	CLA	C3-C5-C6-C7
21	N	608	CHL	C15-C16-C17-C18
25	Y	616	NEX	C11-C12-C13-C14
26	C	520	LHG	C11-C12-C13-C14
26	s	314	LHG	C12-C13-C14-C15
26	S	314	LHG	C12-C13-C14-C15
21	n	605	CHL	O1A-CGA-O2A-C1
21	y	606	CHL	O1A-CGA-O2A-C1
21	G	606	CHL	O1A-CGA-O2A-C1
21	N	605	CHL	O1A-CGA-O2A-C1
35	c	518	DGD	C2G-C3G-O3G-C1D
35	C	519	DGD	C2G-C3G-O3G-C1D
26	G	618	LHG	C32-C33-C34-C35
22	b	605	CLA	C2A-CAA-CBA-CGA
22	B	608	CLA	C2A-CAA-CBA-CGA
26	c	520	LHG	C11-C12-C13-C14
33	l	101	SQD	C9-C10-C11-C12
33	D	402	SQD	C10-C11-C12-C13
33	L	102	SQD	C9-C10-C11-C12
21	r	307	CHL	C4-C3-C5-C6
21	R	306	CHL	C4-C3-C5-C6
22	c	514	CLA	C2-C3-C5-C6
22	C	515	CLA	C2-C3-C5-C6
26	s	314	LHG	O1-C1-C2-C3
26	S	314	LHG	O1-C1-C2-C3
33	d	402	SQD	C10-C11-C12-C13
36	B	601	LMG	C36-C37-C38-C39
36	I	101	LMG	C36-C37-C38-C39
22	C	514	CLA	C13-C15-C16-C17
22	c	513	CLA	C13-C15-C16-C17
24	n	615	XAT	C29-C30-C31-C32
26	N	618	LHG	C18-C19-C20-C21
36	k	103	LMG	C40-C41-C42-C43
36	K	103	LMG	C40-C41-C42-C43
36	d	410	LMG	O10-C28-O8-C9
36	D	411	LMG	O10-C28-O8-C9
21	n	608	CHL	C13-C15-C16-C17
22	g	603	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	y	603	CLA	C5-C6-C7-C8
23	g	616	LUT	C12-C13-C14-C15
23	G	616	LUT	C28-C29-C30-C31
24	Y	615	XAT	C11-C10-C9-C8
31	c	516	BCR	C20-C21-C22-C23
31	B	602	BCR	C16-C17-C18-C19
31	C	517	BCR	C20-C21-C22-C23
31	T	102	BCR	C16-C17-C18-C19
36	M	101	LMG	C22-C23-C24-C25
36	T	101	LMG	C22-C23-C24-C25
22	n	603	CLA	C5-C6-C7-C8
22	G	603	CLA	C5-C6-C7-C8
22	N	603	CLA	C5-C6-C7-C8
22	Y	603	CLA	C5-C6-C7-C8
26	g	619	LHG	O6-C4-C5-O7
26	Y	617	LHG	O6-C4-C5-O7
26	c	521	LHG	O6-C4-C5-O7
26	C	521	LHG	O6-C4-C5-O7
35	h	102	DGD	O6E-C1E-O5D-C6D
35	H	102	DGD	O6E-C1E-O5D-C6D
26	r	302	LHG	C4-C5-C6-O8
26	R	301	LHG	C4-C5-C6-O8
33	d	402	SQD	C44-C45-C46-O48
33	D	402	SQD	C44-C45-C46-O48
37	f	101	HEM	C4B-C3B-CAB-CBB
37	f	101	HEM	C4C-C3C-CAC-CBC
37	F	101	HEM	C4B-C3B-CAB-CBB
37	F	101	HEM	C4C-C3C-CAC-CBC
26	b	619	LHG	C35-C36-C37-C38
26	B	622	LHG	C35-C36-C37-C38
36	B	623	LMG	C42-C43-C44-C45
22	C	512	CLA	O1A-CGA-O2A-C1
26	y	617	LHG	C24-C23-O8-C6
22	a	405	CLA	C4-C3-C5-C6
22	A	406	CLA	C4-C3-C5-C6
32	d	406	PL9	C15-C14-C16-C17
36	b	620	LMG	C42-C43-C44-C45
25	y	616	NEX	C7-C8-C9-C19
25	y	618	NEX	C7-C8-C9-C19
25	r	315	NEX	C7-C8-C9-C19
22	x	101	CLA	C15-C16-C17-C18
22	B	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	k	103	LMG	C11-C12-C13-C14
36	K	103	LMG	C11-C12-C13-C14
26	c	522	LHG	O7-C5-C6-O8
26	C	522	LHG	O7-C5-C6-O8
21	n	606	CHL	C6-C7-C8-C9
21	r	306	CHL	C11-C12-C13-C14
21	R	305	CHL	C11-C12-C13-C14
30	a	407	PHO	C11-C10-C8-C9
30	d	401	PHO	C6-C7-C8-C9
30	A	408	PHO	C11-C10-C8-C9
30	D	401	PHO	C6-C7-C8-C9
22	G	613	CLA	C16-C17-C18-C20
36	I	101	LMG	C31-C32-C33-C34
36	M	101	LMG	C13-C14-C15-C16
26	d	407	LHG	C12-C13-C14-C15
26	D	408	LHG	C12-C13-C14-C15
35	h	102	DGD	C7A-C8A-C9A-CAA
35	C	519	DGD	CAB-CBB-CCB-CDB
35	H	102	DGD	C7A-C8A-C9A-CAA
22	c	511	CLA	O1A-CGA-O2A-C1
35	c	518	DGD	CAB-CBB-CCB-CDB
36	B	601	LMG	C31-C32-C33-C34
36	T	101	LMG	C13-C14-C15-C16
22	R	309	CLA	CBD-CGD-O2D-CED
26	Y	617	LHG	C29-C30-C31-C32
26	s	314	LHG	C28-C29-C30-C31
26	S	314	LHG	C28-C29-C30-C31
36	B	601	LMG	C11-C10-O7-C8
36	I	101	LMG	C11-C10-O7-C8
33	d	402	SQD	O47-C7-C8-C9
33	D	402	SQD	O47-C7-C8-C9
26	Y	617	LHG	C9-C10-C11-C12
23	G	616	LUT	C9-C10-C11-C12
25	y	618	NEX	C13-C14-C15-C35
25	r	315	NEX	C13-C14-C15-C35
21	N	608	CHL	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C20
22	B	607	CLA	C16-C17-C18-C20
32	D	407	PL9	C15-C14-C16-C17
21	r	307	CHL	C2-C3-C5-C6
21	R	306	CHL	C2-C3-C5-C6
22	r	310	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	Y	608	CHL	C16-C17-C18-C19
26	b	619	LHG	C12-C13-C14-C15
26	Y	617	LHG	C28-C29-C30-C31
22	s	309	CLA	C5-C6-C7-C8
26	B	622	LHG	C12-C13-C14-C15
22	Y	609	CLA	C11-C12-C13-C15
22	S	309	CLA	C5-C6-C7-C8
22	c	512	CLA	C13-C15-C16-C17
22	C	513	CLA	C13-C15-C16-C17
22	g	603	CLA	C4B-C3B-CAB-CBB
22	g	610	CLA	C4B-C3B-CAB-CBB
22	n	603	CLA	C4B-C3B-CAB-CBB
22	n	609	CLA	C4B-C3B-CAB-CBB
22	y	603	CLA	C4B-C3B-CAB-CBB
22	y	610	CLA	C4B-C3B-CAB-CBB
22	G	603	CLA	C4B-C3B-CAB-CBB
22	G	610	CLA	C4B-C3B-CAB-CBB
22	N	603	CLA	C4B-C3B-CAB-CBB
22	N	609	CLA	C4B-C3B-CAB-CBB
22	Y	603	CLA	C4B-C3B-CAB-CBB
22	Y	609	CLA	C4B-C3B-CAB-CBB
22	a	406	CLA	C4B-C3B-CAB-CBB
22	b	608	CLA	C4B-C3B-CAB-CBB
22	c	506	CLA	C4B-C3B-CAB-CBB
22	c	511	CLA	C4B-C3B-CAB-CBB
22	A	407	CLA	C4B-C3B-CAB-CBB
22	B	611	CLA	C4B-C3B-CAB-CBB
22	C	507	CLA	C4B-C3B-CAB-CBB
22	C	512	CLA	C4B-C3B-CAB-CBB
22	s	303	CLA	C4B-C3B-CAB-CBB
22	s	304	CLA	C4B-C3B-CAB-CBB
22	S	303	CLA	C4B-C3B-CAB-CBB
22	S	304	CLA	C4B-C3B-CAB-CBB
22	g	612	CLA	C4-C3-C5-C6
22	n	611	CLA	C4-C3-C5-C6
22	G	612	CLA	C4-C3-C5-C6
22	N	611	CLA	C4-C3-C5-C6
22	w	101	CLA	C4-C3-C5-C6
22	W	101	CLA	C4-C3-C5-C6
24	n	615	XAT	C7-C8-C9-C10
25	N	617	NEX	C11-C12-C13-C14
22	y	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	r	303	CLA	C2A-CAA-CBA-CGA
22	R	302	CLA	C2A-CAA-CBA-CGA
36	k	103	LMG	C19-C20-C21-C22
26	d	407	LHG	O6-C4-C5-C6
26	D	408	LHG	O6-C4-C5-C6
26	s	314	LHG	O6-C4-C5-C6
26	S	314	LHG	O6-C4-C5-C6
32	d	406	PL9	C42-C43-C44-C45
36	K	103	LMG	C19-C20-C21-C22
33	D	402	SQD	O49-C7-O47-C45
21	g	601	CHL	C6-C7-C8-C10
21	g	601	CHL	C12-C13-C15-C16
21	n	601	CHL	C6-C7-C8-C10
21	n	601	CHL	C12-C13-C15-C16
21	y	601	CHL	C6-C7-C8-C10
21	y	601	CHL	C12-C13-C15-C16
21	G	601	CHL	C6-C7-C8-C10
21	G	601	CHL	C12-C13-C15-C16
21	N	601	CHL	C6-C7-C8-C10
21	N	601	CHL	C12-C13-C15-C16
21	Y	601	CHL	C6-C7-C8-C10
21	Y	601	CHL	C12-C13-C15-C16
22	b	604	CLA	C12-C13-C15-C16
22	b	607	CLA	C12-C13-C15-C16
22	b	610	CLA	C6-C7-C8-C10
22	b	611	CLA	C12-C13-C15-C16
22	c	502	CLA	C11-C10-C8-C7
22	c	503	CLA	C11-C10-C8-C7
22	c	508	CLA	C11-C12-C13-C15
22	c	514	CLA	C11-C10-C8-C7
22	B	607	CLA	C12-C13-C15-C16
22	B	610	CLA	C12-C13-C15-C16
22	B	613	CLA	C6-C7-C8-C10
22	B	614	CLA	C12-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C7
22	C	504	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C12-C13-C15
22	C	515	CLA	C11-C10-C8-C7
22	r	303	CLA	C11-C10-C8-C7
22	R	302	CLA	C11-C10-C8-C7
21	y	609	CHL	C16-C17-C18-C19
35	c	518	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	d	403	CLA	CBD-CGD-O2D-CED
22	D	404	CLA	CBD-CGD-O2D-CED
26	r	302	LHG	C31-C32-C33-C34
26	R	301	LHG	C31-C32-C33-C34
35	C	519	DGD	C8A-C9A-CAA-CBA
30	d	401	PHO	CBA-CGA-O2A-C1
30	D	401	PHO	CBA-CGA-O2A-C1
26	y	617	LHG	C13-C14-C15-C16
26	c	522	LHG	C2-C3-O3-P
26	C	522	LHG	C2-C3-O3-P
26	D	408	LHG	C10-C11-C12-C13
36	D	411	LMG	C31-C32-C33-C34
22	b	614	CLA	C4-C3-C5-C6
22	B	617	CLA	C4-C3-C5-C6
26	d	407	LHG	C10-C11-C12-C13
36	c	523	LMG	C37-C38-C39-C40
35	c	517	DGD	C6A-C7A-C8A-C9A
35	C	518	DGD	C6A-C7A-C8A-C9A
33	d	402	SQD	O49-C7-O47-C45
32	a	410	PL9	C2-C3-C7-C8
32	A	411	PL9	C2-C3-C7-C8
26	c	520	LHG	O6-C4-C5-O7
26	d	407	LHG	O6-C4-C5-O7
26	C	520	LHG	O6-C4-C5-O7
26	D	408	LHG	O6-C4-C5-O7
26	r	302	LHG	O6-C4-C5-O7
26	R	301	LHG	O6-C4-C5-O7
36	C	523	LMG	C37-C38-C39-C40
26	d	407	LHG	C8-C7-O7-C5
26	d	409	LHG	C8-C7-O7-C5
26	D	408	LHG	C8-C7-O7-C5
26	D	410	LHG	C8-C7-O7-C5
22	c	506	CLA	C2A-CAA-CBA-CGA
22	C	503	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	C2A-CAA-CBA-CGA
22	r	305	CLA	C2A-CAA-CBA-CGA
21	g	607	CHL	C6-C7-C8-C9
21	y	607	CHL	C6-C7-C8-C9
21	G	607	CHL	C6-C7-C8-C9
21	N	606	CHL	C6-C7-C8-C9
21	Y	606	CHL	C6-C7-C8-C9
21	r	306	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	R	305	CHL	C14-C13-C15-C16
22	b	605	CLA	C14-C13-C15-C16
22	b	612	CLA	C14-C13-C15-C16
22	c	509	CLA	C11-C10-C8-C9
22	B	608	CLA	C14-C13-C15-C16
22	B	615	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C9
22	r	310	CLA	C6-C7-C8-C9
22	R	309	CLA	C6-C7-C8-C9
26	y	617	LHG	C11-C12-C13-C14
36	d	410	LMG	C31-C32-C33-C34
24	N	616	XAT	C29-C30-C31-C32
31	k	101	BCR	C15-C16-C17-C18
31	K	101	BCR	C15-C16-C17-C18
35	H	102	DGD	C3A-C4A-C5A-C6A
26	l	102	LHG	C11-C10-C9-C8
35	c	517	DGD	C4B-C5B-C6B-C7B
35	c	519	DGD	C9B-CAB-CBB-CCB
35	h	102	DGD	C3A-C4A-C5A-C6A
21	g	606	CHL	C1-C2-C3-C4
21	n	605	CHL	C1-C2-C3-C4
21	y	606	CHL	C1-C2-C3-C4
21	G	606	CHL	C1-C2-C3-C4
21	N	605	CHL	C1-C2-C3-C4
21	Y	605	CHL	C1-C2-C3-C4
22	s	312	CLA	C1-C2-C3-C4
22	S	312	CLA	C1-C2-C3-C4
33	l	103	SQD	O5-C5-C6-S
33	L	101	SQD	O5-C5-C6-S
32	D	407	PL9	C42-C43-C44-C45
26	L	103	LHG	C11-C10-C9-C8
35	C	518	DGD	C4B-C5B-C6B-C7B
35	J	101	DGD	C9B-CAB-CBB-CCB
21	r	306	CHL	C3-C5-C6-C7
21	R	305	CHL	C3-C5-C6-C7
26	N	618	LHG	O10-C23-O8-C6
26	b	619	LHG	O7-C5-C6-O8
26	B	622	LHG	O7-C5-C6-O8
33	a	411	SQD	O6-C44-C45-O47
33	l	103	SQD	O6-C44-C45-O47
33	A	412	SQD	O6-C44-C45-O47
33	L	101	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
36	k	103	LMG	O1-C7-C8-O7
36	K	103	LMG	O1-C7-C8-O7
26	d	408	LHG	C1-C2-C3-O3
26	D	409	LHG	C1-C2-C3-O3
26	r	302	LHG	C15-C16-C17-C18
22	G	613	CLA	C16-C17-C18-C19
33	l	101	SQD	C44-C45-C46-O48
33	L	102	SQD	C44-C45-C46-O48
35	c	517	DGD	O1G-C1G-C2G-C3G
35	C	518	DGD	O1G-C1G-C2G-C3G
36	w	102	LMG	O1-C7-C8-C9
36	C	502	LMG	O1-C7-C8-C9
22	b	605	CLA	C10-C11-C12-C13
22	B	608	CLA	C10-C11-C12-C13
22	C	514	CLA	C8-C10-C11-C12
21	s	306	CHL	CAD-CBD-CGD-O2D
21	S	306	CHL	CAD-CBD-CGD-O2D
22	g	613	CLA	CAD-CBD-CGD-O2D
22	n	612	CLA	CAD-CBD-CGD-O2D
22	y	612	CLA	CAD-CBD-CGD-O2D
22	G	613	CLA	CAD-CBD-CGD-O2D
22	N	612	CLA	CAD-CBD-CGD-O2D
22	Y	611	CLA	CAD-CBD-CGD-O2D
22	b	603	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	B	606	CLA	CAD-CBD-CGD-O2D
22	B	616	CLA	CAD-CBD-CGD-O2D
22	s	304	CLA	CAD-CBD-CGD-O2D
22	S	304	CLA	CAD-CBD-CGD-O2D
22	c	513	CLA	C8-C10-C11-C12
26	R	301	LHG	C15-C16-C17-C18
26	L	103	LHG	O10-C23-O8-C6
22	b	605	CLA	C15-C16-C17-C18
22	B	608	CLA	C15-C16-C17-C18
22	c	502	CLA	C2A-CAA-CBA-CGA
22	R	304	CLA	C2A-CAA-CBA-CGA
26	l	102	LHG	O10-C23-O8-C6
36	b	620	LMG	C4-C5-C6-O5
36	B	623	LMG	C4-C5-C6-O5
30	d	401	PHO	O1A-CGA-O2A-C1
30	D	401	PHO	O1A-CGA-O2A-C1
21	g	605	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	g	607	CHL	CHA-CBD-CGD-O2D
21	n	606	CHL	CHA-CBD-CGD-O1D
21	n	606	CHL	CHA-CBD-CGD-O2D
21	y	605	CHL	CHA-CBD-CGD-O2D
21	y	607	CHL	CHA-CBD-CGD-O2D
21	G	605	CHL	CHA-CBD-CGD-O2D
21	G	607	CHL	CHA-CBD-CGD-O1D
21	G	607	CHL	CHA-CBD-CGD-O2D
21	N	606	CHL	CHA-CBD-CGD-O1D
21	N	606	CHL	CHA-CBD-CGD-O2D
21	Y	606	CHL	CHA-CBD-CGD-O1D
21	Y	606	CHL	CHA-CBD-CGD-O2D
21	r	301	CHL	CHA-CBD-CGD-O2D
21	s	301	CHL	CHA-CBD-CGD-O2D
21	s	306	CHL	CAD-CBD-CGD-O1D
21	S	301	CHL	CHA-CBD-CGD-O2D
21	S	306	CHL	CAD-CBD-CGD-O1D
22	g	613	CLA	CAD-CBD-CGD-O1D
22	n	612	CLA	CAD-CBD-CGD-O1D
22	y	612	CLA	CAD-CBD-CGD-O1D
22	G	613	CLA	CAD-CBD-CGD-O1D
22	N	612	CLA	CAD-CBD-CGD-O1D
22	Y	611	CLA	CAD-CBD-CGD-O1D
22	b	603	CLA	CAD-CBD-CGD-O1D
22	b	613	CLA	CAD-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CAD-CBD-CGD-O1D
22	B	616	CLA	CAD-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	r	312	CLA	CHA-CBD-CGD-O1D
22	r	312	CLA	CHA-CBD-CGD-O2D
22	s	304	CLA	CAD-CBD-CGD-O1D
22	s	305	CLA	CHA-CBD-CGD-O1D
22	s	305	CLA	CHA-CBD-CGD-O2D
22	S	304	CLA	CAD-CBD-CGD-O1D
22	S	305	CLA	CHA-CBD-CGD-O1D
22	S	305	CLA	CHA-CBD-CGD-O2D
22	R	311	CLA	CHA-CBD-CGD-O1D
22	R	311	CLA	CHA-CBD-CGD-O2D
24	y	615	XAT	C29-C30-C31-C32
24	N	616	XAT	C33-C34-C35-C15
24	Y	615	XAT	C33-C34-C35-C15

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Mol	Chain	Res	Type	Atoms
24	r	314	XAT	C13-C14-C15-C35
24	R	313	XAT	C13-C14-C15-C35
26	G	618	LHG	C3-O3-P-O5
26	Y	617	LHG	C3-O3-P-O5
26	b	619	LHG	C4-O6-P-O3
26	c	520	LHG	C4-O6-P-O5
26	d	409	LHG	C3-O3-P-O6
26	l	102	LHG	C3-O3-P-O6
26	B	622	LHG	C4-O6-P-O3
26	C	520	LHG	C4-O6-P-O5
26	D	408	LHG	C3-O3-P-O6
26	D	410	LHG	C3-O3-P-O6
26	L	103	LHG	C3-O3-P-O6
26	s	314	LHG	C4-O6-P-O3
26	S	314	LHG	C4-O6-P-O3
30	d	401	PHO	CHA-CBD-CGD-O2D
30	D	401	PHO	CHA-CBD-CGD-O2D
21	g	601	CHL	CBD-CGD-O2D-CED
21	N	601	CHL	CBD-CGD-O2D-CED
22	r	310	CLA	O1D-CGD-O2D-CED
31	B	602	BCR	C14-C15-C16-C17
26	n	617	LHG	O10-C23-O8-C6
36	M	101	LMG	C21-C22-C23-C24
36	T	101	LMG	C21-C22-C23-C24
22	c	506	CLA	C2B-C3B-CAB-CBB
22	c	511	CLA	C2B-C3B-CAB-CBB
22	C	507	CLA	C2B-C3B-CAB-CBB
22	C	512	CLA	C2B-C3B-CAB-CBB
22	s	303	CLA	C2B-C3B-CAB-CBB
22	S	303	CLA	C2B-C3B-CAB-CBB
23	N	615	LUT	C1-C6-C7-C8
31	a	409	BCR	C1-C6-C7-C8
31	c	515	BCR	C23-C24-C25-C30
31	c	516	BCR	C23-C24-C25-C30
31	d	405	BCR	C23-C24-C25-C30
31	h	101	BCR	C1-C6-C7-C8
31	k	101	BCR	C1-C6-C7-C8
31	A	410	BCR	C1-C6-C7-C8
31	C	516	BCR	C23-C24-C25-C30
31	C	517	BCR	C23-C24-C25-C30
31	D	406	BCR	C23-C24-C25-C30
31	H	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	K	101	BCR	C1-C6-C7-C8
26	d	409	LHG	C14-C15-C16-C17
22	a	405	CLA	C2-C3-C5-C6
22	A	406	CLA	C2-C3-C5-C6
26	D	410	LHG	C14-C15-C16-C17
23	G	616	LUT	C31-C32-C33-C40
26	c	521	LHG	C5-C4-O6-P
26	d	407	LHG	C2-C3-O3-P
26	d	407	LHG	C5-C4-O6-P
26	C	521	LHG	C5-C4-O6-P
26	D	408	LHG	C2-C3-O3-P
26	D	408	LHG	C5-C4-O6-P
22	r	304	CLA	C5-C6-C7-C8
26	c	520	LHG	C23-C24-C25-C26
26	C	520	LHG	C23-C24-C25-C26
26	L	103	LHG	C10-C11-C12-C13
36	k	103	LMG	C37-C38-C39-C40
26	N	618	LHG	C35-C36-C37-C38
26	l	102	LHG	C10-C11-C12-C13
36	K	103	LMG	C37-C38-C39-C40
26	c	521	LHG	O1-C1-C2-C3
26	C	521	LHG	O1-C1-C2-C3
22	R	303	CLA	C5-C6-C7-C8
35	c	518	DGD	C3G-C2G-O2G-C1B
35	C	519	DGD	C3G-C2G-O2G-C1B
26	S	314	LHG	C31-C32-C33-C34
23	g	615	LUT	C10-C11-C12-C13
23	n	614	LUT	C10-C11-C12-C13
23	y	614	LUT	C10-C11-C12-C13
23	G	615	LUT	C10-C11-C12-C13
23	N	614	LUT	C10-C11-C12-C13
23	Y	613	LUT	C10-C11-C12-C13
23	r	313	LUT	C10-C11-C12-C13
23	R	312	LUT	C10-C11-C12-C13
25	g	618	NEX	C30-C31-C32-C33
25	n	616	NEX	C30-C31-C32-C33
25	y	616	NEX	C30-C31-C32-C33
25	N	617	NEX	C30-C31-C32-C33
25	Y	616	NEX	C30-C31-C32-C33
26	s	314	LHG	C31-C32-C33-C34
36	c	523	LMG	C4-C5-C6-O5
22	G	610	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	R	309	CLA	O1D-CGD-O2D-CED
21	g	601	CHL	C16-C17-C18-C20
21	n	601	CHL	C16-C17-C18-C20
21	y	601	CHL	C16-C17-C18-C20
21	G	601	CHL	C16-C17-C18-C20
21	N	601	CHL	C16-C17-C18-C20
21	Y	601	CHL	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C20
22	B	607	CLA	C16-C17-C18-C19
22	C	504	CLA	C16-C17-C18-C20
36	b	620	LMG	C41-C42-C43-C44
36	B	623	LMG	C41-C42-C43-C44
36	C	523	LMG	C4-C5-C6-O5
26	g	619	LHG	O6-C4-C5-C6
21	g	608	CHL	C6-C7-C8-C9
21	n	607	CHL	C6-C7-C8-C9
21	y	608	CHL	C6-C7-C8-C9
21	G	608	CHL	C6-C7-C8-C9
21	N	607	CHL	C6-C7-C8-C9
21	Y	607	CHL	C6-C7-C8-C9
22	g	602	CLA	C11-C10-C8-C9
22	n	602	CLA	C11-C10-C8-C9
22	y	602	CLA	C11-C10-C8-C9
22	y	612	CLA	C14-C13-C15-C16
22	G	602	CLA	C11-C10-C8-C9
22	N	602	CLA	C11-C10-C8-C9
22	Y	602	CLA	C11-C10-C8-C9
22	b	610	CLA	C14-C13-C15-C16
22	b	614	CLA	C14-C13-C15-C16
22	c	502	CLA	C11-C10-C8-C9
22	c	508	CLA	C11-C12-C13-C14
22	d	403	CLA	C11-C12-C13-C14
22	B	613	CLA	C14-C13-C15-C16
22	B	617	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C12-C13-C14
22	D	404	CLA	C11-C12-C13-C14
22	s	303	CLA	C6-C7-C8-C9
22	S	303	CLA	C6-C7-C8-C9
21	n	608	CHL	C11-C12-C13-C15
22	g	611	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	n	610	CLA	C6-C7-C8-C10
22	y	611	CLA	C6-C7-C8-C10
22	G	611	CLA	C6-C7-C8-C10
22	N	610	CLA	C6-C7-C8-C10
22	Y	610	CLA	C6-C7-C8-C10
21	G	601	CHL	CBD-CGD-O2D-CED
31	T	102	BCR	C14-C15-C16-C17
35	h	102	DGD	C2E-C1E-O5D-C6D
35	H	102	DGD	C2E-C1E-O5D-C6D
35	C	518	DGD	C4D-C5D-C6D-O5D
21	r	306	CHL	C4-C3-C5-C6
21	R	305	CHL	C4-C3-C5-C6
26	y	617	LHG	C23-C24-C25-C26
21	n	606	CHL	C10-C11-C12-C13
21	N	606	CHL	C10-C11-C12-C13
36	d	410	LMG	C32-C33-C34-C35
36	D	411	LMG	C32-C33-C34-C35
35	c	517	DGD	C4D-C5D-C6D-O5D
26	y	617	LHG	C35-C36-C37-C38
36	B	601	LMG	O7-C8-C9-O8
36	I	101	LMG	O7-C8-C9-O8
21	y	601	CHL	CBD-CGD-O2D-CED
21	g	607	CHL	C10-C11-C12-C13
21	y	607	CHL	C10-C11-C12-C13
21	G	607	CHL	C10-C11-C12-C13
36	w	102	LMG	C16-C17-C18-C19
36	C	502	LMG	C16-C17-C18-C19
21	Y	606	CHL	C10-C11-C12-C13
22	c	510	CLA	CAA-CBA-CGA-O2A
22	C	511	CLA	CAA-CBA-CGA-O2A
26	y	617	LHG	C11-C10-C9-C8
36	c	523	LMG	C35-C36-C37-C38
36	C	523	LMG	C35-C36-C37-C38
22	r	310	CLA	C16-C17-C18-C20
22	R	309	CLA	C16-C17-C18-C20
33	a	411	SQD	O6-C44-C45-C46
33	A	412	SQD	O6-C44-C45-C46
33	D	402	SQD	C11-C10-C9-C8
33	d	402	SQD	C11-C10-C9-C8
35	C	518	DGD	C2A-C3A-C4A-C5A
24	G	617	XAT	C7-C8-C9-C10
21	n	601	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	B	601	LMG	C8-C7-O1-C1
36	I	101	LMG	C8-C7-O1-C1
35	c	517	DGD	C2A-C3A-C4A-C5A
22	b	601	CLA	C5-C6-C7-C8
22	B	604	CLA	C5-C6-C7-C8
30	d	401	PHO	C2A-CAA-CBA-CGA
30	D	401	PHO	C2A-CAA-CBA-CGA
23	r	313	LUT	C29-C30-C31-C32
23	R	312	LUT	C29-C30-C31-C32
26	c	520	LHG	C31-C32-C33-C34
26	C	520	LHG	C31-C32-C33-C34
36	c	523	LMG	C16-C17-C18-C19
36	C	523	LMG	C16-C17-C18-C19
22	b	604	CLA	C4-C3-C5-C6
22	B	607	CLA	C4-C3-C5-C6
21	G	601	CHL	C8-C10-C11-C12
21	Y	601	CHL	C8-C10-C11-C12
36	d	410	LMG	C14-C15-C16-C17
22	C	511	CLA	C4C-C3C-CAC-CBC
26	C	522	LHG	C14-C15-C16-C17
36	D	411	LMG	C14-C15-C16-C17
26	D	408	LHG	O10-C23-O8-C6
22	c	510	CLA	C4C-C3C-CAC-CBC
21	y	601	CHL	C8-C10-C11-C12
21	g	606	CHL	CAA-CBA-CGA-O1A
21	n	605	CHL	CAA-CBA-CGA-O1A
21	y	606	CHL	CAA-CBA-CGA-O1A
21	G	606	CHL	CAA-CBA-CGA-O1A
21	N	605	CHL	CAA-CBA-CGA-O1A
21	Y	605	CHL	CAA-CBA-CGA-O1A
22	D	404	CLA	O1D-CGD-O2D-CED
26	c	522	LHG	C14-C15-C16-C17
21	r	308	CHL	C6-C7-C8-C9
21	R	307	CHL	C6-C7-C8-C9
22	b	604	CLA	C14-C13-C15-C16
22	b	607	CLA	C14-C13-C15-C16
22	b	610	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C12-C13-C14
22	c	513	CLA	C11-C12-C13-C14
22	B	607	CLA	C14-C13-C15-C16
22	B	610	CLA	C14-C13-C15-C16
22	B	613	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	C11-C12-C13-C14
22	C	514	CLA	C11-C12-C13-C14
22	g	614	CLA	CBA-CGA-O2A-C1
22	n	613	CLA	CBA-CGA-O2A-C1
22	y	613	CLA	CBA-CGA-O2A-C1
22	G	614	CLA	CBA-CGA-O2A-C1
22	N	613	CLA	CBA-CGA-O2A-C1
22	Y	612	CLA	CBA-CGA-O2A-C1
21	g	601	CHL	C8-C10-C11-C12
22	x	101	CLA	C13-C15-C16-C17
26	d	407	LHG	O10-C23-O8-C6
22	d	403	CLA	O1D-CGD-O2D-CED
22	s	308	CLA	C4B-C3B-CAB-CBB
22	S	308	CLA	C4B-C3B-CAB-CBB
21	N	601	CHL	C8-C10-C11-C12
21	n	601	CHL	C8-C10-C11-C12
22	B	603	CLA	C13-C15-C16-C17
26	N	618	LHG	C19-C20-C21-C22
26	Y	617	LHG	C24-C23-O8-C6
21	r	306	CHL	C2-C3-C5-C6
21	R	305	CHL	C2-C3-C5-C6
33	d	402	SQD	C30-C31-C32-C33
33	D	402	SQD	C30-C31-C32-C33
26	n	617	LHG	O6-C4-C5-C6
21	G	601	CHL	O1D-CGD-O2D-CED
21	N	601	CHL	O1D-CGD-O2D-CED
22	g	610	CLA	C6-C7-C8-C10
22	n	609	CLA	C6-C7-C8-C10
22	y	610	CLA	C6-C7-C8-C10
22	G	610	CLA	C6-C7-C8-C10
22	N	609	CLA	C6-C7-C8-C10
22	Y	609	CLA	C6-C7-C8-C10
22	b	610	CLA	C11-C10-C8-C7
22	B	613	CLA	C11-C10-C8-C7
21	Y	601	CHL	CBD-CGD-O2D-CED
26	c	520	LHG	C26-C27-C28-C29
26	C	520	LHG	C26-C27-C28-C29
22	y	613	CLA	O1A-CGA-O2A-C1
22	N	613	CLA	O1A-CGA-O2A-C1
21	g	601	CHL	O1D-CGD-O2D-CED
22	y	610	CLA	C11-C12-C13-C14
22	Y	609	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	C16-C17-C18-C20
22	C	504	CLA	C16-C17-C18-C19
26	L	103	LHG	C28-C29-C30-C31
33	D	402	SQD	O49-C7-C8-C9
22	a	405	CLA	C15-C16-C17-C18
22	A	406	CLA	C15-C16-C17-C18
22	g	614	CLA	O1A-CGA-O2A-C1
22	n	613	CLA	O1A-CGA-O2A-C1
22	G	614	CLA	O1A-CGA-O2A-C1
22	Y	612	CLA	O1A-CGA-O2A-C1
26	l	102	LHG	C28-C29-C30-C31
35	c	517	DGD	O1G-C1G-C2G-O2G
35	C	518	DGD	O1G-C1G-C2G-O2G
21	g	608	CHL	C3A-C2A-CAA-CBA
21	n	607	CHL	C3A-C2A-CAA-CBA
21	y	608	CHL	C3A-C2A-CAA-CBA
21	G	608	CHL	C3A-C2A-CAA-CBA
21	N	607	CHL	C3A-C2A-CAA-CBA
21	Y	607	CHL	C3A-C2A-CAA-CBA
22	b	607	CLA	C3A-C2A-CAA-CBA
22	c	509	CLA	C4-C3-C5-C6
22	B	610	CLA	C3A-C2A-CAA-CBA
22	C	510	CLA	C4-C3-C5-C6
21	y	601	CHL	O1D-CGD-O2D-CED
36	B	601	LMG	C33-C34-C35-C36
22	c	503	CLA	C16-C17-C18-C19
36	I	101	LMG	C33-C34-C35-C36
25	Y	616	NEX	C39-C29-C30-C31
36	k	103	LMG	O6-C1-O1-C7
36	K	103	LMG	O6-C1-O1-C7
33	d	402	SQD	O49-C7-C8-C9
24	Y	615	XAT	C29-C30-C31-C32
25	n	616	NEX	C29-C30-C31-C32
25	n	616	NEX	C33-C34-C35-C15
22	b	602	CLA	C16-C17-C18-C20
36	C	502	LMG	O6-C5-C6-O5
36	M	101	LMG	C19-C20-C21-C22
36	T	101	LMG	C19-C20-C21-C22
36	B	601	LMG	C37-C38-C39-C40
36	B	623	LMG	C29-C30-C31-C32
36	I	101	LMG	C37-C38-C39-C40
21	Y	601	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	R	307	CHL	C5-C6-C7-C8
22	C	508	CLA	C5-C6-C7-C8
22	b	614	CLA	C2-C3-C5-C6
22	B	617	CLA	C2-C3-C5-C6
22	c	507	CLA	C5-C6-C7-C8
36	b	620	LMG	C29-C30-C31-C32
21	s	306	CHL	C2A-CAA-CBA-CGA
36	w	102	LMG	O6-C5-C6-O5
21	n	601	CHL	O1D-CGD-O2D-CED
26	y	617	LHG	C30-C31-C32-C33
21	r	308	CHL	C5-C6-C7-C8
36	k	103	LMG	C39-C40-C41-C42
36	K	103	LMG	C39-C40-C41-C42
22	s	304	CLA	CAA-CBA-CGA-O1A
22	S	304	CLA	CAA-CBA-CGA-O1A
26	G	618	LHG	O10-C23-O8-C6
22	g	610	CLA	C6-C7-C8-C9
22	n	609	CLA	C6-C7-C8-C9
22	y	610	CLA	C6-C7-C8-C9
22	G	610	CLA	C6-C7-C8-C9
22	N	609	CLA	C6-C7-C8-C9
22	Y	609	CLA	C6-C7-C8-C9
22	b	601	CLA	C11-C12-C13-C14
22	b	603	CLA	C11-C12-C13-C14
22	b	610	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C12-C13-C14
22	d	403	CLA	C6-C7-C8-C9
22	B	604	CLA	C11-C12-C13-C14
22	B	606	CLA	C11-C12-C13-C14
22	B	613	CLA	C11-C10-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C12-C13-C14
22	D	404	CLA	C6-C7-C8-C9
33	d	402	SQD	C23-C24-C25-C26
33	D	402	SQD	C23-C24-C25-C26
22	c	506	CLA	C15-C16-C17-C18
22	C	507	CLA	C15-C16-C17-C18
26	G	618	LHG	O9-C7-O7-C5
21	g	608	CHL	C1A-C2A-CAA-CBA
21	n	607	CHL	C1A-C2A-CAA-CBA
21	y	608	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	G	608	CHL	C1A-C2A-CAA-CBA
21	N	607	CHL	C1A-C2A-CAA-CBA
21	Y	607	CHL	C1A-C2A-CAA-CBA
21	s	307	CHL	C1A-C2A-CAA-CBA
21	S	306	CHL	CAA-CBA-CGA-O1A
22	n	611	CLA	C2-C3-C5-C6
22	N	611	CLA	C2-C3-C5-C6
22	W	101	CLA	C2-C3-C5-C6
36	C	502	LMG	C4-C5-C6-O5
22	B	605	CLA	C2A-CAA-CBA-CGA
26	g	619	LHG	C27-C28-C29-C30
35	c	518	DGD	O2G-C1B-C2B-C3B
35	C	519	DGD	O2G-C1B-C2B-C3B
22	b	602	CLA	C1A-C2A-CAA-CBA
22	b	605	CLA	C1A-C2A-CAA-CBA
22	c	502	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C1A-C2A-CAA-CBA
22	C	503	CLA	C1A-C2A-CAA-CBA
24	r	314	XAT	C32-C33-C34-C35
24	R	313	XAT	C32-C33-C34-C35
36	w	102	LMG	C4-C5-C6-O5
22	g	610	CLA	C2B-C3B-CAB-CBB
22	n	609	CLA	C2B-C3B-CAB-CBB
22	y	610	CLA	C2B-C3B-CAB-CBB
22	G	610	CLA	C2B-C3B-CAB-CBB
22	N	609	CLA	C2B-C3B-CAB-CBB
22	Y	609	CLA	C2B-C3B-CAB-CBB
22	a	406	CLA	C2B-C3B-CAB-CBB
22	b	606	CLA	C2B-C3B-CAB-CBB
22	b	608	CLA	C2B-C3B-CAB-CBB
22	A	407	CLA	C2B-C3B-CAB-CBB
22	B	609	CLA	C2B-C3B-CAB-CBB
22	B	611	CLA	C2B-C3B-CAB-CBB
22	r	304	CLA	C2B-C3B-CAB-CBB
22	r	311	CLA	C2B-C3B-CAB-CBB
22	s	304	CLA	C2B-C3B-CAB-CBB
22	s	308	CLA	C2B-C3B-CAB-CBB
22	S	304	CLA	C2B-C3B-CAB-CBB
22	S	308	CLA	C2B-C3B-CAB-CBB
22	R	303	CLA	C2B-C3B-CAB-CBB
22	R	310	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	a	409	BCR	C23-C24-C25-C30
31	b	616	BCR	C5-C6-C7-C8
31	b	617	BCR	C1-C6-C7-C8
31	c	515	BCR	C5-C6-C7-C8
31	c	516	BCR	C1-C6-C7-C8
31	d	405	BCR	C5-C6-C7-C8
31	h	101	BCR	C23-C24-C25-C30
31	k	101	BCR	C23-C24-C25-C30
31	k	102	BCR	C5-C6-C7-C8
31	k	102	BCR	C23-C24-C25-C30
31	A	410	BCR	C5-C6-C7-C8
31	A	410	BCR	C23-C24-C25-C30
31	B	602	BCR	C5-C6-C7-C8
31	B	619	BCR	C5-C6-C7-C8
31	B	620	BCR	C1-C6-C7-C8
31	C	516	BCR	C5-C6-C7-C8
31	C	517	BCR	C1-C6-C7-C8
31	D	406	BCR	C5-C6-C7-C8
31	H	101	BCR	C23-C24-C25-C30
31	K	101	BCR	C23-C24-C25-C30
31	K	102	BCR	C5-C6-C7-C8
31	K	102	BCR	C23-C24-C25-C30
31	T	102	BCR	C5-C6-C7-C8
21	S	302	CHL	CAA-CBA-CGA-O2A
22	S	304	CLA	CAA-CBA-CGA-O2A
26	c	522	LHG	C11-C10-C9-C8
26	C	522	LHG	C11-C10-C9-C8
21	s	302	CHL	CAA-CBA-CGA-O2A
21	S	306	CHL	CAA-CBA-CGA-O2A
22	s	304	CLA	CAA-CBA-CGA-O2A
32	d	406	PL9	C35-C34-C36-C37
32	D	407	PL9	C35-C34-C36-C37
22	g	612	CLA	C2-C3-C5-C6
22	G	612	CLA	C2-C3-C5-C6
22	w	101	CLA	C2-C3-C5-C6
36	B	623	LMG	C39-C40-C41-C42
22	s	312	CLA	O2A-C1-C2-C3
22	S	312	CLA	O2A-C1-C2-C3
21	s	306	CHL	CAA-CBA-CGA-O2A
36	b	620	LMG	C39-C40-C41-C42
21	N	608	CHL	C11-C12-C13-C15
21	r	308	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	R	307	CHL	C6-C7-C8-C10
22	g	612	CLA	C6-C7-C8-C10
22	n	611	CLA	C6-C7-C8-C10
22	G	612	CLA	C6-C7-C8-C10
22	N	611	CLA	C6-C7-C8-C10
22	a	405	CLA	C6-C7-C8-C10
22	b	603	CLA	C6-C7-C8-C10
22	b	613	CLA	C12-C13-C15-C16
22	b	614	CLA	C12-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C15
22	w	101	CLA	C6-C7-C8-C10
22	A	406	CLA	C6-C7-C8-C10
22	B	606	CLA	C6-C7-C8-C10
22	B	616	CLA	C12-C13-C15-C16
22	B	617	CLA	C12-C13-C15-C16
22	C	512	CLA	C11-C12-C13-C15
22	W	101	CLA	C6-C7-C8-C10
22	b	614	CLA	C16-C17-C18-C20
22	B	617	CLA	C16-C17-C18-C20
22	r	310	CLA	C16-C17-C18-C19
22	R	309	CLA	C16-C17-C18-C19
21	S	306	CHL	C2A-CAA-CBA-CGA
22	b	602	CLA	C2A-CAA-CBA-CGA
22	s	312	CLA	C2A-CAA-CBA-CGA
22	S	312	CLA	C2A-CAA-CBA-CGA
35	a	413	DGD	O2G-C2G-C3G-O3G
35	A	401	DGD	O2G-C2G-C3G-O3G
21	s	306	CHL	CAA-CBA-CGA-O1A
35	a	413	DGD	C6A-C7A-C8A-C9A
35	h	102	DGD	C7B-C8B-C9B-CAB
35	A	401	DGD	C6A-C7A-C8A-C9A
35	H	102	DGD	C7B-C8B-C9B-CAB
36	d	410	LMG	C35-C36-C37-C38
36	D	411	LMG	C35-C36-C37-C38
36	K	103	LMG	O9-C10-O7-C8
22	s	311	CLA	C11-C10-C8-C7
22	S	311	CLA	C11-C10-C8-C7
30	d	401	PHO	C4-C3-C5-C6
30	D	401	PHO	C4-C3-C5-C6
21	g	608	CHL	CAA-CBA-CGA-O2A
22	s	311	CLA	CAA-CBA-CGA-O2A
22	S	311	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
35	c	518	DGD	C3B-C4B-C5B-C6B
35	C	519	DGD	C3B-C4B-C5B-C6B
35	c	519	DGD	O6D-C5D-C6D-O5D
35	J	101	DGD	O6D-C5D-C6D-O5D
22	g	604	CLA	C2-C1-O2A-CGA
22	n	604	CLA	C2-C1-O2A-CGA
22	y	604	CLA	C2-C1-O2A-CGA
22	G	604	CLA	C2-C1-O2A-CGA
22	N	604	CLA	C2-C1-O2A-CGA
22	Y	604	CLA	C2-C1-O2A-CGA
22	d	404	CLA	C14-C13-C15-C16
22	D	405	CLA	C14-C13-C15-C16
36	k	103	LMG	O9-C10-O7-C8
21	n	607	CHL	CAA-CBA-CGA-O2A
21	G	608	CHL	CAA-CBA-CGA-O2A
21	N	607	CHL	CAA-CBA-CGA-O2A
22	b	604	CLA	CBA-CGA-O2A-C1
22	c	504	CLA	C4-C3-C5-C6
22	C	505	CLA	C4-C3-C5-C6
26	r	302	LHG	C5-C4-O6-P
26	R	301	LHG	C5-C4-O6-P
21	y	608	CHL	CAA-CBA-CGA-O2A
21	Y	607	CHL	CAA-CBA-CGA-O2A
22	s	310	CLA	C2-C3-C5-C6
22	S	310	CLA	C2-C3-C5-C6
21	g	601	CHL	C16-C17-C18-C19
21	n	601	CHL	C16-C17-C18-C19
21	y	601	CHL	C16-C17-C18-C19
21	G	601	CHL	C16-C17-C18-C19
21	N	601	CHL	C16-C17-C18-C19
21	Y	601	CHL	C16-C17-C18-C19
22	B	607	CLA	CBA-CGA-O2A-C1
21	S	302	CHL	CAA-CBA-CGA-O1A
22	s	308	CLA	CAA-CBA-CGA-O2A
22	S	308	CLA	CAA-CBA-CGA-O2A
22	b	604	CLA	O1A-CGA-O2A-C1
22	B	607	CLA	O1A-CGA-O2A-C1
26	Y	617	LHG	C23-C24-C25-C26
35	a	413	DGD	C1G-C2G-C3G-O3G
35	c	517	DGD	C1G-C2G-C3G-O3G
35	A	401	DGD	C1G-C2G-C3G-O3G
35	C	518	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
36	c	523	LMG	O1-C7-C8-C9
36	C	523	LMG	O1-C7-C8-C9
26	c	521	LHG	C19-C20-C21-C22
26	C	521	LHG	C19-C20-C21-C22
21	s	302	CHL	CAA-CBA-CGA-O1A
36	C	502	LMG	C38-C39-C40-C41
21	r	308	CHL	C4-C3-C5-C6
21	R	307	CHL	C4-C3-C5-C6
36	w	102	LMG	C38-C39-C40-C41
22	b	602	CLA	C4B-C3B-CAB-CBB
22	b	604	CLA	C4B-C3B-CAB-CBB
22	b	606	CLA	C4B-C3B-CAB-CBB
22	B	605	CLA	C4B-C3B-CAB-CBB
22	B	607	CLA	C4B-C3B-CAB-CBB
22	B	609	CLA	C4B-C3B-CAB-CBB
22	r	305	CLA	C4B-C3B-CAB-CBB
22	r	311	CLA	C4B-C3B-CAB-CBB
22	r	312	CLA	C4B-C3B-CAB-CBB
22	R	304	CLA	C4B-C3B-CAB-CBB
22	R	310	CLA	C4B-C3B-CAB-CBB
22	R	311	CLA	C4B-C3B-CAB-CBB
26	s	314	LHG	O10-C23-O8-C6
26	S	314	LHG	O10-C23-O8-C6
22	g	614	CLA	CAA-CBA-CGA-O2A
22	n	613	CLA	CAA-CBA-CGA-O2A
22	y	613	CLA	CAA-CBA-CGA-O2A
22	G	614	CLA	CAA-CBA-CGA-O2A
22	N	613	CLA	CAA-CBA-CGA-O2A
22	Y	612	CLA	CAA-CBA-CGA-O2A
22	R	302	CLA	C10-C11-C12-C13
26	c	521	LHG	C1-C2-C3-O3
26	C	521	LHG	C1-C2-C3-O3
21	g	605	CHL	CHA-CBD-CGD-O1D
21	g	607	CHL	CHA-CBD-CGD-O1D
21	y	607	CHL	CHA-CBD-CGD-O1D
21	G	605	CHL	CHA-CBD-CGD-O1D
21	s	301	CHL	CHA-CBD-CGD-O1D
22	b	613	CLA	C15-C16-C17-C18
22	B	616	CLA	C15-C16-C17-C18
22	r	303	CLA	C10-C11-C12-C13
22	A	406	CLA	C2A-CAA-CBA-CGA
26	r	302	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	R	301	LHG	C10-C11-C12-C13
26	N	618	LHG	O6-C4-C5-C6
26	c	520	LHG	O6-C4-C5-C6
26	C	520	LHG	O6-C4-C5-C6
22	s	303	CLA	C5-C6-C7-C8
22	S	303	CLA	C5-C6-C7-C8
26	c	522	LHG	C28-C29-C30-C31
21	Y	608	CHL	C12-C13-C15-C16
22	g	610	CLA	C11-C12-C13-C15
22	N	609	CLA	C11-C12-C13-C15
22	c	514	CLA	C12-C13-C15-C16
22	C	515	CLA	C12-C13-C15-C16
26	g	619	LHG	C14-C15-C16-C17
26	Y	617	LHG	C10-C11-C12-C13
26	C	522	LHG	C28-C29-C30-C31
26	n	617	LHG	C34-C35-C36-C37
21	g	605	CHL	CAA-CBA-CGA-O2A
26	c	521	LHG	C24-C23-O8-C6
26	C	521	LHG	C24-C23-O8-C6
22	g	612	CLA	C11-C10-C8-C9
22	n	611	CLA	C11-C10-C8-C9
22	G	612	CLA	C11-C10-C8-C9
22	N	611	CLA	C11-C10-C8-C9
22	c	505	CLA	C11-C10-C8-C9
22	w	101	CLA	C11-C10-C8-C9
22	C	506	CLA	C11-C10-C8-C9
22	W	101	CLA	C11-C10-C8-C9
30	d	401	PHO	C11-C10-C8-C9
30	d	401	PHO	C14-C13-C15-C16
30	D	401	PHO	C11-C10-C8-C9
30	D	401	PHO	C14-C13-C15-C16
35	c	519	DGD	C5D-C6D-O5D-C1E
35	h	102	DGD	C2G-C3G-O3G-C1D
35	H	102	DGD	C2G-C3G-O3G-C1D
35	J	101	DGD	C5D-C6D-O5D-C1E
26	c	520	LHG	C35-C36-C37-C38
21	G	605	CHL	CAA-CBA-CGA-O2A
22	g	602	CLA	C2A-CAA-CBA-CGA
22	n	602	CLA	C2A-CAA-CBA-CGA
22	y	602	CLA	C2A-CAA-CBA-CGA
22	G	602	CLA	C2A-CAA-CBA-CGA
22	N	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	Y	602	CLA	C2A-CAA-CBA-CGA
22	a	405	CLA	C2A-CAA-CBA-CGA
21	g	608	CHL	C2-C1-O2A-CGA
21	n	607	CHL	C2-C1-O2A-CGA
21	y	608	CHL	C2-C1-O2A-CGA
21	G	608	CHL	C2-C1-O2A-CGA
21	N	607	CHL	C2-C1-O2A-CGA
21	Y	607	CHL	C2-C1-O2A-CGA
22	b	601	CLA	C2-C1-O2A-CGA
22	b	609	CLA	C2-C1-O2A-CGA
22	c	508	CLA	C2-C1-O2A-CGA
22	B	604	CLA	C2-C1-O2A-CGA
22	B	612	CLA	C2-C1-O2A-CGA
22	C	509	CLA	C2-C1-O2A-CGA
22	s	312	CLA	C2-C1-O2A-CGA
22	S	312	CLA	C2-C1-O2A-CGA
26	g	619	LHG	C35-C36-C37-C38
22	c	514	CLA	C3A-C2A-CAA-CBA
22	C	515	CLA	C3A-C2A-CAA-CBA
30	d	401	PHO	C3A-C2A-CAA-CBA
30	D	401	PHO	C3A-C2A-CAA-CBA
26	C	520	LHG	C35-C36-C37-C38
26	b	619	LHG	C13-C14-C15-C16
36	M	101	LMG	O8-C28-C29-C30
36	T	101	LMG	O8-C28-C29-C30
30	d	401	PHO	C2-C3-C5-C6
26	B	622	LHG	C13-C14-C15-C16
35	h	102	DGD	C2A-C3A-C4A-C5A
35	H	102	DGD	C2A-C3A-C4A-C5A
35	c	517	DGD	O2G-C1B-C2B-C3B
35	C	518	DGD	O2G-C1B-C2B-C3B
22	b	601	CLA	C16-C17-C18-C20
22	B	604	CLA	C16-C17-C18-C20
22	s	308	CLA	CAA-CBA-CGA-O1A
22	S	308	CLA	CAA-CBA-CGA-O1A
22	B	618	CLA	C3-C5-C6-C7
30	D	401	PHO	C2-C3-C5-C6
35	c	517	DGD	O6D-C5D-C6D-O5D
24	y	615	XAT	O4-C6-C7-C8
24	Y	615	XAT	O4-C6-C7-C8
31	T	102	BCR	C12-C13-C14-C15
22	b	615	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	c	521	LHG	O7-C7-C8-C9
26	D	408	LHG	C15-C16-C17-C18
35	C	518	DGD	O6D-C5D-C6D-O5D
22	Y	611	CLA	C15-C16-C17-C18
26	d	407	LHG	C15-C16-C17-C18
35	a	413	DGD	O1G-C1G-C2G-C3G
35	A	401	DGD	O1G-C1G-C2G-C3G
22	G	603	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	C8-C10-C11-C12
26	C	521	LHG	O7-C7-C8-C9
22	b	614	CLA	O1D-CGD-O2D-CED
33	A	412	SQD	C27-C28-C29-C30
21	g	605	CHL	CAA-CBA-CGA-O1A
21	G	605	CHL	CAA-CBA-CGA-O1A
33	a	411	SQD	C27-C28-C29-C30
26	B	622	LHG	C10-C11-C12-C13
26	b	619	LHG	O7-C7-C8-C9
22	g	603	CLA	CBD-CGD-O2D-CED
26	b	619	LHG	C10-C11-C12-C13
25	Y	616	NEX	C7-C8-C9-C19
22	c	504	CLA	C8-C10-C11-C12
22	y	603	CLA	CBD-CGD-O2D-CED
22	N	603	CLA	CBD-CGD-O2D-CED
22	Y	603	CLA	CBD-CGD-O2D-CED
26	N	618	LHG	O8-C23-C24-C25
26	B	622	LHG	O7-C7-C8-C9
26	Y	617	LHG	C31-C32-C33-C34
35	c	517	DGD	O2G-C2G-C3G-O3G
35	C	518	DGD	O2G-C2G-C3G-O3G
22	b	611	CLA	C14-C13-C15-C16
22	c	510	CLA	C11-C12-C13-C14
22	B	614	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14
22	r	303	CLA	C11-C10-C8-C9
22	R	302	CLA	C11-C10-C8-C9
26	d	408	LHG	C31-C32-C33-C34
26	D	409	LHG	C31-C32-C33-C34
22	n	612	CLA	CAA-CBA-CGA-O2A
22	c	514	CLA	C13-C15-C16-C17
22	C	515	CLA	C13-C15-C16-C17
22	n	603	CLA	CBD-CGD-O2D-CED
35	c	517	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
22	g	613	CLA	CAA-CBA-CGA-O2A
22	y	612	CLA	CAA-CBA-CGA-O2A
22	G	613	CLA	CAA-CBA-CGA-O2A
22	N	612	CLA	CAA-CBA-CGA-O2A
22	Y	611	CLA	CAA-CBA-CGA-O2A
22	B	617	CLA	O1D-CGD-O2D-CED
22	g	603	CLA	C6-C7-C8-C10
22	n	603	CLA	C6-C7-C8-C10
22	n	609	CLA	C11-C12-C13-C15
22	y	603	CLA	C6-C7-C8-C10
22	G	610	CLA	C11-C12-C13-C15
22	N	603	CLA	C6-C7-C8-C10
22	Y	603	CLA	C6-C7-C8-C10
22	b	602	CLA	C11-C12-C13-C15
22	b	614	CLA	C6-C7-C8-C10
22	c	505	CLA	C11-C10-C8-C7
22	d	404	CLA	C12-C13-C15-C16
22	B	605	CLA	C11-C12-C13-C15
22	B	617	CLA	C6-C7-C8-C10
22	C	506	CLA	C11-C10-C8-C7
22	D	405	CLA	C12-C13-C15-C16
30	d	401	PHO	C11-C10-C8-C7
30	d	401	PHO	C12-C13-C15-C16
30	D	401	PHO	C11-C10-C8-C7
30	D	401	PHO	C12-C13-C15-C16
22	g	602	CLA	C2B-C3B-CAB-CBB
22	n	602	CLA	C2B-C3B-CAB-CBB
22	y	602	CLA	C2B-C3B-CAB-CBB
22	G	602	CLA	C2B-C3B-CAB-CBB
22	N	602	CLA	C2B-C3B-CAB-CBB
22	Y	602	CLA	C2B-C3B-CAB-CBB
22	b	601	CLA	C2B-C3B-CAB-CBB
22	b	604	CLA	C2B-C3B-CAB-CBB
22	b	615	CLA	C2B-C3B-CAB-CBB
22	c	509	CLA	C2B-C3B-CAB-CBB
22	B	604	CLA	C2B-C3B-CAB-CBB
22	B	607	CLA	C2B-C3B-CAB-CBB
22	B	618	CLA	C2B-C3B-CAB-CBB
22	C	510	CLA	C2B-C3B-CAB-CBB
22	r	305	CLA	C2B-C3B-CAB-CBB
22	R	304	CLA	C2B-C3B-CAB-CBB
31	a	409	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	a	409	BCR	C23-C24-C25-C26
31	b	617	BCR	C5-C6-C7-C8
31	c	515	BCR	C23-C24-C25-C26
31	c	516	BCR	C5-C6-C7-C8
31	c	516	BCR	C23-C24-C25-C26
31	d	405	BCR	C23-C24-C25-C26
31	h	101	BCR	C5-C6-C7-C8
31	h	101	BCR	C23-C24-C25-C26
31	k	101	BCR	C5-C6-C7-C8
31	k	101	BCR	C23-C24-C25-C26
31	k	102	BCR	C23-C24-C25-C26
31	A	410	BCR	C23-C24-C25-C26
31	B	620	BCR	C5-C6-C7-C8
31	C	516	BCR	C23-C24-C25-C26
31	C	517	BCR	C5-C6-C7-C8
31	C	517	BCR	C23-C24-C25-C26
31	D	406	BCR	C23-C24-C25-C26
31	H	101	BCR	C5-C6-C7-C8
31	H	101	BCR	C23-C24-C25-C26
31	K	101	BCR	C5-C6-C7-C8
31	K	101	BCR	C23-C24-C25-C26
31	K	102	BCR	C23-C24-C25-C26
35	C	518	DGD	C3B-C4B-C5B-C6B
36	k	103	LMG	C11-C10-O7-C8
36	K	103	LMG	C11-C10-O7-C8
35	J	101	DGD	C4B-C5B-C6B-C7B
21	r	308	CHL	C2-C1-O2A-CGA
21	R	307	CHL	C2-C1-O2A-CGA
22	c	514	CLA	C2-C1-O2A-CGA
22	C	515	CLA	C2-C1-O2A-CGA
22	r	312	CLA	C2-C1-O2A-CGA
22	R	311	CLA	C2-C1-O2A-CGA
26	B	622	LHG	C17-C18-C19-C20
21	r	308	CHL	C11-C12-C13-C14
22	s	310	CLA	C6-C7-C8-C9
26	L	103	LHG	C31-C32-C33-C34
35	c	519	DGD	C4B-C5B-C6B-C7B
36	C	523	LMG	C30-C31-C32-C33
22	r	304	CLA	CAA-CBA-CGA-O2A
26	b	619	LHG	C17-C18-C19-C20
26	l	102	LHG	C31-C32-C33-C34
36	c	523	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
21	R	307	CHL	C11-C12-C13-C14
22	S	310	CLA	C6-C7-C8-C9
22	c	506	CLA	CAA-CBA-CGA-O2A
22	C	507	CLA	CAA-CBA-CGA-O2A
22	s	305	CLA	CAA-CBA-CGA-O2A
22	S	305	CLA	CAA-CBA-CGA-O2A
22	R	303	CLA	CAA-CBA-CGA-O2A
22	Y	603	CLA	C15-C16-C17-C18
22	b	613	CLA	C8-C10-C11-C12
22	B	614	CLA	C15-C16-C17-C18
22	B	616	CLA	C8-C10-C11-C12
21	r	306	CHL	C2A-CAA-CBA-CGA
22	g	603	CLA	C15-C16-C17-C18
22	y	603	CLA	C15-C16-C17-C18
22	G	603	CLA	C15-C16-C17-C18
22	b	611	CLA	C15-C16-C17-C18
21	g	601	CHL	CAA-CBA-CGA-O2A
21	n	601	CHL	CAA-CBA-CGA-O2A
21	y	601	CHL	CAA-CBA-CGA-O2A
21	G	601	CHL	CAA-CBA-CGA-O2A
21	N	601	CHL	CAA-CBA-CGA-O2A
21	Y	601	CHL	CAA-CBA-CGA-O2A
36	M	101	LMG	C38-C39-C40-C41
36	T	101	LMG	C38-C39-C40-C41
35	H	102	DGD	C9B-CAB-CBB-CCB
35	h	102	DGD	C9B-CAB-CBB-CCB
22	n	603	CLA	C15-C16-C17-C18
22	N	603	CLA	C15-C16-C17-C18
33	a	411	SQD	C4-C5-C6-S
33	A	412	SQD	C4-C5-C6-S
22	c	502	CLA	CAA-CBA-CGA-O2A
22	C	503	CLA	CAA-CBA-CGA-O2A
22	b	604	CLA	C2-C3-C5-C6
22	c	509	CLA	C2-C3-C5-C6
22	B	607	CLA	C2-C3-C5-C6
22	C	510	CLA	C2-C3-C5-C6
26	g	619	LHG	C7-C8-C9-C10
21	R	305	CHL	C2A-CAA-CBA-CGA
26	d	408	LHG	C28-C29-C30-C31
26	D	409	LHG	C28-C29-C30-C31
22	b	615	CLA	C8-C10-C11-C12
26	b	619	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	B	622	LHG	C31-C32-C33-C34
21	g	601	CHL	C6-C7-C8-C9
21	n	601	CHL	C6-C7-C8-C9
21	y	601	CHL	C6-C7-C8-C9
21	G	601	CHL	C6-C7-C8-C9
21	N	601	CHL	C6-C7-C8-C9
21	Y	601	CHL	C6-C7-C8-C9
22	b	603	CLA	C6-C7-C8-C9
22	B	606	CLA	C6-C7-C8-C9
22	x	101	CLA	C5-C6-C7-C8
22	B	603	CLA	C5-C6-C7-C8
22	c	513	CLA	CAA-CBA-CGA-O2A
22	C	514	CLA	CAA-CBA-CGA-O2A
35	c	519	DGD	O2G-C1B-C2B-C3B
26	S	314	LHG	C9-C10-C11-C12
26	c	521	LHG	O2-C2-C3-O3
26	C	521	LHG	O2-C2-C3-O3
35	h	102	DGD	C1G-C2G-C3G-O3G
35	H	102	DGD	C1G-C2G-C3G-O3G
26	C	521	LHG	C9-C10-C11-C12
22	g	602	CLA	C4B-C3B-CAB-CBB
22	n	602	CLA	C4B-C3B-CAB-CBB
22	y	602	CLA	C4B-C3B-CAB-CBB
22	G	602	CLA	C4B-C3B-CAB-CBB
22	N	602	CLA	C4B-C3B-CAB-CBB
22	Y	602	CLA	C4B-C3B-CAB-CBB
22	b	607	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	d	403	CLA	C4B-C3B-CAB-CBB
22	B	610	CLA	C1A-C2A-CAA-CBA
22	C	514	CLA	C1A-C2A-CAA-CBA
22	D	404	CLA	C4B-C3B-CAB-CBB
26	s	314	LHG	C9-C10-C11-C12
22	b	614	CLA	CBD-CGD-O2D-CED
26	R	301	LHG	C29-C30-C31-C32
31	c	515	BCR	C6-C7-C8-C9
31	C	516	BCR	C6-C7-C8-C9
21	y	605	CHL	CAA-CBA-CGA-O2A
22	b	607	CLA	CAA-CBA-CGA-O2A
22	B	610	CLA	CAA-CBA-CGA-O2A
22	r	312	CLA	CAA-CBA-CGA-O2A
22	s	310	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	s	313	CLA	CAA-CBA-CGA-O2A
22	S	310	CLA	CAA-CBA-CGA-O2A
22	S	313	CLA	CAA-CBA-CGA-O2A
22	R	311	CLA	CAA-CBA-CGA-O2A
26	G	618	LHG	O7-C7-C8-C9
26	r	302	LHG	C29-C30-C31-C32
24	g	617	XAT	C7-C8-C9-C10
22	B	618	CLA	C8-C10-C11-C12
22	B	617	CLA	CBD-CGD-O2D-CED
26	c	521	LHG	C9-C10-C11-C12
26	d	409	LHG	C24-C23-O8-C6
26	D	410	LHG	C24-C23-O8-C6
22	n	603	CLA	O1D-CGD-O2D-CED
22	g	610	CLA	CAA-CBA-CGA-O2A
22	n	609	CLA	CAA-CBA-CGA-O2A
22	y	610	CLA	CAA-CBA-CGA-O2A
22	Y	609	CLA	CAA-CBA-CGA-O2A
22	r	303	CLA	CAA-CBA-CGA-O2A
22	r	309	CLA	CAA-CBA-CGA-O2A
22	R	302	CLA	CAA-CBA-CGA-O2A
22	R	308	CLA	CAA-CBA-CGA-O2A
35	J	101	DGD	O2G-C1B-C2B-C3B
22	B	610	CLA	C2A-CAA-CBA-CGA
22	G	610	CLA	CAA-CBA-CGA-O2A
22	N	609	CLA	CAA-CBA-CGA-O2A
22	N	603	CLA	O1D-CGD-O2D-CED
33	a	411	SQD	C5-C6-S-O7
33	d	402	SQD	C5-C6-S-O9
33	A	412	SQD	C5-C6-S-O7
33	D	402	SQD	C5-C6-S-O9
35	C	519	DGD	C4B-C5B-C6B-C7B
21	g	601	CHL	C2-C1-O2A-CGA
21	n	601	CHL	C2-C1-O2A-CGA
21	y	601	CHL	C2-C1-O2A-CGA
21	G	601	CHL	C2-C1-O2A-CGA
21	Y	601	CHL	C2-C1-O2A-CGA
36	k	103	LMG	O7-C10-C11-C12
36	K	103	LMG	O7-C10-C11-C12
22	Y	603	CLA	O1D-CGD-O2D-CED
21	y	609	CHL	C11-C12-C13-C15
22	G	603	CLA	C6-C7-C8-C10
22	b	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C11-C12-C13-C15
22	B	613	CLA	C11-C12-C13-C15
22	C	507	CLA	C11-C12-C13-C15
22	s	303	CLA	C11-C12-C13-C15
22	S	303	CLA	C11-C12-C13-C15
35	c	518	DGD	C4B-C5B-C6B-C7B
33	d	402	SQD	C7-C8-C9-C10
33	D	402	SQD	C7-C8-C9-C10
36	w	102	LMG	C11-C12-C13-C14
22	G	603	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	CAA-CBA-CGA-O2A
22	y	612	CLA	C13-C15-C16-C17
22	b	604	CLA	C5-C6-C7-C8
22	B	607	CLA	C5-C6-C7-C8
22	d	403	CLA	C3-C5-C6-C7
35	h	102	DGD	C6A-C7A-C8A-C9A
36	C	502	LMG	C11-C12-C13-C14
21	s	307	CHL	C2A-CAA-CBA-CGA
22	b	607	CLA	C2A-CAA-CBA-CGA
22	b	613	CLA	C2A-CAA-CBA-CGA
22	B	616	CLA	C2A-CAA-CBA-CGA
35	H	102	DGD	C6A-C7A-C8A-C9A
32	a	410	PL9	C7-C8-C9-C11
32	A	411	PL9	C7-C8-C9-C11
22	B	604	CLA	CAA-CBA-CGA-O2A
21	s	307	CHL	CAA-CBA-CGA-O1A
21	S	307	CHL	CAA-CBA-CGA-O1A
22	c	513	CLA	C3A-C2A-CAA-CBA
22	C	514	CLA	C3A-C2A-CAA-CBA
22	s	303	CLA	C3A-C2A-CAA-CBA
22	S	303	CLA	C3A-C2A-CAA-CBA
22	N	602	CLA	CAA-CBA-CGA-O2A
31	B	602	BCR	C12-C13-C14-C15
22	d	404	CLA	C15-C16-C17-C18
22	D	405	CLA	C15-C16-C17-C18
22	D	404	CLA	C3-C5-C6-C7
26	y	617	LHG	C15-C16-C17-C18
22	n	612	CLA	CAA-CBA-CGA-O1A
22	S	305	CLA	CAA-CBA-CGA-O1A
26	G	618	LHG	O9-C7-C8-C9
22	y	603	CLA	O1D-CGD-O2D-CED
22	G	602	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
35	a	413	DGD	O2G-C1B-C2B-C3B
35	A	401	DGD	O2G-C1B-C2B-C3B
21	g	601	CHL	CAA-CBA-CGA-O1A
21	G	601	CHL	CAA-CBA-CGA-O1A
21	N	601	CHL	CAA-CBA-CGA-O1A
22	g	613	CLA	CAA-CBA-CGA-O1A
22	y	612	CLA	CAA-CBA-CGA-O1A
22	G	613	CLA	CAA-CBA-CGA-O1A
22	N	612	CLA	CAA-CBA-CGA-O1A
22	Y	611	CLA	CAA-CBA-CGA-O1A
22	c	506	CLA	CAA-CBA-CGA-O1A
22	C	507	CLA	CAA-CBA-CGA-O1A
22	s	305	CLA	CAA-CBA-CGA-O1A
21	n	608	CHL	C11-C12-C13-C14
21	y	609	CHL	C11-C12-C13-C14
21	N	608	CHL	C11-C12-C13-C14
22	b	615	CLA	C6-C7-C8-C9
22	c	514	CLA	C14-C13-C15-C16
22	B	618	CLA	C6-C7-C8-C9
22	C	507	CLA	C11-C12-C13-C14
22	C	509	CLA	C11-C10-C8-C9
22	C	515	CLA	C14-C13-C15-C16
22	g	602	CLA	CAA-CBA-CGA-O2A
22	n	602	CLA	CAA-CBA-CGA-O2A
22	y	602	CLA	CAA-CBA-CGA-O2A
22	Y	602	CLA	CAA-CBA-CGA-O2A
25	Y	616	NEX	C13-C14-C15-C35
26	d	407	LHG	C26-C27-C28-C29
22	b	613	CLA	C10-C11-C12-C13
31	K	102	BCR	C11-C12-C13-C35
21	n	601	CHL	CAA-CBA-CGA-O1A
21	y	601	CHL	CAA-CBA-CGA-O1A
21	Y	601	CHL	CAA-CBA-CGA-O1A
26	b	619	LHG	O9-C7-C8-C9
26	D	408	LHG	C26-C27-C28-C29
25	y	616	NEX	C7-C8-C9-C10
25	y	618	NEX	C7-C8-C9-C10
25	y	618	NEX	C21-C26-C27-C28
25	Y	616	NEX	C21-C26-C27-C28
25	r	315	NEX	C7-C8-C9-C10
25	r	315	NEX	C21-C26-C27-C28
33	a	411	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
33	A	412	SQD	O5-C5-C6-S
22	r	309	CLA	CAA-CBA-CGA-O1A
22	S	313	CLA	CAA-CBA-CGA-O1A
22	g	603	CLA	O1D-CGD-O2D-CED
22	B	616	CLA	C10-C11-C12-C13
22	G	612	CLA	CAA-CBA-CGA-O2A
22	N	611	CLA	CAA-CBA-CGA-O2A
22	w	101	CLA	CAA-CBA-CGA-O2A
22	r	311	CLA	CAA-CBA-CGA-O2A
22	R	310	CLA	CAA-CBA-CGA-O2A
22	b	607	CLA	CAA-CBA-CGA-O1A
22	B	610	CLA	CAA-CBA-CGA-O1A
22	s	313	CLA	CAA-CBA-CGA-O1A
22	R	303	CLA	CAA-CBA-CGA-O1A
22	R	308	CLA	CAA-CBA-CGA-O1A
26	B	622	LHG	O9-C7-C8-C9
33	l	103	SQD	O10-C23-C24-C25
33	L	101	SQD	O10-C23-C24-C25
22	r	304	CLA	CAA-CBA-CGA-O1A
22	s	310	CLA	CAA-CBA-CGA-O1A
22	S	310	CLA	CAA-CBA-CGA-O1A
22	R	311	CLA	CAA-CBA-CGA-O1A
33	l	101	SQD	O49-C7-C8-C9
33	L	102	SQD	O49-C7-C8-C9
36	B	601	LMG	O10-C28-C29-C30
36	I	101	LMG	O10-C28-C29-C30
22	g	612	CLA	CAA-CBA-CGA-O2A
22	n	611	CLA	CAA-CBA-CGA-O2A
22	W	101	CLA	CAA-CBA-CGA-O2A
36	M	101	LMG	C35-C36-C37-C38
36	T	101	LMG	C35-C36-C37-C38
21	y	605	CHL	CAA-CBA-CGA-O1A
22	G	610	CLA	CAA-CBA-CGA-O1A
22	r	312	CLA	CAA-CBA-CGA-O1A
36	K	103	LMG	O9-C10-C11-C12
36	w	102	LMG	C34-C35-C36-C37
22	c	513	CLA	C10-C11-C12-C13
22	C	514	CLA	C10-C11-C12-C13
22	c	507	CLA	CAA-CBA-CGA-O2A
22	C	508	CLA	CAA-CBA-CGA-O2A
36	k	103	LMG	C15-C16-C17-C18
36	K	103	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	g	610	CLA	CAA-CBA-CGA-O1A
22	n	609	CLA	CAA-CBA-CGA-O1A
22	y	610	CLA	CAA-CBA-CGA-O1A
22	N	609	CLA	CAA-CBA-CGA-O1A
22	Y	609	CLA	CAA-CBA-CGA-O1A
36	C	502	LMG	C34-C35-C36-C37
22	s	309	CLA	CAD-CBD-CGD-O2D
22	s	311	CLA	CAD-CBD-CGD-O2D
22	s	312	CLA	CAD-CBD-CGD-O2D
22	S	309	CLA	CAD-CBD-CGD-O2D
22	S	311	CLA	CAD-CBD-CGD-O2D
22	S	312	CLA	CAD-CBD-CGD-O2D
21	S	301	CHL	CAA-CBA-CGA-O2A
22	n	603	CLA	CAA-CBA-CGA-O2A
22	G	603	CLA	CAA-CBA-CGA-O2A
22	Y	603	CLA	CAA-CBA-CGA-O2A
22	b	605	CLA	C3-C5-C6-C7
22	C	503	CLA	CAA-CBA-CGA-O1A
36	k	103	LMG	O9-C10-C11-C12
21	S	301	CHL	O1A-CGA-O2A-C1
22	c	502	CLA	CAA-CBA-CGA-O1A
22	g	603	CLA	CAA-CBA-CGA-O2A
22	y	603	CLA	CAA-CBA-CGA-O2A
22	N	603	CLA	CAA-CBA-CGA-O2A
22	d	403	CLA	CAA-CBA-CGA-O2A
33	L	102	SQD	O47-C7-C8-C9
22	B	608	CLA	C3-C5-C6-C7
33	l	103	SQD	O49-C7-C8-C9
33	L	101	SQD	O49-C7-C8-C9
22	n	610	CLA	C11-C10-C8-C7
22	y	611	CLA	C11-C10-C8-C7
22	N	610	CLA	C11-C10-C8-C7
21	r	307	CHL	CAA-CBA-CGA-O2A
21	R	306	CHL	CAA-CBA-CGA-O2A
22	b	615	CLA	CAA-CBA-CGA-O2A
22	D	404	CLA	CAA-CBA-CGA-O2A
33	l	101	SQD	O47-C7-C8-C9
36	B	601	LMG	O8-C28-C29-C30
36	I	101	LMG	O8-C28-C29-C30
22	a	408	CLA	C2-C3-C5-C6
21	S	307	CHL	CAA-CBA-CGA-O2A
22	R	302	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	S	301	CHL	C2-C1-O2A-CGA
22	B	618	CLA	CAA-CBA-CGA-O2A
26	g	619	LHG	O8-C23-C24-C25
26	D	409	LHG	O8-C23-C24-C25
33	l	103	SQD	O47-C7-C8-C9
33	L	101	SQD	O47-C7-C8-C9
22	D	404	CLA	CAA-CBA-CGA-O1A
22	r	303	CLA	CAA-CBA-CGA-O1A
22	r	311	CLA	CAA-CBA-CGA-O1A
22	R	310	CLA	CAA-CBA-CGA-O1A
35	J	101	DGD	O1B-C1B-C2B-C3B

There are no ring outliers.

311 monomers are involved in 2203 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	509	CLA	2	0
25	Y	616	NEX	9	0
22	b	610	CLA	1	0
25	y	616	NEX	7	0
22	b	603	CLA	6	0
21	n	608	CHL	28	0
21	R	305	CHL	33	0
22	r	303	CLA	2	0
21	y	609	CHL	26	0
26	n	617	LHG	10	0
22	g	611	CLA	2	0
22	c	507	CLA	1	0
22	G	614	CLA	3	0
22	C	512	CLA	5	0
23	Y	613	LUT	16	0
22	n	612	CLA	18	0
22	B	614	CLA	4	0
22	y	610	CLA	6	0
36	d	410	LMG	4	0
22	y	603	CLA	3	0
32	a	410	PL9	2	0
22	N	602	CLA	4	0
22	N	610	CLA	2	0
31	C	517	BCR	2	0
25	y	618	NEX	9	0
22	y	613	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	G	616	LUT	11	0
22	G	612	CLA	6	0
21	S	301	CHL	48	0
21	y	607	CHL	19	0
22	B	604	CLA	3	0
22	c	509	CLA	3	0
22	n	613	CLA	1	0
22	A	405	CLA	3	0
31	B	621	BCR	1	0
22	g	613	CLA	18	0
22	b	604	CLA	2	0
22	B	611	CLA	1	0
31	A	410	BCR	2	0
22	B	606	CLA	6	0
22	S	304	CLA	1	0
22	Y	612	CLA	3	0
22	b	605	CLA	2	0
21	G	608	CHL	35	0
31	k	102	BCR	4	0
22	y	604	CLA	13	0
31	b	616	BCR	4	0
26	N	618	LHG	9	0
31	B	620	BCR	2	0
21	r	308	CHL	4	0
22	C	513	CLA	4	0
26	c	520	LHG	4	0
22	C	507	CLA	4	0
22	w	101	CLA	5	0
22	y	612	CLA	21	0
22	B	607	CLA	4	0
31	b	618	BCR	3	0
22	B	613	CLA	1	0
21	y	605	CHL	26	0
22	N	609	CLA	7	0
22	W	101	CLA	16	0
22	B	603	CLA	2	0
22	b	613	CLA	3	0
22	d	403	CLA	4	0
22	n	603	CLA	3	0
21	y	608	CHL	37	0
22	g	614	CLA	1	0
21	N	605	CHL	24	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	617	CLA	3	0
22	R	310	CLA	3	0
22	c	514	CLA	7	0
26	c	521	LHG	2	0
22	b	606	CLA	3	0
22	r	312	CLA	4	0
22	S	303	CLA	3	0
26	C	521	LHG	5	0
21	R	307	CHL	4	0
22	C	503	CLA	4	0
22	N	603	CLA	9	0
35	H	102	DGD	8	0
32	A	411	PL9	2	0
22	C	504	CLA	3	0
22	n	602	CLA	4	0
21	R	306	CHL	39	0
21	s	302	CHL	19	0
21	n	601	CHL	28	0
21	N	606	CHL	23	0
26	d	409	LHG	5	0
22	c	513	CLA	4	0
32	d	406	PL9	3	0
36	D	411	LMG	2	0
22	B	605	CLA	7	0
36	B	601	LMG	5	0
26	Y	617	LHG	10	0
21	G	606	CHL	23	0
21	Y	606	CHL	24	0
33	L	102	SQD	5	0
25	n	616	NEX	12	0
22	n	604	CLA	16	0
21	Y	605	CHL	29	0
22	Y	611	CLA	21	0
22	b	614	CLA	3	0
23	g	616	LUT	13	0
32	D	407	PL9	3	0
26	d	408	LHG	7	0
22	Y	602	CLA	5	0
22	N	613	CLA	3	0
22	C	508	CLA	1	0
26	S	314	LHG	6	0
23	Y	614	LUT	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	g	612	CLA	7	0
33	d	402	SQD	3	0
22	R	309	CLA	5	0
22	C	506	CLA	6	0
22	s	313	CLA	5	0
31	c	515	BCR	7	0
36	k	103	LMG	1	0
22	C	514	CLA	5	0
22	B	616	CLA	3	0
21	Y	607	CHL	37	0
22	C	505	CLA	5	0
26	c	522	LHG	3	0
22	g	610	CLA	6	0
23	G	615	LUT	14	0
26	G	618	LHG	13	0
21	n	607	CHL	38	0
21	g	609	CHL	25	0
21	r	306	CHL	25	0
22	C	515	CLA	8	0
35	J	101	DGD	6	0
22	s	310	CLA	6	0
26	C	522	LHG	3	0
22	c	508	CLA	4	0
36	C	502	LMG	2	0
22	G	611	CLA	2	0
22	b	611	CLA	3	0
26	b	619	LHG	1	0
30	D	401	PHO	6	0
22	y	602	CLA	3	0
37	f	101	HEM	20	0
22	b	612	CLA	3	0
22	c	511	CLA	5	0
35	C	518	DGD	1	0
21	S	306	CHL	16	0
26	D	410	LHG	4	0
22	C	510	CLA	4	0
30	A	408	PHO	4	0
26	r	302	LHG	3	0
36	C	523	LMG	3	0
22	R	308	CLA	8	0
24	R	313	XAT	5	0
22	a	406	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	k	101	BCR	2	0
21	s	301	CHL	51	0
22	D	404	CLA	2	0
26	s	314	LHG	7	0
22	S	308	CLA	2	0
22	b	601	CLA	6	0
22	g	604	CLA	13	0
22	c	510	CLA	21	0
22	c	512	CLA	5	0
22	r	310	CLA	3	0
21	G	609	CHL	34	0
21	G	601	CHL	42	0
22	c	505	CLA	6	0
36	K	103	LMG	1	0
21	n	605	CHL	31	0
22	b	615	CLA	1	0
22	A	407	CLA	2	0
22	S	313	CLA	5	0
31	B	619	BCR	4	0
22	S	305	CLA	9	0
33	l	101	SQD	3	0
36	I	101	LMG	6	0
22	x	101	CLA	2	0
22	B	612	CLA	3	0
22	s	311	CLA	2	0
22	R	304	CLA	3	0
24	Y	615	XAT	2	0
21	Y	601	CHL	23	0
23	R	312	LUT	2	0
21	r	301	CHL	26	0
21	y	601	CHL	26	0
33	L	101	SQD	4	0
22	G	602	CLA	4	0
35	h	102	DGD	4	0
35	c	518	DGD	10	0
22	Y	609	CLA	6	0
26	C	520	LHG	7	0
22	C	511	CLA	21	0
36	c	523	LMG	3	0
22	G	610	CLA	7	0
22	G	603	CLA	6	0
21	s	306	CHL	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	g	601	CHL	23	0
31	K	101	BCR	2	0
22	S	311	CLA	3	0
21	N	607	CHL	41	0
31	h	101	BCR	5	0
22	g	603	CLA	7	0
22	y	611	CLA	2	0
21	n	606	CHL	17	0
22	r	305	CLA	2	0
22	d	404	CLA	3	0
22	S	310	CLA	8	0
22	R	303	CLA	5	0
31	H	101	BCR	3	0
22	r	309	CLA	6	0
22	a	404	CLA	4	0
23	y	614	LUT	11	0
22	n	611	CLA	7	0
21	g	606	CHL	28	0
22	Y	610	CLA	4	0
22	s	308	CLA	2	0
26	y	617	LHG	9	0
25	N	617	NEX	9	0
22	Y	603	CLA	14	0
21	y	606	CHL	28	0
22	A	406	CLA	3	0
36	T	101	LMG	5	0
22	B	610	CLA	2	0
35	a	413	DGD	7	0
22	N	604	CLA	13	0
26	L	103	LHG	2	0
21	s	307	CHL	24	0
33	D	402	SQD	3	0
22	c	502	CLA	7	0
22	N	612	CLA	17	0
31	B	602	BCR	2	0
22	B	615	CLA	3	0
35	c	517	DGD	1	0
22	G	604	CLA	12	0
22	B	608	CLA	2	0
24	r	314	XAT	5	0
23	g	615	LUT	16	0
22	b	608	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	B	623	LMG	53	0
31	b	617	BCR	1	0
21	g	607	CHL	22	0
33	a	411	SQD	4	0
30	a	407	PHO	5	0
21	S	307	CHL	25	0
22	g	602	CLA	3	0
22	c	503	CLA	3	0
23	N	614	LUT	16	0
35	c	519	DGD	4	0
31	d	405	BCR	4	0
22	s	304	CLA	1	0
22	R	302	CLA	2	0
23	r	313	LUT	2	0
33	A	412	SQD	4	0
21	S	302	CHL	17	0
22	c	504	CLA	5	0
22	Y	604	CLA	14	0
22	B	618	CLA	3	0
24	G	617	XAT	1	0
22	D	405	CLA	3	0
21	G	605	CHL	20	0
23	N	615	LUT	17	0
22	B	609	CLA	2	0
22	S	309	CLA	3	0
22	n	609	CLA	6	0
22	s	305	CLA	8	0
22	c	506	CLA	5	0
34	a	412	BCT	4	0
22	r	304	CLA	5	0
25	g	618	NEX	8	0
26	B	622	LHG	1	0
22	r	311	CLA	3	0
21	N	601	CHL	32	0
26	R	301	LHG	5	0
22	b	607	CLA	2	0
22	G	613	CLA	18	0
34	D	403	BCT	4	0
31	T	102	BCR	2	0
26	D	409	LHG	4	0
36	w	102	LMG	3	0
36	M	101	LMG	5	0

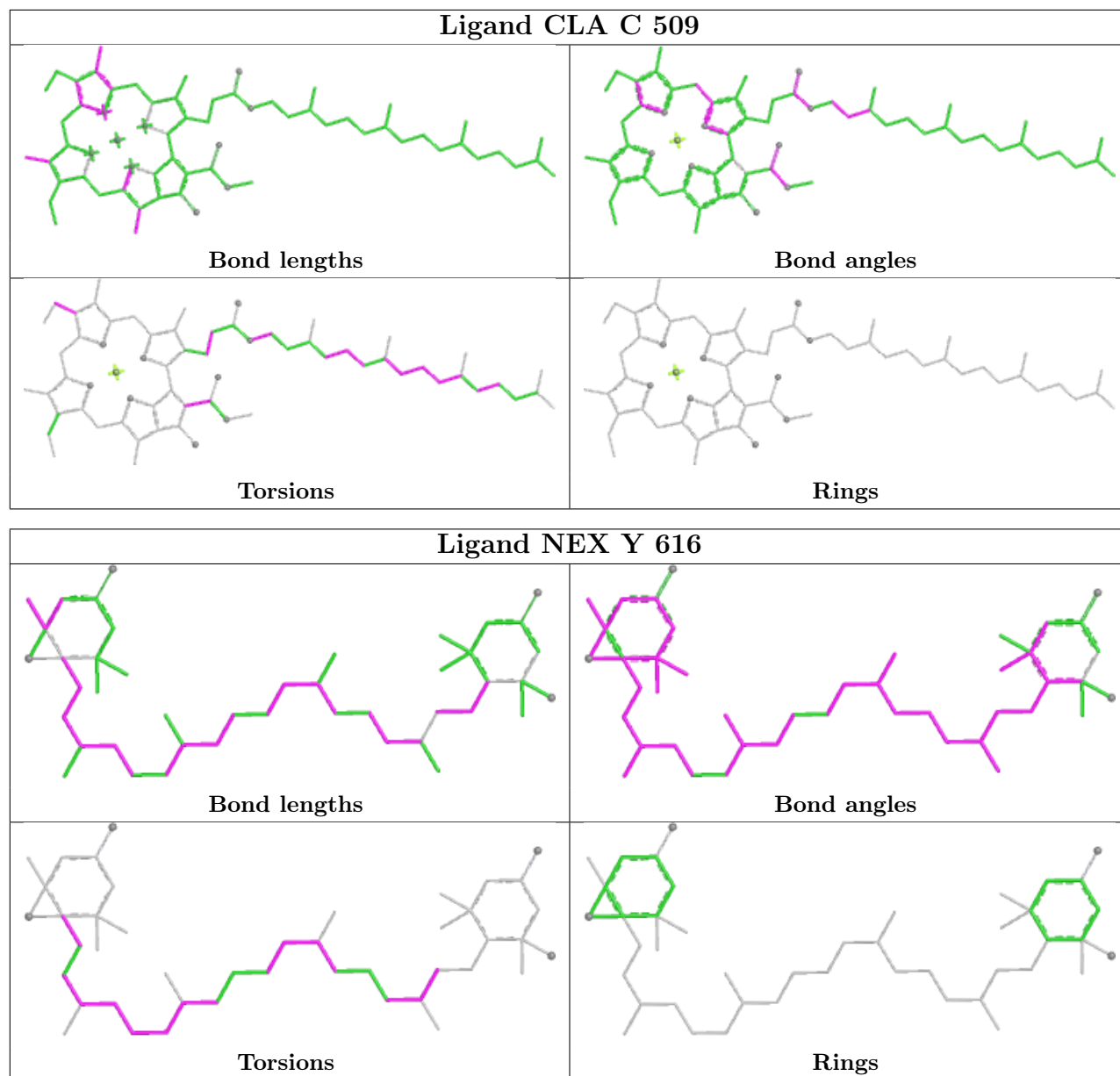
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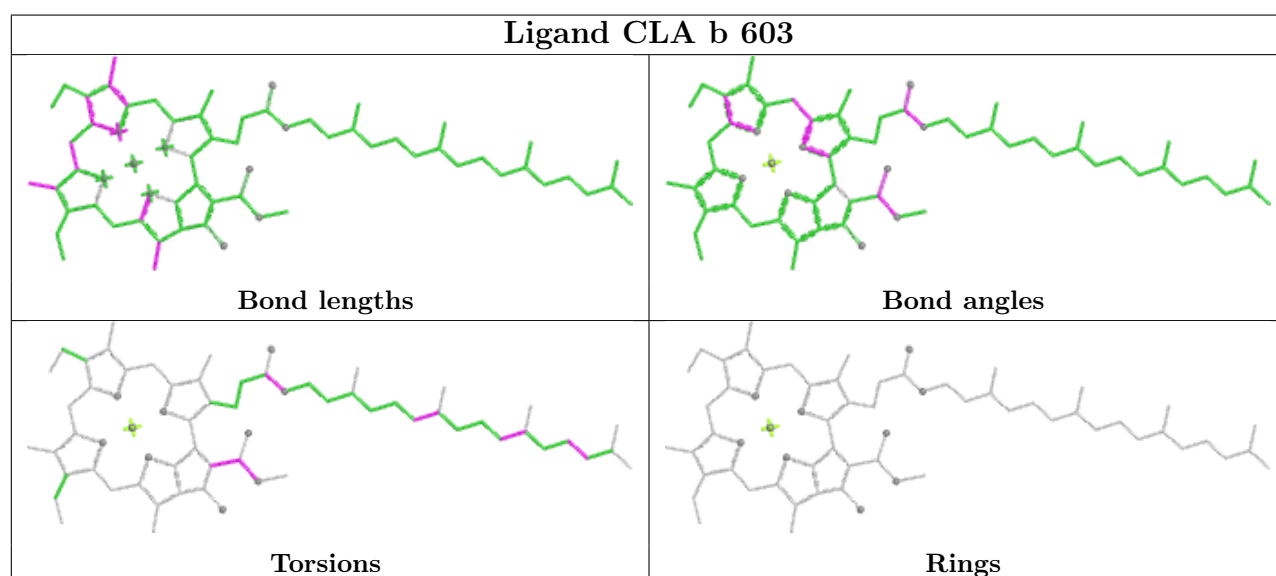
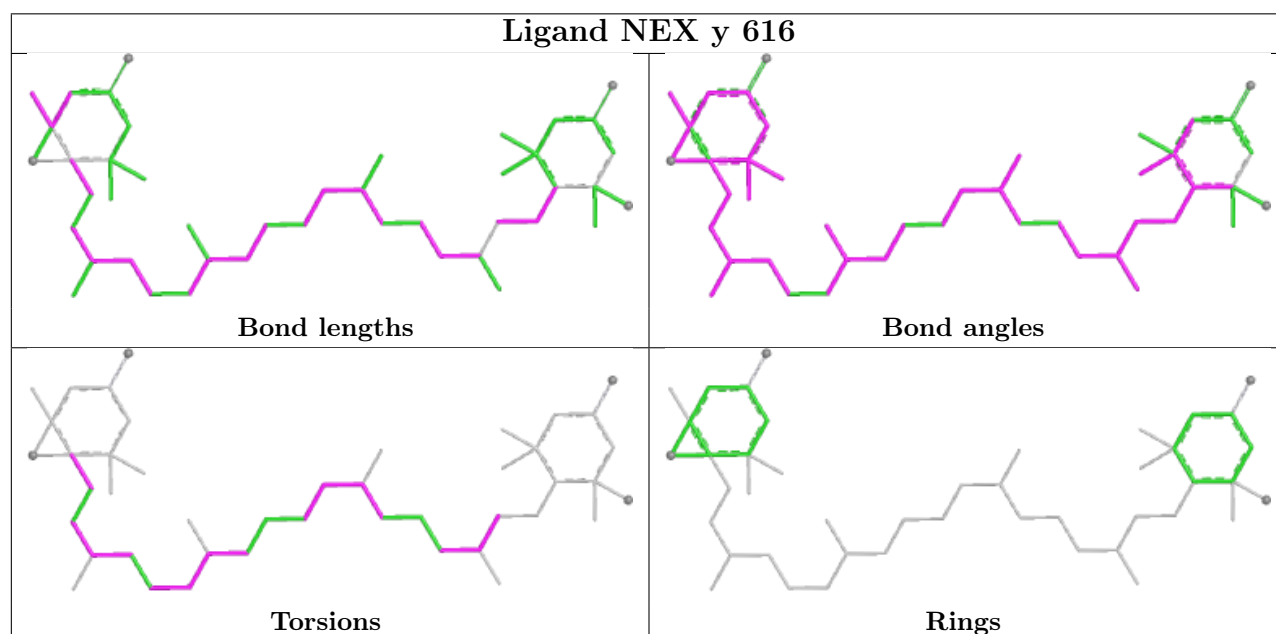
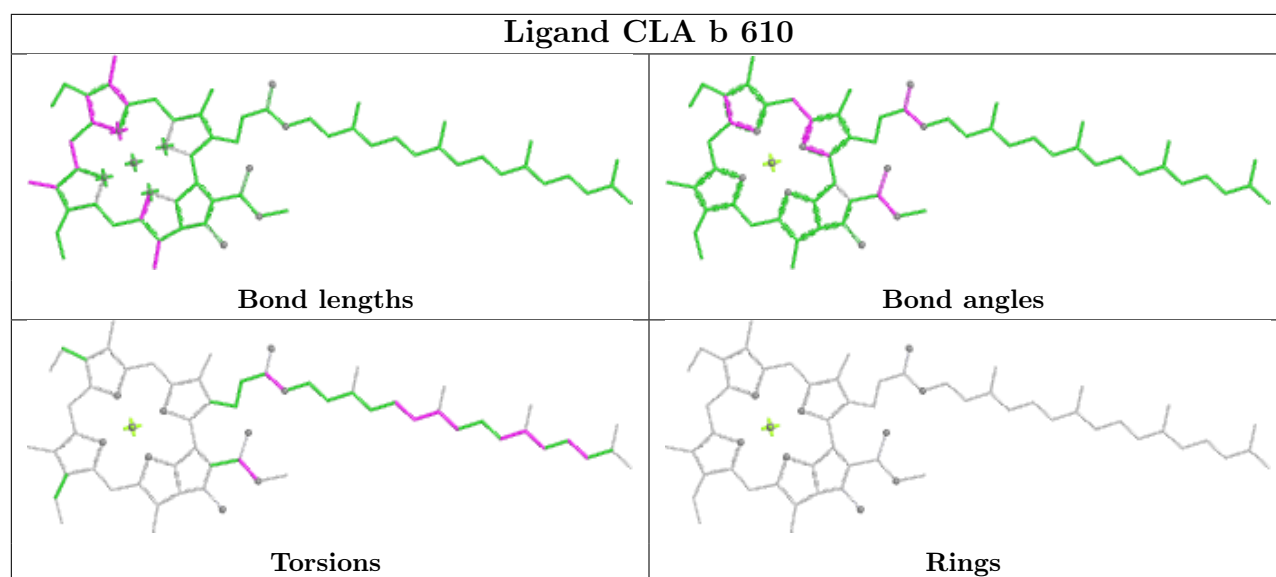
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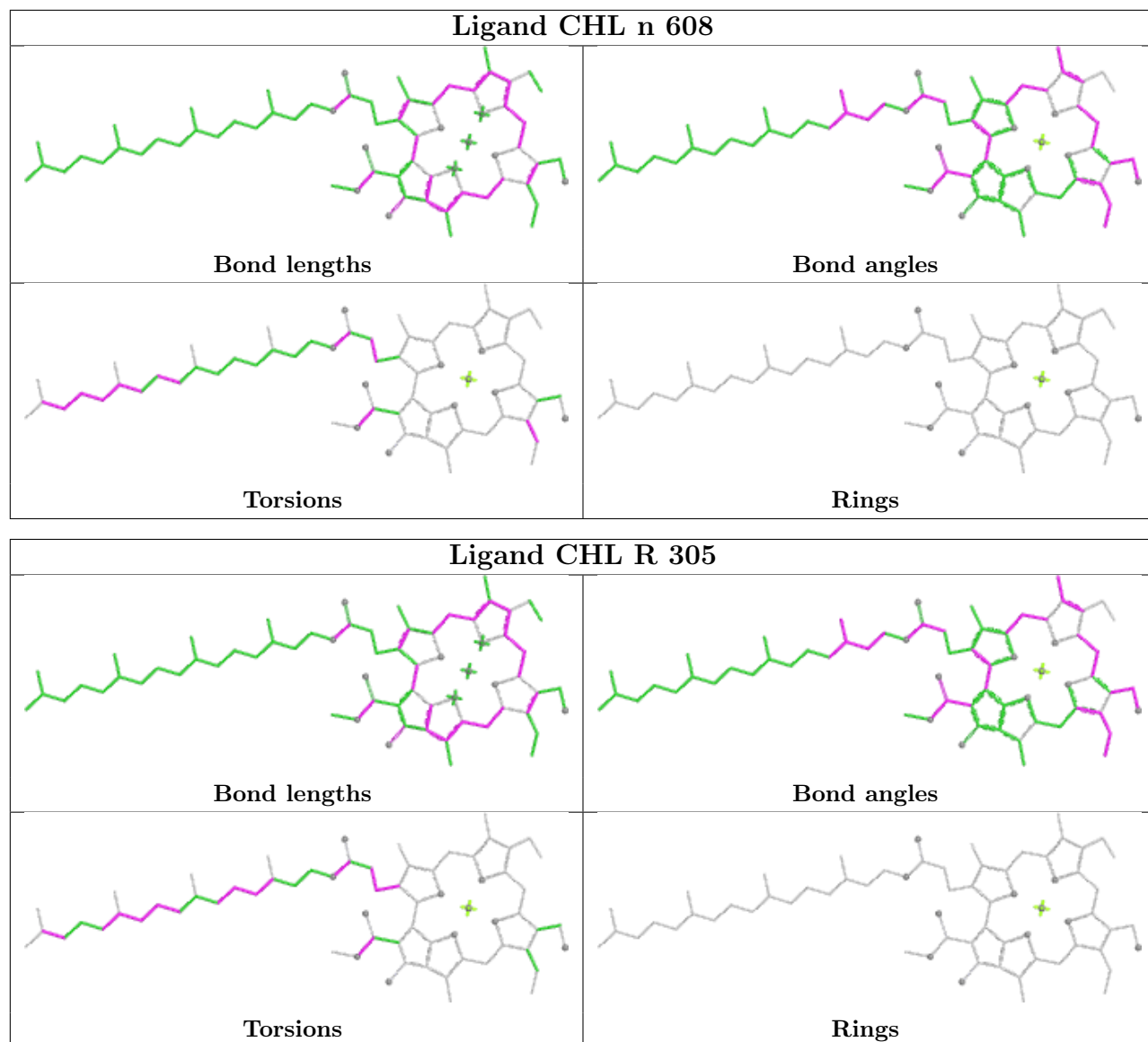
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	N	616	XAT	2	0
31	C	516	BCR	6	0
33	l	103	SQD	4	0
26	g	619	LHG	6	0
22	A	409	CLA	2	0
21	N	608	CHL	27	0
30	d	401	PHO	6	0
23	n	614	LUT	12	0
22	s	303	CLA	4	0
22	a	408	CLA	3	0
21	G	607	CHL	22	0
26	D	408	LHG	1	0
35	A	401	DGD	7	0
22	n	610	CLA	2	0
21	g	605	CHL	20	0
21	Y	608	CHL	32	0
22	b	609	CLA	3	0
22	s	309	CLA	2	0
37	F	101	HEM	17	0
24	y	615	XAT	2	0
21	r	307	CHL	28	0
22	R	311	CLA	5	0
22	N	611	CLA	8	0
35	C	519	DGD	9	0
22	a	405	CLA	3	0
25	r	315	NEX	8	0
21	g	608	CHL	35	0
22	b	602	CLA	5	0
31	D	406	BCR	4	0
36	b	620	LMG	36	0
24	n	615	XAT	2	0
31	a	409	BCR	1	0
31	K	102	BCR	4	0

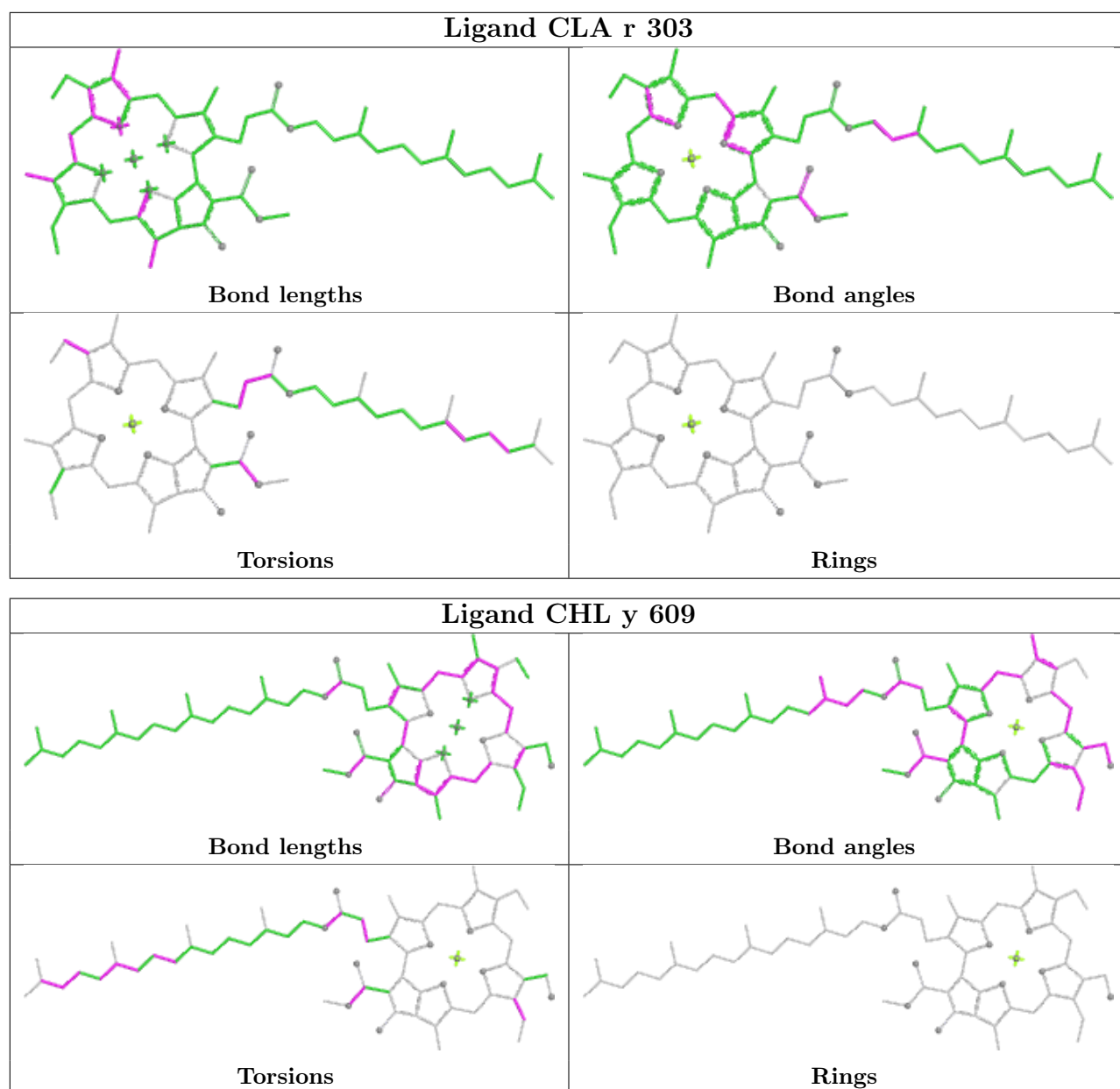
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

