



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:41 AM UTC

PDB ID : 3JCU / pdb_00003jcu
EMDB ID : EMD-6617
Title : Cryo-EM structure of spinach PSII-LHCII supercomplex at 3.2 Angstrom resolution
Authors : Wei, X.P.; Zhang, X.Z.; Su, X.D.; Cao, P.; Liu, X.Y.; Li, M.; Chang, W.R.; Liu, Z.F.
Deposited on : 2016-03-10
Resolution : 3.20 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

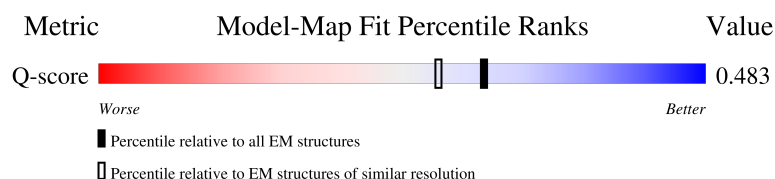
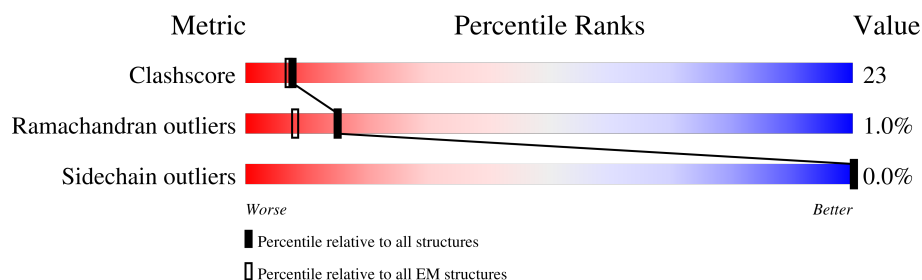
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	344	9% 57% 39% ..
1	a	344	9% 58% 38% ..
2	B	508	8% 55% 40% ..
2	b	508	8% 55% 40% ..

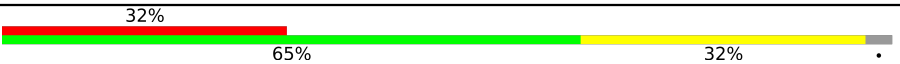
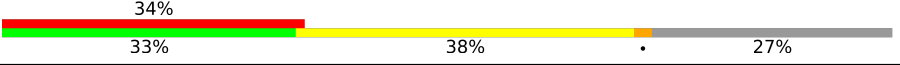
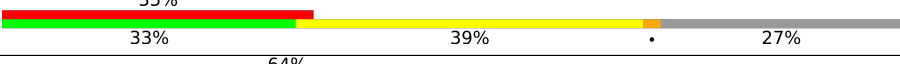
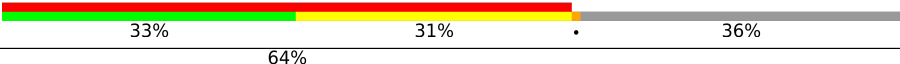
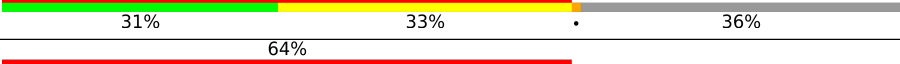
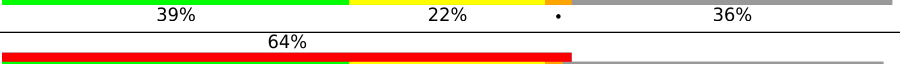
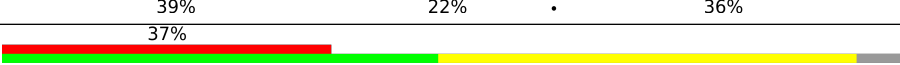
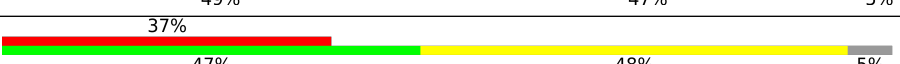
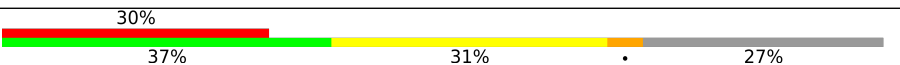
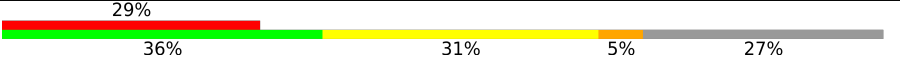
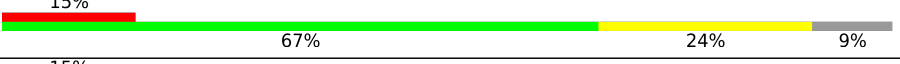
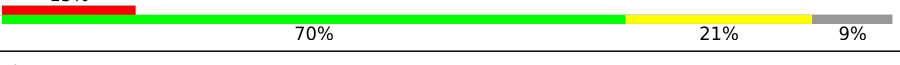
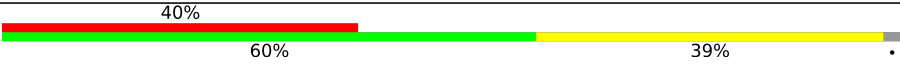
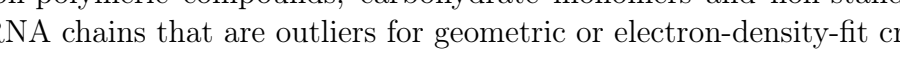
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Mol	Chain	Length	Quality of chain
3	C	473	
3	c	473	
4	D	353	
4	d	353	
5	E	83	
5	e	83	
6	F	39	
6	f	39	
7	G	267	
7	N	267	
7	Y	267	
7	g	267	
7	n	267	
7	y	267	
8	H	73	
8	h	73	
9	I	36	
9	i	36	
10	J	40	
10	j	40	
11	K	59	
11	k	59	
12	L	38	
12	l	38	
13	M	34	

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Mol	Chain	Length	Quality of chain
13	m	34	
14	O	332	
14	o	332	
15	P	267	
15	p	267	
16	Q	232	
16	q	232	
17	R	243	
17	r	243	
18	S	295	
18	s	295	
19	T	33	
19	t	33	
20	U	99	
20	u	99	
21	W	137	
21	w	137	
22	X	117	
22	x	117	
23	Z	62	
23	z	62	

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
27	CLA	A	405	X	-	-	-
27	CLA	A	406	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	407	X	-	-	-
27	CLA	A	410	X	-	-	-
27	CLA	B	602	X	-	-	-
27	CLA	B	603	X	-	-	-
27	CLA	B	604	X	-	-	-
27	CLA	B	605	X	-	-	-
27	CLA	B	606	X	-	-	-
27	CLA	B	607	X	-	-	-
27	CLA	B	608	X	-	-	-
27	CLA	B	609	X	-	-	-
27	CLA	B	610	X	-	-	-
27	CLA	B	611	X	-	-	-
27	CLA	B	612	X	-	-	-
27	CLA	B	613	X	-	-	-
27	CLA	B	614	X	-	-	-
27	CLA	B	615	X	-	-	-
27	CLA	B	616	X	-	-	-
27	CLA	B	617	X	-	-	-
27	CLA	C	501	X	-	-	-
27	CLA	C	502	X	-	-	-
27	CLA	C	503	X	-	-	-
27	CLA	C	504	X	-	-	-
27	CLA	C	505	X	-	-	-
27	CLA	C	506	X	-	-	-
27	CLA	C	507	X	-	-	-
27	CLA	C	508	X	-	-	-
27	CLA	C	509	X	-	-	-
27	CLA	C	510	X	-	-	-
27	CLA	C	511	X	-	-	-
27	CLA	C	512	X	-	-	-
27	CLA	C	513	X	-	-	-
27	CLA	D	402	X	-	-	-
27	CLA	D	403	X	-	-	-
27	CLA	G	602	X	-	-	-
27	CLA	G	603	X	-	-	-
27	CLA	G	604	X	-	-	-
27	CLA	G	610	X	-	-	-
27	CLA	G	611	X	-	-	-
27	CLA	G	612	X	-	-	-
27	CLA	G	613	X	-	-	-
27	CLA	G	614	X	-	-	-
27	CLA	N	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	N	603	X	-	-	-
27	CLA	N	604	X	-	-	-
27	CLA	N	610	X	-	-	-
27	CLA	N	611	X	-	-	-
27	CLA	N	612	X	-	-	-
27	CLA	N	613	X	-	-	-
27	CLA	N	614	X	-	-	-
27	CLA	R	601	X	-	-	-
27	CLA	R	602	X	-	-	-
27	CLA	R	603	X	-	-	-
27	CLA	R	604	X	-	-	-
27	CLA	R	609	X	-	-	-
27	CLA	R	610	X	-	-	-
27	CLA	R	611	X	-	-	-
27	CLA	R	612	X	-	-	-
27	CLA	R	613	X	-	-	-
27	CLA	R	616	X	-	-	-
27	CLA	S	602	X	-	-	-
27	CLA	S	604	X	-	-	-
27	CLA	S	609	X	-	-	-
27	CLA	S	610	X	-	-	-
27	CLA	S	611	X	-	-	-
27	CLA	S	612	X	-	-	-
27	CLA	S	613	X	-	-	-
27	CLA	S	614	X	-	-	-
27	CLA	Y	602	X	-	-	-
27	CLA	Y	603	X	-	-	-
27	CLA	Y	604	X	-	-	-
27	CLA	Y	610	X	-	-	-
27	CLA	Y	611	X	-	-	-
27	CLA	Y	612	X	-	-	-
27	CLA	Y	613	X	-	-	-
27	CLA	Y	614	X	-	-	-
27	CLA	a	405	X	-	-	-
27	CLA	a	406	X	-	-	-
27	CLA	a	407	X	-	-	-
27	CLA	a	410	X	-	-	-
27	CLA	b	602	X	-	-	-
27	CLA	b	603	X	-	-	-
27	CLA	b	604	X	-	-	-
27	CLA	b	605	X	-	-	-
27	CLA	b	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	607	X	-	-	-
27	CLA	b	608	X	-	-	-
27	CLA	b	609	X	-	-	-
27	CLA	b	610	X	-	-	-
27	CLA	b	611	X	-	-	-
27	CLA	b	612	X	-	-	-
27	CLA	b	613	X	-	-	-
27	CLA	b	614	X	-	-	-
27	CLA	b	615	X	-	-	-
27	CLA	b	616	X	-	-	-
27	CLA	b	617	X	-	-	-
27	CLA	c	501	X	-	-	-
27	CLA	c	502	X	-	-	-
27	CLA	c	503	X	-	-	-
27	CLA	c	504	X	-	-	-
27	CLA	c	505	X	-	-	-
27	CLA	c	506	X	-	-	-
27	CLA	c	507	X	-	-	-
27	CLA	c	508	X	-	-	-
27	CLA	c	509	X	-	-	-
27	CLA	c	510	X	-	-	-
27	CLA	c	511	X	-	-	-
27	CLA	c	512	X	-	-	-
27	CLA	c	513	X	-	-	-
27	CLA	d	402	X	-	-	-
27	CLA	d	403	X	-	-	-
27	CLA	g	602	X	-	-	-
27	CLA	g	603	X	-	-	-
27	CLA	g	604	X	-	-	-
27	CLA	g	610	X	-	-	-
27	CLA	g	611	X	-	-	-
27	CLA	g	612	X	-	-	-
27	CLA	g	613	X	-	-	-
27	CLA	g	614	X	-	-	-
27	CLA	n	602	X	-	-	-
27	CLA	n	603	X	-	-	-
27	CLA	n	604	X	-	-	-
27	CLA	n	610	X	-	-	-
27	CLA	n	611	X	-	-	-
27	CLA	n	612	X	-	-	-
27	CLA	n	613	X	-	-	-
27	CLA	n	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	r	601	X	-	-	-
27	CLA	r	602	X	-	-	-
27	CLA	r	603	X	-	-	-
27	CLA	r	604	X	-	-	-
27	CLA	r	609	X	-	-	-
27	CLA	r	610	X	-	-	-
27	CLA	r	611	X	-	-	-
27	CLA	r	612	X	-	-	-
27	CLA	r	613	X	-	-	-
27	CLA	r	616	X	-	-	-
27	CLA	s	602	X	-	-	-
27	CLA	s	604	X	-	-	-
27	CLA	s	609	X	-	-	-
27	CLA	s	610	X	-	-	-
27	CLA	s	611	X	-	-	-
27	CLA	s	612	X	-	-	-
27	CLA	s	613	X	-	-	-
27	CLA	s	614	X	-	-	-
27	CLA	y	602	X	-	-	-
27	CLA	y	603	X	-	-	-
27	CLA	y	604	X	-	-	-
27	CLA	y	610	X	-	-	-
27	CLA	y	611	X	-	-	-
27	CLA	y	612	X	-	-	-
27	CLA	y	613	X	-	-	-
27	CLA	y	614	X	-	-	-
33	BCT	D	401	-	-	X	-
33	BCT	d	401	-	-	X	-
37	CHL	G	601	X	-	-	-
37	CHL	G	605	X	-	-	-
37	CHL	G	606	X	-	-	-
37	CHL	G	607	X	-	-	-
37	CHL	G	608	X	-	-	-
37	CHL	G	609	X	-	-	-
37	CHL	N	601	X	-	-	-
37	CHL	N	605	X	-	-	-
37	CHL	N	606	X	-	-	-
37	CHL	N	607	X	-	-	-
37	CHL	N	608	X	-	-	-
37	CHL	N	609	X	-	-	-
37	CHL	R	606	X	-	-	-
37	CHL	R	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CHL	R	608	X	-	-	-
37	CHL	S	601	X	-	-	-
37	CHL	S	606	X	-	-	-
37	CHL	S	607	X	-	-	-
37	CHL	S	608	X	-	-	-
37	CHL	Y	601	X	-	-	-
37	CHL	Y	605	X	-	-	-
37	CHL	Y	606	X	-	-	-
37	CHL	Y	607	X	-	-	-
37	CHL	Y	608	X	-	-	-
37	CHL	Y	609	X	-	-	-
37	CHL	g	601	X	-	-	-
37	CHL	g	605	X	-	-	-
37	CHL	g	606	X	-	-	-
37	CHL	g	607	X	-	-	-
37	CHL	g	608	X	-	-	-
37	CHL	g	609	X	-	-	-
37	CHL	n	601	X	-	-	-
37	CHL	n	605	X	-	-	-
37	CHL	n	606	X	-	-	-
37	CHL	n	607	X	-	-	-
37	CHL	n	608	X	-	-	-
37	CHL	n	609	X	-	-	-
37	CHL	r	606	X	-	-	-
37	CHL	r	607	X	-	-	-
37	CHL	r	608	X	-	-	-
37	CHL	s	601	X	-	-	-
37	CHL	s	606	X	-	-	-
37	CHL	s	607	X	-	-	-
37	CHL	s	608	X	-	-	-
37	CHL	y	601	X	-	-	-
37	CHL	y	605	X	-	-	-
37	CHL	y	606	X	-	-	-
37	CHL	y	607	X	-	-	-
37	CHL	y	608	X	-	-	-
37	CHL	y	609	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 75994 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 Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2614	1707	430	464	13		
1	a	334	Total	C	N	O	S	0	0
			2614	1707	430	464	13		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	487	Total	C	N	O	S	0	0
			3820	2501	640	667	12		
2	b	487	Total	C	N	O	S	0	0
			3820	2501	640	667	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3475	2284	581	599	11		
3	c	449	Total	C	N	O	S	0	0
			3475	2284	581	599	11		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	340	Total	C	N	O	S	0	0
			2703	1786	443	462	12		
4	d	340	Total	C	N	O	S	0	0
			2703	1786	443	462	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	79	Total	C	N	O	0	0
			636	412	104	120		
5	e	79	Total	C	N	O	0	0
			636	412	104	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	32	Total	C	N	O	S	0	0
			257	174	43	39	1		
6	f	32	Total	C	N	O	S	0	0
			257	174	43	39	1		

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	N	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	Y	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	g	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	n	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	y	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total	C	N	O	S	0	0
			434	288	65	78	3		
8	h	59	Total	C	N	O	S	0	0
			434	288	65	78	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	34	Total	C	N	O		0	0
			247	168	38	41			
10	j	34	Total	C	N	O		0	0
			247	168	38	41			

- 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
			307	217	43	46	1		
11	k	37	Total	C	N	O	S	0	0
			307	217	43	46	1		

- Molecule 12 is a protein called Protein 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		0	0
			258	176	37	45			
13	m	33	Total	C	N	O		0	0
			258	176	37	45			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	243	Total	C	N	O	S	0	0
			1844	1164	301	376	3		
14	o	243	Total	C	N	O	S	0	0
			1844	1164	301	376	3		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	172	Total	C	N	O	S	0	0
			1324	841	215	266	2		
15	p	172	Total	C	N	O	S	0	0
			1324	841	215	266	2		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O		0	0
			1162	736	202	224			
16	q	148	Total	C	N	O		0	0
			1162	736	202	224			

- Molecule 17 is a protein called Chlorophyll A-B Binding protein 29 kD (CP29).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	232	Total	C	N	O	S	0	0
			1806	1170	293	339	4		
17	r	232	Total	C	N	O	S	0	0
			1806	1170	293	339	4		

- Molecule 18 is a protein called Chlorophyll A-B Binding protein 26 kD (CP26).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	214	Total	C	N	O	S	0	0
			1653	1080	269	299	5		
18	s	214	Total	C	N	O	S	0	0
			1653	1080	269	299	5		

- Molecule 19 is a protein called Photosystem II Reaction Center protein Tc.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	30	Total	C	N	O	S	0	0
			245	171	34	39	1		
19	t	30	Total	C	N	O	S	0	0
			245	171	34	39	1		

- Molecule 20 is a protein called Photosystem II Reaction Center Tn protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	25	Total	C	N	O	S	0	0
			193	123	35	32	3		
20	u	25	Total	C	N	O	S	0	0
			193	123	35	32	3		

- Molecule 21 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	54	Total	C	N	O	S	0	0
			419	276	61	81	1		
21	w	54	Total	C	N	O	S	0	0
			419	276	61	81	1		

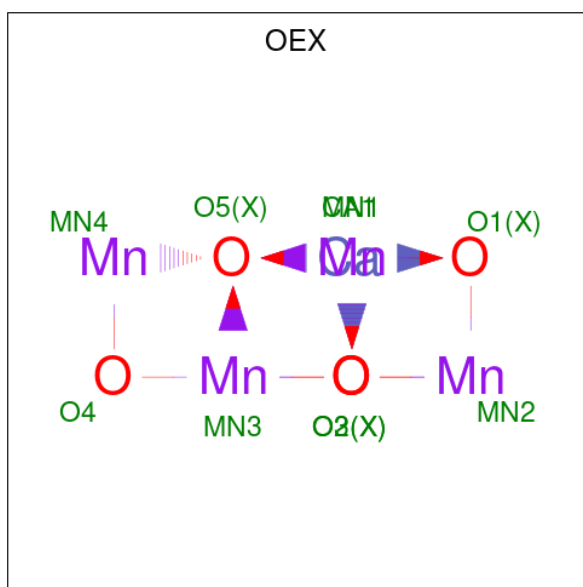
- Molecule 22 is a protein called Photosystem II Reaction Center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	35	Total	C	N	O	0	0
			246	163	38	45		
22	x	35	Total	C	N	O	0	0
			246	163	38	45		

- Molecule 23 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Z	61	Total	C	N	O	0	0
			454	306	68	80		
23	z	61	Total	C	N	O	0	0
			454	306	68	80		

- Molecule 24 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

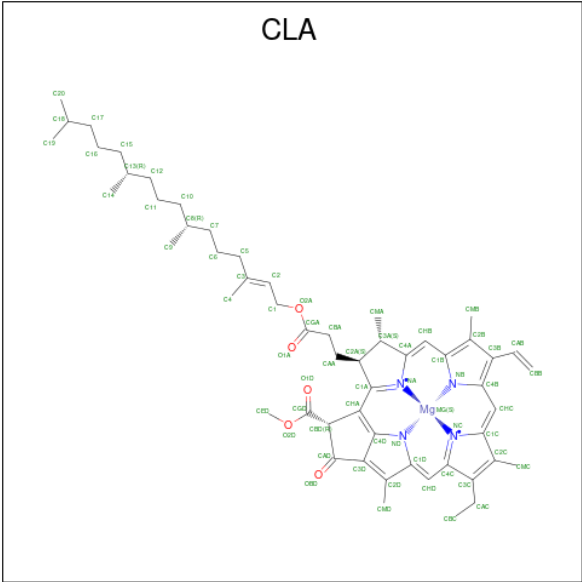
- Molecule 25 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 26 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Cl	0
			2	2	
26	a	2	Total	Cl	0
			2	2	

- Molecule 27 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Y	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	Y	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	Y	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0

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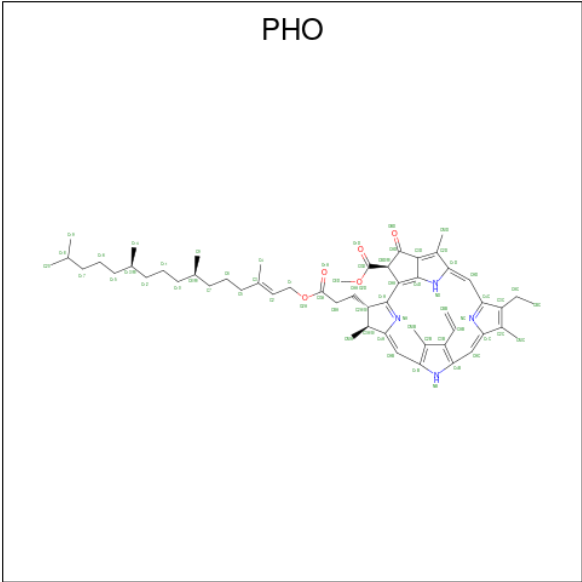
Mol	Chain	Residues	Atoms					AltConf
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0

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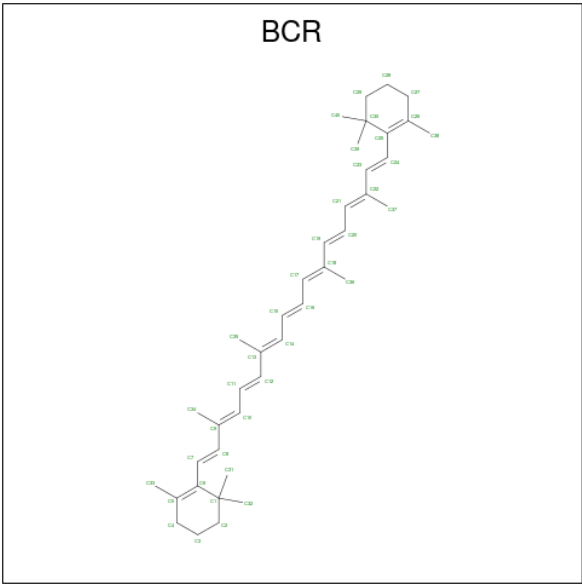
Mol	Chain	Residues	Atoms					AltConf
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	y	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	y	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	y	1	Total 49	C 39	Mg 1	N 4	O 5	0

- Molecule 28 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



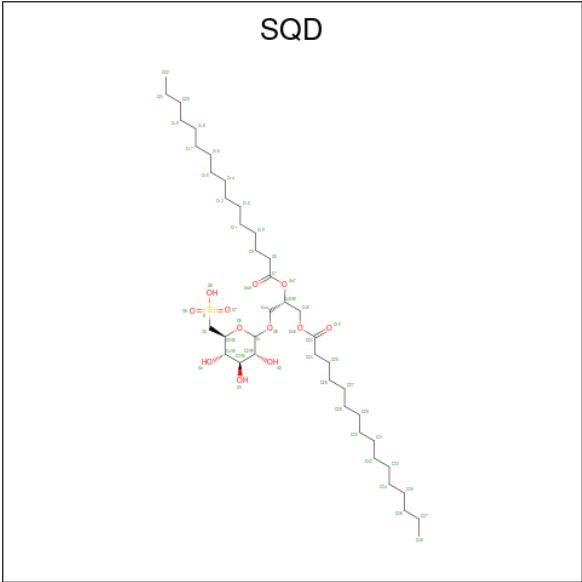
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	N	O	0
			64	55	4	5	
28	A	1	Total	C	N	O	0
			64	55	4	5	
28	a	1	Total	C	N	O	0
			64	55	4	5	
28	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



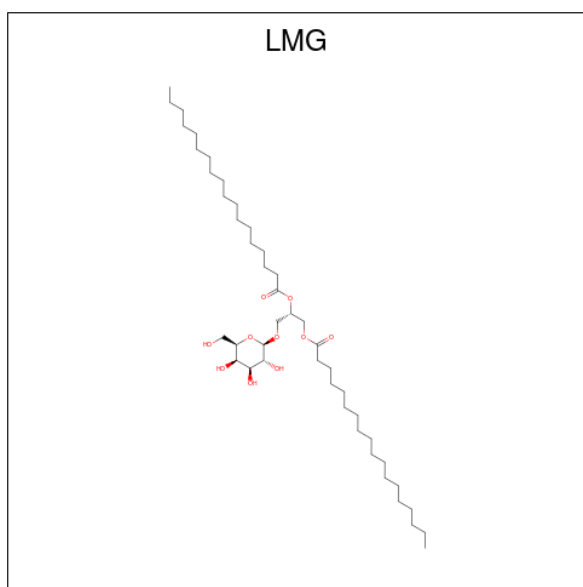
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	D	1	Total C 40 40	0
29	H	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	d	1	Total C 40 40	0
29	h	1	Total C 40 40	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



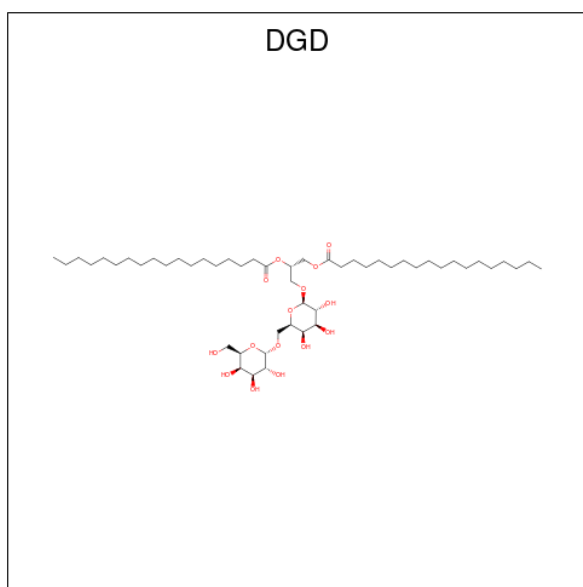
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	b	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



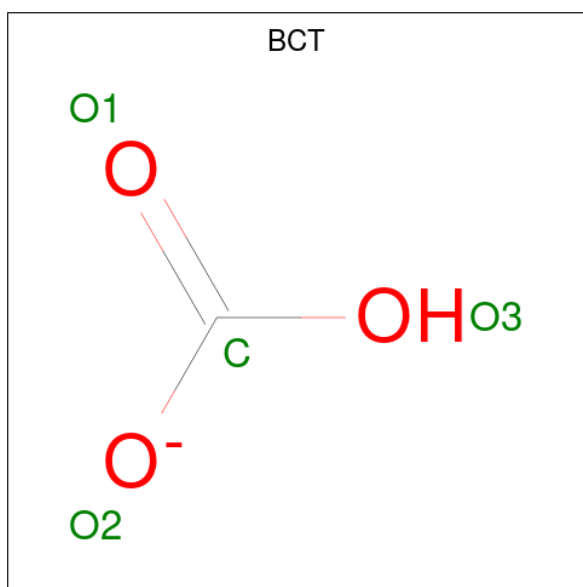
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			48	38	10	
31	B	1	Total	C	O	0
			51	41	10	
31	C	1	Total	C	O	0
			51	41	10	
31	D	1	Total	C	O	0
			46	36	10	
31	Z	1	Total	C	O	0
			51	41	10	
31	a	1	Total	C	O	0
			48	38	10	
31	b	1	Total	C	O	0
			51	41	10	
31	c	1	Total	C	O	0
			51	41	10	
31	d	1	Total	C	O	0
			46	36	10	
31	z	1	Total	C	O	0
			51	41	10	

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



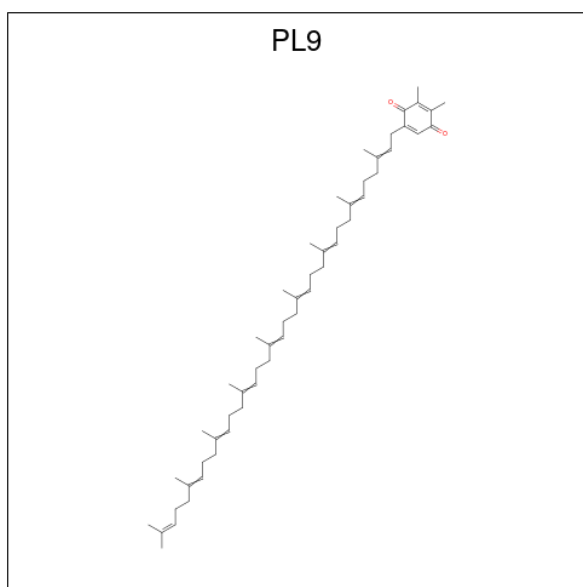
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			55	40	15	
32	C	1	Total	C	O	0
			62	47	15	
32	C	1	Total	C	O	0
			62	47	15	
32	H	1	Total	C	O	0
			62	47	15	
32	c	1	Total	C	O	0
			55	40	15	
32	c	1	Total	C	O	0
			62	47	15	
32	c	1	Total	C	O	0
			62	47	15	
32	h	1	Total	C	O	0
			62	47	15	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
33	D	1	Total	C	O	0
			4	1	3	
33	d	1	Total	C	O	0
			4	1	3	

- Molecule 34 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: C₅₃H₈₀O₂).



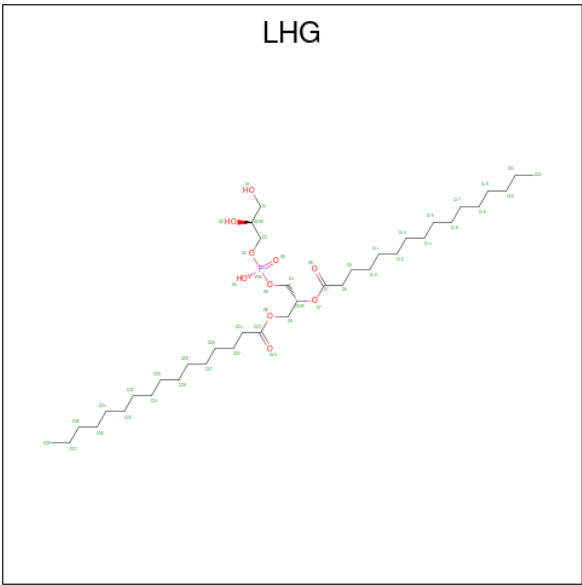
Mol	Chain	Residues	Atoms			AltConf
34	D	1	Total	C	O	0
			55	53	2	

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Mol	Chain	Residues	Atoms			AltConf
34	d	1	Total	C	O	0
			55	53	2	

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
35	D	1	Total	C	O	P	0
			43	32	10	1	
35	D	1	Total	C	O	P	0
			49	38	10	1	
35	D	1	Total	C	O	P	0
			37	26	10	1	
35	G	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	N	1	Total	C	O	P	0
			49	38	10	1	
35	R	1	Total	C	O	P	0
			49	38	10	1	
35	S	1	Total	C	O	P	0
			49	38	10	1	
35	Y	1	Total	C	O	P	0
			49	38	10	1	
35	d	1	Total	C	O	P	0
			43	32	10	1	

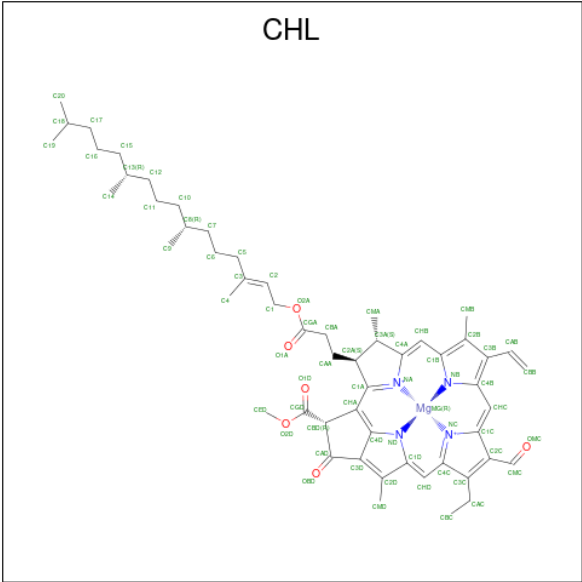
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Mol	Chain	Residues	Atoms				AltConf
35	d	1	Total 49	C 38	O 10	P 1	0
35	d	1	Total 37	C 26	O 10	P 1	0
35	g	1	Total 49	C 38	O 10	P 1	0
35	l	1	Total 49	C 38	O 10	P 1	0
35	n	1	Total 49	C 38	O 10	P 1	0
35	r	1	Total 49	C 38	O 10	P 1	0
35	s	1	Total 49	C 38	O 10	P 1	0
35	y	1	Total 49	C 38	O 10	P 1	0

- # HEM



WORLD WIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms						AltConf
37	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
37	G	1	Total	C	Mg	N	O		0
			48	37	1	4	6		
37	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
37	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
37	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
37	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
37	N	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
37	N	1	Total	C	Mg	N	O		0
			48	37	1	4	6		
37	N	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
37	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
37	N	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
37	N	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
37	R	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
37	R	1	Total	C	Mg	N	O		0
			50	39	1	4	6		

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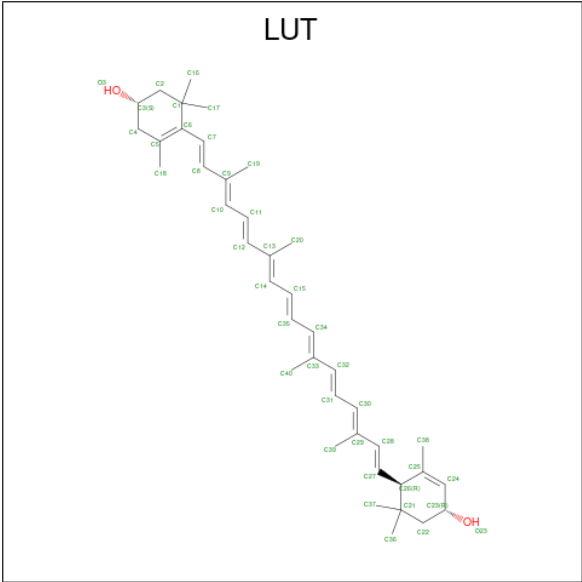
Mol	Chain	Residues	Atoms					AltConf
37	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	S	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
37	S	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	S	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	S	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	g	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
37	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
37	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
37	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	s	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
37	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 38 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



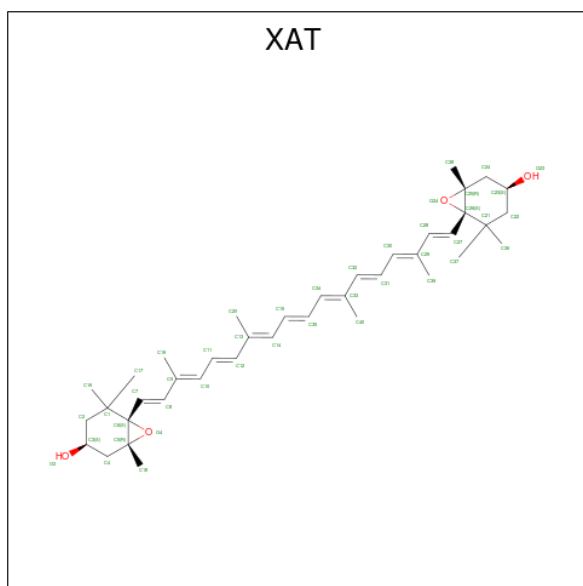
Mol	Chain	Residues	Atoms			AltConf
38	G	1	Total	C	O	0
			42	40	2	
38	G	1	Total	C	O	0
			42	40	2	
38	N	1	Total	C	O	0
			42	40	2	
38	N	1	Total	C	O	0
			42	40	2	
38	R	1	Total	C	O	0
			42	40	2	
38	S	1	Total	C	O	0
			42	40	2	
38	S	1	Total	C	O	0
			42	40	2	
38	Y	1	Total	C	O	0
			42	40	2	
38	Y	1	Total	C	O	0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

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Mol	Chain	Residues	Atoms			AltConf
38	s	1	Total	C	O	0
			42	40	2	
38	s	1	Total	C	O	0
			42	40	2	
38	y	1	Total	C	O	0
			42	40	2	
38	y	1	Total	C	O	0
			42	40	2	

- Molecule 39 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).



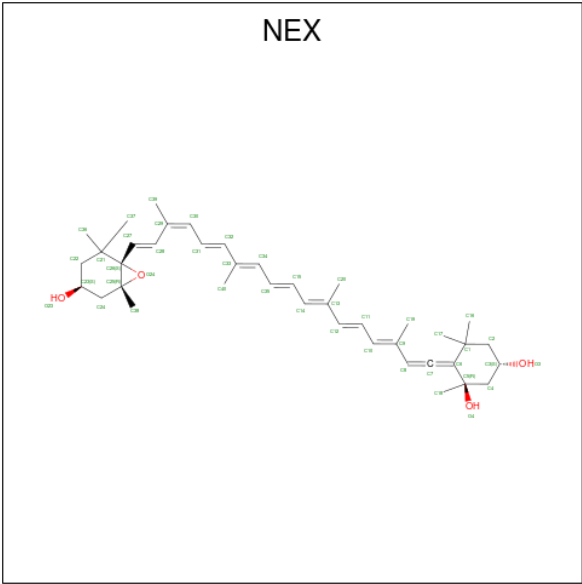
Mol	Chain	Residues	Atoms			AltConf
39	G	1	Total	C	O	0
			44	40	4	
39	N	1	Total	C	O	0
			44	40	4	
39	R	1	Total	C	O	0
			44	40	4	
39	Y	1	Total	C	O	0
			44	40	4	
39	g	1	Total	C	O	0
			44	40	4	
39	n	1	Total	C	O	0
			44	40	4	
39	r	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
39	y	1	Total	C	O	0
			44	40	4	

- Molecule 40 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
40	G	1	Total	C	O	0
			44	40	4	
40	N	1	Total	C	O	0
			44	40	4	
40	R	1	Total	C	O	0
			44	40	4	
40	S	1	Total	C	O	0
			44	40	4	
40	Y	1	Total	C	O	0
			44	40	4	
40	g	1	Total	C	O	0
			44	40	4	
40	n	1	Total	C	O	0
			44	40	4	
40	r	1	Total	C	O	0
			44	40	4	
40	s	1	Total	C	O	0
			44	40	4	

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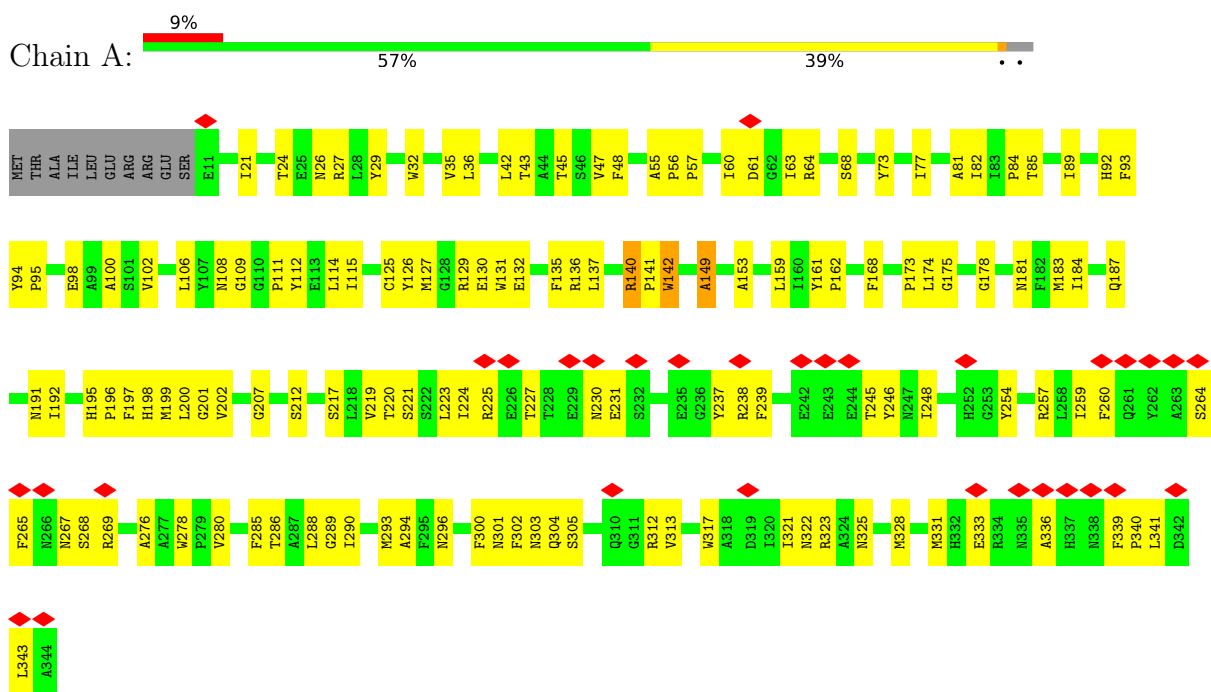
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	y	1	44	40	4	0

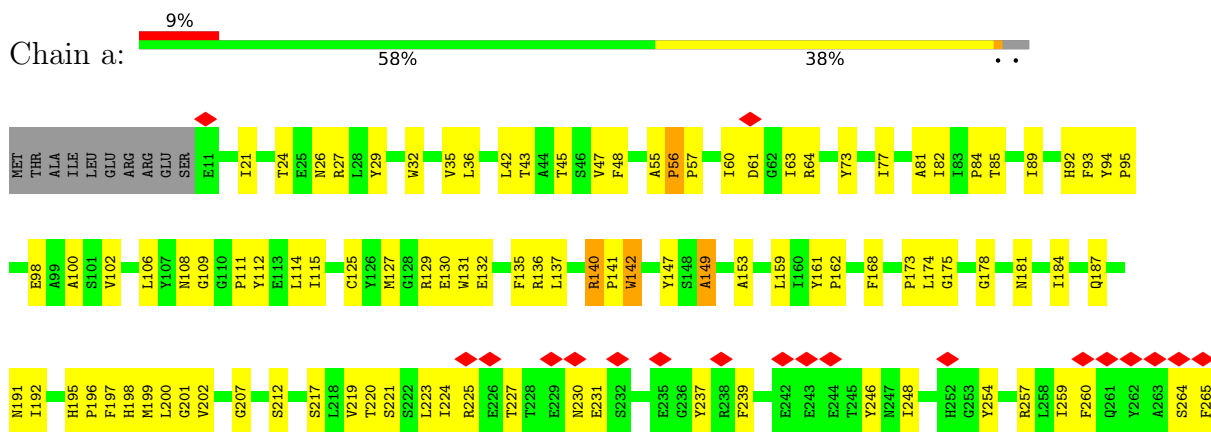
3 Residue-property plots

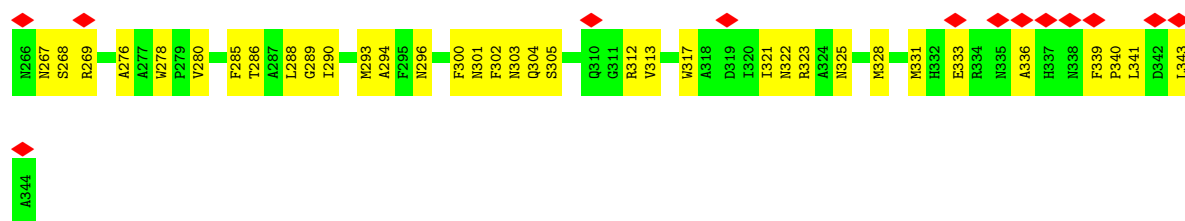
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Photosystem II protein D1

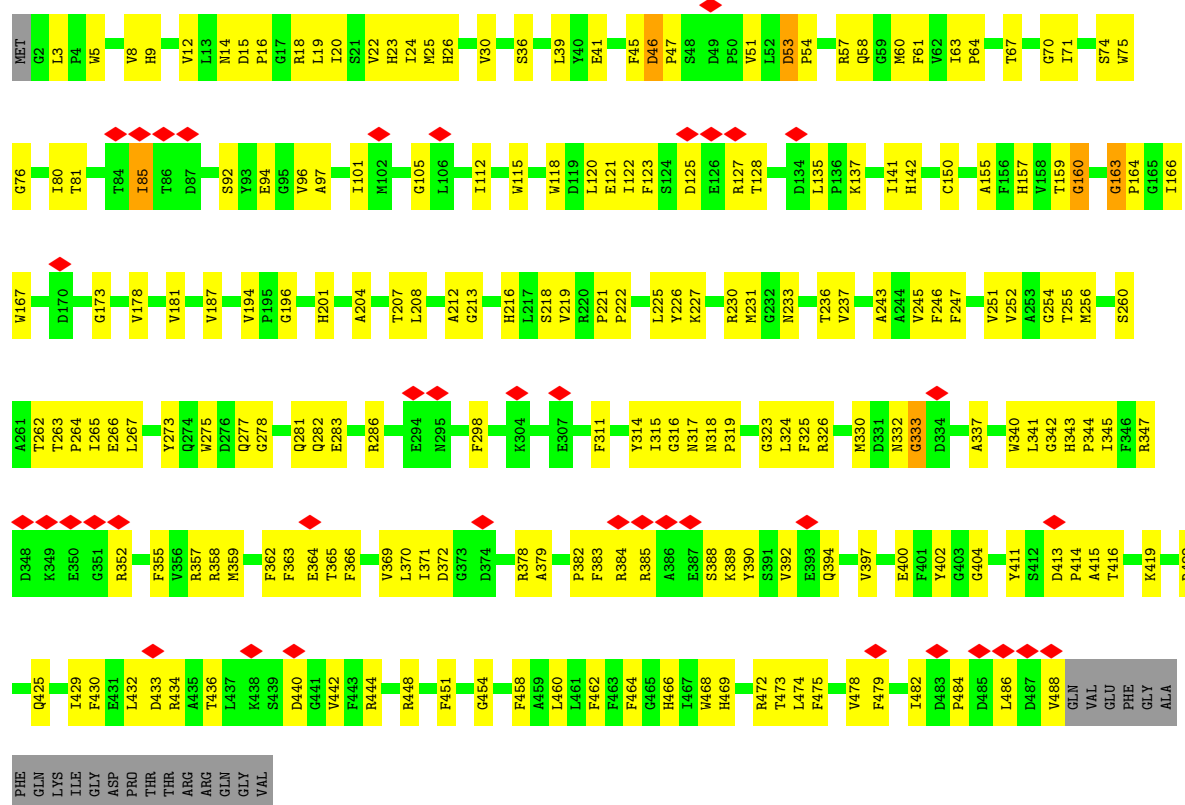


• Molecule 1: Photosystem II protein D1

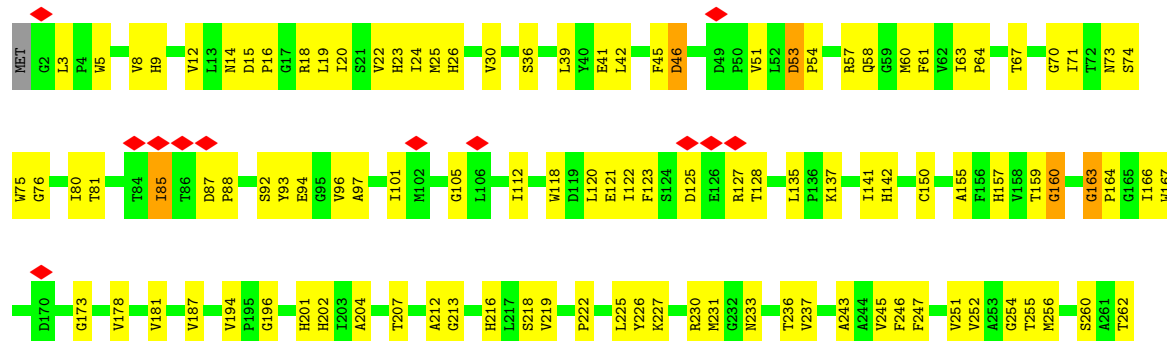


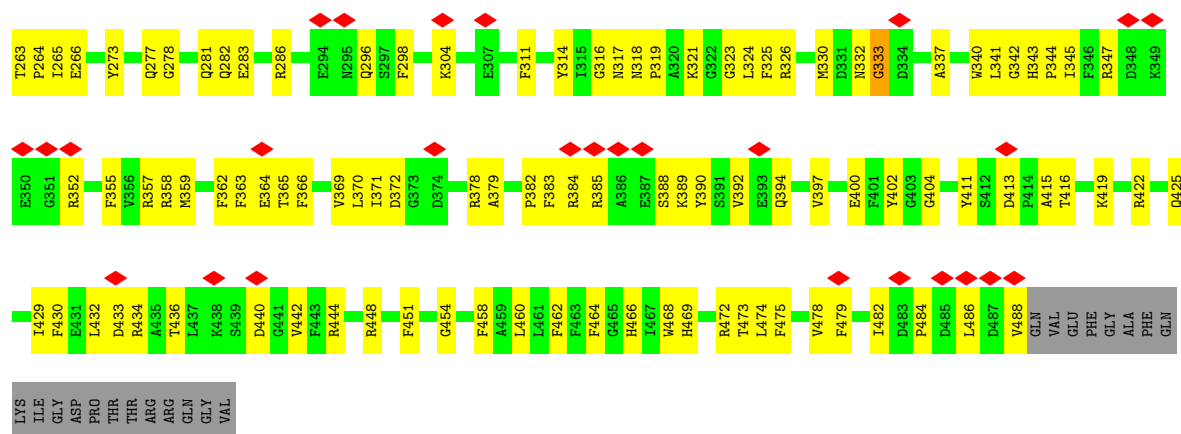


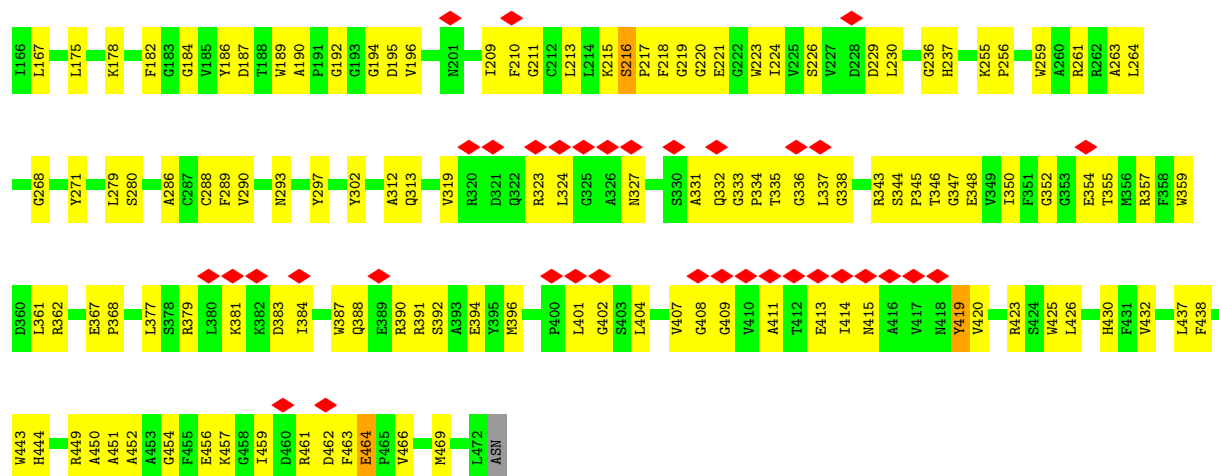
• Molecule 2: Photosystem II CP47 reaction center protein



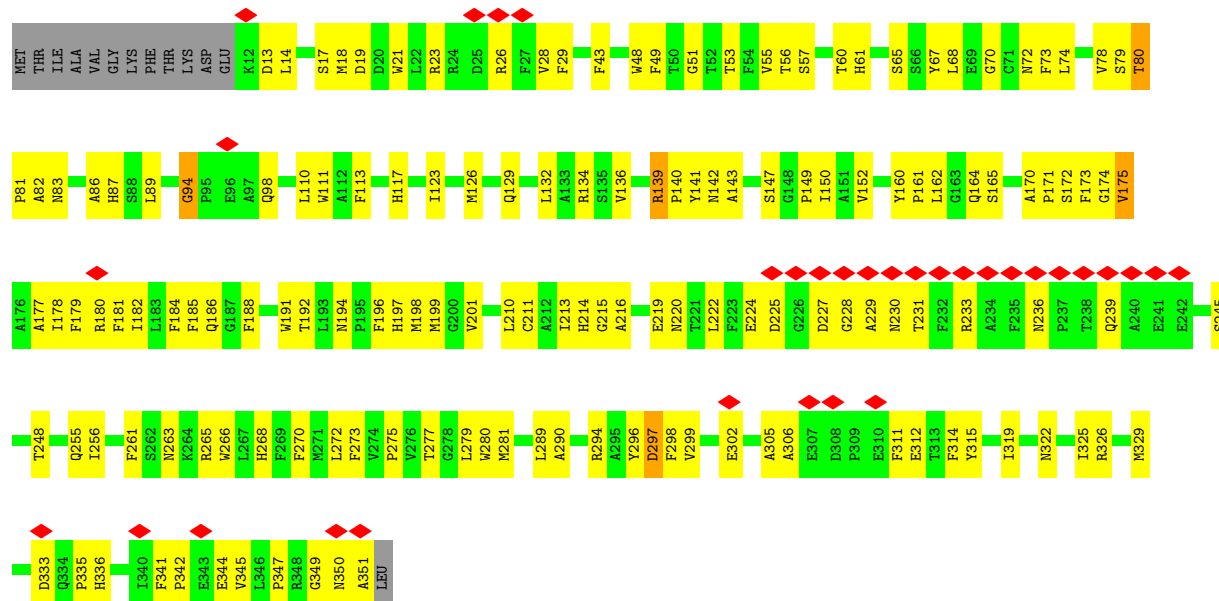
• Molecule 2: Photosystem II CP47 reaction center protein



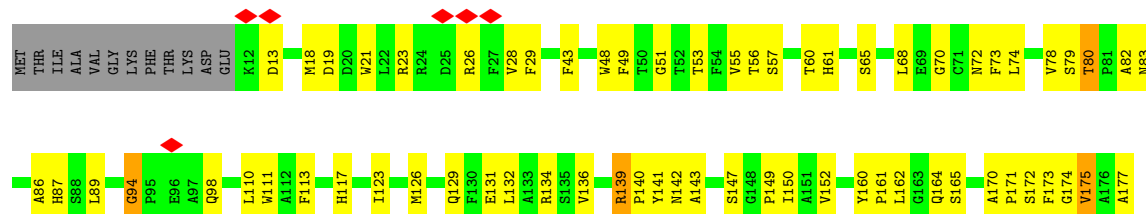


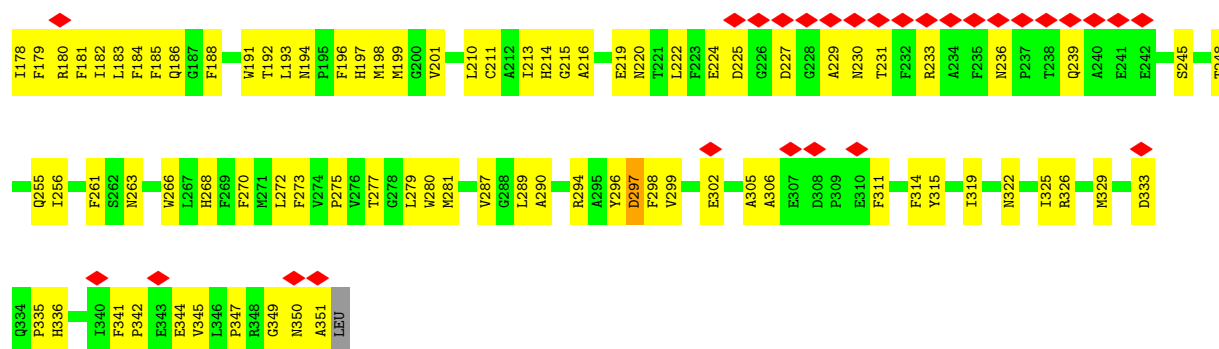


• Molecule 4: Photosystem II D2 protein

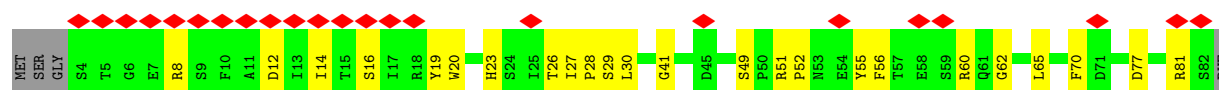


• Molecule 4: Photosystem II D2 protein

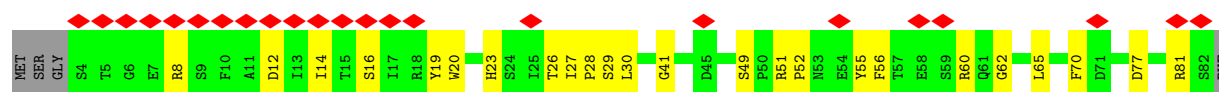




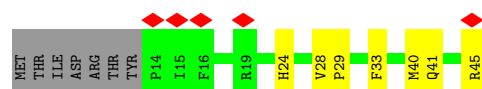
• Molecule 5: Cytochrome b559 subunit alpha



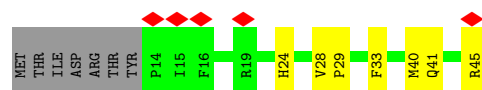
• Molecule 5: Cytochrome b559 subunit alpha



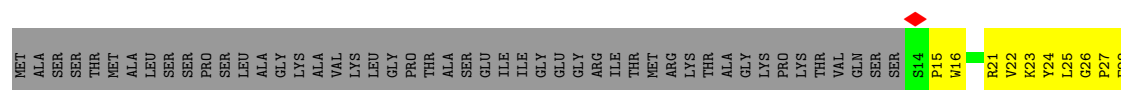
• Molecule 6: Cytochrome b559 subunit beta

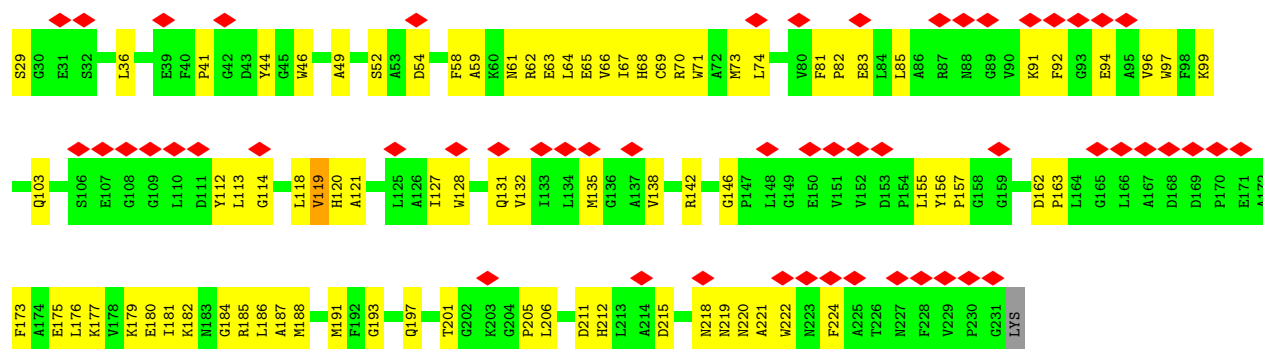


• Molecule 6: Cytochrome b559 subunit beta

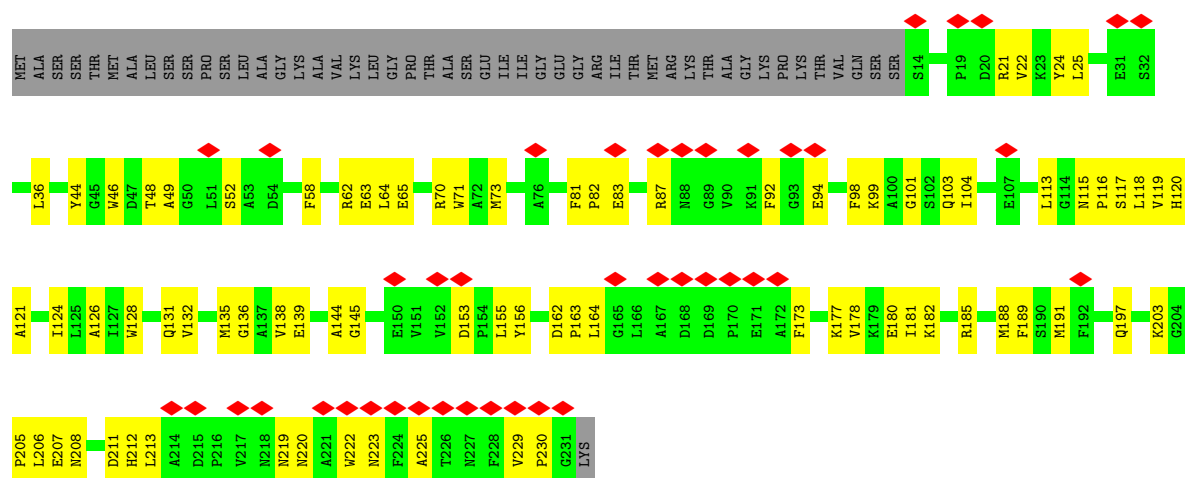


• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

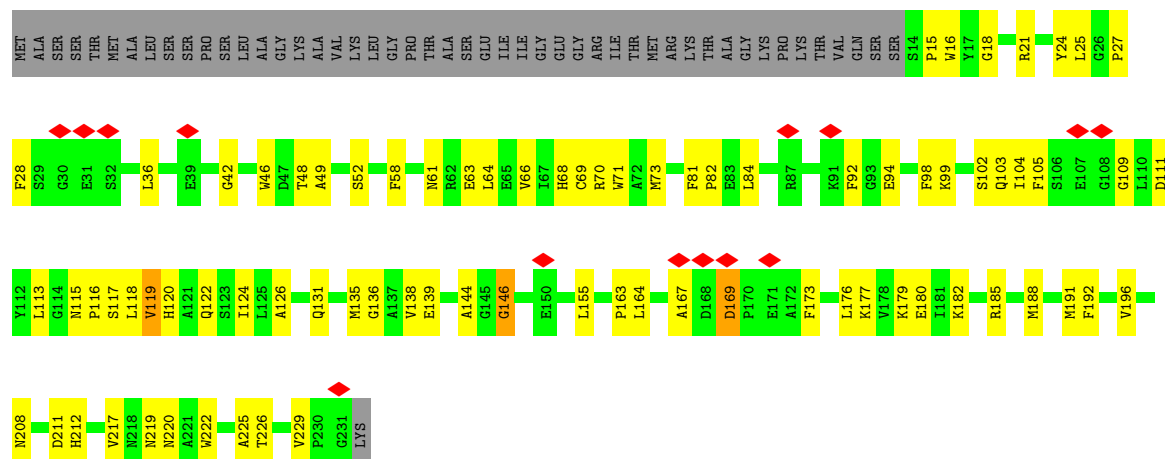




• Molecule 7: Chlorophyll a-b binding protein, chloroplastic



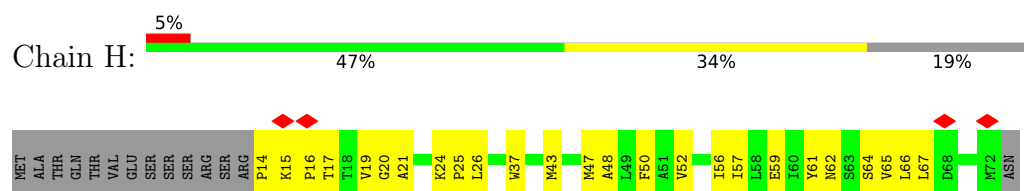
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic



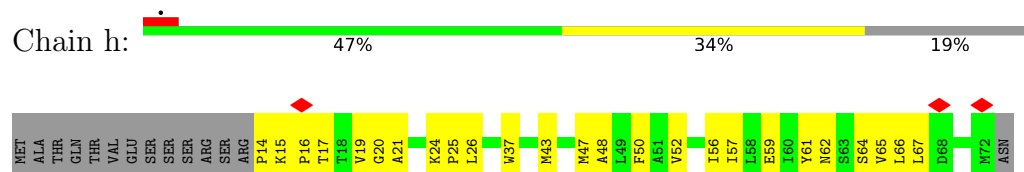
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic



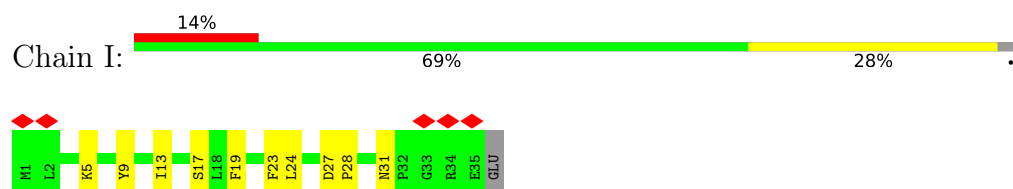
- Molecule 8: Photosystem II reaction center protein H



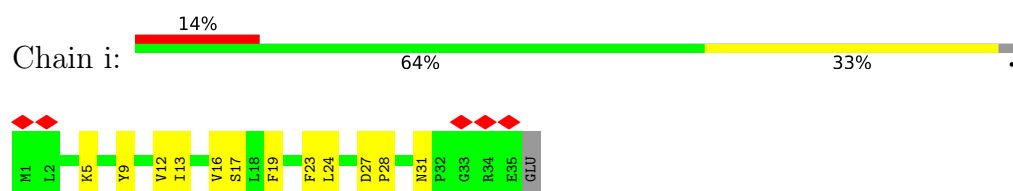
- Molecule 8: Photosystem II reaction center protein H



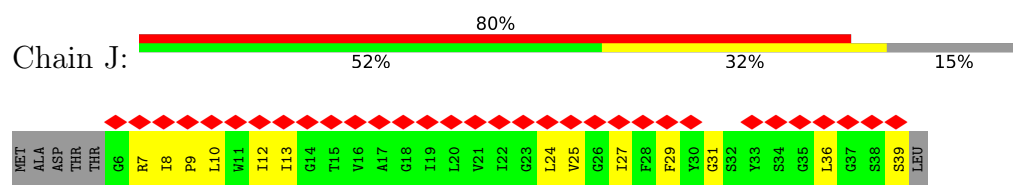
- Molecule 9: Protein Photosystem II reaction center protein I



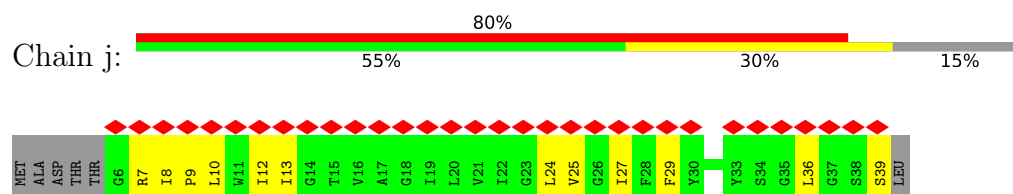
- Molecule 9: Protein Photosystem II reaction center protein I



- Molecule 10: Photosystem II reaction center protein J

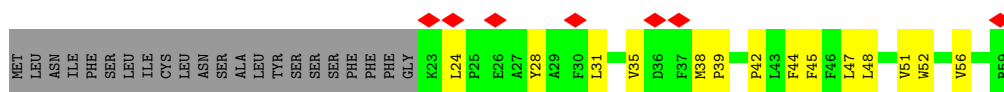


- Molecule 10: Photosystem II reaction center protein J

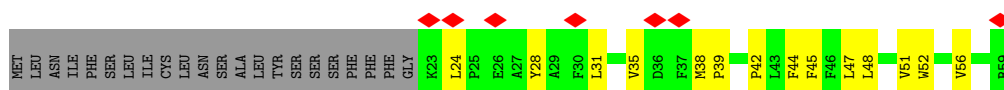
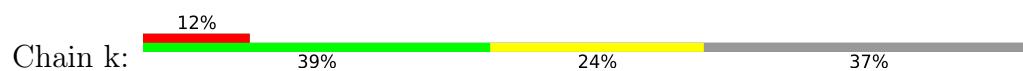


- Molecule 11: Photosystem II reaction center protein K

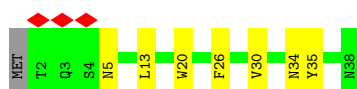




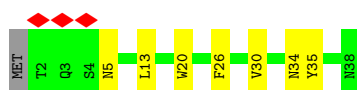
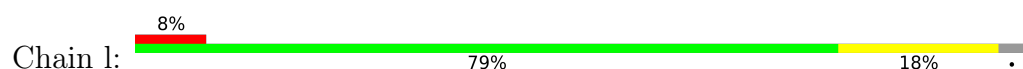
- Molecule 11: Photosystem II reaction center protein K



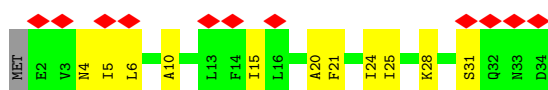
- Molecule 12: Protein Photosystem II reaction center protein L



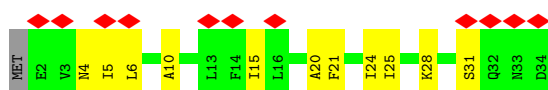
- Molecule 12: Protein Photosystem II reaction center protein L



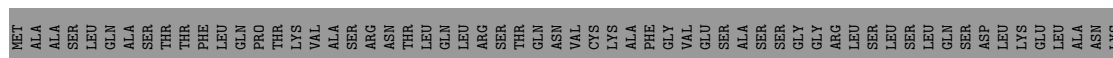
- Molecule 13: Photosystem II reaction center protein M

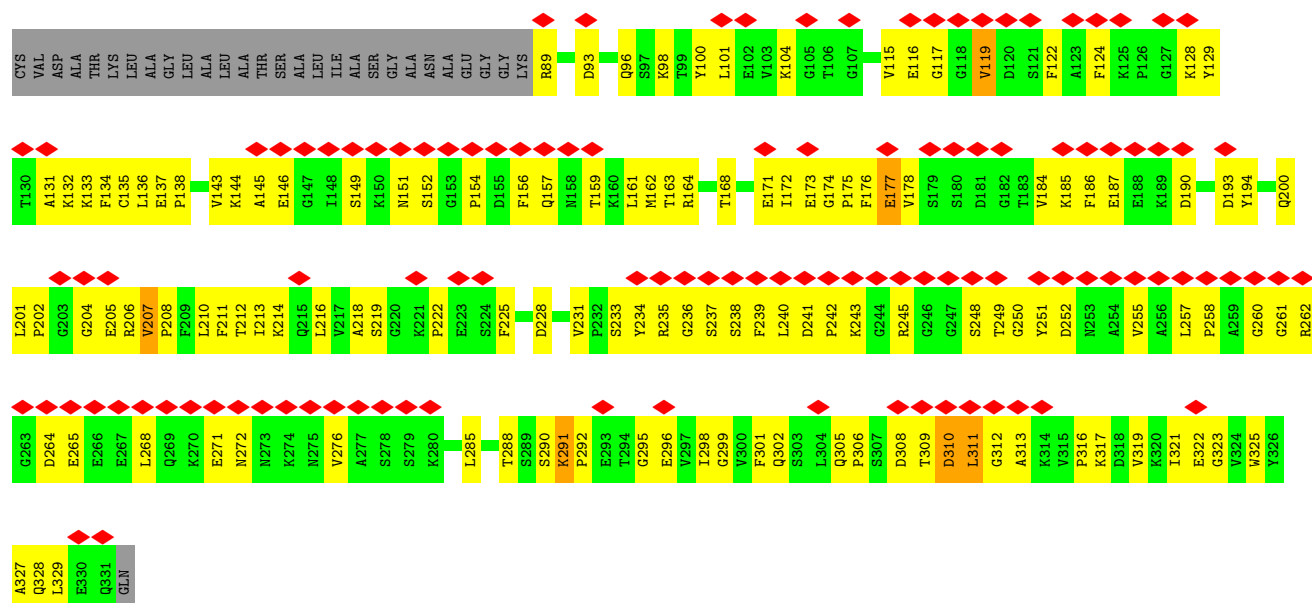


- Molecule 13: Photosystem II reaction center protein M

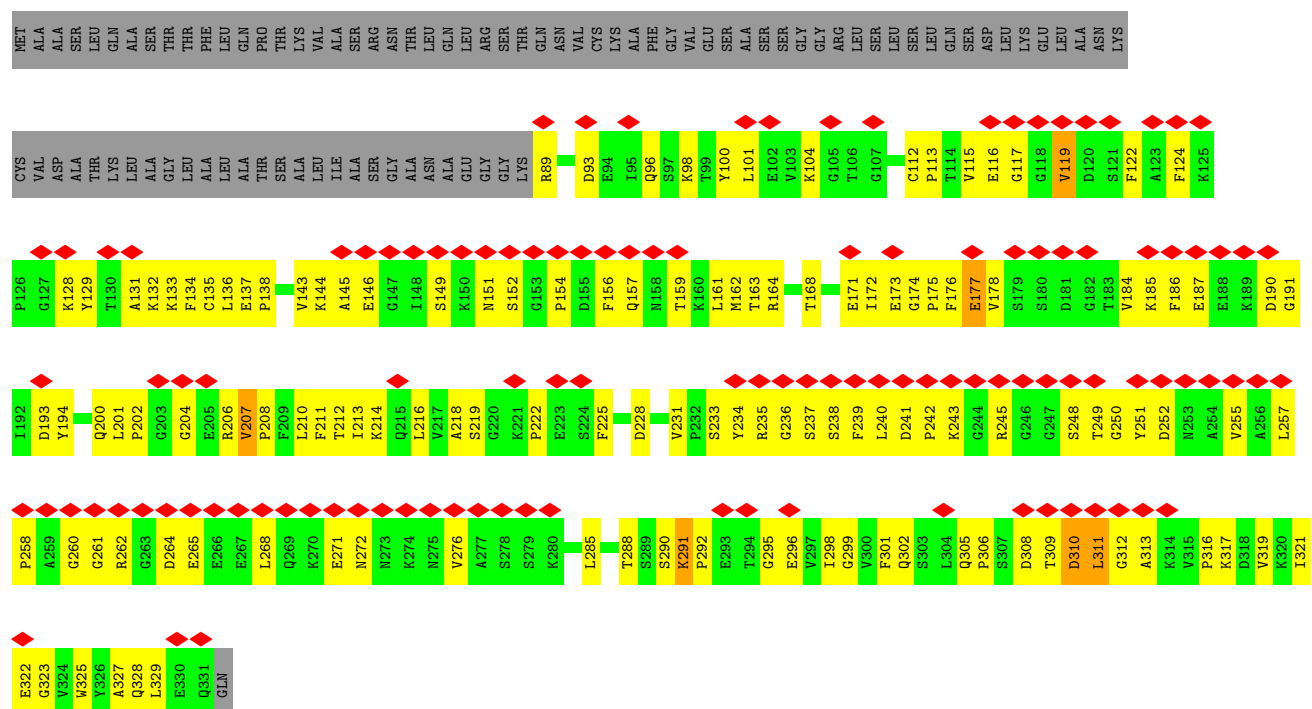


- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

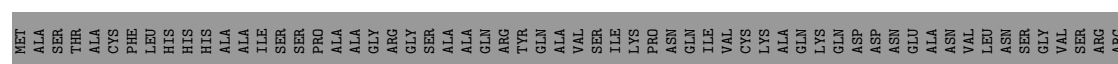




• Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

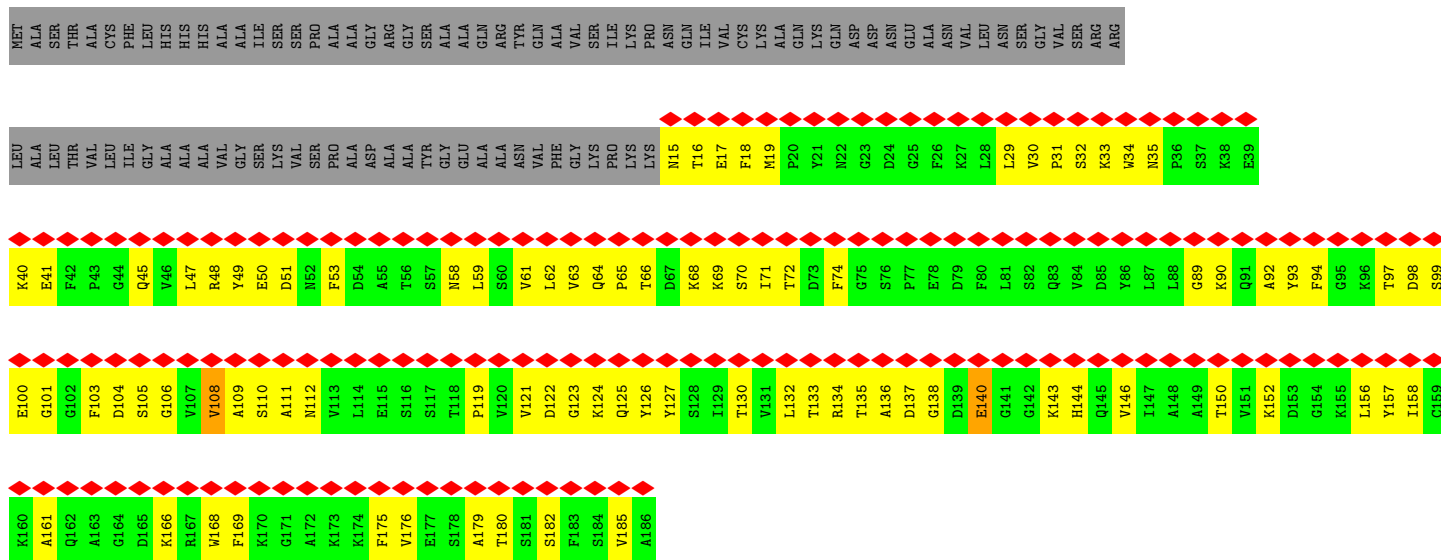
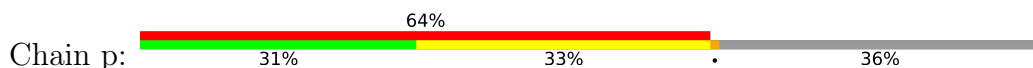


• Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

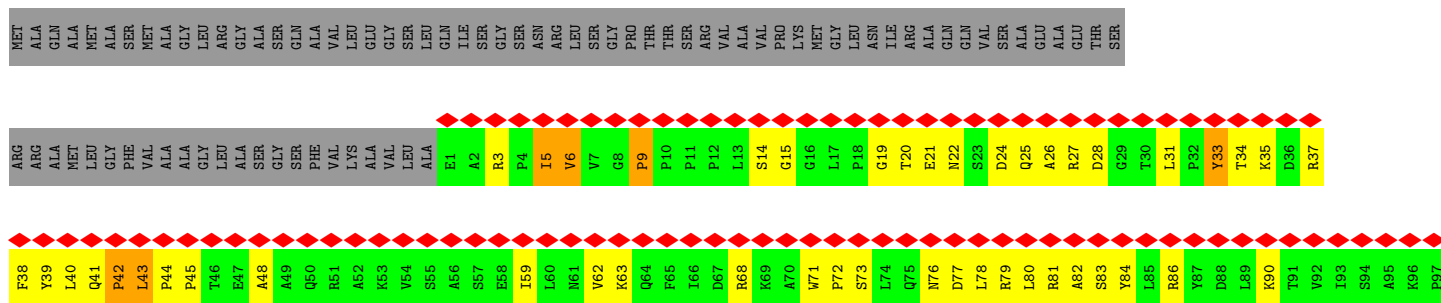
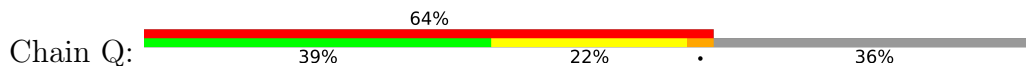


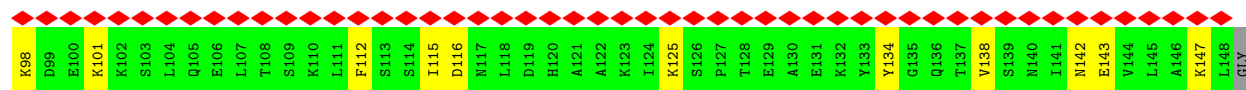


• Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

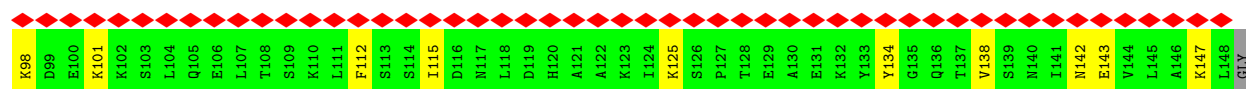
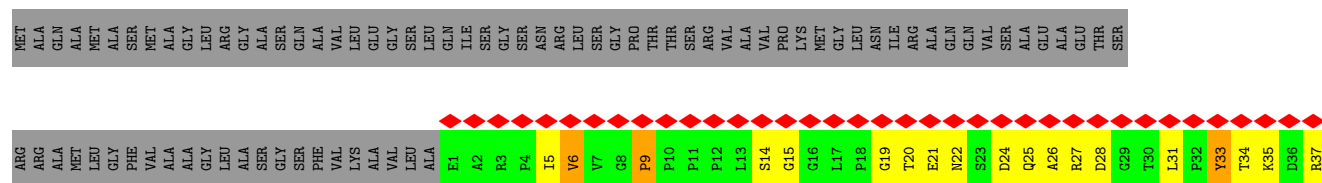
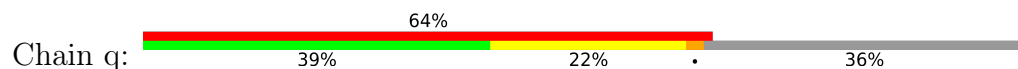


• Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

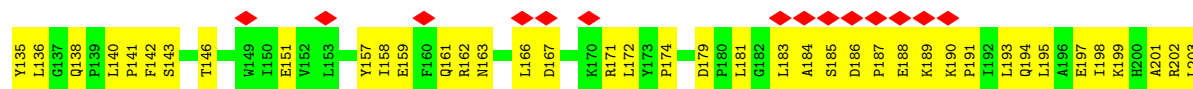
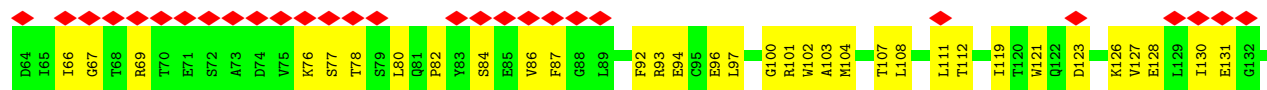
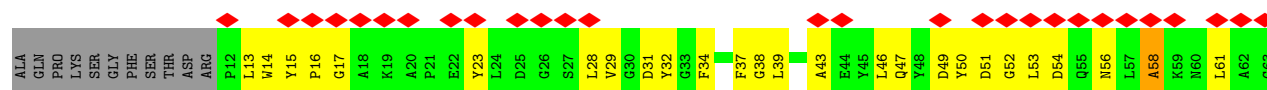




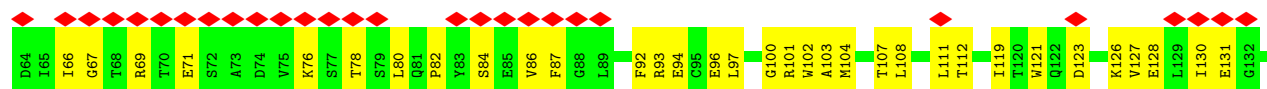
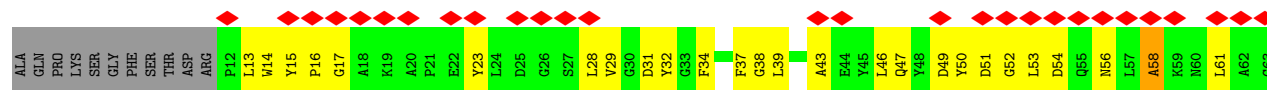
- Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic



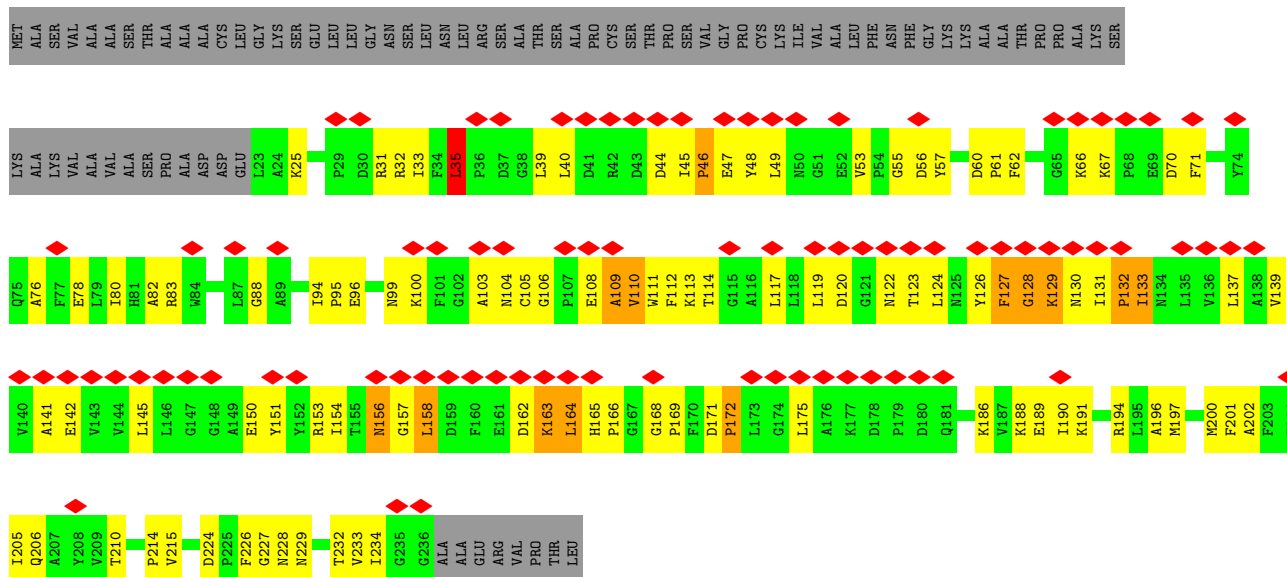
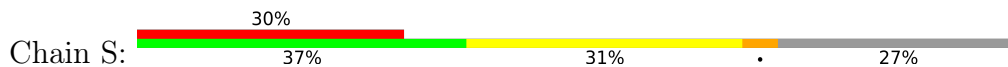
- Molecule 17: Chlorophyll A-B Binding protein 29 kD (CP29)



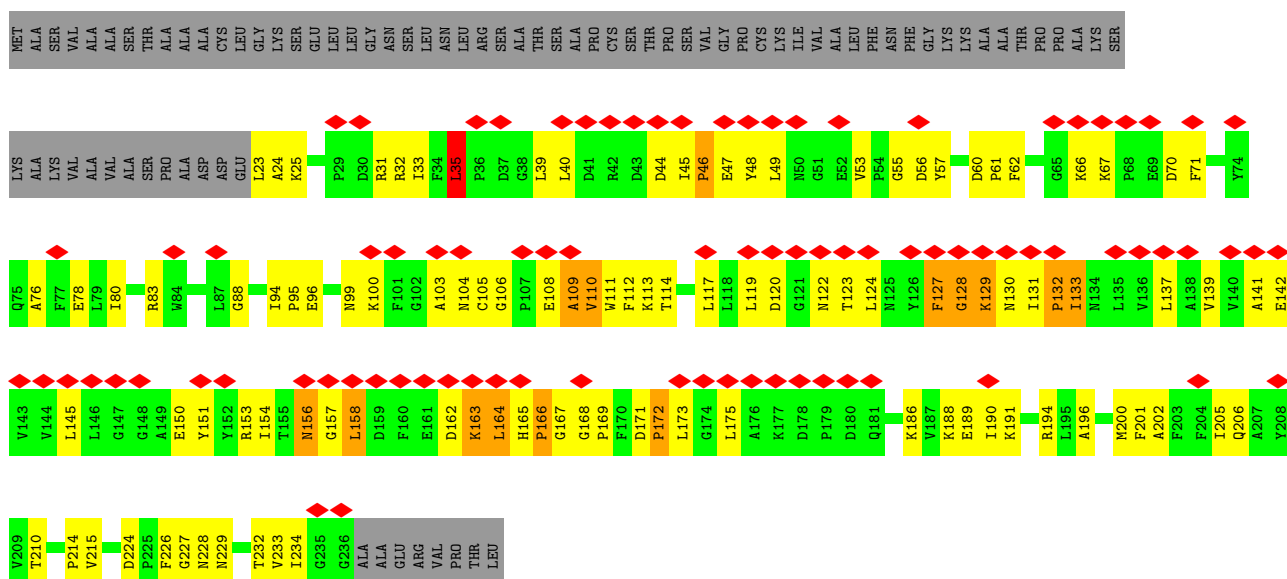
- Molecule 17: Chlorophyll A-B Binding protein 29 kD (CP29)



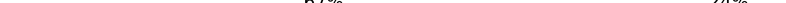
- Molecule 18: Chlorophyll A-B Binding protein 26 kD (CP26)

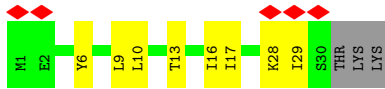


- Molecule 18: Chlorophyll A-B Binding protein 26 kD (CP26)



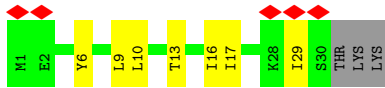
- Molecule 19: Photosystem II Reaction Center protein Tc

Chain T:  15% 67% 24% 9%

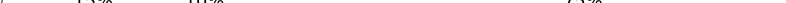


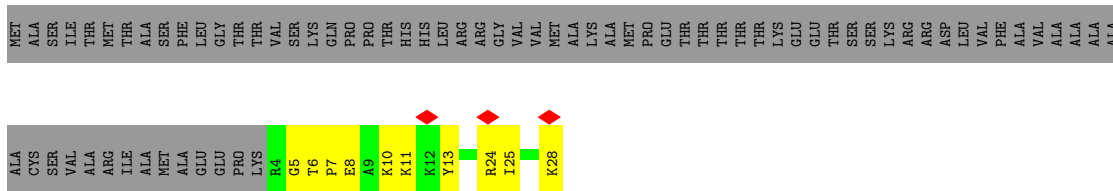
- Molecule 19: Photosystem II Reaction Center protein Tc

Chain t:  15% 70% 21% 9%

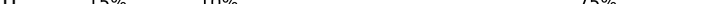


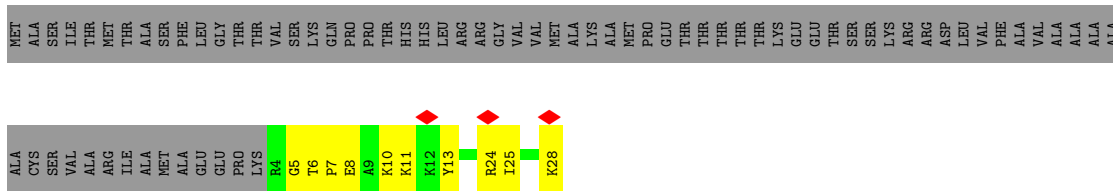
- Molecule 20: Photosystem II Reaction Center Tn protein

Chain U:  15% 10% 75%

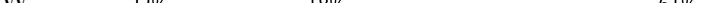


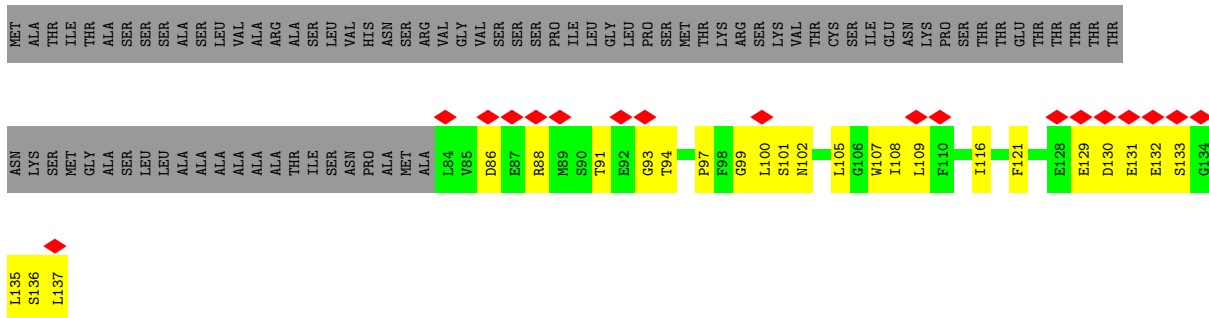
- Molecule 20: Photosystem II Reaction Center Tn protein

Chain u: 



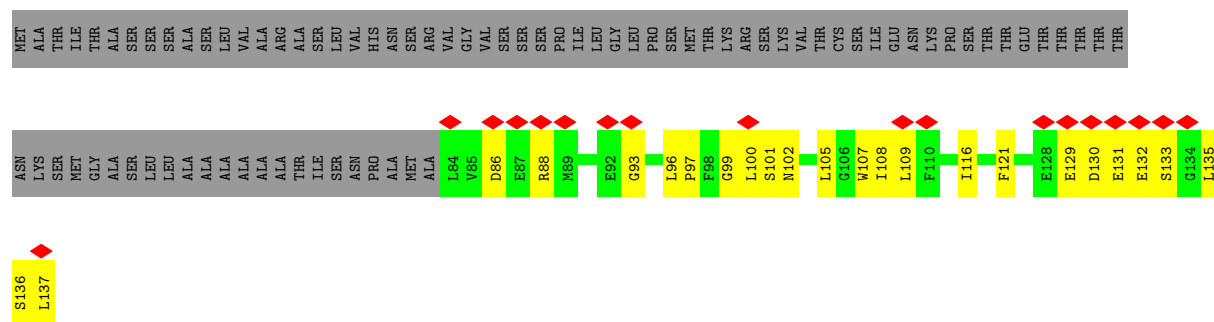
- Molecule 21: Photosystem II reaction center W protein, chloroplastic

Chain W: 

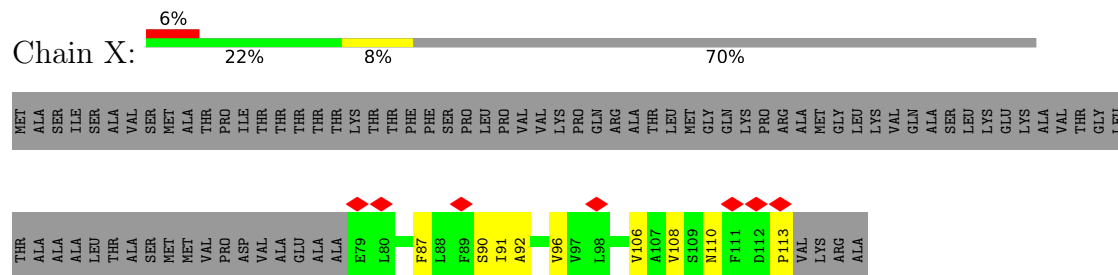


- Molecule 21: Photosystem II reaction center W protein, chloroplatic

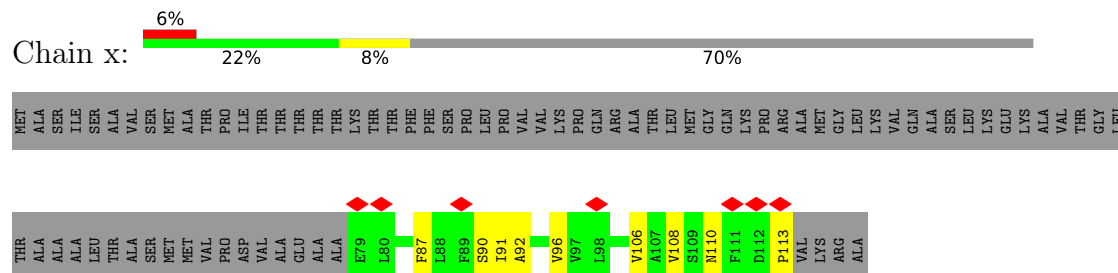
Chain w: 13% 23% 17% 61%



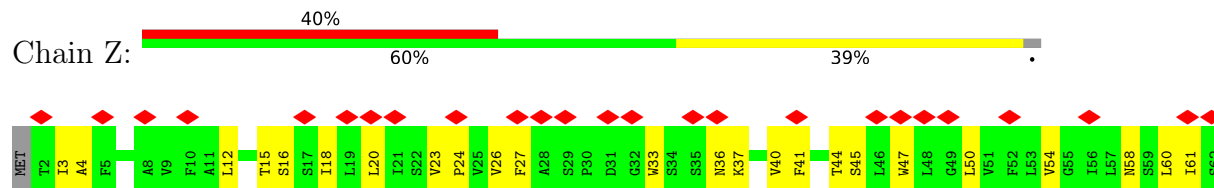
• Molecule 22: Photosystem II Reaction Center X protein



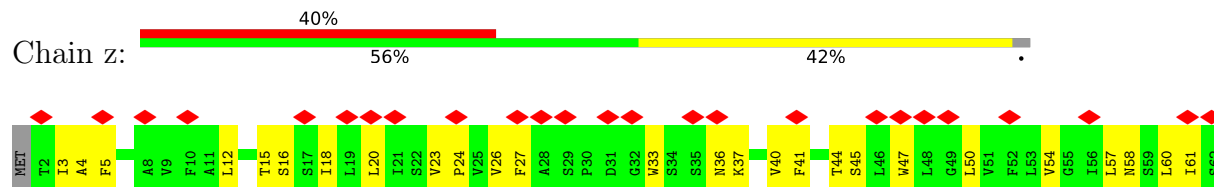
• Molecule 22: Photosystem II Reaction Center X protein



• Molecule 23: Photosystem II reaction center protein Z



• Molecule 23: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	109042	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	59000	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.393	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	337.5, 337.5, 216.0	wwPDB
Map dimensions	250, 250, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.77	0/2695	0.91	9/3674 (0.2%)
1	a	0.77	0/2695	0.91	10/3674 (0.3%)
2	B	0.75	0/3951	0.92	12/5379 (0.2%)
2	b	0.75	0/3951	0.92	12/5379 (0.2%)
3	C	0.72	0/3589	0.84	3/4891 (0.1%)
3	c	0.72	0/3589	0.84	5/4891 (0.1%)
4	D	0.78	0/2796	0.87	10/3811 (0.3%)
4	d	0.78	0/2796	0.87	10/3811 (0.3%)
5	E	0.53	0/654	0.76	0/889
5	e	0.53	0/654	0.77	0/889
6	F	0.59	0/265	0.82	0/358
6	f	0.59	0/265	0.81	0/358
7	G	0.54	0/1713	0.84	2/2333 (0.1%)
7	N	0.53	0/1713	0.82	0/2333
7	Y	0.65	0/1713	0.86	9/2333 (0.4%)
7	g	0.54	0/1713	0.84	2/2333 (0.1%)
7	n	0.53	0/1713	0.82	0/2333
7	y	0.65	0/1713	0.86	9/2333 (0.4%)
8	H	0.64	0/444	0.81	0/605
8	h	0.64	0/444	0.81	0/605
9	I	0.75	0/294	0.80	0/397
9	i	0.75	0/294	0.80	0/397
10	J	0.34	0/253	0.71	1/343 (0.3%)
10	j	0.34	0/253	0.71	0/343
11	K	0.63	0/320	0.79	0/436
11	k	0.63	0/320	0.80	0/436
12	L	0.73	0/319	0.67	0/434
12	l	0.73	0/319	0.68	0/434
13	M	0.71	0/262	0.77	0/359
13	m	0.71	0/262	0.77	0/359
14	O	0.47	0/1880	0.84	6/2541 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	o	0.47	0/1880	0.84	6/2541 (0.2%)
15	P	0.35	0/1353	0.78	2/1828 (0.1%)
15	p	0.35	0/1353	0.78	1/1828 (0.1%)
16	Q	0.40	0/1186	0.85	6/1609 (0.4%)
16	q	0.40	0/1186	0.85	6/1609 (0.4%)
17	R	0.53	0/1853	0.86	1/2522 (0.0%)
17	r	0.53	0/1853	0.86	1/2522 (0.0%)
18	S	0.53	0/1700	1.00	11/2310 (0.5%)
18	s	0.52	0/1700	1.00	11/2310 (0.5%)
19	T	0.76	0/252	0.92	0/341
19	t	0.75	0/252	0.92	0/341
20	U	0.59	0/197	0.85	0/264
20	u	0.59	0/197	0.86	0/264
21	W	0.59	0/429	0.83	0/582
21	w	0.59	0/429	0.83	0/582
22	X	0.60	0/250	0.76	0/342
22	x	0.61	0/250	0.76	0/342
23	Z	0.55	0/464	0.91	1/636 (0.2%)
23	z	0.54	0/464	0.91	1/636 (0.2%)
All	All	0.64	0/61090	0.86	147/83100 (0.2%)

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	A	0	1
1	a	0	1
18	S	0	1
18	s	0	1
All	All	0	4

There are no bond length outliers.