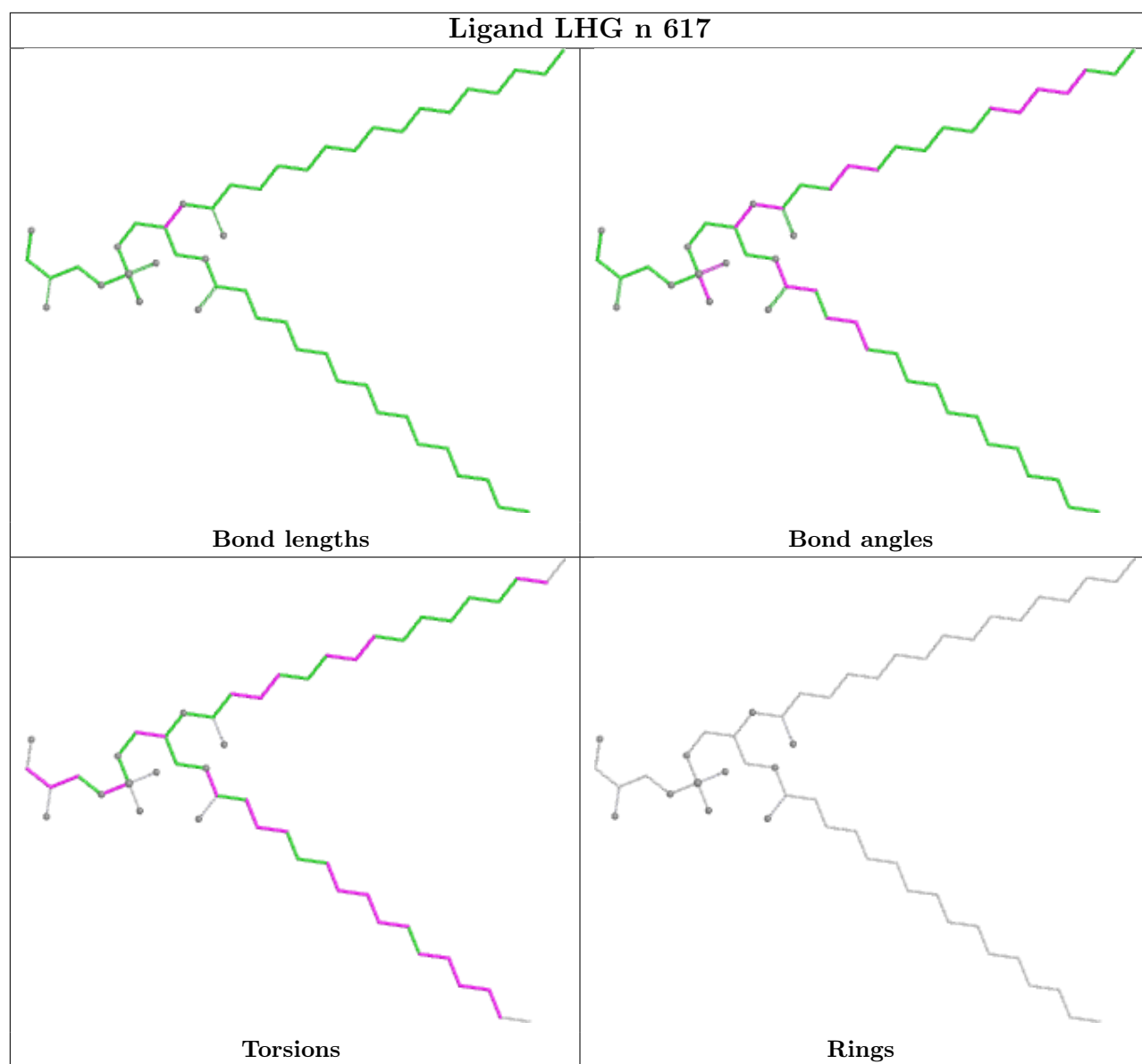
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

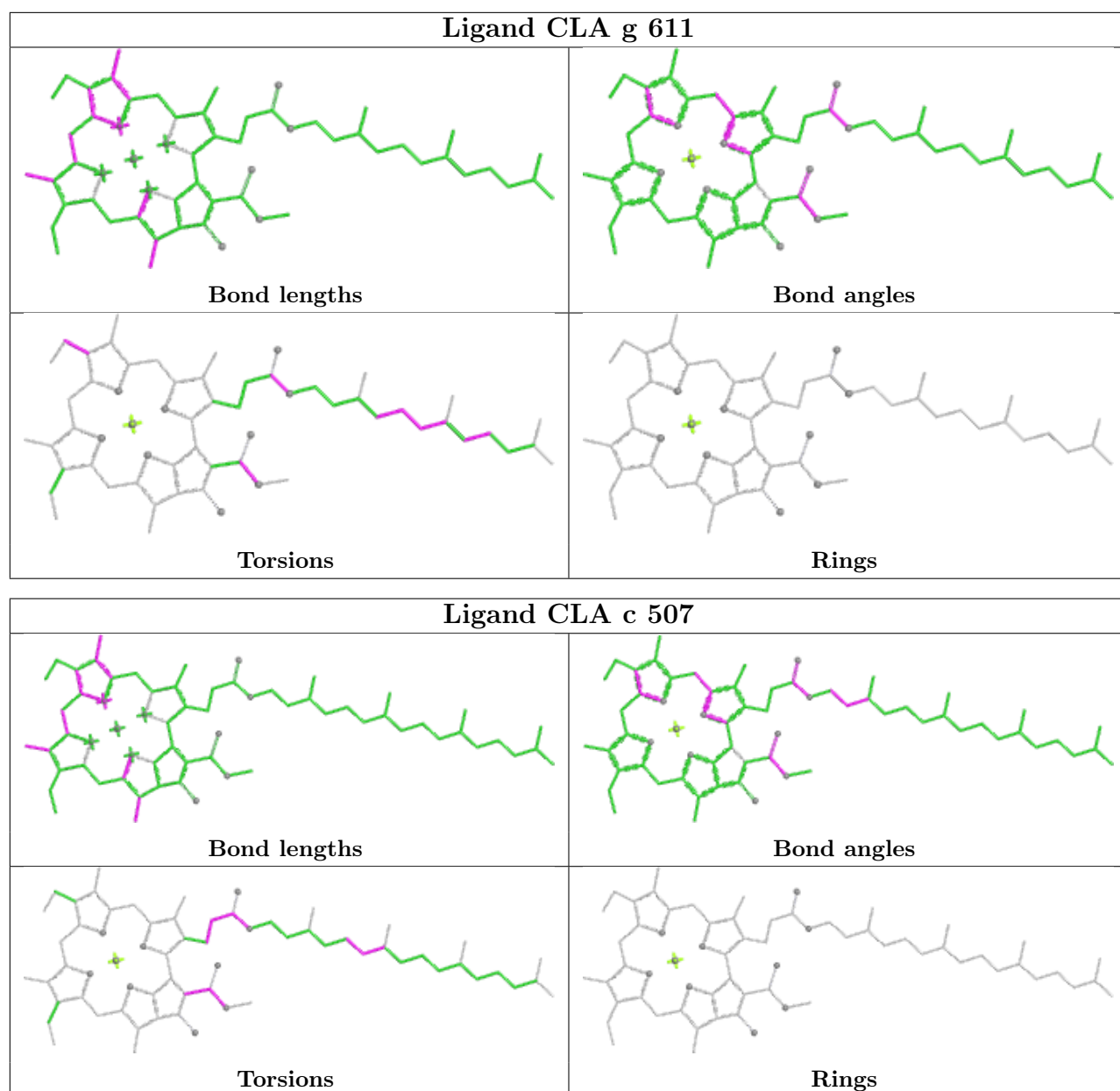




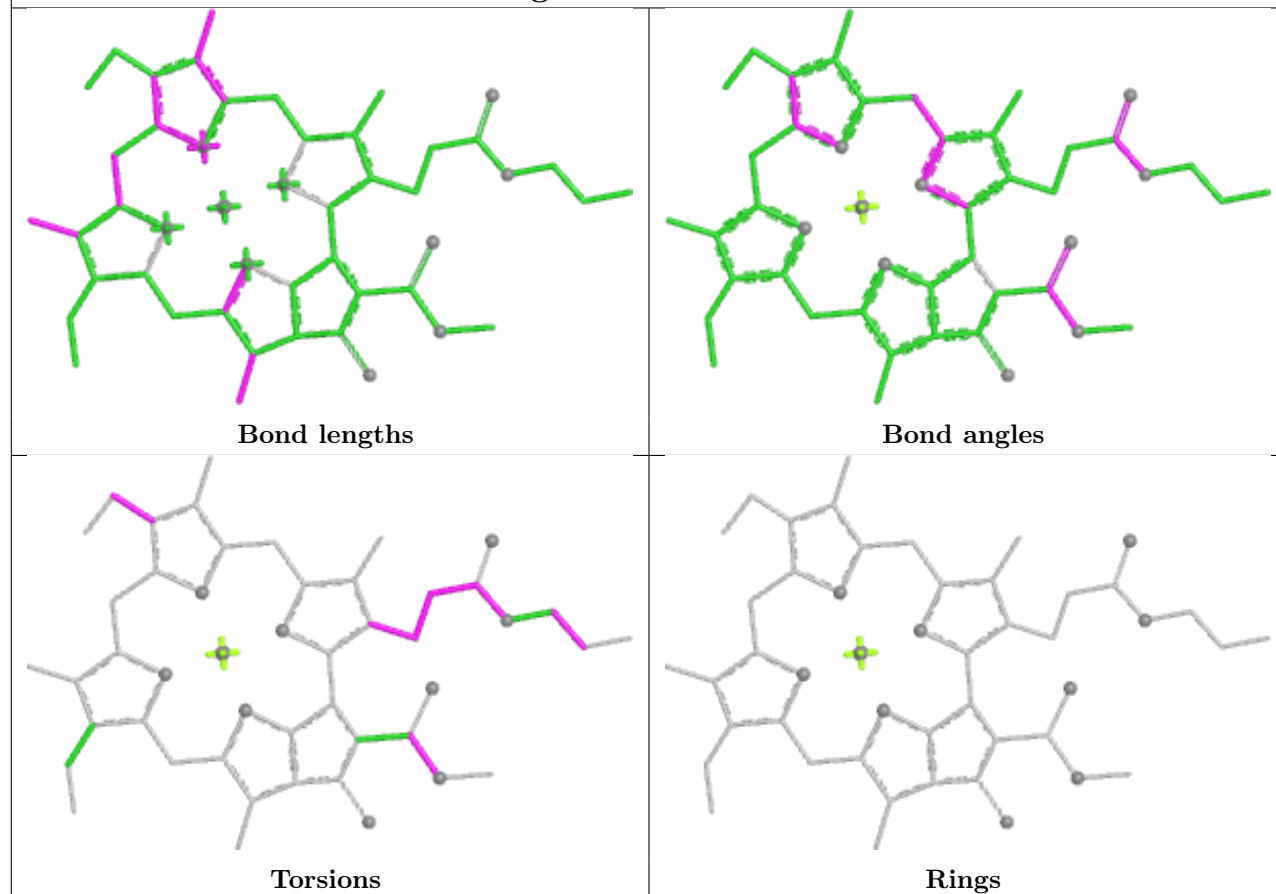




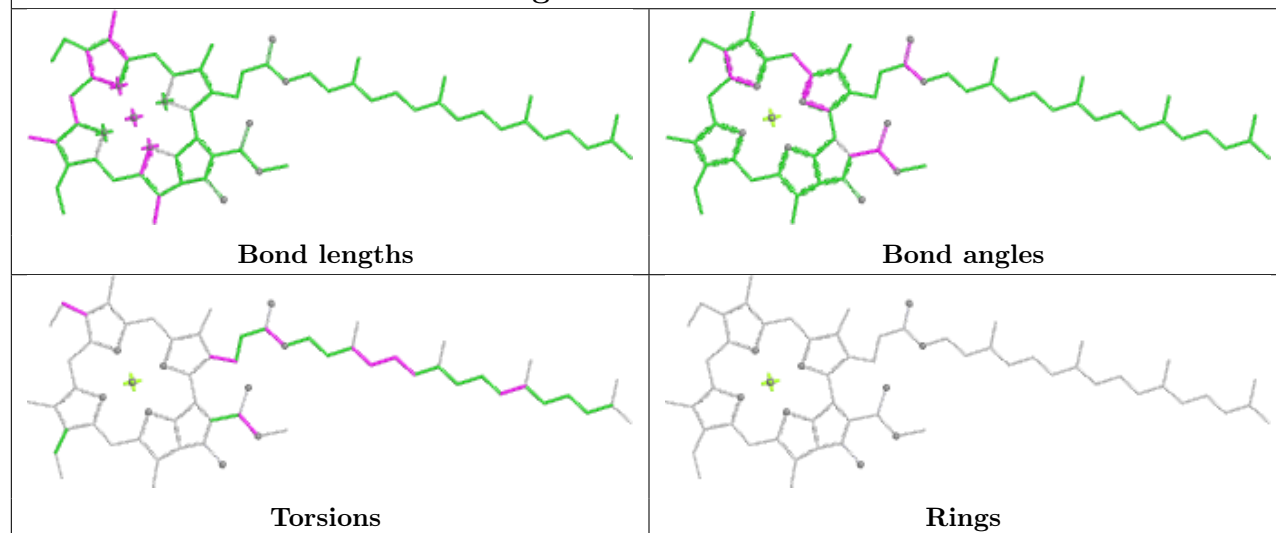


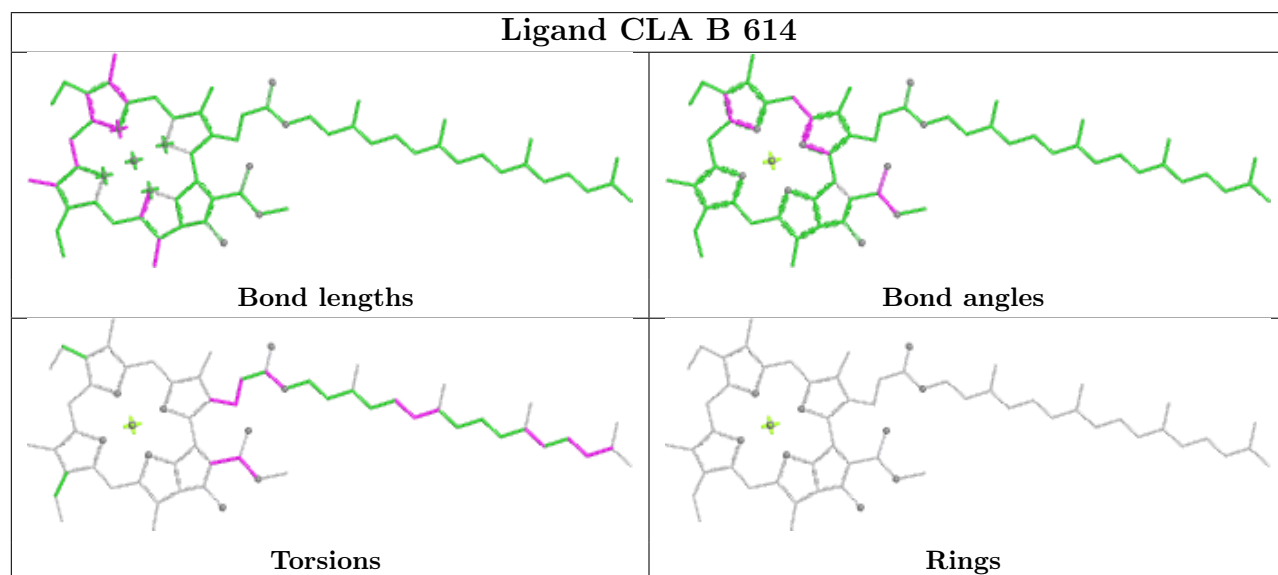
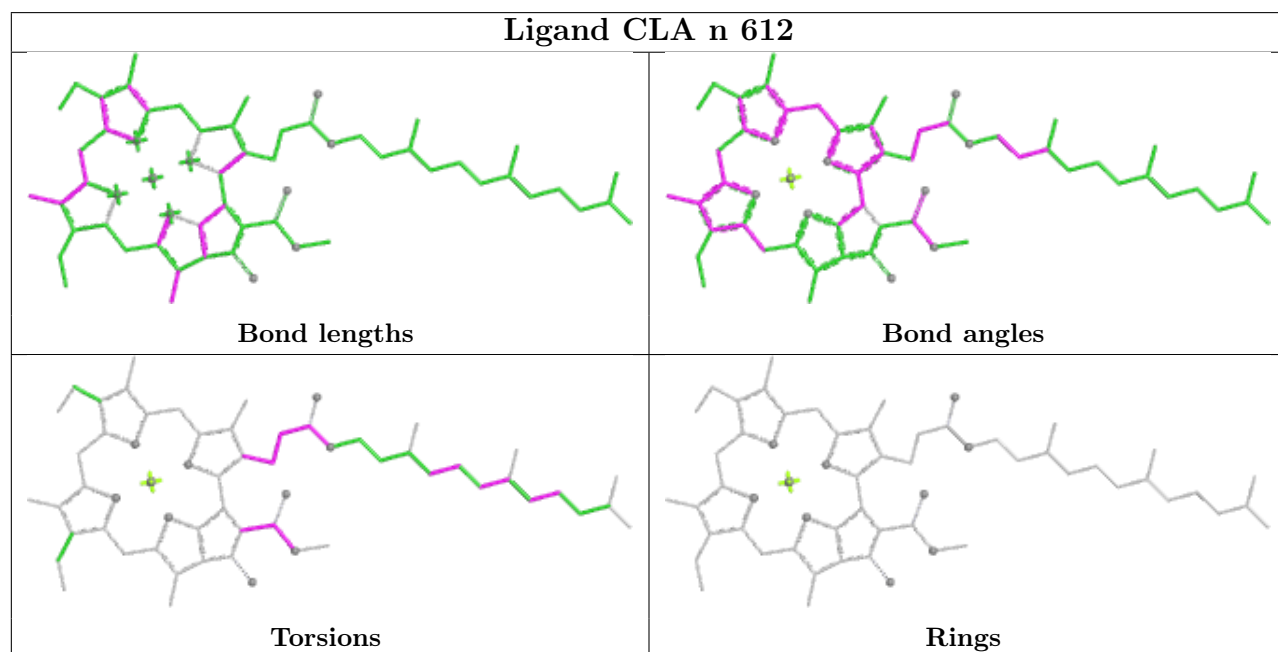
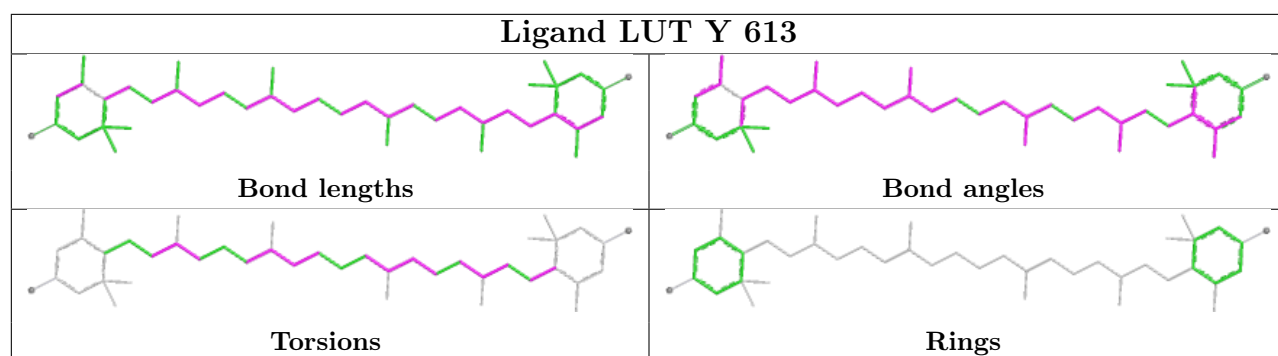


Ligand CLA G 614

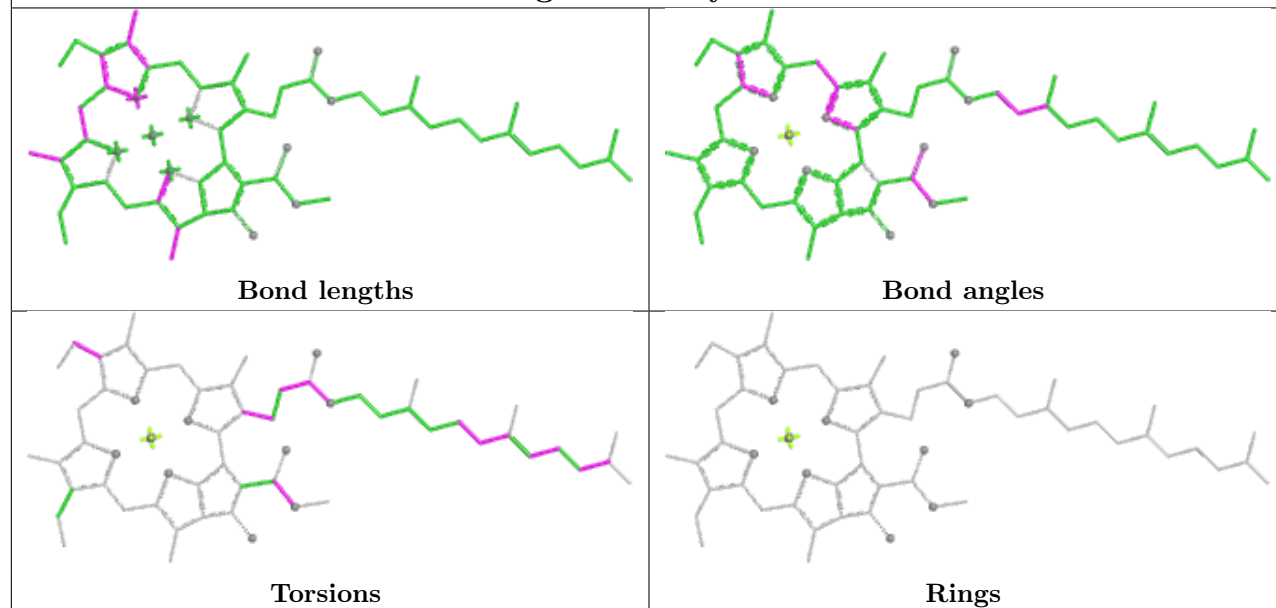


Ligand CLA C 512





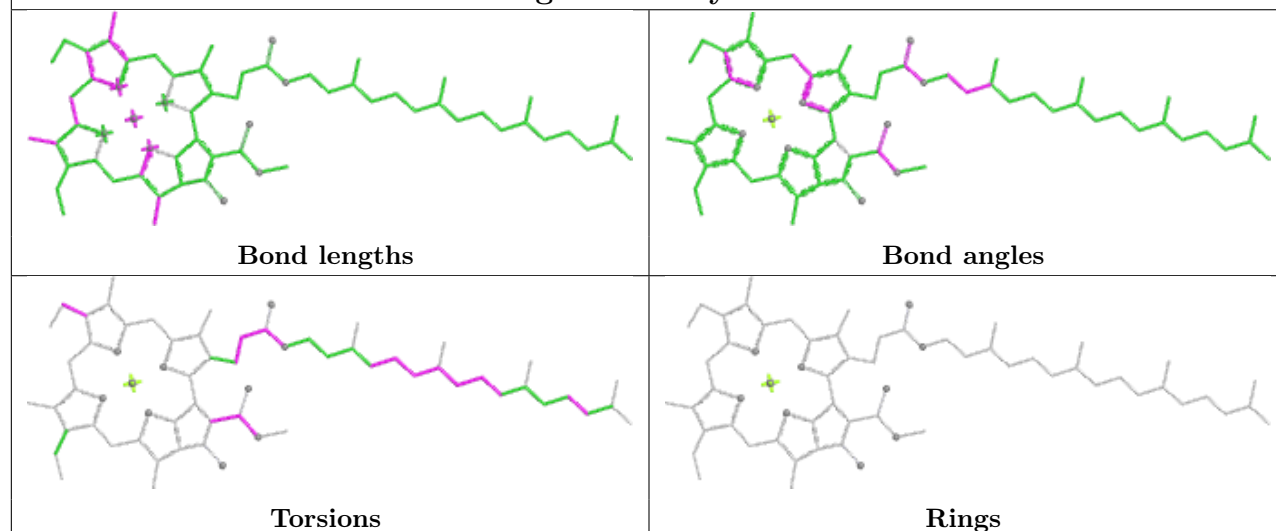
Ligand CLA y 610

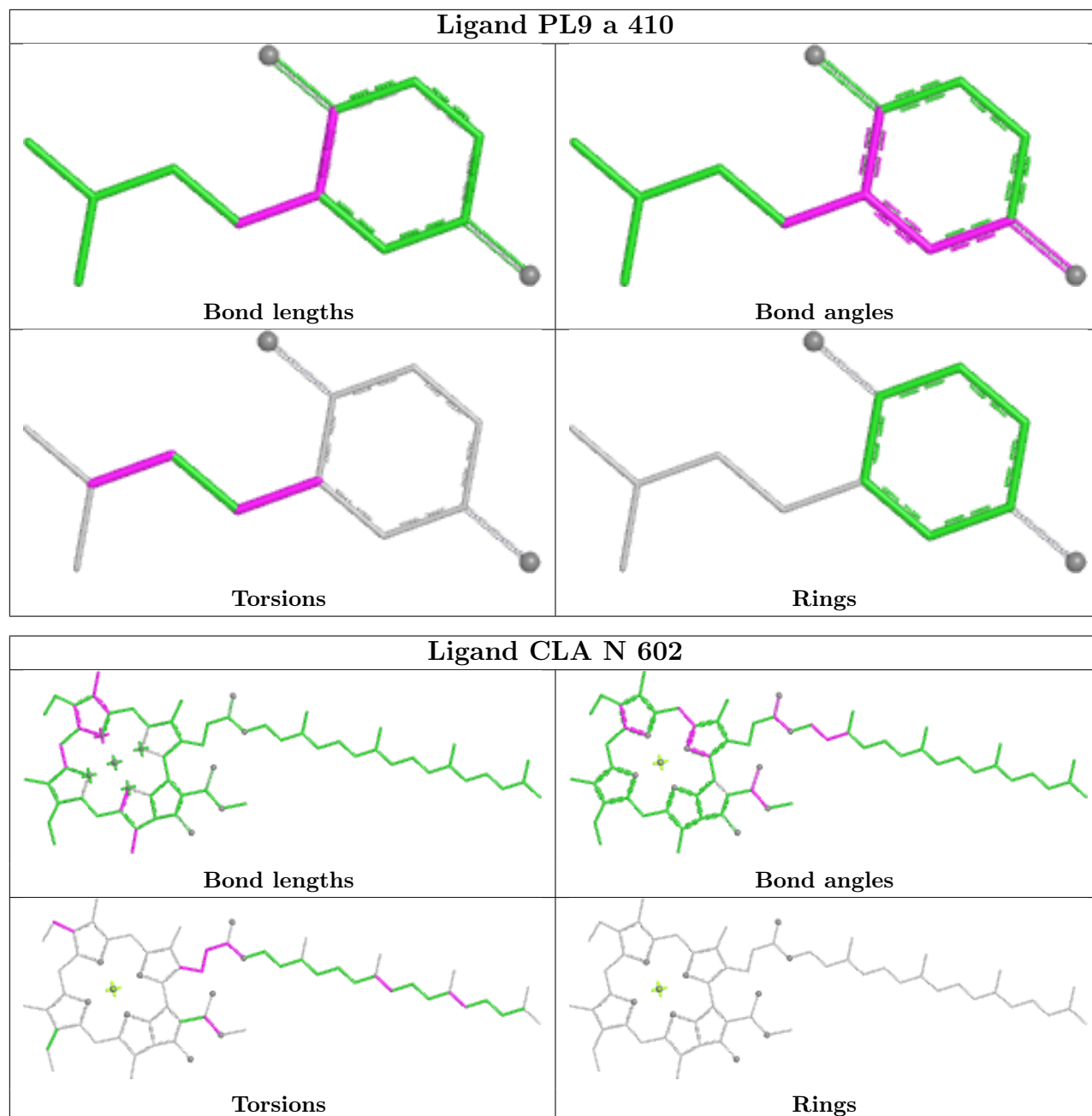


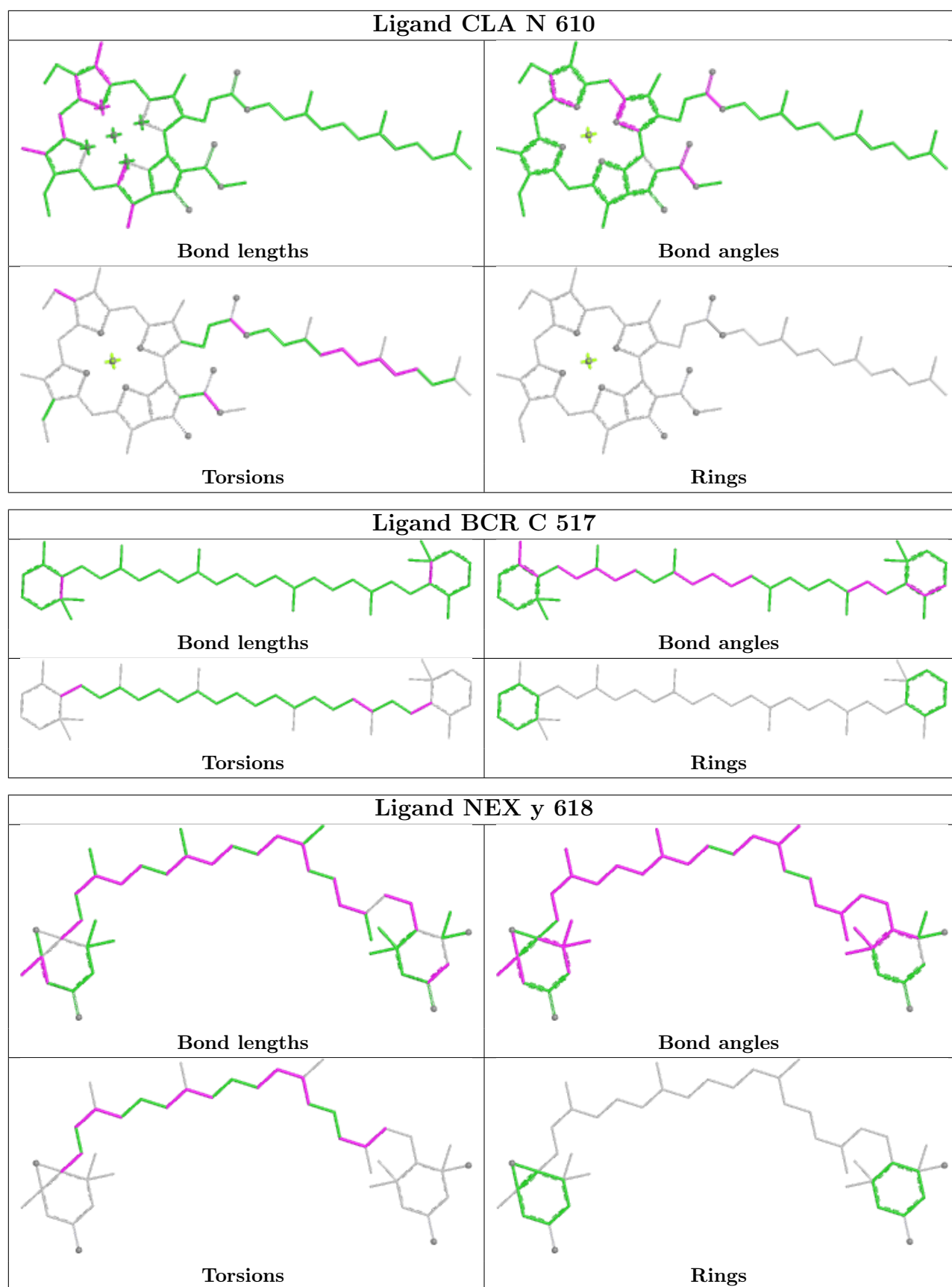
Ligand LMG d 410



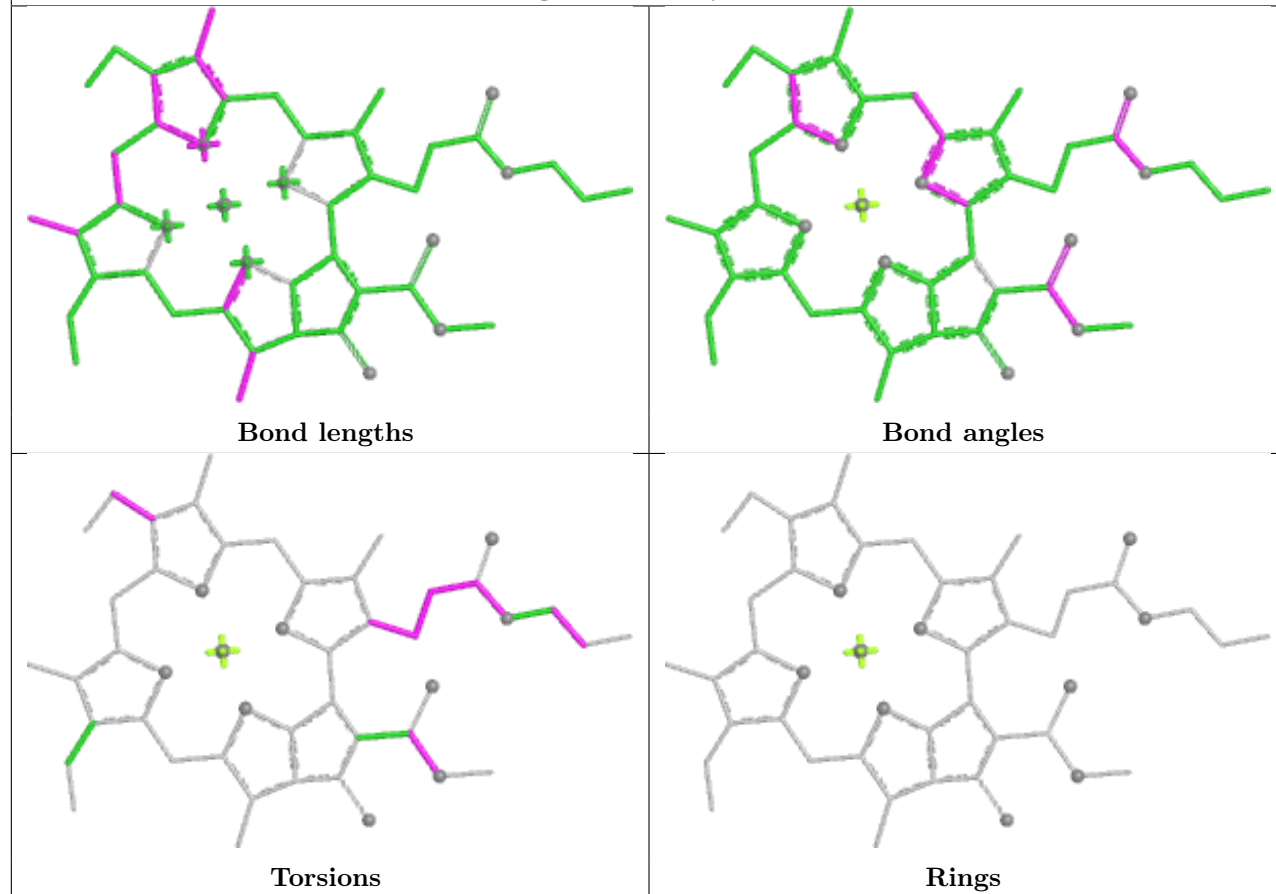
Ligand CLA y 603



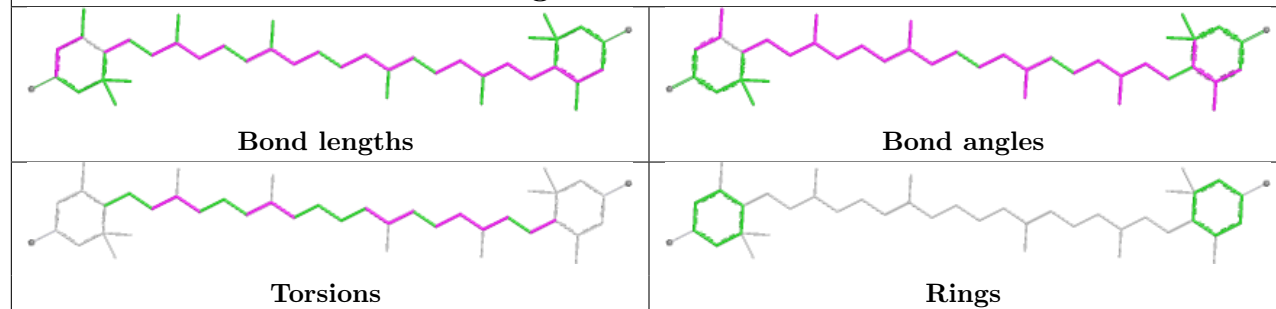


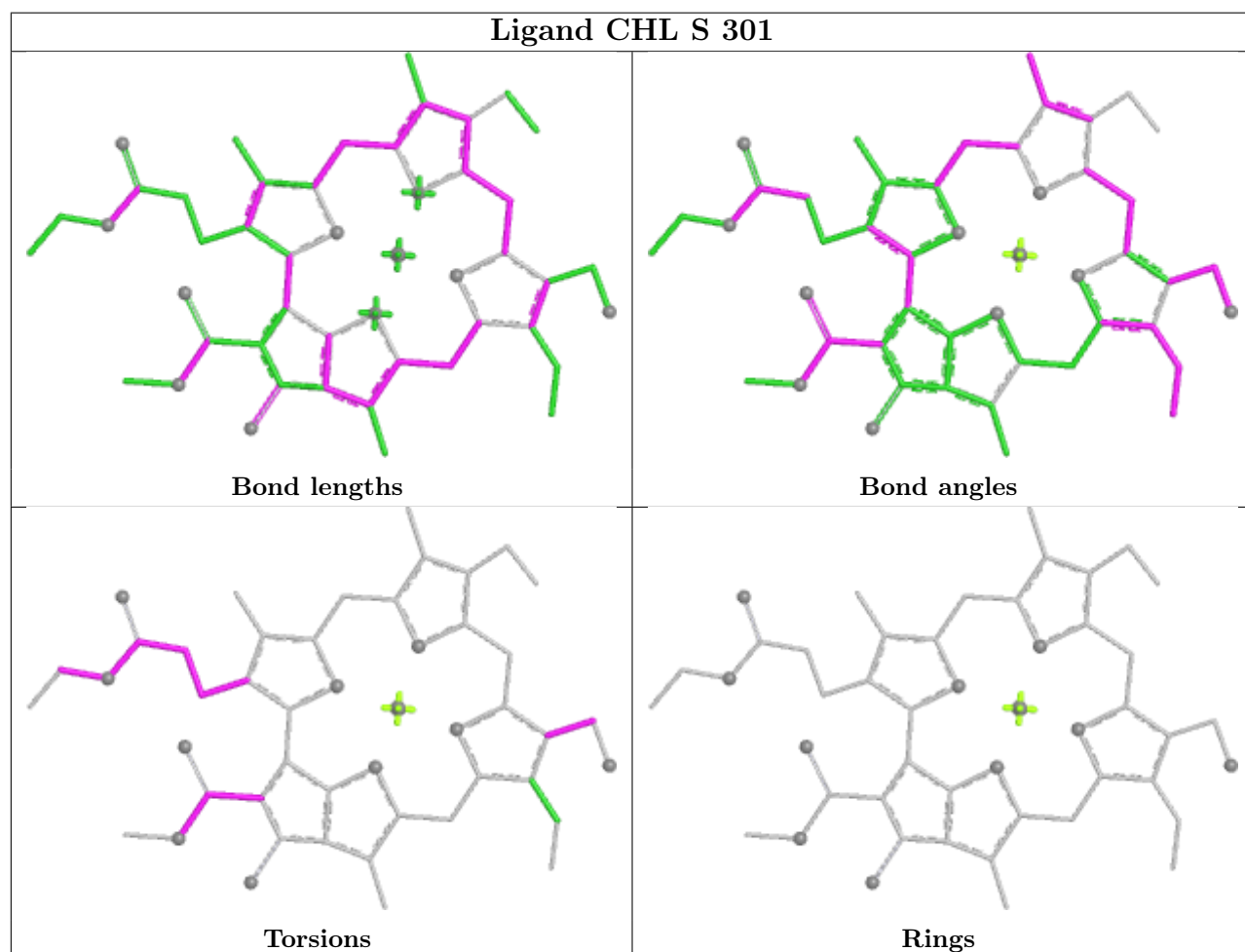
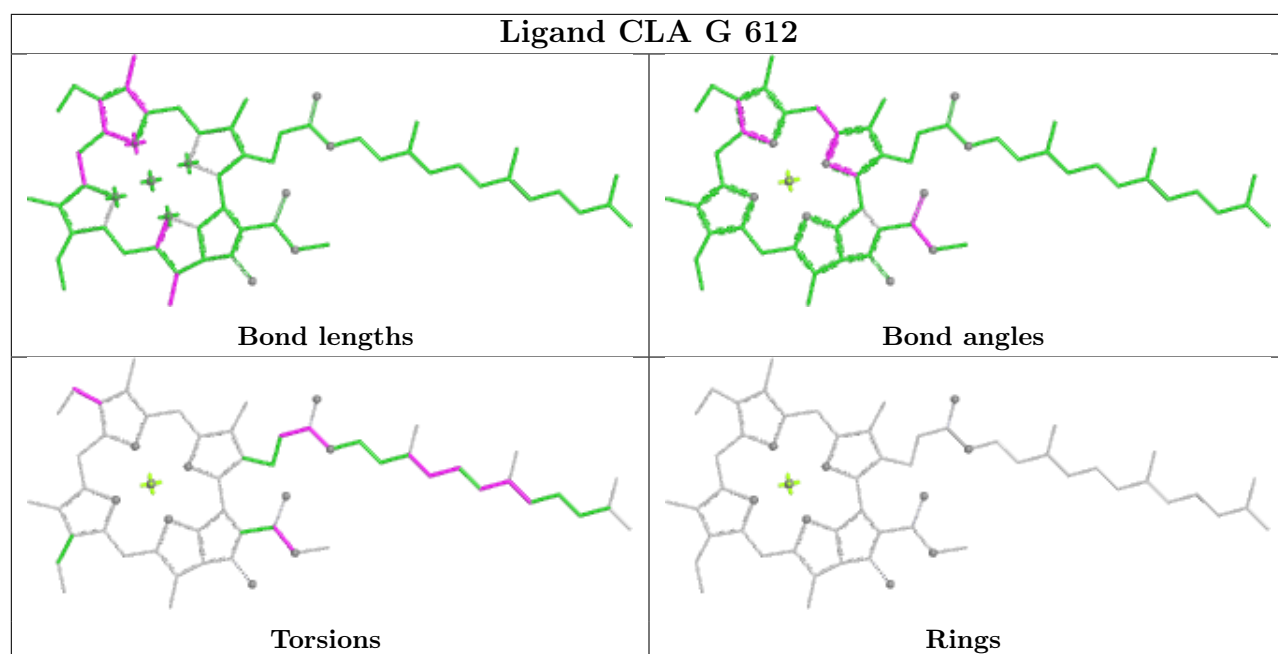


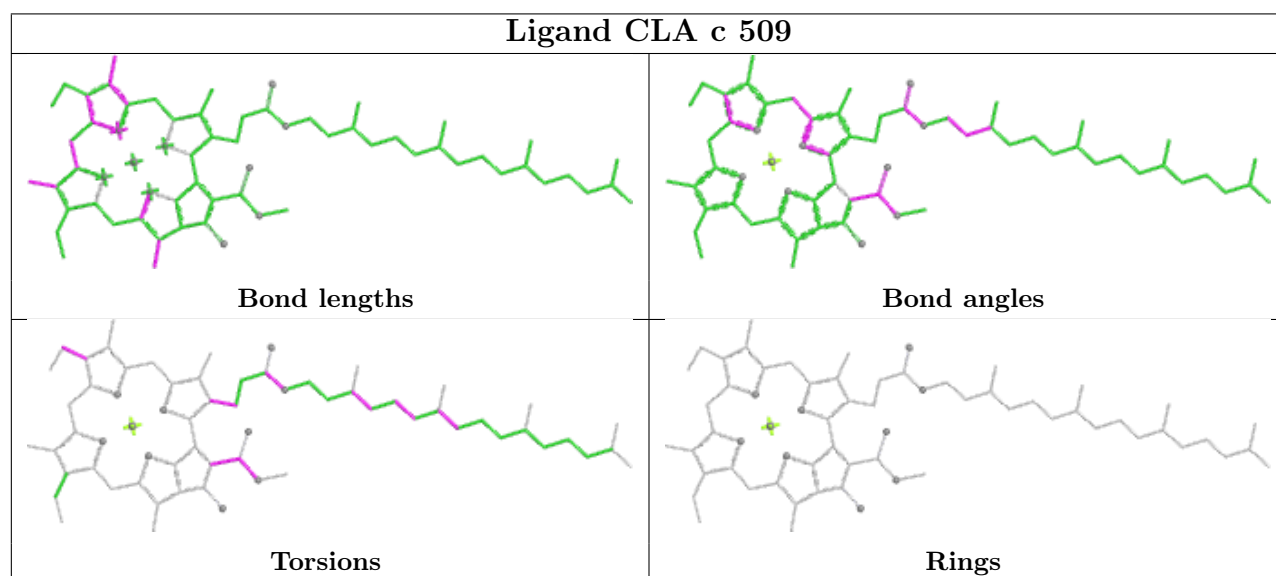
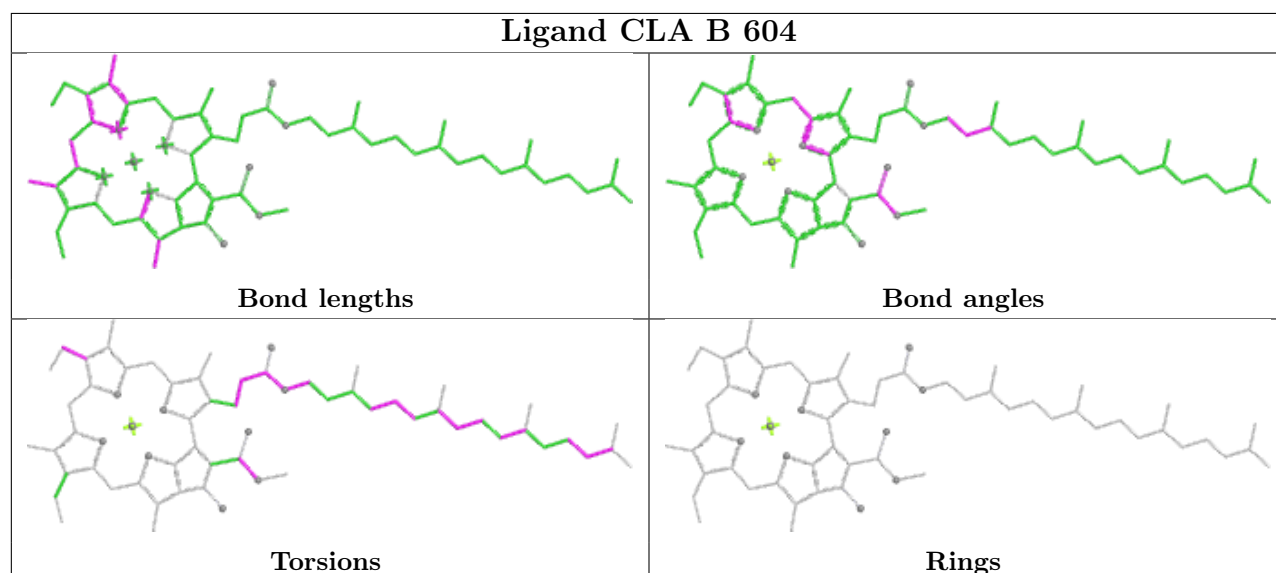
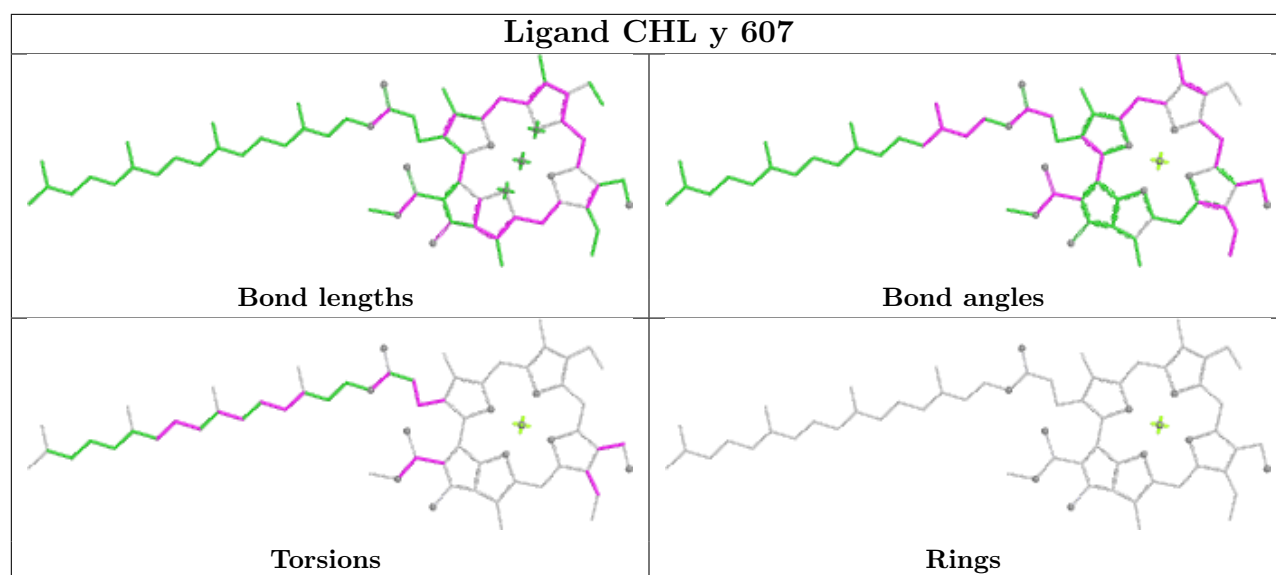
Ligand CLA y 613



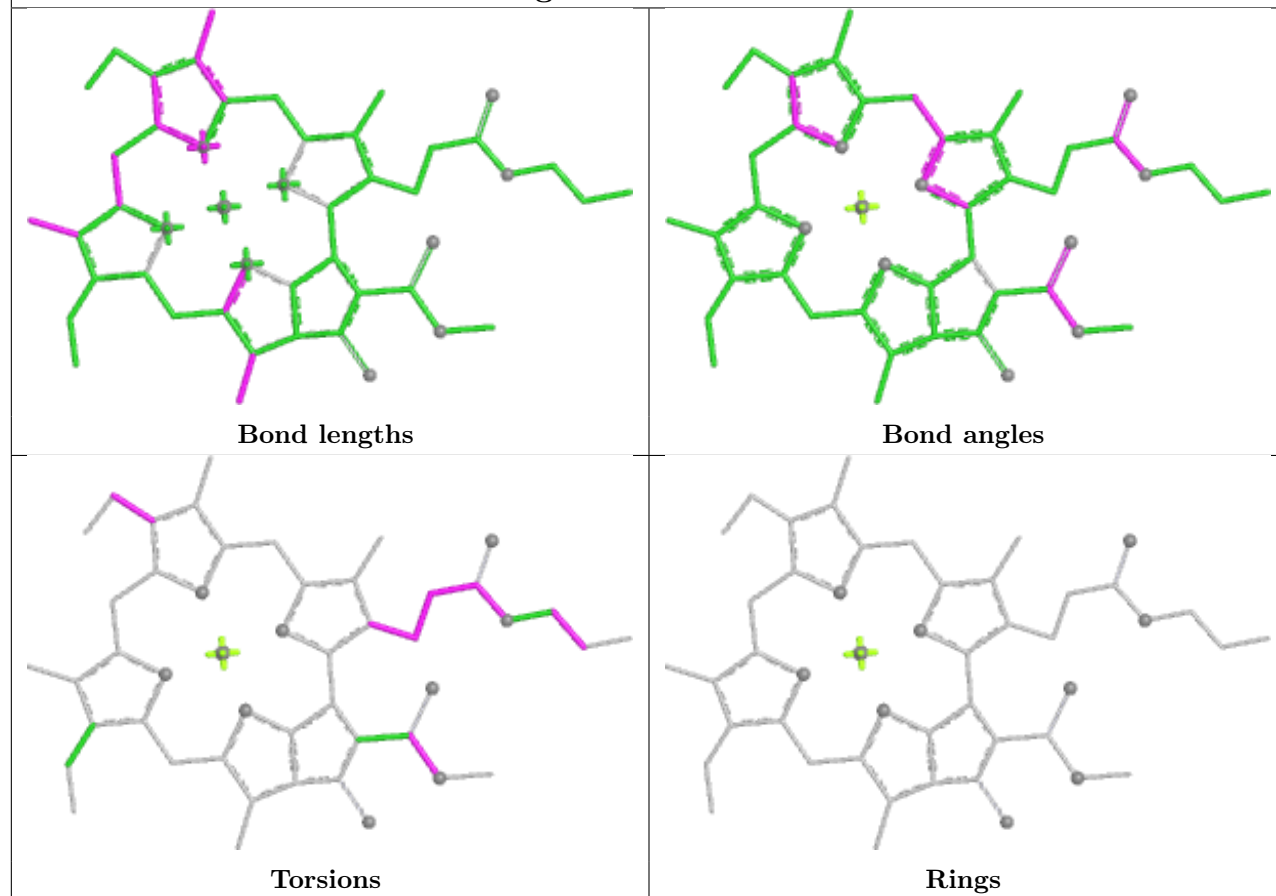
Ligand LUT G 616



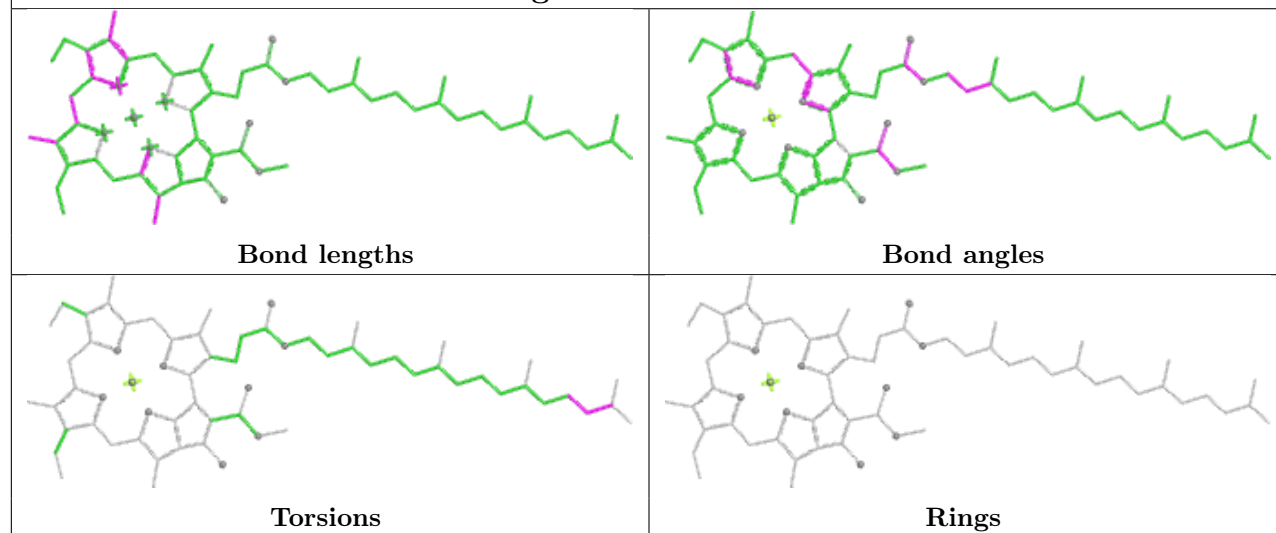


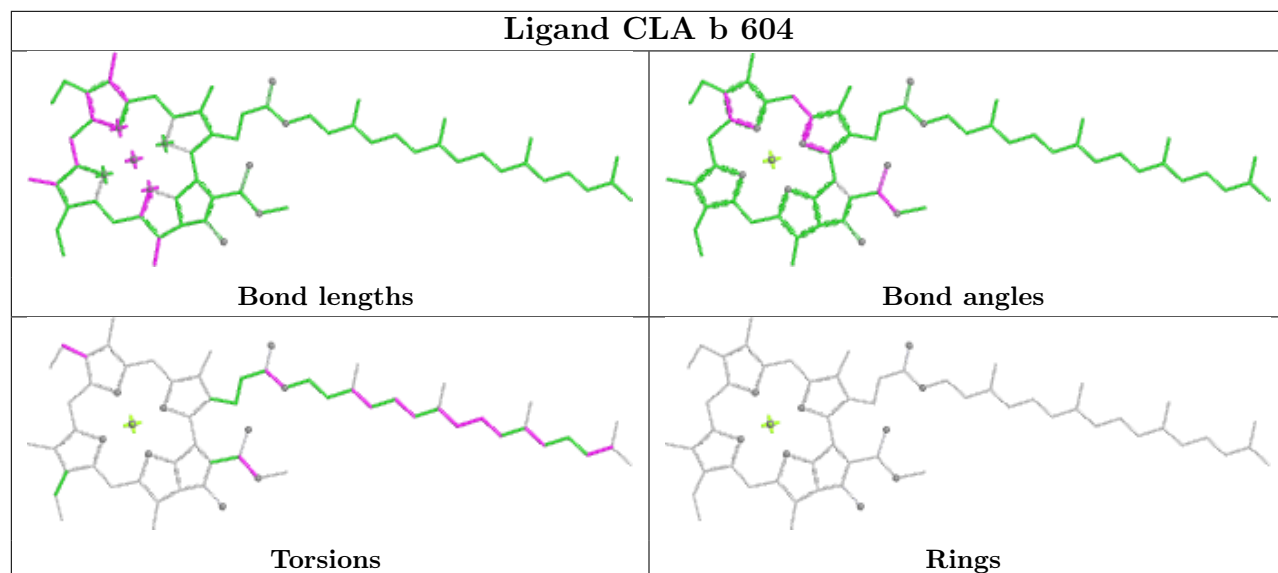
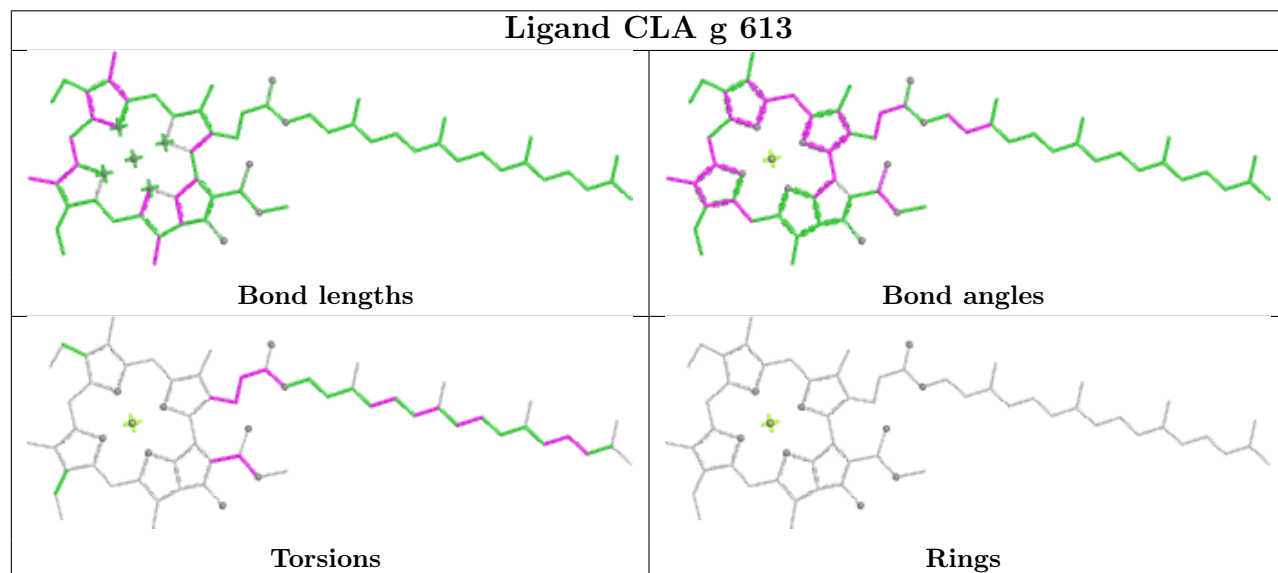
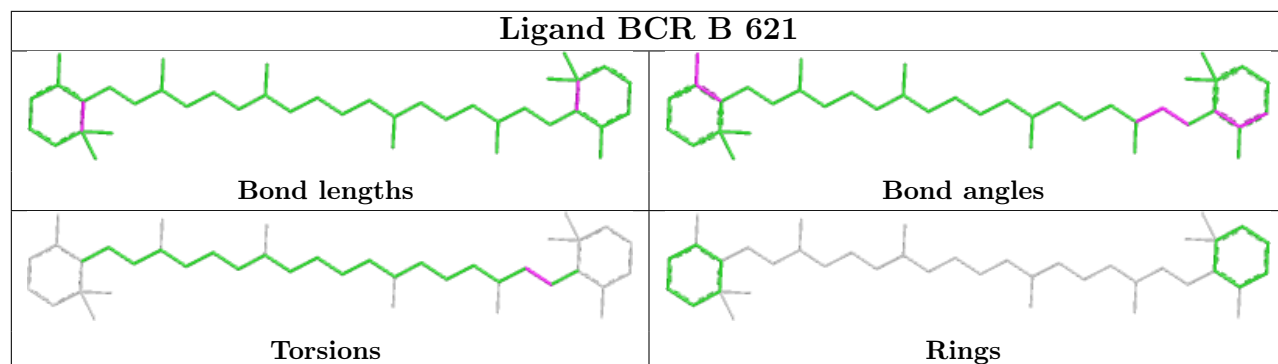


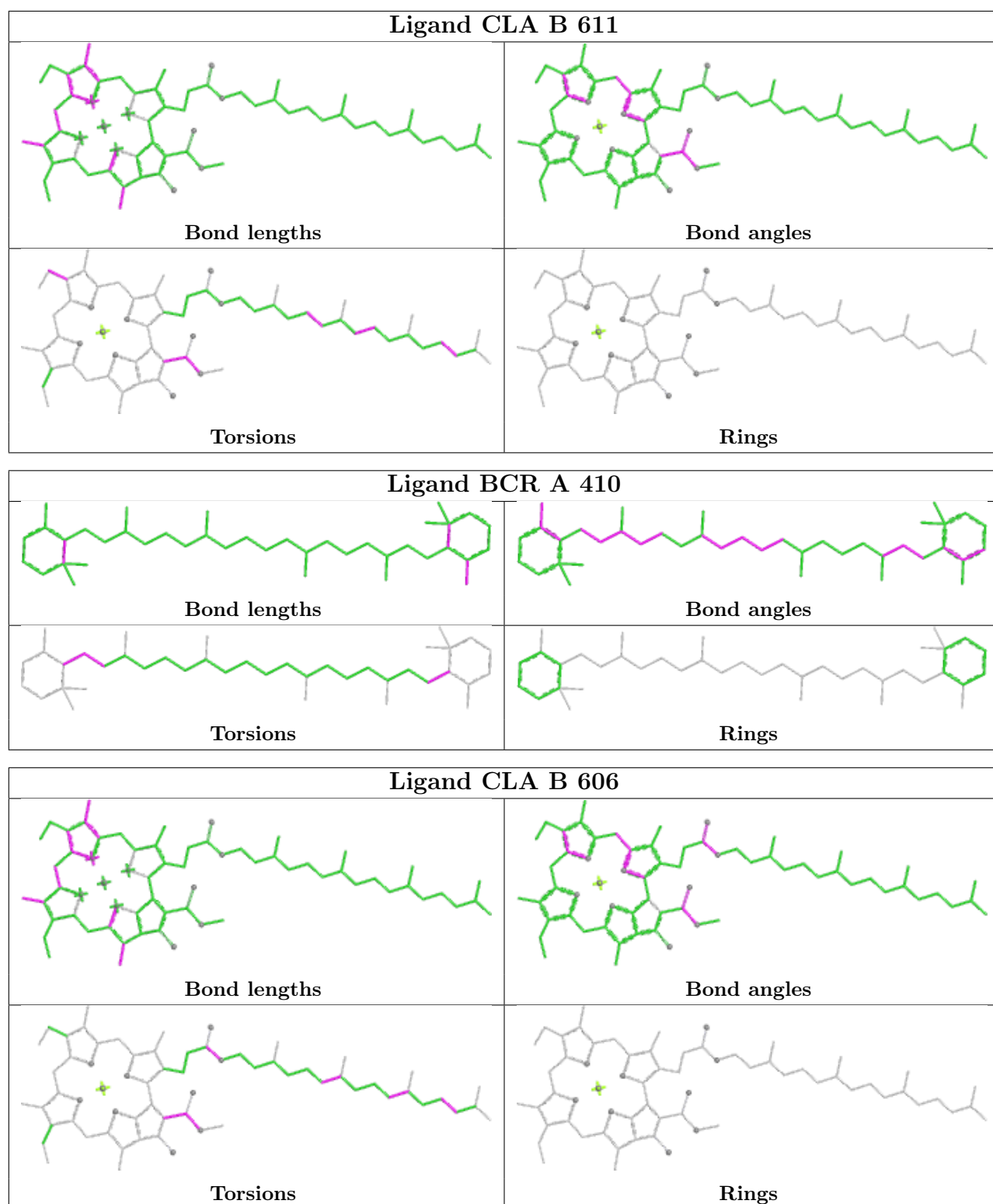
Ligand CLA n 613



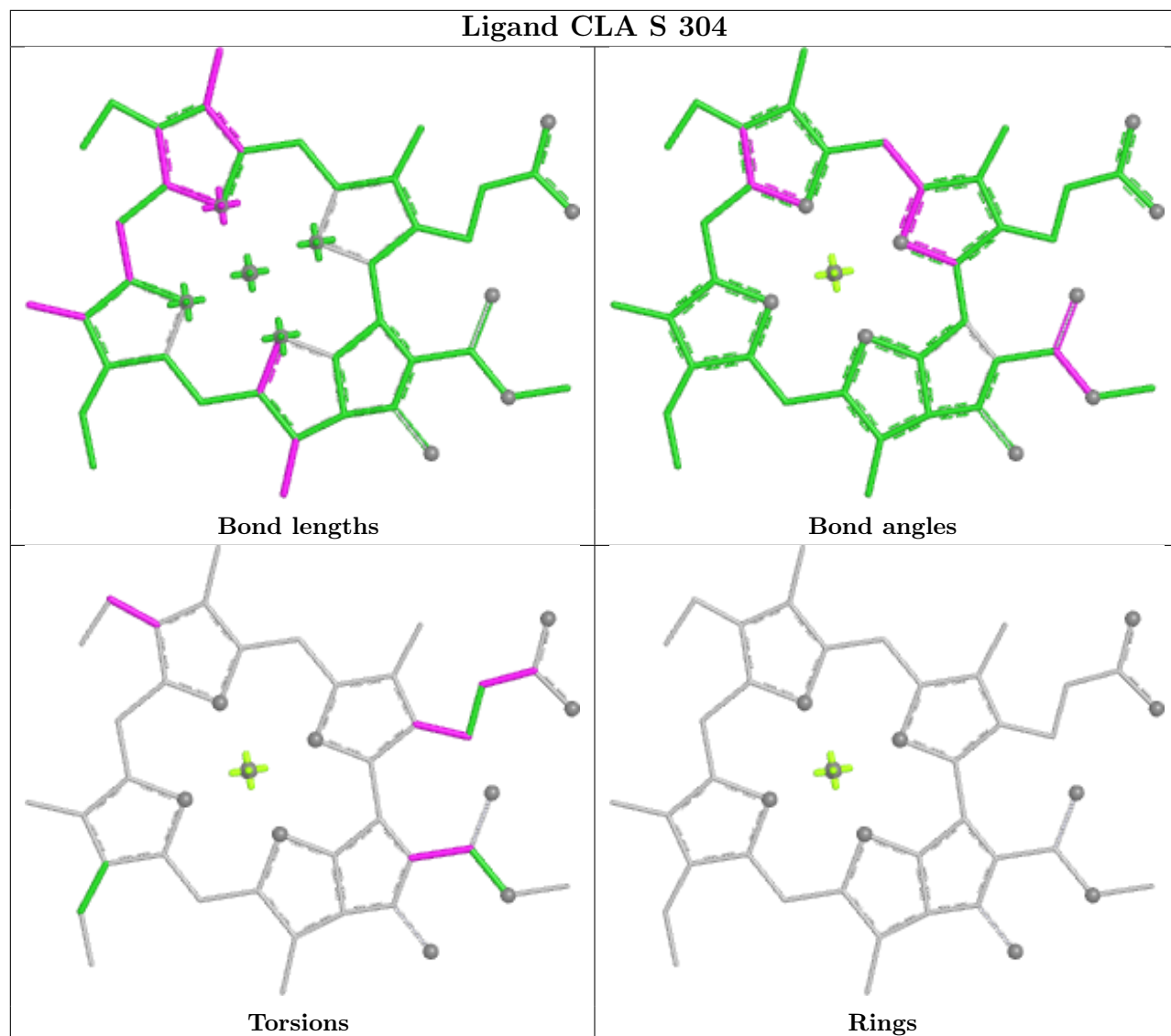
Ligand CLA A 405



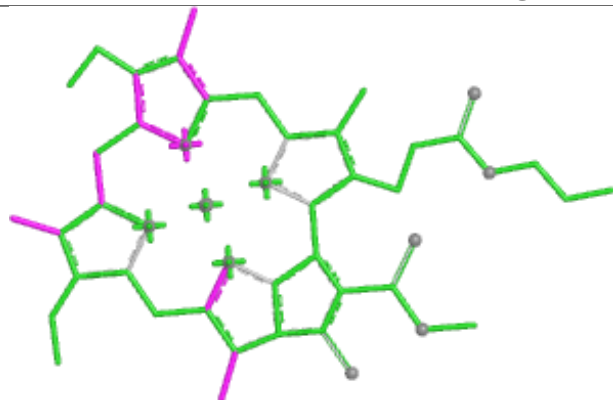




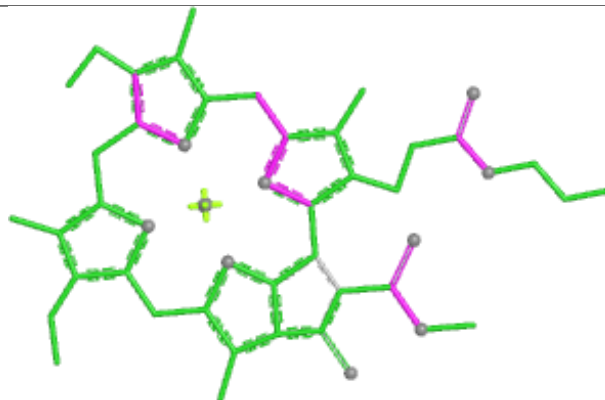
Ligand CLA S 304



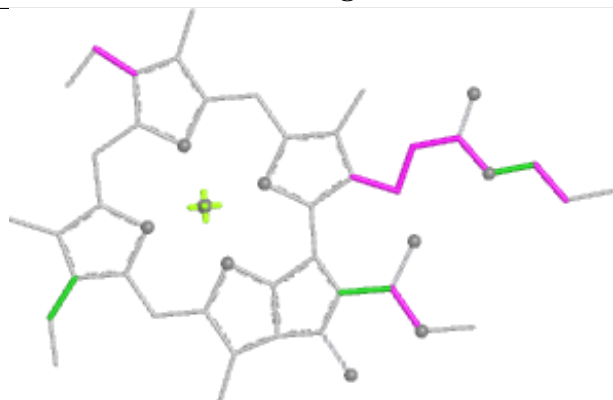
Ligand CLA Y 612



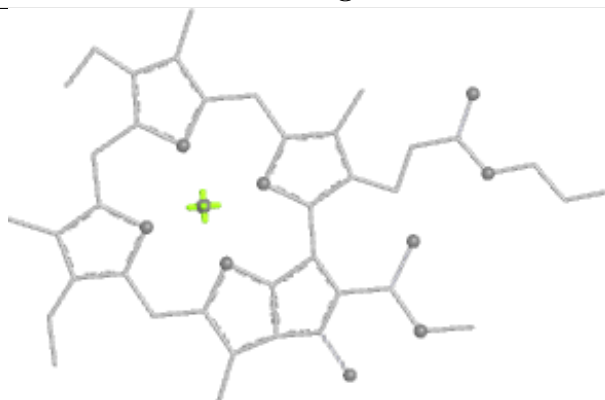
Bond lengths



Bond angles

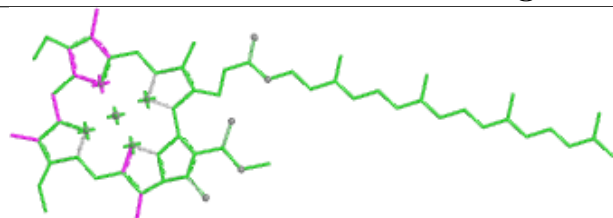


Torsions

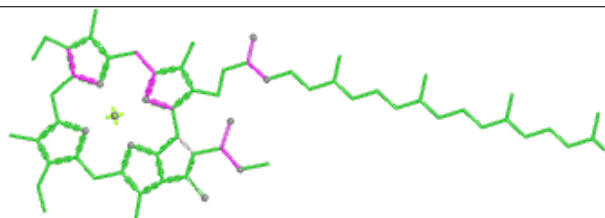


Rings

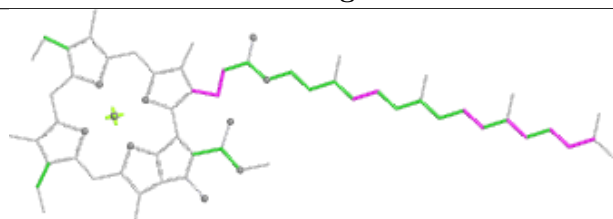
Ligand CLA b 605



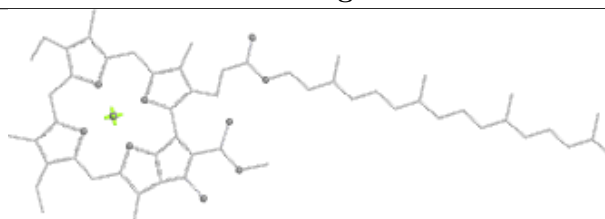
Bond lengths



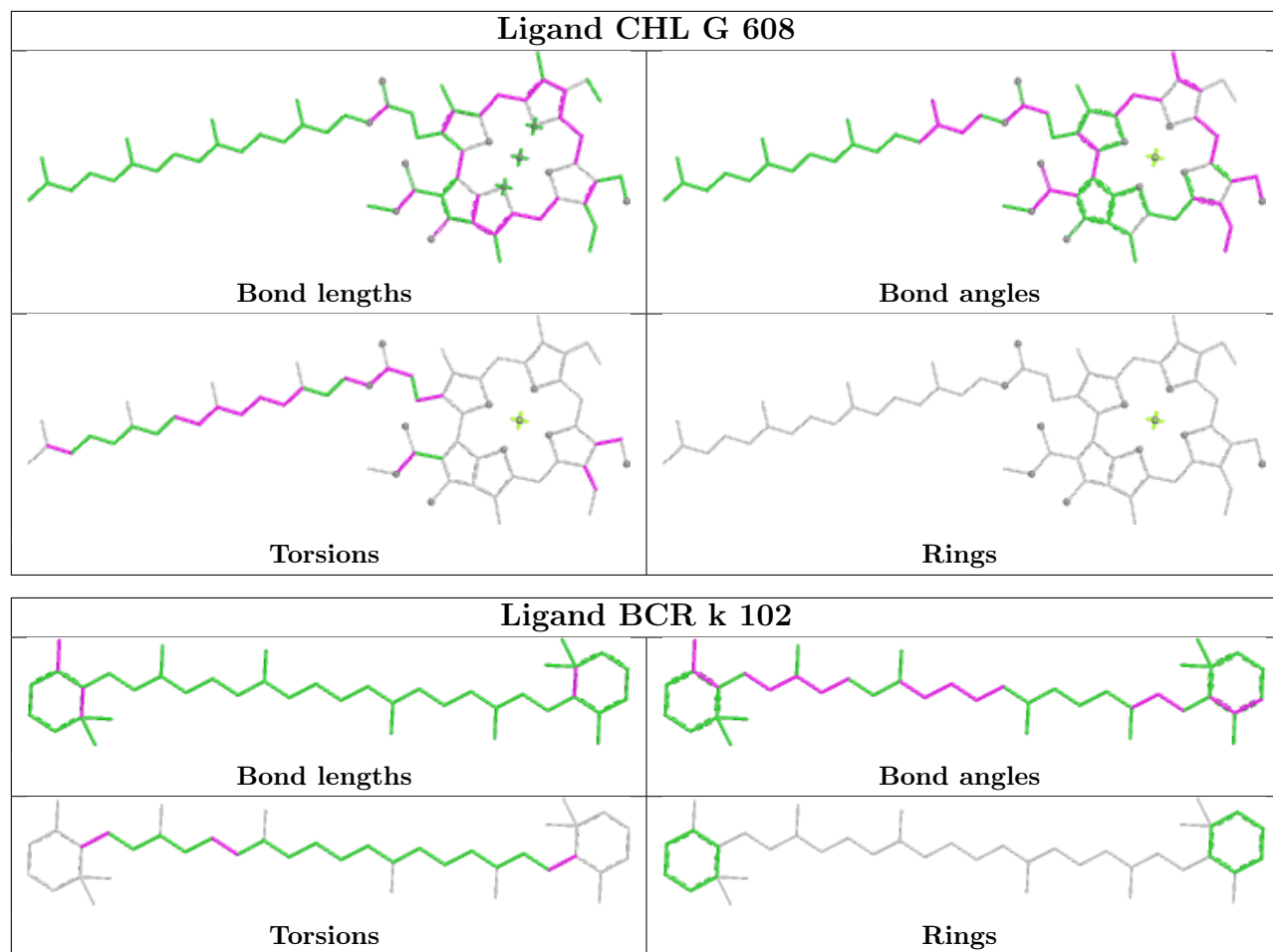
Bond angles



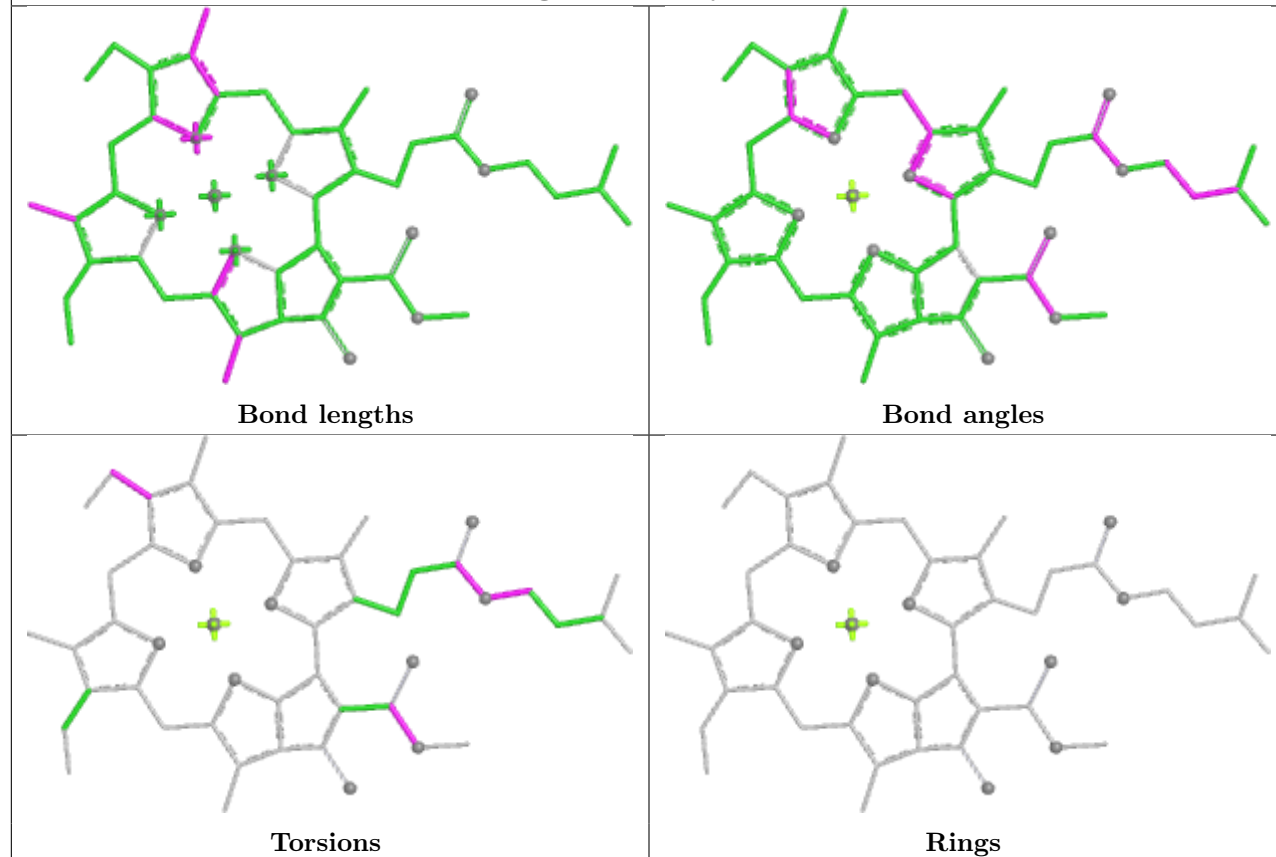
Torsions



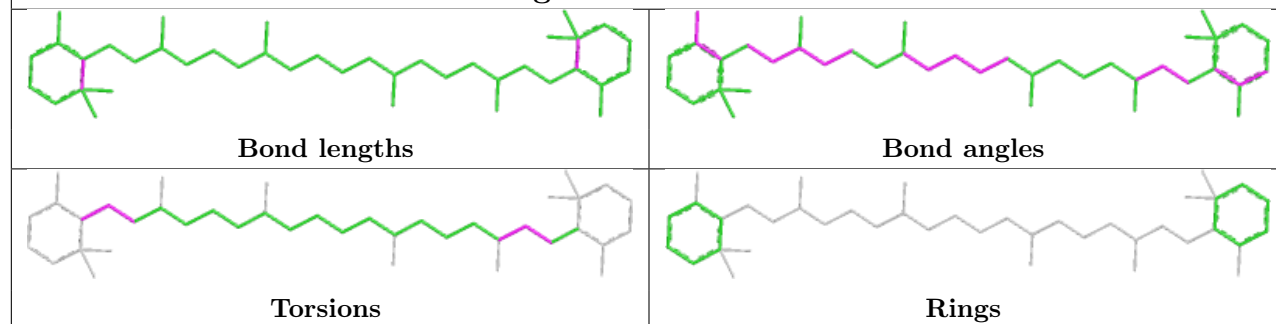
Rings

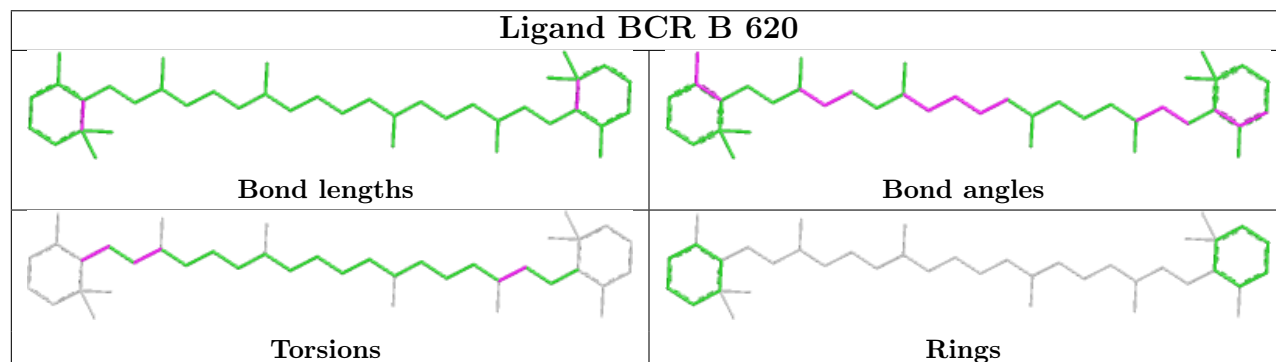
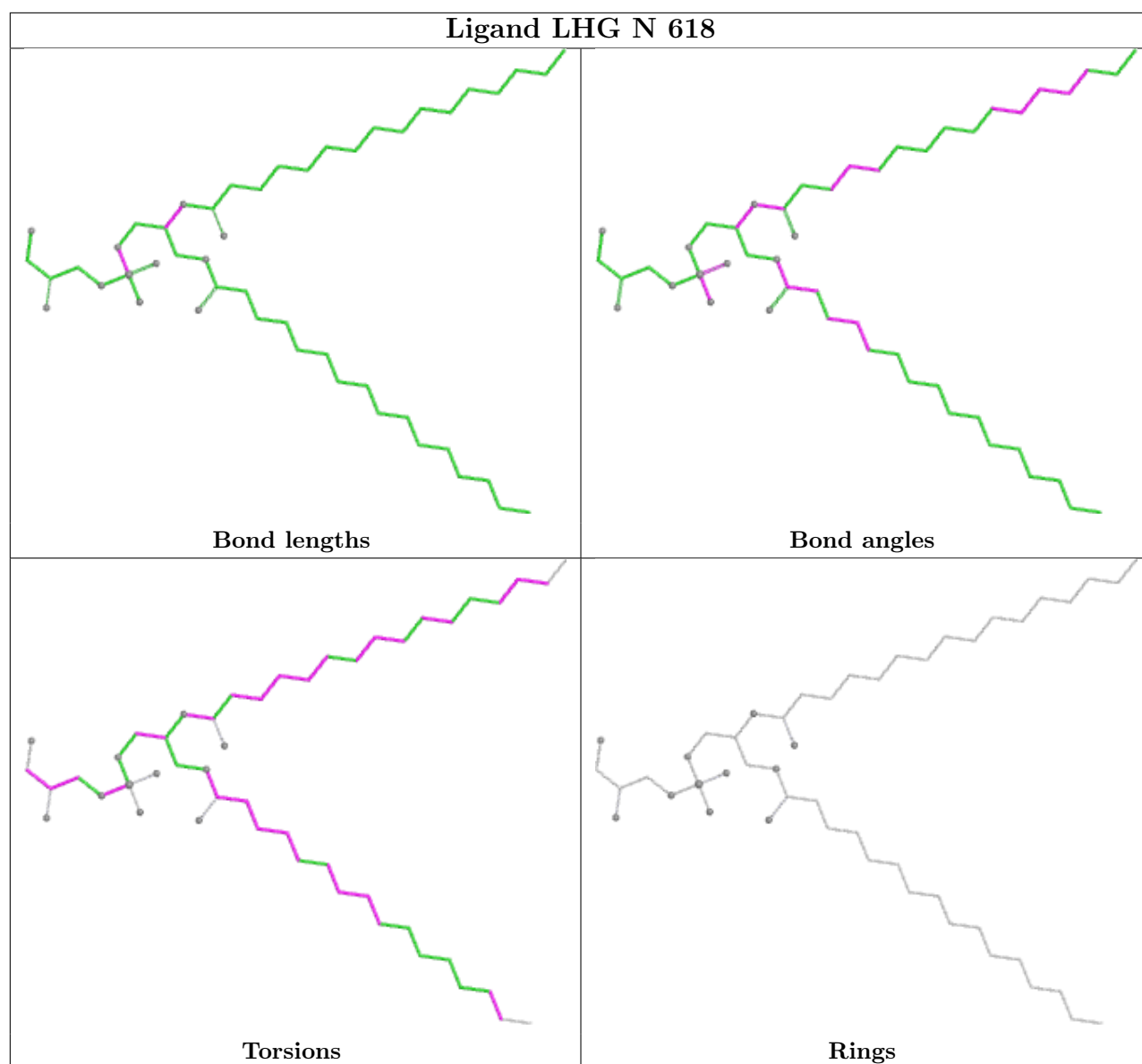


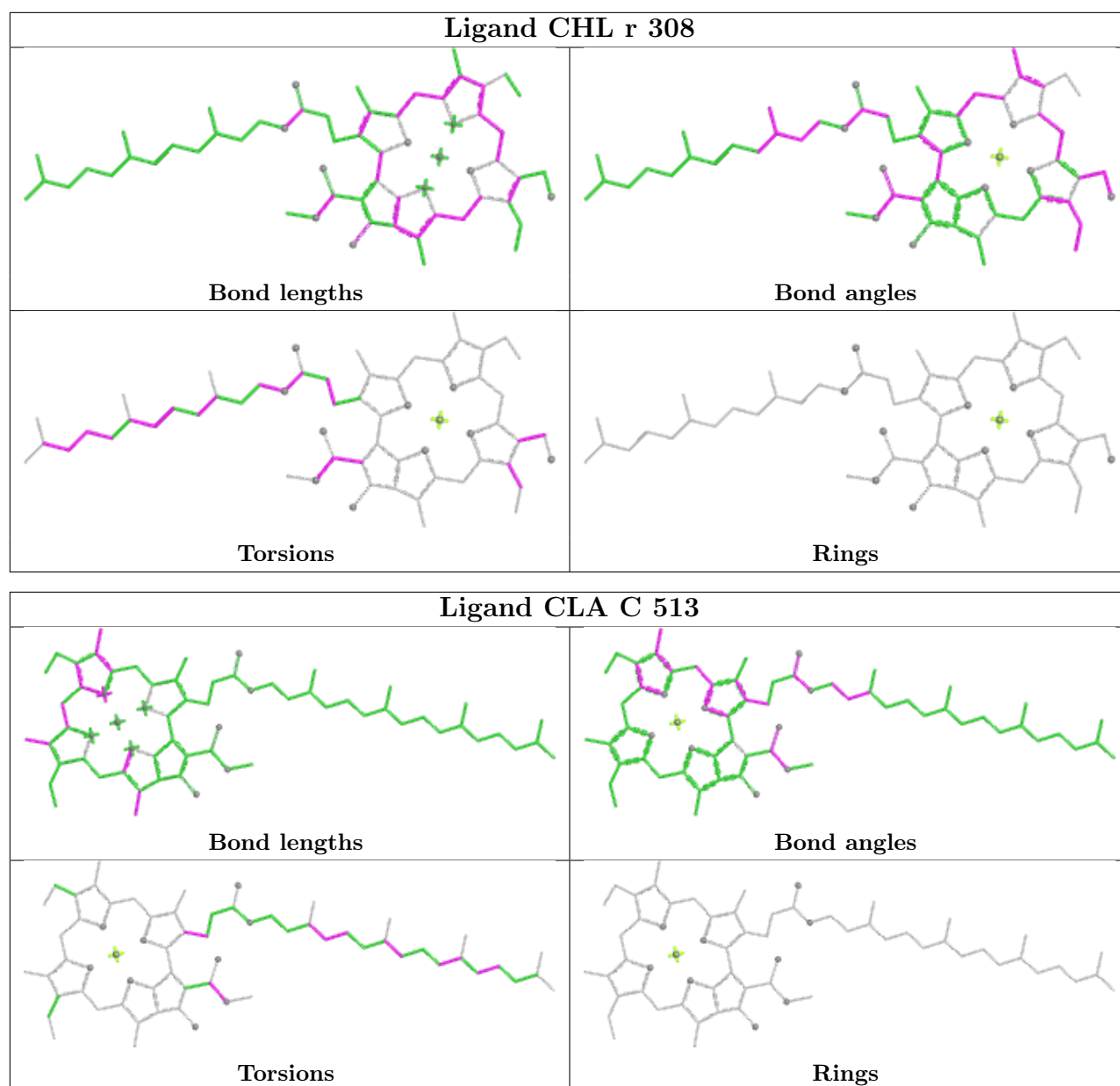
Ligand CLA y 604

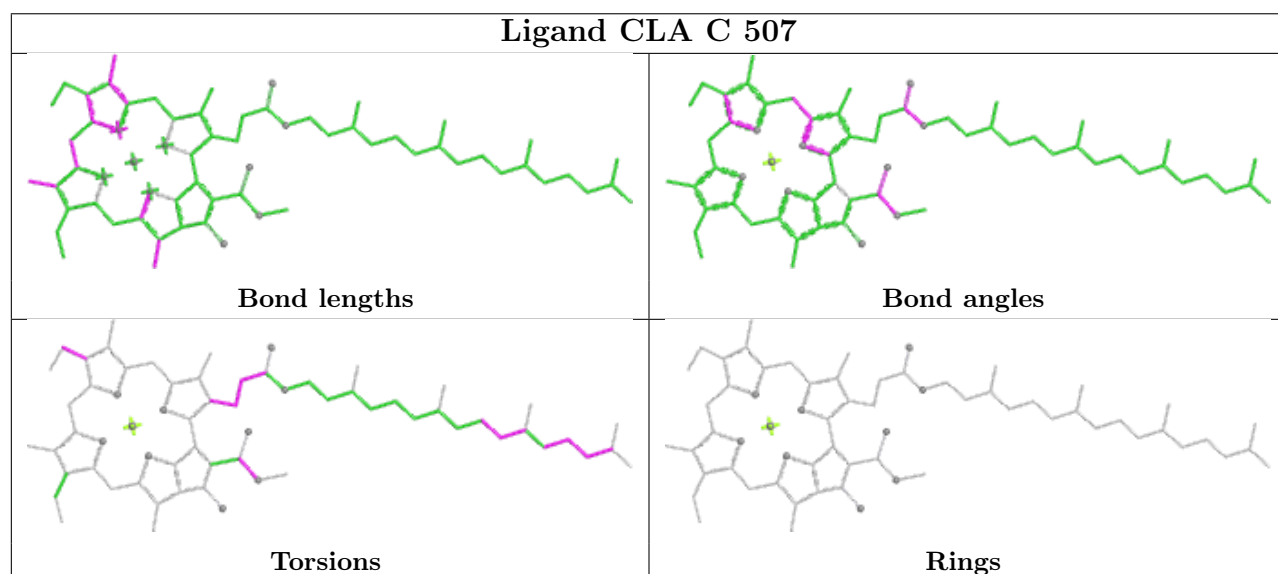
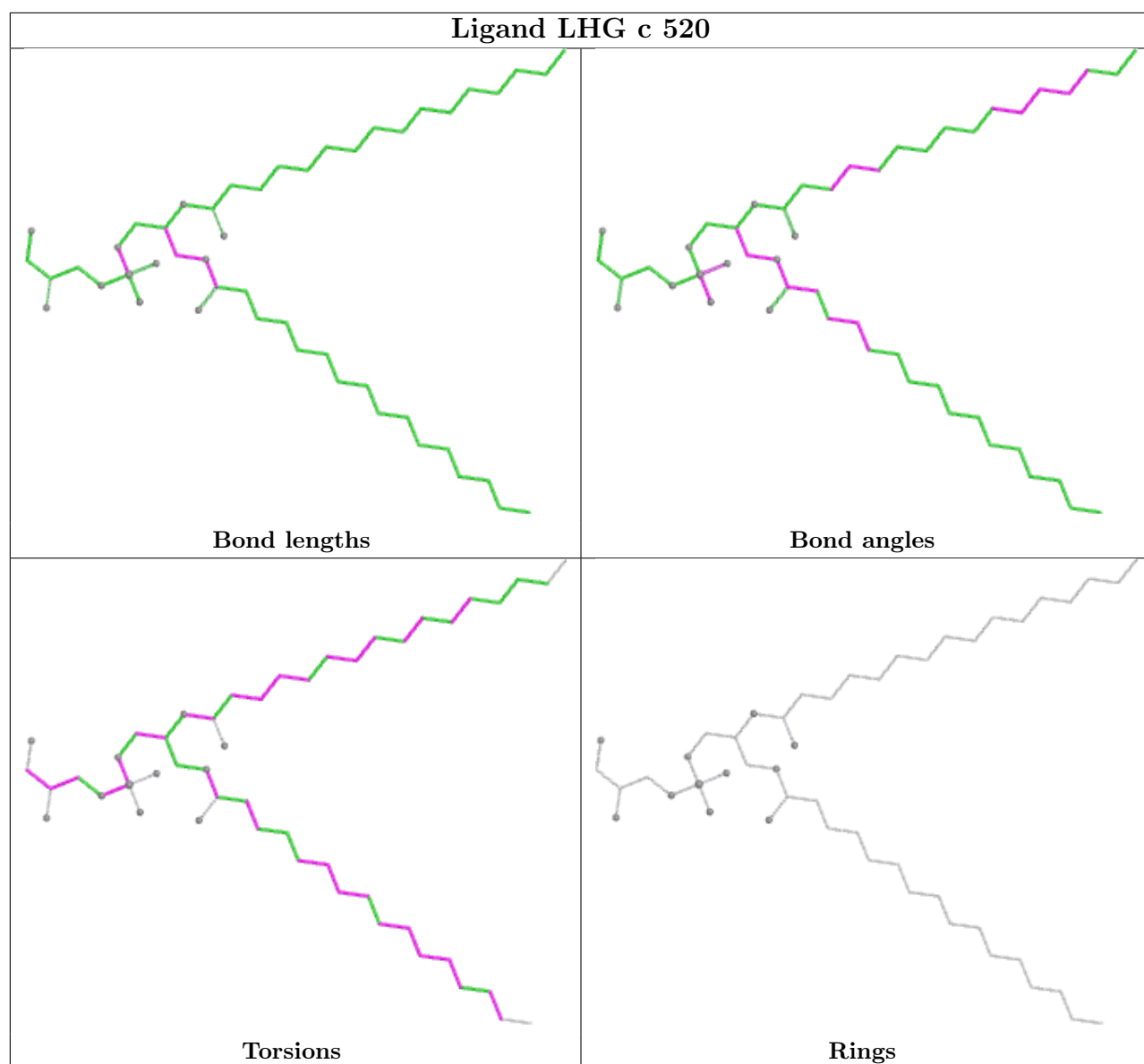


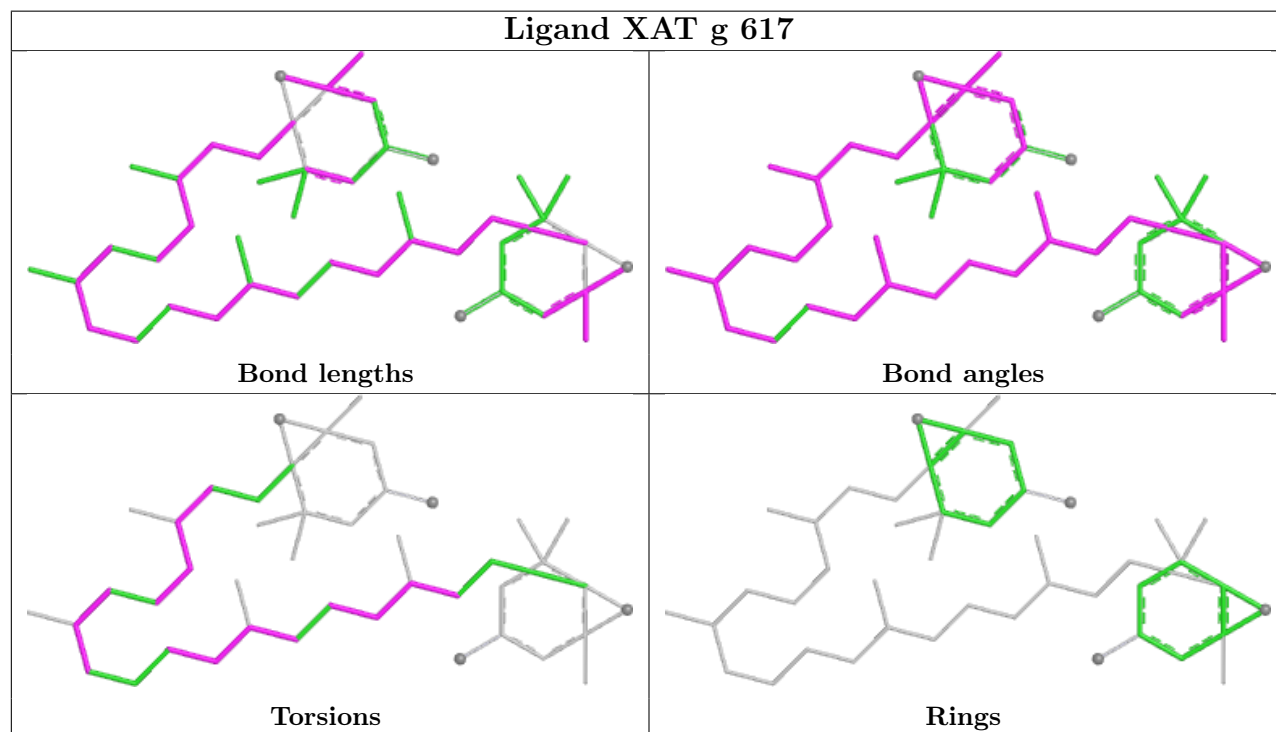
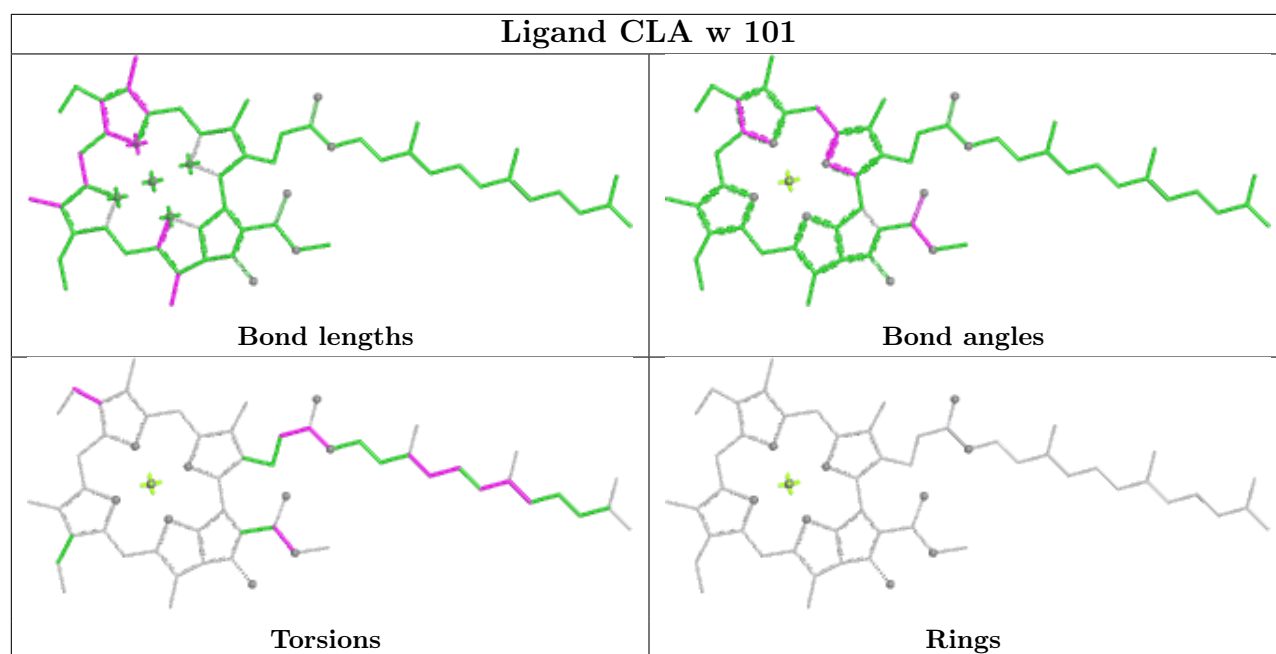
Ligand BCR b 616

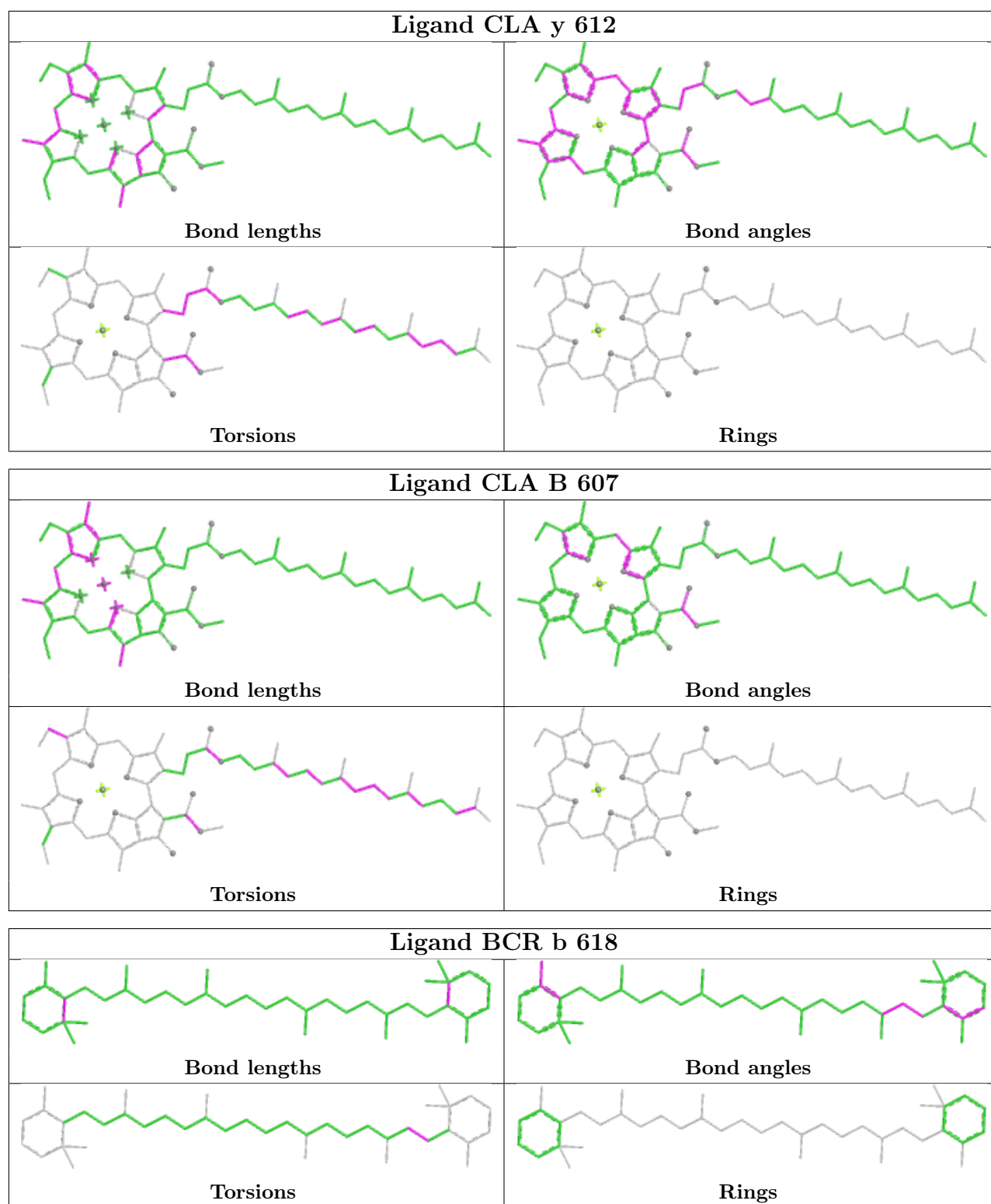


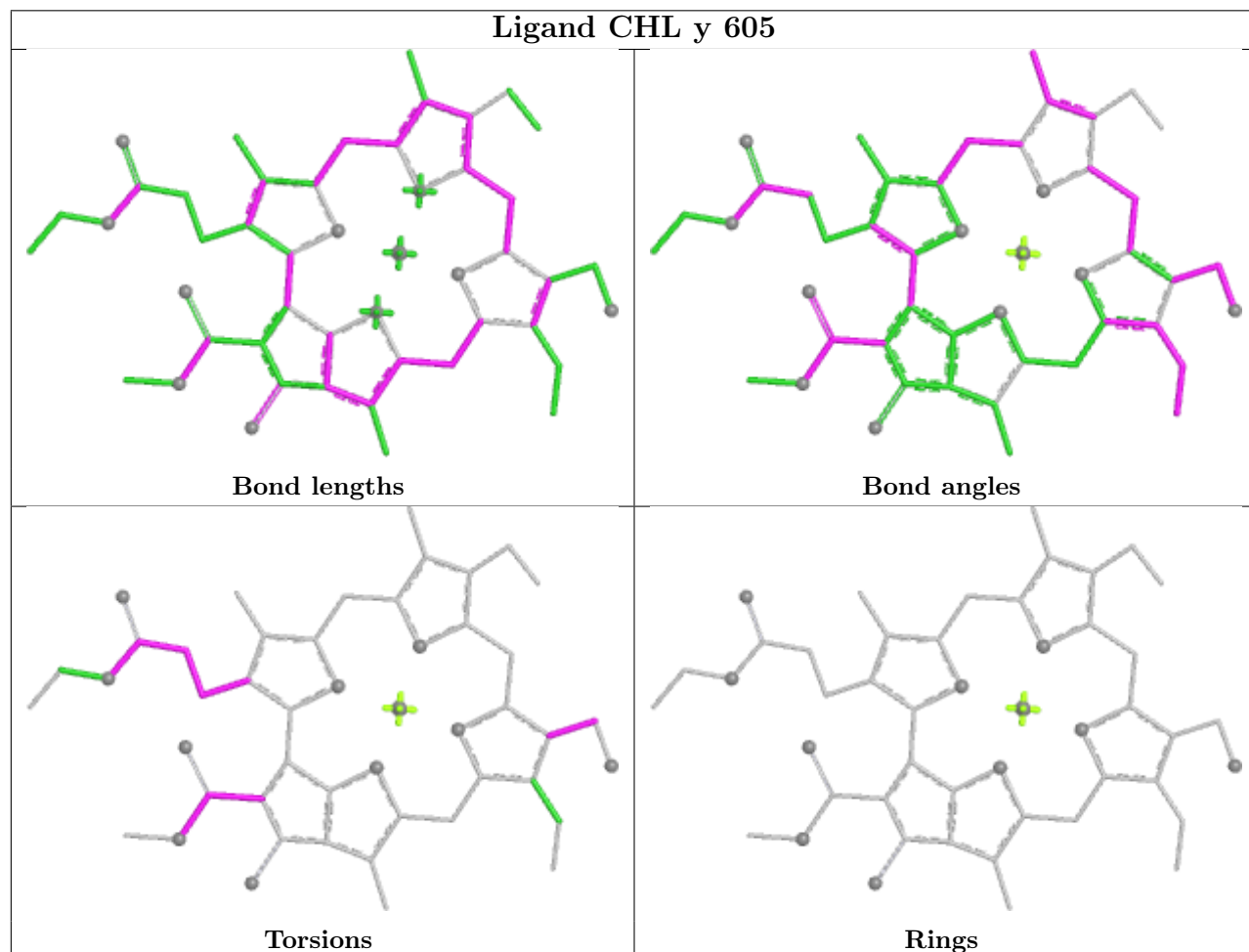
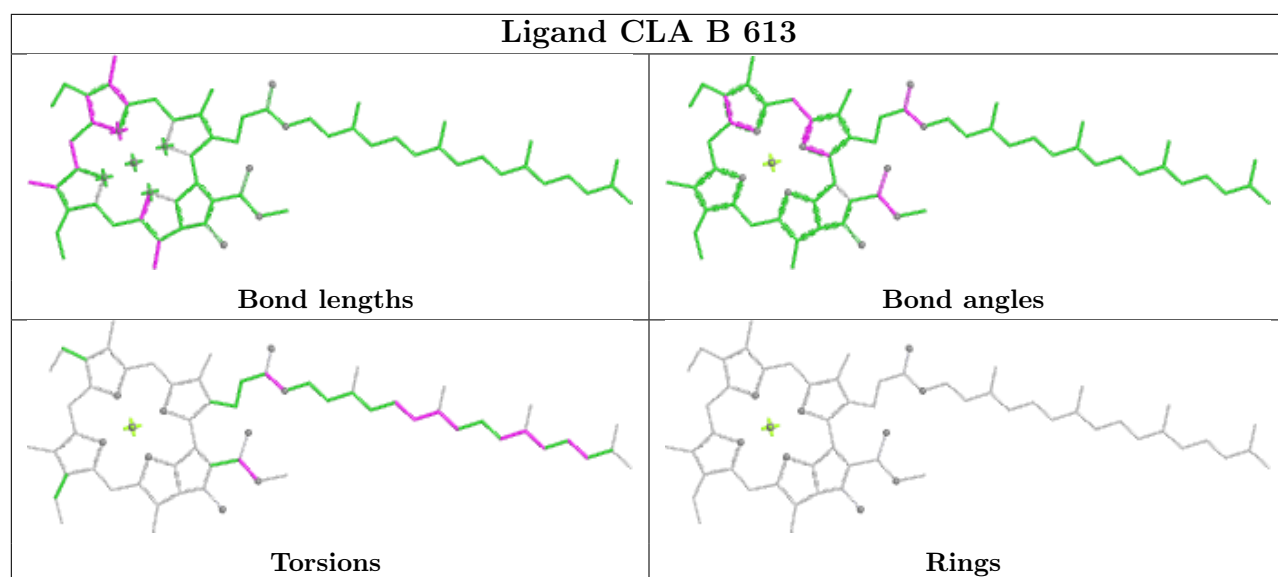


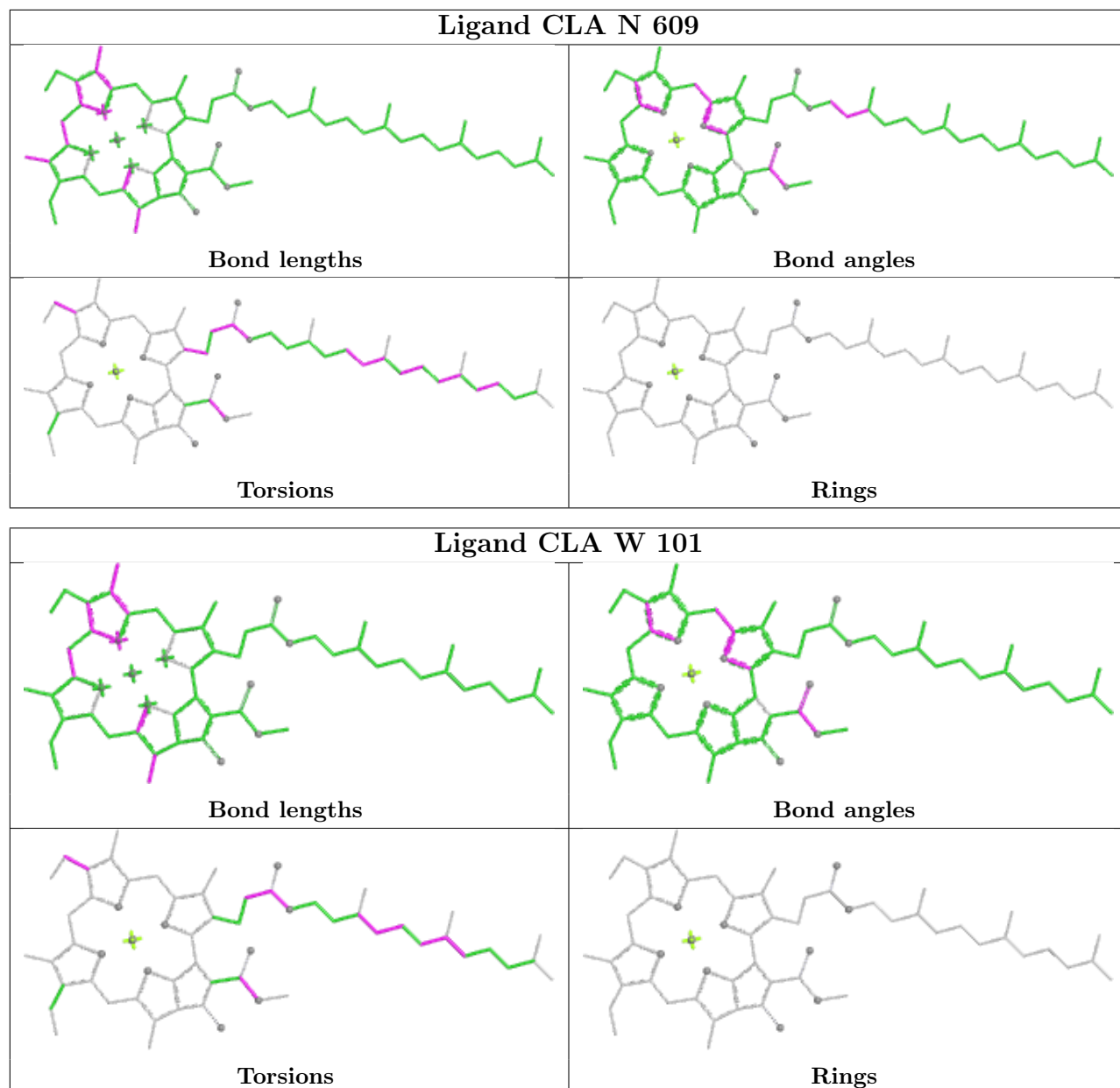


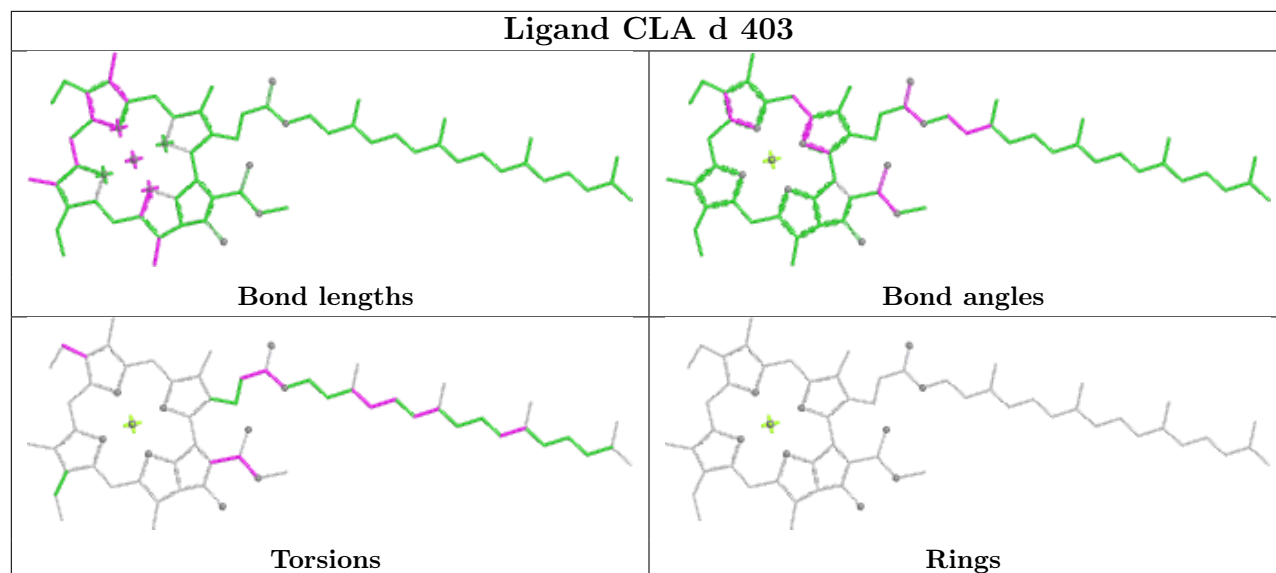
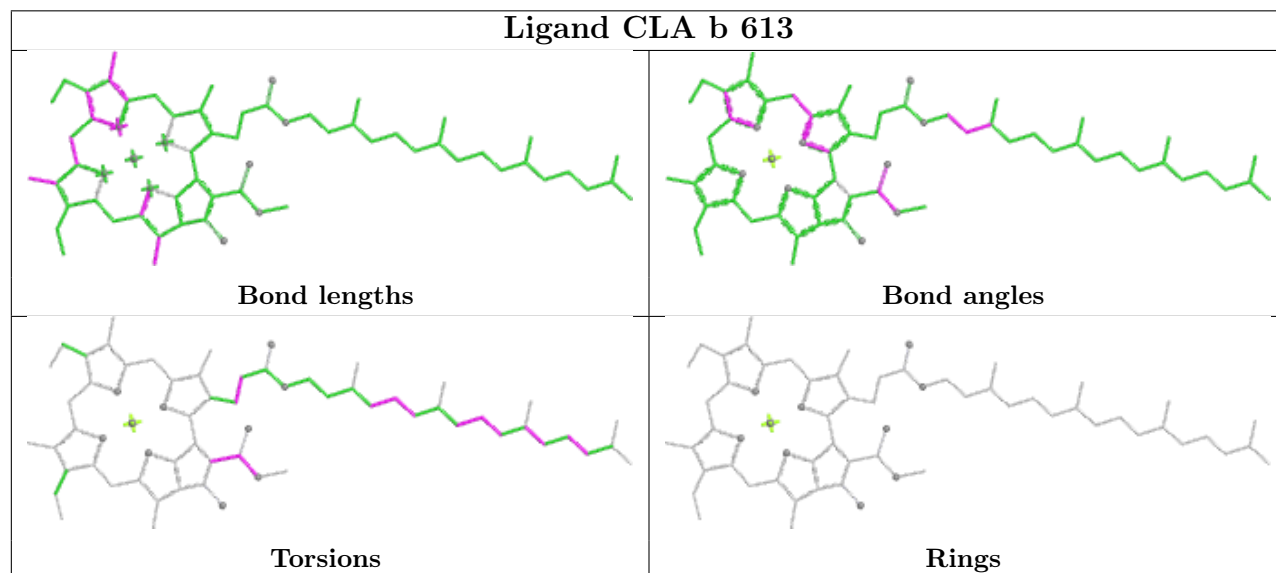
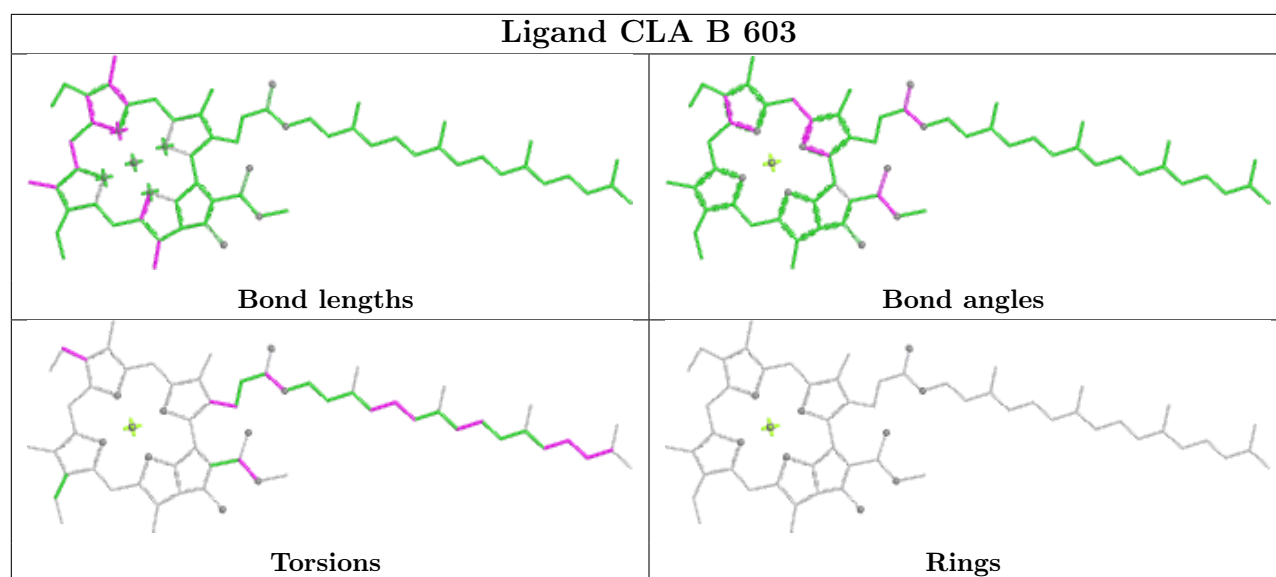


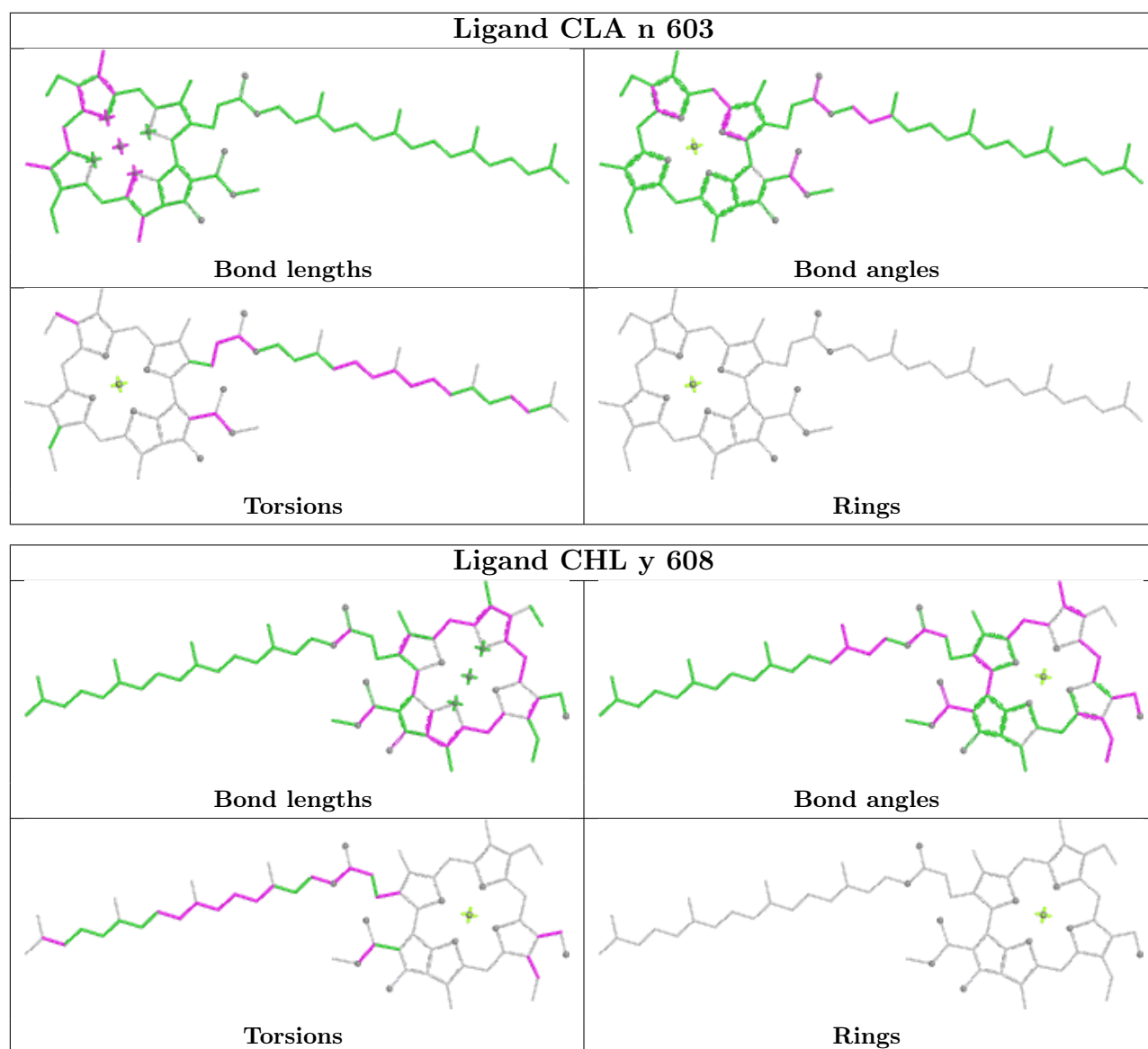


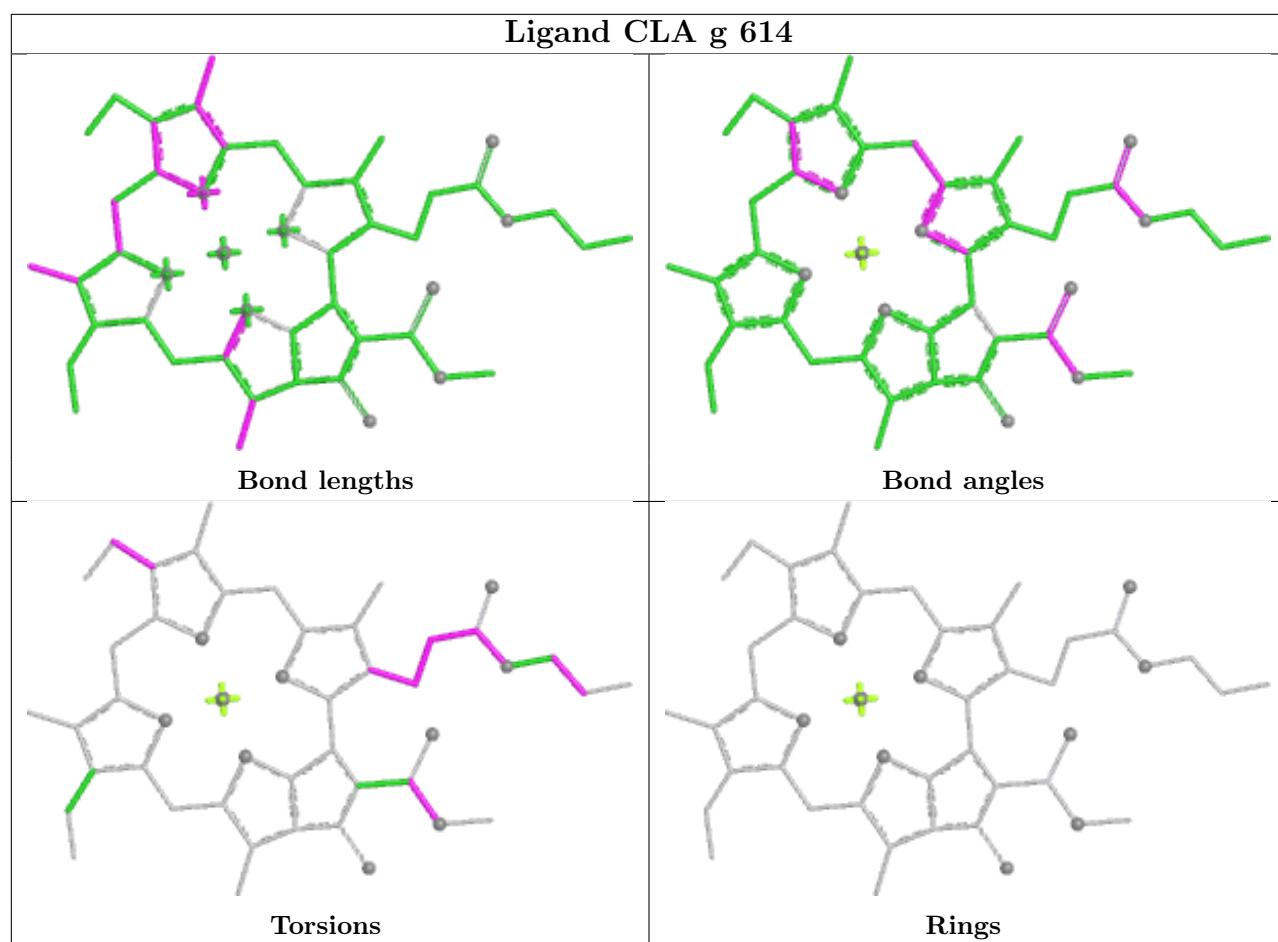


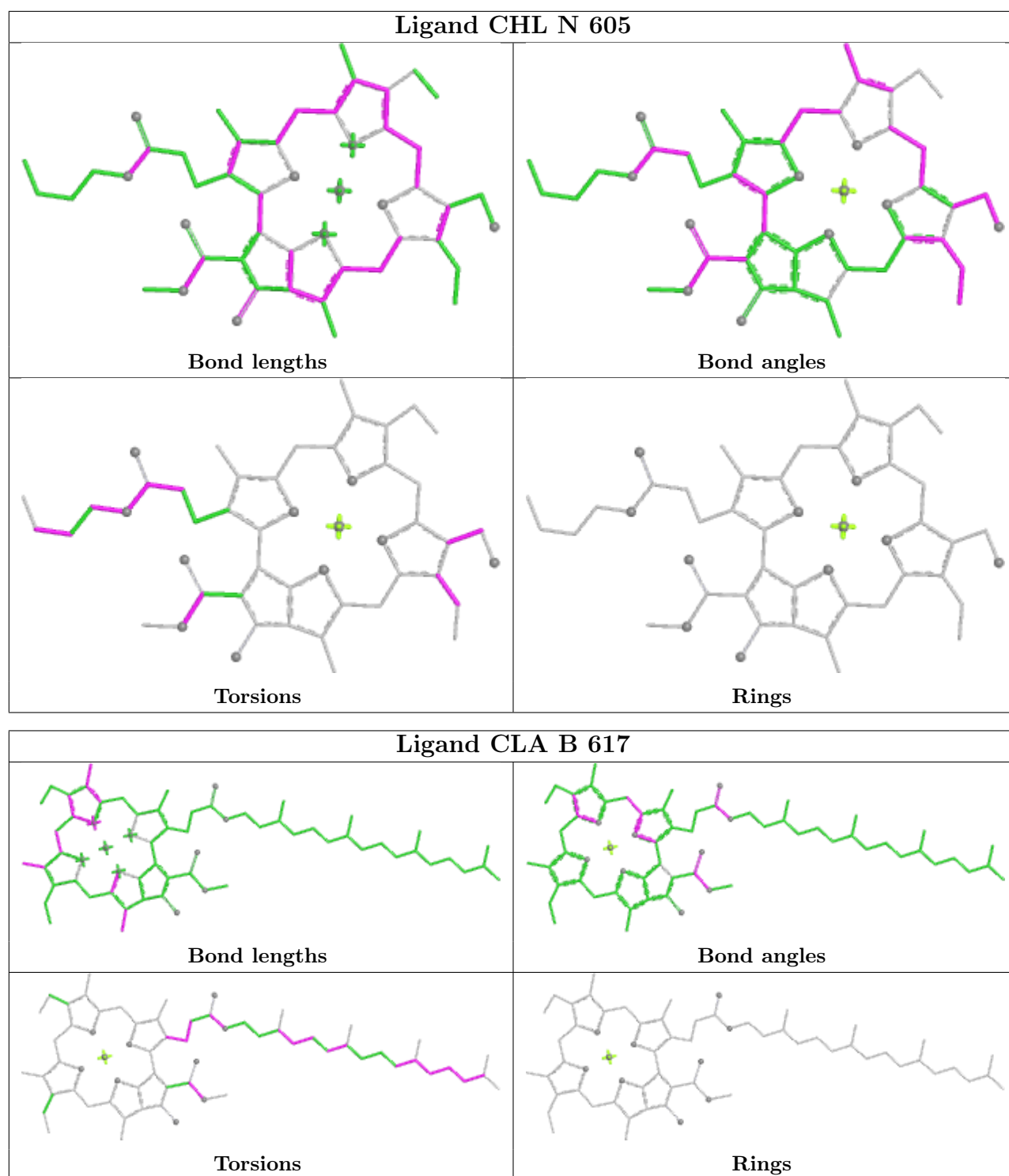




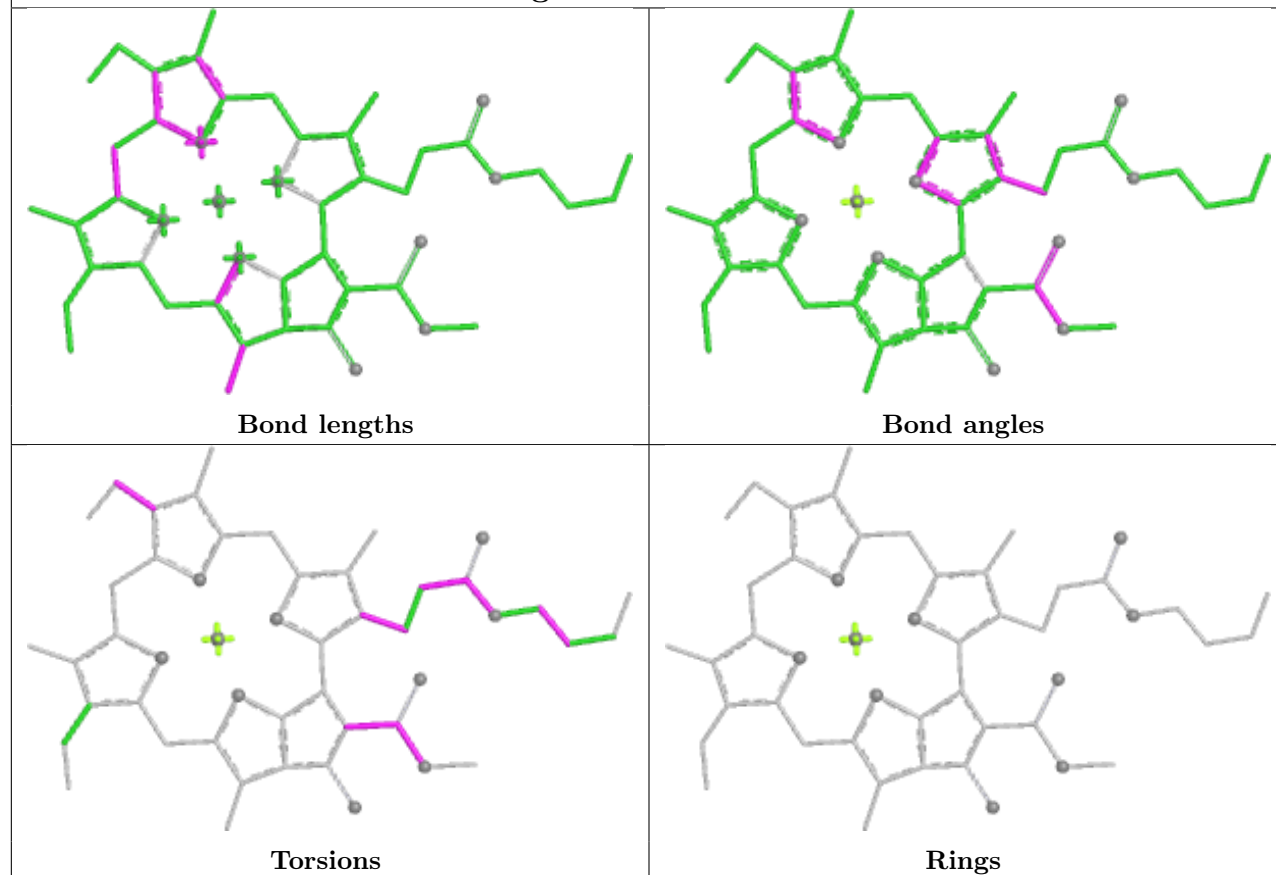




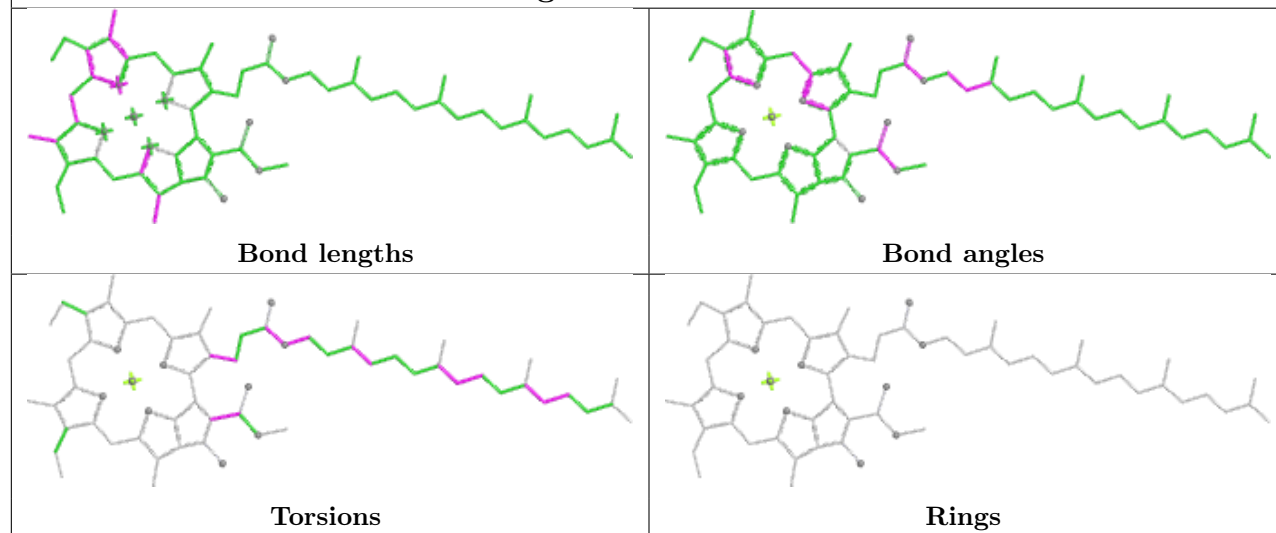


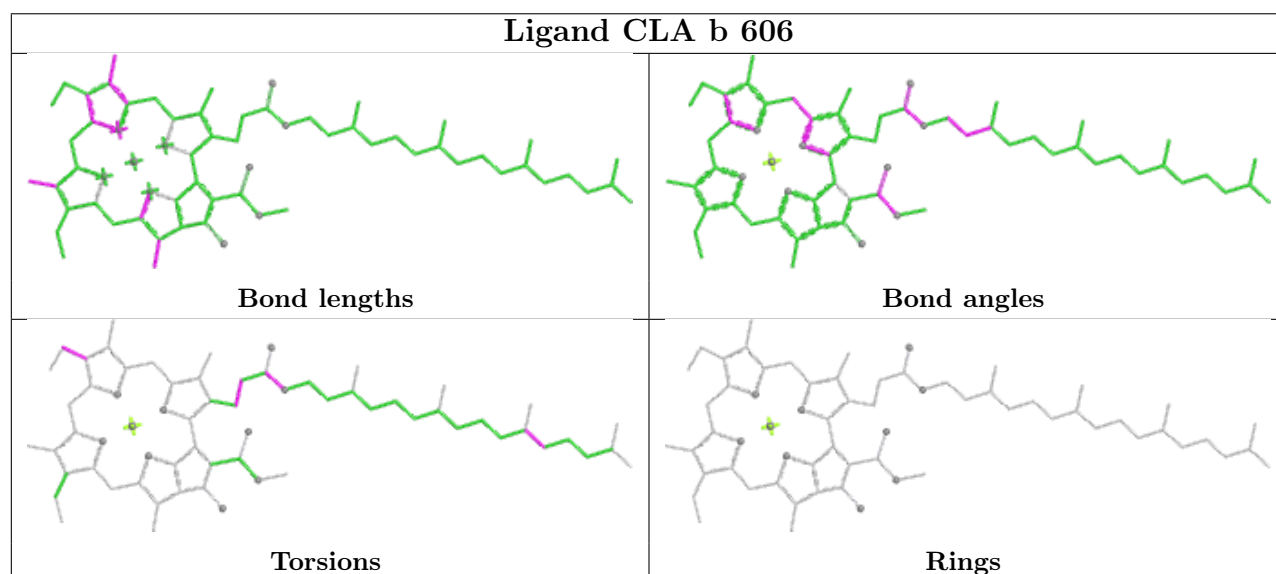
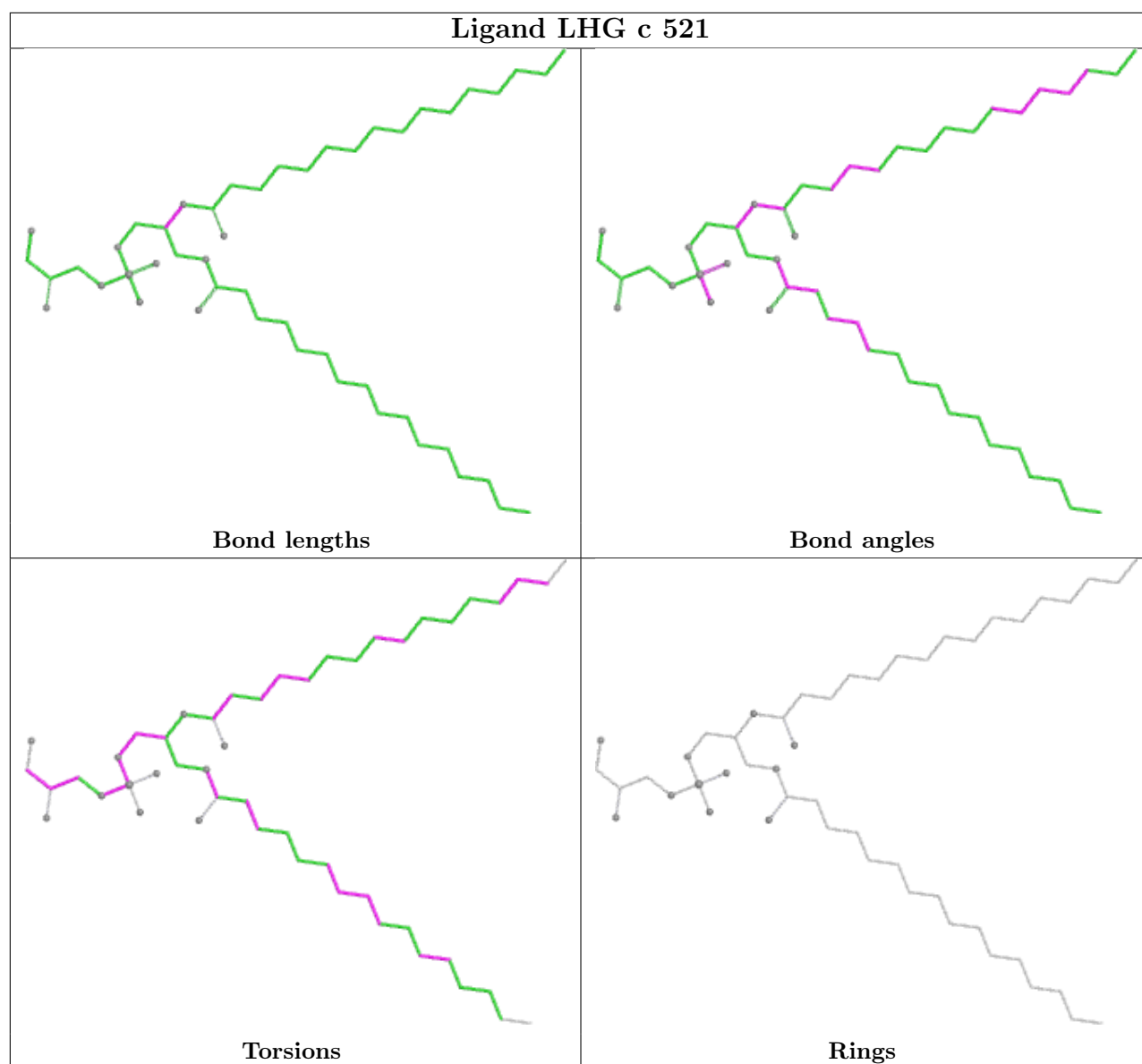


Ligand CLA R 310

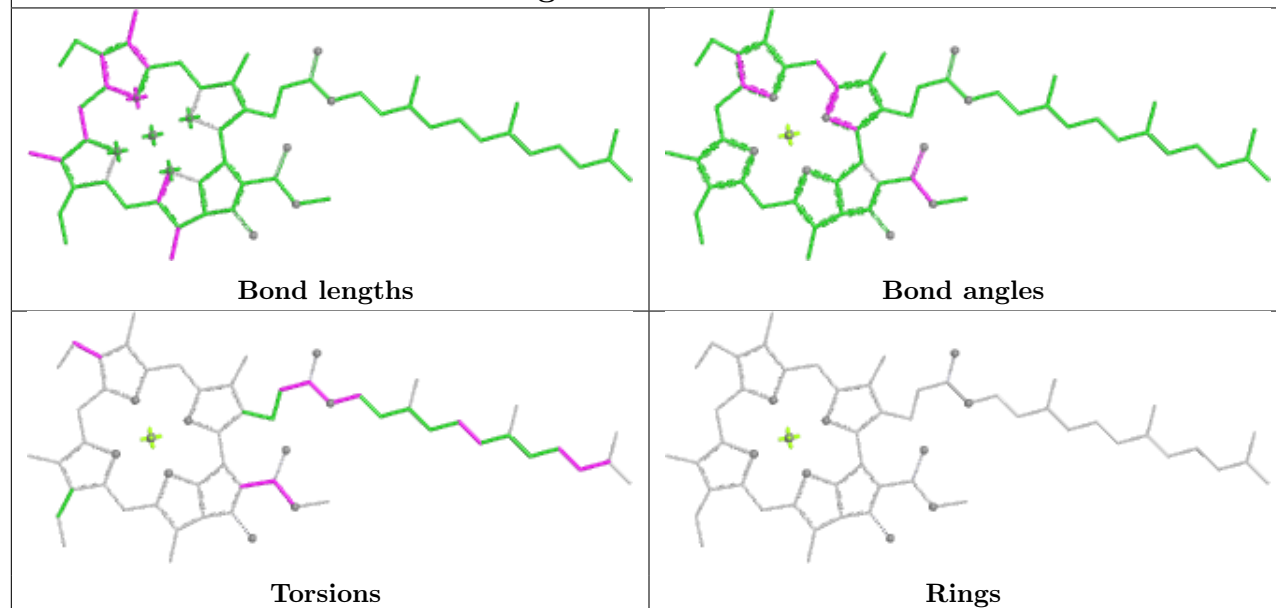


Ligand CLA c 514

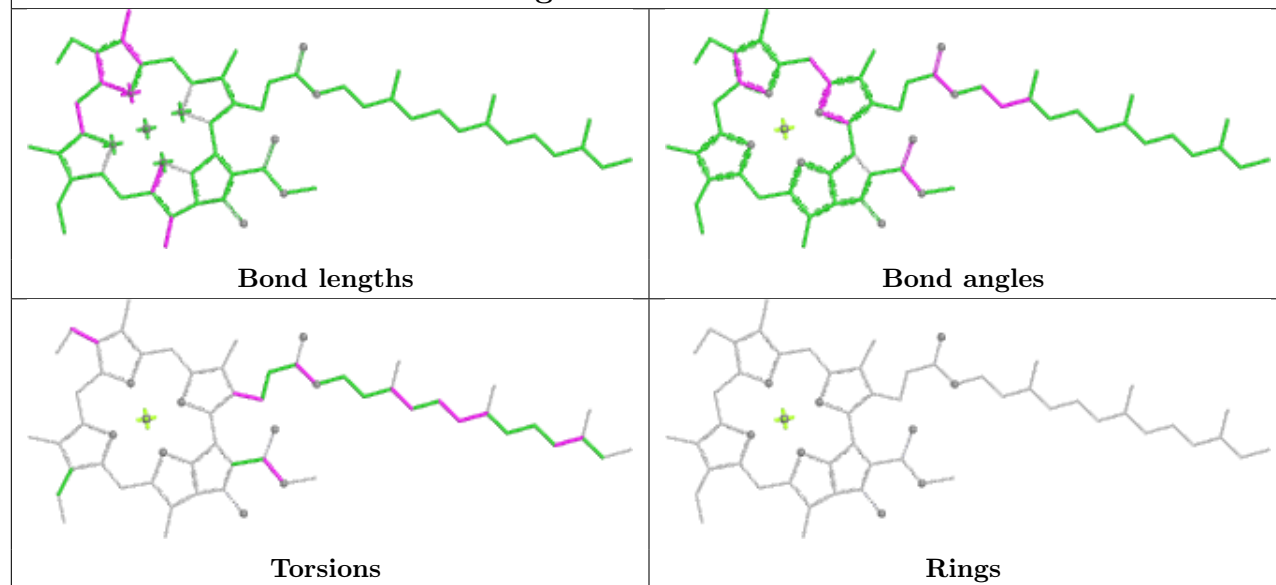


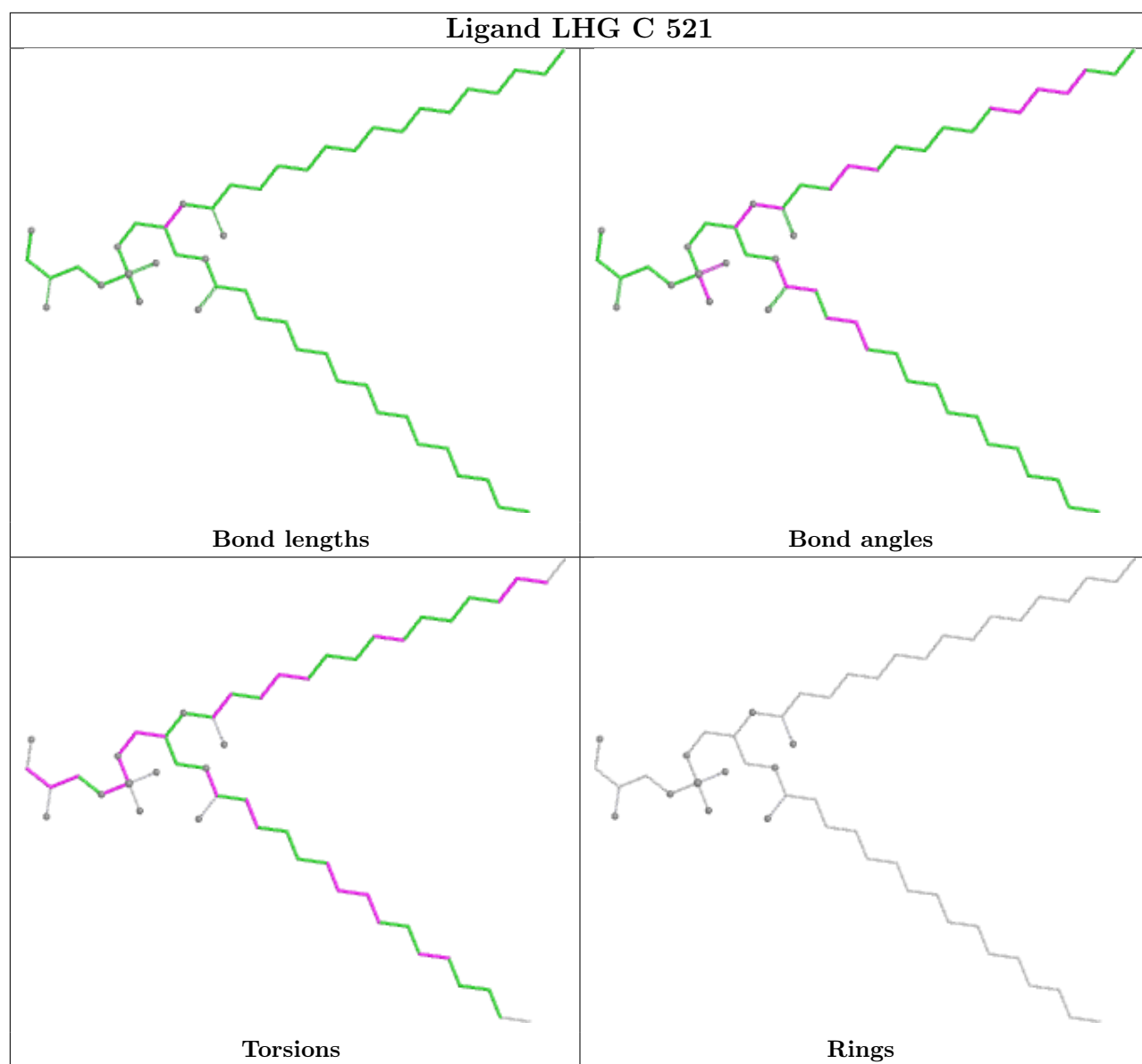


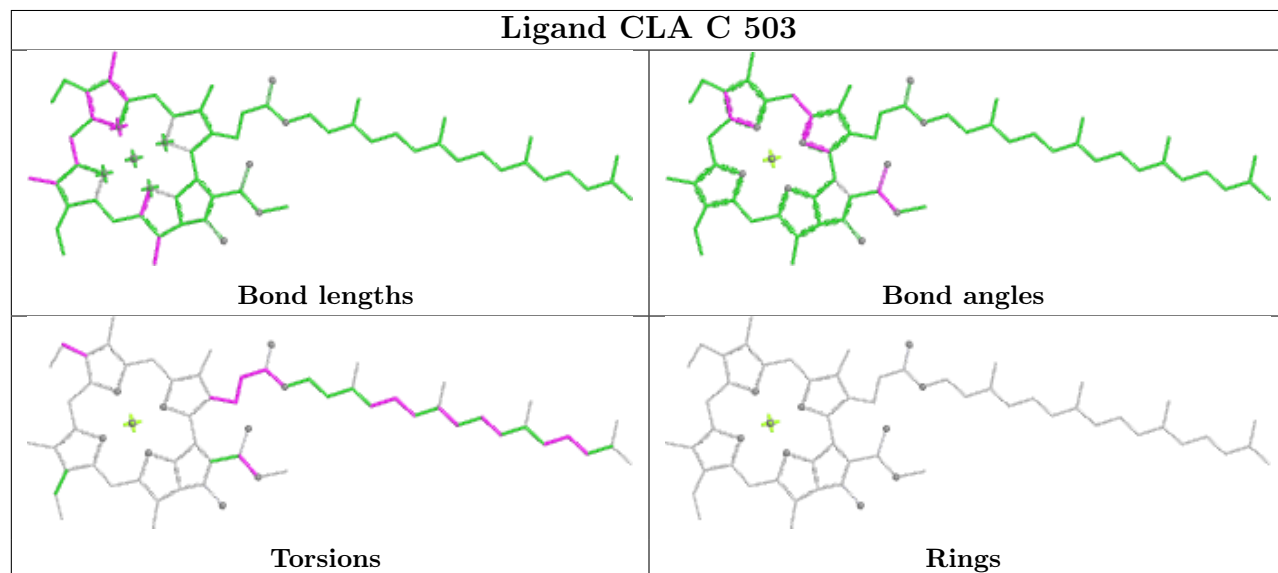
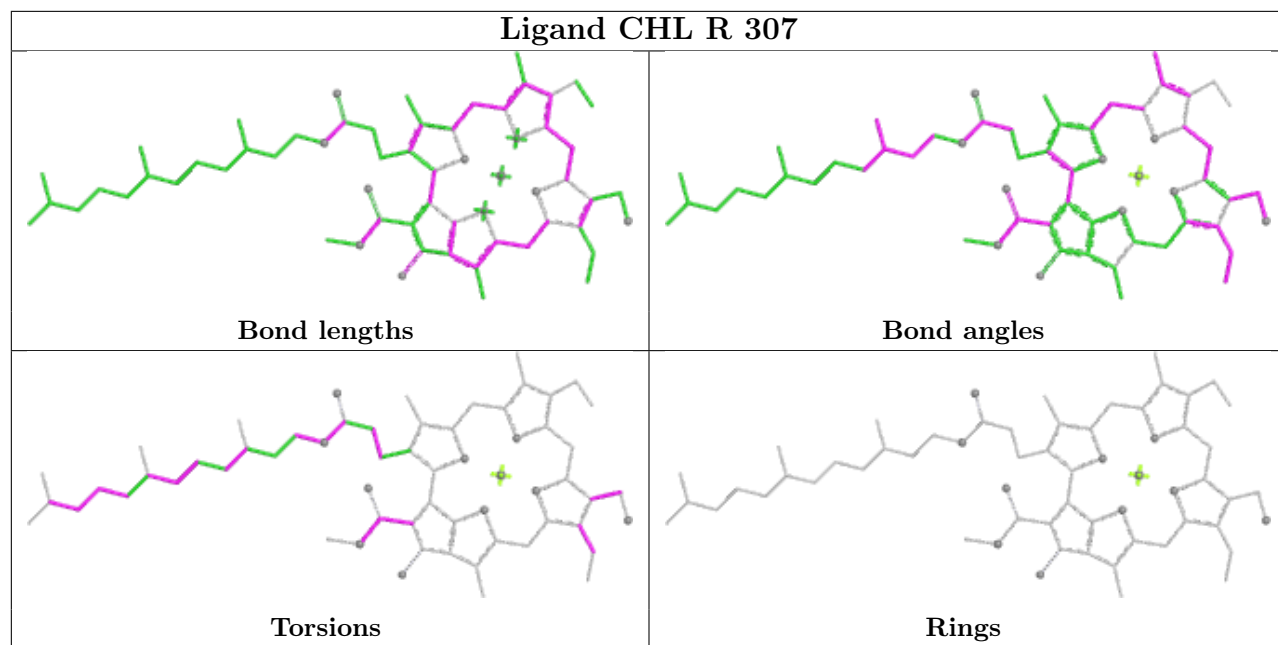
Ligand CLA r 312

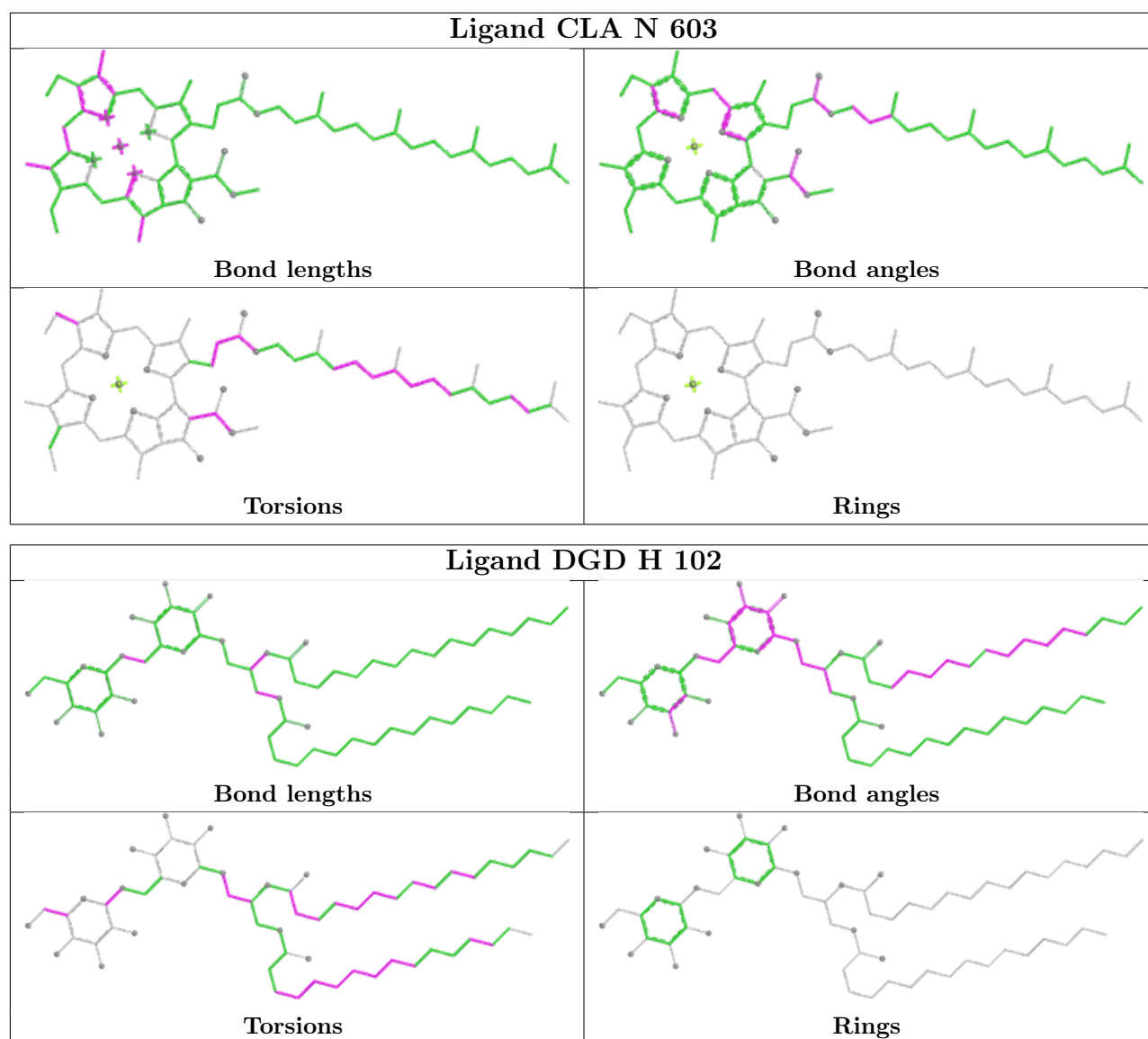


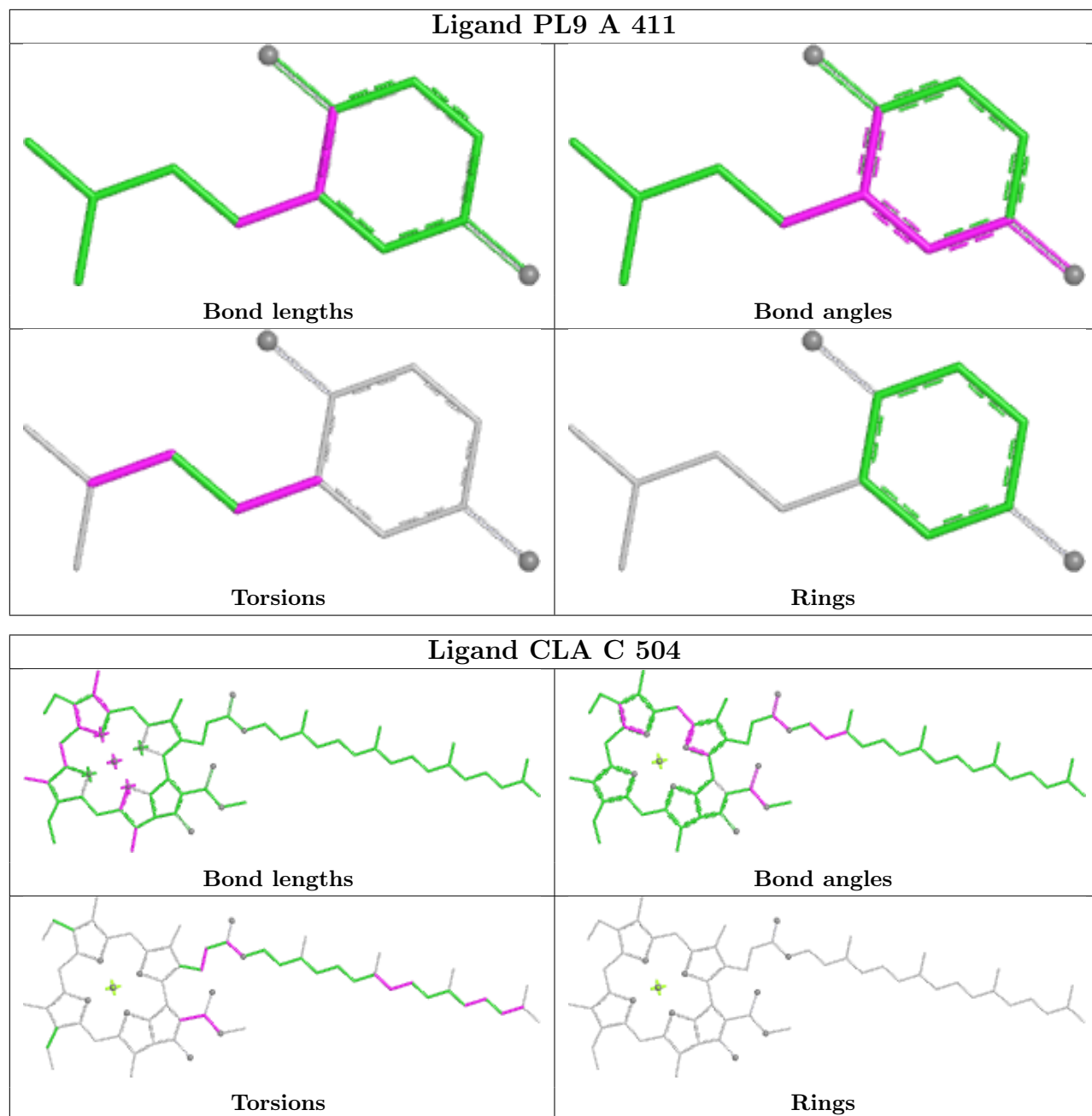
Ligand CLA S 303



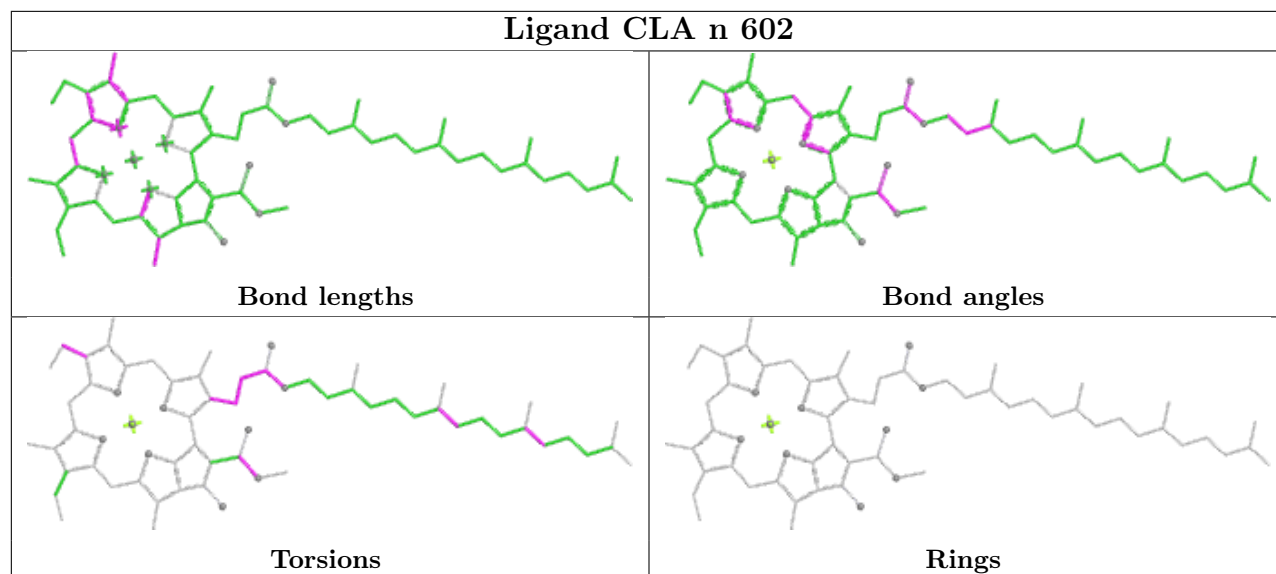




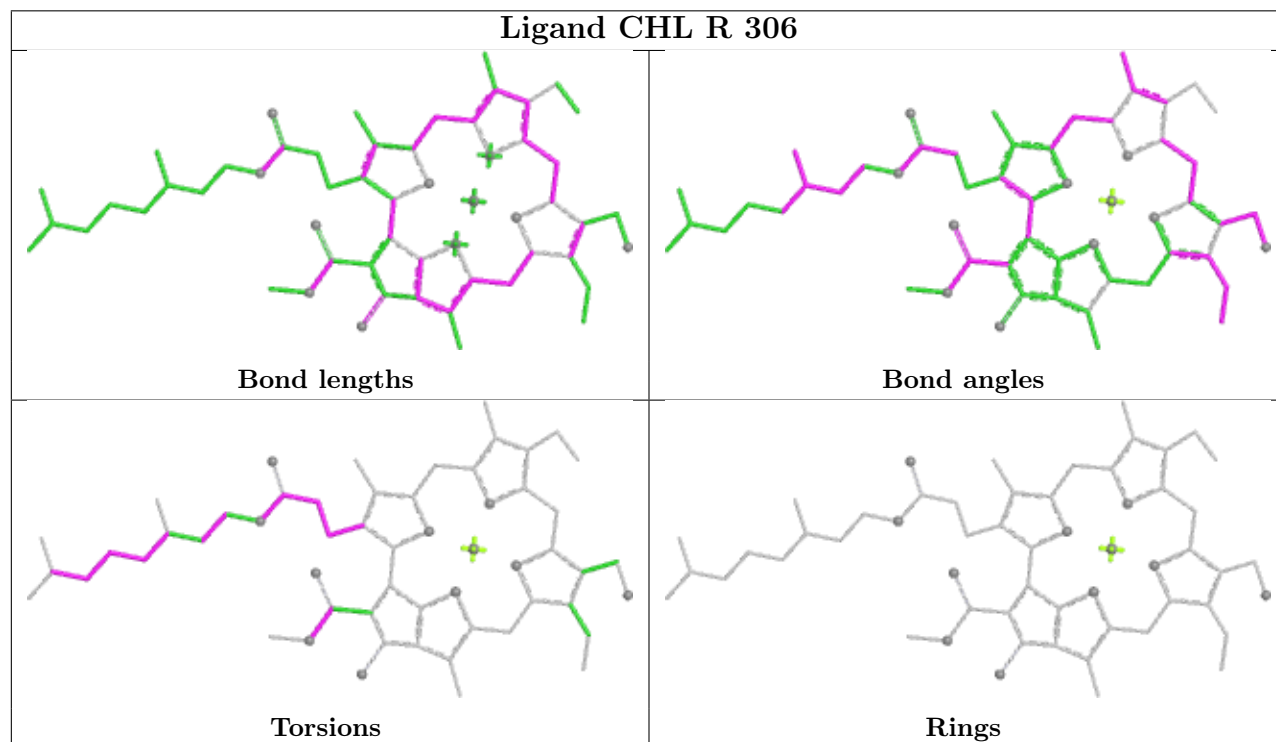




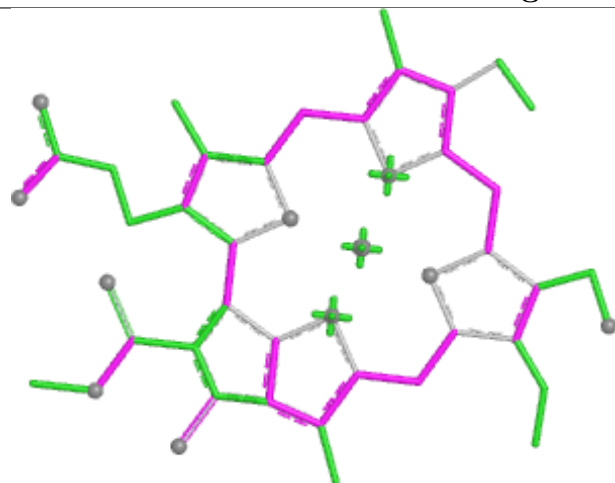
Ligand CLA n 602



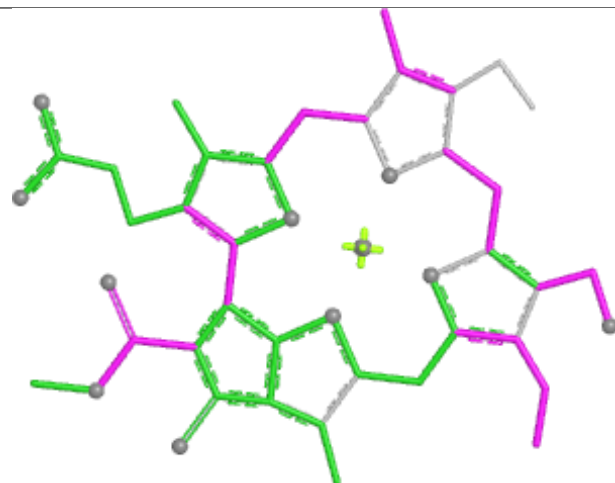
Ligand CHL R 306



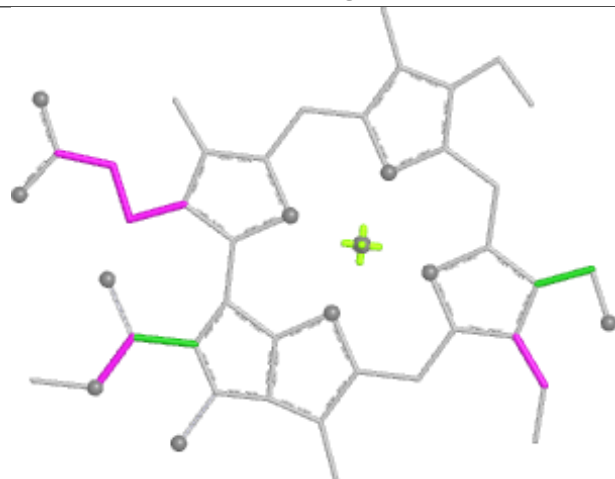
Ligand CHL s 302



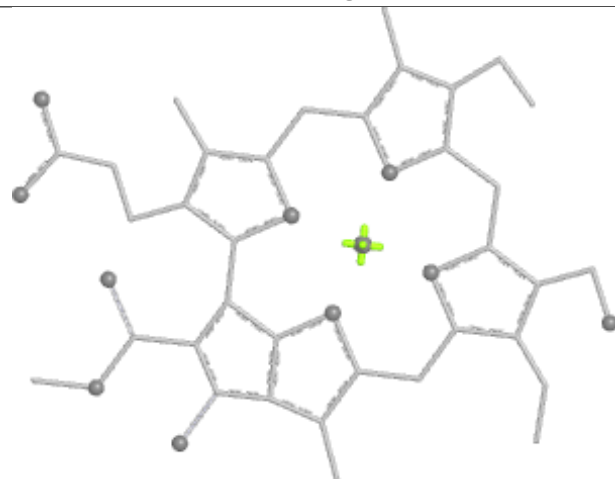
Bond lengths



Bond angles

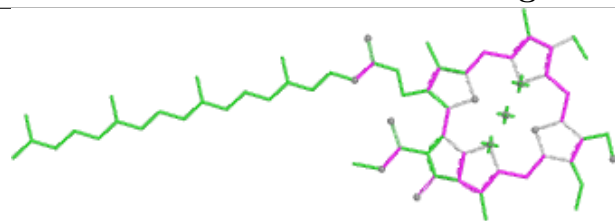


Torsions

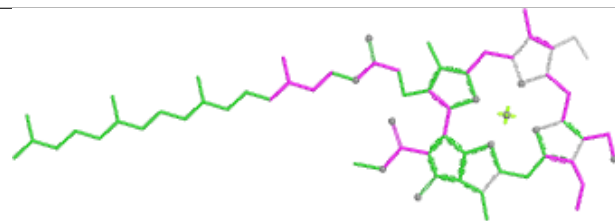


Rings

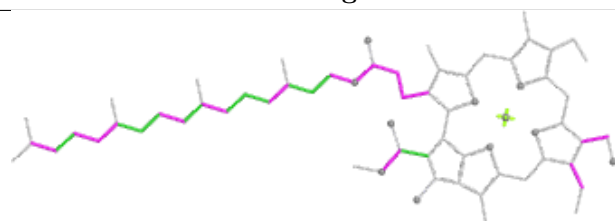
Ligand CHL n 601



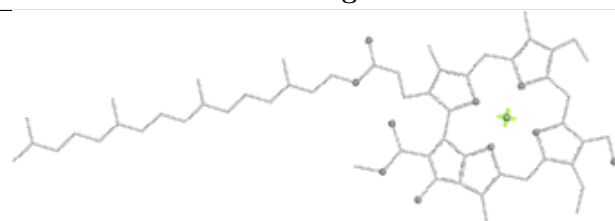
Bond lengths



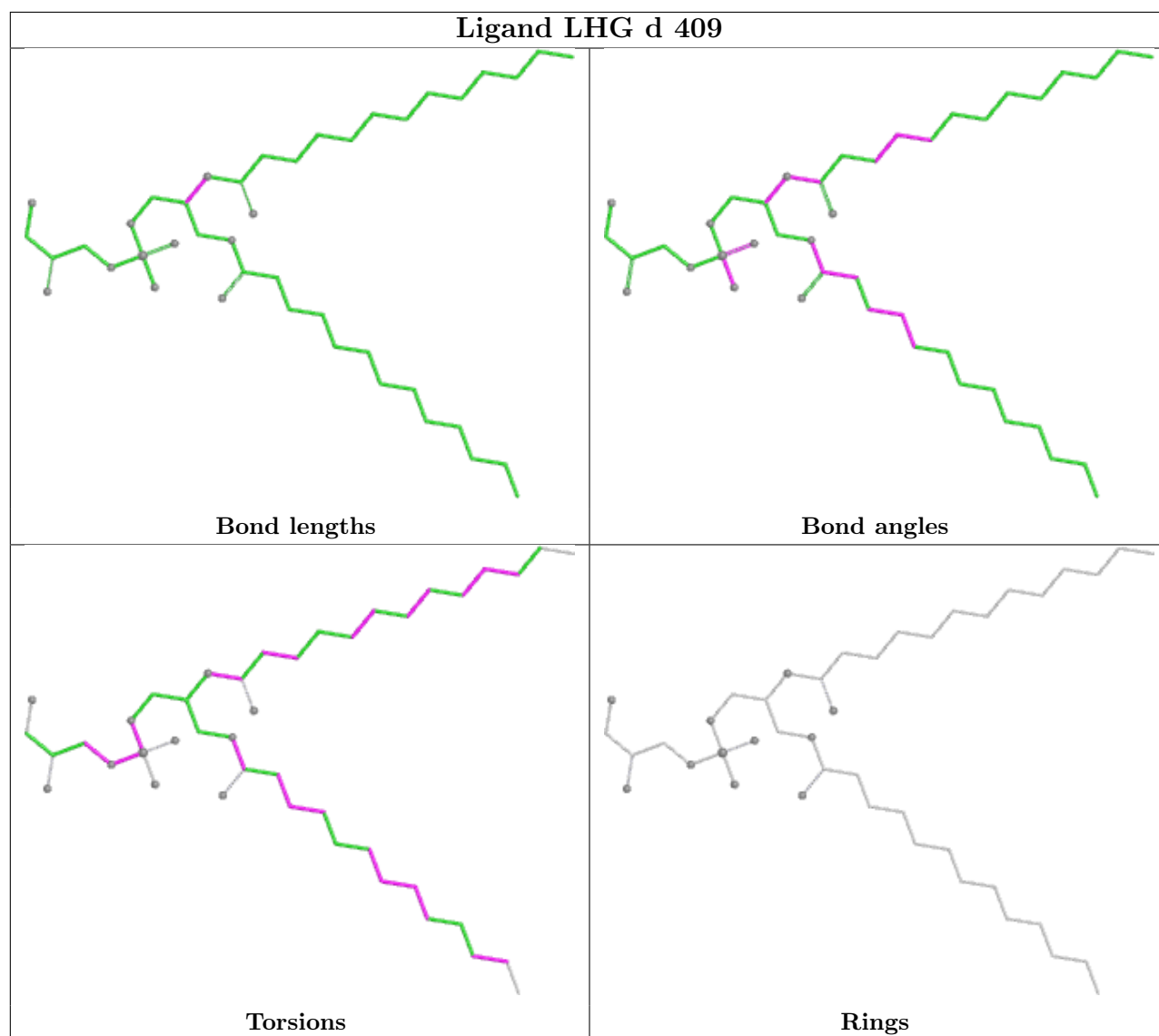
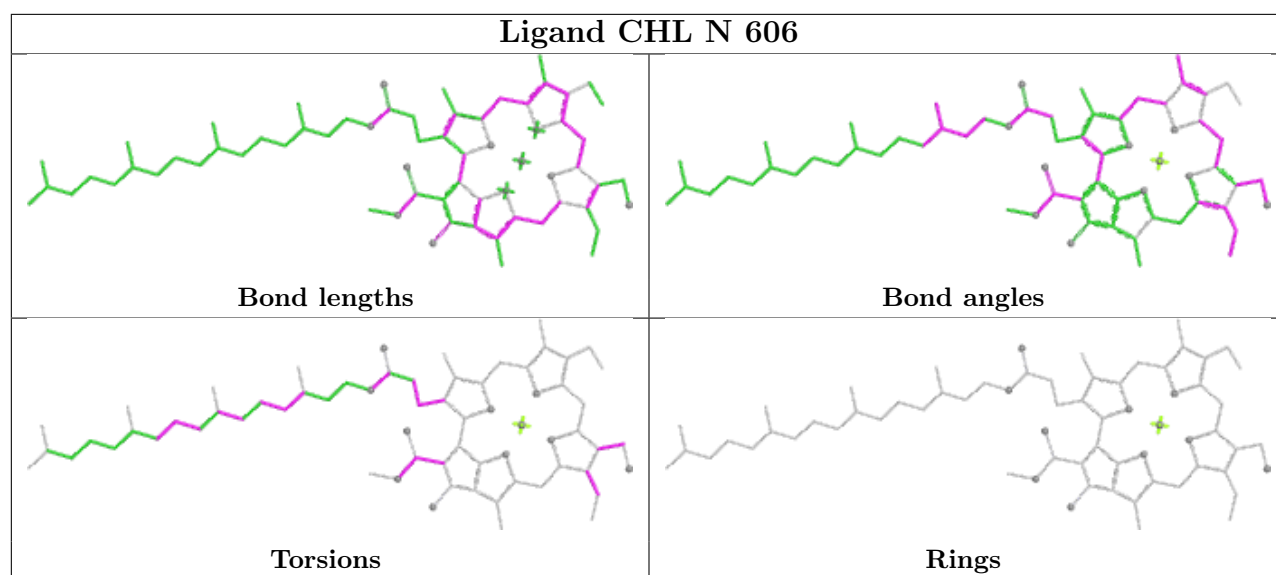
Bond angles

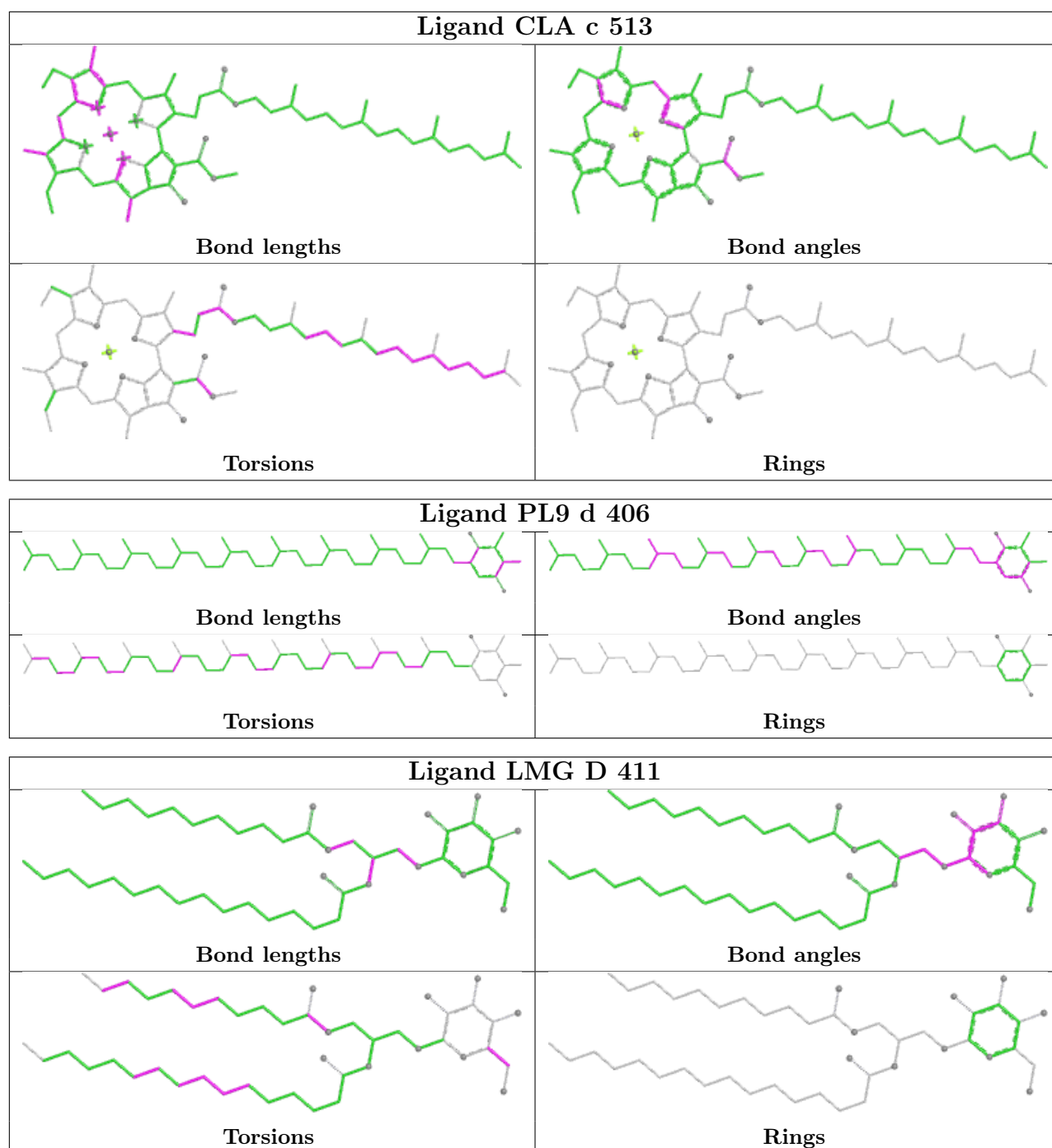


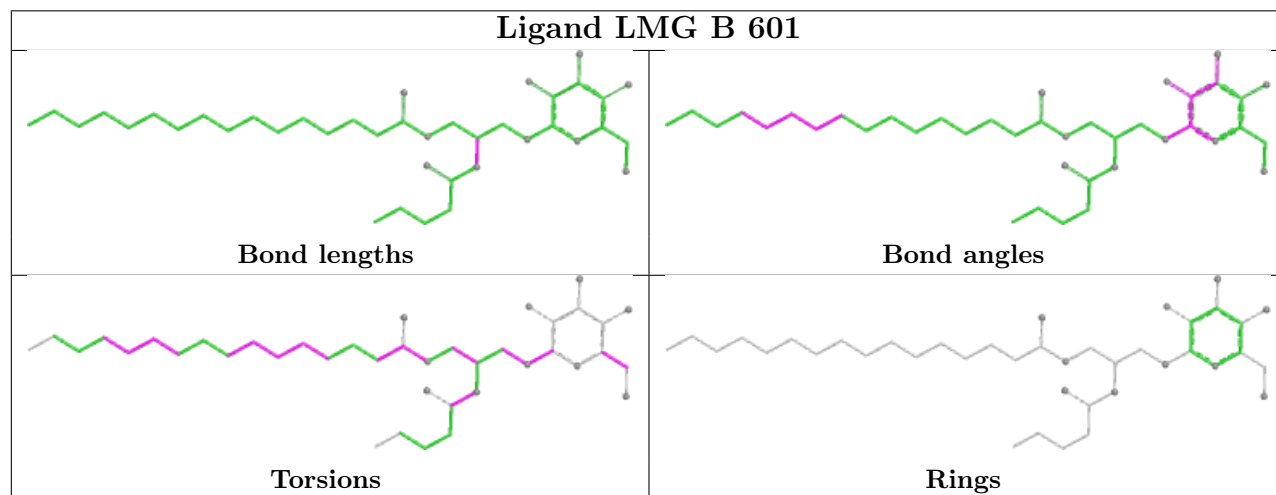
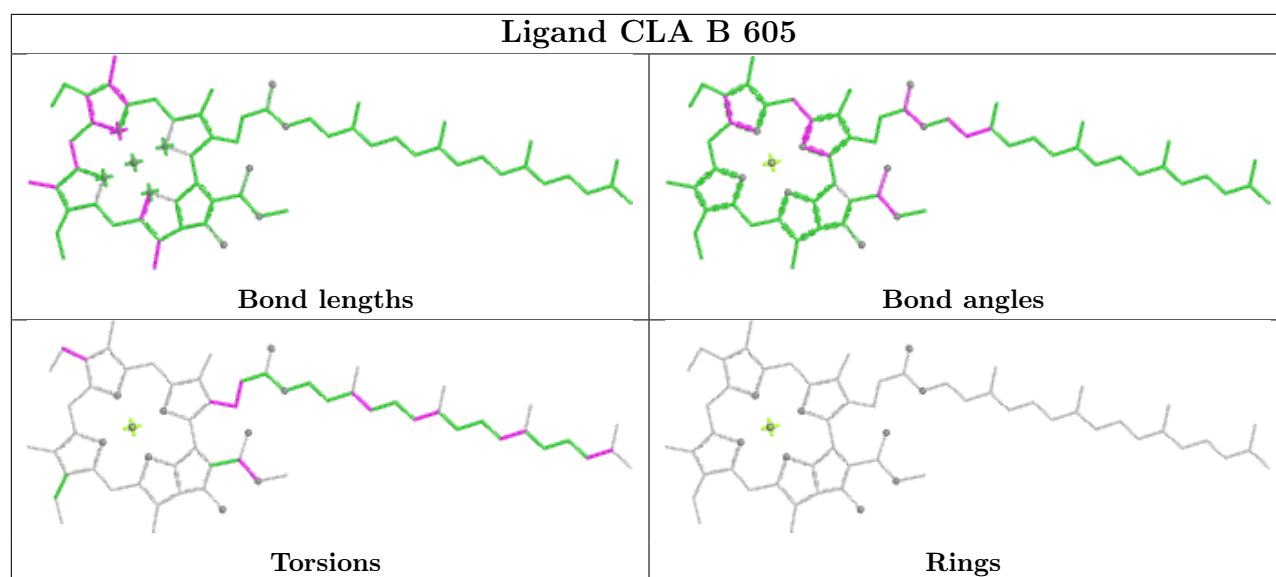
Torsions

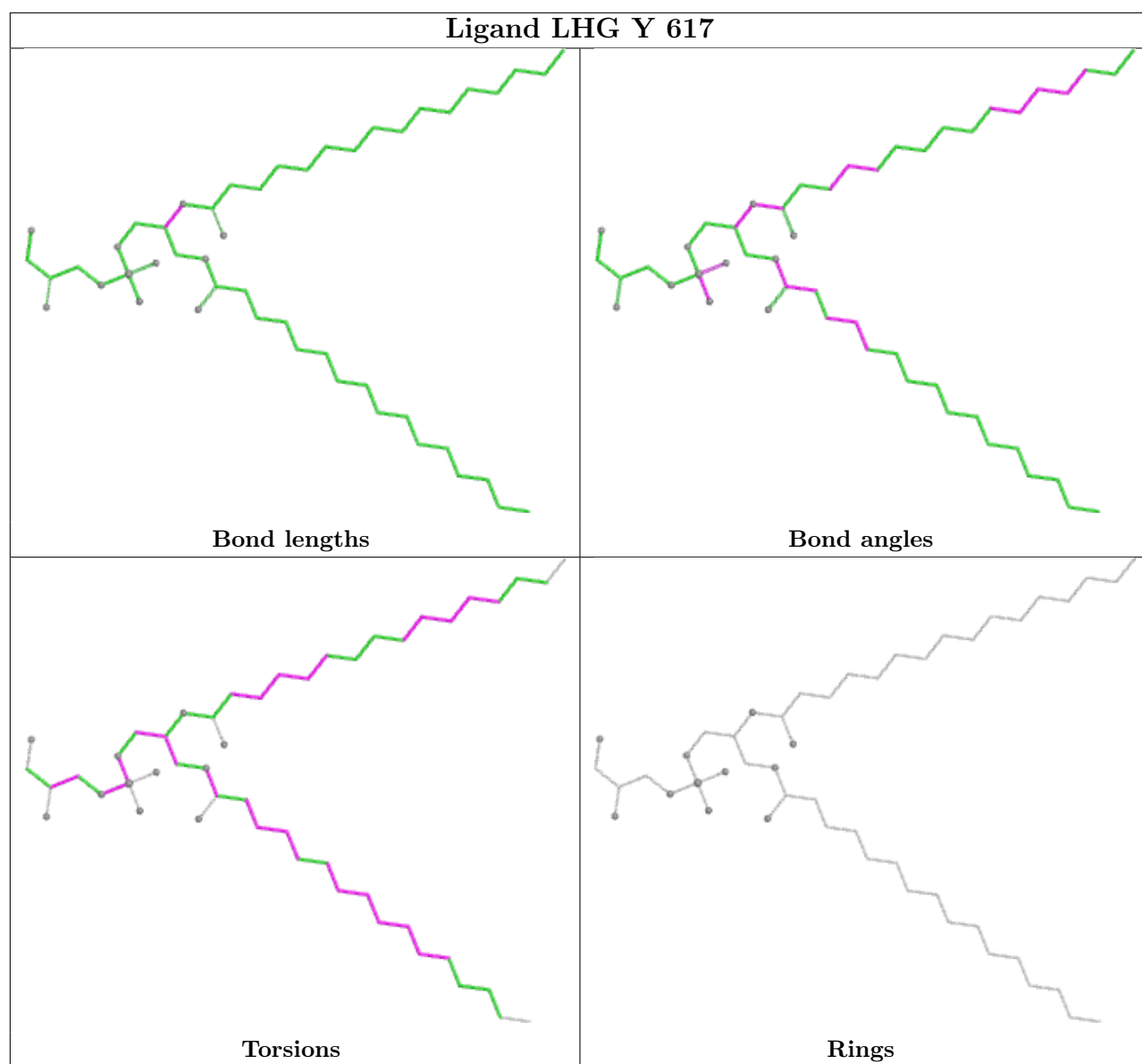


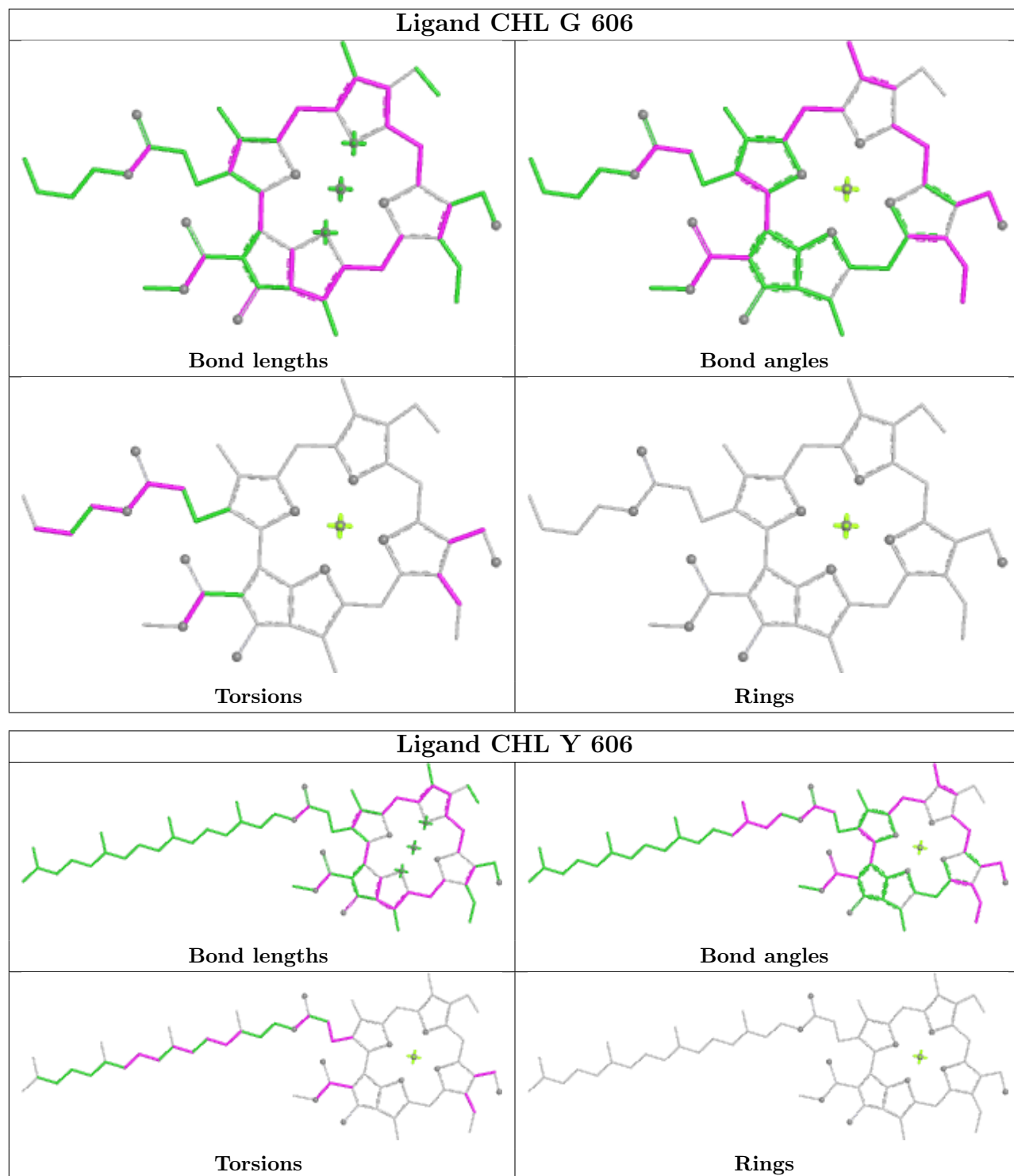
Rings



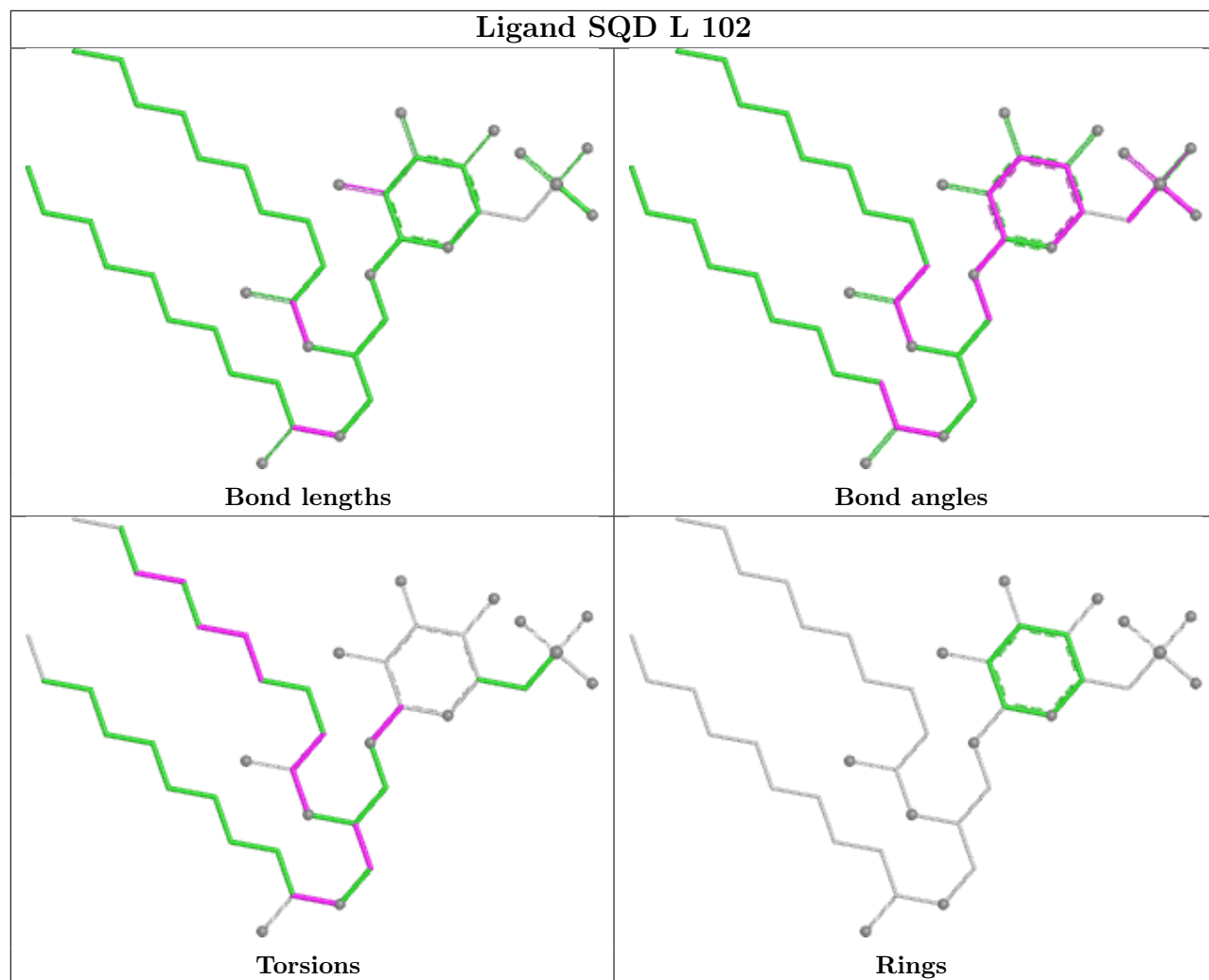




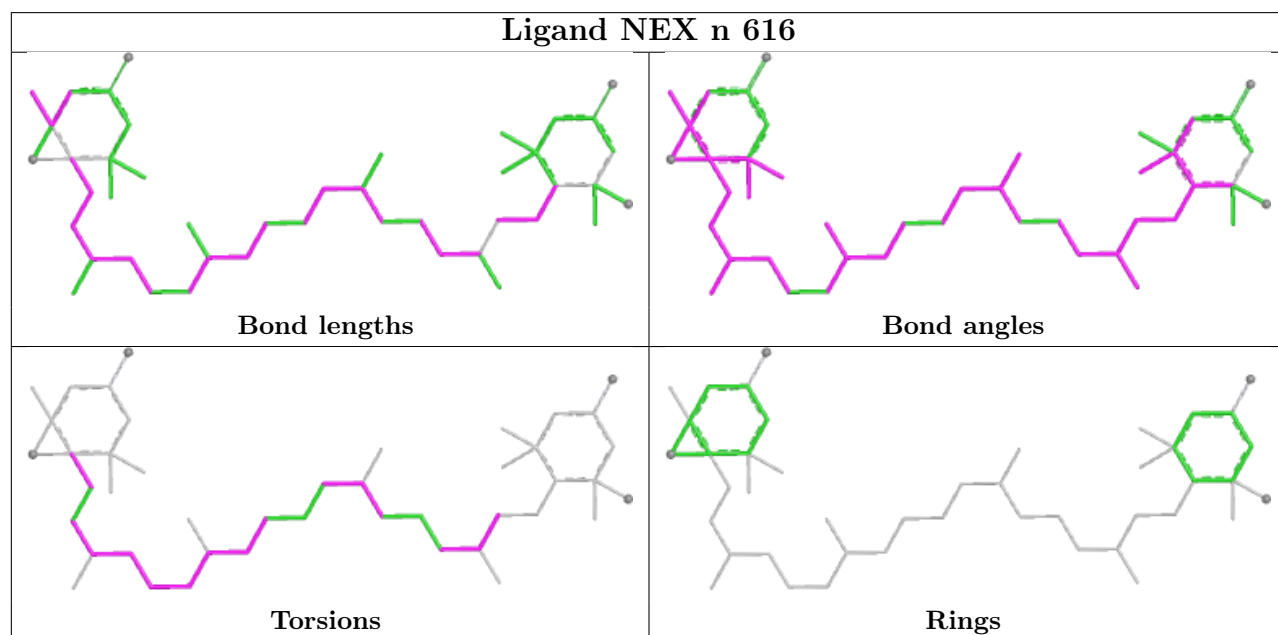




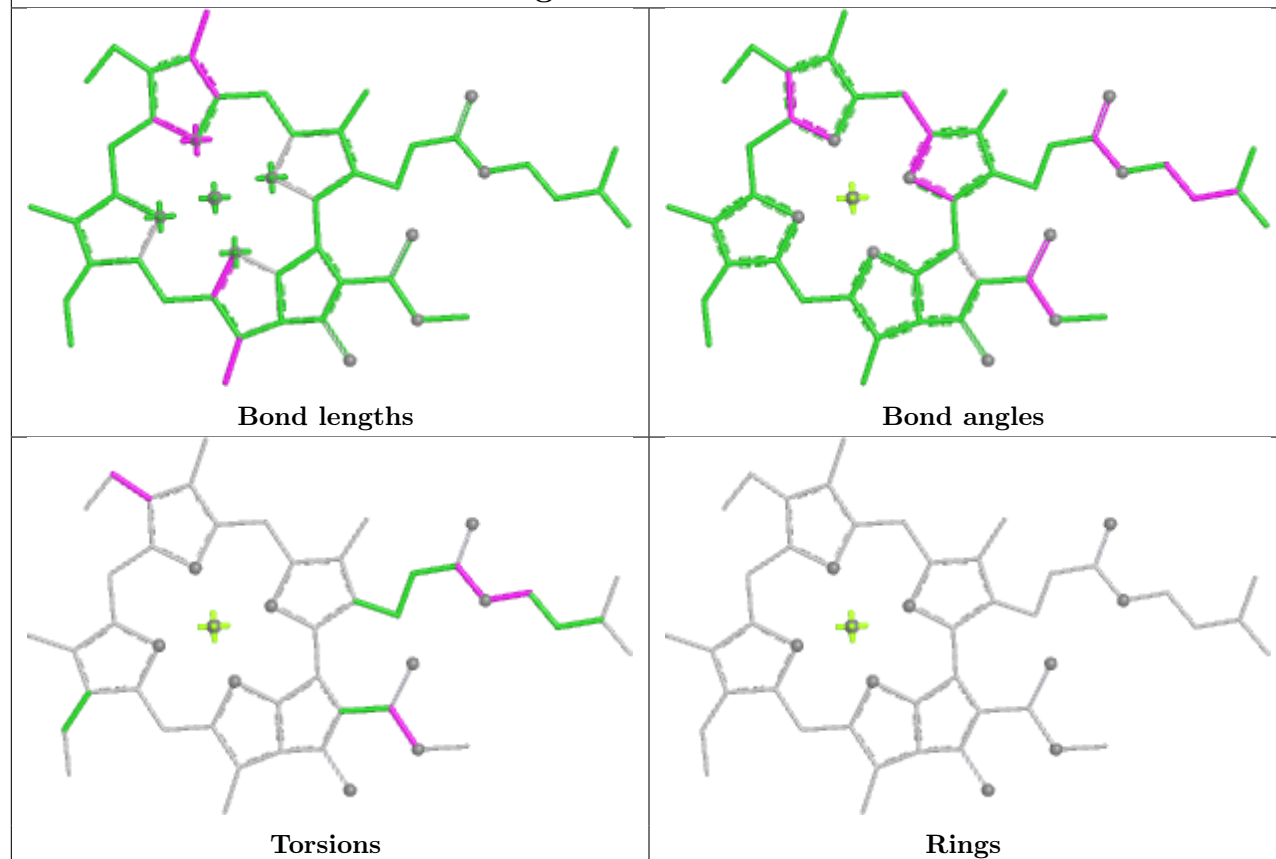
Ligand SQD L 102



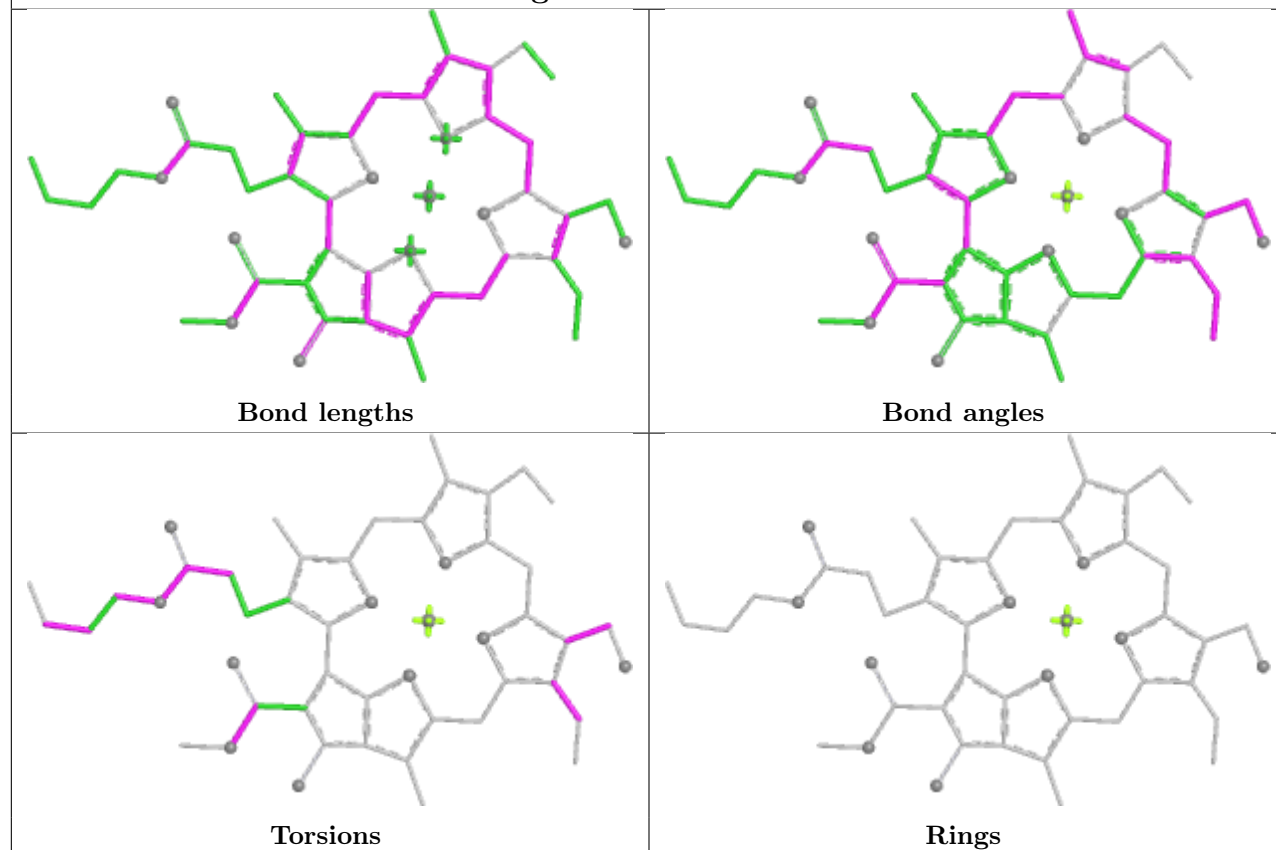
Ligand NEX n 616

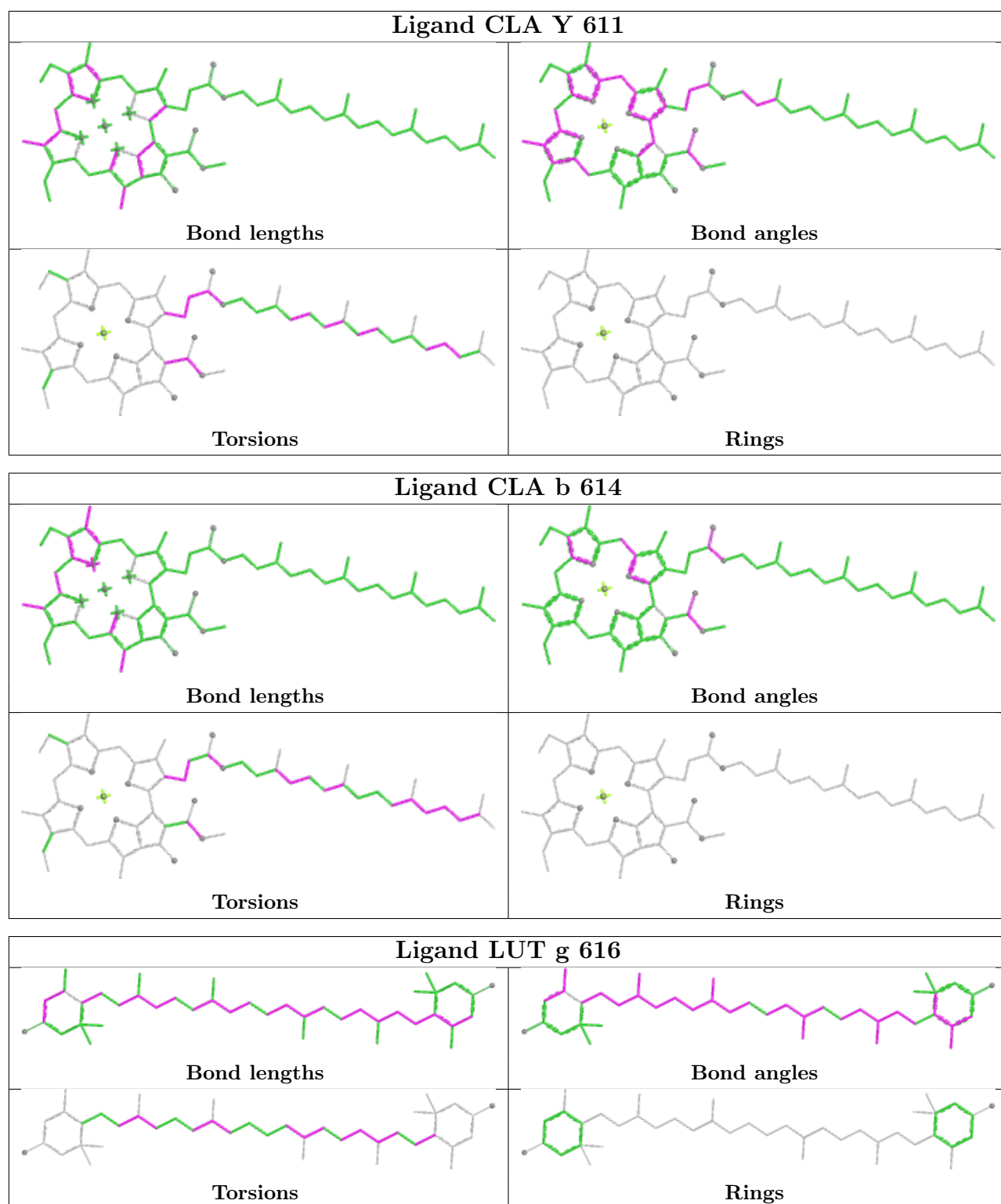


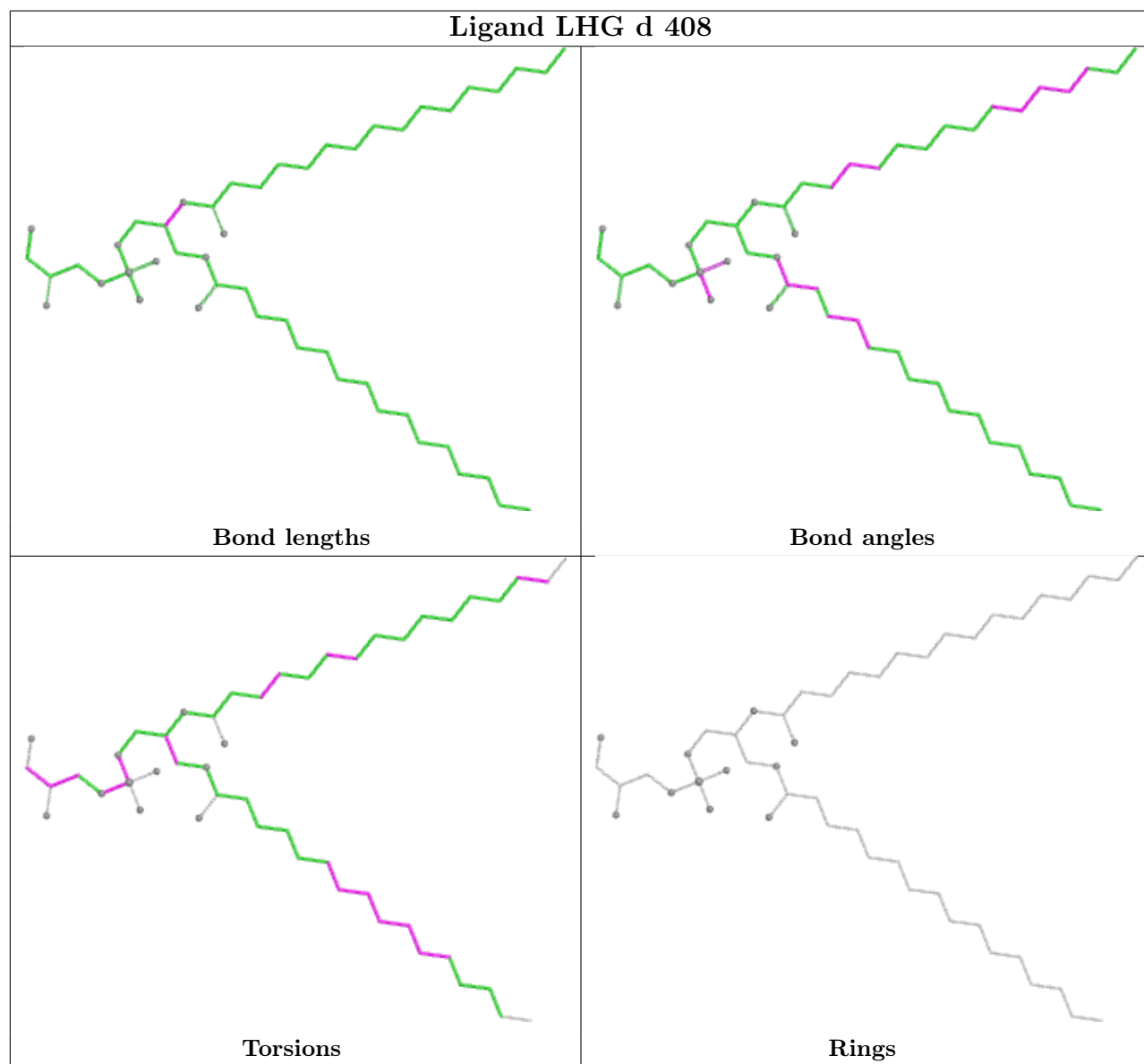
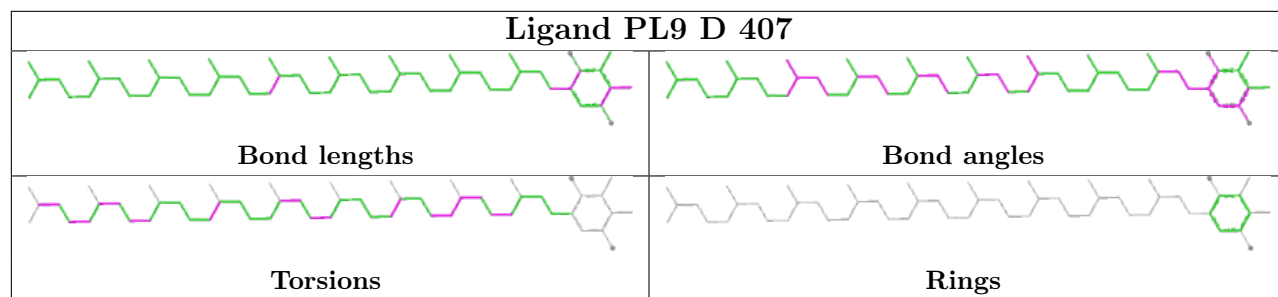
Ligand CLA n 604