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	46	ASP	CA-C-N	8.53	128.66	119.28
2	B	46	ASP	C-N-CA	8.53	128.66	119.28
2	b	46	ASP	CA-C-N	8.44	128.56	119.28
2	b	46	ASP	C-N-CA	8.44	128.56	119.28
1	A	140	ARG	CA-C-N	7.66	127.70	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	C-N-CA	7.66	127.70	119.28
1	a	55	ALA	CA-C-N	7.65	125.17	119.66
1	a	55	ALA	C-N-CA	7.65	125.17	119.66
1	a	140	ARG	CA-C-N	7.61	127.65	119.28
1	a	140	ARG	C-N-CA	7.61	127.65	119.28
1	A	55	ALA	CA-C-N	7.59	125.20	119.66
1	A	55	ALA	C-N-CA	7.59	125.20	119.66
18	S	128	GLY	N-CA-C	-7.47	105.50	115.21
18	s	128	GLY	N-CA-C	-7.47	105.50	115.21
4	d	139	ARG	CA-C-N	7.19	126.89	119.56
4	d	139	ARG	C-N-CA	7.19	126.89	119.56
4	D	139	ARG	CA-C-N	7.14	126.84	119.56
4	D	139	ARG	C-N-CA	7.14	126.84	119.56
16	Q	42	PRO	CA-C-N	6.98	134.26	121.70
16	Q	42	PRO	C-N-CA	6.98	134.26	121.70
16	q	42	PRO	CA-C-N	6.95	134.22	121.70
16	q	42	PRO	C-N-CA	6.95	134.22	121.70
7	G	146	GLY	CA-C-N	6.91	126.72	119.05
7	G	146	GLY	C-N-CA	6.91	126.72	119.05
7	g	146	GLY	CA-C-N	6.90	126.71	119.05
7	g	146	GLY	C-N-CA	6.90	126.71	119.05
14	O	207	VAL	CA-C-N	6.85	126.84	119.78
14	O	207	VAL	C-N-CA	6.85	126.84	119.78
14	o	207	VAL	CA-C-N	6.84	126.83	119.78
14	o	207	VAL	C-N-CA	6.84	126.83	119.78
23	Z	4	ALA	N-CA-C	-6.75	105.02	113.18
23	z	4	ALA	N-CA-C	-6.74	105.02	113.18
18	s	35	LEU	CA-C-N	6.72	126.51	119.05
18	s	35	LEU	C-N-CA	6.72	126.51	119.05
4	D	297	ASP	N-CA-C	6.71	119.06	108.79
4	d	297	ASP	N-CA-C	6.70	119.04	108.79
18	S	35	LEU	CA-C-N	6.68	126.47	119.05
18	S	35	LEU	C-N-CA	6.68	126.47	119.05
1	A	94	TYR	CA-C-N	6.60	126.55	120.21
1	A	94	TYR	C-N-CA	6.60	126.55	120.21
1	a	94	TYR	CA-C-N	6.57	126.52	120.21
1	a	94	TYR	C-N-CA	6.57	126.52	120.21
7	Y	169	ASP	CA-C-N	6.52	126.29	119.05
7	Y	169	ASP	C-N-CA	6.52	126.29	119.05
7	y	169	ASP	CA-C-N	6.49	126.26	119.05
7	y	169	ASP	C-N-CA	6.49	126.26	119.05
16	Q	42	PRO	CA-C-O	-6.49	109.74	119.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	q	42	PRO	CA-C-O	-6.49	109.74	119.86
2	B	76	GLY	N-CA-C	-6.43	106.89	115.32
2	b	76	GLY	N-CA-C	-6.43	106.90	115.32
4	d	80	THR	CA-C-N	6.40	126.37	119.78
4	d	80	THR	C-N-CA	6.40	126.37	119.78
4	D	80	THR	CA-C-N	6.37	126.34	119.78
4	D	80	THR	C-N-CA	6.37	126.34	119.78
16	Q	42	PRO	N-CA-C	6.16	122.09	113.53
16	q	42	PRO	N-CA-C	6.14	122.07	113.53
3	C	216	SER	CA-C-N	6.10	125.99	119.28
3	C	216	SER	C-N-CA	6.10	125.99	119.28
3	c	216	SER	CA-C-N	6.07	125.96	119.28
3	c	216	SER	C-N-CA	6.07	125.96	119.28
18	S	164	LEU	CA-C-N	6.01	132.52	121.70
18	S	164	LEU	C-N-CA	6.01	132.52	121.70
18	s	164	LEU	CA-C-N	5.98	132.47	121.70
18	s	164	LEU	C-N-CA	5.98	132.47	121.70
2	b	122	ILE	CB-CA-C	-5.78	104.58	111.81
14	o	291	LYS	CA-C-N	5.75	125.60	119.28
14	o	291	LYS	C-N-CA	5.75	125.60	119.28
2	B	122	ILE	CB-CA-C	-5.72	104.65	111.81
14	O	291	LYS	CA-C-N	5.72	125.58	119.28
14	O	291	LYS	C-N-CA	5.72	125.58	119.28
7	Y	192	PHE	N-CA-C	-5.72	105.13	111.71
7	y	192	PHE	N-CA-C	-5.72	105.13	111.71
2	B	163	GLY	CA-C-N	5.58	125.42	119.28
2	B	163	GLY	C-N-CA	5.58	125.42	119.28
2	b	163	GLY	CA-C-N	5.57	125.41	119.28
2	b	163	GLY	C-N-CA	5.57	125.41	119.28
7	Y	18	GLY	CA-C-N	5.54	125.38	119.28
7	Y	18	GLY	C-N-CA	5.54	125.38	119.28
7	y	18	GLY	CA-C-N	5.52	125.35	119.28
7	y	18	GLY	C-N-CA	5.52	125.35	119.28
18	S	129	LYS	N-CA-C	-5.51	106.51	113.18
18	s	129	LYS	N-CA-C	-5.51	106.51	113.18
3	C	419	TYR	N-CA-C	5.46	116.34	107.23
3	c	419	TYR	N-CA-C	5.45	116.33	107.23
18	s	156	ASN	CB-CA-C	-5.44	109.32	115.79
2	b	160	GLY	N-CA-C	-5.42	107.77	115.30
4	D	194	ASN	CA-C-N	5.42	125.24	119.28
4	D	194	ASN	C-N-CA	5.42	125.24	119.28
4	d	194	ASN	CA-C-N	5.42	125.24	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	194	ASN	C-N-CA	5.42	125.24	119.28
2	B	160	GLY	N-CA-C	-5.39	107.81	115.30
4	d	86	ALA	CB-CA-C	-5.38	110.39	116.63
14	o	310	ASP	N-CA-C	-5.38	102.43	110.23
4	D	86	ALA	CB-CA-C	-5.38	110.39	116.63
14	O	310	ASP	N-CA-C	-5.37	102.44	110.23
18	S	156	ASN	CB-CA-C	-5.37	109.40	115.79
2	B	194	VAL	CA-C-N	5.35	125.17	119.28
2	B	194	VAL	C-N-CA	5.35	125.17	119.28
2	b	194	VAL	CA-C-N	5.35	125.17	119.28
2	b	194	VAL	C-N-CA	5.35	125.17	119.28
1	a	149	ALA	CA-C-N	-5.35	113.15	119.84
1	a	149	ALA	C-N-CA	-5.35	113.15	119.84
1	A	149	ALA	CA-C-N	-5.33	113.18	119.84
1	A	149	ALA	C-N-CA	-5.33	113.18	119.84
7	y	146	GLY	CA-C-N	5.29	124.92	119.05
7	y	146	GLY	C-N-CA	5.29	124.92	119.05
18	s	109	ALA	CA-C-N	5.23	131.12	121.70
18	s	109	ALA	C-N-CA	5.23	131.12	121.70
18	S	109	ALA	CA-C-N	5.23	131.12	121.70
18	S	109	ALA	C-N-CA	5.23	131.12	121.70
17	r	207	GLY	N-CA-C	-5.23	106.43	112.50
2	b	213	GLY	N-CA-C	-5.23	106.44	112.50
15	P	140	GLU	N-CA-C	-5.21	104.52	111.87
17	R	207	GLY	N-CA-C	-5.21	106.45	112.50
15	p	140	GLU	N-CA-C	-5.21	104.52	111.87
7	Y	115	ASN	CA-C-N	5.21	125.01	119.28
7	Y	115	ASN	C-N-CA	5.21	125.01	119.28
7	Y	146	GLY	CA-C-N	5.20	125.00	119.28
7	Y	146	GLY	C-N-CA	5.20	125.00	119.28
3	c	464	GLU	CA-C-N	5.19	124.81	119.05
3	c	464	GLU	C-N-CA	5.19	124.81	119.05
2	B	213	GLY	N-CA-C	-5.17	106.51	112.50
18	S	168	GLY	CA-C-N	5.14	124.94	119.28
18	S	168	GLY	C-N-CA	5.14	124.94	119.28
7	y	115	ASN	CA-C-N	5.12	124.91	119.28
7	y	115	ASN	C-N-CA	5.12	124.91	119.28
4	D	94	GLY	CA-C-N	5.12	124.91	119.28
4	D	94	GLY	C-N-CA	5.12	124.91	119.28
18	s	168	GLY	CA-C-N	5.10	124.89	119.28
18	s	168	GLY	C-N-CA	5.10	124.89	119.28
1	A	142	TRP	N-CA-C	5.08	118.62	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	94	GLY	CA-C-N	5.08	124.87	119.28
4	d	94	GLY	C-N-CA	5.08	124.87	119.28
2	b	53	ASP	CA-C-N	5.05	125.03	120.03
2	b	53	ASP	C-N-CA	5.05	125.03	120.03
1	a	56	PRO	O-C-N	5.04	123.52	121.15
1	a	142	TRP	N-CA-C	5.04	118.57	112.93
14	o	212	THR	N-CA-C	5.04	116.49	108.79
15	P	121	VAL	N-CA-C	-5.03	107.02	112.80
16	Q	9	PRO	CA-C-N	-5.02	116.04	119.66
16	Q	9	PRO	C-N-CA	-5.02	116.04	119.66
16	q	9	PRO	CA-C-N	-5.02	116.04	119.66
16	q	9	PRO	C-N-CA	-5.02	116.04	119.66
2	B	53	ASP	CA-C-N	5.02	125.00	120.03
2	B	53	ASP	C-N-CA	5.02	125.00	120.03
10	J	31	GLY	N-CA-C	-5.02	108.75	115.32
14	O	212	THR	N-CA-C	5.02	116.47	108.79

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	PRO	Peptide
18	S	35	LEU	Peptide
1	a	141	PRO	Peptide
18	s	35	LEU	Peptide

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	A	2614	0	2521	161	0
1	a	2614	0	2521	152	0
2	B	3820	0	3690	193	0
2	b	3820	0	3690	193	0
3	C	3475	0	3416	200	0
3	c	3475	0	3416	193	0
4	D	2703	0	2592	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	d	2703	0	2592	147	0
5	E	636	0	612	19	0
5	e	636	0	612	19	0
6	F	257	0	267	10	0
6	f	257	0	267	10	0
7	G	1661	0	1592	92	0
7	N	1661	0	1592	77	0
7	Y	1661	0	1592	75	0
7	g	1661	0	1592	97	0
7	n	1661	0	1592	82	0
7	y	1661	0	1592	77	0
8	H	434	0	459	23	0
8	h	434	0	459	24	0
9	I	286	0	295	10	0
9	i	286	0	295	10	0
10	J	247	0	258	9	0
10	j	247	0	258	9	0
11	K	307	0	310	16	0
11	k	307	0	310	16	0
12	L	311	0	299	10	0
12	l	311	0	299	11	0
13	M	258	0	277	10	0
13	m	258	0	277	10	0
14	O	1844	0	1812	121	0
14	o	1844	0	1812	120	0
15	P	1324	0	1283	79	0
15	p	1324	0	1283	80	0
16	Q	1162	0	1190	64	0
16	q	1162	0	1190	61	0
17	R	1806	0	1784	117	0
17	r	1806	0	1784	120	0
18	S	1653	0	1620	117	0
18	s	1653	0	1620	115	0
19	T	245	0	260	9	0
19	t	245	0	260	8	0
20	U	193	0	205	10	0
20	u	193	0	205	10	0
21	W	419	0	401	30	0
21	w	419	0	401	30	0
22	X	246	0	256	7	0
22	x	246	0	256	7	0
23	Z	454	0	479	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	z	454	0	479	21	0
24	A	10	0	0	2	0
24	a	10	0	0	2	0
25	A	1	0	0	0	0
25	a	1	0	0	0	0
26	A	2	0	0	1	0
26	a	2	0	0	1	0
27	A	239	0	242	26	0
27	B	1040	0	1152	79	0
27	C	829	0	903	64	0
27	D	130	0	144	15	0
27	G	424	0	378	37	0
27	N	424	0	378	23	0
27	R	522	0	456	47	0
27	S	441	0	351	27	0
27	Y	472	0	477	37	0
27	a	239	0	242	23	0
27	b	1040	0	1152	81	0
27	c	829	0	903	63	0
27	d	130	0	144	15	0
27	g	424	0	378	36	0
27	n	424	0	378	25	0
27	r	522	0	456	50	0
27	s	441	0	351	27	0
27	y	472	0	477	39	0
28	A	128	0	148	10	0
28	a	128	0	148	9	0
29	A	40	0	56	6	0
29	B	120	0	168	15	0
29	C	160	0	224	30	0
29	D	40	0	56	5	0
29	H	40	0	56	6	0
29	a	40	0	56	4	0
29	b	120	0	168	15	0
29	c	160	0	224	29	0
29	d	40	0	56	5	0
29	h	40	0	56	6	0
30	A	108	0	155	6	0
30	B	54	0	77	3	0
30	a	108	0	154	6	0
30	b	54	0	77	3	0
31	A	48	0	66	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	B	51	0	72	10	0
31	C	51	0	72	4	0
31	D	46	0	62	4	0
31	Z	51	0	72	6	0
31	a	48	0	66	8	0
31	b	51	0	72	9	0
31	c	51	0	72	5	0
31	d	46	0	62	4	0
31	z	51	0	72	4	0
32	C	179	0	232	30	0
32	H	62	0	82	10	0
32	c	179	0	232	28	0
32	h	62	0	82	9	0
33	D	4	0	0	4	0
33	d	4	0	0	4	0
34	D	55	0	80	7	0
34	d	55	0	80	9	0
35	D	129	0	177	13	0
35	G	49	0	74	14	0
35	L	49	0	74	6	0
35	N	49	0	74	7	0
35	R	49	0	74	3	0
35	S	49	0	74	2	0
35	Y	49	0	74	7	0
35	d	129	0	177	12	0
35	g	49	0	74	13	0
35	l	49	0	74	7	0
35	n	49	0	74	7	0
35	r	49	0	74	3	0
35	s	49	0	74	3	0
35	y	49	0	74	8	0
36	F	43	0	30	5	0
36	f	43	0	30	5	0
37	G	314	0	251	34	0
37	N	314	0	251	35	0
37	R	150	0	111	19	0
37	S	201	0	147	12	0
37	Y	330	0	284	28	0
37	g	314	0	251	36	0
37	n	314	0	251	35	0
37	r	150	0	111	16	0
37	s	201	0	147	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	y	330	0	284	25	0
38	G	84	0	112	15	0
38	N	84	0	112	16	0
38	R	42	0	56	11	0
38	S	84	0	112	17	0
38	Y	84	0	112	14	0
38	g	84	0	112	13	0
38	n	84	0	112	16	0
38	r	42	0	56	10	0
38	s	84	0	112	17	0
38	y	84	0	112	17	0
39	G	44	0	56	7	0
39	N	44	0	56	7	0
39	R	44	0	56	7	0
39	Y	44	0	56	9	0
39	g	44	0	56	6	0
39	n	44	0	56	6	0
39	r	44	0	56	7	0
39	y	44	0	56	9	0
40	G	44	0	56	3	0
40	N	44	0	56	3	0
40	R	44	0	56	6	0
40	S	44	0	56	4	0
40	Y	44	0	56	4	0
40	g	44	0	56	3	0
40	n	44	0	56	3	0
40	r	44	0	56	6	0
40	s	44	0	56	4	0
40	y	44	0	56	3	0
All	All	75994	0	75847	3448	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 23.