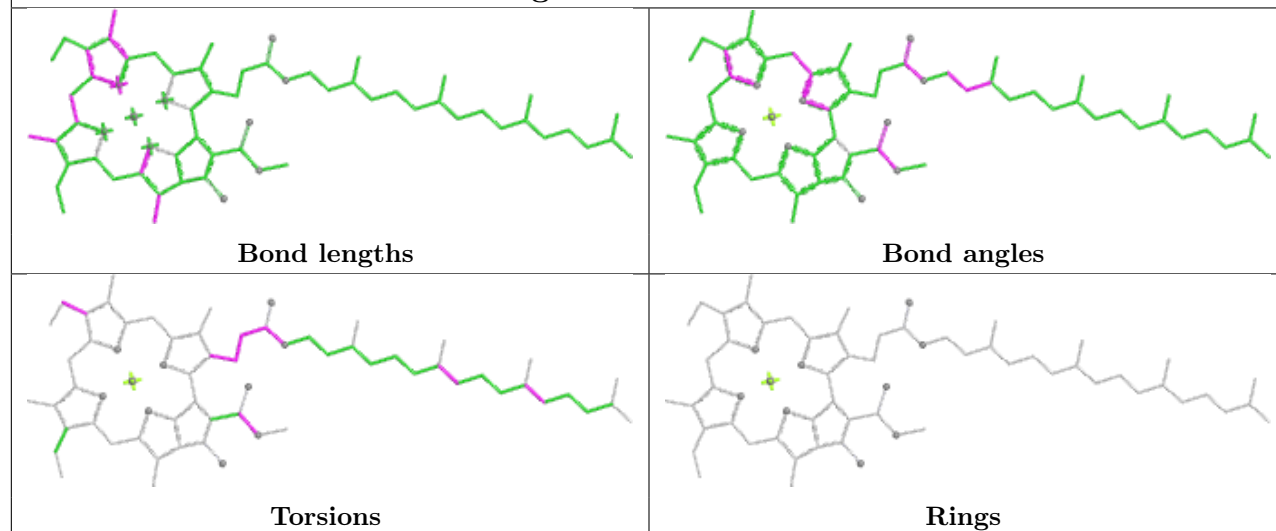
Ligand CHL Y 605



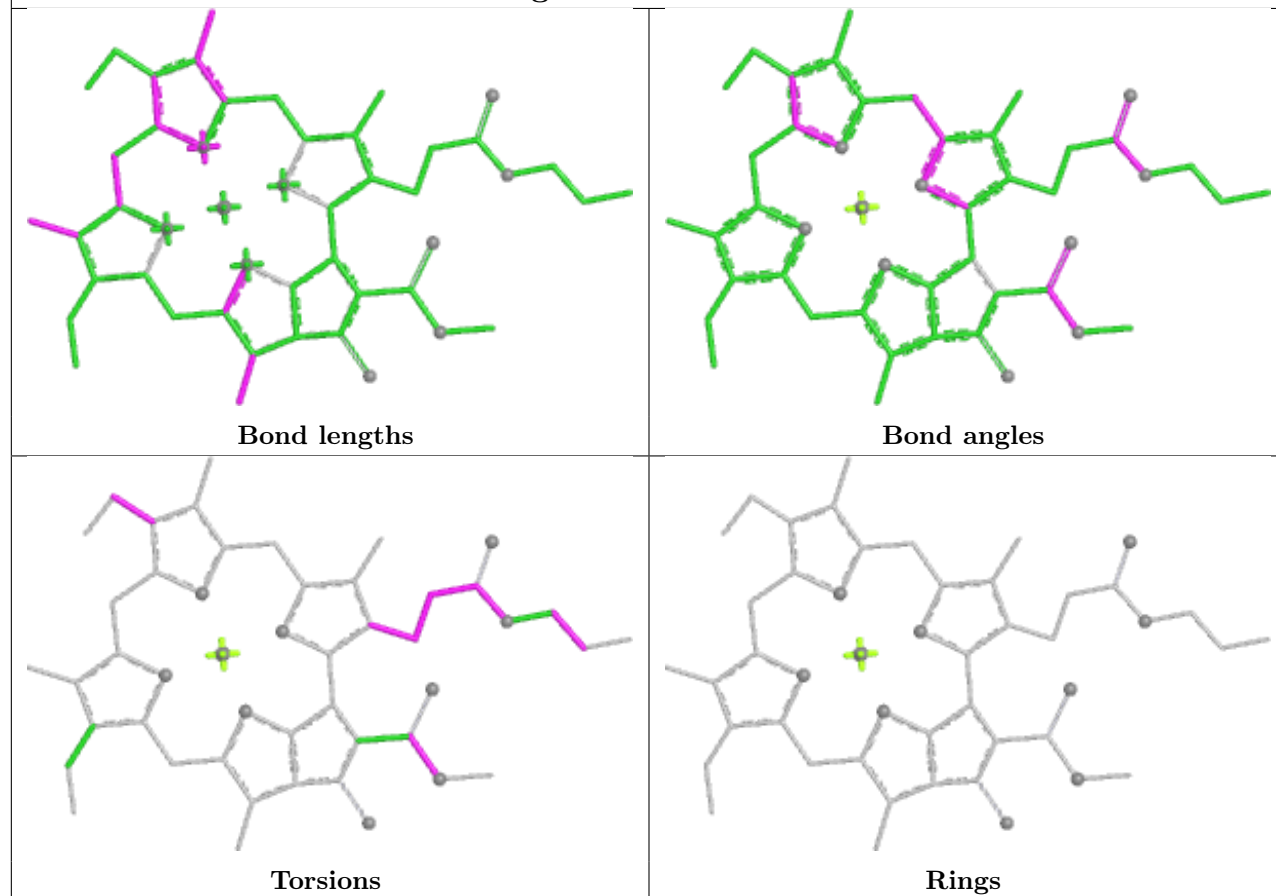


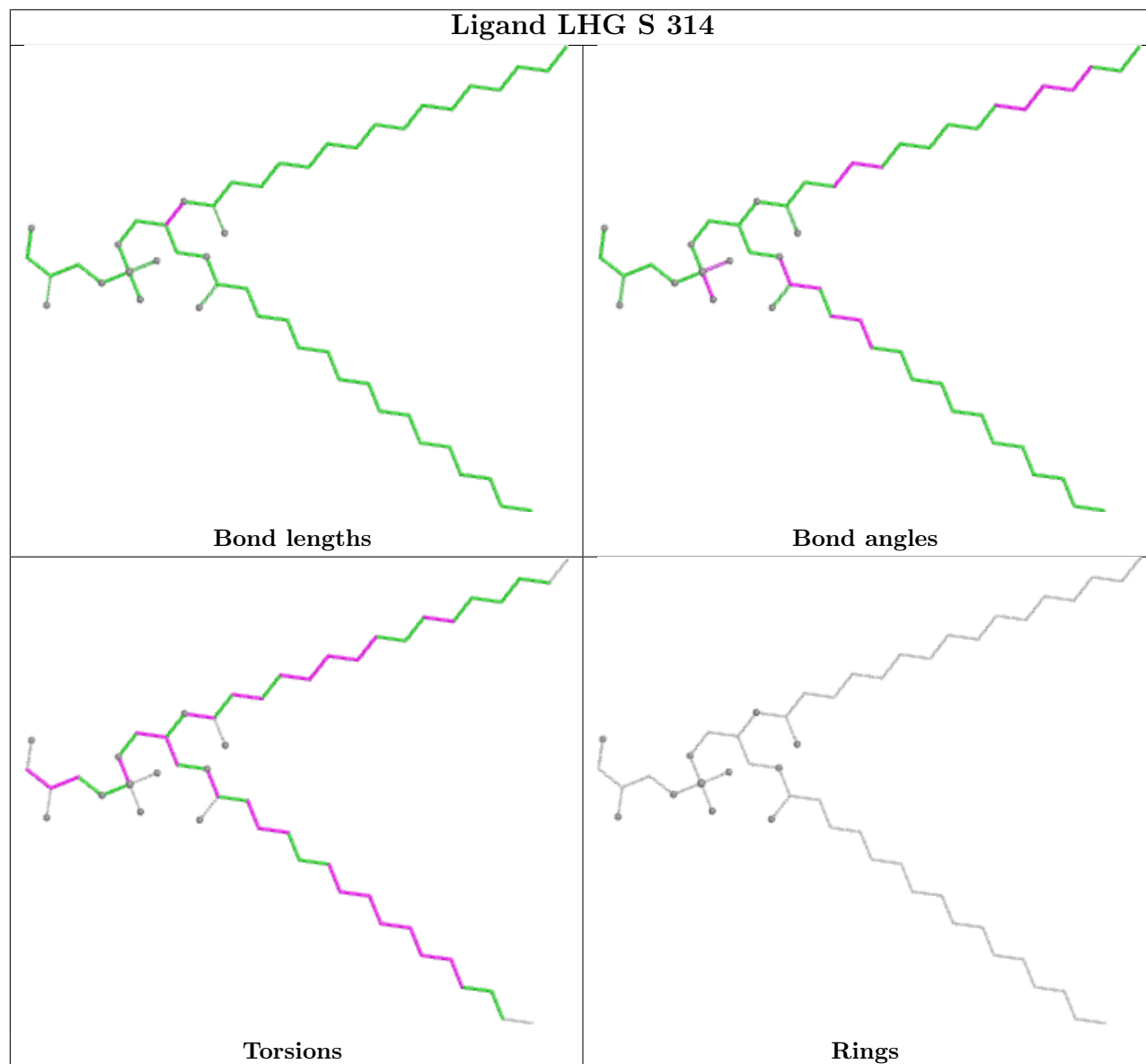
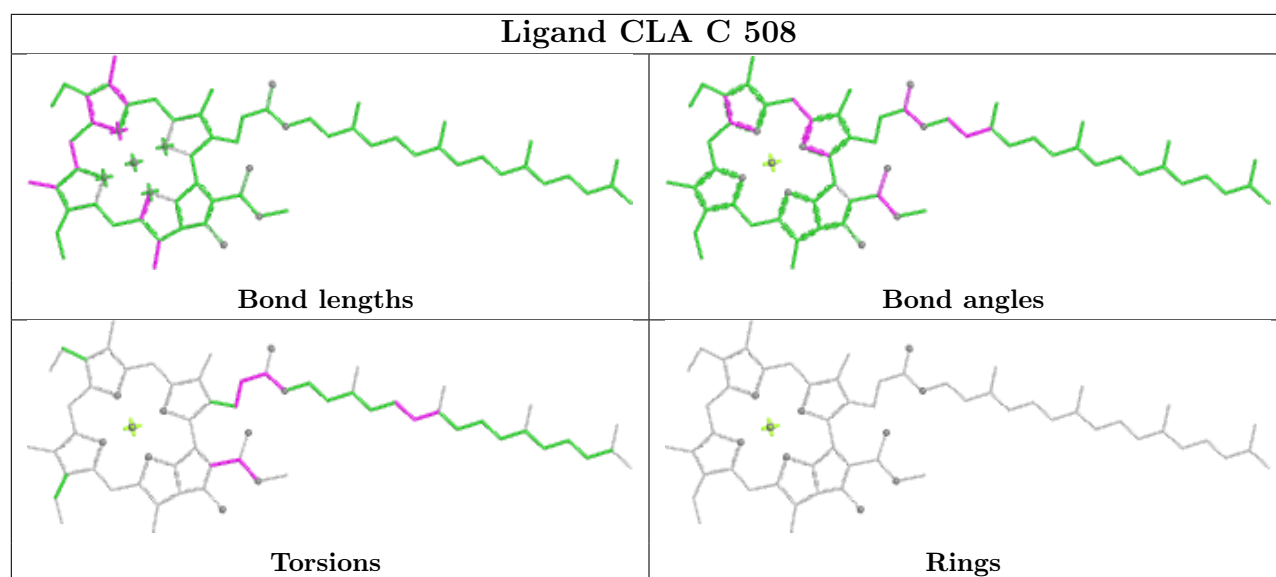


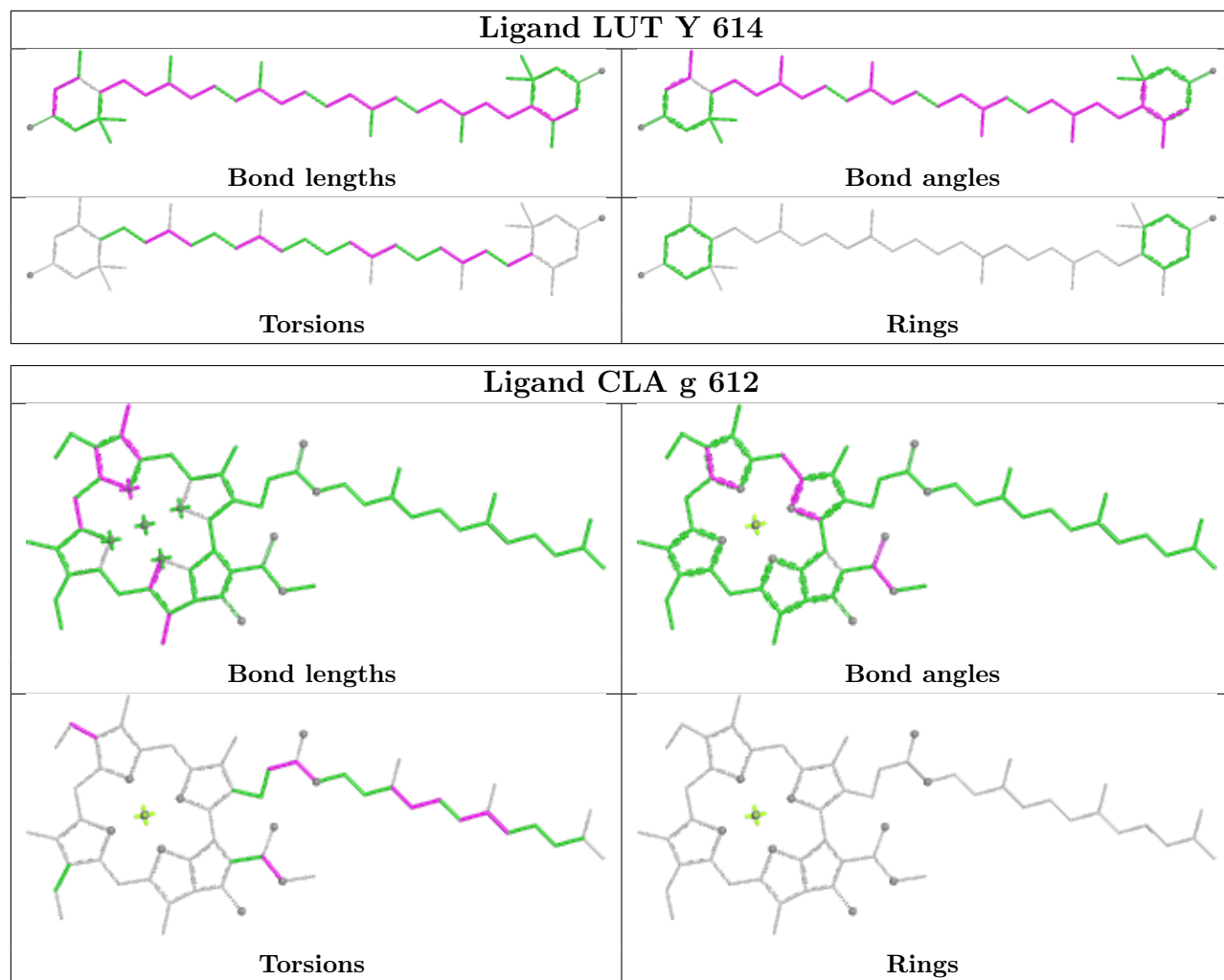
Ligand CLA Y 602

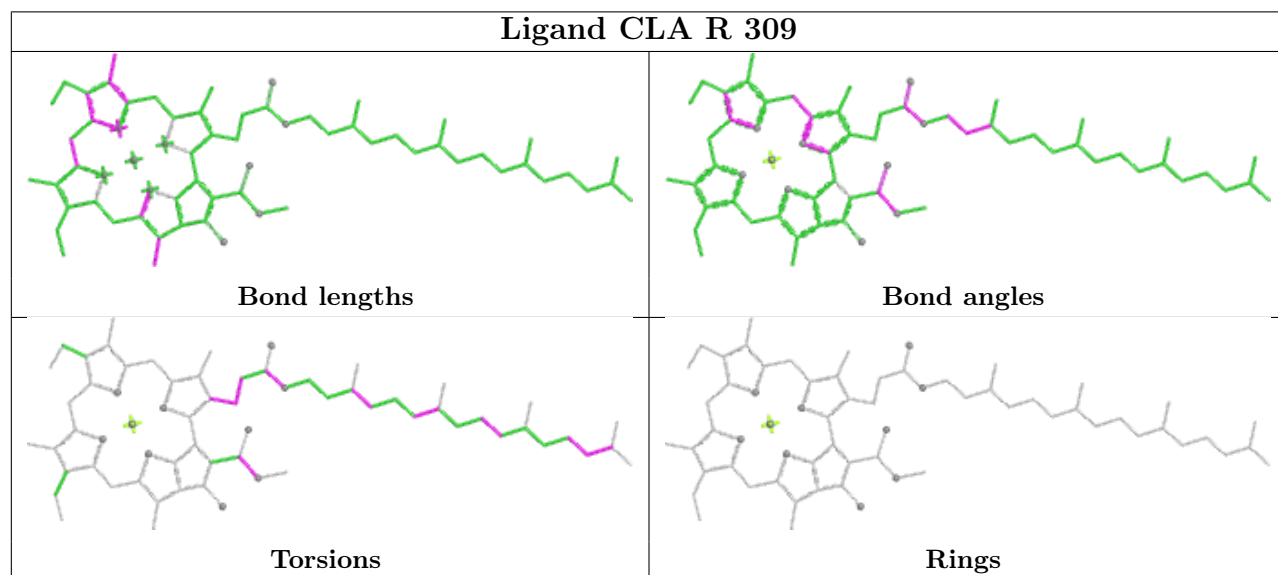
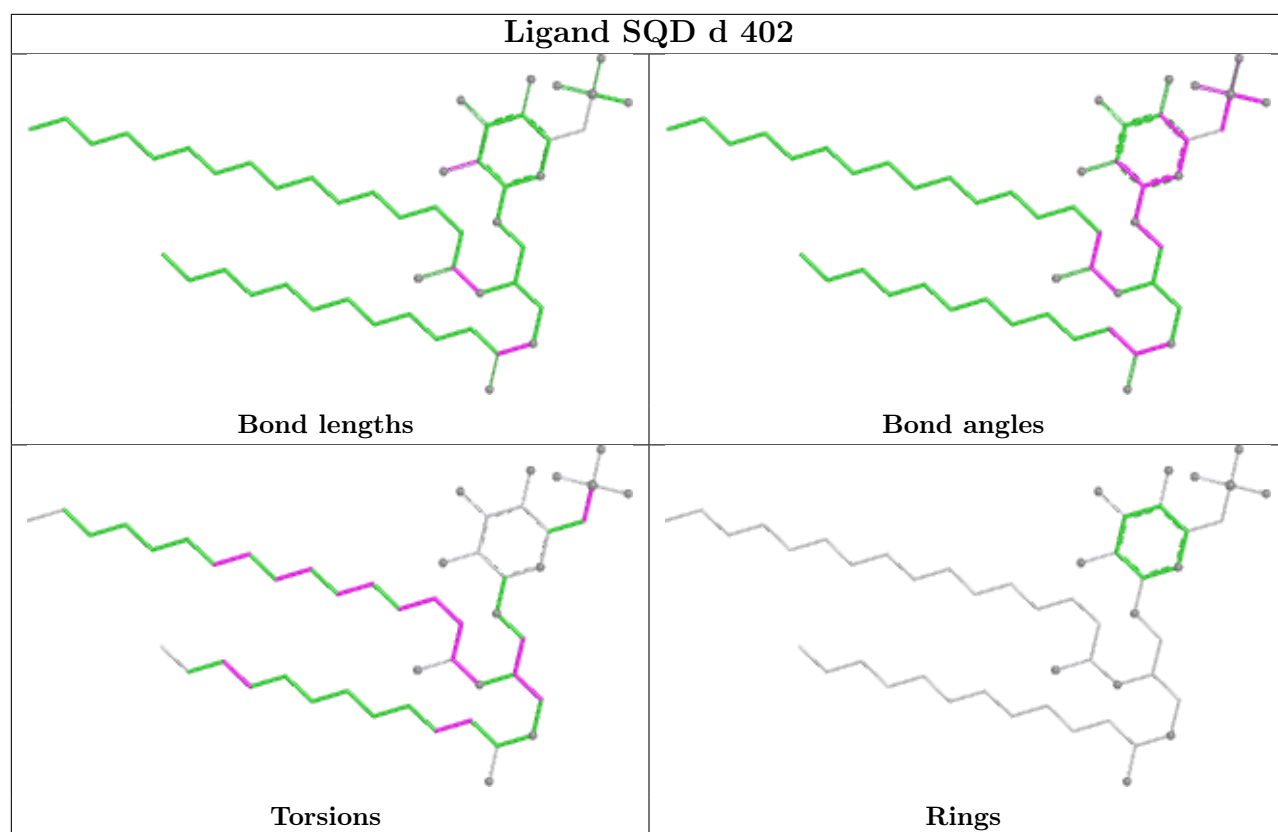


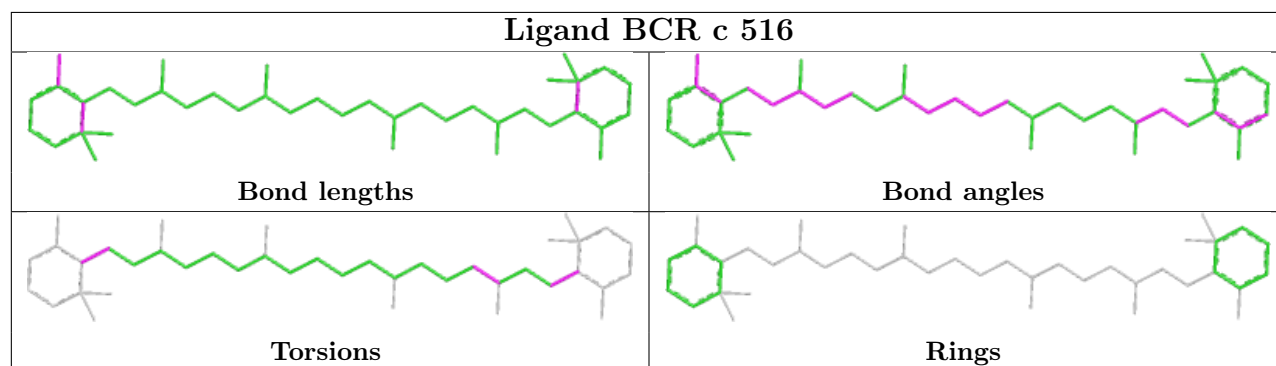
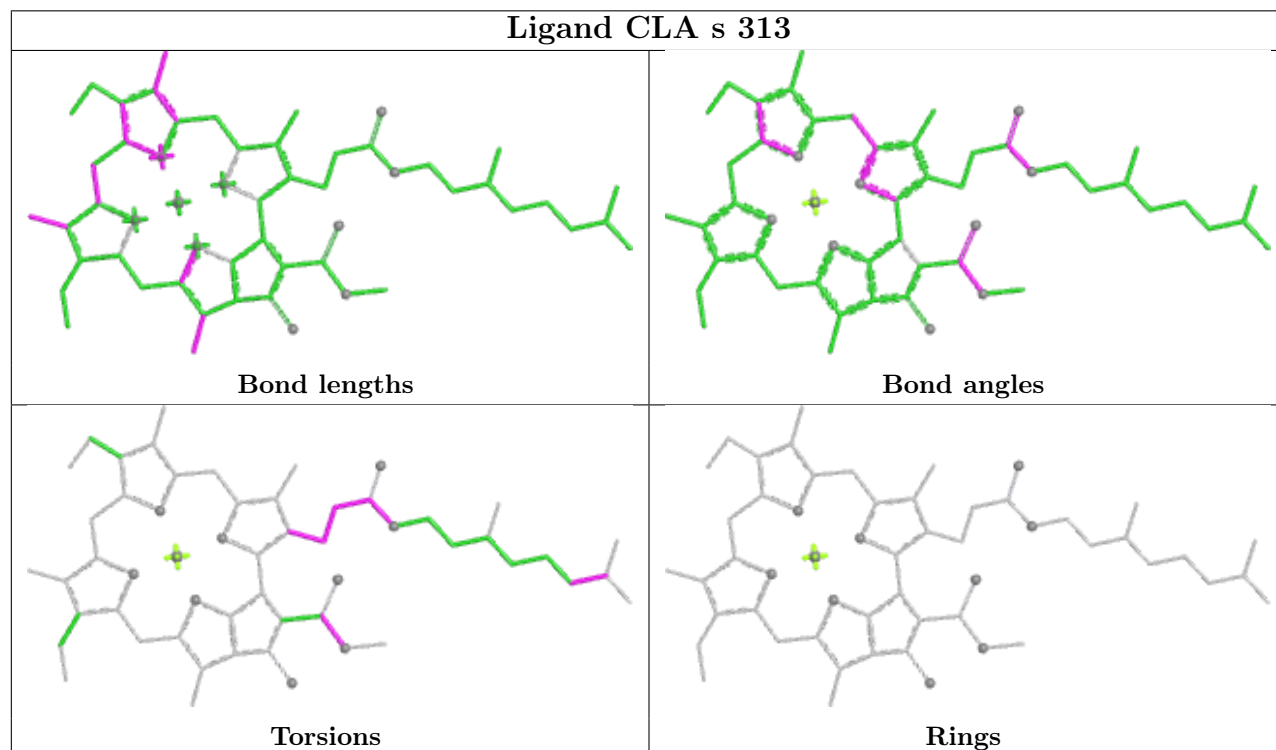
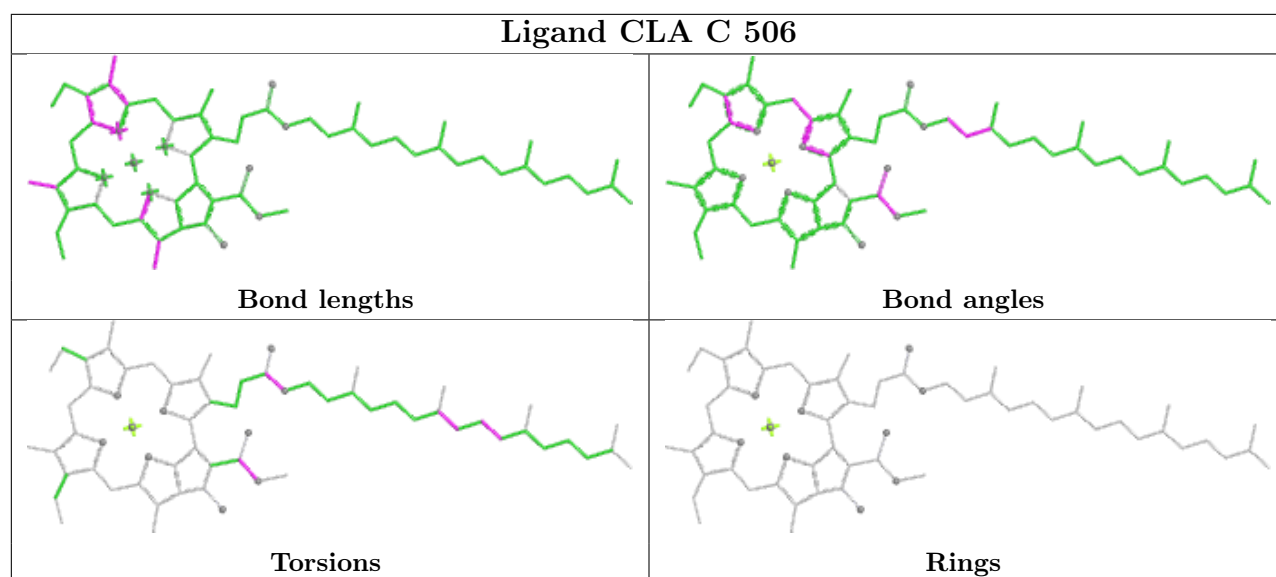
Ligand CLA N 613

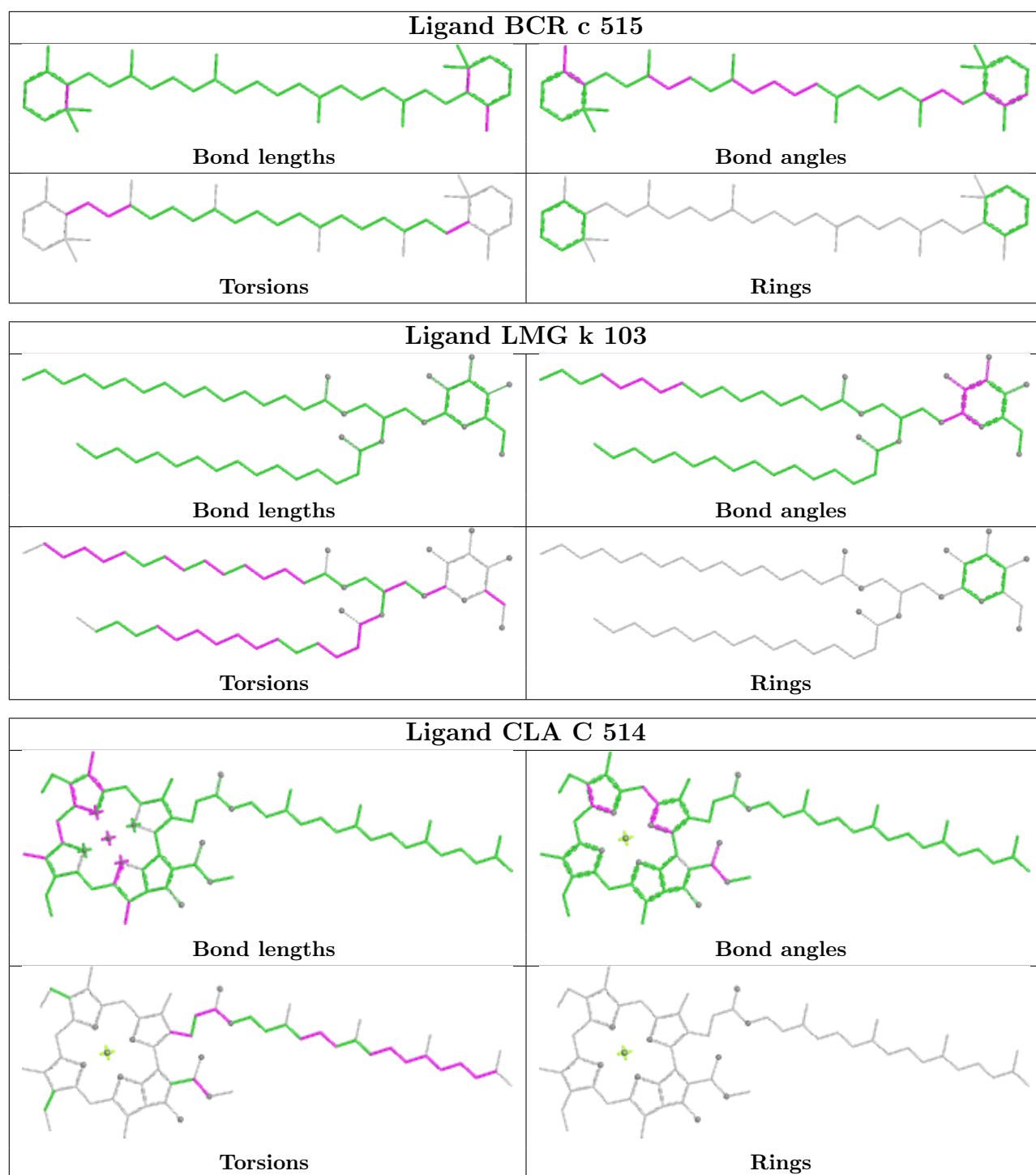


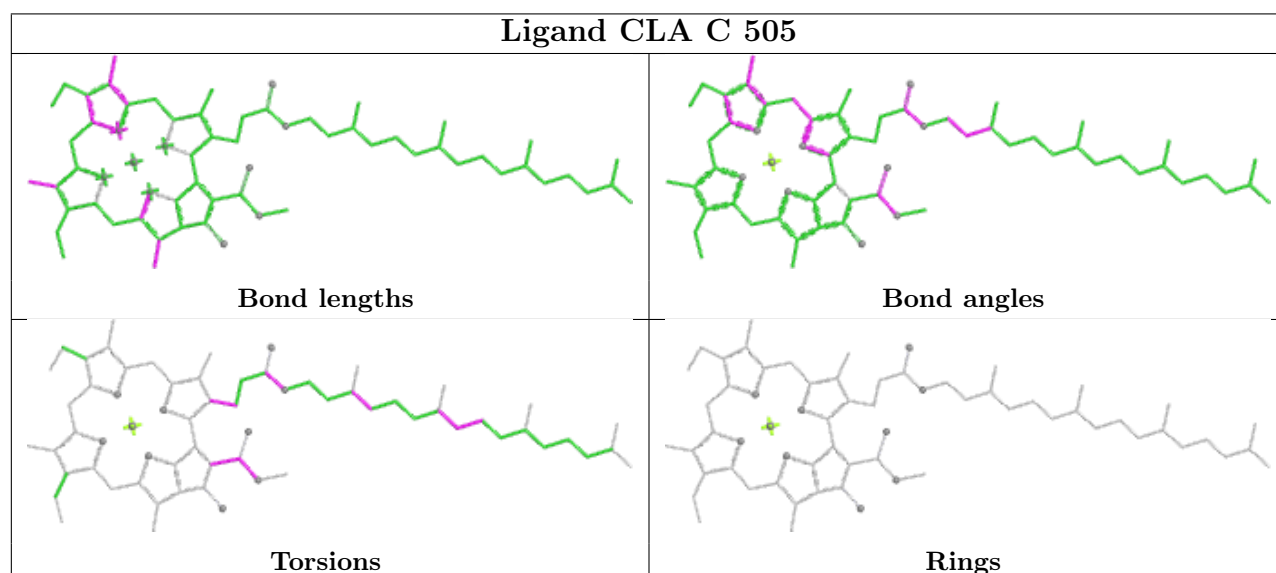
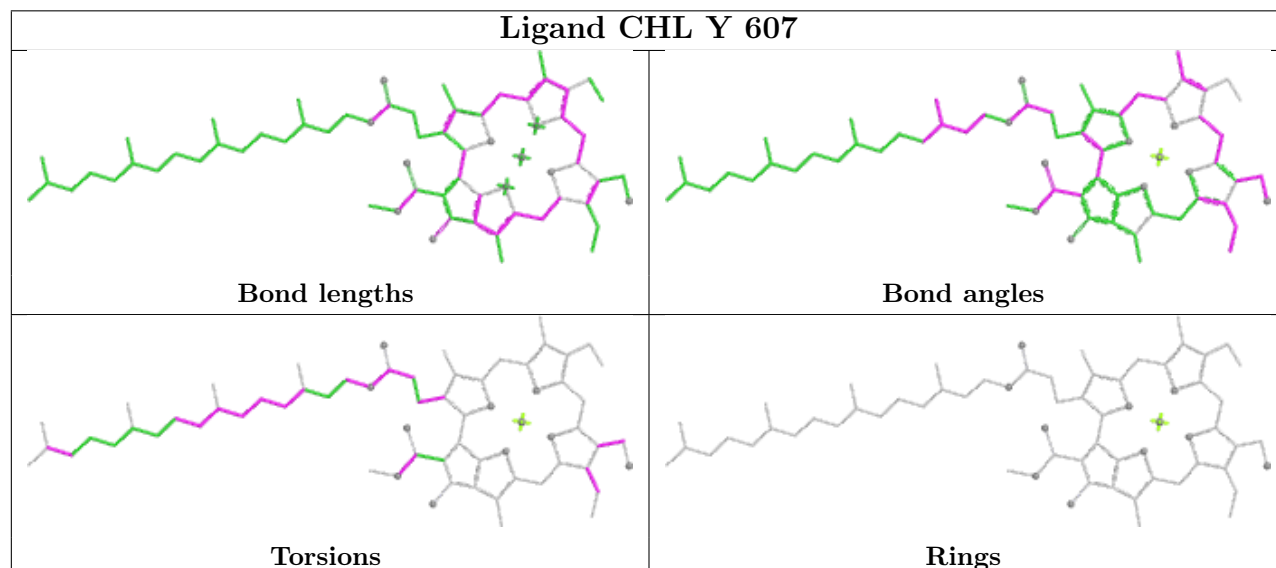
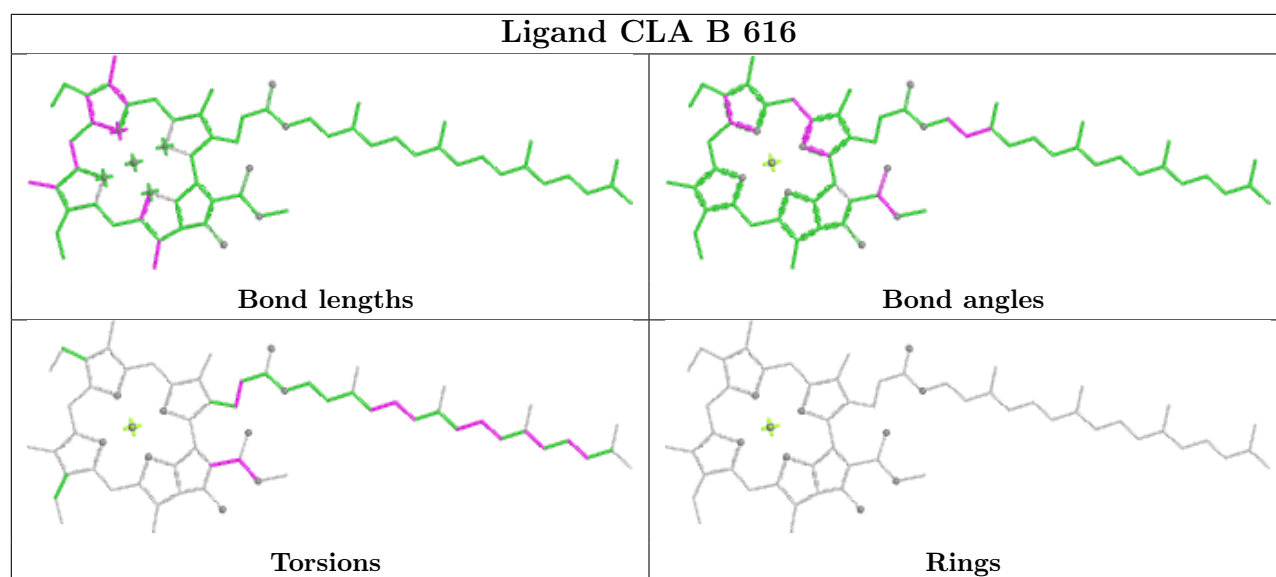


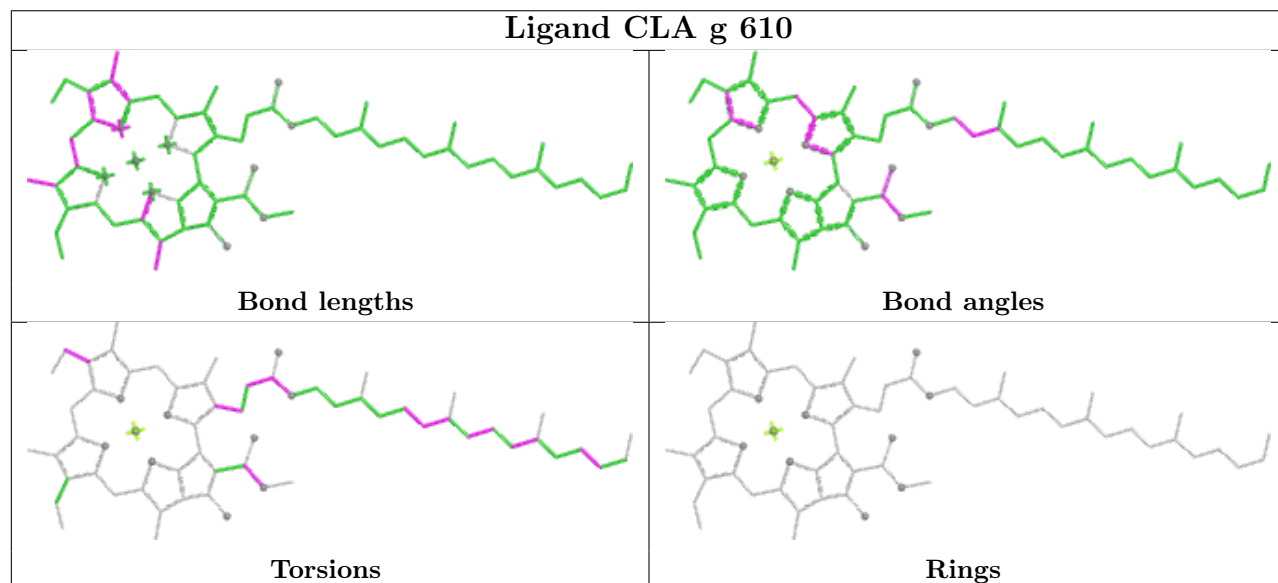
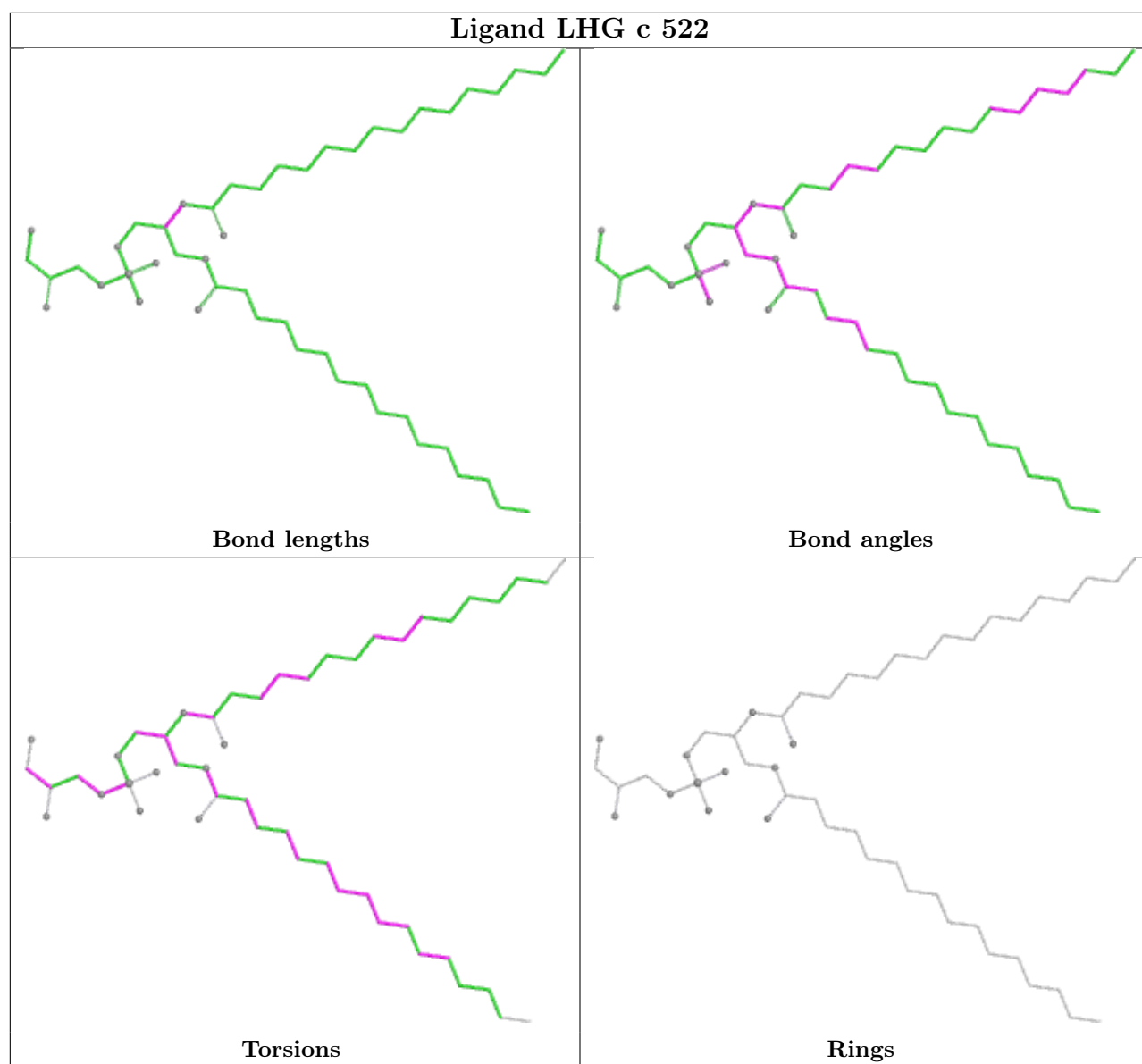


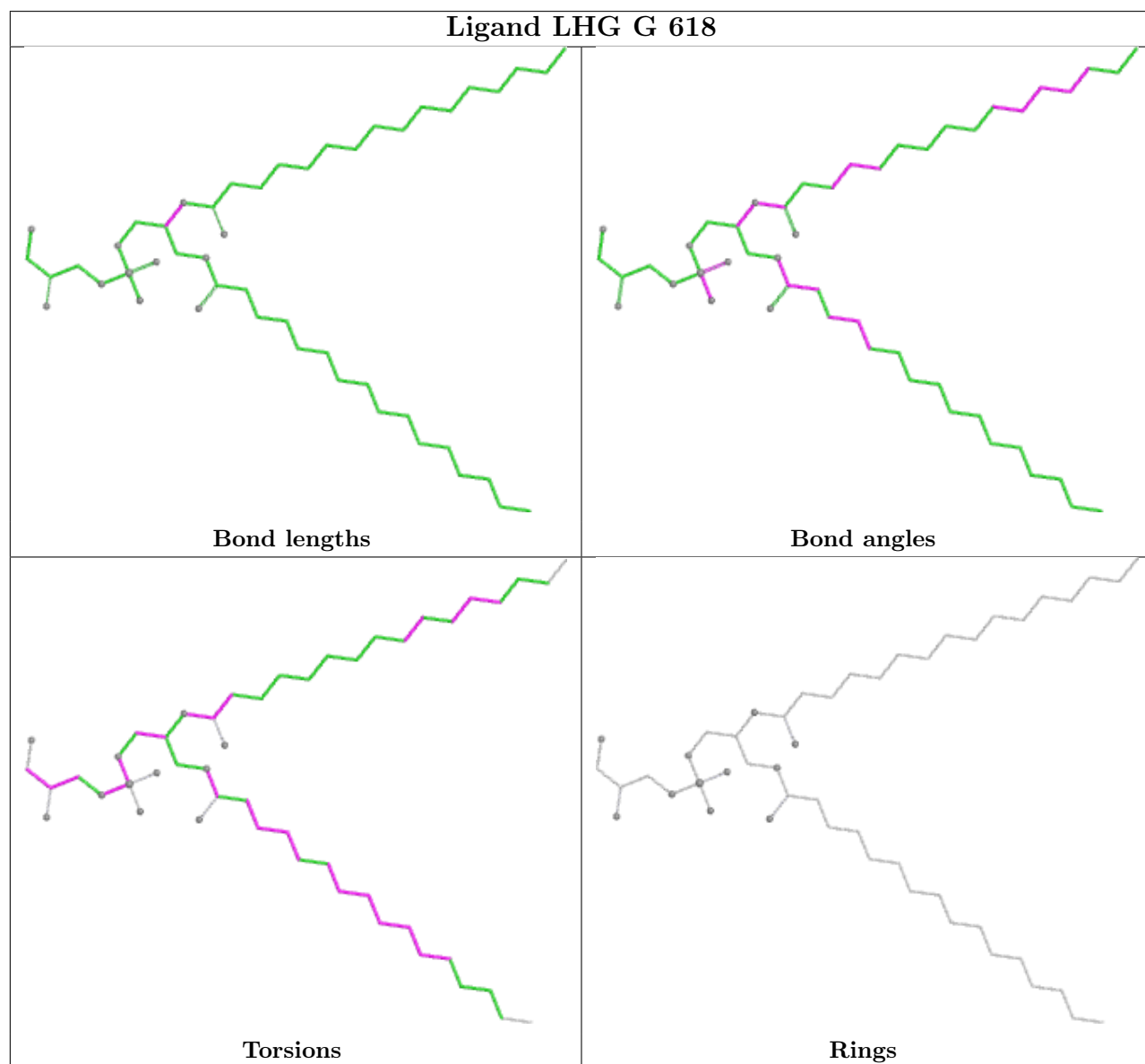
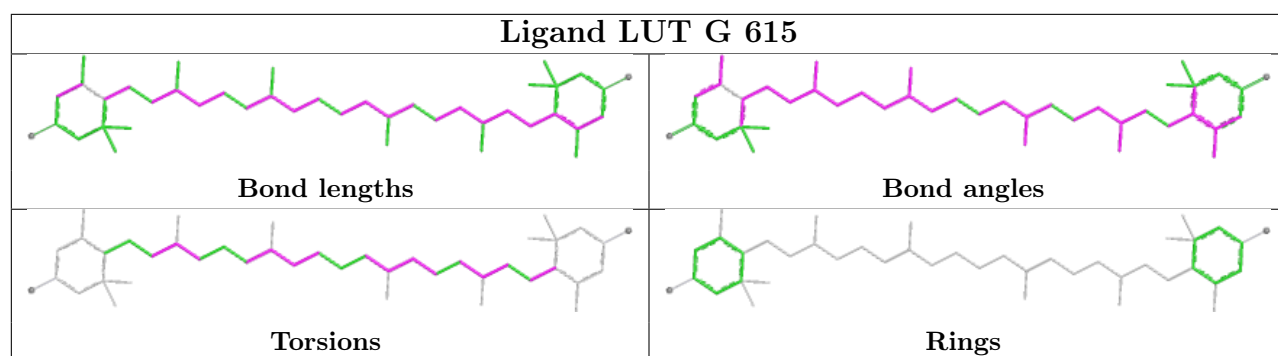


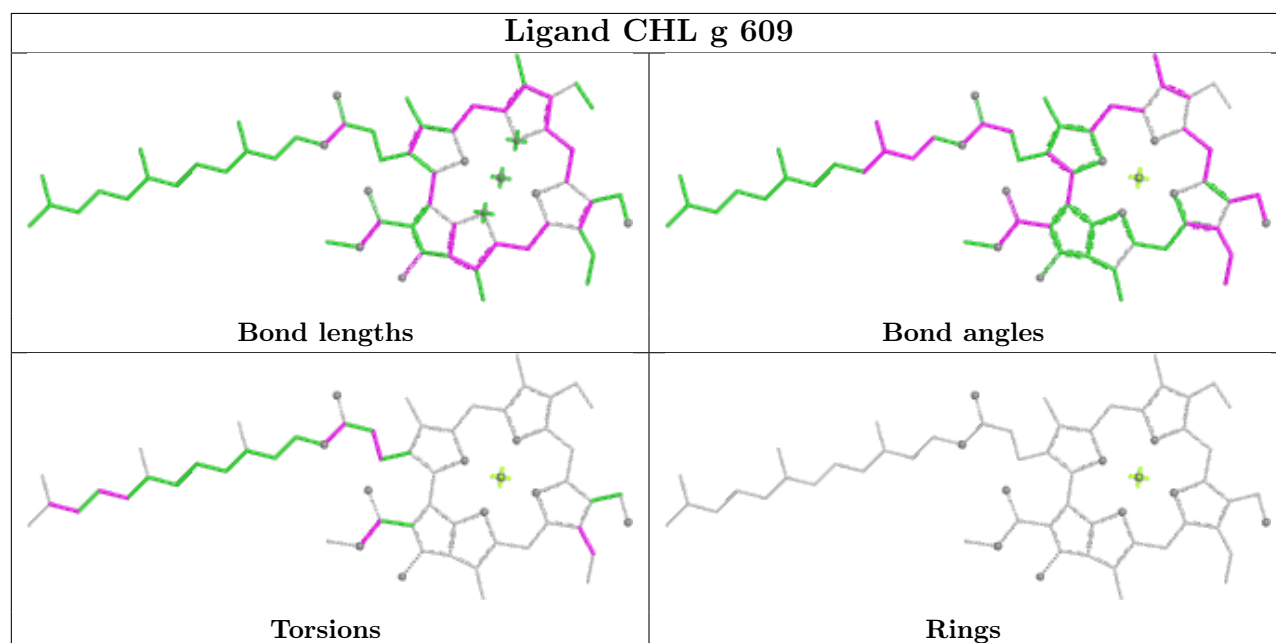
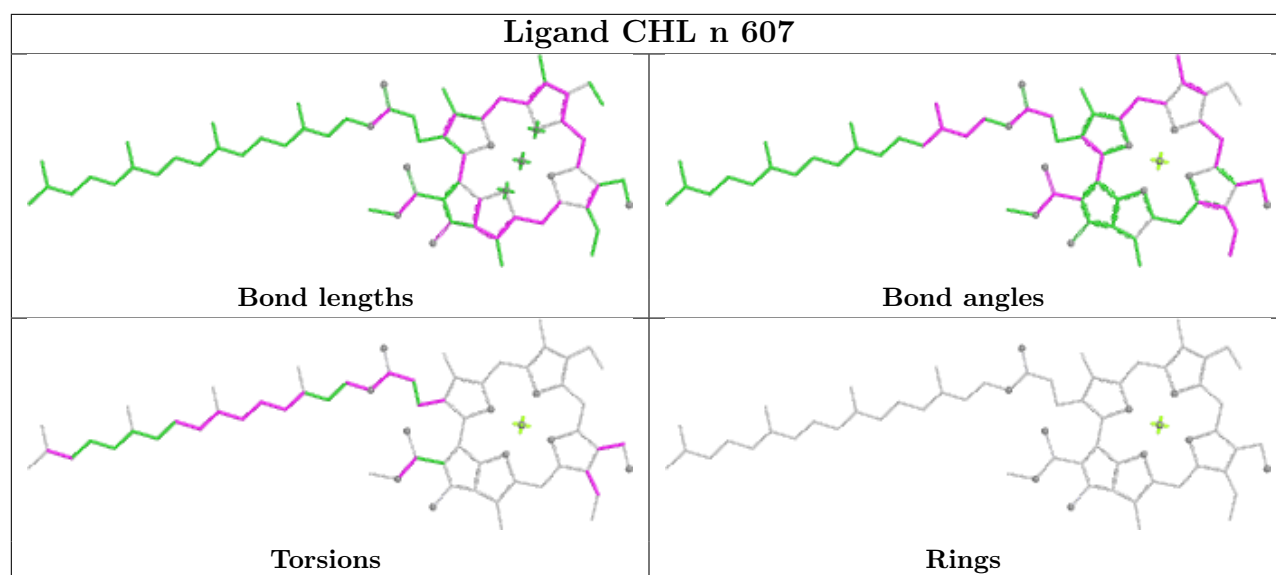


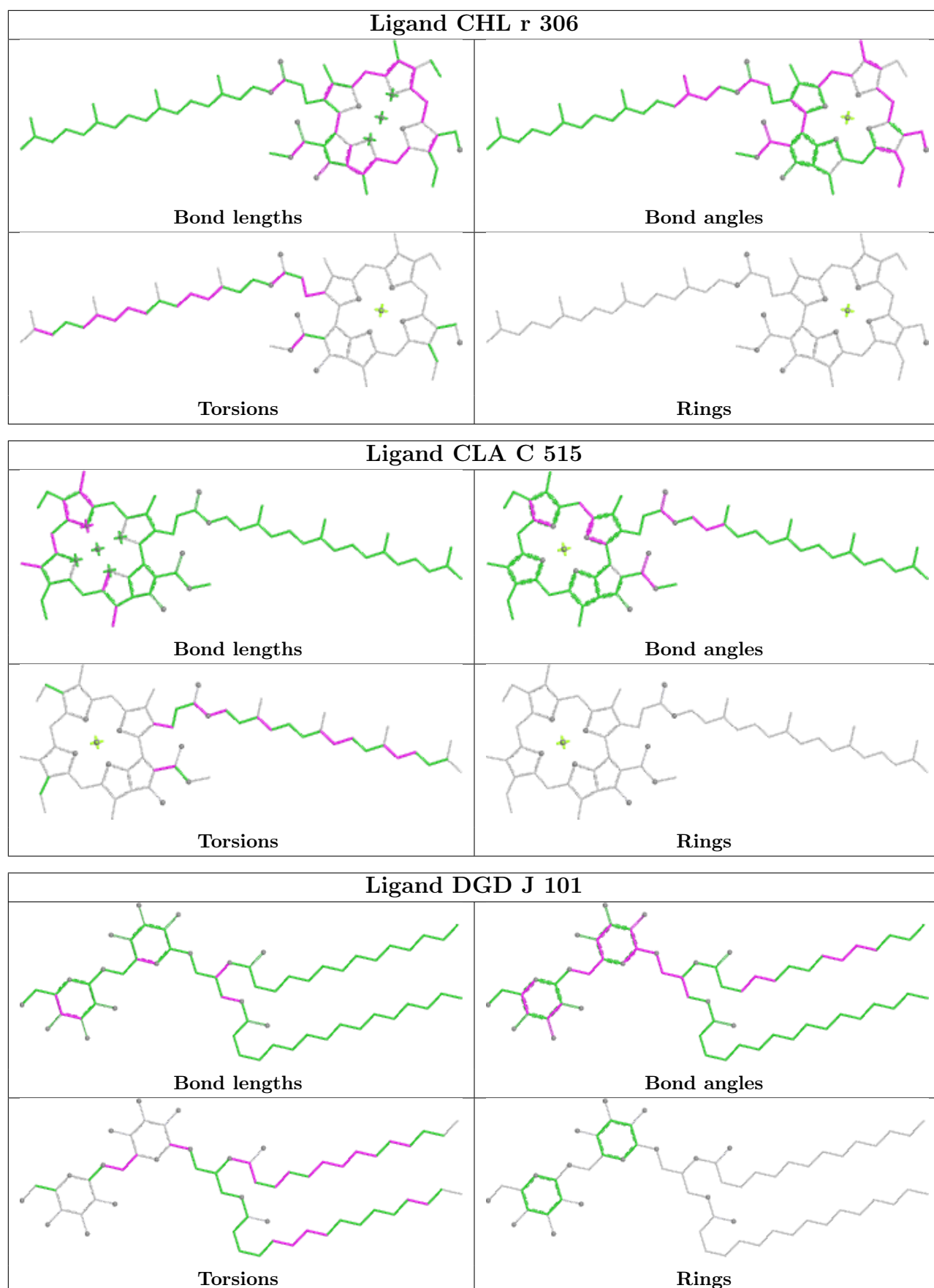


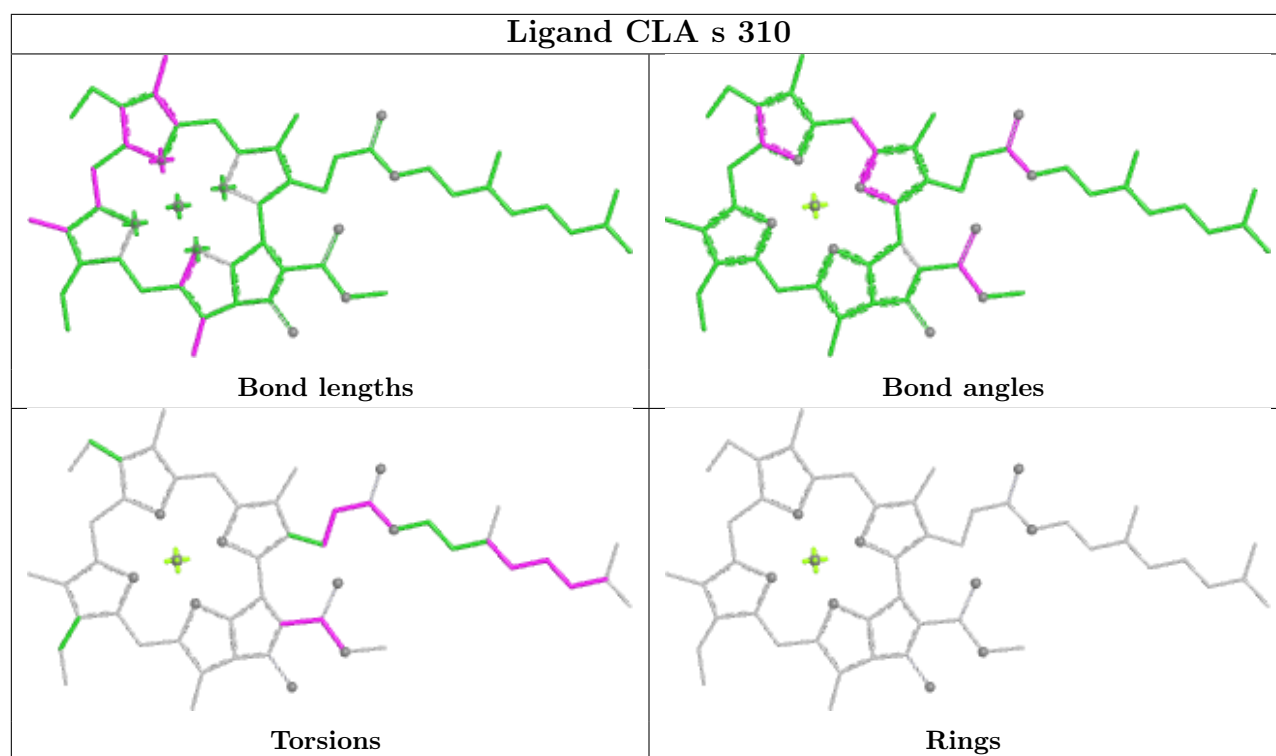


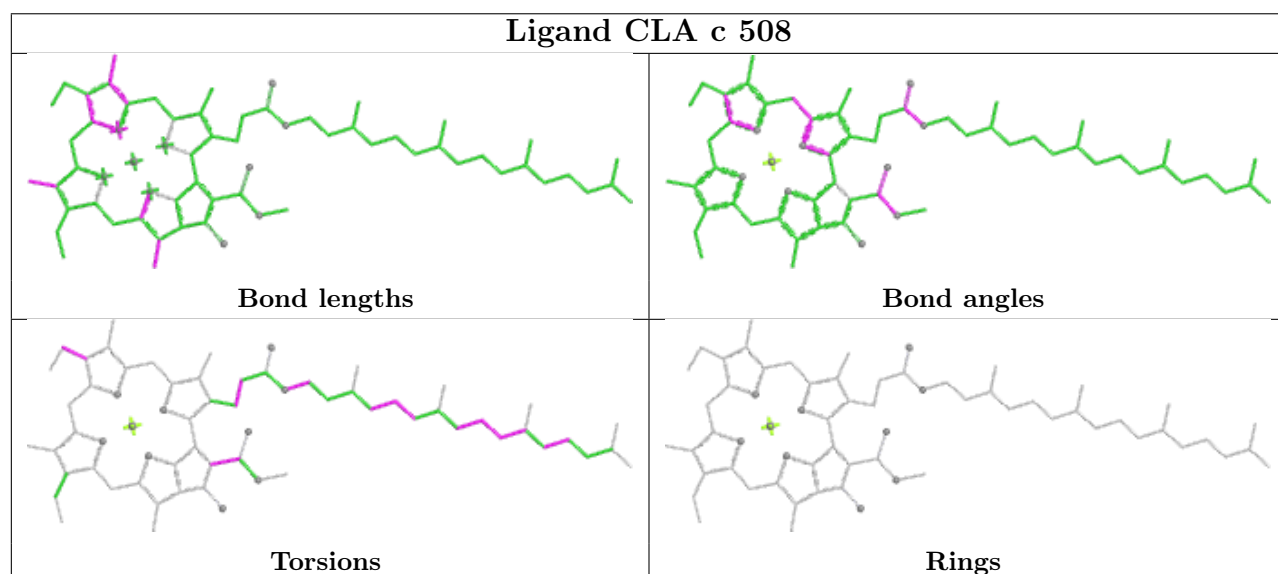
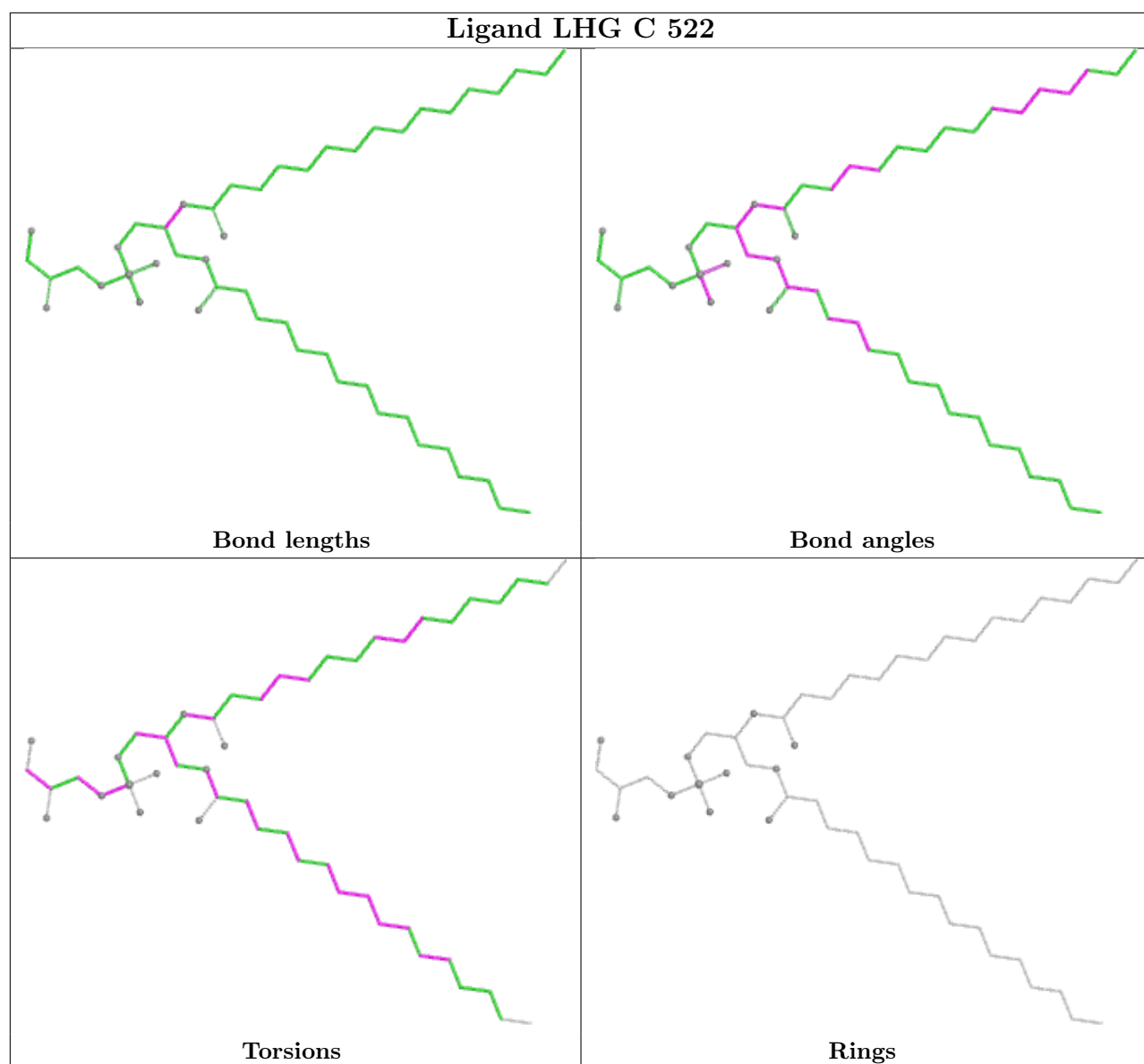


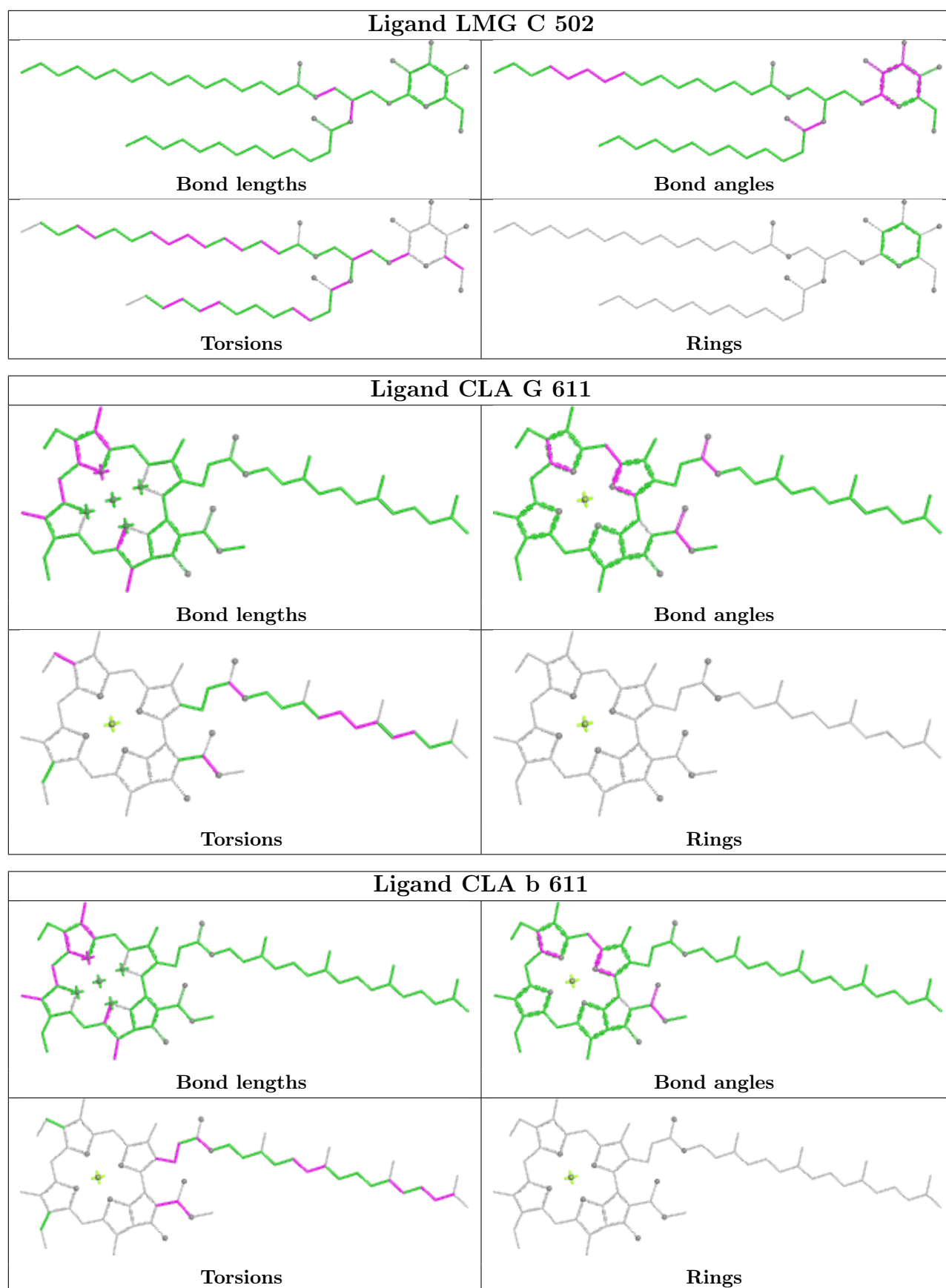


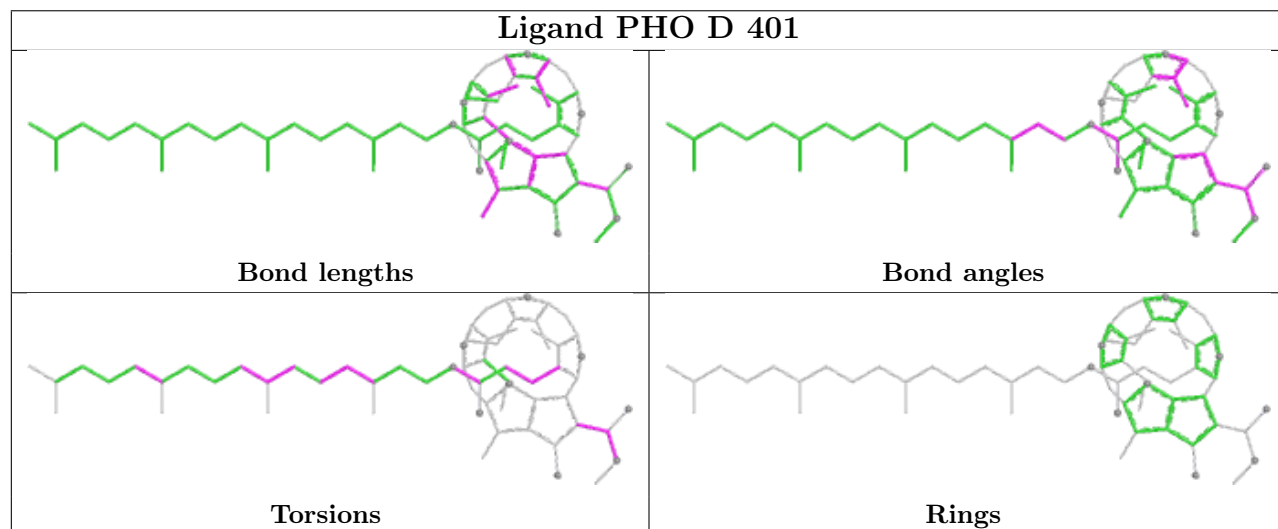
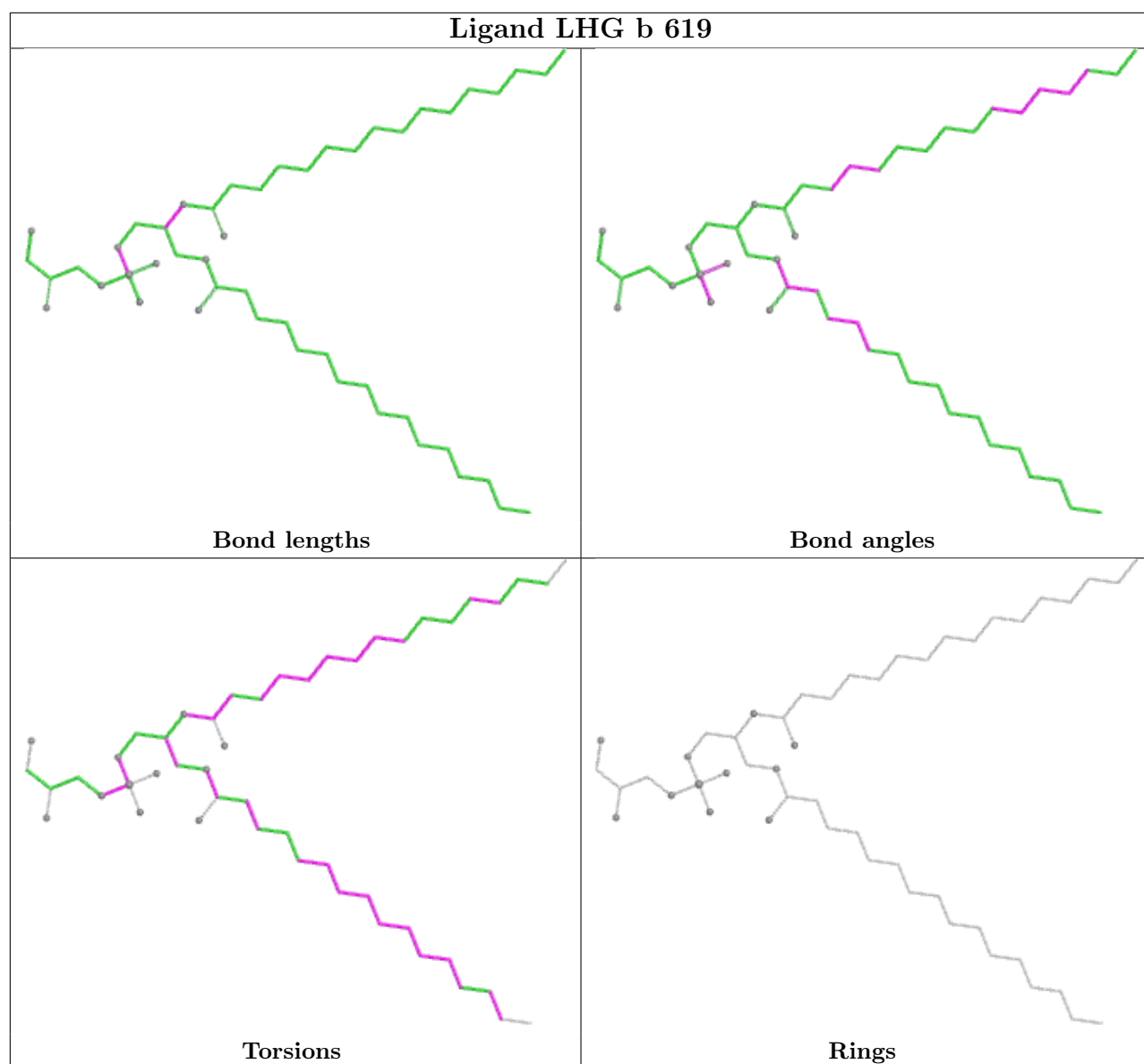




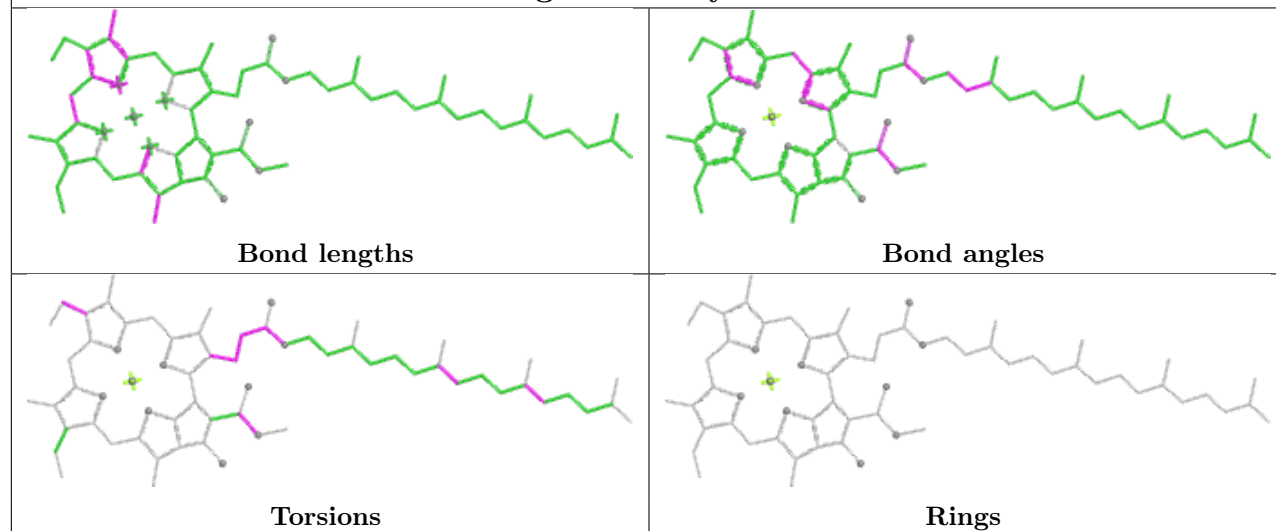




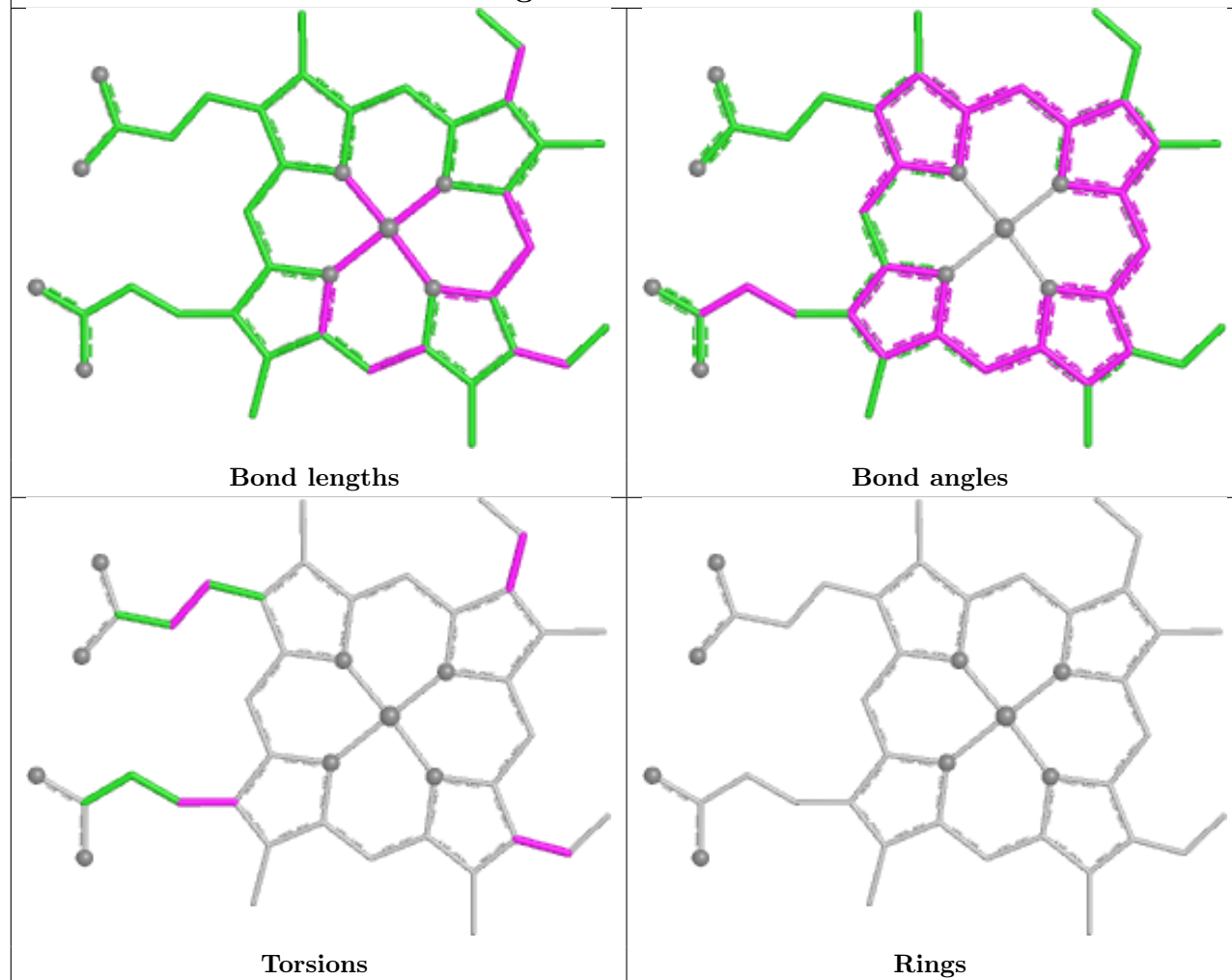


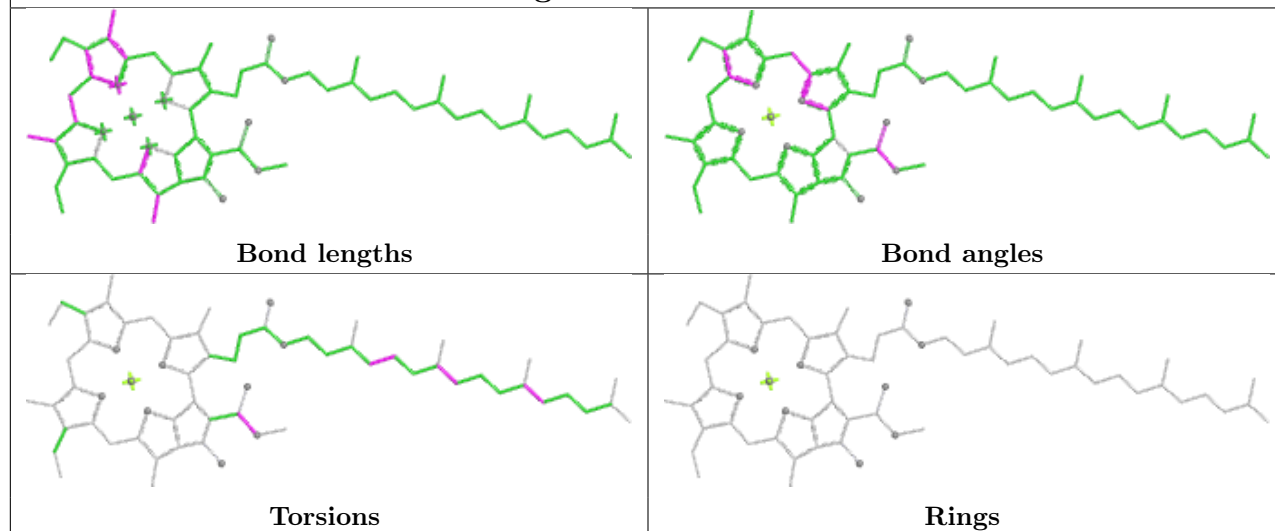
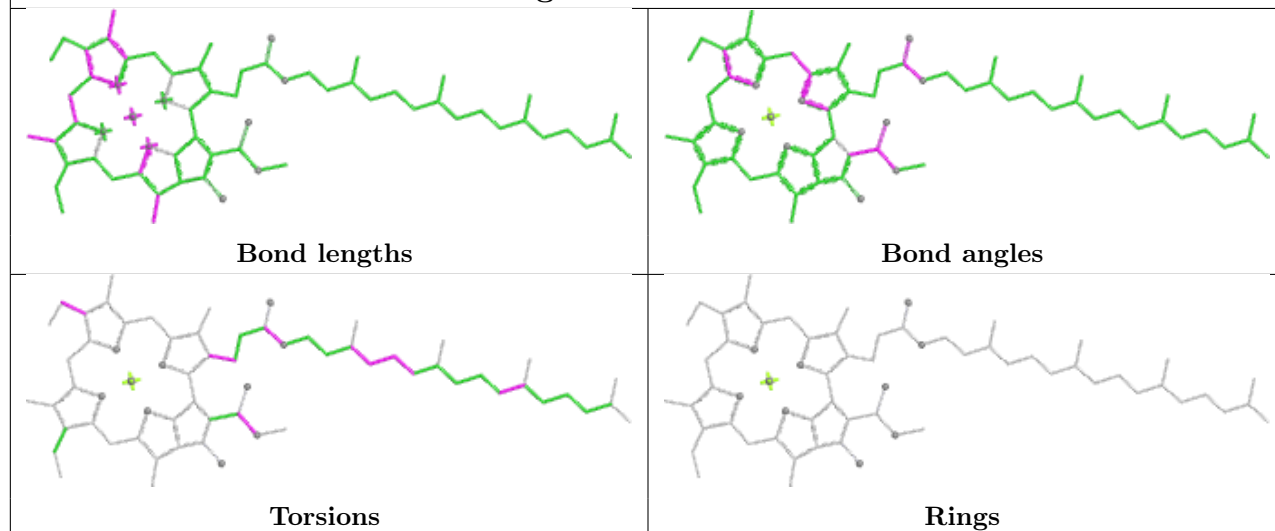
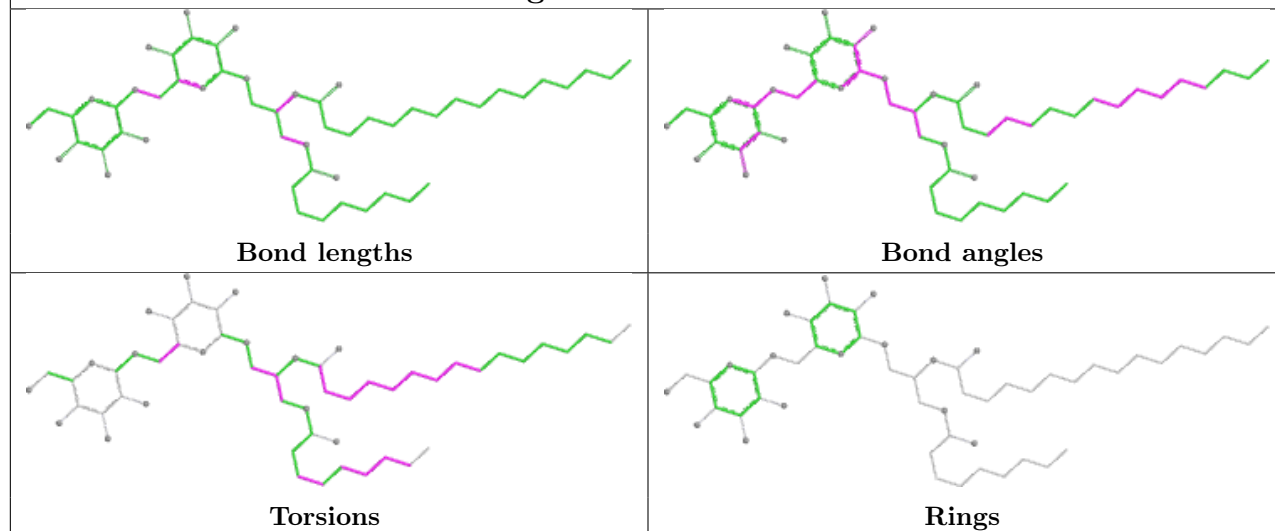


Ligand CLA y 602

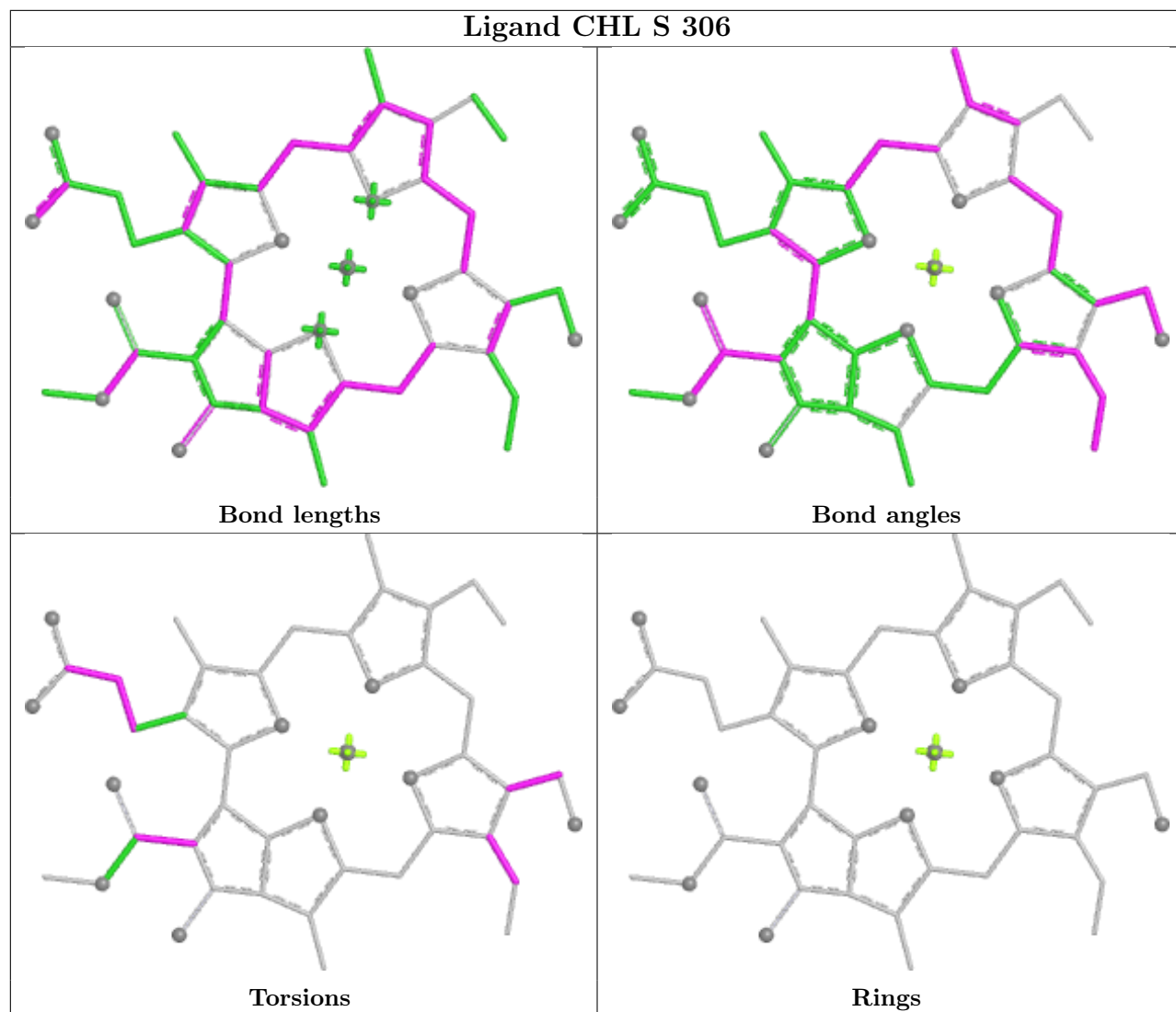


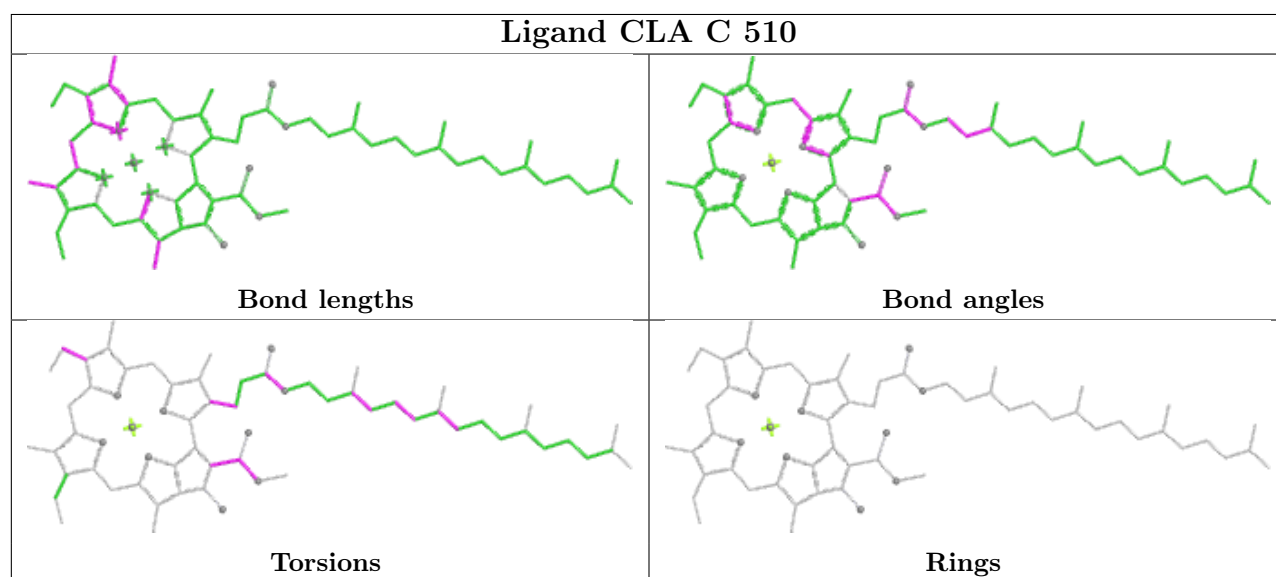
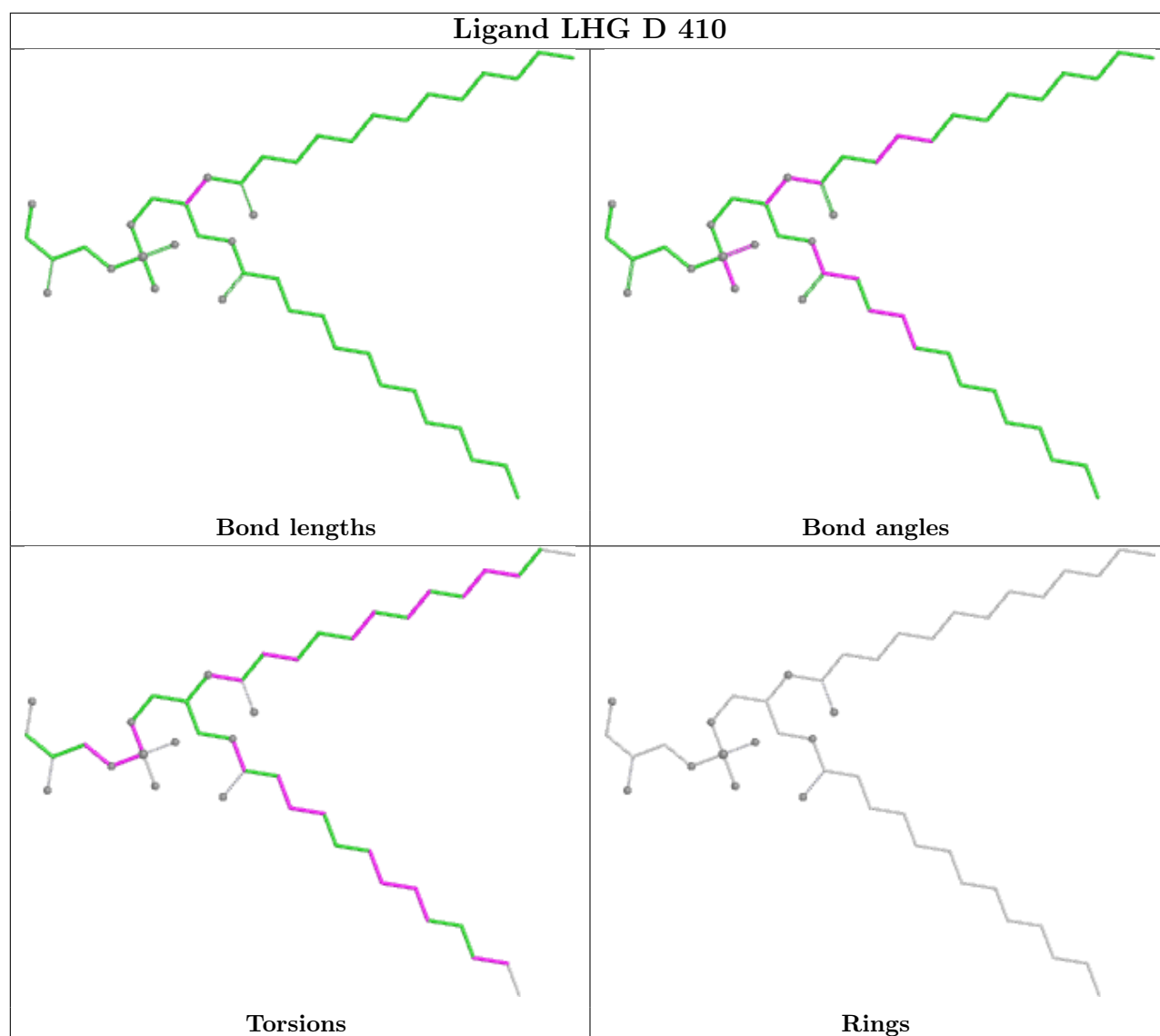
Ligand HEM f 101