All (3448) 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)
27:G:611:CLA:NB	35:G:2630:LHG:O4	1.78	1.15
27:g:611:CLA:NB	35:g:2630:LHG:O4	1.78	1.15
1:a:317:TRP:HE3	4:d:180:ARG:HD3	1.26	0.98
1:A:317:TRP:HE3	4:D:180:ARG:HD3	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:162:MET:HE3	14:O:200:GLN:HB2	1.51	0.91
14:o:162:MET:HE3	14:o:200:GLN:HB2	1.51	0.91
1:A:303:ASN:O	3:C:415:ASN:ND2	2.05	0.90
17:R:158:ILE:HD11	40:R:623:NEX:H34	1.53	0.90
7:n:191:MET:HE2	38:n:1621:LUT:H10	1.52	0.90
1:a:303:ASN:O	3:c:415:ASN:ND2	2.04	0.90
17:r:158:ILE:HD11	40:r:623:NEX:H34	1.53	0.89
2:b:277:GLN:HB3	20:u:24:ARG:HG3	1.55	0.89
7:N:191:MET:HE2	38:N:1621:LUT:H10	1.52	0.88
2:B:277:GLN:HB3	20:U:24:ARG:HG3	1.55	0.87
2:B:382:PRO:O	2:B:385:ARG:NH2	2.07	0.87
7:G:191:MET:HE2	38:G:1621:LUT:H10	1.56	0.87
2:b:382:PRO:O	2:b:385:ARG:NH2	2.07	0.87
18:S:205:ILE:HG21	27:S:613:CLA:HAC2	1.57	0.86
3:C:345:PRO:HB3	14:O:164:ARG:HE	1.41	0.85
7:g:191:MET:HE2	38:g:1621:LUT:H10	1.56	0.85
18:s:205:ILE:HG21	27:s:613:CLA:HAC2	1.57	0.85
4:d:180:ARG:NH2	4:d:333:ASP:OD1	2.09	0.85
4:D:180:ARG:NH2	4:D:333:ASP:OD1	2.09	0.85
17:R:208:PHE:HA	17:R:211:PHE:HD2	1.42	0.84
3:c:345:PRO:HB3	14:o:164:ARG:HE	1.41	0.84
15:P:99:SER:H	15:P:106:GLY:H	1.23	0.84
14:O:200:GLN:HE21	14:O:204:GLY:HA2	1.42	0.84
18:s:200:MET:HE2	38:s:1621:LUT:H10	1.60	0.84
18:S:200:MET:HE2	38:S:1621:LUT:H10	1.60	0.84
14:O:225:PHE:HB2	14:O:285:LEU:HB2	1.60	0.83
17:r:208:PHE:HA	17:r:211:PHE:HD2	1.42	0.83
15:p:99:SER:H	15:p:106:GLY:H	1.23	0.83
14:O:89:ARG:NH1	14:O:137:GLU:OE2	2.12	0.83
14:o:89:ARG:NH1	14:o:137:GLU:OE2	2.12	0.82
14:o:200:GLN:HE21	14:o:204:GLY:HA2	1.42	0.82
1:a:48:PHE:HE2	34:d:405:PL9:H48	1.43	0.82
7:Y:191:MET:HE2	38:Y:1621:LUT:H10	1.62	0.82
7:y:191:MET:HE2	38:y:1621:LUT:H10	1.62	0.82
14:o:225:PHE:HB2	14:o:285:LEU:HB2	1.60	0.81
1:A:48:PHE:HE2	34:D:405:PL9:H48	1.43	0.81
1:a:82:ILE:HD11	1:a:111:PRO:HB2	1.61	0.81
37:n:601:CHL:HBB1	37:n:601:CHL:HHC	1.63	0.81
37:N:601:CHL:HBB1	37:N:601:CHL:HHC	1.63	0.80
1:a:317:TRP:CE3	4:d:180:ARG:HD3	2.16	0.80
3:C:78:GLU:HB2	16:Q:33:TYR:HA	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD11	1:A:111:PRO:HB2	1.61	0.80
18:s:99:ASN:ND2	18:s:108:GLU:OE2	2.14	0.79
3:c:332:GLN:HB3	15:p:101:GLY:H	1.47	0.79
1:A:317:TRP:CE3	4:D:180:ARG:HD3	2.16	0.79
18:S:99:ASN:ND2	18:S:108:GLU:OE2	2.14	0.79
3:C:31:THR:HG23	3:C:33:PHE:H	1.45	0.79
3:C:332:GLN:HB3	15:P:101:GLY:H	1.47	0.79
26:a:404:CL:CL	3:c:354:GLU:N	2.53	0.78
7:G:41:PRO:HB2	7:G:181:ILE:HD12	1.64	0.78
3:c:31:THR:HG23	3:c:33:PHE:H	1.45	0.78
37:N:609:CHL:HBB1	37:Y:601:CHL:H51	1.65	0.78
3:c:78:GLU:HB2	16:q:33:TYR:HA	1.64	0.78
26:A:404:CL:CL	3:C:354:GLU:N	2.53	0.78
37:n:609:CHL:HBB1	37:y:601:CHL:H51	1.65	0.78
7:N:94:GLU:H	7:N:103:GLN:HE21	1.32	0.77
7:n:94:GLU:H	7:n:103:GLN:HE21	1.32	0.77
3:c:331:ALA:O	14:o:194:TYR:OH	2.02	0.77
7:g:41:PRO:HB2	7:g:181:ILE:HD12	1.63	0.77
1:A:333:GLU:OE2	24:A:401:OEX:O5	2.03	0.77
27:b:613:CLA:H13	27:b:614:CLA:HAB	1.67	0.77
3:C:331:ALA:O	14:O:194:TYR:OH	2.02	0.76
1:a:333:GLU:OE2	24:a:401:OEX:O5	2.03	0.76
7:G:220:ASN:HB2	27:G:614:CLA:HED3	1.68	0.76
4:d:57:SER:HG	4:d:65:SER:HG	1.25	0.76
27:g:602:CLA:H2	38:g:1621:LUT:H26	1.68	0.76
17:r:97:LEU:HD23	17:r:172:LEU:HD22	1.68	0.76
3:C:76:VAL:O	3:C:84:GLN:NE2	2.18	0.76
7:G:182:LYS:NZ	35:G:2630:LHG:O5	2.19	0.76
3:c:76:VAL:O	3:c:84:GLN:NE2	2.18	0.76
7:g:220:ASN:HB2	27:g:614:CLA:HED3	1.68	0.76
39:n:1622:XAT:H393	35:y:2630:LHG:H101	1.68	0.76
18:s:57:TYR:OH	18:s:191:LYS:NZ	2.16	0.76
2:b:389:LYS:NZ	15:p:41:GLU:OE2	2.19	0.75
1:A:29:TYR:O	1:A:129:ARG:NH2	2.17	0.75
2:B:385:ARG:HD2	15:P:93:TYR:H	1.51	0.75
27:B:613:CLA:H13	27:B:614:CLA:HAB	1.67	0.75
39:N:1622:XAT:H393	35:Y:2630:LHG:H101	1.68	0.75
4:d:26:ARG:HG3	4:d:28:VAL:H	1.51	0.75
17:R:97:LEU:HD23	17:R:172:LEU:HD22	1.68	0.75
4:D:26:ARG:HG3	4:D:28:VAL:H	1.51	0.75
7:g:182:LYS:NZ	35:g:2630:LHG:O5	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:N:606:CHL:HHC	37:N:606:CHL:HBB1	1.69	0.74
27:G:602:CLA:H2	38:G:1621:LUT:H26	1.68	0.74
3:c:148:GLY:O	3:c:156:LYS:NZ	2.21	0.74
2:B:389:LYS:NZ	15:P:41:GLU:OE2	2.19	0.74
7:Y:126:ALA:HB3	37:Y:605:CHL:HMC	1.70	0.74
2:b:385:ARG:HD2	15:p:93:TYR:H	1.51	0.74
1:a:64:ARG:HH21	14:o:163:THR:HB	1.53	0.74
3:c:189:TRP:O	16:q:79:ARG:NH1	2.21	0.74
28:A:409:PHO:HBC3	4:D:279:LEU:HD22	1.70	0.74
2:B:422:ARG:HD3	14:O:262:ARG:HE	1.53	0.74
18:S:57:TYR:OH	18:S:191:LYS:NZ	2.16	0.74
16:q:112:PHE:HA	16:q:115:ILE:HG22	1.70	0.73
16:q:42:PRO:HB2	16:q:43:LEU:HB2	1.70	0.73
1:A:64:ARG:HH21	14:O:163:THR:HB	1.53	0.73
16:Q:112:PHE:HA	16:Q:115:ILE:HG22	1.70	0.73
7:y:126:ALA:HB3	37:y:605:CHL:HMC	1.70	0.73
2:b:422:ARG:HD3	14:o:262:ARG:HE	1.53	0.73
29:B:618:BCR:HC31	31:B:622:LMG:H291	1.71	0.73
3:C:189:TRP:O	16:Q:79:ARG:NH1	2.21	0.73
7:y:94:GLU:H	7:y:103:GLN:HE21	1.36	0.73
28:a:409:PHO:HBC3	4:d:279:LEU:HD22	1.70	0.72
37:n:606:CHL:HHC	37:n:606:CHL:HBB1	1.69	0.72
2:b:260:SER:HG	2:b:262:THR:HG1	1.36	0.72
14:o:296:GLU:HG2	14:o:328:GLN:HG2	1.70	0.72
1:a:29:TYR:O	1:a:129:ARG:NH2	2.17	0.72
1:a:259:ILE:HG22	1:a:260:PHE:H	1.55	0.72
1:a:301:ASN:HB3	3:c:407:VAL:HG21	1.72	0.72
17:R:94:GLU:HA	17:R:172:LEU:HD21	1.70	0.72
27:b:602:CLA:H93	29:h:101:BCR:H402	1.72	0.72
3:C:148:GLY:O	3:C:156:LYS:NZ	2.21	0.72
29:b:618:BCR:HC31	31:b:622:LMG:H291	1.71	0.72
16:Q:42:PRO:HB2	16:Q:43:LEU:HB2	1.70	0.71
1:A:301:ASN:HB3	3:C:407:VAL:HG21	1.72	0.71
27:B:602:CLA:H93	29:H:101:BCR:H402	1.72	0.71
18:S:189:GLU:OE1	27:S:610:CLA:NA	2.24	0.71
2:B:53:ASP:OD2	2:B:58:GLN:NE2	2.23	0.71
1:a:153:ALA:HB1	27:a:405:CLA:HED1	1.73	0.71
1:A:259:ILE:HG22	1:A:260:PHE:H	1.55	0.71
2:B:260:SER:HG	2:B:262:THR:HG1	1.38	0.71
3:c:45:LEU:HD22	3:c:138:GLU:HB3	1.73	0.71
27:c:504:CLA:H71	32:c:520:DGD:HBW2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:225:ALA:HA	39:y:1622:XAT:H22	1.73	0.71
14:O:276:VAL:HG22	14:O:311:LEU:HD11	1.73	0.71
15:P:108:VAL:HG23	15:P:109:ALA:H	1.55	0.71
2:b:53:ASP:OD2	2:b:58:GLN:NE2	2.23	0.71
7:g:52:SER:HB3	7:g:58:PHE:HD1	1.56	0.71
17:R:229:HIS:ND1	17:R:236:THR:OG1	2.20	0.71
23:Z:26:VAL:HG13	23:Z:36:ASN:HB3	1.72	0.71
7:g:118:LEU:O	7:g:120:HIS:N	2.24	0.71
14:o:276:VAL:HG22	14:o:311:LEU:HD11	1.72	0.71
14:O:178:VAL:HA	14:O:184:VAL:HG22	1.73	0.71
14:O:302:GLN:HG2	14:O:322:GLU:HG2	1.73	0.71
32:c:519:DGD:HA31	31:c:521:LMG:H331	1.73	0.71
23:z:26:VAL:HG13	23:z:36:ASN:HB3	1.72	0.71
14:O:296:GLU:HG2	14:O:328:GLN:HG2	1.70	0.71
3:C:45:LEU:HD22	3:C:138:GLU:HB3	1.73	0.70
3:C:95:LEU:O	3:C:178:LYS:NZ	2.20	0.70
37:n:608:CHL:HHC	37:n:608:CHL:HBB1	1.72	0.70
18:s:164:LEU:HB3	18:s:165:HIS:HB3	1.72	0.70
32:C:519:DGD:HA31	31:C:521:LMG:H331	1.73	0.70
7:N:211:ASP:O	7:N:219:ASN:ND2	2.24	0.70
3:c:95:LEU:O	3:c:178:LYS:NZ	2.20	0.70
17:r:94:GLU:HA	17:r:172:LEU:HD21	1.70	0.70
37:s:606:CHL:HHC	37:s:606:CHL:HBB1	1.72	0.70
10:j:7:ARG:HG3	10:j:8:ILE:HD12	1.74	0.70
37:N:608:CHL:HHC	37:N:608:CHL:HBB1	1.72	0.70
15:p:108:VAL:HG23	15:p:109:ALA:H	1.55	0.70
2:B:317:ASN:HA	2:B:330:MET:HE1	1.74	0.70
29:D:404:BCR:H401	10:J:25:VAL:HG22	1.74	0.70
18:s:189:GLU:OE1	27:s:610:CLA:NA	2.24	0.70
1:a:85:THR:HG22	1:a:168:PHE:HB2	1.74	0.70
1:a:296:ASN:HB3	3:c:401:LEU:HA	1.73	0.70
37:n:607:CHL:H142	37:y:601:CHL:H18	1.74	0.70
1:A:153:ALA:HB1	27:A:405:CLA:HED1	1.73	0.70
7:G:52:SER:HB3	7:G:58:PHE:HD1	1.56	0.70
2:b:317:ASN:HA	2:b:330:MET:HE1	1.74	0.70
3:c:297:TYR:O	3:c:423:ARG:NH2	2.25	0.70
12:L:30:VAL:O	12:L:34:ASN:ND2	2.25	0.70
1:a:195:HIS:HD2	1:a:196:PRO:HD2	1.57	0.70
12:l:30:VAL:O	12:l:34:ASN:ND2	2.25	0.70
27:C:504:CLA:H71	32:C:520:DGD:HBW2	1.73	0.69
7:G:118:LEU:O	7:G:120:HIS:N	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Y:607:CHL:HHC	37:Y:607:CHL:HBB1	1.74	0.69
14:O:132:LYS:HG3	14:O:133:LYS:H	1.58	0.69
20:U:5:GLY:O	20:U:10:LYS:NZ	2.25	0.69
18:S:164:LEU:HB3	18:S:165:HIS:HB3	1.72	0.69
3:c:261:ARG:NH2	21:w:131:GLU:OE1	2.25	0.69
14:o:302:GLN:HG2	14:o:322:GLU:HG2	1.73	0.69
17:r:229:HIS:ND1	17:r:236:THR:OG1	2.20	0.69
7:y:24:TYR:CG	7:y:46:TRP:HB2	2.28	0.69
1:A:85:THR:HG22	1:A:168:PHE:HB2	1.74	0.69
3:C:297:TYR:O	3:C:423:ARG:NH2	2.25	0.69
7:G:179:LYS:HD3	27:G:612:CLA:HAA2	1.73	0.69
7:N:225:ALA:HA	39:Y:1622:XAT:H22	1.72	0.69
37:S:606:CHL:HHC	37:S:606:CHL:HBB1	1.72	0.69
3:c:332:GLN:HG3	3:c:336:GLY:HA2	1.72	0.69
3:C:332:GLN:HG3	3:C:336:GLY:HA2	1.72	0.69
37:y:607:CHL:HHC	37:y:607:CHL:HBB1	1.74	0.69
10:J:7:ARG:HG3	10:J:8:ILE:HD12	1.74	0.69
7:n:211:ASP:O	7:n:219:ASN:ND2	2.24	0.69
37:N:607:CHL:H142	37:Y:601:CHL:H18	1.74	0.69
7:Y:94:GLU:H	7:Y:103:GLN:HE21	1.36	0.69
2:b:157:HIS:HE1	27:b:607:CLA:NA	1.89	0.69
7:g:179:LYS:HD3	27:g:612:CLA:HAA2	1.73	0.69
14:o:178:VAL:HA	14:o:184:VAL:HG22	1.73	0.69
3:C:261:ARG:NH2	21:W:131:GLU:OE1	2.25	0.69
29:D:404:BCR:H14C	6:F:33:PHE:CD2	2.28	0.69
17:R:29:VAL:HG21	17:R:194:GLN:HE21	1.57	0.69
7:Y:24:TYR:CG	7:Y:46:TRP:HB2	2.28	0.69
29:d:404:BCR:H401	10:j:25:VAL:HG22	1.74	0.69
37:N:607:CHL:HMA3	37:N:607:CHL:H43	1.75	0.69
20:u:5:GLY:O	20:u:10:LYS:NZ	2.25	0.69
13:M:5:ILE:HG23	13:m:5:ILE:HG23	1.74	0.68
7:y:21:ARG:NH2	7:y:36:LEU:O	2.26	0.68
1:A:296:ASN:HB3	3:C:401:LEU:HA	1.73	0.68
7:Y:21:ARG:NH2	7:Y:36:LEU:O	2.26	0.68
1:a:221:SER:HA	4:d:139:ARG:HB2	1.76	0.68
27:g:610:CLA:H2	38:g:1620:LUT:H28	1.75	0.68
37:r:608:CHL:H12	38:r:620:LUT:H383	1.74	0.68
7:Y:52:SER:OG	7:Y:61:ASN:ND2	2.26	0.68
14:o:164:ARG:HA	21:w:88:ARG:HH22	1.58	0.68
27:y:602:CLA:HAB	38:y:1621:LUT:H32	1.76	0.68
29:d:404:BCR:H14C	6:f:33:PHE:CD2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p:68:LYS:HA	15:p:69:LYS:HB2	1.75	0.68
17:r:29:VAL:HG21	17:r:194:GLN:HE21	1.57	0.68
17:r:96:GLU:OE2	17:r:202:ARG:NE	2.27	0.68
27:G:610:CLA:H2	38:G:1620:LUT:H28	1.75	0.68
35:d:408:LHG:H351	35:d:408:LHG:H101	1.76	0.68
1:A:195:HIS:HD2	1:A:196:PRO:HD2	1.57	0.67
1:A:221:SER:HA	4:D:139:ARG:HB2	1.76	0.67
15:P:68:LYS:HA	15:P:69:LYS:HB2	1.75	0.67
37:R:608:CHL:H12	38:R:620:LUT:H383	1.74	0.67
14:o:132:LYS:HG3	14:o:133:LYS:H	1.58	0.67
17:R:93:ARG:HH12	27:R:602:CLA:HED1	1.58	0.67
7:Y:212:HIS:CG	27:Y:613:CLA:HAA2	2.29	0.67
23:Z:33:TRP:O	23:Z:37:LYS:N	2.27	0.67
27:g:602:CLA:HBA1	38:g:1621:LUT:H382	1.76	0.67
23:z:33:TRP:O	23:z:37:LYS:N	2.27	0.67
18:S:35:LEU:HD13	18:S:39:LEU:HB3	1.77	0.67
4:d:186:GLN:HB2	27:d:402:CLA:HBC1	1.76	0.67
37:n:607:CHL:H43	37:n:607:CHL:HMA3	1.75	0.67
27:b:615:CLA:H102	35:l:101:LHG:H372	1.76	0.67
1:A:82:ILE:HG22	1:A:174:LEU:HB2	1.76	0.67
7:N:99:LYS:HA	37:N:607:CHL:HED2	1.77	0.67
18:s:35:LEU:HD13	18:s:39:LEU:HB3	1.77	0.67
27:B:603:CLA:HBD	27:B:603:CLA:HBA2	1.76	0.67
15:P:30:VAL:HG13	15:P:59:LEU:HD21	1.76	0.67
17:r:191:PRO:O	17:r:194:GLN:HG2	1.95	0.67
18:s:123:THR:HG23	18:s:130:ASN:HD21	1.60	0.67
35:D:408:LHG:H351	35:D:408:LHG:H101	1.76	0.67
5:E:19:TYR:O	5:E:23:HIS:ND1	2.24	0.67
3:C:387:TRP:NE1	16:Q:80:LEU:O	2.26	0.67
3:c:387:TRP:NE1	16:q:80:LEU:O	2.26	0.67
14:o:143:VAL:HG22	14:o:319:VAL:HG22	1.76	0.67
1:A:196:PRO:HA	1:A:199:MET:HG3	1.77	0.67
14:O:143:VAL:HG22	14:O:319:VAL:HG22	1.77	0.67
27:Y:602:CLA:HAB	38:Y:1621:LUT:H32	1.76	0.67
1:A:57:PRO:O	14:O:206:ARG:NH1	2.25	0.66
3:C:66:ALA:HB1	11:K:38:MET:HB3	1.78	0.66
14:O:164:ARG:HA	21:W:88:ARG:HH22	1.58	0.66
18:S:145:LEU:HD22	37:S:606:CHL:HMA2	1.77	0.66
15:p:30:VAL:HG13	15:p:59:LEU:HD21	1.76	0.66
7:y:212:HIS:CG	27:y:613:CLA:HAA2	2.29	0.66
27:B:615:CLA:H102	35:L:101:LHG:H372	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:186:GLN:HB2	27:D:402:CLA:HBC1	1.76	0.66
24:a:401:OEX:O4	3:c:357:ARG:NH2	2.28	0.66
17:r:93:ARG:HH12	27:r:602:CLA:HED1	1.59	0.66
2:B:370:LEU:HB2	2:B:379:ALA:HB3	1.76	0.66
37:N:606:CHL:HBA2	37:N:606:CHL:HBD	1.76	0.66
4:d:192:THR:HG23	27:d:402:CLA:HBC2	1.77	0.66
14:O:124:PHE:HE2	14:O:329:LEU:HD12	1.60	0.66
17:R:191:PRO:O	17:R:194:GLN:HG2	1.95	0.66
18:S:46:PRO:HB2	18:S:49:LEU:HB2	1.77	0.66
1:a:199:MET:HG2	32:c:520:DGD:HAE2	1.76	0.66
3:c:66:ALA:HB1	11:k:38:MET:HB3	1.78	0.66
18:s:145:LEU:HD22	37:s:606:CHL:HMA2	1.77	0.66
21:w:97:PRO:HG2	21:w:100:LEU:HD12	1.76	0.66
1:A:257:ARG:HH21	4:D:136:VAL:HG22	1.60	0.66
27:G:602:CLA:HBA1	38:G:1621:LUT:H382	1.76	0.66
7:n:99:LYS:HA	37:n:607:CHL:HED2	1.77	0.66
37:n:606:CHL:HBA2	37:n:606:CHL:HBD	1.76	0.66
21:W:97:PRO:HG2	21:W:100:LEU:HD12	1.76	0.66
16:q:138:VAL:O	16:q:142:ASN:ND2	2.27	0.66
17:R:96:GLU:OE2	17:R:202:ARG:NE	2.27	0.66
18:S:123:THR:HG23	18:S:130:ASN:HD21	1.60	0.66
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.78	0.66
15:p:111:ALA:HA	15:p:133:THR:HA	1.78	0.66
3:C:256:PRO:HA	27:C:506:CLA:HED3	1.78	0.66
2:b:71:ILE:HD13	2:b:96:VAL:HG21	1.77	0.66
1:A:149:ALA:HB2	1:A:280:VAL:HG13	1.78	0.66
1:a:196:PRO:HA	1:a:199:MET:HG3	1.77	0.66
1:a:246:TYR:CE2	1:a:248:ILE:HG22	2.31	0.66
2:b:370:LEU:HB2	2:b:379:ALA:HB3	1.76	0.66
7:g:26:GLY:O	7:g:29:SER:OG	2.12	0.66
2:b:227:LYS:O	2:b:230:ARG:NH1	2.29	0.66
3:c:464:GLU:OE2	4:d:248:THR:OG1	2.14	0.66
14:o:241:ASP:OD1	14:o:245:ARG:N	2.29	0.66
17:r:222:PRO:HA	17:r:225:ASN:HD22	1.61	0.66
18:s:234:ILE:HG13	23:z:60:LEU:HD21	1.77	0.66
2:B:71:ILE:HD13	2:B:96:VAL:HG21	1.77	0.65
15:P:111:ALA:HA	15:P:133:THR:HA	1.78	0.65
3:c:256:PRO:HA	27:c:506:CLA:HED3	1.78	0.65
1:A:199:MET:HG2	32:C:520:DGD:HAE2	1.76	0.65
1:a:257:ARG:HH21	4:d:136:VAL:HG22	1.60	0.65
27:b:603:CLA:HBD	27:b:603:CLA:HBA2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:604:CLA:H192	27:b:610:CLA:H91	1.78	0.65
29:b:618:BCR:H322	31:b:622:LMG:H111	1.77	0.65
3:c:38:GLY:HA3	27:c:511:CLA:HMD2	1.78	0.65
3:c:110:PRO:HB3	31:z:101:LMG:H142	1.78	0.65
24:A:401:OEX:O4	3:C:357:ARG:NH2	2.28	0.65
28:A:408:PHO:H41	30:A:418:SQD:H192	1.79	0.65
4:D:139:ARG:NH2	4:D:141:TYR:OH	2.30	0.65
7:G:21:ARG:NH2	7:G:36:LEU:O	2.29	0.65
18:S:139:VAL:HG22	37:S:607:CHL:HBC1	1.77	0.65
1:a:82:ILE:HG22	1:a:174:LEU:HB2	1.75	0.65
28:a:408:PHO:H41	30:a:418:SQD:H192	1.79	0.65
2:B:157:HIS:HE1	27:B:607:CLA:NA	1.89	0.65
3:C:26:ARG:O	3:C:41:ARG:NH1	2.29	0.65
7:G:26:GLY:O	7:G:29:SER:OG	2.12	0.65
14:O:173:GLU:N	14:O:190:ASP:O	2.28	0.65
1:a:149:ALA:HB2	1:a:280:VAL:HG13	1.78	0.65
4:d:19:ASP:OD2	4:d:23:ARG:NH2	2.26	0.65
7:g:21:ARG:NH2	7:g:36:LEU:O	2.28	0.65
3:C:42:LEU:HD21	27:C:511:CLA:H2A	1.77	0.65
28:a:409:PHO:OBD	4:d:129:GLN:NE2	2.29	0.65
6:f:24:HIS:NE2	36:f:101:HEM:NA	2.45	0.65
2:B:254:GLY:HA3	32:H:102:DGD:HB61	1.78	0.65
14:O:241:ASP:OD1	14:O:245:ARG:N	2.29	0.65
17:R:222:PRO:HA	17:R:225:ASN:HD22	1.61	0.65
18:S:127:PHE:HB3	18:S:129:LYS:H	1.61	0.65
17:r:208:PHE:HA	17:r:211:PHE:CD2	2.30	0.65
18:s:139:VAL:HG22	37:s:607:CHL:HBC1	1.77	0.65
28:A:409:PHO:OBD	4:D:129:GLN:NE2	2.29	0.65
3:c:26:ARG:O	3:c:41:ARG:NH1	2.29	0.65
3:c:42:LEU:HD21	27:c:511:CLA:H2A	1.77	0.65
29:B:618:BCR:H322	31:B:622:LMG:H111	1.77	0.65
3:C:110:PRO:HB3	31:Z:101:LMG:H142	1.78	0.65
3:C:459:ILE:HG22	3:C:461:ARG:H	1.62	0.65
4:D:18:MET:HE1	22:X:106:VAL:HA	1.78	0.65
14:o:124:PHE:HE2	14:o:329:LEU:HD12	1.60	0.65
3:C:409:GLY:HA3	3:C:413:GLU:HG2	1.79	0.65
29:d:404:BCR:H14C	6:f:33:PHE:CE2	2.32	0.65
7:g:44:TYR:HD2	27:g:602:CLA:HMD2	1.61	0.65
7:y:179:LYS:HD3	27:y:612:CLA:HAA2	1.79	0.65
37:y:601:CHL:HBB1	37:y:601:CHL:HHC	1.78	0.65
1:A:246:TYR:CE2	1:A:248:ILE:HG22	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:192:THR:HG23	27:D:402:CLA:HBC2	1.78	0.65
18:S:210:THR:HG22	18:S:233:VAL:HG11	1.79	0.65
2:b:254:GLY:HA3	32:h:102:DGD:HB61	1.78	0.65
37:Y:601:CHL:HHC	37:Y:601:CHL:HBB1	1.78	0.64
17:r:127:VAL:O	17:r:131:GLU:HG2	1.97	0.64
18:s:210:THR:HG22	18:s:233:VAL:HG11	1.79	0.64
2:B:227:LYS:O	2:B:230:ARG:NH1	2.29	0.64
3:C:264:LEU:HD11	29:C:515:BCR:H322	1.79	0.64
1:a:57:PRO:O	14:o:206:ARG:NH1	2.25	0.64
29:D:404:BCR:H14C	6:F:33:PHE:CE2	2.32	0.64
18:S:234:ILE:HG13	23:Z:60:LEU:HD21	1.77	0.64
1:a:323:ARG:NH1	15:p:53:PHE:O	2.31	0.64
3:c:264:LEU:HD11	29:c:515:BCR:H322	1.79	0.64
7:g:63:GLU:HA	7:g:155:LEU:HD21	1.79	0.64
1:A:323:ARG:NH1	15:P:53:PHE:O	2.31	0.64
6:F:24:HIS:NE2	36:F:101:HEM:NA	2.45	0.64
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.78	0.64
2:b:469:HIS:HE1	27:b:612:CLA:NA	1.96	0.64
27:B:604:CLA:H192	27:B:610:CLA:H91	1.78	0.64
3:C:38:GLY:HA3	27:C:511:CLA:HMD2	1.78	0.64
3:C:464:GLU:OE2	4:D:248:THR:OG1	2.14	0.64
14:O:310:ASP:O	14:O:313:ALA:N	2.25	0.64
4:d:18:MET:HE1	22:x:106:VAL:HA	1.78	0.64
18:S:153:ARG:HB2	37:S:608:CHL:CHD	2.28	0.64
1:a:61:ASP:HB2	1:a:63:ILE:HG12	1.78	0.64
5:e:19:TYR:O	5:e:23:HIS:ND1	2.24	0.64
14:o:173:GLU:N	14:o:190:ASP:O	2.28	0.64
1:a:24:THR:O	4:d:255:GLN:NE2	2.28	0.64
16:q:40:LEU:HD13	16:q:41:GLN:HG3	1.79	0.64
18:s:46:PRO:HB2	18:s:49:LEU:HB2	1.77	0.64
1:A:246:TYR:OH	33:D:401:BCT:O2	2.16	0.64
7:G:44:TYR:HD2	27:G:602:CLA:HMD2	1.61	0.64
15:p:146:VAL:HG12	15:p:180:THR:HG21	1.80	0.64
2:B:383:PHE:O	14:O:250:GLY:N	2.31	0.64
2:B:469:HIS:HE1	27:B:612:CLA:NA	1.96	0.64
16:Q:40:LEU:HD13	16:Q:41:GLN:HG3	1.79	0.64
18:S:78:GLU:OE2	18:S:194:ARG:NE	2.30	0.64
7:Y:179:LYS:HD3	27:Y:612:CLA:HAA2	1.79	0.64
27:B:603:CLA:H171	32:H:102:DGD:HAF2	1.80	0.63
18:S:53:VAL:HG21	18:S:71:PHE:HE2	1.63	0.63
27:b:603:CLA:H171	32:h:102:DGD:HAF2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:139:ARG:NH2	4:d:141:TYR:OH	2.30	0.63
18:s:31:ARG:NE	18:s:56:ASP:OD2	2.31	0.63
18:s:127:PHE:HB3	18:s:129:LYS:H	1.61	0.63
37:y:608:CHL:HHC	37:y:608:CHL:HBB1	1.80	0.63
2:B:75:TRP:CD1	2:B:92:SER:HG	2.16	0.63
3:c:333:GLY:H	15:p:101:GLY:HA2	1.63	0.63
1:A:61:ASP:HB2	1:A:63:ILE:HG12	1.78	0.63
35:G:2630:LHG:H102	35:G:2630:LHG:H282	1.80	0.63
17:R:127:VAL:O	17:R:131:GLU:HG2	1.97	0.63
2:b:383:PHE:O	14:o:250:GLY:N	2.31	0.63
2:b:392:VAL:HG13	2:b:397:VAL:HB	1.81	0.63
7:G:63:GLU:HA	7:G:155:LEU:HD21	1.79	0.63
18:S:31:ARG:NE	18:S:56:ASP:OD2	2.31	0.63
4:d:141:TYR:OH	35:d:408:LHG:O4	2.10	0.63
14:o:144:LYS:HA	14:o:156:PHE:HA	1.81	0.63
18:s:157:GLY:HA2	18:s:158:LEU:HB3	1.80	0.63
14:O:235:ARG:HB2	14:O:311:LEU:HD13	1.81	0.63
16:Q:138:VAL:O	16:Q:142:ASN:ND2	2.27	0.63
3:c:86:LEU:HD13	3:c:89:LEU:HD12	1.80	0.63
3:c:409:GLY:HA3	3:c:413:GLU:HG2	1.79	0.63
14:o:291:LYS:O	14:o:295:GLY:N	2.30	0.63
15:p:48:ARG:HH12	15:p:50:GLU:HB3	1.64	0.63
18:s:78:GLU:OE2	18:s:194:ARG:NE	2.30	0.63
7:N:163:PRO:HD2	38:N:1620:LUT:H23	1.81	0.63
3:c:459:ILE:HG22	3:c:461:ARG:H	1.62	0.63
18:s:53:VAL:HG21	18:s:71:PHE:HE2	1.63	0.63
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.17	0.63
14:O:124:PHE:CE2	14:O:329:LEU:HD12	2.34	0.63
14:O:149:SER:HB3	14:O:154:PRO:HG3	1.81	0.63
31:d:411:LMG:O4	31:d:411:LMG:O5	2.16	0.63
7:n:63:GLU:HA	7:n:155:LEU:HD21	1.81	0.63
7:y:52:SER:OG	7:y:61:ASN:ND2	2.26	0.63
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.34	0.63
14:O:146:GLU:HG2	14:O:317:LYS:HE3	1.81	0.63
15:P:146:VAL:HG12	15:P:180:THR:HG21	1.80	0.62
18:S:157:GLY:HA2	18:S:158:LEU:HB3	1.81	0.62
3:c:387:TRP:HA	3:c:390:ARG:HG3	1.81	0.62
18:s:153:ARG:HB2	37:s:608:CHL:CHD	2.28	0.62
3:C:387:TRP:HA	3:C:390:ARG:HG3	1.81	0.62
4:D:57:SER:OG	4:D:65:SER:OG	2.08	0.62
7:Y:99:LYS:HA	37:Y:607:CHL:HED2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:217:VAL:O	7:Y:220:ASN:ND2	2.32	0.62
37:Y:608:CHL:HHC	37:Y:608:CHL:HBB1	1.80	0.62
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.34	0.62
37:s:601:CHL:HHC	37:s:601:CHL:HBB1	1.81	0.62
27:C:503:CLA:HMA1	31:Z:101:LMG:H191	1.81	0.62
15:P:48:ARG:HH12	15:P:50:GLU:HB3	1.64	0.62
1:a:136:ARG:NH1	9:i:27:ASP:OD1	2.29	0.62
7:g:211:ASP:O	7:g:219:ASN:ND2	2.27	0.62
14:o:146:GLU:HG2	14:o:317:LYS:HE3	1.81	0.62
14:o:211:PHE:HA	14:o:305:GLN:HE22	1.64	0.62
7:N:135:MET:HA	7:N:138:VAL:HG22	1.80	0.62
7:g:193:GLY:O	7:g:197:GLN:HB2	2.00	0.62
7:n:118:LEU:HD23	37:n:605:CHL:HED2	1.81	0.62
18:s:83:ARG:NH2	18:s:189:GLU:OE2	2.32	0.62
14:O:211:PHE:HA	14:O:305:GLN:HE22	1.64	0.62
2:B:233:ASN:O	2:B:236:THR:HG22	2.00	0.62
2:B:347:ARG:NH1	2:B:400:GLU:OE1	2.32	0.62
3:C:333:GLY:H	15:P:101:GLY:HA2	1.63	0.62
17:R:208:PHE:HA	17:R:211:PHE:CD2	2.30	0.62
37:R:606:CHL:HMB3	27:R:609:CLA:HBC2	1.81	0.62
18:S:60:ASP:OD1	38:S:1621:LUT:O23	2.18	0.62
37:S:601:CHL:HBB1	37:S:601:CHL:HHC	1.82	0.62
1:A:136:ARG:NH1	9:I:27:ASP:OD1	2.29	0.62
7:N:118:LEU:HD23	37:N:605:CHL:HED2	1.81	0.62
14:O:144:LYS:HA	14:O:156:PHE:HA	1.80	0.62
2:b:433:ASP:OD2	2:b:436:THR:OG1	2.17	0.62
7:y:99:LYS:HA	37:y:607:CHL:HED2	1.81	0.62
7:N:21:ARG:NH2	7:N:36:LEU:O	2.32	0.62
14:o:149:SER:HB3	14:o:154:PRO:HG3	1.81	0.62
3:C:86:LEU:HD13	3:C:89:LEU:HD12	1.80	0.62
35:g:2630:LHG:H282	35:g:2630:LHG:H102	1.80	0.62
14:o:124:PHE:CE2	14:o:329:LEU:HD12	2.34	0.62
5:E:8:ARG:NH2	5:E:12:ASP:O	2.33	0.62
7:N:63:GLU:HA	7:N:155:LEU:HD21	1.81	0.62
37:N:608:CHL:H12	38:N:1620:LUT:H383	1.82	0.62
5:e:8:ARG:NH2	5:e:12:ASP:O	2.33	0.62
1:A:100:ALA:HB2	21:W:88:ARG:HD3	1.82	0.61
2:b:347:ARG:NH1	2:b:400:GLU:OE1	2.32	0.61
7:n:135:MET:HA	7:n:138:VAL:HG22	1.80	0.61
7:y:217:VAL:O	7:y:220:ASN:ND2	2.32	0.61
1:A:24:THR:O	4:D:255:GLN:NE2	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:21:ARG:NH2	7:n:36:LEU:O	2.32	0.61
7:n:182:LYS:HZ1	35:n:2630:LHG:P	2.24	0.61
7:y:94:GLU:N	7:y:103:GLN:HE21	1.97	0.61
2:B:392:VAL:HG13	2:B:397:VAL:HB	1.81	0.61
7:N:212:HIS:HB2	27:N:613:CLA:HAA2	1.83	0.61
7:Y:94:GLU:N	7:Y:103:GLN:HE21	1.97	0.61
37:r:606:CHL:HMB3	27:r:609:CLA:HBC2	1.81	0.61
1:a:77:ILE:HD11	19:t:6:TYR:HB3	1.83	0.61
1:a:220:THR:HA	1:a:223:LEU:HD13	1.82	0.61
34:d:405:PL9:H122	35:d:409:LHG:HC92	1.82	0.61
7:n:163:PRO:HD2	38:n:1620:LUT:H23	1.81	0.61
37:n:608:CHL:H12	38:n:1620:LUT:H383	1.82	0.61
7:y:182:LYS:NZ	27:y:611:CLA:O1D	2.27	0.61
29:c:516:BCR:HC7	23:z:20:LEU:HD11	1.82	0.61
1:a:100:ALA:HB2	21:w:88:ARG:HD3	1.82	0.61
32:c:520:DGD:HAT1	4:d:74:LEU:HD22	1.82	0.61
7:n:212:HIS:HB2	27:n:613:CLA:HAA2	1.83	0.61
17:r:195:LEU:HD21	17:r:199:LYS:HE3	1.83	0.61
1:A:77:ILE:HD11	19:T:6:TYR:HB3	1.83	0.61
31:C:521:LMG:H311	31:C:521:LMG:H212	1.83	0.61
14:o:310:ASP:O	14:o:313:ALA:N	2.25	0.61
1:A:140:ARG:HH21	1:A:142:TRP:HZ3	1.49	0.61
14:O:129:TYR:HB2	14:O:176:PHE:HB3	1.83	0.61
2:b:233:ASN:O	2:b:236:THR:HG22	2.00	0.61
14:o:134:PHE:HB3	14:o:172:ILE:HB	1.83	0.61
18:s:60:ASP:OD1	38:s:1621:LUT:O23	2.18	0.61
32:C:520:DGD:HAT1	4:D:74:LEU:HD22	1.82	0.61
13:M:31:SER:OG	13:m:31:SER:OG	2.08	0.61
17:R:195:LEU:HD21	17:R:199:LYS:HE3	1.83	0.61
2:B:125:ASP:OD2	2:B:128:THR:N	2.34	0.61
3:C:209:ILE:HG23	29:C:515:BCR:H403	1.83	0.61
3:C:319:VAL:HG22	3:C:384:ILE:HD13	1.83	0.61
29:C:516:BCR:HC7	23:Z:20:LEU:HD11	1.82	0.61
31:c:521:LMG:H311	31:c:521:LMG:H212	1.83	0.61
14:o:235:ARG:HB2	14:o:311:LEU:HD13	1.81	0.61
17:r:181:LEU:HD12	38:r:620:LUT:H222	1.83	0.61
18:s:123:THR:O	18:s:130:ASN:ND2	2.34	0.61
37:G:608:CHL:H12	38:G:1620:LUT:H383	1.84	0.60
27:G:610:CLA:H2	38:G:1620:LUT:H26	1.83	0.60
7:N:180:GLU:HB2	27:N:610:CLA:C1B	2.31	0.60
14:O:175:PRO:HG2	14:O:187:GLU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:83:ARG:NH2	18:S:189:GLU:OE2	2.32	0.60
1:a:302:PHE:HE2	4:d:74:LEU:HD12	1.66	0.60
27:c:503:CLA:HMA1	31:z:101:LMG:H191	1.81	0.60
27:n:614:CLA:O1A	27:n:614:CLA:H3A	2.01	0.60
14:o:175:PRO:HG2	14:o:187:GLU:HB2	1.82	0.60
15:p:41:GLU:HB3	15:p:45:GLN:HE22	1.66	0.60
14:O:291:LYS:O	14:O:295:GLY:N	2.30	0.60
1:A:302:PHE:HE2	4:D:74:LEU:HD12	1.66	0.60
34:D:405:PL9:H122	35:D:409:LHG:HC92	1.82	0.60
7:G:193:GLY:O	7:G:197:GLN:HB2	2.00	0.60
7:N:182:LYS:HZ1	35:N:2630:LHG:P	2.23	0.60
14:O:131:ALA:HB2	14:O:186:PHE:HE1	1.67	0.60
27:R:611:CLA:HBC3	35:R:2630:LHG:HC62	1.83	0.60
2:b:311:PHE:O	2:b:317:ASN:ND2	2.35	0.60
3:C:346:THR:OG1	3:C:348:GLU:OE1	2.15	0.60
37:g:608:CHL:H12	38:g:1620:LUT:H383	1.84	0.60
14:o:131:ALA:HB2	14:o:186:PHE:HE1	1.67	0.60
15:P:41:GLU:HB3	15:P:45:GLN:HE22	1.66	0.60
3:c:346:THR:OG1	3:c:348:GLU:OE1	2.15	0.60
23:z:16:SER:HB2	23:z:47:TRP:HE1	1.67	0.60
27:N:614:CLA:O1A	27:N:614:CLA:H3A	2.01	0.60
14:O:143:VAL:HB	14:O:201:LEU:HD21	1.84	0.60
18:S:78:GLU:HB2	27:S:602:CLA:C1B	2.32	0.60
27:b:613:CLA:H151	27:b:614:CLA:HBB2	1.84	0.60
14:O:234:TYR:H	14:O:308:ASP:CG	2.09	0.60
27:g:610:CLA:H2	38:g:1620:LUT:H26	1.83	0.60
18:S:171:ASP:OD1	38:S:1620:LUT:O23	2.20	0.60
3:c:319:VAL:HG22	3:c:384:ILE:HD13	1.83	0.60
7:g:215:ASP:OD2	7:g:218:ASN:ND2	2.31	0.60
7:n:70:ARG:NE	7:n:180:GLU:OE2	2.33	0.60
2:B:311:PHE:O	2:B:317:ASN:ND2	2.35	0.60
3:c:132:HIS:CE1	27:c:513:CLA:NA	2.70	0.60
7:n:118:LEU:O	7:n:120:HIS:N	2.35	0.60
7:n:164:LEU:HD12	38:n:1620:LUT:H222	1.82	0.60
14:o:129:TYR:HB2	14:o:176:PHE:HB3	1.83	0.60
14:o:234:TYR:H	14:O:308:ASP:CG	2.09	0.60
18:s:78:GLU:HB2	27:s:602:CLA:C1B	2.32	0.60
1:A:220:THR:HA	1:A:223:LEU:HD13	1.82	0.60
2:B:340:TRP:HA	2:B:430:PHE:HD1	1.67	0.60
4:d:55:VAL:HG21	4:d:110:LEU:HD12	1.84	0.60
14:o:143:VAL:HB	14:O:201:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:HIS:CE1	27:B:610:CLA:NA	2.70	0.59
7:N:164:LEU:HD12	38:N:1620:LUT:H222	1.82	0.59
4:d:72:ASN:HA	31:d:411:LMG:HC1	1.83	0.59
7:n:180:GLU:HB2	27:n:610:CLA:C1B	2.31	0.59
3:C:223:TRP:CG	3:C:224:ILE:H	2.21	0.59
32:C:519:DGD:HA41	10:J:29:PHE:HD2	1.67	0.59
14:O:134:PHE:HB3	14:O:172:ILE:HB	1.83	0.59
1:a:246:TYR:OH	33:d:401:BCT:O2	2.16	0.59
27:a:407:CLA:HMB2	27:d:402:CLA:H102	1.85	0.59
2:b:75:TRP:CD1	2:b:92:SER:HG	2.20	0.59
3:C:377:LEU:HD11	3:C:381:LYS:HE3	1.84	0.59
31:D:411:LMG:O4	31:D:411:LMG:O5	2.16	0.59
7:G:24:TYR:CG	7:G:46:TRP:HB2	2.37	0.59
7:N:70:ARG:NE	7:N:180:GLU:OE2	2.34	0.59
16:Q:33:TYR:HB3	16:Q:35:LYS:HG2	1.84	0.59
17:R:87:PHE:HA	17:R:92:PHE:CE2	2.38	0.59
2:b:15:ASP:OD2	12:l:5:ASN:ND2	2.35	0.59
2:b:340:TRP:HA	2:b:430:PHE:HD1	1.67	0.59
3:c:223:TRP:CG	3:c:224:ILE:H	2.21	0.59
7:g:24:TYR:CG	7:g:46:TRP:HB2	2.37	0.59
7:n:126:ALA:HB3	37:n:605:CHL:HMC	1.85	0.59
7:N:118:LEU:O	7:N:120:HIS:N	2.35	0.59
17:R:140:LEU:HD12	37:R:606:CHL:HMD3	1.85	0.59
1:a:106:LEU:HD11	29:a:411:BCR:H402	1.84	0.59
16:q:33:TYR:HB3	16:q:35:LYS:HG2	1.84	0.59
18:s:171:ASP:OD1	38:s:1620:LUT:O23	2.20	0.59
4:D:72:ASN:HA	31:D:411:LMG:HC1	1.83	0.59
2:b:125:ASP:OD2	2:b:128:THR:N	2.34	0.59
3:c:107:ASP:OD2	31:z:101:LMG:O2	2.20	0.59
7:y:24:TYR:CD1	7:y:46:TRP:HB2	2.37	0.59
7:G:211:ASP:O	7:G:219:ASN:ND2	2.27	0.59
1:a:305:SER:HA	10:j:39:SER:HB3	1.85	0.59
27:c:502:CLA:H12	27:c:503:CLA:H42	1.85	0.59
16:q:43:LEU:HD22	16:q:45:PRO:HD3	1.84	0.59
27:D:403:CLA:H152	22:X:91:ILE:HG22	1.85	0.59
7:N:126:ALA:HB3	37:N:605:CHL:HMC	1.85	0.59
16:Q:43:LEU:HD22	16:Q:45:PRO:HD3	1.84	0.59
17:R:181:LEU:HD12	38:R:620:LUT:H222	1.83	0.59
2:b:357:ARG:NH1	2:b:358:ARG:O	2.36	0.59
3:c:377:LEU:HD11	3:c:381:LYS:HE3	1.84	0.59
32:c:518:DGD:O5E	32:c:518:DGD:O4E	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:350:ASN:OD1	4:d:351:ALA:N	2.36	0.59
7:y:63:GLU:HA	7:y:155:LEU:HD21	1.85	0.59
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.85	0.59
2:B:394:GLN:HE21	15:P:90:LYS:HB2	1.68	0.59
27:C:502:CLA:H12	27:C:503:CLA:H42	1.85	0.59
4:D:350:ASN:OD1	4:D:351:ALA:N	2.36	0.59
3:c:209:ILE:HG23	29:c:515:BCR:H403	1.83	0.59
1:a:140:ARG:HH21	1:a:142:TRP:HZ3	1.49	0.59
3:C:216:SER:HB3	3:C:221:GLU:OE1	2.02	0.59
16:Q:76:ASN:OD1	16:Q:77:ASP:N	2.36	0.59
2:b:394:GLN:HE21	15:p:90:LYS:HB2	1.68	0.59
7:g:24:TYR:CD1	7:g:46:TRP:HB2	2.37	0.59
14:o:138:PRO:HA	14:o:323:GLY:HA3	1.85	0.59
16:q:76:ASN:OD1	16:q:77:ASP:N	2.36	0.59
27:r:611:CLA:HBC3	35:r:2630:LHG:HC62	1.83	0.59
4:D:19:ASP:OD2	4:D:23:ARG:NH2	2.26	0.58
7:Y:24:TYR:CD1	7:Y:46:TRP:HB2	2.37	0.58
7:Y:63:GLU:HA	7:Y:155:LEU:HD21	1.85	0.58
1:a:131:TRP:CZ3	27:c:505:CLA:HAA2	2.38	0.58
2:b:46:ASP:HB3	2:b:58:GLN:HE22	1.68	0.58
7:y:182:LYS:HZ3	27:y:611:CLA:CGD	2.14	0.58
4:D:55:VAL:HG21	4:D:110:LEU:HD12	1.84	0.58
18:S:123:THR:O	18:S:130:ASN:ND2	2.34	0.58
1:A:131:TRP:CZ3	27:C:505:CLA:HAA2	2.38	0.58
27:B:613:CLA:H151	27:B:614:CLA:HBB2	1.84	0.58
7:G:24:TYR:CD1	7:G:46:TRP:HB2	2.37	0.58
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.85	0.58
27:b:604:CLA:H143	27:b:609:CLA:HAC1	1.85	0.58
32:c:519:DGD:HA41	10:j:29:PHE:HD2	1.67	0.58
14:o:238:SER:HB2	15:p:137:ASP:H	1.68	0.58
15:p:35:ASN:N	15:p:50:GLU:O	2.36	0.58
17:r:87:PHE:HA	17:r:92:PHE:CE2	2.38	0.58
1:A:106:LEU:HD11	29:A:411:BCR:H402	1.84	0.58
15:P:35:ASN:N	15:P:50:GLU:O	2.36	0.58
27:R:601:CLA:HBC3	27:R:601:CLA:HHD	1.85	0.58
2:b:216:HIS:CE1	27:b:610:CLA:NA	2.70	0.58
3:c:216:SER:HB3	3:c:221:GLU:OE1	2.02	0.58
17:r:87:PHE:HA	17:r:92:PHE:HE2	1.69	0.58
27:r:601:CLA:HBC3	27:r:601:CLA:HHD	1.85	0.58
1:A:207:GLY:HA3	1:A:278:TRP:NE1	2.19	0.58
2:B:388:SER:O	2:B:394:GLN:NE2	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:116:VAL:HG11	29:c:514:BCR:HC32	1.86	0.58
14:O:145:ALA:HB2	14:O:157:GLN:HE22	1.69	0.58
18:S:142:GLU:HG2	37:S:606:CHL:CHB	2.34	0.58
7:g:121:ALA:HA	37:g:605:CHL:C1C	2.34	0.58
1:A:302:PHE:CE2	4:D:74:LEU:HD12	2.39	0.58
2:B:15:ASP:OD2	12:L:5:ASN:ND2	2.35	0.58
2:B:46:ASP:HB3	2:B:58:GLN:HE22	1.68	0.58
3:C:48:LYS:HE2	3:C:138:GLU:HG2	1.85	0.58
3:C:107:ASP:OD2	31:Z:101:LMG:O2	2.20	0.58
14:O:138:PRO:HA	14:O:323:GLY:HA3	1.85	0.58
17:R:162:ARG:HA	37:R:608:CHL:HBC2	1.85	0.58
23:Z:16:SER:HB2	23:Z:47:TRP:HE1	1.67	0.58
1:a:302:PHE:CE2	4:d:74:LEU:HD12	2.39	0.58
14:o:145:ALA:HB2	14:o:157:GLN:HE22	1.69	0.58
1:A:27:ARG:NH1	1:A:27:ARG:O	2.37	0.58
1:A:135:PHE:CZ	9:I:31:ASN:HB3	2.39	0.58
2:b:46:ASP:HB3	2:b:58:GLN:NE2	2.18	0.58
2:b:201:HIS:HE2	27:b:604:CLA:C2B	2.16	0.58
2:b:311:PHE:HA	2:b:430:PHE:CZ	2.39	0.58
27:c:511:CLA:HBA1	29:c:517:BCR:H271	1.86	0.58
7:g:163:PRO:HD2	38:g:1620:LUT:H23	1.85	0.58
3:C:132:HIS:CE1	27:C:513:CLA:NA	2.70	0.58
27:d:403:CLA:H152	22:x:91:ILE:HG22	1.85	0.58
17:r:208:PHE:CZ	39:r:622:XAT:H10	2.39	0.58
7:y:131:GLN:OE1	37:y:607:CHL:HMC	2.04	0.58
2:B:201:HIS:HE2	27:B:604:CLA:C2B	2.16	0.58
4:D:149:PRO:HB3	27:D:402:CLA:H41	1.86	0.58
37:N:607:CHL:HHC	37:N:607:CHL:HBB1	1.85	0.58
14:O:238:SER:HB2	15:P:137:ASP:H	1.68	0.58
16:Q:80:LEU:HD12	16:Q:81:ARG:HG3	1.86	0.58
17:R:208:PHE:CZ	39:R:622:XAT:H10	2.39	0.58
17:r:140:LEU:HD12	37:r:606:CHL:HMD3	1.85	0.58
27:A:407:CLA:HMB2	27:D:402:CLA:H102	1.85	0.57
5:E:27:ILE:HG12	36:F:101:HEM:HMC3	1.86	0.57
7:G:121:ALA:HA	37:G:605:CHL:C1C	2.34	0.57
37:R:606:CHL:HBA2	40:R:623:NEX:H403	1.86	0.57
1:a:135:PHE:CZ	9:i:31:ASN:HB3	2.39	0.57
7:y:139:GLU:HG3	37:y:609:CHL:C4B	2.34	0.57
1:A:305:SER:HA	10:J:39:SER:HB3	1.85	0.57
2:B:46:ASP:HB3	2:B:58:GLN:NE2	2.18	0.57
2:B:357:ARG:NH1	2:B:358:ARG:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:40:LEU:HB2	16:Q:41:GLN:HG3	1.86	0.57
1:a:207:GLY:HA3	1:a:278:TRP:NE1	2.19	0.57
1:a:267:ASN:OD1	1:a:269:ARG:N	2.37	0.57
32:h:102:DGD:O4D	32:h:102:DGD:O5D	2.20	0.57
7:n:24:TYR:CD1	7:n:46:TRP:HB2	2.39	0.57
14:o:164:ARG:HA	21:w:88:ARG:NH2	2.19	0.57
1:A:63:ILE:HB	3:C:335:THR:HG21	1.86	0.57
2:B:22:VAL:HG13	27:B:615:CLA:HMB2	1.86	0.57
27:C:511:CLA:HBA1	29:C:517:BCR:H271	1.86	0.57
4:D:270:PHE:HZ	34:D:405:PL9:H203	1.69	0.57
7:G:180:GLU:HB2	27:G:610:CLA:C1B	2.35	0.57
1:a:63:ILE:HB	3:c:335:THR:HG21	1.86	0.57
5:e:27:ILE:HG12	36:f:101:HEM:HMC3	1.86	0.57
1:A:93:PHE:HZ	27:A:410:CLA:HAA1	1.69	0.57
2:B:388:SER:C	2:B:394:GLN:HE22	2.11	0.57
7:G:92:PHE:HE1	7:G:113:LEU:HA	1.69	0.57
7:G:163:PRO:HD2	38:G:1620:LUT:H23	1.85	0.57
7:g:119:VAL:N	37:g:605:CHL:O1D	2.37	0.57
27:n:610:CLA:HBB1	27:n:610:CLA:H51	1.85	0.57
15:p:19:MET:HE2	15:p:32:SER:HA	1.87	0.57
27:A:410:CLA:H13	27:C:506:CLA:H152	1.86	0.57
2:B:155:ALA:O	2:B:159:THR:OG1	2.22	0.57
27:B:604:CLA:H143	27:B:609:CLA:HAC1	1.85	0.57
27:B:605:CLA:HBD	27:B:605:CLA:HBA1	1.87	0.57
3:C:71:GLU:O	3:C:75:PHE:N	2.38	0.57
7:Y:131:GLN:OE1	37:Y:607:CHL:HMC	2.04	0.57
1:a:93:PHE:HZ	27:a:410:CLA:HAA1	1.69	0.57
37:n:607:CHL:HHC	37:n:607:CHL:HBB1	1.85	0.57
16:q:80:LEU:HD12	16:q:81:ARG:HG3	1.86	0.57
18:s:142:GLU:HG2	37:s:606:CHL:CHB	2.34	0.57
1:A:63:ILE:HA	3:C:337:LEU:HD13	1.86	0.57
7:N:24:TYR:CD1	7:N:46:TRP:HB2	2.39	0.57
17:R:101:ARG:NE	17:R:197:GLU:OE2	2.38	0.57
27:a:410:CLA:H13	27:c:506:CLA:H152	1.86	0.57
4:d:149:PRO:HB3	27:d:402:CLA:H41	1.86	0.57
7:y:118:LEU:O	7:y:120:HIS:N	2.38	0.57
1:A:267:ASN:OD1	1:A:269:ARG:N	2.37	0.57
2:B:332:ASN:ND2	31:B:622:LMG:O4	2.38	0.57
7:N:87:ARG:HH21	7:N:207:GLU:HA	1.70	0.57
27:y:613:CLA:H112	35:y:2630:LHG:H322	1.86	0.57
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:182:LYS:NZ	27:Y:611:CLA:O1D	2.27	0.57
2:b:155:ALA:O	2:b:159:THR:OG1	2.22	0.57
2:b:332:ASN:ND2	31:b:622:LMG:O4	2.38	0.57
3:c:48:LYS:HE2	3:c:138:GLU:HG2	1.85	0.57
17:R:210:GLY:O	17:R:214:GLN:HG2	2.05	0.57
2:b:282:GLN:HE22	20:u:24:ARG:HB2	1.70	0.57
2:b:422:ARG:NH2	14:o:252:ASP:OD1	2.38	0.57
17:r:162:ARG:HA	37:r:608:CHL:HBC2	1.85	0.57
29:C:516:BCR:H373	11:K:47:LEU:HB3	1.87	0.57
7:G:66:VAL:HB	7:G:155:LEU:HD22	1.87	0.57
27:N:610:CLA:HBB1	27:N:610:CLA:H51	1.85	0.57
19:T:10:LEU:O	19:T:13:THR:OG1	2.21	0.57
27:Y:602:CLA:HBA1	38:Y:1621:LUT:H382	1.87	0.57
27:b:605:CLA:HBD	27:b:605:CLA:HBA1	1.87	0.57
29:b:618:BCR:H282	30:b:621:SQD:H82	1.87	0.57
7:n:87:ARG:HH21	7:n:207:GLU:HA	1.70	0.57
14:o:310:ASP:O	14:o:312:GLY:N	2.38	0.57
7:G:119:VAL:N	37:G:605:CHL:O1D	2.37	0.56
1:a:341:LEU:HD11	15:p:169:PHE:HZ	1.69	0.56
7:g:162:ASP:OD1	38:g:1620:LUT:O23	2.23	0.56
7:g:180:GLU:HB2	27:g:610:CLA:C1B	2.35	0.56
17:r:101:ARG:NE	17:r:197:GLU:OE2	2.38	0.56
37:r:606:CHL:HBA2	40:r:623:NEX:H403	1.86	0.56
1:A:140:ARG:NH1	4:D:222:LEU:HD12	2.20	0.56
14:O:164:ARG:HA	21:W:88:ARG:NH2	2.19	0.56
17:R:47:GLN:HB3	17:R:66:ILE:HB	1.88	0.56
17:R:92:PHE:HB3	27:R:602:CLA:HHB	1.87	0.56
17:R:211:PHE:CZ	38:R:620:LUT:H8	2.40	0.56
3:c:71:GLU:O	3:c:75:PHE:N	2.38	0.56
37:n:601:CHL:HED3	35:n:2630:LHG:H142	1.87	0.56
39:n:1622:XAT:H22	7:y:225:ALA:HA	1.87	0.56
7:y:135:MET:HA	7:y:138:VAL:HG22	1.86	0.56
1:A:254:TYR:HE2	4:D:142:ASN:HD22	1.53	0.56
2:B:422:ARG:NH2	14:O:252:ASP:OD1	2.38	0.56
3:C:113:VAL:O	3:C:117:LEU:HG	2.05	0.56
3:C:116:VAL:HG11	29:C:514:BCR:HC32	1.86	0.56
3:C:437:LEU:HA	27:C:508:CLA:HMC2	1.87	0.56
9:I:28:PRO:HB3	21:W:135:LEU:HD12	1.87	0.56
18:S:123:THR:HG23	18:S:130:ASN:ND2	2.20	0.56
1:a:63:ILE:HA	3:c:337:LEU:HD13	1.86	0.56
1:a:140:ARG:NH1	4:d:222:LEU:HD12	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:112:ILE:HG21	29:b:620:BCR:H272	1.85	0.56
3:c:113:VAL:O	3:c:117:LEU:HG	2.05	0.56
3:c:151:TRP:HB2	21:w:137:LEU:HD23	1.87	0.56
7:g:66:VAL:HB	7:g:155:LEU:HD22	1.87	0.56
15:p:99:SER:HB2	15:p:108:VAL:H	1.71	0.56
14:O:310:ASP:O	14:O:312:GLY:N	2.38	0.56
16:Q:78:LEU:HD11	16:Q:115:ILE:HD11	1.87	0.56
40:S:1623:NEX:H192	40:S:1623:NEX:H183	1.87	0.56
7:Y:92:PHE:CE1	7:Y:113:LEU:HA	2.40	0.56
7:Y:135:MET:HA	7:Y:138:VAL:HG22	1.86	0.56
1:a:27:ARG:NH1	1:a:27:ARG:O	2.37	0.56
2:b:388:SER:C	2:b:394:GLN:HE22	2.10	0.56
3:c:437:LEU:HA	27:c:508:CLA:HMC2	1.88	0.56
4:d:270:PHE:HZ	34:d:405:PL9:H203	1.69	0.56
16:q:40:LEU:HB2	16:q:41:GLN:HG3	1.86	0.56
40:s:1623:NEX:H183	40:s:1623:NEX:H192	1.87	0.56
2:B:112:ILE:HG21	29:B:620:BCR:H272	1.85	0.56
29:B:618:BCR:H282	30:B:621:SQD:H82	1.87	0.56
15:P:19:MET:HE2	15:P:32:SER:HA	1.87	0.56
17:R:87:PHE:HA	17:R:92:PHE:HE2	1.69	0.56
18:S:32:ARG:NH1	35:S:2630:LHG:O1	2.39	0.56
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.87	0.56
18:s:78:GLU:OE1	27:s:602:CLA:C4A	2.51	0.56
7:G:52:SER:OG	7:G:61:ASN:ND2	2.36	0.56
7:Y:118:LEU:O	7:Y:120:HIS:N	2.38	0.56
1:a:85:THR:HA	1:a:109:GLY:HA3	1.87	0.56
17:r:96:GLU:HB2	27:r:602:CLA:C1B	2.36	0.56
1:A:85:THR:HA	1:A:109:GLY:HA3	1.87	0.56
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.87	0.56
27:A:407:CLA:HED1	4:D:175:VAL:HG22	1.88	0.56
2:B:282:GLN:HE22	20:U:24:ARG:HB2	1.69	0.56
7:Y:139:GLU:HG3	37:Y:609:CHL:C4B	2.34	0.56
27:Y:613:CLA:H112	35:Y:2630:LHG:H322	1.86	0.56
2:b:388:SER:O	2:b:394:GLN:NE2	2.27	0.56
7:n:188:MET:SD	27:n:602:CLA:HBB1	2.46	0.56
16:q:78:LEU:HD11	16:q:115:ILE:HD11	1.87	0.56
17:r:119:ILE:HD13	17:r:127:VAL:HG21	1.87	0.56
17:r:210:GLY:O	17:r:214:GLN:HG2	2.05	0.56
7:y:173:PHE:CE2	7:y:177:LYS:HE3	2.41	0.56
1:A:341:LEU:HD11	15:P:169:PHE:HZ	1.69	0.56
3:C:271:TYR:CE1	27:C:507:CLA:HAC2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:315:TYR:CE2	4:D:319:ILE:HD11	2.41	0.56
27:G:611:CLA:C1B	35:G:2630:LHG:O4	2.53	0.56
15:P:169:PHE:HB2	16:Q:28:ASP:HB3	1.88	0.56
17:R:96:GLU:HB2	27:R:602:CLA:C1B	2.36	0.56
37:Y:605:CHL:HHB	17:r:138:GLN:HE21	1.70	0.56
3:c:464:GLU:OE2	4:d:245:SER:OG	2.18	0.56
4:d:315:TYR:CE2	4:d:319:ILE:HD11	2.41	0.56
17:r:211:PHE:CZ	38:r:620:LUT:H8	2.40	0.56
18:s:122:ASN:HB2	18:s:132:PRO:HB2	1.87	0.56
18:s:202:ALA:O	18:s:206:GLN:HG2	2.06	0.56
7:y:92:PHE:CE1	7:y:113:LEU:HA	2.40	0.56
3:C:255:LYS:NZ	21:W:132:GLU:OE2	2.39	0.56
15:P:74:PHE:HB2	15:P:127:TYR:HE2	1.71	0.56
18:S:202:ALA:O	18:S:206:GLN:HG2	2.06	0.56
7:g:92:PHE:HE1	7:g:113:LEU:HA	1.69	0.56
9:i:28:PRO:HB3	21:w:135:LEU:HD12	1.87	0.56
7:n:173:PHE:CE2	7:n:177:LYS:HE3	2.41	0.56
39:N:1622:XAT:H22	7:Y:225:ALA:HA	1.87	0.56
16:Q:86:ARG:O	16:Q:90:LYS:HG2	2.06	0.56
27:a:407:CLA:HED1	4:d:175:VAL:HG22	1.88	0.56
2:b:204:ALA:O	2:b:207:THR:OG1	2.21	0.56
3:c:255:LYS:NZ	21:w:132:GLU:OE2	2.39	0.56
29:c:516:BCR:H373	11:k:47:LEU:HB3	1.87	0.56
18:s:123:THR:HG23	18:s:130:ASN:ND2	2.20	0.56
3:C:464:GLU:OE2	4:D:245:SER:OG	2.18	0.55
4:D:13:ASP:OD2	8:H:37:TRP:NE1	2.38	0.55
37:G:601:CHL:HED3	35:G:2630:LHG:H121	1.89	0.55
7:N:145:GLY:HA2	37:N:608:CHL:HAC1	1.88	0.55
17:R:138:GLN:HE21	37:y:605:CHL:HHB	1.70	0.55
37:g:601:CHL:HED3	35:g:2630:LHG:H121	1.88	0.55
15:p:169:PHE:HB2	16:q:28:ASP:HB3	1.88	0.55
17:r:159:GLU:OE1	27:r:609:CLA:NA	2.39	0.55
12:L:30:VAL:HG22	19:T:9:LEU:HB3	1.88	0.55
17:R:119:ILE:HD13	17:R:127:VAL:HG21	1.87	0.55
37:g:601:CHL:H122	35:g:2630:LHG:H212	1.88	0.55
17:r:92:PHE:HB3	27:r:602:CLA:HHB	1.87	0.55
18:s:32:ARG:NH1	35:s:2630:LHG:O1	2.39	0.55
27:y:602:CLA:HBA1	38:y:1621:LUT:H382	1.87	0.55
2:B:464:PHE:HD2	27:B:612:CLA:HAC2	1.71	0.55
35:D:409:LHG:H302	19:T:17:ILE:HG23	1.87	0.55
7:G:24:TYR:CE2	7:G:25:LEU:HG	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:G:611:CLA:C4B	35:G:2630:LHG:O4	2.53	0.55
7:Y:103:GLN:HE22	27:Y:604:CLA:HED3	1.71	0.55
1:a:254:TYR:HE2	4:d:142:ASN:HD22	1.53	0.55
3:c:141:GLU:OE2	3:c:149:TYR:N	2.39	0.55
3:c:271:TYR:CE1	27:c:507:CLA:HAC2	2.41	0.55
4:d:13:ASP:OD2	8:h:37:TRP:NE1	2.38	0.55
4:d:216:ALA:O	4:d:220:ASN:ND2	2.29	0.55
17:r:126:LYS:HB2	37:r:607:CHL:CGD	2.37	0.55
1:A:43:THR:HG23	29:A:411:BCR:H362	1.89	0.55
3:C:211:GLY:O	3:C:215:LYS:HG3	2.06	0.55
7:G:97:TRP:HE1	7:G:205:PRO:HD3	1.72	0.55
7:N:173:PHE:CE2	7:N:177:LYS:HE3	2.41	0.55
18:S:122:ASN:HB2	18:S:132:PRO:HB2	1.87	0.55
1:a:43:THR:HG23	29:a:411:BCR:H362	1.89	0.55
2:b:41:GLU:OE1	2:b:63:ILE:HG12	2.07	0.55
2:b:464:PHE:HD2	27:b:612:CLA:HAC2	1.71	0.55
14:o:159:THR:HG22	14:o:201:LEU:HD23	1.89	0.55
7:y:103:GLN:HE22	27:y:604:CLA:HED3	1.71	0.55
7:y:136:GLY:HA2	37:y:609:CHL:HAB	1.88	0.55
1:A:47:VAL:HG13	1:A:115:ILE:HG12	1.89	0.55
3:C:151:TRP:HB2	21:W:137:LEU:HD23	1.87	0.55
3:c:211:GLY:O	3:c:215:LYS:HG3	2.06	0.55
7:g:97:TRP:HE1	7:g:205:PRO:HD3	1.72	0.55
12:l:30:VAL:HG22	19:t:9:LEU:HB3	1.88	0.55
21:w:100:LEU:O	21:w:101:SER:OG	2.21	0.55
1:A:202:VAL:HG11	27:A:407:CLA:C3D	2.37	0.55
7:N:188:MET:SD	27:N:602:CLA:HBB1	2.45	0.55
7:Y:173:PHE:CE2	7:Y:177:LYS:HE3	2.41	0.55
1:a:47:VAL:HG11	1:a:114:LEU:HD22	1.88	0.55
27:c:503:CLA:H2	27:c:501:CLA:C2D	2.37	0.55
7:g:131:GLN:OE1	37:g:607:CHL:HMC	2.07	0.55
17:r:121:TRP:HE1	17:r:222:PRO:HG2	1.72	0.55
18:s:55:GLY:HA3	18:s:190:ILE:HD11	1.89	0.55
1:A:140:ARG:HH12	4:D:222:LEU:HD12	1.71	0.55
2:B:222:PRO:HG2	2:B:225:LEU:HD12	1.89	0.55
2:B:256:MET:O	2:B:448:ARG:NH1	2.39	0.55
3:C:141:GLU:OE2	3:C:149:TYR:N	2.39	0.55
9:I:13:ILE:HD13	21:W:109:LEU:HA	1.89	0.55
37:N:607:CHL:HBC2	7:Y:222:TRP:CH2	2.41	0.55
15:P:34:TRP:HA	15:P:51:ASP:HA	1.89	0.55
15:P:99:SER:HB2	15:P:108:VAL:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:121:TRP:HE1	17:R:222:PRO:HG2	1.71	0.55
17:R:126:LYS:HB2	37:R:607:CHL:CGD	2.37	0.55
4:d:188:PHE:CD1	4:d:326:ARG:HG2	2.42	0.55
35:d:409:LHG:H302	19:t:17:ILE:HG23	1.87	0.55
37:n:607:CHL:HBC2	7:y:222:TRP:CH2	2.41	0.55
17:r:47:GLN:HB3	17:r:66:ILE:HB	1.88	0.55
18:s:162:ASP:HB2	18:s:164:LEU:HD13	1.88	0.55
18:s:189:GLU:HB2	27:s:610:CLA:C1B	2.37	0.55
4:D:83:ASN:HD22	4:D:336:HIS:CD2	2.25	0.55
7:G:162:ASP:OD1	38:G:1620:LUT:O23	2.23	0.55
37:N:601:CHL:HED3	35:N:2630:LHG:H142	1.87	0.55
17:R:14:TRP:CD2	17:R:34:PHE:HD1	2.25	0.55
27:S:611:CLA:H3A	27:S:611:CLA:CGA	2.37	0.55
7:g:24:TYR:CE2	7:g:25:LEU:HG	2.42	0.55
7:g:94:GLU:O	7:g:103:GLN:NE2	2.40	0.55
27:g:611:CLA:C1B	35:g:2630:LHG:O4	2.52	0.55
15:p:74:PHE:HB2	15:p:127:TYR:HE2	1.71	0.55
7:y:180:GLU:OE1	27:y:610:CLA:C4A	2.54	0.55
29:C:516:BCR:H332	11:K:38:MET:HE1	1.88	0.55
5:E:26:THR:O	5:E:29:SER:OG	2.22	0.55
7:G:94:GLU:O	7:G:103:GLN:NE2	2.40	0.55
17:R:179:ASP:HA	38:R:620:LUT:H24	1.88	0.55
17:R:208:PHE:CD2	39:R:622:XAT:H12	2.42	0.55
3:c:29:GLU:HA	4:d:233:ARG:HH12	1.72	0.55
3:c:263:ALA:HB2	9:i:24:LEU:HD23	1.89	0.55
7:n:70:ARG:NH1	37:n:608:CHL:OBD	2.33	0.55
18:s:47:GLU:N	18:s:48:TYR:HB2	2.22	0.55
3:C:29:GLU:HA	4:D:233:ARG:HH12	1.72	0.55
27:C:503:CLA:H2	27:C:501:CLA:C2D	2.37	0.55
7:N:162:ASP:OD1	38:N:1620:LUT:O23	2.25	0.55
17:R:159:GLU:OE1	27:R:609:CLA:NA	2.39	0.55
37:S:606:CHL:HBA2	37:S:606:CHL:HBD	1.89	0.55
15:p:34:TRP:HA	15:p:51:ASP:HA	1.89	0.55
18:s:57:TYR:HD2	27:s:602:CLA:HMD1	1.72	0.55
27:B:609:CLA:H172	27:B:610:CLA:H192	1.89	0.54
29:C:516:BCR:H19C	11:K:51:VAL:HG21	1.89	0.54
18:S:172:PRO:HD2	38:S:1620:LUT:H23	1.89	0.54
18:S:206:GLN:NE2	38:S:1620:LUT:H42	2.22	0.54
1:a:202:VAL:HG11	27:a:407:CLA:C3D	2.37	0.54
10:j:9:PRO:HD2	10:j:12:ILE:HD12	1.89	0.54
16:q:86:ARG:O	16:q:90:LYS:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:188:PHE:CD1	4:D:326:ARG:HG2	2.42	0.54
7:G:131:GLN:OE1	37:G:607:CHL:HMC	2.07	0.54
17:R:127:VAL:HG23	17:R:128:GLU:HG3	1.90	0.54
17:R:143:SER:O	17:R:146:THR:OG1	2.24	0.54
18:S:47:GLU:N	18:S:48:TYR:HB2	2.22	0.54
18:S:154:ILE:HD11	27:S:609:CLA:HMA1	1.89	0.54
1:a:47:VAL:HG13	1:a:115:ILE:HG12	1.89	0.54
28:a:409:PHO:H3A	27:d:402:CLA:H121	1.89	0.54
2:b:30:VAL:HG11	27:b:613:CLA:H112	1.89	0.54
2:b:245:VAL:HG21	27:b:613:CLA:HED3	1.90	0.54
11:k:28:TYR:O	11:k:31:LEU:HG	2.08	0.54
17:r:214:GLN:HG3	38:r:620:LUT:H42	1.88	0.54
18:s:172:PRO:HD2	38:s:1620:LUT:H23	1.89	0.54
17:R:179:ASP:OD1	38:R:620:LUT:O23	2.23	0.54
17:R:214:GLN:HG3	38:R:620:LUT:H42	1.88	0.54
18:S:55:GLY:HA3	18:S:190:ILE:HD11	1.89	0.54
2:b:222:PRO:HG2	2:b:225:LEU:HD12	1.89	0.54
9:i:13:ILE:HD13	21:w:109:LEU:HA	1.89	0.54
7:y:104:ILE:HG21	7:y:124:ILE:HD13	1.88	0.54
3:C:362:ARG:HD2	14:O:101:LEU:HD21	1.89	0.54
11:K:28:TYR:O	11:K:31:LEU:HG	2.08	0.54
14:O:159:THR:HG22	14:O:201:LEU:HD23	1.89	0.54
17:R:195:LEU:O	17:R:198:ILE:HG22	2.07	0.54
18:S:57:TYR:HD2	27:S:602:CLA:HMD1	1.72	0.54
29:c:516:BCR:H332	11:k:38:MET:HE1	1.88	0.54
27:g:611:CLA:C4B	35:g:2630:LHG:O4	2.53	0.54
14:o:309:THR:HG22	14:o:316:PRO:HD3	1.90	0.54
17:r:179:ASP:HA	38:r:620:LUT:H24	1.88	0.54
7:y:70:ARG:NE	7:y:180:GLU:OE2	2.37	0.54
2:B:245:VAL:HG21	27:B:613:CLA:HED3	1.90	0.54
4:D:294:ARG:HG3	4:D:296:TYR:HB2	1.88	0.54
37:G:601:CHL:H122	35:G:2630:LHG:H212	1.89	0.54
13:M:31:SER:HB3	13:m:28:LYS:HG3	1.90	0.54
7:N:203:LYS:HB2	7:N:208:ASN:HD21	1.72	0.54
17:R:96:GLU:OE1	27:R:602:CLA:C4A	2.54	0.54
18:S:162:ASP:HB2	18:S:164:LEU:HD13	1.88	0.54
18:S:189:GLU:HB2	27:S:610:CLA:C1B	2.37	0.54
1:a:201:GLY:HA3	1:a:286:THR:HG23	1.89	0.54
2:b:366:PHE:HD2	2:b:425:GLN:HE21	1.55	0.54
3:c:345:PRO:HB3	14:o:164:ARG:NE	2.19	0.54
4:d:61:HIS:CD2	4:d:79:SER:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:52:SER:OG	7:g:61:ASN:ND2	2.36	0.54
17:r:127:VAL:HG23	17:r:128:GLU:HG3	1.90	0.54
18:s:206:GLN:NE2	38:s:1620:LUT:H42	2.22	0.54
1:A:196:PRO:HB3	1:A:199:MET:HE2	1.90	0.54
2:B:41:GLU:OE1	2:B:63:ILE:HG12	2.07	0.54
2:B:366:PHE:HD2	2:B:425:GLN:HE21	1.55	0.54
4:D:335:PRO:HB2	5:E:65:LEU:HD22	1.89	0.54
7:G:215:ASP:OD2	7:G:218:ASN:ND2	2.31	0.54
14:O:299:GLY:HA3	14:O:325:TRP:CE2	2.43	0.54
14:O:309:THR:HG22	14:O:316:PRO:HD3	1.90	0.54
17:R:214:GLN:OE1	27:R:613:CLA:C4D	2.38	0.54
7:Y:104:ILE:HG21	7:Y:124:ILE:HD13	1.88	0.54
7:Y:182:LYS:HZ3	27:Y:611:CLA:CGD	2.15	0.54
4:d:83:ASN:HD22	4:d:336:HIS:CD2	2.25	0.54
14:o:128:LYS:HG2	14:o:177:GLU:HG2	1.90	0.54
17:r:163:ASN:HD22	27:r:616:CLA:HBC3	1.73	0.54
1:A:47:VAL:HG11	1:A:114:LEU:HD22	1.88	0.54
7:G:83:GLU:HB3	7:G:206:LEU:HD12	1.89	0.54
1:a:322:ASN:HD21	15:p:53:PHE:HE1	1.56	0.54
2:b:256:MET:O	2:b:448:ARG:NH1	2.39	0.54
3:c:450:ALA:O	3:c:454:GLY:N	2.40	0.54
7:n:145:GLY:HA2	37:n:608:CHL:HAC1	1.88	0.54
14:o:299:GLY:HA3	14:o:325:TRP:CE2	2.43	0.54
1:A:312:ARG:HA	15:P:33:LYS:HA	1.89	0.54
2:B:64:PRO:HA	2:B:67:THR:HG22	1.90	0.54
3:C:152:LYS:HZ2	21:W:137:LEU:HD11	1.73	0.54
3:C:368:PRO:HG3	16:Q:79:ARG:HB2	1.90	0.54
13:M:28:LYS:HG3	13:m:31:SER:HB3	1.90	0.54
7:Y:136:GLY:HA2	37:Y:609:CHL:HAB	1.88	0.54
27:b:610:CLA:H2	8:h:47:MET:HE1	1.90	0.54
3:c:407:VAL:HG13	3:c:415:ASN:HA	1.90	0.54
27:c:506:CLA:H12	29:c:515:BCR:H323	1.90	0.54
4:d:294:ARG:HG3	4:d:296:TYR:HB2	1.88	0.54
17:r:208:PHE:CD2	39:r:622:XAT:H12	2.42	0.54
2:B:30:VAL:HG12	27:B:606:CLA:HHD	1.90	0.54
3:C:450:ALA:O	3:C:454:GLY:N	2.40	0.54
27:C:506:CLA:H12	29:C:515:BCR:H323	1.90	0.54
4:D:61:HIS:CD2	4:D:79:SER:HB3	2.43	0.54
7:N:71:TRP:CE2	37:N:608:CHL:HED2	2.43	0.54
27:N:610:CLA:CBB	38:N:1620:LUT:H32	2.38	0.54
21:W:100:LEU:O	21:W:101:SER:OG	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:140:ARG:HH12	4:d:222:LEU:HD12	1.71	0.54
31:a:413:LMG:HC61	21:w:99:GLY:HA2	1.90	0.54
3:c:286:ALA:HB2	27:c:502:CLA:HMD2	1.89	0.54
7:g:188:MET:SD	27:g:602:CLA:HMC3	2.48	0.54
37:s:606:CHL:HBD	37:s:606:CHL:HBA2	1.89	0.54
2:B:204:ALA:O	2:B:207:THR:OG1	2.21	0.54
27:B:610:CLA:H2	8:H:47:MET:HE1	1.90	0.54
27:C:511:CLA:H141	23:Z:20:LEU:HD22	1.89	0.54
7:G:188:MET:SD	27:G:602:CLA:HMC3	2.48	0.54
8:H:50:PHE:HB2	29:H:101:BCR:C10	2.38	0.54
14:O:128:LYS:HG2	14:O:177:GLU:HG2	1.89	0.54
18:S:78:GLU:OE1	27:S:602:CLA:C4A	2.50	0.54
7:Y:180:GLU:OE1	27:Y:610:CLA:C4A	2.54	0.54
27:c:511:CLA:H141	23:z:20:LEU:HD22	1.89	0.54
29:c:516:BCR:H19C	11:k:51:VAL:HG21	1.89	0.54
7:g:83:GLU:HB3	7:g:206:LEU:HD12	1.89	0.54
27:n:610:CLA:CBB	38:n:1620:LUT:H32	2.38	0.54
17:r:14:TRP:CD2	17:r:34:PHE:HD1	2.25	0.54
17:r:31:ASP:HA	27:r:602:CLA:HED2	1.89	0.54
18:s:154:ILE:HD11	27:s:609:CLA:HMA1	1.89	0.54
27:s:611:CLA:H3A	27:s:611:CLA:CGA	2.37	0.54
19:t:10:LEU:O	19:t:13:THR:OG1	2.21	0.54
31:A:413:LMG:HC61	21:W:99:GLY:HA2	1.90	0.53
7:G:173:PHE:CE2	7:G:177:LYS:HE3	2.43	0.53
17:R:104:MET:HE3	27:R:610:CLA:HMC2	1.90	0.53
17:R:214:GLN:HE22	27:R:613:CLA:C1A	2.21	0.53
4:d:335:PRO:HB2	5:e:65:LEU:HD22	1.89	0.53
17:r:104:MET:HE3	27:r:610:CLA:HMC2	1.90	0.53
2:B:30:VAL:HG11	27:B:613:CLA:H112	1.89	0.53
27:S:604:CLA:C1C	40:S:1623:NEX:H222	2.38	0.53
27:b:609:CLA:H172	27:b:610:CLA:H192	1.89	0.53
3:c:362:ARG:HD2	14:o:101:LEU:HD21	1.89	0.53
27:r:602:CLA:HAB	39:r:622:XAT:H32	1.89	0.53
1:A:191:ASN:HB2	3:C:411:ALA:HB1	1.91	0.53
1:A:322:ASN:HD21	15:P:53:PHE:HE1	1.56	0.53
28:A:409:PHO:H3A	27:D:402:CLA:H121	1.89	0.53
27:N:611:CLA:O1A	27:N:611:CLA:H3A	2.08	0.53
17:R:31:ASP:HA	27:R:602:CLA:HED2	1.89	0.53
7:g:27:PRO:HD2	37:g:601:CHL:HBB1	1.91	0.53
27:s:604:CLA:C1C	40:s:1623:NEX:H222	2.38	0.53
1:A:201:GLY:HA3	1:A:286:THR:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:80:LEU:HD12	16:Q:81:ARG:H	1.74	0.53
17:R:14:TRP:CD2	17:R:16:PRO:HD3	2.44	0.53
29:c:514:BCR:HC21	23:z:58:ASN:HD22	1.74	0.53
7:g:173:PHE:CE2	7:g:177:LYS:HE3	2.43	0.53
8:h:50:PHE:HB2	29:h:101:BCR:C10	2.38	0.53
7:n:203:LYS:HB2	7:n:208:ASN:HD21	1.72	0.53
14:o:235:ARG:HD2	14:o:239:PHE:CG	2.44	0.53
17:r:96:GLU:OE1	27:r:602:CLA:C4A	2.54	0.53
2:B:355:PHE:N	2:B:371:ILE:O	2.37	0.53
3:C:189:TRP:HZ3	3:C:367:GLU:HG3	1.74	0.53
3:C:263:ALA:HB2	9:I:24:LEU:HD23	1.89	0.53
7:G:27:PRO:HD2	37:G:601:CHL:HBB1	1.91	0.53
17:R:184:ALA:HB3	27:R:610:CLA:HAA2	1.91	0.53
27:R:602:CLA:HAB	39:R:622:XAT:H32	1.89	0.53
18:S:94:ILE:HG21	27:S:604:CLA:HAC2	1.90	0.53
7:Y:196:VAL:HB	27:Y:613:CLA:HAC2	1.91	0.53
2:b:22:VAL:HG13	27:b:615:CLA:HMB3	1.90	0.53
3:c:152:LYS:HZ2	21:w:137:LEU:HD11	1.72	0.53
3:c:189:TRP:HZ3	3:c:367:GLU:HG3	1.74	0.53
27:n:611:CLA:H2A	27:n:611:CLA:O1D	2.09	0.53
17:r:204:ALA:O	17:r:208:PHE:N	2.37	0.53
18:s:94:ILE:HG21	27:s:604:CLA:HAC2	1.90	0.53
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.90	0.53
10:J:9:PRO:HD2	10:J:12:ILE:HD12	1.89	0.53
11:K:35:VAL:HA	11:K:38:MET:HG2	1.91	0.53
15:P:161:ALA:HB3	15:P:176:VAL:HG13	1.91	0.53
7:Y:70:ARG:NE	7:Y:180:GLU:OE2	2.37	0.53
3:c:350:ILE:HG21	3:c:359:TRP:HB2	1.90	0.53
7:n:162:ASP:OD1	38:n:1620:LUT:O23	2.25	0.53
17:r:14:TRP:CD2	17:r:16:PRO:HD3	2.44	0.53
17:r:214:GLN:HE22	27:r:613:CLA:C1A	2.21	0.53
7:N:94:GLU:N	7:N:103:GLN:HE21	2.04	0.53
1:a:43:THR:O	1:a:47:VAL:HG12	2.08	0.53
5:e:41:GLY:O	5:e:51:ARG:NH2	2.42	0.53
31:D:411:LMG:O6	6:F:41:GLN:NE2	2.40	0.53
21:W:102:ASN:HB3	21:W:105:LEU:HD13	1.90	0.53
2:b:30:VAL:HG12	27:b:606:CLA:HHD	1.90	0.53
2:b:137:LYS:HD2	8:h:26:LEU:O	2.09	0.53
17:r:195:LEU:O	17:r:198:ILE:HG22	2.08	0.53
8:H:25:PRO:HG2	17:R:78:THR:HG21	1.90	0.53
3:c:78:GLU:O	16:q:34:THR:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:394:GLU:HB2	16:q:27:ARG:NE	2.24	0.53
27:n:610:CLA:H2A	27:n:610:CLA:O1D	2.09	0.53
16:q:80:LEU:HD12	16:q:81:ARG:H	1.74	0.53
2:B:187:VAL:HG13	27:B:602:CLA:HMD2	1.91	0.53
27:N:610:CLA:O1D	27:N:610:CLA:H2A	2.09	0.53
16:Q:31:LEU:O	16:Q:37:ARG:NH2	2.42	0.53
17:R:163:ASN:HD22	27:R:616:CLA:HBC3	1.73	0.53
1:a:312:ARG:HA	15:p:33:LYS:HA	1.89	0.53
8:h:25:PRO:HG2	17:r:78:THR:HG21	1.90	0.53
27:n:610:CLA:H2	38:n:1620:LUT:H28	1.91	0.53
17:r:184:ALA:HB3	27:r:610:CLA:HAA2	1.91	0.53
18:s:158:LEU:HG	18:s:163:LYS:HG2	1.91	0.53
2:B:45:PHE:HD1	2:B:60:MET:HG3	1.74	0.52
7:N:70:ARG:NH1	37:N:608:CHL:OBD	2.33	0.52
14:O:268:LEU:O	14:O:272:ASN:N	2.40	0.52
1:a:64:ARG:HH11	3:c:337:LEU:HD11	1.74	0.52
1:a:191:ASN:HB2	3:c:411:ALA:HB1	1.91	0.52
4:d:325:ILE:O	4:d:329:MET:HG2	2.09	0.52
21:w:102:ASN:HB3	21:w:105:LEU:HD13	1.90	0.52
2:B:105:GLY:HA3	29:B:619:BCR:H282	1.92	0.52
2:B:120:LEU:HB2	2:B:123:PHE:CE2	2.44	0.52
27:C:511:CLA:H161	29:C:517:BCR:H19C	1.91	0.52
4:D:216:ALA:O	4:D:220:ASN:ND2	2.29	0.52
4:D:325:ILE:O	4:D:329:MET:HG2	2.09	0.52
1:a:26:ASN:OD1	30:a:418:SQD:O3	2.18	0.52
7:y:196:VAL:HB	27:y:613:CLA:HAC2	1.91	0.52
1:A:43:THR:O	1:A:47:VAL:HG12	2.08	0.52
1:A:290:ILE:HG13	27:A:405:CLA:HED3	1.92	0.52
3:C:78:GLU:O	16:Q:34:THR:N	2.42	0.52
7:G:138:VAL:O	7:G:142:ARG:HG3	2.09	0.52
7:N:87:ARG:NH2	7:N:207:GLU:HA	2.24	0.52
1:a:196:PRO:HB3	1:a:199:MET:HE2	1.90	0.52
3:c:457:LYS:HB3	4:d:224:GLU:HG2	1.91	0.52
7:n:94:GLU:N	7:n:103:GLN:HE21	2.04	0.52
27:n:611:CLA:H3A	27:n:611:CLA:O1A	2.08	0.52
7:y:164:LEU:HD12	38:y:1620:LUT:H222	1.92	0.52
2:B:394:GLN:NE2	15:P:90:LYS:HB2	2.24	0.52
31:B:622:LMG:O10	13:M:4:ASN:ND2	2.43	0.52
14:O:237:SER:HA	14:O:276:VAL:HG21	1.92	0.52
18:S:142:GLU:OE2	37:S:607:CHL:HMC	2.09	0.52
1:a:199:MET:CG	32:c:520:DGD:HA92	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:45:PHE:HD1	2:b:60:MET:HG3	1.74	0.52
2:b:64:PRO:HA	2:b:67:THR:HG22	1.90	0.52
3:c:368:PRO:HG3	16:q:79:ARG:HB2	1.90	0.52
3:c:466:VAL:HG21	4:d:248:THR:HG23	1.92	0.52
37:g:601:CHL:HMA1	39:g:1622:XAT:H403	1.92	0.52
7:n:71:TRP:CE2	37:n:608:CHL:HED2	2.43	0.52
7:n:131:GLN:OE1	37:n:607:CHL:HMC	2.10	0.52
2:B:137:LYS:HD2	8:H:26:LEU:O	2.09	0.52
31:B:622:LMG:H351	13:M:10:ALA:HB1	1.91	0.52
29:C:514:BCR:HC21	23:Z:58:ASN:HD22	1.74	0.52
5:E:8:ARG:HE	5:E:12:ASP:HB3	1.75	0.52
27:N:611:CLA:H2A	27:N:611:CLA:O1D	2.08	0.52
18:S:76:ALA:O	18:S:80:ILE:HG12	2.10	0.52
20:U:5:GLY:HA3	20:U:28:LYS:HA	1.92	0.52
27:b:609:CLA:H62	27:b:610:CLA:H121	1.92	0.52
7:n:87:ARG:NH2	7:n:207:GLU:HA	2.24	0.52
14:o:119:VAL:HB	14:o:290:SER:O	2.10	0.52
16:q:31:LEU:O	16:q:37:ARG:NH2	2.42	0.52
7:y:73:MET:SD	27:y:610:CLA:HAB	2.50	0.52
2:B:422:ARG:HD3	14:O:262:ARG:NE	2.23	0.52
27:B:615:CLA:H2	30:B:621:SQD:H121	1.92	0.52
3:C:87:ILE:C	3:C:90:PRO:HD2	2.35	0.52
3:C:394:GLU:HB2	16:Q:27:ARG:NE	2.24	0.52
3:C:407:VAL:HG13	3:C:415:ASN:HA	1.90	0.52
29:C:517:BCR:H312	11:K:31:LEU:HD22	1.92	0.52
1:a:131:TRP:CZ2	3:c:449:ARG:HG2	2.45	0.52
2:b:120:LEU:HB2	2:b:123:PHE:CE2	2.44	0.52
27:c:511:CLA:H161	29:c:517:BCR:H19C	1.91	0.52
9:i:9:TYR:OH	21:w:99:GLY:HA3	2.10	0.52
16:q:80:LEU:HD12	16:q:81:ARG:N	2.25	0.52
7:G:221:ALA:N	27:G:613:CLA:O1A	2.43	0.52
37:G:601:CHL:HMA1	39:G:1622:XAT:H403	1.92	0.52
7:N:131:GLN:OE1	37:N:607:CHL:HMC	2.10	0.52
14:O:310:ASP:HB3	14:O:313:ALA:HB3	1.92	0.52
16:Q:80:LEU:HD12	16:Q:81:ARG:N	2.25	0.52
17:R:102:TRP:CE2	37:R:608:CHL:HED2	2.45	0.52
1:a:32:TRP:O	1:a:35:VAL:HG22	2.10	0.52
1:a:36:LEU:HD22	1:a:125:CYS:SG	2.50	0.52
1:a:290:ILE:HG13	27:a:405:CLA:HED3	1.92	0.52
2:b:105:GLY:HA3	29:b:619:BCR:H282	1.92	0.52
14:o:245:ARG:HD2	14:o:272:ASN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p:161:ALA:HB3	15:p:176:VAL:HG13	1.91	0.52
18:s:162:ASP:O	18:s:164:LEU:HA	2.10	0.52
1:A:276:ALA:HB2	4:D:215:GLY:C	2.35	0.52
27:C:511:CLA:H8	23:Z:24:PRO:HB3	1.92	0.52
7:N:92:PHE:HE1	7:N:113:LEU:HA	1.75	0.52
27:N:610:CLA:H2	38:N:1620:LUT:H28	1.91	0.52
14:O:241:ASP:OD2	14:O:245:ARG:HB2	2.10	0.52
14:O:245:ARG:HD2	14:O:272:ASN:HA	1.91	0.52
18:S:162:ASP:O	18:S:164:LEU:HA	2.10	0.52
31:b:622:LMG:O10	13:m:4:ASN:ND2	2.43	0.52
14:o:237:SER:HA	14:o:276:VAL:HG21	1.92	0.52
18:s:142:GLU:OE2	37:s:607:CHL:HMC	2.09	0.52
21:w:107:TRP:HH2	7:y:84:LEU:HD21	1.75	0.52
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.91	0.52
2:B:458:PHE:CE2	31:B:622:LMG:H212	2.45	0.52
3:C:466:VAL:HG21	4:D:248:THR:HG23	1.92	0.52
14:O:235:ARG:HD2	14:O:239:PHE:CG	2.44	0.52