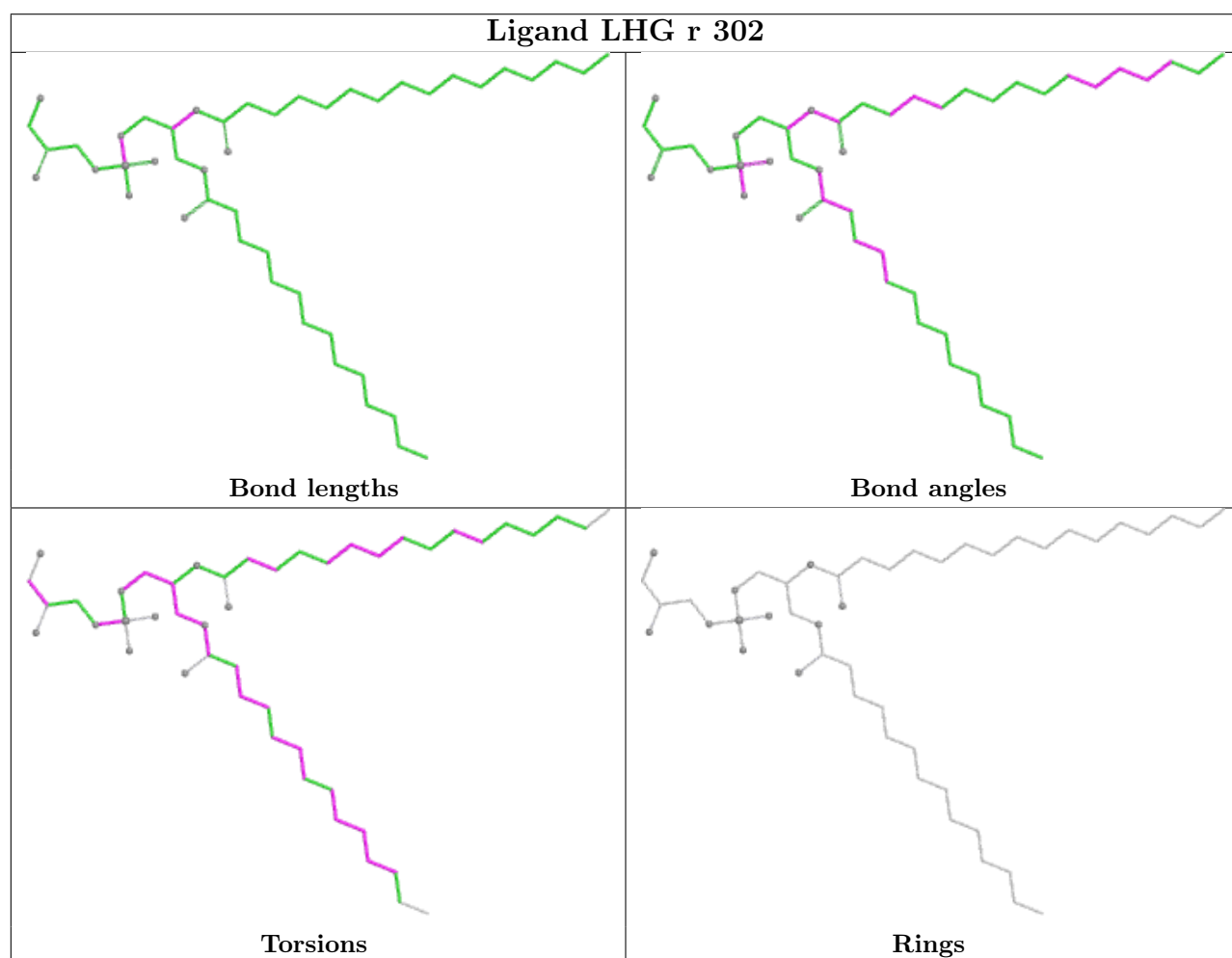
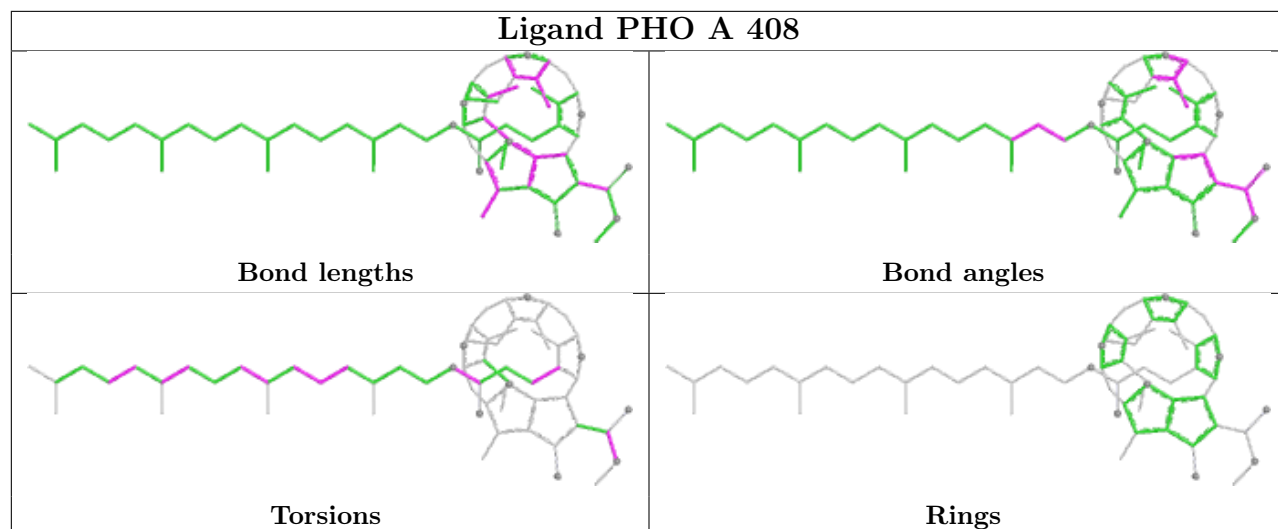


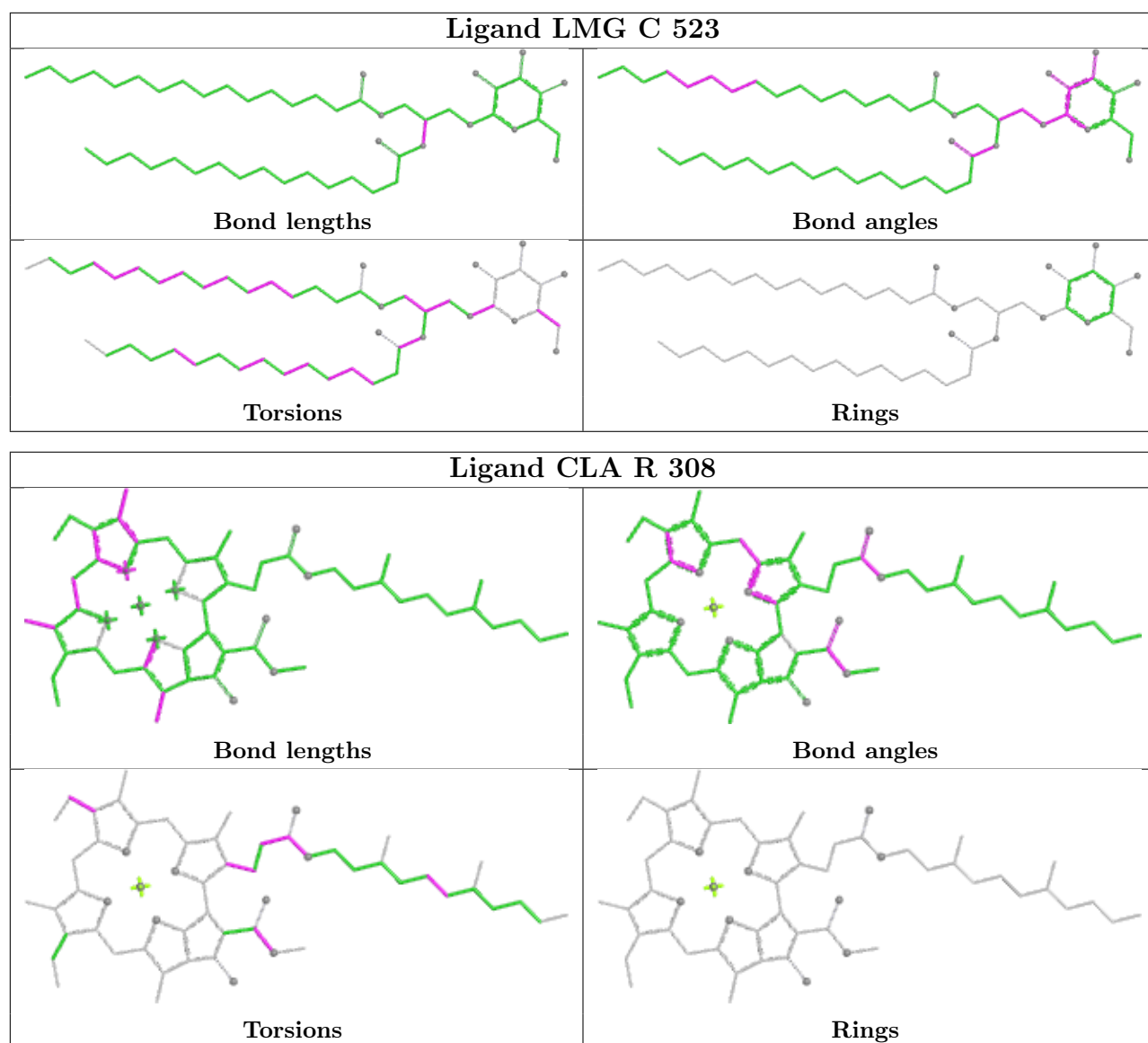
Ligand CLA b 612**Ligand CLA c 511****Ligand DGD C 518**

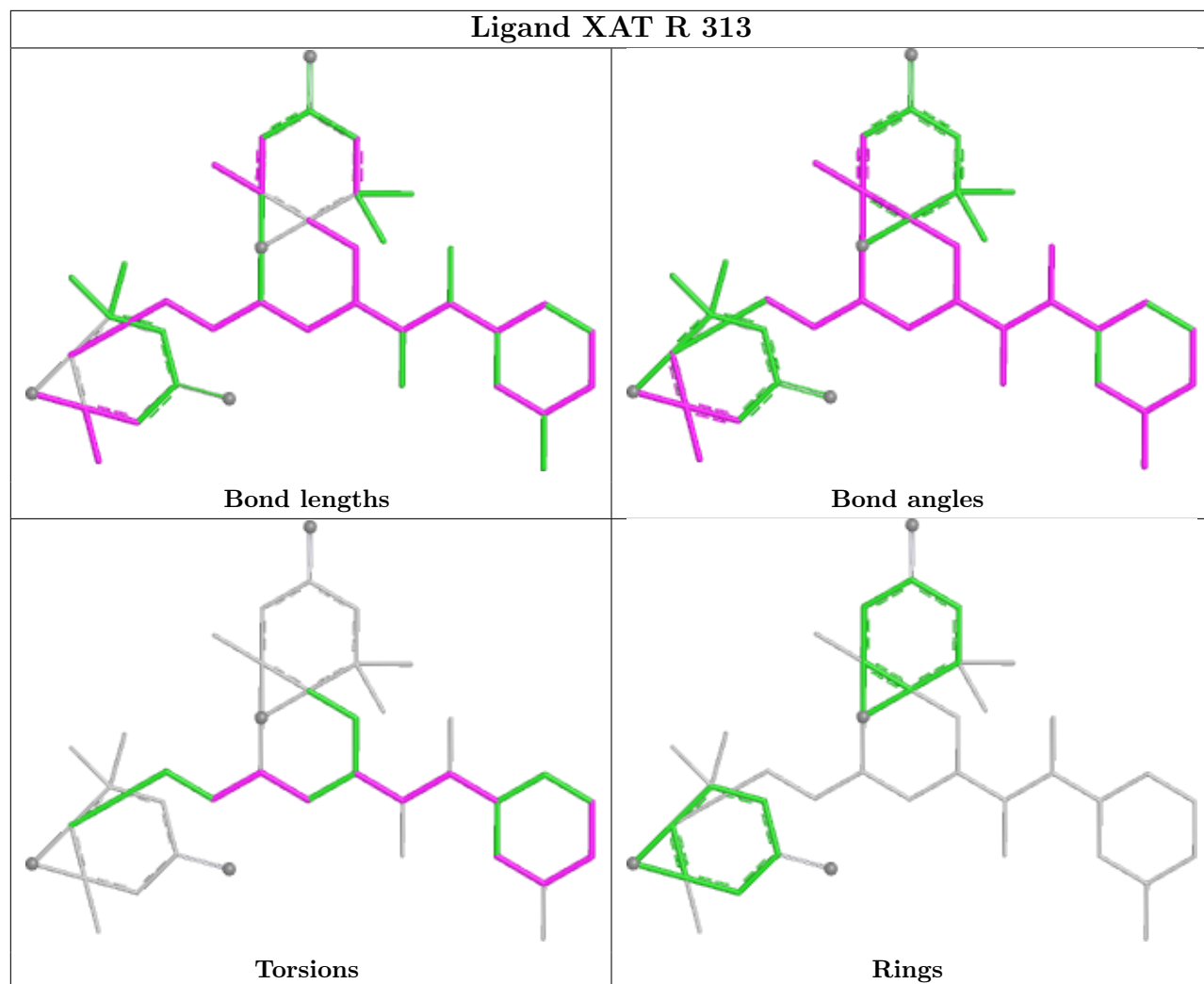
Ligand CHL S 306



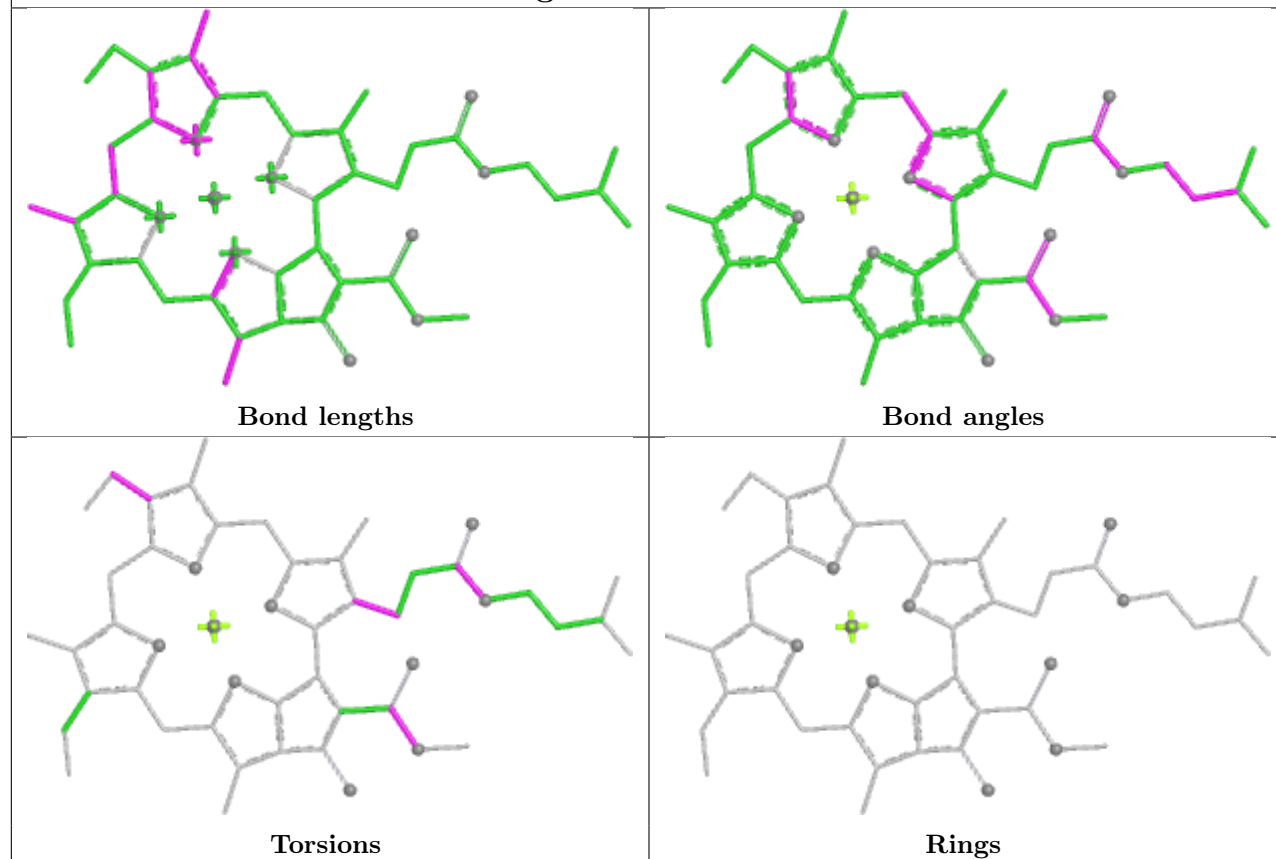




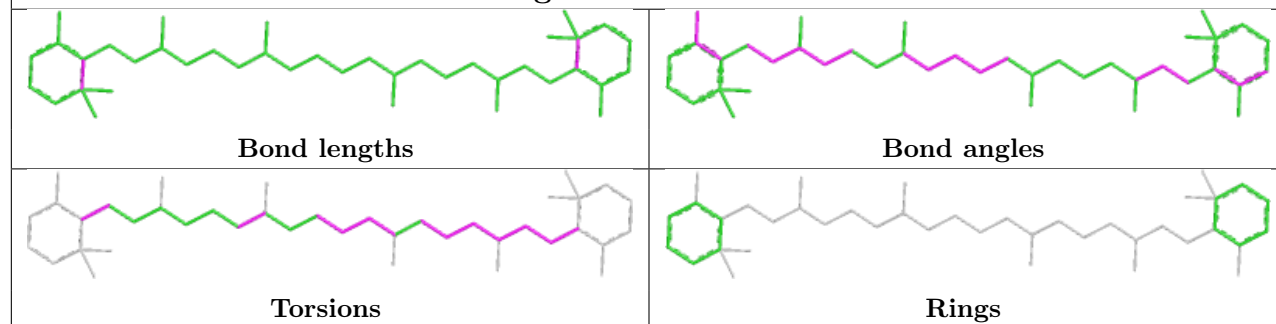




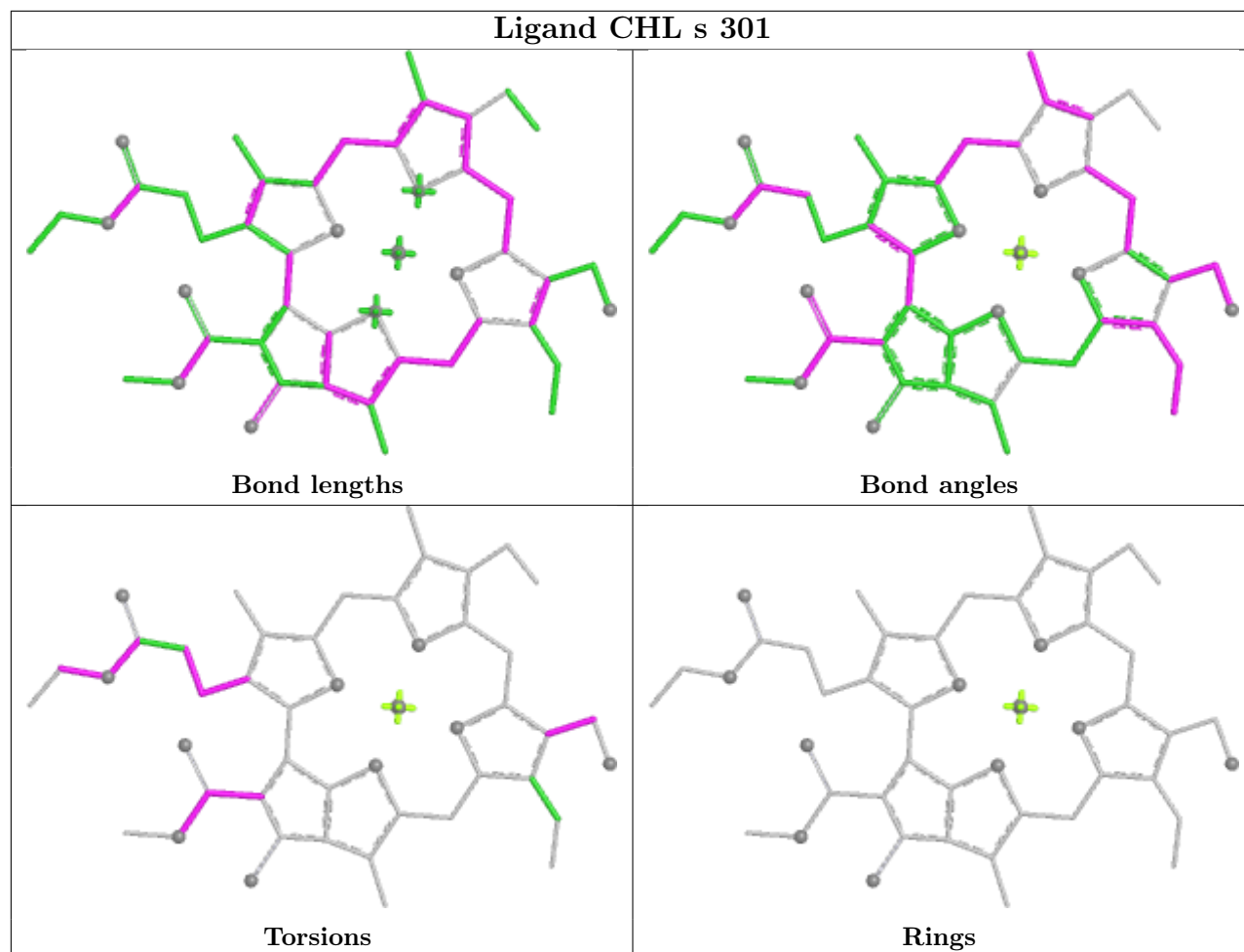
Ligand CLA a 406



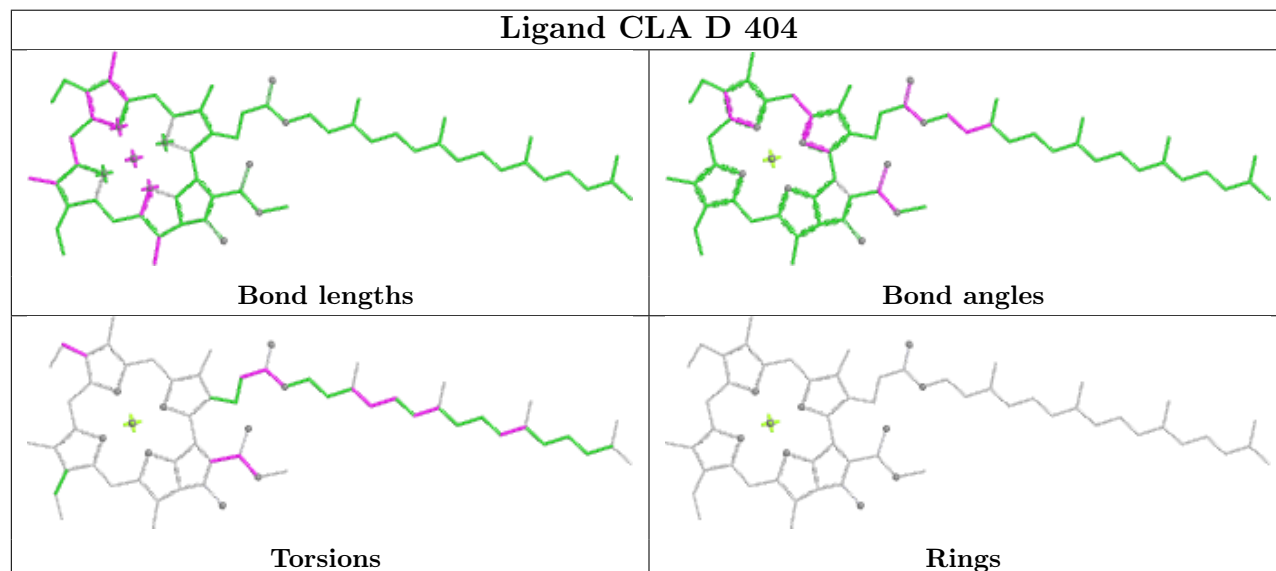
Ligand BCR k 101

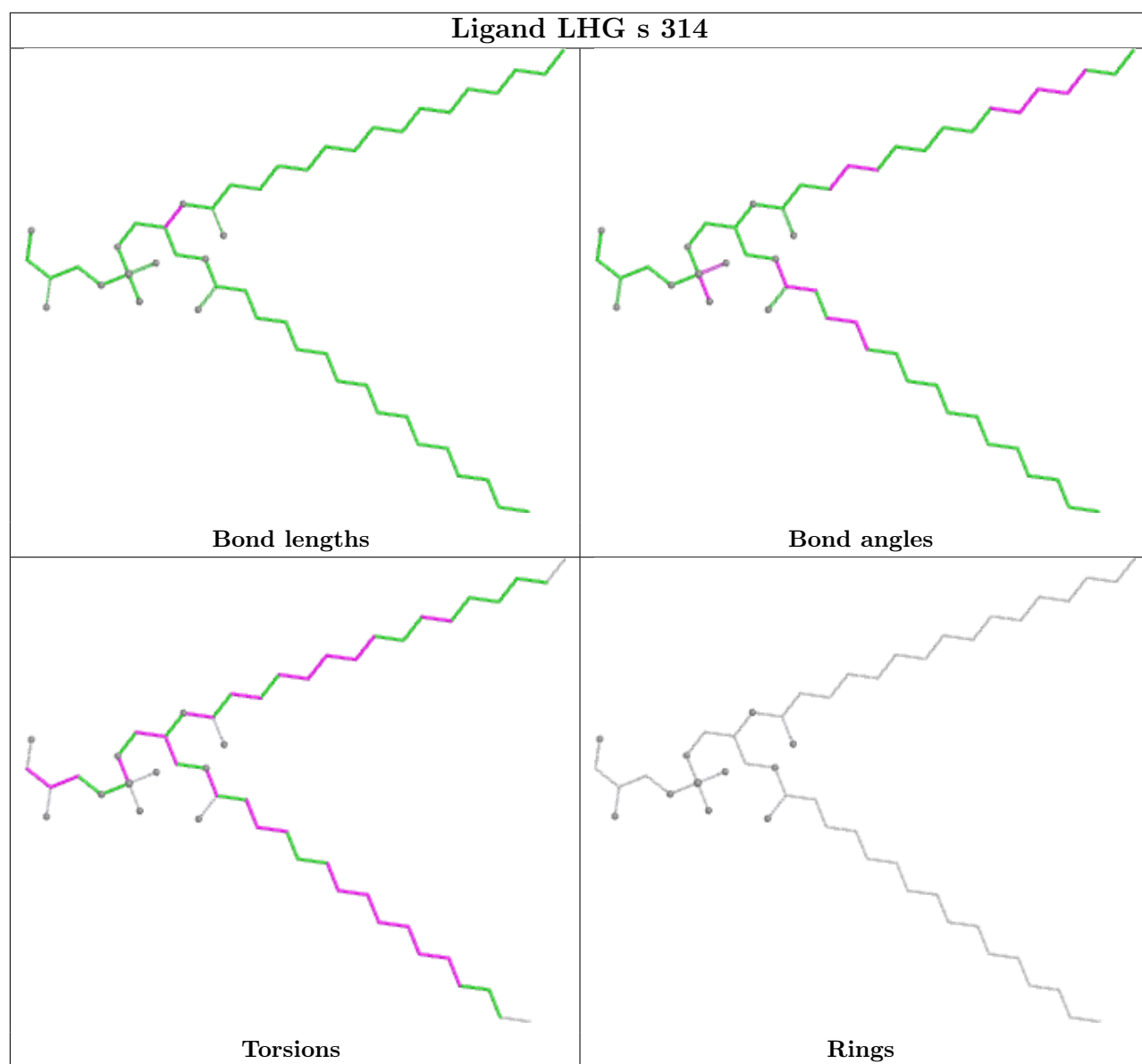


Ligand CHL s 301

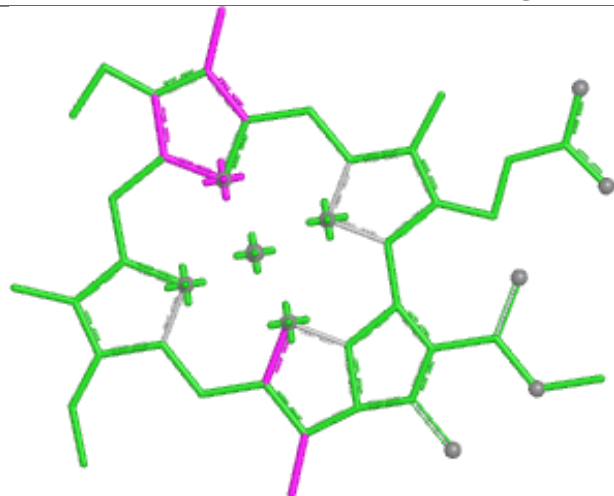


Ligand CLA D 404

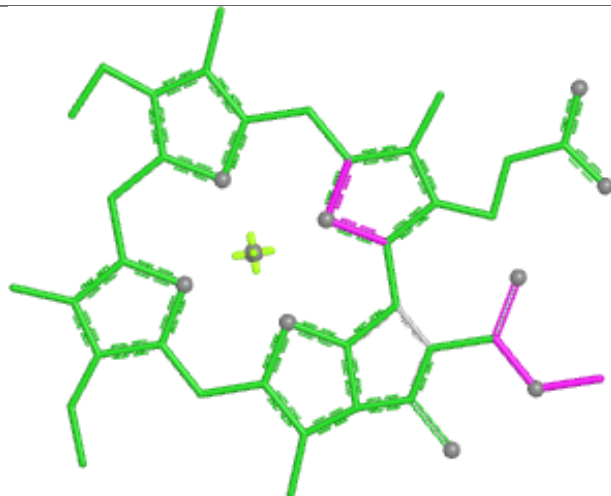




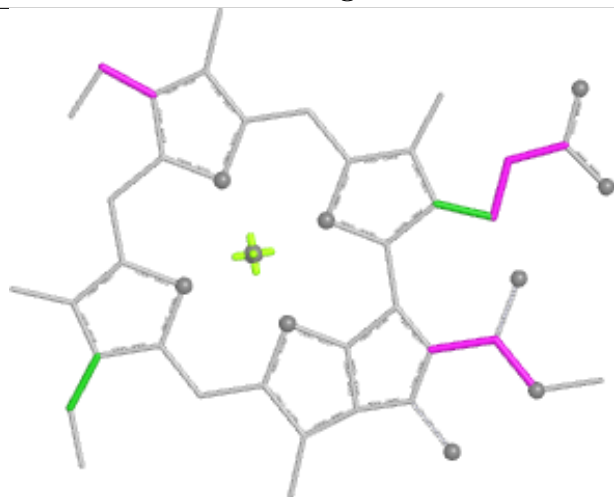
Ligand CLA S 308



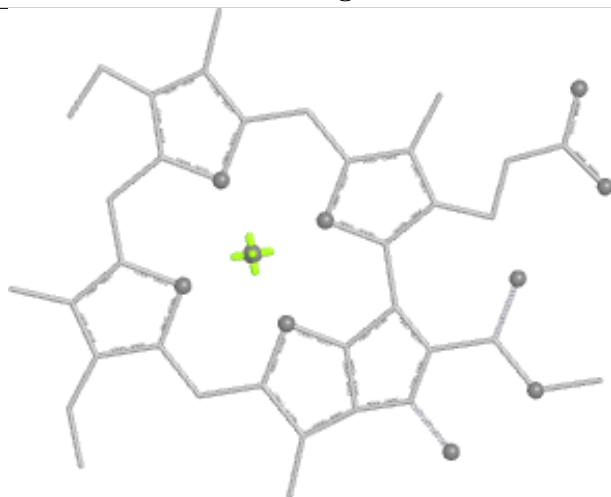
Bond lengths



Bond angles

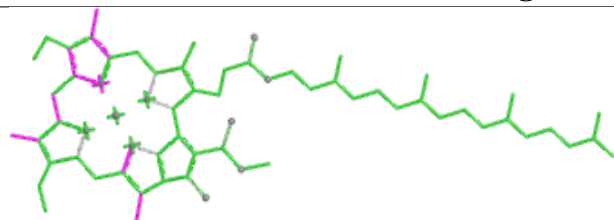


Torsions

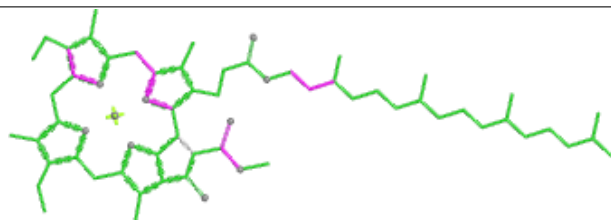


Rings

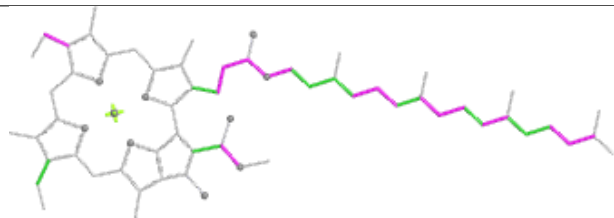
Ligand CLA b 601



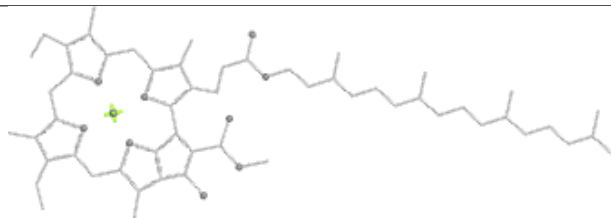
Bond lengths



Bond angles

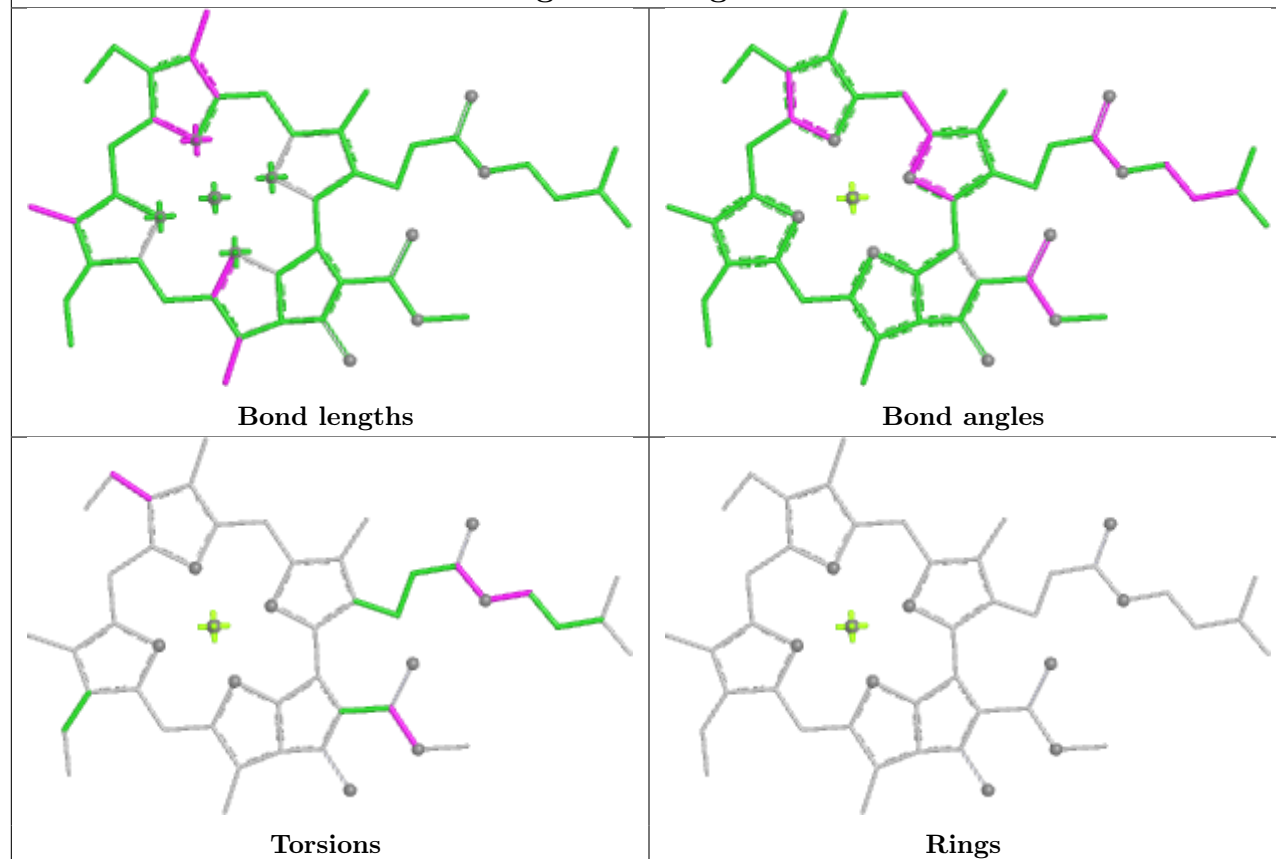


Torsions

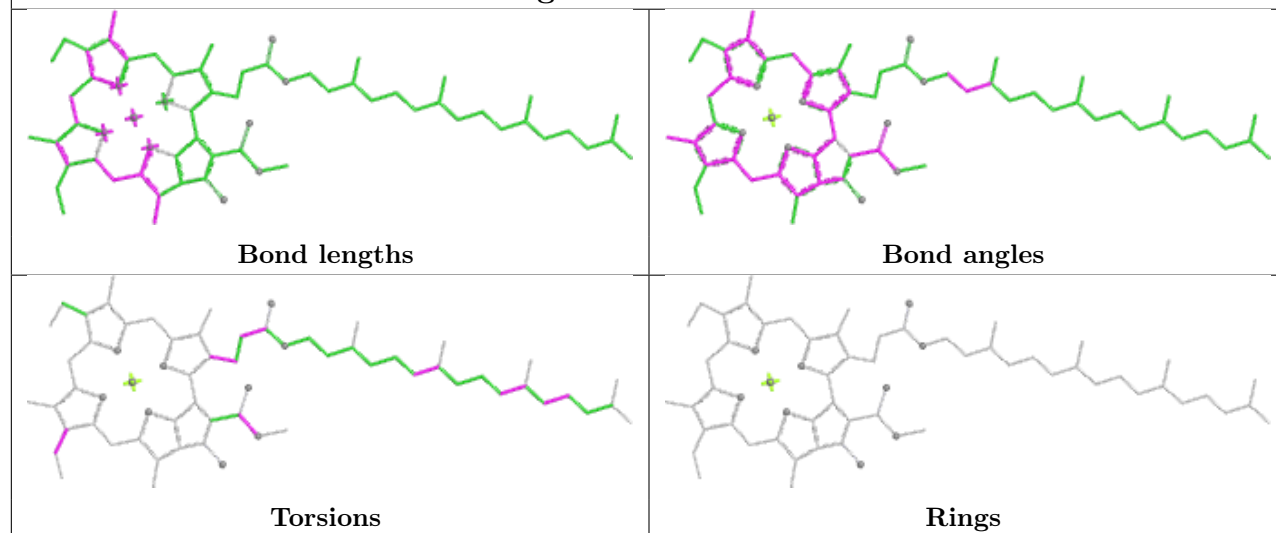


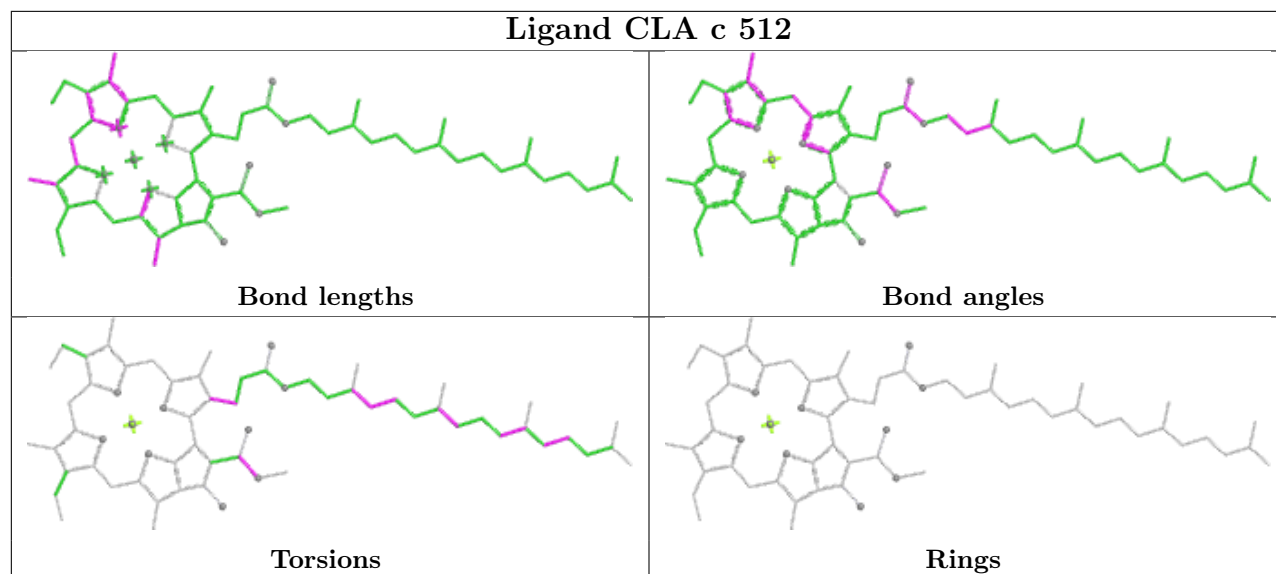
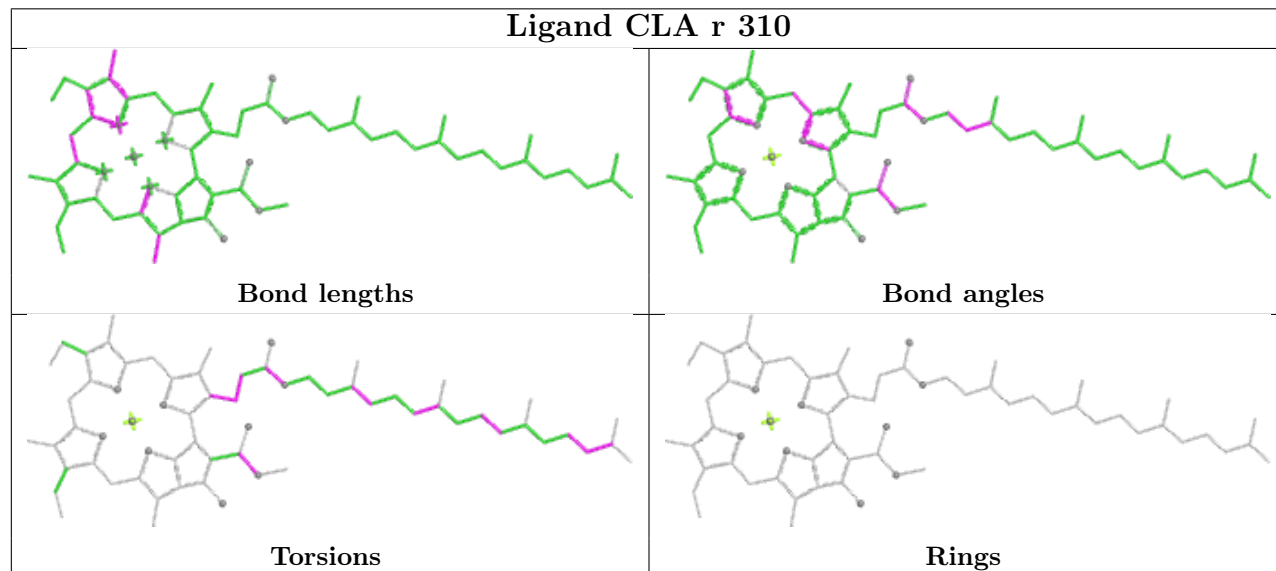
Rings

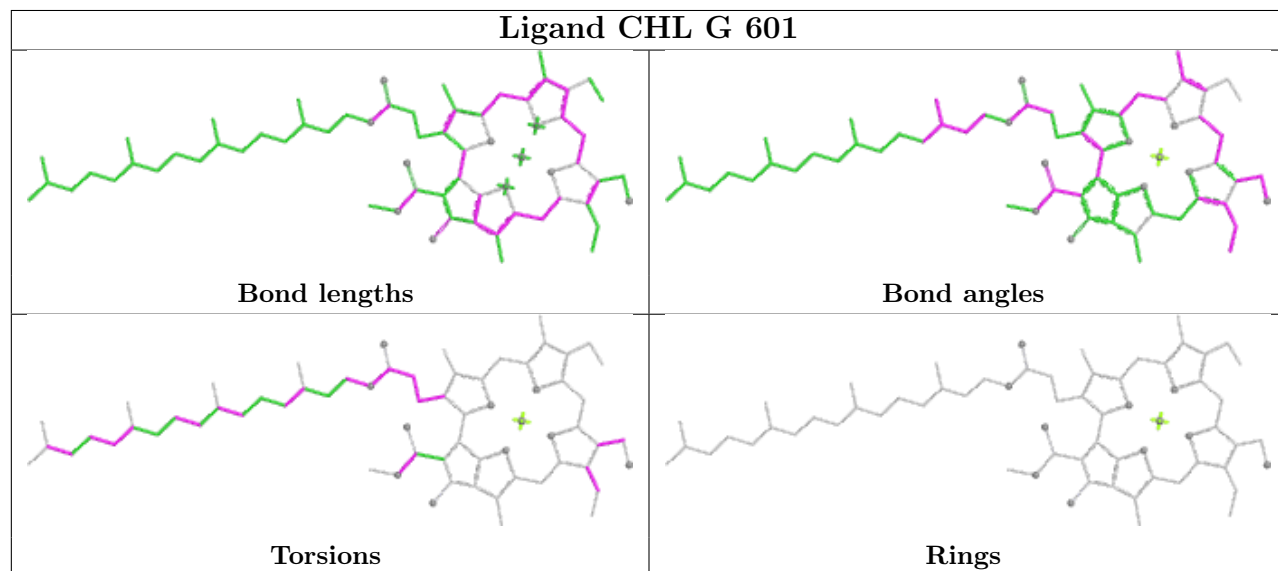
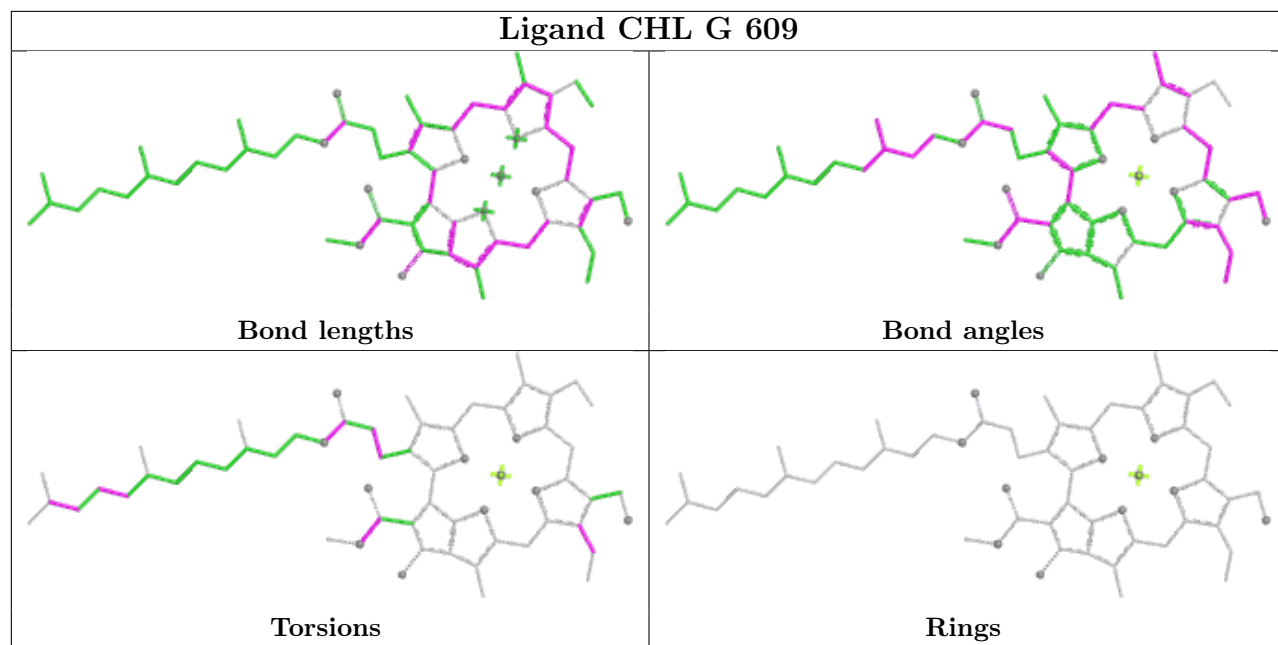
Ligand CLA g 604

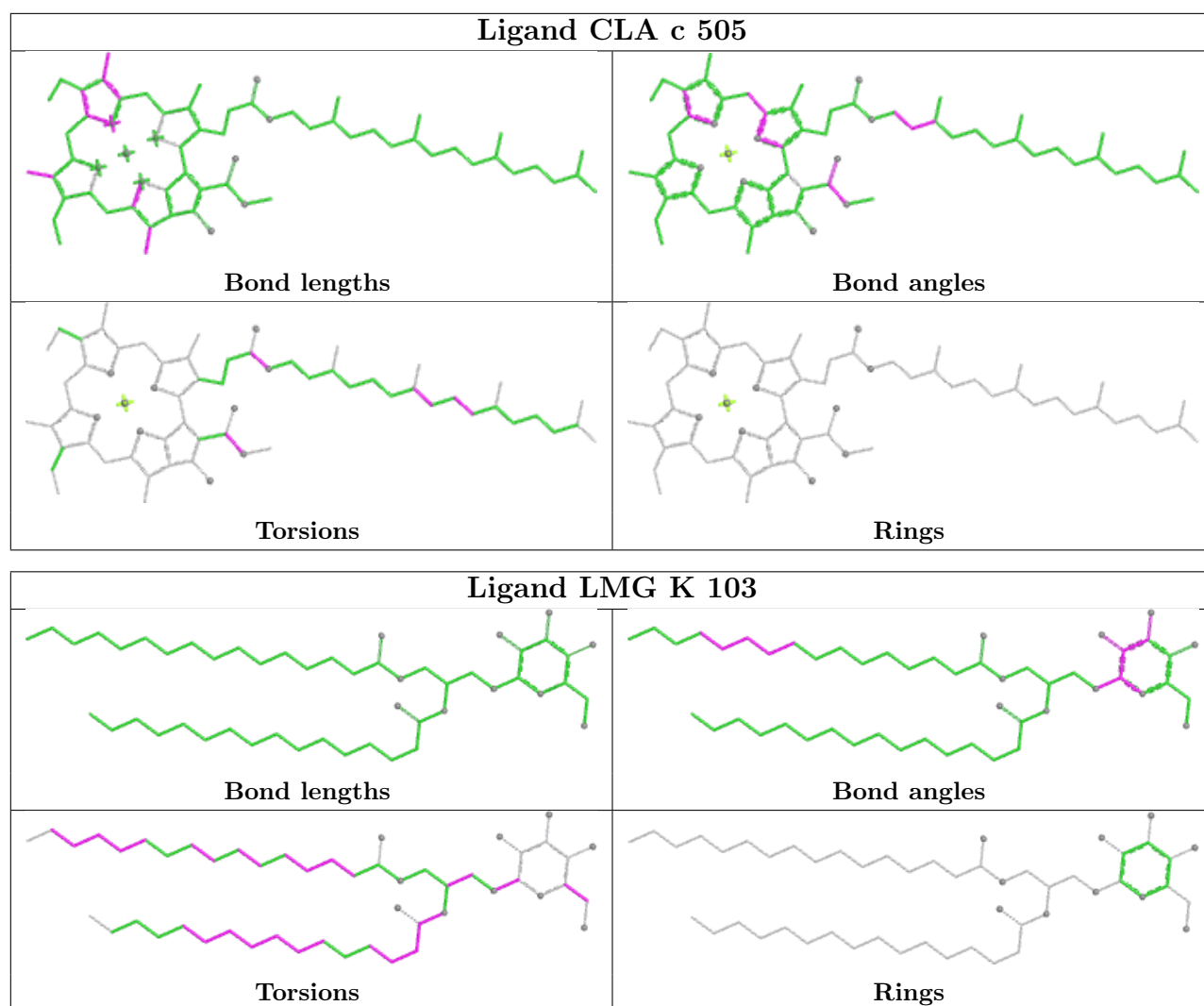


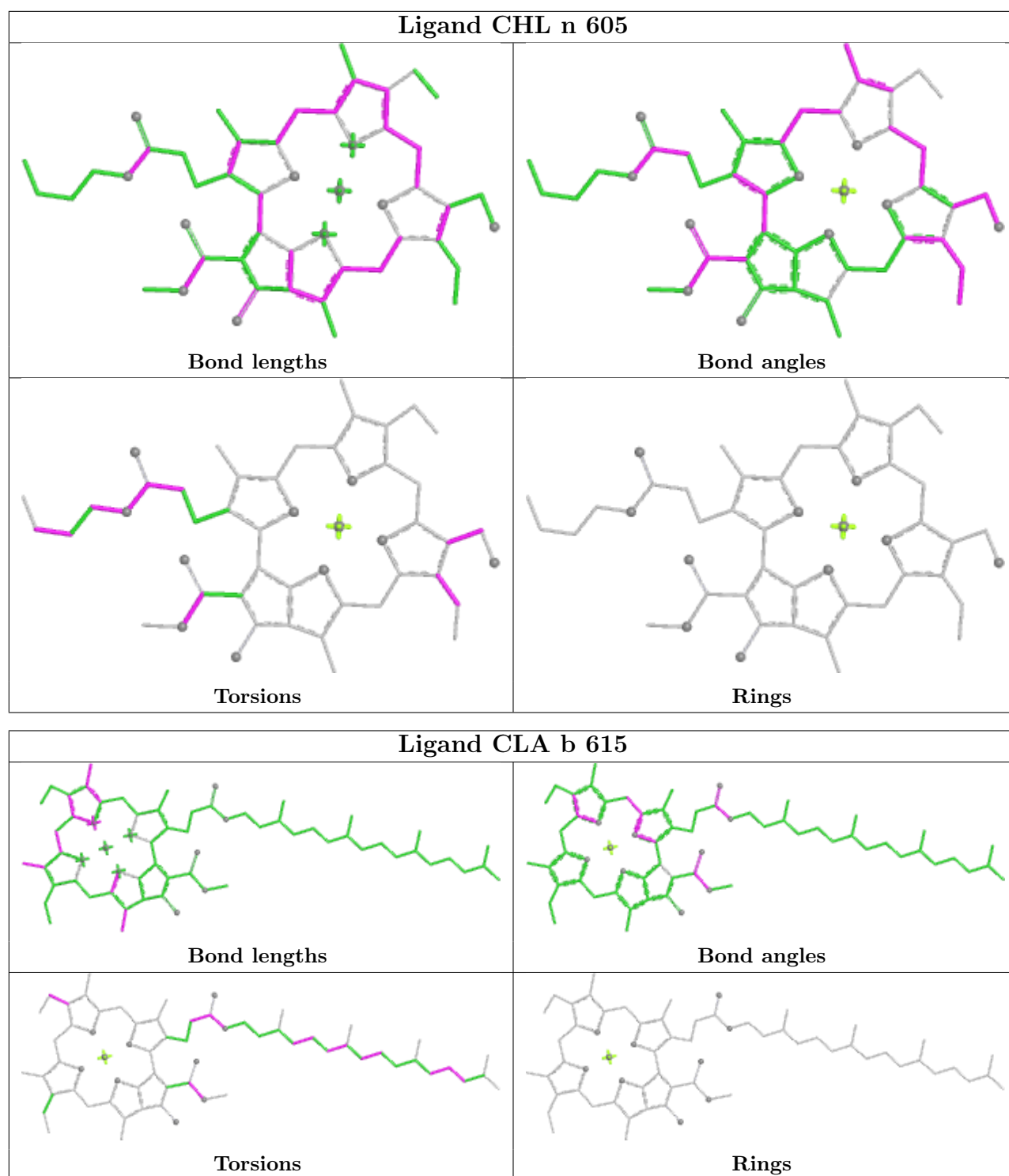
Ligand CLA c 510



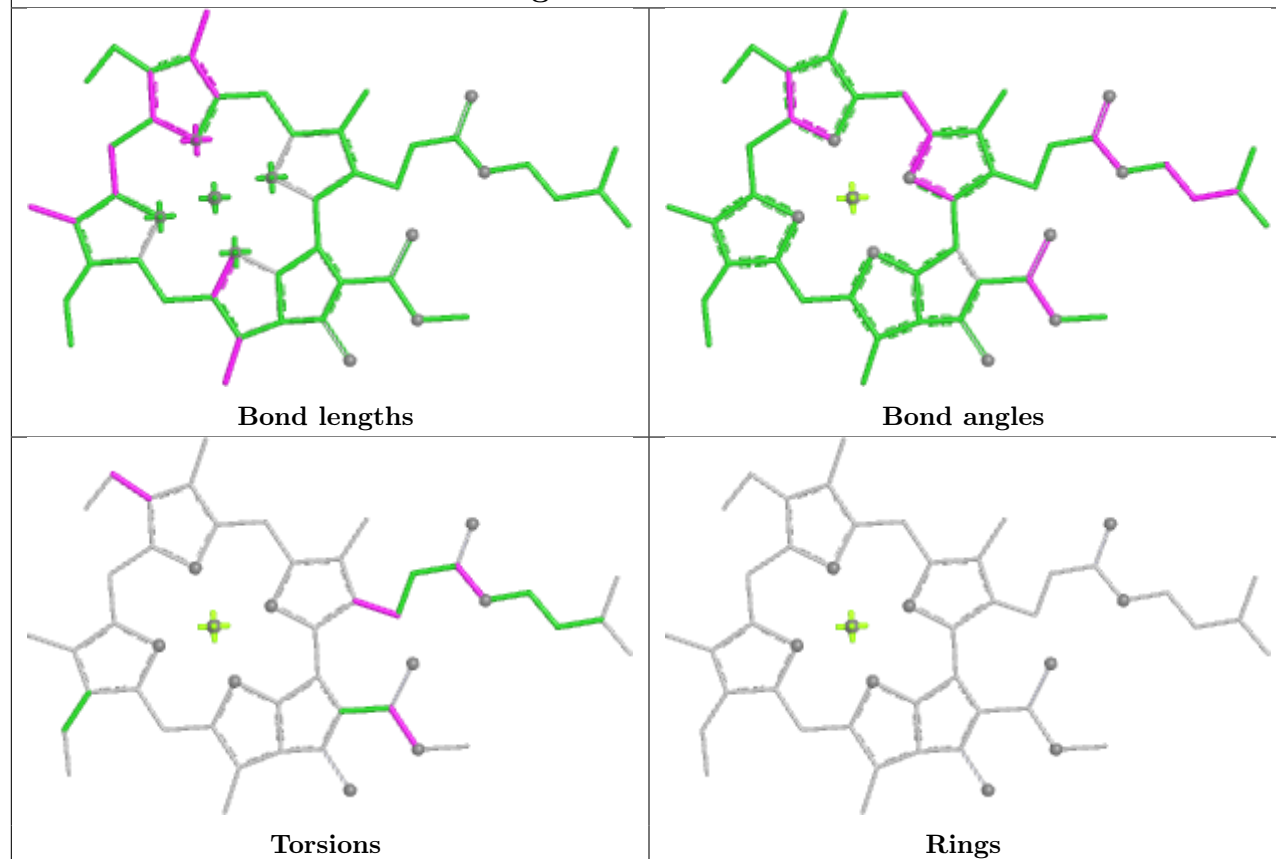
Ligand CLA c 512**Ligand CLA r 310**



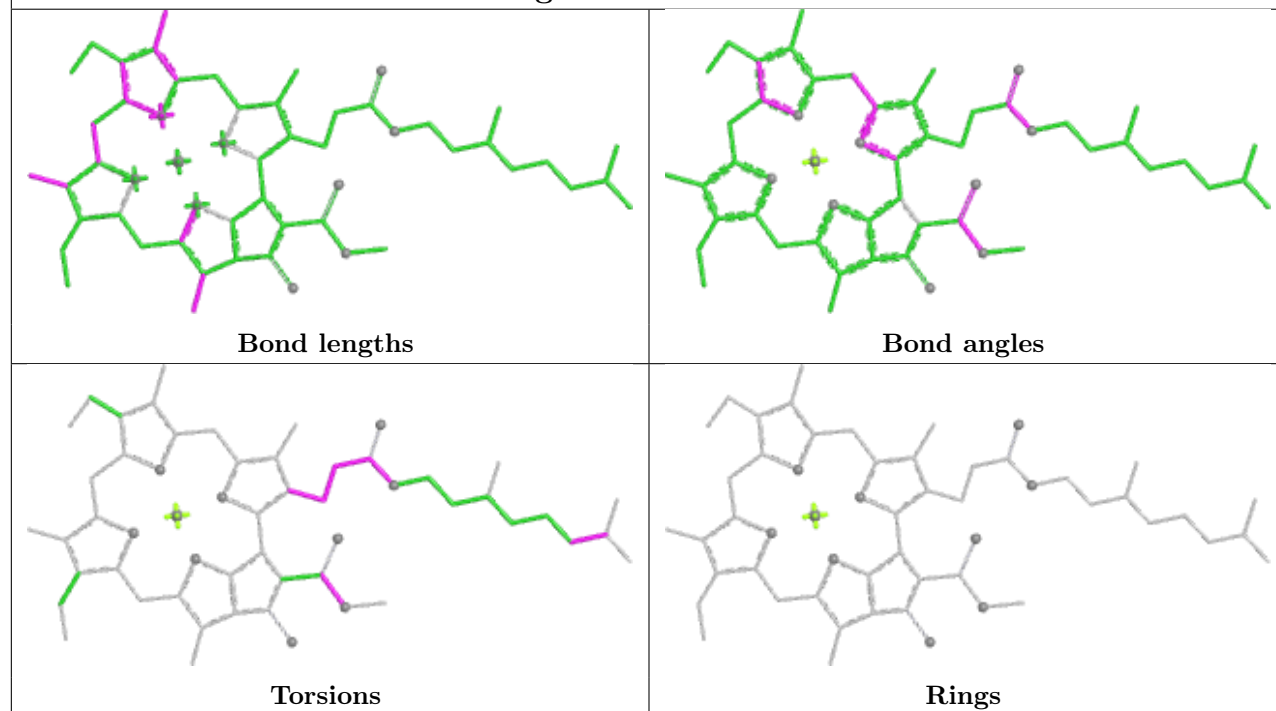


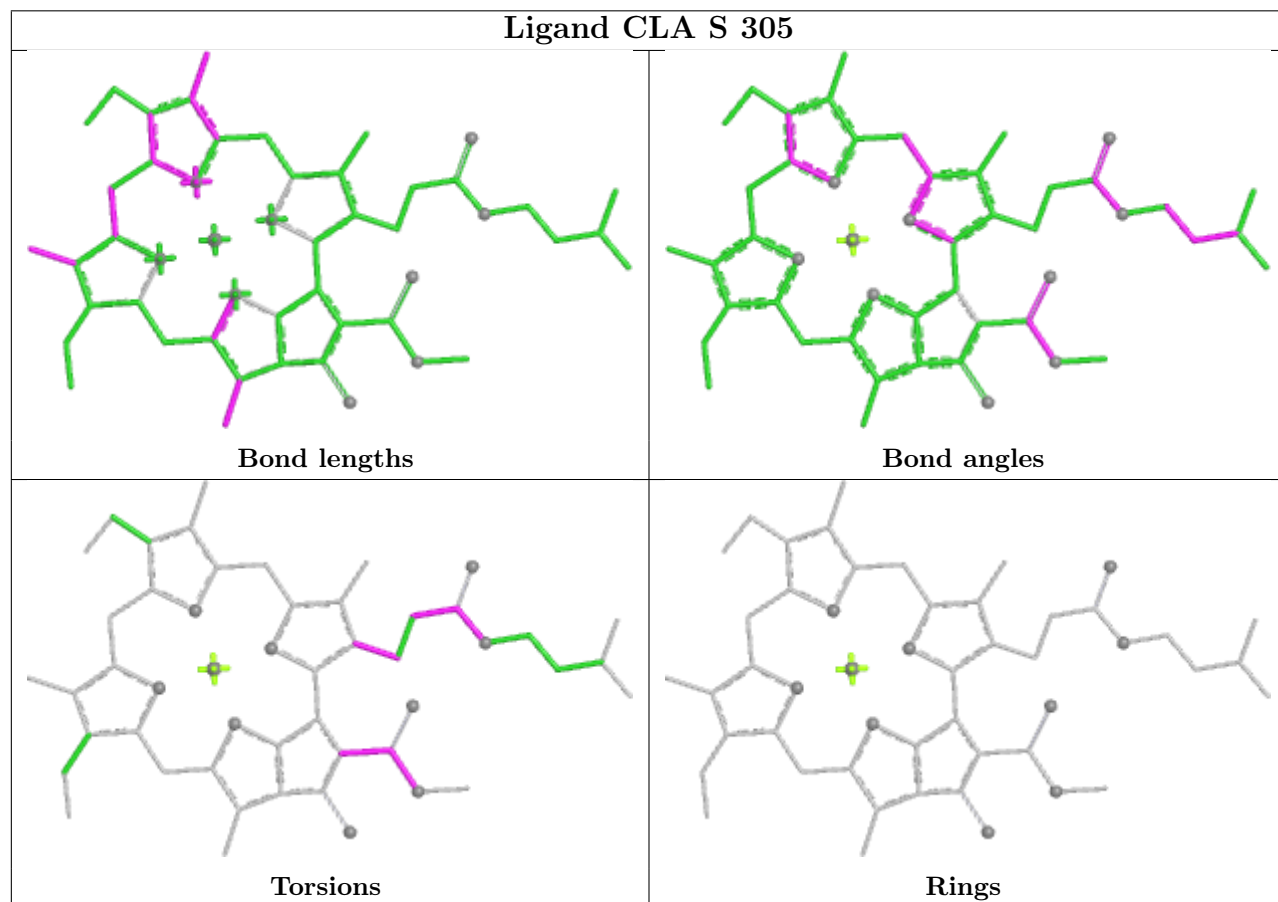
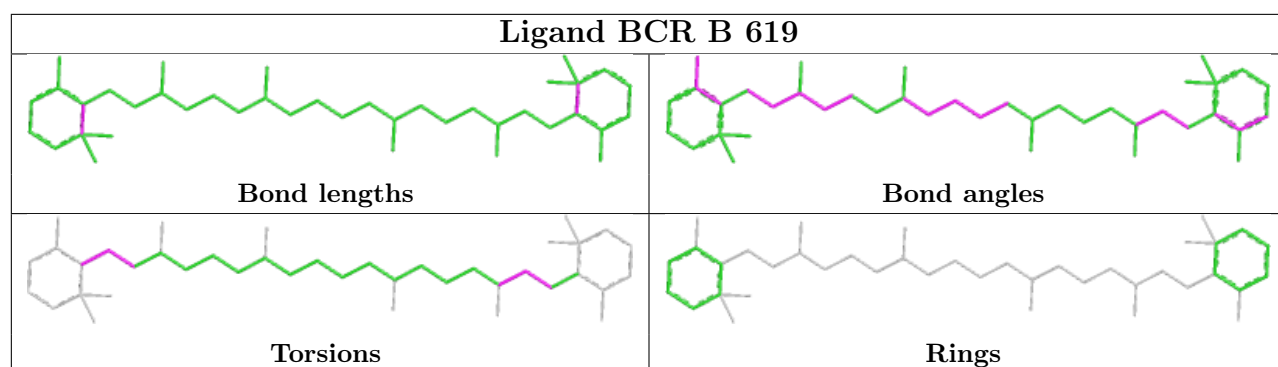


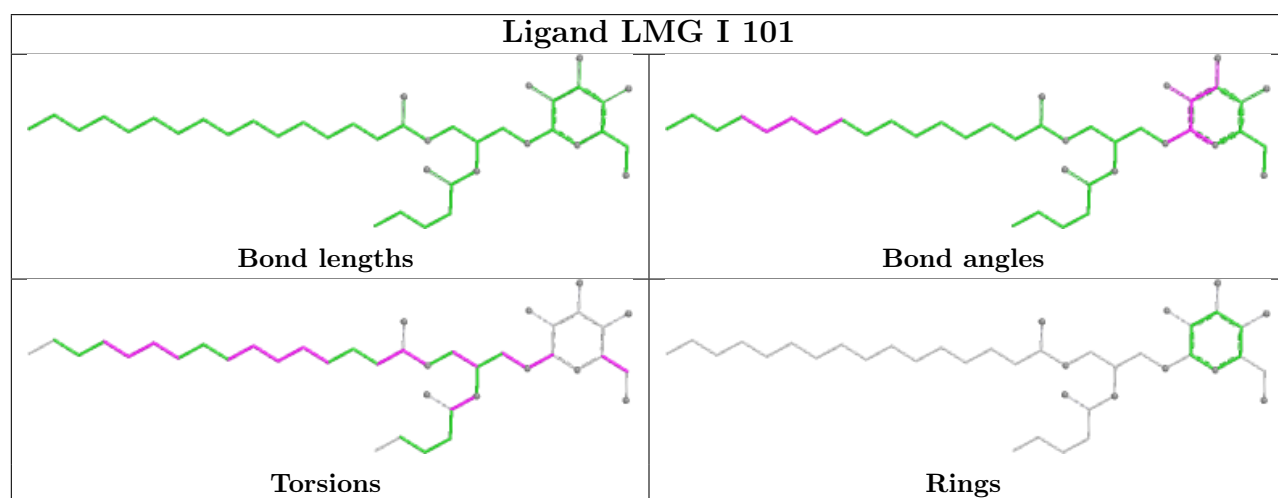
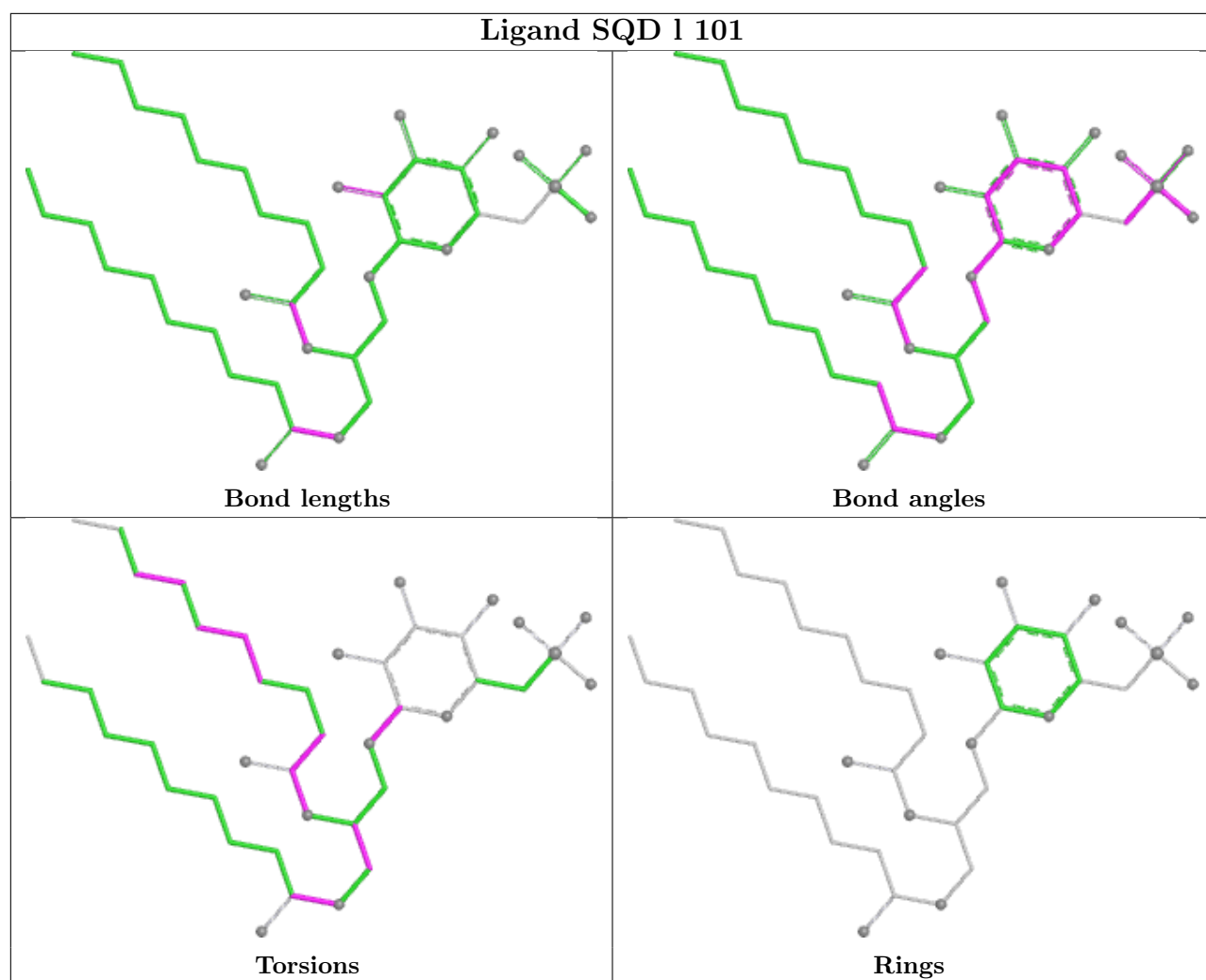
Ligand CLA A 407

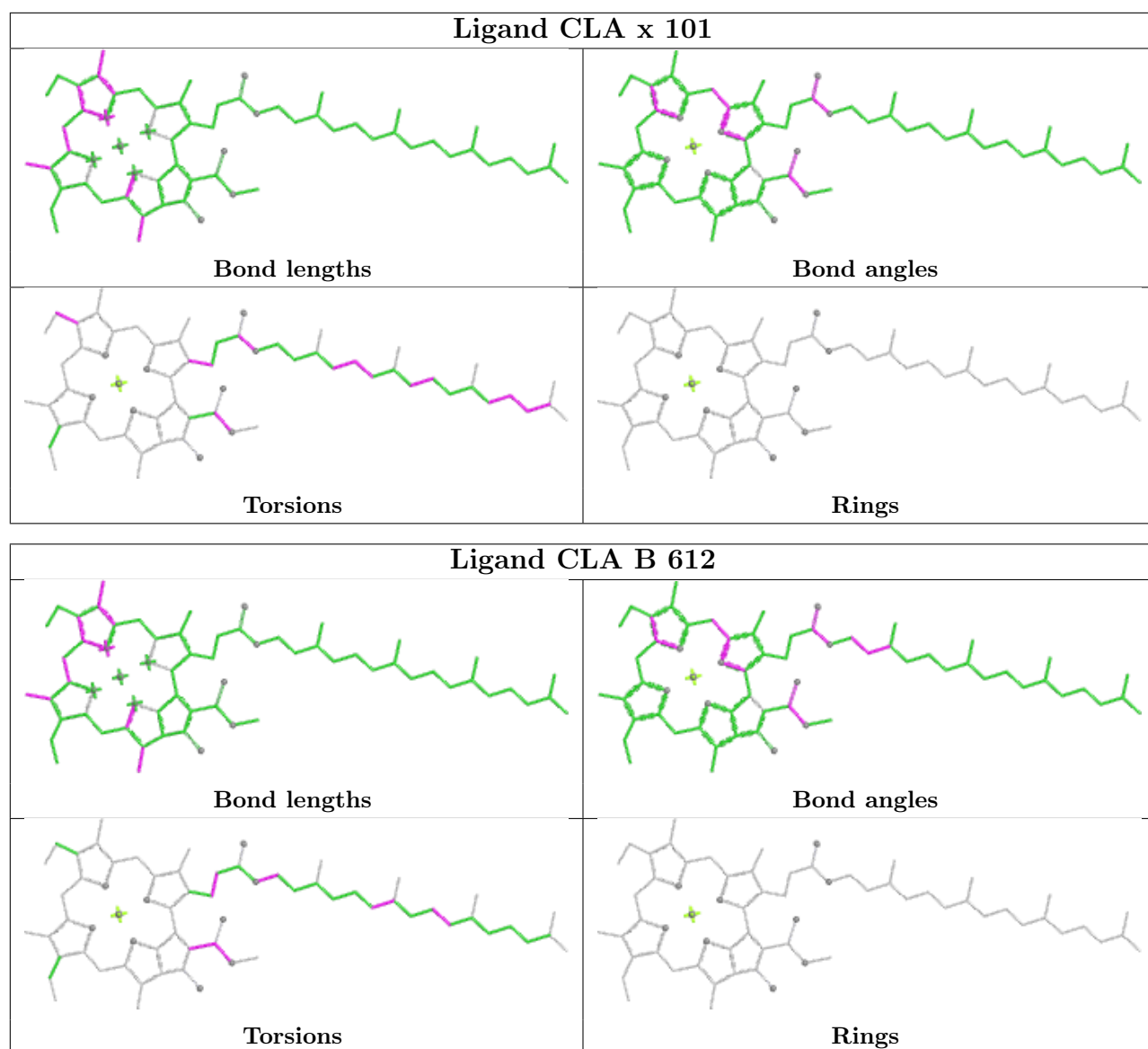


Ligand CLA S 313

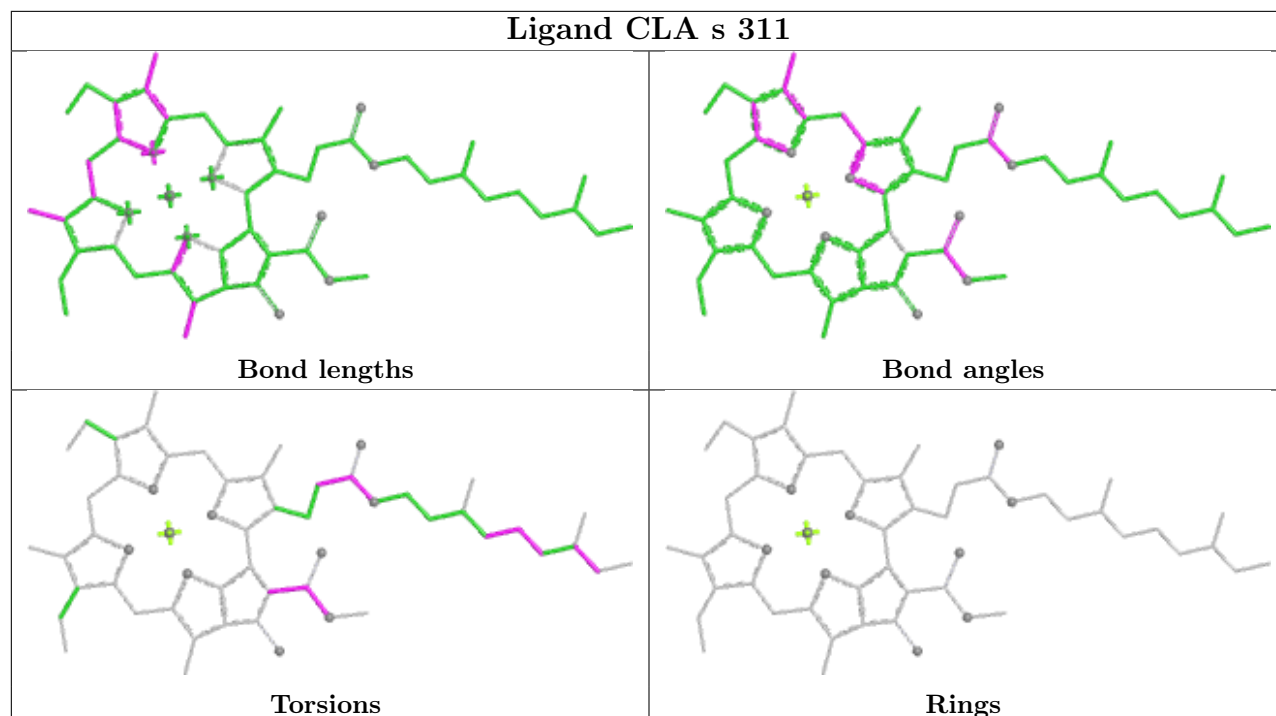




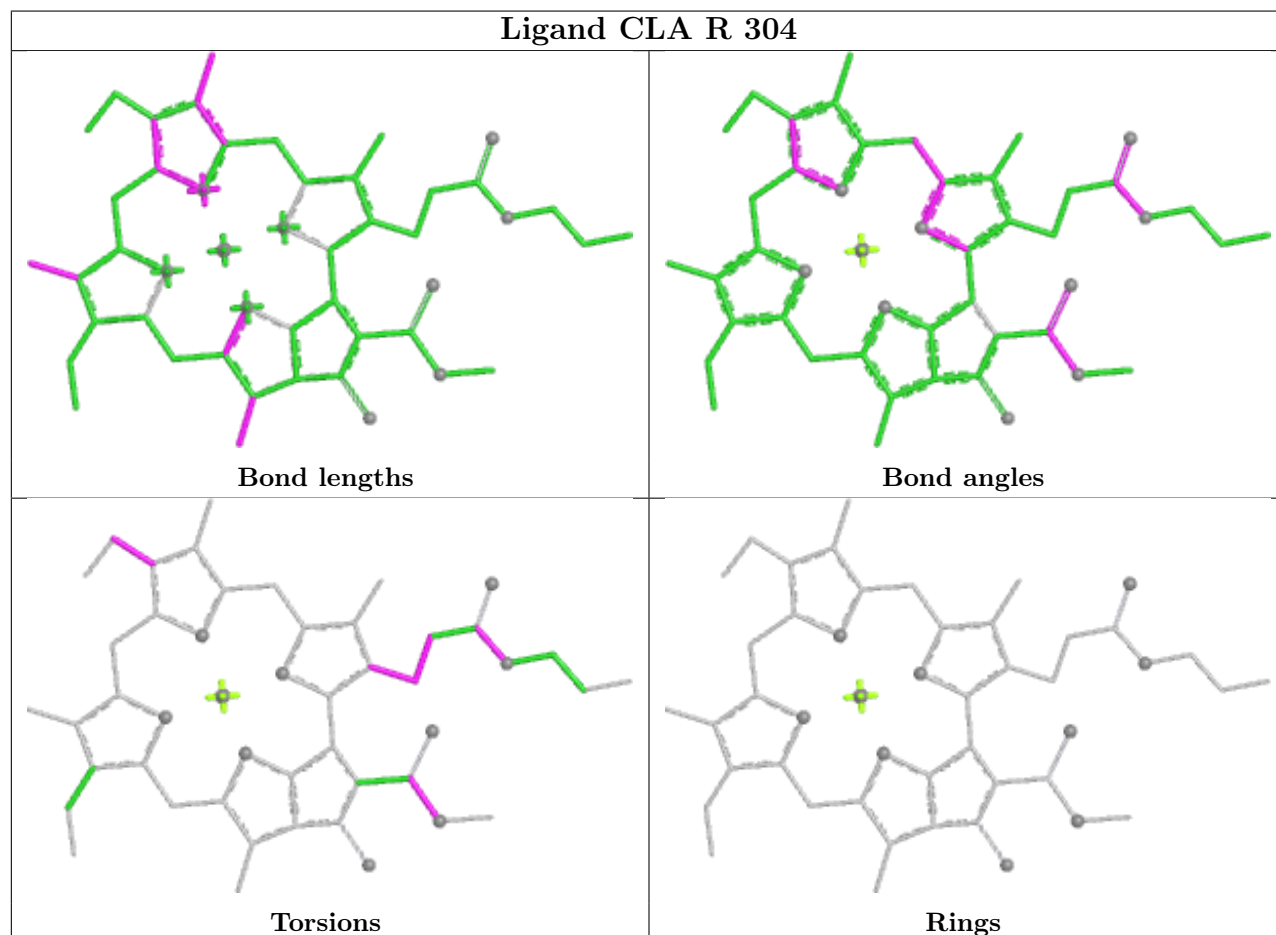


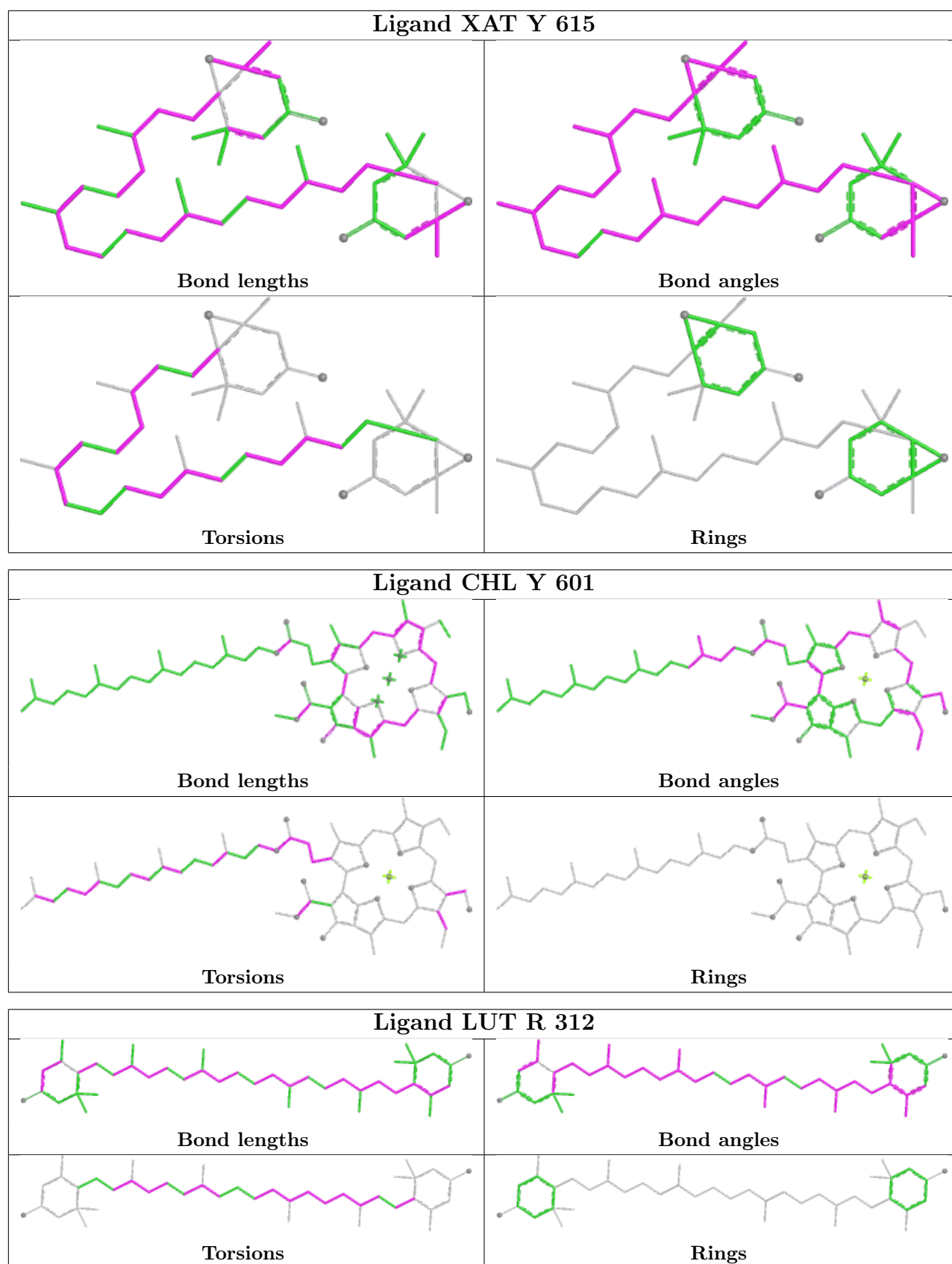


Ligand CLA s 311

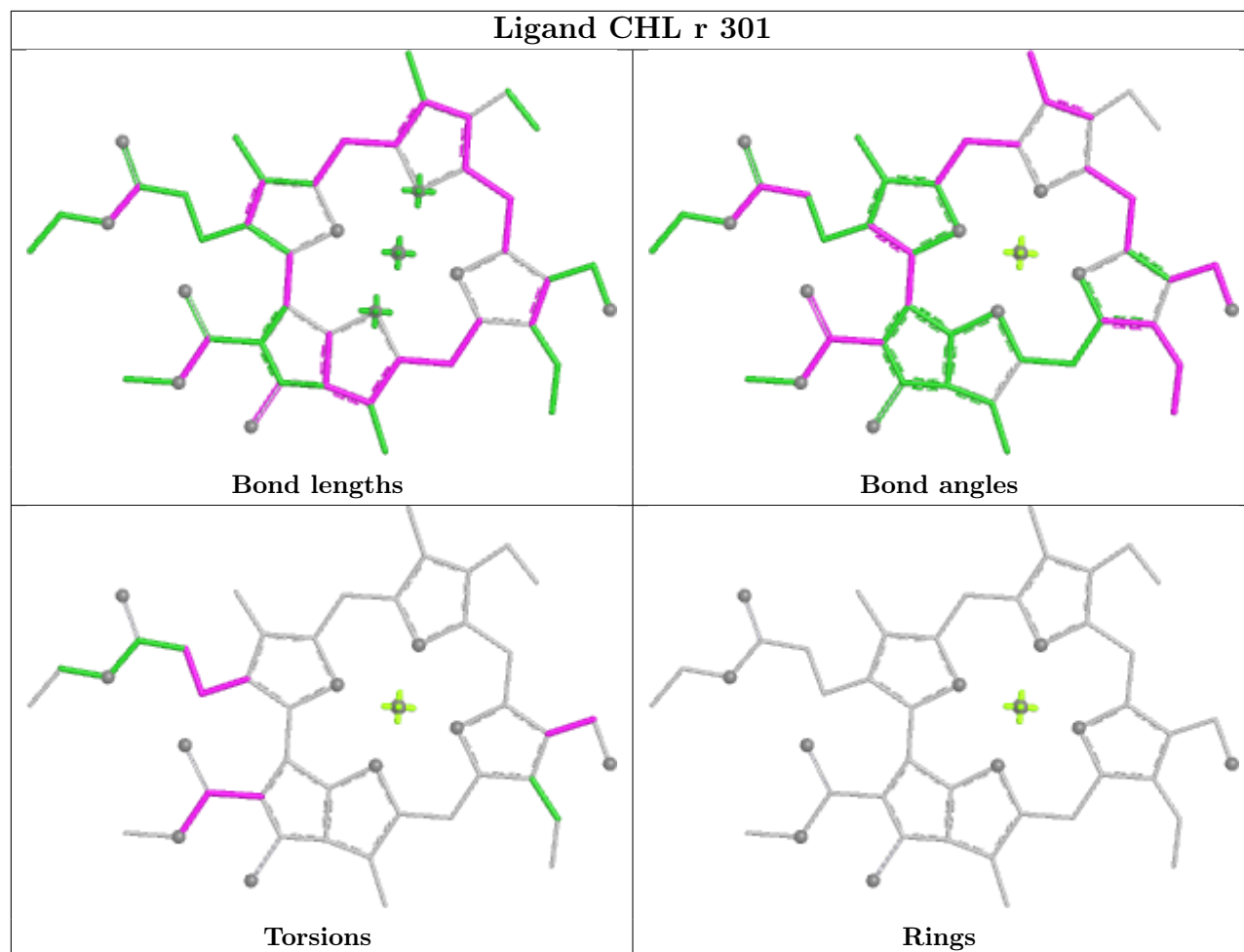


Ligand CLA R 304

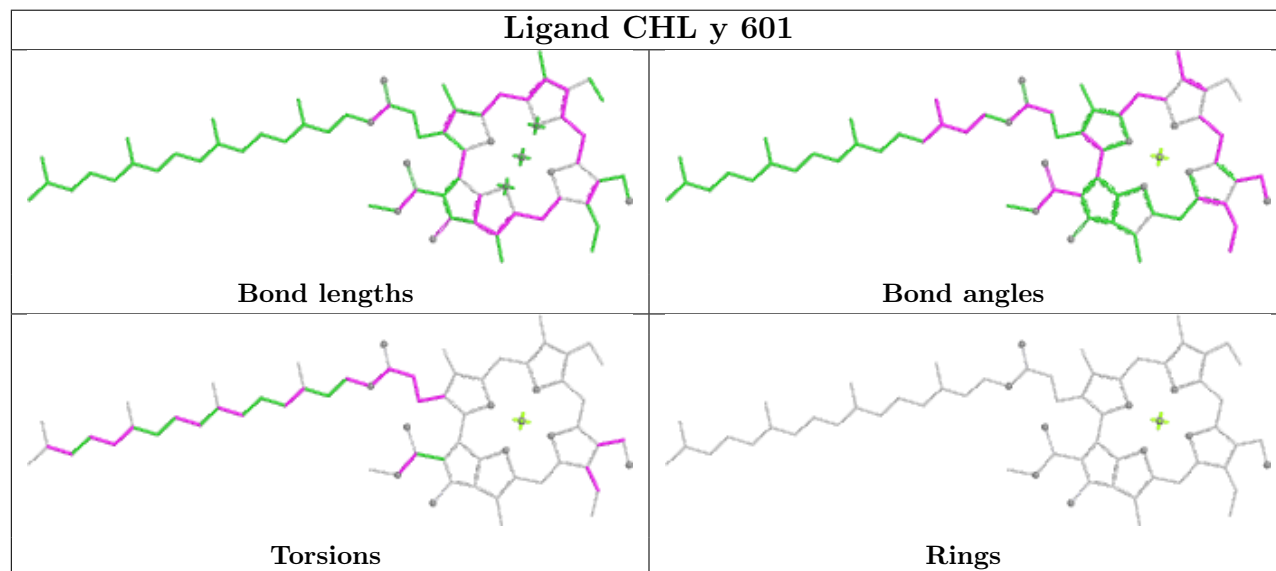


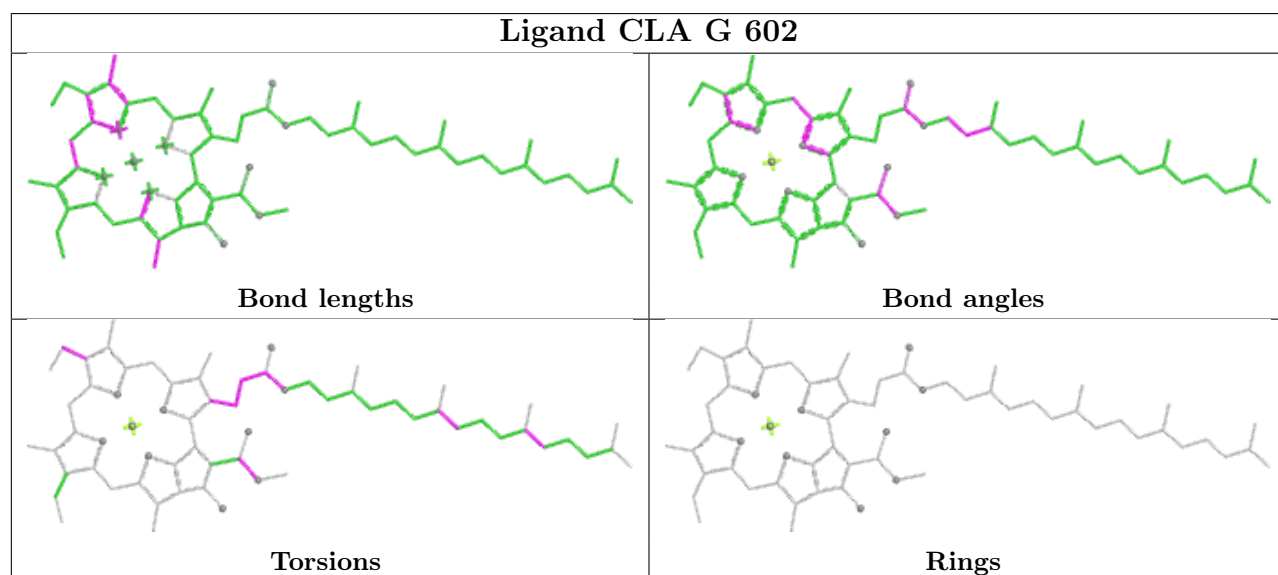
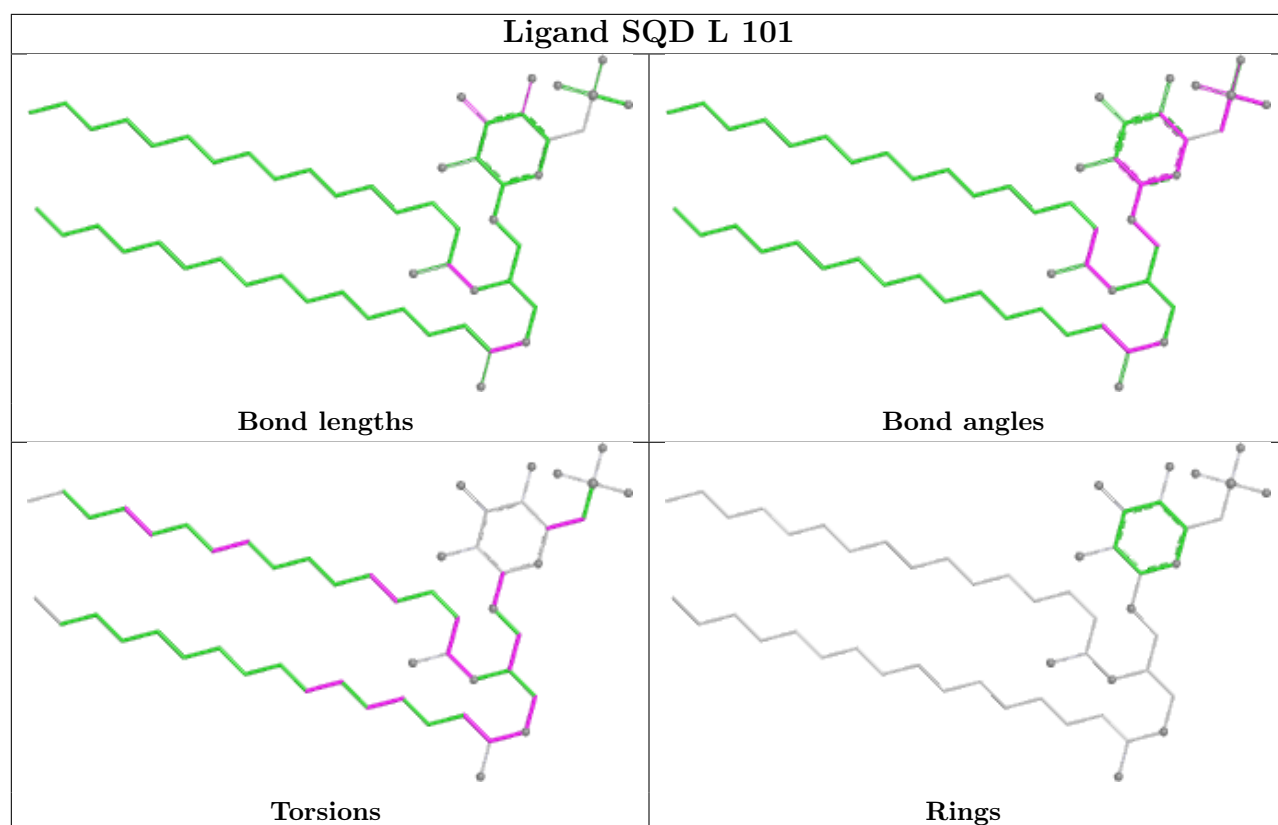


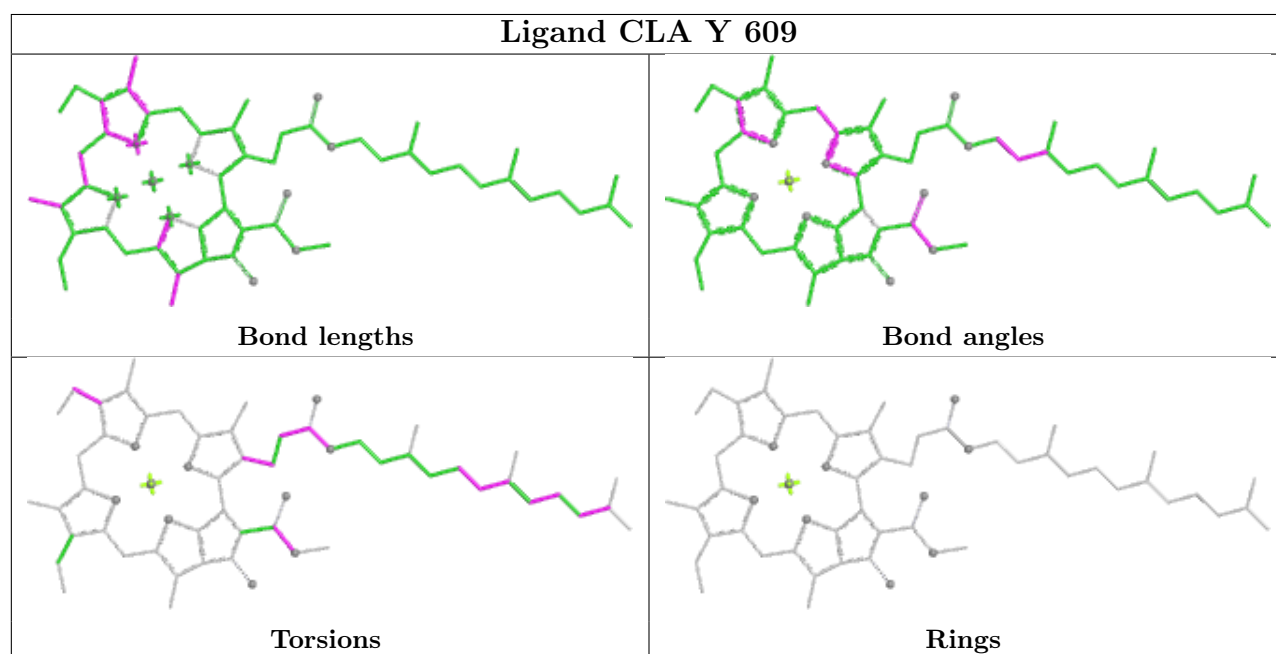
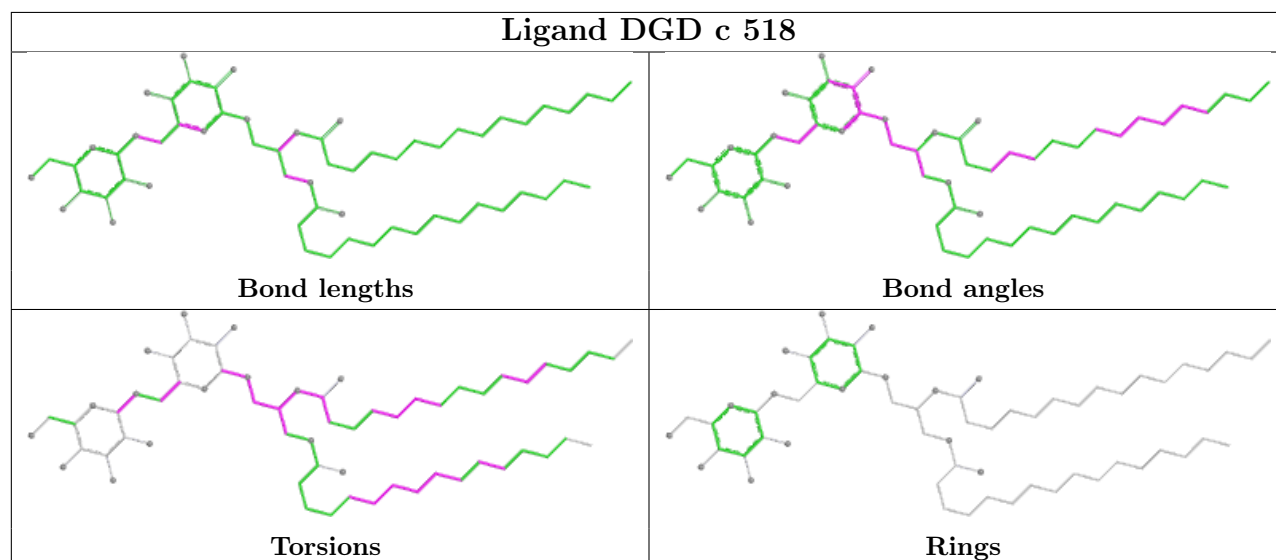
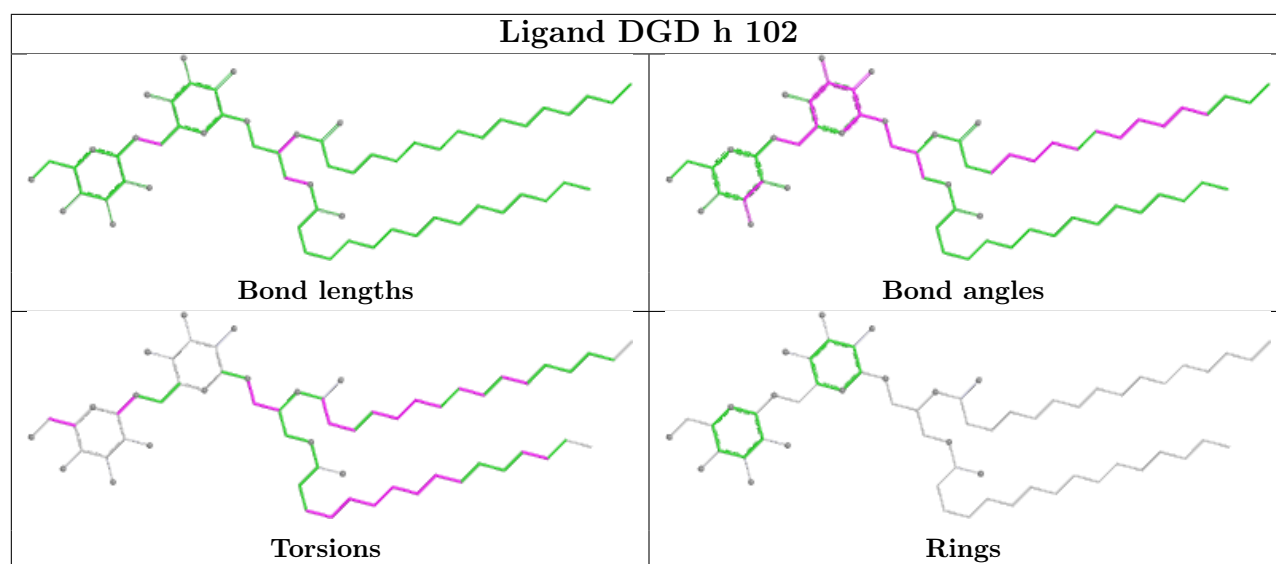
Ligand CHL r 301