14:O:257:LEU:O	14:O:262:ARG:HG2	2.10	0.52
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.92	0.52
11:k:35:VAL:HA	11:k:38:MET:HG2	1.91	0.52
7:n:92:PHE:HE1	7:n:113:LEU:HA	1.75	0.52
39:n:1622:XAT:H363	35:y:2630:LHG:HC41	1.92	0.52
17:r:102:TRP:CE2	37:r:608:CHL:HED2	2.45	0.52
17:r:159:GLU:OE1	17:r:162:ARG:NH2	2.43	0.52
32:C:520:DGD:HAW2	4:D:74:LEU:CD2	2.40	0.52
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.92	0.52
15:P:74:PHE:HE2	15:P:156:LEU:HD21	1.75	0.52
7:Y:73:MET:SD	27:Y:610:CLA:HAB	2.50	0.52
1:a:276:ALA:HB2	4:d:215:GLY:C	2.35	0.52
27:b:615:CLA:H2	30:b:621:SQD:H121	1.92	0.52
31:b:622:LMG:H351	13:m:10:ALA:HB1	1.91	0.52
3:c:119:LEU:O	3:c:122:SER:OG	2.20	0.52
27:c:511:CLA:H8	23:z:24:PRO:HB3	1.92	0.52
16:q:79:ARG:O	16:q:83:SER:HB3	2.09	0.52
1:A:26:ASN:OD1	30:A:418:SQD:O3	2.18	0.51
1:A:131:TRP:CZ2	3:C:449:ARG:HG2	2.45	0.51
3:C:178:LYS:NZ	3:C:184:GLY:O	2.43	0.51
5:E:41:GLY:O	5:E:51:ARG:NH2	2.42	0.51
14:O:235:ARG:HD2	14:O:239:PHE:CD2	2.45	0.51
16:Q:42:PRO:CB	16:Q:43:LEU:HB2	2.39	0.51
2:b:355:PHE:N	2:b:371:ILE:O	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:o:93:ASP:OD1	16:q:68:ARG:NH2	2.43	0.51
15:p:47:LEU:HB3	15:p:61:VAL:HB	1.92	0.51
16:q:42:PRO:CB	16:q:43:LEU:HB2	2.39	0.51
1:A:199:MET:CG	32:C:520:DGD:HA92	2.39	0.51
14:O:211:PHE:HD1	14:O:321:ILE:HD13	1.74	0.51
15:P:31:PRO:HD3	15:P:179:ALA:HB2	1.92	0.51
16:Q:22:ASN:O	16:Q:26:ALA:N	2.40	0.51
16:Q:42:PRO:HB2	16:Q:43:LEU:CB	2.40	0.51
18:S:158:LEU:HG	18:S:163:LYS:HG2	1.91	0.51
23:Z:12:LEU:HD13	23:Z:50:LEU:HB2	1.92	0.51
2:b:187:VAL:HG13	27:b:602:CLA:HMD2	1.91	0.51
29:b:619:BCR:H333	31:b:622:LMG:H382	1.93	0.51
3:c:73:ALA:HA	11:k:24:LEU:HG	1.92	0.51
27:c:504:CLA:H72	32:c:519:DGD:HB1	1.92	0.51
29:c:517:BCR:H312	11:k:31:LEU:HD22	1.92	0.51
7:g:138:VAL:O	7:g:142:ARG:HG3	2.09	0.51
7:n:24:TYR:CE2	7:n:25:LEU:HG	2.45	0.51
17:r:100:GLY:HA3	17:r:201:ALA:HB1	1.92	0.51
14:O:144:LYS:HB2	14:O:156:PHE:HB3	1.93	0.51
21:W:107:TRP:HH2	7:Y:84:LEU:HD21	1.75	0.51
1:a:199:MET:SD	32:c:520:DGD:HA92	2.50	0.51
2:b:458:PHE:CE2	31:b:622:LMG:H212	2.45	0.51
29:c:517:BCR:H313	11:k:31:LEU:HD13	1.93	0.51
7:g:221:ALA:N	27:g:613:CLA:O1A	2.43	0.51
37:n:609:CHL:HAA2	7:y:48:THR:HG21	1.91	0.51
14:o:241:ASP:OD2	14:o:245:ARG:HB2	2.10	0.51
17:r:214:GLN:OE1	27:r:613:CLA:C4D	2.38	0.51
18:s:83:ARG:HD3	27:s:610:CLA:HAC2	1.92	0.51
7:y:119:VAL:N	37:y:605:CHL:O1D	2.40	0.51
7:G:71:TRP:CE2	37:G:608:CHL:HED2	2.46	0.51
7:N:24:TYR:CE2	7:N:25:LEU:HG	2.45	0.51
37:N:601:CHL:HHD	35:N:2630:LHG:HC41	1.92	0.51
14:O:119:VAL:HB	14:O:290:SER:O	2.10	0.51
16:Q:79:ARG:O	16:Q:83:SER:HB3	2.10	0.51
17:R:32:TYR:HD2	27:R:602:CLA:HMD2	1.75	0.51
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.92	0.51
1:a:197:PHE:CZ	32:c:520:DGD:HBH1	2.46	0.51
1:a:340:PRO:HB2	15:p:166:LYS:HB2	1.92	0.51
2:b:365:THR:HG1	4:d:326:ARG:HH21	1.57	0.51
14:o:257:LEU:O	14:o:262:ARG:HG2	2.10	0.51
17:r:32:TYR:HD2	27:r:602:CLA:HMD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:76:ALA:O	18:s:80:ILE:HG12	2.10	0.51
1:A:36:LEU:HD22	1:A:125:CYS:SG	2.50	0.51
4:D:48:TRP:NE1	4:D:173:PHE:O	2.28	0.51
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.46	0.51
7:N:220:ASN:OD1	7:N:223:ASN:N	2.44	0.51
39:N:1622:XAT:H363	35:Y:2630:LHG:HC41	1.92	0.51
15:P:47:LEU:HB3	15:P:61:VAL:HB	1.93	0.51
17:R:159:GLU:OE1	17:R:162:ARG:NH2	2.43	0.51
32:c:520:DGD:HAW2	4:d:74:LEU:CD2	2.40	0.51
14:o:211:PHE:HD1	14:o:321:ILE:HD13	1.74	0.51
17:r:158:ILE:HD13	37:r:608:CHL:HMA1	1.93	0.51
27:A:406:CLA:H203	28:A:408:PHO:H101	1.93	0.51
27:B:604:CLA:H192	27:B:610:CLA:H112	1.93	0.51
3:C:457:LYS:HB3	4:D:224:GLU:HG2	1.91	0.51
7:G:119:VAL:HA	37:G:605:CHL:C4D	2.40	0.51
9:I:9:TYR:OH	21:W:99:GLY:HA3	2.10	0.51
17:R:112:THR:HG21	27:R:604:CLA:HAC2	1.92	0.51
18:S:189:GLU:OE1	27:S:610:CLA:C4A	2.59	0.51
14:o:176:PHE:CZ	14:o:184:VAL:HG11	2.46	0.51
15:p:71:ILE:HD12	15:p:150:THR:HA	1.93	0.51
1:A:32:TRP:O	1:A:35:VAL:HG22	2.10	0.51
2:B:472:ARG:HA	2:B:479:PHE:CE2	2.46	0.51
7:G:69:CYS:SG	7:G:188:MET:HE3	2.50	0.51
37:N:609:CHL:HAA2	7:Y:48:THR:HG21	1.91	0.51
17:R:204:ALA:O	17:R:208:PHE:N	2.37	0.51
7:Y:27:PRO:HD2	37:Y:601:CHL:HBB1	1.93	0.51
3:c:87:ILE:C	3:c:90:PRO:HD2	2.35	0.51
29:d:404:BCR:H16C	6:f:33:PHE:HD2	1.76	0.51
7:g:71:TRP:CE2	37:g:608:CHL:HED2	2.46	0.51
37:n:601:CHL:HHH	35:n:2630:LHG:HC41	1.92	0.51
14:o:235:ARG:HD2	14:o:239:PHE:CD2	2.45	0.51
14:o:310:ASP:HB3	14:o:313:ALA:HB3	1.92	0.51
37:y:601:CHL:HMA3	35:y:2630:LHG:H121	1.93	0.51
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.92	0.51
1:A:199:MET:SD	32:C:520:DGD:HA92	2.50	0.51
21:W:121:PHE:CE2	27:Y:612:CLA:H11	2.46	0.51
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.91	0.51
3:c:338:GLY:HA2	14:o:194:TYR:OH	2.11	0.51
37:g:601:CHL:HAC2	35:g:2630:LHG:HC41	1.93	0.51
39:g:1622:XAT:H10	35:g:2630:LHG:H212	1.93	0.51
14:o:184:VAL:HB	14:o:225:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:39:LEU:HD13	27:r:602:CLA:H42	1.93	0.51
1:A:64:ARG:HH11	3:C:337:LEU:HD11	1.74	0.51
2:B:121:GLU:OE1	8:H:14:PRO:HB2	2.11	0.51
3:C:73:ALA:HA	11:K:24:LEU:HG	1.92	0.51
32:C:518:DGD:O4E	32:C:518:DGD:O5E	2.19	0.51
14:O:184:VAL:HB	14:O:225:PHE:CE1	2.46	0.51
15:P:71:ILE:HD12	15:P:150:THR:HA	1.93	0.51
2:b:157:HIS:HE1	27:b:607:CLA:C1A	2.24	0.51
4:d:87:HIS:CD2	4:d:162:LEU:HA	2.46	0.51
7:g:119:VAL:HA	37:g:605:CHL:C4D	2.41	0.51
15:p:31:PRO:HD3	15:p:179:ALA:HB2	1.92	0.51
17:r:112:THR:HG21	27:r:604:CLA:HAC2	1.92	0.51
18:s:188:LYS:HD3	27:s:612:CLA:HAA2	1.93	0.51
1:A:340:PRO:HB2	15:P:166:LYS:HB2	1.92	0.51
27:B:609:CLA:H62	27:B:610:CLA:H121	1.92	0.51
3:C:345:PRO:HB3	14:O:164:ARG:NE	2.19	0.51
29:C:517:BCR:H313	11:K:31:LEU:HD13	1.93	0.51
15:P:103:PHE:CE2	15:P:136:ALA:HB2	2.46	0.51
17:R:39:LEU:HD13	27:R:602:CLA:H42	1.93	0.51
17:R:202:ARG:HH22	27:R:602:CLA:CED	2.23	0.51
2:b:394:GLN:NE2	15:p:90:LYS:HB2	2.24	0.51
29:b:618:BCR:H383	30:b:621:SQD:H101	1.93	0.51
3:c:290:VAL:O	3:c:423:ARG:NH1	2.43	0.51
3:c:443:TRP:HH2	35:d:410:LHG:HC61	1.76	0.51
7:g:70:ARG:NE	7:g:180:GLU:OE2	2.43	0.51
18:s:49:LEU:HD21	27:s:602:CLA:HBD	1.93	0.51
1:A:197:PHE:CZ	32:C:520:DGD:HBH1	2.46	0.50
3:C:368:PRO:O	16:Q:76:ASN:HB2	2.11	0.50
3:C:456:GLU:OE1	3:C:456:GLU:N	2.38	0.50
27:C:504:CLA:H72	32:C:519:DGD:HBH1	1.92	0.50
14:O:193:ASP:OD2	14:O:214:LYS:HG2	2.11	0.50
7:Y:164:LEU:HD12	38:Y:1620:LUT:H222	1.92	0.50
2:b:472:ARG:HA	2:b:479:PHE:CE2	2.46	0.50
36:f:101:HEM:HMC1	36:f:101:HEM:HBC2	1.93	0.50
15:p:74:PHE:HE2	15:p:156:LEU:HD21	1.75	0.50
15:p:103:PHE:CE2	15:p:136:ALA:HB2	2.46	0.50
17:r:202:ARG:HH22	27:r:602:CLA:CED	2.23	0.50
7:y:71:TRP:CE2	37:y:608:CHL:HED2	2.47	0.50
1:A:82:ILE:CG2	1:A:174:LEU:HB2	2.41	0.50
2:B:157:HIS:HE1	27:B:607:CLA:C1A	2.24	0.50
3:C:443:TRP:HH2	35:D:410:LHG:HC61	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:42:PRO:HA	11:K:45:PHE:HD2	1.76	0.50
17:R:185:SER:HB2	17:R:186:ASP:HB3	1.93	0.50
23:Z:15:THR:HA	23:Z:18:ILE:HD12	1.93	0.50
3:c:368:PRO:O	16:q:76:ASN:HB2	2.11	0.50
5:e:8:ARG:HE	5:e:12:ASP:HB3	1.75	0.50
37:g:607:CHL:H43	7:n:230:PRO:HB3	1.93	0.50
20:u:5:GLY:HA3	20:u:28:LYS:HA	1.92	0.50
23:z:12:LEU:HD13	23:z:50:LEU:HB2	1.93	0.50
3:C:279:LEU:HD11	27:C:507:CLA:HBA1	1.92	0.50
29:D:404:BCR:H16C	6:F:33:PHE:HD2	1.76	0.50
7:G:70:ARG:NE	7:G:180:GLU:OE2	2.43	0.50
39:G:1622:XAT:H10	35:G:2630:LHG:H212	1.93	0.50
39:N:1622:XAT:H221	35:Y:2630:LHG:HC32	1.93	0.50
17:R:158:ILE:HD13	37:R:608:CHL:HMA1	1.93	0.50
18:S:206:GLN:OE1	27:S:613:CLA:C4D	2.47	0.50
2:b:323:GLY:N	2:b:326:ARG:HD2	2.27	0.50
27:b:606:CLA:H193	27:b:610:CLA:HBB2	1.93	0.50
29:c:514:BCR:HC21	23:z:58:ASN:ND2	2.27	0.50
7:n:136:GLY:HA2	37:n:609:CHL:HAB	1.93	0.50
15:p:47:LEU:HD11	15:p:49:TYR:CE2	2.46	0.50
29:C:514:BCR:HC21	23:Z:58:ASN:ND2	2.27	0.50
37:G:607:CHL:H43	7:N:230:PRO:HB3	1.93	0.50
15:P:47:LEU:HD11	15:P:49:TYR:CE2	2.46	0.50
18:S:83:ARG:HD3	27:S:610:CLA:HAC2	1.92	0.50
2:b:71:ILE:HG13	27:b:607:CLA:HMA2	1.94	0.50
3:c:80:PRO:HD2	3:c:83:GLU:OE1	2.11	0.50
7:g:69:CYS:SG	7:g:188:MET:HE3	2.51	0.50
11:k:39:PRO:O	11:k:42:PRO:HD2	2.11	0.50
14:o:144:LYS:HB2	14:o:156:PHE:HB3	1.93	0.50
2:B:71:ILE:HG13	27:B:607:CLA:HMA2	1.94	0.50
27:B:606:CLA:H193	27:B:610:CLA:HBB2	1.93	0.50
14:O:122:PHE:CZ	14:O:124:PHE:HB2	2.46	0.50
18:S:150:GLU:O	18:S:153:ARG:HG2	2.12	0.50
18:S:188:LYS:HD3	27:S:612:CLA:HAA2	1.93	0.50
1:a:82:ILE:HD13	1:a:115:ILE:HD12	1.93	0.50
2:b:226:TYR:CD1	2:b:231:MET:HB2	2.47	0.50
2:b:247:PHE:CE1	27:b:603:CLA:H8	2.46	0.50
3:c:236:GLY:C	29:c:515:BCR:H383	2.37	0.50
14:o:268:LEU:O	14:o:272:ASN:N	2.40	0.50
3:C:236:GLY:C	29:C:515:BCR:H383	2.37	0.50
7:G:46:TRP:O	38:G:1621:LUT:H24	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:406:CLA:H203	28:a:408:PHO:H101	1.93	0.50
3:c:178:LYS:NZ	3:c:184:GLY:O	2.43	0.50
11:k:42:PRO:HA	11:k:45:PHE:HD2	1.76	0.50
18:s:62:PHE:HD2	38:s:1621:LUT:H222	1.76	0.50
21:w:121:PHE:CE2	27:y:612:CLA:H11	2.46	0.50
1:A:201:GLY:HA3	1:A:286:THR:CG2	2.42	0.50
1:A:217:SER:HB2	4:D:142:ASN:HA	1.94	0.50
2:B:474:LEU:HD11	27:B:609:CLA:HAA2	1.94	0.50
29:B:619:BCR:H333	31:B:622:LMG:H382	1.93	0.50
4:D:68:LEU:HD13	6:F:40:MET:HE2	1.93	0.50
11:K:39:PRO:O	11:K:42:PRO:HD2	2.11	0.50
14:O:93:ASP:OD1	16:Q:68:ARG:NH2	2.43	0.50
2:b:121:GLU:OE1	8:h:14:PRO:HB2	2.11	0.50
2:b:475:PHE:O	2:b:478:VAL:HG22	2.12	0.50
27:b:604:CLA:H192	27:b:610:CLA:H112	1.93	0.50
3:c:279:LEU:HD11	27:c:507:CLA:HBA1	1.92	0.50
12:l:26:PHE:O	12:l:30:VAL:HG23	2.11	0.50
18:s:189:GLU:OE1	27:s:610:CLA:C4A	2.59	0.50
7:y:173:PHE:CZ	7:y:177:LYS:HE3	2.47	0.50
37:y:601:CHL:H43	37:y:601:CHL:HMA2	1.94	0.50
1:A:48:PHE:CE2	34:D:405:PL9:H48	2.35	0.50
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.94	0.50
1:A:82:ILE:HD13	1:A:115:ILE:HD12	1.93	0.50
2:B:247:PHE:CE1	27:B:603:CLA:H8	2.46	0.50
2:B:251:VAL:HG22	27:B:603:CLA:H92	1.94	0.50
27:B:616:CLA:H71	27:B:617:CLA:H162	1.94	0.50
36:F:101:HEM:HBC2	36:F:101:HEM:HMC1	1.93	0.50
7:N:121:ALA:HA	37:N:605:CHL:CHC	2.42	0.50
14:O:176:PHE:CZ	14:O:184:VAL:HG11	2.46	0.50
17:R:100:GLY:HA3	17:R:201:ALA:HB1	1.92	0.50
18:S:62:PHE:HD2	38:S:1621:LUT:H222	1.76	0.50
7:Y:173:PHE:CZ	7:Y:177:LYS:HE3	2.47	0.50
1:a:42:LEU:HB3	29:a:411:BCR:H353	1.94	0.50
2:b:25:MET:HE3	29:b:618:BCR:H23C	1.94	0.50
2:B:19:LEU:HD11	2:B:23:HIS:CE1	2.47	0.50
2:B:475:PHE:O	2:B:478:VAL:HG22	2.12	0.50
7:Y:119:VAL:N	37:Y:605:CHL:O1D	2.40	0.50
17:r:28:LEU:HB3	17:r:93:ARG:HH11	1.77	0.50
23:z:15:THR:HA	23:z:18:ILE:HD12	1.93	0.50
2:B:323:GLY:N	2:B:326:ARG:HD2	2.27	0.49
3:C:338:GLY:HA2	14:O:194:TYR:OH	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:131:ALA:N	14:O:174:GLY:O	2.44	0.49
15:P:126:TYR:CD1	15:P:150:THR:HB	2.47	0.49
7:Y:71:TRP:CE2	37:Y:608:CHL:HED2	2.47	0.49
14:o:122:PHE:CZ	14:o:124:PHE:HB2	2.46	0.49
1:a:60:ILE:HD12	1:a:84:PRO:HD2	1.93	0.49
1:a:201:GLY:HA3	1:a:286:THR:CG2	2.42	0.49
2:b:422:ARG:HD3	14:o:262:ARG:NE	2.23	0.49
2:b:474:LEU:HD11	27:b:609:CLA:HAA2	1.94	0.49
7:g:46:TRP:O	38:g:1621:LUT:H24	2.11	0.49
7:g:63:GLU:O	7:g:67:ILE:HG12	2.12	0.49
17:r:185:SER:HB2	17:r:186:ASP:HB3	1.93	0.49
1:A:264:SER:OG	1:A:265:PHE:N	2.44	0.49
2:B:25:MET:HE3	29:B:618:BCR:H23C	1.94	0.49
3:C:28:GLN:HE21	4:D:230:ASN:ND2	2.11	0.49
4:D:227:ASP:OD2	4:D:233:ARG:NH1	2.45	0.49
7:G:118:LEU:HD23	37:G:605:CHL:HED2	1.94	0.49
37:G:601:CHL:HAC2	35:G:2630:LHG:HC41	1.93	0.49
12:L:26:PHE:O	12:L:30:VAL:HG23	2.12	0.49
7:N:136:GLY:HA2	37:N:609:CHL:HAB	1.93	0.49
37:Y:601:CHL:HMA3	35:Y:2630:LHG:H121	1.93	0.49
2:b:251:VAL:HG22	27:b:603:CLA:H92	1.93	0.49
3:c:130:ILE:HD12	23:z:27:PHE:HE2	1.77	0.49
3:c:390:ARG:HG2	16:q:39:TYR:C	2.37	0.49
4:d:322:ASN:O	4:d:326:ARG:HG3	2.12	0.49
34:d:405:PL9:H472	19:t:10:LEU:HD22	1.94	0.49
36:f:101:HEM:HBB2	36:f:101:HEM:HMB1	1.95	0.49
15:p:126:TYR:CD1	15:p:150:THR:HB	2.47	0.49
30:A:412:SQD:H301	29:C:516:BCR:H291	1.95	0.49
27:B:608:CLA:C4A	27:B:608:CLA:HBA2	2.43	0.49
12:L:26:PHE:CD2	19:T:16:ILE:HD11	2.47	0.49
7:N:189:PHE:CD1	27:N:602:CLA:H201	2.47	0.49
16:Q:63:LYS:HB2	16:Q:134:TYR:CZ	2.47	0.49
1:a:341:LEU:HB3	1:a:343:LEU:HG	1.94	0.49
27:b:616:CLA:H71	27:b:617:CLA:H162	1.94	0.49
3:c:430:HIS:CD2	27:c:502:CLA:ND	2.80	0.49
7:g:96:VAL:HG12	7:g:99:LYS:H	1.78	0.49
7:y:211:ASP:O	7:y:219:ASN:ND2	2.42	0.49
2:B:226:TYR:CD1	2:B:231:MET:HB2	2.47	0.49
3:C:130:ILE:HD12	23:Z:27:PHE:HE2	1.77	0.49
3:C:430:HIS:CD2	27:C:502:CLA:ND	2.80	0.49
15:P:49:TYR:HB2	15:P:59:LEU:HG	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:180:GLU:HB2	27:Y:610:CLA:C1B	2.42	0.49
7:g:175:GLU:HG3	27:g:611:CLA:HED1	1.95	0.49
14:o:222:PRO:HA	14:o:225:PHE:CE1	2.48	0.49
17:r:143:SER:O	17:r:146:THR:OG1	2.24	0.49
17:r:211:PHE:HZ	38:r:620:LUT:H8	1.78	0.49
18:s:111:TRP:O	18:s:114:THR:HG22	2.12	0.49
18:s:150:GLU:O	18:s:153:ARG:HG2	2.12	0.49
1:A:56:PRO:HA	1:A:73:TYR:CE2	2.48	0.49
1:A:325:ASN:HA	1:A:328:MET:HE3	1.93	0.49
2:B:366:PHE:O	2:B:425:GLN:NE2	2.30	0.49
34:D:405:PL9:H472	19:T:10:LEU:HD22	1.94	0.49
12:L:13:LEU:HA	35:L:101:LHG:HC11	1.94	0.49
37:R:608:CHL:HBB1	37:R:608:CHL:HHC	1.94	0.49
18:S:49:LEU:HD21	27:S:602:CLA:HBD	1.93	0.49
1:a:81:ALA:HB2	1:a:175:GLY:HA3	1.94	0.49
4:d:48:TRP:NE1	4:d:173:PHE:O	2.29	0.49
4:d:94:GLY:O	4:d:98:GLN:N	2.41	0.49
7:n:24:TYR:CE1	7:n:46:TRP:HB2	2.48	0.49
14:o:131:ALA:N	14:o:174:GLY:O	2.44	0.49
37:r:608:CHL:HBB1	37:r:608:CHL:HHC	1.94	0.49
1:A:135:PHE:CE1	3:C:449:ARG:HG3	2.48	0.49
2:B:475:PHE:HD2	4:D:140:PRO:HD3	1.77	0.49
3:C:390:ARG:HG2	16:Q:39:TYR:C	2.37	0.49
18:S:111:TRP:O	18:S:114:THR:HG22	2.12	0.49
18:S:165:HIS:CD2	18:S:186:LYS:HE2	2.48	0.49
2:b:18:ARG:NH1	12:l:5:ASN:HD22	2.11	0.49
2:b:366:PHE:O	2:b:425:GLN:NE2	2.30	0.49
35:d:409:LHG:H192	19:t:17:ILE:HD11	1.95	0.49
7:n:220:ASN:OD1	7:n:223:ASN:N	2.43	0.49
14:o:193:ASP:OD2	14:o:214:LYS:HG2	2.11	0.49
16:q:42:PRO:HB2	16:q:43:LEU:CB	2.40	0.49
17:r:163:ASN:O	17:r:171:ARG:NH2	2.46	0.49
17:r:197:GLU:OE1	27:r:610:CLA:NA	2.46	0.49
1:A:42:LEU:HB3	29:A:411:BCR:H353	1.94	0.49
1:A:341:LEU:HB3	1:A:343:LEU:HG	1.94	0.49
2:B:18:ARG:NH1	12:L:5:ASN:HD22	2.11	0.49
3:C:80:PRO:HD2	3:C:83:GLU:OE1	2.11	0.49
3:C:348:GLU:OE1	3:C:348:GLU:N	2.42	0.49
14:O:143:VAL:HG21	14:O:207:VAL:HG11	1.95	0.49
1:a:264:SER:OG	1:a:265:PHE:N	2.44	0.49
4:d:227:ASP:OD2	4:d:233:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:n:607:CHL:H142	37:y:601:CHL:H161	1.95	0.49
16:q:63:LYS:HB2	16:q:134:TYR:CZ	2.47	0.49
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.93	0.49
31:A:413:LMG:H292	31:A:413:LMG:H321	1.59	0.49
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.95	0.49
16:Q:40:LEU:HB2	16:Q:41:GLN:CG	2.42	0.49
17:R:197:GLU:OE1	27:R:610:CLA:NA	2.46	0.49
21:W:121:PHE:CD2	27:Y:612:CLA:H42	2.48	0.49
37:Y:601:CHL:H43	37:Y:601:CHL:HMA2	1.94	0.49
2:b:19:LEU:HD11	2:b:23:HIS:CE1	2.46	0.49
2:b:61:PHE:CZ	27:b:605:CLA:HMA1	2.48	0.49
3:c:348:GLU:OE1	3:c:348:GLU:N	2.42	0.49
7:g:35:TYR:OH	7:g:47:ASP:OD2	2.27	0.49
7:g:69:CYS:HB3	7:g:184:GLY:HA3	1.95	0.49
12:l:13:LEU:HA	35:l:101:LHG:HC11	1.94	0.49
12:l:26:PHE:HE1	13:m:15:ILE:HG23	1.78	0.49
3:C:119:LEU:O	3:C:122:SER:OG	2.20	0.49
3:C:319:VAL:O	3:C:323:ARG:HG2	2.13	0.49
4:D:322:ASN:O	4:D:326:ARG:HG3	2.12	0.49
7:N:24:TYR:CE1	7:N:46:TRP:HB2	2.48	0.49
14:O:96:GLN:OE1	16:Q:68:ARG:NE	2.32	0.49
15:P:17:GLU:HG3	15:P:18:PHE:CD2	2.48	0.49
16:Q:19:GLY:HA2	16:Q:20:THR:HA	1.54	0.49
18:S:66:LYS:HG3	18:S:67:LYS:H	1.78	0.49
2:b:167:TRP:CD1	2:b:264:PRO:HG2	2.47	0.49
3:c:213:LEU:O	3:c:223:TRP:NE1	2.46	0.49
7:g:118:LEU:HD23	37:g:605:CHL:HED2	1.94	0.49
37:n:601:CHL:C1D	35:n:2630:LHG:HC82	2.42	0.49
7:y:27:PRO:HD2	37:y:601:CHL:HBB1	1.93	0.49
29:B:618:BCR:H383	30:B:621:SQD:H101	1.93	0.48
3:C:408:GLY:HA3	3:C:419:TYR:H	1.77	0.48
4:D:236:ASN:O	4:D:239:GLN:HG2	2.13	0.48
7:G:44:TYR:N	27:G:602:CLA:OBD	2.46	0.48
12:L:26:PHE:HE1	13:M:15:ILE:HG23	1.78	0.48
14:O:222:PRO:HA	14:O:225:PHE:CE1	2.48	0.48
14:O:255:VAL:HG13	14:O:262:ARG:HD3	1.95	0.48
15:P:130:THR:HG22	15:P:146:VAL:HG13	1.95	0.48
17:R:211:PHE:HZ	38:R:620:LUT:H8	1.78	0.48
18:S:112:PHE:CE2	18:S:113:LYS:HE2	2.48	0.48
7:Y:163:PRO:HD2	38:Y:1620:LUT:H23	1.95	0.48
23:Z:41:PHE:O	23:Z:45:SER:OG	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:212:SER:OG	4:d:211:CYS:HB2	2.13	0.48
1:a:325:ASN:HA	1:a:328:MET:HE3	1.93	0.48
30:a:412:SQD:H301	29:c:516:BCR:H291	1.95	0.48
2:b:390:TYR:HB2	4:d:344:GLU:OE2	2.13	0.48
2:b:475:PHE:HD2	4:d:140:PRO:HD3	1.77	0.48
3:c:130:ILE:HD12	23:z:27:PHE:CE2	2.48	0.48
4:d:56:THR:HB	5:e:49:SER:HA	1.95	0.48
7:n:178:VAL:O	7:n:181:ILE:HG22	2.13	0.48
39:n:1622:XAT:H221	35:y:2630:LHG:HC32	1.93	0.48
35:D:409:LHG:H192	19:T:17:ILE:HD11	1.95	0.48
7:G:65:GLU:OE2	7:G:185:ARG:NE	2.46	0.48
27:G:610:CLA:H2A	27:G:610:CLA:O1D	2.14	0.48
14:O:245:ARG:HA	14:O:251:TYR:O	2.13	0.48
17:R:223:LEU:O	17:R:227:VAL:HG23	2.13	0.48
7:g:44:TYR:N	27:g:602:CLA:OBD	2.46	0.48
12:l:26:PHE:CD2	19:t:16:ILE:HD11	2.47	0.48
7:n:121:ALA:HA	37:n:605:CHL:CHC	2.42	0.48
7:y:15:PRO:HG2	7:y:16:TRP:CD1	2.48	0.48
27:B:605:CLA:HBA1	27:B:605:CLA:CHA	2.43	0.48
3:C:343:ARG:NH1	3:C:347:GLY:O	2.45	0.48
7:G:222:TRP:CH2	37:Y:607:CHL:HBC2	2.48	0.48
8:H:17:THR:O	8:H:21:ALA:N	2.45	0.48
7:N:178:VAL:O	7:N:181:ILE:HG22	2.13	0.48
37:N:607:CHL:H142	37:Y:601:CHL:H161	1.95	0.48
16:Q:59:ILE:O	16:Q:62:VAL:HG22	2.13	0.48
17:R:163:ASN:O	17:R:171:ARG:NH2	2.46	0.48
7:Y:15:PRO:HG2	7:Y:16:TRP:CD1	2.48	0.48
1:a:56:PRO:HA	1:a:73:TYR:CE2	2.48	0.48
3:c:61:VAL:HG12	3:c:118:HIS:O	2.13	0.48
7:g:65:GLU:OE2	7:g:185:ARG:NE	2.46	0.48
35:n:2630:LHG:H211	39:y:1622:XAT:H10	1.95	0.48
16:q:22:ASN:HA	16:q:25:GLN:HB3	1.96	0.48
18:s:156:ASN:O	18:s:158:LEU:HB3	2.13	0.48
18:s:165:HIS:CD2	18:s:186:LYS:HE2	2.48	0.48
7:y:163:PRO:HD2	38:y:1620:LUT:H23	1.95	0.48
27:y:611:CLA:NA	35:y:2630:LHG:O4	2.46	0.48
27:A:407:CLA:O2D	32:C:520:DGD:HAH2	2.13	0.48
2:B:61:PHE:CZ	27:B:605:CLA:HMA1	2.48	0.48
2:B:167:TRP:CD1	2:B:264:PRO:HG2	2.47	0.48
2:B:390:TYR:HB2	4:D:344:GLU:OE2	2.13	0.48
37:G:601:CHL:HBA2	37:Y:609:CHL:HBA1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:187:GLN:NE2	1:a:191:ASN:HA	2.28	0.48
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.95	0.48
2:b:475:PHE:CE1	4:d:134:ARG:HB2	2.49	0.48
3:c:456:GLU:OE1	3:c:456:GLU:N	2.38	0.48
4:d:306:ALA:HA	14:o:243:LYS:HG3	1.95	0.48
27:g:610:CLA:HBA1	27:g:610:CLA:CHA	2.40	0.48
15:p:17:GLU:HG3	15:p:18:PHE:CD2	2.48	0.48
15:p:74:PHE:CE2	15:p:156:LEU:HD21	2.49	0.48
2:B:254:GLY:HA2	32:H:102:DGD:HBW1	1.94	0.48
2:B:434:ARG:NH1	14:O:260:GLY:HA2	2.29	0.48
4:D:51:GLY:HA3	4:D:78:VAL:HG22	1.95	0.48
7:G:63:GLU:O	7:G:67:ILE:HG12	2.12	0.48
1:a:82:ILE:CG2	1:a:174:LEU:HB2	2.41	0.48
1:a:135:PHE:CE1	3:c:449:ARG:HG3	2.48	0.48
2:b:383:PHE:HD1	14:o:251:TYR:CE1	2.32	0.48
2:b:383:PHE:CG	4:d:347:PRO:HA	2.49	0.48
27:b:607:CLA:H61	27:b:607:CLA:H102	1.56	0.48
3:c:319:VAL:O	3:c:323:ARG:HG2	2.13	0.48
7:n:189:PHE:CD1	27:n:602:CLA:H201	2.47	0.48
14:o:116:GLU:HA	14:o:117:GLY:HA2	1.51	0.48
21:w:129:GLU:HB3	21:w:130:ASP:HB2	1.95	0.48
7:y:24:TYR:CE2	7:y:25:LEU:HG	2.49	0.48
7:G:96:VAL:HG12	7:G:99:LYS:H	1.78	0.48
17:R:28:LEU:HB3	17:R:93:ARG:HH11	1.77	0.48
18:S:156:ASN:O	18:S:158:LEU:HB3	2.13	0.48
2:b:383:PHE:CD2	4:d:347:PRO:HA	2.49	0.48
2:b:434:ARG:NH1	14:o:260:GLY:HA2	2.29	0.48
4:d:236:ASN:O	4:d:239:GLN:HG2	2.13	0.48
37:g:601:CHL:HBB1	37:g:601:CHL:HHC	1.96	0.48
37:g:606:CHL:HMB1	37:g:609:CHL:HAC1	1.96	0.48
35:n:2630:LHG:HC81	39:y:1622:XAT:H361	1.96	0.48
14:o:157:GLN:HE21	14:o:201:LEU:HD22	1.79	0.48
16:q:40:LEU:HB2	16:q:41:GLN:CG	2.42	0.48
7:y:180:GLU:HB2	27:y:610:CLA:C1B	2.42	0.48
1:A:207:GLY:HA3	1:A:278:TRP:HE1	1.78	0.48
2:B:39:LEU:HG	2:B:97:ALA:HB1	1.96	0.48
2:B:345:ILE:HD12	2:B:402:TYR:CE2	2.49	0.48
2:B:383:PHE:CG	4:D:347:PRO:HA	2.49	0.48
3:C:130:ILE:HD12	23:Z:27:PHE:CE2	2.48	0.48
36:F:101:HEM:HBB2	36:F:101:HEM:HMB1	1.95	0.48
7:G:54:ASP:O	7:G:58:PHE:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:69:CYS:HB3	7:G:184:GLY:HA3	1.95	0.48
37:N:601:CHL:C1D	35:N:2630:LHG:HC82	2.42	0.48
14:O:157:GLN:HE21	14:O:201:LEU:HD22	1.79	0.48
16:Q:73:SER:HA	16:Q:76:ASN:ND2	2.29	0.48
18:S:114:THR:HG21	38:S:1621:LUT:O3	2.14	0.48
38:S:1620:LUT:H35	38:S:1620:LUT:H401	1.70	0.48
7:Y:24:TYR:CE2	7:Y:25:LEU:HG	2.49	0.48
7:Y:99:LYS:O	7:Y:102:SER:OG	2.31	0.48
1:a:207:GLY:HA3	1:a:278:TRP:HE1	1.78	0.48
27:b:605:CLA:HBA1	27:b:605:CLA:CHA	2.43	0.48
4:d:68:LEU:HD13	6:f:40:MET:HE2	1.93	0.48
15:p:104:ASP:OD1	15:p:105:SER:N	2.45	0.48
16:q:59:ILE:O	16:q:62:VAL:HG22	2.13	0.48
18:s:66:LYS:HG3	18:s:67:LYS:H	1.78	0.48
18:s:112:PHE:CE2	18:s:113:LYS:HE2	2.48	0.48
1:A:197:PHE:HB3	1:A:285:PHE:O	2.13	0.48
1:A:212:SER:OG	4:D:211:CYS:HB2	2.13	0.48
3:C:327:ASN:HD21	14:O:190:ASP:HB3	1.79	0.48
4:D:306:ALA:HA	14:O:243:LYS:HG3	1.95	0.48
8:H:65:VAL:HG12	8:H:67:LEU:HG	1.95	0.48
35:N:2630:LHG:H211	39:Y:1622:XAT:H10	1.95	0.48
14:O:218:ALA:HB1	14:O:225:PHE:HB3	1.96	0.48
14:O:255:VAL:HA	14:O:262:ARG:HD3	1.96	0.48
17:R:47:GLN:HB3	17:R:67:GLY:H	1.79	0.48
1:a:217:SER:HB2	4:d:142:ASN:HA	1.94	0.48
17:r:223:LEU:O	17:r:227:VAL:HG23	2.14	0.48
7:y:69:CYS:SG	7:y:188:MET:HE2	2.54	0.48
23:z:41:PHE:O	23:z:45:SER:OG	2.27	0.48
1:A:187:GLN:NE2	1:A:191:ASN:HA	2.28	0.48
1:A:230:ASN:O	2:B:3:LEU:HD23	2.14	0.48
2:B:36:SER:OG	29:B:619:BCR:H362	2.14	0.48
2:B:255:THR:HG21	27:B:603:CLA:HED1	1.96	0.48
3:C:56:HIS:HB2	27:C:509:CLA:HMB1	1.96	0.48
3:C:192:GLY:HA2	16:Q:82:ALA:O	2.14	0.48
7:G:180:GLU:OE1	27:G:610:CLA:C4A	2.59	0.48
9:I:5:LYS:HE2	9:I:9:TYR:HE2	1.79	0.48
14:O:245:ARG:NE	14:O:271:GLU:O	2.45	0.48
17:R:29:VAL:HG21	17:R:194:GLN:NE2	2.27	0.48
27:R:601:CLA:HBC2	35:R:2630:LHG:O7	2.14	0.48
1:a:63:ILE:HG21	1:a:336:ALA:HA	1.96	0.48
1:a:197:PHE:HB3	1:a:285:PHE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:407:CLA:O2D	32:c:520:DGD:HAH2	2.13	0.48
29:a:411:BCR:H351	29:a:411:BCR:H15C	1.71	0.48
3:c:192:GLY:HA2	16:q:82:ALA:O	2.14	0.48
3:c:280:SER:OG	3:c:438:PHE:HB2	2.14	0.48
27:c:504:CLA:C3D	32:c:519:DGD:HB21	2.44	0.48
7:g:222:TRP:CH2	37:y:607:CHL:HBC2	2.48	0.48
27:g:610:CLA:H2A	27:g:610:CLA:O1D	2.14	0.48
14:o:143:VAL:HG21	14:o:207:VAL:HG11	1.95	0.48
14:o:255:VAL:HG13	14:o:262:ARG:HD3	1.95	0.48
16:q:73:SER:HA	16:q:76:ASN:ND2	2.29	0.48
2:B:166:ILE:HG22	2:B:167:TRP:O	2.14	0.48
2:B:371:ILE:HG22	2:B:372:ASP:O	2.14	0.48
2:B:475:PHE:CE1	4:D:134:ARG:HB2	2.49	0.48
3:C:61:VAL:HG12	3:C:118:HIS:O	2.13	0.48
3:C:132:HIS:HE1	27:C:513:CLA:NA	2.11	0.48
40:G:1623:NEX:H11	40:G:1623:NEX:H191	1.71	0.48
21:W:129:GLU:HB3	21:W:130:ASP:HB2	1.95	0.48
27:Y:611:CLA:NA	35:Y:2630:LHG:O4	2.46	0.48
1:a:230:ASN:O	2:b:3:LEU:HD23	2.14	0.48
2:b:36:SER:OG	29:b:619:BCR:H362	2.14	0.48
3:c:28:GLN:HE21	4:d:230:ASN:ND2	2.11	0.48
8:h:20:GLY:O	8:h:24:LYS:HG3	2.14	0.48
7:n:70:ARG:HA	7:n:73:MET:HE3	1.96	0.48
15:p:130:THR:HG22	15:p:146:VAL:HG13	1.95	0.48
17:r:47:GLN:HB3	17:r:67:GLY:H	1.79	0.48
27:y:603:CLA:C3D	37:y:609:CHL:H2	2.44	0.48
1:A:224:ILE:HG23	2:B:484:PRO:HA	1.96	0.47
2:B:16:PRO:HB2	2:B:123:PHE:CD1	2.49	0.47
4:D:342:PRO:O	4:D:345:VAL:HG22	2.14	0.47
5:E:60:ARG:NH1	5:E:62:GLY:O	2.47	0.47
2:b:166:ILE:HG22	2:b:167:TRP:O	2.14	0.47
2:b:254:GLY:HA2	32:h:102:DGD:HBW1	1.94	0.47
2:b:364:GLU:HG2	4:d:296:TYR:CE2	2.49	0.47
2:b:365:THR:OG1	4:d:326:ARG:NH2	2.34	0.47
3:c:56:HIS:HB2	27:c:509:CLA:HMB1	1.96	0.47
3:c:186:TYR:HA	3:c:196:VAL:HA	1.96	0.47
3:c:344:SER:OG	3:c:348:GLU:OE1	2.31	0.47
3:c:408:GLY:HA3	3:c:419:TYR:H	1.78	0.47
7:g:74:LEU:HD11	27:g:610:CLA:HBC1	1.96	0.47
8:h:65:VAL:HG12	8:h:67:LEU:HG	1.95	0.47
2:B:364:GLU:HG2	4:D:296:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:VAL:HG21	4:D:299:VAL:HG22	1.97	0.47
3:C:452:ALA:HB1	21:W:135:LEU:HB3	1.96	0.47
37:G:606:CHL:HMB1	37:G:609:CHL:HAC1	1.96	0.47
14:O:98:LYS:O	16:Q:72:PRO:HG3	2.14	0.47
7:Y:211:ASP:O	7:Y:219:ASN:ND2	2.42	0.47
2:b:16:PRO:HB2	2:b:123:PHE:CD1	2.49	0.47
27:b:608:CLA:HBA2	27:b:608:CLA:C4A	2.43	0.47
3:c:288:CYS:SG	32:c:518:DGD:HB22	2.54	0.47
29:c:516:BCR:C7	23:z:20:LEU:HD11	2.44	0.47
18:s:114:THR:HG21	38:s:1621:LUT:O3	2.14	0.47
30:A:412:SQD:H322	29:C:516:BCR:H391	1.96	0.47
2:B:311:PHE:HA	2:B:430:PHE:HZ	1.79	0.47
2:B:383:PHE:HD1	14:O:251:TYR:CE1	2.32	0.47
2:B:383:PHE:CD2	4:D:347:PRO:HA	2.49	0.47
27:B:603:CLA:H42	32:H:102:DGD:HB22	1.96	0.47
3:C:182:PHE:CZ	27:S:614:CLA:HBB1	2.50	0.47
15:P:104:ASP:OD1	15:P:105:SER:N	2.45	0.47
15:P:136:ALA:HA	15:P:137:ASP:OD1	2.14	0.47
3:c:444:HIS:CE1	27:c:508:CLA:NA	2.82	0.47
4:d:70:GLY:HA3	10:j:36:LEU:HB3	1.96	0.47
4:d:273:PHE:HZ	35:d:408:LHG:H122	1.78	0.47
15:p:49:TYR:HB2	15:p:59:LEU:HG	1.95	0.47
15:p:136:ALA:HA	15:p:137:ASP:OD1	2.14	0.47
27:r:601:CLA:HBC2	35:r:2630:LHG:O7	2.14	0.47
1:A:63:ILE:HG21	1:A:336:ALA:HA	1.96	0.47
1:A:140:ARG:NH1	4:D:231:THR:HG21	2.30	0.47
28:A:408:PHO:HBC2	28:A:408:PHO:HHH	1.96	0.47
3:C:186:TYR:HA	3:C:196:VAL:HA	1.96	0.47
3:C:391:ARG:NE	16:Q:84:TYR:OH	2.48	0.47
27:C:504:CLA:C3D	32:C:519:DGD:HB21	2.44	0.47
29:C:516:BCR:C7	23:Z:20:LEU:HD11	2.44	0.47
4:D:273:PHE:HZ	35:D:408:LHG:H122	1.78	0.47
7:G:81:PHE:HB3	7:G:82:PRO:HD3	1.96	0.47
27:G:611:CLA:H3A	27:G:611:CLA:HBA1	1.41	0.47
10:J:24:LEU:O	10:J:27:ILE:HG22	2.15	0.47
7:N:52:SER:HB3	7:N:58:PHE:HD1	1.80	0.47
1:a:246:TYR:CE1	33:d:401:BCT:O1	2.68	0.47
2:b:345:ILE:HD12	2:b:402:TYR:CE2	2.49	0.47
2:b:454:GLY:HA2	31:b:622:LMG:H211	1.96	0.47
3:c:327:ASN:HD21	14:o:190:ASP:HB3	1.79	0.47
5:e:23:HIS:NE2	36:f:101:HEM:ND	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:601:CHL:HBA2	37:y:609:CHL:HBA1	1.96	0.47
9:i:19:PHE:CE1	9:i:23:PHE:HE2	2.32	0.47
14:o:132:LYS:HG3	14:o:133:LYS:N	2.29	0.47
14:o:245:ARG:HA	14:o:251:TYR:O	2.13	0.47
15:p:97:THR:OG1	15:p:98:ASP:HB3	2.15	0.47
20:u:6:THR:HG22	20:u:10:LYS:HZ3	1.80	0.47
1:A:321:ILE:HG12	4:D:180:ARG:HB3	1.97	0.47
2:B:454:GLY:HA2	31:B:622:LMG:H211	1.96	0.47
37:G:601:CHL:HBB1	37:G:601:CHL:HHC	1.96	0.47
14:O:237:SER:HB3	15:P:98:ASP:O	2.14	0.47
17:R:188:GLU:O	17:R:190:LYS:N	2.48	0.47
37:Y:607:CHL:HBB2	37:Y:609:CHL:HBC1	1.97	0.47
23:Z:3:ILE:H	23:Z:61:ILE:HG21	1.79	0.47
3:c:101:PRO:HB3	16:q:86:ARG:HB3	1.96	0.47
14:o:237:SER:HB3	15:p:98:ASP:O	2.15	0.47
15:p:45:GLN:HA	15:p:62:LEU:HA	1.96	0.47
15:p:152:LYS:HD2	15:p:185:VAL:HG11	1.97	0.47
1:A:246:TYR:CE1	33:D:401:BCT:O1	2.68	0.47
2:B:434:ARG:NH2	14:O:264:ASP:OD2	2.48	0.47
3:C:288:CYS:SG	32:C:518:DGD:HB22	2.54	0.47
4:D:56:THR:HB	5:E:49:SER:HA	1.95	0.47
5:E:14:ILE:O	5:E:20:TRP:NE1	2.42	0.47
5:E:23:HIS:NE2	36:F:101:HEM:ND	2.63	0.47
7:G:175:GLU:HG3	27:G:611:CLA:HED1	1.95	0.47
7:N:44:TYR:HD2	27:N:602:CLA:HMD1	1.80	0.47
15:P:74:PHE:CE2	15:P:156:LEU:HD21	2.49	0.47
27:Y:603:CLA:C3D	37:Y:609:CHL:H2	2.44	0.47
2:b:442:VAL:HG21	4:d:299:VAL:HG22	1.96	0.47
27:b:602:CLA:H91	27:b:602:CLA:C2D	2.45	0.47
4:d:188:PHE:HD1	4:d:326:ARG:HG2	1.79	0.47
5:e:30:LEU:HD13	6:f:28:VAL:HG13	1.96	0.47
27:g:604:CLA:C2B	40:g:1623:NEX:H383	2.45	0.47
7:n:52:SER:HB3	7:n:58:PHE:HD1	1.80	0.47
15:p:144:HIS:HD1	15:p:168:TRP:CG	2.33	0.47
21:w:121:PHE:CD2	27:y:612:CLA:H42	2.48	0.47
2:B:142:HIS:HB3	27:B:611:CLA:H101	1.97	0.47
27:B:602:CLA:H143	27:B:602:CLA:H161	1.65	0.47
3:C:27:ASP:O	3:C:31:THR:HG22	2.15	0.47
3:C:280:SER:OG	3:C:438:PHE:HB2	2.14	0.47
3:C:444:HIS:CE1	27:C:508:CLA:NA	2.82	0.47
7:G:81:PHE:CE2	7:G:85:LEU:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:2630:LHG:HC81	39:Y:1622:XAT:H361	1.96	0.47
7:Y:185:ARG:HD3	27:Y:602:CLA:CHD	2.45	0.47
37:Y:601:CHL:H102	37:Y:601:CHL:H61	1.46	0.47
40:Y:1623:NEX:H192	40:Y:1623:NEX:H183	1.96	0.47
1:a:131:TRP:HZ2	3:c:449:ARG:HG2	1.79	0.47
1:a:140:ARG:NH1	4:d:231:THR:HG21	2.30	0.47
28:a:408:PHO:HHD	28:a:408:PHO:HBC2	1.95	0.47
30:a:412:SQD:H322	29:c:516:BCR:H391	1.96	0.47
3:c:182:PHE:CZ	27:s:614:CLA:HBB1	2.50	0.47
27:c:509:CLA:H3A	27:c:509:CLA:HBA1	1.55	0.47
4:d:78:VAL:O	4:d:111:TRP:HD1	1.98	0.47
4:d:126:MET:HE1	4:d:147:SER:HB3	1.97	0.47
4:d:229:ALA:O	35:d:410:LHG:O1	2.25	0.47
5:e:60:ARG:NH1	5:e:62:GLY:O	2.47	0.47
7:g:81:PHE:HB3	7:g:82:PRO:HD3	1.96	0.47
7:g:81:PHE:CE2	7:g:85:LEU:HD11	2.50	0.47
7:g:176:LEU:C	27:g:610:CLA:HMA1	2.40	0.47
10:j:24:LEU:O	10:j:27:ILE:HG22	2.15	0.47
40:n:1623:NEX:H35	40:n:1623:NEX:H401	1.77	0.47
40:n:1623:NEX:H11	40:n:1623:NEX:H191	1.72	0.47
14:o:210:LEU:HD23	14:o:234:TYR:HA	1.96	0.47
14:o:245:ARG:NE	14:o:271:GLU:O	2.45	0.47
17:r:183:LEU:HB2	27:r:610:CLA:O1A	2.15	0.47
27:s:604:CLA:H2A	27:s:604:CLA:O1D	2.15	0.47
1:A:131:TRP:HZ2	3:C:449:ARG:HG2	1.79	0.47
27:C:509:CLA:H3A	27:C:509:CLA:HBA1	1.54	0.47
4:D:78:VAL:O	4:D:111:TRP:HD1	1.98	0.47
8:H:20:GLY:O	8:H:24:LYS:HG3	2.14	0.47
7:N:70:ARG:HA	7:N:73:MET:HE3	1.96	0.47
7:N:83:GLU:CD	7:N:206:LEU:HB2	2.40	0.47
7:N:128:TRP:O	7:N:132:VAL:HG23	2.15	0.47
38:N:1620:LUT:H15	38:N:1620:LUT:H201	1.77	0.47
7:Y:169:ASP:O	7:Y:173:PHE:N	2.41	0.47
2:b:167:TRP:HD1	2:b:264:PRO:HG2	1.80	0.47
2:b:255:THR:HG21	27:b:603:CLA:HED1	1.96	0.47
3:c:452:ALA:HB1	21:w:135:LEU:HB3	1.96	0.47
4:d:342:PRO:O	4:d:345:VAL:HG22	2.14	0.47
7:n:44:TYR:HD2	27:n:602:CLA:HMD1	1.80	0.47
23:z:3:ILE:H	23:z:61:ILE:HG21	1.79	0.47
28:A:409:PHO:HAC1	4:D:275:PRO:HB2	1.97	0.47
3:C:101:PRO:HB3	16:Q:86:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:HIS:HE1	27:C:513:CLA:C1A	2.28	0.47
3:C:379:ARG:O	3:C:383:ASP:N	2.45	0.47
7:G:156:TYR:HB3	27:G:610:CLA:HED2	1.97	0.47
15:P:144:HIS:HD1	15:P:168:TRP:CG	2.33	0.47
16:Q:22:ASN:HA	16:Q:25:GLN:HB3	1.96	0.47
27:R:616:CLA:HBA1	27:R:616:CLA:H12	1.44	0.47
7:Y:52:SER:HB3	7:Y:58:PHE:HD1	1.79	0.47
2:b:39:LEU:HG	2:b:97:ALA:HB1	1.96	0.47
2:b:142:HIS:HB3	27:b:611:CLA:H101	1.97	0.47
2:b:371:ILE:HG22	2:b:372:ASP:O	2.14	0.47
2:b:434:ARG:NH2	14:o:264:ASP:OD2	2.48	0.47
3:c:402:GLY:HA3	3:c:420:VAL:HG22	1.97	0.47
5:e:26:THR:O	5:e:29:SER:OG	2.22	0.47
7:g:64:LEU:HD11	7:n:49:ALA:HA	1.97	0.47
7:g:157:PRO:HB3	37:g:608:CHL:HBC2	1.96	0.47
18:s:67:LYS:HB2	18:s:70:ASP:H	1.80	0.47
1:A:173:PRO:HB2	1:A:178:GLY:HA3	1.96	0.47
27:B:602:CLA:H91	27:B:602:CLA:C2D	2.45	0.47
4:D:70:GLY:HA3	10:J:36:LEU:HB3	1.96	0.47
4:D:188:PHE:HD1	4:D:326:ARG:HG2	1.79	0.47
7:G:128:TRP:CD1	7:N:222:TRP:HZ2	2.33	0.47
27:N:602:CLA:HBA1	38:N:1621:LUT:H382	1.96	0.47
18:S:105:CYS:HA	27:S:604:CLA:HED1	1.96	0.47
7:Y:69:CYS:SG	7:Y:188:MET:HE2	2.54	0.47
7:g:173:PHE:HE1	27:g:610:CLA:H2A	1.80	0.47
27:g:611:CLA:H3A	27:g:611:CLA:HBA1	1.41	0.47
14:o:218:ALA:HB1	14:o:225:PHE:HB3	1.96	0.47
17:r:188:GLU:O	17:r:190:LYS:N	2.48	0.47
37:r:608:CHL:HBC3	37:r:608:CHL:HHD	1.97	0.47
7:y:109:GLY:HA3	7:y:122:GLN:NE2	2.30	0.47
1:A:239:PHE:HE2	19:T:29:ILE:HG13	1.80	0.46
2:B:384:ARG:HG3	14:O:249:THR:HG22	1.97	0.46
7:G:74:LEU:HD11	27:G:610:CLA:HBC1	1.96	0.46
15:P:92:ALA:HA	15:P:94:PHE:N	2.30	0.46
27:S:604:CLA:H2A	27:S:604:CLA:O1D	2.15	0.46
1:a:173:PRO:HB2	1:a:178:GLY:HA3	1.97	0.46
1:a:198:HIS:CE1	27:a:405:CLA:NB	2.83	0.46
4:d:51:GLY:HA3	4:d:78:VAL:HG22	1.96	0.46
4:d:161:PRO:HB3	4:d:170:ALA:HB2	1.97	0.46
5:e:70:PHE:HD2	20:u:28:LYS:HD2	1.80	0.46
14:o:161:LEU:HD23	21:w:88:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:162:ASP:C	18:s:164:LEU:HA	2.40	0.46
27:s:609:CLA:H3A	27:s:609:CLA:HBA2	1.37	0.46
27:y:602:CLA:H41	27:y:603:CLA:HBA1	1.97	0.46
1:A:197:PHE:CE2	32:C:520:DGD:HBN2	2.50	0.46
2:B:167:TRP:HD1	2:B:264:PRO:HG2	1.80	0.46
3:C:462:ASP:OD1	3:C:463:PHE:N	2.49	0.46
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.15	0.46
4:D:298:PHE:O	4:D:302:GLU:HG2	2.15	0.46
5:E:70:PHE:HD2	20:U:28:LYS:HD2	1.80	0.46
27:G:602:CLA:H62	27:G:602:CLA:H92	1.77	0.46
27:G:604:CLA:H2	37:G:606:CHL:CAD	2.45	0.46
9:I:19:PHE:CE1	9:I:23:PHE:HE2	2.32	0.46
7:N:197:GLN:NE2	38:N:1620:LUT:O3	2.49	0.46
15:P:45:GLN:HA	15:P:62:LEU:HA	1.96	0.46
15:P:121:VAL:O	15:P:123:GLY:N	2.46	0.46
15:P:133:THR:OG1	15:P:143:LYS:O	2.31	0.46
27:R:611:CLA:HBA2	27:R:611:CLA:H3A	1.45	0.46
27:c:503:CLA:H2	27:c:501:CLA:C3D	2.45	0.46
27:g:613:CLA:C4B	38:g:1620:LUT:H183	2.46	0.46
7:n:139:GLU:HG3	37:n:609:CHL:C4B	2.46	0.46
14:o:98:LYS:O	16:q:72:PRO:HG3	2.14	0.46
14:o:151:ASN:CG	14:o:152:SER:H	2.23	0.46
14:o:255:VAL:HA	14:o:262:ARG:HD3	1.96	0.46
15:p:92:ALA:HA	15:p:94:PHE:N	2.30	0.46
1:A:198:HIS:HA	1:A:286:THR:HG22	1.98	0.46
32:C:520:DGD:HAW2	4:D:74:LEU:HD22	1.96	0.46
4:D:49:PHE:HE1	31:D:411:LMG:H321	1.80	0.46
5:E:30:LEU:HD13	6:F:28:VAL:HG13	1.96	0.46
7:G:212:HIS:CG	27:G:613:CLA:HAA2	2.51	0.46
37:G:607:CHL:HBB1	37:G:607:CHL:HHC	1.97	0.46
37:N:607:CHL:H152	37:N:607:CHL:H111	1.52	0.46
15:P:97:THR:OG1	15:P:98:ASP:HB3	2.15	0.46
15:P:152:LYS:HD2	15:P:185:VAL:HG11	1.97	0.46
17:R:13:LEU:HB2	17:R:15:TYR:CE1	2.51	0.46
17:R:183:LEU:HB2	27:R:610:CLA:O1A	2.15	0.46
18:S:162:ASP:C	18:S:164:LEU:HA	2.40	0.46
21:W:105:LEU:O	21:W:108:ILE:HG13	2.16	0.46
2:b:366:PHE:HD2	2:b:425:GLN:NE2	2.13	0.46
27:b:602:CLA:H92	27:b:602:CLA:H61	1.78	0.46
27:b:607:CLA:H2A	27:b:607:CLA:O1D	2.15	0.46
3:c:178:LYS:HB2	27:c:502:CLA:H203	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:405:PL9:H422	34:d:405:PL9:H401	1.70	0.46
27:g:604:CLA:H2	37:g:606:CHL:CAD	2.45	0.46
37:n:601:CHL:HBB1	37:n:601:CHL:CHC	2.42	0.46
15:p:31:PRO:HG3	15:p:175:PHE:HB3	1.98	0.46
17:r:126:LYS:O	17:r:130:ILE:HG12	2.15	0.46
17:r:179:ASP:OD1	38:r:620:LUT:O23	2.23	0.46
18:s:224:ASP:HB3	18:s:227:GLY:HA3	1.97	0.46
7:y:185:ARG:HD3	27:y:602:CLA:CHD	2.45	0.46
27:C:502:CLA:H193	18:S:226:PHE:HE2	1.80	0.46
7:G:197:GLN:HG3	27:G:613:CLA:C1D	2.46	0.46
7:N:139:GLU:HG3	37:N:609:CHL:C4B	2.46	0.46
17:R:210:GLY:O	17:R:214:GLN:N	2.41	0.46
35:Y:2630:LHG:H272	35:Y:2630:LHG:H242	1.54	0.46
1:a:184:ILE:HG23	1:a:328:MET:SD	2.55	0.46
1:a:224:ILE:HG23	2:b:484:PRO:HA	1.96	0.46
2:b:475:PHE:CD1	4:d:134:ARG:HD3	2.50	0.46
3:c:27:ASP:O	3:c:31:THR:HG22	2.15	0.46
37:g:607:CHL:HBB1	37:g:607:CHL:HHC	1.97	0.46
7:n:128:TRP:O	7:n:132:VAL:HG23	2.15	0.46
27:n:602:CLA:HBA1	38:n:1621:LUT:H382	1.96	0.46
14:o:233:SER:N	15:p:100:GLU:OE2	2.48	0.46
1:A:198:HIS:CE1	27:A:405:CLA:NB	2.83	0.46
27:A:407:CLA:HED2	32:C:520:DGD:HAE1	1.98	0.46
2:B:45:PHE:CD1	2:B:60:MET:HG3	2.50	0.46
27:B:613:CLA:H151	27:B:613:CLA:H18	1.69	0.46
27:B:613:CLA:HBA2	27:B:613:CLA:H3A	1.32	0.46
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.97	0.46
27:C:502:CLA:H141	27:C:502:CLA:H161	1.61	0.46
27:C:508:CLA:HBC3	27:C:510:CLA:H92	1.97	0.46
5:E:8:ARG:HH22	5:E:16:SER:HB3	1.81	0.46
7:G:49:ALA:HA	7:Y:64:LEU:HD11	1.98	0.46
7:G:63:GLU:HA	7:G:155:LEU:HD11	1.97	0.46
27:G:613:CLA:C4B	38:G:1620:LUT:H183	2.46	0.46
32:H:102:DGD:O5D	32:H:102:DGD:O4D	2.20	0.46
40:R:623:NEX:H15	40:R:623:NEX:H201	1.68	0.46
27:Y:602:CLA:H41	27:Y:603:CLA:HBA1	1.97	0.46
1:a:239:PHE:HE2	19:t:29:ILE:HG13	1.80	0.46
2:b:236:THR:HB	2:b:473:THR:HG21	1.97	0.46
27:b:603:CLA:H42	32:h:102:DGD:HB22	1.96	0.46
27:c:502:CLA:H141	27:c:502:CLA:H161	1.61	0.46
27:c:509:CLA:H161	27:c:509:CLA:H141	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:89:LEU:HG	8:h:62:ASN:ND2	2.31	0.46
31:d:411:LMG:O6	6:f:41:GLN:NE2	2.40	0.46
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.98	0.46
7:g:94:GLU:HB3	7:g:103:GLN:HE21	1.81	0.46
37:g:609:CHL:HAA2	7:n:48:THR:HG21	1.97	0.46
9:i:5:LYS:HE2	9:i:9:TYR:HE2	1.79	0.46
18:s:105:CYS:HA	27:s:604:CLA:HED1	1.96	0.46
21:w:105:LEU:O	21:w:108:ILE:HG13	2.15	0.46
7:y:169:ASP:O	7:y:173:PHE:N	2.40	0.46
7:G:157:PRO:HB3	37:G:608:CHL:HBC2	1.96	0.46
37:G:607:CHL:HBC2	7:N:222:TRP:CH2	2.51	0.46
18:S:44:ASP:C	18:S:45:ILE:HG13	2.41	0.46
1:a:197:PHE:CE2	32:c:520:DGD:HBN2	2.50	0.46
1:a:246:TYR:HE1	33:d:401:BCT:O1	1.99	0.46
1:a:321:ILE:HG12	4:d:180:ARG:HB3	1.96	0.46
2:b:324:LEU:HD21	4:d:196:PHE:HE2	1.81	0.46
27:b:613:CLA:H3A	27:b:613:CLA:HBA2	1.31	0.46
3:c:343:ARG:NH1	3:c:347:GLY:O	2.45	0.46
3:c:451:ALA:HA	3:c:456:GLU:OE1	2.16	0.46
3:c:462:ASP:OD1	3:c:463:PHE:N	2.49	0.46
4:d:298:PHE:O	4:d:302:GLU:HG2	2.15	0.46
7:g:44:TYR:CD2	37:g:601:CHL:HMD2	2.51	0.46
7:g:128:TRP:CD1	7:n:222:TRP:HZ2	2.33	0.46
7:n:83:GLU:CD	7:n:206:LEU:HB2	2.40	0.46
17:r:197:GLU:OE1	27:r:610:CLA:NB	2.48	0.46
7:y:52:SER:HB3	7:y:58:PHE:HD1	1.80	0.46
40:y:1623:NEX:H192	40:y:1623:NEX:H183	1.95	0.46
2:B:486:LEU:HD23	2:B:488:VAL:H	1.80	0.46
3:C:213:LEU:HD23	3:C:224:ILE:HG21	1.98	0.46
3:C:425:TRP:HB3	27:C:504:CLA:HHB	1.98	0.46
27:C:503:CLA:H2	27:C:501:CLA:C3D	2.46	0.46
4:D:152:VAL:HG22	27:D:402:CLA:HED3	1.97	0.46
27:G:602:CLA:H93	27:G:602:CLA:H111	1.67	0.46
7:N:121:ALA:HA	37:N:605:CHL:C1C	2.46	0.46
15:P:62:LEU:HD11	15:P:158:ILE:HD12	1.98	0.46
17:R:126:LYS:O	17:R:130:ILE:HG12	2.15	0.46
17:R:197:GLU:OE1	27:R:610:CLA:NB	2.49	0.46
7:Y:117:SER:HB3	17:r:141:PRO:HD3	1.97	0.46
7:Y:208:ASN:HB3	27:Y:613:CLA:O1D	2.16	0.46
27:Y:613:CLA:H8	27:Y:614:CLA:HMD3	1.98	0.46
1:a:92:HIS:CE1	3:c:220:GLY:HA3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:409:PHO:HAC1	4:d:275:PRO:HB2	1.97	0.46
2:b:486:LEU:HD23	2:b:488:VAL:H	1.81	0.46
32:c:520:DGD:HAW2	4:d:74:LEU:HD22	1.96	0.46
4:d:49:PHE:HE1	31:d:411:LMG:H321	1.80	0.46
4:d:79:SER:O	4:d:111:TRP:HB2	2.16	0.46
4:d:129:GLN:OE1	4:d:143:ALA:HA	2.15	0.46
7:g:156:TYR:HB3	27:g:610:CLA:HED2	1.97	0.46
7:g:197:GLN:O	7:g:201:THR:OG1	2.16	0.46
7:n:58:PHE:O	7:n:62:ARG:HG3	2.15	0.46
7:n:121:ALA:HA	37:n:605:CHL:C1C	2.46	0.46
17:r:151:GLU:OE1	37:r:607:CHL:HMC	2.15	0.46
18:s:114:THR:HA	18:s:117:LEU:HD23	1.98	0.46
18:s:124:LEU:HG	18:s:128:GLY:HA2	1.97	0.46
1:A:184:ILE:HG23	1:A:328:MET:SD	2.55	0.46
1:A:312:ARG:HD2	5:E:56:PHE:CE2	2.51	0.46
2:B:366:PHE:HD2	2:B:425:GLN:NE2	2.13	0.46
2:B:475:PHE:CD1	4:D:134:ARG:HD3	2.51	0.46
3:C:210:PHE:HD1	3:C:213:LEU:HD12	1.81	0.46
27:C:505:CLA:HMD3	27:C:507:CLA:HAB	1.98	0.46
4:D:141:TYR:OH	35:D:408:LHG:O4	2.10	0.46
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.98	0.46
7:G:135:MET:HA	7:G:138:VAL:HG22	1.98	0.46
32:H:102:DGD:HB62	32:H:102:DGD:HB91	1.70	0.46
14:O:233:SER:N	15:P:100:GLU:OE2	2.48	0.46
17:R:93:ARG:HH12	27:R:602:CLA:CED	2.26	0.46
27:a:407:CLA:HED2	32:c:520:DGD:HAE1	1.98	0.46
2:b:45:PHE:CD1	2:b:60:MET:HG3	2.50	0.46
3:c:210:PHE:HD1	3:c:213:LEU:HD12	1.81	0.46
3:c:425:TRP:HB3	27:c:504:CLA:HBB	1.98	0.46
27:d:403:CLA:HBB1	27:d:403:CLA:HMB1	1.98	0.46
5:e:8:ARG:HH22	5:e:16:SER:HB3	1.81	0.46
7:g:131:GLN:HE21	37:g:609:CHL:HMC	1.81	0.46
7:g:197:GLN:HG3	27:g:613:CLA:C1D	2.46	0.46
18:s:66:LYS:HG3	18:s:67:LYS:N	2.31	0.46
18:s:133:ILE:HD13	18:s:137:LEU:HB3	1.98	0.46
27:y:610:CLA:H52	38:y:1620:LUT:H30	1.98	0.46
1:A:92:HIS:CE1	3:C:220:GLY:HA3	2.51	0.46
4:D:89:LEU:HG	8:H:62:ASN:ND2	2.31	0.46
7:G:64:LEU:HD11	7:N:49:ALA:HA	1.97	0.46
37:G:607:CHL:HAA2	39:Y:1622:XAT:H41	1.98	0.46
39:G:1622:XAT:H15	39:G:1622:XAT:H201	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:58:PHE:O	7:N:62:ARG:HG3	2.15	0.46
14:O:151:ASN:CG	14:O:152:SER:H	2.23	0.46
14:O:161:LEU:HD23	21:W:88:ARG:NH2	2.30	0.46
17:R:197:GLU:CD	27:R:610:CLA:NB	2.74	0.46
18:S:124:LEU:HG	18:S:128:GLY:HA2	1.97	0.46
27:Y:602:CLA:H52	38:Y:1621:LUT:H28	1.98	0.46
3:c:132:HIS:HE1	27:c:513:CLA:C1A	2.28	0.46
7:g:63:GLU:HA	7:g:155:LEU:HD11	1.97	0.46
7:g:135:MET:HA	7:g:138:VAL:HG22	1.98	0.46
7:n:197:GLN:NE2	38:n:1620:LUT:O3	2.49	0.46
14:o:238:SER:OG	15:p:136:ALA:O	2.34	0.46
18:s:194:ARG:NH2	27:s:602:CLA:O2D	2.49	0.46
18:s:229:ASN:N	18:s:232:THR:OG1	2.49	0.46
1:A:246:TYR:HE1	33:D:401:BCT:O1	1.99	0.46
1:A:331:MET:SD	4:D:347:PRO:HB2	2.56	0.46
3:C:290:VAL:O	3:C:423:ARG:NH1	2.43	0.46
32:C:520:DGD:HB32	32:C:520:DGD:HB61	1.65	0.46
4:D:126:MET:HE3	4:D:143:ALA:O	2.16	0.46
4:D:266:TRP:CH2	35:L:101:LHG:HC82	2.51	0.46
27:D:403:CLA:HBB1	27:D:403:CLA:HMB1	1.98	0.46
7:G:131:GLN:HE21	37:G:609:CHL:HMC	1.81	0.46
7:G:201:THR:HG22	7:G:224:PHE:HE2	1.82	0.46
27:G:604:CLA:C2B	40:G:1623:NEX:H383	2.45	0.46
37:G:609:CHL:HAA2	7:N:48:THR:HG21	1.97	0.46
37:S:608:CHL:H2A	37:S:608:CHL:HED3	1.99	0.46
7:Y:109:GLY:HA3	7:Y:122:GLN:NE2	2.30	0.46
1:a:48:PHE:CE2	34:d:405:PL9:H48	2.35	0.46
1:a:198:HIS:HA	1:a:286:THR:HG22	1.98	0.46
1:a:331:MET:SD	4:d:347:PRO:HB2	2.56	0.46
2:b:411:TYR:CD1	2:b:416:THR:HG21	2.51	0.46
7:g:201:THR:HG22	7:g:224:PHE:HE2	1.81	0.46
17:r:13:LEU:HB2	17:r:15:TYR:CE1	2.51	0.46
17:r:190:LYS:HB3	17:r:193:LEU:HG	1.97	0.46
7:y:208:ASN:HB3	27:y:613:CLA:O1D	2.16	0.46
37:y:607:CHL:HBB2	37:y:609:CHL:HBC1	1.97	0.46
2:B:236:THR:HB	2:B:473:THR:HG21	1.98	0.45
2:B:246:PHE:HB3	2:B:462:PHE:HB2	1.98	0.45
3:C:178:LYS:HB2	27:C:502:CLA:H203	1.98	0.45
3:C:290:VAL:HG21	3:C:426:LEU:HB2	1.98	0.45
7:G:94:GLU:HB3	7:G:103:GLN:HE21	1.81	0.45
7:G:128:TRP:O	7:G:132:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:176:LEU:C	27:G:610:CLA:HMA1	2.40	0.45
8:H:61:TYR:CE1	32:H:102:DGD:HB31	2.51	0.45
14:O:116:GLU:HA	14:O:117:GLY:HA2	1.51	0.45
14:O:210:LEU:HD23	14:O:234:TYR:HA	1.96	0.45
17:R:23:TYR:OH	17:R:38:GLY:HA2	2.15	0.45
17:R:151:GLU:OE1	37:R:607:CHL:HMC	2.15	0.45
18:S:66:LYS:HG3	18:S:67:LYS:N	2.31	0.45
7:Y:64:LEU:HD13	27:Y:603:CLA:HAA2	1.98	0.45
1:a:288:LEU:HD13	3:c:432:VAL:HG13	1.98	0.45
2:b:167:TRP:HA	2:b:178:VAL:HA	1.98	0.45
3:c:334:PRO:HB3	15:p:137:ASP:HB2	1.98	0.45
27:c:502:CLA:H152	27:c:502:CLA:H111	1.86	0.45
7:g:49:ALA:HA	7:y:64:LEU:HD11	1.98	0.45
7:g:128:TRP:O	7:g:132:VAL:HG23	2.16	0.45
39:g:1622:XAT:H31	39:g:1622:XAT:H391	1.83	0.45
27:y:611:CLA:H122	27:y:612:CLA:H143	1.99	0.45
27:y:613:CLA:H8	27:y:614:CLA:HMD3	1.98	0.45
1:A:56:PRO:HB2	14:O:206:ARG:NH2	2.30	0.45
1:A:217:SER:HA	4:D:272:LEU:HD12	1.99	0.45
1:A:237:TYR:CD2	4:D:263:ASN:HA	2.51	0.45
2:B:256:MET:HA	2:B:263:THR:HG21	1.99	0.45
27:B:607:CLA:H2A	27:B:607:CLA:O1D	2.16	0.45
3:C:223:TRP:CG	3:C:224:ILE:N	2.82	0.45
3:C:256:PRO:O	3:C:261:ARG:NH1	2.49	0.45
29:C:517:BCR:H15C	29:C:517:BCR:H351	1.73	0.45
29:C:517:BCR:H24C	29:C:517:BCR:H371	1.71	0.45
4:D:14:LEU:O	4:D:17:SER:OG	2.27	0.45
4:D:21:TRP:CZ2	22:X:108:VAL:HG11	2.52	0.45
37:G:605:CHL:H3A	37:G:605:CHL:HBA2	1.73	0.45
7:N:180:GLU:OE1	27:N:610:CLA:C4A	2.64	0.45
14:O:133:LYS:HZ1	14:O:328:GLN:CD	2.19	0.45
15:P:15:ASN:HA	15:P:16:THR:HA	1.61	0.45
18:S:158:LEU:HB2	37:S:608:CHL:HAC1	1.98	0.45
18:S:224:ASP:O	18:S:228:ASN:N	2.38	0.45
7:Y:63:GLU:HA	7:Y:155:LEU:HD11	1.98	0.45
39:Y:1622:XAT:H31	39:Y:1622:XAT:H391	1.78	0.45
1:a:131:TRP:CH2	27:c:505:CLA:HAA2	2.52	0.45
1:a:339:PHE:HB3	1:a:340:PRO:HD2	1.98	0.45
37:g:607:CHL:HBC2	7:n:222:TRP:CH2	2.51	0.45
16:q:14:SER:HA	16:q:15:GLY:HA3	1.68	0.45
17:r:210:GLY:O	17:r:214:GLN:N	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:r:606:CHL:H43	40:r:623:NEX:H402	1.98	0.45
21:w:129:GLU:HA	21:w:130:ASP:HA	1.76	0.45
7:y:66:VAL:HG21	7:y:155:LEU:HD13	1.98	0.45
7:y:215:ASP:OD2	7:y:218:ASN:ND2	2.39	0.45
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.51	0.45
3:C:167:LEU:HD13	27:C:512:CLA:HBA2	1.98	0.45
31:C:521:LMG:H291	31:C:521:LMG:H182	1.99	0.45
4:D:126:MET:HE1	4:D:147:SER:HB3	1.97	0.45
7:G:92:PHE:CE1	7:G:113:LEU:HA	2.50	0.45
7:G:173:PHE:HE1	27:G:610:CLA:H2A	1.80	0.45
14:O:231:VAL:HG21	14:O:306:PRO:HD2	1.99	0.45
15:P:31:PRO:HG3	15:P:175:PHE:HB3	1.98	0.45
38:R:620:LUT:H15	38:R:620:LUT:H201	1.80	0.45
18:S:67:LYS:HB2	18:S:70:ASP:H	1.80	0.45
7:Y:81:PHE:HB3	7:Y:82:PRO:HD3	1.98	0.45
27:Y:602:CLA:H92	27:Y:603:CLA:HMA1	1.99	0.45
1:a:217:SER:HA	4:d:272:LEU:HD12	1.99	0.45
1:a:312:ARG:HD2	5:e:56:PHE:CE2	2.51	0.45
27:a:407:CLA:O1D	32:c:520:DGD:HAH2	2.16	0.45
2:b:384:ARG:HG3	14:o:249:THR:HG22	1.97	0.45
3:c:167:LEU:HD13	27:c:512:CLA:HBA2	1.98	0.45
29:c:516:BCR:H15C	29:c:516:BCR:H351	1.83	0.45
31:c:521:LMG:H291	31:c:521:LMG:H182	1.99	0.45
37:g:607:CHL:HAA2	39:y:1622:XAT:H41	1.98	0.45
8:h:61:TYR:CE1	32:h:102:DGD:HB31	2.51	0.45
16:q:22:ASN:O	16:q:26:ALA:N	2.40	0.45
17:r:23:TYR:OH	17:r:38:GLY:HA2	2.15	0.45
18:s:206:GLN:OE1	27:s:613:CLA:C4D	2.47	0.45
1:A:131:TRP:CH2	27:C:505:CLA:HAA2	2.52	0.45
2:B:167:TRP:HA	2:B:178:VAL:HA	1.98	0.45
2:B:298:PHE:HB2	2:B:402:TYR:CD1	2.51	0.45
31:B:622:LMG:HC92	13:M:6:LEU:HD12	1.98	0.45
3:C:451:ALA:HA	3:C:456:GLU:OE1	2.16	0.45
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.97	0.45
4:D:261:PHE:HD2	34:D:405:PL9:HC72	1.82	0.45
37:R:608:CHL:HBC3	37:R:608:CHL:HHD	1.97	0.45
18:S:109:ALA:HA	18:S:110:VAL:O	2.17	0.45
18:S:114:THR:HA	18:S:117:LEU:HD23	1.98	0.45
27:Y:610:CLA:H2	38:Y:1620:LUT:H28	1.98	0.45
27:Y:611:CLA:H122	27:Y:612:CLA:H143	1.98	0.45
1:a:56:PRO:HB2	14:o:206:ARG:NH2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:405:CLA:HBB1	27:a:405:CLA:HMB3	1.97	0.45
2:b:166:ILE:HD13	27:b:604:CLA:HED1	1.98	0.45
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.51	0.45
3:c:132:HIS:HE1	27:c:513:CLA:NA	2.11	0.45
27:c:502:CLA:H193	18:s:226:PHE:HE2	1.80	0.45
27:c:508:CLA:H92	27:c:508:CLA:H61	1.78	0.45
27:c:508:CLA:HBC3	27:c:510:CLA:H92	1.97	0.45
27:c:510:CLA:H61	27:c:510:CLA:H2	1.64	0.45
4:d:152:VAL:HG22	27:d:402:CLA:HED3	1.97	0.45
7:g:212:HIS:CG	27:g:613:CLA:HAA2	2.51	0.45
32:h:102:DGD:HB62	32:h:102:DGD:HB32	1.74	0.45
39:n:1622:XAT:H15	39:n:1622:XAT:H201	1.75	0.45
18:s:44:ASP:C	18:s:45:ILE:HG13	2.41	0.45
18:s:109:ALA:HA	18:s:110:VAL:C	2.42	0.45
7:y:81:PHE:HB3	7:y:82:PRO:HD3	1.98	0.45
7:y:118:LEU:HD23	37:y:605:CHL:HED2	1.98	0.45
27:y:602:CLA:H92	27:y:603:CLA:HMA1	1.99	0.45
1:A:269:ARG:HE	4:D:222:LEU:HD13	1.82	0.45
2:B:340:TRP:HB2	2:B:430:PHE:HE1	1.81	0.45
2:B:413:ASP:HA	2:B:414:PRO:HD3	1.83	0.45
17:R:128:GLU:OE2	27:R:604:CLA:HAA1	2.16	0.45
17:R:141:PRO:HD3	7:y:117:SER:HB3	1.96	0.45
18:S:119:LEU:HD12	18:S:120:ASP:OD1	2.16	0.45
18:S:224:ASP:HB3	18:S:227:GLY:HA3	1.96	0.45
20:U:8:GLU:HA	20:U:11:LYS:NZ	2.32	0.45
7:Y:42:GLY:O	7:Y:185:ARG:NH1	2.44	0.45
39:Y:1622:XAT:H35	39:Y:1622:XAT:H401	1.68	0.45
4:d:185:PHE:CD2	27:d:402:CLA:HMD1	2.52	0.45
7:g:23:LYS:HG3	7:g:29:SER:HB3	1.98	0.45
14:o:231:VAL:HG21	14:o:306:PRO:HD2	1.99	0.45
17:r:185:SER:HA	17:r:186:ASP:HA	1.70	0.45
23:z:27:PHE:HE1	23:z:33:TRP:CZ3	2.35	0.45
1:A:227:THR:HB	1:A:231:GLU:HG3	1.98	0.45
27:A:405:CLA:H72	27:A:405:CLA:H111	1.69	0.45
3:C:334:PRO:HB3	15:P:137:ASP:HB2	1.98	0.45
4:D:79:SER:O	4:D:111:TRP:HB2	2.16	0.45
7:G:23:LYS:HG3	7:G:29:SER:HB3	1.98	0.45
7:G:44:TYR:CD2	37:G:601:CHL:HMD2	2.51	0.45
7:G:71:TRP:CD1	37:G:609:CHL:HMD3	2.52	0.45
14:O:207:VAL:HA	14:O:208:PRO:HD2	1.70	0.45
17:R:213:VAL:HG21	27:R:613:CLA:HAC2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:49:LEU:HB3	18:S:56:ASP:OD1	2.17	0.45
18:S:194:ARG:NH2	27:S:602:CLA:O2D	2.49	0.45
7:Y:118:LEU:HD23	37:Y:605:CHL:HED2	1.98	0.45
2:b:298:PHE:HB2	2:b:402:TYR:CD1	2.51	0.45
31:b:622:LMG:HC92	13:m:6:LEU:HD12	1.98	0.45
3:c:69:LEU:HA	3:c:72:VAL:HG12	1.98	0.45
3:c:391:ARG:NE	16:q:84:TYR:OH	2.48	0.45
4:d:349:GLY:HA2	4:d:350:ASN:HA	1.62	0.45
29:h:101:BCR:H371	29:h:101:BCR:H24C	1.79	0.45
17:r:76:LYS:HZ3	17:r:84:SER:HB2	1.82	0.45
18:s:158:LEU:HB2	37:s:608:CHL:HAC1	1.98	0.45
20:u:8:GLU:HA	20:u:11:LYS:NZ	2.32	0.45
2:B:166:ILE:HD13	27:B:604:CLA:HED1	1.98	0.45
2:B:201:HIS:HE1	27:B:603:CLA:C1D	2.30	0.45
3:C:223:TRP:CE3	3:C:224:ILE:HG13	2.52	0.45
3:C:387:TRP:CE2	16:Q:83:SER:OG	2.68	0.45
32:C:519:DGD:HB81	31:C:521:LMG:H421	1.98	0.45
8:H:56:ILE:HG12	22:X:87:PHE:CE2	2.52	0.45
14:O:238:SER:OG	15:P:136:ALA:O	2.34	0.45
17:R:190:LYS:HB3	17:R:193:LEU:HG	1.98	0.45
18:S:88:GLY:HA2	38:S:1621:LUT:H181	1.98	0.45
18:S:94:ILE:HG22	18:S:95:PRO:HD3	1.99	0.45
2:b:246:PHE:HB3	2:b:462:PHE:HB2	1.98	0.45
3:c:213:LEU:HD23	3:c:224:ILE:HG21	1.98	0.45
3:c:361:LEU:HD12	32:c:518:DGD:O3E	2.17	0.45
7:g:71:TRP:CD1	37:g:609:CHL:HMD3	2.52	0.45
7:g:92:PHE:CE1	7:g:113:LEU:HA	2.50	0.45
7:g:213:LEU:HD21	27:g:614:CLA:HMC2	1.99	0.45
7:n:104:ILE:HG21	7:n:124:ILE:HD13	1.97	0.45
17:r:128:GLU:OE2	27:r:604:CLA:HAA1	2.16	0.45
17:r:197:GLU:CD	27:r:610:CLA:NB	2.74	0.45
18:s:49:LEU:HB3	18:s:56:ASP:OD1	2.17	0.45
18:s:119:LEU:HD12	18:s:120:ASP:OD1	2.16	0.45
38:s:1621:LUT:H35	38:s:1621:LUT:H401	1.77	0.45
7:y:63:GLU:HA	7:y:155:LEU:HD11	1.98	0.45
7:y:146:GLY:N	37:y:608:CHL:HMC	2.32	0.45
2:B:14:ASN:OD1	17:R:53:LEU:HB2	2.17	0.45
3:C:187:ASP:HB3	3:C:190:ALA:HB2	1.99	0.45
3:C:390:ARG:NH1	16:Q:40:LEU:O	2.50	0.45
4:D:94:GLY:O	4:D:98:GLN:N	2.41	0.45
7:G:112:TYR:HD2	7:G:118:LEU:HD13	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:104:ILE:HG21	7:N:124:ILE:HD13	1.97	0.45
27:N:610:CLA:H92	27:N:610:CLA:H61	1.78	0.45
38:N:1620:LUT:H35	38:N:1620:LUT:H401	1.78	0.45
15:P:119:PRO:HD2	15:P:126:TYR:O	2.17	0.45
15:P:136:ALA:HA	15:P:137:ASP:HA	1.67	0.45
16:Q:14:SER:HA	16:Q:15:GLY:HA3	1.68	0.45
18:S:133:ILE:HD13	18:S:137:LEU:HB3	1.98	0.45
22:X:110:ASN:O	22:X:113:PRO:HD3	2.17	0.45
1:a:237:TYR:CD2	4:d:263:ASN:HA	2.51	0.45
2:b:247:PHE:HB2	27:b:609:CLA:HBC1	1.99	0.45
2:b:283:GLU:OE2	2:b:286:ARG:NH2	2.50	0.45
3:c:93:ALA:HB1	3:c:99:VAL:HG11	1.99	0.45
7:g:112:TYR:HD2	7:g:118:LEU:HD13	1.81	0.45
15:p:62:LEU:HD11	15:p:158:ILE:HD12	1.98	0.45
15:p:133:THR:OG1	15:p:143:LYS:O	2.31	0.45
27:r:601:CLA:C4C	35:r:2630:LHG:HC82	2.47	0.45
18:s:62:PHE:CD2	38:s:1621:LUT:H222	2.52	0.45
1:A:267:ASN:OD1	1:A:268:SER:N	2.50	0.45
2:B:181:VAL:CG1	2:B:196:GLY:HA2	2.47	0.45
3:C:142:GLU:OE1	3:C:142:GLU:N	2.50	0.45
4:D:266:TRP:HH2	35:L:101:LHG:HC82	1.81	0.45
7:G:59:ALA:HA	7:G:62:ARG:NH1	2.32	0.45
39:G:1622:XAT:H373	39:G:1622:XAT:H23	1.76	0.45
17:R:108:LEU:O	17:R:112:THR:HG22	2.17	0.45
1:a:127:MET:HE3	27:c:505:CLA:HMB2	1.99	0.45
1:a:225:ARG:HD3	17:r:58:ALA:HB1	1.98	0.45
31:a:413:LMG:H411	32:c:518:DGD:HB72	1.99	0.45
2:b:150:CYS:HB2	27:b:604:CLA:CMC	2.47	0.45
2:b:340:TRP:HB2	2:b:430:PHE:HE1	1.81	0.45
3:c:223:TRP:CE3	3:c:224:ILE:HG13	2.52	0.45
32:c:519:DGD:HB81	31:c:521:LMG:H421	1.98	0.45
15:p:109:ALA:HA	15:p:135:THR:HA	1.99	0.45
15:p:119:PRO:HD2	15:p:126:TYR:O	2.17	0.45
18:s:109:ALA:HA	18:s:110:VAL:O	2.17	0.45
7:y:111:ASP:OD1	7:y:120:HIS:ND1	2.40	0.45
1:A:288:LEU:HD13	3:C:432:VAL:HG13	1.98	0.45
3:C:69:LEU:HA	3:C:72:VAL:HG12	1.98	0.45
3:C:213:LEU:O	3:C:223:TRP:NE1	2.46	0.45
3:C:344:SER:OG	3:C:348:GLU:OE1	2.31	0.45
3:C:377:LEU:HB3	14:O:171:GLU:OE1	2.18	0.45
27:C:510:CLA:H2	27:C:510:CLA:H61	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:174:GLY:O	4:D:178:ILE:HG12	2.17	0.45
5:E:77:ASP:O	5:E:81:ARG:HG3	2.17	0.45
13:M:20:ALA:O	13:M:24:ILE:HG13	2.17	0.45
14:O:137:GLU:HA	14:O:168:THR:HG22	1.99	0.45
18:S:44:ASP:N	18:S:44:ASP:OD1	2.49	0.45
21:W:131:GLU:HA	21:W:132:GLU:HA	1.54	0.45
7:Y:92:PHE:HE1	7:Y:113:LEU:HA	1.81	0.45
7:Y:146:GLY:N	37:Y:608:CHL:HMC	2.32	0.45
27:Y:613:CLA:H111	27:Y:613:CLA:H152	1.71	0.45
27:a:406:CLA:H203	27:a:406:CLA:H162	1.74	0.45
2:b:256:MET:HA	2:b:263:THR:HG21	1.99	0.45
2:b:341:LEU:HD12	2:b:429:ILE:HG22	2.00	0.45
27:b:614:CLA:H161	29:b:619:BCR:H312	1.99	0.45
3:c:368:PRO:HA	16:q:76:ASN:HB2	1.99	0.45
4:d:261:PHE:HD2	34:d:405:PL9:HC72	1.82	0.45
4:d:266:TRP:CH2	35:l:101:LHG:HC82	2.51	0.45
4:d:305:ALA:HB3	14:o:243:LYS:HD3	1.98	0.45
27:d:402:CLA:H143	27:d:402:CLA:H161	1.77	0.45
14:o:96:GLN:OE1	16:q:68:ARG:NE	2.32	0.45
17:r:93:ARG:HH12	27:r:602:CLA:CED	2.26	0.45
18:s:214:PRO:O	38:s:1620:LUT:O3	2.33	0.45
37:s:608:CHL:H2A	37:s:608:CHL:HED3	1.98	0.45
27:y:610:CLA:H2	38:y:1620:LUT:H28	1.98	0.45
1:A:130:GLU:HG2	4:D:256:ILE:HG21	1.98	0.44
1:A:259:ILE:HG22	1:A:260:PHE:N	2.29	0.44
27:A:407:CLA:O1D	32:C:520:DGD:HAH2	2.16	0.44
31:A:413:LMG:H411	32:C:518:DGD:HB72	1.99	0.44
2:B:80:ILE:HG13	2:B:81:THR:N	2.32	0.44
2:B:324:LEU:HD21	4:D:196:PHE:HE2	1.81	0.44
2:B:411:TYR:CD1	2:B:416:THR:HG21	2.51	0.44
3:C:93:ALA:HB1	3:C:99:VAL:HG11	1.99	0.44
27:C:505:CLA:CMD	27:C:507:CLA:HAB	2.47	0.44
4:D:305:ALA:HB3	14:O:243:LYS:HD3	1.98	0.44
27:D:402:CLA:H91	27:D:402:CLA:H112	1.82	0.44
7:G:70:ARG:NH1	37:G:608:CHL:OBD	2.37	0.44
40:N:1623:NEX:H35	40:N:1623:NEX:H401	1.77	0.44
27:R:601:CLA:C4C	35:R:2630:LHG:HC82	2.47	0.44
27:a:407:CLA:CED	4:d:175:VAL:HG13	2.47	0.44
30:a:412:SQD:H351	30:a:412:SQD:H382	1.69	0.44
2:b:468:TRP:CH2	35:d:408:LHG:HC42	2.53	0.44
27:b:613:CLA:H61	27:b:613:CLA:H102	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:187:ASP:HB3	3:c:190:ALA:HB2	1.99	0.44
3:c:256:PRO:O	3:c:261:ARG:NH1	2.49	0.44
27:c:505:CLA:HMD3	27:c:507:CLA:HAB	1.98	0.44
27:c:506:CLA:H162	27:c:506:CLA:H122	1.82	0.44
32:c:520:DGD:HBW1	32:c:520:DGD:HB51	1.99	0.44
7:g:127:ILE:HG12	37:g:605:CHL:HAC1	1.99	0.44
39:g:1622:XAT:H373	39:g:1622:XAT:H23	1.76	0.44
14:o:133:LYS:HZ1	14:o:328:GLN:CD	2.18	0.44
16:q:42:PRO:O	16:q:87:TYR:OH	2.28	0.44
17:r:108:LEU:O	17:r:112:THR:HG22	2.17	0.44
18:s:61:PRO:HD2	38:s:1621:LUT:H23	1.99	0.44
18:s:157:GLY:HA2	18:s:158:LEU:O	2.17	0.44
27:y:602:CLA:H52	38:y:1621:LUT:H28	1.98	0.44
1:A:84:PRO:HA	1:A:112:TYR:CG	2.52	0.44
1:A:140:ARG:NH2	1:A:142:TRP:HZ3	2.15	0.44
1:A:339:PHE:HB3	1:A:340:PRO:HD2	1.98	0.44
27:B:614:CLA:H161	29:B:619:BCR:H312	1.99	0.44
3:C:361:LEU:HD12	32:C:518:DGD:O3E	2.17	0.44
3:C:387:TRP:CE3	16:Q:84:TYR:HE2	2.36	0.44
4:D:80:THR:HG21	4:D:170:ALA:O	2.18	0.44
27:G:610:CLA:CHA	27:G:610:CLA:HBA1	2.40	0.44
40:G:1623:NEX:H15	40:G:1623:NEX:H201	1.63	0.44
14:O:164:ARG:HA	21:W:88:ARG:HH12	1.82	0.44
18:S:62:PHE:CD2	38:S:1621:LUT:H222	2.52	0.44
27:Y:610:CLA:H52	38:Y:1620:LUT:H30	1.98	0.44
27:a:406:CLA:HBB1	28:a:408:PHO:H141	1.99	0.44
31:a:413:LMG:H342	3:c:217:PRO:HD3	2.00	0.44
2:b:181:VAL:CG1	2:b:196:GLY:HA2	2.47	0.44
3:c:55:ALA:HB1	29:c:517:BCR:H373	1.99	0.44
4:d:117:HIS:CE1	27:d:403:CLA:NA	2.86	0.44
7:g:52:SER:HB3	7:g:58:PHE:CD1	2.46	0.44
7:g:70:ARG:HA	7:g:73:MET:HE3	1.99	0.44
18:s:88:GLY:HA2	38:s:1621:LUT:H181	1.98	0.44
2:B:85:ILE:HD11	14:o:202:PRO:HD3	1.99	0.44
4:D:311:PHE:O	14:O:242:PRO:HG2	2.18	0.44
14:O:248:SER:OG	14:O:249:THR:N	2.50	0.44
18:S:151:TYR:HA	18:S:154:ILE:HD12	2.00	0.44
18:S:157:GLY:HA2	18:S:158:LEU:O	2.17	0.44
40:Y:1623:NEX:H35	40:Y:1623:NEX:H401	1.80	0.44
3:c:195:ASP:HB2	16:q:86:ARG:HD3	2.00	0.44
4:d:126:MET:HE3	4:d:143:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:59:ALA:HA	7:g:62:ARG:NH1	2.32	0.44
11:k:44:PHE:O	11:k:48:LEU:N	2.47	0.44
14:o:100:TYR:CE2	14:o:104:LYS:HD2	2.53	0.44
15:p:97:THR:HA	15:p:98:ASP:HA	1.67	0.44
18:s:164:LEU:N	18:s:165:HIS:C	2.75	0.44
18:s:224:ASP:O	18:s:228:ASN:N	2.38	0.44
35:s:2630:LHG:H331	35:s:2630:LHG:H361	1.59	0.44
1:A:225:ARG:HD3	17:R:58:ALA:HB1	1.98	0.44
2:B:278:GLY:O	2:B:282:GLN:HG3	2.16	0.44
29:C:515:BCR:H351	29:C:515:BCR:H15C	1.69	0.44
4:D:297:ASP:HA	4:D:315:TYR:OH	2.18	0.44
7:N:24:TYR:HB3	7:N:44:TYR:HB3	2.00	0.44
15:P:99:SER:N	15:P:106:GLY:H	2.03	0.44
18:S:165:HIS:NE2	27:S:610:CLA:HED3	2.33	0.44
18:S:229:ASN:N	18:S:232:THR:OG1	2.49	0.44
7:Y:66:VAL:HG21	7:Y:155:LEU:HD13	1.98	0.44
23:Z:27:PHE:HE1	23:Z:33:TRP:CZ3	2.35	0.44
1:a:227:THR:HB	1:a:231:GLU:HG3	1.98	0.44
1:a:267:ASN:OD1	1:a:268:SER:N	2.50	0.44
2:b:282:GLN:NE2	20:u:25:ILE:HG12	2.33	0.44
29:c:516:BCR:HC41	11:k:38:MET:SD	2.58	0.44
35:d:409:LHG:O1	35:l:101:LHG:O4	2.24	0.44
7:g:180:GLU:OE1	27:g:610:CLA:C4A	2.59	0.44
39:g:1622:XAT:H201	39:g:1622:XAT:H15	1.68	0.44
40:g:1623:NEX:H191	40:g:1623:NEX:H11	1.71	0.44
7:n:64:LEU:HD11	7:y:49:ALA:HA	1.99	0.44
7:n:180:GLU:OE1	27:n:610:CLA:C4A	2.65	0.44
15:p:45:GLN:HG2	15:p:62:LEU:HB3	2.00	0.44
18:s:94:ILE:HG22	18:s:95:PRO:HD3	1.99	0.44
18:s:122:ASN:HB2	18:s:132:PRO:HG2	1.99	0.44
29:A:411:BCR:H20C	29:A:411:BCR:H361	1.83	0.44
2:B:167:TRP:HZ2	2:B:266:GLU:OE1	2.00	0.44
2:B:247:PHE:HB2	27:B:609:CLA:HBC1	1.98	0.44
2:B:282:GLN:NE2	20:U:25:ILE:HG12	2.33	0.44
2:B:468:TRP:CH2	35:D:408:LHG:HC42	2.53	0.44
3:C:55:ALA:HB1	29:C:517:BCR:H373	1.99	0.44
27:C:510:CLA:H192	27:C:510:CLA:H162	1.78	0.44
29:C:516:BCR:HC41	11:K:38:MET:SD	2.58	0.44
35:D:408:LHG:O1	35:L:101:LHG:O5	2.33	0.44
7:G:222:TRP:HB3	7:Y:105:PHE:HZ	1.82	0.44
18:S:83:ARG:HD2	37:S:608:CHL:OBD	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:87:PHE:O	22:X:90:SER:HB3	2.18	0.44
2:b:14:ASN:OD1	17:r:53:LEU:HB2	2.17	0.44
2:b:167:TRP:HZ2	2:b:266:GLU:OE1	2.00	0.44
2:b:201:HIS:HE1	27:b:603:CLA:C1D	2.30	0.44
3:c:57:ALA:O	3:c:61:VAL:HG23	2.18	0.44
3:c:379:ARG:O	3:c:383:ASP:N	2.45	0.44
27:c:505:CLA:CMD	27:c:507:CLA:HAB	2.47	0.44
4:d:21:TRP:CZ2	22:x:108:VAL:HG11	2.52	0.44
4:d:174:GLY:O	4:d:178:ILE:HG12	2.17	0.44
17:r:80:LEU:HD22	27:r:616:CLA:CHC	2.48	0.44
38:r:620:LUT:H15	38:r:620:LUT:H201	1.80	0.44
18:s:83:ARG:HD2	37:s:608:CHL:OBD	2.17	0.44
18:s:165:HIS:NE2	27:s:610:CLA:HED3	2.33	0.44
27:A:407:CLA:CED	4:D:175:VAL:HG13	2.47	0.44
2:B:12:VAL:HB	27:B:613:CLA:HMC2	1.98	0.44
2:B:18:ARG:HG3	2:B:118:TRP:HB3	2.00	0.44
2:B:415:ALA:HB1	2:B:419:LYS:NZ	2.32	0.44
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.00	0.44
9:I:17:SER:HB2	21:W:116:ILE:HD12	1.99	0.44
7:N:136:GLY:CA	37:N:609:CHL:HAB	2.48	0.44
17:R:185:SER:HA	17:R:186:ASP:HA	1.71	0.44
31:Z:101:LMG:HC1	31:Z:101:LMG:HC8	1.87	0.44
1:a:187:GLN:HB2	27:a:405:CLA:CAC	2.48	0.44
1:a:197:PHE:HD2	1:a:289:GLY:HA2	1.83	0.44
2:b:278:GLY:O	2:b:282:GLN:HG3	2.17	0.44
2:b:460:LEU:HG	4:d:280:TRP:HZ3	1.82	0.44
3:c:290:VAL:HG21	3:c:426:LEU:HB2	1.99	0.44
3:c:387:TRP:CE3	16:q:84:TYR:HE2	2.35	0.44
4:d:349:GLY:HA3	14:o:240:LEU:HD11	1.99	0.44
17:r:29:VAL:HG21	17:r:194:GLN:NE2	2.27	0.44
22:x:110:ASN:O	22:x:113:PRO:HD3	2.17	0.44
27:y:613:CLA:H111	27:y:613:CLA:H152	1.71	0.44
35:y:2630:LHG:H272	35:y:2630:LHG:H242	1.54	0.44
1:A:181:ASN:HD22	4:D:314:PHE:HD1	1.66	0.44
2:B:341:LEU:HD12	2:B:429:ILE:HG22	1.99	0.44
2:B:460:LEU:HG	4:D:280:TRP:HZ3	1.82	0.44
27:C:508:CLA:H62	27:C:508:CLA:H41	1.72	0.44
7:G:70:ARG:HA	7:G:73:MET:HE3	1.99	0.44
37:G:601:CHL:HHD	35:G:2630:LHG:HC41	2.00	0.44
7:N:64:LEU:HD11	7:Y:49:ALA:HA	1.99	0.44
14:O:100:TYR:CE2	14:O:104:LYS:HD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:167:ASP:O	17:R:171:ARG:HG3	2.18	0.44
18:S:109:ALA:HA	18:S:110:VAL:C	2.42	0.44
18:S:169:PRO:O	18:S:172:PRO:HD3	2.18	0.44
1:a:45:THR:HG23	27:a:406:CLA:H201	2.00	0.44
2:b:12:VAL:HB	27:b:613:CLA:HMC2	1.98	0.44
2:b:80:ILE:HG13	2:b:81:THR:N	2.32	0.44
2:b:141:ILE:HD13	27:b:616:CLA:HBB1	2.00	0.44
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.53	0.44
2:b:311:PHE:HA	2:b:430:PHE:HZ	1.79	0.44
2:b:343:HIS:HA	2:b:344:PRO:HD2	1.85	0.44
2:b:415:ALA:HB1	2:b:419:LYS:NZ	2.32	0.44
3:c:85:GLY:O	27:c:504:CLA:HMA3	2.18	0.44
35:d:408:LHG:O1	35:l:101:LHG:O5	2.33	0.44
37:n:607:CHL:H152	37:n:607:CHL:H111	1.52	0.44
14:o:207:VAL:HA	14:o:208:PRO:HD2	1.70	0.44
17:r:103:ALA:O	17:r:107:THR:HG23	2.18	0.44
17:r:211:PHE:HD1	17:r:222:PRO:CB	2.30	0.44
17:r:213:VAL:HG21	27:r:613:CLA:HAC2	1.99	0.44
18:s:44:ASP:O	18:s:45:ILE:HG13	2.18	0.44
7:y:64:LEU:HD13	27:y:603:CLA:HAA2	1.98	0.44
38:y:1620:LUT:H35	38:y:1620:LUT:H401	1.85	0.44
1:A:127:MET:HE3	27:C:505:CLA:HMB2	1.99	0.44
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.00	0.44
2:B:283:GLU:OE2	2:B:286:ARG:NH2	2.50	0.44
4:D:197:HIS:O	4:D:201:VAL:HG23	2.18	0.44
4:D:349:GLY:HA3	14:O:240:LEU:HD11	1.99	0.44
7:G:127:ILE:HG12	37:G:605:CHL:HAC1	1.99	0.44
15:P:97:THR:HA	15:P:98:ASP:HA	1.67	0.44
18:S:44:ASP:O	18:S:45:ILE:HG13	2.17	0.44
18:S:175:LEU:HD13	27:S:610:CLA:H11	1.99	0.44
21:W:129:GLU:HA	21:W:130:ASP:HA	1.76	0.44
2:b:74:SER:OG	2:b:94:GLU:OE2	2.36	0.44
2:b:281:GLN:OE1	2:b:358:ARG:NH1	2.51	0.44
27:b:613:CLA:H151	27:b:613:CLA:H18	1.69	0.44
3:c:67:MET:HB3	3:c:88:LEU:HD11	2.00	0.44
3:c:195:ASP:CB	16:q:86:ARG:HD3	2.48	0.44
27:c:504:CLA:H193	27:c:510:CLA:H93	2.00	0.44
5:e:52:PRO:HA	5:e:55:TYR:CE2	2.53	0.44
7:g:222:TRP:HB3	7:y:105:PHE:HZ	1.82	0.44
13:m:20:ALA:O	13:m:24:ILE:HG13	2.17	0.44
18:s:33:ILE:HG21	18:s:40:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:166:PRO:HB2	18:s:167:GLY:H	1.64	0.44
7:y:92:PHE:HE1	7:y:113:LEU:HA	1.81	0.44
1:A:340:PRO:HB3	15:P:140:GLU:C	2.43	0.44
2:B:74:SER:OG	2:B:94:GLU:OE2	2.36	0.44
2:B:150:CYS:HB2	27:B:604:CLA:CMC	2.47	0.44
27:B:617:CLA:H142	27:B:617:CLA:H112	1.85	0.44
29:B:620:BCR:H15C	29:B:620:BCR:H351	1.78	0.44
3:C:53:HIS:CD2	27:C:509:CLA:NA	2.86	0.44
3:C:461:ARG:HH11	4:D:225:ASP:CG	2.26	0.44
4:D:349:GLY:HA2	4:D:350:ASN:HA	1.62	0.44
7:N:173:PHE:HE1	27:N:610:CLA:H2A	1.83	0.44
14:O:202:PRO:HD3	2:b:85:ILE:HD11	2.00	0.44
15:P:45:GLN:HG2	15:P:62:LEU:HB3	2.00	0.44
15:P:109:ALA:HA	15:P:135:THR:HA	1.99	0.44
18:S:164:LEU:N	18:S:165:HIS:C	2.75	0.44
4:d:171:PRO:HG3	4:d:181:PHE:CD1	2.53	0.44
8:h:50:PHE:HB2	29:h:101:BCR:H10C	2.00	0.44
8:h:56:ILE:HG12	22:x:87:PHE:CE2	2.51	0.44
9:i:17:SER:HB2	21:w:116:ILE:HD12	1.99	0.44
7:n:136:GLY:CA	37:n:609:CHL:HAB	2.48	0.44
14:o:124:PHE:HE1	14:o:292:PRO:HA	1.83	0.44
1:A:187:GLN:HB2	27:A:405:CLA:CAC	2.48	0.43
31:A:413:LMG:H331	31:A:413:LMG:H361	1.70	0.43
2:B:359:MET:HE2	2:B:366:PHE:HB3	2.00	0.43
3:C:57:ALA:O	3:C:61:VAL:HG23	2.18	0.43
3:C:195:ASP:CB	16:Q:86:ARG:HD3	2.48	0.43
4:D:179:PHE:O	4:D:182:ILE:HB	2.18	0.43
7:G:15:PRO:O	7:G:21:ARG:HA	2.18	0.43
13:M:21:PHE:CZ	13:M:25:ILE:HD11	2.53	0.43
7:N:225:ALA:HB1	39:Y:1622:XAT:H183	2.00	0.43
37:R:606:CHL:H43	40:R:623:NEX:H402	1.98	0.43
27:Y:613:CLA:H2	27:Y:613:CLA:H61	1.73	0.43
1:a:130:GLU:HG2	4:d:256:ILE:HG21	1.98	0.43
4:d:311:PHE:O	14:o:242:PRO:HG2	2.18	0.43
7:g:142:ARG:HG2	37:g:608:CHL:C1D	2.48	0.43
7:n:225:ALA:HB1	39:y:1622:XAT:H183	2.00	0.43
17:r:167:ASP:O	17:r:171:ARG:HG3	2.18	0.43
40:y:1623:NEX:H35	40:y:1623:NEX:H401	1.80	0.43
27:B:609:CLA:H161	27:B:609:CLA:H141	1.64	0.43
3:C:67:MET:HB3	3:C:88:LEU:HD11	2.00	0.43
3:C:322:GLN:NE2	3:C:380:LEU:O	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:505:CLA:C4A	27:C:505:CLA:HBA2	2.48	0.43
32:C:520:DGD:HB51	32:C:520:DGD:HBW1	1.99	0.43
4:D:123:ILE:HD11	32:H:102:DGD:HAH1	2.00	0.43
4:D:160:TYR:O	4:D:164:GLN:HG2	2.18	0.43
4:D:185:PHE:CD2	27:D:402:CLA:HMD1	2.52	0.43
5:E:52:PRO:HA	5:E:55:TYR:CE2	2.53	0.43
7:G:142:ARG:HG2	37:G:608:CHL:C1D	2.48	0.43
11:K:52:TRP:O	11:K:56:VAL:HG22	2.18	0.43
7:N:101:GLY:HA2	37:N:606:CHL:HAC2	2.00	0.43
40:N:1623:NEX:H11	40:N:1623:NEX:H191	1.72	0.43
17:R:103:ALA:O	17:R:107:THR:HG23	2.18	0.43
17:R:211:PHE:HD1	17:R:222:PRO:CB	2.30	0.43
20:U:13:TYR:CB	20:U:25:ILE:HD12	2.48	0.43
38:Y:1620:LUT:H15	38:Y:1620:LUT:H201	1.86	0.43
27:a:406:CLA:HED2	4:d:198:MET:SD	2.59	0.43
2:b:378:ARG:HE	15:p:40:LYS:NZ	2.16	0.43
2:b:384:ARG:HA	14:o:249:THR:HA	2.00	0.43
3:c:215:LYS:NZ	3:c:226:SER:OG	2.48	0.43
29:c:517:BCR:H371	29:c:517:BCR:H24C	1.71	0.43
4:d:179:PHE:O	4:d:182:ILE:HB	2.18	0.43
4:d:277:THR:O	4:d:281:MET:HG2	2.18	0.43
37:g:601:CHL:HHD	35:g:2630:LHG:HC41	2.00	0.43
27:g:602:CLA:H111	27:g:602:CLA:H93	1.67	0.43
7:n:24:TYR:HB3	7:n:44:TYR:HB3	2.00	0.43
7:n:144:ALA:HB2	7:y:28:PHE:O	2.18	0.43
37:n:607:CHL:H121	37:n:607:CHL:H8	1.82	0.43
18:s:175:LEU:HD13	27:s:610:CLA:H11	1.99	0.43
18:s:189:GLU:CD	27:s:610:CLA:NB	2.77	0.43
7:y:42:GLY:O	7:y:185:ARG:NH1	2.44	0.43
27:y:610:CLA:H92	27:y:610:CLA:H61	1.66	0.43
1:A:45:THR:OG1	28:A:408:PHO:H62	2.17	0.43
27:A:407:CLA:CGD	32:C:520:DGD:HAH2	2.48	0.43
3:C:85:GLY:O	27:C:504:CLA:HMA3	2.18	0.43
3:C:368:PRO:HA	16:Q:76:ASN:HB2	1.99	0.43
29:C:516:BCR:H20C	29:C:516:BCR:H361	1.83	0.43
7:N:144:ALA:HB2	7:Y:28:PHE:O	2.18	0.43
14:O:205:GLU:OE2	14:O:317:LYS:NZ	2.31	0.43
15:P:66:THR:HG21	15:P:156:LEU:HG	2.01	0.43
17:R:80:LEU:HD22	27:R:616:CLA:CHC	2.48	0.43
38:R:620:LUT:H31	38:R:620:LUT:H391	1.87	0.43
18:S:189:GLU:CD	27:S:610:CLA:NB	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Y:607:CHL:HHC	37:Y:607:CHL:CBB	2.47	0.43
1:a:131:TRP:CE3	1:a:132:GLU:HA	2.53	0.43
1:a:269:ARG:HE	4:d:222:LEU:HD13	1.81	0.43
2:b:359:MET:HE2	2:b:366:PHE:HB3	2.00	0.43
3:c:368:PRO:HB3	16:q:80:LEU:HB3	2.00	0.43
29:c:516:BCR:H20C	29:c:516:BCR:H361	1.83	0.43
4:d:266:TRP:HH2	35:l:101:LHG:HC82	1.81	0.43
27:d:403:CLA:H91	8:h:48:ALA:HB1	1.99	0.43
15:p:72:THR:HG23	15:p:125:GLN:HE21	1.84	0.43
15:p:122:ASP:C	15:p:124:LYS:HA	2.43	0.43
17:r:214:GLN:OE1	27:r:613:CLA:C1D	2.48	0.43
18:s:57:TYR:CD2	37:s:601:CHL:HMD2	2.54	0.43
2:B:5:TRP:HA	2:B:8:VAL:HG13	2.00	0.43
2:B:216:HIS:HE1	27:B:610:CLA:C1A	2.32	0.43
2:B:281:GLN:OE1	2:B:358:ARG:NH1	2.51	0.43
31:B:622:LMG:H121	31:B:622:LMG:H152	1.74	0.43
3:C:195:ASP:HB2	16:Q:86:ARG:HD3	2.00	0.43
3:C:387:TRP:CE2	3:C:388:GLN:HG3	2.54	0.43
27:C:504:CLA:H193	27:C:510:CLA:H93	1.99	0.43
27:D:403:CLA:H91	8:H:48:ALA:HB1	1.99	0.43
14:O:185:LYS:HA	14:O:219:SER:HA	2.00	0.43
14:O:288:THR:OG1	14:O:298:ILE:HG23	2.18	0.43
37:Y:609:CHL:H112	37:Y:609:CHL:H152	1.30	0.43
1:a:100:ALA:HB2	21:w:88:ARG:CD	2.48	0.43
27:b:611:CLA:H102	27:b:616:CLA:HAA1	2.01	0.43
4:d:43:PHE:HB3	4:d:113:PHE:CZ	2.54	0.43
4:d:80:THR:HG22	4:d:111:TRP:CE2	2.54	0.43
4:d:80:THR:HG21	4:d:170:ALA:O	2.18	0.43
7:g:28:PHE:HA	7:y:144:ALA:HB2	2.01	0.43
7:n:63:GLU:HA	7:n:155:LEU:HD11	2.00	0.43
7:n:101:GLY:HA2	37:n:606:CHL:HAC2	2.00	0.43
17:r:86:VAL:HG22	27:r:616:CLA:CGA	2.48	0.43
18:s:169:PRO:O	18:s:172:PRO:HD3	2.18	0.43
20:u:13:TYR:CB	20:u:25:ILE:HD12	2.48	0.43
27:y:602:CLA:H2	38:y:1621:LUT:H26	2.00	0.43
3:C:210:PHE:CD1	3:C:213:LEU:HD12	2.54	0.43
4:D:277:THR:O	4:D:281:MET:HG2	2.18	0.43
8:H:15:LYS:HA	8:H:16:PRO:HD2	1.90	0.43
7:N:205:PRO:HB3	38:N:1620:LUT:H41	2.01	0.43
18:S:61:PRO:HD2	38:S:1621:LUT:H23	1.99	0.43
18:S:122:ASN:HB2	18:S:132:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:611:CLA:H142	27:Y:611:CLA:H111	1.80	0.43
1:a:45:THR:OG1	28:a:408:PHO:H62	2.17	0.43
1:a:340:PRO:HB3	15:p:140:GLU:C	2.43	0.43
2:b:54:PRO:HD2	2:b:57:ARG:HG3	2.00	0.43
2:b:97:ALA:O	2:b:101:ILE:HG12	2.18	0.43
27:b:605:CLA:H162	27:b:605:CLA:H193	1.69	0.43
3:c:344:SER:OG	3:c:348:GLU:N	2.51	0.43
32:c:520:DGD:HB61	32:c:520:DGD:HB32	1.65	0.43
4:d:117:HIS:HE1	27:d:403:CLA:C4D	2.31	0.43
4:d:160:TYR:O	4:d:164:GLN:HG2	2.18	0.43
40:g:1623:NEX:H15	40:g:1623:NEX:H201	1.63	0.43
8:h:17:THR:O	8:h:21:ALA:N	2.45	0.43
7:n:46:TRP:CD1	7:n:48:THR:HG23	2.54	0.43
27:r:611:CLA:H3A	27:r:611:CLA:HBA2	1.45	0.43
38:y:1621:LUT:H15	38:y:1621:LUT:H201	1.80	0.43
1:A:21:ILE:HD13	1:A:35:VAL:HG11	2.00	0.43
1:A:45:THR:HG23	27:A:406:CLA:H201	2.00	0.43
1:A:85:THR:CG2	1:A:168:PHE:HB2	2.47	0.43
1:A:92:HIS:HE1	3:C:220:GLY:HA3	1.84	0.43
1:A:100:ALA:HB2	21:W:88:ARG:CD	2.48	0.43
1:A:197:PHE:HD2	1:A:289:GLY:HA2	1.83	0.43
27:A:406:CLA:HBB1	28:A:408:PHO:H141	1.99	0.43
2:B:385:ARG:HB3	15:P:93:TYR:N	2.34	0.43
3:C:368:PRO:HB3	16:Q:80:LEU:HB3	2.00	0.43
27:C:505:CLA:H71	27:C:505:CLA:H112	1.78	0.43
14:O:124:PHE:HE1	14:O:292:PRO:HA	1.83	0.43
18:S:57:TYR:CD2	37:S:601:CHL:HMD2	2.54	0.43
18:S:206:GLN:HE22	38:S:1620:LUT:H42	1.84	0.43
2:b:164:PRO:HG3	27:b:607:CLA:O1D	2.19	0.43
2:b:415:ALA:O	2:b:419:LYS:HG3	2.18	0.43
3:c:312:ALA:HB1	3:c:392:SER:HA	2.01	0.43
29:c:515:BCR:H15C	29:c:515:BCR:H351	1.69	0.43
29:c:514:BCR:H15C	29:c:514:BCR:H351	1.74	0.43
27:d:402:CLA:H91	27:d:402:CLA:H112	1.82	0.43
7:g:15:PRO:O	7:g:21:ARG:HA	2.18	0.43
14:o:137:GLU:HA	14:o:168:THR:HG22	1.99	0.43
14:o:185:LYS:HA	14:o:219:SER:HA	2.00	0.43
18:s:44:ASP:N	18:s:44:ASP:OD1	2.49	0.43
18:s:108:GLU:N	18:s:117:LEU:HD22	2.34	0.43
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.53	0.43
31:A:413:LMG:H342	3:C:217:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ILE:HD13	27:B:616:CLA:HBB1	2.00	0.43
2:B:415:ALA:O	2:B:419:LYS:HG3	2.18	0.43
29:B:619:BCR:H11C	29:B:619:BCR:H341	1.82	0.43
7:G:27:PRO:HD2	37:G:601:CHL:CBB	2.49	0.43
15:P:112:ASN:HA	16:Q:9:PRO:O	2.19	0.43
15:P:124:LYS:HG3	15:P:152:LYS:HE2	2.01	0.43
16:Q:27:ARG:NH1	16:Q:38:PHE:HD1	2.17	0.43
17:R:14:TRP:HB2	27:R:601:CLA:C1D	2.49	0.43
17:R:142:PHE:CE2	37:R:606:CHL:HED3	2.53	0.43
18:S:45:ILE:N	18:S:46:PRO:HD3	2.34	0.43
1:a:84:PRO:HA	1:a:112:TYR:CG	2.52	0.43
1:a:181:ASN:HD22	4:d:314:PHE:HD1	1.66	0.43
2:b:5:TRP:HA	2:b:8:VAL:HG13	2.00	0.43
3:c:53:HIS:CD2	27:c:509:CLA:NA	2.86	0.43
3:c:62:PHE:HE2	11:k:42:PRO:HD3	1.84	0.43
3:c:223:TRP:CG	3:c:224:ILE:N	2.83	0.43
3:c:368:PRO:HG3	16:q:79:ARG:CB	2.49	0.43
5:e:77:ASP:O	5:e:81:ARG:HG3	2.18	0.43
7:g:25:LEU:O	37:g:601:CHL:HBB1	2.19	0.43
14:o:136:LEU:HG	14:o:325:TRP:HB3	2.01	0.43
14:o:164:ARG:HA	21:w:88:ARG:HH12	1.82	0.43
15:p:121:VAL:O	15:p:123:GLY:N	2.46	0.43
39:y:1622:XAT:H31	39:y:1622:XAT:H391	1.79	0.43
1:A:223:LEU:O	2:B:482:ILE:HG12	2.19	0.43
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.53	0.43
2:B:325:PHE:CG	12:L:35:TYR:HB3	2.54	0.43
3:C:215:LYS:HZ3	3:C:226:SER:HG	1.61	0.43
3:C:312:ALA:HB1	3:C:392:SER:HA	2.01	0.43
3:C:368:PRO:HG3	16:Q:79:ARG:CB	2.48	0.43
29:C:516:BCR:H15C	29:C:516:BCR:H351	1.83	0.43
4:D:60:THR:HA	4:D:82:ALA:HB2	2.01	0.43
27:G:610:CLA:C2	38:G:1620:LUT:H26	2.49	0.43
38:G:1620:LUT:H35	38:G:1620:LUT:H401	1.76	0.43
8:H:52:VAL:O	8:H:56:ILE:HG13	2.19	0.43
7:N:46:TRP:CD1	7:N:48:THR:HG23	2.53	0.43
15:P:49:TYR:O	15:P:58:ASN:HB2	2.19	0.43
17:R:14:TRP:HA	27:R:601:CLA:C4C	2.49	0.43
2:b:337:ALA:HA	2:b:432:LEU:HD23	2.01	0.43
3:c:377:LEU:HB3	14:o:171:GLU:OE1	2.18	0.43
3:c:387:TRP:CE2	3:c:388:GLN:HG3	2.54	0.43
4:d:297:ASP:HA	4:d:315:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:r:613:CLA:H2A	27:r:613:CLA:O2D	2.18	0.43
18:s:175:LEU:HD12	38:s:1620:LUT:H221	2.01	0.43
22:x:87:PHE:O	22:x:90:SER:HB3	2.18	0.43
7:y:115:ASN:HA	7:y:116:PRO:HD3	1.87	0.43
2:B:365:THR:OG1	4:D:326:ARG:NH2	2.34	0.43
27:B:611:CLA:H102	27:B:616:CLA:HAA1	2.01	0.43
3:C:95:LEU:HD23	3:C:95:LEU:HA	1.84	0.43
29:C:515:BCR:H11C	29:C:515:BCR:H341	1.78	0.43
4:D:117:HIS:CE1	27:D:403:CLA:NA	2.85	0.43
29:H:101:BCR:H15C	29:H:101:BCR:H351	1.87	0.43
7:N:229:VAL:HA	7:N:230:PRO:HD2	1.92	0.43
14:O:132:LYS:HG3	14:O:133:LYS:N	2.29	0.43
15:P:63:VAL:HG22	15:P:157:TYR:CD1	2.54	0.43
15:P:122:ASP:C	15:P:124:LYS:HA	2.43	0.43
18:S:108:GLU:N	18:S:117:LEU:HD22	2.34	0.43
18:S:119:LEU:HA	18:S:120:ASP:HA	1.78	0.43
3:c:142:GLU:OE1	3:c:142:GLU:N	2.50	0.43
3:c:297:TYR:HD1	3:c:302:TYR:CZ	2.37	0.43
4:d:123:ILE:HD11	32:h:102:DGD:HAH1	2.00	0.43
4:d:210:LEU:HA	4:d:213:ILE:HG22	2.00	0.43
13:m:21:PHE:CZ	13:m:25:ILE:HD11	2.53	0.43
7:n:81:PHE:HB3	7:n:82:PRO:HD3	2.01	0.43
15:p:64:GLN:HA	15:p:65:PRO:HD3	1.88	0.43
15:p:66:THR:HG21	15:p:156:LEU:HG	2.01	0.43
17:r:14:TRP:HD1	17:r:32:TYR:O	2.02	0.43
39:y:1622:XAT:H35	39:y:1622:XAT:H401	1.68	0.43
2:B:97:ALA:O	2:B:101:ILE:HG12	2.18	0.43
2:B:378:ARG:HE	15:P:40:LYS:NZ	2.16	0.43
2:B:384:ARG:HA	14:O:249:THR:HA	2.00	0.43
7:G:28:PHE:HA	7:Y:144:ALA:HB2	2.01	0.43
7:N:22:VAL:HB	37:N:601:CHL:HBC1	2.00	0.43
27:N:602:CLA:H172	27:N:602:CLA:H13	1.82	0.43
27:R:610:CLA:H143	27:R:610:CLA:H111	1.77	0.43
21:W:91:THR:O	21:W:94:THR:OG1	2.23	0.43
27:Y:602:CLA:H2	38:Y:1621:LUT:H26	2.00	0.43
1:a:223:LEU:O	2:b:482:ILE:HG12	2.19	0.43
27:a:407:CLA:CGD	32:c:520:DGD:HAH2	2.48	0.43
27:a:410:CLA:H12	31:a:413:LMG:H112	2.00	0.43
2:b:218:SER:OG	2:b:219:VAL:N	2.52	0.43
2:b:325:PHE:CG	12:l:35:TYR:HB3	2.54	0.43
4:d:197:HIS:O	4:d:201:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:187:ALA:O	7:g:191:MET:HG2	2.19	0.43
27:r:616:CLA:H12	27:r:616:CLA:HBA1	1.44	0.43
27:A:406:CLA:HED2	4:D:198:MET:SD	2.59	0.42
2:B:440:ASP:CG	2:B:444:ARG:HH12	2.27	0.42
2:B:475:PHE:CE1	4:D:134:ARG:HD3	2.54	0.42
3:C:348:GLU:OE2	14:O:104:LYS:HA	2.19	0.42
27:C:503:CLA:H62	27:C:503:CLA:H101	1.86	0.42
32:C:520:DGD:HBT1	32:C:520:DGD:HB71	1.65	0.42
4:D:80:THR:HG22	4:D:111:TRP:CE2	2.53	0.42
4:D:214:HIS:HA	34:D:405:PL9:O2	2.19	0.42
38:G:1620:LUT:H15	38:G:1620:LUT:H201	1.87	0.42
7:N:153:ASP:OD2	7:N:156:TYR:HB2	2.19	0.42
38:N:1621:LUT:H35	38:N:1621:LUT:H401	1.81	0.42
15:P:34:TRP:CD1	15:P:51:ASP:HA	2.54	0.42
18:S:33:ILE:HG21	18:S:40:LEU:HD21	2.00	0.42
38:S:1621:LUT:H15	38:S:1621:LUT:H201	1.91	0.42
39:Y:1622:XAT:H11	39:Y:1622:XAT:H191	1.84	0.42
1:a:246:TYR:HH	33:d:401:BCT:C	2.26	0.42
2:b:440:ASP:CG	2:b:444:ARG:HH12	2.27	0.42
29:b:619:BCR:H20C	29:b:619:BCR:H361	1.88	0.42
3:c:461:ARG:NH1	4:d:225:ASP:OD2	2.46	0.42
27:c:503:CLA:CHB	31:z:101:LMG:H212	2.49	0.42
4:d:188:PHE:HE1	4:d:326:ARG:HA	1.84	0.42
15:p:63:VAL:HG22	15:p:157:TYR:CD1	2.54	0.42
16:q:44:PRO:HG2	16:q:48:ALA:N	2.34	0.42
17:r:142:PHE:CE2	37:r:606:CHL:HED3	2.53	0.42
18:s:108:GLU:HG3	18:s:110:VAL:HG22	2.01	0.42
27:s:604:CLA:H3A	27:s:604:CLA:HBA2	1.54	0.42
21:w:130:ASP:HB3	21:w:133:SER:HB2	2.01	0.42
7:y:220:ASN:HB2	27:y:614:CLA:HED1	2.01	0.42
37:y:607:CHL:HHC	37:y:607:CHL:CBB	2.47	0.42
27:A:410:CLA:H93	27:A:410:CLA:H112	1.83	0.42
2:B:164:PRO:HG3	27:B:607:CLA:O1D	2.19	0.42
2:B:383:PHE:HE2	4:D:349:GLY:H	1.67	0.42
27:C:508:CLA:H92	27:C:508:CLA:H61	1.78	0.42
32:C:520:DGD:HAH1	4:D:73:PHE:HE2	1.84	0.42
7:G:25:LEU:O	37:G:601:CHL:HBB1	2.19	0.42
7:N:63:GLU:HA	7:N:155:LEU:HD11	2.00	0.42
40:N:1623:NEX:H15	40:N:1623:NEX:H201	1.74	0.42
27:R:613:CLA:H2A	27:R:613:CLA:O2D	2.18	0.42
18:S:162:ASP:O	18:S:163:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:S:1620:LUT:H15	38:S:1620:LUT:H201	1.90	0.42
2:b:18:ARG:HG3	2:b:118:TRP:HB3	2.00	0.42
2:b:475:PHE:CE1	4:d:134:ARG:HD3	2.54	0.42
3:c:229:ASP:OD1	3:c:230:LEU:N	2.52	0.42
7:g:27:PRO:HD2	37:g:601:CHL:CBB	2.49	0.42
38:n:1621:LUT:H15	38:n:1621:LUT:H201	1.77	0.42
15:p:110:SER:N	15:p:134:ARG:O	2.46	0.42
16:q:40:LEU:CD1	16:q:41:GLN:HG3	2.48	0.42
18:s:151:TYR:HA	18:s:154:ILE:HD12	2.00	0.42
35:s:2630:LHG:H292	35:s:2630:LHG:H262	1.81	0.42
38:y:1621:LUT:H35	38:y:1621:LUT:H401	1.81	0.42
1:A:137:LEU:HD23	3:C:469:MET:HE1	2.01	0.42
1:A:159:LEU:C	1:A:162:PRO:HD2	2.44	0.42
27:A:410:CLA:H12	31:A:413:LMG:H112	2.00	0.42
2:B:127:ARG:HH11	17:R:69:ARG:HD2	1.84	0.42
2:B:337:ALA:HA	2:B:432:LEU:HD23	2.01	0.42
3:C:165:LEU:HD21	27:C:506:CLA:CAB	2.49	0.42
3:C:387:TRP:O	3:C:390:ARG:HB2	2.19	0.42
4:D:117:HIS:HE1	27:D:403:CLA:C4D	2.31	0.42
17:R:76:LYS:HZ3	17:R:84:SER:HB2	1.83	0.42
17:R:198:ILE:HD12	17:R:198:ILE:HA	1.96	0.42
18:S:141:ALA:O	18:S:145:LEU:HB2	2.20	0.42
1:a:21:ILE:HD13	1:a:35:VAL:HG11	2.00	0.42
1:a:92:HIS:HE1	3:c:220:GLY:HA3	1.84	0.42
2:b:8:VAL:HG23	2:b:9:HIS:CD2	2.54	0.42
2:b:135:LEU:HD22	2:b:237:VAL:HG21	2.02	0.42
2:b:385:ARG:HB3	15:p:93:TYR:N	2.34	0.42
3:c:259:TRP:HH2	27:c:507:CLA:H201	1.84	0.42
3:c:313:GLN:HG3	3:c:396:MET:HE3	2.01	0.42
3:c:348:GLU:OE2	14:o:104:LYS:HA	2.19	0.42
3:c:390:ARG:NH1	16:q:40:LEU:O	2.50	0.42
29:d:404:BCR:H11C	29:d:404:BCR:H341	1.76	0.42
8:h:52:VAL:O	8:h:56:ILE:HG13	2.19	0.42
7:n:14:SER:HA	7:n:15:PRO:HD2	1.88	0.42
7:n:22:VAL:HB	37:n:601:CHL:HBC1	2.00	0.42
14:o:248:SER:OG	14:o:249:THR:N	2.50	0.42
14:o:249:THR:HG21	15:p:138:GLY:HA3	2.01	0.42
14:o:288:THR:OG1	14:o:298:ILE:HG23	2.18	0.42
15:p:112:ASN:HA	16:q:9:PRO:O	2.19	0.42
15:p:124:LYS:HG3	15:p:152:LYS:HE2	2.01	0.42
17:r:242:PHE:CD2	17:r:243:LEU:HG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:103:ALA:HB1	18:s:104:ASN:HA	2.01	0.42
27:y:602:CLA:H93	27:y:602:CLA:H111	1.81	0.42
1:A:84:PRO:HD2	4:D:314:PHE:HZ	1.85	0.42
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.55	0.42
2:B:383:PHE:CZ	14:O:250:GLY:HA2	2.54	0.42
4:D:53:THR:HG22	6:F:40:MET:HE1	2.02	0.42
7:G:187:ALA:O	7:G:191:MET:HG2	2.19	0.42
7:N:81:PHE:HB3	7:N:82:PRO:HD3	2.01	0.42
15:P:72:THR:HG23	15:P:125:GLN:HE21	1.84	0.42
37:Y:601:CHL:H92	37:Y:601:CHL:H112	1.69	0.42
23:Z:40:VAL:O	23:Z:44:THR:N	2.51	0.42
2:b:383:PHE:HE2	4:d:349:GLY:H	1.67	0.42
27:b:607:CLA:H142	27:b:607:CLA:H111	1.86	0.42
4:d:199:MET:HE3	4:d:281:MET:HB3	2.02	0.42
40:n:1623:NEX:H15	40:n:1623:NEX:H201	1.74	0.42
15:p:49:TYR:O	15:p:58:ASN:HB2	2.19	0.42
15:p:121:VAL:HG21	15:p:126:TYR:CE2	2.54	0.42
18:s:141:ALA:O	18:s:145:LEU:HB2	2.20	0.42
2:B:46:ASP:HA	2:B:47:PRO:HD2	1.80	0.42
3:C:219:GLY:HA2	32:C:518:DGD:C2D	2.49	0.42
3:C:426:LEU:HD23	27:C:504:CLA:HMB1	2.01	0.42
27:C:503:CLA:CHB	31:Z:101:LMG:H212	2.49	0.42
29:C:514:BCR:H20C	29:C:514:BCR:H361	1.86	0.42
4:D:199:MET:HE3	4:D:281:MET:HB3	2.02	0.42
15:P:110:SER:N	15:P:134:ARG:O	2.46	0.42
39:R:622:XAT:H15	39:R:622:XAT:H201	1.92	0.42
18:S:175:LEU:HD12	38:S:1620:LUT:H221	2.01	0.42
18:S:214:PRO:O	38:S:1620:LUT:O3	2.33	0.42
7:Y:176:LEU:C	27:Y:610:CLA:HMA1	2.45	0.42
1:a:223:LEU:O	2:b:482:ILE:N	2.40	0.42
27:b:617:CLA:H11	27:b:617:CLA:H51	1.81	0.42
8:h:59:GLU:HB3	8:h:64:SER:HB2	2.02	0.42
15:p:34:TRP:CD1	15:p:51:ASP:HA	2.54	0.42
15:p:136:ALA:HA	15:p:137:ASP:HA	1.68	0.42
17:r:174:PRO:HD2	27:r:610:CLA:OBD	2.20	0.42
7:y:111:ASP:CG	7:y:116:PRO:HA	2.45	0.42
27:A:406:CLA:H161	27:A:406:CLA:H141	1.81	0.42
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.54	0.42
27:B:603:CLA:HBA1	8:H:57:ILE:HB	2.01	0.42
27:B:606:CLA:H61	27:B:606:CLA:H41	1.93	0.42
27:B:606:CLA:H152	27:B:606:CLA:H18	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:PHE:HB3	4:D:113:PHE:CZ	2.54	0.42
7:N:213:LEU:HD21	27:N:614:CLA:HMC2	2.01	0.42
15:P:121:VAL:HG21	15:P:126:TYR:CE2	2.55	0.42
17:R:86:VAL:HG22	27:R:616:CLA:CGA	2.48	0.42
17:R:242:PHE:CD2	17:R:243:LEU:HG	2.54	0.42
1:a:84:PRO:HD2	4:d:314:PHE:HZ	1.85	0.42
2:b:383:PHE:CZ	14:o:250:GLY:HA2	2.54	0.42
3:c:210:PHE:CD1	3:c:213:LEU:HD12	2.54	0.42
27:c:505:CLA:H62	27:c:505:CLA:H92	1.81	0.42
32:c:520:DGD:HAH1	4:d:73:PHE:HE2	1.84	0.42
4:d:214:HIS:HA	34:d:405:PL9:O2	2.19	0.42
37:g:601:CHL:HBA1	37:g:601:CHL:H3A	1.77	0.42
37:g:605:CHL:HBA2	37:g:605:CHL:H3A	1.72	0.42
37:g:608:CHL:C4A	37:g:608:CHL:HBA2	2.49	0.42
11:k:52:TRP:O	11:k:56:VAL:HG22	2.18	0.42
7:n:173:PHE:HE1	27:n:610:CLA:H2A	1.83	0.42
16:q:19:GLY:HA2	16:q:20:THR:HA	1.54	0.42
16:q:71:TRP:CD1	16:q:125:LYS:HB2	2.55	0.42
17:r:14:TRP:HA	27:r:601:CLA:C4C	2.49	0.42
17:r:14:TRP:HB2	27:r:601:CLA:C1D	2.49	0.42
18:s:162:ASP:O	18:s:163:LYS:HB2	2.20	0.42
38:s:1620:LUT:H11	38:s:1620:LUT:H191	1.92	0.42
27:y:610:CLA:H141	27:y:610:CLA:H162	1.81	0.42
1:A:300:PHE:HE2	32:C:520:DGD:HA71	1.85	0.42
29:A:411:BCR:H351	29:A:411:BCR:H15C	1.71	0.42
2:B:70:GLY:HA2	2:B:178:VAL:CG2	2.49	0.42
3:C:164:HIS:HA	3:C:167:LEU:HG	2.01	0.42
3:C:344:SER:OG	3:C:348:GLU:N	2.51	0.42
27:C:505:CLA:HMB3	27:C:505:CLA:HBB1	2.02	0.42
27:C:509:CLA:H141	27:C:509:CLA:H161	1.58	0.42
32:H:102:DGD:HB62	32:H:102:DGD:HB32	1.75	0.42
27:N:602:CLA:H2	38:N:1621:LUT:H26	2.02	0.42
14:O:115:VAL:HG22	14:O:296:GLU:HB3	2.01	0.42
14:O:216:LEU:HA	14:O:228:ASP:O	2.20	0.42
20:U:6:THR:HG22	20:U:10:LYS:HZ3	1.85	0.42
7:Y:226:THR:O	7:Y:229:VAL:HG23	2.19	0.42
2:b:160:GLY:HA2	2:b:163:GLY:O	2.19	0.42
3:c:404:LEU:HD21	32:c:520:DGD:HB51	2.02	0.42
27:c:503:CLA:H101	27:c:503:CLA:H62	1.86	0.42
27:c:510:CLA:H192	27:c:510:CLA:H162	1.79	0.42
7:n:42:GLY:O	7:n:185:ARG:NH1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:153:ASP:OD2	7:n:156:TYR:HB2	2.19	0.42
14:o:193:ASP:HB2	14:o:213:ILE:O	2.20	0.42
17:r:49:ASP:OD1	17:r:50:TYR:N	2.53	0.42
17:r:197:GLU:HB2	27:r:610:CLA:C1B	2.50	0.42
7:y:176:LEU:C	27:y:610:CLA:HMA1	2.45	0.42
1:A:304:GLN:NE2	1:A:313:VAL:HG21	2.35	0.42
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.02	0.42
29:B:619:BCR:H351	29:B:619:BCR:H15C	1.74	0.42
3:C:182:PHE:CD2	27:C:502:CLA:H201	2.55	0.42
3:C:297:TYR:HD1	3:C:302:TYR:CZ	2.37	0.42
14:O:136:LEU:HG	14:O:325:TRP:HB3	2.01	0.42
15:P:89:GLY:O	16:Q:6:VAL:HG23	2.19	0.42
17:R:66:ILE:HG21	17:R:69:ARG:NH1	2.35	0.42
17:R:135:TYR:HD1	27:R:604:CLA:HBA1	1.85	0.42
18:S:103:ALA:HB1	18:S:104:ASN:HA	2.01	0.42
18:S:108:GLU:HG3	18:S:110:VAL:HG22	2.01	0.42
1:a:159:LEU:C	1:a:162:PRO:HD2	2.44	0.42
29:b:618:BCR:H11C	29:b:618:BCR:H341	1.78	0.42
3:c:165:LEU:HD21	27:c:506:CLA:CAB	2.49	0.42
3:c:387:TRP:HZ2	16:q:80:LEU:HA	1.85	0.42
3:c:461:ARG:HH11	4:d:225:ASP:CG	2.26	0.42
27:c:508:CLA:H62	27:c:508:CLA:H41	1.72	0.42
5:e:14:ILE:O	5:e:20:TRP:NE1	2.43	0.42
7:n:24:TYR:O	37:n:601:CHL:C1C	2.39	0.42
7:n:169:ASP:HA	7:n:170:PRO:HD3	1.89	0.42
14:o:190:ASP:HA	14:o:191:GLY:HA2	1.80	0.42
40:s:1623:NEX:H35	40:s:1623:NEX:H401	1.88	0.42
7:y:119:VAL:HA	37:y:605:CHL:C4D	2.50	0.42
27:y:604:CLA:C4A	27:y:604:CLA:HBA2	2.49	0.42
2:B:160:GLY:HA2	2:B:163:GLY:O	2.19	0.42
27:B:606:CLA:H61	27:B:606:CLA:H92	1.86	0.42
3:C:112:PHE:HE2	29:C:514:BCR:HC31	1.85	0.42
3:C:152:LYS:HG2	21:W:136:SER:HB3	2.02	0.42
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.55	0.42
3:C:259:TRP:HH2	27:C:507:CLA:H201	1.84	0.42
4:D:171:PRO:HG3	4:D:181:PHE:CD1	2.53	0.42
29:D:404:BCR:H11C	29:D:404:BCR:H341	1.76	0.42
7:G:91:LYS:O	7:G:114:GLY:HA3	2.20	0.42
37:G:601:CHL:C1D	35:G:2630:LHG:HC82	2.50	0.42
29:H:101:BCR:H371	29:H:101:BCR:H24C	1.79	0.42
14:O:135:CYS:C	14:O:136:LEU:HD12	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:193:ASP:HB2	14:O:213:ILE:O	2.20	0.42
17:R:14:TRP:HD1	17:R:32:TYR:O	2.02	0.42
17:R:123:ASP:HA	37:R:607:CHL:HED2	2.02	0.42
37:R:608:CHL:H3A	37:R:608:CHL:HBA2	1.85	0.42
21:W:130:ASP:HB3	21:W:133:SER:HB2	2.01	0.42
23:Z:23:VAL:HB	23:Z:24:PRO:HD3	2.02	0.42
1:a:187:GLN:HB2	27:a:405:CLA:HAC2	2.02	0.42
2:b:127:ARG:HH11	17:r:69:ARG:HD2	1.84	0.42
2:b:342:GLY:N	2:b:404:GLY:HA3	2.35	0.42
3:c:387:TRP:O	3:c:390:ARG:HB2	2.19	0.42
7:g:68:HIS:HB3	7:g:188:MET:HE2	2.01	0.42
7:n:205:PRO:HB3	38:n:1620:LUT:H41	2.01	0.42
14:o:136:LEU:HD23	14:o:301:PHE:CZ	2.55	0.42
15:p:89:GLY:O	16:q:6:VAL:HG23	2.19	0.42
15:p:112:ASN:O	15:p:132:LEU:N	2.43	0.42
16:q:27:ARG:NH1	16:q:38:PHE:HD1	2.17	0.42
17:r:37:PHE:CD2	39:r:622:XAT:H372	2.55	0.42
17:r:193:LEU:HD22	27:r:612:CLA:HBA2	2.02	0.42
18:s:25:LYS:O	18:s:31:ARG:HA	2.20	0.42
18:s:109:ALA:HB3	27:s:604:CLA:HED3	2.02	0.42
38:s:1620:LUT:H15	38:s:1620:LUT:H201	1.90	0.42
2:B:283:GLU:CD	2:B:286:ARG:HH21	2.27	0.42
27:B:602:CLA:HAC1	29:H:101:BCR:H383	2.02	0.42
27:B:611:CLA:H202	27:B:611:CLA:H161	1.77	0.42
3:C:62:PHE:HE2	11:K:42:PRO:HD3	1.84	0.42
3:C:387:TRP:HZ2	16:Q:80:LEU:HA	1.85	0.42
3:C:404:LEU:HD21	32:C:520:DGD:HB51	2.02	0.42
7:G:186:LEU:HA	35:G:2630:LHG:H261	2.02	0.42
32:H:102:DGD:HB91	32:H:102:DGD:HBW2	1.76	0.42
17:R:112:THR:HG21	27:R:604:CLA:CAC	2.50	0.42
17:R:136:LEU:HD23	17:R:136:LEU:O	2.20	0.42
17:R:203:LEU:HD13	27:R:611:CLA:HBC1	2.02	0.42
7:Y:81:PHE:CD2	27:Y:604:CLA:HAC2	2.55	0.42
7:Y:119:VAL:HA	37:Y:605:CHL:C4D	2.50	0.42
40:Y:1623:NEX:H191	40:Y:1623:NEX:H11	1.72	0.42
1:a:137:LEU:HD23	3:c:469:MET:HE1	2.00	0.42
1:a:230:ASN:HB2	17:r:56:ASN:HA	2.02	0.42
1:a:304:GLN:NE2	1:a:313:VAL:HG21	2.35	0.42
2:b:20:ILE:O	2:b:24:ILE:HG13	2.20	0.42
2:b:70:GLY:HA2	2:b:178:VAL:CG2	2.49	0.42
27:b:603:CLA:HBA1	8:h:57:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:504:CLA:H92	27:c:504:CLA:H62	1.81	0.42
27:c:505:CLA:C4A	27:c:505:CLA:HBA2	2.48	0.42
4:d:60:THR:HA	4:d:82:ALA:HB2	2.00	0.42
7:g:68:HIS:CE1	27:g:603:CLA:ND	2.87	0.42
37:n:605:CHL:H11	18:s:100:LYS:HD2	2.02	0.42
38:n:1620:LUT:H35	38:n:1620:LUT:H401	1.78	0.42
35:n:2630:LHG:H211	39:y:1622:XAT:H12	2.02	0.42
14:o:115:VAL:HG22	14:o:296:GLU:HB3	2.01	0.42
14:o:236:GLY:HA2	15:p:100:GLU:OE1	2.20	0.42
17:r:136:LEU:HD23	17:r:136:LEU:O	2.20	0.42
17:r:157:TYR:O	17:r:161:GLN:HG2	2.20	0.42
17:r:203:LEU:HD13	27:r:611:CLA:HBC1	2.02	0.42
1:A:238:ARG:NH1	19:T:28:LYS:O	2.31	0.41
2:B:340:TRP:HA	2:B:430:PHE:CD1	2.51	0.41
2:B:342:GLY:N	2:B:404:GLY:HA3	2.35	0.41
4:D:172:SER:HB2	4:D:177:ALA:CB	2.49	0.41
7:G:96:VAL:HB	7:G:99:LYS:HB2	2.02	0.41
27:G:603:CLA:HBB1	38:G:1621:LUT:C14	2.50	0.41
37:G:608:CHL:C4A	37:G:608:CHL:HBA2	2.49	0.41
38:G:1621:LUT:H15	38:G:1621:LUT:H201	1.88	0.41
14:O:136:LEU:HD23	14:O:301:PHE:CZ	2.55	0.41
16:Q:71:TRP:CD1	16:Q:125:LYS:HB2	2.55	0.41
17:R:49:ASP:OD1	17:R:50:TYR:N	2.53	0.41
18:S:126:TYR:CG	18:S:127:PHE:N	2.88	0.41
7:Y:220:ASN:HB2	27:Y:614:CLA:HED1	2.00	0.41
38:Y:1620:LUT:H11	38:Y:1620:LUT:H191	1.93	0.41
38:Y:1621:LUT:H201	38:Y:1621:LUT:H15	1.80	0.41
1:a:219:VAL:HG21	4:d:268:HIS:CD2	2.54	0.41
3:c:175:LEU:HD23	3:c:237:HIS:CG	2.55	0.41
3:c:352:GLY:O	3:c:355:THR:HG22	2.20	0.41
27:c:505:CLA:HMB3	27:c:505:CLA:HBB1	2.02	0.41
4:d:43:PHE:CE2	27:d:403:CLA:C2C	3.03	0.41
7:g:54:ASP:O	7:g:58:PHE:N	2.44	0.41
7:g:96:VAL:HB	7:g:99:LYS:HB2	2.02	0.41
7:n:117:SER:O	37:n:605:CHL:HMA2	2.20	0.41
27:n:602:CLA:HBB2	38:n:1621:LUT:H34	2.03	0.41
40:r:623:NEX:H201	40:r:623:NEX:H15	1.68	0.41
18:s:44:ASP:OD1	18:s:46:PRO:HD3	2.20	0.41
18:s:45:ILE:N	18:s:46:PRO:HD3	2.34	0.41
38:y:1620:LUT:H15	38:y:1620:LUT:H201	1.86	0.41
23:z:50:LEU:O	23:z:54:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PRO:HG2	1:A:98:GLU:HG2	2.01	0.41
1:A:161:TYR:HA	1:A:294:ALA:CB	2.50	0.41
27:B:603:CLA:H93	27:B:603:CLA:H61	1.69	0.41
8:H:50:PHE:HB2	29:H:101:BCR:H10C	2.00	0.41
8:H:59:GLU:HB3	8:H:64:SER:HB2	2.02	0.41
7:N:24:TYR:O	37:N:601:CHL:C1C	2.39	0.41
7:N:117:SER:O	37:N:605:CHL:HMA2	2.20	0.41
14:O:249:THR:HG21	15:P:138:GLY:HA3	2.01	0.41
17:R:161:GLN:HB3	37:R:608:CHL:CMC	2.51	0.41
18:S:131:ILE:HB	18:S:133:ILE:H	1.85	0.41
7:Y:111:ASP:CG	7:Y:116:PRO:HA	2.45	0.41
1:a:161:TYR:HA	1:a:294:ALA:CB	2.50	0.41
1:a:259:ILE:HG22	1:a:260:PHE:N	2.29	0.41
2:b:216:HIS:HE1	27:b:610:CLA:C1A	2.32	0.41
2:b:462:PHE:CE2	27:b:605:CLA:HAC2	2.55	0.41
27:b:608:CLA:HBC2	29:b:618:BCR:H321	2.02	0.41
3:c:80:PRO:HD3	16:q:37:ARG:NH1	2.34	0.41
3:c:118:HIS:HE1	27:c:503:CLA:C4A	2.33	0.41
3:c:164:HIS:HA	3:c:167:LEU:HG	2.01	0.41
3:c:219:GLY:HA2	32:c:518:DGD:C2D	2.49	0.41
3:c:268:GLY:HA2	3:c:271:TYR:CD2	2.55	0.41
8:h:25:PRO:CG	17:r:78:THR:HG21	2.50	0.41
15:p:15:ASN:HA	15:p:16:THR:HA	1.61	0.41
18:s:172:PRO:HA	18:s:173:LEU:HA	1.86	0.41
40:s:1623:NEX:H11	40:s:1623:NEX:H191	1.82	0.41
21:w:131:GLU:HA	21:w:132:GLU:HA	1.54	0.41
7:y:226:THR:O	7:y:229:VAL:HG23	2.19	0.41
1:A:93:PHE:HB2	3:C:218:PHE:CB	2.50	0.41
1:A:230:ASN:HB2	17:R:56:ASN:HA	2.02	0.41
1:A:304:GLN:HG3	3:C:414:ILE:HG22	2.03	0.41
3:C:221:GLU:HG3	21:W:93:GLY:HA2	2.03	0.41
3:C:344:SER:N	3:C:348:GLU:O	2.38	0.41
3:C:459:ILE:O	4:D:224:GLU:N	2.37	0.41
27:C:502:CLA:HBB2	27:C:510:CLA:H151	2.01	0.41
7:N:24:TYR:O	37:N:601:CHL:C4C	2.47	0.41
39:N:1622:XAT:H201	39:N:1622:XAT:H15	1.75	0.41
27:Y:604:CLA:HBA2	27:Y:604:CLA:C4A	2.49	0.41
23:Z:50:LEU:O	23:Z:54:VAL:HG23	2.20	0.41
1:a:196:PRO:HG3	1:a:300:PHE:HE2	1.85	0.41
27:a:405:CLA:H92	27:a:405:CLA:H62	1.81	0.41
2:b:26:HIS:O	2:b:30:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:152:LYS:HG2	21:w:136:SER:HB3	2.02	0.41
3:c:390:ARG:HG2	16:q:39:TYR:O	2.20	0.41
4:d:53:THR:HG22	6:f:40:MET:HE1	2.02	0.41
27:n:602:CLA:H172	27:n:602:CLA:H13	1.82	0.41
17:r:66:ILE:HG21	17:r:69:ARG:NH1	2.35	0.41
17:r:112:THR:HG21	27:r:604:CLA:CAC	2.50	0.41
17:r:161:GLN:HB3	37:r:608:CHL:CMC	2.51	0.41
27:r:602:CLA:H161	27:r:602:CLA:H141	1.83	0.41
38:y:1621:LUT:H31	38:y:1621:LUT:H391	1.90	0.41
2:B:369:VAL:HG21	4:D:341:PHE:CE1	2.55	0.41
27:B:613:CLA:H162	27:B:613:CLA:H122	1.75	0.41
3:C:80:PRO:HD3	16:Q:37:ARG:NH1	2.34	0.41
3:C:289:PHE:HB3	3:C:297:TYR:CE2	2.55	0.41
3:C:352:GLY:O	3:C:355:THR:HG22	2.20	0.41
32:C:519:DGD:HA81	32:C:519:DGD:HAE2	1.88	0.41
5:E:70:PHE:CZ	8:H:66:LEU:HD21	2.56	0.41
27:G:610:CLA:H62	27:G:610:CLA:H41	1.87	0.41
39:G:1622:XAT:H173	39:G:1622:XAT:H3	1.83	0.41
16:Q:44:PRO:HG2	16:Q:48:ALA:N	2.34	0.41
16:Q:143:GLU:O	16:Q:147:LYS:HG2	2.21	0.41
18:S:109:ALA:HB3	27:S:604:CLA:HED3	2.02	0.41
1:a:93:PHE:HB2	3:c:218:PHE:CG	2.56	0.41
31:a:413:LMG:H331	31:a:413:LMG:H361	1.70	0.41
2:b:369:VAL:HG21	4:d:341:PHE:CE1	2.55	0.41
29:b:618:BCR:H24C	29:b:618:BCR:H371	1.90	0.41
3:c:289:PHE:HB3	3:c:297:TYR:CE2	2.55	0.41
27:c:502:CLA:HBB2	27:c:510:CLA:H151	2.01	0.41
4:d:193:LEU:O	12:l:35:TYR:OH	2.28	0.41
39:g:1622:XAT:H173	39:g:1622:XAT:H3	1.83	0.41
7:n:24:TYR:CD2	7:n:25:LEU:HG	2.56	0.41
38:n:1621:LUT:H401	38:n:1621:LUT:H35	1.81	0.41
18:s:23:LEU:HA	18:s:24:ALA:HA	1.70	0.41
1:A:89:ILE:HD11	1:A:108:ASN:HB3	2.03	0.41
1:A:93:PHE:HB2	3:C:218:PHE:CG	2.55	0.41
1:A:102:VAL:O	1:A:106:LEU:HG	2.20	0.41
1:A:245:THR:OG1	4:D:265:ARG:NE	2.38	0.41
1:A:246:TYR:OH	33:D:401:BCT:C	2.68	0.41
2:B:252:VAL:HG12	27:B:604:CLA:O1A	2.20	0.41
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.56	0.41
2:B:345:ILE:HD12	2:B:402:TYR:CD2	2.55	0.41
27:B:605:CLA:HBA1	27:B:605:CLA:CBD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:313:GLN:HG3	3:C:396:MET:HE3	2.01	0.41
27:C:502:CLA:HMD2	27:C:503:CLA:H102	2.01	0.41
7:G:68:HIS:CE1	27:G:603:CLA:ND	2.87	0.41
7:G:68:HIS:HB3	7:G:188:MET:HE2	2.01	0.41
39:G:1622:XAT:H393	35:G:2630:LHG:HC92	2.03	0.41
7:N:115:ASN:HA	7:N:116:PRO:HD2	1.90	0.41
27:N:602:CLA:H193	27:N:602:CLA:H161	1.83	0.41
35:N:2630:LHG:H211	39:Y:1622:XAT:H12	2.02	0.41
17:R:158:ILE:HG21	37:R:608:CHL:HMA3	2.02	0.41
27:S:610:CLA:HBB1	27:S:612:CLA:HAA1	2.03	0.41
7:Y:68:HIS:CE1	27:Y:603:CLA:ND	2.88	0.41
38:Y:1621:LUT:H35	38:Y:1621:LUT:H401	1.81	0.41
1:a:89:ILE:HD11	1:a:108:ASN:HB3	2.03	0.41
1:a:200:LEU:HD23	1:a:200:LEU:HA	1.86	0.41
2:b:352:ARG:CD	2:b:378:ARG:HH12	2.34	0.41
2:b:466:HIS:CE1	27:b:609:CLA:ND	2.88	0.41
3:c:221:GLU:HG3	21:w:93:GLY:HA2	2.03	0.41
3:c:289:PHE:HD1	3:c:293:ASN:HD22	1.67	0.41
5:e:70:PHE:CZ	8:h:66:LEU:HD21	2.56	0.41
7:g:70:ARG:NH1	37:g:608:CHL:OBD	2.36	0.41
8:h:59:GLU:O	8:h:64:SER:N	2.53	0.41
7:n:213:LEU:HD21	27:n:614:CLA:HMC2	2.01	0.41
27:n:602:CLA:H101	38:n:1621:LUT:H371	2.02	0.41
39:n:1622:XAT:H31	39:n:1622:XAT:H391	1.88	0.41
17:r:158:ILE:HG21	37:r:608:CHL:HMA3	2.02	0.41
2:B:282:GLN:NE2	20:U:25:ILE:H	2.18	0.41
2:B:458:PHE:HB3	27:B:605:CLA:HBC2	2.03	0.41
27:B:608:CLA:HBC2	29:B:618:BCR:H321	2.02	0.41
4:D:43:PHE:HE2	27:D:403:CLA:C2C	2.34	0.41
14:O:236:GLY:HA2	15:P:100:GLU:OE1	2.20	0.41
17:R:37:PHE:CD2	39:R:622:XAT:H372	2.55	0.41
18:S:163:LYS:HB2	18:S:164:LEU:HA	2.02	0.41
18:S:226:PHE:HB3	31:Z:101:LMG:H132	2.03	0.41
27:b:604:CLA:H41	27:b:604:CLA:H61	1.74	0.41
27:b:616:CLA:H161	8:h:19:VAL:HG11	2.02	0.41
29:b:618:BCR:H15C	29:b:618:BCR:H351	1.79	0.41
3:c:182:PHE:CD2	27:c:502:CLA:H201	2.55	0.41
3:c:324:LEU:HD13	15:p:134:ARG:NH2	2.36	0.41
7:g:22:VAL:HG23	7:g:44:TYR:HE1	1.85	0.41
8:h:15:LYS:HA	8:h:16:PRO:HD2	1.90	0.41
14:o:134:PHE:HD1	14:o:327:ALA:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:34:PHE:CD2	39:r:622:XAT:H383	2.55	0.41
17:r:51:ASP:N	17:r:52:GLY:HA2	2.36	0.41
18:s:196:ALA:O	18:s:200:MET:HG2	2.21	0.41
7:y:68:HIS:CE1	27:y:603:CLA:ND	2.88	0.41
1:A:196:PRO:HG3	1:A:300:PHE:HE2	1.85	0.41
29:A:411:BCR:H341	29:A:411:BCR:H11C	1.82	0.41
2:B:333:GLY:HA2	2:B:444:ARG:HH11	1.86	0.41
27:B:603:CLA:HBA2	27:B:603:CLA:CBD	2.48	0.41
3:C:191:PRO:HD2	16:Q:116:ASP:OD1	2.21	0.41
27:C:502:CLA:H152	27:C:502:CLA:H111	1.86	0.41
27:C:509:CLA:H192	27:C:512:CLA:HMD1	2.03	0.41
7:G:112:TYR:HB3	7:G:118:LEU:HB3	2.03	0.41
27:G:611:CLA:C4C	35:G:2630:LHG:HC62	2.51	0.41
17:R:157:TYR:O	17:R:161:GLN:HG2	2.20	0.41
17:R:174:PRO:HD2	27:R:610:CLA:OBD	2.20	0.41
37:R:608:CHL:HBD	37:R:608:CHL:HAA1	2.03	0.41
18:S:106:GLY:O	18:S:124:LEU:HB2	2.21	0.41
27:S:604:CLA:HBA2	27:S:604:CLA:H3A	1.54	0.41
31:a:413:LMG:H332	3:c:223:TRP:NE1	2.36	0.41
2:b:256:MET:HG2	2:b:451:PHE:CD2	2.56	0.41
2:b:296:GLN:HE22	2:b:304:LYS:NZ	2.19	0.41
2:b:363:PHE:HB3	2:b:365:THR:O	2.21	0.41
31:c:521:LMG:H211	31:c:521:LMG:H181	1.90	0.41
4:d:29:PHE:CG	4:d:132:LEU:HD21	2.56	0.41
37:g:601:CHL:C1D	35:g:2630:LHG:HC82	2.50	0.41
27:g:610:CLA:C2	38:g:1620:LUT:H26	2.49	0.41
27:g:611:CLA:C4C	35:g:2630:LHG:HC62	2.51	0.41
7:n:115:ASN:HA	7:n:116:PRO:HD2	1.90	0.41
15:p:29:LEU:HB3	15:p:182:SER:HB3	2.03	0.41
39:r:622:XAT:H15	39:r:622:XAT:H201	1.92	0.41
38:s:1620:LUT:H35	38:s:1620:LUT:H401	1.70	0.41
22:x:92:ALA:O	22:x:96:VAL:HG23	2.20	0.41
7:y:81:PHE:CD2	27:y:604:CLA:HAC2	2.55	0.41
27:A:406:CLA:H203	27:A:406:CLA:H162	1.74	0.41
31:A:413:LMG:H332	3:C:223:TRP:NE1	2.36	0.41
2:B:20:ILE:O	2:B:24:ILE:HG13	2.20	0.41
2:B:208:LEU:HD23	2:B:208:LEU:HA	1.94	0.41
2:B:212:ALA:HB2	27:B:610:CLA:HMC3	2.02	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.96	0.41
2:B:352:ARG:CD	2:B:378:ARG:HH12	2.34	0.41
27:B:615:CLA:HBA2	27:B:615:CLA:H11	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:324:LEU:HD13	15:P:134:ARG:NH2	2.36	0.41
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.56	0.41
4:D:219:GLU:HG2	35:D:410:LHG:C23	2.51	0.41
12:L:20:TRP:CE3	35:L:101:LHG:H132	2.56	0.41
7:N:64:LEU:HD13	27:N:603:CLA:HBA1	2.01	0.41
27:R:613:CLA:H3A	27:R:613:CLA:HBA2	1.82	0.41
18:S:25:LYS:O	18:S:31:ARG:HA	2.20	0.41
27:S:614:CLA:C4D	27:S:614:CLA:H12	2.50	0.41
22:X:92:ALA:O	22:X:96:VAL:HG23	2.20	0.41
2:b:283:GLU:CD	2:b:286:ARG:HH21	2.27	0.41
2:b:460:LEU:HD22	4:d:287:VAL:HG21	2.03	0.41
27:b:615:CLA:HBA2	27:b:615:CLA:H11	1.66	0.41
3:c:112:PHE:HE2	29:c:514:BCR:HC31	1.85	0.41
27:g:603:CLA:HBB1	38:g:1621:LUT:C14	2.50	0.41
9:i:12:VAL:O	9:i:16:VAL:HG23	2.21	0.41
11:k:35:VAL:HA	11:k:38:MET:CG	2.50	0.41
7:n:104:ILE:HD12	7:n:104:ILE:HA	1.91	0.41
14:o:265:GLU:N	14:o:265:GLU:OE1	2.54	0.41
27:r:609:CLA:HHC	27:r:609:CLA:HBB1	2.01	0.41
39:r:622:XAT:H35	39:r:622:XAT:H401	1.90	0.41
40:r:623:NEX:H11	40:r:623:NEX:H191	1.77	0.41
27:s:610:CLA:HBB1	27:s:612:CLA:HAA1	2.03	0.41
27:s:614:CLA:C4D	27:s:614:CLA:H12	2.50	0.41
23:z:23:VAL:HB	23:z:24:PRO:HD3	2.02	0.41
1:A:68:SER:N	4:D:312:GLU:O	2.54	0.41
1:A:142:TRP:HZ2	3:C:447:ARG:HB2	1.86	0.41
2:B:318:ASN:HA	2:B:319:PRO:HD2	1.86	0.41
2:B:343:HIS:HA	2:B:344:PRO:HD2	1.85	0.41
27:B:610:CLA:C3D	8:H:43:MET:HB2	2.51	0.41
27:B:616:CLA:H112	27:B:616:CLA:H152	1.92	0.41
27:B:616:CLA:H161	8:H:19:VAL:HG11	2.02	0.41
29:B:618:BCR:H11C	29:B:618:BCR:H341	1.78	0.41
3:C:174:LEU:HD11	27:C:512:CLA:H61	2.02	0.41
3:C:216:SER:OG	3:C:218:PHE:HD2	2.04	0.41
3:C:331:ALA:C	14:O:194:TYR:HH	2.22	0.41
3:C:390:ARG:HG2	16:Q:39:TYR:O	2.20	0.41
4:D:29:PHE:CG	4:D:132:LEU:HD21	2.56	0.41
4:D:43:PHE:CE2	27:D:403:CLA:C2C	3.03	0.41
4:D:53:THR:HA	4:D:67:TYR:CD2	2.56	0.41
4:D:188:PHE:HE1	4:D:326:ARG:HA	1.84	0.41
7:N:24:TYR:CD2	7:N:25:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:65:GLU:OE2	7:N:185:ARG:NE	2.53	0.41
37:N:605:CHL:H11	18:S:100:LYS:HD2	2.02	0.41
15:P:91:GLN:HB3	16:Q:3:ARG:O	2.21	0.41
17:R:77:SER:HA	17:R:166:LEU:HD21	2.03	0.41
17:R:193:LEU:HD22	27:R:612:CLA:HBA2	2.02	0.41
17:R:202:ARG:HH22	27:R:602:CLA:HED3	1.86	0.41
18:S:44:ASP:OD1	18:S:46:PRO:HD3	2.20	0.41
18:S:123:THR:O	18:S:124:LEU:HD12	2.21	0.41
40:S:1623:NEX:H15	40:S:1623:NEX:H201	1.67	0.41
40:S:1623:NEX:H191	40:S:1623:NEX:H11	1.82	0.41
7:Y:66:VAL:HB	7:Y:155:LEU:HD22	2.03	0.41
7:Y:98:PHE:CD1	7:Y:99:LYS:HG3	2.56	0.41
1:a:95:PRO:HG2	1:a:98:GLU:HG2	2.01	0.41
1:a:127:MET:HB2	1:a:147:TYR:HD2	1.85	0.41
1:a:300:PHE:HE2	32:c:520:DGD:HA71	1.85	0.41
30:a:418:SQD:H191	30:a:418:SQD:H161	1.76	0.41
2:b:273:TYR:HE1	4:d:165:SER:HA	1.85	0.41
2:b:282:GLN:NE2	20:u:25:ILE:H	2.18	0.41
2:b:318:ASN:HA	2:b:319:PRO:HD2	1.86	0.41
2:b:345:ILE:HD12	2:b:402:TYR:CD2	2.55	0.41
2:b:413:ASP:N	2:b:413:ASP:OD1	2.52	0.41
27:b:602:CLA:HAC1	29:h:101:BCR:H383	2.02	0.41
27:b:605:CLA:HBA1	27:b:605:CLA:CBD	2.50	0.41
27:b:615:CLA:H62	27:b:615:CLA:H41	1.87	0.41
27:b:616:CLA:H91	27:b:616:CLA:H112	1.75	0.41
3:c:456:GLU:OE2	3:c:457:LYS:NZ	2.42	0.41
27:c:501:CLA:H193	27:c:506:CLA:C1B	2.51	0.41
27:c:509:CLA:H192	27:c:512:CLA:HMD1	2.03	0.41
29:c:517:BCR:H11C	29:c:517:BCR:H341	1.88	0.41
4:d:181:PHE:O	4:d:184:PHE:HB3	2.21	0.41
7:g:54:ASP:HB3	7:g:57:THR:HB	2.03	0.41
7:g:91:LYS:O	7:g:114:GLY:HA3	2.20	0.41
7:g:186:LEU:HA	35:g:2630:LHG:H261	2.02	0.41
32:h:102:DGD:HB62	32:h:102:DGD:HB91	1.70	0.41
7:n:98:PHE:CE1	7:n:99:LYS:HE3	2.56	0.41
27:n:602:CLA:H2	38:n:1621:LUT:H26	2.02	0.41
27:n:610:CLA:H143	27:n:610:CLA:H111	1.87	0.41
16:q:143:GLU:O	16:q:147:LYS:HG2	2.21	0.41
17:r:123:ASP:HA	37:r:607:CHL:HED2	2.02	0.41
17:r:135:TYR:HD1	27:r:604:CLA:HBA1	1.85	0.41
27:r:602:CLA:H62	27:r:602:CLA:H41	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:r:610:CLA:H52	38:r:620:LUT:H30	2.03	0.41
18:s:127:PHE:HB3	18:s:129:LYS:HB3	2.03	0.41
18:s:131:ILE:HB	18:s:133:ILE:H	1.85	0.41
7:y:98:PHE:CD1	7:y:99:LYS:HG3	2.56	0.41
23:z:40:VAL:O	23:z:44:THR:N	2.51	0.41
1:A:126:TYR:OH	28:A:408:PHO:O1D	2.34	0.41
1:A:187:GLN:HB2	27:A:405:CLA:HAC2	2.02	0.41
1:A:200:LEU:HA	1:A:200:LEU:HD23	1.86	0.41
1:A:276:ALA:HB1	35:D:410:LHG:H262	2.03	0.41
1:A:317:TRP:HZ3	4:D:180:ARG:NH1	2.19	0.41
1:A:317:TRP:HZ2	4:D:79:SER:OG	2.04	0.41
30:A:418:SQD:H191	30:A:418:SQD:H161	1.76	0.41
2:B:26:HIS:O	2:B:30:VAL:HG23	2.20	0.41
2:B:363:PHE:HB3	2:B:365:THR:O	2.21	0.41
2:B:466:HIS:CE1	27:B:609:CLA:ND	2.88	0.41
27:B:602:CLA:H92	27:B:602:CLA:H61	1.78	0.41
27:B:613:CLA:H61	27:B:613:CLA:H102	1.68	0.41
3:C:229:ASP:OD1	3:C:230:LEU:N	2.52	0.41
3:C:354:GLU:O	3:C:357:ARG:HG2	2.21	0.41
4:D:80:THR:HA	4:D:81:PRO:HD3	1.85	0.41
6:F:45:ARG:HB3	10:J:36:LEU:HD23	2.03	0.41
7:G:22:VAL:HG23	7:G:44:TYR:HE1	1.85	0.41
7:G:155:LEU:HA	7:G:155:LEU:HD23	1.88	0.41
39:G:1622:XAT:H35	39:G:1622:XAT:H401	1.82	0.41
8:H:59:GLU:O	8:H:64:SER:N	2.53	0.41
27:N:602:CLA:HBB2	38:N:1621:LUT:H34	2.03	0.41
14:O:265:GLU:OE1	14:O:265:GLU:N	2.54	0.41
17:R:197:GLU:HB2	27:R:610:CLA:C1B	2.50	0.41
27:R:604:CLA:CHC	40:R:623:NEX:H222	2.51	0.41
27:R:609:CLA:HHC	27:R:609:CLA:HBB1	2.02	0.41
35:S:2630:LHG:H331	35:S:2630:LHG:H361	1.59	0.41
7:Y:180:GLU:HB2	27:Y:610:CLA:CHB	2.51	0.41
1:a:93:PHE:HB2	3:c:218:PHE:CB	2.50	0.41
2:b:8:VAL:HG22	27:b:612:CLA:H11	2.03	0.41
2:b:362:PHE:CE2	4:d:184:PHE:HZ	2.39	0.41
27:b:610:CLA:C3D	8:h:43:MET:HB2	2.51	0.41
29:c:515:BCR:H341	29:c:515:BCR:H11C	1.77	0.41
34:d:405:PL9:H121	34:d:405:PL9:H101	1.66	0.41
7:g:112:TYR:HB3	7:g:118:LEU:HB3	2.03	0.41
7:n:65:GLU:OE2	7:n:185:ARG:NE	2.53	0.41
16:q:134:TYR:O	16:q:138:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:111:LEU:HD11	17:r:211:PHE:CZ	2.56	0.41
27:r:604:CLA:CHC	40:r:623:NEX:H222	2.51	0.41
18:s:163:LYS:HB2	18:s:164:LEU:HA	2.02	0.41
3:C:118:HIS:HE1	27:C:503:CLA:C4A	2.33	0.40
3:C:268:GLY:HA2	3:C:271:TYR:CD2	2.55	0.40
3:C:443:TRP:CH2	35:D:410:LHG:HC61	2.55	0.40
27:C:503:CLA:H151	27:C:510:CLA:HBB2	2.04	0.40
27:C:501:CLA:H193	27:C:506:CLA:C1B	2.51	0.40
4:D:229:ALA:O	35:D:410:LHG:O1	2.25	0.40
10:J:10:LEU:HA	10:J:13:ILE:HD12	2.03	0.40
11:K:35:VAL:HA	11:K:38:MET:CG	2.50	0.40
37:N:601:CHL:HBB1	37:N:601:CHL:CHC	2.42	0.40
27:N:602:CLA:H101	38:N:1621:LUT:H371	2.02	0.40
16:Q:21:GLU:HB2	16:Q:24:ASP:HB2	2.02	0.40
16:Q:98:LYS:O	16:Q:101:LYS:HG2	2.21	0.40
17:R:34:PHE:CD2	39:R:622:XAT:H383	2.55	0.40
18:S:127:PHE:C	18:S:129:LYS:H	2.29	0.40
18:S:196:ALA:O	18:S:200:MET:HG2	2.21	0.40
7:Y:46:TRP:CE3	38:Y:1621:LUT:H383	2.56	0.40
27:Y:610:CLA:H162	27:Y:610:CLA:H141	1.81	0.40
1:a:102:VAL:O	1:a:106:LEU:HG	2.20	0.40
1:a:304:GLN:HG3	3:c:414:ILE:HG22	2.03	0.40
2:b:321:LYS:HD3	2:b:321:LYS:HA	1.89	0.40
27:b:609:CLA:H161	27:b:609:CLA:H141	1.64	0.40
4:d:126:MET:SD	4:d:150:ILE:HD12	2.62	0.40
4:d:164:GLN:HE21	4:d:290:ALA:HA	1.86	0.40
4:d:219:GLU:HG2	35:d:410:LHG:C23	2.51	0.40
27:g:614:CLA:HBA1	27:g:614:CLA:H3A	1.86	0.40
38:g:1621:LUT:H35	38:g:1621:LUT:H401	1.83	0.40
12:l:20:TRP:CE3	35:l:101:LHG:H132	2.56	0.40
7:n:64:LEU:HD13	27:n:603:CLA:HBA1	2.01	0.40
15:p:99:SER:N	15:p:106:GLY:H	2.03	0.40
1:A:64:ARG:NH2	14:O:163:THR:HB	2.29	0.40
27:A:405:CLA:H92	27:A:405:CLA:H62	1.81	0.40
2:B:273:TYR:HE1	4:D:165:SER:HA	1.86	0.40
3:C:112:PHE:CE2	29:C:514:BCR:HC31	2.56	0.40
3:C:379:ARG:NH2	16:Q:73:SER:OG	2.54	0.40
3:C:385:GLN:HB3	3:C:386:PRO:HD2	2.02	0.40
3:C:457:LYS:HE3	4:D:228:GLY:HA3	2.03	0.40
27:C:506:CLA:H41	27:C:506:CLA:H62	1.71	0.40
4:D:164:GLN:HE21	4:D:290:ALA:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:16:TRP:NE1	27:G:611:CLA:HED3	2.37	0.40
8:H:25:PRO:CG	17:R:78:THR:HG21	2.50	0.40
39:N:1622:XAT:H11	39:N:1622:XAT:H191	1.86	0.40
39:N:1622:XAT:H3	39:N:1622:XAT:H173	1.89	0.40
16:Q:134:TYR:O	16:Q:138:VAL:HG23	2.22	0.40
17:R:121:TRP:HE3	39:R:622:XAT:H173	1.87	0.40
37:R:607:CHL:HHC	37:R:607:CHL:HBB1	2.04	0.40
27:R:610:CLA:H62	27:R:610:CLA:H41	1.83	0.40
38:R:620:LUT:H11	38:R:620:LUT:H191	1.95	0.40
38:R:620:LUT:H35	38:R:620:LUT:H401	1.95	0.40
18:S:82:ALA:HB2	18:S:197:MET:HE2	2.04	0.40
18:S:224:ASP:O	18:S:227:GLY:N	2.55	0.40
2:b:42:LEU:HD11	2:b:93:TYR:HB3	2.02	0.40
2:b:73:ASN:HB3	2:b:88:PRO:HA	2.03	0.40
2:b:252:VAL:HG12	27:b:604:CLA:O1A	2.20	0.40
27:b:602:CLA:H161	27:b:602:CLA:H143	1.65	0.40
27:b:604:CLA:H141	27:b:610:CLA:H8	2.03	0.40
27:b:611:CLA:H161	27:b:611:CLA:H202	1.77	0.40
3:c:408:GLY:HA2	3:c:419:TYR:O	2.21	0.40
3:c:426:LEU:HD23	27:c:504:CLA:HMB1	2.01	0.40
27:c:502:CLA:H161	27:c:502:CLA:H192	1.81	0.40
7:g:145:GLY:C	37:g:608:CHL:HMC	2.47	0.40
7:n:52:SER:O	7:n:58:PHE:HB2	2.20	0.40
27:n:610:CLA:H43	27:n:612:CLA:HBA1	2.03	0.40
14:o:112:CYS:HA	14:o:113:PRO:HD3	1.98	0.40
16:q:98:LYS:O	16:q:101:LYS:HG2	2.21	0.40
17:r:214:GLN:HE22	27:r:613:CLA:CHA	2.34	0.40
18:s:201:PHE:O	18:s:205:ILE:HG22	2.22	0.40
38:y:1620:LUT:H31	38:y:1620:LUT:H391	1.90	0.40
23:z:5:PHE:HD1	23:z:57:LEU:HB2	1.87	0.40
1:A:183:MET:HA	27:A:405:CLA:HMD2	2.04	0.40
1:A:223:LEU:O	2:B:482:ILE:N	2.40	0.40
30:A:412:SQD:H382	30:A:412:SQD:H351	1.69	0.40
2:B:256:MET:HG2	2:B:451:PHE:CD2	2.56	0.40
2:B:275:TRP:CZ2	2:B:315:ILE:HB	2.57	0.40
3:C:471:PRO:O	3:C:472:LEU:HB2	2.21	0.40
27:C:502:CLA:H161	27:C:502:CLA:H192	1.82	0.40
29:C:514:BCR:H15C	29:C:514:BCR:H351	1.74	0.40
4:D:191:TRP:NE1	4:D:197:HIS:CD2	2.90	0.40
27:G:602:CLA:H41	27:G:602:CLA:H61	1.83	0.40
9:I:5:LYS:HE2	9:I:9:TYR:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:52:SER:O	7:N:58:PHE:HB2	2.20	0.40
7:N:98:PHE:CE1	7:N:99:LYS:HE3	2.56	0.40
15:P:90:LYS:HG2	16:Q:5:ILE:HG13	2.03	0.40
17:R:51:ASP:N	17:R:52:GLY:HA2	2.36	0.40
18:S:201:PHE:O	18:S:205:ILE:HG22	2.22	0.40
7:Y:167:ALA:HA	7:Y:173:PHE:HB2	2.03	0.40
40:Y:1623:NEX:H15	40:Y:1623:NEX:H201	1.73	0.40
1:a:140:ARG:NH2	1:a:142:TRP:HZ3	2.15	0.40
27:b:609:CLA:H91	27:b:609:CLA:H142	2.02	0.40
27:b:616:CLA:HBA1	27:b:616:CLA:H3A	1.84	0.40
3:c:112:PHE:CE2	29:c:514:BCR:HC31	2.56	0.40
4:d:191:TRP:NE1	4:d:197:HIS:CD2	2.90	0.40
7:n:115:ASN:HB3	7:n:118:LEU:HD12	2.03	0.40
27:n:610:CLA:H92	27:n:610:CLA:H61	1.78	0.40
14:o:135:CYS:C	14:o:136:LEU:HD12	2.45	0.40
14:o:216:LEU:HA	14:o:228:ASP:O	2.20	0.40
18:s:106:GLY:O	18:s:124:LEU:HB2	2.21	0.40
18:s:206:GLN:HE22	38:s:1620:LUT:H42	1.84	0.40
7:y:66:VAL:HB	7:y:155:LEU:HD22	2.03	0.40
7:y:180:GLU:HB2	27:y:610:CLA:CHB	2.51	0.40
27:y:611:CLA:CHD	35:y:2630:LHG:HC62	2.52	0.40
38:y:1621:LUT:H11	38:y:1621:LUT:H191	1.92	0.40
39:y:1622:XAT:H173	39:y:1622:XAT:H3	1.86	0.40
2:B:8:VAL:HG22	27:B:612:CLA:H11	2.03	0.40
2:B:18:ARG:HD3	2:B:115:TRP:CH2	2.57	0.40
2:B:75:TRP:NE1	2:B:92:SER:HG	2.18	0.40
2:B:218:SER:OG	2:B:219:VAL:N	2.52	0.40
2:B:264:PRO:HD2	2:B:267:LEU:HD12	2.04	0.40
2:B:413:ASP:OD1	2:B:413:ASP:N	2.52	0.40
27:B:613:CLA:CMB	27:B:615:CLA:HBB1	2.52	0.40
4:D:181:PHE:O	4:D:184:PHE:HB3	2.21	0.40
11:K:44:PHE:O	11:K:48:LEU:N	2.47	0.40
14:O:134:PHE:HD1	14:O:327:ALA:HB2	1.85	0.40
17:R:111:LEU:HD11	17:R:211:PHE:CZ	2.56	0.40
18:S:96:GLU:CD	18:S:215:VAL:HB	2.46	0.40
31:a:413:LMG:H292	31:a:413:LMG:H321	1.59	0.40
31:a:413:LMG:HC62	21:w:96:LEU:HB2	2.02	0.40
2:b:87:ASP:HA	2:b:88:PRO:HD2	1.94	0.40
2:b:340:TRP:HA	2:b:430:PHE:CD1	2.51	0.40
3:c:187:ASP:O	3:c:194:GLY:HA2	2.22	0.40
3:c:216:SER:OG	3:c:218:PHE:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:354:GLU:O	3:c:357:ARG:HG2	2.21	0.40
4:d:29:PHE:HZ	4:d:131:GLU:HG2	1.86	0.40
4:d:183:LEU:HD23	4:d:183:LEU:HA	1.93	0.40
7:g:22:VAL:HG23	7:g:44:TYR:CE1	2.57	0.40
29:h:101:BCR:H20C	29:h:101:BCR:H361	1.90	0.40
17:r:69:ARG:O	17:r:71:GLU:HG3	2.22	0.40
17:r:192:ILE:O	17:r:195:LEU:HB3	2.21	0.40
17:r:201:ALA:O	17:r:205:MET:HB2	2.22	0.40
17:r:202:ARG:HH22	27:r:602:CLA:HED3	1.86	0.40
18:s:96:GLU:CD	18:s:215:VAL:HB	2.46	0.40
7:y:46:TRP:CE3	38:y:1621:LUT:H383	2.56	0.40
7:y:167:ALA:HA	7:y:173:PHE:HB2	2.03	0.40
2:B:362:PHE:CE2	4:D:184:PHE:HZ	2.39	0.40
2:B:382:PRO:HG2	2:B:385:ARG:HH21	1.87	0.40
27:B:609:CLA:H91	27:B:609:CLA:H142	2.02	0.40
27:B:617:CLA:H11	27:B:617:CLA:H51	1.81	0.40
4:D:126:MET:SD	4:D:150:ILE:HD12	2.62	0.40
40:R:623:NEX:H11	40:R:623:NEX:H191	1.77	0.40
27:S:609:CLA:H3A	27:S:609:CLA:HBA2	1.37	0.40
38:S:1620:LUT:H11	38:S:1620:LUT:H191	1.92	0.40
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.03	0.40
2:b:150:CYS:O	2:b:202:HIS:HB3	2.22	0.40
2:b:212:ALA:HB2	27:b:610:CLA:HMC3	2.02	0.40
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.56	0.40
2:b:333:GLY:HA2	2:b:444:ARG:HH11	1.86	0.40
2:b:382:PRO:HG2	2:b:385:ARG:HH21	1.87	0.40
27:b:604:CLA:H152	8:h:50:PHE:HE2	1.87	0.40
27:b:610:CLA:H93	27:b:610:CLA:H62	1.95	0.40
27:b:613:CLA:CMB	27:b:615:CLA:HBB1	2.52	0.40
3:c:344:SER:N	3:c:348:GLU:O	2.38	0.40
6:f:45:ARG:HB3	10:j:36:LEU:HD23	2.03	0.40
27:g:602:CLA:H92	27:g:602:CLA:H62	1.77	0.40
10:j:10:LEU:HA	10:j:13:ILE:HD12	2.03	0.40
7:n:143:ILE:O	7:n:151:VAL:HG21	2.21	0.40
7:n:189:PHE:HD1	27:n:602:CLA:H201	1.87	0.40
16:q:21:GLU:HB2	16:q:24:ASP:HB2	2.02	0.40
17:r:226:TRP:CH2	17:r:230:LEU:HD22	2.57	0.40
27:r:611:CLA:HBA1	27:r:611:CLA:H12	1.79	0.40
38:r:620:LUT:H11	38:r:620:LUT:H191	1.95	0.40
18:s:224:ASP:O	18:s:227:GLY:N	2.55	0.40
27:y:604:CLA:O2A	40:y:1623:NEX:H241	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
1	a	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
2	B	485/508 (96%)	469 (97%)	13 (3%)	3 (1%)	21	56
2	b	485/508 (96%)	469 (97%)	13 (3%)	3 (1%)	21	56
3	C	447/473 (94%)	424 (95%)	23 (5%)	0	100	100
3	c	447/473 (94%)	424 (95%)	23 (5%)	0	100	100
4	D	338/353 (96%)	317 (94%)	20 (6%)	1 (0%)	36	68
4	d	338/353 (96%)	317 (94%)	20 (6%)	1 (0%)	36	68
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
6	F	30/39 (77%)	30 (100%)	0	0	100	100
6	f	30/39 (77%)	30 (100%)	0	0	100	100
7	G	216/267 (81%)	208 (96%)	7 (3%)	1 (0%)	24	59
7	N	216/267 (81%)	210 (97%)	5 (2%)	1 (0%)	24	59
7	Y	216/267 (81%)	205 (95%)	10 (5%)	1 (0%)	24	59
7	g	216/267 (81%)	208 (96%)	7 (3%)	1 (0%)	24	59
7	n	216/267 (81%)	210 (97%)	5 (2%)	1 (0%)	24	59
7	y	216/267 (81%)	205 (95%)	10 (5%)	1 (0%)	24	59
8	H	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
8	h	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
9	I	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
9	i	33/36 (92%)	30 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	32/40 (80%)	32 (100%)	0	0	100	100
10	j	32/40 (80%)	32 (100%)	0	0	100	100
11	K	35/59 (59%)	35 (100%)	0	0	100	100
11	k	35/59 (59%)	35 (100%)	0	0	100	100
12	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
12	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
13	M	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
13	m	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
14	O	241/332 (73%)	210 (87%)	26 (11%)	5 (2%)	5	31
14	o	241/332 (73%)	210 (87%)	26 (11%)	5 (2%)	5	31
15	P	170/267 (64%)	148 (87%)	20 (12%)	2 (1%)	10	42
15	p	170/267 (64%)	148 (87%)	20 (12%)	2 (1%)	10	42
16	Q	146/232 (63%)	134 (92%)	8 (6%)	4 (3%)	4	25
16	q	146/232 (63%)	134 (92%)	8 (6%)	4 (3%)	4	25
17	R	230/243 (95%)	211 (92%)	10 (4%)	9 (4%)	2	18
17	r	230/243 (95%)	211 (92%)	10 (4%)	9 (4%)	2	18
18	S	212/295 (72%)	187 (88%)	17 (8%)	8 (4%)	2	18
18	s	212/295 (72%)	187 (88%)	17 (8%)	8 (4%)	2	18
19	T	28/33 (85%)	28 (100%)	0	0	100	100
19	t	28/33 (85%)	28 (100%)	0	0	100	100
20	U	23/99 (23%)	21 (91%)	1 (4%)	1 (4%)	2	16
20	u	23/99 (23%)	21 (91%)	1 (4%)	1 (4%)	2	16
21	W	52/137 (38%)	46 (88%)	5 (10%)	1 (2%)	6	33
21	w	52/137 (38%)	46 (88%)	5 (10%)	1 (2%)	6	33
22	X	33/117 (28%)	33 (100%)	0	0	100	100
22	x	33/117 (28%)	33 (100%)	0	0	100	100
23	Z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
23	z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
All	All	7548/9396 (80%)	7100 (94%)	374 (5%)	74 (1%)	15	45