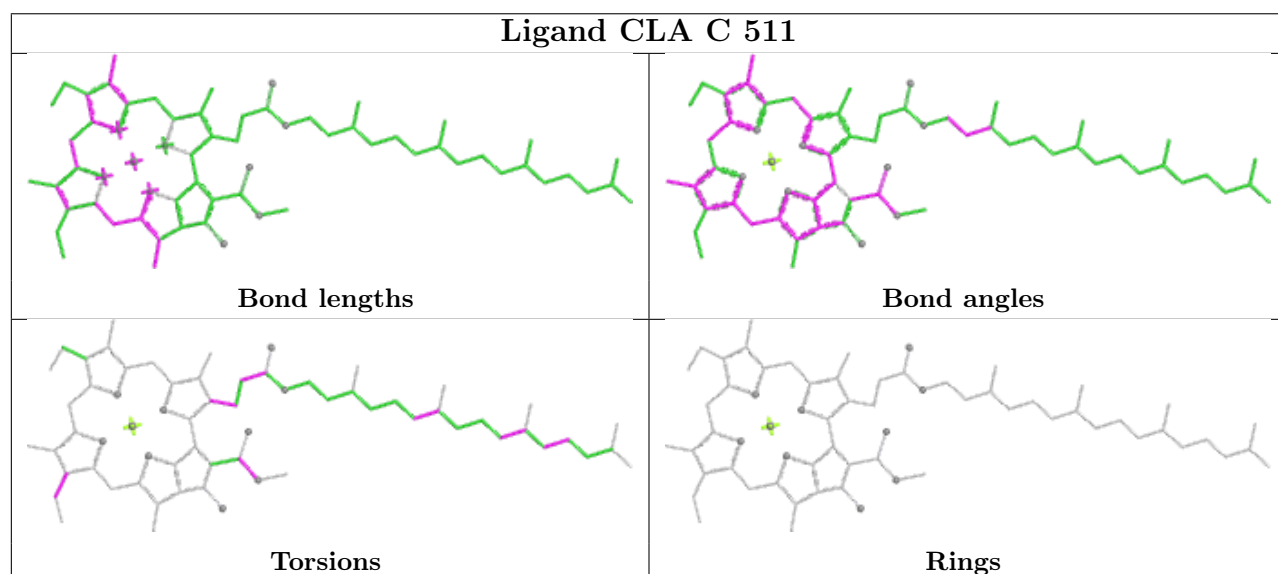
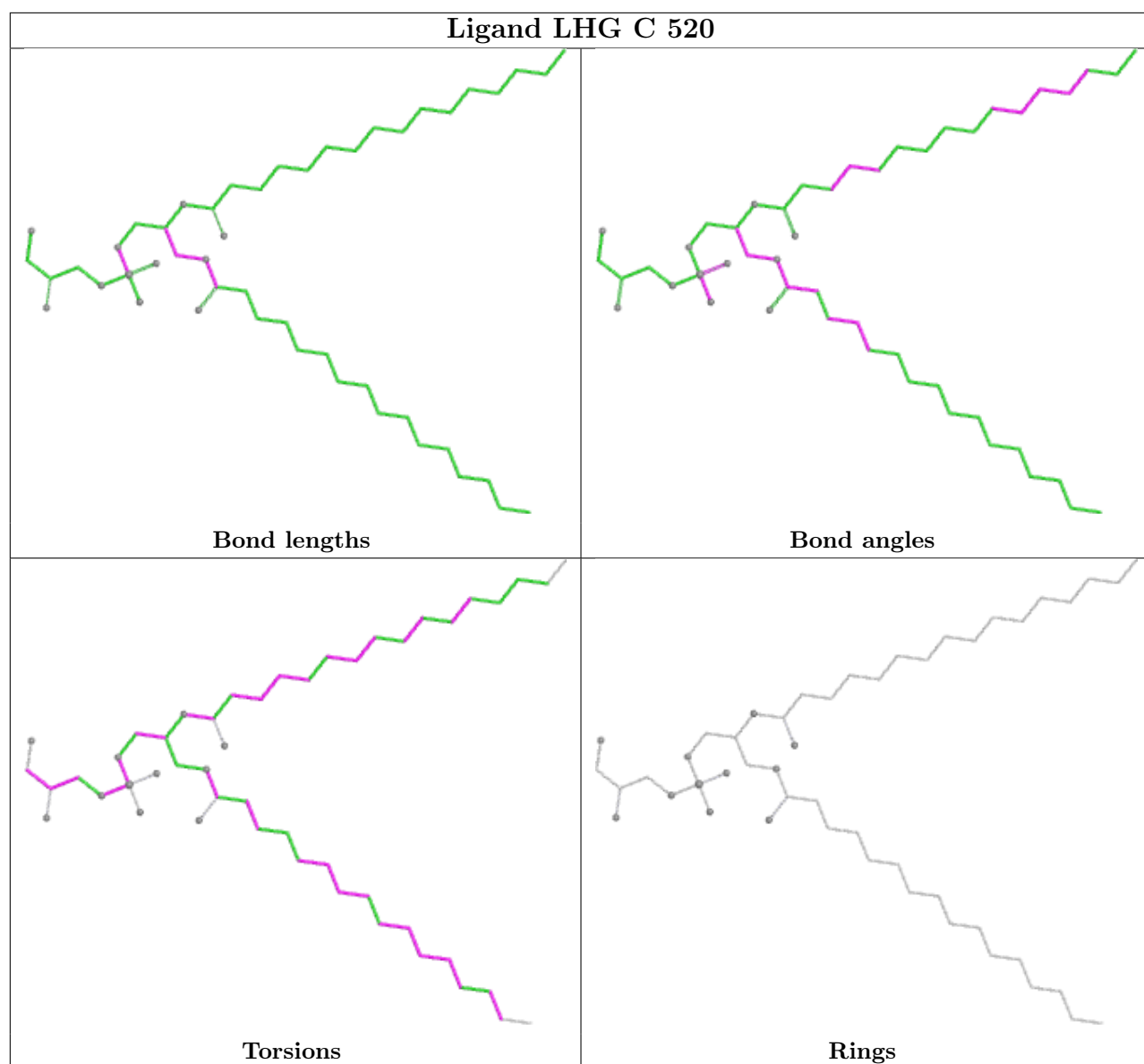


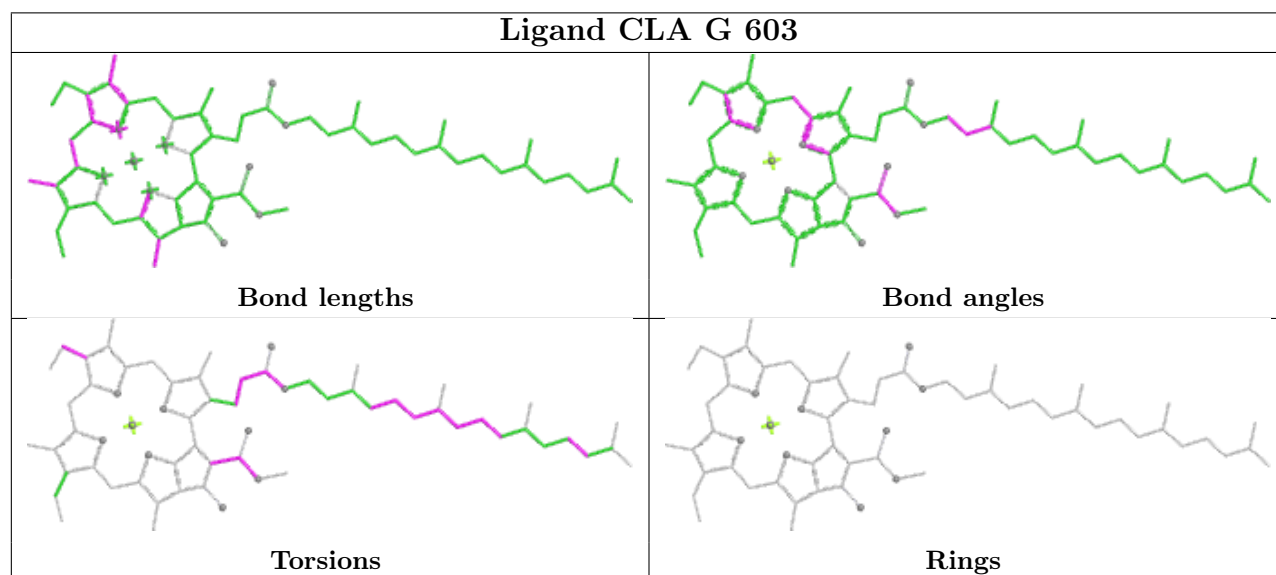
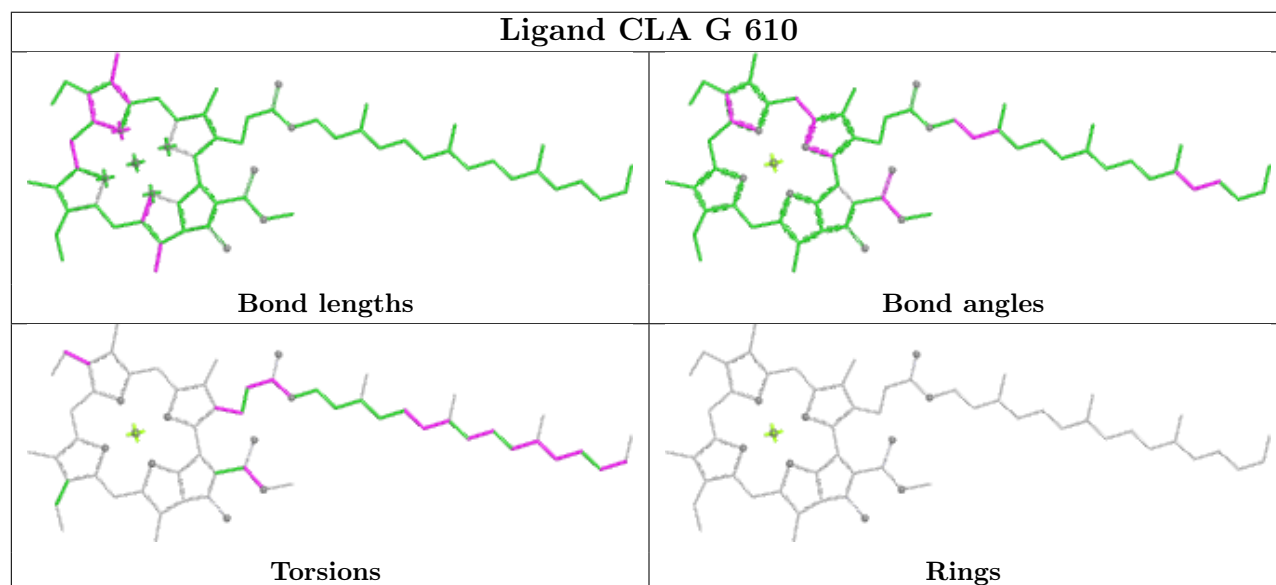
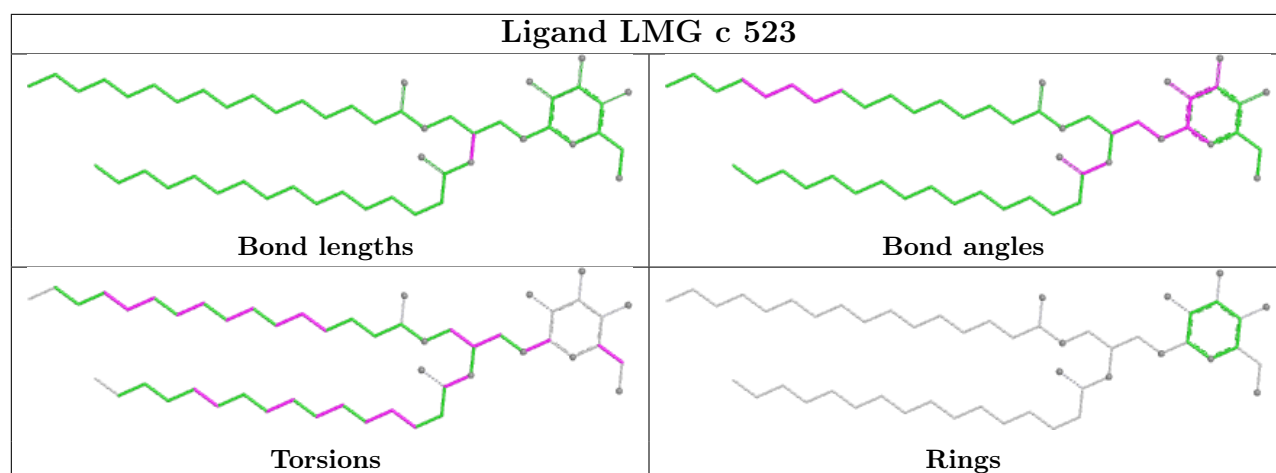
Ligand CHL y 601



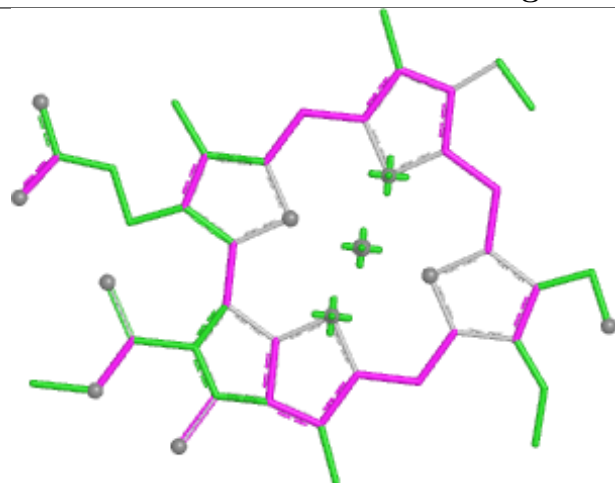




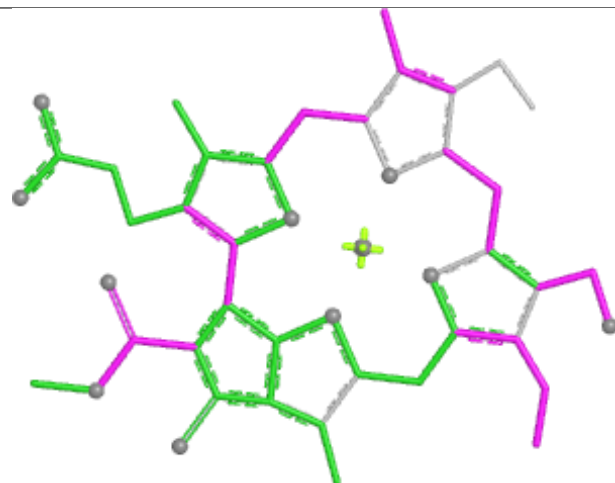




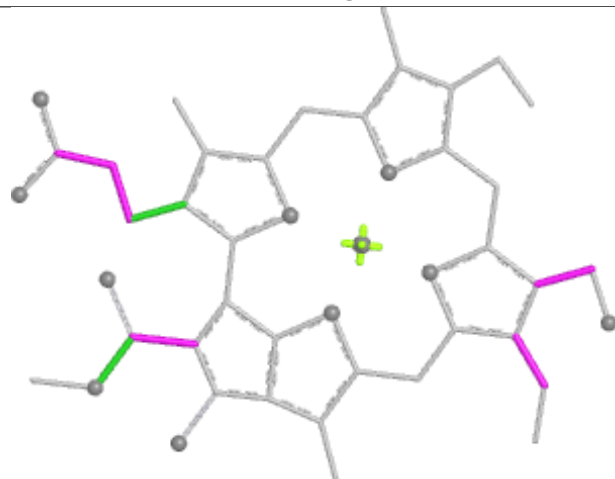
Ligand CHL s 306



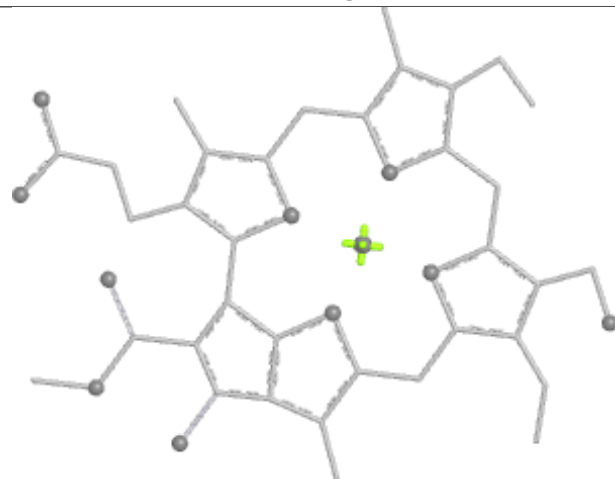
Bond lengths



Bond angles

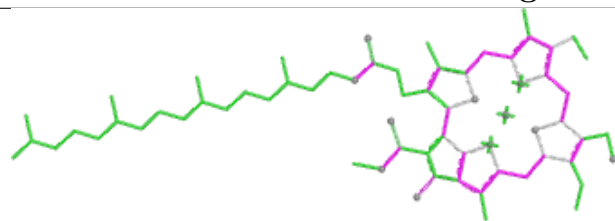


Torsions

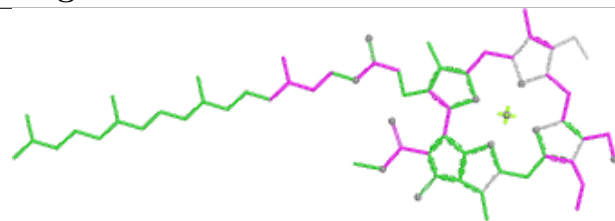


Rings

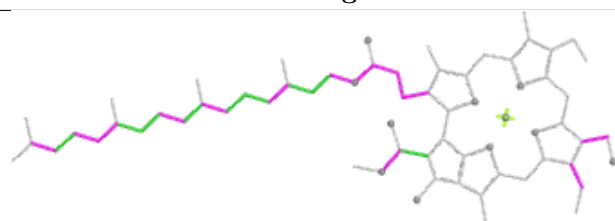
Ligand CHL g 601



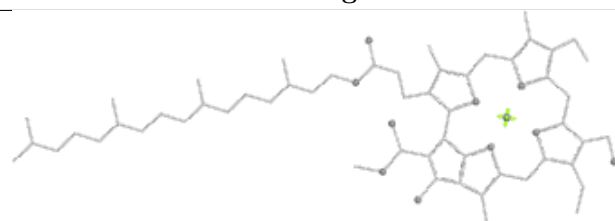
Bond lengths



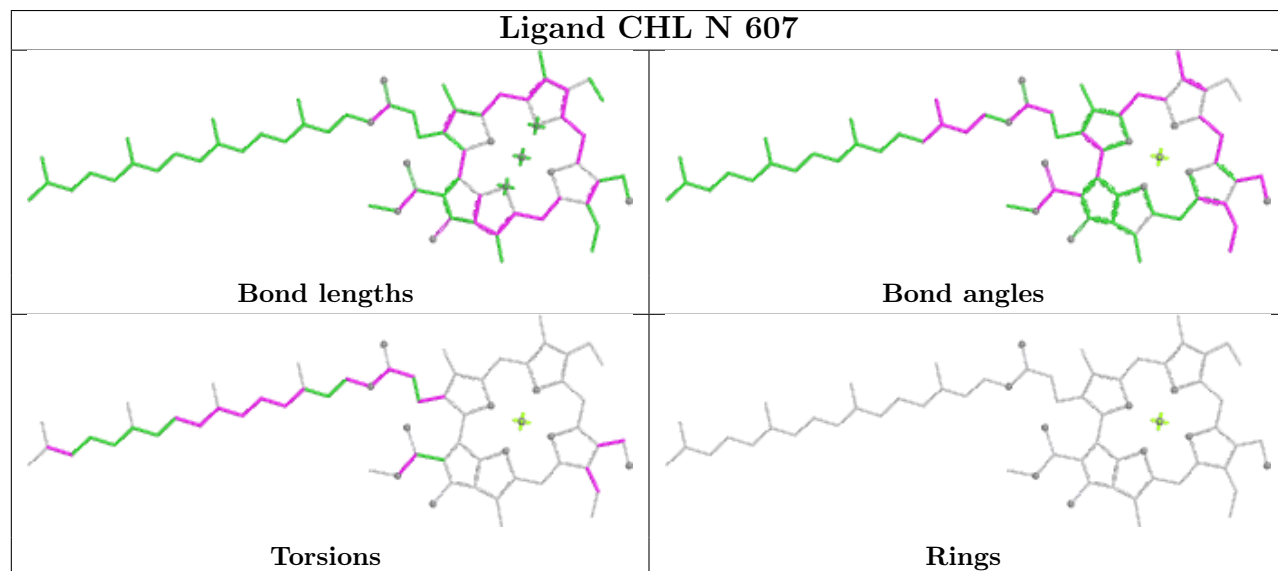
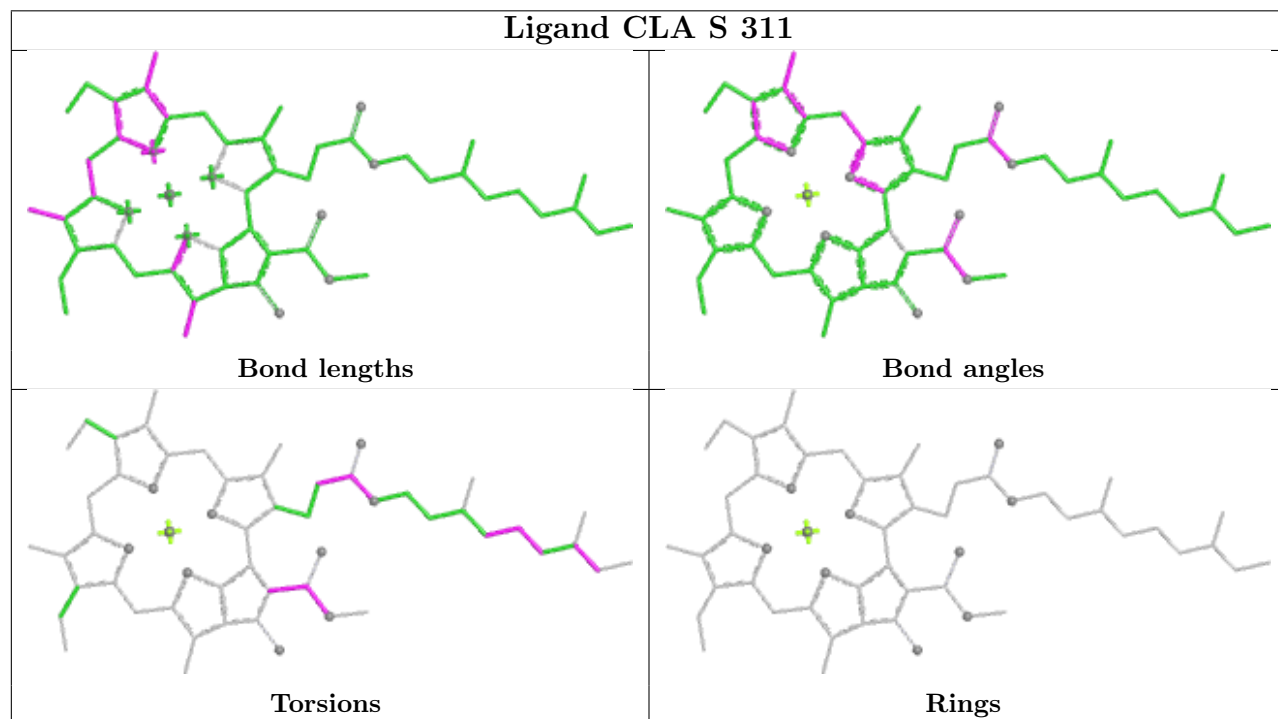
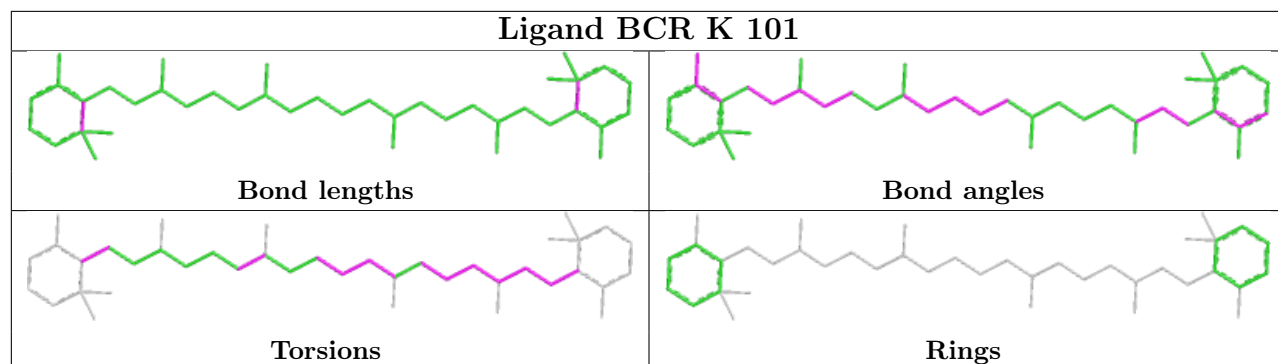
Bond angles

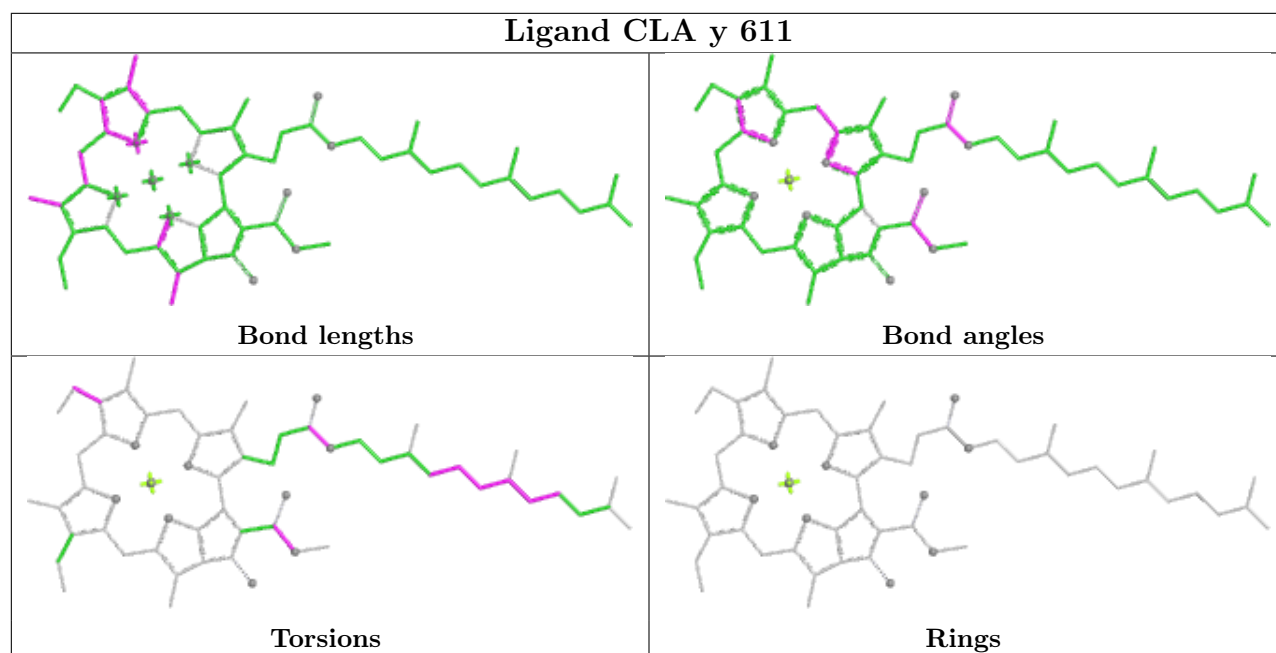
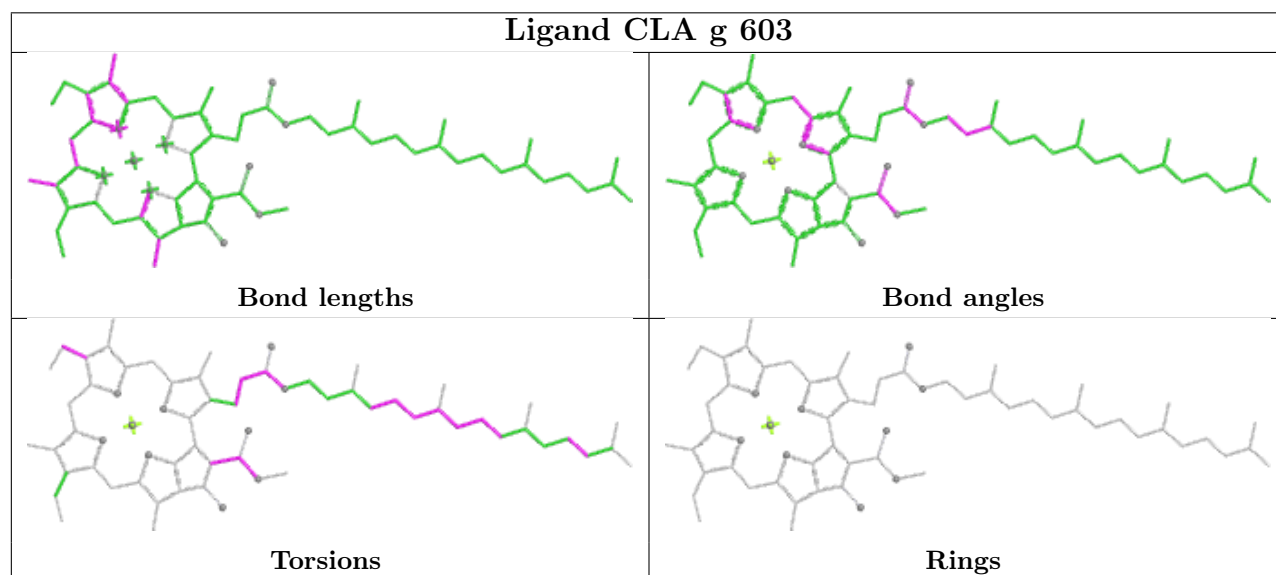
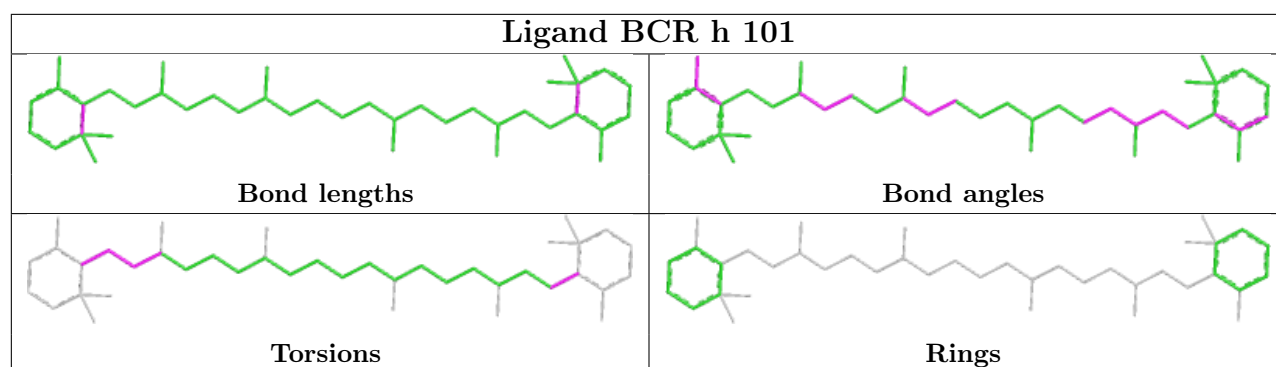


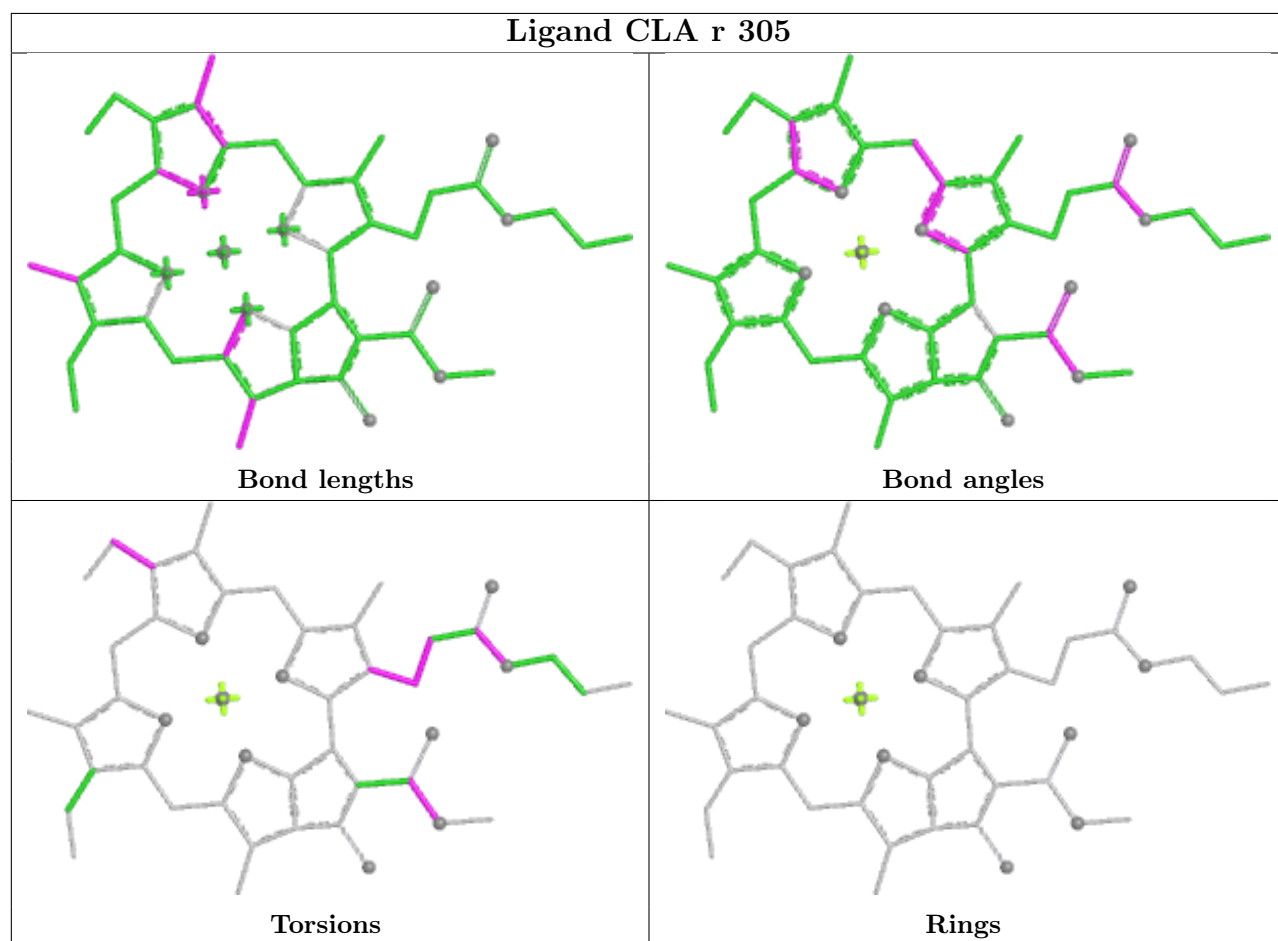
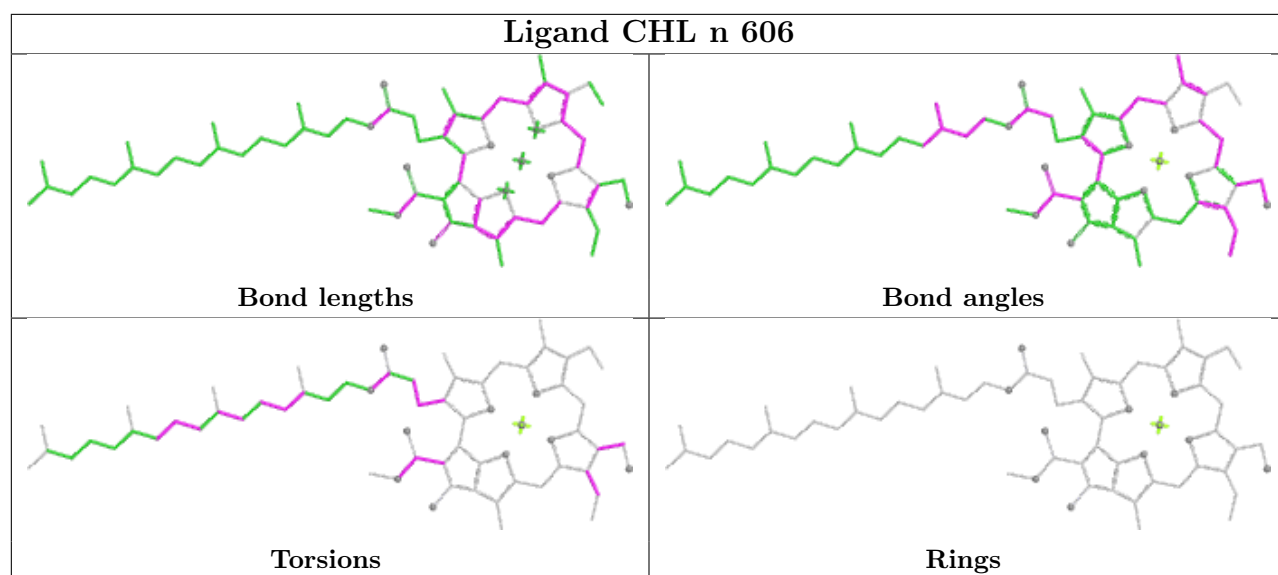
Torsions



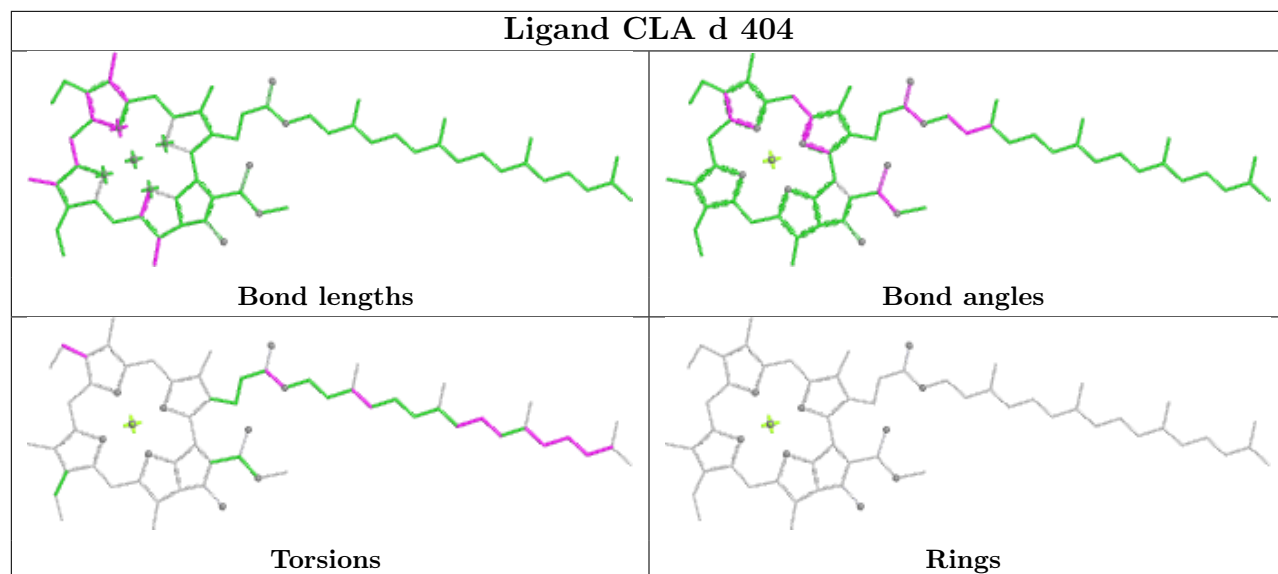
Rings



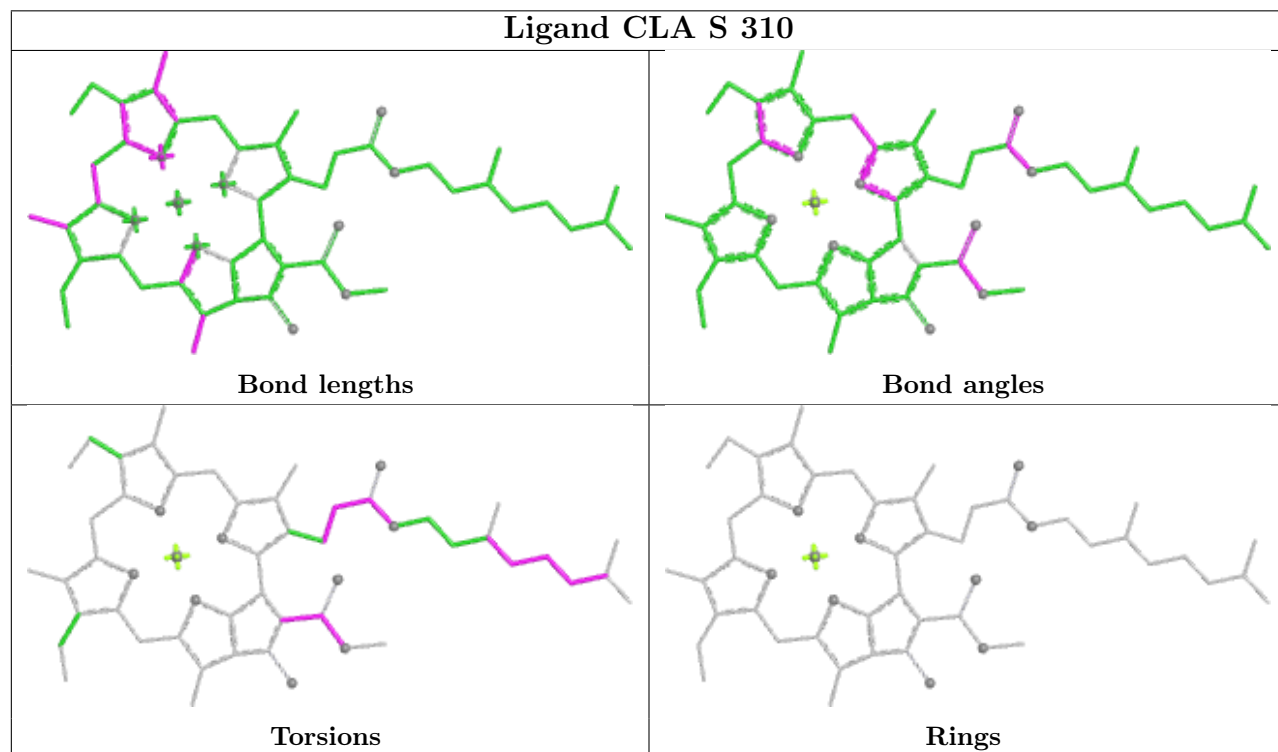


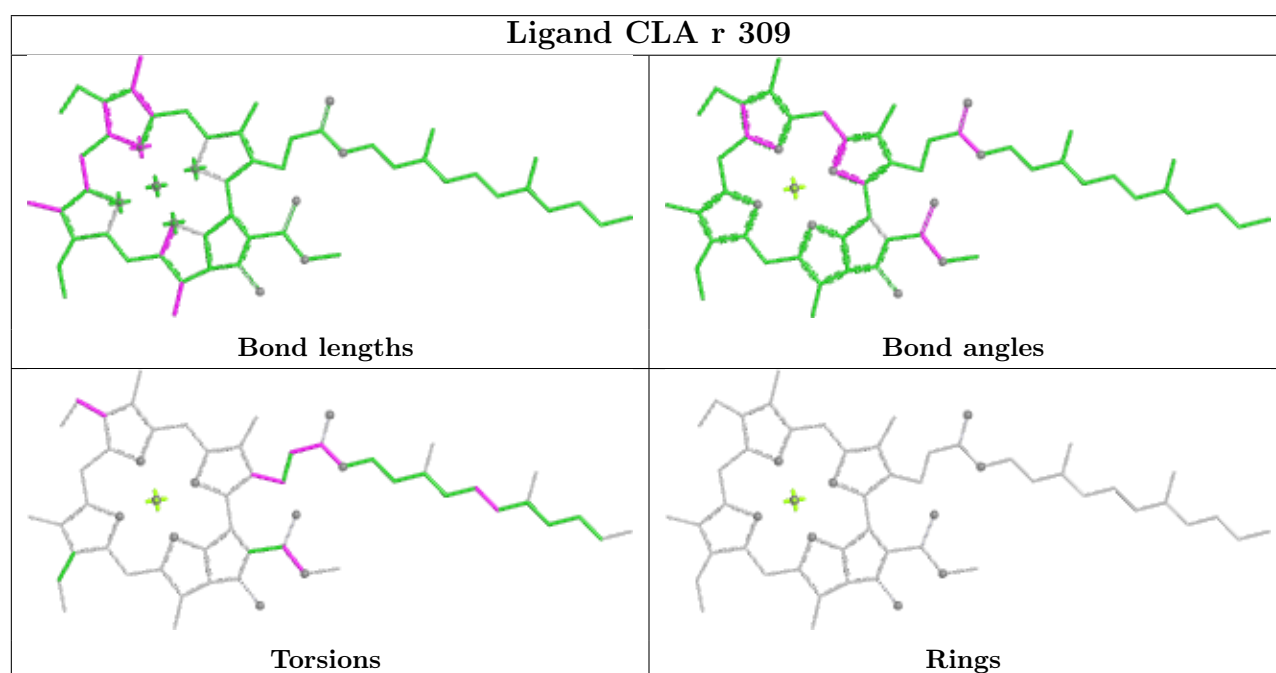
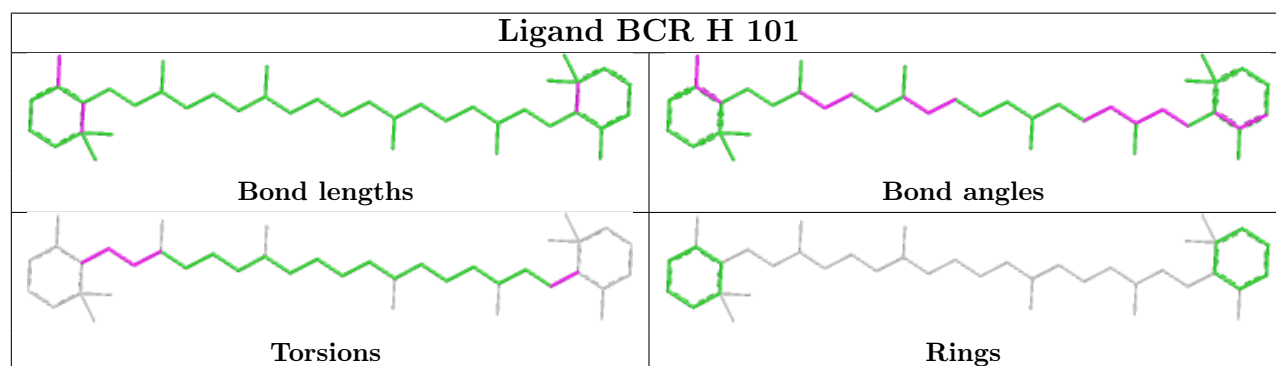
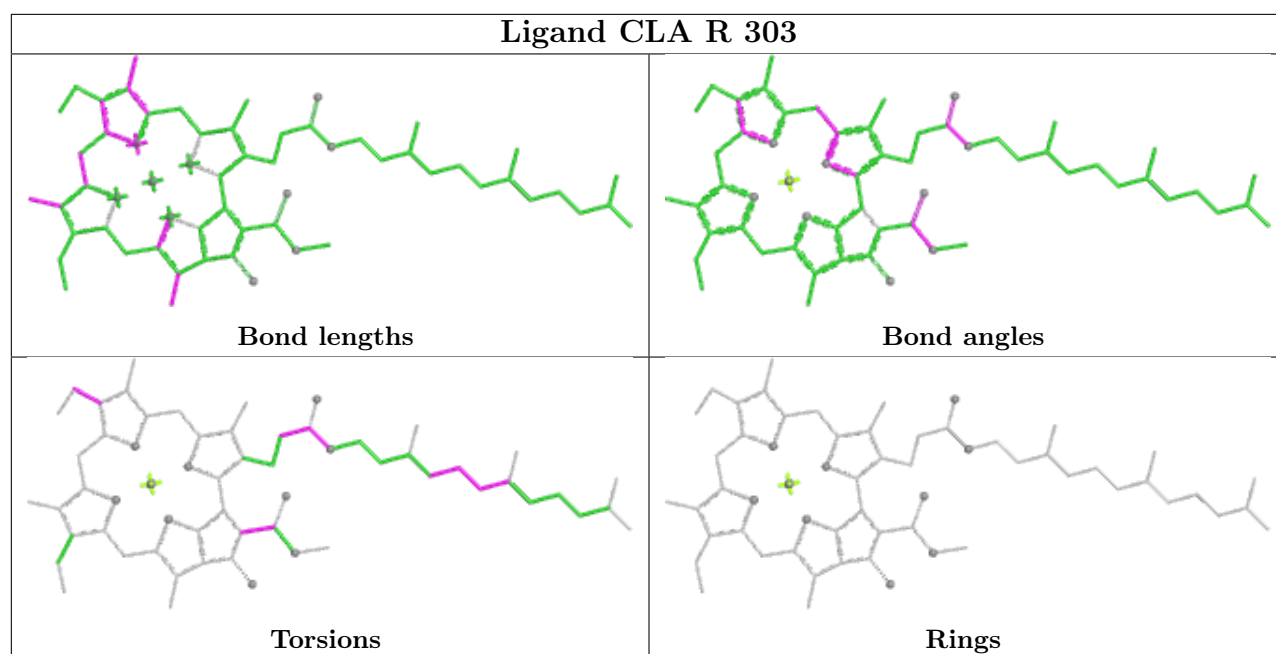


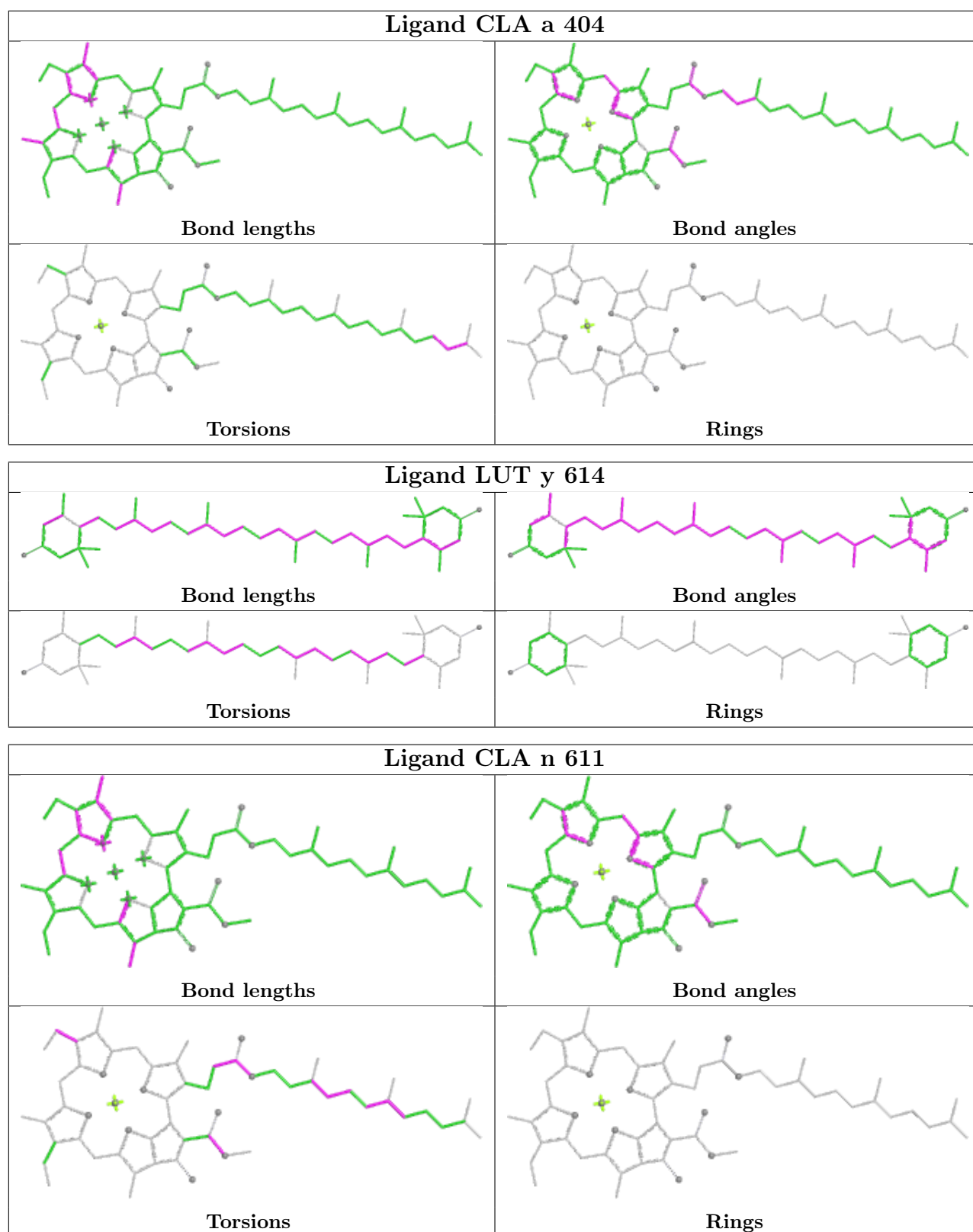
Ligand CLA d 404

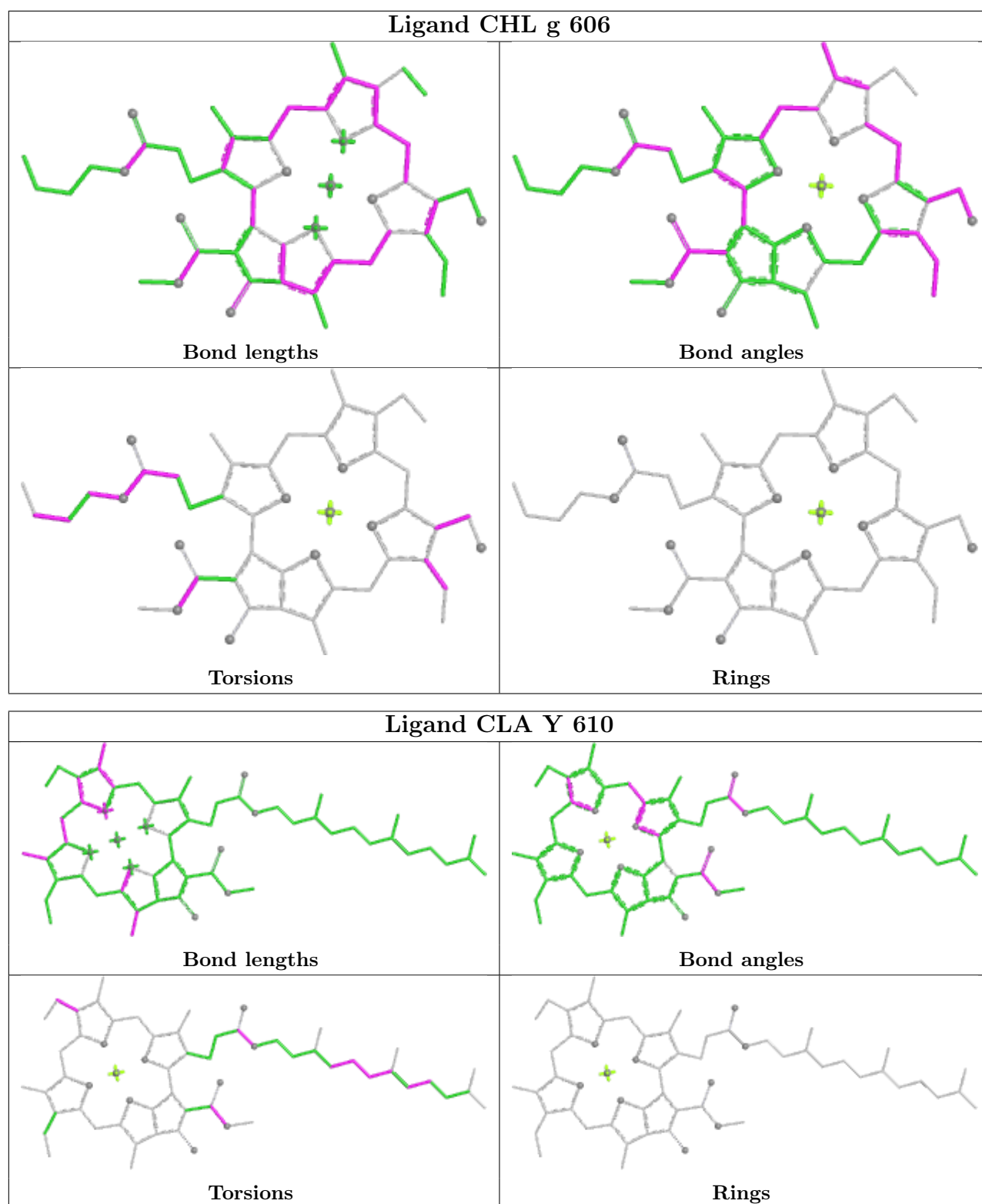


Ligand CLA S 310

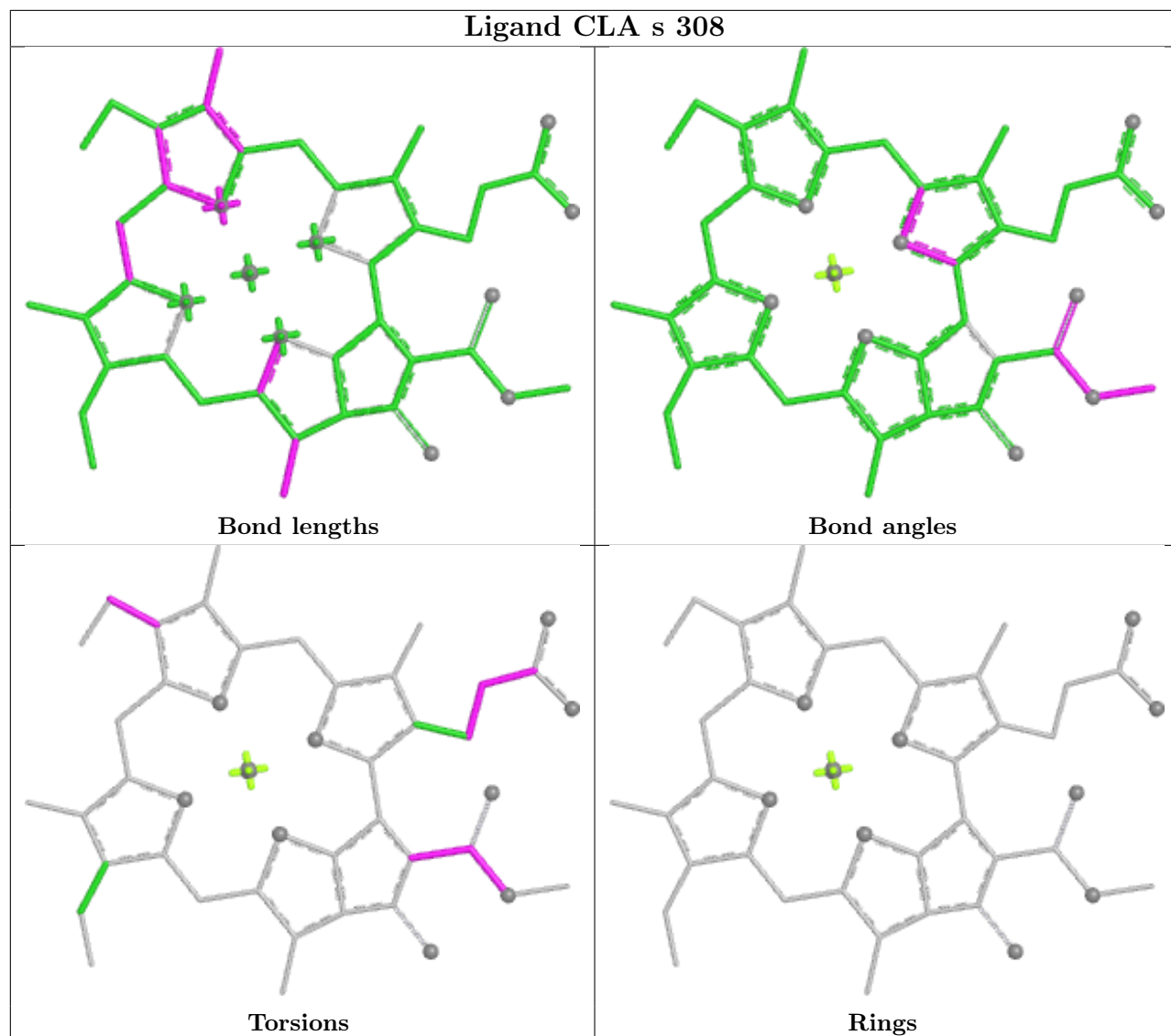


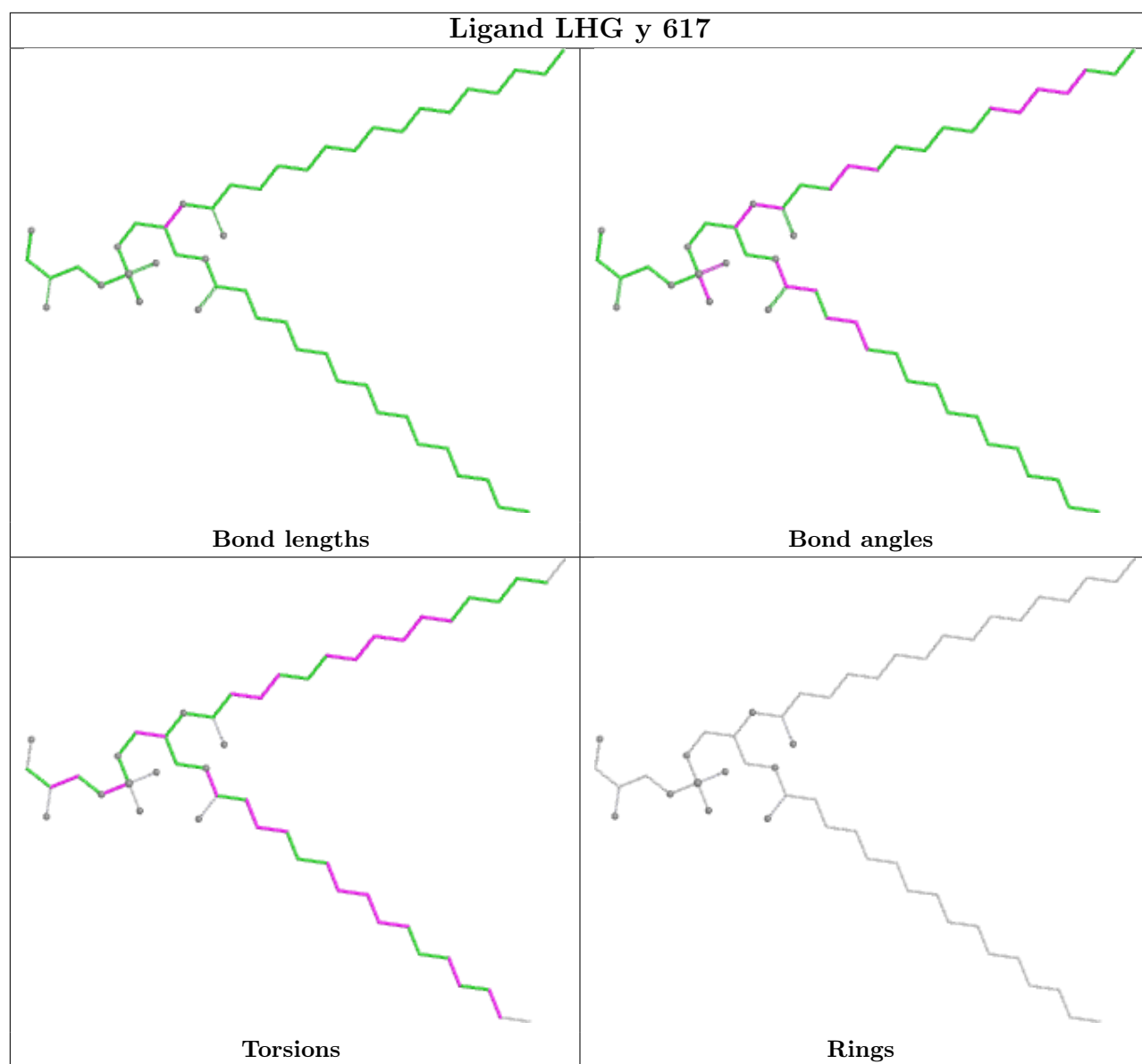


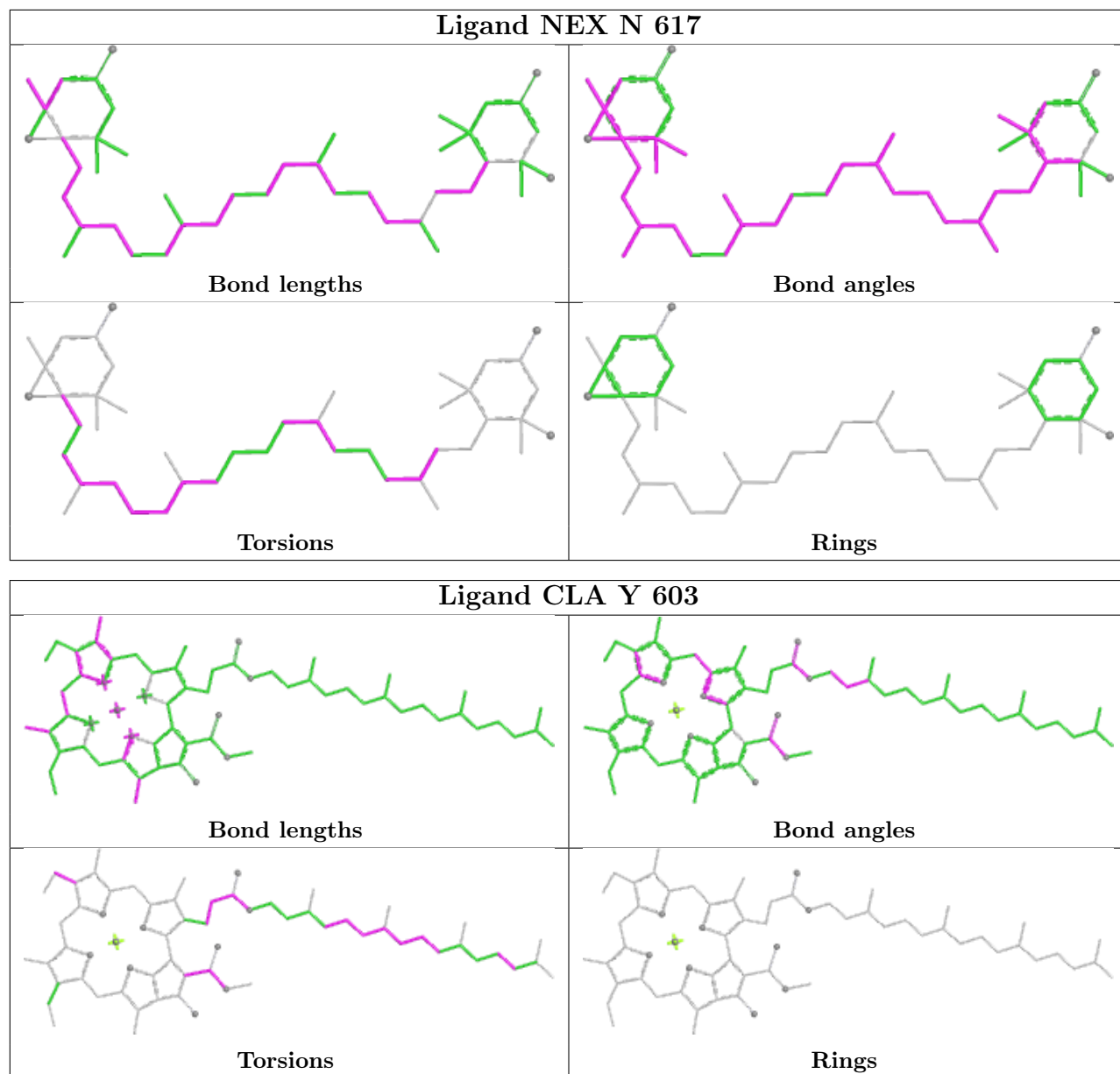


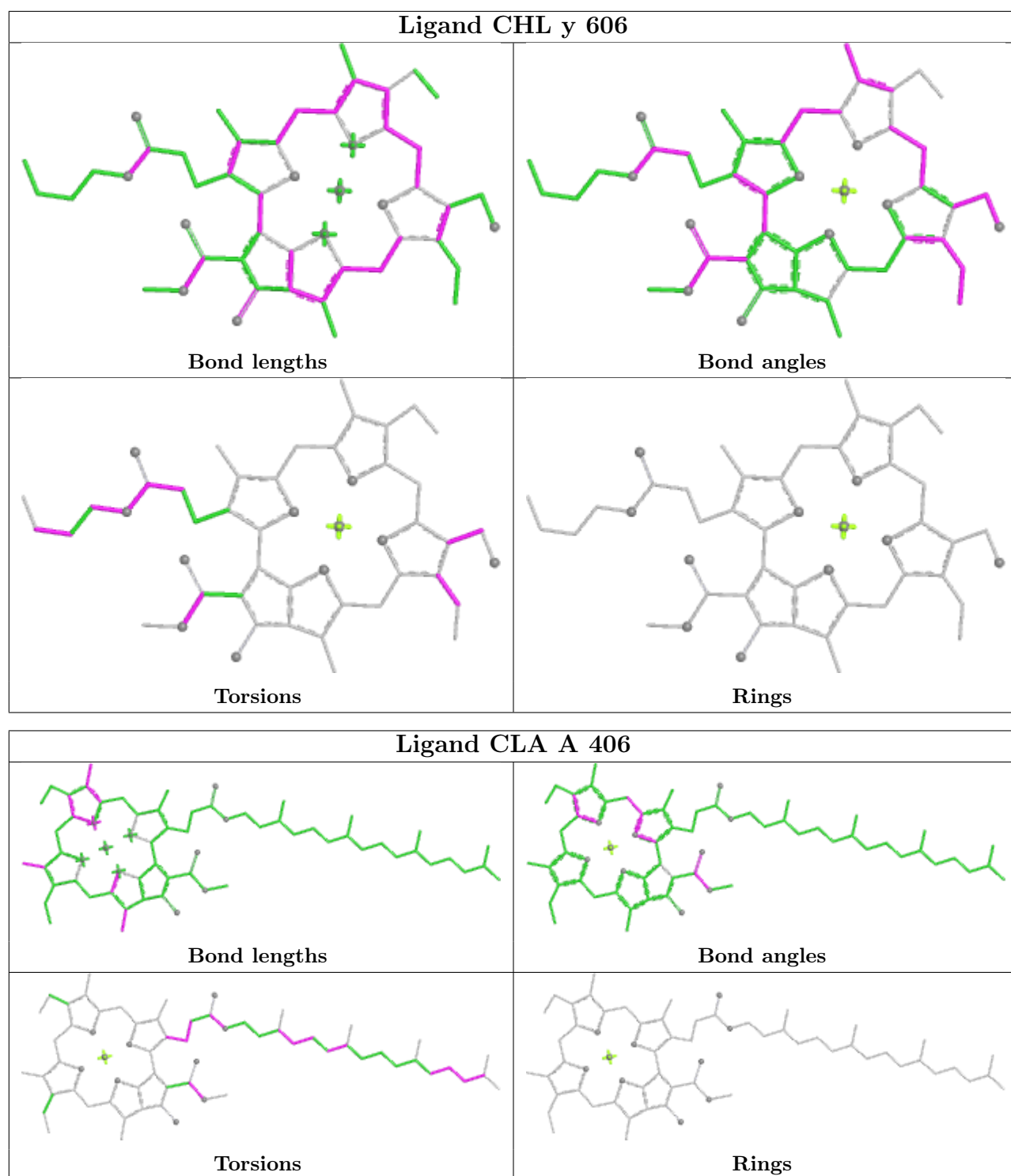


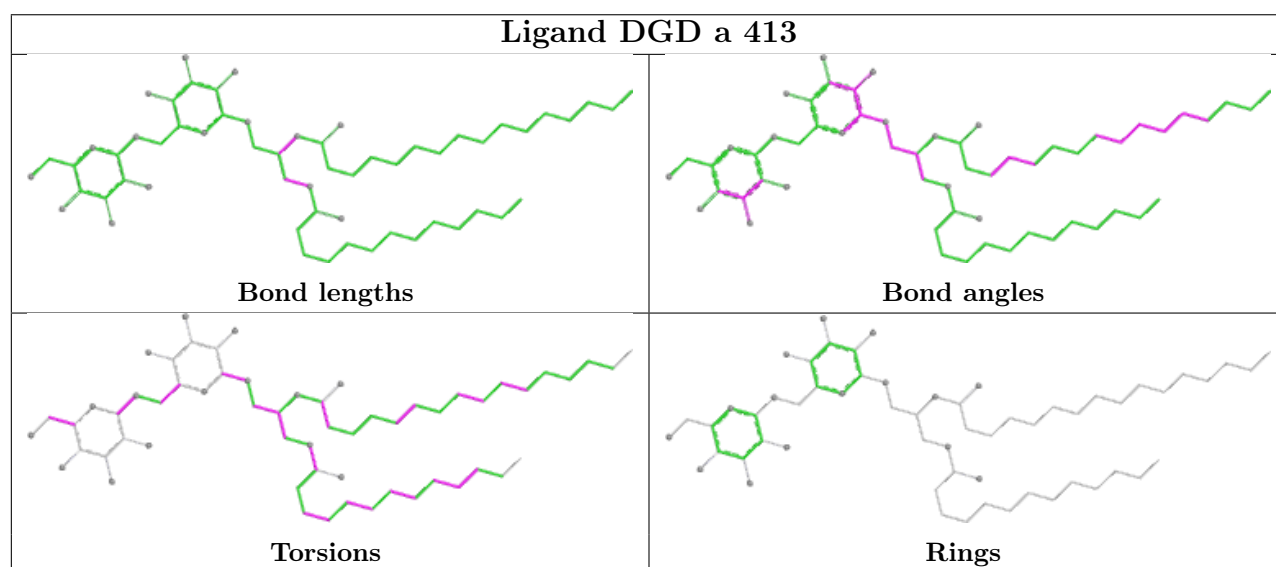
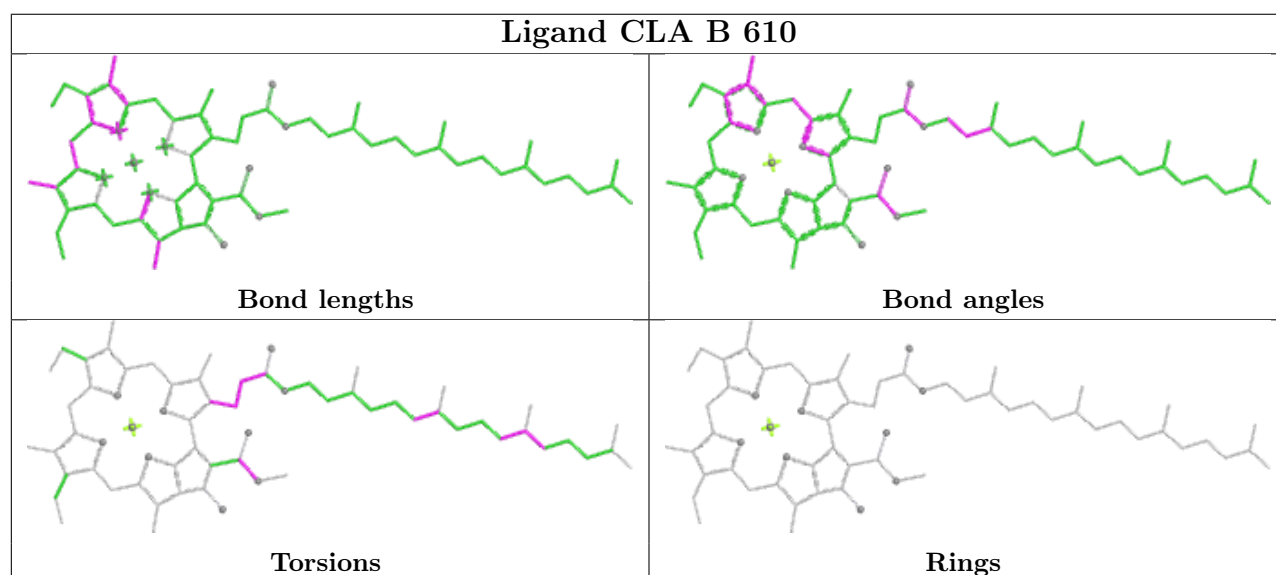
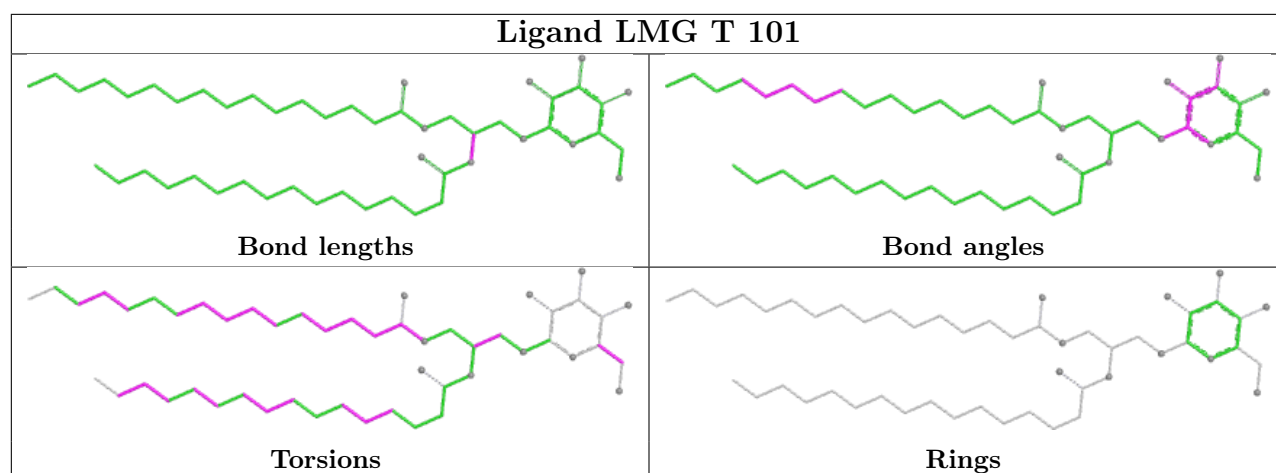
Ligand CLA s 308



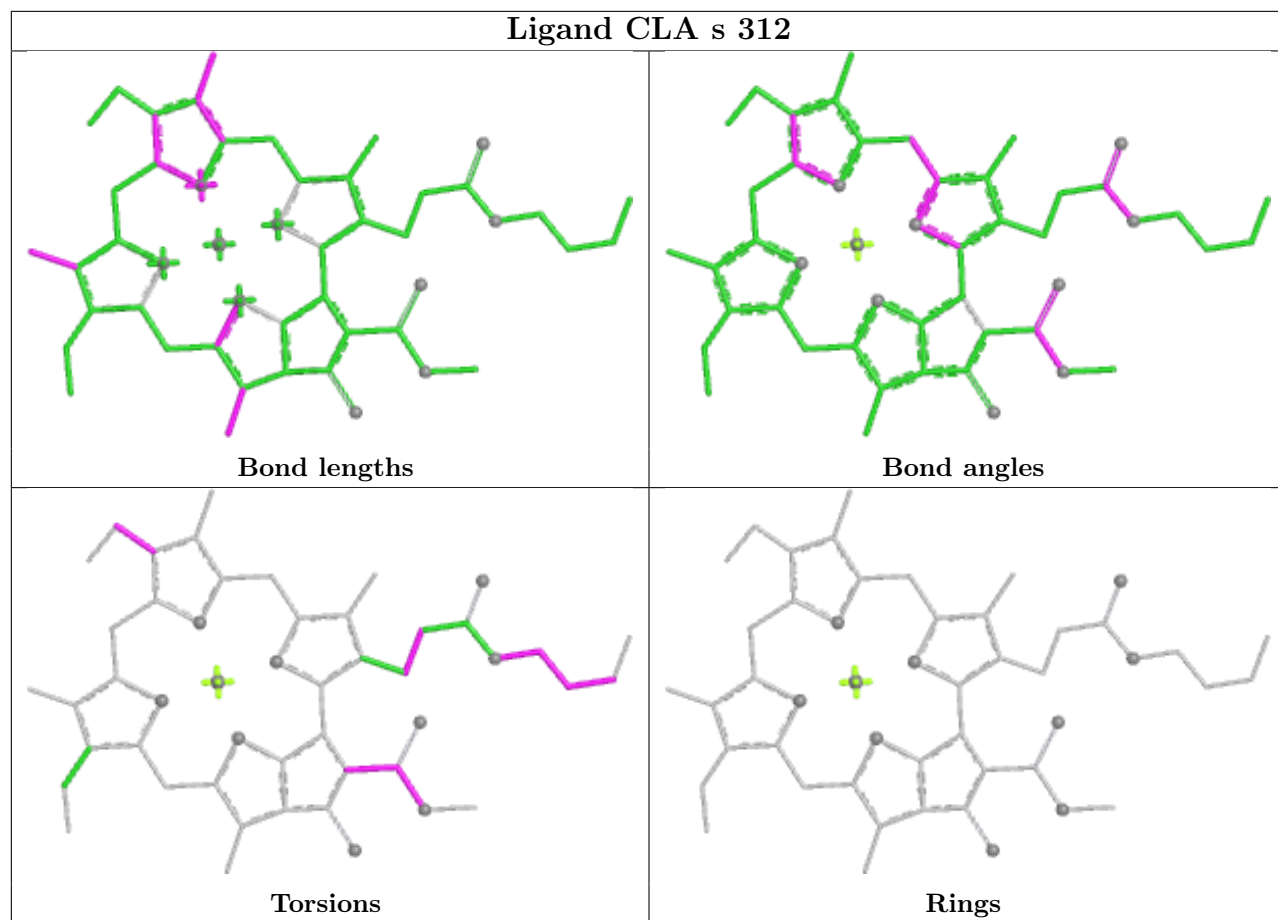


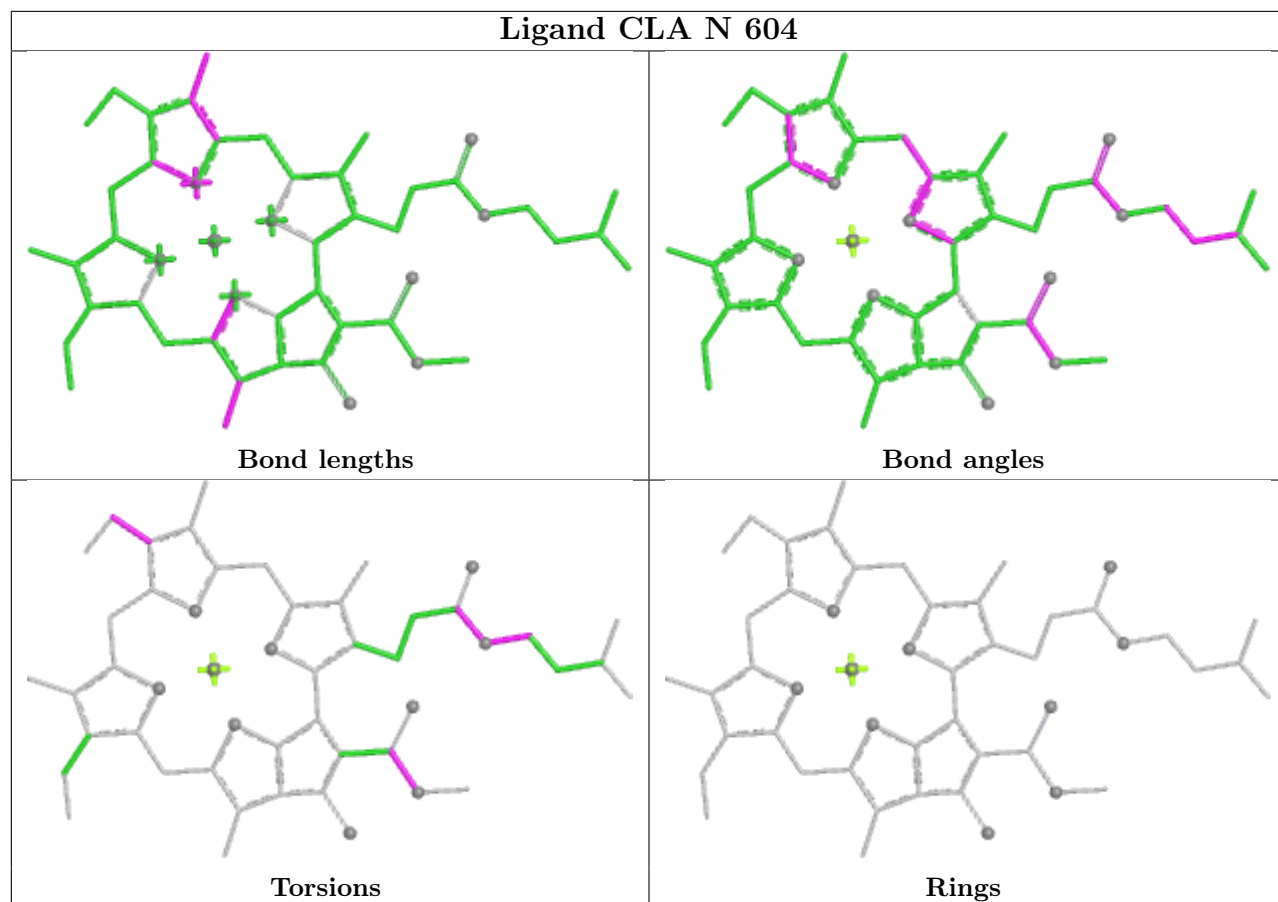


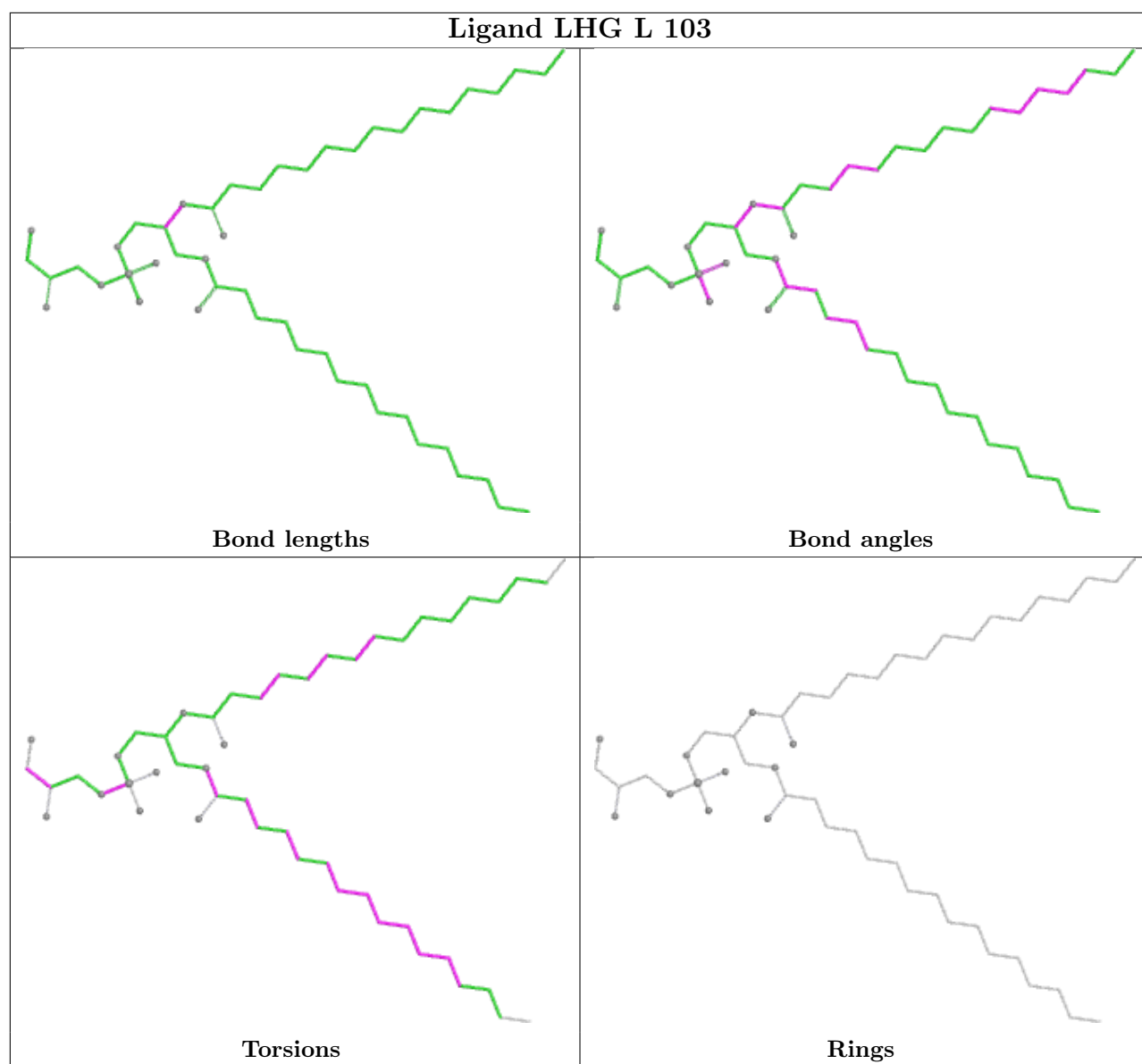




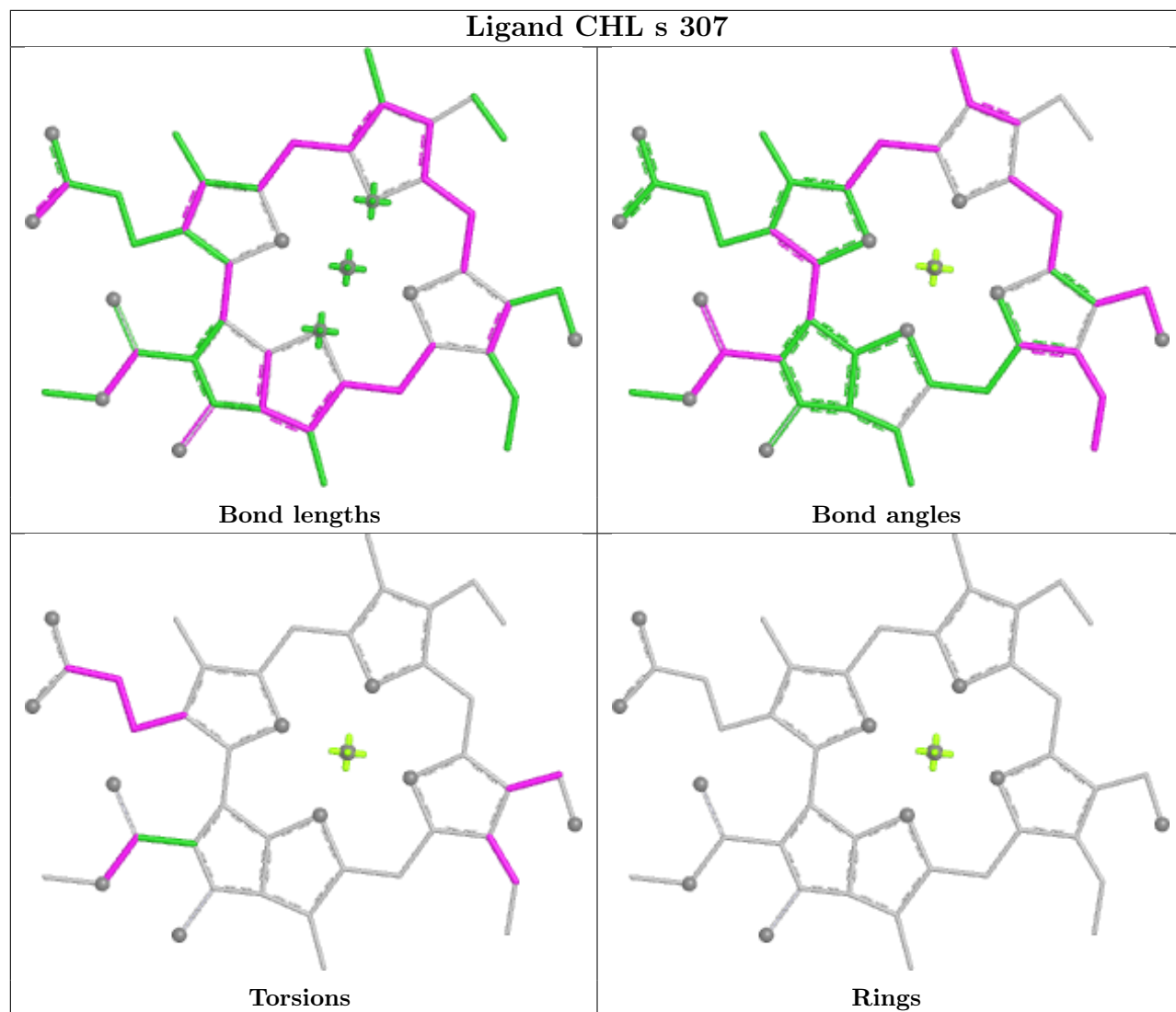
Ligand CLA s 312

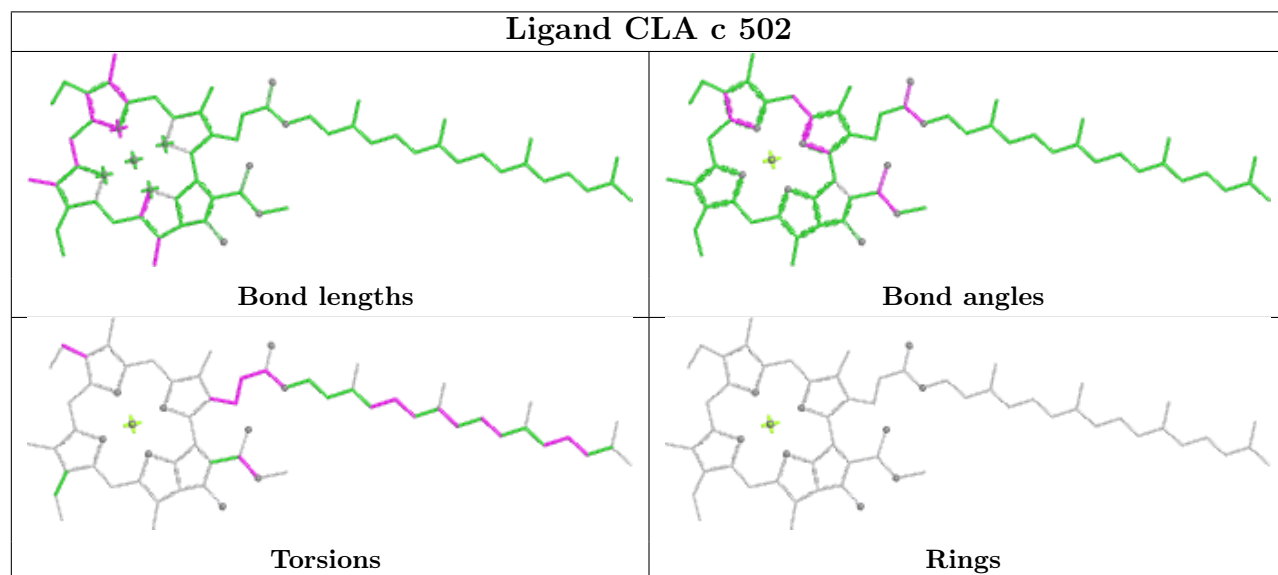
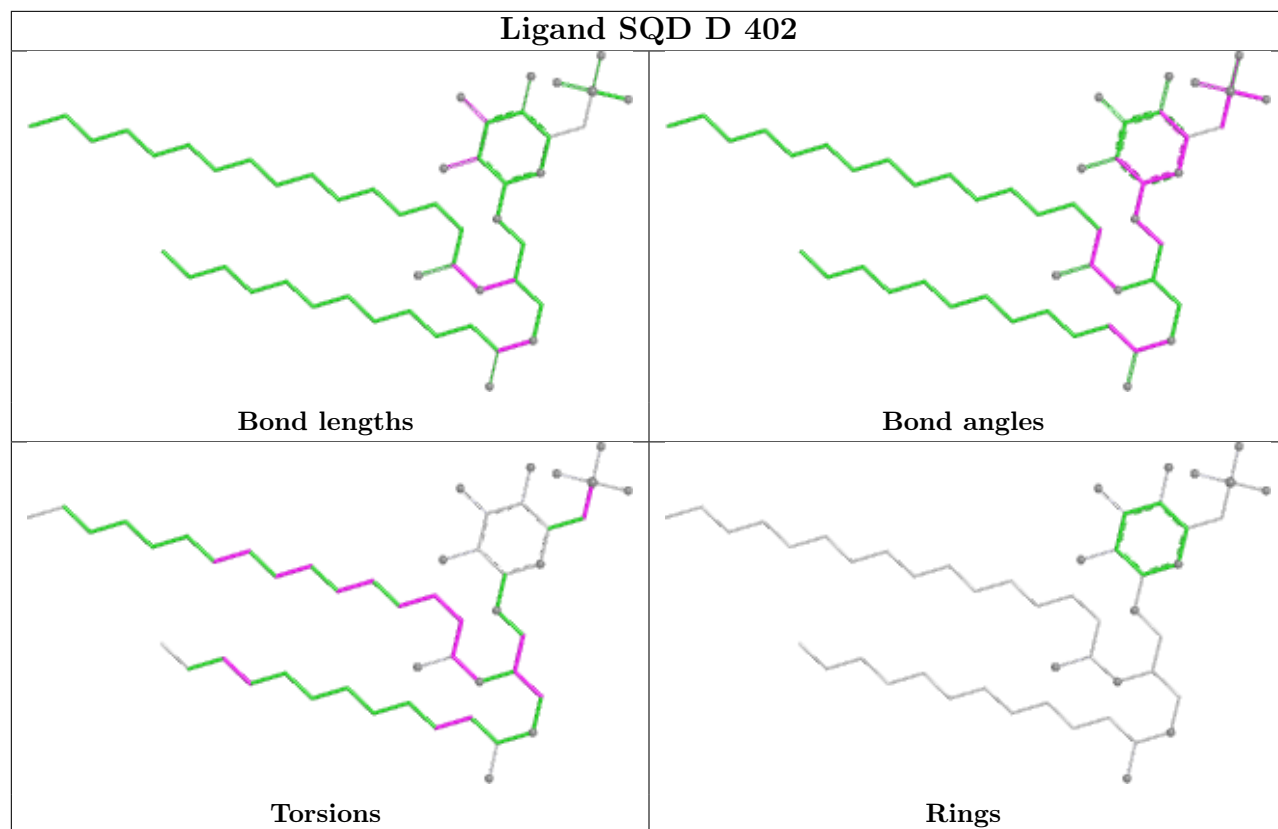