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	85	ILE
14	O	258	PRO
14	O	311	LEU
15	P	108	VAL
18	S	110	VAL
18	S	163	LYS
2	b	85	ILE
14	o	258	PRO
14	o	311	LEU
15	p	108	VAL
18	s	110	VAL
18	s	163	LYS
7	G	119	VAL
14	O	261	GLY
16	Q	5	ILE
17	R	43	ALA
17	R	58	ALA
18	S	166	PRO
21	W	86	ASP
7	g	119	VAL
14	o	261	GLY
16	q	5	ILE
17	r	43	ALA
17	r	58	ALA
18	s	166	PRO
21	w	86	ASP
2	B	51	VAL
17	R	17	GLY
17	R	189	LYS
18	S	127	PHE
2	b	51	VAL
17	r	17	GLY
17	r	189	LYS
18	s	127	PHE
14	O	119	VAL
15	P	70	SER
17	R	54	ASP
17	R	61	LEU
18	S	158	LEU
14	o	119	VAL
15	p	70	SER
17	r	54	ASP
17	r	61	LEU

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Mol	Chain	Res	Type
18	s	158	LEU
2	B	333	GLY
7	N	119	VAL
14	O	177	GLU
16	Q	33	TYR
17	R	46	LEU
17	R	82	PRO
18	S	46	PRO
18	S	132	PRO
2	b	333	GLY
7	n	119	VAL
16	q	33	TYR
17	r	46	LEU
17	r	82	PRO
18	s	46	PRO
18	s	132	PRO
17	R	187	PRO
7	Y	119	VAL
14	o	177	GLU
17	r	187	PRO
7	y	119	VAL
4	D	175	VAL
16	Q	43	LEU
4	d	175	VAL
16	q	43	LEU
16	Q	6	VAL
18	S	172	PRO
20	U	7	PRO
16	q	6	VAL
18	s	172	PRO
20	u	7	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/279 (97%)	270 (100%)	0	100	100
1	a	270/279 (97%)	270 (100%)	0	100	100
2	B	389/406 (96%)	389 (100%)	0	100	100
2	b	389/406 (96%)	389 (100%)	0	100	100
3	C	351/374 (94%)	351 (100%)	0	100	100
3	c	351/374 (94%)	351 (100%)	0	100	100
4	D	272/283 (96%)	272 (100%)	0	100	100
4	d	272/283 (96%)	272 (100%)	0	100	100
5	E	70/73 (96%)	70 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	27/34 (79%)	27 (100%)	0	100	100
6	f	27/34 (79%)	27 (100%)	0	100	100
7	G	168/206 (82%)	168 (100%)	0	100	100
7	N	168/206 (82%)	168 (100%)	0	100	100
7	Y	168/206 (82%)	168 (100%)	0	100	100
7	g	168/206 (82%)	168 (100%)	0	100	100
7	n	168/206 (82%)	168 (100%)	0	100	100
7	y	168/206 (82%)	168 (100%)	0	100	100
8	H	48/61 (79%)	48 (100%)	0	100	100
8	h	48/61 (79%)	48 (100%)	0	100	100
9	I	32/33 (97%)	32 (100%)	0	100	100
9	i	32/33 (97%)	32 (100%)	0	100	100
10	J	25/30 (83%)	25 (100%)	0	100	100
10	j	25/30 (83%)	25 (100%)	0	100	100
11	K	32/52 (62%)	32 (100%)	0	100	100
11	k	32/52 (62%)	32 (100%)	0	100	100
12	L	35/36 (97%)	35 (100%)	0	100	100
12	l	35/36 (97%)	35 (100%)	0	100	100
13	M	29/30 (97%)	29 (100%)	0	100	100
13	m	29/30 (97%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	202/269 (75%)	202 (100%)	0	100	100
14	o	202/269 (75%)	202 (100%)	0	100	100
15	P	144/212 (68%)	144 (100%)	0	100	100
15	p	144/212 (68%)	144 (100%)	0	100	100
16	Q	129/187 (69%)	129 (100%)	0	100	100
16	q	129/187 (69%)	129 (100%)	0	100	100
17	R	189/198 (96%)	189 (100%)	0	100	100
17	r	189/198 (96%)	189 (100%)	0	100	100
18	S	167/226 (74%)	166 (99%)	1 (1%)	78	84
18	s	167/226 (74%)	166 (99%)	1 (1%)	78	84
19	T	27/30 (90%)	27 (100%)	0	100	100
19	t	27/30 (90%)	27 (100%)	0	100	100
20	U	21/80 (26%)	21 (100%)	0	100	100
20	u	21/80 (26%)	21 (100%)	0	100	100
21	W	44/110 (40%)	44 (100%)	0	100	100
21	w	44/110 (40%)	44 (100%)	0	100	100
22	X	26/90 (29%)	26 (100%)	0	100	100
22	x	26/90 (29%)	26 (100%)	0	100	100
23	Z	52/53 (98%)	52 (100%)	0	100	100
23	z	52/53 (98%)	52 (100%)	0	100	100
All	All	6170/7528 (82%)	6168 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	S	133	ILE
18	s	133	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	GLN
2	B	157	HIS
2	B	216	HIS

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Mol	Chain	Res	Type
2	B	282	GLN
2	B	296	GLN
2	B	343	HIS
3	C	28	GLN
3	C	68	ASN
3	C	201	ASN
3	C	327	ASN
3	C	418	ASN
4	D	83	ASN
4	D	142	ASN
4	D	164	GLN
4	D	186	GLN
4	D	322	ASN
7	G	88	ASN
7	G	103	GLN
7	G	197	GLN
11	K	53	GLN
7	N	88	ASN
7	N	103	GLN
7	N	208	ASN
14	O	157	GLN
14	O	305	GLN
14	O	331	GLN
17	R	138	GLN
17	R	194	GLN
18	S	81	HIS
18	S	104	ASN
7	Y	103	GLN
7	Y	122	GLN
7	Y	208	ASN
23	Z	58	ASN
1	a	304	GLN
2	b	157	HIS
2	b	216	HIS
2	b	282	GLN
2	b	296	GLN
2	b	343	HIS
3	c	28	GLN
3	c	68	ASN
3	c	201	ASN
3	c	327	ASN
3	c	332	GLN

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Mol	Chain	Res	Type
3	c	418	ASN
4	d	83	ASN
4	d	142	ASN
4	d	164	GLN
4	d	186	GLN
4	d	301	GLN
4	d	322	ASN
7	g	88	ASN
7	g	103	GLN
7	g	197	GLN
11	k	53	GLN
7	n	88	ASN
7	n	103	GLN
7	n	208	ASN
14	o	157	GLN
14	o	200	GLN
14	o	305	GLN
14	o	331	GLN
17	r	55	GLN
17	r	138	GLN
17	r	194	GLN
18	s	81	HIS
18	s	104	ASN
7	y	103	GLN
7	y	208	ASN
23	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 322 ligands modelled in this entry, 6 are monoatomic - leaving 316 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$
29	BCR	c	516	-	41,41,41	0.73	1 (2%)	56,56,56	2.32	18 (32%)
38	LUT	S	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.92	18 (35%)
27	CLA	S	604	-	53,57,73	1.29	8 (15%)	61,93,113	1.52	5 (8%)
39	XAT	r	622	-	41,47,47	0.95	2 (4%)	54,74,74	2.75	22 (40%)
27	CLA	y	604	-	53,57,73	1.29	8 (15%)	61,93,113	1.47	6 (9%)
37	CHL	S	608	-	43,57,74	4.05	19 (44%)	37,93,114	2.14	9 (24%)
27	CLA	n	613	7	53,57,73	1.29	8 (15%)	61,93,113	1.44	4 (6%)
27	CLA	r	611	35	53,57,73	1.29	7 (13%)	61,93,113	1.37	6 (9%)
29	BCR	b	618	-	41,41,41	0.83	2 (4%)	56,56,56	2.22	19 (33%)
29	BCR	b	620	-	41,41,41	0.91	2 (4%)	56,56,56	2.14	17 (30%)
38	LUT	g	1620	-	42,43,43	0.80	1 (2%)	51,60,60	1.96	16 (31%)
27	CLA	N	602	7	69,73,73	1.16	9 (13%)	82,113,113	1.31	4 (4%)
27	CLA	c	509	-	69,73,73	1.16	10 (14%)	82,113,113	1.44	11 (13%)
29	BCR	a	411	-	41,41,41	0.83	2 (4%)	56,56,56	2.11	19 (33%)
37	CHL	R	608	-	44,58,74	3.82	19 (43%)	37,94,114	2.26	13 (35%)
27	CLA	d	403	-	69,73,73	1.14	9 (13%)	82,113,113	1.33	7 (8%)
37	CHL	g	608	-	44,58,74	3.83	19 (43%)	37,94,114	2.24	13 (35%)
29	BCR	C	514	-	41,41,41	0.82	1 (2%)	56,56,56	2.05	18 (32%)
29	BCR	B	618	-	41,41,41	0.83	2 (4%)	56,56,56	2.21	19 (33%)
28	PHO	A	408	-	58,69,69	2.03	11 (18%)	55,99,99	1.48	5 (9%)
35	LHG	l	101	-	48,48,48	0.75	1 (2%)	51,54,54	1.34	7 (13%)
27	CLA	N	604	-	53,57,73	1.29	10 (18%)	61,93,113	1.47	5 (8%)
27	CLA	C	506	-	69,73,73	1.17	8 (11%)	82,113,113	1.35	9 (10%)
35	LHG	s	2630	27	48,48,48	0.65	1 (2%)	51,54,54	1.30	6 (11%)
38	LUT	s	1620	-	42,43,43	0.82	2 (4%)	51,60,60	2.07	16 (31%)
28	PHO	a	409	-	58,69,69	2.03	12 (20%)	55,99,99	1.54	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	C	508	-	69,73,73	1.20	7 (10%)	82,113,113	1.42	5 (6%)
27	CLA	S	613	18	53,57,73	1.28	8 (15%)	61,93,113	1.42	5 (8%)
27	CLA	B	609	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	7 (8%)
27	CLA	y	613	7	69,73,73	1.15	8 (11%)	82,113,113	1.32	6 (7%)
27	CLA	B	607	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	8 (9%)
37	CHL	y	605	7	42,56,74	3.85	19 (45%)	36,92,114	2.54	12 (33%)
27	CLA	c	511	3	69,73,73	1.16	10 (14%)	82,113,113	1.39	7 (8%)
37	CHL	r	607	-	44,58,74	3.80	20 (45%)	37,94,114	2.65	12 (32%)
27	CLA	C	502	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	7 (8%)
27	CLA	A	405	-	69,73,73	1.19	8 (11%)	82,113,113	1.36	8 (9%)
27	CLA	N	610	7	69,73,73	1.15	9 (13%)	82,113,113	1.35	8 (9%)
37	CHL	n	609	7	44,58,74	3.77	19 (43%)	37,94,114	2.60	12 (32%)
31	LMG	z	101	-	51,51,55	0.72	1 (1%)	59,59,63	1.35	6 (10%)
27	CLA	b	604	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
27	CLA	b	607	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	8 (9%)
27	CLA	b	602	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	5 (6%)
27	CLA	Y	603	-	53,57,73	1.31	9 (16%)	61,93,113	1.39	5 (8%)
27	CLA	s	604	-	53,57,73	1.29	8 (15%)	61,93,113	1.52	5 (8%)
37	CHL	y	606	-	44,58,74	3.73	20 (45%)	37,94,114	2.78	12 (32%)
27	CLA	N	613	7	53,57,73	1.30	8 (15%)	61,93,113	1.44	4 (6%)
37	CHL	r	608	-	44,58,74	3.82	19 (43%)	37,94,114	2.25	12 (32%)
37	CHL	g	601	7	60,74,74	3.23	19 (31%)	58,114,114	2.37	14 (24%)
31	LMG	b	622	-	51,51,55	0.81	1 (1%)	59,59,63	1.45	7 (11%)
27	CLA	C	504	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	4 (4%)
27	CLA	c	501	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
27	CLA	s	602	18	53,57,73	1.31	9 (16%)	61,93,113	1.44	5 (8%)
31	LMG	A	413	-	48,48,55	0.82	2 (4%)	56,56,63	1.57	13 (23%)
38	LUT	N	1621	-	42,43,43	0.89	2 (4%)	51,60,60	1.86	15 (29%)
27	CLA	B	605	-	69,73,73	1.17	10 (14%)	82,113,113	1.52	8 (9%)
35	LHG	L	101	-	48,48,48	0.75	1 (2%)	51,54,54	1.34	7 (13%)
27	CLA	G	613	7	53,57,73	1.31	9 (16%)	61,93,113	1.45	6 (9%)
27	CLA	a	406	-	69,73,73	1.15	7 (10%)	82,113,113	1.38	7 (8%)
27	CLA	Y	614	-	53,57,73	1.26	8 (15%)	61,93,113	1.43	5 (8%)
33	BCT	d	401	-	3,3,3	1.13	0	2,3,3	1.11	0
37	CHL	N	606	-	44,58,74	3.82	20 (45%)	37,94,114	2.76	12 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMG	D	411	-	46,46,55	0.84	4 (8%)	54,54,63	1.42	9 (16%)
30	SQD	A	418	-	52,54,54	0.99	4 (7%)	62,65,65	1.43	9 (14%)
37	CHL	g	607	-	44,58,74	3.80	19 (43%)	37,94,114	2.71	12 (32%)
37	CHL	R	607	-	44,58,74	3.80	20 (45%)	37,94,114	2.66	12 (32%)
33	BCT	D	401	-	3,3,3	1.13	0	2,3,3	1.11	0
27	CLA	Y	602	7	69,73,73	1.17	8 (11%)	82,113,113	1.37	6 (7%)
37	CHL	Y	606	-	44,58,74	3.73	20 (45%)	37,94,114	2.77	12 (32%)
27	CLA	b	613	-	69,73,73	1.17	8 (11%)	82,113,113	1.43	9 (10%)
38	LUT	R	620	-	42,43,43	0.78	2 (4%)	51,60,60	1.80	16 (31%)
27	CLA	n	603	-	53,57,73	1.29	8 (15%)	61,93,113	1.43	4 (6%)
27	CLA	C	512	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	5 (6%)
27	CLA	n	602	7	69,73,73	1.17	8 (11%)	82,113,113	1.30	4 (4%)
24	OEX	A	401	3,1	0,15,15	-	-	-	-	-
27	CLA	S	614	-	53,57,73	1.30	10 (18%)	61,93,113	1.40	5 (8%)
27	CLA	Y	612	7	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
29	BCR	d	404	-	41,41,41	0.74	1 (2%)	56,56,56	2.22	15 (26%)
37	CHL	s	601	18	46,60,74	3.71	20 (43%)	40,97,114	2.50	15 (37%)
27	CLA	n	610	7	69,73,73	1.16	10 (14%)	82,113,113	1.34	8 (9%)
38	LUT	S	1620	-	42,43,43	0.82	1 (2%)	51,60,60	2.07	16 (31%)
27	CLA	C	505	-	69,73,73	1.18	9 (13%)	82,113,113	1.40	7 (8%)
37	CHL	N	605	7	42,56,74	3.95	20 (47%)	36,92,114	2.41	12 (33%)
27	CLA	G	610	7	69,73,73	1.15	8 (11%)	82,113,113	1.32	7 (8%)
29	BCR	c	515	-	41,41,41	0.84	2 (4%)	56,56,56	2.17	20 (35%)
27	CLA	y	603	-	53,57,73	1.31	9 (16%)	61,93,113	1.40	4 (6%)
27	CLA	D	403	-	69,73,73	1.14	9 (13%)	82,113,113	1.33	7 (8%)
28	PHO	a	408	-	58,69,69	2.03	12 (20%)	55,99,99	1.49	5 (9%)
27	CLA	S	602	18	53,57,73	1.31	9 (16%)	61,93,113	1.45	5 (8%)
27	CLA	y	614	-	53,57,73	1.27	8 (15%)	61,93,113	1.45	5 (8%)
27	CLA	n	604	-	53,57,73	1.29	10 (18%)	61,93,113	1.47	5 (8%)
29	BCR	B	620	-	41,41,41	0.91	2 (4%)	56,56,56	2.14	17 (30%)
38	LUT	G	1621	-	42,43,43	0.87	1 (2%)	51,60,60	1.95	18 (35%)
37	CHL	s	606	-	44,58,74	3.90	19 (43%)	37,94,114	2.27	12 (32%)
29	BCR	B	619	-	41,41,41	0.81	2 (4%)	56,56,56	2.11	17 (30%)
35	LHG	D	410	-	36,36,48	0.71	0	39,42,54	1.30	4 (10%)
27	CLA	a	407	-	53,57,73	1.31	9 (16%)	61,93,113	1.44	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	611	-	69,73,73	1.18	8 (11%)	82,113,113	1.36	7 (8%)
35	LHG	r	2630	27	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
27	CLA	R	616	17	53,57,73	1.31	8 (15%)	61,93,113	1.44	6 (9%)
31	LMG	c	521	-	51,51,55	0.75	0	59,59,63	1.39	7 (11%)
27	CLA	D	402	-	69,73,73	1.18	8 (11%)	82,113,113	1.40	7 (8%)
35	LHG	g	2630	27	48,48,48	0.63	1 (2%)	51,54,54	1.31	7 (13%)
30	SQD	B	621	-	52,54,54	0.95	4 (7%)	62,65,65	1.49	9 (14%)
27	CLA	N	603	-	53,57,73	1.29	9 (16%)	61,93,113	1.43	4 (6%)
27	CLA	c	508	-	69,73,73	1.20	8 (11%)	82,113,113	1.43	5 (6%)
27	CLA	G	614	-	53,57,73	1.30	9 (16%)	61,93,113	1.44	5 (8%)
27	CLA	R	610	17	69,73,73	1.15	8 (11%)	82,113,113	1.33	5 (6%)
27	CLA	b	616	-	69,73,73	1.17	10 (14%)	82,113,113	1.29	5 (6%)
27	CLA	c	502	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
32	DGD	c	519	-	63,63,67	1.00	4 (6%)	77,77,81	1.51	13 (16%)
27	CLA	B	608	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	8 (9%)
40	NEX	g	1623	-	40,46,46	1.13	3 (7%)	50,70,70	2.46	15 (30%)
27	CLA	c	513	-	53,57,73	1.31	9 (16%)	61,93,113	1.51	7 (11%)
27	CLA	B	617	-	69,73,73	1.17	11 (15%)	82,113,113	1.31	6 (7%)
37	CHL	N	607	-	60,74,74	3.22	19 (31%)	58,114,114	2.16	16 (27%)
27	CLA	r	612	-	53,57,73	1.30	9 (16%)	61,93,113	1.37	5 (8%)
27	CLA	B	604	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
27	CLA	N	614	-	53,57,73	1.29	9 (16%)	61,93,113	1.47	6 (9%)
37	CHL	Y	608	-	44,58,74	3.76	19 (43%)	37,94,114	2.50	10 (27%)
38	LUT	r	620	-	42,43,43	0.78	2 (4%)	51,60,60	1.80	16 (31%)
27	CLA	C	503	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	7 (8%)
27	CLA	R	604	-	53,57,73	1.30	8 (15%)	61,93,113	1.49	5 (8%)
27	CLA	S	610	18	53,57,73	1.28	7 (13%)	61,93,113	1.44	8 (13%)
27	CLA	B	614	-	69,73,73	1.19	9 (13%)	82,113,113	1.25	6 (7%)
27	CLA	R	602	17	69,73,73	1.14	8 (11%)	82,113,113	1.29	5 (6%)
27	CLA	c	504	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	4 (4%)
29	BCR	A	411	-	41,41,41	0.83	2 (4%)	56,56,56	2.11	19 (33%)
37	CHL	S	601	18	46,60,74	3.71	20 (43%)	40,97,114	2.51	15 (37%)
40	NEX	G	1623	-	40,46,46	1.13	3 (7%)	50,70,70	2.46	15 (30%)
29	BCR	D	404	-	41,41,41	0.73	1 (2%)	56,56,56	2.22	15 (26%)
27	CLA	b	606	-	69,73,73	1.19	10 (14%)	82,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PL9	D	405	-	55,55,55	1.86	12 (21%)	68,69,69	1.53	12 (17%)
37	CHL	Y	607	-	44,58,74	3.71	19 (43%)	37,94,114	2.78	12 (32%)
29	BCR	c	514	-	41,41,41	0.81	1 (2%)	56,56,56	2.05	18 (32%)
27	CLA	y	611	35	69,73,73	1.15	9 (13%)	82,113,113	1.26	5 (6%)
27	CLA	b	609	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	7 (8%)
27	CLA	a	405	-	69,73,73	1.19	8 (11%)	82,113,113	1.37	8 (9%)
40	NEX	s	1623	-	40,46,46	1.07	4 (10%)	50,70,70	2.36	14 (28%)
27	CLA	r	610	17	69,73,73	1.15	8 (11%)	82,113,113	1.33	5 (6%)
32	DGD	h	102	-	63,63,67	0.99	4 (6%)	77,77,81	1.48	8 (10%)
27	CLA	B	606	-	69,73,73	1.19	10 (14%)	82,113,113	1.27	6 (7%)
35	LHG	d	410	-	36,36,48	0.72	0	39,42,54	1.30	4 (10%)
28	PHO	A	409	-	58,69,69	2.03	12 (20%)	55,99,99	1.54	7 (12%)
37	CHL	G	607	-	44,58,74	3.80	19 (43%)	37,94,114	2.71	12 (32%)
39	XAT	y	1622	-	41,47,47	0.90	1 (2%)	54,74,74	2.84	20 (37%)
35	LHG	y	2630	27	48,48,48	0.76	1 (2%)	51,54,54	1.33	6 (11%)
37	CHL	s	608	-	43,57,74	4.05	19 (44%)	37,93,114	2.14	9 (24%)
35	LHG	D	408	-	42,42,48	0.80	1 (2%)	45,48,54	1.31	5 (11%)
37	CHL	n	605	7	42,56,74	3.96	20 (47%)	36,92,114	2.41	12 (33%)
27	CLA	G	612	7	53,57,73	1.32	10 (18%)	61,93,113	1.41	5 (8%)
27	CLA	g	610	7	69,73,73	1.15	8 (11%)	82,113,113	1.33	7 (8%)
27	CLA	G	603	-	53,57,73	1.30	8 (15%)	61,93,113	1.44	4 (6%)
27	CLA	G	602	7	69,73,73	1.17	9 (13%)	82,113,113	1.32	5 (6%)
27	CLA	c	512	-	69,73,73	1.14	10 (14%)	82,113,113	1.31	5 (6%)
27	CLA	r	602	17	69,73,73	1.14	8 (11%)	82,113,113	1.30	5 (6%)
30	SQD	a	418	-	52,54,54	0.99	4 (7%)	62,65,65	1.43	9 (14%)
37	CHL	G	609	7	44,58,74	3.84	20 (45%)	37,94,114	2.34	11 (29%)
27	CLA	g	613	7	53,57,73	1.31	9 (16%)	61,93,113	1.45	6 (9%)
27	CLA	g	612	7	53,57,73	1.32	10 (18%)	61,93,113	1.42	5 (8%)
32	DGD	C	519	-	63,63,67	1.00	4 (6%)	77,77,81	1.51	13 (16%)
37	CHL	n	601	7	44,58,74	3.89	20 (45%)	37,94,114	2.39	12 (32%)
37	CHL	g	609	7	44,58,74	3.84	20 (45%)	37,94,114	2.33	11 (29%)
27	CLA	N	611	35	53,57,73	1.29	8 (15%)	61,93,113	1.45	6 (9%)
27	CLA	g	611	35	53,57,73	1.30	10 (18%)	61,93,113	1.46	6 (9%)
27	CLA	r	604	-	53,57,73	1.28	8 (15%)	61,93,113	1.48	5 (8%)
27	CLA	r	613	17	53,57,73	1.29	9 (16%)	61,93,113	1.47	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	b	612	-	69,73,73	1.20	11 (15%)	82,113,113	1.39	9 (10%)
27	CLA	C	513	-	53,57,73	1.31	9 (16%)	61,93,113	1.51	7 (11%)
37	CHL	y	607	-	44,58,74	3.71	19 (43%)	37,94,114	2.77	12 (32%)
39	XAT	Y	1622	-	41,47,47	0.91	1 (2%)	54,74,74	2.84	20 (37%)
27	CLA	A	406	-	69,73,73	1.15	7 (10%)	82,113,113	1.40	8 (9%)
27	CLA	b	615	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	4 (4%)
29	BCR	C	516	-	41,41,41	0.74	1 (2%)	56,56,56	2.32	18 (32%)
37	CHL	R	606	-	44,58,74	3.71	19 (43%)	37,94,114	2.69	13 (35%)
32	DGD	c	518	-	56,56,67	1.14	6 (10%)	70,70,81	1.71	15 (21%)
35	LHG	S	2630	27	48,48,48	0.66	1 (2%)	51,54,54	1.30	6 (11%)
27	CLA	A	410	-	64,68,73	1.19	8 (12%)	76,107,113	1.43	7 (9%)
27	CLA	C	509	-	69,73,73	1.16	8 (11%)	82,113,113	1.44	11 (13%)
30	SQD	a	412	-	52,54,54	0.97	3 (5%)	62,65,65	1.38	10 (16%)
38	LUT	g	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.95	18 (35%)
27	CLA	g	604	-	53,57,73	1.30	8 (15%)	61,93,113	1.39	5 (8%)
27	CLA	R	603	-	53,57,73	1.29	9 (16%)	61,93,113	1.39	5 (8%)
37	CHL	n	607	-	60,74,74	3.22	19 (31%)	58,114,114	2.16	16 (27%)
38	LUT	y	1620	-	42,43,43	0.83	2 (4%)	51,60,60	1.98	18 (35%)
31	LMG	a	413	-	48,48,55	0.82	2 (4%)	56,56,63	1.56	13 (23%)
27	CLA	s	611	35	53,57,73	1.29	9 (16%)	61,93,113	1.41	5 (8%)
27	CLA	n	614	-	53,57,73	1.29	8 (15%)	61,93,113	1.46	6 (9%)
27	CLA	s	610	18	53,57,73	1.29	8 (15%)	61,93,113	1.45	8 (13%)
29	BCR	c	517	-	41,41,41	0.86	2 (4%)	56,56,56	2.36	16 (28%)
27	CLA	a	410	-	64,68,73	1.20	8 (12%)	76,107,113	1.43	7 (9%)
27	CLA	C	511	3	69,73,73	1.16	9 (13%)	82,113,113	1.40	7 (8%)
31	LMG	B	622	-	51,51,55	0.81	1 (1%)	59,59,63	1.45	7 (11%)
34	PL9	d	405	-	55,55,55	1.85	13 (23%)	68,69,69	1.52	12 (17%)
27	CLA	b	617	-	69,73,73	1.17	10 (14%)	82,113,113	1.31	7 (8%)
37	CHL	S	607	-	44,58,74	3.91	19 (43%)	37,94,114	2.35	12 (32%)
32	DGD	c	520	-	63,63,67	0.98	5 (7%)	77,77,81	1.50	11 (14%)
31	LMG	d	411	-	46,46,55	0.85	4 (8%)	54,54,63	1.42	9 (16%)
37	CHL	y	608	-	44,58,74	3.75	19 (43%)	37,94,114	2.50	9 (24%)
32	DGD	H	102	-	63,63,67	0.99	4 (6%)	77,77,81	1.48	8 (10%)
27	CLA	r	616	17	53,57,73	1.31	8 (15%)	61,93,113	1.43	6 (9%)
35	LHG	N	2630	27	48,48,48	0.62	1 (2%)	51,54,54	1.30	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	H	101	-	41,41,41	0.78	1 (2%)	56,56,56	2.04	18 (32%)
27	CLA	B	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
27	CLA	s	613	18	53,57,73	1.29	8 (15%)	61,93,113	1.43	5 (8%)
27	CLA	s	612	18	53,57,73	1.29	9 (16%)	61,93,113	1.38	5 (8%)
27	CLA	b	605	-	69,73,73	1.17	10 (14%)	82,113,113	1.52	8 (9%)
27	CLA	b	611	-	69,73,73	1.18	8 (11%)	82,113,113	1.36	7 (8%)
38	LUT	Y	1620	-	42,43,43	0.84	2 (4%)	51,60,60	1.97	18 (35%)
27	CLA	y	612	7	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
35	LHG	d	409	-	48,48,48	0.79	1 (2%)	51,54,54	1.38	9 (17%)
35	LHG	Y	2630	27	48,48,48	0.77	2 (4%)	51,54,54	1.33	6 (11%)
40	NEX	R	623	-	40,46,46	1.23	3 (7%)	50,70,70	2.35	19 (38%)
38	LUT	y	1621	-	42,43,43	0.95	2 (4%)	51,60,60	2.00	16 (31%)
31	LMG	Z	101	-	51,51,55	0.72	1 (1%)	59,59,63	1.35	6 (10%)
40	NEX	N	1623	-	40,46,46	1.14	3 (7%)	50,70,70	2.46	17 (34%)
38	LUT	N	1620	-	42,43,43	0.79	2 (4%)	51,60,60	1.99	16 (31%)
29	BCR	C	517	-	41,41,41	0.87	2 (4%)	56,56,56	2.36	16 (28%)
27	CLA	Y	611	35	69,73,73	1.15	9 (13%)	82,113,113	1.26	4 (4%)
38	LUT	G	1620	-	42,43,43	0.81	1 (2%)	51,60,60	1.95	16 (31%)
37	CHL	r	606	-	44,58,74	3.71	19 (43%)	37,94,114	2.70	13 (35%)
35	LHG	G	2630	27	48,48,48	0.63	1 (2%)	51,54,54	1.30	7 (13%)
27	CLA	b	614	-	69,73,73	1.19	9 (13%)	82,113,113	1.25	6 (7%)
27	CLA	g	603	-	53,57,73	1.30	8 (15%)	61,93,113	1.44	4 (6%)
36	HEM	F	101	6,5	50,50,50	1.78	7 (14%)	67,82,82	1.09	2 (2%)
35	LHG	D	409	-	48,48,48	0.79	1 (2%)	51,54,54	1.38	9 (17%)
27	CLA	g	602	7	69,73,73	1.17	9 (13%)	82,113,113	1.32	5 (6%)
27	CLA	c	507	-	69,73,73	1.18	10 (14%)	82,113,113	1.29	6 (7%)
27	CLA	G	611	35	53,57,73	1.29	10 (18%)	61,93,113	1.45	6 (9%)
27	CLA	c	510	-	69,73,73	1.17	9 (13%)	82,113,113	1.34	6 (7%)
30	SQD	b	621	-	52,54,54	0.95	4 (7%)	62,65,65	1.49	9 (14%)
40	NEX	Y	1623	-	40,46,46	1.24	3 (7%)	50,70,70	2.42	17 (34%)
27	CLA	s	603	-	53,57,73	1.30	7 (13%)	61,93,113	1.37	5 (8%)
38	LUT	s	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.92	18 (35%)
27	CLA	N	612	7	53,57,73	1.30	7 (13%)	61,93,113	1.45	5 (8%)
27	CLA	n	611	35	53,57,73	1.28	8 (15%)	61,93,113	1.46	6 (9%)
37	CHL	y	601	7	60,74,74	3.23	20 (33%)	58,114,114	2.27	14 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	g	614	-	53,57,73	1.30	8 (15%)	61,93,113	1.44	5 (8%)
27	CLA	c	505	-	69,73,73	1.17	8 (11%)	82,113,113	1.39	7 (8%)
27	CLA	S	609	18	53,57,73	1.32	8 (15%)	61,93,113	1.37	4 (6%)
27	CLA	B	612	-	69,73,73	1.19	11 (15%)	82,113,113	1.40	9 (10%)
37	CHL	N	608	-	44,58,74	3.78	19 (43%)	37,94,114	2.66	12 (32%)
27	CLA	S	611	35	53,57,73	1.30	10 (18%)	61,93,113	1.41	5 (8%)
27	CLA	r	603	-	53,57,73	1.29	9 (16%)	61,93,113	1.41	5 (8%)
27	CLA	s	614	-	53,57,73	1.30	9 (16%)	61,93,113	1.39	5 (8%)
36	HEM	f	101	6,5	50,50,50	1.77	7 (14%)	67,82,82	1.09	2 (2%)
27	CLA	r	601	17	53,57,73	1.30	8 (15%)	61,93,113	1.46	7 (11%)
27	CLA	Y	604	-	53,57,73	1.31	8 (15%)	61,93,113	1.47	6 (9%)
40	NEX	r	623	-	40,46,46	1.24	3 (7%)	50,70,70	2.35	19 (38%)
29	BCR	C	515	-	41,41,41	0.84	2 (4%)	56,56,56	2.17	20 (35%)
27	CLA	Y	610	7	69,73,73	1.16	8 (11%)	82,113,113	1.34	9 (10%)
29	BCR	h	101	-	41,41,41	0.79	1 (2%)	56,56,56	2.03	18 (32%)
27	CLA	G	604	-	53,57,73	1.30	8 (15%)	61,93,113	1.39	5 (8%)
37	CHL	y	609	7	60,74,74	3.17	19 (31%)	58,114,114	2.22	16 (27%)
27	CLA	b	610	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	8 (9%)
27	CLA	c	503	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	8 (9%)
32	DGD	C	520	-	63,63,67	0.98	5 (7%)	77,77,81	1.50	11 (14%)
27	CLA	R	612	-	53,57,73	1.30	9 (16%)	61,93,113	1.37	5 (8%)
27	CLA	b	608	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	8 (9%)
27	CLA	B	602	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
31	LMG	C	521	-	51,51,55	0.75	0	59,59,63	1.39	7 (11%)
27	CLA	R	601	17	53,57,73	1.30	8 (15%)	61,93,113	1.46	7 (11%)
27	CLA	R	609	17	53,57,73	1.28	8 (15%)	61,93,113	1.42	5 (8%)
37	CHL	Y	601	7	60,74,74	3.22	20 (33%)	58,114,114	2.27	14 (24%)
37	CHL	Y	609	7	60,74,74	3.17	19 (31%)	58,114,114	2.23	16 (27%)
39	XAT	n	1622	-	41,47,47	0.93	2 (4%)	54,74,74	2.94	24 (44%)
27	CLA	R	613	17	53,57,73	1.29	9 (16%)	61,93,113	1.45	5 (8%)
27	CLA	B	610	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	8 (9%)
27	CLA	d	402	-	69,73,73	1.19	8 (11%)	82,113,113	1.40	7 (8%)
37	CHL	G	608	-	44,58,74	3.81	19 (43%)	37,94,114	2.24	13 (35%)
32	DGD	C	518	-	56,56,67	1.15	7 (12%)	70,70,81	1.71	15 (21%)
27	CLA	b	603	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	A	407	-	53,57,73	1.30	9 (16%)	61,93,113	1.45	7 (11%)
27	CLA	C	501	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
37	CHL	N	609	7	44,58,74	3.77	19 (43%)	37,94,114	2.60	12 (32%)
27	CLA	s	609	18	53,57,73	1.31	8 (15%)	61,93,113	1.37	4 (6%)
37	CHL	G	601	7	60,74,74	3.22	19 (31%)	58,114,114	2.36	14 (24%)
30	SQD	A	412	-	52,54,54	0.98	4 (7%)	62,65,65	1.38	10 (16%)
39	XAT	g	1622	-	41,47,47	0.95	2 (4%)	54,74,74	2.76	18 (33%)
37	CHL	g	606	-	44,58,74	3.88	20 (45%)	37,94,114	2.53	12 (32%)
37	CHL	G	605	7	42,56,74	4.05	19 (45%)	36,92,114	2.27	11 (30%)
35	LHG	n	2630	27	48,48,48	0.63	1 (2%)	51,54,54	1.30	6 (11%)
27	CLA	c	506	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	9 (10%)
35	LHG	R	2630	27	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
39	XAT	R	622	-	41,47,47	0.94	3 (7%)	54,74,74	2.75	22 (40%)
27	CLA	C	510	-	69,73,73	1.17	9 (13%)	82,113,113	1.34	6 (7%)
38	LUT	n	1620	-	42,43,43	0.78	2 (4%)	51,60,60	2.00	16 (31%)
27	CLA	y	610	7	69,73,73	1.16	8 (11%)	82,113,113	1.33	9 (10%)
27	CLA	Y	613	7	69,73,73	1.16	8 (11%)	82,113,113	1.32	6 (7%)
27	CLA	R	611	35	53,57,73	1.29	7 (13%)	61,93,113	1.37	6 (9%)
37	CHL	Y	605	7	42,56,74	3.85	19 (45%)	36,92,114	2.53	12 (33%)
37	CHL	s	607	-	44,58,74	3.92	19 (43%)	37,94,114	2.35	12 (32%)
38	LUT	Y	1621	-	42,43,43	0.94	2 (4%)	51,60,60	2.00	16 (31%)
24	OEX	a	401	3,1	0,15,15	-	-	-	-	-
40	NEX	n	1623	-	40,46,46	1.14	3 (7%)	50,70,70	2.45	17 (34%)
37	CHL	N	601	7	44,58,74	3.89	20 (45%)	37,94,114	2.40	12 (32%)
27	CLA	S	603	-	53,57,73	1.30	7 (13%)	61,93,113	1.38	5 (8%)
27	CLA	r	609	17	53,57,73	1.29	8 (15%)	61,93,113	1.43	5 (8%)
37	CHL	G	606	-	44,58,74	3.89	20 (45%)	37,94,114	2.52	12 (32%)
27	CLA	B	613	-	69,73,73	1.17	8 (11%)	82,113,113	1.42	9 (10%)
39	XAT	N	1622	-	41,47,47	0.93	2 (4%)	54,74,74	2.95	24 (44%)
40	NEX	S	1623	-	40,46,46	1.08	4 (10%)	50,70,70	2.36	14 (28%)
37	CHL	n	606	-	44,58,74	3.81	20 (45%)	37,94,114	2.76	13 (35%)
27	CLA	B	616	-	69,73,73	1.16	10 (14%)	82,113,113	1.30	4 (4%)
27	CLA	B	615	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	4 (4%)
37	CHL	g	605	7	42,56,74	4.04	19 (45%)	36,92,114	2.27	11 (30%)
27	CLA	n	612	7	53,57,73	1.30	7 (13%)	61,93,113	1.45	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	y	602	7	69,73,73	1.16	8 (11%)	82,113,113	1.37	6 (7%)
27	CLA	C	507	-	69,73,73	1.18	10 (14%)	82,113,113	1.29	6 (7%)
29	BCR	b	619	-	41,41,41	0.82	2 (4%)	56,56,56	2.11	17 (30%)
38	LUT	n	1621	-	42,43,43	0.88	2 (4%)	51,60,60	1.87	15 (29%)
37	CHL	S	606	-	44,58,74	3.89	19 (43%)	37,94,114	2.28	12 (32%)
40	NEX	y	1623	-	40,46,46	1.23	3 (7%)	50,70,70	2.42	17 (34%)
35	LHG	d	408	-	42,42,48	0.80	1 (2%)	45,48,54	1.31	5 (11%)
37	CHL	n	608	-	44,58,74	3.76	19 (43%)	37,94,114	2.66	12 (32%)
39	XAT	G	1622	-	41,47,47	0.95	2 (4%)	54,74,74	2.76	18 (33%)
27	CLA	S	612	18	53,57,73	1.29	9 (16%)	61,93,113	1.38	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
29	BCR	c	516	-	-	5/29/63/63	0/2/2/2
38	LUT	S	1621	-	-	3/29/67/67	0/2/2/2
27	CLA	S	604	-	1/1/11/20	11/20/96/115	-
39	XAT	r	622	-	-	2/31/93/93	0/4/4/4
27	CLA	y	604	-	1/1/11/20	6/20/96/115	-
37	CHL	S	608	-	3/3/16/26	5/19/117/137	-
27	CLA	n	613	7	1/1/11/20	7/20/96/115	-
27	CLA	r	611	35	1/1/11/20	9/20/96/115	-
29	BCR	b	618	-	-	4/29/63/63	0/2/2/2
29	BCR	b	620	-	-	6/29/63/63	0/2/2/2
38	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	N	602	7	1/1/15/20	12/39/115/115	-
27	CLA	c	509	-	1/1/15/20	7/39/115/115	-
29	BCR	a	411	-	-	0/29/63/63	0/2/2/2
37	CHL	R	608	-	3/3/16/26	10/20/118/137	-
27	CLA	d	403	-	1/1/15/20	9/39/115/115	-
37	CHL	g	608	-	3/3/16/26	9/20/118/137	-
29	BCR	C	514	-	-	2/29/63/63	0/2/2/2
29	BCR	B	618	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PHO	A	408	-	-	9/37/103/103	0/5/6/6
35	LHG	l	101	-	-	26/53/53/53	-
27	CLA	N	604	-	1/1/11/20	6/20/96/115	-
27	CLA	C	506	-	1/1/15/20	15/39/115/115	-
35	LHG	s	2630	27	-	22/53/53/53	-
38	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
28	PHO	a	409	-	-	14/37/103/103	0/5/6/6
27	CLA	C	508	-	1/1/15/20	11/39/115/115	-
27	CLA	S	613	18	1/1/11/20	5/20/96/115	-
27	CLA	B	609	-	1/1/15/20	15/39/115/115	-
27	CLA	y	613	7	1/1/15/20	15/39/115/115	-
27	CLA	B	607	-	1/1/15/20	7/39/115/115	-
37	CHL	y	605	7	3/3/16/26	8/18/116/137	-
27	CLA	c	511	3	1/1/15/20	7/39/115/115	-
37	CHL	r	607	-	3/3/16/26	9/20/118/137	-
27	CLA	C	502	-	1/1/15/20	14/39/115/115	-
27	CLA	A	405	-	1/1/15/20	13/39/115/115	-
27	CLA	N	610	7	1/1/15/20	12/39/115/115	-
37	CHL	n	609	7	3/3/16/26	10/20/118/137	-
31	LMG	z	101	-	-	21/46/66/70	0/1/1/1
27	CLA	b	604	-	1/1/15/20	14/39/115/115	-
27	CLA	b	607	-	1/1/15/20	6/39/115/115	-
27	CLA	b	602	-	1/1/15/20	18/39/115/115	-
27	CLA	Y	603	-	1/1/11/20	5/20/96/115	-
27	CLA	s	604	-	1/1/11/20	11/20/96/115	-
37	CHL	y	606	-	3/3/16/26	5/20/118/137	-
27	CLA	N	613	7	1/1/11/20	7/20/96/115	-
37	CHL	r	608	-	3/3/16/26	10/20/118/137	-
37	CHL	g	601	7	4/4/20/26	16/39/137/137	-
31	LMG	b	622	-	-	23/46/66/70	0/1/1/1
27	CLA	C	504	-	1/1/15/20	16/39/115/115	-
27	CLA	c	501	-	1/1/15/20	11/39/115/115	-
27	CLA	s	602	18	1/1/11/20	7/20/96/115	-
31	LMG	A	413	-	-	15/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LUT	N	1621	-	-	3/29/67/67	0/2/2/2
27	CLA	B	605	-	1/1/15/20	17/39/115/115	-
35	LHG	L	101	-	-	26/53/53/53	-
27	CLA	G	613	7	1/1/11/20	8/20/96/115	-
27	CLA	a	406	-	1/1/15/20	10/39/115/115	-
27	CLA	Y	614	-	1/1/11/20	10/20/96/115	-
37	CHL	N	606	-	3/3/16/26	5/20/118/137	-
31	LMG	D	411	-	-	13/41/61/70	0/1/1/1
30	SQD	A	418	-	-	19/49/69/69	0/1/1/1
37	CHL	g	607	-	3/3/16/26	9/20/118/137	-
37	CHL	R	607	-	3/3/16/26	9/20/118/137	-
27	CLA	Y	602	7	1/1/15/20	14/39/115/115	-
37	CHL	Y	606	-	3/3/16/26	5/20/118/137	-
27	CLA	b	613	-	1/1/15/20	16/39/115/115	-
38	LUT	R	620	-	-	2/29/67/67	0/2/2/2
27	CLA	n	603	-	1/1/11/20	11/20/96/115	-
27	CLA	C	512	-	1/1/15/20	15/39/115/115	-
27	CLA	n	602	7	1/1/15/20	12/39/115/115	-
27	CLA	S	614	-	1/1/11/20	9/20/96/115	-
27	CLA	Y	612	7	1/1/15/20	12/39/115/115	-
29	BCR	d	404	-	-	9/29/63/63	0/2/2/2
37	CHL	s	601	18	3/3/17/26	8/23/121/137	-
27	CLA	n	610	7	1/1/15/20	12/39/115/115	-
38	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	C	505	-	1/1/15/20	9/39/115/115	-
37	CHL	N	605	7	3/3/16/26	9/18/116/137	-
27	CLA	G	610	7	1/1/15/20	14/39/115/115	-
29	BCR	c	515	-	-	0/29/63/63	0/2/2/2
27	CLA	y	603	-	1/1/11/20	5/20/96/115	-
27	CLA	D	403	-	1/1/15/20	9/39/115/115	-
28	PHO	a	408	-	-	9/37/103/103	0/5/6/6
27	CLA	S	602	18	1/1/11/20	7/20/96/115	-
27	CLA	y	614	-	1/1/11/20	10/20/96/115	-
27	CLA	n	604	-	1/1/11/20	6/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	B	620	-	-	6/29/63/63	0/2/2/2
38	LUT	G	1621	-	-	0/29/67/67	0/2/2/2
37	CHL	s	606	-	3/3/16/26	8/20/118/137	-
29	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	LHG	D	410	-	-	20/41/41/53	-
27	CLA	a	407	-	1/1/11/20	6/20/96/115	-
27	CLA	B	611	-	1/1/15/20	11/39/115/115	-
35	LHG	r	2630	27	-	13/53/53/53	-
27	CLA	R	616	17	1/1/11/20	9/20/96/115	-
31	LMG	c	521	-	-	20/46/66/70	0/1/1/1
27	CLA	D	402	-	1/1/15/20	8/39/115/115	-
35	LHG	g	2630	27	-	30/53/53/53	-
30	SQD	B	621	-	-	22/49/69/69	0/1/1/1
27	CLA	N	603	-	1/1/11/20	11/20/96/115	-
27	CLA	c	508	-	1/1/15/20	11/39/115/115	-
27	CLA	G	614	-	1/1/11/20	8/20/96/115	-
27	CLA	R	610	17	1/1/15/20	13/39/115/115	-
27	CLA	b	616	-	1/1/15/20	8/39/115/115	-
27	CLA	c	502	-	1/1/15/20	14/39/115/115	-
32	DGD	c	519	-	-	22/51/91/95	0/2/2/2
27	CLA	B	608	-	1/1/15/20	8/39/115/115	-
40	NEX	g	1623	-	-	5/27/83/83	0/3/3/3
27	CLA	c	513	-	1/1/11/20	5/20/96/115	-
27	CLA	B	617	-	1/1/15/20	15/39/115/115	-
37	CHL	N	607	-	4/4/20/26	15/39/137/137	-
27	CLA	r	612	-	1/1/11/20	4/20/96/115	-
27	CLA	B	604	-	1/1/15/20	14/39/115/115	-
27	CLA	N	614	-	1/1/11/20	11/20/96/115	-
37	CHL	Y	608	-	3/3/16/26	6/20/118/137	-
38	LUT	r	620	-	-	2/29/67/67	0/2/2/2
27	CLA	C	503	-	1/1/15/20	14/39/115/115	-
27	CLA	R	604	-	1/1/11/20	9/20/96/115	-
27	CLA	S	610	18	1/1/11/20	3/20/96/115	-
27	CLA	B	614	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	R	602	17	1/1/15/20	16/39/115/115	-
27	CLA	c	504	-	1/1/15/20	16/39/115/115	-
29	BCR	A	411	-	-	0/29/63/63	0/2/2/2
37	CHL	S	601	18	3/3/17/26	8/23/121/137	-
40	NEX	G	1623	-	-	5/27/83/83	0/3/3/3
29	BCR	D	404	-	-	9/29/63/63	0/2/2/2
27	CLA	b	606	-	1/1/15/20	14/39/115/115	-
37	CHL	Y	607	-	3/3/16/26	7/20/118/137	-
34	PL9	D	405	-	-	14/53/73/73	0/1/1/1
29	BCR	c	514	-	-	2/29/63/63	0/2/2/2
27	CLA	y	611	35	1/1/15/20	8/39/115/115	-
27	CLA	b	609	-	1/1/15/20	14/39/115/115	-
27	CLA	a	405	-	1/1/15/20	13/39/115/115	-
40	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
27	CLA	r	610	17	1/1/15/20	13/39/115/115	-
32	DGD	h	102	-	-	20/51/91/95	0/2/2/2
27	CLA	B	606	-	1/1/15/20	14/39/115/115	-
37	CHL	G	607	-	3/3/16/26	9/20/118/137	-
28	PHO	A	409	-	-	14/37/103/103	0/5/6/6
35	LHG	d	410	-	-	20/41/41/53	-
39	XAT	y	1622	-	-	3/31/93/93	0/4/4/4
37	CHL	s	608	-	3/3/16/26	5/19/117/137	-
35	LHG	y	2630	27	-	20/53/53/53	-
35	LHG	D	408	-	-	20/47/47/53	-
37	CHL	n	605	7	3/3/16/26	9/18/116/137	-
27	CLA	G	612	7	1/1/11/20	8/20/96/115	-
27	CLA	g	610	7	1/1/15/20	14/39/115/115	-
27	CLA	G	603	-	1/1/11/20	8/20/96/115	-
27	CLA	G	602	7	1/1/15/20	13/39/115/115	-
27	CLA	c	512	-	1/1/15/20	15/39/115/115	-
27	CLA	r	602	17	1/1/15/20	16/39/115/115	-
30	SQD	a	418	-	-	19/49/69/69	0/1/1/1
37	CHL	G	609	7	3/3/16/26	10/20/118/137	-
27	CLA	g	613	7	1/1/11/20	8/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	g	612	7	1/1/11/20	8/20/96/115	-
32	DGD	C	519	-	-	22/51/91/95	0/2/2/2
37	CHL	n	601	7	3/3/16/26	7/20/118/137	-
37	CHL	g	609	7	3/3/16/26	10/20/118/137	-
27	CLA	N	611	35	1/1/11/20	9/20/96/115	-
27	CLA	g	611	35	1/1/11/20	8/20/96/115	-
27	CLA	r	604	-	1/1/11/20	9/20/96/115	-
27	CLA	r	613	17	1/1/11/20	6/20/96/115	-
27	CLA	b	612	-	1/1/15/20	15/39/115/115	-
27	CLA	C	513	-	1/1/11/20	5/20/96/115	-
37	CHL	y	607	-	3/3/16/26	7/20/118/137	-
39	XAT	Y	1622	-	-	3/31/93/93	0/4/4/4
27	CLA	A	406	-	1/1/15/20	10/39/115/115	-
27	CLA	b	615	-	1/1/15/20	15/39/115/115	-
29	BCR	C	516	-	-	5/29/63/63	0/2/2/2
37	CHL	R	606	-	3/3/16/26	9/20/118/137	-
32	DGD	c	518	-	-	17/44/84/95	0/2/2/2
35	LHG	S	2630	27	-	22/53/53/53	-
27	CLA	A	410	-	1/1/14/20	11/33/109/115	-
27	CLA	C	509	-	1/1/15/20	7/39/115/115	-
30	SQD	a	412	-	-	29/49/69/69	0/1/1/1
38	LUT	g	1621	-	-	0/29/67/67	0/2/2/2
27	CLA	g	604	-	1/1/11/20	12/20/96/115	-
27	CLA	R	603	-	1/1/11/20	6/20/96/115	-
37	CHL	n	607	-	4/4/20/26	15/39/137/137	-
38	LUT	y	1620	-	-	0/29/67/67	0/2/2/2
31	LMG	a	413	-	-	15/43/63/70	0/1/1/1
27	CLA	s	611	35	1/1/11/20	7/20/96/115	-
27	CLA	n	614	-	1/1/11/20	11/20/96/115	-
27	CLA	s	610	18	1/1/11/20	3/20/96/115	-
29	BCR	c	517	-	-	1/29/63/63	0/2/2/2
27	CLA	a	410	-	1/1/14/20	11/33/109/115	-
27	CLA	C	511	3	1/1/15/20	7/39/115/115	-
31	LMG	B	622	-	-	23/46/66/70	0/1/1/1
34	PL9	d	405	-	-	14/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	617	-	1/1/15/20	15/39/115/115	-
37	CHL	S	607	-	3/3/16/26	9/20/118/137	-
32	DGD	c	520	-	-	14/51/91/95	0/2/2/2
31	LMG	d	411	-	-	13/41/61/70	0/1/1/1
37	CHL	y	608	-	3/3/16/26	6/20/118/137	-
32	DGD	H	102	-	-	20/51/91/95	0/2/2/2
27	CLA	r	616	17	1/1/11/20	9/20/96/115	-
35	LHG	N	2630	27	-	24/53/53/53	-
29	BCR	H	101	-	-	3/29/63/63	0/2/2/2
27	CLA	B	603	-	1/1/15/20	15/39/115/115	-
27	CLA	s	613	18	1/1/11/20	5/20/96/115	-
27	CLA	s	612	18	1/1/11/20	3/20/96/115	-
27	CLA	b	605	-	1/1/15/20	17/39/115/115	-
27	CLA	b	611	-	1/1/15/20	11/39/115/115	-
38	LUT	Y	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	y	612	7	1/1/15/20	12/39/115/115	-
35	LHG	d	409	-	-	13/53/53/53	-
35	LHG	Y	2630	27	-	20/53/53/53	-
40	NEX	R	623	-	-	3/27/83/83	0/3/3/3
38	LUT	y	1621	-	-	0/29/67/67	0/2/2/2
31	LMG	Z	101	-	-	21/46/66/70	0/1/1/1
40	NEX	N	1623	-	-	5/27/83/83	0/3/3/3
38	LUT	N	1620	-	-	1/29/67/67	0/2/2/2
29	BCR	C	517	-	-	1/29/63/63	0/2/2/2
27	CLA	Y	611	35	1/1/15/20	8/39/115/115	-
38	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
37	CHL	r	606	-	3/3/16/26	9/20/118/137	-
35	LHG	G	2630	27	-	30/53/53/53	-
27	CLA	b	614	-	1/1/15/20	8/39/115/115	-
27	CLA	g	603	-	1/1/11/20	8/20/96/115	-
36	HEM	F	101	6,5	-	0/14/54/54	-
35	LHG	D	409	-	-	13/53/53/53	-
27	CLA	g	602	7	1/1/15/20	13/39/115/115	-
27	CLA	c	507	-	1/1/15/20	14/39/115/115	-
27	CLA	G	611	35	1/1/11/20	8/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	c	510	-	1/1/15/20	16/39/115/115	-
40	NEX	Y	1623	-	-	3/27/83/83	0/3/3/3
30	SQD	b	621	-	-	22/49/69/69	0/1/1/1
27	CLA	s	603	-	-	10/20/96/115	-
38	LUT	s	1621	-	-	3/29/67/67	0/2/2/2
27	CLA	N	612	7	1/1/11/20	11/20/96/115	-
27	CLA	n	611	35	1/1/11/20	9/20/96/115	-
37	CHL	y	601	7	4/4/20/26	17/39/137/137	-
27	CLA	g	614	-	1/1/11/20	8/20/96/115	-
27	CLA	c	505	-	1/1/15/20	9/39/115/115	-
27	CLA	S	609	18	1/1/11/20	10/20/96/115	-
27	CLA	B	612	-	1/1/15/20	15/39/115/115	-
37	CHL	N	608	-	3/3/16/26	6/20/118/137	-
27	CLA	S	611	35	1/1/11/20	7/20/96/115	-
27	CLA	r	603	-	1/1/11/20	6/20/96/115	-
27	CLA	s	614	-	1/1/11/20	9/20/96/115	-
36	HEM	f	101	6,5	-	0/14/54/54	-
27	CLA	r	601	17	1/1/11/20	12/20/96/115	-
27	CLA	Y	604	-	1/1/11/20	6/20/96/115	-
40	NEX	r	623	-	-	3/27/83/83	0/3/3/3
29	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	CLA	Y	610	7	1/1/15/20	14/39/115/115	-
29	BCR	h	101	-	-	3/29/63/63	0/2/2/2
27	CLA	G	604	-	1/1/11/20	12/20/96/115	-
37	CHL	y	609	7	4/4/20/26	21/39/137/137	-
27	CLA	b	610	-	1/1/15/20	11/39/115/115	-
27	CLA	c	503	-	1/1/15/20	14/39/115/115	-
32	DGD	C	520	-	-	14/51/91/95	0/2/2/2
27	CLA	R	612	-	1/1/11/20	4/20/96/115	-
27	CLA	b	608	-	1/1/15/20	8/39/115/115	-
27	CLA	B	602	-	1/1/15/20	18/39/115/115	-
31	LMG	C	521	-	-	20/46/66/70	0/1/1/1
27	CLA	R	601	17	1/1/11/20	12/20/96/115	-
27	CLA	R	609	17	1/1/11/20	8/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CHL	Y	601	7	4/4/20/26	17/39/137/137	-
37	CHL	Y	609	7	4/4/20/26	21/39/137/137	-
39	XAT	n	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	R	613	17	1/1/11/20	6/20/96/115	-
27	CLA	B	610	-	1/1/15/20	11/39/115/115	-
27	CLA	d	402	-	1/1/15/20	8/39/115/115	-
37	CHL	G	608	-	3/3/16/26	9/20/118/137	-
32	DGD	C	518	-	-	17/44/84/95	0/2/2/2
27	CLA	b	603	-	1/1/15/20	15/39/115/115	-
27	CLA	A	407	-	1/1/11/20	6/20/96/115	-
27	CLA	C	501	-	1/1/15/20	11/39/115/115	-
37	CHL	N	609	7	3/3/16/26	10/20/118/137	-
27	CLA	s	609	18	1/1/11/20	10/20/96/115	-
37	CHL	G	601	7	4/4/20/26	16/39/137/137	-
30	SQD	A	412	-	-	29/49/69/69	0/1/1/1
39	XAT	g	1622	-	-	3/31/93/93	0/4/4/4
37	CHL	g	606	-	3/3/16/26	3/20/118/137	-
37	CHL	G	605	7	3/3/16/26	5/18/116/137	-
35	LHG	n	2630	27	-	24/53/53/53	-
27	CLA	c	506	-	1/1/15/20	15/39/115/115	-
35	LHG	R	2630	27	-	13/53/53/53	-
39	XAT	R	622	-	-	2/31/93/93	0/4/4/4
27	CLA	C	510	-	1/1/15/20	16/39/115/115	-
38	LUT	n	1620	-	-	1/29/67/67	0/2/2/2
27	CLA	y	610	7	1/1/15/20	14/39/115/115	-
27	CLA	Y	613	7	1/1/15/20	15/39/115/115	-
27	CLA	R	611	35	1/1/11/20	9/20/96/115	-
37	CHL	Y	605	7	3/3/16/26	8/18/116/137	-
37	CHL	s	607	-	3/3/16/26	9/20/118/137	-
38	LUT	Y	1621	-	-	0/29/67/67	0/2/2/2
40	NEX	n	1623	-	-	5/27/83/83	0/3/3/3
37	CHL	N	601	7	3/3/16/26	7/20/118/137	-
27	CLA	S	603	-	-	10/20/96/115	-
27	CLA	r	609	17	1/1/11/20	8/20/96/115	-
37	CHL	G	606	-	3/3/16/26	3/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	613	-	1/1/15/20	16/39/115/115	-
39	XAT	N	1622	-	-	1/31/93/93	0/4/4/4
40	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
37	CHL	n	606	-	3/3/16/26	5/20/118/137	-
27	CLA	B	616	-	1/1/15/20	8/39/115/115	-
27	CLA	B	615	-	1/1/15/20	15/39/115/115	-
37	CHL	g	605	7	3/3/16/26	5/18/116/137	-
27	CLA	n	612	7	1/1/11/20	11/20/96/115	-
27	CLA	y	602	7	1/1/15/20	14/39/115/115	-
27	CLA	C	507	-	1/1/15/20	14/39/115/115	-
29	BCR	b	619	-	-	0/29/63/63	0/2/2/2
38	LUT	n	1621	-	-	3/29/67/67	0/2/2/2
37	CHL	S	606	-	3/3/16/26	8/20/118/137	-
40	NEX	y	1623	-	-	3/27/83/83	0/3/3/3
35	LHG	d	408	-	-	20/47/47/53	-
37	CHL	n	608	-	3/3/16/26	6/20/118/137	-
39	XAT	G	1622	-	-	3/31/93/93	0/4/4/4
27	CLA	S	612	18	1/1/11/20	3/20/96/115	-