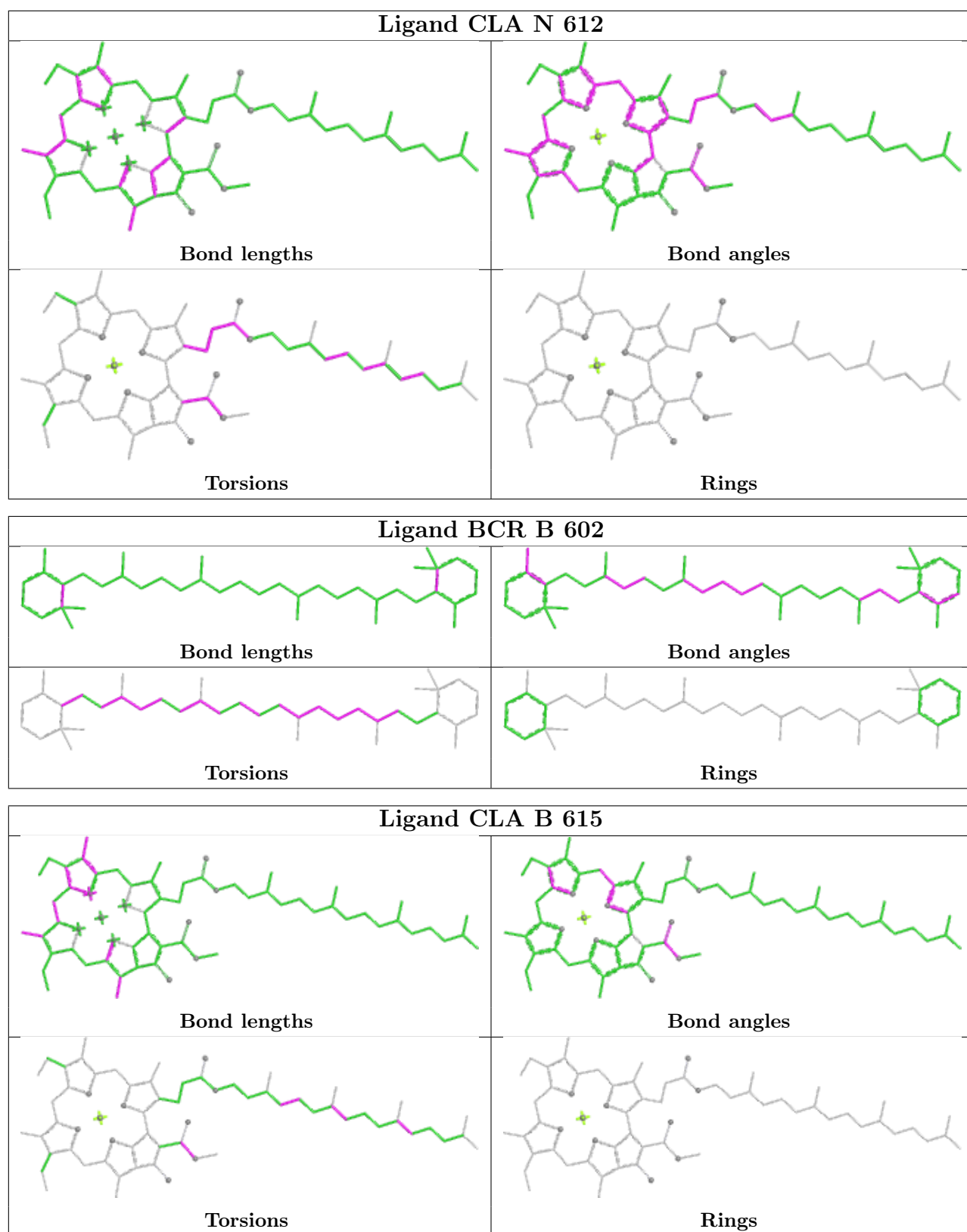




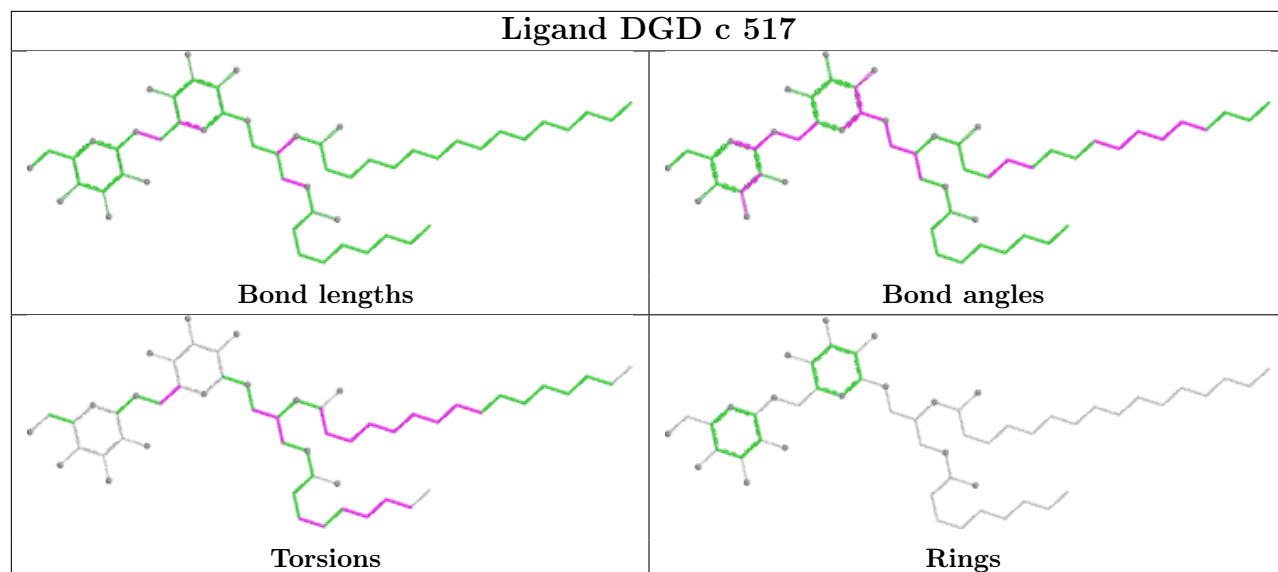
Ligand CHL s 307



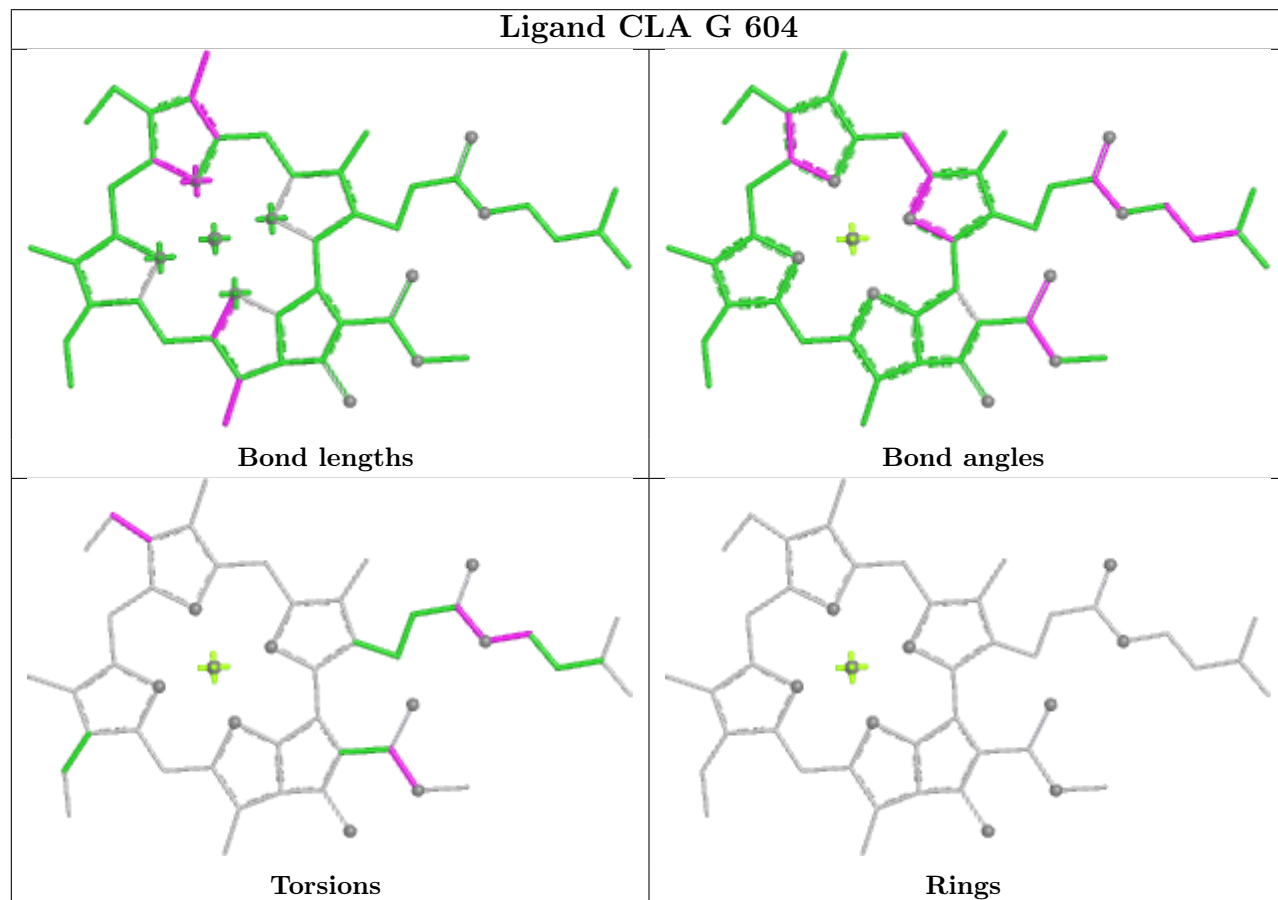




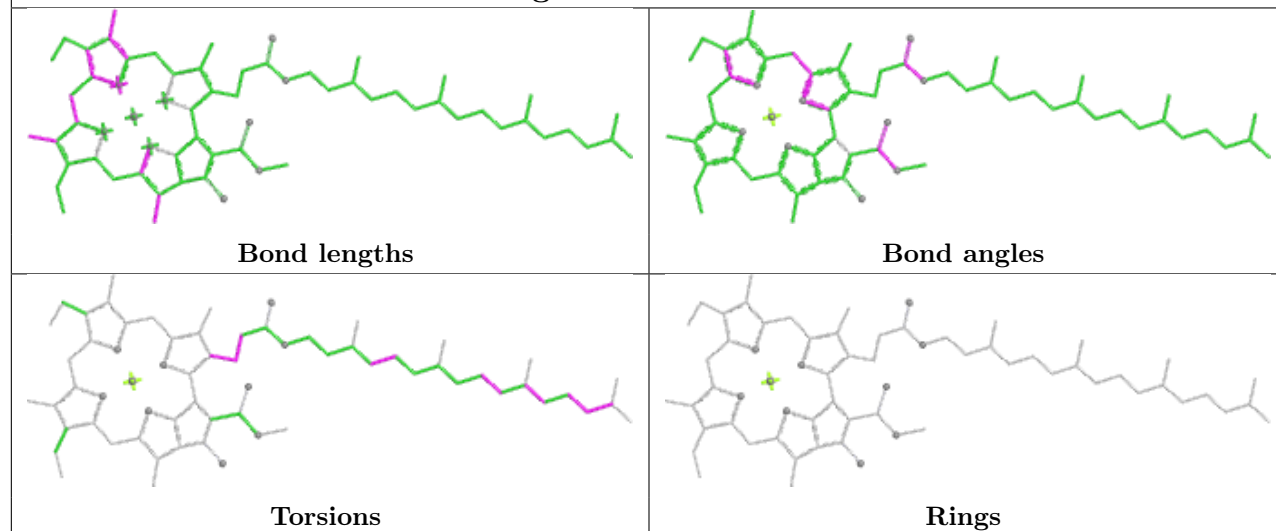
Ligand DGD c 517



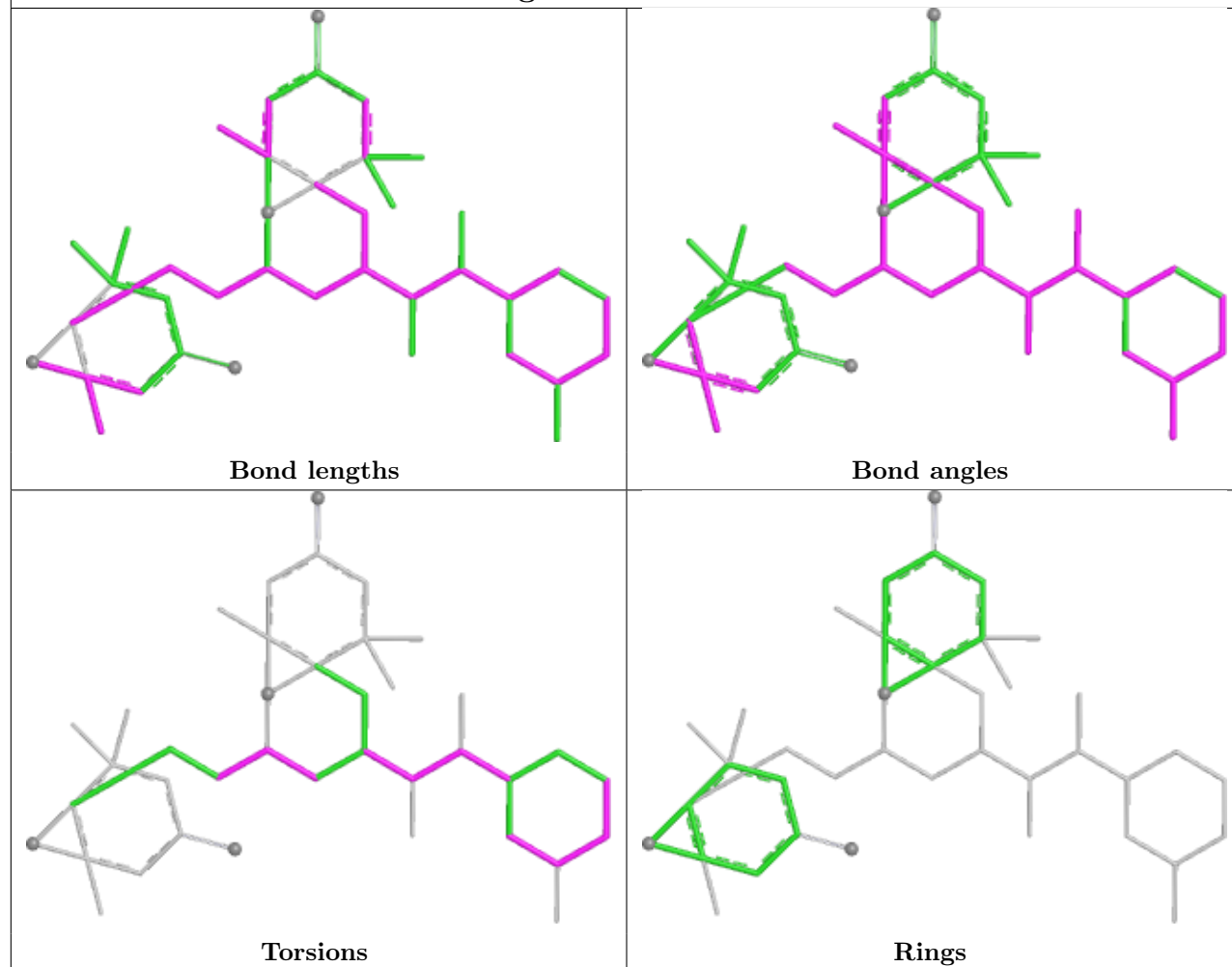
Ligand CLA G 604



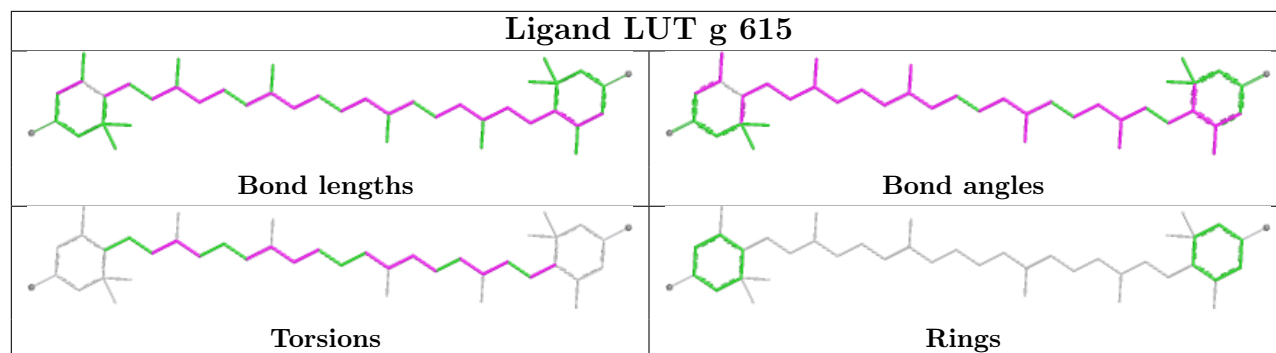
Ligand CLA B 608



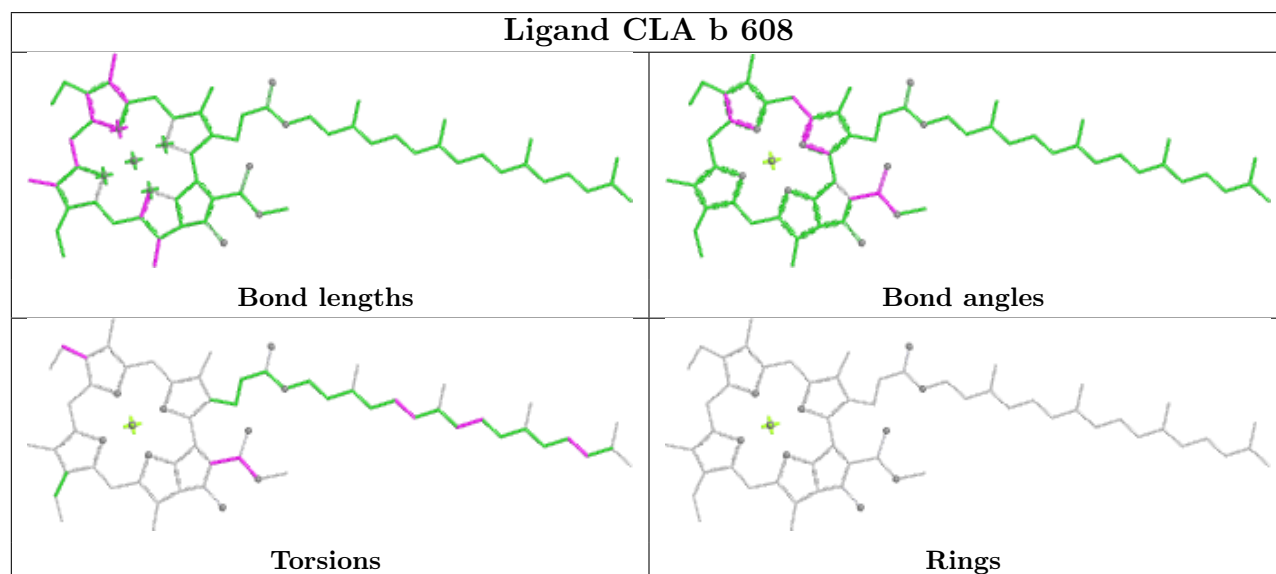
Ligand XAT r 314



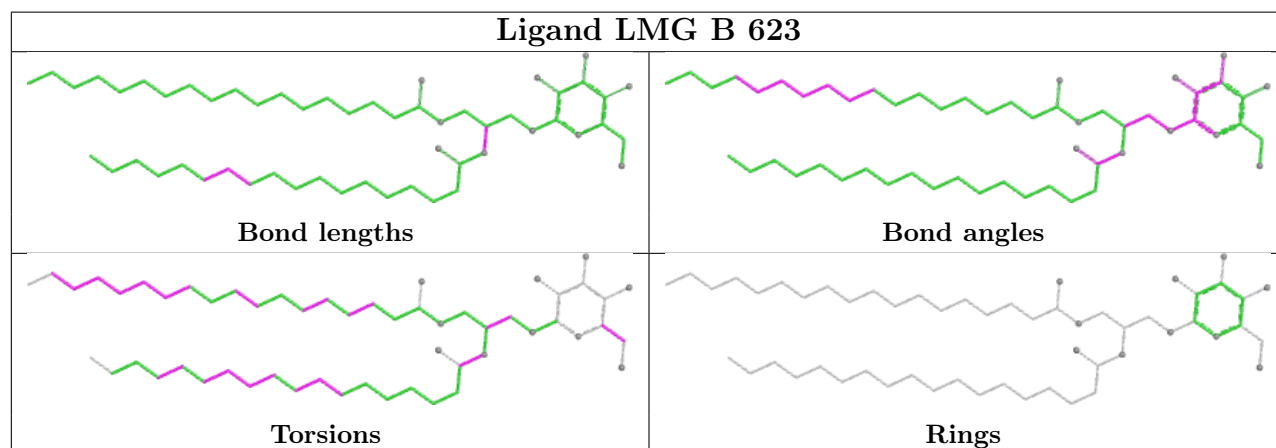
Ligand LUT g 615



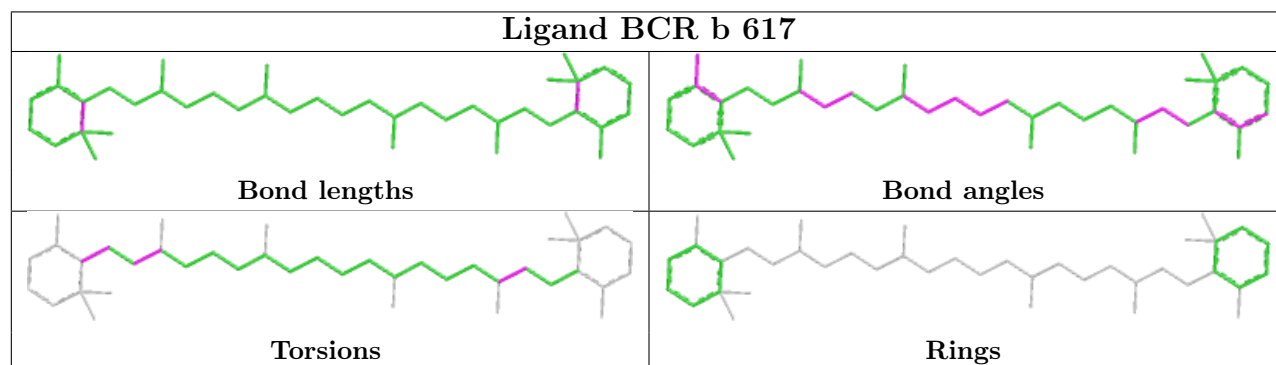
Ligand CLA b 608

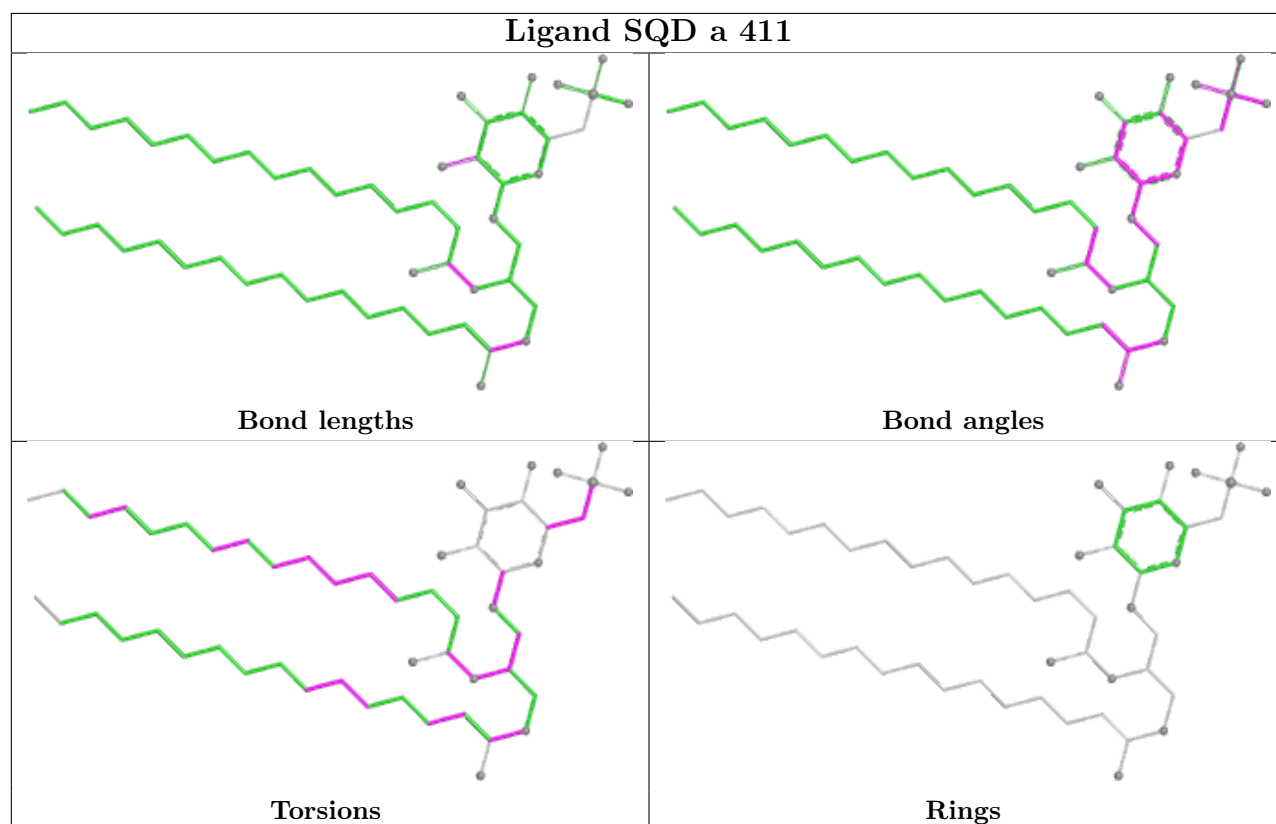
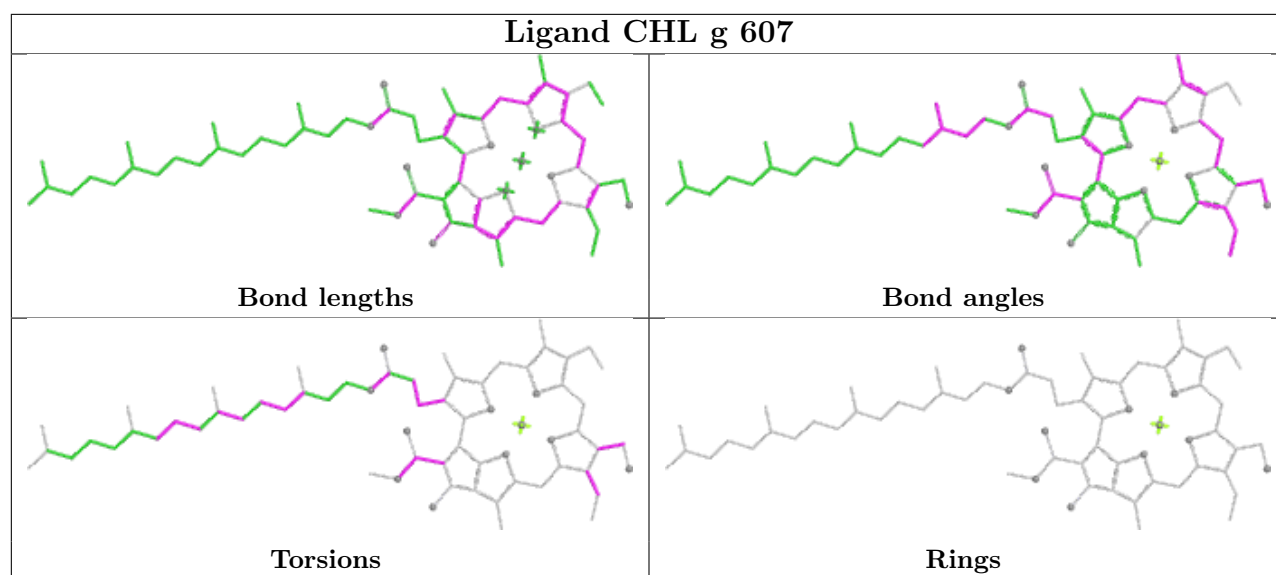


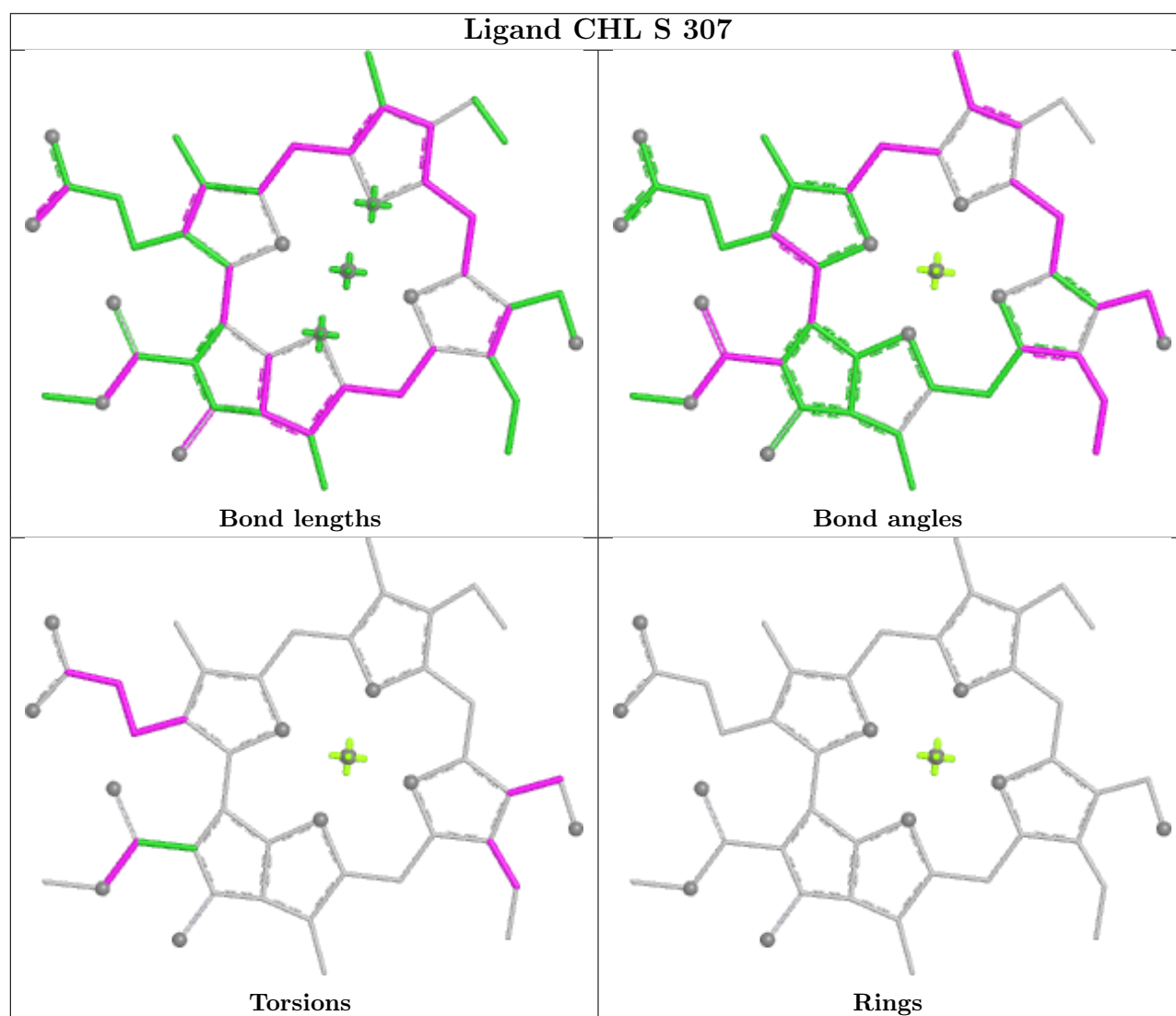
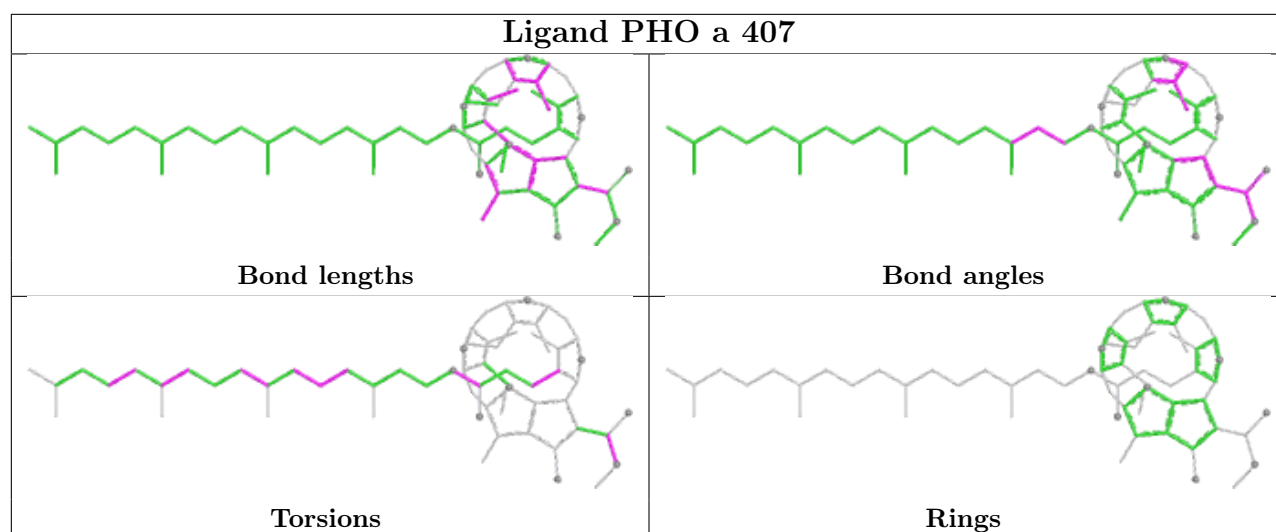
Ligand LMG B 623

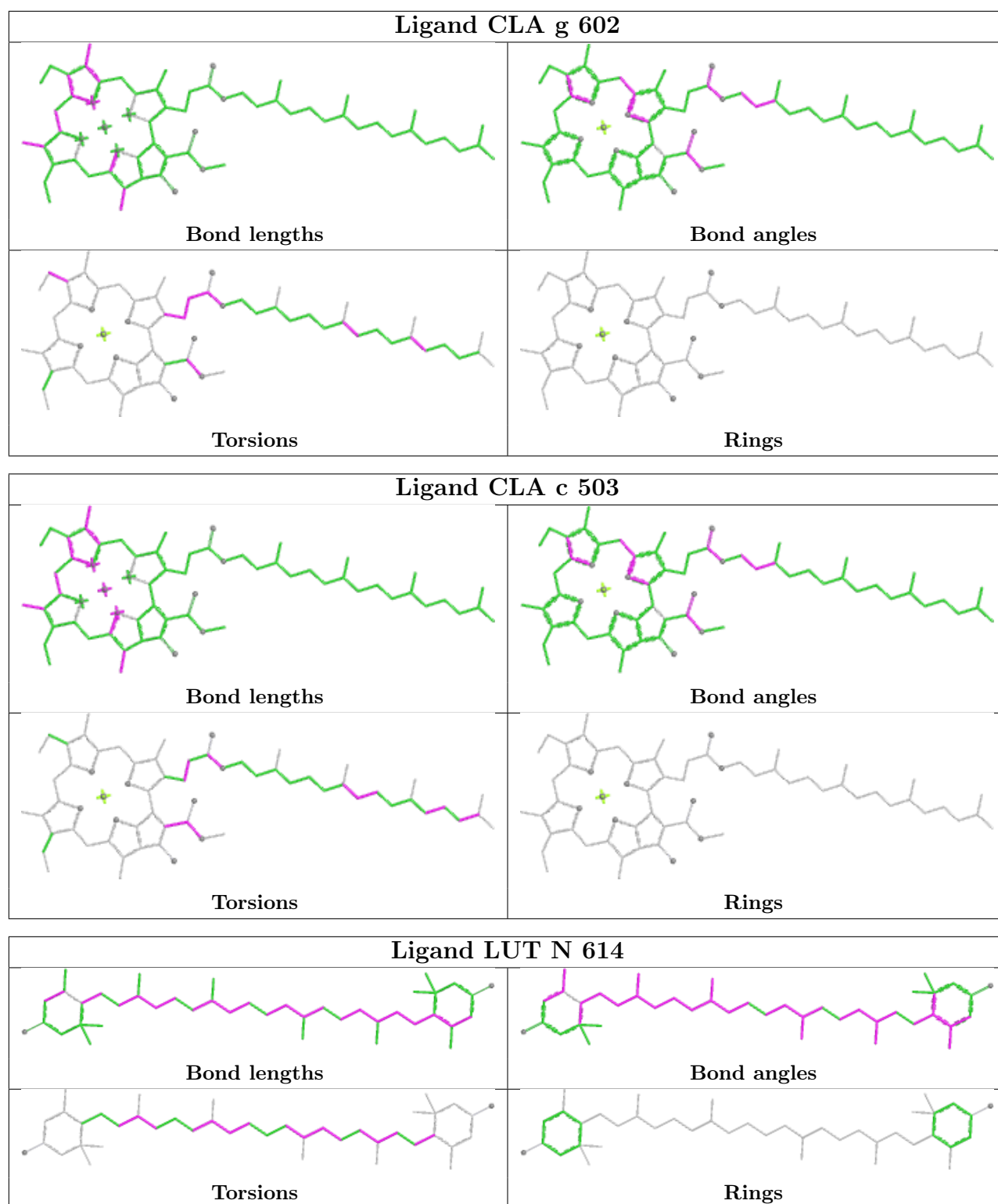


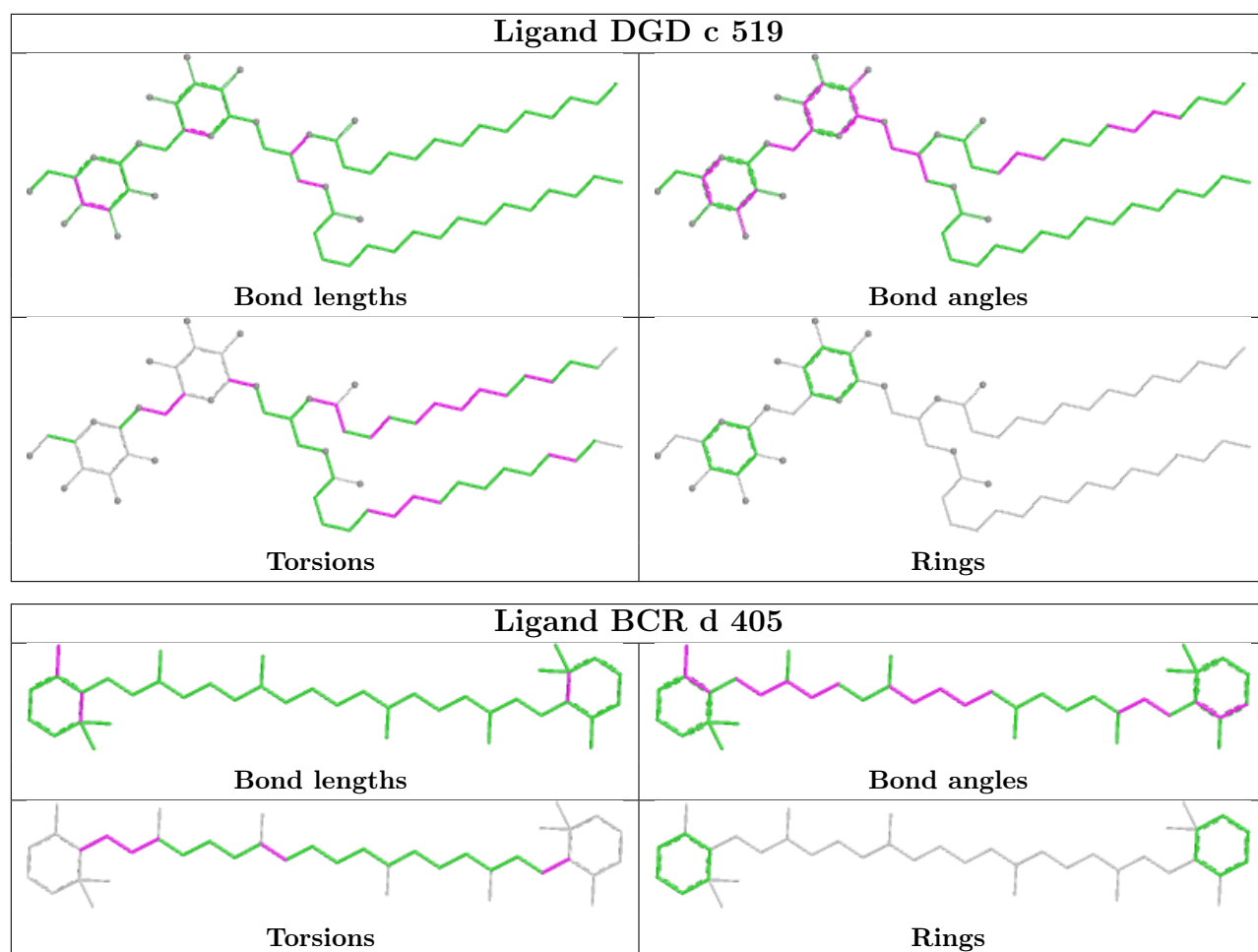
Ligand BCR b 617



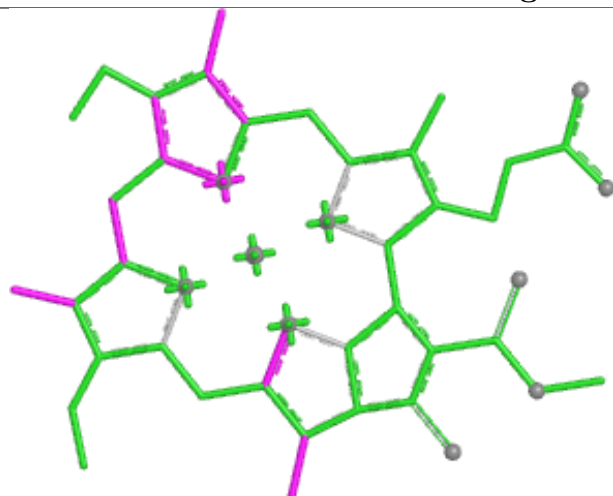




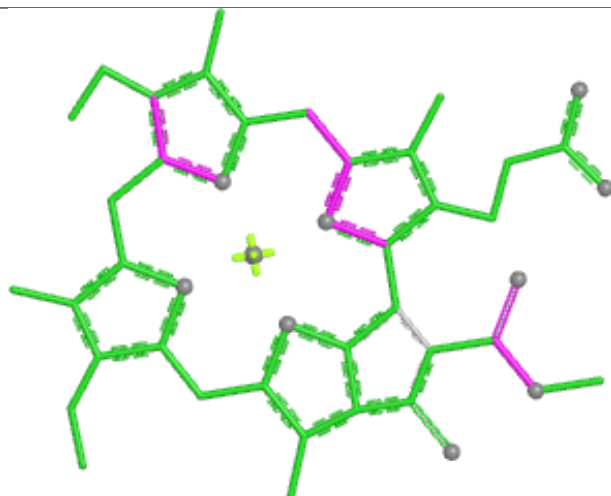




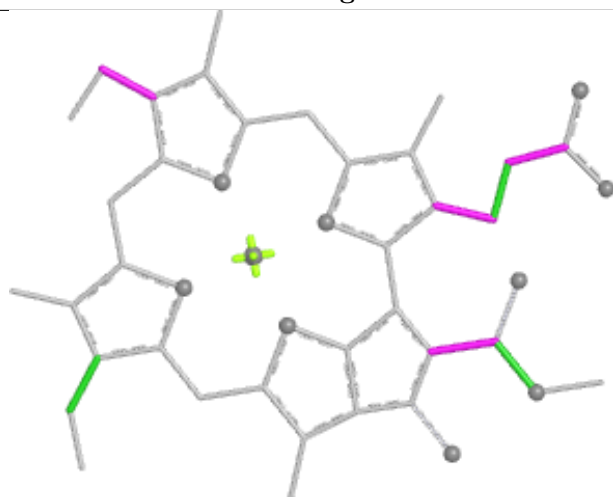
Ligand CLA s 304



Bond lengths



Bond angles

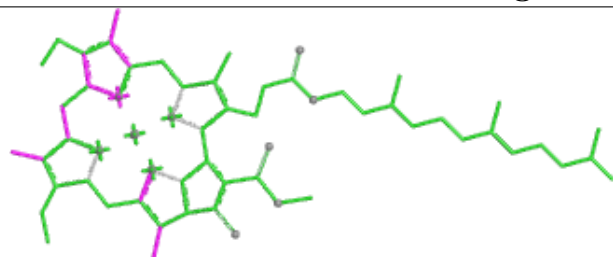


Torsions

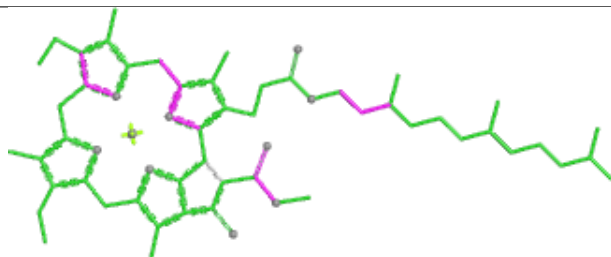


Rings

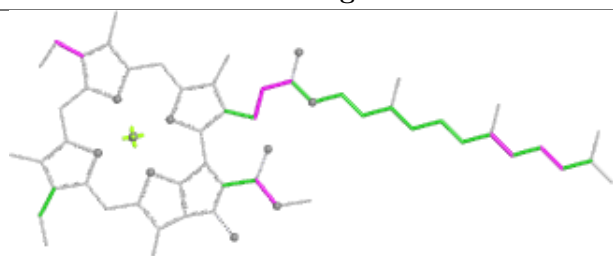
Ligand CLA R 302



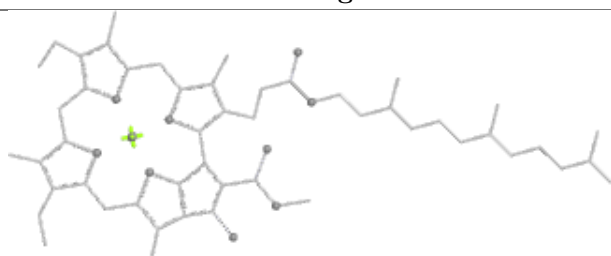
Bond lengths



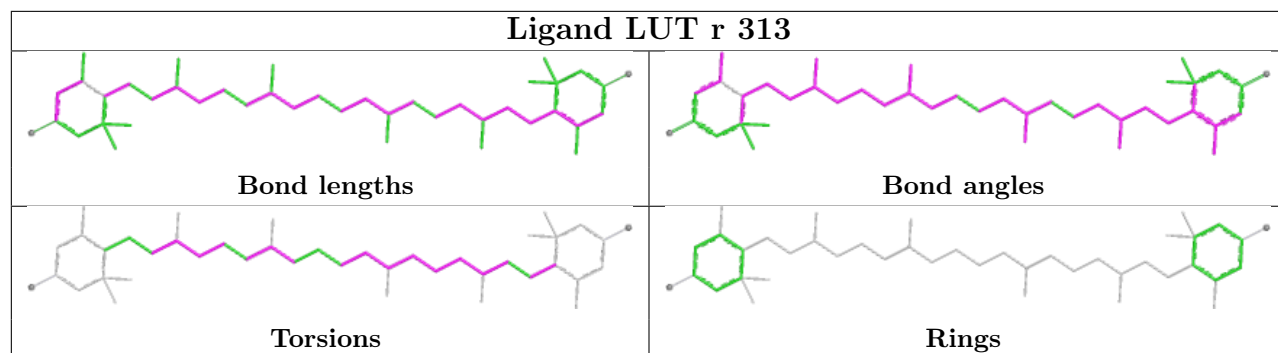
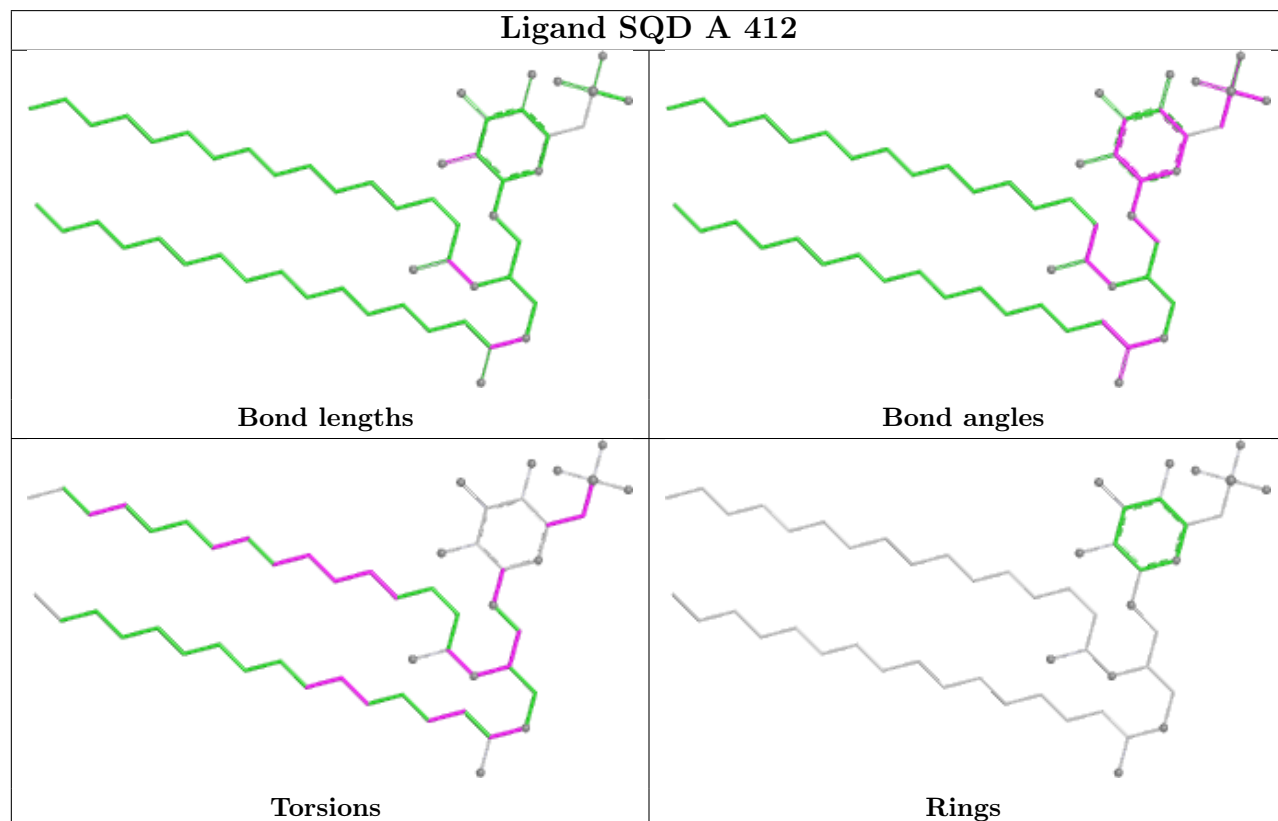
Bond angles



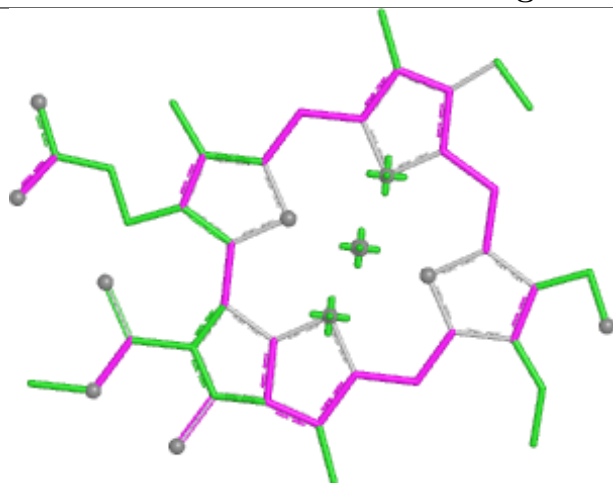
Torsions



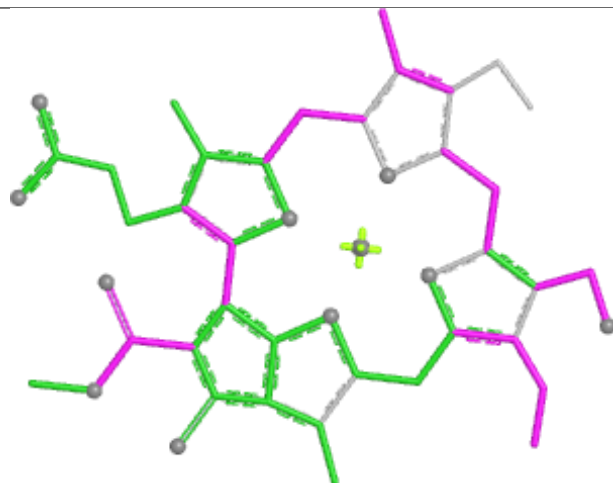
Rings

Ligand LUT r 313**Ligand SQD A 412**

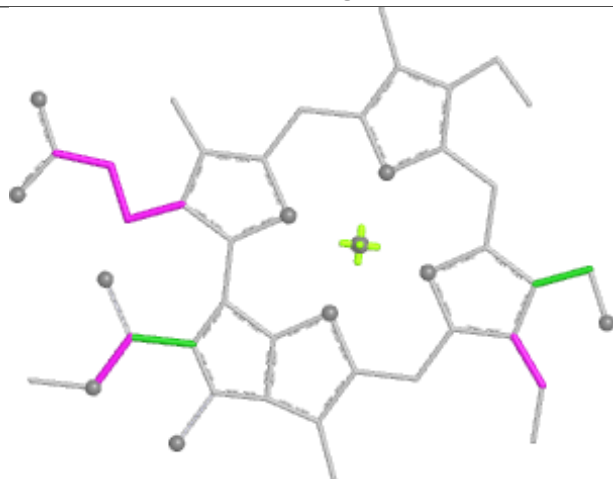
Ligand CHL S 302



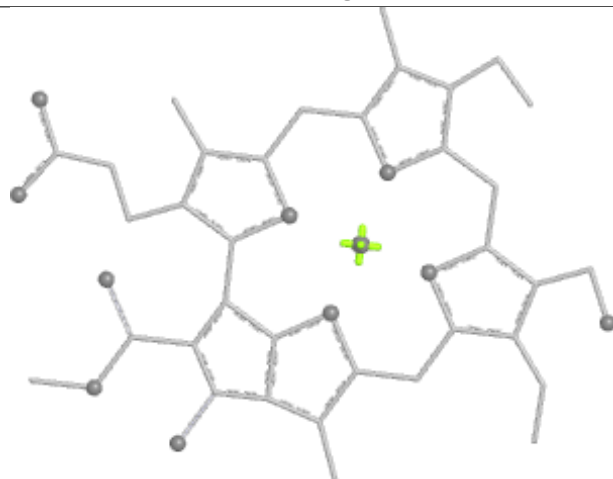
Bond lengths



Bond angles

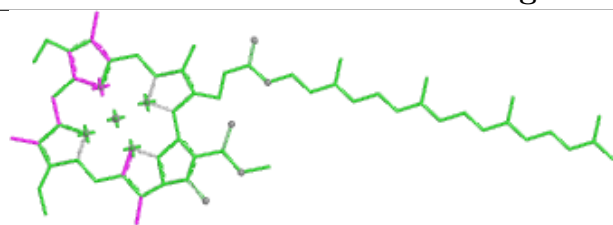


Torsions

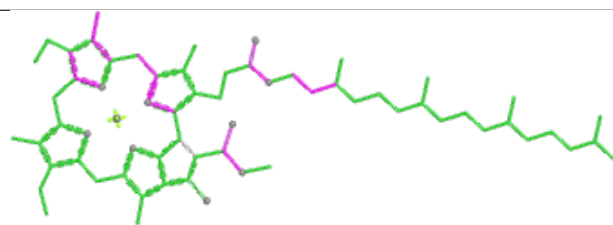


Rings

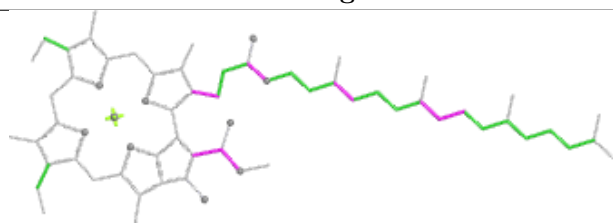
Ligand CLA c 504



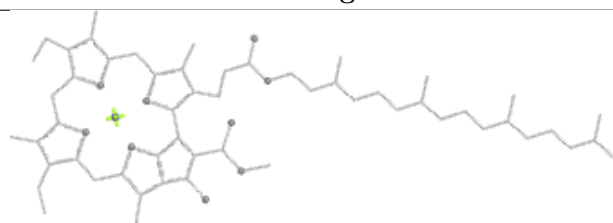
Bond lengths



Bond angles

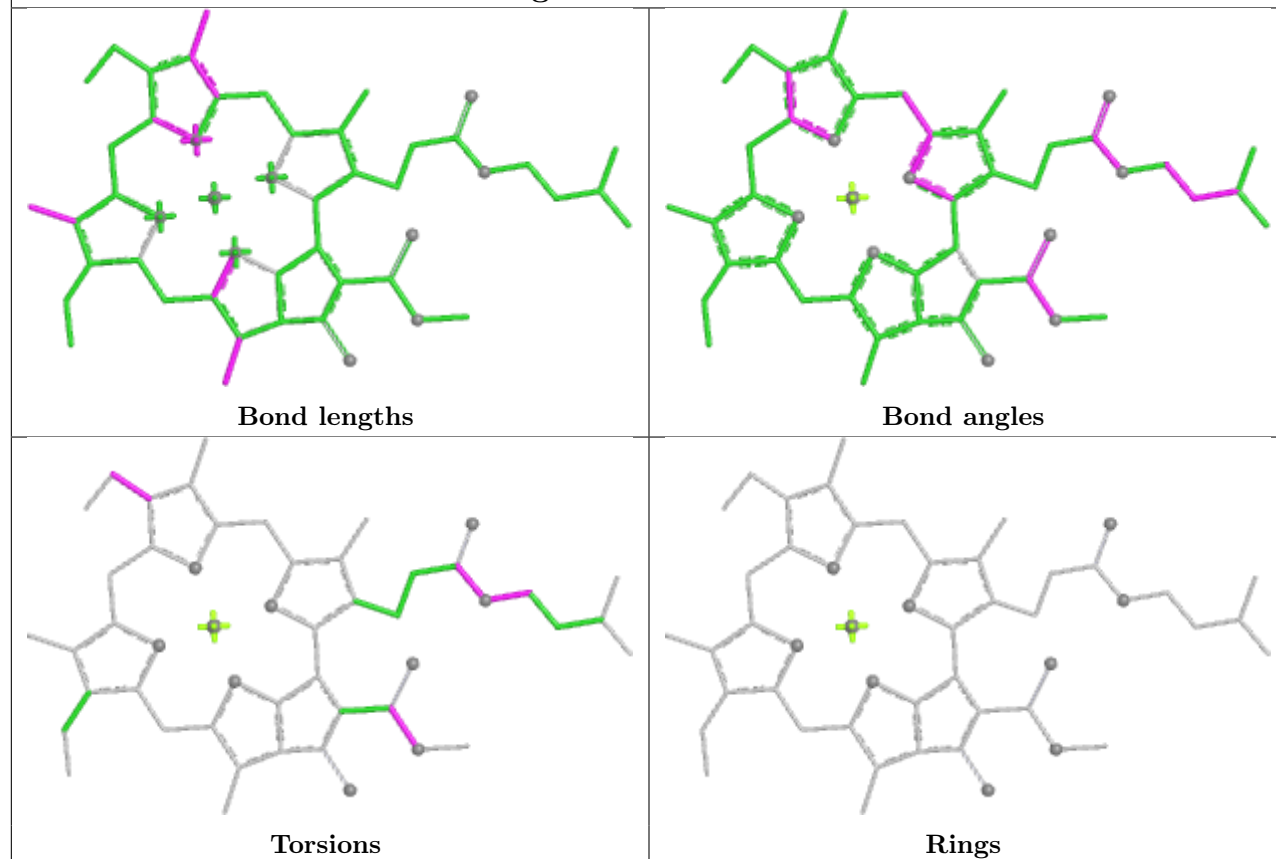


Torsions

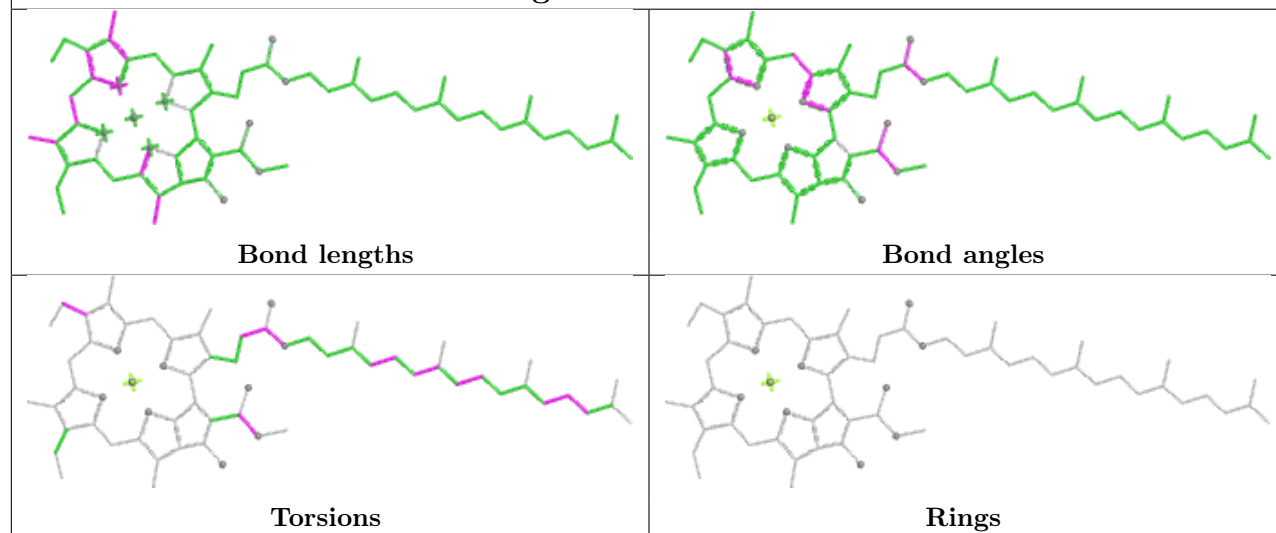


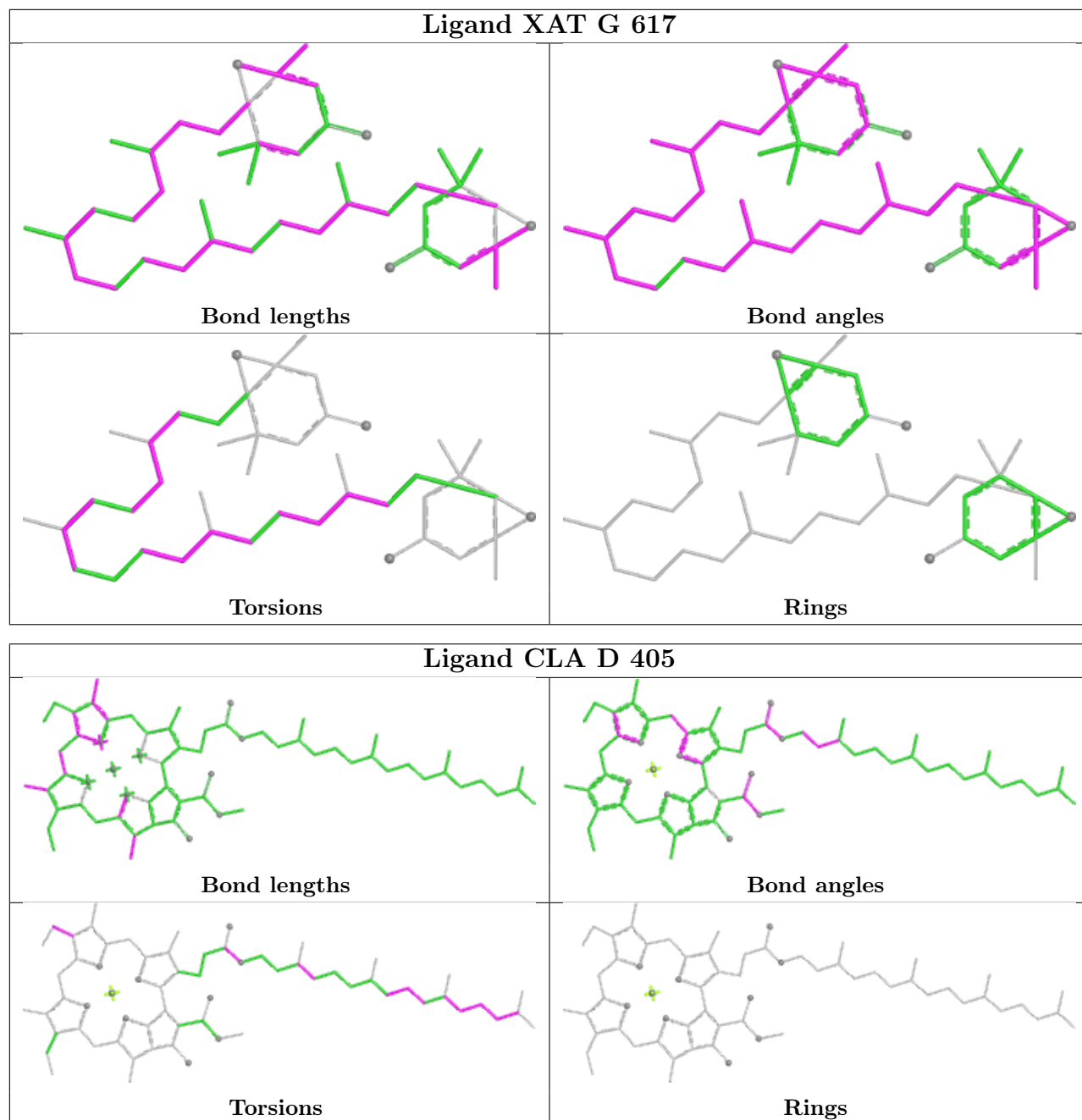
Rings

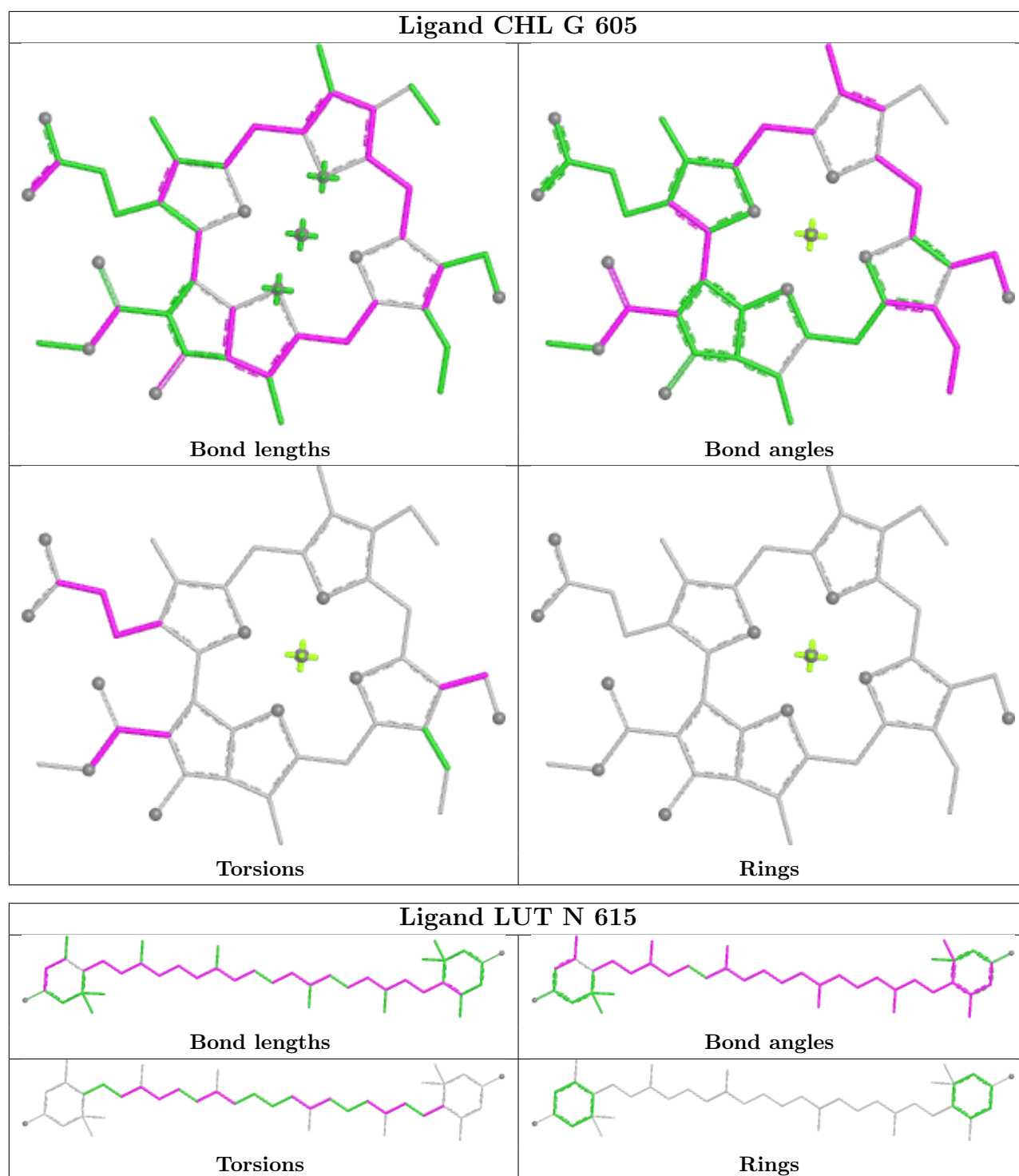
Ligand CLA Y 604



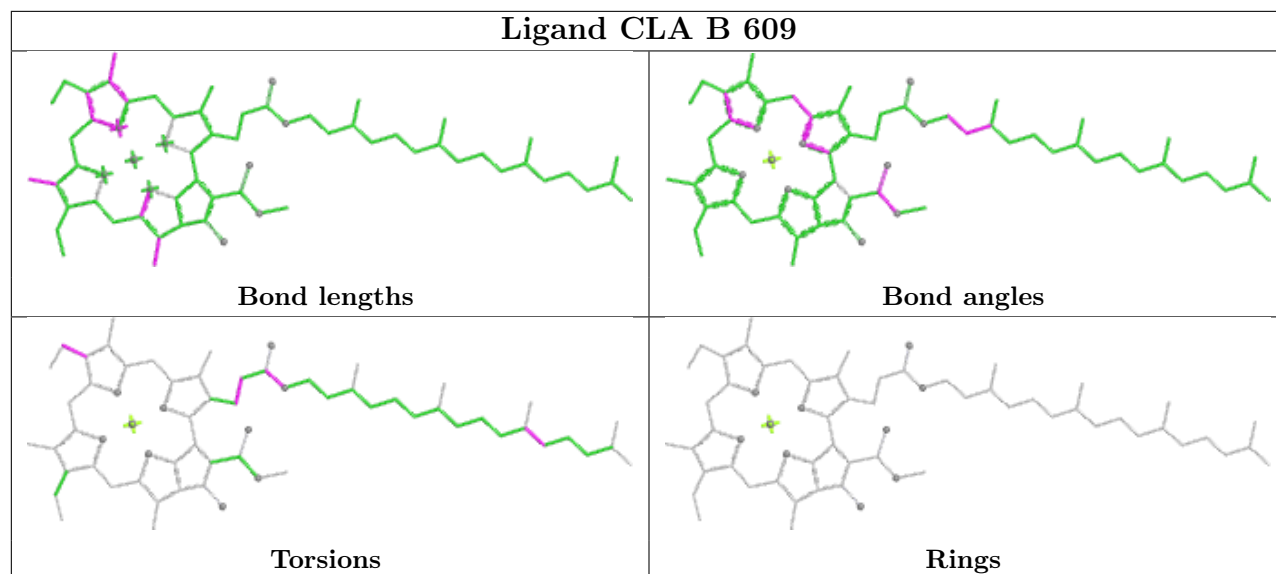
Ligand CLA B 618



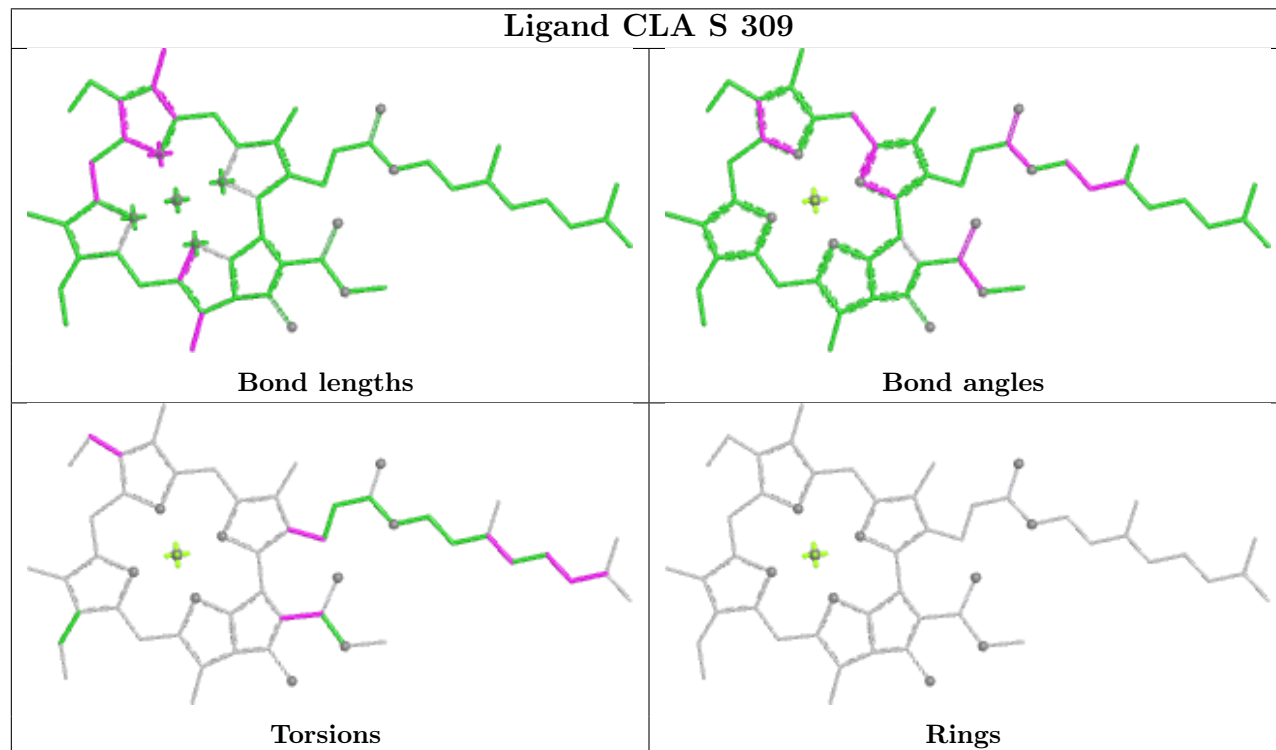




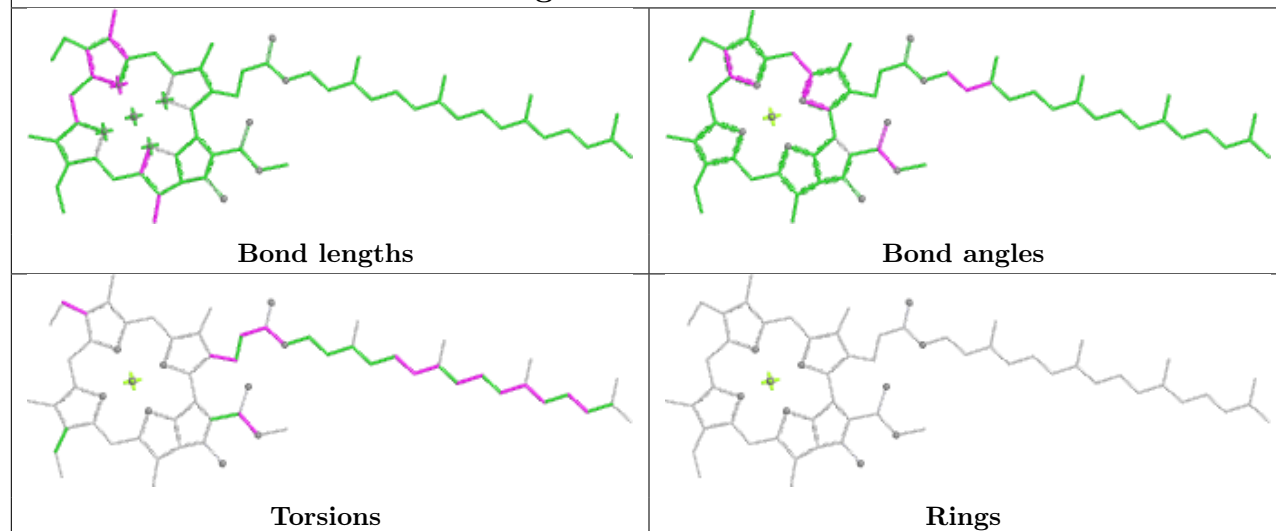
Ligand CLA B 609



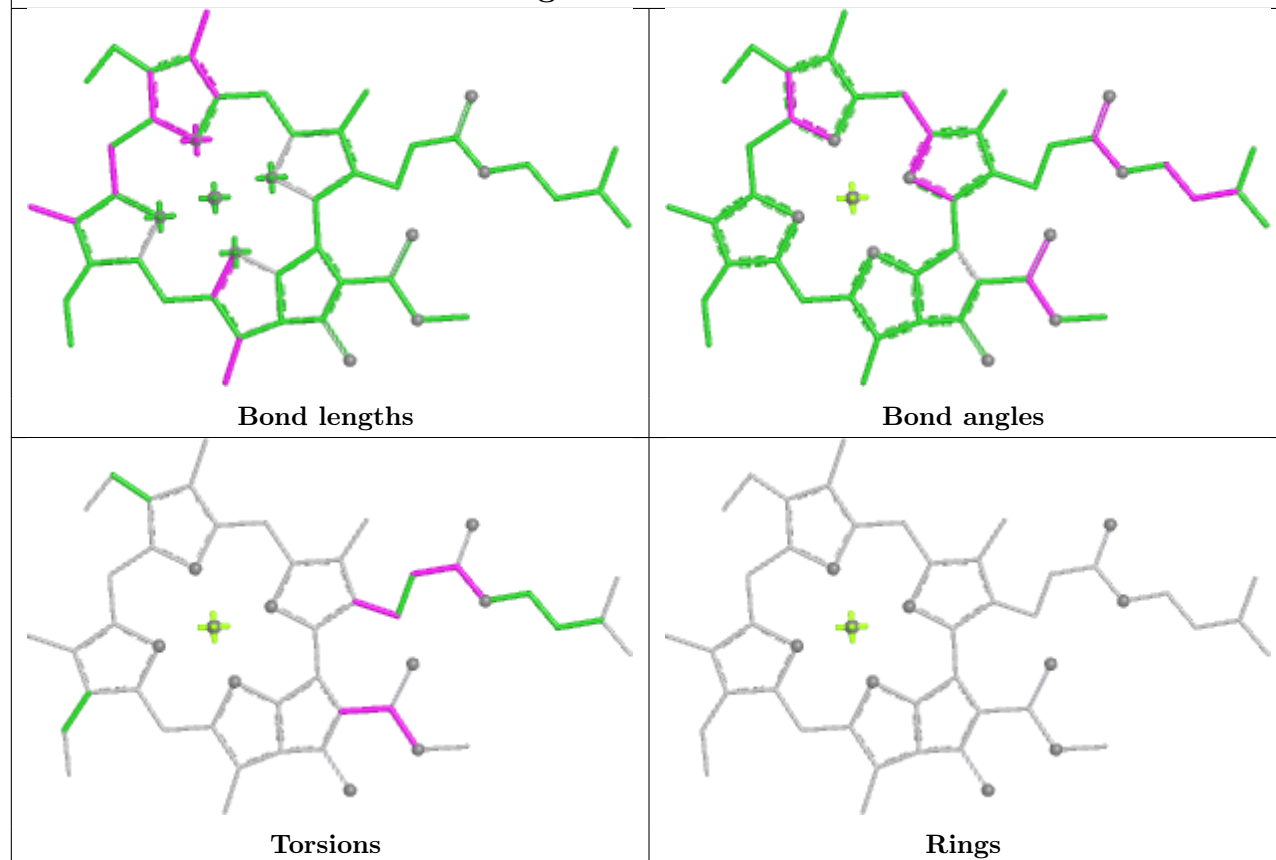
Ligand CLA S 309

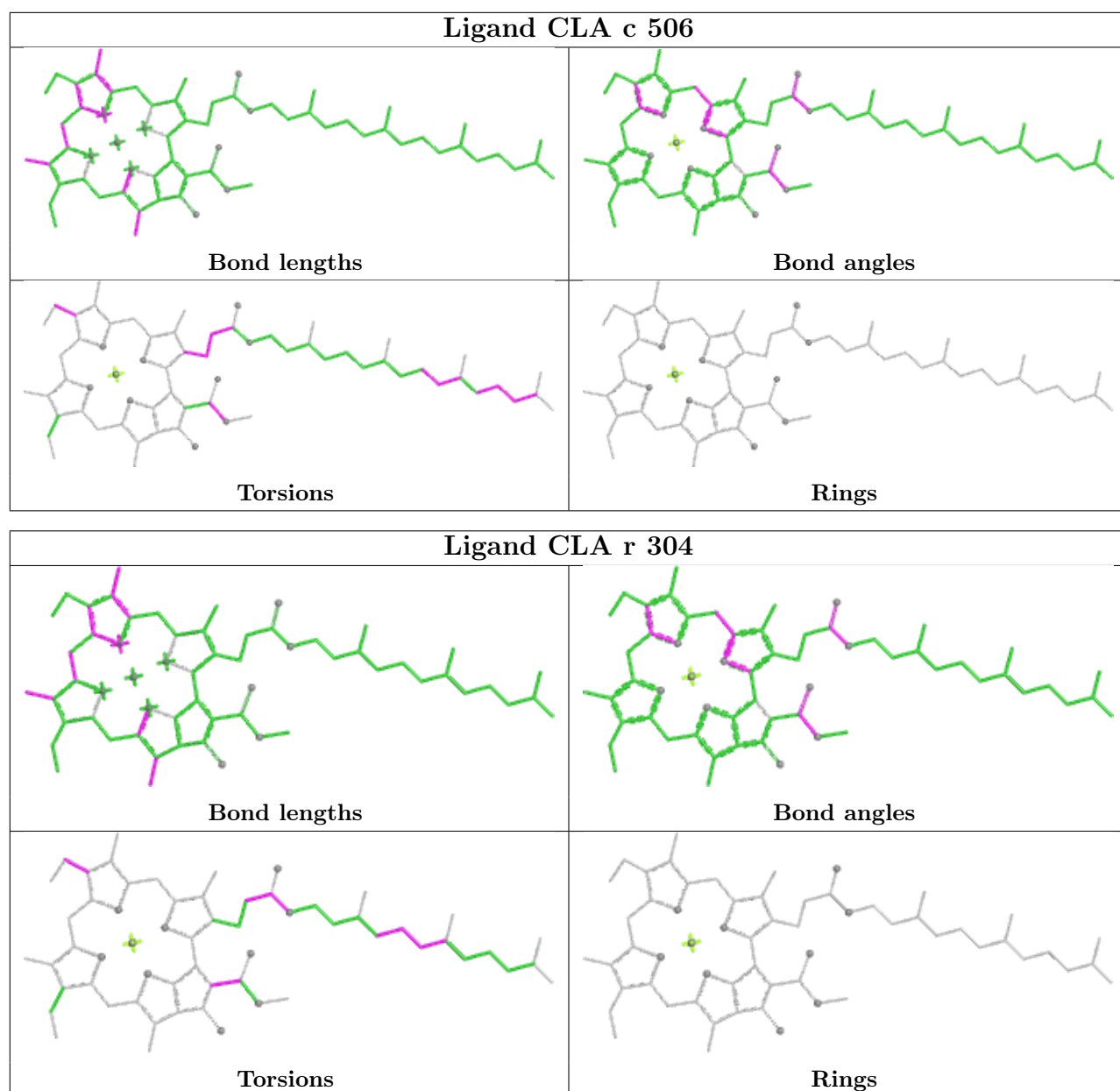


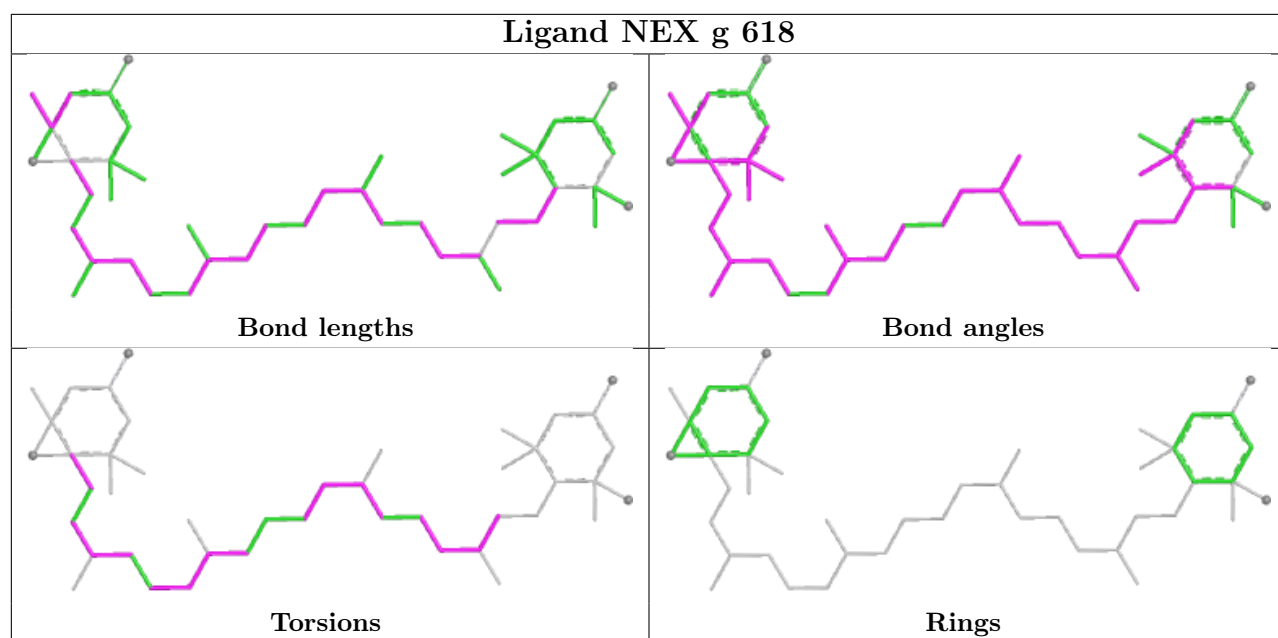
Ligand CLA n 609

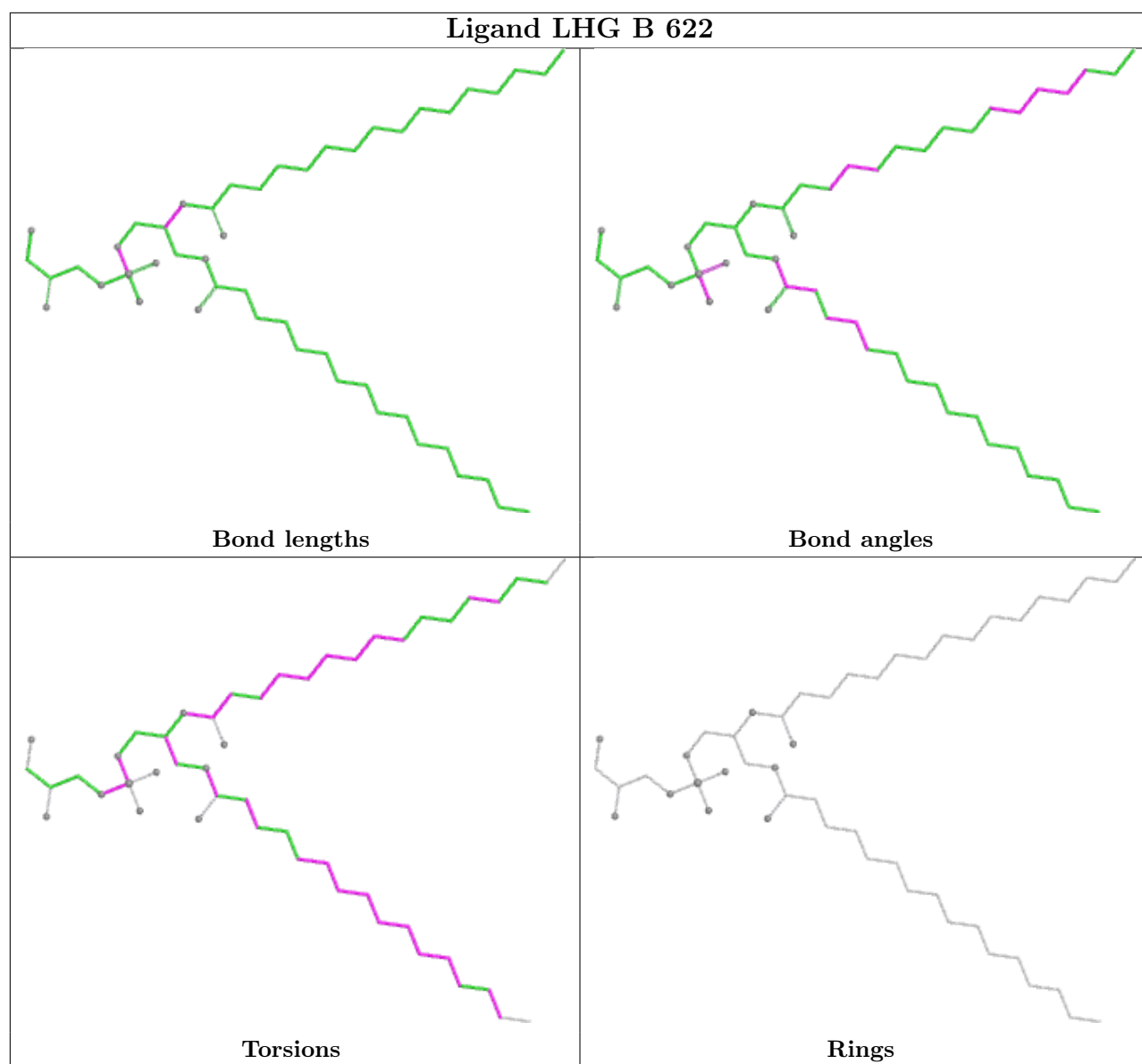


Ligand CLA s 305

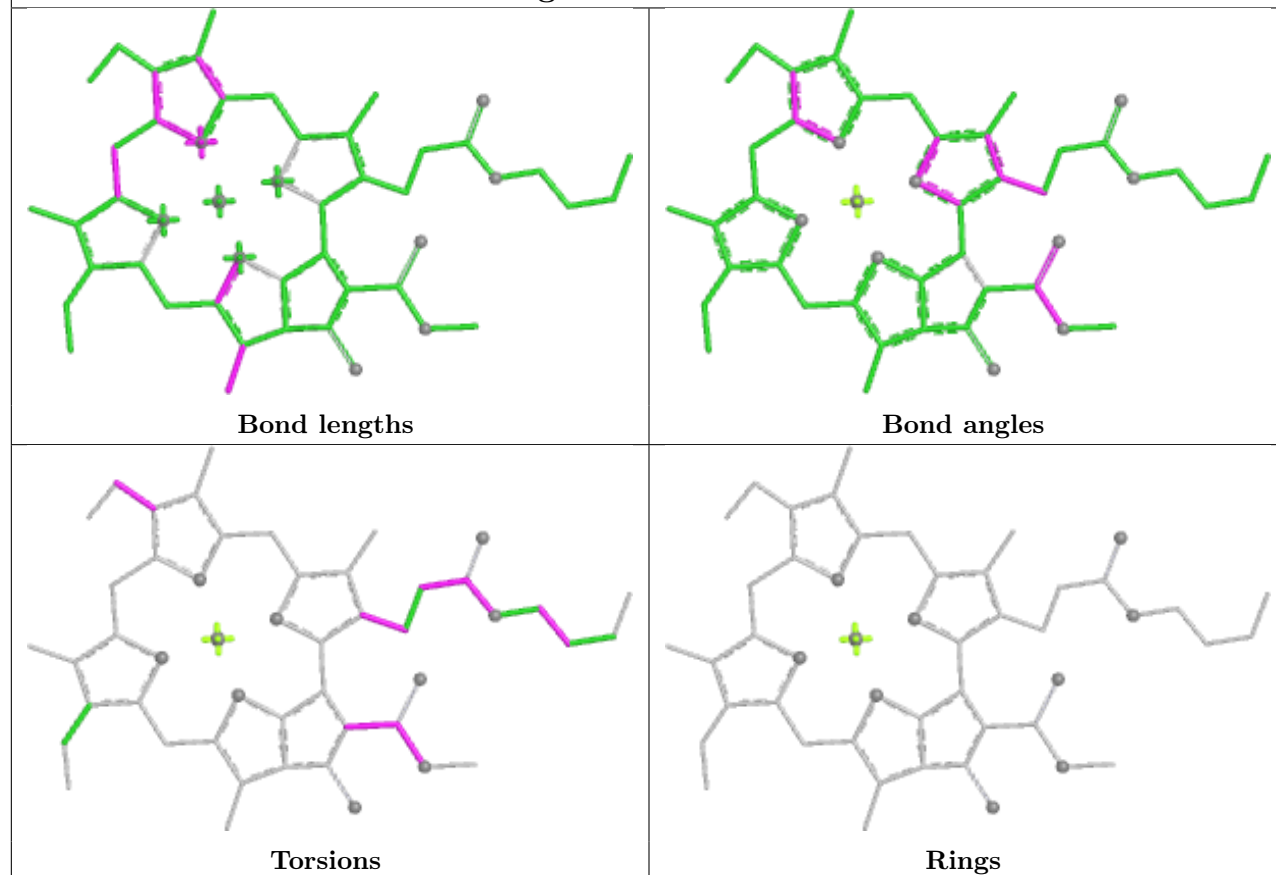




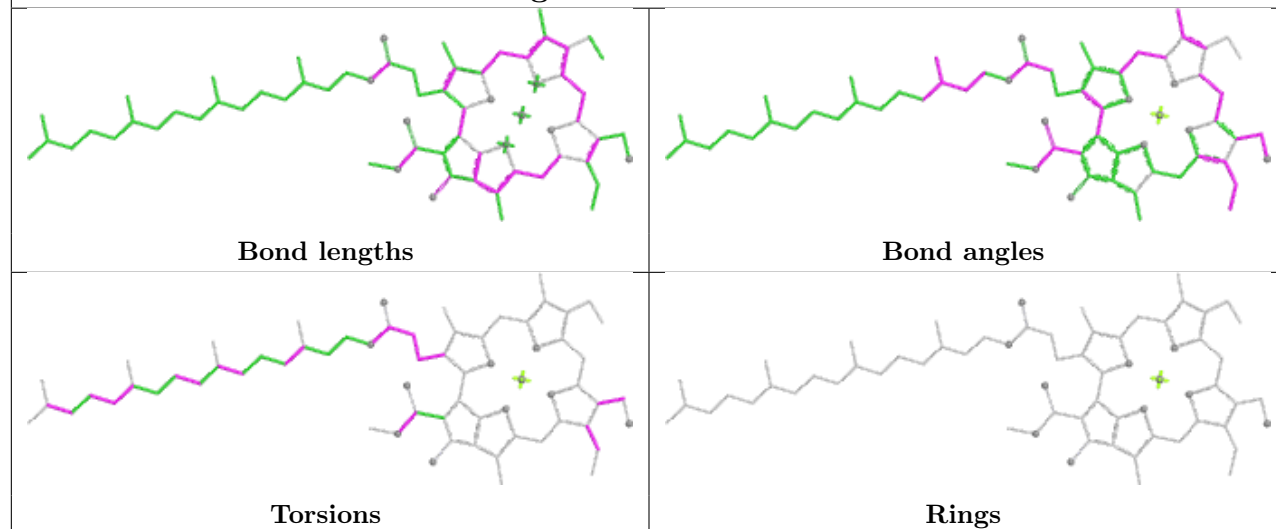


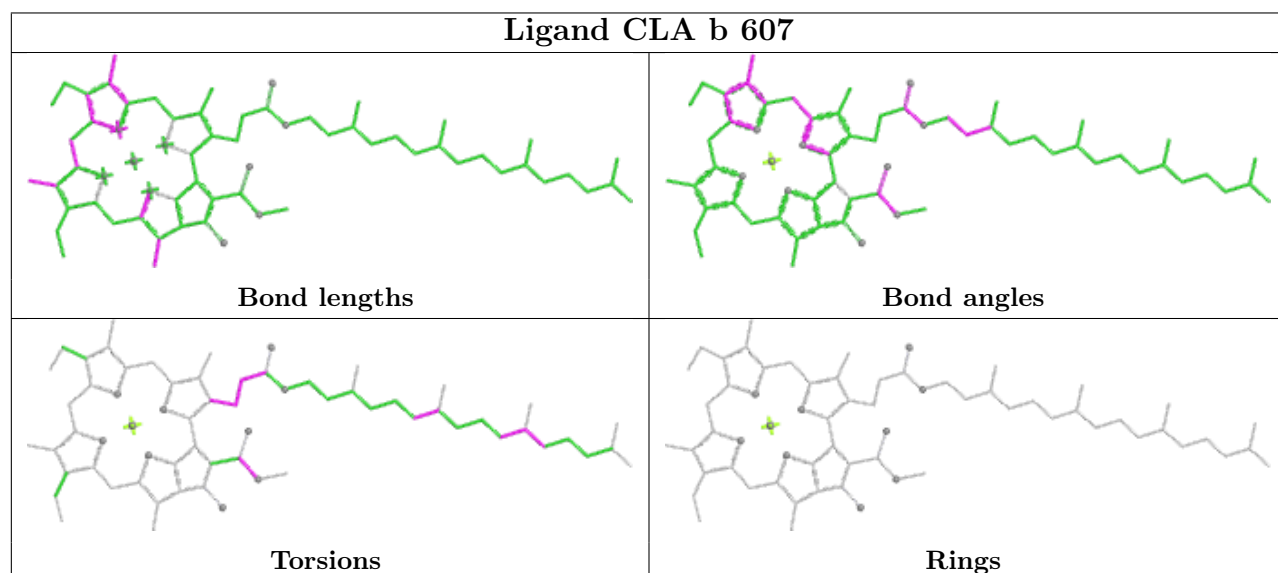
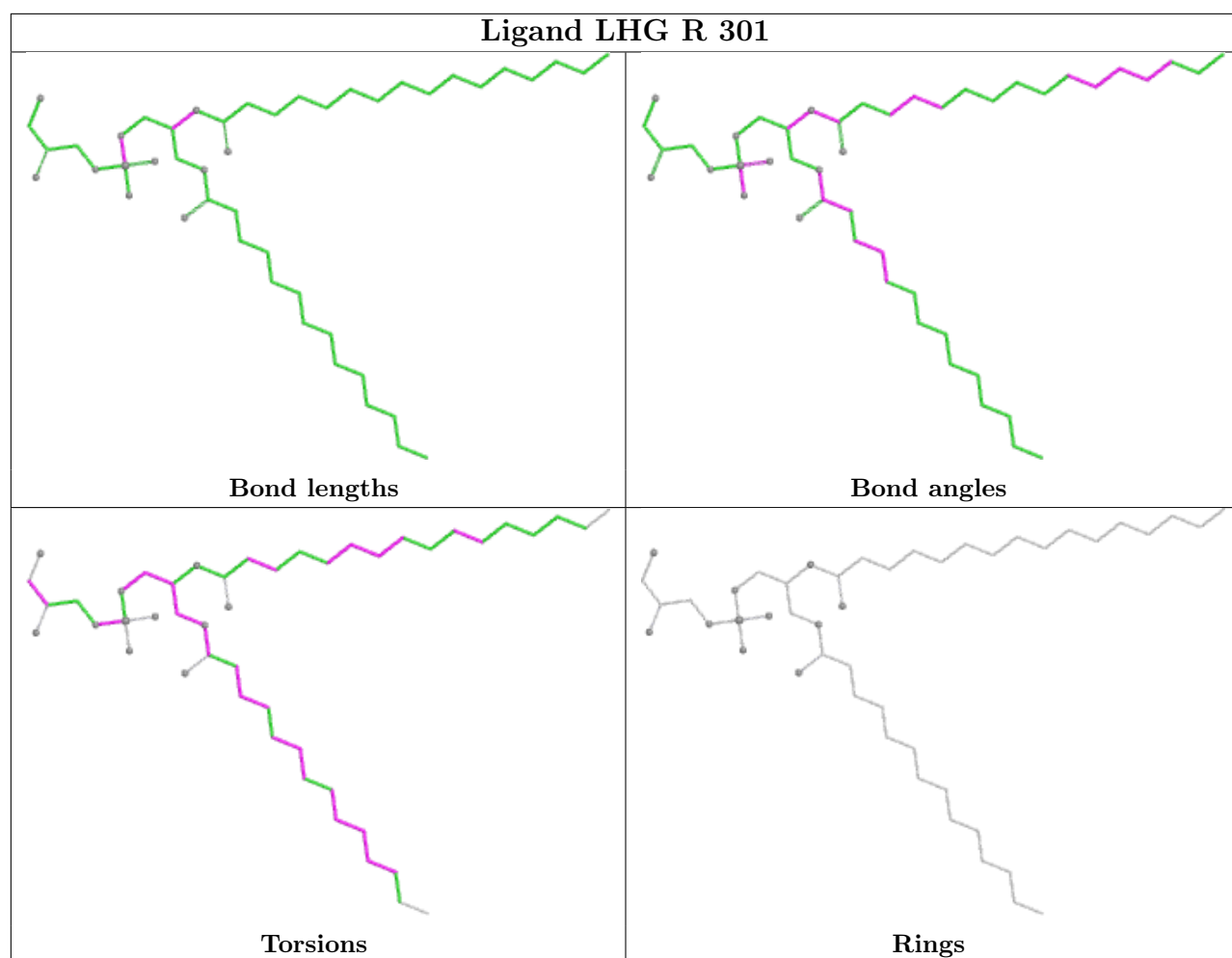


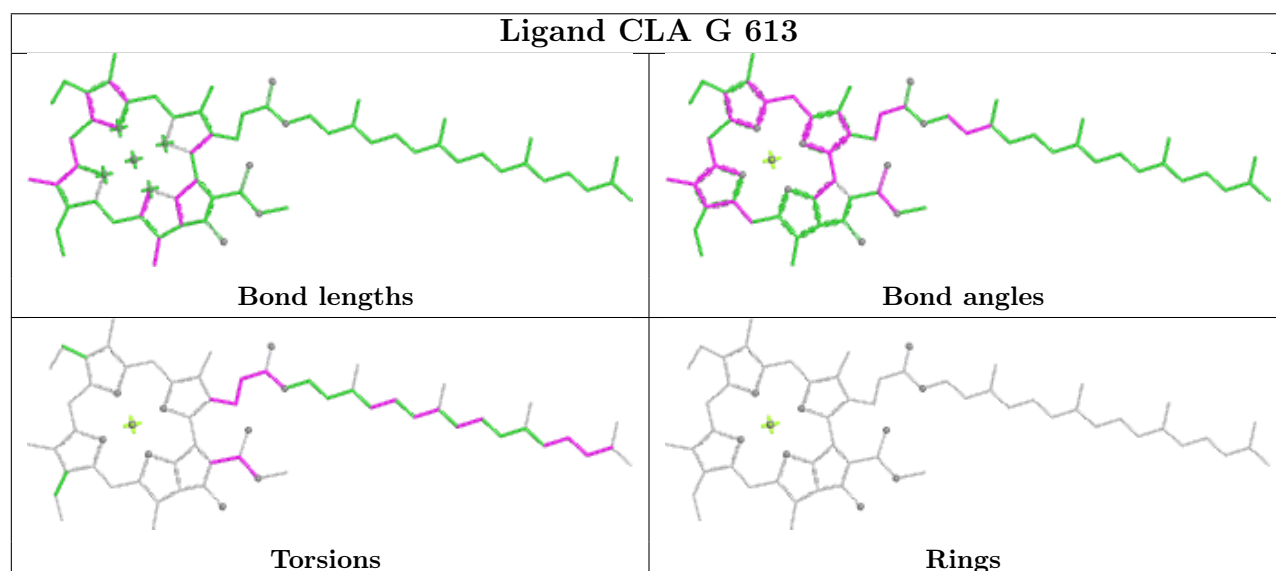
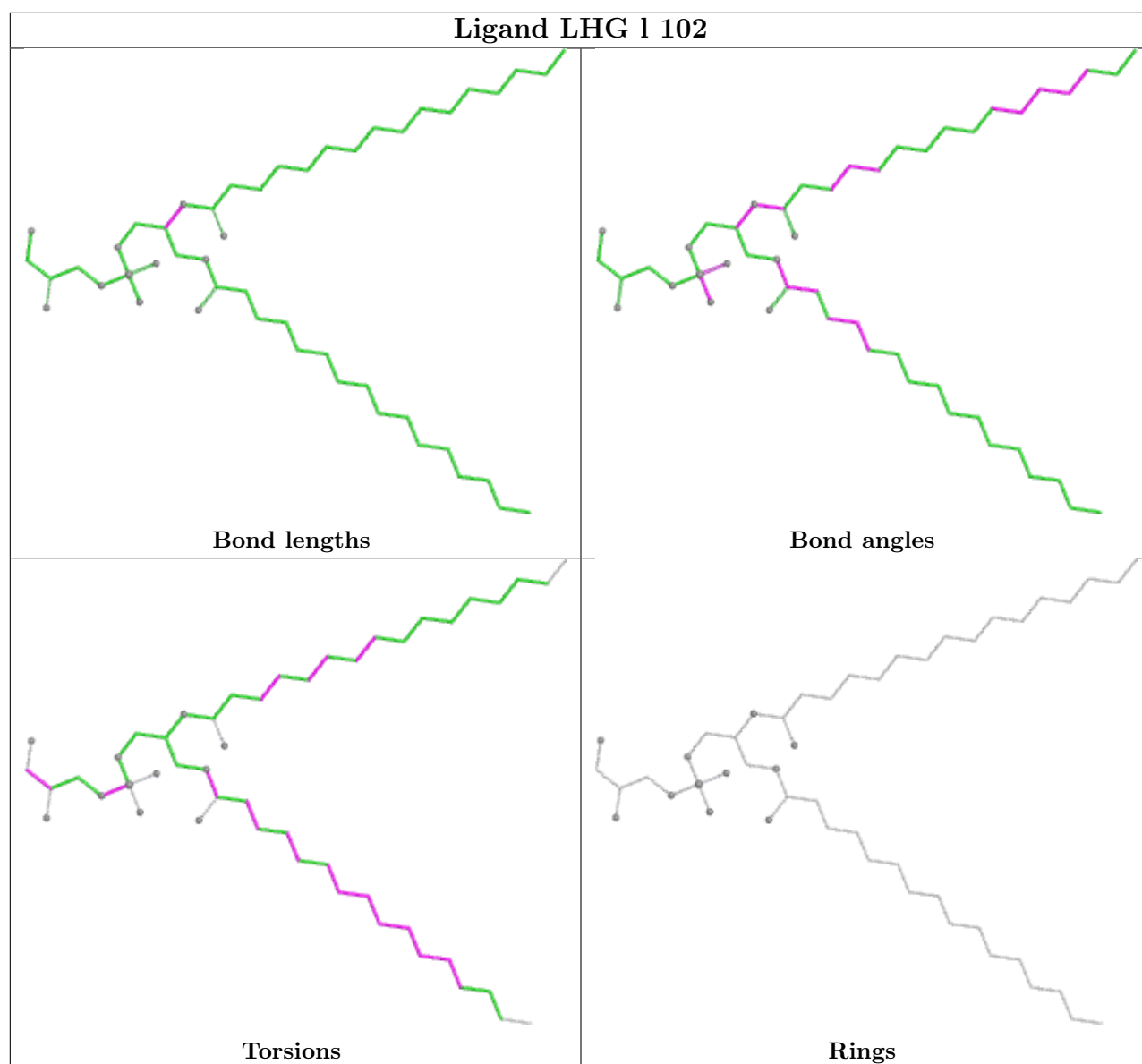
Ligand CLA r 311

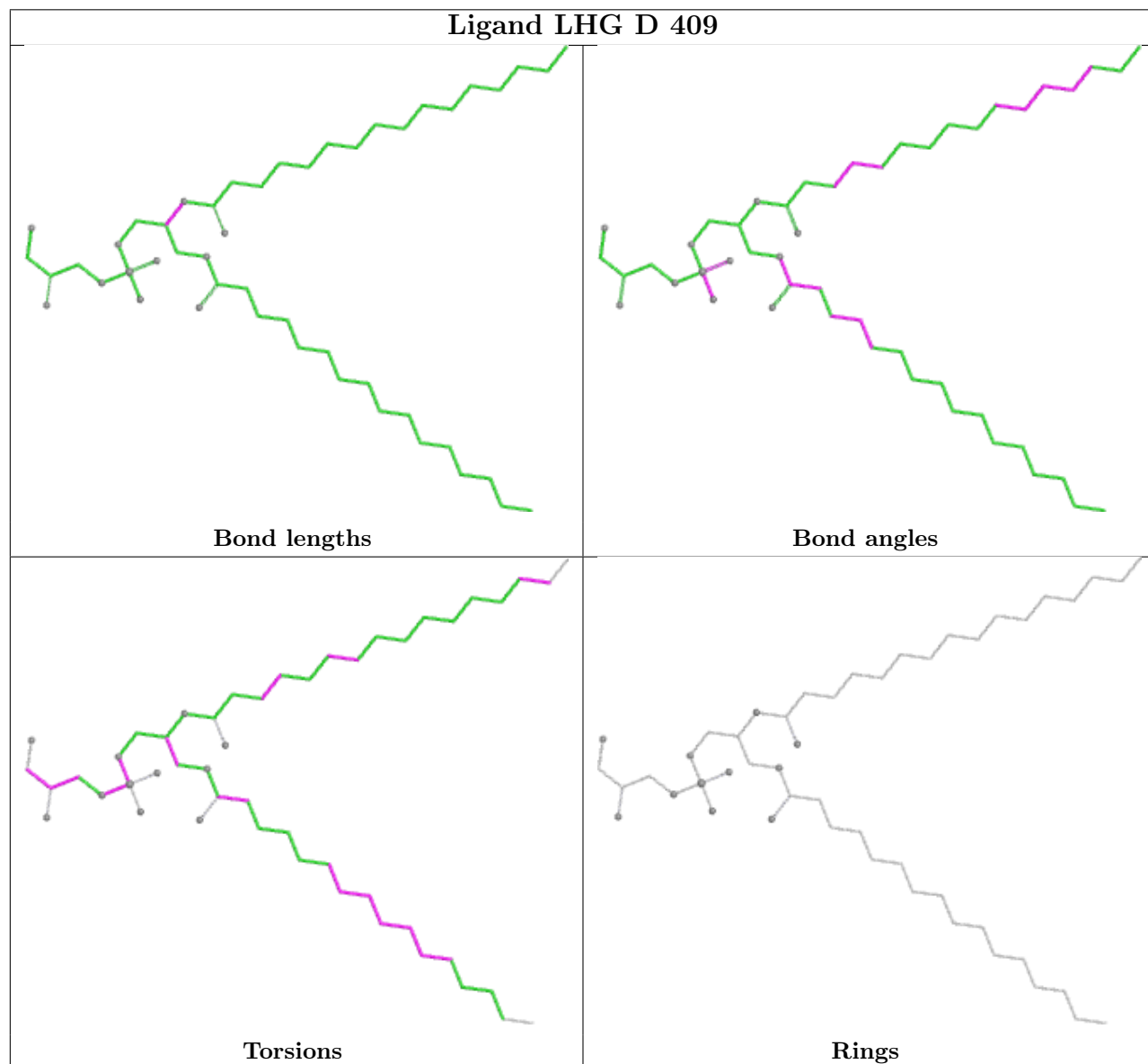
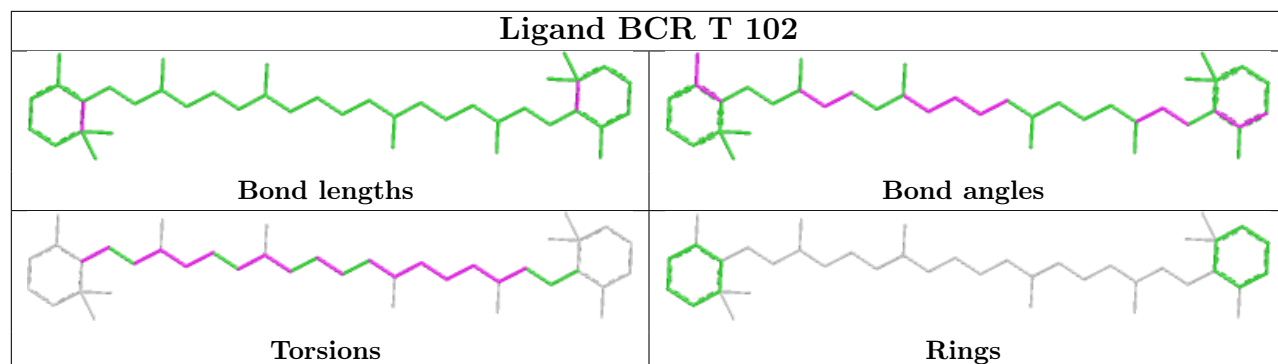