All (2602) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	S	608	CHL	C2C-C3C	10.72	1.46	1.36
37	s	608	CHL	C2C-C3C	10.70	1.46	1.36
37	G	605	CHL	C2C-C3C	10.63	1.46	1.36
37	g	605	CHL	C2C-C3C	10.63	1.46	1.36
37	N	601	CHL	C2C-C3C	10.57	1.46	1.36
37	n	601	CHL	C2C-C3C	10.57	1.46	1.36
37	R	608	CHL	C2C-C3C	10.18	1.46	1.36
37	r	608	CHL	C2C-C3C	10.13	1.46	1.36
37	g	608	CHL	C2C-C3C	10.11	1.46	1.36
37	N	605	CHL	C2C-C3C	10.10	1.46	1.36
37	G	609	CHL	C1D-C2D	10.09	1.51	1.39
37	G	608	CHL	C2C-C3C	10.09	1.46	1.36
37	n	605	CHL	C2C-C3C	10.08	1.46	1.36
37	G	605	CHL	C1D-C2D	10.05	1.51	1.39
37	g	609	CHL	C1D-C2D	10.03	1.51	1.39
37	S	606	CHL	C1D-C2D	10.02	1.51	1.39
37	s	607	CHL	C2C-C3C	10.00	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	g	609	CHL	C2C-C3C	9.99	1.46	1.36
37	G	609	CHL	C2C-C3C	9.95	1.46	1.36
37	s	606	CHL	C1D-C2D	9.94	1.50	1.39
37	G	606	CHL	C1D-C2D	9.94	1.50	1.39
37	g	605	CHL	C1D-C2D	9.93	1.50	1.39
37	S	607	CHL	C2C-C3C	9.92	1.46	1.36
37	g	606	CHL	C1D-C2D	9.91	1.50	1.39
37	n	605	CHL	C1D-C2D	9.89	1.50	1.39
37	N	605	CHL	C1D-C2D	9.87	1.50	1.39
37	N	608	CHL	C2C-C3C	9.85	1.45	1.36
37	G	607	CHL	C2C-C3C	9.84	1.45	1.36
37	g	607	CHL	C2C-C3C	9.84	1.45	1.36
37	s	607	CHL	C1D-C2D	9.83	1.50	1.39
37	s	608	CHL	C1D-C2D	9.81	1.50	1.39
37	S	608	CHL	C1D-C2D	9.79	1.50	1.39
37	y	605	CHL	C2C-C3C	9.79	1.45	1.36
37	G	606	CHL	C2C-C3C	9.77	1.45	1.36
37	g	606	CHL	C2C-C3C	9.77	1.45	1.36
37	r	607	CHL	C2C-C3C	9.77	1.45	1.36
37	R	607	CHL	C2C-C3C	9.76	1.45	1.36
37	S	607	CHL	C1D-C2D	9.76	1.50	1.39
37	Y	605	CHL	C2C-C3C	9.75	1.45	1.36
37	S	606	CHL	C2C-C3C	9.72	1.45	1.36
37	s	606	CHL	C2C-C3C	9.72	1.45	1.36
37	n	601	CHL	C1D-C2D	9.68	1.50	1.39
37	N	601	CHL	C1D-C2D	9.68	1.50	1.39
37	n	608	CHL	C2C-C3C	9.68	1.45	1.36
37	N	606	CHL	C2C-C3C	9.67	1.45	1.36
37	n	606	CHL	C2C-C3C	9.67	1.45	1.36
37	s	601	CHL	C1D-C2D	9.65	1.50	1.39
37	Y	605	CHL	C1D-C2D	9.65	1.50	1.39
37	y	605	CHL	C1D-C2D	9.65	1.50	1.39
37	N	609	CHL	C2C-C3C	9.60	1.45	1.36
37	n	609	CHL	C2C-C3C	9.60	1.45	1.36
37	N	606	CHL	C1D-C2D	9.60	1.50	1.39
37	n	606	CHL	C1D-C2D	9.60	1.50	1.39
37	g	608	CHL	C1D-C2D	9.59	1.50	1.39
37	N	607	CHL	C2C-C3C	9.58	1.45	1.36
37	n	607	CHL	C2C-C3C	9.55	1.45	1.36
37	S	601	CHL	C1D-C2D	9.53	1.50	1.39
37	y	608	CHL	C2C-C3C	9.53	1.45	1.36
37	y	601	CHL	C1D-C2D	9.51	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	608	CHL	C2C-C3C	9.49	1.45	1.36
37	G	608	CHL	C1D-C2D	9.47	1.50	1.39
37	g	601	CHL	C1D-C2D	9.46	1.50	1.39
37	N	608	CHL	C1D-C2D	9.45	1.50	1.39
37	Y	601	CHL	C1D-C2D	9.40	1.50	1.39
37	G	601	CHL	C1D-C2D	9.39	1.50	1.39
37	g	601	CHL	C2C-C3C	9.39	1.45	1.36
37	g	607	CHL	C1D-C2D	9.39	1.50	1.39
37	n	608	CHL	C1D-C2D	9.37	1.50	1.39
37	G	607	CHL	C1D-C2D	9.37	1.50	1.39
37	G	601	CHL	C2C-C3C	9.35	1.45	1.36
37	R	607	CHL	C1D-C2D	9.35	1.50	1.39
37	r	607	CHL	C1D-C2D	9.35	1.50	1.39
37	S	601	CHL	C2C-C3C	9.35	1.45	1.36
37	r	606	CHL	C1D-C2D	9.32	1.50	1.39
37	R	606	CHL	C2C-C3C	9.31	1.45	1.36
37	r	606	CHL	C2C-C3C	9.31	1.45	1.36
37	R	606	CHL	C1D-C2D	9.31	1.50	1.39
37	Y	609	CHL	C1D-C2D	9.31	1.50	1.39
37	y	609	CHL	C1D-C2D	9.29	1.50	1.39
37	s	601	CHL	C2C-C3C	9.28	1.45	1.36
37	N	609	CHL	C1D-C2D	9.27	1.50	1.39
37	n	609	CHL	C1D-C2D	9.25	1.50	1.39
37	r	608	CHL	C1D-C2D	9.24	1.50	1.39
37	R	608	CHL	C1D-C2D	9.23	1.50	1.39
37	Y	601	CHL	C2C-C3C	9.20	1.45	1.36
37	y	601	CHL	C2C-C3C	9.20	1.45	1.36
37	Y	609	CHL	C2C-C3C	9.18	1.45	1.36
37	y	607	CHL	C2C-C3C	9.12	1.45	1.36
37	Y	607	CHL	C2C-C3C	9.11	1.45	1.36
37	y	609	CHL	C2C-C3C	9.04	1.45	1.36
37	Y	606	CHL	C1D-C2D	9.04	1.49	1.39
37	y	606	CHL	C1D-C2D	9.04	1.49	1.39
37	Y	608	CHL	C1D-C2D	9.03	1.49	1.39
37	y	608	CHL	C1D-C2D	9.03	1.49	1.39
37	Y	606	CHL	C2C-C3C	9.01	1.45	1.36
37	y	606	CHL	C2C-C3C	9.01	1.45	1.36
37	y	607	CHL	C1D-C2D	8.83	1.49	1.39
37	Y	607	CHL	C1D-C2D	8.82	1.49	1.39
28	A	408	PHO	C1B-C2B	8.79	1.49	1.39
28	a	408	PHO	C1B-C2B	8.79	1.49	1.39
37	n	607	CHL	C1D-C2D	8.77	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	607	CHL	C1D-C2D	8.75	1.49	1.39
28	A	409	PHO	C1B-C2B	8.55	1.48	1.39
28	a	409	PHO	C1B-C2B	8.51	1.48	1.39
37	S	608	CHL	C1B-C2B	8.51	1.49	1.39
37	s	608	CHL	C1B-C2B	8.51	1.49	1.39
37	G	605	CHL	C1B-C2B	8.27	1.49	1.39
37	g	605	CHL	C1B-C2B	8.27	1.49	1.39
37	G	609	CHL	C1B-C2B	8.12	1.48	1.39
37	g	609	CHL	C1B-C2B	8.10	1.48	1.39
37	g	601	CHL	C1B-C2B	8.09	1.48	1.39
37	Y	605	CHL	C1B-C2B	8.09	1.48	1.39
37	R	608	CHL	C1B-C2B	8.08	1.48	1.39
37	s	607	CHL	C1B-C2B	8.08	1.48	1.39
37	r	608	CHL	C1B-C2B	8.07	1.48	1.39
37	S	607	CHL	C1B-C2B	8.05	1.48	1.39
37	G	601	CHL	C1B-C2B	8.03	1.48	1.39
37	G	607	CHL	C1B-C2B	8.02	1.48	1.39
37	g	607	CHL	C1B-C2B	8.02	1.48	1.39
37	N	605	CHL	C1B-C2B	8.02	1.48	1.39
37	n	605	CHL	C1B-C2B	8.02	1.48	1.39
37	R	607	CHL	C1B-C2B	8.01	1.48	1.39
37	y	605	CHL	C1B-C2B	8.01	1.48	1.39
37	r	607	CHL	C1B-C2B	8.00	1.48	1.39
37	S	601	CHL	C1B-C2B	7.96	1.48	1.39
37	s	606	CHL	C3B-C4B	7.91	1.49	1.41
37	s	601	CHL	C1B-C2B	7.89	1.48	1.39
37	N	607	CHL	C1B-C2B	7.86	1.48	1.39
37	S	606	CHL	C3B-C4B	7.86	1.49	1.41
28	A	409	PHO	C3B-C4B	7.83	1.49	1.41
28	a	409	PHO	C3B-C4B	7.83	1.49	1.41
37	n	607	CHL	C1B-C2B	7.82	1.48	1.39
37	n	601	CHL	C1B-C2B	7.82	1.48	1.39
37	G	608	CHL	C1B-C2B	7.81	1.48	1.39
37	Y	608	CHL	C1B-C2B	7.80	1.48	1.39
37	N	601	CHL	C1B-C2B	7.80	1.48	1.39
37	g	608	CHL	C1B-C2B	7.77	1.48	1.39
37	n	606	CHL	C3B-C4B	7.75	1.48	1.41
37	R	606	CHL	C1B-C2B	7.74	1.48	1.39
37	y	608	CHL	C1B-C2B	7.72	1.48	1.39
37	Y	609	CHL	C1B-C2B	7.70	1.48	1.39
37	N	609	CHL	C1B-C2B	7.67	1.48	1.39
37	n	609	CHL	C1B-C2B	7.67	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	606	CHL	C3B-C4B	7.67	1.48	1.41
37	Y	601	CHL	C1B-C2B	7.67	1.48	1.39
37	y	609	CHL	C1B-C2B	7.67	1.48	1.39
37	y	601	CHL	C1B-C2B	7.66	1.48	1.39
37	G	606	CHL	C3B-C4B	7.62	1.48	1.41
37	g	606	CHL	C3B-C4B	7.62	1.48	1.41
36	F	101	HEM	C3D-C2D	7.62	1.53	1.36
28	A	408	PHO	C3B-C4B	7.61	1.49	1.41
36	f	101	HEM	C3D-C2D	7.61	1.53	1.36
37	N	606	CHL	C1B-C2B	7.59	1.48	1.39
37	n	606	CHL	C1B-C2B	7.59	1.48	1.39
37	r	606	CHL	C1B-C2B	7.59	1.48	1.39
37	S	608	CHL	C3B-C4B	7.54	1.48	1.41
37	s	608	CHL	C3B-C4B	7.53	1.48	1.41
28	a	408	PHO	C3B-C4B	7.53	1.49	1.41
37	g	606	CHL	C1B-C2B	7.53	1.48	1.39
37	N	608	CHL	C1B-C2B	7.52	1.48	1.39
37	n	608	CHL	C1B-C2B	7.52	1.48	1.39
37	G	606	CHL	C1B-C2B	7.51	1.48	1.39
37	Y	606	CHL	C3B-C4B	7.51	1.48	1.41
37	Y	607	CHL	C1B-C2B	7.48	1.48	1.39
37	y	607	CHL	C1B-C2B	7.48	1.48	1.39
37	N	608	CHL	C3B-C4B	7.48	1.48	1.41
37	y	606	CHL	C1B-C2B	7.46	1.48	1.39
37	y	608	CHL	C3B-C4B	7.45	1.48	1.41
37	g	608	CHL	C3B-C4B	7.44	1.48	1.41
37	Y	606	CHL	C1B-C2B	7.43	1.48	1.39
37	s	606	CHL	C1B-C2B	7.42	1.48	1.39
37	N	601	CHL	C3B-C4B	7.41	1.48	1.41
37	n	608	CHL	C3B-C4B	7.41	1.48	1.41
37	y	606	CHL	C3B-C4B	7.40	1.48	1.41
37	n	601	CHL	C3B-C4B	7.39	1.48	1.41
37	Y	608	CHL	C3B-C4B	7.39	1.48	1.41
37	S	606	CHL	C1B-C2B	7.37	1.47	1.39
37	r	608	CHL	C3B-C4B	7.36	1.48	1.41
37	G	608	CHL	C3B-C4B	7.32	1.48	1.41
37	S	601	CHL	C3B-C4B	7.32	1.48	1.41
37	G	605	CHL	C3B-C4B	7.29	1.48	1.41
37	g	605	CHL	C3B-C4B	7.29	1.48	1.41
37	R	608	CHL	C3B-C4B	7.29	1.48	1.41
37	S	608	CHL	C1A-CHA	7.29	1.48	1.40
37	g	601	CHL	C3B-C4B	7.25	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	G	605	CHL	C1A-CHA	7.24	1.48	1.40
37	g	605	CHL	C1A-CHA	7.24	1.48	1.40
37	S	607	CHL	C1A-CHA	7.24	1.48	1.40
37	s	607	CHL	C1A-CHA	7.24	1.48	1.40
37	s	601	CHL	C3B-C4B	7.23	1.48	1.41
37	s	608	CHL	C1A-CHA	7.21	1.48	1.40
37	G	601	CHL	C3B-C4B	7.20	1.48	1.41
37	S	607	CHL	C3B-C4B	7.13	1.48	1.41
37	s	607	CHL	C3B-C4B	7.13	1.48	1.41
37	Y	601	CHL	C3B-C4B	7.10	1.48	1.41
37	y	601	CHL	C3B-C4B	7.10	1.48	1.41
37	N	607	CHL	C3B-C4B	7.04	1.48	1.41
37	N	605	CHL	C3B-C4B	7.02	1.48	1.41
37	n	607	CHL	C3B-C4B	7.02	1.48	1.41
37	n	605	CHL	C3B-C4B	7.02	1.48	1.41
37	G	607	CHL	C3B-C4B	6.98	1.48	1.41
37	r	607	CHL	C3B-C4B	6.98	1.48	1.41
37	Y	607	CHL	C3B-C4B	6.98	1.48	1.41
37	y	607	CHL	C3B-C4B	6.97	1.48	1.41
37	R	607	CHL	C3B-C4B	6.96	1.48	1.41
37	G	607	CHL	C1A-CHA	6.93	1.47	1.40
37	g	607	CHL	C1A-CHA	6.93	1.47	1.40
37	g	607	CHL	C3B-C4B	6.93	1.48	1.41
37	R	606	CHL	C3B-C4B	6.87	1.48	1.41
37	r	606	CHL	C3B-C4B	6.84	1.48	1.41
37	R	608	CHL	C1A-CHA	6.82	1.47	1.40
37	r	608	CHL	C1A-CHA	6.81	1.47	1.40
37	y	607	CHL	C1A-CHA	6.80	1.47	1.40
37	N	607	CHL	C1A-CHA	6.80	1.47	1.40
37	s	606	CHL	C1A-CHA	6.78	1.47	1.40
37	n	607	CHL	C1A-CHA	6.77	1.47	1.40
37	Y	607	CHL	C1A-CHA	6.75	1.47	1.40
37	Y	605	CHL	C3B-C4B	6.72	1.47	1.41
37	y	605	CHL	C1A-CHA	6.71	1.47	1.40
37	G	608	CHL	C1A-CHA	6.71	1.47	1.40
37	g	608	CHL	C1A-CHA	6.71	1.47	1.40
37	y	605	CHL	C3B-C4B	6.70	1.47	1.41
37	S	606	CHL	C1A-CHA	6.66	1.47	1.40
37	Y	605	CHL	C1A-CHA	6.63	1.47	1.40
37	Y	608	CHL	C1A-CHA	6.61	1.47	1.40
37	r	606	CHL	C1A-CHA	6.60	1.47	1.40
37	y	608	CHL	C1A-CHA	6.55	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	R	606	CHL	C1A-CHA	6.53	1.47	1.40
34	D	405	PL9	C3-C4	-6.39	1.39	1.49
37	N	608	CHL	C1A-CHA	6.39	1.47	1.40
37	N	601	CHL	C1A-CHA	6.39	1.47	1.40
37	n	601	CHL	C1A-CHA	6.39	1.47	1.40
34	d	405	PL9	C3-C4	-6.37	1.39	1.49
37	G	609	CHL	C3B-C4B	6.36	1.47	1.41
37	y	609	CHL	C1A-CHA	6.36	1.47	1.40
37	g	609	CHL	C3B-C4B	6.35	1.47	1.41
37	N	609	CHL	C1A-CHA	6.29	1.47	1.40
37	n	609	CHL	C1A-CHA	6.29	1.47	1.40
37	n	608	CHL	C1A-CHA	6.28	1.47	1.40
37	Y	609	CHL	C1A-CHA	6.27	1.47	1.40
37	N	606	CHL	C1A-CHA	6.27	1.47	1.40
37	n	606	CHL	C1A-CHA	6.27	1.47	1.40
37	Y	601	CHL	C1A-CHA	6.26	1.47	1.40
37	y	601	CHL	C1A-CHA	6.24	1.47	1.40
37	R	607	CHL	C1A-CHA	6.20	1.47	1.40
37	g	601	CHL	C1A-CHA	6.19	1.47	1.40
37	G	609	CHL	C1A-CHA	6.19	1.47	1.40
37	g	609	CHL	C1A-CHA	6.19	1.47	1.40
37	G	601	CHL	C1A-CHA	6.14	1.47	1.40
37	r	607	CHL	C1A-CHA	6.13	1.47	1.40
37	N	609	CHL	C3B-C4B	6.13	1.47	1.41
37	n	609	CHL	C3B-C4B	6.11	1.47	1.41
37	S	601	CHL	C1A-CHA	6.08	1.46	1.40
37	N	609	CHL	C3A-C2A	-6.08	1.49	1.54
37	Y	606	CHL	C1A-CHA	6.06	1.46	1.40
37	y	606	CHL	C1A-CHA	6.06	1.46	1.40
37	n	609	CHL	C3A-C2A	-6.05	1.49	1.54
37	G	606	CHL	C1A-CHA	6.00	1.46	1.40
37	g	606	CHL	C1A-CHA	6.00	1.46	1.40
37	s	601	CHL	C1A-CHA	5.99	1.46	1.40
37	y	609	CHL	C3B-C4B	5.97	1.47	1.41
37	G	601	CHL	C3D-C4D	-5.95	1.32	1.41
37	Y	609	CHL	C3B-C4B	5.93	1.47	1.41
37	g	601	CHL	C3D-C4D	-5.92	1.32	1.41
37	N	605	CHL	C1A-CHA	5.90	1.46	1.40
37	R	608	CHL	C3D-C4D	-5.87	1.32	1.41
37	r	608	CHL	C3D-C4D	-5.87	1.32	1.41
37	Y	608	CHL	C3D-C4D	-5.86	1.32	1.41
37	n	605	CHL	C1A-CHA	5.86	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	601	CHL	C3D-C4D	-5.86	1.32	1.41
37	y	601	CHL	C3D-C4D	-5.85	1.32	1.41
37	n	605	CHL	C3D-C4D	-5.84	1.32	1.41
37	y	608	CHL	C3D-C4D	-5.83	1.32	1.41
37	y	609	CHL	C3D-C4D	-5.83	1.32	1.41
37	y	606	CHL	C3D-C4D	-5.81	1.32	1.41
37	n	608	CHL	C3D-C4D	-5.81	1.32	1.41
37	g	608	CHL	C3D-C4D	-5.81	1.32	1.41
37	Y	606	CHL	C3D-C4D	-5.80	1.32	1.41
37	Y	609	CHL	C3D-C4D	-5.80	1.32	1.41
37	N	607	CHL	C3D-C4D	-5.79	1.32	1.41
37	n	607	CHL	C3D-C4D	-5.77	1.32	1.41
37	N	609	CHL	C3D-C4D	-5.77	1.32	1.41
37	n	609	CHL	C3D-C4D	-5.77	1.32	1.41
37	N	608	CHL	C3D-C4D	-5.76	1.32	1.41
37	Y	607	CHL	C3D-C4D	-5.76	1.32	1.41
37	y	607	CHL	C3D-C4D	-5.75	1.32	1.41
37	N	605	CHL	C3D-C4D	-5.75	1.32	1.41
37	G	608	CHL	C3D-C4D	-5.73	1.32	1.41
37	G	609	CHL	C3D-C4D	-5.72	1.32	1.41
37	S	601	CHL	C3D-C4D	-5.72	1.32	1.41
37	G	606	CHL	C3D-C4D	-5.71	1.32	1.41
37	N	601	CHL	C3D-C4D	-5.71	1.32	1.41
37	n	601	CHL	C3D-C4D	-5.69	1.32	1.41
37	g	609	CHL	C3D-C4D	-5.69	1.32	1.41
37	g	606	CHL	CHB-C4A	-5.68	1.31	1.38
37	s	601	CHL	C3D-C4D	-5.67	1.32	1.41
37	Y	607	CHL	CHB-C4A	-5.67	1.31	1.38
37	g	606	CHL	C3D-C4D	-5.67	1.32	1.41
37	R	607	CHL	C3D-C4D	-5.66	1.32	1.41
37	r	607	CHL	C3D-C4D	-5.66	1.32	1.41
37	S	606	CHL	C3D-C4D	-5.66	1.32	1.41
37	s	606	CHL	C3D-C4D	-5.66	1.32	1.41
37	N	606	CHL	C3D-C4D	-5.65	1.32	1.41
37	G	606	CHL	CHB-C4A	-5.65	1.31	1.38
37	n	605	CHL	C3A-C2A	-5.62	1.49	1.54
37	y	607	CHL	C3A-C2A	-5.61	1.49	1.54
37	n	606	CHL	C3D-C4D	-5.60	1.33	1.41
37	Y	606	CHL	C3A-C2A	-5.60	1.49	1.54
37	R	606	CHL	C3D-C4D	-5.59	1.33	1.41
37	y	607	CHL	CHB-C4A	-5.59	1.31	1.38
37	G	606	CHL	C3A-C2A	-5.58	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	S	607	CHL	C3D-C4D	-5.56	1.33	1.41
37	Y	609	CHL	C3A-C2A	-5.56	1.49	1.54
37	y	609	CHL	C3A-C2A	-5.56	1.49	1.54
37	Y	607	CHL	C3A-C2A	-5.54	1.49	1.54
37	s	607	CHL	C3D-C4D	-5.54	1.33	1.41
37	N	605	CHL	C3A-C2A	-5.52	1.49	1.54
37	y	606	CHL	C3A-C2A	-5.52	1.49	1.54
37	S	608	CHL	C3D-C4D	-5.52	1.33	1.41
37	s	608	CHL	C3D-C4D	-5.52	1.33	1.41
37	r	606	CHL	C3D-C4D	-5.52	1.33	1.41
37	g	606	CHL	C3A-C2A	-5.50	1.50	1.54
37	S	608	CHL	C3B-C2B	5.46	1.47	1.40
37	s	608	CHL	C3B-C2B	5.46	1.47	1.40
37	y	605	CHL	C3D-C4D	-5.46	1.33	1.41
37	G	607	CHL	C3A-C2A	-5.45	1.50	1.54
37	g	607	CHL	C3A-C2A	-5.45	1.50	1.54
37	G	605	CHL	C3D-C4D	-5.44	1.33	1.41
37	G	607	CHL	C3D-C4D	-5.44	1.33	1.41
37	g	607	CHL	C3D-C4D	-5.44	1.33	1.41
37	Y	605	CHL	C3D-C4D	-5.44	1.33	1.41
37	N	607	CHL	CHB-C4A	-5.41	1.32	1.38
37	g	605	CHL	C3D-C4D	-5.41	1.33	1.41
37	y	606	CHL	CHB-C4A	-5.40	1.32	1.38
37	Y	606	CHL	CHB-C4A	-5.40	1.32	1.38
37	n	607	CHL	CHB-C4A	-5.39	1.32	1.38
37	N	608	CHL	CHB-C4A	-5.38	1.32	1.38
37	S	601	CHL	CHB-C4A	-5.38	1.32	1.38
37	s	601	CHL	CHB-C4A	-5.38	1.32	1.38
37	N	609	CHL	CHB-C4A	-5.38	1.32	1.38
37	n	609	CHL	CHB-C4A	-5.38	1.32	1.38
37	N	606	CHL	CHB-C4A	-5.35	1.32	1.38
37	n	608	CHL	CHB-C4A	-5.34	1.32	1.38
37	y	608	CHL	CHB-C4A	-5.34	1.32	1.38
37	Y	608	CHL	CHB-C4A	-5.32	1.32	1.38
37	n	608	CHL	C3A-C2A	-5.32	1.50	1.54
37	N	606	CHL	C3A-C2A	-5.32	1.50	1.54
37	n	606	CHL	C3A-C2A	-5.32	1.50	1.54
37	n	606	CHL	CHB-C4A	-5.31	1.32	1.38
37	y	605	CHL	C3A-C2A	-5.28	1.50	1.54
37	R	607	CHL	CHB-C4A	-5.26	1.32	1.38
37	r	607	CHL	CHB-C4A	-5.26	1.32	1.38
37	G	607	CHL	CHB-C4A	-5.26	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	605	CHL	C3A-C2A	-5.23	1.50	1.54
37	N	608	CHL	C3A-C2A	-5.22	1.50	1.54
37	S	608	CHL	CHC-C4B	5.21	1.48	1.39
37	g	607	CHL	CHB-C4A	-5.20	1.32	1.38
37	R	606	CHL	C3A-C2A	-5.18	1.50	1.54
37	Y	608	CHL	C3A-C2A	-5.18	1.50	1.54
37	s	601	CHL	C3A-C2A	-5.17	1.50	1.54
37	s	608	CHL	CHC-C4B	5.15	1.48	1.39
37	Y	601	CHL	C3A-C2A	-5.14	1.50	1.54
37	y	601	CHL	C3A-C2A	-5.14	1.50	1.54
37	G	608	CHL	CHB-C4A	-5.13	1.32	1.38
37	r	606	CHL	C3A-C2A	-5.12	1.50	1.54
37	y	601	CHL	CHB-C4A	-5.10	1.32	1.38
37	Y	609	CHL	CHB-C4A	-5.10	1.32	1.38
37	y	609	CHL	CHB-C4A	-5.10	1.32	1.38
37	r	606	CHL	CHB-C4A	-5.08	1.32	1.38
37	y	608	CHL	C3A-C2A	-5.08	1.50	1.54
37	S	608	CHL	O2D-CGD	5.07	1.45	1.33
37	n	605	CHL	CHB-C4A	-5.07	1.32	1.38
37	N	607	CHL	C3A-C2A	-5.07	1.50	1.54
37	G	601	CHL	C3A-C2A	-5.06	1.50	1.54
37	g	601	CHL	C3A-C2A	-5.06	1.50	1.54
37	s	608	CHL	O2D-CGD	5.05	1.45	1.33
37	g	608	CHL	CHB-C4A	-5.05	1.32	1.38
37	R	606	CHL	CHB-C4A	-5.05	1.32	1.38
37	S	608	CHL	CHD-C4C	5.04	1.49	1.39
37	N	605	CHL	CHB-C4A	-5.03	1.32	1.38
37	S	607	CHL	O2D-CGD	5.03	1.45	1.33
37	s	607	CHL	O2D-CGD	5.03	1.45	1.33
37	s	608	CHL	CHD-C4C	5.03	1.49	1.39
37	Y	601	CHL	CHB-C4A	-5.03	1.32	1.38
37	S	606	CHL	O2D-CGD	5.03	1.45	1.33
37	S	606	CHL	CHB-C4A	-5.02	1.32	1.38
37	s	606	CHL	CHB-C4A	-5.02	1.32	1.38
37	G	605	CHL	O2D-CGD	5.01	1.45	1.33
37	g	609	CHL	C3A-C2A	-5.01	1.50	1.54
37	s	606	CHL	O2D-CGD	5.01	1.45	1.33
37	g	601	CHL	CHB-C4A	-4.99	1.32	1.38
37	S	601	CHL	C3A-C2A	-4.99	1.50	1.54
37	n	607	CHL	C3A-C2A	-4.99	1.50	1.54
37	s	608	CHL	CHB-C1B	4.98	1.47	1.39
37	g	605	CHL	O2D-CGD	4.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	405	PL9	C7-C3	-4.95	1.44	1.51
37	s	607	CHL	C3B-C2B	4.95	1.47	1.40
37	G	601	CHL	CHB-C4A	-4.94	1.32	1.38
37	g	601	CHL	O2D-CGD	4.94	1.45	1.33
37	R	607	CHL	C3A-C2A	-4.93	1.50	1.54
37	G	608	CHL	O2D-CGD	4.93	1.45	1.33
37	g	608	CHL	O2D-CGD	4.93	1.45	1.33
37	R	607	CHL	OBD-CAD	4.93	1.28	1.22
37	G	609	CHL	C3A-C2A	-4.93	1.50	1.54
37	G	607	CHL	O2D-CGD	4.92	1.45	1.33
37	g	607	CHL	O2D-CGD	4.92	1.45	1.33
37	N	601	CHL	C3B-C2B	4.92	1.47	1.40
37	r	607	CHL	O2D-CGD	4.92	1.45	1.33
37	n	601	CHL	C3B-C2B	4.91	1.47	1.40
34	d	405	PL9	C7-C3	-4.91	1.44	1.51
37	g	606	CHL	O2D-CGD	4.91	1.45	1.33
37	S	601	CHL	O2D-CGD	4.91	1.45	1.33
37	s	601	CHL	O2D-CGD	4.91	1.45	1.33
37	r	607	CHL	OBD-CAD	4.91	1.28	1.22
37	G	606	CHL	O2D-CGD	4.90	1.45	1.33
37	r	607	CHL	C3A-C2A	-4.90	1.50	1.54
37	s	606	CHL	OBD-CAD	4.90	1.28	1.22
37	S	608	CHL	CHB-C1B	4.90	1.47	1.39
37	n	605	CHL	O2D-CGD	4.90	1.45	1.33
37	R	608	CHL	O2D-CGD	4.89	1.45	1.33
37	R	608	CHL	C3A-C2A	-4.89	1.50	1.54
37	r	608	CHL	C3A-C2A	-4.89	1.50	1.54
37	r	608	CHL	CHB-C4A	-4.89	1.32	1.38
37	Y	605	CHL	O2D-CGD	4.89	1.45	1.33
37	N	606	CHL	CHC-C4B	4.89	1.47	1.39
37	r	608	CHL	O2D-CGD	4.88	1.45	1.33
37	S	607	CHL	C3B-C2B	4.88	1.47	1.40
37	R	607	CHL	O2D-CGD	4.88	1.45	1.33
37	S	606	CHL	OBD-CAD	4.88	1.28	1.22
37	R	608	CHL	CHB-C4A	-4.88	1.32	1.38
37	G	609	CHL	O2D-CGD	4.87	1.45	1.33
37	g	609	CHL	O2D-CGD	4.87	1.45	1.33
37	y	601	CHL	O2D-CGD	4.87	1.45	1.33
37	G	601	CHL	O2D-CGD	4.87	1.45	1.33
37	Y	601	CHL	O2D-CGD	4.86	1.45	1.33
37	g	609	CHL	C3B-C2B	4.86	1.46	1.40
37	N	601	CHL	O2D-CGD	4.85	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	605	CHL	O2D-CGD	4.85	1.45	1.33
37	y	605	CHL	O2D-CGD	4.85	1.45	1.33
37	N	609	CHL	O2D-CGD	4.84	1.45	1.33
37	n	609	CHL	O2D-CGD	4.84	1.45	1.33
37	g	606	CHL	CHC-C4B	4.84	1.47	1.39
37	n	601	CHL	CHC-C4B	4.83	1.47	1.39
37	n	601	CHL	O2D-CGD	4.83	1.45	1.33
37	G	606	CHL	CHC-C4B	4.83	1.47	1.39
37	Y	606	CHL	O2D-CGD	4.82	1.45	1.33
37	y	606	CHL	O2D-CGD	4.82	1.45	1.33
37	n	606	CHL	CHC-C4B	4.81	1.47	1.39
37	s	606	CHL	CHC-C4B	4.81	1.47	1.39
37	s	607	CHL	OBD-CAD	4.80	1.28	1.22
37	G	607	CHL	OBD-CAD	4.80	1.28	1.22
37	g	607	CHL	OBD-CAD	4.80	1.28	1.22
37	G	605	CHL	OBD-CAD	4.80	1.28	1.22
37	g	605	CHL	OBD-CAD	4.80	1.28	1.22
37	N	607	CHL	O2D-CGD	4.80	1.45	1.33
37	n	607	CHL	O2D-CGD	4.79	1.45	1.33
37	N	601	CHL	CHC-C4B	4.79	1.47	1.39
37	S	606	CHL	CHC-C4B	4.78	1.47	1.39
37	S	607	CHL	CHB-C4A	-4.78	1.32	1.38
37	s	607	CHL	CHB-C4A	-4.78	1.32	1.38
37	S	607	CHL	OBD-CAD	4.78	1.28	1.22
37	s	607	CHL	CHD-C4C	4.77	1.48	1.39
37	Y	605	CHL	CHB-C4A	-4.77	1.32	1.38
37	y	605	CHL	CHB-C4A	-4.77	1.32	1.38
37	G	609	CHL	C3B-C2B	4.77	1.46	1.40
37	s	608	CHL	CHC-C1C	4.77	1.48	1.39
37	G	605	CHL	CHD-C4C	4.77	1.48	1.39
37	N	601	CHL	CHB-C4A	-4.76	1.32	1.38
37	S	606	CHL	C3A-C2A	-4.76	1.50	1.54
37	S	607	CHL	CHD-C1D	4.76	1.47	1.39
37	S	607	CHL	CHC-C4B	4.75	1.47	1.39
37	s	607	CHL	CHC-C4B	4.75	1.47	1.39
37	s	606	CHL	C3A-C2A	-4.75	1.50	1.54
37	S	608	CHL	CHC-C1C	4.75	1.48	1.39
37	G	609	CHL	CHB-C4A	-4.74	1.32	1.38
37	g	609	CHL	CHB-C4A	-4.74	1.32	1.38
37	Y	606	CHL	CHC-C4B	4.74	1.47	1.39
37	y	606	CHL	CHC-C4B	4.74	1.47	1.39
37	n	601	CHL	CHB-C4A	-4.74	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	n	606	CHL	O2D-CGD	4.74	1.44	1.33
37	G	606	CHL	OBD-CAD	4.74	1.28	1.22
37	r	606	CHL	O2D-CGD	4.74	1.44	1.33
37	n	608	CHL	O2D-CGD	4.74	1.44	1.33
37	s	606	CHL	CHD-C1D	4.73	1.47	1.39
37	G	605	CHL	CHB-C4A	-4.73	1.32	1.38
37	g	605	CHL	CHB-C4A	-4.73	1.32	1.38
37	g	605	CHL	CHD-C4C	4.73	1.48	1.39
37	S	607	CHL	CHD-C4C	4.73	1.48	1.39
37	N	609	CHL	OBD-CAD	4.73	1.28	1.22
37	n	609	CHL	OBD-CAD	4.73	1.28	1.22
37	y	609	CHL	O2D-CGD	4.73	1.44	1.33
37	R	606	CHL	O2D-CGD	4.72	1.44	1.33
37	N	608	CHL	O2D-CGD	4.72	1.44	1.33
37	y	607	CHL	O2D-CGD	4.72	1.44	1.33
37	Y	607	CHL	O2D-CGD	4.71	1.44	1.33
37	N	606	CHL	O2D-CGD	4.71	1.44	1.33
37	Y	609	CHL	O2D-CGD	4.71	1.44	1.33
37	G	605	CHL	C3B-C2B	4.71	1.46	1.40
37	g	605	CHL	C3B-C2B	4.71	1.46	1.40
37	s	607	CHL	CHD-C1D	4.71	1.47	1.39
37	g	605	CHL	CHC-C4B	4.70	1.47	1.39
37	Y	609	CHL	OBD-CAD	4.69	1.28	1.22
37	y	609	CHL	OBD-CAD	4.69	1.28	1.22
37	S	606	CHL	CHD-C1D	4.69	1.47	1.39
37	S	606	CHL	CHD-C4C	4.68	1.48	1.39
37	G	605	CHL	CHC-C4B	4.67	1.47	1.39
37	g	606	CHL	OBD-CAD	4.67	1.28	1.22
37	G	608	CHL	C3A-C2A	-4.67	1.50	1.54
37	g	608	CHL	C3A-C2A	-4.67	1.50	1.54
37	N	606	CHL	OBD-CAD	4.66	1.28	1.22
37	s	606	CHL	CHD-C4C	4.65	1.48	1.39
37	n	605	CHL	CHD-C4C	4.65	1.48	1.39
37	G	609	CHL	OBD-CAD	4.65	1.28	1.22
37	g	609	CHL	OBD-CAD	4.65	1.28	1.22
37	n	607	CHL	OBD-CAD	4.65	1.28	1.22
37	N	605	CHL	CHD-C4C	4.65	1.48	1.39
37	r	608	CHL	C3B-C2B	4.65	1.46	1.40
37	Y	608	CHL	O2D-CGD	4.65	1.44	1.33
37	y	608	CHL	O2D-CGD	4.65	1.44	1.33
34	D	405	PL9	C6-C1	-4.65	1.40	1.48
37	N	605	CHL	OBD-CAD	4.64	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	s	601	CHL	OBD-CAD	4.64	1.28	1.22
34	d	405	PL9	C6-C1	-4.62	1.40	1.48
37	N	607	CHL	OBD-CAD	4.62	1.28	1.22
37	G	601	CHL	OBD-CAD	4.61	1.28	1.22
37	g	608	CHL	C3B-C2B	4.61	1.46	1.40
37	S	601	CHL	OBD-CAD	4.61	1.28	1.22
37	Y	607	CHL	OBD-CAD	4.61	1.28	1.22
37	n	605	CHL	OBD-CAD	4.61	1.28	1.22
37	g	608	CHL	CHD-C4C	4.60	1.48	1.39
37	N	601	CHL	OBD-CAD	4.60	1.28	1.22
37	n	601	CHL	OBD-CAD	4.60	1.28	1.22
37	R	608	CHL	CHB-C1B	4.59	1.47	1.39
37	R	608	CHL	C3B-C2B	4.59	1.46	1.40
37	n	606	CHL	OBD-CAD	4.58	1.28	1.22
37	G	608	CHL	CHD-C4C	4.57	1.48	1.39
37	G	608	CHL	C3B-C2B	4.57	1.46	1.40
37	y	608	CHL	OBD-CAD	4.57	1.28	1.22
37	S	607	CHL	C3D-C2D	4.57	1.47	1.39
37	y	607	CHL	OBD-CAD	4.57	1.28	1.22
37	g	601	CHL	OBD-CAD	4.56	1.28	1.22
37	y	606	CHL	OBD-CAD	4.56	1.28	1.22
37	r	606	CHL	OBD-CAD	4.56	1.28	1.22
37	N	601	CHL	CHB-C1B	4.55	1.47	1.39
37	n	601	CHL	CHB-C1B	4.55	1.47	1.39
37	s	607	CHL	C3D-C2D	4.55	1.47	1.39
37	R	606	CHL	OBD-CAD	4.55	1.28	1.22
37	S	608	CHL	C3D-C2D	4.53	1.47	1.39
37	r	608	CHL	CHB-C1B	4.52	1.46	1.39
37	Y	606	CHL	OBD-CAD	4.52	1.28	1.22
37	g	609	CHL	CHB-C1B	4.51	1.46	1.39
37	N	601	CHL	CHD-C4C	4.51	1.48	1.39
37	n	601	CHL	CHD-C4C	4.50	1.48	1.39
37	s	608	CHL	C3D-C2D	4.50	1.47	1.39
37	R	607	CHL	C3B-C2B	4.50	1.46	1.40
37	Y	608	CHL	OBD-CAD	4.50	1.28	1.22
37	r	607	CHL	C3B-C2B	4.50	1.46	1.40
37	s	606	CHL	CHB-C1B	4.49	1.46	1.39
37	G	605	CHL	CHB-C1B	4.47	1.46	1.39
37	G	609	CHL	CHB-C1B	4.47	1.46	1.39
37	g	605	CHL	CHD-C1D	4.47	1.46	1.39
37	s	608	CHL	OBD-CAD	4.47	1.28	1.22
37	y	601	CHL	OBD-CAD	4.46	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	R	606	CHL	CHC-C4B	4.46	1.46	1.39
37	N	608	CHL	CHC-C4B	4.45	1.46	1.39
37	S	608	CHL	CHD-C1D	4.45	1.46	1.39
37	r	606	CHL	CHC-C4B	4.45	1.46	1.39
37	Y	606	CHL	O2A-CGA	4.45	1.46	1.33
37	y	606	CHL	O2A-CGA	4.45	1.46	1.33
37	g	605	CHL	CHB-C1B	4.44	1.46	1.39
37	R	608	CHL	CHC-C4B	4.44	1.46	1.39
37	G	606	CHL	CHD-C4C	4.44	1.47	1.39
37	g	606	CHL	CHD-C4C	4.44	1.47	1.39
37	G	605	CHL	CHD-C1D	4.43	1.46	1.39
37	G	608	CHL	CHD-C1D	4.43	1.46	1.39
37	N	605	CHL	CHC-C4B	4.43	1.46	1.39
37	n	605	CHL	CHC-C4B	4.43	1.46	1.39
37	s	608	CHL	CHD-C1D	4.43	1.46	1.39
37	Y	601	CHL	CHC-C4B	4.42	1.46	1.39
37	y	601	CHL	CHC-C4B	4.42	1.46	1.39
37	s	606	CHL	O2A-CGA	4.42	1.46	1.33
37	S	607	CHL	CHB-C1B	4.42	1.46	1.39
37	s	607	CHL	CHB-C1B	4.42	1.46	1.39
37	s	601	CHL	CHC-C4B	4.41	1.46	1.39
37	N	607	CHL	C3B-C2B	4.41	1.46	1.40
37	G	609	CHL	CHD-C4C	4.41	1.47	1.39
37	g	609	CHL	CHD-C4C	4.41	1.47	1.39
37	S	606	CHL	CHB-C1B	4.41	1.46	1.39
37	g	608	CHL	OBD-CAD	4.41	1.28	1.22
37	Y	601	CHL	CHD-C4C	4.40	1.47	1.39
37	S	606	CHL	O2A-CGA	4.40	1.46	1.33
37	S	608	CHL	OBD-CAD	4.40	1.28	1.22
37	Y	605	CHL	OBD-CAD	4.40	1.28	1.22
37	y	605	CHL	OBD-CAD	4.40	1.28	1.22
37	N	607	CHL	O2A-CGA	4.39	1.46	1.33
37	s	601	CHL	C3B-C2B	4.39	1.46	1.40
37	r	608	CHL	CHC-C4B	4.39	1.46	1.39
37	S	606	CHL	C3B-C2B	4.39	1.46	1.40
37	s	606	CHL	C3B-C2B	4.39	1.46	1.40
37	G	607	CHL	O2A-CGA	4.39	1.46	1.33
37	g	607	CHL	O2A-CGA	4.39	1.46	1.33
37	g	609	CHL	CHC-C4B	4.38	1.46	1.39
37	n	608	CHL	CHC-C4B	4.38	1.46	1.39
37	G	605	CHL	C3A-C2A	-4.38	1.50	1.54
37	n	607	CHL	C3B-C2B	4.38	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	s	607	CHL	O2A-CGA	4.38	1.46	1.33
37	Y	601	CHL	OBD-CAD	4.37	1.28	1.22
37	G	606	CHL	C3B-C2B	4.37	1.46	1.40
37	S	608	CHL	O2A-CGA	4.37	1.46	1.33
37	G	608	CHL	OBD-CAD	4.37	1.28	1.22
37	r	607	CHL	O2A-CGA	4.37	1.46	1.33
37	S	601	CHL	CHC-C4B	4.37	1.46	1.39
37	n	601	CHL	C3A-C2A	-4.36	1.50	1.54
37	G	609	CHL	O2A-CGA	4.36	1.46	1.33
37	y	607	CHL	O2A-CGA	4.36	1.46	1.33
37	n	608	CHL	OBD-CAD	4.36	1.28	1.22
37	g	608	CHL	CHC-C4B	4.36	1.46	1.39
37	n	607	CHL	O2A-CGA	4.36	1.46	1.33
37	N	609	CHL	O2A-CGA	4.35	1.46	1.33
37	n	609	CHL	O2A-CGA	4.35	1.46	1.33
37	g	606	CHL	C3B-C2B	4.35	1.46	1.40
37	G	609	CHL	CHC-C4B	4.35	1.46	1.39
37	G	609	CHL	CHD-C1D	4.35	1.46	1.39
37	g	609	CHL	CHD-C1D	4.35	1.46	1.39
37	g	609	CHL	O2A-CGA	4.35	1.46	1.33
37	Y	607	CHL	O2A-CGA	4.35	1.46	1.33
37	n	606	CHL	O2A-CGA	4.35	1.46	1.33
37	y	601	CHL	CHD-C4C	4.34	1.47	1.39
37	G	601	CHL	CHC-C4B	4.34	1.46	1.39
37	N	608	CHL	OBD-CAD	4.34	1.28	1.22
37	S	607	CHL	O2A-CGA	4.34	1.46	1.33
37	n	607	CHL	CHC-C4B	4.34	1.46	1.39
37	R	607	CHL	CHC-C4B	4.34	1.46	1.39
37	R	607	CHL	O2A-CGA	4.34	1.46	1.33
37	r	607	CHL	CHD-C4C	4.33	1.47	1.39
37	s	608	CHL	O2A-CGA	4.33	1.46	1.33
37	S	607	CHL	CHC-C1C	4.33	1.47	1.39
37	G	606	CHL	CHD-C1D	4.33	1.46	1.39
37	r	607	CHL	CHC-C4B	4.33	1.46	1.39
37	N	606	CHL	O2A-CGA	4.33	1.46	1.33
37	g	608	CHL	CHD-C1D	4.33	1.46	1.39
37	y	601	CHL	C3B-C2B	4.33	1.46	1.40
37	Y	601	CHL	C3B-C2B	4.33	1.46	1.40
37	R	607	CHL	CHD-C4C	4.33	1.47	1.39
37	S	601	CHL	C3B-C2B	4.32	1.46	1.40
37	n	609	CHL	CHC-C4B	4.32	1.46	1.39
37	g	607	CHL	C3B-C2B	4.32	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	n	601	CHL	O2A-CGA	4.32	1.45	1.33
37	Y	608	CHL	O2A-CGA	4.32	1.45	1.33
37	y	608	CHL	O2A-CGA	4.32	1.45	1.33
37	G	605	CHL	O2A-CGA	4.31	1.45	1.33
37	g	605	CHL	O2A-CGA	4.31	1.45	1.33
37	n	605	CHL	C3B-C2B	4.31	1.46	1.40
37	G	605	CHL	C3D-C2D	4.31	1.47	1.39
37	N	608	CHL	O2A-CGA	4.31	1.45	1.33
37	Y	605	CHL	O2A-CGA	4.31	1.45	1.33
37	G	606	CHL	CHC-C1C	4.31	1.47	1.39
37	g	606	CHL	CHC-C1C	4.31	1.47	1.39
37	G	608	CHL	CHC-C4B	4.30	1.46	1.39
37	g	605	CHL	C3D-C2D	4.30	1.47	1.39
37	N	601	CHL	O2A-CGA	4.30	1.45	1.33
37	n	608	CHL	CHD-C4C	4.30	1.47	1.39
37	g	606	CHL	CHD-C1D	4.30	1.46	1.39
37	s	607	CHL	CHC-C1C	4.30	1.47	1.39
37	S	601	CHL	O2A-CGA	4.29	1.45	1.33
37	n	608	CHL	O2A-CGA	4.29	1.45	1.33
37	G	607	CHL	C3B-C2B	4.29	1.46	1.40
37	N	609	CHL	CHD-C4C	4.29	1.47	1.39
37	S	601	CHL	CHD-C4C	4.29	1.47	1.39
37	n	609	CHL	CHD-C4C	4.29	1.47	1.39
37	g	605	CHL	C3A-C2A	-4.29	1.51	1.54
37	s	601	CHL	O2A-CGA	4.29	1.45	1.33
37	G	605	CHL	CHC-C1C	4.29	1.47	1.39
37	G	606	CHL	O2A-CGA	4.28	1.45	1.33
37	g	606	CHL	O2A-CGA	4.28	1.45	1.33
37	y	605	CHL	O2A-CGA	4.28	1.45	1.33
37	G	601	CHL	O2A-CGA	4.28	1.45	1.33
37	g	601	CHL	CHC-C4B	4.27	1.46	1.39
37	N	608	CHL	CHD-C4C	4.27	1.47	1.39
37	n	605	CHL	CHD-C1D	4.27	1.46	1.39
37	N	609	CHL	CHC-C4B	4.27	1.46	1.39
37	y	609	CHL	CHC-C4B	4.27	1.46	1.39
37	g	608	CHL	O2A-CGA	4.27	1.45	1.33
37	Y	608	CHL	CHD-C4C	4.26	1.47	1.39
37	y	608	CHL	CHD-C4C	4.26	1.47	1.39
37	N	607	CHL	CHC-C4B	4.26	1.46	1.39
37	Y	609	CHL	O2A-CGA	4.26	1.45	1.33
37	y	609	CHL	O2A-CGA	4.26	1.45	1.33
37	s	601	CHL	CHD-C4C	4.26	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	605	CHL	CHD-C1D	4.26	1.46	1.39
40	y	1623	NEX	C7-C6	-4.26	1.25	1.30
37	G	601	CHL	C3B-C2B	4.26	1.46	1.40
37	g	601	CHL	CHD-C4C	4.26	1.47	1.39
37	N	608	CHL	C3B-C2B	4.25	1.46	1.40
37	g	601	CHL	O2A-CGA	4.25	1.45	1.33
37	y	609	CHL	C3B-C2B	4.25	1.46	1.40
37	y	601	CHL	CHB-C1B	4.25	1.46	1.39
37	Y	609	CHL	C3B-C2B	4.25	1.46	1.40
37	R	606	CHL	O2A-CGA	4.25	1.45	1.33
37	y	607	CHL	CHC-C4B	4.24	1.46	1.39
37	G	608	CHL	O2A-CGA	4.24	1.45	1.33
37	Y	607	CHL	CHC-C4B	4.24	1.46	1.39
37	Y	609	CHL	CHC-C4B	4.24	1.46	1.39
37	r	606	CHL	O2A-CGA	4.24	1.45	1.33
37	N	605	CHL	C3B-C2B	4.24	1.46	1.40
37	N	605	CHL	O2A-CGA	4.24	1.45	1.33
37	n	605	CHL	O2A-CGA	4.24	1.45	1.33
37	g	605	CHL	CHC-C1C	4.24	1.47	1.39
37	N	601	CHL	CHD-C1D	4.24	1.46	1.39
37	n	601	CHL	CHD-C1D	4.24	1.46	1.39
37	y	608	CHL	C3B-C2B	4.23	1.46	1.40
37	Y	601	CHL	O2A-CGA	4.23	1.45	1.33
37	y	601	CHL	O2A-CGA	4.23	1.45	1.33
37	Y	609	CHL	CHD-C4C	4.23	1.47	1.39
37	y	609	CHL	CHD-C4C	4.23	1.47	1.39
37	N	601	CHL	C3A-C2A	-4.22	1.51	1.54
40	Y	1623	NEX	C7-C6	-4.22	1.25	1.30
37	n	608	CHL	C3B-C2B	4.22	1.46	1.40
37	S	601	CHL	C3D-C2D	4.22	1.46	1.39
37	G	601	CHL	CHD-C4C	4.22	1.47	1.39
37	Y	601	CHL	CHB-C1B	4.22	1.46	1.39
37	G	601	CHL	CHB-C1B	4.21	1.46	1.39
37	y	608	CHL	CHC-C4B	4.21	1.46	1.39
37	g	601	CHL	CHB-C1B	4.21	1.46	1.39
37	g	601	CHL	C3B-C2B	4.21	1.46	1.40
37	Y	608	CHL	C3B-C2B	4.21	1.46	1.40
37	Y	605	CHL	CHB-C1B	4.20	1.46	1.39
37	Y	609	CHL	CHB-C1B	4.20	1.46	1.39
37	y	609	CHL	CHB-C1B	4.20	1.46	1.39
37	Y	605	CHL	C3B-C2B	4.20	1.46	1.40
37	y	605	CHL	C3B-C2B	4.20	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	601	CHL	CHC-C1C	4.20	1.47	1.39
37	n	609	CHL	CHD-C1D	4.19	1.46	1.39
37	N	606	CHL	C3B-C2B	4.19	1.46	1.40
37	n	606	CHL	C3B-C2B	4.19	1.46	1.40
37	n	601	CHL	CHC-C1C	4.19	1.47	1.39
37	N	606	CHL	CHD-C4C	4.18	1.47	1.39
37	n	606	CHL	CHD-C4C	4.18	1.47	1.39
37	G	608	CHL	CHB-C1B	4.18	1.46	1.39
37	Y	605	CHL	CHC-C4B	4.18	1.46	1.39
37	y	605	CHL	CHC-C4B	4.18	1.46	1.39
37	s	606	CHL	CHC-C1C	4.18	1.47	1.39
37	y	605	CHL	CHB-C1B	4.18	1.46	1.39
37	G	607	CHL	CHD-C4C	4.18	1.47	1.39
37	s	601	CHL	C3D-C2D	4.17	1.46	1.39
37	n	609	CHL	C3B-C2B	4.17	1.46	1.40
37	g	607	CHL	CHD-C4C	4.17	1.47	1.39
37	y	606	CHL	CHC-C1C	4.17	1.47	1.39
37	s	606	CHL	C3D-C2D	4.16	1.46	1.39
37	N	609	CHL	CHD-C1D	4.16	1.46	1.39
37	g	608	CHL	CHB-C1B	4.16	1.46	1.39
37	S	606	CHL	CHC-C1C	4.16	1.47	1.39
37	N	605	CHL	CHB-C1B	4.16	1.46	1.39
37	N	606	CHL	CHB-C1B	4.16	1.46	1.39
37	n	605	CHL	CHB-C1B	4.16	1.46	1.39
37	S	606	CHL	C3D-C2D	4.15	1.46	1.39
37	G	606	CHL	CHB-C1B	4.15	1.46	1.39
37	y	605	CHL	CHD-C4C	4.14	1.47	1.39
37	N	609	CHL	C3B-C2B	4.14	1.46	1.40
37	Y	606	CHL	C3B-C2B	4.14	1.46	1.40
37	R	607	CHL	CHB-C1B	4.14	1.46	1.39
37	r	607	CHL	CHB-C1B	4.14	1.46	1.39
37	r	608	CHL	O2A-CGA	4.14	1.45	1.33
37	N	605	CHL	CHC-C1C	4.14	1.47	1.39
37	n	605	CHL	CHC-C1C	4.14	1.47	1.39
37	Y	601	CHL	C3D-C2D	4.13	1.46	1.39
37	N	601	CHL	C3D-C2D	4.13	1.46	1.39
37	Y	608	CHL	CHC-C4B	4.13	1.46	1.39
37	N	607	CHL	CHD-C4C	4.12	1.47	1.39
37	n	606	CHL	CHB-C1B	4.12	1.46	1.39
37	N	606	CHL	CHC-C1C	4.12	1.47	1.39
37	r	606	CHL	CHD-C4C	4.12	1.47	1.39
37	y	601	CHL	C3D-C2D	4.12	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	R	607	CHL	CHD-C1D	4.12	1.46	1.39
37	r	607	CHL	CHD-C1D	4.12	1.46	1.39
37	r	608	CHL	CHD-C4C	4.11	1.47	1.39
37	G	606	CHL	C3D-C2D	4.11	1.46	1.39
37	g	609	CHL	C3D-C2D	4.11	1.46	1.39
37	g	607	CHL	CHC-C4B	4.11	1.46	1.39
37	R	608	CHL	OBD-CAD	4.11	1.27	1.22
37	n	601	CHL	C3D-C2D	4.11	1.46	1.39
37	R	606	CHL	CHD-C4C	4.11	1.47	1.39
37	Y	605	CHL	CHD-C4C	4.10	1.47	1.39
37	g	606	CHL	CHB-C1B	4.10	1.46	1.39
37	Y	607	CHL	C3B-C2B	4.10	1.45	1.40
37	Y	606	CHL	CHC-C1C	4.10	1.47	1.39
37	R	606	CHL	CHB-C1B	4.10	1.46	1.39
37	y	607	CHL	C3B-C2B	4.10	1.45	1.40
37	R	608	CHL	CHD-C4C	4.10	1.47	1.39
37	R	608	CHL	O2A-CGA	4.10	1.45	1.33
37	r	606	CHL	CHB-C1B	4.10	1.46	1.39
37	g	607	CHL	C3D-C2D	4.10	1.46	1.39
37	n	605	CHL	C3D-C2D	4.10	1.46	1.39
37	y	606	CHL	C3B-C2B	4.09	1.45	1.40
37	Y	601	CHL	CHD-C1D	4.09	1.46	1.39
37	G	609	CHL	C3D-C2D	4.09	1.46	1.39
37	s	608	CHL	CHB-C4A	-4.09	1.33	1.38
37	r	608	CHL	OBD-CAD	4.09	1.27	1.22
37	n	607	CHL	CHD-C4C	4.09	1.47	1.39
37	S	601	CHL	CHD-C1D	4.09	1.46	1.39
37	s	601	CHL	CHD-C1D	4.09	1.46	1.39
37	G	607	CHL	CHC-C4B	4.08	1.46	1.39
37	n	606	CHL	CHC-C1C	4.08	1.47	1.39
37	Y	605	CHL	CHD-C1D	4.08	1.46	1.39
37	y	605	CHL	CHD-C1D	4.08	1.46	1.39
37	N	607	CHL	CHB-C1B	4.07	1.46	1.39
37	n	607	CHL	CHD-C1D	4.07	1.46	1.39
37	G	607	CHL	C3D-C2D	4.07	1.46	1.39
37	S	601	CHL	CHB-C1B	4.07	1.46	1.39
37	s	601	CHL	CHB-C1B	4.07	1.46	1.39
37	N	605	CHL	C3D-C2D	4.07	1.46	1.39
37	R	607	CHL	C3D-C2D	4.07	1.46	1.39
37	r	607	CHL	C3D-C2D	4.07	1.46	1.39
37	R	606	CHL	CHC-C1C	4.06	1.47	1.39
37	y	601	CHL	CHD-C1D	4.06	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	r	623	NEX	C7-C6	-4.06	1.25	1.30
40	Y	1623	NEX	C7-C8	-4.06	1.25	1.31
37	n	607	CHL	CHB-C1B	4.05	1.46	1.39
37	r	606	CHL	CHC-C1C	4.04	1.47	1.39
37	g	606	CHL	C3D-C2D	4.03	1.46	1.39
37	S	607	CHL	C3A-C2A	-4.03	1.51	1.54
37	G	608	CHL	CHC-C1C	4.02	1.47	1.39
37	g	608	CHL	CHC-C1C	4.02	1.47	1.39
37	y	607	CHL	CHD-C4C	4.02	1.47	1.39
37	S	608	CHL	CHB-C4A	-4.02	1.33	1.38
37	Y	606	CHL	CHD-C4C	4.02	1.47	1.39
37	Y	607	CHL	CHD-C4C	4.01	1.47	1.39
37	r	607	CHL	CHC-C1C	4.00	1.47	1.39
37	R	607	CHL	CHC-C1C	4.00	1.47	1.39
37	y	606	CHL	CHD-C4C	4.00	1.47	1.39
37	N	609	CHL	CHB-C1B	4.00	1.46	1.39
37	n	609	CHL	CHB-C1B	4.00	1.46	1.39
37	Y	608	CHL	CHD-C1D	4.00	1.46	1.39
37	y	608	CHL	CHD-C1D	4.00	1.46	1.39
37	Y	607	CHL	CHD-C1D	3.99	1.46	1.39
37	y	607	CHL	CHD-C1D	3.99	1.46	1.39
37	r	606	CHL	C3B-C2B	3.99	1.45	1.40
40	y	1623	NEX	C7-C8	-3.98	1.25	1.31
37	G	601	CHL	CHD-C1D	3.98	1.46	1.39
37	G	607	CHL	CHD-C1D	3.98	1.46	1.39
37	g	607	CHL	CHD-C1D	3.98	1.46	1.39
37	Y	609	CHL	CHD-C1D	3.98	1.46	1.39
37	s	607	CHL	C3A-C2A	-3.98	1.51	1.54
37	Y	609	CHL	CHC-C1C	3.98	1.47	1.39
37	g	607	CHL	CHB-C1B	3.97	1.46	1.39
37	N	607	CHL	CHD-C1D	3.97	1.46	1.39
40	R	623	NEX	C7-C6	-3.96	1.26	1.30
37	R	606	CHL	CHD-C1D	3.96	1.46	1.39
37	g	601	CHL	CHD-C1D	3.96	1.46	1.39
37	y	609	CHL	CHD-C1D	3.96	1.46	1.39
37	Y	606	CHL	CHB-C1B	3.96	1.46	1.39
37	R	606	CHL	C3D-C2D	3.95	1.46	1.39
37	G	607	CHL	CHB-C1B	3.95	1.46	1.39
37	s	601	CHL	CHC-C1C	3.95	1.46	1.39
37	S	601	CHL	CHC-C1C	3.95	1.46	1.39
37	y	609	CHL	CHC-C1C	3.95	1.46	1.39
37	N	609	CHL	C3D-C2D	3.94	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	n	609	CHL	C3D-C2D	3.94	1.46	1.39
37	N	608	CHL	CHB-C1B	3.94	1.46	1.39
37	G	609	CHL	CHC-C1C	3.94	1.46	1.39
37	y	606	CHL	CHB-C1B	3.94	1.46	1.39
37	y	605	CHL	C3D-C2D	3.94	1.46	1.39
37	Y	608	CHL	CHB-C1B	3.94	1.46	1.39
37	y	608	CHL	CHB-C1B	3.94	1.46	1.39
37	R	606	CHL	C3B-C2B	3.94	1.45	1.40
37	n	608	CHL	CHB-C1B	3.93	1.46	1.39
37	R	608	CHL	CHC-C1C	3.93	1.46	1.39
37	r	608	CHL	CHC-C1C	3.93	1.46	1.39
37	Y	609	CHL	C3D-C2D	3.92	1.46	1.39
37	y	609	CHL	C3D-C2D	3.92	1.46	1.39
36	F	101	HEM	FE-ND	3.92	2.07	1.94
37	r	606	CHL	C3D-C2D	3.90	1.46	1.39
36	f	101	HEM	FE-ND	3.90	2.06	1.94
37	g	601	CHL	CHC-C1C	3.90	1.46	1.39
37	Y	605	CHL	C3D-C2D	3.90	1.46	1.39
37	g	609	CHL	CHC-C1C	3.89	1.46	1.39
37	r	606	CHL	CHD-C1D	3.89	1.45	1.39
37	N	607	CHL	CHC-C1C	3.88	1.46	1.39
37	n	608	CHL	CHC-C1C	3.87	1.46	1.39
37	N	606	CHL	C3D-C2D	3.86	1.46	1.39
37	G	601	CHL	CHC-C1C	3.86	1.46	1.39
37	N	607	CHL	C3D-C2D	3.86	1.46	1.39
37	n	607	CHL	C3D-C2D	3.86	1.46	1.39
37	r	608	CHL	CHD-C1D	3.85	1.45	1.39
37	N	608	CHL	CHD-C1D	3.83	1.45	1.39
37	n	608	CHL	CHD-C1D	3.83	1.45	1.39
37	N	608	CHL	CHC-C1C	3.83	1.46	1.39
37	n	607	CHL	CHC-C1C	3.83	1.46	1.39
37	N	609	CHL	CHC-C1C	3.81	1.46	1.39
37	n	609	CHL	CHC-C1C	3.81	1.46	1.39
37	n	606	CHL	C3D-C2D	3.81	1.46	1.39
37	Y	606	CHL	CHD-C1D	3.81	1.45	1.39
40	R	623	NEX	C7-C8	-3.81	1.25	1.31
37	G	608	CHL	C3D-C2D	3.80	1.46	1.39
37	g	608	CHL	C3D-C2D	3.79	1.46	1.39
40	r	623	NEX	C7-C8	-3.78	1.25	1.31
37	N	606	CHL	CHD-C1D	3.78	1.45	1.39
37	n	606	CHL	CHD-C1D	3.78	1.45	1.39
37	y	601	CHL	CHC-C1C	3.78	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	R	608	CHL	CHD-C1D	3.78	1.45	1.39
37	y	606	CHL	CHD-C1D	3.78	1.45	1.39
37	Y	601	CHL	CHC-C1C	3.77	1.46	1.39
37	y	607	CHL	CHB-C1B	3.77	1.45	1.39
37	Y	607	CHL	CHB-C1B	3.77	1.45	1.39
37	Y	607	CHL	C3D-C2D	3.76	1.46	1.39
37	y	607	CHL	C3D-C2D	3.76	1.46	1.39
37	r	608	CHL	C3D-C2D	3.76	1.46	1.39
37	g	607	CHL	CHC-C1C	3.76	1.46	1.39
35	D	409	LHG	O7-C5	-3.75	1.37	1.46
35	d	409	LHG	O7-C5	-3.75	1.37	1.46
37	G	607	CHL	CHC-C1C	3.73	1.46	1.39
37	R	608	CHL	C3D-C2D	3.73	1.46	1.39
37	Y	608	CHL	CHC-C1C	3.72	1.46	1.39
37	y	608	CHL	CHC-C1C	3.72	1.46	1.39
37	Y	605	CHL	CHC-C1C	3.71	1.46	1.39
37	G	601	CHL	C3D-C2D	3.71	1.46	1.39
37	g	601	CHL	C3D-C2D	3.70	1.45	1.39
37	y	605	CHL	CHC-C1C	3.67	1.46	1.39
37	y	606	CHL	C3D-C2D	3.65	1.45	1.39
37	Y	608	CHL	C3D-C2D	3.59	1.45	1.39
37	Y	607	CHL	CHC-C1C	3.59	1.46	1.39
37	y	607	CHL	CHC-C1C	3.59	1.46	1.39
37	N	608	CHL	C3D-C2D	3.58	1.45	1.39
37	n	608	CHL	C3D-C2D	3.58	1.45	1.39
37	Y	606	CHL	C3D-C2D	3.57	1.45	1.39
37	y	608	CHL	C3D-C2D	3.56	1.45	1.39
40	n	1623	NEX	C7-C6	-3.56	1.26	1.30
40	g	1623	NEX	C7-C8	-3.53	1.26	1.31
40	N	1623	NEX	C7-C6	-3.52	1.26	1.30
40	N	1623	NEX	C7-C8	-3.52	1.26	1.31
40	G	1623	NEX	C7-C8	-3.51	1.26	1.31
40	n	1623	NEX	C7-C8	-3.47	1.26	1.31
27	R	611	CLA	C1D-ND	3.42	1.42	1.37
27	S	603	CLA	C1D-ND	3.40	1.42	1.37
40	G	1623	NEX	C7-C6	-3.39	1.26	1.30
37	Y	608	CHL	CBD-CGD	-3.38	1.48	1.52
37	y	608	CHL	CBD-CGD	-3.38	1.48	1.52
27	r	611	CLA	C1D-ND	3.38	1.42	1.37
27	s	603	CLA	C1D-ND	3.38	1.42	1.37
40	g	1623	NEX	C7-C6	-3.38	1.26	1.30
27	S	609	CLA	C1D-ND	3.36	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	612	CLA	CMC-C2C	-3.35	1.43	1.50
32	C	519	DGD	O2G-C2G	-3.35	1.38	1.46
27	B	612	CLA	CMC-C2C	-3.33	1.43	1.50
32	c	519	DGD	O2G-C2G	-3.32	1.38	1.46
35	d	408	LHG	O7-C5	-3.32	1.38	1.46
27	s	609	CLA	C1D-ND	3.31	1.42	1.37
27	R	601	CLA	C1D-ND	3.31	1.42	1.37
27	r	601	CLA	C1D-ND	3.31	1.42	1.37
27	N	611	CLA	C1D-ND	3.31	1.42	1.37
37	s	608	CHL	C3A-C2A	-3.29	1.51	1.54
35	D	408	LHG	O7-C5	-3.29	1.38	1.46
30	a	412	SQD	O48-C23	3.23	1.42	1.33
28	a	408	PHO	CMC-C2C	-3.23	1.45	1.50
30	a	418	SQD	O48-C23	3.23	1.42	1.33
27	G	610	CLA	C1D-ND	3.22	1.42	1.37
27	g	610	CLA	C1D-ND	3.22	1.42	1.37
27	n	612	CLA	C1D-ND	3.22	1.42	1.37
30	A	412	SQD	O48-C23	3.21	1.42	1.33
30	A	418	SQD	O48-C23	3.21	1.42	1.33
28	A	409	PHO	C1D-C2D	3.21	1.43	1.39
28	a	409	PHO	C1D-C2D	3.21	1.43	1.39
27	n	611	CLA	C1D-ND	3.21	1.42	1.37
28	A	408	PHO	CMC-C2C	-3.20	1.45	1.50
40	S	1623	NEX	C7-C6	-3.20	1.26	1.30
27	R	616	CLA	C1D-ND	3.20	1.42	1.37
27	r	616	CLA	C1D-ND	3.20	1.42	1.37
37	S	608	CHL	C3A-C2A	-3.20	1.52	1.54
29	B	620	BCR	C1-C6	-3.19	1.49	1.53
40	s	1623	NEX	C7-C8	-3.19	1.26	1.31
37	Y	601	CHL	CBD-CGD	-3.19	1.48	1.52
37	y	601	CHL	CBD-CGD	-3.18	1.48	1.52
27	N	614	CLA	C1D-ND	3.18	1.42	1.37
40	s	1623	NEX	C7-C6	-3.18	1.26	1.30
40	S	1623	NEX	C7-C8	-3.18	1.26	1.31
29	b	620	BCR	C1-C6	-3.17	1.49	1.53
35	l	101	LHG	O7-C5	-3.17	1.39	1.46
27	n	610	CLA	C1D-ND	3.16	1.42	1.37
27	s	604	CLA	C1D-ND	3.16	1.42	1.37
35	L	101	LHG	O7-C5	-3.16	1.39	1.46
27	N	612	CLA	C1D-ND	3.16	1.42	1.37
27	S	604	CLA	C1D-ND	3.16	1.42	1.37
32	c	518	DGD	O1G-C1G	-3.15	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	518	DGD	O1G-C1G	-3.14	1.38	1.45
27	n	614	CLA	C1D-ND	3.14	1.42	1.37
27	R	613	CLA	C1D-ND	3.14	1.42	1.37
27	R	604	CLA	C1D-ND	3.14	1.42	1.37
27	r	613	CLA	C1D-ND	3.14	1.42	1.37
34	d	405	PL9	C52-C5	-3.13	1.44	1.50
27	r	609	CLA	C1D-ND	3.13	1.42	1.37
27	G	611	CLA	C1D-ND	3.13	1.42	1.37
27	R	610	CLA	C1D-ND	3.13	1.42	1.37
27	r	610	CLA	C1D-ND	3.13	1.42	1.37
34	D	405	PL9	C52-C5	-3.13	1.44	1.50
32	H	102	DGD	O1G-C1G	-3.12	1.38	1.45
32	h	102	DGD	O1G-C1G	-3.12	1.38	1.45
27	G	614	CLA	C1D-ND	3.12	1.42	1.37
27	g	614	CLA	C1D-ND	3.12	1.42	1.37
27	S	610	CLA	C1D-ND	3.11	1.41	1.37
27	g	603	CLA	C1D-ND	3.11	1.41	1.37
28	a	409	PHO	CMC-C2C	-3.10	1.45	1.50
27	R	602	CLA	C1D-ND	3.09	1.41	1.37
27	R	609	CLA	C1D-ND	3.09	1.41	1.37
28	A	409	PHO	CMC-C2C	-3.09	1.45	1.50
28	A	408	PHO	C1D-C2D	3.09	1.43	1.39
27	G	603	CLA	C1D-ND	3.09	1.41	1.37
27	r	612	CLA	C1D-ND	3.08	1.41	1.37
27	g	611	CLA	C1D-ND	3.08	1.41	1.37
34	d	405	PL9	C53-C6	-3.08	1.44	1.50
27	R	612	CLA	C1D-ND	3.07	1.41	1.37
27	S	611	CLA	C1D-ND	3.07	1.41	1.37
27	s	610	CLA	C1D-ND	3.06	1.41	1.37
27	N	610	CLA	C1D-ND	3.06	1.41	1.37
27	r	604	CLA	C1D-ND	3.06	1.41	1.37
27	C	508	CLA	CMB-C2B	-3.06	1.44	1.50
27	Y	602	CLA	C1D-ND	3.05	1.41	1.37
27	s	611	CLA	C1D-ND	3.05	1.41	1.37
27	r	602	CLA	C1D-ND	3.04	1.41	1.37
27	c	508	CLA	CMB-C2B	-3.04	1.44	1.50
28	a	408	PHO	C1D-C2D	3.04	1.42	1.39
27	s	602	CLA	C1D-ND	3.03	1.41	1.37
34	D	405	PL9	C53-C6	-3.03	1.44	1.50
27	g	612	CLA	C1D-ND	3.02	1.41	1.37
27	n	613	CLA	C1D-ND	3.02	1.41	1.37
27	R	603	CLA	C1D-ND	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	r	603	CLA	C1D-ND	3.02	1.41	1.37
27	S	602	CLA	C1D-ND	3.01	1.41	1.37
37	N	609	CHL	CBD-CGD	-3.01	1.48	1.52
37	n	607	CHL	CBD-CGD	-3.01	1.48	1.52
37	n	609	CHL	CBD-CGD	-3.01	1.48	1.52
35	Y	2630	LHG	O7-C5	-3.00	1.39	1.46
35	y	2630	LHG	O7-C5	-3.00	1.39	1.46
27	G	613	CLA	C1D-ND	3.00	1.41	1.37
27	S	609	CLA	C4B-NB	3.00	1.41	1.37
30	B	621	SQD	O48-C23	2.99	1.42	1.33
27	N	613	CLA	C1D-ND	2.99	1.41	1.37
37	N	607	CHL	CBD-CGD	-2.99	1.48	1.52
36	f	101	HEM	FE-NB	2.99	2.04	1.94
27	y	602	CLA	C1D-ND	2.98	1.41	1.37
30	b	621	SQD	O48-C23	2.97	1.42	1.33
27	B	611	CLA	MG-NB	-2.96	1.99	2.05
27	b	611	CLA	MG-NB	-2.96	1.99	2.05
32	C	518	DGD	O2G-C2G	-2.96	1.39	1.46
32	c	518	DGD	O2G-C2G	-2.96	1.39	1.46
36	F	101	HEM	FE-NB	2.96	2.04	1.94
27	g	613	CLA	C1D-ND	2.96	1.41	1.37
27	C	501	CLA	C1D-ND	2.96	1.41	1.37
27	c	501	CLA	C1D-ND	2.96	1.41	1.37
27	s	609	CLA	C4B-NB	2.96	1.41	1.37
27	s	612	CLA	C1D-ND	2.96	1.41	1.37
37	N	606	CHL	CBD-CGD	-2.95	1.48	1.52
27	Y	610	CLA	C1D-ND	2.95	1.41	1.37
27	G	612	CLA	C1D-ND	2.95	1.41	1.37
27	C	504	CLA	C1D-ND	2.95	1.41	1.37
37	Y	607	CHL	CBD-CGD	-2.95	1.48	1.52
37	y	607	CHL	CBD-CGD	-2.95	1.48	1.52
36	F	101	HEM	CAB-C3B	2.94	1.55	1.47
37	G	601	CHL	CBD-CGD	-2.94	1.48	1.52
37	g	601	CHL	CBD-CGD	-2.94	1.48	1.52
28	a	409	PHO	CBD-CGD	-2.94	1.48	1.52
27	b	610	CLA	MG-NB	-2.93	2.00	2.05
28	A	409	PHO	CAC-C3C	-2.93	1.46	1.51
27	B	602	CLA	C1D-ND	2.93	1.41	1.37
27	b	602	CLA	C1D-ND	2.93	1.41	1.37
27	b	608	CLA	C1D-ND	2.93	1.41	1.37
27	S	612	CLA	C1D-ND	2.93	1.41	1.37
30	A	418	SQD	O47-C7	2.92	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	610	CLA	MG-NB	-2.92	2.00	2.05
27	a	410	CLA	MG-NB	-2.92	2.00	2.05
37	R	607	CHL	CBD-CGD	-2.91	1.48	1.52
27	s	613	CLA	C1D-ND	2.91	1.41	1.37
27	C	506	CLA	MG-NB	-2.91	2.00	2.05
27	c	506	CLA	MG-NB	-2.91	2.00	2.05
27	y	610	CLA	C1D-ND	2.91	1.41	1.37
36	f	101	HEM	CAB-C3B	2.90	1.55	1.47
30	a	418	SQD	O47-C7	2.90	1.42	1.34
27	c	504	CLA	C1D-ND	2.90	1.41	1.37
37	Y	605	CHL	CBD-CGD	-2.90	1.48	1.52
37	s	601	CHL	CBD-CGD	-2.90	1.48	1.52
37	S	601	CHL	CBD-CGD	-2.89	1.48	1.52
37	Y	609	CHL	CBD-CGD	-2.89	1.48	1.52
27	A	410	CLA	MG-NB	-2.89	2.00	2.05
36	F	101	HEM	CAC-C3C	2.89	1.55	1.47
37	Y	606	CHL	CBD-CGD	-2.89	1.48	1.52
37	y	606	CHL	CBD-CGD	-2.89	1.48	1.52
36	f	101	HEM	CAC-C3C	2.88	1.55	1.47
28	a	409	PHO	CAC-C3C	-2.88	1.46	1.51
37	N	601	CHL	CBD-CGD	-2.88	1.48	1.52
37	n	601	CHL	CBD-CGD	-2.88	1.48	1.52
27	Y	611	CLA	C1D-ND	2.88	1.41	1.37
27	C	510	CLA	MG-NB	-2.88	2.00	2.05
27	c	505	CLA	MG-NB	-2.87	2.00	2.05
28	A	408	PHO	C4D-ND	-2.87	1.34	1.38
28	a	408	PHO	C4D-ND	-2.87	1.34	1.38
27	G	604	CLA	C1D-ND	2.87	1.41	1.37
27	B	604	CLA	MG-NB	-2.87	2.00	2.05
27	b	604	CLA	MG-NB	-2.87	2.00	2.05
38	G	1621	LUT	C22-C21	-2.87	1.51	1.54
37	N	608	CHL	CBD-CGD	-2.86	1.48	1.52
27	B	608	CLA	C1D-ND	2.86	1.41	1.37
27	B	613	CLA	MG-NB	-2.86	2.00	2.05
37	n	608	CHL	CBD-CGD	-2.86	1.48	1.52
27	C	505	CLA	MG-NB	-2.86	2.00	2.05
32	C	518	DGD	O5D-C6D	-2.86	1.38	1.43
37	y	609	CHL	CBD-CGD	-2.86	1.48	1.52
28	A	409	PHO	CBD-CGD	-2.85	1.48	1.52
27	D	402	CLA	CMD-C2D	-2.85	1.44	1.50
28	A	408	PHO	CMB-C2B	-2.85	1.45	1.51
28	a	408	PHO	CMB-C2B	-2.85	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	r	607	CHL	CBD-CGD	-2.85	1.48	1.52
27	Y	604	CLA	C1D-ND	2.85	1.41	1.37
37	n	605	CHL	CBD-CGD	-2.85	1.48	1.52
27	B	609	CLA	C1D-ND	2.84	1.41	1.37
27	b	609	CLA	C1D-ND	2.84	1.41	1.37
27	b	604	CLA	CMB-C2B	-2.84	1.44	1.50
27	g	604	CLA	C1D-ND	2.84	1.41	1.37
37	n	606	CHL	CBD-CGD	-2.84	1.48	1.52
37	R	608	CHL	CBD-CGD	-2.84	1.48	1.52
30	B	621	SQD	O47-C7	2.84	1.42	1.34
30	b	621	SQD	O47-C7	2.84	1.42	1.34
37	y	605	CHL	CBD-CGD	-2.84	1.48	1.52
27	C	509	CLA	MG-NB	-2.83	2.00	2.05
27	B	614	CLA	MG-NB	-2.83	2.00	2.05
34	D	405	PL9	C36-C34	-2.83	1.45	1.51
34	d	405	PL9	C36-C34	-2.83	1.45	1.51
27	N	602	CLA	C1D-ND	2.83	1.41	1.37
27	c	510	CLA	MG-NB	-2.83	2.00	2.05
27	b	617	CLA	C1D-ND	2.83	1.41	1.37
27	y	611	CLA	C1D-ND	2.83	1.41	1.37
27	c	508	CLA	C1D-ND	2.82	1.41	1.37
27	b	613	CLA	MG-NB	-2.82	2.00	2.05
27	Y	613	CLA	MG-NB	-2.82	2.00	2.05
27	C	511	CLA	C1D-ND	2.82	1.41	1.37
27	B	603	CLA	MG-NB	-2.82	2.00	2.05
27	b	603	CLA	MG-NB	-2.82	2.00	2.05
27	b	614	CLA	MG-NB	-2.82	2.00	2.05
27	S	613	CLA	C1D-ND	2.82	1.41	1.37
27	y	612	CLA	MG-NB	-2.81	2.00	2.05
28	A	408	PHO	CAC-C3C	-2.81	1.46	1.51
28	a	408	PHO	CAC-C3C	-2.81	1.46	1.51
27	d	402	CLA	CMD-C2D	-2.81	1.45	1.50
27	g	602	CLA	MG-NB	-2.81	2.00	2.05
27	R	601	CLA	C4B-NB	2.81	1.41	1.37
27	n	602	CLA	C1D-ND	2.81	1.41	1.37
27	r	601	CLA	C4B-NB	2.81	1.41	1.37
27	c	511	CLA	C1D-ND	2.80	1.41	1.37
27	b	615	CLA	C1D-ND	2.80	1.41	1.37
38	g	1621	LUT	C22-C21	-2.80	1.51	1.54
27	c	509	CLA	MG-NB	-2.80	2.00	2.05
37	G	609	CHL	CBD-CGD	-2.80	1.49	1.52
37	g	609	CHL	CBD-CGD	-2.80	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	n	602	CLA	C4B-NB	2.79	1.41	1.37
27	r	611	CLA	C4B-NB	2.79	1.41	1.37
27	c	505	CLA	CMD-C2D	-2.79	1.45	1.50
27	A	405	CLA	MG-NB	-2.79	2.00	2.05
27	Y	603	CLA	C1D-ND	2.79	1.41	1.37
27	y	603	CLA	C1D-ND	2.79	1.41	1.37
37	r	608	CHL	CBD-CGD	-2.79	1.49	1.52
27	G	602	CLA	MG-NB	-2.79	2.00	2.05
27	R	611	CLA	C4B-NB	2.79	1.41	1.37
30	A	412	SQD	O47-C7	2.79	1.42	1.34
30	a	412	SQD	O47-C7	2.79	1.42	1.34
27	a	405	CLA	MG-NB	-2.78	2.00	2.05
27	y	613	CLA	MG-NB	-2.78	2.00	2.05
27	S	614	CLA	C1D-ND	2.78	1.41	1.37
27	s	614	CLA	C1D-ND	2.78	1.41	1.37
27	Y	612	CLA	MG-NB	-2.78	2.00	2.05
27	C	513	CLA	C1D-ND	2.78	1.41	1.37
27	c	513	CLA	C1D-ND	2.78	1.41	1.37
27	g	611	CLA	C4B-NB	2.78	1.41	1.37
27	B	617	CLA	C1D-ND	2.78	1.41	1.37
32	C	520	DGD	O2G-C2G	-2.78	1.40	1.46
27	B	604	CLA	CMB-C2B	-2.78	1.45	1.50
28	A	408	PHO	CMD-C2D	-2.78	1.46	1.51
27	C	512	CLA	MG-NB	-2.78	2.00	2.05
27	c	512	CLA	MG-NB	-2.78	2.00	2.05
32	c	518	DGD	O5D-C6D	-2.78	1.38	1.43
27	C	508	CLA	C1D-ND	2.78	1.41	1.37
27	G	612	CLA	C4B-NB	2.78	1.41	1.37
37	r	606	CHL	CBD-CGD	-2.78	1.49	1.52
32	c	520	DGD	O2G-C2G	-2.77	1.40	1.46
27	y	604	CLA	C1D-ND	2.77	1.41	1.37
27	C	502	CLA	MG-NB	-2.77	2.00	2.05
27	S	602	CLA	C4B-NB	2.77	1.41	1.37
27	s	602	CLA	C4B-NB	2.77	1.41	1.37
28	A	409	PHO	C4D-CHA	2.77	1.43	1.39
28	a	409	PHO	C4D-CHA	2.77	1.43	1.39
27	d	402	CLA	MG-NB	-2.77	2.00	2.05
27	C	505	CLA	CMD-C2D	-2.77	1.45	1.50
38	Y	1621	LUT	C1-C6	-2.77	1.50	1.53
38	y	1621	LUT	C1-C6	-2.77	1.50	1.53
27	a	406	CLA	C1D-ND	2.77	1.41	1.37
27	B	613	CLA	CMD-C2D	-2.77	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	G	614	CLA	C4B-NB	2.76	1.41	1.37
27	g	614	CLA	C4B-NB	2.76	1.41	1.37
28	A	409	PHO	CMD-C2D	-2.76	1.46	1.51
27	Y	613	CLA	C1D-ND	2.76	1.41	1.37
27	y	613	CLA	C1D-ND	2.76	1.41	1.37
28	a	409	PHO	CMD-C2D	-2.76	1.46	1.51
27	C	503	CLA	MG-NB	-2.76	2.00	2.05
27	c	503	CLA	MG-NB	-2.76	2.00	2.05
27	C	502	CLA	C1D-ND	2.76	1.41	1.37
37	N	605	CHL	CBD-CGD	-2.75	1.49	1.52
27	c	506	CLA	CMB-C2B	-2.75	1.45	1.50
27	R	616	CLA	C4B-NB	2.75	1.41	1.37
27	b	613	CLA	CMD-C2D	-2.75	1.45	1.50
27	b	606	CLA	C1D-ND	2.75	1.41	1.37
27	B	612	CLA	CMB-C2B	-2.75	1.45	1.50
27	B	612	CLA	MG-NB	-2.74	2.00	2.05
27	b	612	CLA	MG-NB	-2.74	2.00	2.05
28	a	408	PHO	CMD-C2D	-2.74	1.46	1.51
27	c	508	CLA	MG-NB	-2.74	2.00	2.05
27	r	616	CLA	C4B-NB	2.74	1.41	1.37
32	C	520	DGD	O5D-C6D	-2.74	1.39	1.43
27	b	614	CLA	C1D-ND	2.74	1.41	1.37
27	Y	612	CLA	C1D-ND	2.73	1.41	1.37
27	n	614	CLA	C4B-NB	2.73	1.41	1.37
27	D	402	CLA	MG-NB	-2.73	2.00	2.05
27	d	403	CLA	MG-NB	-2.73	2.00	2.05
27	B	615	CLA	C1D-ND	2.73	1.41	1.37
27	N	611	CLA	C4B-NB	2.72	1.41	1.37
27	A	407	CLA	MG-NB	-2.72	2.00	2.05
27	a	407	CLA	MG-NB	-2.72	2.00	2.05
27	g	602	CLA	C1D-ND	2.72	1.41	1.37
27	B	614	CLA	C1D-ND	2.72	1.41	1.37
27	N	602	CLA	C4B-NB	2.72	1.41	1.37
27	A	405	CLA	CMD-C2D	-2.72	1.45	1.50
27	c	502	CLA	MG-NB	-2.72	2.00	2.05
32	c	520	DGD	O5D-C6D	-2.72	1.39	1.43
27	b	612	CLA	CMB-C2B	-2.72	1.45	1.50
27	n	603	CLA	C1D-ND	2.72	1.41	1.37
27	b	606	CLA	MG-NB	-2.71	2.00	2.05
27	b	608	CLA	MG-NB	-2.71	2.00	2.05
27	y	612	CLA	C1D-ND	2.71	1.41	1.37
27	G	611	CLA	C4B-NB	2.71	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	R	606	CHL	CBD-CGD	-2.71	1.49	1.52
27	C	508	CLA	MG-NB	-2.71	2.00	2.05
27	S	603	CLA	C1B-C2B	2.71	1.49	1.43
27	g	612	CLA	C4B-NB	2.71	1.41	1.37
27	r	612	CLA	C4B-NB	2.71	1.41	1.37
27	b	615	CLA	MG-NB	-2.70	2.00	2.05
27	y	610	CLA	MG-NB	-2.70	2.00	2.05
27	c	503	CLA	C1D-ND	2.70	1.41	1.37
27	D	403	CLA	MG-NB	-2.70	2.00	2.05
27	b	610	CLA	C1D-ND	2.70	1.41	1.37
27	C	506	CLA	CMB-C2B	-2.70	1.45	1.50
27	s	614	CLA	MG-NB	-2.70	2.00	2.05
27	c	502	CLA	C1D-ND	2.70	1.41	1.37
27	B	606	CLA	C1D-ND	2.70	1.41	1.37
27	a	405	CLA	C1D-ND	2.70	1.41	1.37
27	C	507	CLA	MG-NB	-2.70	2.00	2.05
27	c	508	CLA	CMC-C2C	-2.70	1.45	1.50
27	G	602	CLA	C1D-ND	2.69	1.41	1.37
27	n	611	CLA	C4B-NB	2.69	1.41	1.37
35	n	2630	LHG	O7-C5	-2.69	1.40	1.46
27	N	603	CLA	C1D-ND	2.69	1.41	1.37
27	r	610	CLA	C4B-NB	2.68	1.41	1.37
34	d	405	PL9	C31-C29	-2.68	1.45	1.51
27	s	603	CLA	C1B-C2B	2.68	1.49	1.43
27	B	610	CLA	C1D-ND	2.68	1.41	1.37
27	A	406	CLA	CMD-C2D	-2.68	1.45	1.50
27	C	513	CLA	MG-NB	-2.68	2.00	2.05
27	c	513	CLA	MG-NB	-2.68	2.00	2.05
27	a	405	CLA	CMD-C2D	-2.68	1.45	1.50
27	S	614	CLA	MG-NB	-2.68	2.00	2.05
27	G	603	CLA	C4B-NB	2.68	1.41	1.37
27	G	613	CLA	C4B-NB	2.68	1.41	1.37
27	g	603	CLA	C4B-NB	2.68	1.41	1.37
27	g	613	CLA	C4B-NB	2.68	1.41	1.37
27	a	406	CLA	CMD-C2D	-2.67	1.45	1.50
27	B	608	CLA	MG-NB	-2.67	2.00	2.05
27	A	406	CLA	C1D-ND	2.67	1.41	1.37
27	c	506	CLA	C1D-ND	2.67	1.41	1.37
27	B	605	CLA	C1D-ND	2.67	1.41	1.37
27	b	605	CLA	C1D-ND	2.67	1.41	1.37
27	C	512	CLA	C1D-ND	2.67	1.41	1.37
27	c	512	CLA	C1D-ND	2.67	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	N	2630	LHG	O7-C5	-2.67	1.40	1.46
27	G	613	CLA	MG-NB	-2.66	2.00	2.05
27	g	613	CLA	MG-NB	-2.66	2.00	2.05
27	B	615	CLA	MG-NB	-2.66	2.00	2.05
27	B	607	CLA	C1D-ND	2.66	1.41	1.37
27	C	506	CLA	C1D-ND	2.66	1.41	1.37
27	G	610	CLA	C4B-NB	2.66	1.41	1.37
27	s	602	CLA	C1B-C2B	2.66	1.49	1.43
27	B	606	CLA	C4B-NB	2.66	1.41	1.37
27	C	503	CLA	C1D-ND	2.66	1.41	1.37
27	B	606	CLA	MG-NB	-2.65	2.00	2.05
27	C	507	CLA	C1D-ND	2.65	1.41	1.37
27	C	508	CLA	CMC-C2C	-2.65	1.45	1.50
34	D	405	PL9	C31-C29	-2.65	1.45	1.51
27	c	507	CLA	MG-NB	-2.65	2.00	2.05
27	R	610	CLA	C4B-NB	2.65	1.41	1.37
27	g	610	CLA	C4B-NB	2.65	1.41	1.37
27	Y	610	CLA	MG-NB	-2.65	2.00	2.05
27	b	607	CLA	C1D-ND	2.65	1.41	1.37
27	N	612	CLA	C4B-NB	2.64	1.41	1.37
27	R	613	CLA	C4B-NB	2.64	1.41	1.37
31	D	411	LMG	O7-C8	-2.64	1.40	1.46
31	d	411	LMG	O7-C8	-2.64	1.40	1.46
27	N	614	CLA	C4B-NB	2.64	1.41	1.37
27	B	605	CLA	MG-NB	-2.64	2.00	2.05
27	b	605	CLA	MG-NB	-2.64	2.00	2.05
27	S	602	CLA	C1B-C2B	2.64	1.49	1.43
37	G	606	CHL	CBD-CGD	-2.64	1.49	1.52
27	R	612	CLA	C4B-NB	2.64	1.41	1.37
27	N	602	CLA	C1B-C2B	2.64	1.49	1.43
27	n	602	CLA	C1B-C2B	2.64	1.49	1.43
27	a	407	CLA	C1D-ND	2.63	1.41	1.37
27	C	510	CLA	C1D-ND	2.63	1.41	1.37
27	n	612	CLA	C4B-NB	2.63	1.41	1.37
27	N	603	CLA	C4B-NB	2.63	1.41	1.37
27	n	603	CLA	C4B-NB	2.63	1.41	1.37
27	c	507	CLA	C1D-ND	2.63	1.41	1.37
27	b	603	CLA	C1D-ND	2.63	1.41	1.37
27	B	603	CLA	C1D-ND	2.63	1.41	1.37
27	B	609	CLA	MG-NB	-2.63	2.00	2.05
27	G	610	CLA	C1B-C2B	2.62	1.49	1.43
27	A	405	CLA	C1D-ND	2.62	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	604	CLA	MG-NB	-2.62	2.00	2.05
27	n	604	CLA	MG-NB	-2.62	2.00	2.05
27	b	616	CLA	C1D-ND	2.62	1.41	1.37
29	c	515	BCR	C30-C25	-2.62	1.50	1.53
32	h	102	DGD	O2G-C2G	-2.61	1.40	1.46
27	s	612	CLA	C4B-NB	2.61	1.41	1.37
27	Y	610	CLA	CMB-C2B	-2.61	1.45	1.50
27	a	406	CLA	MG-NB	-2.61	2.00	2.05
27	B	617	CLA	CMD-C2D	-2.61	1.45	1.50
27	b	617	CLA	CMD-C2D	-2.61	1.45	1.50
29	C	515	BCR	C30-C25	-2.61	1.50	1.53
35	S	2630	LHG	O7-C5	-2.61	1.40	1.46
32	c	520	DGD	O6D-C5D	-2.61	1.38	1.44
27	c	513	CLA	CMC-C2C	-2.61	1.45	1.50
27	B	602	CLA	C4B-NB	2.61	1.41	1.37
27	b	602	CLA	C4B-NB	2.61	1.41	1.37
27	b	602	CLA	MG-NB	-2.60	2.00	2.05
37	g	606	CHL	CBD-CGD	-2.60	1.49	1.52
27	r	613	CLA	C1B-C2B	2.60	1.49	1.43
27	N	610	CLA	MG-NB	-2.60	2.00	2.05
27	R	604	CLA	C4B-NB	2.60	1.41	1.37
27	R	602	CLA	MG-NB	-2.60	2.00	2.05
27	c	510	CLA	C1D-ND	2.60	1.41	1.37
27	C	511	CLA	MG-NB	-2.60	2.00	2.05
27	c	511	CLA	MG-NB	-2.60	2.00	2.05
27	g	610	CLA	C1B-C2B	2.60	1.49	1.43
27	N	604	CLA	C1D-ND	2.60	1.41	1.37
27	y	602	CLA	MG-NB	-2.60	2.00	2.05
32	H	102	DGD	O2G-C2G	-2.60	1.40	1.46
27	y	603	CLA	C4B-NB	2.60	1.41	1.37
27	y	610	CLA	CMB-C2B	-2.60	1.45	1.50
27	Y	604	CLA	MG-NB	-2.60	2.00	2.05
28	A	409	PHO	CMB-C2B	-2.59	1.46	1.51
27	G	604	CLA	MG-NB	-2.59	2.00	2.05
27	g	604	CLA	MG-NB	-2.59	2.00	2.05
27	n	604	CLA	C1D-ND	2.59	1.41	1.37
27	r	613	CLA	C4B-NB	2.59	1.41	1.37
27	r	616	CLA	C1B-C2B	2.59	1.49	1.43
27	A	407	CLA	C1D-ND	2.59	1.41	1.37
27	Y	604	CLA	CMB-C2B	-2.59	1.45	1.50
27	C	513	CLA	CMC-C2C	-2.59	1.45	1.50
27	N	612	CLA	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	n	612	CLA	C1B-C2B	2.59	1.49	1.43
27	Y	603	CLA	C4B-NB	2.59	1.41	1.37
27	b	607	CLA	MG-NB	-2.59	2.00	2.05
32	C	520	DGD	O6D-C5D	-2.59	1.38	1.44
27	G	602	CLA	CMD-C2D	-2.59	1.45	1.50
27	Y	602	CLA	MG-NB	-2.59	2.00	2.05
27	b	609	CLA	MG-NB	-2.59	2.00	2.05
27	b	606	CLA	C4B-NB	2.59	1.41	1.37
27	r	602	CLA	C1B-C2B	2.59	1.49	1.43
38	N	1621	LUT	C1-C6	-2.59	1.50	1.53
27	N	604	CLA	C4B-NB	2.58	1.41	1.37
27	R	609	CLA	C4B-NB	2.58	1.41	1.37
27	r	609	CLA	C4B-NB	2.58	1.41	1.37
27	y	604	CLA	CMB-C2B	-2.58	1.45	1.50
27	r	603	CLA	C4B-NB	2.58	1.41	1.37
28	A	408	PHO	CBD-CGD	-2.58	1.49	1.52
28	a	408	PHO	CBD-CGD	-2.58	1.49	1.52
27	D	403	CLA	C1D-ND	2.58	1.41	1.37
27	d	403	CLA	C1D-ND	2.58	1.41	1.37
28	A	409	PHO	C4D-ND	-2.58	1.34	1.38
27	g	602	CLA	CMD-C2D	-2.58	1.45	1.50
27	B	616	CLA	C1D-ND	2.57	1.41	1.37
35	s	2630	LHG	O7-C5	-2.57	1.40	1.46
27	s	604	CLA	C1B-C2B	2.57	1.49	1.43
27	G	604	CLA	C4B-NB	2.57	1.41	1.37
27	g	604	CLA	C4B-NB	2.57	1.41	1.37
28	a	409	PHO	CMB-C2B	-2.57	1.46	1.51
27	r	602	CLA	MG-NB	-2.57	2.00	2.05
27	Y	614	CLA	C1D-ND	2.57	1.41	1.37
28	a	409	PHO	C4D-ND	-2.57	1.34	1.38
27	R	616	CLA	C1B-C2B	2.57	1.49	1.43
31	B	622	LMG	O7-C8	-2.57	1.40	1.46
31	b	622	LMG	O7-C8	-2.57	1.40	1.46
27	R	613	CLA	C1B-C2B	2.57	1.49	1.43
27	S	612	CLA	C4B-NB	2.57	1.41	1.37
27	y	614	CLA	C1D-ND	2.57	1.41	1.37
27	R	602	CLA	C1B-C2B	2.57	1.49	1.43
27	A	410	CLA	CMD-C2D	-2.57	1.45	1.50
27	a	410	CLA	CMD-C2D	-2.57	1.45	1.50
27	B	607	CLA	MG-NB	-2.56	2.00	2.05
27	s	603	CLA	C4B-NB	2.56	1.41	1.37
27	y	614	CLA	MG-NB	-2.56	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	602	CLA	MG-NB	-2.56	2.00	2.05
27	C	501	CLA	CMD-C2D	-2.56	1.45	1.50
27	c	501	CLA	CMD-C2D	-2.56	1.45	1.50
27	B	617	CLA	CMC-C2C	-2.56	1.45	1.50
27	n	610	CLA	MG-NB	-2.56	2.00	2.05
27	B	617	CLA	MG-NB	-2.56	2.00	2.05
27	b	617	CLA	MG-NB	-2.56	2.00	2.05
27	A	407	CLA	CMD-C2D	-2.56	1.45	1.50
27	s	610	CLA	C4B-NB	2.56	1.41	1.37
27	R	610	CLA	C1B-C2B	2.56	1.49	1.43
27	r	610	CLA	C1B-C2B	2.56	1.49	1.43
27	A	406	CLA	MG-NB	-2.56	2.00	2.05
27	B	611	CLA	C1D-ND	2.55	1.41	1.37
27	b	611	CLA	C1D-ND	2.55	1.41	1.37
28	a	408	PHO	C4D-CHA	2.55	1.43	1.39
27	Y	602	CLA	CMD-C2D	-2.55	1.45	1.50
27	y	604	CLA	MG-NB	-2.55	2.00	2.05
27	B	616	CLA	MG-NB	-2.55	2.00	2.05
27	B	617	CLA	C4B-NB	2.55	1.41	1.37
27	b	617	CLA	C4B-NB	2.55	1.41	1.37
27	N	613	CLA	C1B-C2B	2.55	1.49	1.43
27	G	604	CLA	C1B-C2B	2.54	1.49	1.43
27	g	604	CLA	C1B-C2B	2.54	1.49	1.43
27	Y	611	CLA	C1B-C2B	2.54	1.49	1.43
27	S	603	CLA	C4B-NB	2.54	1.41	1.37
27	b	617	CLA	CMC-C2C	-2.54	1.45	1.50
27	B	602	CLA	C1B-C2B	2.54	1.49	1.43
27	b	602	CLA	C1B-C2B	2.54	1.49	1.43
27	S	604	CLA	C1B-C2B	2.54	1.49	1.43
27	B	605	CLA	CMB-C2B	-2.54	1.45	1.50
27	b	605	CLA	CMB-C2B	-2.54	1.45	1.50
27	Y	611	CLA	MG-NB	-2.54	2.00	2.05
38	N	1621	LUT	C22-C21	-2.54	1.51	1.54
27	D	402	CLA	MG-ND	-2.53	2.00	2.05
27	d	402	CLA	MG-ND	-2.53	2.00	2.05
27	A	410	CLA	CMB-C2B	-2.53	1.45	1.50
27	a	410	CLA	CMB-C2B	-2.53	1.45	1.50
27	r	604	CLA	C4B-NB	2.53	1.41	1.37
27	S	612	CLA	C1B-C2B	2.53	1.49	1.43
27	s	612	CLA	C1B-C2B	2.53	1.49	1.43
37	S	608	CHL	CBD-CGD	-2.53	1.49	1.52
27	S	613	CLA	MG-NB	-2.53	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	601	CLA	C1B-C2B	2.53	1.49	1.43
27	C	505	CLA	C1D-ND	2.53	1.41	1.37
27	Y	614	CLA	MG-NB	-2.53	2.00	2.05
27	a	407	CLA	CMD-C2D	-2.53	1.45	1.50
27	y	611	CLA	C1B-C2B	2.53	1.49	1.43
38	y	1621	LUT	C22-C21	-2.53	1.51	1.54
27	y	602	CLA	CMD-C2D	-2.53	1.45	1.50
27	b	606	CLA	CMB-C2B	-2.53	1.45	1.50
38	Y	1621	LUT	C22-C21	-2.52	1.51	1.54
27	B	605	CLA	C1B-C2B	2.52	1.49	1.43
27	b	605	CLA	C1B-C2B	2.52	1.49	1.43
27	n	613	CLA	C1B-C2B	2.52	1.49	1.43
29	C	517	BCR	C1-C6	-2.52	1.50	1.53
27	y	611	CLA	MG-NB	-2.52	2.00	2.05
31	A	413	LMG	O8-C9	-2.52	1.39	1.45
27	S	610	CLA	C4B-NB	2.52	1.41	1.37
27	C	507	CLA	CMB-C2B	-2.52	1.45	1.50
27	y	603	CLA	MG-NB	-2.52	2.00	2.05
27	r	601	CLA	C1B-C2B	2.52	1.49	1.43
27	a	405	CLA	CMC-C2C	-2.51	1.45	1.50
27	G	610	CLA	MG-NB	-2.51	2.00	2.05
27	S	614	CLA	CMD-C2D	-2.51	1.45	1.50
27	s	614	CLA	CMD-C2D	-2.51	1.45	1.50
27	n	613	CLA	C4B-NB	2.51	1.41	1.37
27	b	613	CLA	CMC-C2C	-2.51	1.45	1.50
27	R	603	CLA	C4B-NB	2.51	1.41	1.37
27	n	604	CLA	C4B-NB	2.51	1.41	1.37
38	n	1621	LUT	C1-C6	-2.51	1.50	1.53
28	A	408	PHO	C3B-C2B	-2.51	1.37	1.40
28	a	408	PHO	C3B-C2B	-2.51	1.37	1.40
27	n	613	CLA	MG-NB	-2.51	2.00	2.05
27	n	611	CLA	C1B-C2B	2.51	1.49	1.43
27	r	612	CLA	C1B-C2B	2.51	1.49	1.43
27	S	614	CLA	C1B-C2B	2.51	1.49	1.43
27	s	614	CLA	C1B-C2B	2.51	1.49	1.43
27	y	611	CLA	C4B-NB	2.51	1.41	1.37
31	a	413	LMG	O8-C9	-2.51	1.39	1.45
27	B	606	CLA	CMC-C2C	-2.51	1.45	1.50
27	b	606	CLA	CMC-C2C	-2.51	1.45	1.50
27	N	613	CLA	MG-NB	-2.50	2.00	2.05
27	R	602	CLA	C4B-NB	2.50	1.41	1.37
27	N	612	CLA	MG-NB	-2.50	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	n	612	CLA	MG-NB	-2.50	2.00	2.05
27	S	609	CLA	C1B-C2B	2.50	1.49	1.43
27	s	609	CLA	C1B-C2B	2.50	1.49	1.43
27	r	602	CLA	C4B-NB	2.50	1.41	1.37
27	B	603	CLA	MG-ND	-2.50	2.00	2.05
27	b	603	CLA	MG-ND	-2.50	2.00	2.05
27	R	612	CLA	MG-NB	-2.50	2.00	2.05
27	r	612	CLA	MG-NB	-2.50	2.00	2.05
27	s	613	CLA	MG-NB	-2.50	2.00	2.05
27	c	513	CLA	MG-ND	-2.50	2.00	2.05
27	b	616	CLA	MG-NB	-2.50	2.00	2.05
39	n	1622	XAT	O4-C5	-2.50	1.43	1.46
27	Y	611	CLA	C4B-NB	2.50	1.41	1.37
27	c	507	CLA	CMB-C2B	-2.50	1.45	1.50
27	c	509	CLA	CMD-C2D	-2.49	1.45	1.50
38	n	1621	LUT	C22-C21	-2.49	1.51	1.54
27	c	509	CLA	CMB-C2B	-2.49	1.45	1.50
27	g	611	CLA	MG-NB	-2.49	2.00	2.05
27	c	505	CLA	C1D-ND	2.49	1.41	1.37
27	c	506	CLA	CMD-C2D	-2.49	1.45	1.50
27	S	611	CLA	C4B-NB	2.49	1.41	1.37
27	s	611	CLA	C4B-NB	2.49	1.41	1.37
27	y	610	CLA	C4B-NB	2.49	1.41	1.37
28	A	408	PHO	C4D-CHA	2.49	1.43	1.39
27	R	604	CLA	MG-NB	-2.49	2.00	2.05
32	h	102	DGD	O5D-C6D	-2.49	1.39	1.43
27	A	405	CLA	CMC-C2C	-2.49	1.45	1.50
27	C	509	CLA	CMD-C2D	-2.49	1.45	1.50
27	G	613	CLA	C1B-C2B	2.49	1.49	1.43
27	N	611	CLA	C1B-C2B	2.49	1.49	1.43
27	g	613	CLA	C1B-C2B	2.49	1.49	1.43
27	C	511	CLA	CMD-C2D	-2.48	1.45	1.50
27	c	504	CLA	MG-NB	-2.48	2.00	2.05
27	B	612	CLA	C1D-ND	2.48	1.41	1.37
27	b	612	CLA	C1D-ND	2.48	1.41	1.37
27	C	513	CLA	MG-ND	-2.48	2.00	2.05
27	B	604	CLA	MG-ND	-2.48	2.00	2.05
27	R	611	CLA	C1B-C2B	2.48	1.48	1.43
27	r	611	CLA	C1B-C2B	2.48	1.48	1.43
27	B	613	CLA	CMC-C2C	-2.48	1.45	1.50
27	C	507	CLA	CMD-C2D	-2.47	1.45	1.50
37	S	606	CHL	CBD-CGD	-2.47	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	513	CLA	CMD-C2D	-2.47	1.45	1.50
27	b	607	CLA	CMC-C2C	-2.47	1.45	1.50
27	c	513	CLA	CMD-C2D	-2.47	1.45	1.50
27	R	612	CLA	C1B-C2B	2.47	1.48	1.43
27	Y	603	CLA	MG-NB	-2.47	2.00	2.05
27	B	604	CLA	CMD-C2D	-2.47	1.45	1.50
27	b	604	CLA	CMD-C2D	-2.47	1.45	1.50
27	C	504	CLA	MG-NB	-2.47	2.00	2.05
27	C	505	CLA	MG-ND	-2.47	2.00	2.05
27	c	505	CLA	MG-ND	-2.47	2.00	2.05
27	g	611	CLA	C1B-C2B	2.47	1.48	1.43
27	g	610	CLA	MG-NB	-2.47	2.00	2.05
27	R	603	CLA	MG-NB	-2.47	2.00	2.05
27	r	603	CLA	MG-NB	-2.47	2.00	2.05
27	C	504	CLA	CMD-C2D	-2.47	1.45	1.50
27	A	410	CLA	C1D-ND	2.47	1.41	1.37
27	a	410	CLA	C1D-ND	2.47	1.41	1.37
27	N	602	CLA	MG-NB	-2.47	2.00	2.05
27	n	602	CLA	MG-NB	-2.47	2.00	2.05
29	c	517	BCR	C1-C6	-2.47	1.50	1.53
27	S	612	CLA	MG-NB	-2.47	2.00	2.05
29	C	514	BCR	C30-C25	-2.46	1.50	1.53
39	N	1622	XAT	O4-C5	-2.46	1.43	1.46
27	Y	610	CLA	C4B-NB	2.46	1.41	1.37
37	s	608	CHL	CBD-CGD	-2.46	1.49	1.52
27	R	604	CLA	C1B-C2B	2.46	1.48	1.43
27	s	602	CLA	CMD-C2D	-2.46	1.45	1.50
27	C	501	CLA	MG-NB	-2.46	2.00	2.05
27	c	501	CLA	MG-NB	-2.46	2.00	2.05
27	N	613	CLA	C4B-NB	2.46	1.41	1.37
27	b	607	CLA	CMD-C2D	-2.46	1.45	1.50
27	B	606	CLA	CMB-C2B	-2.46	1.45	1.50
27	G	612	CLA	MG-NB	-2.46	2.00	2.05
27	y	602	CLA	C1B-C2B	2.46	1.48	1.43
27	n	610	CLA	C4B-NB	2.46	1.41	1.37
27	s	610	CLA	MG-NB	-2.46	2.00	2.05
27	C	501	CLA	C4B-NB	2.46	1.41	1.37
27	c	501	CLA	C4B-NB	2.46	1.41	1.37
37	N	605	CHL	CHA-CBD	-2.46	1.48	1.51
27	c	507	CLA	C1B-NB	-2.45	1.34	1.37
27	G	603	CLA	C1B-C2B	2.45	1.48	1.43
27	B	613	CLA	C1D-ND	2.45	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	409	PHO	C3B-C2B	-2.45	1.37	1.40
32	c	519	DGD	O1G-C1G	-2.45	1.39	1.45
27	Y	602	CLA	C1B-C2B	2.45	1.48	1.43
27	g	603	CLA	C1B-C2B	2.45	1.48	1.43
32	H	102	DGD	O5D-C6D	-2.45	1.39	1.43
27	D	402	CLA	CMB-C2B	-2.45	1.45	1.50
27	b	614	CLA	CMC-C2C	-2.45	1.45	1.50
27	d	402	CLA	CMB-C2B	-2.45	1.45	1.50
27	C	508	CLA	CMD-C2D	-2.45	1.45	1.50
27	c	508	CLA	CMD-C2D	-2.45	1.45	1.50
27	B	609	CLA	CMD-C2D	-2.45	1.45	1.50
27	B	614	CLA	CMB-C2B	-2.45	1.45	1.50
27	r	610	CLA	MG-NB	-2.45	2.00	2.05
27	B	603	CLA	C1B-C2B	2.45	1.48	1.43
27	C	509	CLA	CMB-C2B	-2.45	1.45	1.50
39	G	1622	XAT	O4-C5	-2.45	1.43	1.46
29	b	620	BCR	C30-C25	-2.45	1.50	1.53
27	C	504	CLA	CMB-C2B	-2.45	1.45	1.50
27	c	504	CLA	CMB-C2B	-2.45	1.45	1.50
27	r	604	CLA	MG-NB	-2.45	2.00	2.05
27	C	506	CLA	CMD-C2D	-2.45	1.45	1.50
27	g	602	CLA	C1B-C2B	2.45	1.48	1.43
27	r	604	CLA	C1B-C2B	2.45	1.48	1.43
27	b	616	CLA	CMD-C2D	-2.44	1.45	1.50
27	c	511	CLA	CMD-C2D	-2.44	1.45	1.50
32	C	519	DGD	O1G-C1G	-2.44	1.39	1.45
27	S	610	CLA	MG-NB	-2.44	2.00	2.05
29	B	620	BCR	C30-C25	-2.44	1.50	1.53
27	s	612	CLA	MG-NB	-2.44	2.00	2.05
27	b	603	CLA	C1B-C2B	2.44	1.48	1.43
27	c	504	CLA	CMD-C2D	-2.44	1.45	1.50
27	n	604	CLA	CMB-C2B	-2.44	1.45	1.50
27	G	611	CLA	C1B-C2B	2.44	1.48	1.43
37	G	607	CHL	CBD-CGD	-2.44	1.49	1.52
29	a	411	BCR	C1-C6	-2.44	1.50	1.53
27	b	613	CLA	C1D-ND	2.44	1.41	1.37
27	y	613	CLA	CMB-C2B	-2.44	1.45	1.50
27	S	614	CLA	C4B-NB	2.44	1.41	1.37
37	g	607	CHL	CBD-CGD	-2.44	1.49	1.52
27	N	614	CLA	C1B-C2B	2.44	1.48	1.43
27	n	614	CLA	C1B-C2B	2.44	1.48	1.43
27	c	510	CLA	CMD-C2D	-2.44	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	n	610	CLA	CMB-C2B	-2.44	1.45	1.50
27	C	507	CLA	C1B-NB	-2.44	1.34	1.37
27	B	607	CLA	CMC-C2C	-2.44	1.45	1.50
27	Y	604	CLA	C4B-NB	2.44	1.41	1.37
27	C	502	CLA	CMB-C2B	-2.44	1.45	1.50
27	c	508	CLA	C1B-NB	-2.44	1.34	1.37
38	G	1620	LUT	C1-C6	-2.43	1.50	1.53
38	g	1620	LUT	C1-C6	-2.43	1.50	1.53
27	C	507	CLA	MG-ND	-2.43	2.01	2.05
27	S	602	CLA	MG-NB	-2.43	2.01	2.05
27	c	507	CLA	MG-ND	-2.43	2.01	2.05
27	b	614	CLA	CMB-C2B	-2.43	1.45	1.50
39	g	1622	XAT	O4-C5	-2.43	1.43	1.46
28	a	409	PHO	C3B-C2B	-2.43	1.37	1.40
27	b	604	CLA	MG-ND	-2.43	2.01	2.05
27	c	507	CLA	CMD-C2D	-2.43	1.45	1.50
27	g	612	CLA	MG-NB	-2.43	2.01	2.05
27	s	614	CLA	C4B-NB	2.43	1.41	1.37
27	b	609	CLA	CMD-C2D	-2.43	1.45	1.50
27	a	407	CLA	MG-ND	-2.43	2.01	2.05
27	Y	610	CLA	CMC-C2C	-2.43	1.45	1.50
27	y	610	CLA	CMC-C2C	-2.43	1.45	1.50
27	s	613	CLA	C4B-NB	2.43	1.41	1.37
27	G	611	CLA	MG-NB	-2.43	2.01	2.05
27	D	402	CLA	C1B-C2B	2.43	1.48	1.43
27	d	402	CLA	C1B-C2B	2.43	1.48	1.43
37	R	607	CHL	CHA-CBD	-2.42	1.48	1.51
27	B	614	CLA	CMD-C2D	-2.42	1.45	1.50
27	b	614	CLA	CMD-C2D	-2.42	1.45	1.50
27	g	612	CLA	C1B-C2B	2.42	1.48	1.43
27	a	407	CLA	CMB-C2B	-2.42	1.45	1.50
29	h	101	BCR	C1-C6	-2.42	1.50	1.53
27	B	614	CLA	CMC-C2C	-2.42	1.45	1.50
27	s	602	CLA	MG-NB	-2.42	2.01	2.05
29	c	514	BCR	C30-C25	-2.42	1.50	1.53
27	G	602	CLA	C1B-C2B	2.42	1.48	1.43
27	D	403	CLA	CMD-C2D	-2.42	1.45	1.50
27	c	511	CLA	CMC-C2C	-2.42	1.45	1.50
27	B	604	CLA	CMC-C2C	-2.42	1.45	1.50
27	c	502	CLA	CMB-C2B	-2.42	1.45	1.50
27	b	614	CLA	MG-ND	-2.42	2.01	2.05
27	y	614	CLA	C1B-C2B	2.42	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	607	CLA	CMD-C2D	-2.41	1.45	1.50
27	A	406	CLA	C1B-C2B	2.41	1.48	1.43
27	S	602	CLA	CMD-C2D	-2.41	1.45	1.50
27	B	616	CLA	CMD-C2D	-2.41	1.45	1.50
27	N	603	CLA	MG-NB	-2.41	2.01	2.05
27	B	605	CLA	C4B-NB	2.41	1.41	1.37
27	S	613	CLA	C4B-NB	2.41	1.41	1.37
27	b	605	CLA	C4B-NB	2.41	1.41	1.37
37	r	607	CHL	CHA-CBD	-2.41	1.48	1.51
29	C	517	BCR	C30-C25	-2.41	1.50	1.53
27	b	615	CLA	CMB-C2B	-2.41	1.45	1.50
27	C	512	CLA	CMD-C2D	-2.41	1.45	1.50
29	A	411	BCR	C1-C6	-2.41	1.50	1.53
27	B	610	CLA	CMD-C2D	-2.41	1.45	1.50
27	G	612	CLA	C1B-C2B	2.41	1.48	1.43
37	n	605	CHL	CHA-CBD	-2.41	1.48	1.51
27	n	603	CLA	MG-NB	-2.41	2.01	2.05
27	N	610	CLA	C4B-NB	2.41	1.41	1.37
29	c	517	BCR	C30-C25	-2.41	1.50	1.53
27	b	610	CLA	CMD-C2D	-2.40	1.45	1.50
27	N	603	CLA	C1B-C2B	2.40	1.48	1.43
27	n	603	CLA	C1B-C2B	2.40	1.48	1.43
27	C	501	CLA	CMB-C2B	-2.40	1.45	1.50
27	N	604	CLA	CMB-C2B	-2.40	1.45	1.50
27	N	610	CLA	CMB-C2B	-2.40	1.45	1.50
27	b	611	CLA	CMD-C2D	-2.40	1.45	1.50
27	c	501	CLA	CMB-C2B	-2.40	1.45	1.50
31	D	411	LMG	O8-C9	-2.40	1.39	1.45
31	d	411	LMG	O8-C9	-2.40	1.39	1.45
37	G	609	CHL	CHA-CBD	-2.40	1.48	1.51
37	g	609	CHL	CHA-CBD	-2.40	1.48	1.51
27	Y	602	CLA	CMC-C2C	-2.40	1.45	1.50
27	g	602	CLA	C4B-NB	2.40	1.41	1.37
27	B	615	CLA	CMB-C2B	-2.40	1.45	1.50
27	Y	602	CLA	CMB-C2B	-2.40	1.45	1.50
27	S	611	CLA	MG-NB	-2.40	2.01	2.05
27	s	611	CLA	MG-NB	-2.40	2.01	2.05
27	s	610	CLA	C1B-C2B	2.40	1.48	1.43
27	Y	603	CLA	CMD-C2D	-2.40	1.45	1.50
38	S	1620	LUT	C1-C6	-2.40	1.50	1.53
38	s	1620	LUT	C1-C6	-2.40	1.50	1.53
27	n	610	CLA	CMD-C2D	-2.40	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	G	614	CLA	C1B-C2B	2.40	1.48	1.43
27	g	614	CLA	C1B-C2B	2.40	1.48	1.43
27	a	407	CLA	C1B-NB	-2.40	1.34	1.37
27	c	503	CLA	CMB-C2B	-2.39	1.45	1.50
27	s	604	CLA	CMB-C2B	-2.39	1.45	1.50
27	R	610	CLA	MG-NB	-2.39	2.01	2.05
27	b	605	CLA	CMC-C2C	-2.39	1.45	1.50
32	c	519	DGD	O6D-C5D	-2.39	1.38	1.44
27	C	511	CLA	CMC-C2C	-2.39	1.45	1.50
27	N	604	CLA	C1B-C2B	2.39	1.48	1.43
27	B	605	CLA	MG-ND	-2.39	2.01	2.05
27	b	605	CLA	MG-ND	-2.39	2.01	2.05
27	B	605	CLA	CMC-C2C	-2.39	1.45	1.50
32	C	519	DGD	O6D-C5D	-2.39	1.38	1.44
27	B	605	CLA	CMD-C2D	-2.39	1.45	1.50
27	b	605	CLA	CMD-C2D	-2.39	1.45	1.50
27	a	405	CLA	CMB-C2B	-2.39	1.45	1.50
27	y	614	CLA	CMD-C2D	-2.39	1.45	1.50
37	s	607	CHL	CBD-CGD	-2.39	1.49	1.52
27	y	602	CLA	CMB-C2B	-2.39	1.45	1.50
27	S	613	CLA	C1B-C2B	2.39	1.48	1.43
27	C	508	CLA	C1B-NB	-2.39	1.34	1.37
27	A	407	CLA	MG-ND	-2.38	2.01	2.05
27	B	615	CLA	C1B-C2B	2.38	1.48	1.43
27	y	602	CLA	CMC-C2C	-2.38	1.45	1.50
27	B	604	CLA	C1D-ND	2.38	1.41	1.37
27	b	604	CLA	C1D-ND	2.38	1.41	1.37
27	S	604	CLA	CMB-C2B	-2.38	1.45	1.50
27	b	611	CLA	CMB-C2B	-2.38	1.45	1.50
29	b	618	BCR	C30-C25	-2.38	1.50	1.53
27	Y	613	CLA	CMB-C2B	-2.38	1.45	1.50
27	A	405	CLA	C1B-C2B	2.38	1.48	1.43
27	a	405	CLA	C1B-C2B	2.38	1.48	1.43
27	B	615	CLA	CMD-C2D	-2.38	1.45	1.50
27	Y	612	CLA	CMD-C2D	-2.38	1.45	1.50
27	b	615	CLA	CMD-C2D	-2.38	1.45	1.50
27	y	612	CLA	CMD-C2D	-2.38	1.45	1.50
27	n	610	CLA	C1B-C2B	2.38	1.48	1.43
27	Y	614	CLA	CMD-C2D	-2.38	1.45	1.50
27	b	612	CLA	CMD-C2D	-2.38	1.45	1.50
27	y	612	CLA	MG-ND	-2.38	2.01	2.05
32	C	520	DGD	O1G-C1G	-2.38	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	520	DGD	O1G-C1G	-2.38	1.39	1.45
27	b	604	CLA	CMC-C2C	-2.38	1.45	1.50
27	G	614	CLA	MG-NB	-2.38	2.01	2.05
27	g	614	CLA	MG-NB	-2.38	2.01	2.05
27	Y	614	CLA	C1B-C2B	2.38	1.48	1.43
27	N	610	CLA	CMC-C2C	-2.38	1.45	1.50
27	c	510	CLA	CMB-C2B	-2.38	1.45	1.50
37	G	605	CHL	CBD-CGD	-2.38	1.49	1.52
27	B	611	CLA	CMD-C2D	-2.38	1.45	1.50
27	b	607	CLA	CMB-C2B	-2.38	1.45	1.50
27	c	512	CLA	CMD-C2D	-2.37	1.45	1.50
27	d	402	CLA	CMC-C2C	-2.37	1.45	1.50
27	d	403	CLA	CMD-C2D	-2.37	1.45	1.50
27	B	614	CLA	MG-ND	-2.37	2.01	2.05
27	a	406	CLA	C1B-C2B	2.37	1.48	1.43
27	c	507	CLA	C4B-NB	2.37	1.41	1.37
27	C	510	CLA	CMD-C2D	-2.37	1.45	1.50
37	s	606	CHL	CBD-CGD	-2.37	1.49	1.52
27	B	612	CLA	CMD-C2D	-2.37	1.45	1.50
27	B	613	CLA	CMB-C2B	-2.37	1.45	1.50
27	S	604	CLA	MG-NB	-2.37	2.01	2.05
27	s	604	CLA	MG-NB	-2.37	2.01	2.05
27	b	606	CLA	CMD-C2D	-2.37	1.45	1.50
27	b	610	CLA	CMB-C2B	-2.37	1.45	1.50
27	c	503	CLA	C1B-C2B	2.37	1.48	1.43
27	B	607	CLA	CMB-C2B	-2.37	1.45	1.50
37	S	607	CHL	CBD-CGD	-2.37	1.49	1.52
27	D	402	CLA	CMC-C2C	-2.37	1.45	1.50
27	A	407	CLA	C1B-NB	-2.37	1.34	1.37
27	C	508	CLA	MG-ND	-2.37	2.01	2.05
27	B	616	CLA	CMC-C2C	-2.37	1.45	1.50
27	b	616	CLA	CMC-C2C	-2.37	1.45	1.50
27	s	613	CLA	C1B-C2B	2.37	1.48	1.43
27	Y	612	CLA	MG-ND	-2.37	2.01	2.05
27	A	407	CLA	CMB-C2B	-2.37	1.45	1.50
27	C	509	CLA	C1D-ND	2.37	1.41	1.37
27	c	509	CLA	C1D-ND	2.37	1.41	1.37
27	C	510	CLA	CMB-C2B	-2.36	1.45	1.50
27	B	606	CLA	CMD-C2D	-2.36	1.45	1.50
27	N	611	CLA	MG-NB	-2.36	2.01	2.05
27	n	602	CLA	CMD-C2D	-2.36	1.45	1.50
27	b	615	CLA	C1B-C2B	2.36	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	101	BCR	C1-C6	-2.36	1.50	1.53
34	d	405	PL9	C46-C44	-2.36	1.46	1.51
27	r	602	CLA	CMC-C2C	-2.36	1.45	1.50
27	n	604	CLA	C1B-C2B	2.36	1.48	1.43
27	n	614	CLA	MG-NB	-2.36	2.01	2.05
27	C	513	CLA	C1B-C2B	2.36	1.48	1.43
27	c	513	CLA	C1B-C2B	2.36	1.48	1.43
27	B	612	CLA	C1B-NB	-2.36	1.34	1.37
27	b	612	CLA	C1B-NB	-2.36	1.34	1.37
27	B	611	CLA	MG-ND	-2.36	2.01	2.05
27	b	611	CLA	MG-ND	-2.36	2.01	2.05
27	R	609	CLA	MG-NB	-2.35	2.01	2.05
27	r	609	CLA	MG-NB	-2.35	2.01	2.05
27	b	613	CLA	MG-ND	-2.35	2.01	2.05
27	b	616	CLA	CMB-C2B	-2.35	1.45	1.50
27	N	610	CLA	C1B-C2B	2.35	1.48	1.43
27	C	511	CLA	C4B-NB	2.35	1.41	1.37
27	S	611	CLA	CMD-C2D	-2.35	1.46	1.50
27	s	611	CLA	CMD-C2D	-2.35	1.46	1.50
27	y	603	CLA	CMD-C2D	-2.35	1.46	1.50
27	N	614	CLA	MG-NB	-2.35	2.01	2.05
27	b	613	CLA	CMB-C2B	-2.35	1.46	1.50
27	S	610	CLA	C1B-C2B	2.35	1.48	1.43
27	n	611	CLA	MG-NB	-2.35	2.01	2.05
27	B	616	CLA	C4B-NB	2.35	1.40	1.37
27	b	616	CLA	C4B-NB	2.35	1.40	1.37
27	A	410	CLA	MG-ND	-2.35	2.01	2.05
27	C	504	CLA	C4B-NB	2.35	1.40	1.37
27	c	504	CLA	C4B-NB	2.35	1.40	1.37
29	b	619	BCR	C1-C6	-2.35	1.50	1.53
27	R	602	CLA	CMC-C2C	-2.35	1.46	1.50
27	C	503	CLA	C1B-C2B	2.35	1.48	1.43
39	r	622	XAT	O4-C5	-2.35	1.43	1.46
27	B	616	CLA	CMB-C2B	-2.35	1.46	1.50
27	n	604	CLA	CMD-C2D	-2.35	1.46	1.50
27	g	610	CLA	CMD-C2D	-2.34	1.46	1.50
27	g	612	CLA	CMB-C2B	-2.34	1.46	1.50
27	A	405	CLA	CMB-C2B	-2.34	1.46	1.50
27	c	506	CLA	MG-ND	-2.34	2.01	2.05
27	Y	603	CLA	CMB-C2B	-2.34	1.46	1.50
27	y	604	CLA	C4B-NB	2.34	1.40	1.37
27	Y	603	CLA	C1B-C2B	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	y	603	CLA	C1B-C2B	2.34	1.48	1.43
27	N	610	CLA	CMD-C2D	-2.34	1.46	1.50
27	B	611	CLA	CMB-C2B	-2.34	1.46	1.50
27	a	406	CLA	CMC-C2C	-2.34	1.46	1.50
27	c	508	CLA	MG-ND	-2.34	2.01	2.05
27	y	603	CLA	CMB-C2B	-2.34	1.46	1.50
27	S	604	CLA	C4B-NB	2.34	1.40	1.37
27	s	604	CLA	C4B-NB	2.34	1.40	1.37
27	G	602	CLA	MG-ND	-2.34	2.01	2.05
27	g	602	CLA	MG-ND	-2.34	2.01	2.05
27	R	609	CLA	C1B-C2B	2.34	1.48	1.43
27	r	609	CLA	C1B-C2B	2.34	1.48	1.43
27	c	504	CLA	CMC-C2C	-2.34	1.46	1.50
27	S	609	CLA	MG-NB	-2.34	2.01	2.05
27	B	603	CLA	CMB-C2B	-2.34	1.46	1.50
27	N	602	CLA	CMD-C2D	-2.34	1.46	1.50
27	Y	610	CLA	C1B-C2B	2.34	1.48	1.43
27	N	604	CLA	CMD-C2D	-2.34	1.46	1.50
27	b	615	CLA	CMC-C2C	-2.34	1.46	1.50
27	C	507	CLA	C4B-NB	2.33	1.40	1.37
27	G	610	CLA	CMD-C2D	-2.33	1.46	1.50
27	Y	611	CLA	CMC-C2C	-2.33	1.46	1.50
27	b	602	CLA	CMD-C2D	-2.33	1.46	1.50
27	Y	610	CLA	CMD-C2D	-2.33	1.46	1.50
34	D	405	PL9	C46-C44	-2.33	1.46	1.51
27	R	603	CLA	CMB-C2B	-2.33	1.46	1.50
27	r	603	CLA	CMB-C2B	-2.33	1.46	1.50
27	B	615	CLA	CMC-C2C	-2.33	1.46	1.50
27	b	607	CLA	C4B-NB	2.33	1.40	1.37
27	B	610	CLA	CMB-C2B	-2.33	1.46	1.50
34	D	405	PL9	C21-C19	-2.33	1.46	1.51
27	y	610	CLA	CMD-C2D	-2.33	1.46	1.50
27	G	602	CLA	C4B-NB	2.33	1.40	1.37
27	c	511	CLA	C4B-NB	2.33	1.40	1.37
29	B	618	BCR	C30-C25	-2.33	1.50	1.53
36	F	101	HEM	FE-NA	2.33	2.02	1.95
38	Y	1620	LUT	C22-C21	-2.33	1.51	1.54
27	N	603	CLA	CMD-C2D	-2.33	1.46	1.50
27	a	410	CLA	MG-ND	-2.32	2.01	2.05
27	Y	611	CLA	CMD-C2D	-2.32	1.46	1.50
27	B	610	CLA	C4B-NB	2.32	1.40	1.37
27	b	610	CLA	C4B-NB	2.32	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	512	CLA	MG-ND	-2.32	2.01	2.05
27	R	610	CLA	CMD-C2D	-2.32	1.46	1.50
40	g	1623	NEX	O24-C25	-2.32	1.43	1.46
27	C	503	CLA	CMB-C2B	-2.32	1.46	1.50
27	G	602	CLA	CMC-C2C	-2.32	1.46	1.50
27	g	602	CLA	CMC-C2C	-2.32	1.46	1.50
27	S	609	CLA	C3B-C4B	2.32	1.49	1.42
27	n	610	CLA	CMC-C2C	-2.32	1.46	1.50
27	N	602	CLA	CMB-C2B	-2.32	1.46	1.50
27	n	602	CLA	CMB-C2B	-2.32	1.46	1.50
27	R	616	CLA	MG-NB	-2.32	2.01	2.05
27	A	406	CLA	CMC-C2C	-2.32	1.46	1.50
27	y	613	CLA	MG-ND	-2.32	2.01	2.05
27	B	613	CLA	MG-ND	-2.32	2.01	2.05
27	C	510	CLA	CMC-C2C	-2.31	1.46	1.50
27	Y	604	CLA	CMC-C2C	-2.31	1.46	1.50
27	c	510	CLA	CMC-C2C	-2.31	1.46	1.50
27	R	603	CLA	C3B-C4B	2.31	1.49	1.42
39	R	622	XAT	O4-C5	-2.31	1.43	1.46
27	C	511	CLA	C1B-C2B	2.31	1.48	1.43
27	C	509	CLA	CMC-C2C	-2.31	1.46	1.50
27	c	509	CLA	CMC-C2C	-2.31	1.46	1.50
27	S	611	CLA	C1B-C2B	2.31	1.48	1.43
27	s	611	CLA	C1B-C2B	2.31	1.48	1.43
27	C	506	CLA	MG-ND	-2.31	2.01	2.05
27	B	608	CLA	CMD-C2D	-2.31	1.46	1.50
27	B	603	CLA	CMC-C2C	-2.31	1.46	1.50
27	b	603	CLA	CMC-C2C	-2.31	1.46	1.50
27	s	610	CLA	CMB-C2B	-2.31	1.46	1.50
27	r	603	CLA	C3B-C4B	2.31	1.49	1.42
40	G	1623	NEX	O24-C25	-2.31	1.43	1.46
27	b	603	CLA	CMD-C2D	-2.31	1.46	1.50
27	c	510	CLA	C1B-C2B	2.31	1.48	1.43
36	f	101	HEM	FE-NA	2.31	2.02	1.95
27	y	603	CLA	CMC-C2C	-2.31	1.46	1.50
27	R	609	CLA	C3B-C4B	2.30	1.49	1.42
27	r	609	CLA	C3B-C4B	2.30	1.49	1.42
27	D	403	CLA	MG-ND	-2.30	2.01	2.05
27	d	403	CLA	MG-ND	-2.30	2.01	2.05
27	r	616	CLA	CMD-C2D	-2.30	1.46	1.50
27	G	613	CLA	CMB-C2B	-2.30	1.46	1.50
27	R	609	CLA	CMD-C2D	-2.30	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	g	605	CHL	CBD-CGD	-2.30	1.49	1.52
27	c	509	CLA	MG-ND	-2.30	2.01	2.05
27	B	617	CLA	CMB-C2B	-2.30	1.46	1.50
27	b	617	CLA	CMB-C2B	-2.30	1.46	1.50
27	c	505	CLA	CMC-C2C	-2.30	1.46	1.50
27	B	602	CLA	MG-ND	-2.30	2.01	2.05
29	B	619	BCR	C1-C6	-2.30	1.50	1.53
27	Y	613	CLA	CMD-C2D	-2.30	1.46	1.50
27	c	503	CLA	CMD-C2D	-2.30	1.46	1.50
27	b	608	CLA	CMD-C2D	-2.30	1.46	1.50
27	r	610	CLA	CMD-C2D	-2.30	1.46	1.50
27	s	613	CLA	CMD-C2D	-2.30	1.46	1.50
27	C	510	CLA	C1B-C2B	2.30	1.48	1.43
27	B	602	CLA	CMD-C2D	-2.30	1.46	1.50
27	B	608	CLA	CMB-C2B	-2.30	1.46	1.50
27	G	604	CLA	CMB-C2B	-2.30	1.46	1.50
27	g	604	CLA	CMB-C2B	-2.30	1.46	1.50
34	d	405	PL9	C21-C19	-2.30	1.46	1.51
27	R	613	CLA	MG-NB	-2.30	2.01	2.05
27	n	614	CLA	C3B-C4B	2.30	1.49	1.42
27	y	610	CLA	C1B-C2B	2.29	1.48	1.43
27	s	609	CLA	C3B-C4B	2.29	1.49	1.42
27	C	505	CLA	CMC-C2C	-2.29	1.46	1.50
27	C	512	CLA	CMC-C2C	-2.29	1.46	1.50
27	S	602	CLA	CMC-C2C	-2.29	1.46	1.50
27	y	611	CLA	CMC-C2C	-2.29	1.46	1.50
35	G	2630	LHG	O7-C5	-2.29	1.41	1.46
27	S	613	CLA	CMD-C2D	-2.29	1.46	1.50
27	y	611	CLA	CMD-C2D	-2.29	1.46	1.50
27	R	616	CLA	CMD-C2D	-2.29	1.46	1.50
27	B	609	CLA	CMB-C2B	-2.29	1.46	1.50
27	b	609	CLA	CMB-C2B	-2.29	1.46	1.50
27	B	616	CLA	C1B-C2B	2.29	1.48	1.43
27	y	613	CLA	CMD-C2D	-2.29	1.46	1.50
27	N	614	CLA	C3B-C4B	2.29	1.49	1.42
27	B	608	CLA	C1B-C2B	2.29	1.48	1.43
27	a	407	CLA	C4B-NB	2.29	1.40	1.37
27	b	616	CLA	C1B-C2B	2.29	1.48	1.43
27	B	603	CLA	CMD-C2D	-2.28	1.46	1.50
27	y	614	CLA	CMB-C2B	-2.28	1.46	1.50
29	b	619	BCR	C30-C25	-2.28	1.50	1.53
27	r	613	CLA	MG-NB	-2.28	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	503	CLA	CMC-C2C	-2.28	1.46	1.50
27	n	603	CLA	CMD-C2D	-2.28	1.46	1.50
27	c	511	CLA	CMB-C2B	-2.28	1.46	1.50
27	G	602	CLA	CMB-C2B	-2.28	1.46	1.50
27	g	602	CLA	CMB-C2B	-2.28	1.46	1.50
27	Y	613	CLA	MG-ND	-2.28	2.01	2.05
27	C	505	CLA	CMB-C2B	-2.28	1.46	1.50
27	c	505	CLA	CMB-C2B	-2.28	1.46	1.50
27	G	612	CLA	CMB-C2B	-2.28	1.46	1.50
27	C	503	CLA	CMD-C2D	-2.28	1.46	1.50
27	Y	603	CLA	CMC-C2C	-2.28	1.46	1.50
27	A	410	CLA	CMC-C2C	-2.28	1.46	1.50
27	a	410	CLA	CMC-C2C	-2.28	1.46	1.50
27	B	606	CLA	MG-ND	-2.28	2.01	2.05
27	r	609	CLA	CMD-C2D	-2.28	1.46	1.50
27	y	604	CLA	CMD-C2D	-2.28	1.46	1.50
37	S	601	CHL	CHA-CBD	-2.28	1.49	1.51
27	C	504	CLA	CMC-C2C	-2.28	1.46	1.50
27	g	604	CLA	CMD-C2D	-2.28	1.46	1.50
27	b	603	CLA	CMB-C2B	-2.28	1.46	1.50
27	B	610	CLA	MG-ND	-2.27	2.01	2.05
27	B	602	CLA	CMB-C2B	-2.27	1.46	1.50
27	b	602	CLA	CMB-C2B	-2.27	1.46	1.50
27	c	512	CLA	MG-ND	-2.27	2.01	2.05
27	R	610	CLA	CMC-C2C	-2.27	1.46	1.50
27	r	610	CLA	CMC-C2C	-2.27	1.46	1.50
27	b	616	CLA	C1B-NB	-2.27	1.34	1.37
27	B	607	CLA	C4B-NB	2.27	1.40	1.37
27	C	503	CLA	C4B-NB	2.27	1.40	1.37
27	c	503	CLA	C4B-NB	2.27	1.40	1.37
27	c	511	CLA	C1B-C2B	2.27	1.48	1.43
27	b	613	CLA	C1B-NB	-2.27	1.34	1.37
27	y	612	CLA	C1B-C2B	2.27	1.48	1.43
32	C	519	DGD	O5D-C6D	-2.27	1.39	1.43
27	G	603	CLA	CMD-C2D	-2.27	1.46	1.50
27	g	603	CLA	CMD-C2D	-2.27	1.46	1.50
27	r	604	CLA	CMD-C2D	-2.27	1.46	1.50
27	C	509	CLA	MG-ND	-2.27	2.01	2.05
27	s	609	CLA	MG-NB	-2.27	2.01	2.05
39	g	1622	XAT	O24-C25	-2.27	1.43	1.46
27	b	608	CLA	CMB-C2B	-2.27	1.46	1.50
27	B	611	CLA	CMC-C2C	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	611	CLA	CMC-C2C	-2.26	1.46	1.50
27	G	603	CLA	MG-NB	-2.26	2.01	2.05
27	g	603	CLA	MG-NB	-2.26	2.01	2.05
27	S	610	CLA	CMB-C2B	-2.26	1.46	1.50
27	r	613	CLA	CMD-C2D	-2.26	1.46	1.50
27	g	613	CLA	CMB-C2B	-2.26	1.46	1.50
27	c	507	CLA	CMC-C2C	-2.26	1.46	1.50
27	r	616	CLA	MG-NB	-2.26	2.01	2.05
27	C	503	CLA	CMC-C2C	-2.26	1.46	1.50
27	R	601	CLA	MG-NB	-2.26	2.01	2.05
27	r	601	CLA	MG-NB	-2.26	2.01	2.05
27	b	602	CLA	MG-ND	-2.26	2.01	2.05
27	c	512	CLA	C1B-C2B	2.26	1.48	1.43
27	C	512	CLA	CMB-C2B	-2.26	1.46	1.50
27	c	512	CLA	CMB-C2B	-2.26	1.46	1.50
27	c	512	CLA	CMC-C2C	-2.26	1.46	1.50
27	g	611	CLA	CMB-C2B	-2.26	1.46	1.50
27	y	604	CLA	CMC-C2C	-2.26	1.46	1.50
27	R	601	CLA	C3B-C4B	2.26	1.49	1.42
27	r	601	CLA	C3B-C4B	2.26	1.49	1.42
29	B	619	BCR	C30-C25	-2.26	1.50	1.53
38	y	1620	LUT	C22-C21	-2.26	1.52	1.54
27	y	614	CLA	C4B-NB	2.25	1.40	1.37
27	n	602	CLA	CMC-C2C	-2.25	1.46	1.50
27	G	611	CLA	CMB-C2B	-2.25	1.46	1.50
27	c	502	CLA	CMD-C2D	-2.25	1.46	1.50
27	n	611	CLA	C3B-C4B	2.25	1.49	1.42
27	s	614	CLA	CMB-C2B	-2.25	1.46	1.50
27	G	614	CLA	CHC-C1C	2.25	1.43	1.38
27	S	613	CLA	CMB-C2B	-2.25	1.46	1.50
27	s	613	CLA	CMB-C2B	-2.25	1.46	1.50
36	F	101	HEM	C2A-C3A	-2.25	1.33	1.38
39	G	1622	XAT	O24-C25	-2.25	1.43	1.46
27	R	613	CLA	CMD-C2D	-2.25	1.46	1.50
27	c	502	CLA	MG-ND	-2.25	2.01	2.05
35	R	2630	LHG	O7-C5	-2.25	1.41	1.46
27	R	611	CLA	C3B-C4B	2.25	1.49	1.42
27	r	611	CLA	C3B-C4B	2.25	1.49	1.42
27	A	407	CLA	CMC-C2C	-2.25	1.46	1.50
27	G	604	CLA	CMD-C2D	-2.25	1.46	1.50
27	b	608	CLA	C1B-C2B	2.25	1.48	1.43
27	N	611	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	612	CLA	C3B-C4B	2.25	1.49	1.42
35	r	2630	LHG	O7-C5	-2.25	1.41	1.46
37	y	606	CHL	CHA-CBD	-2.24	1.49	1.51
27	R	609	CLA	CMB-C2B	-2.24	1.46	1.50
27	n	603	CLA	CMC-C2C	-2.24	1.46	1.50
27	r	609	CLA	CMB-C2B	-2.24	1.46	1.50
27	N	614	CLA	CMD-C2D	-2.24	1.46	1.50
27	C	503	CLA	MG-ND	-2.24	2.01	2.05
27	R	603	CLA	CMD-C2D	-2.24	1.46	1.50
27	Y	614	CLA	CMB-C2B	-2.24	1.46	1.50
27	D	403	CLA	C1B-NB	-2.24	1.34	1.37
27	b	609	CLA	C1B-NB	-2.24	1.34	1.37
27	b	610	CLA	MG-ND	-2.24	2.01	2.05
27	Y	604	CLA	CMD-C2D	-2.24	1.46	1.50
27	R	602	CLA	CMD-C2D	-2.24	1.46	1.50
27	b	609	CLA	MG-ND	-2.24	2.01	2.05
27	B	613	CLA	C1B-NB	-2.24	1.34	1.37
27	C	502	CLA	CMD-C2D	-2.24	1.46	1.50
27	r	609	CLA	CMC-C2C	-2.24	1.46	1.50
27	Y	611	CLA	MG-ND	-2.24	2.01	2.05
27	y	611	CLA	MG-ND	-2.24	2.01	2.05
27	S	613	CLA	CMC-C2C	-2.24	1.46	1.50
27	C	507	CLA	CMC-C2C	-2.24	1.46	1.50
37	Y	601	CHL	CHA-CBD	-2.24	1.49	1.51
27	R	616	CLA	C3B-C4B	2.24	1.49	1.42
27	C	512	CLA	C4B-NB	2.24	1.40	1.37
27	c	503	CLA	MG-ND	-2.24	2.01	2.05
27	A	406	CLA	CMB-C2B	-2.24	1.46	1.50
27	N	613	CLA	CMB-C2B	-2.24	1.46	1.50
27	Y	612	CLA	C1B-C2B	2.24	1.48	1.43
27	b	609	CLA	C1B-C2B	2.24	1.48	1.43
27	Y	613	CLA	CMC-C2C	-2.24	1.46	1.50
27	B	616	CLA	MG-ND	-2.24	2.01	2.05
27	b	616	CLA	MG-ND	-2.24	2.01	2.05
27	c	510	CLA	C1B-NB	-2.24	1.34	1.37
27	G	603	CLA	C3B-C4B	2.24	1.49	1.42
27	g	603	CLA	C3B-C4B	2.24	1.49	1.42
40	R	623	NEX	O24-C25	-2.23	1.43	1.46
27	C	501	CLA	CMC-C2C	-2.23	1.46	1.50
27	C	511	CLA	CMB-C2B	-2.23	1.46	1.50
27	S	603	CLA	MG-NB	-2.23	2.01	2.05
35	g	2630	LHG	O7-C5	-2.23	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	s	603	CLA	MG-NB	-2.23	2.01	2.05
27	s	613	CLA	CMC-C2C	-2.23	1.46	1.50
37	Y	606	CHL	CHA-CBD	-2.23	1.49	1.51
27	R	604	CLA	CMD-C2D	-2.23	1.46	1.50
27	s	602	CLA	CMC-C2C	-2.23	1.46	1.50
27	y	603	CLA	C3B-C4B	2.23	1.49	1.42
40	N	1623	NEX	O24-C25	-2.23	1.43	1.46
40	Y	1623	NEX	O24-C25	-2.23	1.43	1.46
40	y	1623	NEX	O24-C25	-2.23	1.43	1.46
27	B	608	CLA	CMC-C2C	-2.23	1.46	1.50
27	r	612	CLA	C3B-C4B	2.23	1.49	1.42
27	C	502	CLA	CMC-C2C	-2.23	1.46	1.50
27	c	502	CLA	CMC-C2C	-2.23	1.46	1.50
27	r	603	CLA	CMD-C2D	-2.23	1.46	1.50
36	f	101	HEM	C2A-C3A	-2.23	1.33	1.38
27	B	610	CLA	CMC-C2C	-2.23	1.46	1.50
32	C	518	DGD	O3E-C3E	-2.23	1.37	1.43
27	Y	603	CLA	C3B-C4B	2.23	1.49	1.42
27	s	612	CLA	CMC-C2C	-2.23	1.46	1.50
27	C	511	CLA	MG-ND	-2.23	2.01	2.05
27	C	512	CLA	C1B-C2B	2.23	1.48	1.43
27	B	607	CLA	MG-ND	-2.23	2.01	2.05
27	c	510	CLA	MG-ND	-2.23	2.01	2.05
27	C	502	CLA	C1B-C2B	2.23	1.48	1.43
27	d	403	CLA	C1B-C2B	2.22	1.48	1.43
27	N	611	CLA	CMB-C2B	-2.22	1.46	1.50
27	A	407	CLA	C4B-NB	2.22	1.40	1.37
27	b	606	CLA	MG-ND	-2.22	2.01	2.05
27	N	603	CLA	CMC-C2C	-2.22	1.46	1.50
37	n	606	CHL	CHA-CBD	-2.22	1.49	1.51
27	B	611	CLA	C1B-NB	-2.22	1.34	1.37
27	b	611	CLA	C1B-NB	-2.22	1.34	1.37
27	Y	612	CLA	CMB-C2B	-2.22	1.46	1.50
27	y	612	CLA	CMB-C2B	-2.22	1.46	1.50
29	b	618	BCR	C1-C6	-2.22	1.50	1.53
27	B	609	CLA	CMC-C2C	-2.22	1.46	1.50
27	b	608	CLA	CMC-C2C	-2.22	1.46	1.50
27	b	610	CLA	CMC-C2C	-2.22	1.46	1.50
27	Y	613	CLA	C4B-NB	2.22	1.40	1.37
27	d	403	CLA	CMB-C2B	-2.22	1.46	1.50
27	C	513	CLA	CMB-C2B	-2.22	1.46	1.50
27	b	608	CLA	C4B-NB	2.22	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	506	CLA	C4B-NB	2.22	1.40	1.37
27	c	506	CLA	C4B-NB	2.22	1.40	1.37
32	c	519	DGD	O5D-C6D	-2.22	1.39	1.43
27	C	502	CLA	MG-ND	-2.22	2.01	2.05
27	B	609	CLA	C1B-NB	-2.22	1.34	1.37
27	r	616	CLA	C3B-C4B	2.22	1.49	1.42
27	c	501	CLA	CMC-C2C	-2.22	1.46	1.50
27	B	609	CLA	MG-ND	-2.22	2.01	2.05
37	y	601	CHL	CHA-CBD	-2.21	1.49	1.51
27	N	602	CLA	CMC-C2C	-2.21	1.46	1.50
27	n	613	CLA	MG-ND	-2.21	2.01	2.05
27	S	604	CLA	CMC-C2C	-2.21	1.46	1.50
27	S	611	CLA	CMB-C2B	-2.21	1.46	1.50
27	s	611	CLA	CMB-C2B	-2.21	1.46	1.50
27	C	504	CLA	C1B-C2B	2.21	1.48	1.43
27	c	504	CLA	C1B-C2B	2.21	1.48	1.43
37	s	601	CHL	CHA-CBD	-2.21	1.49	1.51
27	B	608	CLA	C3B-C4B	2.21	1.49	1.42
27	b	608	CLA	C3B-C4B	2.21	1.49	1.42
27	C	506	CLA	CMC-C2C	-2.21	1.46	1.50
27	r	603	CLA	C1B-C2B	2.21	1.48	1.43
27	Y	614	CLA	MG-ND	-2.21	2.01	2.05
27	n	603	CLA	MG-ND	-2.21	2.01	2.05
27	y	614	CLA	MG-ND	-2.21	2.01	2.05
27	b	611	CLA	C1B-C2B	2.21	1.48	1.43
27	y	613	CLA	CMC-C2C	-2.21	1.46	1.50
27	g	614	CLA	CHC-C1C	2.21	1.42	1.38
27	B	611	CLA	C1B-C2B	2.21	1.48	1.43
27	B	617	CLA	C1B-C2B	2.21	1.48	1.43
27	b	617	CLA	C1B-C2B	2.21	1.48	1.43
27	Y	612	CLA	CMC-C2C	-2.21	1.46	1.50
27	y	612	CLA	CMC-C2C	-2.21	1.46	1.50
39	Y	1622	XAT	O4-C5	-2.21	1.43	1.46
39	y	1622	XAT	O4-C5	-2.21	1.43	1.46
27	B	608	CLA	C4B-NB	2.21	1.40	1.37
27	S	612	CLA	CMC-C2C	-2.21	1.46	1.50
27	c	513	CLA	CMB-C2B	-2.21	1.46	1.50
27	a	405	CLA	C4B-NB	2.21	1.40	1.37
27	G	614	CLA	CMB-C2B	-2.21	1.46	1.50
27	S	612	CLA	CMB-C2B	-2.21	1.46	1.50
27	a	407	CLA	CMC-C2C	-2.21	1.46	1.50
27	B	609	CLA	C1B-C2B	2.21	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	s	604	CLA	CMD-C2D	-2.20	1.46	1.50
27	b	612	CLA	C4B-NB	2.20	1.40	1.37
27	c	505	CLA	C4B-NB	2.20	1.40	1.37
27	b	613	CLA	C1B-C2B	2.20	1.48	1.43
27	R	602	CLA	CMB-C2B	-2.20	1.46	1.50
27	r	602	CLA	CMB-C2B	-2.20	1.46	1.50
39	r	622	XAT	O24-C25	-2.20	1.43	1.46
27	N	603	CLA	MG-ND	-2.20	2.01	2.05
27	D	403	CLA	CMB-C2B	-2.20	1.46	1.50
27	G	612	CLA	CMC-C2C	-2.20	1.46	1.50
27	G	614	CLA	CMD-C2D	-2.20	1.46	1.50
27	R	612	CLA	CMD-C2D	-2.20	1.46	1.50
27	s	612	CLA	CMB-C2B	-2.20	1.46	1.50
27	N	603	CLA	CMB-C2B	-2.20	1.46	1.50
27	C	505	CLA	C4B-NB	2.20	1.40	1.37
27	R	604	CLA	CMB-C2B	-2.20	1.46	1.50
27	g	612	CLA	CMD-C2D	-2.20	1.46	1.50
27	n	603	CLA	CMB-C2B	-2.20	1.46	1.50
27	r	604	CLA	CMB-C2B	-2.20	1.46	1.50
37	G	608	CHL	CBD-CGD	-2.20	1.49	1.52
27	R	609	CLA	CMC-C2C	-2.20	1.46	1.50
27	b	607	CLA	MG-ND	-2.20	2.01	2.05
27	r	602	CLA	CMD-C2D	-2.20	1.46	1.50
27	S	614	CLA	CMB-C2B	-2.20	1.46	1.50
27	Y	610	CLA	MG-ND	-2.20	2.01	2.05
27	N	612	CLA	CMB-C2B	-2.20	1.46	1.50
27	c	502	CLA	C1B-C2B	2.20	1.48	1.43
27	B	616	CLA	C3B-C4B	2.20	1.49	1.42
27	s	612	CLA	CMD-C2D	-2.19	1.46	1.50
27	c	512	CLA	C1B-NB	-2.19	1.35	1.37
27	S	604	CLA	CMD-C2D	-2.19	1.46	1.50
27	c	511	CLA	MG-ND	-2.19	2.01	2.05
32	c	518	DGD	O3E-C3E	-2.19	1.37	1.43
27	S	602	CLA	CHC-C1C	2.19	1.42	1.38
27	C	510	CLA	MG-ND	-2.19	2.01	2.05
27	N	604	CLA	CMC-C2C	-2.19	1.46	1.50
27	s	603	CLA	CMD-C2D	-2.19	1.46	1.50
27	G	611	CLA	C3B-C4B	2.19	1.49	1.42
27	g	611	CLA	C3B-C4B	2.19	1.49	1.42
27	c	512	CLA	C4B-NB	2.19	1.40	1.37
27	G	610	CLA	CMC-C2C	-2.19	1.46	1.50
27	g	610	CLA	CMB-C2B	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Y	604	CLA	C1B-C2B	2.19	1.48	1.43
40	S	1623	NEX	O24-C25	-2.19	1.43	1.46
37	N	606	CHL	CHA-CBD	-2.19	1.49	1.51
27	A	410	CLA	C1B-NB	-2.19	1.35	1.37
27	n	611	CLA	CMB-C2B	-2.19	1.46	1.50
27	Y	613	CLA	C1B-C2B	2.19	1.48	1.43
27	y	613	CLA	C1B-C2B	2.19	1.48	1.43
27	g	614	CLA	CMB-C2B	-2.19	1.46	1.50
27	s	610	CLA	CMC-C2C	-2.19	1.46	1.50
27	d	402	CLA	C4B-NB	2.19	1.40	1.37
29	B	618	BCR	C1-C6	-2.19	1.51	1.53
27	s	614	CLA	CMC-C2C	-2.19	1.46	1.50
27	R	603	CLA	C1B-C2B	2.18	1.48	1.43
27	n	604	CLA	CMC-C2C	-2.18	1.46	1.50
38	Y	1620	LUT	C1-C6	-2.18	1.51	1.53
38	y	1620	LUT	C1-C6	-2.18	1.51	1.53
27	C	501	CLA	C3B-C4B	2.18	1.49	1.42
27	C	510	CLA	C1B-NB	-2.18	1.35	1.37
27	G	613	CLA	CMD-C2D	-2.18	1.46	1.50
27	g	613	CLA	CMD-C2D	-2.18	1.46	1.50
27	c	501	CLA	C3B-C4B	2.18	1.49	1.42
27	s	604	CLA	CMC-C2C	-2.18	1.46	1.50
27	a	406	CLA	CMB-C2B	-2.18	1.46	1.50
40	n	1623	NEX	O24-C25	-2.18	1.43	1.46
27	g	613	CLA	CMC-C2C	-2.18	1.46	1.50
27	s	609	CLA	CMD-C2D	-2.18	1.46	1.50
27	D	403	CLA	C1B-C2B	2.18	1.48	1.43
27	R	604	CLA	CMC-C2C	-2.18	1.46	1.50
27	g	610	CLA	CMC-C2C	-2.18	1.46	1.50
27	g	614	CLA	CMD-C2D	-2.18	1.46	1.50
27	S	612	CLA	CMD-C2D	-2.18	1.46	1.50
27	y	610	CLA	MG-ND	-2.18	2.01	2.05
27	Y	611	CLA	CMB-C2B	-2.18	1.46	1.50
27	y	611	CLA	CMB-C2B	-2.18	1.46	1.50
27	B	616	CLA	C1B-NB	-2.18	1.35	1.37
27	a	410	CLA	C1B-NB	-2.18	1.35	1.37
40	r	623	NEX	O24-C25	-2.18	1.43	1.46
40	s	1623	NEX	O24-C25	-2.18	1.43	1.46
27	G	603	CLA	CMC-C2C	-2.18	1.46	1.50
27	S	603	CLA	CMD-C2D	-2.18	1.46	1.50
27	g	603	CLA	CMC-C2C	-2.18	1.46	1.50
27	n	614	CLA	CMD-C2D	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	612	CLA	MG-ND	-2.18	2.01	2.05
27	g	603	CLA	CMB-C2B	-2.18	1.46	1.50
27	y	604	CLA	C1B-C2B	2.18	1.48	1.43
27	b	609	CLA	CMC-C2C	-2.18	1.46	1.50
27	c	506	CLA	CMC-C2C	-2.18	1.46	1.50
27	B	602	CLA	CMC-C2C	-2.17	1.46	1.50
27	N	613	CLA	CMD-C2D	-2.17	1.46	1.50
27	b	602	CLA	CMC-C2C	-2.17	1.46	1.50
27	G	604	CLA	MG-ND	-2.17	2.01	2.05
27	g	604	CLA	MG-ND	-2.17	2.01	2.05
27	G	613	CLA	CMC-C2C	-2.17	1.46	1.50
38	N	1620	LUT	C22-C21	-2.17	1.52	1.54
27	A	405	CLA	C4B-NB	2.17	1.40	1.37
27	G	610	CLA	CMB-C2B	-2.17	1.46	1.50
27	B	613	CLA	C1B-C2B	2.17	1.48	1.43
27	n	613	CLA	CMB-C2B	-2.17	1.46	1.50
27	N	613	CLA	MG-ND	-2.17	2.01	2.05
27	B	612	CLA	C3B-C4B	2.17	1.49	1.42
27	d	403	CLA	C1B-NB	-2.17	1.35	1.37
27	B	609	CLA	C4B-NB	2.17	1.40	1.37
27	b	609	CLA	C4B-NB	2.17	1.40	1.37
27	N	611	CLA	CMD-C2D	-2.17	1.46	1.50
27	n	611	CLA	CMD-C2D	-2.17	1.46	1.50
27	r	612	CLA	CMB-C2B	-2.17	1.46	1.50
27	b	616	CLA	C3B-C4B	2.17	1.49	1.42
27	r	610	CLA	CMB-C2B	-2.17	1.46	1.50
27	S	611	CLA	C3B-C4B	2.17	1.49	1.42
27	R	612	CLA	CMB-C2B	-2.17	1.46	1.50
27	S	610	CLA	CMC-C2C	-2.16	1.46	1.50
27	c	501	CLA	C1B-C2B	2.16	1.48	1.43
27	r	612	CLA	CMD-C2D	-2.16	1.46	1.50
27	s	613	CLA	MG-ND	-2.16	2.01	2.05
27	G	612	CLA	CMD-C2D	-2.16	1.46	1.50
38	S	1621	LUT	C1-C6	-2.16	1.51	1.53
38	s	1621	LUT	C1-C6	-2.16	1.51	1.53
27	B	612	CLA	MG-ND	-2.16	2.01	2.05
39	R	622	XAT	O24-C25	-2.16	1.43	1.46
27	C	512	CLA	C1B-NB	-2.16	1.35	1.37
27	G	603	CLA	CMB-C2B	-2.16	1.46	1.50
27	R	611	CLA	MG-NB	-2.16	2.01	2.05
27	r	611	CLA	MG-NB	-2.16	2.01	2.05
27	n	612	CLA	CMB-C2B	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	611	CLA	CMD-C2D	-2.16	1.46	1.50
27	C	507	CLA	C3B-C4B	2.16	1.49	1.42
27	G	611	CLA	MG-ND	-2.16	2.01	2.05
27	B	614	CLA	C4B-NB	2.16	1.40	1.37
27	B	606	CLA	C3B-C4B	2.15	1.49	1.42
27	b	606	CLA	C3B-C4B	2.15	1.49	1.42
27	y	604	CLA	MG-ND	-2.15	2.01	2.05
27	N	613	CLA	CMC-C2C	-2.15	1.46	1.50
38	n	1620	LUT	C22-C21	-2.15	1.52	1.54
27	S	609	CLA	CMD-C2D	-2.15	1.46	1.50
27	g	611	CLA	CMD-C2D	-2.15	1.46	1.50
27	R	610	CLA	CMB-C2B	-2.15	1.46	1.50
27	C	501	CLA	C1B-C2B	2.15	1.48	1.43
27	R	601	CLA	CHC-C1C	2.15	1.42	1.38
27	r	601	CLA	CHC-C1C	2.15	1.42	1.38
27	B	604	CLA	C4B-NB	2.15	1.40	1.37
27	b	614	CLA	C4B-NB	2.15	1.40	1.37
31	d	411	LMG	O1-C7	-2.15	1.40	1.43
27	Y	614	CLA	C4B-NB	2.15	1.40	1.37
27	S	614	CLA	CMC-C2C	-2.15	1.46	1.50
27	B	608	CLA	MG-ND	-2.15	2.01	2.05
27	b	608	CLA	MG-ND	-2.15	2.01	2.05
37	g	608	CHL	CBD-CGD	-2.15	1.49	1.52
31	D	411	LMG	O1-C7	-2.15	1.40	1.43
27	y	612	CLA	C4B-NB	2.15	1.40	1.37
27	y	602	CLA	C4B-NB	2.14	1.40	1.37
29	A	411	BCR	C30-C25	-2.14	1.51	1.53
34	D	405	PL9	C35-C34	-2.14	1.45	1.50
27	Y	602	CLA	C4B-NB	2.14	1.40	1.37
27	G	611	CLA	CMD-C2D	-2.14	1.46	1.50
27	G	612	CLA	C3B-C4B	2.14	1.49	1.42
27	S	609	CLA	CMB-C2B	-2.14	1.46	1.50
38	N	1620	LUT	C1-C6	-2.14	1.51	1.53
27	s	611	CLA	C3B-C4B	2.14	1.49	1.42
27	b	612	CLA	C3B-C4B	2.14	1.49	1.42
27	c	504	CLA	C3B-C4B	2.14	1.49	1.42
27	r	613	CLA	C3B-C4B	2.13	1.49	1.42
27	y	613	CLA	C4B-NB	2.13	1.40	1.37
27	s	612	CLA	MG-ND	-2.13	2.01	2.05
27	r	611	CLA	CMD-C2D	-2.13	1.46	1.50
27	b	604	CLA	C4B-NB	2.13	1.40	1.37
27	S	603	CLA	CMC-C2C	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	611	CLA	CMC-C2C	-2.13	1.46	1.50
27	g	612	CLA	CMC-C2C	-2.13	1.46	1.50
27	n	611	CLA	CMC-C2C	-2.13	1.46	1.50
27	G	604	CLA	CMC-C2C	-2.13	1.46	1.50
34	d	405	PL9	C35-C34	-2.13	1.45	1.50
32	C	518	DGD	O3D-C3D	-2.13	1.37	1.43
27	S	611	CLA	MG-ND	-2.13	2.01	2.05
27	N	602	CLA	C3B-C4B	2.13	1.48	1.42
40	S	1623	NEX	C1-C6	-2.13	1.51	1.54
27	c	507	CLA	C3B-C4B	2.13	1.48	1.42
27	n	602	CLA	C3B-C4B	2.13	1.48	1.42
27	C	501	CLA	MG-ND	-2.13	2.01	2.05
27	c	501	CLA	MG-ND	-2.13	2.01	2.05
27	R	613	CLA	CMC-C2C	-2.13	1.46	1.50
37	N	601	CHL	CHA-CBD	-2.13	1.49	1.51
37	n	601	CHL	CHA-CBD	-2.13	1.49	1.51
27	g	611	CLA	CMC-C2C	-2.13	1.46	1.50
27	r	603	CLA	CMC-C2C	-2.13	1.46	1.50
27	r	604	CLA	CMC-C2C	-2.13	1.46	1.50
27	g	611	CLA	MG-ND	-2.12	2.01	2.05
38	R	620	LUT	C22-C21	-2.12	1.52	1.54
27	a	405	CLA	MG-ND	-2.12	2.01	2.05
27	g	612	CLA	C3B-C4B	2.12	1.48	1.42
27	N	614	CLA	CMB-C2B	-2.12	1.46	1.50
27	n	614	CLA	CMB-C2B	-2.12	1.46	1.50
27	B	614	CLA	C1B-C2B	2.12	1.48	1.43
27	r	616	CLA	CMB-C2B	-2.12	1.46	1.50
27	Y	604	CLA	MG-ND	-2.12	2.01	2.05
32	c	518	DGD	O3D-C3D	-2.12	1.37	1.43
27	s	603	CLA	CMC-C2C	-2.12	1.46	1.50
27	b	617	CLA	C1B-NB	-2.12	1.35	1.37
27	s	602	CLA	CHC-C1C	2.12	1.42	1.38
27	a	407	CLA	C1B-C2B	2.12	1.48	1.43
27	D	402	CLA	C4B-NB	2.12	1.40	1.37
27	g	604	CLA	CMC-C2C	-2.12	1.46	1.50
40	s	1623	NEX	C1-C6	-2.12	1.51	1.54
27	R	616	CLA	CMB-C2B	-2.12	1.46	1.50
27	A	405	CLA	MG-ND	-2.12	2.01	2.05
27	N	604	CLA	C3B-C4B	2.11	1.48	1.42
27	N	612	CLA	CMD-C2D	-2.11	1.46	1.50
27	A	407	CLA	C1B-C2B	2.11	1.48	1.43
27	S	613	CLA	MG-ND	-2.11	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	G	613	CLA	MG-ND	-2.11	2.01	2.05
27	S	612	CLA	MG-ND	-2.11	2.01	2.05
27	g	613	CLA	MG-ND	-2.11	2.01	2.05
27	G	612	CLA	CHC-C1C	2.11	1.42	1.38
27	r	601	CLA	CMD-C2D	-2.11	1.46	1.50
27	B	612	CLA	C4B-NB	2.11	1.40	1.37
32	C	518	DGD	O6D-C5D	-2.11	1.39	1.44
32	c	518	DGD	O6D-C5D	-2.11	1.39	1.44
27	g	614	CLA	C3B-C4B	2.11	1.48	1.42
27	r	604	CLA	MG-ND	-2.11	2.01	2.05
27	C	504	CLA	C3B-C4B	2.11	1.48	1.42
27	G	614	CLA	C3B-C4B	2.11	1.48	1.42
27	R	603	CLA	CMC-C2C	-2.11	1.46	1.50
29	a	411	BCR	C30-C25	-2.11	1.51	1.53
27	R	601	CLA	CMD-C2D	-2.11	1.46	1.50
27	s	610	CLA	CMD-C2D	-2.11	1.46	1.50
27	B	607	CLA	C3B-C4B	2.11	1.48	1.42
27	B	604	CLA	C1B-NB	-2.10	1.35	1.37
27	b	604	CLA	C1B-NB	-2.10	1.35	1.37
27	c	511	CLA	C1B-NB	-2.10	1.35	1.37
27	g	612	CLA	MG-ND	-2.10	2.01	2.05
27	s	611	CLA	CMC-C2C	-2.10	1.46	1.50
27	n	604	CLA	C3B-C4B	2.10	1.48	1.42
27	c	513	CLA	C4B-NB	2.10	1.40	1.37
27	S	611	CLA	CMC-C2C	-2.10	1.46	1.50
27	n	613	CLA	CMD-C2D	-2.10	1.46	1.50
27	S	603	CLA	C3B-C4B	2.10	1.48	1.42
27	n	610	CLA	C3B-C4B	2.10	1.48	1.42
27	B	605	CLA	C1B-NB	-2.10	1.35	1.37
27	C	502	CLA	C4B-NB	2.10	1.40	1.37
27	b	605	CLA	C1B-NB	-2.10	1.35	1.37
27	G	611	CLA	CMC-C2C	-2.10	1.46	1.50
27	n	613	CLA	CMC-C2C	-2.10	1.46	1.50
27	s	602	CLA	C3B-C4B	2.10	1.48	1.42
31	D	411	LMG	O4-C4	-2.10	1.37	1.43
31	d	411	LMG	O4-C4	-2.10	1.37	1.43
27	S	602	CLA	C3B-C4B	2.09	1.48	1.42
27	b	607	CLA	C3B-C4B	2.09	1.48	1.42
27	N	612	CLA	CMC-C2C	-2.09	1.46	1.50
27	A	406	CLA	MG-ND	-2.09	2.01	2.05
27	a	406	CLA	MG-ND	-2.09	2.01	2.05
27	A	410	CLA	C1B-C2B	2.09	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	410	CLA	C1B-C2B	2.09	1.48	1.43
31	Z	101	LMG	O7-C8	-2.09	1.41	1.46
30	B	621	SQD	O2-C2	-2.09	1.37	1.43
27	B	615	CLA	MG-ND	-2.09	2.01	2.05
27	b	615	CLA	MG-ND	-2.09	2.01	2.05
27	R	613	CLA	C3B-C4B	2.09	1.48	1.42
27	S	614	CLA	MG-ND	-2.09	2.01	2.05
27	s	614	CLA	MG-ND	-2.09	2.01	2.05
27	B	615	CLA	C1B-NB	-2.09	1.35	1.37
37	g	606	CHL	CHA-CBD	-2.09	1.49	1.51
34	D	405	PL9	C7-C8	-2.09	1.47	1.50
34	d	405	PL9	C7-C8	-2.09	1.47	1.50
27	s	611	CLA	MG-ND	-2.09	2.01	2.05
27	b	614	CLA	C1B-C2B	2.09	1.48	1.43
31	a	413	LMG	O7-C8	-2.09	1.41	1.46
27	c	513	CLA	C1B-NB	-2.09	1.35	1.37
27	r	613	CLA	CMB-C2B	-2.09	1.46	1.50
27	R	611	CLA	CMB-C2B	-2.08	1.46	1.50
27	r	611	CLA	CMB-C2B	-2.08	1.46	1.50
38	R	620	LUT	C1-C6	-2.08	1.51	1.53
38	r	620	LUT	C1-C6	-2.08	1.51	1.53
27	C	513	CLA	C4B-NB	2.08	1.40	1.37
27	D	403	CLA	C4B-NB	2.08	1.40	1.37
38	n	1620	LUT	C1-C6	-2.08	1.51	1.53
27	S	602	CLA	CMB-C2B	-2.08	1.46	1.50
27	r	613	CLA	CMC-C2C	-2.08	1.46	1.50
27	s	602	CLA	CMB-C2B	-2.08	1.46	1.50
38	r	620	LUT	C22-C21	-2.08	1.52	1.54
39	N	1622	XAT	O24-C25	-2.08	1.43	1.46
30	A	412	SQD	O2-C2	-2.08	1.37	1.43
30	a	412	SQD	O2-C2	-2.08	1.37	1.43
27	B	617	CLA	CHC-C1C	2.08	1.42	1.38
27	C	509	CLA	C4B-NB	2.08	1.40	1.37
27	g	612	CLA	CHC-C1C	2.08	1.42	1.38
27	s	609	CLA	CMB-C2B	-2.08	1.46	1.50
27	G	612	CLA	MG-ND	-2.08	2.01	2.05
27	R	616	CLA	CMC-C2C	-2.08	1.46	1.50
37	G	606	CHL	CHA-CBD	-2.08	1.49	1.51
27	C	511	CLA	C1B-NB	-2.08	1.35	1.37
27	b	614	CLA	C1B-NB	-2.08	1.35	1.37
31	z	101	LMG	O7-C8	-2.07	1.41	1.46
27	Y	612	CLA	C4B-NB	2.07	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	604	CLA	MG-ND	-2.07	2.01	2.05
27	n	610	CLA	CHC-C1C	2.07	1.42	1.38
27	S	610	CLA	CMD-C2D	-2.07	1.46	1.50
27	b	610	CLA	C1B-C2B	2.07	1.48	1.43
27	s	603	CLA	C3B-C4B	2.07	1.48	1.42
27	C	506	CLA	C1B-NB	-2.07	1.35	1.37
27	c	506	CLA	C1B-NB	-2.07	1.35	1.37
27	R	601	CLA	CMC-C2C	-2.07	1.46	1.50
27	r	616	CLA	CMC-C2C	-2.07	1.46	1.50
27	R	613	CLA	MG-ND	-2.07	2.01	2.05
27	R	602	CLA	C3B-C4B	2.07	1.48	1.42
27	r	612	CLA	CMC-C2C	-2.07	1.46	1.50
27	b	606	CLA	C1B-C2B	2.06	1.48	1.43
27	B	617	CLA	MG-ND	-2.06	2.01	2.05
27	b	617	CLA	MG-ND	-2.06	2.01	2.05
30	b	621	SQD	O2-C2	-2.06	1.37	1.43
27	B	617	CLA	C1B-NB	-2.06	1.35	1.37
27	N	610	CLA	C3B-C4B	2.06	1.48	1.42
27	B	610	CLA	C3B-C4B	2.06	1.48	1.42
27	b	610	CLA	C3B-C4B	2.06	1.48	1.42
27	C	504	CLA	MG-ND	-2.06	2.01	2.05
27	c	504	CLA	MG-ND	-2.06	2.01	2.05
34	D	405	PL9	C16-C14	-2.06	1.47	1.51
34	d	405	PL9	C16-C14	-2.06	1.47	1.51
27	B	610	CLA	C1B-C2B	2.06	1.48	1.43
27	c	510	CLA	C4B-NB	2.06	1.40	1.37
27	N	610	CLA	CHC-C1C	2.06	1.42	1.38
27	c	502	CLA	C4B-NB	2.06	1.40	1.37
27	B	606	CLA	C1B-C2B	2.05	1.47	1.43
27	Y	614	CLA	CMC-C2C	-2.05	1.46	1.50
27	S	609	CLA	CHC-C1C	2.05	1.42	1.38
27	s	609	CLA	CHC-C1C	2.05	1.42	1.38
27	b	617	CLA	CHC-C1C	2.05	1.42	1.38
27	N	614	CLA	CHC-C1C	2.05	1.42	1.38
27	n	614	CLA	CHC-C1C	2.05	1.42	1.38
27	C	513	CLA	C1B-NB	-2.05	1.35	1.37
27	Y	603	CLA	MG-ND	-2.05	2.01	2.05
27	y	603	CLA	MG-ND	-2.05	2.01	2.05
28	a	409	PHO	CAA-C2A	-2.05	1.49	1.54
29	c	515	BCR	C1-C6	-2.05	1.51	1.53
27	n	612	CLA	CMD-C2D	-2.05	1.46	1.50
27	c	502	CLA	C1B-NB	-2.05	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	413	LMG	O7-C8	-2.05	1.41	1.46
27	d	403	CLA	C4B-NB	2.05	1.40	1.37
29	D	404	BCR	C30-C25	-2.05	1.51	1.53
29	d	404	BCR	C30-C25	-2.05	1.51	1.53
27	S	611	CLA	CHC-C1C	2.05	1.42	1.38
27	R	612	CLA	CMC-C2C	-2.05	1.46	1.50
27	S	604	CLA	MG-ND	-2.04	2.01	2.05
27	s	604	CLA	MG-ND	-2.04	2.01	2.05
27	G	611	CLA	CHC-C1C	2.04	1.42	1.38
27	r	601	CLA	CMC-C2C	-2.04	1.46	1.50
27	r	602	CLA	C3B-C4B	2.04	1.48	1.42
29	C	516	BCR	C30-C25	-2.04	1.51	1.53
27	G	602	CLA	C3B-C4B	2.04	1.48	1.42
27	G	613	CLA	C3B-C4B	2.04	1.48	1.42
27	g	613	CLA	C3B-C4B	2.04	1.48	1.42
27	R	603	CLA	MG-ND	-2.04	2.01	2.05
27	r	603	CLA	MG-ND	-2.04	2.01	2.05
27	c	508	CLA	C4B-NB	2.04	1.40	1.37
27	C	510	CLA	C4B-NB	2.04	1.40	1.37
27	c	509	CLA	C4B-NB	2.04	1.40	1.37
27	R	612	CLA	CHC-C1C	2.04	1.42	1.38
27	r	612	CLA	CHC-C1C	2.04	1.42	1.38
27	b	607	CLA	C1B-C2B	2.04	1.47	1.43
29	c	516	BCR	C30-C25	-2.04	1.51	1.53
27	r	610	CLA	C3B-C4B	2.04	1.48	1.42
27	R	610	CLA	C3B-C4B	2.04	1.48	1.42
30	b	621	SQD	O3-C3	-2.04	1.37	1.43
27	b	615	CLA	C1B-NB	-2.03	1.35	1.37
27	Y	602	CLA	MG-ND	-2.03	2.01	2.05
27	c	509	CLA	C1B-C2B	2.03	1.47	1.43
27	b	606	CLA	C1B-NB	-2.03	1.35	1.37
27	C	505	CLA	C1B-C2B	2.03	1.47	1.43
27	c	505	CLA	C1B-C2B	2.03	1.47	1.43
27	B	606	CLA	C1B-NB	-2.03	1.35	1.37
27	B	614	CLA	C1B-NB	-2.03	1.35	1.37
30	a	418	SQD	O4-C4	-2.03	1.37	1.43
27	G	614	CLA	CMC-C2C	-2.03	1.46	1.50
27	N	604	CLA	MG-ND	-2.03	2.01	2.05
27	n	604	CLA	MG-ND	-2.03	2.01	2.05
27	R	613	CLA	CMB-C2B	-2.03	1.46	1.50
27	C	507	CLA	C1B-C2B	2.03	1.47	1.43
27	c	507	CLA	C1B-C2B	2.03	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	409	PHO	CAA-C2A	-2.03	1.50	1.54
32	H	102	DGD	O6D-C5D	-2.03	1.39	1.44
32	h	102	DGD	O6D-C5D	-2.03	1.39	1.44
27	C	502	CLA	C1B-NB	-2.03	1.35	1.37
27	s	614	CLA	C3B-C4B	2.03	1.48	1.42
30	B	621	SQD	O3-C3	-2.03	1.37	1.43
27	y	614	CLA	CMC-C2C	-2.03	1.46	1.50
32	C	518	DGD	O2E-C2E	-2.02	1.37	1.43
27	B	612	CLA	CAC-C3C	-2.02	1.45	1.51
27	b	612	CLA	CAC-C3C	-2.02	1.45	1.51
27	S	612	CLA	C3B-C4B	2.02	1.48	1.42
27	B	607	CLA	C1B-C2B	2.02	1.47	1.43
27	c	509	CLA	CHC-C1C	2.02	1.42	1.38
32	C	520	DGD	O3G-C3G	-2.02	1.40	1.43
32	c	520	DGD	O3G-C3G	-2.02	1.40	1.43
27	C	509	CLA	C1B-C2B	2.02	1.47	1.43
27	n	612	CLA	CMC-C2C	-2.02	1.46	1.50
27	c	512	CLA	C3B-C4B	2.02	1.48	1.42
38	s	1620	LUT	C22-C21	-2.02	1.52	1.54
29	C	515	BCR	C1-C6	-2.02	1.51	1.53
27	B	617	CLA	C3B-C4B	2.02	1.48	1.42
27	n	610	CLA	MG-ND	-2.02	2.01	2.05
27	N	603	CLA	C3B-C4B	2.01	1.48	1.42
27	g	610	CLA	C3B-C4B	2.01	1.48	1.42
30	A	418	SQD	O4-C4	-2.01	1.38	1.43
27	c	506	CLA	C1B-C2B	2.01	1.47	1.43
27	C	505	CLA	C1B-NB	-2.01	1.35	1.37
28	a	408	PHO	CAA-C2A	-2.01	1.50	1.54
27	b	603	CLA	C4B-NB	2.01	1.40	1.37
27	s	612	CLA	C3B-C4B	2.01	1.48	1.42
27	y	602	CLA	MG-ND	-2.01	2.01	2.05
27	D	402	CLA	C1D-ND	2.01	1.40	1.37
27	Y	611	CLA	C1B-NB	-2.01	1.35	1.37
27	d	402	CLA	C1D-ND	2.01	1.40	1.37
27	y	611	CLA	C1B-NB	-2.01	1.35	1.37
27	b	605	CLA	CAC-C3C	-2.01	1.45	1.51
27	c	511	CLA	C3B-C4B	2.01	1.48	1.42
27	r	613	CLA	MG-ND	-2.01	2.01	2.05
39	n	1622	XAT	O24-C25	-2.01	1.43	1.46
34	d	405	PL9	C20-C19	-2.01	1.45	1.50
27	B	605	CLA	CAC-C3C	-2.01	1.46	1.51
27	B	612	CLA	CHC-C1C	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	612	CLA	CHC-C1C	2.01	1.42	1.38
30	a	418	SQD	O2-C2	-2.01	1.38	1.43
27	S	614	CLA	CHC-C1C	2.01	1.42	1.38
27	B	602	CLA	C3B-C4B	2.01	1.48	1.42
27	b	602	CLA	C3B-C4B	2.01	1.48	1.42
27	g	602	CLA	C3B-C4B	2.01	1.48	1.42
27	D	403	CLA	CMC-C2C	-2.01	1.46	1.50
27	d	403	CLA	CMC-C2C	-2.01	1.46	1.50
27	N	614	CLA	MG-ND	-2.01	2.01	2.05
27	Y	612	CLA	C1B-NB	-2.01	1.35	1.37
27	y	612	CLA	C1B-NB	-2.01	1.35	1.37
27	c	509	CLA	C1B-NB	-2.00	1.35	1.37
35	Y	2630	LHG	C8-C7	-2.00	1.44	1.50
27	S	614	CLA	C3B-C4B	2.00	1.48	1.42
27	s	610	CLA	CHC-C1C	2.00	1.42	1.38
27	N	604	CLA	C1B-NB	-2.00	1.35	1.37
27	n	604	CLA	C1B-NB	-2.00	1.35	1.37
27	G	610	CLA	C3B-C4B	2.00	1.48	1.42
30	A	412	SQD	O3-C3	-2.00	1.38	1.43
27	N	602	CLA	CHC-C1C	2.00	1.42	1.38
39	R	622	XAT	C2-C1	-2.00	1.51	1.54
30	A	418	SQD	O47-C45	-2.00	1.41	1.46
27	g	611	CLA	CHC-C1C	2.00	1.42	1.38