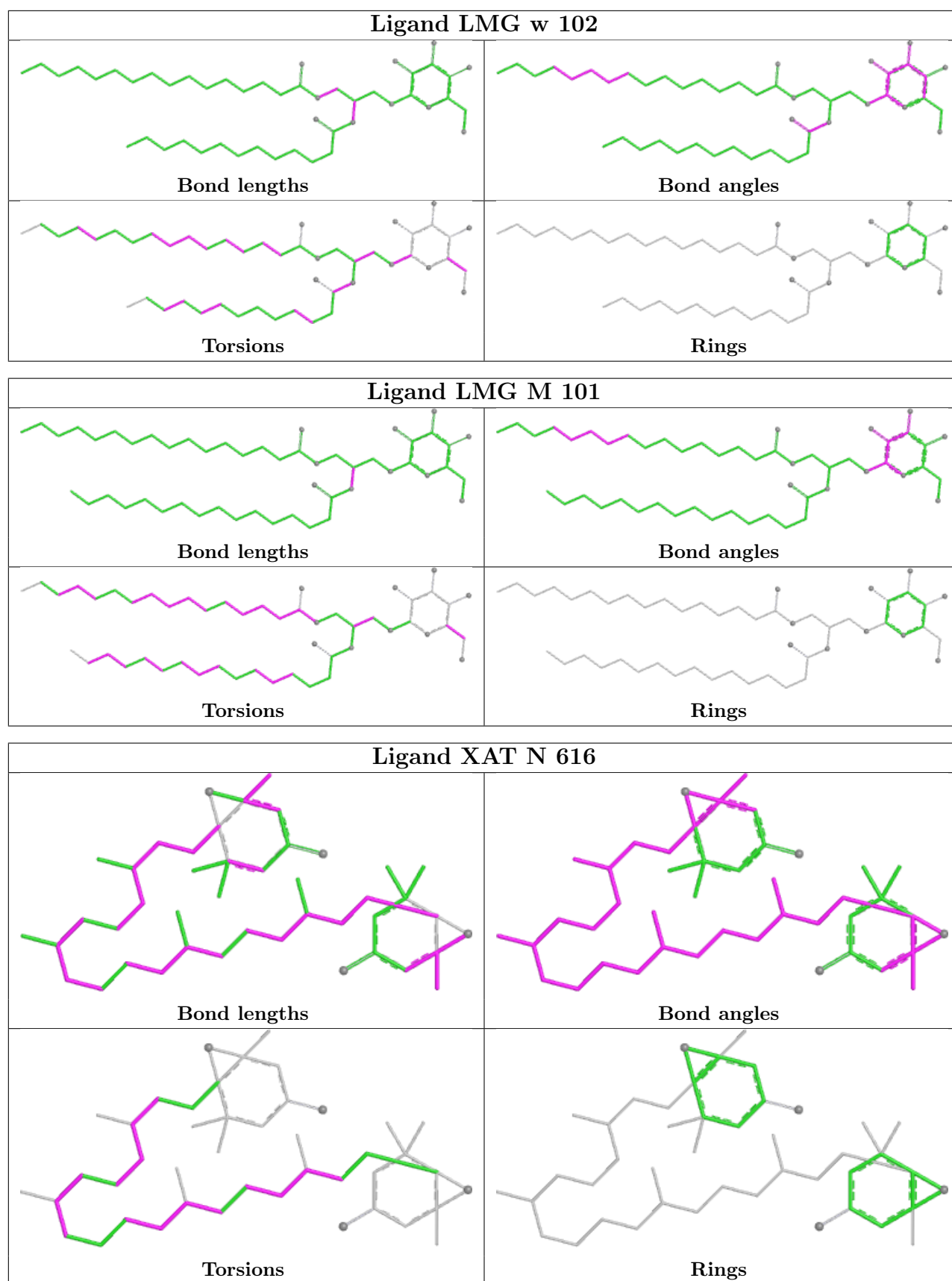
Ligand CHL N 601

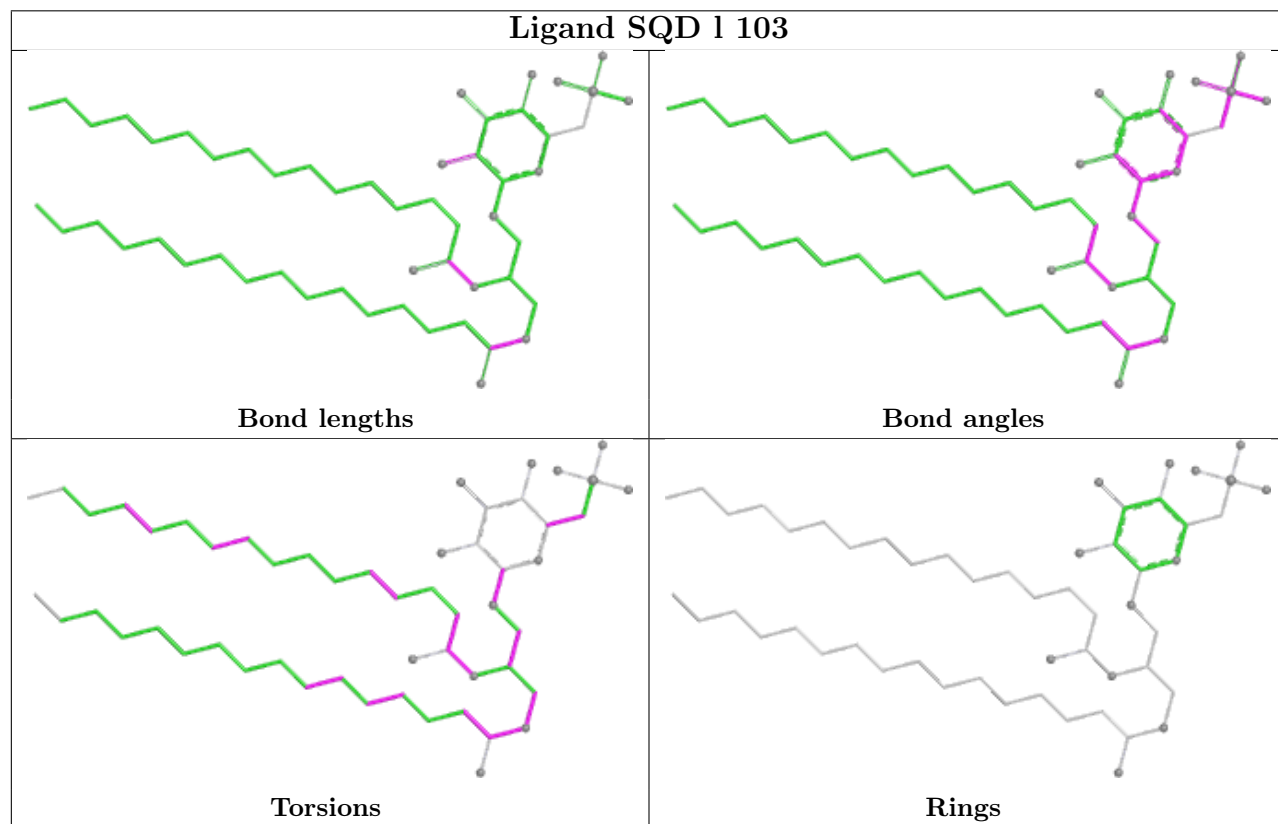
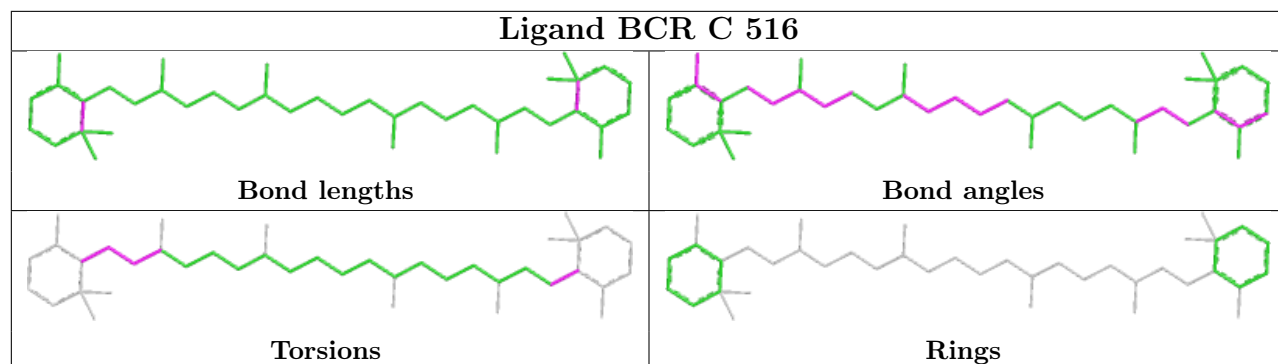


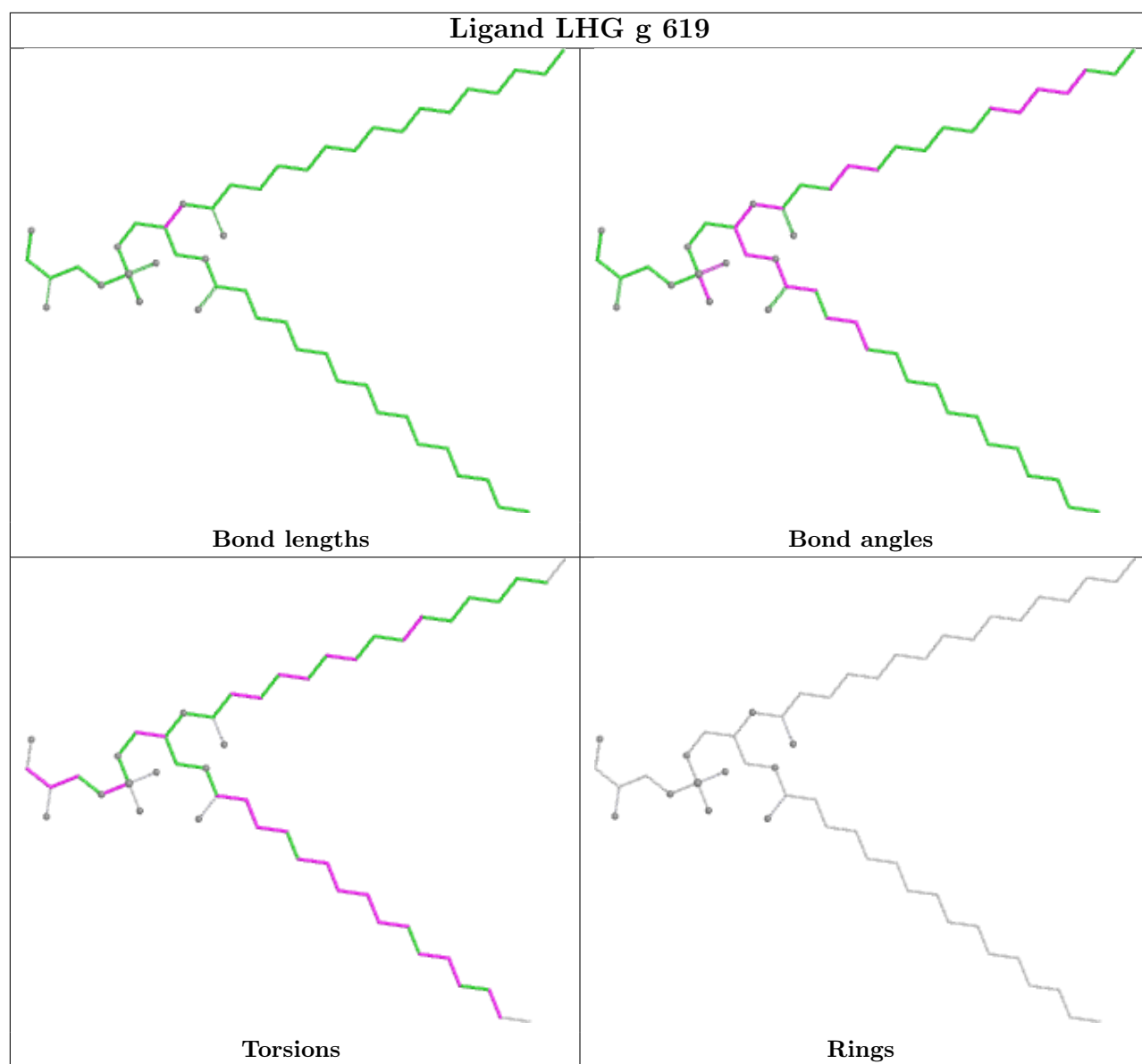


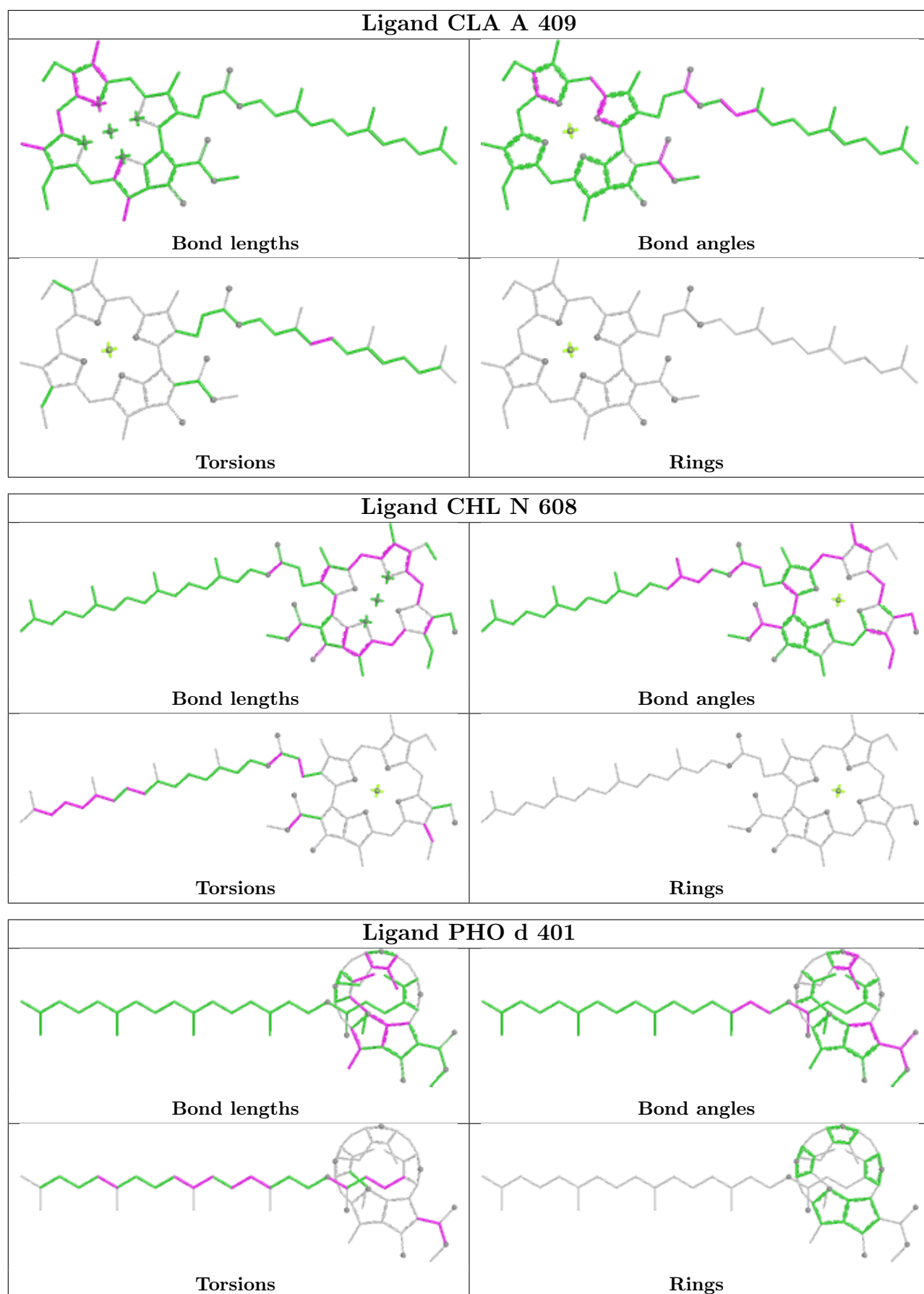




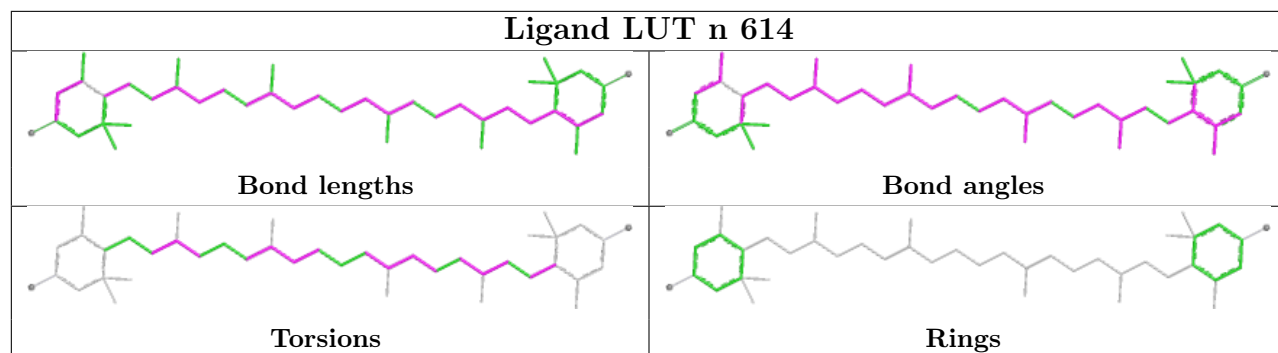




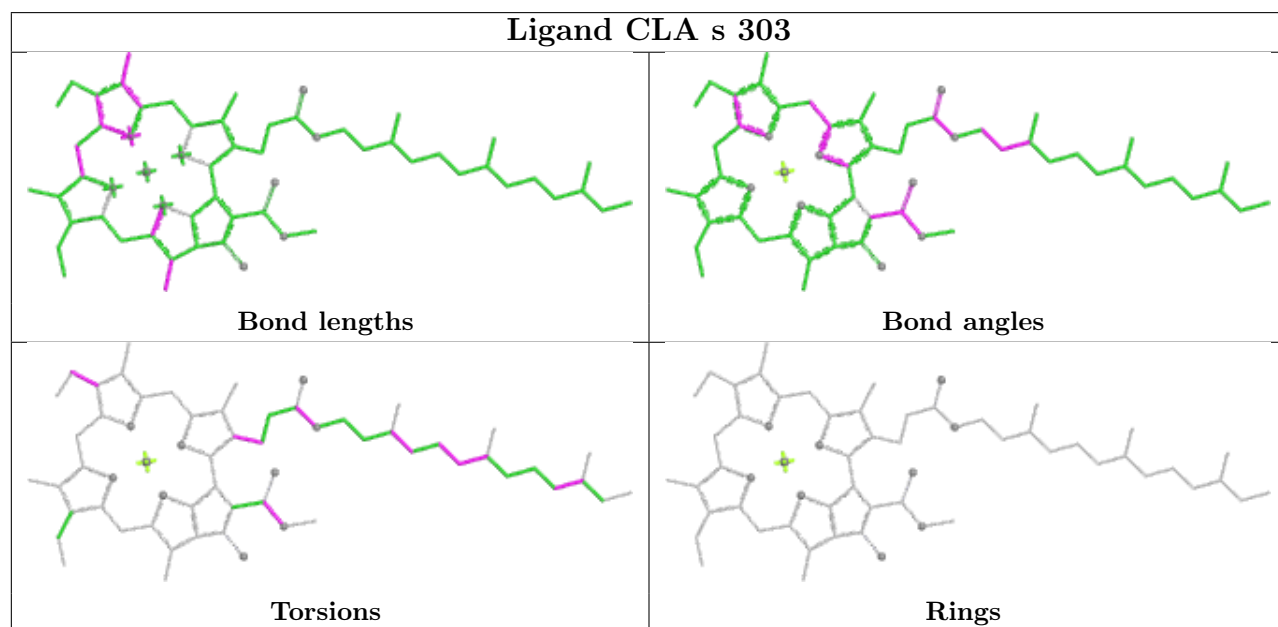




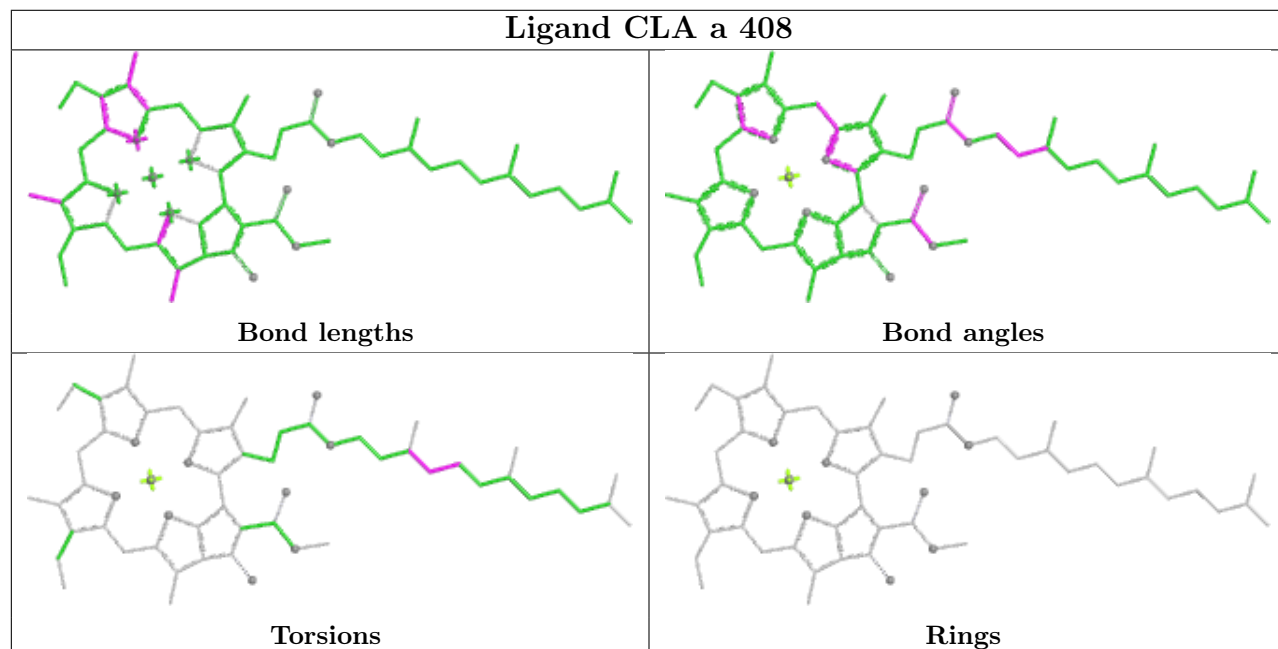
Ligand LUT n 614

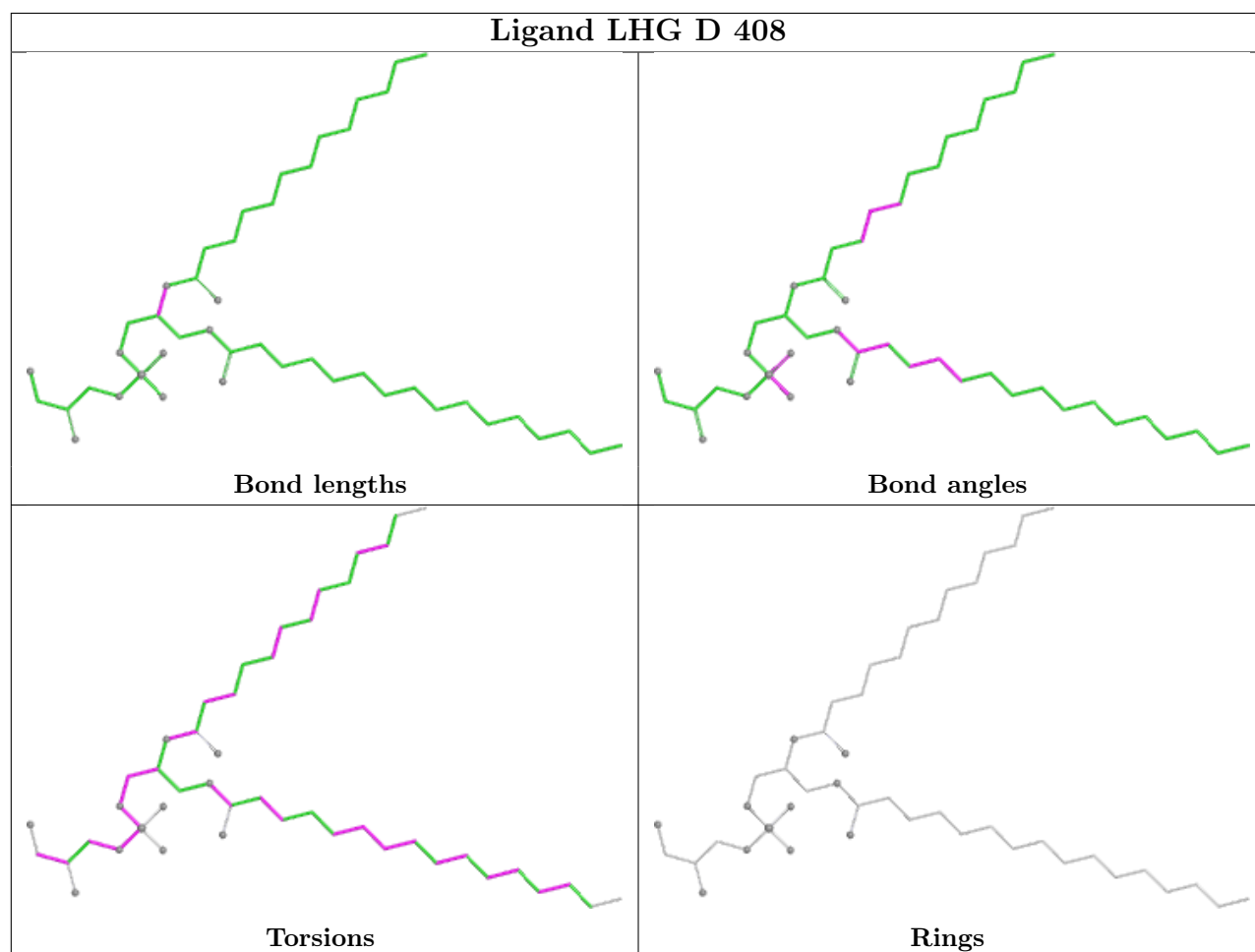
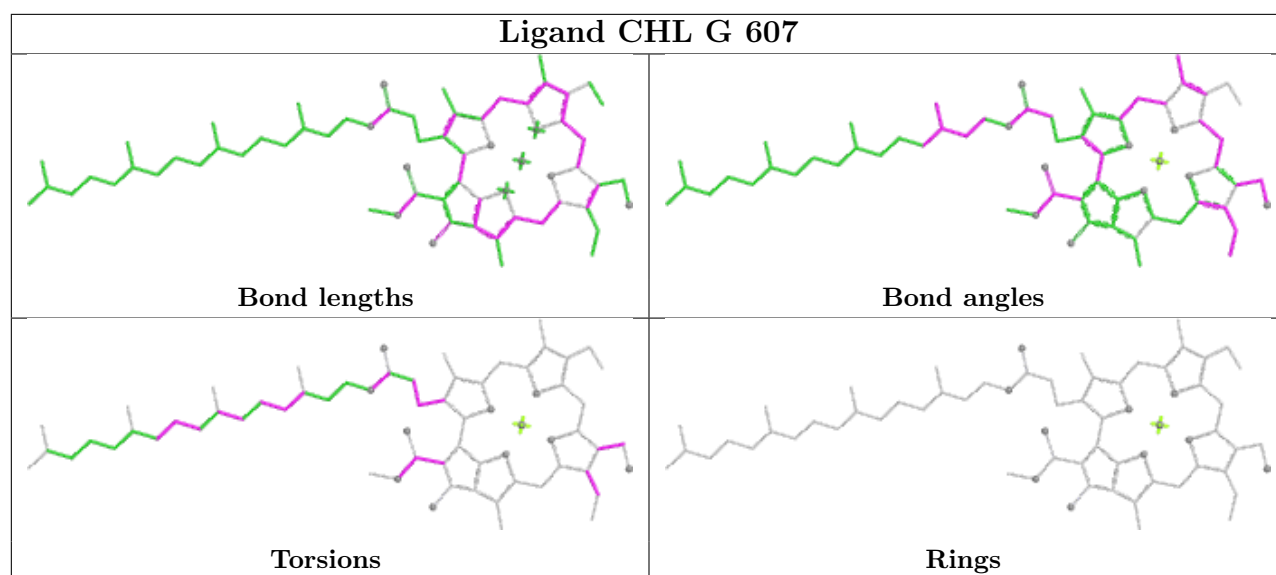


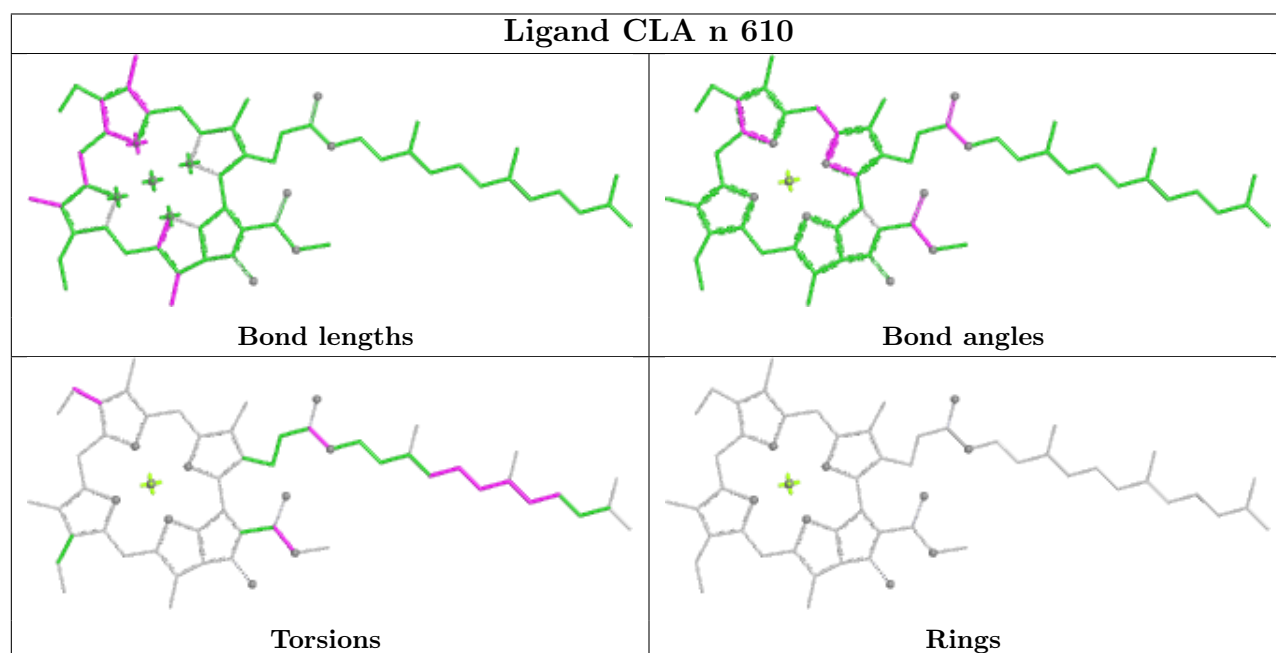
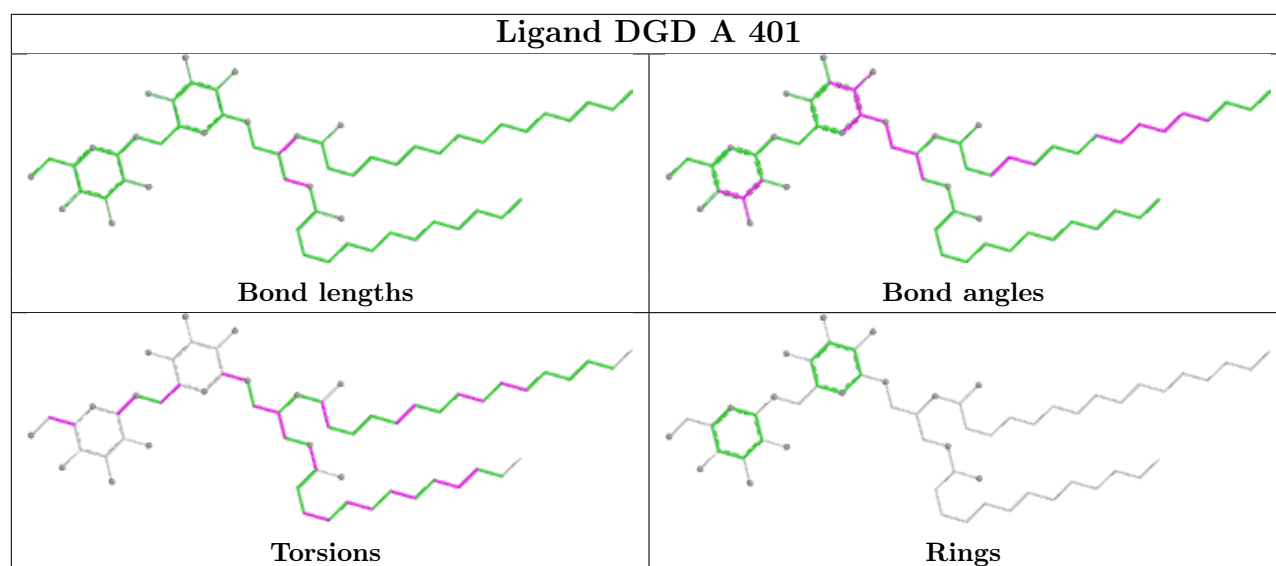
Ligand CLA s 303



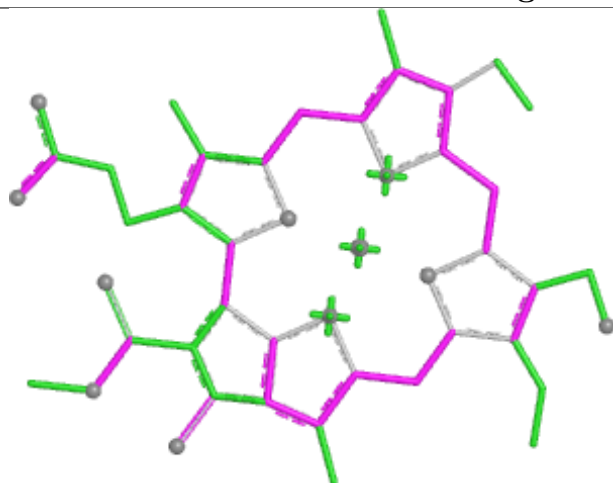
Ligand CLA a 408



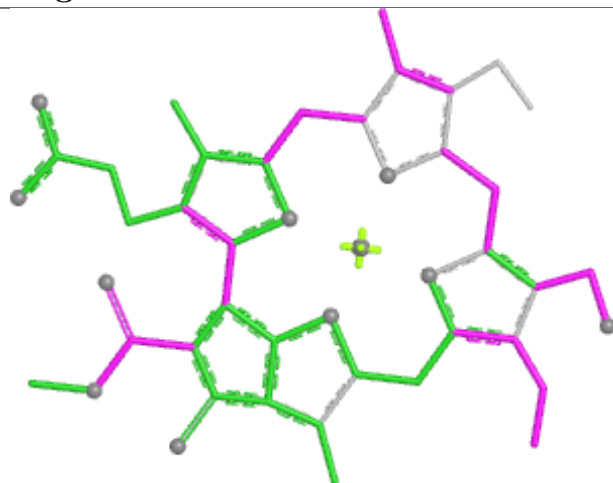




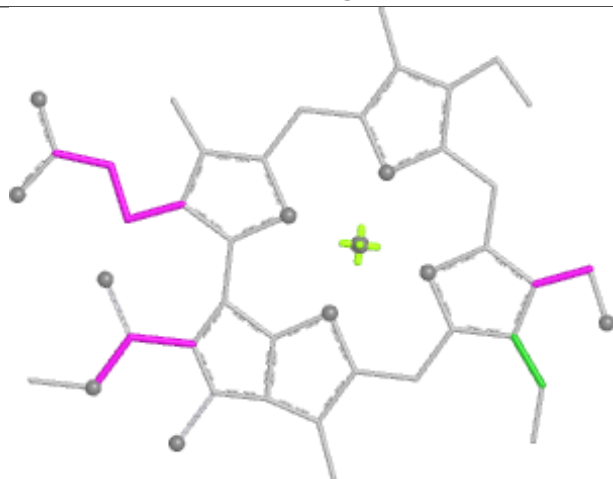
Ligand CHL g 605



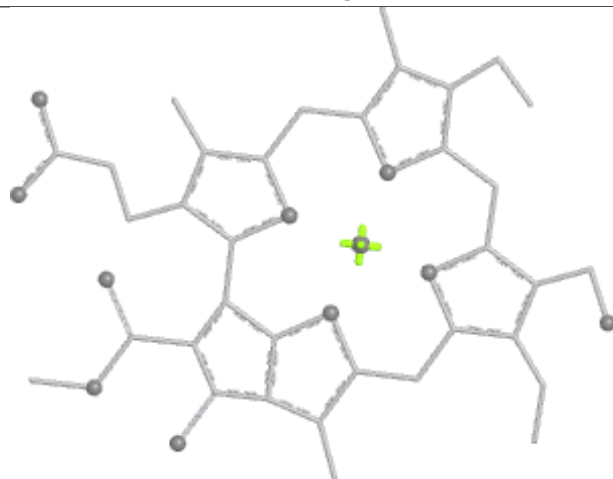
Bond lengths



Bond angles

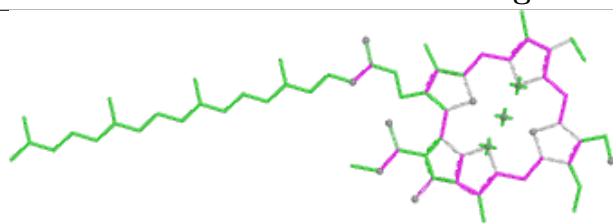


Torsions

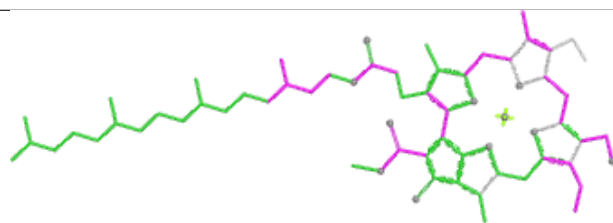


Rings

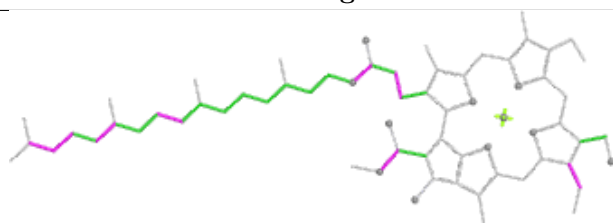
Ligand CHL Y 608



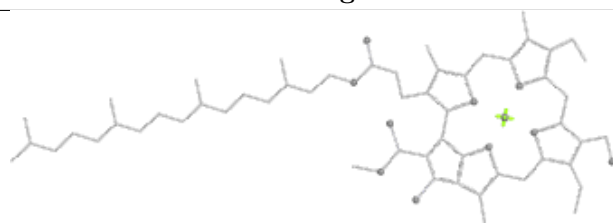
Bond lengths



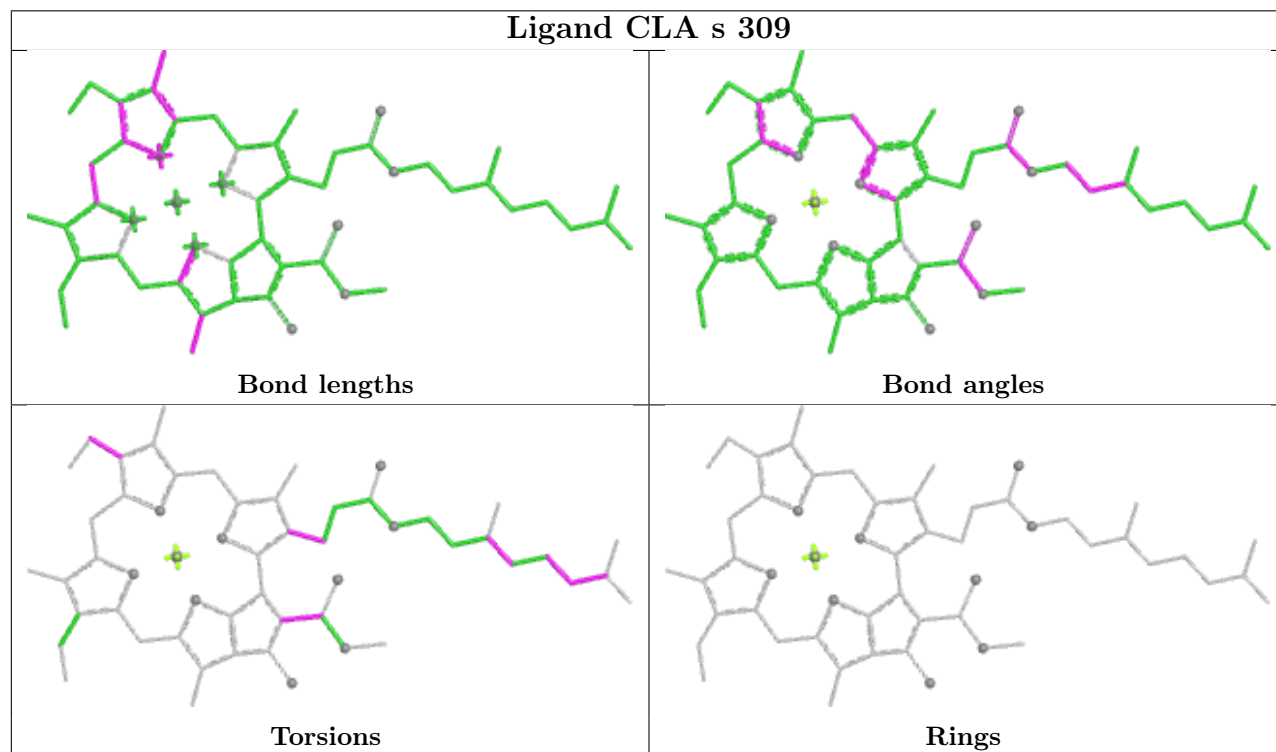
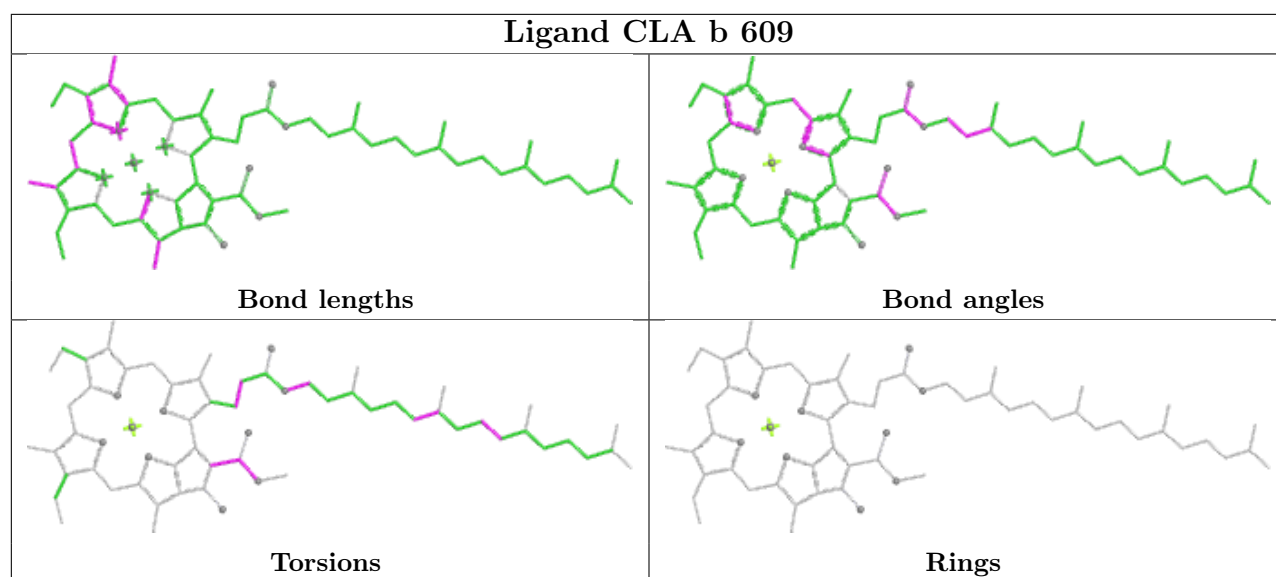
Bond angles

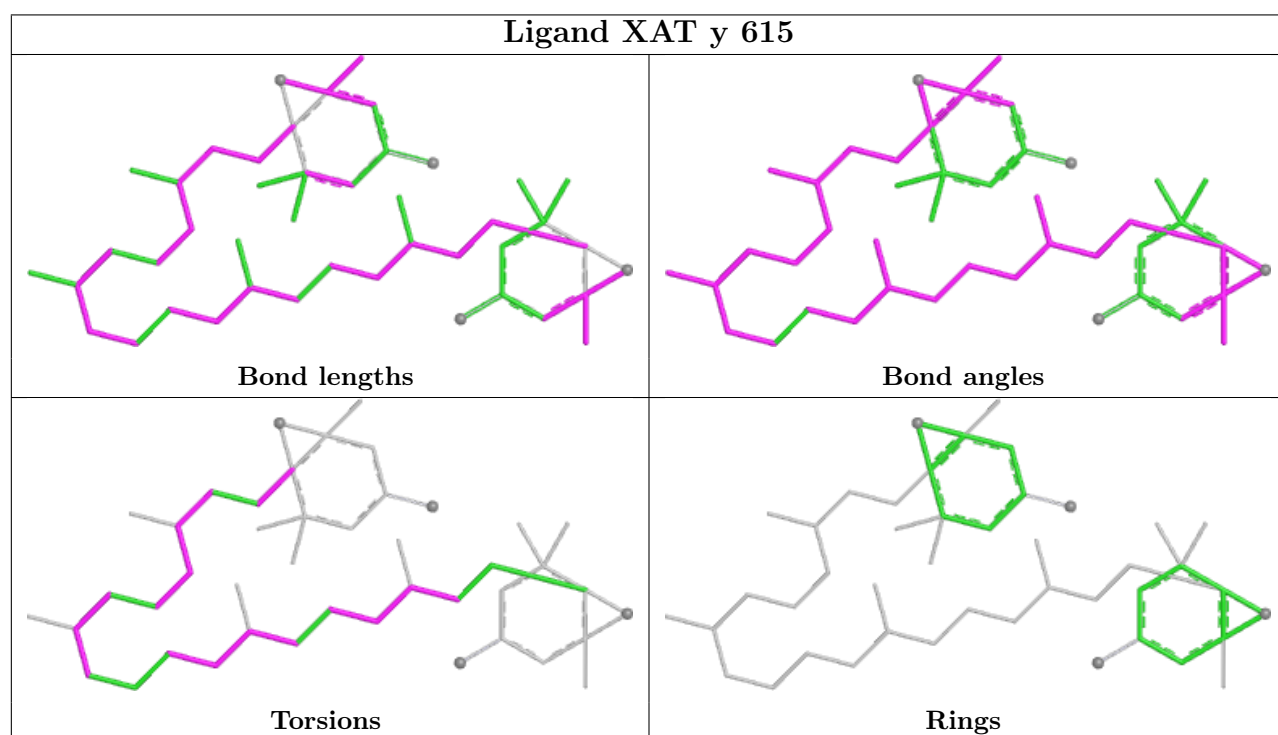
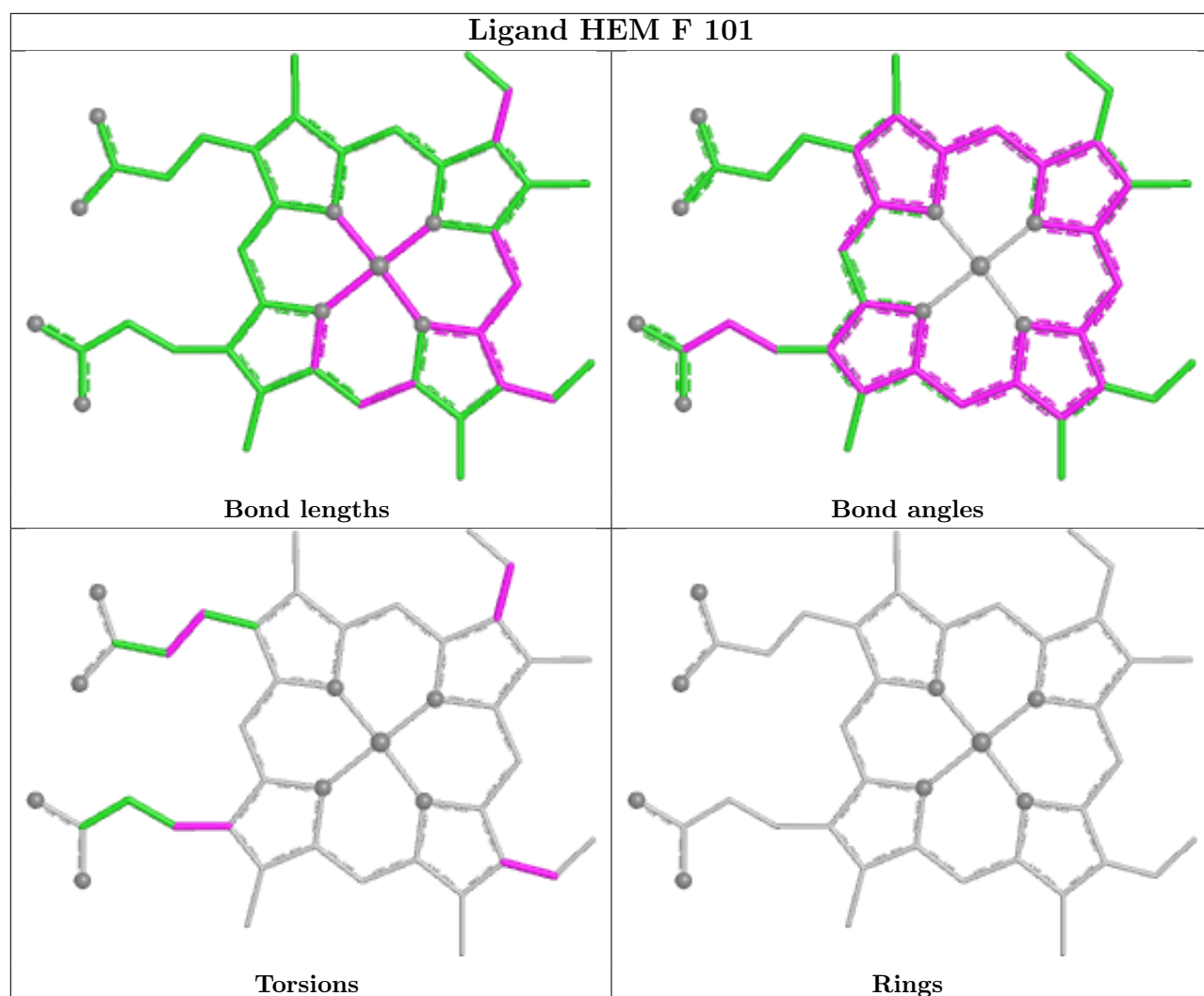


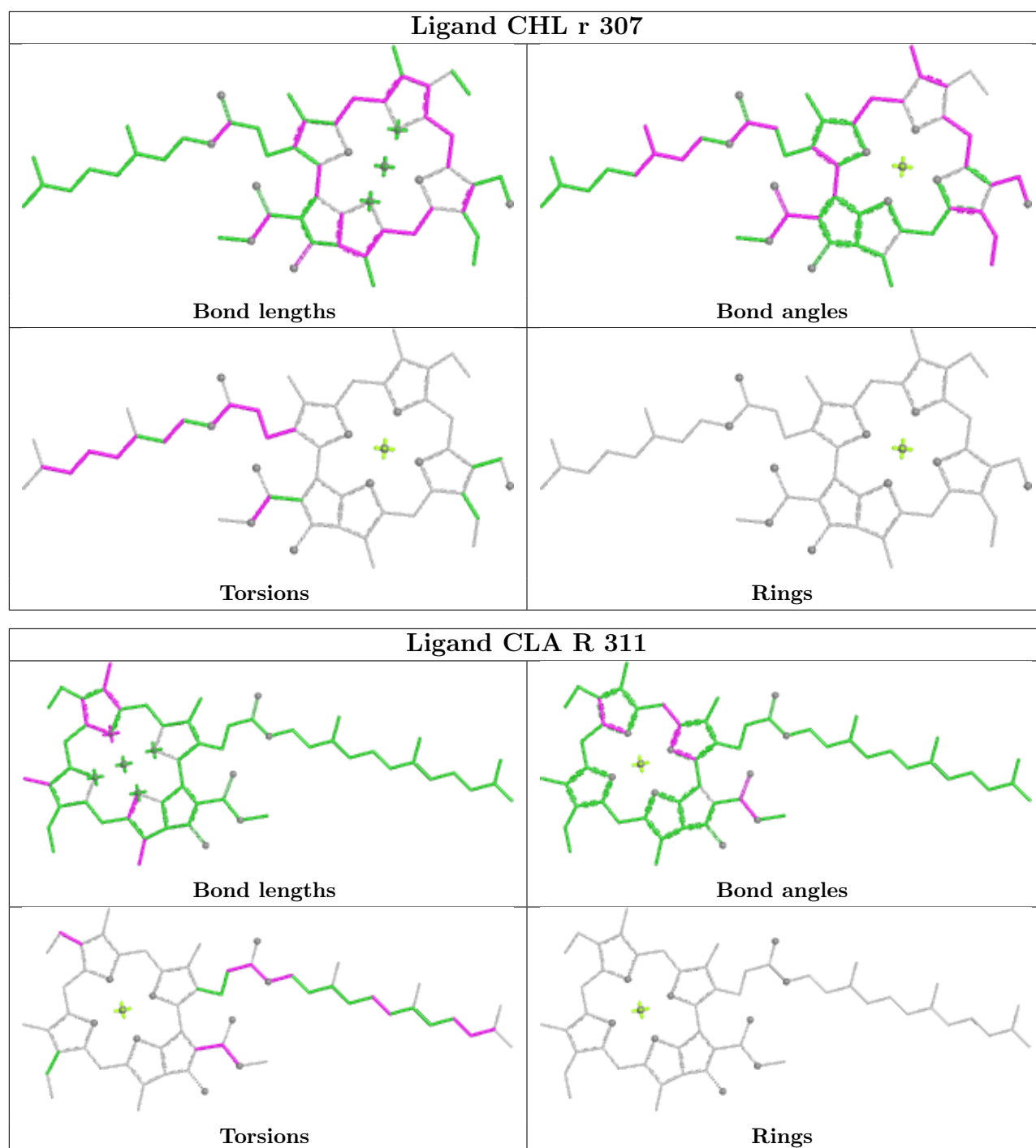
Torsions

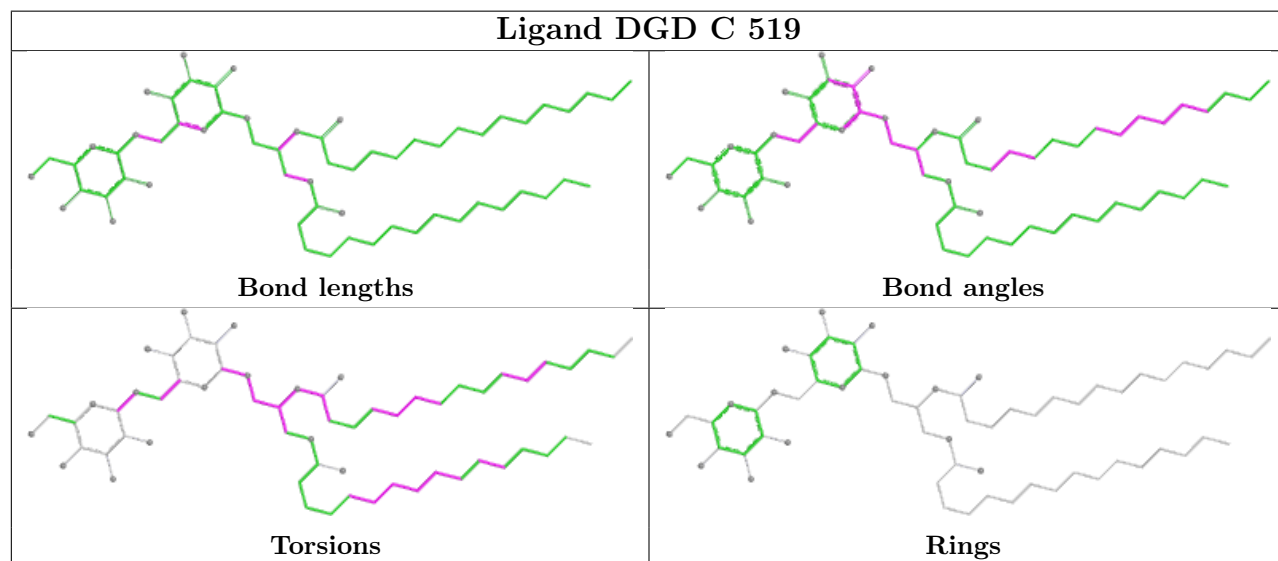
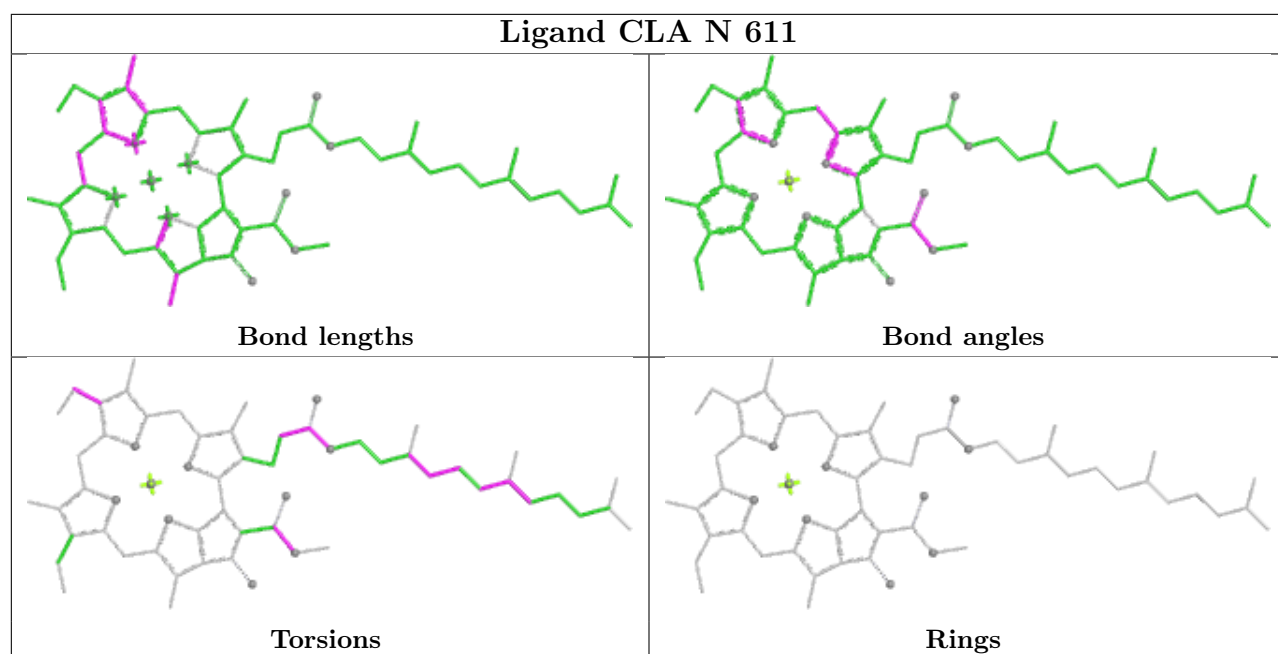


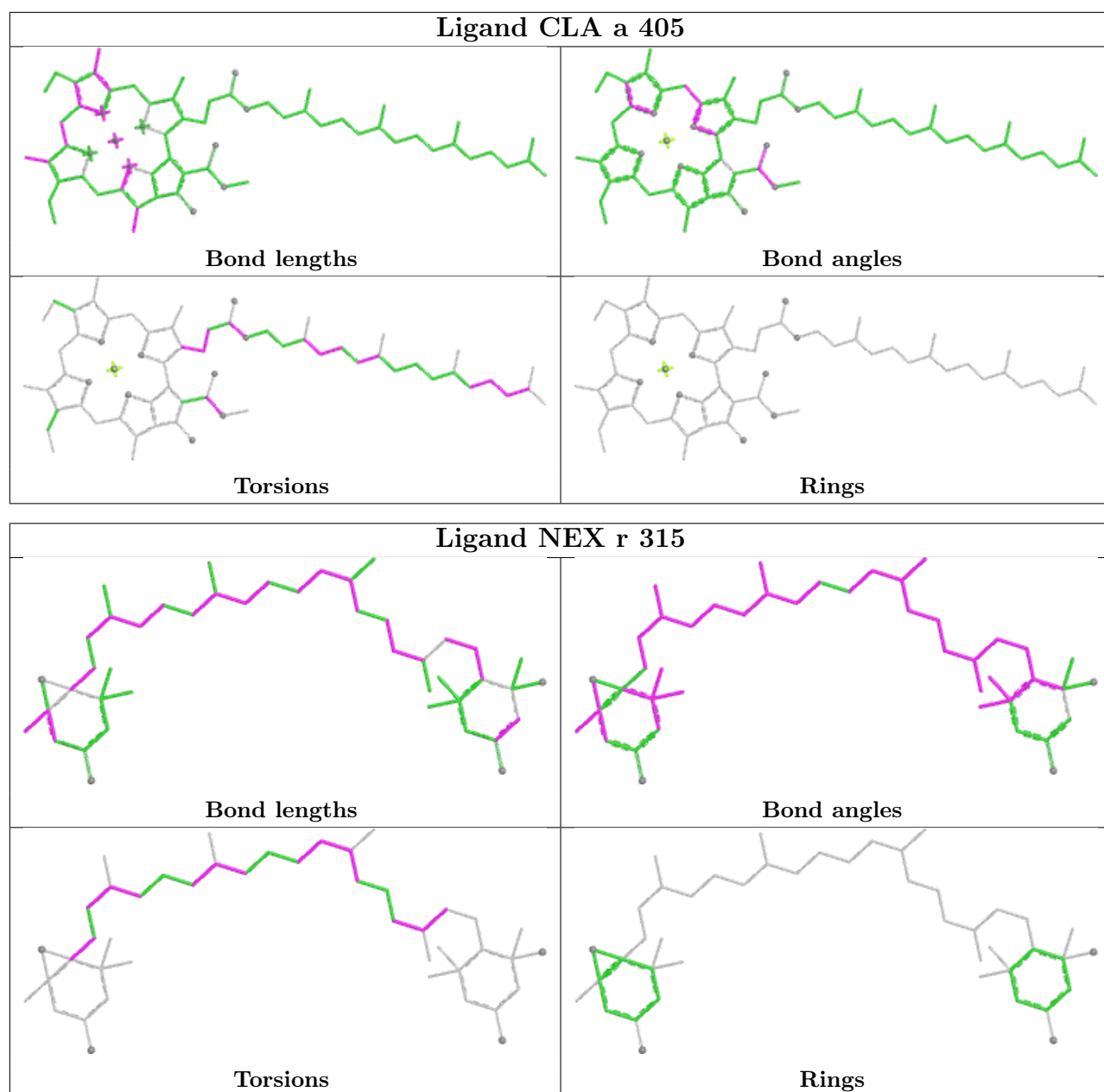
Rings



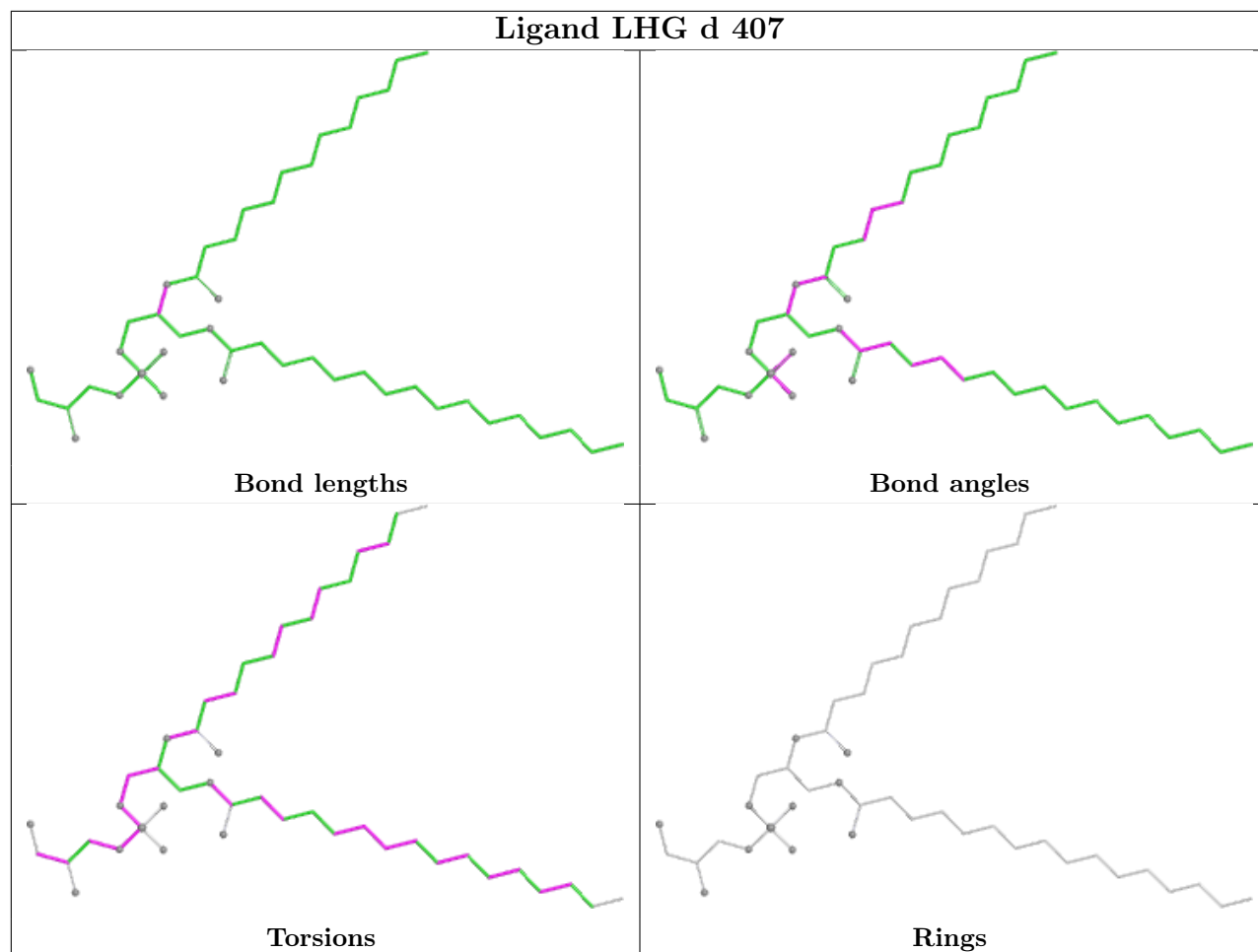




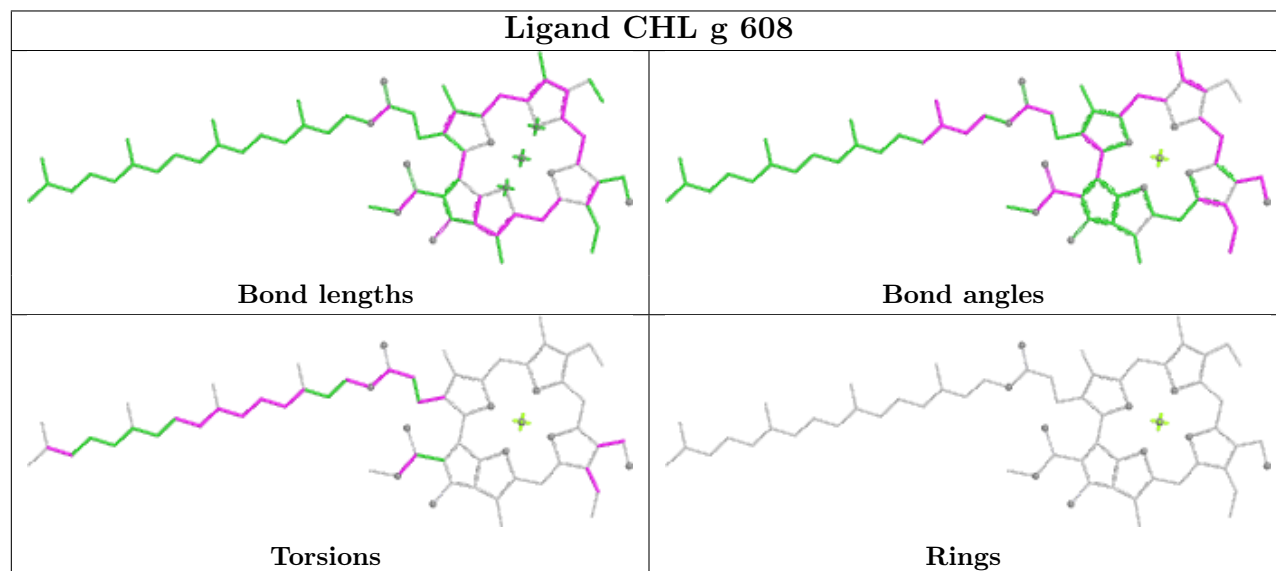


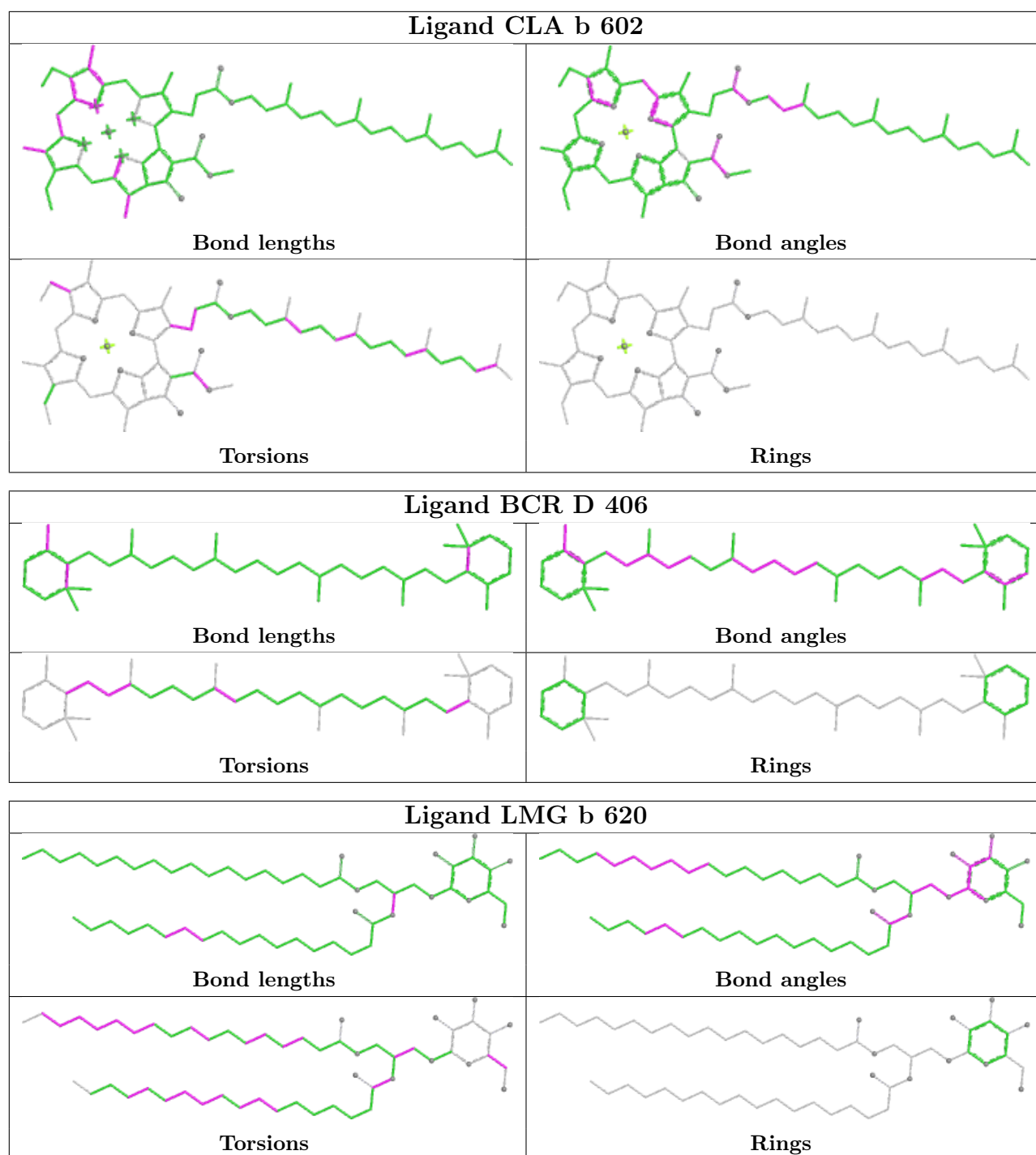


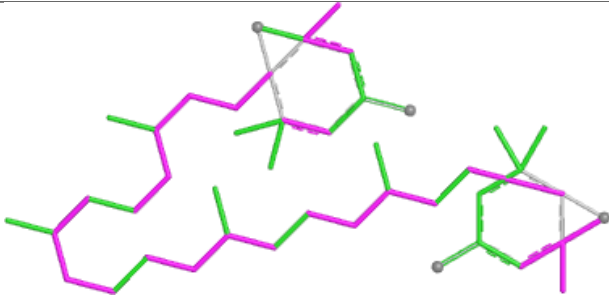
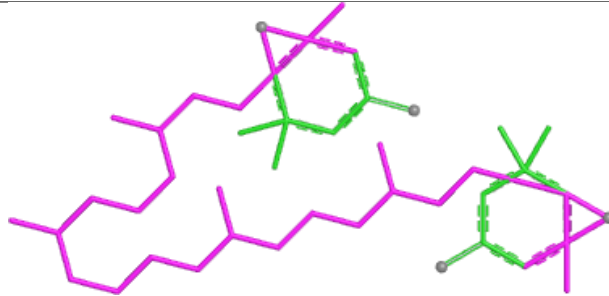
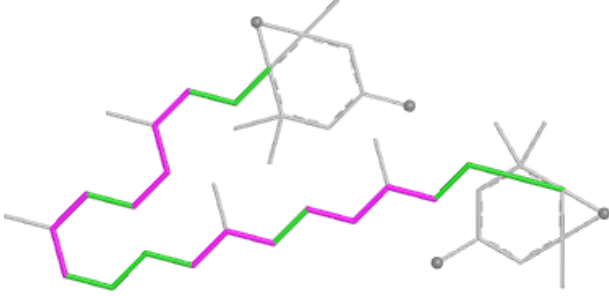
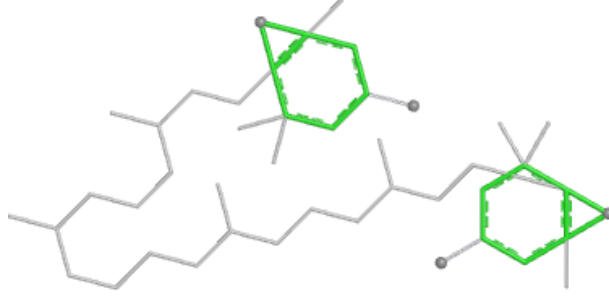
Ligand LHG d 407

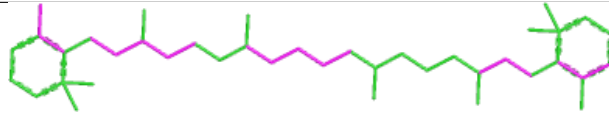
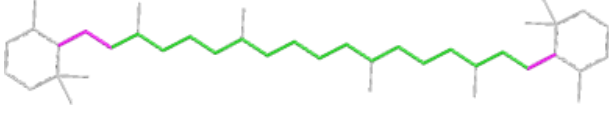
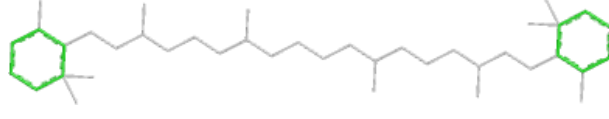


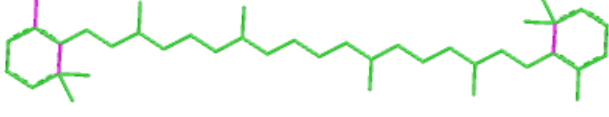
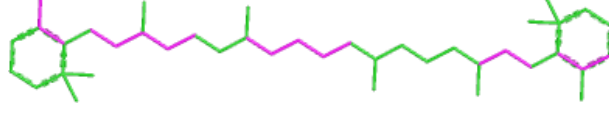
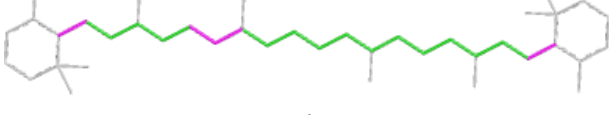
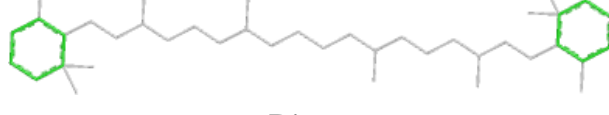
Ligand CHL g 608

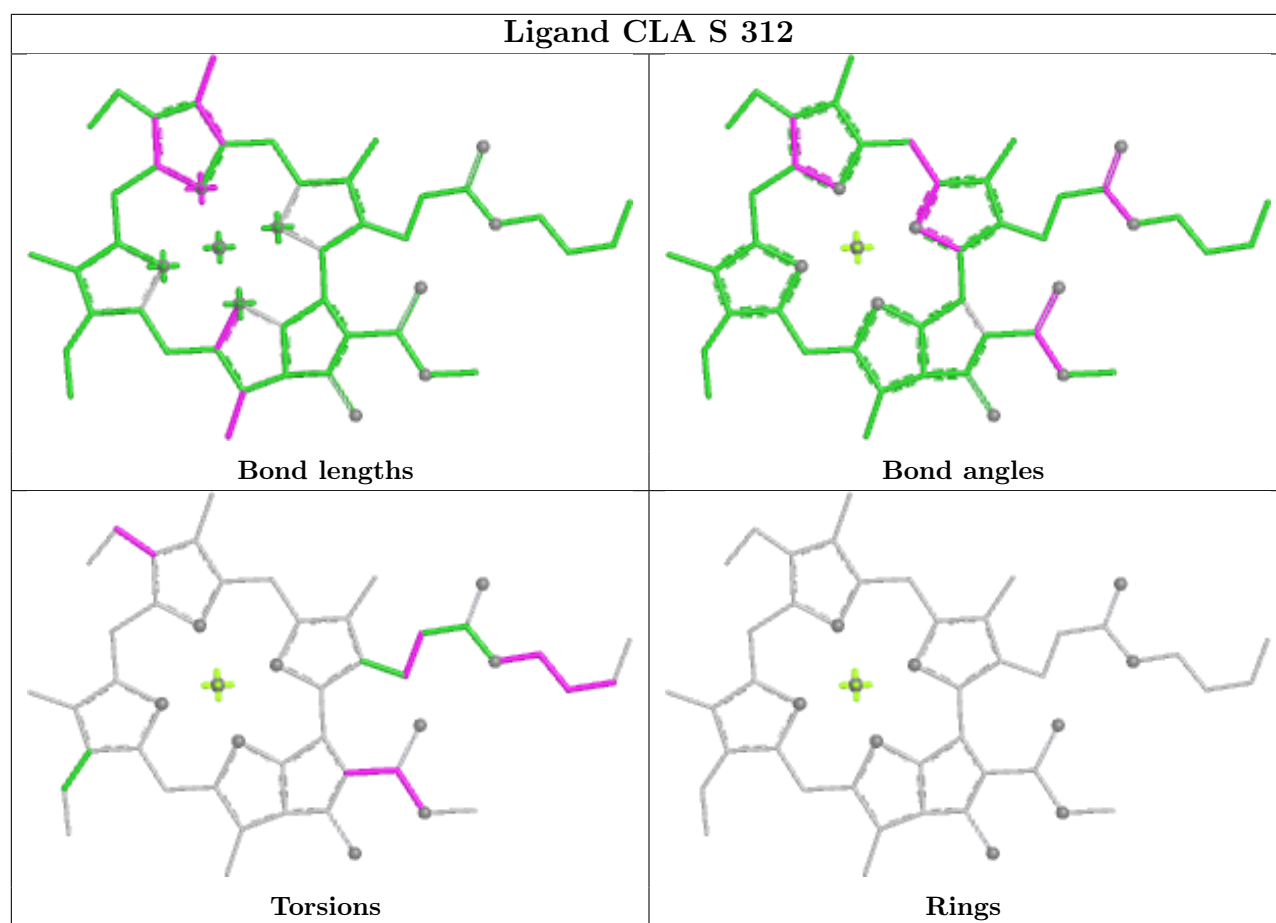




Ligand XAT n 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR K 102	
	
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.

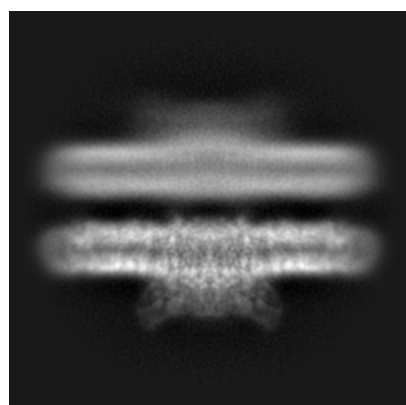
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10865. These allow visual inspection of the internal detail of the map and identification of artifacts.

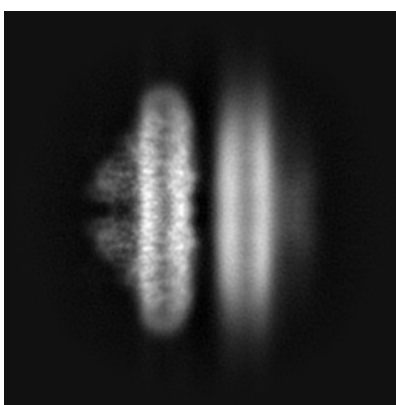
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

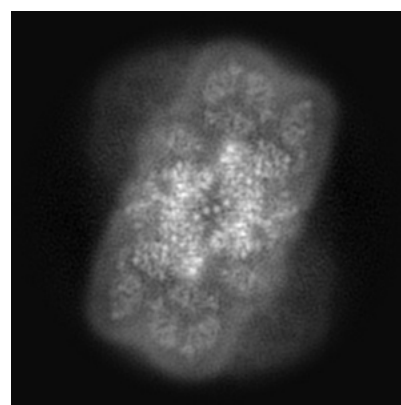
6.1.1 Primary map



X



Y

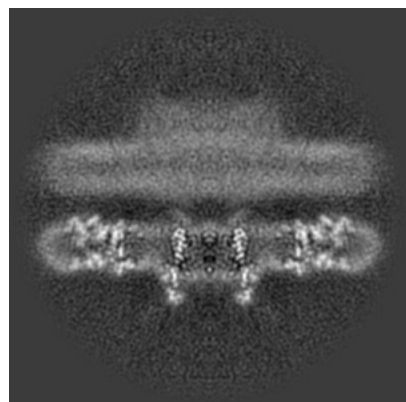


Z

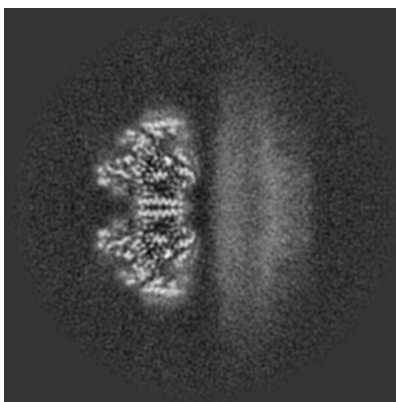
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

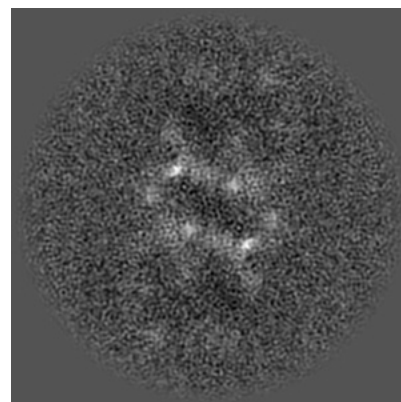
6.2.1 Primary map



X Index: 170



Y Index: 170

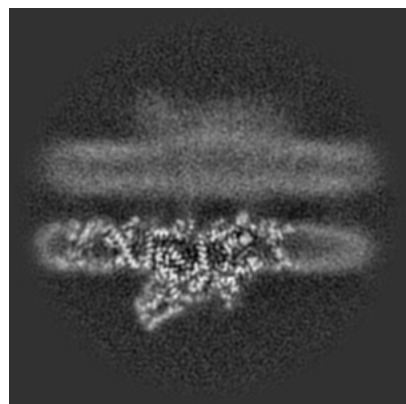


Z Index: 170

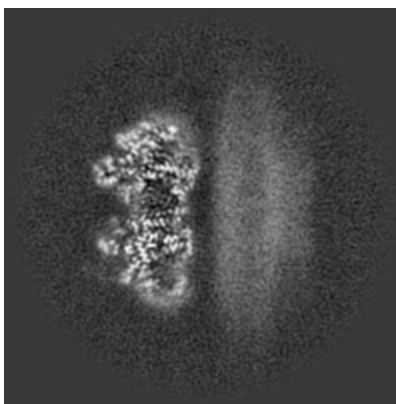
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

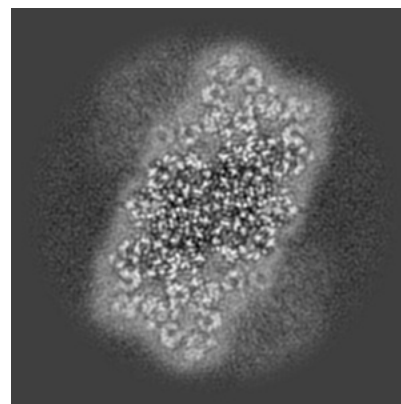
6.3.1 Primary map



X Index: 156



Y Index: 166

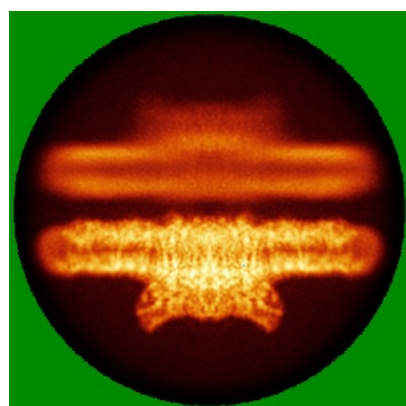


Z Index: 121

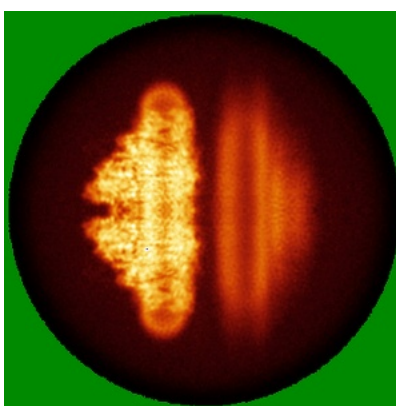
The images above show the largest variance slices of the map in three orthogonal directions.

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

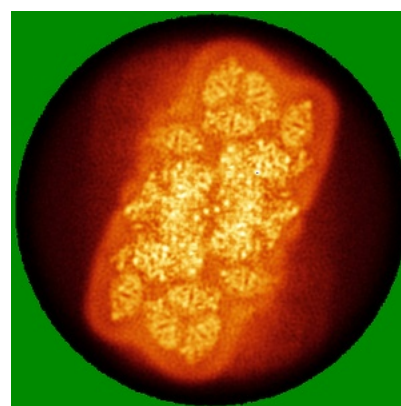
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

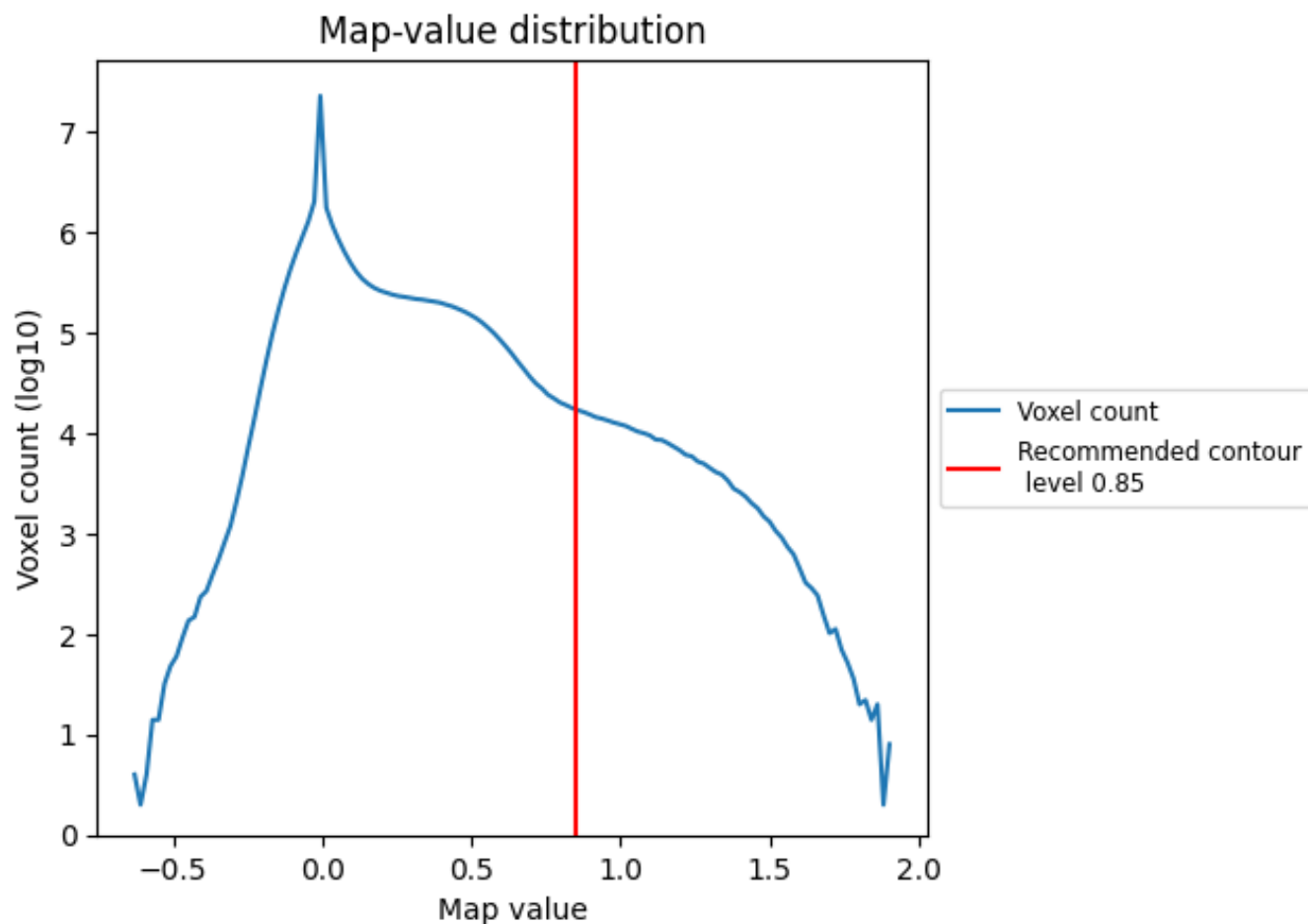
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

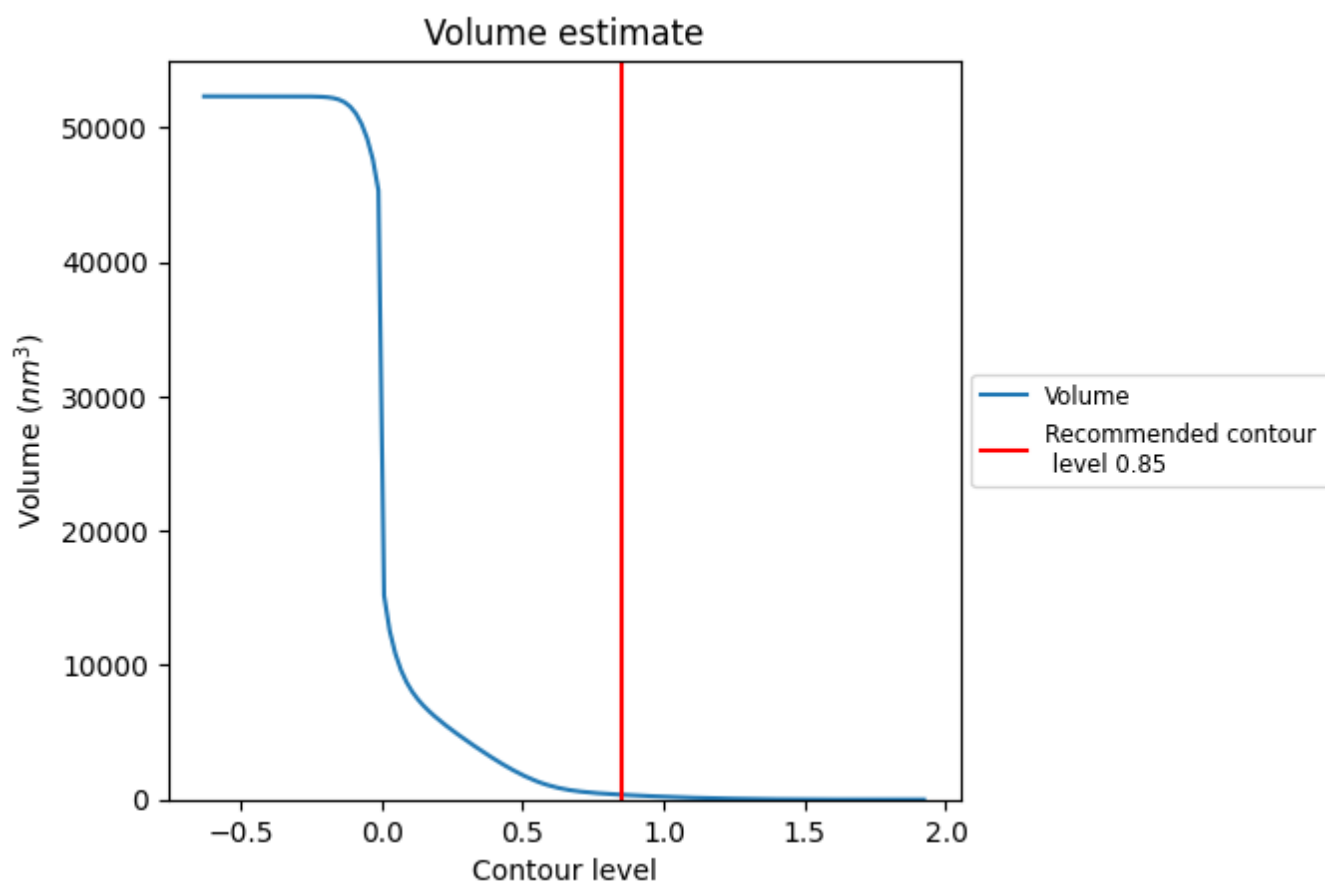
This section contains the results of statistical analysis of the map.

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.

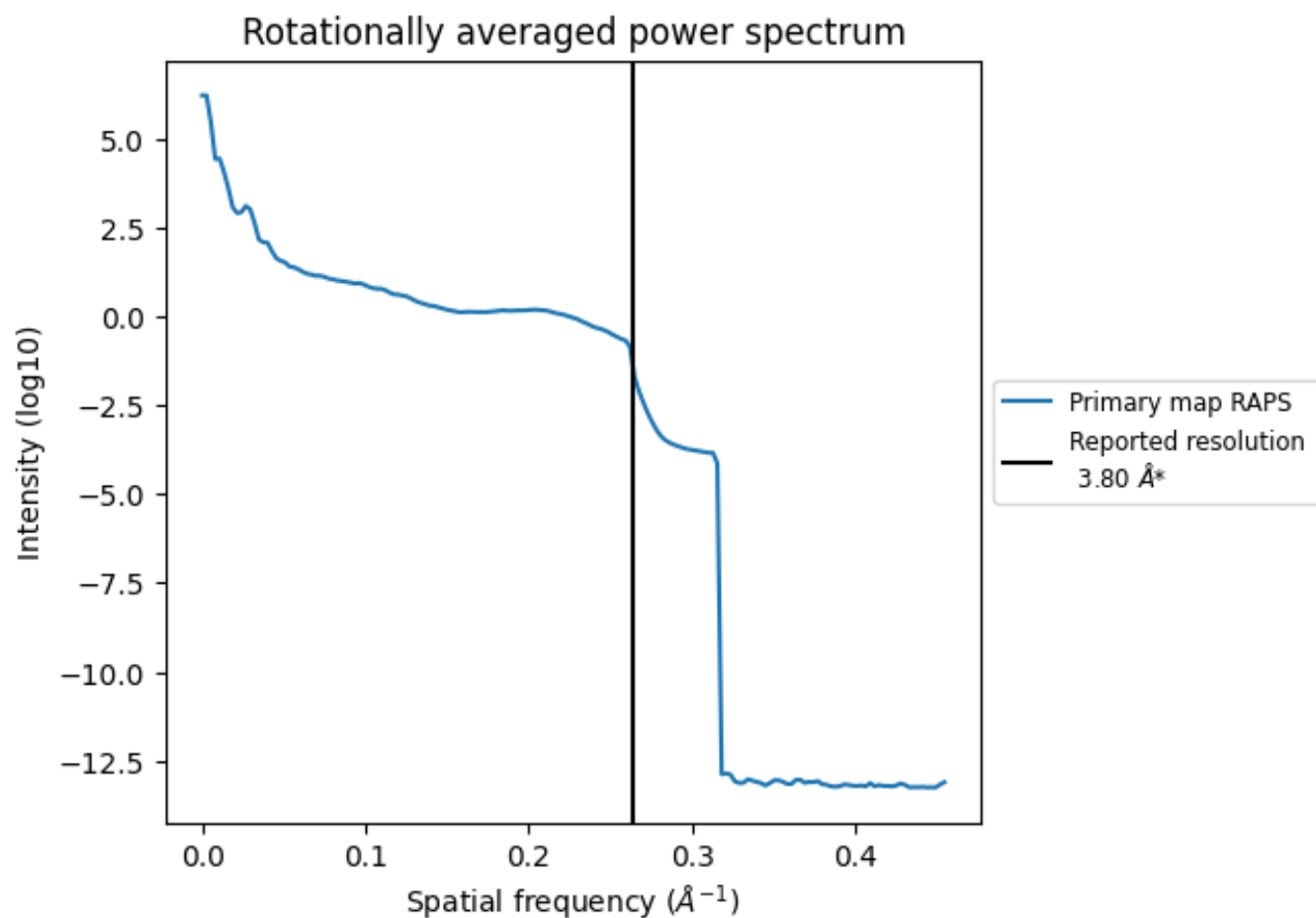
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 360 nm³; this corresponds to an approximate mass of 325 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 0.263 Å⁻¹

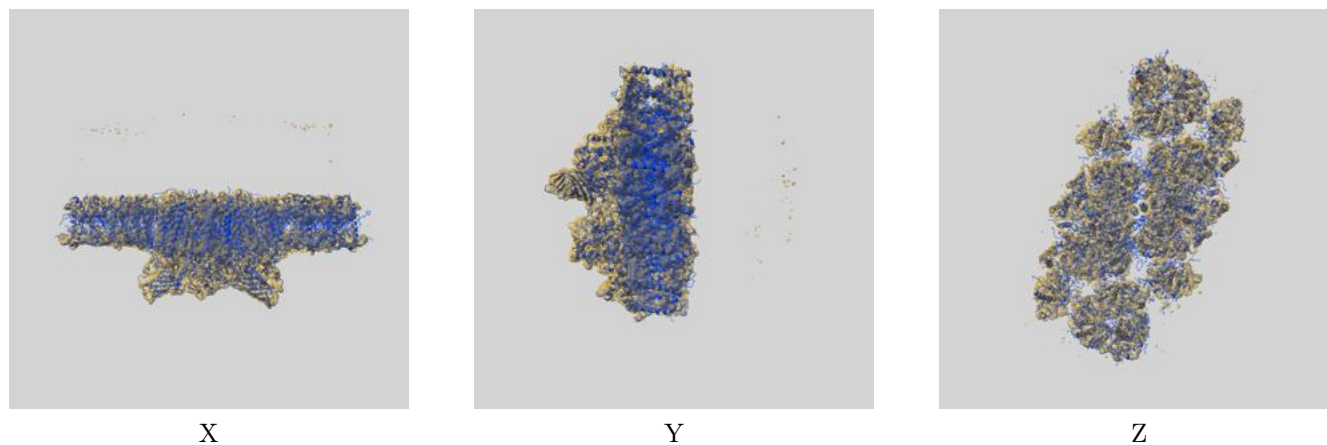
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

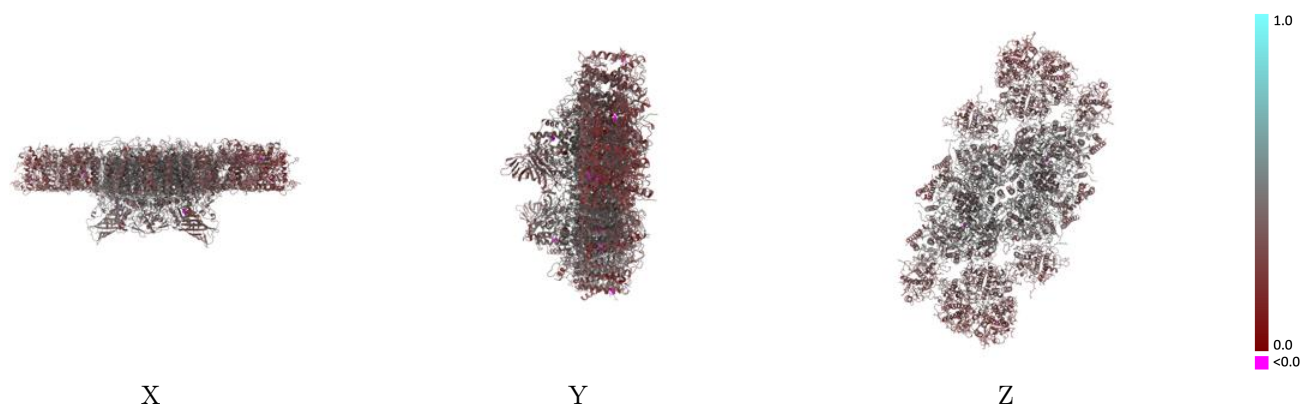
This section contains information regarding the fit between EMDB map EMD-10865 and PDB model 6YP7. Per-residue inclusion information can be found in section [3](#) on page [38](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.85 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](#)

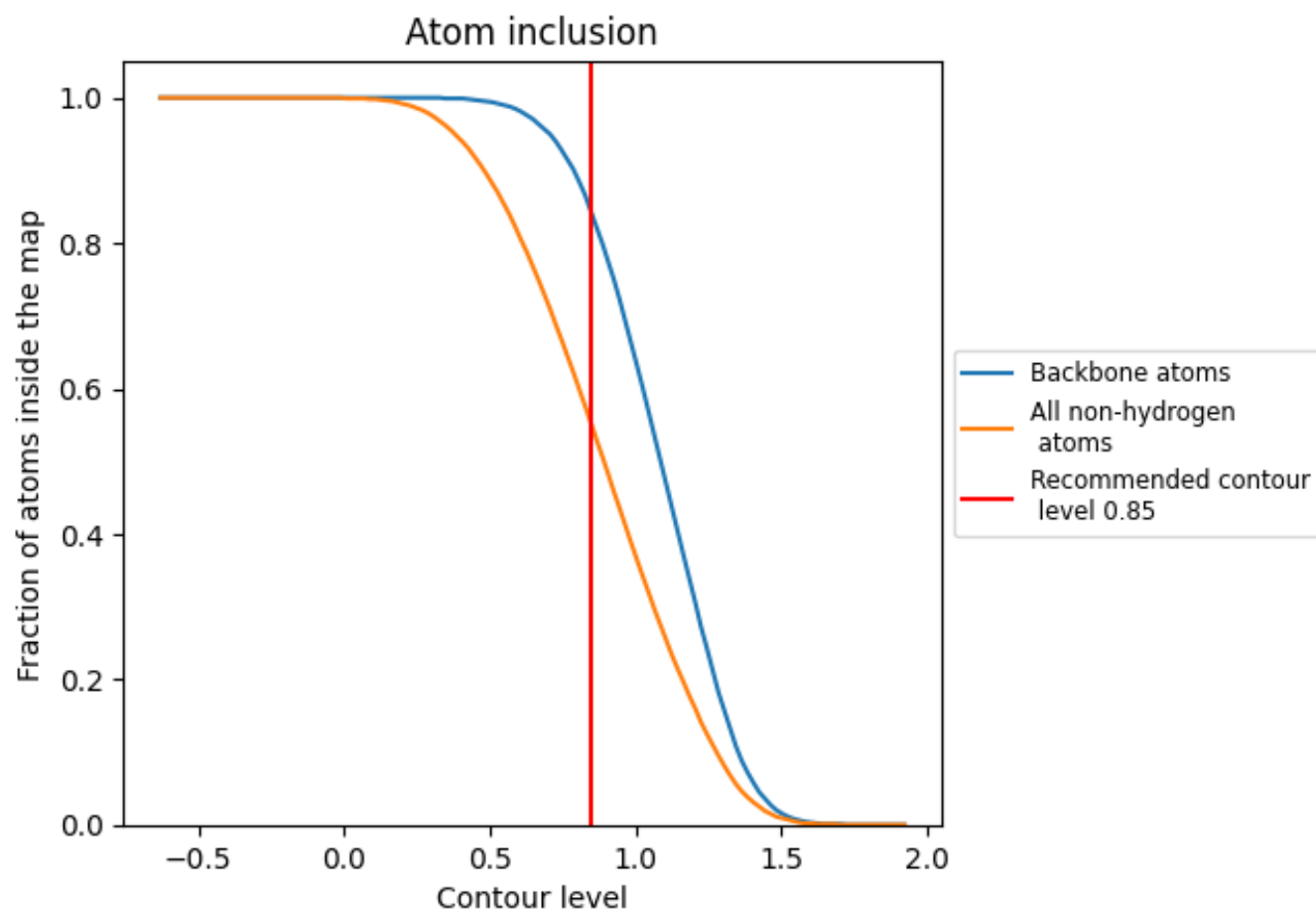


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 55% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5490	 0.3820
A	 0.6070	 0.4440
B	 0.6110	 0.4330
C	 0.6010	 0.4200
D	 0.5870	 0.4380
E	 0.6390	 0.3060
F	 0.5960	 0.3180
G	 0.4520	 0.2780
H	 0.5190	 0.3920
I	 0.5270	 0.4460
J	 0.2670	 0.3740
K	 0.4340	 0.4020
L	 0.4010	 0.4420
M	 0.3530	 0.3940
N	 0.4790	 0.2880
O	 0.5690	 0.4020
R	 0.4710	 0.3470
S	 0.5430	 0.3340
T	 0.3670	 0.4390
W	 0.4440	 0.3460
X	 0.5220	 0.3380
Y	 0.5450	 0.3440
Z	 0.5280	 0.3270
a	 0.6190	 0.4440
b	 0.6220	 0.4350
c	 0.6050	 0.4220
d	 0.5890	 0.4410
e	 0.6740	 0.3500
f	 0.5960	 0.3260
g	 0.4420	 0.2710
h	 0.5360	 0.4140
i	 0.6040	 0.4440
j	 0.2790	 0.3520
k	 0.4300	 0.4000
l	 0.3950	 0.4490



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Chain	Atom inclusion	Q-score
m	 0.4160	 0.3850
n	 0.4890	 0.2920
o	 0.5420	 0.3560
r	 0.4680	 0.3520
s	 0.5430	 0.3330
t	 0.4960	 0.4360
w	 0.4700	 0.4050
x	 0.5250	 0.3640
y	 0.5440	 0.3470
z	 0.5410	 0.3310