All (2944) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	R	607	CHL	O2D-CGD-CBD	9.77	121.68	110.95
37	r	607	CHL	O2D-CGD-CBD	9.75	121.66	110.95
37	y	601	CHL	O2D-CGD-CBD	9.62	121.52	110.95
37	Y	601	CHL	O2D-CGD-CBD	9.55	121.44	110.95
37	N	606	CHL	O2D-CGD-CBD	9.47	121.35	110.95
37	n	606	CHL	O2D-CGD-CBD	9.44	121.32	110.95
39	Y	1622	XAT	O4-C5-C4	9.41	122.31	113.49
39	y	1622	XAT	O4-C5-C4	9.38	122.28	113.49
37	Y	607	CHL	O2D-CGD-CBD	9.13	120.98	110.95
37	y	607	CHL	O2D-CGD-CBD	9.10	120.95	110.95
37	r	606	CHL	C1B-CHB-C4A	8.97	127.09	121.32
37	N	601	CHL	O2D-CGD-CBD	8.91	120.74	110.95
37	n	601	CHL	O2D-CGD-CBD	8.88	120.70	110.95
37	n	605	CHL	O2D-CGD-CBD	8.87	120.69	110.95
37	N	605	CHL	O2D-CGD-CBD	8.85	120.67	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	607	CHL	C1B-CHB-C4A	8.85	127.01	121.32
37	g	607	CHL	C1B-CHB-C4A	8.84	127.01	121.32
37	R	606	CHL	C1B-CHB-C4A	8.83	127.01	121.32
37	g	601	CHL	O2D-CGD-CBD	8.81	120.63	110.95
37	G	601	CHL	O2D-CGD-CBD	8.80	120.62	110.95
37	G	605	CHL	O2D-CGD-CBD	8.78	120.59	110.95
37	S	601	CHL	O2D-CGD-CBD	8.76	120.58	110.95
37	g	605	CHL	O2D-CGD-CBD	8.75	120.56	110.95
37	s	601	CHL	O2D-CGD-CBD	8.73	120.54	110.95
37	S	607	CHL	O2D-CGD-CBD	8.55	120.34	110.95
39	G	1622	XAT	O4-C5-C4	8.54	121.50	113.49
37	s	607	CHL	O2D-CGD-CBD	8.53	120.32	110.95
39	g	1622	XAT	O4-C5-C4	8.51	121.47	113.49
37	G	607	CHL	O2D-CGD-CBD	8.49	120.27	110.95
37	Y	607	CHL	C1B-CHB-C4A	8.48	126.78	121.32
37	g	607	CHL	O2D-CGD-CBD	8.46	120.25	110.95
37	y	607	CHL	C1B-CHB-C4A	8.46	126.76	121.32
37	n	607	CHL	O2D-CGD-CBD	8.44	120.22	110.95
37	g	601	CHL	C1B-CHB-C4A	8.43	126.75	121.32
37	N	607	CHL	O2D-CGD-CBD	8.42	120.20	110.95
37	Y	606	CHL	O2D-CGD-CBD	8.40	120.18	110.95
37	y	606	CHL	O2D-CGD-CBD	8.40	120.18	110.95
37	Y	609	CHL	O2D-CGD-CBD	8.39	120.17	110.95
37	G	601	CHL	C1B-CHB-C4A	8.35	126.69	121.32
37	y	609	CHL	O2D-CGD-CBD	8.34	120.11	110.95
37	N	608	CHL	O2D-CGD-CBD	8.31	120.08	110.95
37	y	606	CHL	C1B-CHB-C4A	8.30	126.66	121.32
37	n	608	CHL	O2D-CGD-CBD	8.30	120.06	110.95
37	Y	606	CHL	C1B-CHB-C4A	8.25	126.63	121.32
37	N	609	CHL	O2D-CGD-CBD	8.25	120.01	110.95
37	n	609	CHL	O2D-CGD-CBD	8.25	120.01	110.95
37	Y	605	CHL	C1B-CHB-C4A	8.03	126.49	121.32
37	y	605	CHL	C1B-CHB-C4A	8.02	126.48	121.32
37	g	606	CHL	O2D-CGD-CBD	8.02	119.76	110.95
37	G	606	CHL	O2D-CGD-CBD	8.01	119.75	110.95
37	r	606	CHL	O2D-CGD-CBD	7.89	119.62	110.95
37	R	606	CHL	O2D-CGD-CBD	7.87	119.59	110.95
27	B	605	CLA	C4A-NA-C1A	7.84	110.26	106.68
27	b	605	CLA	C4A-NA-C1A	7.84	110.26	106.68
37	n	606	CHL	C1B-CHB-C4A	7.79	126.33	121.32
37	N	606	CHL	C1B-CHB-C4A	7.77	126.32	121.32
37	G	609	CHL	O2D-CGD-CBD	7.70	119.40	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	609	CHL	O2D-CGD-CBD	7.70	119.40	110.95
37	s	608	CHL	O2D-CGD-CBD	7.69	119.39	110.95
37	N	608	CHL	C1B-CHB-C4A	7.68	126.27	121.32
37	R	608	CHL	O2D-CGD-CBD	7.68	119.39	110.95
37	S	608	CHL	O2D-CGD-CBD	7.64	119.34	110.95
37	n	608	CHL	C1B-CHB-C4A	7.63	126.23	121.32
37	r	608	CHL	O2D-CGD-CBD	7.61	119.31	110.95
27	S	604	CLA	C4A-NA-C1A	7.53	110.11	106.68
37	y	608	CHL	C1B-CHB-C4A	7.53	126.16	121.32
27	d	402	CLA	C4A-NA-C1A	7.49	110.10	106.68
40	G	1623	NEX	O24-C25-C24	7.47	120.49	113.49
27	D	402	CLA	C4A-NA-C1A	7.45	110.08	106.68
27	s	604	CLA	C4A-NA-C1A	7.44	110.07	106.68
39	g	1622	XAT	O24-C25-C24	7.43	120.45	113.49
40	g	1623	NEX	O24-C25-C24	7.43	120.45	113.49
37	Y	608	CHL	C1B-CHB-C4A	7.42	126.09	121.32
27	C	511	CLA	C4A-NA-C1A	7.41	110.06	106.68
39	G	1622	XAT	O24-C25-C24	7.38	120.41	113.49
37	Y	608	CHL	O2D-CGD-CBD	7.36	119.03	110.95
37	y	608	CHL	O2D-CGD-CBD	7.36	119.03	110.95
27	a	410	CLA	C4A-NA-C1A	7.35	110.03	106.68
39	N	1622	XAT	O4-C5-C4	7.34	120.37	113.49
39	n	1622	XAT	O4-C5-C4	7.34	120.37	113.49
27	A	410	CLA	C4A-NA-C1A	7.30	110.01	106.68
27	R	610	CLA	C4A-NA-C1A	7.28	110.00	106.68
27	r	610	CLA	C4A-NA-C1A	7.28	110.00	106.68
27	c	508	CLA	C4A-NA-C1A	7.24	109.98	106.68
27	c	511	CLA	C4A-NA-C1A	7.24	109.98	106.68
37	G	608	CHL	O2D-CGD-CBD	7.22	118.88	110.95
37	g	608	CHL	O2D-CGD-CBD	7.22	118.88	110.95
37	S	606	CHL	O2D-CGD-CBD	7.20	118.86	110.95
37	s	606	CHL	O2D-CGD-CBD	7.20	118.86	110.95
27	B	613	CLA	C4A-NA-C1A	7.17	109.95	106.68
27	A	406	CLA	C4A-NA-C1A	7.17	109.95	106.68
27	b	613	CLA	C4A-NA-C1A	7.17	109.95	106.68
39	N	1622	XAT	C31-C30-C29	-7.15	117.25	127.28
39	n	1622	XAT	C31-C30-C29	-7.14	117.26	127.28
27	n	604	CLA	C4A-NA-C1A	7.13	109.93	106.68
27	Y	604	CLA	C4A-NA-C1A	7.13	109.93	106.68
27	y	604	CLA	C4A-NA-C1A	7.13	109.93	106.68
27	C	504	CLA	C4A-NA-C1A	7.12	109.93	106.68
27	a	405	CLA	C4A-NA-C1A	7.12	109.93	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	622	XAT	C18-C5-C6	-7.11	110.59	122.30
27	C	508	CLA	C4A-NA-C1A	7.11	109.92	106.68
40	S	1623	NEX	C38-C25-C26	-7.10	110.61	122.30
40	s	1623	NEX	C38-C25-C26	-7.10	110.61	122.30
39	r	622	XAT	C18-C5-C6	-7.10	110.62	122.30
27	c	513	CLA	C4A-NA-C1A	7.09	109.91	106.68
39	N	1622	XAT	C38-C25-C26	-7.08	110.66	122.30
39	n	1622	XAT	C38-C25-C26	-7.08	110.66	122.30
27	c	512	CLA	C4A-NA-C1A	7.06	109.90	106.68
40	r	623	NEX	C38-C25-C26	-7.05	110.69	122.30
27	r	613	CLA	C4A-NA-C1A	7.05	109.89	106.68
27	N	604	CLA	C4A-NA-C1A	7.05	109.89	106.68
40	R	623	NEX	C38-C25-C26	-7.04	110.71	122.30
27	r	609	CLA	C4A-NA-C1A	7.04	109.89	106.68
27	c	504	CLA	C4A-NA-C1A	7.04	109.89	106.68
27	g	611	CLA	C4A-NA-C1A	7.03	109.89	106.68
27	C	512	CLA	C4A-NA-C1A	7.03	109.88	106.68
37	y	605	CHL	O2D-CGD-CBD	7.02	118.66	110.95
27	N	602	CLA	C4A-NA-C1A	7.02	109.88	106.68
37	Y	605	CHL	O2D-CGD-CBD	7.00	118.63	110.95
27	n	603	CLA	C4A-NA-C1A	6.99	109.87	106.68
27	S	602	CLA	C4A-NA-C1A	6.99	109.87	106.68
27	y	602	CLA	C4A-NA-C1A	6.99	109.87	106.68
27	C	513	CLA	C4A-NA-C1A	6.98	109.86	106.68
27	A	405	CLA	C4A-NA-C1A	6.97	109.86	106.68
27	R	613	CLA	C4A-NA-C1A	6.97	109.86	106.68
27	N	614	CLA	C4A-NA-C1A	6.96	109.85	106.68
27	N	612	CLA	C4A-NA-C1A	6.95	109.85	106.68
40	y	1623	NEX	C38-C25-C26	-6.95	110.87	122.30
40	Y	1623	NEX	C38-C25-C26	-6.94	110.88	122.30
27	R	609	CLA	C4A-NA-C1A	6.94	109.84	106.68
27	c	509	CLA	C4A-NA-C1A	6.94	109.84	106.68
27	r	602	CLA	C4A-NA-C1A	6.94	109.84	106.68
27	R	602	CLA	C4A-NA-C1A	6.93	109.84	106.68
27	G	611	CLA	C4A-NA-C1A	6.92	109.84	106.68
27	a	406	CLA	C4A-NA-C1A	6.92	109.84	106.68
27	R	604	CLA	C4A-NA-C1A	6.92	109.83	106.68
27	r	604	CLA	C4A-NA-C1A	6.92	109.83	106.68
40	N	1623	NEX	C38-C25-C26	-6.91	110.92	122.30
39	y	1622	XAT	C38-C25-C26	-6.91	110.92	122.30
27	G	614	CLA	C4A-NA-C1A	6.91	109.83	106.68
27	C	509	CLA	C4A-NA-C1A	6.91	109.83	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	g	614	CLA	C4A-NA-C1A	6.91	109.83	106.68
27	n	614	CLA	C4A-NA-C1A	6.90	109.83	106.68
39	Y	1622	XAT	C38-C25-C26	-6.89	110.96	122.30
27	N	603	CLA	C4A-NA-C1A	6.89	109.82	106.68
27	n	611	CLA	C4A-NA-C1A	6.88	109.82	106.68
40	n	1623	NEX	C38-C25-C26	-6.87	111.00	122.30
27	n	612	CLA	C4A-NA-C1A	6.87	109.81	106.68
27	s	602	CLA	C4A-NA-C1A	6.86	109.81	106.68
27	n	602	CLA	C4A-NA-C1A	6.85	109.81	106.68
27	Y	602	CLA	C4A-NA-C1A	6.85	109.81	106.68
27	N	611	CLA	C4A-NA-C1A	6.85	109.80	106.68
27	Y	610	CLA	C4A-NA-C1A	6.85	109.80	106.68
39	R	622	XAT	C38-C25-C26	-6.82	111.08	122.30
27	y	614	CLA	C4A-NA-C1A	6.79	109.78	106.68
39	r	622	XAT	C38-C25-C26	-6.79	111.12	122.30
27	n	613	CLA	C4A-NA-C1A	6.77	109.77	106.68
27	y	610	CLA	C4A-NA-C1A	6.76	109.76	106.68
27	N	613	CLA	C4A-NA-C1A	6.74	109.76	106.68
27	g	610	CLA	C4A-NA-C1A	6.72	109.75	106.68
27	A	407	CLA	C4A-NA-C1A	6.71	109.74	106.68
29	C	516	BCR	C24-C23-C22	-6.71	116.30	126.23
27	G	610	CLA	C4A-NA-C1A	6.70	109.74	106.68
27	g	603	CLA	C4A-NA-C1A	6.70	109.73	106.68
29	c	516	BCR	C24-C23-C22	-6.69	116.33	126.23
27	B	611	CLA	C4A-NA-C1A	6.69	109.73	106.68
27	b	611	CLA	C4A-NA-C1A	6.69	109.73	106.68
27	g	612	CLA	C4A-NA-C1A	6.67	109.72	106.68
27	G	603	CLA	C4A-NA-C1A	6.66	109.72	106.68
29	D	404	BCR	C11-C10-C9	-6.66	117.94	127.28
29	d	404	BCR	C11-C10-C9	-6.66	117.94	127.28
27	S	610	CLA	C4A-NA-C1A	6.64	109.71	106.68
27	B	617	CLA	C4A-NA-C1A	6.63	109.71	106.68
27	s	610	CLA	C4A-NA-C1A	6.61	109.69	106.68
39	Y	1622	XAT	C35-C34-C33	-6.61	118.01	127.28
27	Y	611	CLA	C4A-NA-C1A	6.60	109.69	106.68
27	a	407	CLA	C4A-NA-C1A	6.60	109.69	106.68
27	y	611	CLA	C4A-NA-C1A	6.60	109.69	106.68
27	Y	614	CLA	C4A-NA-C1A	6.59	109.68	106.68
27	G	612	CLA	C4A-NA-C1A	6.58	109.68	106.68
29	C	516	BCR	C16-C17-C18	-6.58	118.05	127.28
39	y	1622	XAT	C35-C34-C33	-6.58	118.06	127.28
27	b	617	CLA	C4A-NA-C1A	6.57	109.68	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	g	1622	XAT	C38-C25-C26	-6.57	111.49	122.30
27	C	505	CLA	C4A-NA-C1A	6.56	109.67	106.68
39	G	1622	XAT	C38-C25-C26	-6.55	111.52	122.30
29	c	516	BCR	C16-C17-C18	-6.54	118.11	127.28
29	C	517	BCR	C7-C8-C9	-6.52	116.58	126.23
27	B	609	CLA	C4A-NA-C1A	6.52	109.65	106.68
29	c	517	BCR	C7-C8-C9	-6.52	116.59	126.23
27	b	602	CLA	C4A-NA-C1A	6.51	109.65	106.68
27	B	602	CLA	C4A-NA-C1A	6.49	109.64	106.68
27	B	615	CLA	C4A-NA-C1A	6.49	109.64	106.68
27	b	615	CLA	C4A-NA-C1A	6.49	109.64	106.68
27	R	611	CLA	C4A-NA-C1A	6.49	109.64	106.68
27	r	611	CLA	C4A-NA-C1A	6.49	109.64	106.68
27	B	612	CLA	C4A-NA-C1A	6.48	109.64	106.68
27	N	610	CLA	C4A-NA-C1A	6.48	109.64	106.68
27	b	612	CLA	C4A-NA-C1A	6.48	109.64	106.68
27	c	505	CLA	C4A-NA-C1A	6.48	109.64	106.68
27	b	609	CLA	C4A-NA-C1A	6.48	109.64	106.68
27	S	614	CLA	C4A-NA-C1A	6.45	109.62	106.68
27	s	614	CLA	C4A-NA-C1A	6.43	109.61	106.68
27	G	602	CLA	C4A-NA-C1A	6.42	109.61	106.68
28	a	408	PHO	C4D-CHA-CBD	-6.41	105.38	108.45
27	C	507	CLA	C4A-NA-C1A	6.40	109.60	106.68
27	g	602	CLA	C4A-NA-C1A	6.40	109.60	106.68
27	r	603	CLA	C4A-NA-C1A	6.39	109.59	106.68
27	s	612	CLA	C4A-NA-C1A	6.38	109.59	106.68
40	G	1623	NEX	C38-C25-C26	-6.37	111.81	122.30
27	B	616	CLA	C4A-NA-C1A	6.37	109.58	106.68
27	D	403	CLA	C4A-NA-C1A	6.36	109.58	106.68
27	R	612	CLA	C4A-NA-C1A	6.36	109.58	106.68
27	d	403	CLA	C4A-NA-C1A	6.36	109.58	106.68
37	N	609	CHL	C1B-CHB-C4A	6.36	125.41	121.32
37	n	609	CHL	C1B-CHB-C4A	6.36	125.41	121.32
27	c	507	CLA	C4A-NA-C1A	6.35	109.57	106.68
27	n	610	CLA	C4A-NA-C1A	6.34	109.57	106.68
40	g	1623	NEX	C38-C25-C26	-6.34	111.87	122.30
27	S	612	CLA	C4A-NA-C1A	6.33	109.57	106.68
28	A	408	PHO	C4D-CHA-CBD	-6.33	105.42	108.45
27	B	610	CLA	C4A-NA-C1A	6.31	109.56	106.68
27	c	502	CLA	C4A-NA-C1A	6.31	109.56	106.68
27	G	604	CLA	C4A-NA-C1A	6.30	109.55	106.68
27	g	604	CLA	C4A-NA-C1A	6.30	109.55	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	Y	601	CHL	C1B-CHB-C4A	6.30	125.38	121.32
27	R	616	CLA	C4A-NA-C1A	6.29	109.55	106.68
27	b	610	CLA	C4A-NA-C1A	6.28	109.54	106.68
37	y	601	CHL	C1B-CHB-C4A	6.28	125.36	121.32
27	r	612	CLA	C4A-NA-C1A	6.27	109.54	106.68
27	r	601	CLA	C4A-NA-C1A	6.27	109.54	106.68
37	g	606	CHL	C1B-CHB-C4A	6.26	125.35	121.32
27	b	616	CLA	C4A-NA-C1A	6.26	109.53	106.68
27	S	613	CLA	C4A-NA-C1A	6.25	109.53	106.68
27	s	613	CLA	C4A-NA-C1A	6.25	109.53	106.68
27	C	502	CLA	C4A-NA-C1A	6.23	109.52	106.68
27	R	601	CLA	C4A-NA-C1A	6.23	109.52	106.68
27	R	603	CLA	C4A-NA-C1A	6.22	109.52	106.68
37	Y	606	CHL	CHA-C1A-C2A	-6.21	118.72	133.31
37	y	606	CHL	CHA-C1A-C2A	-6.21	118.72	133.31
27	b	608	CLA	C4A-NA-C1A	6.20	109.51	106.68
27	s	611	CLA	C4A-NA-C1A	6.20	109.51	106.68
37	Y	609	CHL	C1B-CHB-C4A	6.20	125.31	121.32
37	y	609	CHL	C1B-CHB-C4A	6.20	125.31	121.32
27	B	608	CLA	C4A-NA-C1A	6.19	109.50	106.68
27	S	611	CLA	C4A-NA-C1A	6.19	109.50	106.68
37	n	607	CHL	C1B-CHB-C4A	6.19	125.30	121.32
37	R	607	CHL	C1B-CHB-C4A	6.18	125.30	121.32
37	r	607	CHL	C1B-CHB-C4A	6.18	125.30	121.32
27	c	506	CLA	C4A-NA-C1A	6.17	109.49	106.68
27	c	510	CLA	C4A-NA-C1A	6.16	109.49	106.68
27	r	616	CLA	C4A-NA-C1A	6.16	109.49	106.68
27	C	510	CLA	C4A-NA-C1A	6.15	109.48	106.68
39	G	1622	XAT	C18-C5-C6	-6.15	112.18	122.30
37	r	606	CHL	CHA-C1A-C2A	-6.15	118.88	133.31
37	R	606	CHL	CHA-C1A-C2A	-6.15	118.88	133.31
27	y	613	CLA	C4A-NA-C1A	6.13	109.48	106.68
37	N	607	CHL	C1B-CHB-C4A	6.12	125.26	121.32
39	g	1622	XAT	C18-C5-C6	-6.12	112.24	122.30
37	G	606	CHL	C1B-CHB-C4A	6.11	125.25	121.32
27	s	609	CLA	C4A-NA-C1A	6.10	109.46	106.68
27	b	607	CLA	C4A-NA-C1A	6.10	109.46	106.68
27	B	607	CLA	C4A-NA-C1A	6.09	109.46	106.68
27	S	609	CLA	C4A-NA-C1A	6.08	109.45	106.68
40	G	1623	NEX	C15-C14-C13	-6.06	118.78	127.28
27	y	603	CLA	C4A-NA-C1A	6.06	109.44	106.68
37	G	601	CHL	CHA-C1A-C2A	-6.06	119.09	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	601	CHL	CHA-C1A-C2A	-6.05	119.11	133.31
27	C	506	CLA	C4A-NA-C1A	6.04	109.43	106.68
40	g	1623	NEX	C15-C14-C13	-6.02	118.84	127.28
37	Y	609	CHL	CHA-C1A-C2A	-6.02	119.18	133.31
27	Y	613	CLA	C4A-NA-C1A	6.02	109.42	106.68
37	G	606	CHL	CHA-C1A-C2A	-6.02	119.18	133.31
37	g	606	CHL	CHA-C1A-C2A	-6.02	119.18	133.31
27	C	501	CLA	C4A-NA-C1A	6.01	109.42	106.68
27	c	501	CLA	C4A-NA-C1A	6.01	109.42	106.68
37	y	609	CHL	CHA-C1A-C2A	-6.01	119.19	133.31
27	s	603	CLA	C4A-NA-C1A	5.99	109.41	106.68
27	Y	603	CLA	C4A-NA-C1A	5.98	109.41	106.68
27	S	603	CLA	C4A-NA-C1A	5.98	109.41	106.68
40	N	1623	NEX	O24-C25-C24	5.96	119.08	113.49
27	g	613	CLA	C4A-NA-C1A	5.96	109.40	106.68
37	N	606	CHL	CHA-C1A-C2A	-5.96	119.33	133.31
37	n	606	CHL	CHA-C1A-C2A	-5.96	119.33	133.31
39	r	622	XAT	C26-C27-C28	-5.95	113.41	125.99
27	G	613	CLA	C4A-NA-C1A	5.95	109.39	106.68
39	R	622	XAT	C26-C27-C28	-5.94	113.44	125.99
40	n	1623	NEX	O24-C25-C24	5.94	119.06	113.49
29	C	515	BCR	C15-C14-C13	-5.94	118.95	127.28
37	N	609	CHL	CHA-C1A-C2A	-5.94	119.37	133.31
37	n	609	CHL	CHA-C1A-C2A	-5.94	119.37	133.31
39	Y	1622	XAT	C18-C5-C6	-5.94	112.53	122.30
39	y	1622	XAT	C18-C5-C6	-5.94	112.53	122.30
39	R	622	XAT	O24-C25-C24	5.93	119.05	113.49
39	r	622	XAT	O24-C25-C24	5.93	119.05	113.49
37	N	608	CHL	CHA-C1A-C2A	-5.92	119.41	133.31
27	Y	612	CLA	C4A-NA-C1A	5.92	109.38	106.68
29	c	515	BCR	C15-C14-C13	-5.91	118.99	127.28
37	y	605	CHL	CHA-C1A-C2A	-5.91	119.43	133.31
40	s	1623	NEX	C15-C14-C13	-5.91	119.00	127.28
37	n	608	CHL	CHA-C1A-C2A	-5.90	119.44	133.31
37	Y	605	CHL	CHA-C1A-C2A	-5.90	119.46	133.31
40	S	1623	NEX	C15-C14-C13	-5.88	119.03	127.28
37	R	607	CHL	CHA-C1A-C2A	-5.88	119.51	133.31
28	A	409	PHO	C4D-CHA-CBD	-5.88	105.64	108.45
37	g	607	CHL	CHA-C1A-C2A	-5.87	119.52	133.31
39	g	1622	XAT	C15-C14-C13	-5.87	119.05	127.28
37	G	607	CHL	CHA-C1A-C2A	-5.87	119.53	133.31
39	G	1622	XAT	C15-C14-C13	-5.86	119.06	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	r	607	CHL	CHA-C1A-C2A	-5.84	119.59	133.31
27	y	612	CLA	C4A-NA-C1A	5.83	109.34	106.68
37	G	609	CHL	CHA-C1A-C2A	-5.81	119.67	133.31
28	a	409	PHO	C4D-CHA-CBD	-5.80	105.67	108.45
37	g	609	CHL	CHA-C1A-C2A	-5.80	119.69	133.31
37	y	601	CHL	CHA-C1A-C2A	-5.77	119.76	133.31
39	N	1622	XAT	C18-C5-C6	-5.76	112.82	122.30
37	S	601	CHL	CHA-C1A-C2A	-5.76	119.79	133.31
39	n	1622	XAT	C18-C5-C6	-5.75	112.83	122.30
29	H	101	BCR	C16-C17-C18	-5.75	119.22	127.28
27	c	503	CLA	C4A-NA-C1A	5.74	109.30	106.68
37	Y	601	CHL	CHA-C1A-C2A	-5.73	119.85	133.31
29	D	404	BCR	C7-C8-C9	-5.72	117.77	126.23
29	d	404	BCR	C7-C8-C9	-5.72	117.77	126.23
37	Y	608	CHL	CHA-C1A-C2A	-5.72	119.88	133.31
29	h	101	BCR	C16-C17-C18	-5.72	119.26	127.28
37	s	601	CHL	CHA-C1A-C2A	-5.72	119.88	133.31
29	c	517	BCR	C11-C10-C9	-5.71	119.27	127.28
37	y	608	CHL	CHA-C1A-C2A	-5.71	119.91	133.31
29	C	517	BCR	C11-C10-C9	-5.71	119.28	127.28
29	D	404	BCR	C24-C23-C22	-5.70	117.80	126.23
29	d	404	BCR	C24-C23-C22	-5.70	117.80	126.23
37	y	607	CHL	CHA-C1A-C2A	-5.70	119.93	133.31
37	Y	607	CHL	CHA-C1A-C2A	-5.69	119.95	133.31
40	Y	1623	NEX	C15-C14-C13	-5.65	119.35	127.28
29	b	620	BCR	C16-C17-C18	-5.64	119.37	127.28
39	r	622	XAT	O4-C5-C4	5.63	118.77	113.49
39	R	622	XAT	O4-C5-C4	5.62	118.76	113.49
27	C	503	CLA	C4A-NA-C1A	5.62	109.24	106.68
29	C	517	BCR	C15-C14-C13	-5.59	119.44	127.28
29	c	517	BCR	C15-C14-C13	-5.59	119.44	127.28
29	B	620	BCR	C16-C17-C18	-5.59	119.44	127.28
39	y	1622	XAT	O24-C25-C24	5.59	118.73	113.49
40	y	1623	NEX	C15-C14-C13	-5.59	119.44	127.28
27	b	603	CLA	C4A-NA-C1A	5.59	109.23	106.68
27	B	603	CLA	C4A-NA-C1A	5.58	109.22	106.68
27	b	604	CLA	C4A-NA-C1A	5.57	109.22	106.68
37	N	601	CHL	CHA-C1A-C2A	-5.57	120.23	133.31
37	n	601	CHL	CHA-C1A-C2A	-5.57	120.23	133.31
40	r	623	NEX	C15-C14-C13	-5.56	119.49	127.28
39	Y	1622	XAT	O24-C25-C24	5.55	118.70	113.49
40	R	623	NEX	C15-C14-C13	-5.55	119.49	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	604	CLA	C4A-NA-C1A	5.54	109.21	106.68
29	B	620	BCR	C7-C8-C9	-5.53	118.05	126.23
29	b	620	BCR	C7-C8-C9	-5.53	118.05	126.23
37	N	607	CHL	CHA-C1A-C2A	-5.53	120.32	133.31
40	G	1623	NEX	C11-C10-C9	-5.53	119.52	127.28
40	g	1623	NEX	C11-C10-C9	-5.53	119.52	127.28
37	n	607	CHL	CHA-C1A-C2A	-5.51	120.36	133.31
38	S	1620	LUT	C26-C27-C28	-5.49	116.03	124.58
29	b	619	BCR	C15-C14-C13	-5.48	119.59	127.28
29	B	619	BCR	C15-C14-C13	-5.48	119.59	127.28
29	a	411	BCR	C15-C14-C13	-5.48	119.60	127.28
38	s	1620	LUT	C26-C27-C28	-5.47	116.07	124.58
29	A	411	BCR	C15-C14-C13	-5.47	119.61	127.28
29	C	517	BCR	C24-C23-C22	-5.45	118.18	126.23
29	c	517	BCR	C24-C23-C22	-5.45	118.18	126.23
27	B	614	CLA	C4A-NA-C1A	5.44	109.16	106.68
27	b	614	CLA	C4A-NA-C1A	5.43	109.16	106.68
37	G	608	CHL	CHA-C1A-C2A	-5.43	120.57	133.31
37	g	608	CHL	CHA-C1A-C2A	-5.43	120.57	133.31
32	c	518	DGD	O3G-C3G-C2G	-5.41	97.65	110.82
32	C	518	DGD	O3G-C3G-C2G	-5.41	97.65	110.82
37	R	608	CHL	CHA-C1A-C2A	-5.40	120.64	133.31
40	R	623	NEX	O24-C25-C24	5.39	118.54	113.49
37	r	608	CHL	CHA-C1A-C2A	-5.39	120.66	133.31
39	n	1622	XAT	C15-C14-C13	-5.36	119.76	127.28
37	s	606	CHL	CHA-C1A-C2A	-5.36	120.72	133.31
37	S	606	CHL	CHA-C1A-C2A	-5.35	120.74	133.31
38	S	1620	LUT	C35-C34-C33	-5.34	119.79	127.28
38	s	1620	LUT	C35-C34-C33	-5.32	119.81	127.28
40	r	623	NEX	O24-C25-C24	5.32	118.48	113.49
39	N	1622	XAT	C15-C14-C13	-5.31	119.83	127.28
40	y	1623	NEX	O24-C25-C24	5.31	118.46	113.49
37	N	605	CHL	CHA-C1A-C2A	-5.29	120.89	133.31
37	n	605	CHL	CHA-C1A-C2A	-5.29	120.89	133.31
40	Y	1623	NEX	O24-C25-C24	5.28	118.44	113.49
29	b	618	BCR	C7-C8-C9	-5.28	118.43	126.23
29	C	516	BCR	C20-C21-C22	-5.26	119.90	127.28
27	b	606	CLA	C4A-NA-C1A	5.24	109.07	106.68
40	n	1623	NEX	C11-C10-C9	-5.23	119.94	127.28
29	B	618	BCR	C7-C8-C9	-5.23	118.50	126.23
29	c	516	BCR	C20-C21-C22	-5.22	119.96	127.28
40	N	1623	NEX	C11-C10-C9	-5.22	119.96	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	514	BCR	C15-C14-C13	-5.20	119.99	127.28
40	s	1623	NEX	O24-C25-C38	5.19	120.84	115.05
39	N	1622	XAT	O24-C25-C38	5.18	120.84	115.05
29	b	618	BCR	C28-C27-C26	-5.18	104.81	114.06
39	n	1622	XAT	O24-C25-C38	5.17	120.83	115.05
27	B	606	CLA	C4A-NA-C1A	5.17	109.04	106.68
29	B	618	BCR	C28-C27-C26	-5.17	104.84	114.06
38	S	1620	LUT	C7-C8-C9	-5.17	118.59	126.23
29	C	514	BCR	C15-C14-C13	-5.15	120.05	127.28
40	S	1623	NEX	O24-C25-C38	5.15	120.80	115.05
39	n	1622	XAT	O24-C25-C24	5.14	118.30	113.49
38	s	1620	LUT	C7-C8-C9	-5.13	118.64	126.23
40	S	1623	NEX	O24-C25-C24	5.13	118.30	113.49
39	N	1622	XAT	O24-C25-C24	5.12	118.29	113.49
40	s	1623	NEX	O24-C25-C24	5.10	118.27	113.49
29	a	411	BCR	C16-C17-C18	-5.03	120.22	127.28
29	A	411	BCR	C16-C17-C18	-5.01	120.25	127.28
37	g	605	CHL	CHA-C1A-C2A	-5.01	121.55	133.31
37	G	605	CHL	CHA-C1A-C2A	-5.00	121.58	133.31
40	Y	1623	NEX	O24-C25-C38	4.98	120.61	115.05
40	y	1623	NEX	O24-C25-C38	4.98	120.61	115.05
29	c	515	BCR	C11-C10-C9	-4.97	120.30	127.28
29	C	515	BCR	C11-C10-C9	-4.94	120.35	127.28
40	N	1623	NEX	C35-C34-C33	-4.93	120.37	127.28
39	R	622	XAT	O4-C5-C18	4.92	120.55	115.05
39	r	622	XAT	O4-C5-C18	4.92	120.55	115.05
40	n	1623	NEX	C15-C14-C13	-4.91	120.39	127.28
29	C	514	BCR	C16-C17-C18	-4.89	120.41	127.28
29	c	515	BCR	C3-C4-C5	-4.88	105.36	114.06
40	n	1623	NEX	C35-C34-C33	-4.87	120.44	127.28
29	c	514	BCR	C16-C17-C18	-4.87	120.44	127.28
38	s	1621	LUT	C26-C27-C28	-4.87	117.00	124.58
40	n	1623	NEX	O24-C25-C38	4.87	120.49	115.05
39	n	1622	XAT	C27-C28-C29	-4.87	117.98	125.53
38	g	1620	LUT	C26-C27-C28	-4.86	117.02	124.58
29	C	515	BCR	C3-C4-C5	-4.86	105.39	114.06
38	S	1621	LUT	C26-C27-C28	-4.85	117.03	124.58
40	N	1623	NEX	C15-C14-C13	-4.85	120.47	127.28
37	S	601	CHL	C1B-CHB-C4A	4.85	124.44	121.32
37	s	601	CHL	C1B-CHB-C4A	4.85	124.44	121.32
39	N	1622	XAT	C27-C28-C29	-4.84	118.02	125.53
38	G	1620	LUT	C26-C27-C28	-4.83	117.06	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	N	1623	NEX	O24-C25-C38	4.83	120.44	115.05
39	Y	1622	XAT	O24-C25-C38	4.83	120.44	115.05
39	y	1622	XAT	O24-C25-C38	4.83	120.44	115.05
40	g	1623	NEX	C27-C28-C29	-4.82	118.05	125.53
40	G	1623	NEX	C27-C28-C29	-4.80	118.08	125.53
39	R	622	XAT	C6-C7-C8	-4.77	115.91	125.99
39	r	622	XAT	C6-C7-C8	-4.77	115.92	125.99
32	c	519	DGD	O3G-C3G-C2G	-4.75	99.28	110.82
32	C	519	DGD	O3G-C3G-C2G	-4.72	99.33	110.82
38	n	1620	LUT	C26-C27-C28	-4.71	117.25	124.58
40	y	1623	NEX	C27-C28-C29	-4.69	118.25	125.53
29	b	618	BCR	C11-C10-C9	-4.68	120.71	127.28
38	n	1620	LUT	C15-C14-C13	-4.68	120.71	127.28
40	Y	1623	NEX	C27-C28-C29	-4.66	118.29	125.53
29	B	618	BCR	C11-C10-C9	-4.66	120.74	127.28
38	N	1620	LUT	C15-C14-C13	-4.66	120.74	127.28
29	B	618	BCR	C15-C14-C13	-4.65	120.75	127.28
29	b	618	BCR	C15-C14-C13	-4.65	120.75	127.28
40	R	623	NEX	O24-C25-C38	4.65	120.25	115.05
38	N	1620	LUT	C26-C27-C28	-4.65	117.34	124.58
38	G	1620	LUT	C35-C34-C33	-4.65	120.76	127.28
38	g	1620	LUT	C35-C34-C33	-4.65	120.76	127.28
29	b	619	BCR	C24-C23-C22	-4.64	119.37	126.23
40	r	623	NEX	O24-C25-C38	4.64	120.23	115.05
32	c	520	DGD	O3G-C3G-C2G	-4.62	99.58	110.82
29	C	516	BCR	C33-C5-C6	-4.62	119.44	124.48
29	c	516	BCR	C33-C5-C6	-4.62	119.44	124.48
32	C	520	DGD	O3G-C3G-C2G	-4.61	99.61	110.82
40	Y	1623	NEX	C35-C34-C33	-4.60	120.83	127.28
40	y	1623	NEX	C35-C34-C33	-4.60	120.83	127.28
35	S	2630	LHG	O4-P-O5	4.59	133.79	112.44
29	B	619	BCR	C24-C23-C22	-4.59	119.45	126.23
35	s	2630	LHG	O4-P-O5	4.58	133.76	112.44
38	n	1620	LUT	C35-C34-C33	-4.58	120.85	127.28
38	s	1621	LUT	C35-C34-C33	-4.58	120.85	127.28
29	B	620	BCR	C15-C14-C13	-4.58	120.86	127.28
29	b	620	BCR	C15-C14-C13	-4.58	120.86	127.28
37	Y	609	CHL	CBC-CAC-C3C	-4.57	106.33	112.87
37	y	609	CHL	CBC-CAC-C3C	-4.57	106.33	112.87
29	C	515	BCR	C7-C8-C9	-4.56	119.50	126.23
38	N	1620	LUT	C35-C34-C33	-4.55	120.89	127.28
29	c	515	BCR	C7-C8-C9	-4.53	119.53	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	S	1621	LUT	C35-C34-C33	-4.53	120.93	127.28
29	b	619	BCR	C20-C21-C22	-4.53	120.93	127.28
29	B	619	BCR	C20-C21-C22	-4.52	120.94	127.28
35	d	408	LHG	O4-P-O5	4.52	133.45	112.44
36	F	101	HEM	C4D-ND-C1D	4.51	110.54	105.21
35	D	408	LHG	O4-P-O5	4.50	133.39	112.44
36	f	101	HEM	C4D-ND-C1D	4.50	110.54	105.21
38	y	1621	LUT	C21-C26-C27	-4.50	107.65	112.83
35	g	2630	LHG	O4-P-O5	4.50	133.37	112.44
35	y	2630	LHG	O4-P-O5	4.50	133.36	112.44
35	Y	2630	LHG	O4-P-O5	4.49	133.35	112.44
29	C	517	BCR	C20-C21-C22	-4.49	120.98	127.28
29	c	517	BCR	C20-C21-C22	-4.49	120.98	127.28
29	b	618	BCR	C33-C5-C6	-4.49	119.59	124.48
35	G	2630	LHG	O4-P-O5	4.49	133.32	112.44
29	C	515	BCR	C24-C23-C22	-4.49	119.60	126.23
35	R	2630	LHG	O4-P-O5	4.48	133.28	112.44
29	B	618	BCR	C33-C5-C6	-4.48	119.60	124.48
35	r	2630	LHG	O4-P-O5	4.48	133.27	112.44
38	Y	1621	LUT	C21-C26-C27	-4.48	107.68	112.83
35	D	409	LHG	O4-P-O5	4.47	133.25	112.44
35	d	409	LHG	O4-P-O5	4.47	133.23	112.44
40	s	1623	NEX	C27-C28-C29	-4.47	118.60	125.53
29	c	515	BCR	C24-C23-C22	-4.46	119.63	126.23
35	l	101	LHG	O4-P-O5	4.46	133.18	112.44
35	L	101	LHG	O4-P-O5	4.45	133.14	112.44
40	S	1623	NEX	C27-C28-C29	-4.45	118.63	125.53
38	Y	1621	LUT	C15-C14-C13	-4.44	121.05	127.28
38	y	1621	LUT	C15-C14-C13	-4.44	121.05	127.28
35	D	410	LHG	O4-P-O5	4.43	133.07	112.44
35	d	410	LHG	O4-P-O5	4.43	133.07	112.44
39	N	1622	XAT	C6-C7-C8	-4.42	116.64	125.99
29	B	619	BCR	C16-C17-C18	-4.42	121.08	127.28
29	b	619	BCR	C16-C17-C18	-4.42	121.08	127.28
37	G	609	CHL	C1B-CHB-C4A	4.41	124.16	121.32
37	S	608	CHL	CHA-C1A-C2A	-4.40	122.98	133.31
38	y	1620	LUT	C26-C27-C28	-4.38	117.76	124.58
39	n	1622	XAT	C6-C7-C8	-4.38	116.73	125.99
37	s	608	CHL	CHA-C1A-C2A	-4.37	123.03	133.31
35	N	2630	LHG	O4-P-O5	4.37	132.78	112.44
35	n	2630	LHG	O4-P-O5	4.37	132.78	112.44
29	b	618	BCR	C24-C23-C22	-4.37	119.77	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	R	623	NEX	C27-C28-C29	-4.37	118.75	125.53
40	N	1623	NEX	C27-C28-C29	-4.36	118.76	125.53
37	S	607	CHL	CBC-CAC-C3C	-4.35	106.64	112.87
29	c	514	BCR	C11-C10-C9	-4.35	121.17	127.28
38	Y	1620	LUT	C26-C27-C28	-4.35	117.81	124.58
37	s	607	CHL	CBC-CAC-C3C	-4.35	106.65	112.87
29	B	618	BCR	C24-C23-C22	-4.34	119.81	126.23
40	r	623	NEX	C27-C28-C29	-4.34	118.79	125.53
37	g	609	CHL	C1B-CHB-C4A	4.34	124.11	121.32
40	n	1623	NEX	C27-C28-C29	-4.34	118.80	125.53
29	C	514	BCR	C11-C10-C9	-4.34	121.20	127.28
39	Y	1622	XAT	C7-C8-C9	-4.32	118.83	125.53
29	C	516	BCR	C7-C8-C9	-4.32	119.85	126.23
29	c	516	BCR	C7-C8-C9	-4.30	119.87	126.23
39	y	1622	XAT	C31-C30-C29	-4.30	121.25	127.28
39	y	1622	XAT	C7-C8-C9	-4.29	118.87	125.53
29	A	411	BCR	C7-C8-C9	-4.29	119.89	126.23
30	B	621	SQD	O9-S-C6	4.29	113.16	106.76
29	a	411	BCR	C33-C5-C6	-4.29	119.81	124.48
39	Y	1622	XAT	C31-C30-C29	-4.28	121.28	127.28
29	a	411	BCR	C7-C8-C9	-4.27	119.92	126.23
30	b	621	SQD	O9-S-C6	4.27	113.12	106.76
38	N	1621	LUT	C15-C14-C13	-4.26	121.30	127.28
38	n	1621	LUT	C15-C14-C13	-4.26	121.31	127.28
29	B	619	BCR	C11-C10-C9	-4.23	121.34	127.28
29	A	411	BCR	C33-C5-C6	-4.23	119.87	124.48
40	g	1623	NEX	C35-C34-C33	-4.23	121.34	127.28
39	r	622	XAT	O24-C25-C38	4.23	119.78	115.05
39	G	1622	XAT	C31-C30-C29	-4.22	121.35	127.28
37	S	606	CHL	C1B-CHB-C4A	4.22	124.04	121.32
34	D	405	PL9	C7-C3-C4	4.22	120.39	116.91
40	G	1623	NEX	C35-C34-C33	-4.22	121.36	127.28
29	b	619	BCR	C11-C10-C9	-4.22	121.36	127.28
37	s	606	CHL	C1B-CHB-C4A	4.19	124.02	121.32
29	c	517	BCR	C33-C5-C6	-4.19	119.91	124.48
39	g	1622	XAT	C31-C30-C29	-4.19	121.40	127.28
38	n	1621	LUT	C26-C27-C28	-4.19	118.06	124.58
37	S	607	CHL	CHA-C1A-C2A	-4.19	123.48	133.31
37	s	607	CHL	CHA-C1A-C2A	-4.19	123.48	133.31
38	G	1621	LUT	C21-C26-C27	-4.18	108.02	112.83
37	G	601	CHL	CBC-CAC-C3C	-4.17	106.90	112.87
38	g	1621	LUT	C21-C26-C27	-4.16	108.04	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	622	XAT	O24-C25-C38	4.16	119.70	115.05
38	N	1621	LUT	C26-C27-C28	-4.16	118.10	124.58
29	C	517	BCR	C33-C5-C6	-4.16	119.94	124.48
34	d	405	PL9	C7-C3-C4	4.14	120.32	116.91
37	S	608	CHL	CBC-CAC-C3C	-4.13	106.96	112.87
37	g	601	CHL	CBC-CAC-C3C	-4.13	106.96	112.87
39	R	622	XAT	C35-C15-C14	-4.12	115.09	123.52
39	r	622	XAT	C35-C15-C14	-4.11	115.10	123.52
37	s	608	CHL	CBC-CAC-C3C	-4.11	106.98	112.87
38	n	1621	LUT	C35-C34-C33	-4.11	121.51	127.28
38	N	1621	LUT	C35-C34-C33	-4.11	121.52	127.28
29	d	404	BCR	C33-C5-C6	-4.11	120.00	124.48
29	d	404	BCR	C38-C26-C25	-4.10	120.01	124.48
39	Y	1622	XAT	C26-C27-C28	-4.09	117.35	125.99
29	D	404	BCR	C38-C26-C25	-4.08	120.03	124.48
29	H	101	BCR	C24-C23-C22	-4.08	120.20	126.23
39	y	1622	XAT	C26-C27-C28	-4.08	117.38	125.99
29	h	101	BCR	C20-C21-C22	-4.07	121.56	127.28
29	D	404	BCR	C33-C5-C6	-4.07	120.04	124.48
29	B	618	BCR	C20-C21-C22	-4.06	121.58	127.28
29	b	618	BCR	C20-C21-C22	-4.06	121.58	127.28
29	H	101	BCR	C20-C21-C22	-4.06	121.59	127.28
29	D	404	BCR	C16-C17-C18	-4.05	121.60	127.28
37	g	608	CHL	C1B-CHB-C4A	4.05	123.93	121.32
37	G	608	CHL	C1B-CHB-C4A	4.05	123.93	121.32
29	h	101	BCR	C24-C23-C22	-4.05	120.25	126.23
39	R	622	XAT	C35-C34-C33	-4.04	121.61	127.28
38	R	620	LUT	C26-C27-C28	-4.03	118.30	124.58
29	d	404	BCR	C16-C17-C18	-4.03	121.62	127.28
38	r	620	LUT	C26-C27-C28	-4.03	118.31	124.58
37	r	608	CHL	C1B-CHB-C4A	4.02	123.91	121.32
39	g	1622	XAT	C26-C27-C28	-4.01	117.51	125.99
39	Y	1622	XAT	C11-C10-C9	-4.01	121.66	127.28
39	G	1622	XAT	C26-C27-C28	-4.01	117.52	125.99
29	H	101	BCR	C10-C11-C12	-3.99	111.62	123.20
30	B	621	SQD	O9-S-O7	-3.99	100.84	113.82
39	r	622	XAT	C35-C34-C33	-3.99	121.68	127.28
39	y	1622	XAT	C11-C10-C9	-3.99	121.69	127.28
30	b	621	SQD	O9-S-O7	-3.99	100.86	113.82
29	h	101	BCR	C10-C11-C12	-3.98	111.65	123.20
37	R	608	CHL	C1B-CHB-C4A	3.98	123.89	121.32
30	a	418	SQD	O9-S-O7	-3.98	100.87	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	418	SQD	O9-S-O7	-3.98	100.88	113.82
32	H	102	DGD	O3G-C3G-C2G	-3.97	101.16	110.82
38	R	620	LUT	C15-C14-C13	-3.97	121.72	127.28
38	r	620	LUT	C15-C14-C13	-3.97	121.72	127.28
32	h	102	DGD	O3G-C3G-C2G	-3.97	101.17	110.82
29	H	101	BCR	C7-C8-C9	-3.96	120.37	126.23
29	h	101	BCR	C7-C8-C9	-3.96	120.37	126.23
29	a	411	BCR	C11-C10-C9	-3.95	121.73	127.28
37	N	609	CHL	CBC-CAC-C3C	-3.94	107.23	112.87
38	y	1621	LUT	C35-C34-C33	-3.92	121.78	127.28
37	n	609	CHL	CBC-CAC-C3C	-3.91	107.28	112.87
38	g	1621	LUT	C26-C27-C28	-3.91	118.50	124.58
40	y	1623	NEX	C11-C10-C9	-3.91	121.80	127.28
40	Y	1623	NEX	C11-C10-C9	-3.90	121.80	127.28
38	G	1621	LUT	C26-C27-C28	-3.90	118.50	124.58
30	a	412	SQD	O9-S-O7	-3.90	101.13	113.82
38	Y	1621	LUT	C35-C34-C33	-3.90	121.81	127.28
29	B	619	BCR	C33-C5-C6	-3.90	120.23	124.48
29	A	411	BCR	C11-C10-C9	-3.90	121.81	127.28
29	b	619	BCR	C33-C5-C6	-3.89	120.23	124.48
38	N	1620	LUT	C8-C7-C6	-3.89	116.60	127.00
29	B	619	BCR	C8-C7-C6	-3.88	116.64	127.00
38	n	1620	LUT	C8-C7-C6	-3.88	116.64	127.00
30	A	412	SQD	O9-S-O7	-3.87	101.22	113.82
29	b	619	BCR	C8-C7-C6	-3.87	116.65	127.00
29	c	514	BCR	C24-C23-C22	-3.85	120.53	126.23
29	c	517	BCR	C16-C17-C18	-3.85	121.87	127.28
38	Y	1620	LUT	C18-C5-C6	-3.84	120.29	124.48
38	y	1620	LUT	C18-C5-C6	-3.84	120.29	124.48
40	s	1623	NEX	C11-C10-C9	-3.84	121.89	127.28
40	S	1623	NEX	C11-C10-C9	-3.84	121.89	127.28
29	C	514	BCR	C24-C23-C22	-3.83	120.56	126.23
29	B	618	BCR	C16-C17-C18	-3.83	121.91	127.28
29	b	618	BCR	C16-C17-C18	-3.83	121.91	127.28
37	N	605	CHL	C1B-CHB-C4A	3.83	123.79	121.32
29	C	517	BCR	C16-C17-C18	-3.82	121.92	127.28
29	C	517	BCR	C38-C26-C25	-3.82	120.32	124.48
29	c	516	BCR	C15-C14-C13	-3.82	121.93	127.28
40	r	623	NEX	C11-C10-C9	-3.81	121.93	127.28
29	C	516	BCR	C15-C14-C13	-3.80	121.95	127.28
29	c	517	BCR	C38-C26-C25	-3.80	120.34	124.48
38	G	1621	LUT	C35-C34-C33	-3.79	121.97	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	R	623	NEX	C11-C10-C9	-3.78	121.97	127.28
38	g	1621	LUT	C35-C34-C33	-3.78	121.98	127.28
30	A	418	SQD	O47-C7-C8	3.77	119.65	111.48
37	N	607	CHL	C1-C2-C3	-3.77	120.01	126.20
37	Y	601	CHL	CBC-CAC-C3C	-3.77	107.47	112.87
38	s	1621	LUT	C21-C26-C27	-3.77	108.49	112.83
37	n	605	CHL	C1B-CHB-C4A	3.77	123.75	121.32
29	A	411	BCR	C20-C21-C22	-3.77	122.00	127.28
29	a	411	BCR	C20-C21-C22	-3.77	122.00	127.28
30	a	418	SQD	O47-C7-C8	3.76	119.62	111.48
38	n	1621	LUT	C8-C7-C6	-3.76	116.97	127.00
38	y	1621	LUT	C26-C27-C28	-3.75	118.75	124.58
38	S	1621	LUT	C21-C26-C27	-3.74	108.53	112.83
37	y	601	CHL	CBC-CAC-C3C	-3.74	107.52	112.87
37	n	607	CHL	C1-C2-C3	-3.73	120.08	126.20
38	Y	1621	LUT	C26-C27-C28	-3.73	118.77	124.58
32	C	520	DGD	O6D-C1D-O3G	-3.73	101.23	110.04
27	n	611	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
38	N	1621	LUT	C8-C7-C6	-3.73	117.04	127.00
29	H	101	BCR	C15-C14-C13	-3.73	122.05	127.28
29	h	101	BCR	C15-C14-C13	-3.73	122.05	127.28
27	N	611	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
39	G	1622	XAT	C6-C7-C8	-3.72	118.13	125.99
32	c	520	DGD	O6D-C1D-O3G	-3.72	101.25	110.04
39	g	1622	XAT	C6-C7-C8	-3.72	118.13	125.99
39	N	1622	XAT	C15-C35-C34	-3.71	115.92	123.52
27	B	603	CLA	CAA-C2A-C3A	-3.70	103.01	113.00
38	S	1620	LUT	C11-C10-C9	-3.69	122.11	127.28
38	g	1620	LUT	C7-C8-C9	-3.69	120.78	126.23
38	G	1620	LUT	C7-C8-C9	-3.69	120.78	126.23
38	Y	1620	LUT	C35-C34-C33	-3.68	122.12	127.28
38	y	1620	LUT	C35-C34-C33	-3.68	122.12	127.28
29	c	515	BCR	C21-C20-C19	-3.67	112.55	123.20
27	b	603	CLA	CAA-C2A-C3A	-3.67	103.08	113.00
39	n	1622	XAT	C15-C35-C34	-3.67	116.02	123.52
32	C	519	DGD	O6D-C1D-O3G	-3.66	101.39	110.04
27	c	507	CLA	C3B-C4B-NB	-3.66	107.26	110.53
29	C	515	BCR	C21-C20-C19	-3.66	112.58	123.20
29	B	620	BCR	C24-C23-C22	-3.66	120.82	126.23
29	d	404	BCR	C20-C21-C22	-3.66	122.15	127.28
32	c	519	DGD	O6D-C1D-O3G	-3.66	101.40	110.04
29	b	620	BCR	C24-C23-C22	-3.65	120.83	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	N	1622	XAT	C26-C27-C28	-3.65	118.28	125.99
39	n	1622	XAT	C26-C27-C28	-3.64	118.30	125.99
38	s	1620	LUT	C11-C10-C9	-3.63	122.18	127.28
40	R	623	NEX	C26-C27-C28	-3.63	118.31	125.99
29	c	514	BCR	C20-C21-C22	-3.63	122.19	127.28
27	B	605	CLA	CAA-C2A-C3A	-3.62	103.22	113.00
27	b	605	CLA	CAA-C2A-C3A	-3.62	103.22	113.00
40	r	623	NEX	C26-C27-C28	-3.61	118.35	125.99
29	C	514	BCR	C20-C21-C22	-3.61	122.22	127.28
29	D	404	BCR	C20-C21-C22	-3.61	122.22	127.28
38	Y	1620	LUT	C15-C14-C13	-3.60	122.23	127.28
38	y	1620	LUT	C15-C14-C13	-3.60	122.23	127.28
37	g	601	CHL	C1-C2-C3	-3.60	120.30	126.20
37	n	608	CHL	CBC-CAC-C3C	-3.60	107.72	112.87
27	C	507	CLA	C3B-C4B-NB	-3.60	107.32	110.53
38	n	1621	LUT	C18-C5-C6	-3.60	120.56	124.48
38	y	1620	LUT	C7-C8-C9	-3.59	120.92	126.23
38	y	1621	LUT	C10-C11-C12	-3.59	112.79	123.20
38	Y	1621	LUT	C10-C11-C12	-3.59	112.79	123.20
39	N	1622	XAT	O4-C5-C18	3.59	119.06	115.05
38	y	1620	LUT	C21-C26-C27	-3.59	108.70	112.83
30	A	412	SQD	O47-C7-C8	3.59	119.25	111.48
30	a	412	SQD	O47-C7-C8	3.59	119.25	111.48
38	N	1621	LUT	C18-C5-C6	-3.59	120.57	124.48
37	G	601	CHL	C1-C2-C3	-3.58	120.33	126.20
37	N	608	CHL	CBC-CAC-C3C	-3.58	107.75	112.87
38	n	1620	LUT	C21-C26-C27	-3.57	108.72	112.83
29	C	516	BCR	C16-C15-C14	-3.57	116.21	123.52
29	c	516	BCR	C16-C15-C14	-3.57	116.21	123.52
38	Y	1620	LUT	C7-C8-C9	-3.57	120.95	126.23
37	y	601	CHL	C1-C2-C3	-3.57	120.35	126.20
37	y	601	CHL	O1D-CGD-CBD	-3.56	119.32	124.72
34	D	405	PL9	C7-C3-C2	-3.56	119.20	123.39
27	b	607	CLA	C3B-C4B-NB	-3.55	107.36	110.53
37	Y	601	CHL	C1-C2-C3	-3.55	120.39	126.20
38	N	1620	LUT	C21-C26-C27	-3.54	108.75	112.83
39	G	1622	XAT	C35-C34-C33	-3.54	122.31	127.28
29	a	411	BCR	C24-C23-C22	-3.54	121.00	126.23
38	S	1621	LUT	C8-C7-C6	-3.54	117.54	127.00
39	N	1622	XAT	C11-C10-C9	-3.54	122.32	127.28
37	Y	601	CHL	O1D-CGD-CBD	-3.54	119.36	124.72
39	n	1622	XAT	O4-C5-C18	3.53	119.00	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	s	1621	LUT	C8-C7-C6	-3.53	117.56	127.00
34	d	405	PL9	C7-C3-C2	-3.53	119.23	123.39
39	g	1622	XAT	C35-C34-C33	-3.52	122.33	127.28
38	Y	1620	LUT	C21-C26-C27	-3.52	108.77	112.83
27	B	607	CLA	C3B-C4B-NB	-3.52	107.39	110.53
29	A	411	BCR	C24-C23-C22	-3.52	121.03	126.23
29	A	411	BCR	C38-C26-C25	-3.51	120.65	124.48
38	y	1621	LUT	C8-C7-C6	-3.51	117.63	127.00
29	B	619	BCR	C15-C16-C17	-3.49	116.37	123.52
29	b	619	BCR	C15-C16-C17	-3.49	116.38	123.52
29	c	516	BCR	C28-C27-C26	-3.49	107.83	114.06
38	Y	1621	LUT	C8-C7-C6	-3.49	117.68	127.00
39	n	1622	XAT	C11-C10-C9	-3.49	122.39	127.28
37	N	601	CHL	C1B-CHB-C4A	3.48	123.56	121.32
29	c	517	BCR	C15-C16-C17	-3.48	116.41	123.52
27	B	607	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
32	C	518	DGD	O6D-C1D-O3G	-3.47	101.85	110.04
29	C	516	BCR	C28-C27-C26	-3.47	107.87	114.06
28	A	409	PHO	CMB-C2B-C3B	3.47	131.61	124.68
39	G	1622	XAT	O24-C25-C38	3.46	118.92	115.05
29	C	517	BCR	C15-C16-C17	-3.46	116.45	123.52
27	b	607	CLA	O2D-CGD-O1D	-3.45	117.12	123.85
27	R	604	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
32	c	518	DGD	O6D-C1D-O3G	-3.45	101.89	110.04
39	g	1622	XAT	O24-C25-C38	3.45	118.91	115.05
30	a	418	SQD	O7-S-C6	3.45	111.91	106.76
29	a	411	BCR	C38-C26-C25	-3.45	120.72	124.48
37	Y	606	CHL	CBC-CAC-C3C	-3.44	107.95	112.87
37	y	606	CHL	CBC-CAC-C3C	-3.44	107.95	112.87
29	B	620	BCR	C1-C6-C5	-3.44	117.94	122.64
30	A	418	SQD	O7-S-C6	3.44	111.89	106.76
28	a	409	PHO	CMB-C2B-C3B	3.43	131.54	124.68
29	b	620	BCR	C1-C6-C5	-3.43	117.95	122.64
38	G	1621	LUT	C8-C7-C6	-3.43	117.84	127.00
29	H	101	BCR	C28-C27-C26	-3.43	107.94	114.06
37	n	601	CHL	C1B-CHB-C4A	3.42	123.53	121.32
38	g	1621	LUT	C8-C7-C6	-3.42	117.86	127.00
37	S	601	CHL	O1D-CGD-CBD	-3.42	119.54	124.72
27	r	604	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
38	S	1620	LUT	C35-C15-C14	-3.41	116.53	123.52
29	h	101	BCR	C28-C27-C26	-3.41	107.98	114.06
37	R	607	CHL	O1D-CGD-CBD	-3.41	119.56	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	n	610	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
40	y	1623	NEX	C24-C23-C22	-3.40	104.42	110.79
28	a	409	PHO	O1D-CGD-CBD	3.40	129.88	124.72
27	N	610	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
38	Y	1620	LUT	C10-C11-C12	-3.40	113.35	123.20
37	s	601	CHL	O1D-CGD-CBD	-3.39	119.58	124.72
38	y	1620	LUT	C10-C11-C12	-3.39	113.37	123.20
40	Y	1623	NEX	C24-C23-C22	-3.39	104.44	110.79
29	C	515	BCR	C15-C16-C17	-3.39	116.58	123.52
38	r	620	LUT	C21-C26-C27	-3.39	108.93	112.83
29	d	404	BCR	C16-C15-C14	-3.39	116.59	123.52
27	Y	612	CLA	C3B-C4B-NB	-3.38	107.51	110.53
29	c	515	BCR	C15-C16-C17	-3.38	116.60	123.52
27	y	612	CLA	C3B-C4B-NB	-3.38	107.51	110.53
37	r	607	CHL	O1D-CGD-CBD	-3.37	119.61	124.72
38	g	1621	LUT	C15-C14-C13	-3.37	122.55	127.28
38	s	1620	LUT	C35-C15-C14	-3.37	116.63	123.52
27	Y	612	CLA	C1-C2-C3	-3.37	120.68	126.20
27	c	508	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
40	y	1623	NEX	C26-C27-C28	-3.36	118.90	125.99
27	y	612	CLA	C1-C2-C3	-3.34	120.72	126.20
29	D	404	BCR	C16-C15-C14	-3.34	116.68	123.52
29	c	514	BCR	C3-C4-C5	-3.34	108.09	114.06
37	N	606	CHL	O1D-CGD-CBD	-3.34	119.65	124.72
38	G	1621	LUT	C15-C14-C13	-3.34	122.59	127.28
39	r	622	XAT	C15-C14-C13	-3.34	122.59	127.28
28	A	409	PHO	O1D-CGD-CBD	3.34	129.79	124.72
27	C	508	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
38	G	1620	LUT	C18-C5-C6	-3.33	120.84	124.48
40	Y	1623	NEX	C26-C27-C28	-3.33	118.95	125.99
34	D	405	PL9	C40-C39-C41	3.33	121.01	115.23
38	g	1620	LUT	C18-C5-C6	-3.33	120.85	124.48
37	S	607	CHL	OMC-CMC-C2C	-3.33	119.33	125.12
37	s	607	CHL	OMC-CMC-C2C	-3.33	119.33	125.12
27	A	410	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
27	a	410	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
37	n	606	CHL	O1D-CGD-CBD	-3.33	119.67	124.72
29	b	620	BCR	C11-C10-C9	-3.33	122.61	127.28
39	R	622	XAT	C15-C14-C13	-3.33	122.61	127.28
29	B	619	BCR	C7-C8-C9	-3.33	121.31	126.23
29	b	619	BCR	C7-C8-C9	-3.33	121.31	126.23
29	c	515	BCR	C28-C27-C26	-3.33	108.12	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	514	BCR	C3-C4-C5	-3.32	108.13	114.06
29	B	620	BCR	C38-C26-C25	-3.32	120.86	124.48
29	b	620	BCR	C38-C26-C25	-3.32	120.86	124.48
32	C	518	DGD	C3G-C2G-C1G	-3.32	104.05	111.78
32	c	518	DGD	C3G-C2G-C1G	-3.32	104.05	111.78
38	R	620	LUT	C21-C26-C27	-3.32	109.01	112.83
29	C	515	BCR	C28-C27-C26	-3.32	108.14	114.06
40	s	1623	NEX	C26-C27-C28	-3.31	118.99	125.99
29	C	516	BCR	C11-C10-C9	-3.31	122.64	127.28
38	S	1621	LUT	C15-C14-C13	-3.31	122.64	127.28
29	c	516	BCR	C11-C10-C9	-3.30	122.64	127.28
29	B	620	BCR	C11-C10-C9	-3.30	122.65	127.28
38	s	1621	LUT	C15-C14-C13	-3.30	122.66	127.28
38	S	1620	LUT	C18-C5-C6	-3.30	120.89	124.48
40	S	1623	NEX	C26-C27-C28	-3.30	119.03	125.99
40	n	1623	NEX	C24-C23-C22	-3.30	104.63	110.79
30	B	621	SQD	O47-C7-C8	3.29	118.61	111.48
27	c	509	CLA	C3B-C4B-NB	-3.29	107.59	110.53
34	d	405	PL9	C40-C39-C41	3.29	120.94	115.23
38	n	1620	LUT	C18-C5-C6	-3.29	120.89	124.48
38	s	1620	LUT	C18-C5-C6	-3.29	120.89	124.48
38	g	1621	LUT	C18-C5-C6	-3.28	120.90	124.48
29	H	101	BCR	C16-C15-C14	-3.28	116.80	123.52
29	h	101	BCR	C16-C15-C14	-3.28	116.80	123.52
27	g	614	CLA	C3B-C4B-NB	-3.28	107.60	110.53
40	N	1623	NEX	C24-C23-C22	-3.28	104.66	110.79
29	C	516	BCR	C38-C26-C25	-3.28	120.91	124.48
37	Y	608	CHL	CBC-CAC-C3C	-3.28	108.18	112.87
30	b	621	SQD	O47-C7-C8	3.28	118.57	111.48
27	C	509	CLA	C3B-C4B-NB	-3.27	107.61	110.53
27	B	613	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
39	r	622	XAT	C10-C11-C12	-3.27	113.72	123.20
38	S	1621	LUT	C10-C11-C12	-3.27	113.72	123.20
38	s	1621	LUT	C10-C11-C12	-3.27	113.73	123.20
27	B	606	CLA	C3B-C4B-NB	-3.27	107.61	110.53
29	C	517	BCR	C21-C20-C19	-3.27	113.73	123.20
29	c	517	BCR	C21-C20-C19	-3.27	113.73	123.20
27	b	611	CLA	C3B-C4B-NB	-3.26	107.62	110.53
39	R	622	XAT	C10-C11-C12	-3.26	113.74	123.20
38	R	620	LUT	C8-C7-C6	-3.26	118.28	127.00
38	G	1620	LUT	C21-C26-C27	-3.26	109.08	112.83
38	n	1621	LUT	C21-C26-C27	-3.26	109.08	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	r	620	LUT	C8-C7-C6	-3.26	118.30	127.00
27	b	615	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
38	N	1620	LUT	C18-C5-C6	-3.25	120.93	124.48
31	A	413	LMG	O6-C5-C4	3.25	115.56	109.70
29	c	516	BCR	C3-C4-C5	-3.25	108.26	114.06
37	y	608	CHL	CBC-CAC-C3C	-3.25	108.22	112.87
29	c	516	BCR	C38-C26-C25	-3.25	120.94	124.48
38	G	1621	LUT	C18-C5-C6	-3.25	120.94	124.48
38	g	1620	LUT	C21-C26-C27	-3.25	109.09	112.83
31	D	411	LMG	C1-C2-C3	-3.24	103.19	110.01
30	B	621	SQD	O7-S-C6	3.24	111.60	106.76
38	N	1621	LUT	C21-C26-C27	-3.24	109.10	112.83
27	Y	603	CLA	C3B-C4B-NB	-3.24	107.64	110.53
27	B	615	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
30	b	621	SQD	O7-S-C6	3.24	111.59	106.76
27	G	614	CLA	C3B-C4B-NB	-3.24	107.64	110.53
31	d	411	LMG	C1-C2-C3	-3.24	103.20	110.01
27	b	613	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
31	a	413	LMG	O6-C5-C4	3.24	115.53	109.70
38	y	1621	LUT	C11-C10-C9	-3.23	122.74	127.28
38	g	1620	LUT	C11-C10-C9	-3.23	122.74	127.28
27	B	611	CLA	C3B-C4B-NB	-3.23	107.65	110.53
37	N	601	CHL	O1D-CGD-CBD	-3.23	119.83	124.72
37	n	601	CHL	O1D-CGD-CBD	-3.23	119.83	124.72
29	C	516	BCR	C3-C4-C5	-3.23	108.30	114.06
29	B	620	BCR	C21-C20-C19	-3.22	113.88	123.20
38	Y	1621	LUT	C11-C10-C9	-3.22	122.77	127.28
37	n	606	CHL	C1C-CHC-C4B	3.22	127.58	116.07
40	s	1623	NEX	C31-C30-C29	-3.21	122.77	127.28
38	n	1620	LUT	C30-C31-C32	-3.21	113.89	123.20
29	b	620	BCR	C21-C20-C19	-3.21	113.89	123.20
38	g	1620	LUT	C15-C14-C13	-3.21	122.77	127.28
29	B	620	BCR	C33-C5-C4	3.20	120.43	113.60
29	b	620	BCR	C33-C5-C4	3.20	120.43	113.60
27	S	604	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
27	b	606	CLA	C3B-C4B-NB	-3.20	107.67	110.53
37	N	606	CHL	C1C-CHC-C4B	3.20	127.52	116.07
27	c	501	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
27	s	604	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
27	C	501	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
37	y	607	CHL	O1D-CGD-CBD	-3.19	119.88	124.72
40	S	1623	NEX	C31-C30-C29	-3.19	122.80	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	603	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
27	b	603	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
27	c	510	CLA	C3B-C4B-NB	-3.19	107.68	110.53
38	G	1620	LUT	C11-C10-C9	-3.19	122.81	127.28
37	R	606	CHL	OMC-CMC-C2C	-3.19	119.59	125.12
27	y	603	CLA	C3B-C4B-NB	-3.19	107.69	110.53
38	R	620	LUT	C31-C30-C29	-3.18	122.82	127.28
37	Y	607	CHL	O1D-CGD-CBD	-3.18	119.90	124.72
39	R	622	XAT	C4-C3-C2	-3.18	104.84	110.79
27	C	505	CLA	CMB-C2B-C1B	-3.18	120.58	125.42
27	c	505	CLA	CMB-C2B-C1B	-3.18	120.58	125.42
38	N	1620	LUT	C30-C31-C32	-3.18	113.99	123.20
27	n	610	CLA	C3B-C4B-NB	-3.18	107.69	110.53
38	y	1620	LUT	C30-C31-C32	-3.18	113.99	123.20
37	r	606	CHL	OMC-CMC-C2C	-3.18	119.60	125.12
38	Y	1620	LUT	C30-C31-C32	-3.17	114.00	123.20
32	h	102	DGD	O6D-C1D-O3G	-3.17	102.55	110.04
29	B	620	BCR	C33-C5-C6	-3.17	121.02	124.48
29	b	620	BCR	C33-C5-C6	-3.17	121.02	124.48
32	H	102	DGD	O6D-C1D-O3G	-3.17	102.55	110.04
38	G	1620	LUT	C15-C14-C13	-3.17	122.83	127.28
27	Y	613	CLA	C3B-C4B-NB	-3.16	107.71	110.53
40	g	1623	NEX	O24-C25-C38	3.16	118.58	115.05
27	g	602	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
27	Y	614	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
37	n	608	CHL	C1C-CHC-C4B	3.15	127.36	116.07
29	d	404	BCR	C3-C4-C5	-3.15	108.43	114.06
38	r	620	LUT	C31-C30-C29	-3.15	122.86	127.28
39	r	622	XAT	C4-C3-C2	-3.15	104.89	110.79
38	Y	1620	LUT	C11-C10-C9	-3.15	122.86	127.28
27	R	616	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
27	r	616	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
29	D	404	BCR	C3-C4-C5	-3.14	108.45	114.06
27	c	505	CLA	C1-C2-C3	-3.14	121.05	126.20
38	y	1620	LUT	C11-C10-C9	-3.14	122.88	127.28
37	N	608	CHL	C1C-CHC-C4B	3.14	127.30	116.07
27	c	501	CLA	C3B-C4B-NB	-3.14	107.73	110.53
29	c	514	BCR	C28-C27-C26	-3.14	108.46	114.06
37	S	606	CHL	CBC-CAC-C3C	-3.14	108.38	112.87
27	g	602	CLA	C3B-C4B-NB	-3.14	107.73	110.53
37	s	606	CHL	CBC-CAC-C3C	-3.14	108.38	112.87
27	y	613	CLA	C3B-C4B-NB	-3.13	107.73	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	G	602	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
37	G	601	CHL	O1D-CGD-CBD	-3.13	119.97	124.72
37	g	601	CHL	O1D-CGD-CBD	-3.13	119.97	124.72
27	G	602	CLA	C3B-C4B-NB	-3.13	107.73	110.53
29	C	514	BCR	C28-C27-C26	-3.13	108.48	114.06
27	C	510	CLA	C3B-C4B-NB	-3.12	107.74	110.53
38	G	1621	LUT	C10-C11-C12	-3.12	114.15	123.20
38	g	1621	LUT	C10-C11-C12	-3.12	114.15	123.20
29	B	620	BCR	C4-C5-C6	-3.12	118.48	122.70
29	b	620	BCR	C4-C5-C6	-3.12	118.48	122.70
27	n	610	CLA	C1-C2-C3	-3.12	121.08	126.20
27	N	610	CLA	C1-C2-C3	-3.12	121.08	126.20
27	C	507	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
27	c	507	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
27	C	501	CLA	C3B-C4B-NB	-3.12	107.75	110.53
28	a	408	PHO	O1D-CGD-CBD	3.12	129.45	124.72
27	C	505	CLA	C1-C2-C3	-3.12	121.09	126.20
27	y	614	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
27	n	614	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
27	n	602	CLA	C3B-C4B-NB	-3.11	107.75	110.53
32	c	518	DGD	C4E-C3E-C2E	-3.11	105.37	110.83
32	C	518	DGD	C4E-C3E-C2E	-3.11	105.37	110.83
40	G	1623	NEX	C31-C30-C29	-3.11	122.92	127.28
37	y	606	CHL	O1D-CGD-CBD	-3.11	120.01	124.72
28	A	408	PHO	O1D-CGD-CBD	3.11	129.43	124.72
27	N	614	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
31	A	413	LMG	C1-C2-C3	-3.10	103.48	110.01
27	D	403	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
27	d	403	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
31	a	413	LMG	C1-C2-C3	-3.10	103.48	110.01
29	B	618	BCR	C27-C26-C25	-3.10	118.51	122.70
27	B	610	CLA	C3B-C4B-NB	-3.10	107.76	110.53
27	b	610	CLA	C3B-C4B-NB	-3.10	107.76	110.53
40	N	1623	NEX	C26-C27-C28	-3.10	119.44	125.99
37	Y	606	CHL	O1D-CGD-CBD	-3.10	120.02	124.72
27	y	614	CLA	C3B-C4B-NB	-3.10	107.77	110.53
40	S	1623	NEX	C24-C23-C22	-3.10	105.00	110.79
40	s	1623	NEX	C24-C23-C22	-3.10	105.00	110.79
27	B	604	CLA	C3B-C4B-NB	-3.10	107.77	110.53
29	b	619	BCR	C28-C27-C26	-3.09	108.54	114.06
40	n	1623	NEX	C26-C27-C28	-3.09	119.45	125.99
34	d	405	PL9	C27-C28-C29	-3.09	120.55	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	1622	XAT	C15-C35-C34	-3.09	117.19	123.52
37	Y	606	CHL	C1C-CHC-C4B	3.09	127.12	116.07
27	Y	611	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
27	y	611	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
40	G	1623	NEX	O24-C25-C38	3.09	118.50	115.05
37	y	606	CHL	C1C-CHC-C4B	3.09	127.11	116.07
27	b	612	CLA	C3B-C4B-NB	-3.09	107.78	110.53
29	b	618	BCR	C27-C26-C25	-3.08	118.54	122.70
27	b	604	CLA	C3B-C4B-NB	-3.08	107.78	110.53
40	g	1623	NEX	C31-C30-C29	-3.08	122.96	127.28
38	y	1621	LUT	C7-C8-C9	-3.08	121.68	126.23
27	B	602	CLA	C3B-C4B-NB	-3.08	107.78	110.53
27	b	602	CLA	C3B-C4B-NB	-3.08	107.78	110.53
29	B	619	BCR	C28-C27-C26	-3.08	108.57	114.06
27	B	605	CLA	C1-C2-C3	-3.07	121.16	126.20
27	N	610	CLA	C3B-C4B-NB	-3.07	107.79	110.53
27	R	609	CLA	C3B-C4B-NB	-3.07	107.79	110.53
27	r	602	CLA	C3B-C4B-NB	-3.07	107.79	110.53
27	r	609	CLA	C3B-C4B-NB	-3.07	107.79	110.53
34	D	405	PL9	C27-C28-C29	-3.07	120.59	127.62
27	b	605	CLA	C1-C2-C3	-3.07	121.17	126.20
27	B	612	CLA	C3B-C4B-NB	-3.07	107.79	110.53
39	g	1622	XAT	C15-C35-C34	-3.07	117.25	123.52
27	g	613	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
27	b	605	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
27	b	606	CLA	C1-C2-C3	-3.06	121.18	126.20
27	N	602	CLA	C3B-C4B-NB	-3.06	107.80	110.53
39	N	1622	XAT	C24-C23-C22	-3.06	105.07	110.79
27	B	612	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
38	Y	1621	LUT	C7-C8-C9	-3.05	121.72	126.23
38	n	1621	LUT	C10-C11-C12	-3.05	114.35	123.20
37	S	601	CHL	C1C-CHC-C4B	3.05	126.99	116.07
38	R	620	LUT	C18-C5-C6	-3.05	121.16	124.48
38	r	620	LUT	C18-C5-C6	-3.05	121.16	124.48
37	N	605	CHL	C1C-CHC-C4B	3.05	126.98	116.07
37	n	605	CHL	C1C-CHC-C4B	3.05	126.98	116.07
39	n	1622	XAT	C24-C23-C22	-3.05	105.09	110.79
27	G	613	CLA	C3B-C4B-NB	-3.05	107.81	110.53
27	g	613	CLA	C3B-C4B-NB	-3.05	107.81	110.53
27	B	605	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
29	B	618	BCR	C21-C20-C19	-3.05	114.37	123.20
27	B	611	CLA	O2D-CGD-O1D	-3.05	117.92	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	412	SQD	O7-S-C6	3.05	111.30	106.76
29	b	618	BCR	C21-C20-C19	-3.04	114.38	123.20
37	Y	608	CHL	C1C-CHC-C4B	3.04	126.96	116.07
27	G	613	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
27	b	612	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
37	y	607	CHL	C1C-CHC-C4B	3.04	126.95	116.07
30	A	412	SQD	O7-S-C6	3.04	111.30	106.76
37	Y	607	CHL	C1C-CHC-C4B	3.04	126.95	116.07
27	R	602	CLA	C3B-C4B-NB	-3.04	107.82	110.53
35	S	2630	LHG	O8-C23-C24	3.04	121.09	111.83
38	N	1621	LUT	C10-C11-C12	-3.03	114.41	123.20
37	s	601	CHL	C1C-CHC-C4B	3.03	126.93	116.07
35	s	2630	LHG	O8-C23-C24	3.03	121.08	111.83
27	r	612	CLA	C3B-C4B-NB	-3.03	107.82	110.53
27	Y	614	CLA	C3B-C4B-NB	-3.03	107.83	110.53
37	y	608	CHL	C1C-CHC-C4B	3.03	126.91	116.07
27	D	402	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
37	Y	605	CHL	OMC-CMC-C2C	-3.03	119.86	125.12
35	D	409	LHG	C11-C10-C9	-3.03	99.06	114.37
35	d	409	LHG	C11-C10-C9	-3.03	99.07	114.37
37	S	608	CHL	O2A-CGA-CBA	3.03	121.06	111.83
37	r	607	CHL	O2A-CGA-CBA	3.03	121.06	111.83
29	C	517	BCR	C10-C11-C12	-3.02	114.44	123.20
29	c	517	BCR	C10-C11-C12	-3.02	114.44	123.20
39	Y	1622	XAT	C15-C14-C13	-3.02	123.04	127.28
29	c	514	BCR	C33-C5-C6	-3.02	121.19	124.48
38	s	1620	LUT	C21-C26-C27	-3.02	109.36	112.83
29	a	411	BCR	C23-C24-C25	-3.02	118.94	127.00
37	y	605	CHL	OMC-CMC-C2C	-3.02	119.88	125.12
37	N	609	CHL	CMA-C3A-C4A	-3.02	108.11	114.61
27	B	606	CLA	C1-C2-C3	-3.02	121.26	126.20
37	s	608	CHL	O2A-CGA-CBA	3.01	121.03	111.83
38	G	1621	LUT	C31-C30-C29	-3.01	123.05	127.28
38	g	1621	LUT	C31-C30-C29	-3.01	123.05	127.28
34	D	405	PL9	C7-C8-C9	-3.01	121.64	126.83
34	d	405	PL9	C7-C8-C9	-3.01	121.64	126.83
37	r	607	CHL	C1C-CHC-C4B	3.01	126.85	116.07
31	c	521	LMG	O6-C1-O1	-3.01	102.93	110.04
37	R	607	CHL	C1C-CHC-C4B	3.01	126.85	116.07
40	R	623	NEX	C15-C35-C34	-3.01	117.36	123.52
32	C	519	DGD	O3G-C1D-C2D	-3.01	103.70	108.27
32	c	519	DGD	O3G-C1D-C2D	-3.01	103.70	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	521	LMG	O6-C1-O1	-3.01	102.93	110.04
40	S	1623	NEX	C15-C35-C34	-3.01	117.36	123.52
40	s	1623	NEX	C15-C35-C34	-3.01	117.36	123.52
27	d	402	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
37	R	607	CHL	O2A-CGA-CBA	3.01	121.00	111.83
29	B	620	BCR	C3-C4-C5	-3.01	108.70	114.06
27	R	612	CLA	C3B-C4B-NB	-3.01	107.85	110.53
27	b	616	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
29	A	411	BCR	C23-C24-C25	-3.01	118.97	127.00
27	c	510	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
39	y	1622	XAT	C15-C14-C13	-3.00	123.07	127.28
27	C	506	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
32	c	518	DGD	C1D-C2D-C3D	-3.00	103.69	110.01
38	g	1620	LUT	C35-C15-C14	-3.00	117.38	123.52
40	s	1623	NEX	C35-C34-C33	-3.00	123.07	127.28
32	C	518	DGD	C1D-C2D-C3D	-3.00	103.70	110.01
37	S	606	CHL	C1C-CHC-C4B	3.00	126.79	116.07
27	c	505	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
37	N	609	CHL	O1D-CGD-CBD	-3.00	120.18	124.72
37	n	609	CHL	O1D-CGD-CBD	-3.00	120.18	124.72
37	s	601	CHL	CBC-CAC-C3C	-3.00	108.58	112.87
27	c	506	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
27	b	611	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
27	B	609	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
27	S	603	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
27	s	603	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
27	C	510	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
27	S	602	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
27	s	602	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
37	n	609	CHL	CMA-C3A-C4A	-2.99	108.17	114.61
29	b	620	BCR	C3-C4-C5	-2.99	108.73	114.06
37	g	601	CHL	C1C-CHC-C4B	2.98	126.75	116.07
29	H	101	BCR	C38-C26-C25	-2.98	121.23	124.48
27	b	609	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
37	G	606	CHL	C1C-CHC-C4B	2.98	126.74	116.07
40	r	623	NEX	C15-C35-C34	-2.98	117.42	123.52
37	S	601	CHL	CBC-CAC-C3C	-2.98	108.60	112.87
37	S	607	CHL	O1D-CGD-CBD	-2.98	120.20	124.72
37	Y	609	CHL	C1-C2-C3	-2.98	121.31	126.20
27	N	602	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
40	S	1623	NEX	C35-C34-C33	-2.98	123.10	127.28
27	c	513	CLA	O2D-CGD-O1D	-2.98	118.05	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	606	CHL	C1C-CHC-C4B	2.98	126.73	116.07
37	y	609	CHL	C1-C2-C3	-2.98	121.32	126.20
30	a	412	SQD	O9-S-C6	2.98	111.20	106.76
37	N	609	CHL	C1C-CHC-C4B	2.98	126.73	116.07
27	B	616	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
37	s	606	CHL	C1C-CHC-C4B	2.98	126.72	116.07
29	C	515	BCR	C20-C21-C22	-2.98	123.10	127.28
29	c	515	BCR	C20-C21-C22	-2.98	123.10	127.28
37	N	607	CHL	C1C-CHC-C4B	2.98	126.72	116.07
37	G	601	CHL	C1C-CHC-C4B	2.98	126.72	116.07
27	Y	602	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
37	n	609	CHL	C1C-CHC-C4B	2.97	126.71	116.07
38	G	1620	LUT	C35-C15-C14	-2.97	117.44	123.52
27	C	505	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
37	n	607	CHL	C1C-CHC-C4B	2.97	126.70	116.07
30	A	412	SQD	O9-S-C6	2.97	111.19	106.76
29	C	514	BCR	C33-C5-C6	-2.97	121.24	124.48
32	H	102	DGD	C3G-C2G-C1G	-2.97	104.86	111.78
27	g	610	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
27	y	602	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
27	G	610	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
27	n	602	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
38	y	1621	LUT	C18-C5-C6	-2.96	121.25	124.48
39	Y	1622	XAT	C24-C23-C22	-2.96	105.25	110.79
27	C	506	CLA	C3B-C4B-NB	-2.96	107.89	110.53
37	g	607	CHL	C1C-CHC-C4B	2.96	126.65	116.07
27	B	616	CLA	C3B-C4B-NB	-2.96	107.89	110.53
37	G	607	CHL	C1C-CHC-C4B	2.95	126.64	116.07
37	s	607	CHL	O1D-CGD-CBD	-2.95	120.24	124.72
30	B	621	SQD	O5-C5-C4	2.95	115.02	109.70
30	b	621	SQD	O5-C5-C4	2.95	115.02	109.70
32	C	520	DGD	O5D-C6D-C5D	-2.95	102.76	109.42
32	h	102	DGD	C3G-C2G-C1G	-2.95	104.90	111.78
38	Y	1621	LUT	C18-C5-C6	-2.95	121.26	124.48
29	C	514	BCR	C15-C16-C17	-2.95	117.48	123.52
29	c	514	BCR	C15-C16-C17	-2.95	117.48	123.52
38	S	1620	LUT	C21-C26-C27	-2.95	109.43	112.83
39	G	1622	XAT	C27-C28-C29	-2.95	120.95	125.53
29	h	101	BCR	C38-C26-C25	-2.95	121.27	124.48
31	B	622	LMG	O6-C1-O1	-2.94	103.09	110.04
27	C	513	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
37	y	606	CHL	O2A-CGA-CBA	2.94	120.81	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	Y	1620	LUT	C31-C30-C29	-2.94	123.15	127.28
29	C	514	BCR	C21-C20-C19	-2.94	114.67	123.20
27	S	612	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
27	G	612	CLA	C3B-C4B-NB	-2.94	107.90	110.53
39	y	1622	XAT	C24-C23-C22	-2.94	105.29	110.79
39	g	1622	XAT	C27-C28-C29	-2.94	120.97	125.53
31	b	622	LMG	O6-C1-O1	-2.94	103.10	110.04
37	y	608	CHL	O2A-CGA-CBA	2.94	120.80	111.83
27	n	614	CLA	C3B-C4B-NB	-2.94	107.91	110.53
27	D	402	CLA	C3B-C4B-NB	-2.94	107.91	110.53
27	c	506	CLA	C3B-C4B-NB	-2.94	107.91	110.53
37	Y	606	CHL	O2A-CGA-CBA	2.94	120.79	111.83
37	N	605	CHL	O1D-CGD-CBD	-2.94	120.27	124.72
37	Y	608	CHL	O2A-CGA-CBA	2.93	120.78	111.83
29	c	514	BCR	C21-C20-C19	-2.93	114.71	123.20
38	Y	1620	LUT	C35-C15-C14	-2.93	117.52	123.52
38	y	1620	LUT	C35-C15-C14	-2.93	117.52	123.52
27	G	611	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
37	y	601	CHL	C1C-CHC-C4B	2.93	126.55	116.07
27	g	611	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
38	G	1621	LUT	C11-C10-C9	-2.92	123.18	127.28
38	g	1621	LUT	C11-C10-C9	-2.92	123.18	127.28
27	R	613	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	c	520	DGD	O5D-C6D-C5D	-2.92	102.83	109.42
27	Y	610	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
27	y	610	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
37	Y	601	CHL	C1C-CHC-C4B	2.92	126.52	116.07
38	S	1620	LUT	C15-C14-C13	-2.92	123.18	127.28
40	R	623	NEX	C24-C23-C22	-2.92	105.33	110.79
39	N	1622	XAT	C10-C11-C12	-2.92	114.74	123.20
27	b	613	CLA	C3B-C4B-NB	-2.92	107.92	110.53
27	b	616	CLA	C3B-C4B-NB	-2.92	107.93	110.53
38	s	1620	LUT	C15-C14-C13	-2.91	123.19	127.28
27	s	612	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
37	y	605	CHL	C1C-CHC-C4B	2.91	126.49	116.07
37	Y	605	CHL	C1C-CHC-C4B	2.91	126.49	116.07
27	r	610	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
27	S	614	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
27	s	614	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
30	A	418	SQD	C44-O6-C1	2.91	120.03	113.80
37	g	601	CHL	O2A-CGA-CBA	2.91	120.71	111.83
38	y	1620	LUT	C31-C30-C29	-2.91	123.20	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	618	BCR	C23-C24-C25	-2.91	119.23	127.00
40	r	623	NEX	C24-C23-C22	-2.91	105.35	110.79
37	S	601	CHL	C4-C3-C5	2.91	119.55	116.13
27	Y	613	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
35	D	408	LHG	O8-C23-C24	2.90	120.69	111.83
27	R	601	CLA	CAC-C3C-C4C	2.90	128.57	124.79
39	Y	1622	XAT	C35-C15-C14	-2.90	117.58	123.52
37	g	608	CHL	C1C-CHC-C4B	2.90	126.45	116.07
39	n	1622	XAT	C10-C11-C12	-2.90	114.80	123.20
37	r	608	CHL	OMC-CMC-C2C	-2.90	120.08	125.12
37	G	608	CHL	C1C-CHC-C4B	2.90	126.44	116.07
38	N	1620	LUT	C10-C11-C12	-2.90	114.80	123.20
35	d	408	LHG	O8-C23-C24	2.90	120.67	111.83
27	B	615	CLA	C3B-C4B-NB	-2.90	107.94	110.53
27	r	613	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
29	B	618	BCR	C23-C24-C25	-2.90	119.26	127.00
27	S	614	CLA	C3B-C4B-NB	-2.90	107.94	110.53
29	B	620	BCR	C20-C21-C22	-2.90	123.22	127.28
37	n	605	CHL	O1D-CGD-CBD	-2.89	120.33	124.72
37	G	601	CHL	O2A-CGA-CBA	2.89	120.66	111.83
39	N	1622	XAT	C35-C34-C33	-2.89	123.22	127.28
37	n	608	CHL	O2A-CGA-CBA	2.89	120.66	111.83
37	s	601	CHL	C4-C3-C5	2.89	119.53	116.13
37	S	607	CHL	O2A-CGA-CBA	2.89	120.65	111.83
37	s	607	CHL	O2A-CGA-CBA	2.89	120.65	111.83
40	G	1623	NEX	C11-C12-C13	-2.89	118.44	126.36
27	B	613	CLA	C3B-C4B-NB	-2.89	107.95	110.53
27	s	613	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
30	a	418	SQD	C44-O6-C1	2.89	119.99	113.80
27	d	402	CLA	C3B-C4B-NB	-2.89	107.95	110.53
31	A	413	LMG	C4-C3-C2	-2.89	105.76	110.83
31	a	413	LMG	C4-C3-C2	-2.89	105.76	110.83
39	y	1622	XAT	C35-C15-C14	-2.89	117.61	123.52
27	s	614	CLA	C3B-C4B-NB	-2.89	107.95	110.53
38	n	1620	LUT	C10-C11-C12	-2.89	114.84	123.20
27	g	612	CLA	C3B-C4B-NB	-2.88	107.95	110.53
35	D	410	LHG	O8-C23-C24	2.88	120.63	111.83
35	d	410	LHG	O8-C23-C24	2.88	120.63	111.83
37	y	609	CHL	C1C-CHC-C4B	2.88	126.39	116.07
40	g	1623	NEX	C11-C12-C13	-2.88	118.46	126.36
37	g	608	CHL	O2A-CGA-CBA	2.88	120.62	111.83
37	G	605	CHL	O2A-CGA-CBA	2.88	120.62	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	605	CHL	O2A-CGA-CBA	2.88	120.62	111.83
37	Y	609	CHL	C1C-CHC-C4B	2.88	126.38	116.07
27	R	610	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
29	a	411	BCR	C16-C15-C14	-2.88	117.63	123.52
37	G	608	CHL	O2A-CGA-CBA	2.88	120.61	111.83
27	A	410	CLA	C3B-C4B-NB	-2.88	107.96	110.53
37	N	608	CHL	O2A-CGA-CBA	2.88	120.61	111.83
27	S	613	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
37	R	608	CHL	OMC-CMC-C2C	-2.87	120.13	125.12
27	B	617	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
27	b	617	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
37	G	605	CHL	O1D-CGD-CBD	-2.87	120.37	124.72
37	Y	609	CHL	C4-C3-C5	2.87	120.20	115.23
27	R	601	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
37	g	609	CHL	C1C-CHC-C4B	2.87	126.33	116.07
29	A	411	BCR	C16-C15-C14	-2.87	117.65	123.52
27	B	608	CLA	C3B-C4B-NB	-2.87	107.97	110.53
27	y	613	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
27	S	602	CLA	C3B-C4B-NB	-2.86	107.98	110.53
27	r	601	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
39	n	1622	XAT	C35-C34-C33	-2.86	123.27	127.28
37	g	605	CHL	O1D-CGD-CBD	-2.86	120.39	124.72
28	a	408	PHO	C2B-C1B-NB	-2.86	107.36	109.43
27	Y	610	CLA	CMB-C2B-C1B	-2.86	121.07	125.42
27	r	602	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
27	a	410	CLA	C3B-C4B-NB	-2.86	107.98	110.53
39	N	1622	XAT	C4-C3-C2	-2.86	105.45	110.79
29	b	620	BCR	C20-C21-C22	-2.85	123.28	127.28
37	N	601	CHL	C1C-CHC-C4B	2.85	126.28	116.07
27	b	615	CLA	C3B-C4B-NB	-2.85	107.98	110.53
37	G	609	CHL	C1C-CHC-C4B	2.85	126.28	116.07
29	b	620	BCR	C16-C15-C14	-2.85	117.68	123.52
27	N	614	CLA	C3B-C4B-NB	-2.85	107.98	110.53
37	n	601	CHL	C1C-CHC-C4B	2.85	126.27	116.07
27	B	604	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
27	s	613	CLA	C3B-C4B-NB	-2.85	107.99	110.53
37	y	609	CHL	C4-C3-C5	2.85	120.17	115.23
40	S	1623	NEX	C38-C25-C24	2.85	117.44	114.24
40	s	1623	NEX	C38-C25-C24	2.85	117.44	114.24
29	B	618	BCR	C15-C16-C17	-2.85	117.69	123.52
29	b	618	BCR	C15-C16-C17	-2.85	117.69	123.52
27	R	602	CLA	O2D-CGD-O1D	-2.85	118.31	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	S	606	CHL	CMA-C3A-C4A	-2.85	108.48	114.61
37	s	606	CHL	CMA-C3A-C4A	-2.85	108.48	114.61
27	r	611	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
27	g	611	CLA	CHB-C4A-NA	2.84	128.50	124.40
27	C	503	CLA	C3B-C4B-NB	-2.84	107.99	110.53
27	c	503	CLA	C3B-C4B-NB	-2.84	107.99	110.53
27	s	611	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
37	G	601	CHL	C4-C3-C5	2.84	120.16	115.23
29	A	411	BCR	C8-C7-C6	-2.84	119.42	127.00
27	r	601	CLA	CAC-C3C-C4C	2.84	128.48	124.79
40	G	1623	NEX	C24-C23-C22	-2.84	105.49	110.79
40	g	1623	NEX	C24-C23-C22	-2.84	105.49	110.79
27	S	611	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
32	C	519	DGD	CDB-CCB-CBB	-2.83	100.05	114.37
37	G	609	CHL	O2A-CGA-CBA	2.83	120.47	111.83
32	c	519	DGD	CDB-CCB-CBB	-2.83	100.05	114.37
29	B	620	BCR	C16-C15-C14	-2.83	117.72	123.52
27	R	611	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
38	G	1620	LUT	C8-C7-C6	-2.83	119.44	127.00
27	y	610	CLA	CMB-C2B-C1B	-2.83	121.11	125.42
27	B	607	CLA	CHB-C4A-NA	2.83	128.48	124.40
39	n	1622	XAT	C4-C3-C2	-2.83	105.51	110.79
27	b	604	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
39	N	1622	XAT	C38-C25-C24	2.82	117.41	114.24
39	n	1622	XAT	C38-C25-C24	2.82	117.41	114.24
27	b	608	CLA	C3B-C4B-NB	-2.82	108.01	110.53
37	g	609	CHL	O2A-CGA-CBA	2.82	120.44	111.83
37	N	601	CHL	OMC-CMC-C2C	-2.82	120.22	125.12
37	R	608	CHL	C1C-CHC-C4B	2.82	126.16	116.07
32	c	520	DGD	C3G-C2G-C1G	-2.82	105.21	111.78
27	b	613	CLA	CHB-C4A-NA	2.82	128.47	124.40
29	a	411	BCR	C8-C7-C6	-2.82	119.47	127.00
27	R	603	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
38	g	1620	LUT	C8-C7-C6	-2.82	119.47	127.00
27	y	604	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
27	s	602	CLA	C3B-C4B-NB	-2.82	108.02	110.53
37	g	601	CHL	C4-C3-C5	2.82	120.12	115.23
32	C	520	DGD	C3G-C2G-C1G	-2.82	105.22	111.78
27	b	607	CLA	CHB-C4A-NA	2.82	128.46	124.40
37	r	608	CHL	C1C-CHC-C4B	2.82	126.14	116.07
27	R	601	CLA	C3B-C4B-NB	-2.82	108.02	110.53
27	r	601	CLA	C3B-C4B-NB	-2.82	108.02	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	606	CHL	CMB-C2B-C3B	2.81	130.31	124.68
37	g	606	CHL	CMB-C2B-C3B	2.81	130.31	124.68
37	N	601	CHL	O2A-CGA-CBA	2.81	120.41	111.83
28	A	408	PHO	C2B-C1B-NB	-2.81	107.40	109.43
27	r	603	CLA	C3B-C4B-NB	-2.81	108.02	110.53
37	g	609	CHL	O1D-CGD-CBD	-2.81	120.46	124.72
37	s	601	CHL	OMC-CMC-C2C	-2.81	120.25	125.12
40	Y	1623	NEX	C31-C30-C29	-2.81	123.34	127.28
27	S	613	CLA	C3B-C4B-NB	-2.81	108.03	110.53
37	G	609	CHL	O1D-CGD-CBD	-2.81	120.47	124.72
27	r	603	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
27	D	403	CLA	C3B-C4B-NB	-2.80	108.03	110.53
37	n	601	CHL	OMC-CMC-C2C	-2.80	120.25	125.12
40	r	623	NEX	C38-C25-C24	2.80	117.39	114.24
37	S	601	CHL	OMC-CMC-C2C	-2.80	120.25	125.12
27	Y	604	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
31	B	622	LMG	O1-C7-C8	-2.80	104.01	110.82
38	r	620	LUT	C35-C34-C33	-2.80	123.35	127.28
37	y	607	CHL	CBC-CAC-C3C	-2.80	108.87	112.87
37	Y	607	CHL	CBC-CAC-C3C	-2.80	108.87	112.87
27	b	614	CLA	C3B-C4B-NB	-2.80	108.03	110.53
29	c	514	BCR	C7-C8-C9	-2.80	122.10	126.23
37	n	601	CHL	O2A-CGA-CBA	2.79	120.35	111.83
37	y	607	CHL	CMB-C2B-C3B	2.79	130.26	124.68
27	G	611	CLA	C3B-C4B-NB	-2.79	108.04	110.53
27	b	606	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
27	c	511	CLA	C3B-C4B-NB	-2.79	108.04	110.53
38	S	1620	LUT	C18-C5-C4	2.79	119.55	114.42
38	s	1620	LUT	C18-C5-C4	2.79	119.55	114.42
27	B	613	CLA	CHB-C4A-NA	2.79	128.43	124.40
38	g	1621	LUT	C30-C31-C32	-2.79	115.11	123.20
37	n	607	CHL	O1D-CGD-CBD	-2.79	120.49	124.72
37	R	606	CHL	C1C-CHC-C4B	2.79	126.05	116.07
27	C	511	CLA	CHB-C4A-NA	2.79	128.42	124.40
39	r	622	XAT	C24-C23-C22	-2.79	105.58	110.79
31	b	622	LMG	O1-C7-C8	-2.79	104.04	110.82
27	B	614	CLA	C3B-C4B-NB	-2.78	108.04	110.53
39	N	1622	XAT	C40-C33-C32	2.78	122.34	118.09
27	r	611	CLA	C3B-C4B-NB	-2.78	108.05	110.53
38	G	1621	LUT	C30-C31-C32	-2.78	115.14	123.20
29	C	514	BCR	C7-C8-C9	-2.78	122.12	126.23
27	C	504	CLA	CHB-C4A-NA	2.78	128.42	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	y	605	CHL	CBC-CAC-C3C	-2.78	108.89	112.87
39	g	1622	XAT	O4-C5-C18	2.78	118.16	115.05
27	R	609	CLA	CHB-C4A-NA	2.78	128.41	124.40
27	r	609	CLA	CHB-C4A-NA	2.78	128.41	124.40
37	r	606	CHL	C1C-CHC-C4B	2.78	126.01	116.07
27	C	512	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
27	c	512	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
27	A	406	CLA	CHB-C4A-NA	2.78	128.41	124.40
35	y	2630	LHG	O8-C23-C24	2.77	120.30	111.83
37	N	607	CHL	O1D-CGD-CBD	-2.77	120.52	124.72
35	Y	2630	LHG	O8-C23-C24	2.77	120.29	111.83
38	g	1620	LUT	C31-C30-C29	-2.77	123.39	127.28
37	Y	607	CHL	CMB-C2B-C3B	2.77	130.22	124.68
27	c	511	CLA	CHB-C4A-NA	2.77	128.40	124.40
27	G	611	CLA	CHB-C4A-NA	2.77	128.40	124.40
27	s	610	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
40	y	1623	NEX	C31-C30-C29	-2.77	123.39	127.28
32	C	518	DGD	CDB-CCB-CBB	-2.77	100.37	114.37
27	B	606	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
39	G	1622	XAT	O4-C5-C18	2.77	118.14	115.05
28	a	409	PHO	C1-C2-C3	-2.77	121.67	126.20
27	d	403	CLA	C3B-C4B-NB	-2.76	108.06	110.53
37	S	606	CHL	O2A-CGA-CBA	2.76	120.26	111.83
27	N	612	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
27	n	612	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
32	c	518	DGD	CDB-CCB-CBB	-2.76	100.40	114.37
27	R	603	CLA	C3B-C4B-NB	-2.76	108.06	110.53
28	A	409	PHO	C1-C2-C3	-2.76	121.67	126.20
39	R	622	XAT	C24-C23-C22	-2.76	105.62	110.79
38	R	620	LUT	C10-C11-C12	-2.76	115.20	123.20
38	r	620	LUT	C10-C11-C12	-2.76	115.20	123.20
27	R	604	CLA	CHB-C4A-NA	2.76	128.38	124.40
27	r	604	CLA	CHB-C4A-NA	2.76	128.38	124.40
27	s	609	CLA	C3B-C4B-NB	-2.76	108.07	110.53
38	R	620	LUT	C35-C34-C33	-2.76	123.41	127.28
29	C	514	BCR	C8-C7-C6	-2.76	119.63	127.00
27	c	504	CLA	CHB-C4A-NA	2.76	128.38	124.40
37	S	601	CHL	C1-C2-C3	-2.76	121.68	126.20
37	Y	605	CHL	CBC-CAC-C3C	-2.76	108.93	112.87
27	G	604	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
27	R	610	CLA	C3B-C4B-NB	-2.76	108.07	110.53
29	c	514	BCR	C8-C7-C6	-2.76	119.64	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	608	CHL	OMC-CMC-C2C	-2.75	120.34	125.12
27	S	610	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
27	R	611	CLA	C3B-C4B-NB	-2.75	108.07	110.53
37	n	605	CHL	O2A-CGA-CBA	2.75	120.23	111.83
39	R	622	XAT	C38-C25-C24	2.75	117.33	114.24
27	d	403	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
40	g	1623	NEX	C26-C27-C28	-2.75	120.18	125.99
37	N	605	CHL	O2A-CGA-CBA	2.75	120.22	111.83
37	s	606	CHL	O2A-CGA-CBA	2.75	120.22	111.83
38	G	1620	LUT	C31-C30-C29	-2.75	123.42	127.28
27	g	611	CLA	C3B-C4B-NB	-2.75	108.08	110.53
39	n	1622	XAT	C40-C33-C32	2.75	122.28	118.09
38	S	1620	LUT	C10-C11-C12	-2.74	115.25	123.20
27	B	608	CLA	CHB-C4A-NA	2.74	128.36	124.40
37	G	608	CHL	OMC-CMC-C2C	-2.74	120.36	125.12
27	b	608	CLA	CHB-C4A-NA	2.74	128.36	124.40
40	N	1623	NEX	C8-C7-C6	-2.74	174.43	177.66
37	Y	601	CHL	O2A-CGA-CBA	2.74	120.19	111.83
37	y	601	CHL	O2A-CGA-CBA	2.74	120.19	111.83
30	a	412	SQD	C44-O6-C1	2.74	119.67	113.80
27	S	609	CLA	C3B-C4B-NB	-2.74	108.09	110.53
27	A	407	CLA	C3B-C4B-NB	-2.74	108.09	110.53
37	Y	609	CHL	O2A-CGA-CBA	2.74	120.18	111.83
38	s	1620	LUT	C10-C11-C12	-2.74	115.27	123.20
27	g	604	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
37	y	609	CHL	O1D-CGD-CBD	-2.73	120.58	124.72
27	C	511	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
37	G	607	CHL	O1D-CGD-CBD	-2.73	120.58	124.72
27	C	507	CLA	CHB-C4A-NA	2.73	128.34	124.40
27	Y	610	CLA	C3B-C4B-NB	-2.73	108.09	110.53
27	r	613	CLA	CHB-C4A-NA	2.73	128.34	124.40
27	A	406	CLA	C3B-C4B-NB	-2.73	108.10	110.53
27	a	406	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
37	y	609	CHL	O2A-CGA-CBA	2.72	120.14	111.83
27	D	403	CLA	CMB-C2B-C1B	-2.72	121.27	125.42
38	s	1620	LUT	C30-C31-C32	-2.72	115.31	123.20
27	y	614	CLA	CHB-C4A-NA	2.72	128.33	124.40
30	A	412	SQD	C44-O6-C1	2.72	119.63	113.80
37	Y	609	CHL	O1D-CGD-CBD	-2.72	120.60	124.72
27	a	406	CLA	CHB-C4A-NA	2.72	128.32	124.40
38	y	1620	LUT	C20-C13-C12	2.72	122.24	118.09
27	A	406	CLA	O2D-CGD-O1D	-2.72	118.56	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	S	1620	LUT	C30-C31-C32	-2.72	115.33	123.20
40	n	1623	NEX	C8-C7-C6	-2.72	174.46	177.66
40	R	623	NEX	C38-C25-C24	2.72	117.29	114.24
27	R	610	CLA	CHB-C4A-NA	2.71	128.32	124.40
27	r	610	CLA	CHB-C4A-NA	2.71	128.32	124.40
27	A	410	CLA	C1-C2-C3	-2.71	121.75	126.20
37	s	601	CHL	C1-C2-C3	-2.71	121.75	126.20
27	c	511	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
40	G	1623	NEX	C26-C27-C28	-2.71	120.26	125.99
35	R	2630	LHG	O8-C23-C24	2.71	120.10	111.83
37	G	608	CHL	CBC-CAC-C3C	-2.71	108.99	112.87
27	g	604	CLA	C3B-C4B-NB	-2.71	108.11	110.53
27	a	410	CLA	C1-C2-C3	-2.71	121.76	126.20
35	r	2630	LHG	O8-C23-C24	2.71	120.09	111.83
27	B	605	CLA	C3B-C4B-NB	-2.71	108.11	110.53
27	b	605	CLA	C3B-C4B-NB	-2.71	108.11	110.53
40	N	1623	NEX	C31-C30-C29	-2.71	123.48	127.28
39	r	622	XAT	C38-C25-C24	2.71	117.28	114.24
27	g	612	CLA	CHB-C4A-NA	2.71	128.30	124.40
37	g	607	CHL	O1D-CGD-CBD	-2.70	120.62	124.72
27	N	614	CLA	CHB-C4A-NA	2.70	128.30	124.40
38	N	1621	LUT	C30-C31-C32	-2.70	115.37	123.20
27	a	407	CLA	C3B-C4B-NB	-2.70	108.12	110.53
27	b	602	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
37	s	608	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
27	a	406	CLA	C3B-C4B-NB	-2.70	108.12	110.53
27	b	609	CLA	C3B-C4B-NB	-2.70	108.12	110.53
37	s	607	CHL	CMA-C3A-C4A	-2.70	108.80	114.61
38	Y	1620	LUT	C20-C13-C12	2.70	122.21	118.09
27	S	610	CLA	C3B-C4B-NB	-2.70	108.12	110.53
37	N	605	CHL	OMC-CMC-C2C	-2.70	120.44	125.12
27	S	604	CLA	CHB-C4A-NA	2.70	128.29	124.40
27	c	508	CLA	CHB-C4A-NA	2.70	128.29	124.40
27	C	511	CLA	C3B-C4B-NB	-2.70	108.12	110.53
37	S	608	CHL	O1D-CGD-CBD	-2.70	120.64	124.72
37	Y	607	CHL	O2A-CGA-CBA	2.69	120.05	111.83
27	n	614	CLA	CHB-C4A-NA	2.69	128.29	124.40
37	S	607	CHL	CMA-C3A-C4A	-2.69	108.81	114.61
37	N	607	CHL	CMB-C2B-C3B	2.69	130.07	124.68
40	n	1623	NEX	C31-C30-C29	-2.69	123.50	127.28
27	R	613	CLA	CHB-C4A-NA	2.69	128.28	124.40
37	Y	601	CHL	C4-C3-C5	2.69	119.90	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	507	CLA	CHB-C4A-NA	2.69	128.28	124.40
37	g	605	CHL	C1C-CHC-C4B	2.69	125.68	116.07
37	n	607	CHL	CMB-C2B-C3B	2.68	130.05	124.68
37	y	601	CHL	C4-C3-C5	2.68	119.89	115.23
27	r	610	CLA	C3B-C4B-NB	-2.68	108.13	110.53
37	S	606	CHL	CAC-C3C-C4C	2.68	130.93	124.03
38	n	1621	LUT	C30-C31-C32	-2.68	115.43	123.20
28	A	408	PHO	CMB-C2B-C3B	2.68	130.04	124.68
28	a	408	PHO	CMB-C2B-C3B	2.68	130.04	124.68
27	R	612	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
37	G	606	CHL	O2A-CGA-CBA	2.68	120.01	111.83
27	s	610	CLA	C3B-C4B-NB	-2.68	108.14	110.53
38	N	1621	LUT	C18-C5-C4	2.68	119.35	114.42
39	y	1622	XAT	C31-C32-C33	-2.68	119.02	126.36
37	g	608	CHL	CBC-CAC-C3C	-2.68	109.04	112.87
37	S	607	CHL	C1B-CHB-C4A	-2.68	119.60	121.32
37	s	607	CHL	C1B-CHB-C4A	-2.68	119.60	121.32
27	C	506	CLA	C1-C2-C3	-2.68	121.81	126.20
37	G	605	CHL	C1C-CHC-C4B	2.67	125.64	116.07
27	G	604	CLA	C3B-C4B-NB	-2.67	108.14	110.53
30	B	621	SQD	O48-C23-C24	2.67	119.99	111.83
37	g	606	CHL	O2A-CGA-CBA	2.67	119.99	111.83
29	B	619	BCR	C38-C26-C25	-2.67	121.57	124.48
37	n	605	CHL	OMC-CMC-C2C	-2.67	120.48	125.12
27	r	612	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
27	s	604	CLA	CHB-C4A-NA	2.67	128.25	124.40
27	Y	602	CLA	C3B-C4B-NB	-2.67	108.15	110.53
39	Y	1622	XAT	C31-C32-C33	-2.67	119.05	126.36
27	C	508	CLA	CHB-C4A-NA	2.67	128.25	124.40
37	y	607	CHL	O2A-CGA-CBA	2.67	119.97	111.83
27	y	602	CLA	C3B-C4B-NB	-2.67	108.15	110.53
38	S	1621	LUT	C31-C30-C29	-2.67	123.54	127.28
38	s	1621	LUT	C31-C30-C29	-2.67	123.54	127.28
37	N	607	CHL	CMA-C3A-C4A	-2.66	108.87	114.61
27	c	504	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
27	a	410	CLA	CHB-C4A-NA	2.66	128.24	124.40
38	n	1621	LUT	C18-C5-C4	2.66	119.32	114.42
27	G	614	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
37	r	608	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
32	H	102	DGD	CDB-CCB-CBB	-2.66	100.92	114.37
27	C	509	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
37	n	609	CHL	CMB-C2B-C3B	2.66	129.99	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	s	606	CHL	CAC-C3C-C4C	2.66	130.86	124.03
37	r	608	CHL	CAC-C3C-C4C	2.66	130.86	124.03
27	R	609	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
27	G	612	CLA	CHB-C4A-NA	2.66	128.23	124.40
30	b	621	SQD	O48-C23-C24	2.66	119.93	111.83
37	y	606	CHL	CMA-C3A-C4A	-2.66	108.89	114.61
27	r	609	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
27	n	604	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
27	n	613	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
27	y	610	CLA	C3B-C4B-NB	-2.65	108.16	110.53
37	n	607	CHL	CMA-C3A-C4A	-2.65	108.90	114.61
27	b	617	CLA	C3B-C4B-NB	-2.65	108.16	110.53
32	h	102	DGD	CDB-CCB-CBB	-2.65	100.97	114.37
27	s	611	CLA	CHB-C4A-NA	2.65	128.22	124.40
29	b	619	BCR	C38-C26-C25	-2.65	121.59	124.48
27	B	609	CLA	C3B-C4B-NB	-2.65	108.17	110.53
27	c	506	CLA	C1-C2-C3	-2.65	121.86	126.20
37	N	609	CHL	CMB-C2B-C3B	2.65	129.97	124.68
27	c	502	CLA	C3B-C4B-NB	-2.65	108.17	110.53
37	s	601	CHL	O2A-CGA-CBA	2.65	119.91	111.83
27	A	410	CLA	CHB-C4A-NA	2.65	128.22	124.40
38	S	1621	LUT	C30-C31-C32	-2.65	115.53	123.20
38	s	1621	LUT	C30-C31-C32	-2.65	115.53	123.20
37	Y	606	CHL	CMA-C3A-C4A	-2.65	108.91	114.61
30	a	418	SQD	C4-C3-C2	2.65	115.47	110.83
27	B	617	CLA	C3B-C4B-NB	-2.65	108.17	110.53
37	Y	607	CHL	OMC-CMC-C2C	-2.65	120.53	125.12
27	N	611	CLA	CHB-C4A-NA	2.64	128.22	124.40
27	n	611	CLA	CHB-C4A-NA	2.64	128.22	124.40
27	C	502	CLA	C3B-C4B-NB	-2.64	108.17	110.53
37	g	601	CHL	CMA-C3A-C4A	-2.64	108.92	114.61
35	N	2630	LHG	C11-C10-C9	-2.64	101.01	114.37
29	c	517	BCR	C36-C18-C19	2.64	122.13	118.09
27	c	513	CLA	CHB-C4A-NA	2.64	128.21	124.40
37	S	601	CHL	O2A-CGA-CBA	2.64	119.89	111.83
27	Y	614	CLA	CHB-C4A-NA	2.64	128.21	124.40
27	y	603	CLA	CHB-C4A-NA	2.64	128.21	124.40
28	a	409	PHO	C4A-C3A-C2A	-2.64	100.33	102.84
37	N	608	CHL	O1D-CGD-CBD	-2.64	120.72	124.72
27	r	613	CLA	C3B-C4B-NB	-2.64	108.17	110.53
27	g	614	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
27	c	503	CLA	O2D-CGD-O1D	-2.64	118.71	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	509	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
27	n	604	CLA	C3B-C4B-NB	-2.64	108.17	110.53
37	G	601	CHL	CMA-C3A-C4A	-2.64	108.93	114.61
29	C	515	BCR	C16-C17-C18	-2.64	123.58	127.28
29	c	515	BCR	C16-C17-C18	-2.64	123.58	127.28
37	N	607	CHL	C1-O2A-CGA	2.64	123.03	116.65
31	D	411	LMG	O6-C1-O1	-2.64	103.81	110.04
40	R	623	NEX	C30-C31-C32	-2.64	115.56	123.20
35	n	2630	LHG	C11-C10-C9	-2.64	101.04	114.37
37	R	608	CHL	CAC-C3C-C4C	2.64	130.80	124.03
27	N	613	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
27	n	612	CLA	C3B-C4B-NB	-2.63	108.18	110.53
37	R	608	CHL	O1D-CGD-CBD	-2.63	120.73	124.72
27	N	604	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
37	G	608	CHL	CMB-C2B-C3B	2.63	129.95	124.68
27	C	513	CLA	CHB-C4A-NA	2.63	128.20	124.40
27	B	602	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
37	n	607	CHL	C1-O2A-CGA	2.63	123.02	116.65
27	C	504	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
38	N	1620	LUT	C19-C9-C8	2.63	122.11	118.09
39	n	1622	XAT	C30-C31-C32	-2.63	115.58	123.20
30	A	418	SQD	C4-C3-C2	2.63	115.44	110.83
39	N	1622	XAT	C30-C31-C32	-2.63	115.58	123.20
27	S	611	CLA	CHB-C4A-NA	2.63	128.19	124.40
40	r	623	NEX	C30-C31-C32	-2.63	115.58	123.20
37	r	607	CHL	O2D-CGD-O1D	-2.63	118.73	123.85
27	B	608	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
27	A	407	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
27	b	608	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
32	c	520	DGD	C4E-C3E-C2E	-2.62	106.22	110.83
31	A	413	LMG	O3-C3-C2	-2.62	104.19	110.38
31	d	411	LMG	O6-C1-O1	-2.62	103.85	110.04
27	B	616	CLA	CHB-C4A-NA	2.62	128.18	124.40
29	C	517	BCR	C36-C18-C19	2.62	122.09	118.09
29	d	404	BCR	C33-C5-C4	2.62	119.18	113.60
29	h	101	BCR	C21-C20-C19	-2.62	115.61	123.20
37	g	609	CHL	CMA-C3A-C4A	-2.62	108.97	114.61
27	N	604	CLA	C3B-C4B-NB	-2.62	108.19	110.53
27	a	407	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
37	R	607	CHL	OMC-CMC-C2C	-2.61	120.58	125.12
27	a	405	CLA	C3B-C4B-NB	-2.61	108.20	110.53
38	y	1621	LUT	C15-C35-C34	-2.61	118.17	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	503	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
37	R	607	CHL	O2D-CGD-O1D	-2.61	118.76	123.85
27	C	509	CLA	C11-C12-C13	-2.61	107.28	115.97
27	c	509	CLA	C11-C12-C13	-2.61	107.28	115.97
38	n	1620	LUT	C19-C9-C8	2.61	122.08	118.09
32	C	520	DGD	C4E-C3E-C2E	-2.61	106.24	110.83
37	y	607	CHL	OMC-CMC-C2C	-2.61	120.59	125.12
27	S	602	CLA	CHB-C4A-NA	2.61	128.16	124.40
28	A	409	PHO	C4A-C3A-C2A	-2.61	100.36	102.84
27	B	605	CLA	CHB-C4A-NA	2.61	128.16	124.40
27	b	605	CLA	CHB-C4A-NA	2.61	128.16	124.40
31	a	413	LMG	O3-C3-C2	-2.61	104.23	110.38
37	G	606	CHL	OMC-CMC-C2C	-2.60	120.60	125.12
27	g	614	CLA	CHB-C4A-NA	2.60	128.16	124.40
27	Y	603	CLA	CHB-C4A-NA	2.60	128.16	124.40
37	n	608	CHL	O1D-CGD-CBD	-2.60	120.78	124.72
29	H	101	BCR	C21-C20-C19	-2.60	115.66	123.20
27	N	613	CLA	C3B-C4B-NB	-2.60	108.21	110.53
39	N	1622	XAT	C7-C8-C9	-2.60	121.50	125.53
38	S	1620	LUT	C16-C1-C6	-2.60	106.17	110.24
38	s	1620	LUT	C16-C1-C6	-2.60	106.17	110.24
37	y	605	CHL	O2A-CGA-CBA	2.60	119.76	111.83
37	g	608	CHL	CMB-C2B-C3B	2.60	129.87	124.68
27	S	609	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
27	G	614	CLA	CHB-C4A-NA	2.60	128.15	124.40
27	R	613	CLA	C3B-C4B-NB	-2.60	108.21	110.53
27	n	613	CLA	C3B-C4B-NB	-2.59	108.22	110.53
37	r	607	CHL	OMC-CMC-C2C	-2.59	120.62	125.12
29	D	404	BCR	C33-C5-C4	2.59	119.12	113.60
27	b	616	CLA	CHB-C4A-NA	2.59	128.14	124.40
37	n	606	CHL	O2A-CGA-CBA	2.59	119.73	111.83
37	G	609	CHL	CMA-C3A-C4A	-2.59	109.03	114.61
29	H	101	BCR	C23-C24-C25	-2.59	120.08	127.00
27	N	603	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
27	B	602	CLA	CHB-C4A-NA	2.59	128.14	124.40
37	N	606	CHL	O2A-CGA-CBA	2.59	119.73	111.83
27	C	504	CLA	C3B-C4B-NB	-2.59	108.22	110.53
27	c	504	CLA	C3B-C4B-NB	-2.59	108.22	110.53
27	C	509	CLA	C1-C2-C3	-2.59	121.96	126.20
27	c	509	CLA	C1-C2-C3	-2.59	121.96	126.20
27	b	611	CLA	CAA-CBA-CGA	-2.59	105.86	113.21
27	n	604	CLA	CHB-C4A-NA	2.59	128.13	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	R	604	CLA	C3B-C4B-NB	-2.59	108.22	110.53
27	B	615	CLA	CHB-C4A-NA	2.58	128.13	124.40
40	y	1623	NEX	C11-C12-C13	-2.58	119.28	126.36
38	Y	1621	LUT	C15-C35-C34	-2.58	118.23	123.52
40	r	623	NEX	C8-C7-C6	-2.58	174.61	177.66
27	S	611	CLA	C3B-C4B-NB	-2.58	108.22	110.53
37	Y	605	CHL	O2A-CGA-CBA	2.58	119.71	111.83
38	Y	1621	LUT	C18-C5-C4	2.58	119.17	114.42
39	r	622	XAT	C30-C31-C32	-2.58	115.72	123.20
37	S	607	CHL	C1C-CHC-C4B	2.58	125.30	116.07
37	n	607	CHL	O2A-CGA-CBA	2.58	119.70	111.83
29	h	101	BCR	C23-C24-C25	-2.58	120.11	127.00
27	b	602	CLA	CHB-C4A-NA	2.58	128.12	124.40
27	A	405	CLA	C3B-C4B-NB	-2.58	108.23	110.53
27	r	604	CLA	C3B-C4B-NB	-2.58	108.23	110.53
37	g	606	CHL	OMC-CMC-C2C	-2.58	120.65	125.12
27	B	611	CLA	CAA-CBA-CGA	-2.58	105.90	113.21
37	N	607	CHL	O2A-CGA-CBA	2.57	119.68	111.83
38	G	1621	LUT	C18-C5-C4	2.57	119.15	114.42
38	g	1621	LUT	C18-C5-C4	2.57	119.15	114.42
27	s	609	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
27	y	612	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
37	s	607	CHL	C1C-CHC-C4B	2.57	125.27	116.07
30	a	418	SQD	O48-C23-C24	2.57	119.68	111.83
27	C	508	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
31	b	622	LMG	C38-C37-C36	-2.57	101.37	114.37
31	B	622	LMG	C38-C37-C36	-2.57	101.37	114.37
27	Y	604	CLA	CHB-C4A-NA	2.57	128.11	124.40
27	y	604	CLA	CHB-C4A-NA	2.57	128.11	124.40
40	Y	1623	NEX	C19-C9-C10	-2.57	118.65	122.82
40	y	1623	NEX	C19-C9-C10	-2.57	118.65	122.82
27	s	611	CLA	C3B-C4B-NB	-2.57	108.23	110.53
27	b	608	CLA	C1-C2-C3	-2.57	121.98	126.20
35	l	101	LHG	C5-O7-C7	-2.57	111.64	117.80
27	R	604	CLA	O2D-CGD-CBD	2.57	115.72	111.23
37	N	606	CHL	CBC-CAC-C3C	-2.57	109.19	112.87
27	N	604	CLA	CHB-C4A-NA	2.57	128.11	124.40
27	G	603	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
27	s	602	CLA	CHB-C4A-NA	2.57	128.10	124.40
38	y	1621	LUT	C31-C30-C29	-2.56	123.68	127.28
37	Y	609	CHL	CMB-C2B-C3B	2.56	129.81	124.68
37	N	608	CHL	OMC-CMC-C2C	-2.56	120.67	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	r	602	CLA	CHB-C4A-NA	2.56	128.10	124.40
38	g	1621	LUT	C19-C9-C8	2.56	122.00	118.09
37	n	606	CHL	CBC-CAC-C3C	-2.56	109.20	112.87
27	g	610	CLA	C3B-C4B-NB	-2.56	108.24	110.53
27	N	612	CLA	CHB-C4A-NA	2.56	128.10	124.40
27	r	603	CLA	CHB-C4A-NA	2.56	128.10	124.40
35	L	101	LHG	C5-O7-C7	-2.56	111.67	117.80
27	b	614	CLA	C1-C2-C3	-2.56	122.00	126.20
38	y	1621	LUT	C18-C5-C4	2.56	119.13	114.42
30	A	418	SQD	O48-C23-C24	2.56	119.64	111.83
37	y	606	CHL	CMB-C2B-C3B	2.56	129.80	124.68
27	n	603	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
29	d	404	BCR	C8-C7-C6	-2.56	120.16	127.00
39	r	622	XAT	C31-C30-C29	-2.56	123.69	127.28
27	A	407	CLA	CHB-C4A-NA	2.56	128.09	124.40
27	G	610	CLA	CHB-C4A-NA	2.56	128.09	124.40
40	Y	1623	NEX	C11-C12-C13	-2.56	119.36	126.36
27	A	405	CLA	CMB-C2B-C1B	-2.56	121.53	125.42
27	c	505	CLA	C3B-C4B-NB	-2.56	108.25	110.53
27	b	615	CLA	CHB-C4A-NA	2.55	128.09	124.40
27	g	603	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
27	g	610	CLA	CHB-C4A-NA	2.55	128.09	124.40
37	n	608	CHL	OMC-CMC-C2C	-2.55	120.69	125.12
37	G	606	CHL	O1D-CGD-CBD	-2.55	120.85	124.72
27	N	612	CLA	C3B-C4B-NB	-2.55	108.25	110.53
37	r	606	CHL	O2A-CGA-CBA	2.55	119.61	111.83
38	g	1620	LUT	C10-C11-C12	-2.55	115.81	123.20
39	R	622	XAT	C30-C31-C32	-2.55	115.81	123.20
27	Y	612	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
27	R	616	CLA	C3B-C4B-NB	-2.55	108.25	110.53
27	c	512	CLA	C3B-C4B-NB	-2.55	108.25	110.53
27	a	407	CLA	CHB-C4A-NA	2.55	128.08	124.40
30	B	621	SQD	C1-O5-C5	2.55	118.70	113.72
27	C	505	CLA	C3B-C4B-NB	-2.55	108.25	110.53
35	D	409	LHG	C5-O7-C7	-2.55	111.70	117.80
35	d	409	LHG	C5-O7-C7	-2.55	111.70	117.80
27	g	612	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
27	c	508	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
29	D	404	BCR	C8-C7-C6	-2.55	120.19	127.00
27	r	604	CLA	O2D-CGD-CBD	2.55	115.68	111.23
27	C	511	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
27	a	405	CLA	CMB-C2B-C1B	-2.55	121.54	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	606	CHL	O1D-CGD-CBD	-2.54	120.86	124.72
27	B	608	CLA	C1-C2-C3	-2.54	122.03	126.20
27	R	616	CLA	CHB-C4A-NA	2.54	128.07	124.40
30	b	621	SQD	C1-O5-C5	2.54	118.68	113.72
27	B	614	CLA	C1-C2-C3	-2.54	122.03	126.20
37	Y	609	CHL	CMA-C3A-C4A	-2.54	109.14	114.61
37	y	609	CHL	CMA-C3A-C4A	-2.54	109.14	114.61
39	Y	1622	XAT	C38-C25-C24	2.54	117.09	114.24
27	b	612	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
37	Y	606	CHL	CMB-C2B-C3B	2.54	129.76	124.68
27	B	614	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
37	R	606	CHL	O2A-CGA-CBA	2.54	119.58	111.83
38	G	1620	LUT	C30-C31-C32	-2.54	115.84	123.20
38	G	1621	LUT	C19-C9-C8	2.54	121.97	118.09
27	n	603	CLA	CHB-C4A-NA	2.54	128.06	124.40
38	S	1621	LUT	C18-C5-C6	-2.54	121.72	124.48
40	G	1623	NEX	C15-C35-C34	-2.54	118.33	123.52
39	n	1622	XAT	C7-C8-C9	-2.53	121.60	125.53
27	n	612	CLA	CHB-C4A-NA	2.53	128.06	124.40
35	g	2630	LHG	C20-C19-C18	-2.53	101.56	114.37
37	y	609	CHL	CMB-C2B-C3B	2.53	129.75	124.68
27	B	607	CLA	C1-C2-C3	-2.53	122.05	126.20
27	G	612	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
27	D	402	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
27	G	610	CLA	C3B-C4B-NB	-2.53	108.27	110.53
38	g	1620	LUT	C30-C31-C32	-2.53	115.87	123.20
39	R	622	XAT	C31-C30-C29	-2.53	123.73	127.28
29	B	618	BCR	C16-C15-C14	-2.53	118.34	123.52
29	b	618	BCR	C16-C15-C14	-2.53	118.34	123.52
35	G	2630	LHG	C20-C19-C18	-2.53	101.59	114.37
27	C	502	CLA	CHB-C4A-NA	2.53	128.05	124.40
27	b	614	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
29	C	517	BCR	C8-C7-C6	-2.53	120.25	127.00
27	N	603	CLA	CHB-C4A-NA	2.52	128.04	124.40
29	B	620	BCR	C23-C24-C25	-2.52	120.26	127.00
35	d	409	LHG	C20-C19-C18	-2.52	101.61	114.37
40	g	1623	NEX	C15-C35-C34	-2.52	118.36	123.52
29	H	101	BCR	C8-C7-C6	-2.52	120.26	127.00
38	n	1620	LUT	C35-C15-C14	-2.52	118.36	123.52
40	N	1623	NEX	C30-C31-C32	-2.52	115.89	123.20
29	h	101	BCR	C8-C7-C6	-2.52	120.26	127.00
27	B	612	CLA	CMB-C2B-C1B	-2.52	121.58	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	620	BCR	C23-C24-C25	-2.52	120.27	127.00
32	C	518	DGD	C1E-C2E-C3E	-2.52	104.71	110.01
32	c	518	DGD	C1E-C2E-C3E	-2.52	104.71	110.01
35	G	2630	LHG	C11-C10-C9	-2.52	101.63	114.37
40	r	623	NEX	C16-C1-C6	-2.52	108.22	110.47
27	r	616	CLA	CHB-C4A-NA	2.52	128.04	124.40
35	D	410	LHG	C11-C10-C9	-2.52	101.63	114.37
35	d	410	LHG	C11-C10-C9	-2.52	101.63	114.37
40	R	623	NEX	C8-C7-C6	-2.52	174.69	177.66
32	h	102	DGD	C1D-C2D-C3D	-2.52	104.71	110.01
27	b	607	CLA	C1-C2-C3	-2.52	122.07	126.20
38	Y	1621	LUT	C31-C30-C29	-2.52	123.75	127.28
38	s	1621	LUT	C18-C5-C6	-2.52	121.74	124.48
35	g	2630	LHG	C11-C10-C9	-2.52	101.64	114.37
31	B	622	LMG	C40-C39-C38	-2.52	101.65	114.37
29	c	517	BCR	C8-C7-C6	-2.51	120.28	127.00
27	N	613	CLA	CHB-C4A-NA	2.51	128.03	124.40
35	N	2630	LHG	O8-C23-C24	2.51	119.50	111.83
35	D	409	LHG	C20-C19-C18	-2.51	101.67	114.37
37	r	607	CHL	CMB-C2B-C3B	2.51	129.70	124.68
31	b	622	LMG	C40-C39-C38	-2.51	101.67	114.37
39	y	1622	XAT	C38-C25-C24	2.51	117.06	114.24
40	G	1623	NEX	C39-C29-C30	-2.51	118.75	122.82
38	G	1620	LUT	C10-C11-C12	-2.51	115.93	123.20
27	A	407	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
40	N	1623	NEX	C39-C29-C30	-2.51	118.75	122.82
27	N	610	CLA	CHB-C4A-NA	2.51	128.02	124.40
27	c	502	CLA	CHB-C4A-NA	2.51	128.02	124.40
32	H	102	DGD	C1D-C2D-C3D	-2.51	104.73	110.01
29	C	517	BCR	C33-C5-C4	2.51	118.94	113.60
29	c	517	BCR	C33-C5-C4	2.51	118.94	113.60
38	N	1620	LUT	C35-C15-C14	-2.51	118.39	123.52
40	n	1623	NEX	C30-C31-C32	-2.50	115.94	123.20
27	G	603	CLA	CHB-C4A-NA	2.50	128.01	124.40
27	A	405	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
37	n	605	CHL	O2D-CGD-O1D	-2.50	118.98	123.85
27	R	603	CLA	CHB-C4A-NA	2.50	128.01	124.40
27	r	616	CLA	C3B-C4B-NB	-2.50	108.30	110.53
40	R	623	NEX	C16-C1-C6	-2.50	108.23	110.47
37	R	607	CHL	CMB-C2B-C3B	2.50	129.68	124.68
37	R	606	CHL	O1D-CGD-CBD	-2.50	120.93	124.72
37	G	605	CHL	CBC-CAC-C3C	-2.50	109.30	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	s	608	CHL	C1C-CHC-C4B	2.50	125.01	116.07
35	l	101	LHG	O8-C23-C24	2.50	119.45	111.83
27	s	610	CLA	CHB-C4A-NA	2.50	128.00	124.40
27	b	609	CLA	CHB-C4A-NA	2.50	128.00	124.40
37	y	605	CHL	O1D-CGD-CBD	-2.50	120.94	124.72
27	B	609	CLA	CHB-C4A-NA	2.50	128.00	124.40
35	n	2630	LHG	O8-C23-C24	2.50	119.44	111.83
37	N	606	CHL	O2D-CGD-O1D	-2.49	118.99	123.85
27	G	603	CLA	C3B-C4B-NB	-2.49	108.30	110.53
27	g	603	CLA	C3B-C4B-NB	-2.49	108.30	110.53
35	l	101	LHG	C11-C10-C9	-2.49	101.76	114.37
27	g	603	CLA	CHB-C4A-NA	2.49	128.00	124.40
27	R	602	CLA	CHB-C4A-NA	2.49	128.00	124.40
35	L	101	LHG	C11-C10-C9	-2.49	101.76	114.37
27	Y	604	CLA	C3B-C4B-NB	-2.49	108.30	110.53
38	S	1620	LUT	C31-C30-C29	-2.49	123.78	127.28
37	s	606	CHL	CMD-C2D-C3D	-2.49	119.70	124.68
27	d	402	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
27	c	511	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
37	r	606	CHL	O1D-CGD-CBD	-2.49	120.94	124.72
40	R	623	NEX	C31-C30-C29	-2.49	123.78	127.28
37	S	608	CHL	C1C-CHC-C4B	2.49	124.98	116.07
29	h	101	BCR	C35-C13-C12	2.49	121.89	118.09
32	C	520	DGD	CDB-CCB-CBB	-2.49	101.79	114.37
37	n	606	CHL	O2D-CGD-O1D	-2.49	119.00	123.85
37	y	608	CHL	O1D-CGD-CBD	-2.49	120.95	124.72
37	S	606	CHL	CMD-C2D-C3D	-2.49	119.71	124.68
29	H	101	BCR	C35-C13-C12	2.49	121.89	118.09
27	s	610	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
27	Y	602	CLA	CHB-C4A-NA	2.48	127.99	124.40
38	S	1621	LUT	C35-C15-C14	-2.48	118.44	123.52
40	g	1623	NEX	C39-C29-C30	-2.48	118.79	122.82
27	a	407	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
32	c	520	DGD	CDB-CCB-CBB	-2.48	101.81	114.37
38	g	1620	LUT	C16-C1-C6	-2.48	106.35	110.24
27	a	405	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
32	C	520	DGD	O2D-C2D-C1D	-2.48	104.16	110.08
37	g	605	CHL	CBC-CAC-C3C	-2.48	109.32	112.87
34	D	405	PL9	O1-C4-C3	-2.48	118.11	120.73
29	B	619	BCR	C10-C11-C12	-2.48	116.01	123.20
35	l	101	LHG	C20-C19-C18	-2.48	101.83	114.37
40	r	623	NEX	C31-C30-C29	-2.48	123.80	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	L	101	LHG	O8-C23-C24	2.48	119.40	111.83
29	C	516	BCR	C8-C7-C6	-2.48	120.37	127.00
29	c	516	BCR	C8-C7-C6	-2.48	120.37	127.00
40	n	1623	NEX	C39-C29-C30	-2.48	118.80	122.82
29	b	619	BCR	C10-C11-C12	-2.48	116.02	123.20
27	y	602	CLA	CHB-C4A-NA	2.48	127.97	124.40
37	Y	608	CHL	O1D-CGD-CBD	-2.48	120.97	124.72
31	A	413	LMG	C38-C37-C36	-2.48	101.85	114.37
27	c	506	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
27	b	610	CLA	CHB-C4A-NA	2.48	127.97	124.40
27	R	616	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
27	S	610	CLA	CHB-C4A-NA	2.48	127.97	124.40
40	Y	1623	NEX	C38-C25-C24	2.47	117.02	114.24
27	B	610	CLA	CHB-C4A-NA	2.47	127.97	124.40
37	G	605	CHL	O2D-CGD-O1D	-2.47	119.03	123.85
37	G	609	CHL	CMB-C2B-C3B	2.47	129.63	124.68
35	L	101	LHG	C20-C19-C18	-2.47	101.87	114.37
27	s	609	CLA	CHB-C4A-NA	2.47	127.97	124.40
27	y	610	CLA	C1-C2-C3	-2.47	122.15	126.20
38	s	1620	LUT	C31-C30-C29	-2.47	123.81	127.28
27	C	512	CLA	C3B-C4B-NB	-2.47	108.33	110.53
27	C	511	CLA	CAA-CBA-CGA	-2.47	106.19	113.21
31	b	622	LMG	O7-C10-O9	-2.47	117.93	123.70
27	C	506	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
37	g	605	CHL	O2D-CGD-O1D	-2.47	119.04	123.85
31	A	413	LMG	C40-C39-C38	-2.47	101.89	114.37
35	S	2630	LHG	C11-C10-C9	-2.47	101.89	114.37
31	a	413	LMG	C38-C37-C36	-2.47	101.90	114.37
29	b	618	BCR	C3-C4-C5	-2.47	109.66	114.06
37	N	609	CHL	O2A-CGA-CBA	2.47	119.35	111.83
35	s	2630	LHG	C11-C10-C9	-2.46	101.91	114.37
32	c	520	DGD	O2D-C2D-C1D	-2.46	104.20	110.08
27	y	604	CLA	C3B-C4B-NB	-2.46	108.33	110.53
27	n	613	CLA	CHB-C4A-NA	2.46	127.96	124.40
38	G	1620	LUT	C16-C1-C6	-2.46	106.38	110.24
37	g	607	CHL	O2A-CGA-CBA	2.46	119.35	111.83
31	d	411	LMG	O1-C7-C8	-2.46	104.83	110.82
27	y	603	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
27	C	505	CLA	CMB-C2B-C3B	2.46	132.34	126.55
27	c	505	CLA	CMB-C2B-C3B	2.46	132.34	126.55
27	a	410	CLA	O2D-CGD-CBD	2.46	115.53	111.23
27	S	609	CLA	CHB-C4A-NA	2.46	127.95	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	r	616	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
38	N	1621	LUT	C16-C1-C6	-2.46	106.38	110.24
27	c	511	CLA	CAA-CBA-CGA	-2.46	106.22	113.21
37	N	605	CHL	O2D-CGD-O1D	-2.46	119.06	123.85
27	R	601	CLA	CHB-C4A-NA	2.46	127.95	124.40
35	S	2630	LHG	C20-C19-C18	-2.46	101.94	114.37
27	C	513	CLA	C3B-C4B-NB	-2.46	108.34	110.53
31	a	413	LMG	C40-C39-C38	-2.46	101.94	114.37
37	r	608	CHL	O2A-CGA-CBA	2.46	119.33	111.83
27	Y	603	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
37	R	606	CHL	CMB-C2B-C3B	2.46	129.59	124.68
31	B	622	LMG	O7-C10-O9	-2.46	117.97	123.70
37	R	608	CHL	O2A-CGA-CBA	2.45	119.32	111.83
37	n	609	CHL	O2A-CGA-CBA	2.45	119.32	111.83
27	Y	610	CLA	C1-C2-C3	-2.45	122.18	126.20
38	R	620	LUT	C18-C5-C4	2.45	118.93	114.42
32	c	519	DGD	O5D-C6D-C5D	-2.45	103.89	109.42
37	Y	605	CHL	O1D-CGD-CBD	-2.45	121.00	124.72
37	G	607	CHL	O2A-CGA-CBA	2.45	119.31	111.83
27	n	610	CLA	CHB-C4A-NA	2.45	127.94	124.40
39	R	622	XAT	C40-C33-C32	2.45	121.83	118.09
27	n	611	CLA	O2D-CGD-CBD	2.45	115.51	111.23
32	C	519	DGD	O5D-C6D-C5D	-2.45	103.90	109.42
38	r	620	LUT	C18-C5-C4	2.45	118.92	114.42
29	B	618	BCR	C3-C4-C5	-2.45	109.69	114.06
31	D	411	LMG	O1-C7-C8	-2.45	104.86	110.82
27	S	610	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
40	y	1623	NEX	C38-C25-C24	2.45	116.99	114.24
34	d	405	PL9	O1-C4-C3	-2.45	118.15	120.73
31	a	413	LMG	O7-C10-O9	-2.45	117.98	123.70
37	Y	601	CHL	CMB-C2B-C3B	2.45	129.57	124.68
29	a	411	BCR	C21-C20-C19	-2.45	116.11	123.20
27	C	509	CLA	CHB-C4A-NA	2.45	127.93	124.40
27	c	509	CLA	CHB-C4A-NA	2.45	127.93	124.40
27	s	603	CLA	CHB-C4A-NA	2.45	127.93	124.40
29	c	514	BCR	C10-C11-C12	-2.44	116.12	123.20
35	s	2630	LHG	C20-C19-C18	-2.44	102.01	114.37
37	g	609	CHL	CMB-C2B-C3B	2.44	129.57	124.68
29	C	514	BCR	C10-C11-C12	-2.44	116.12	123.20
29	A	411	BCR	C21-C20-C19	-2.44	116.12	123.20
38	s	1621	LUT	C35-C15-C14	-2.44	118.52	123.52
39	R	622	XAT	C18-C5-C4	2.44	116.98	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Y	611	CLA	O2D-CGD-CBD	2.44	115.50	111.23
35	Y	2630	LHG	C11-C10-C9	-2.44	102.03	114.37
27	y	611	CLA	O2D-CGD-CBD	2.44	115.50	111.23
35	y	2630	LHG	C11-C10-C9	-2.44	102.04	114.37
37	n	601	CHL	CMB-C2B-C3B	2.44	129.56	124.68
38	n	1621	LUT	C16-C1-C6	-2.44	106.42	110.24
27	S	614	CLA	CHB-C4A-NA	2.44	127.92	124.40
27	b	610	CLA	CAA-CBA-CGA	-2.44	106.29	113.21
35	D	408	LHG	C11-C10-C9	-2.44	102.06	114.37
35	d	408	LHG	C11-C10-C9	-2.44	102.06	114.37
35	y	2630	LHG	C20-C19-C18	-2.43	102.06	114.37
37	Y	608	CHL	CMB-C2B-C3B	2.43	129.55	124.68
32	c	519	DGD	C3G-C2G-C1G	-2.43	106.11	111.78
37	Y	607	CHL	O2D-CGD-O1D	-2.43	119.11	123.85
37	S	608	CHL	CMB-C2B-C3B	2.43	129.54	124.68
37	s	608	CHL	CMB-C2B-C3B	2.43	129.54	124.68
37	g	607	CHL	CMB-C2B-C3B	2.43	129.54	124.68
32	C	520	DGD	O3G-C1D-C2D	-2.43	104.58	108.27
37	y	601	CHL	CMB-C2B-C3B	2.43	129.54	124.68
27	s	612	CLA	CHB-C4A-NA	2.43	127.91	124.40
27	A	410	CLA	O2D-CGD-CBD	2.43	115.48	111.23
40	N	1623	NEX	C11-C12-C13	-2.43	119.70	126.36
37	G	606	CHL	CBC-CAC-C3C	-2.43	109.39	112.87
27	b	610	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
32	c	519	DGD	CBB-CAB-C9B	-2.43	102.09	114.37
32	C	519	DGD	C3G-C2G-C1G	-2.43	106.12	111.78
39	r	622	XAT	C40-C33-C32	2.43	121.80	118.09
37	G	608	CHL	CMA-C3A-C4A	-2.43	109.38	114.61
30	a	412	SQD	O8-S-C6	2.42	110.65	105.97
37	g	608	CHL	CMA-C3A-C4A	-2.42	109.39	114.61
32	C	519	DGD	CBB-CAB-C9B	-2.42	102.12	114.37
35	Y	2630	LHG	C20-C19-C18	-2.42	102.12	114.37
37	g	607	CHL	O2D-CGD-O1D	-2.42	119.13	123.85
40	n	1623	NEX	C11-C12-C13	-2.42	119.72	126.36
27	N	611	CLA	O2D-CGD-CBD	2.42	115.46	111.23
40	R	623	NEX	C17-C1-C6	-2.42	108.31	110.47
37	g	606	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
28	a	409	PHO	O2D-CGD-O1D	-2.42	119.14	123.85
27	s	614	CLA	CHB-C4A-NA	2.42	127.89	124.40
27	S	612	CLA	CHB-C4A-NA	2.42	127.89	124.40
37	G	607	CHL	CMB-C2B-C3B	2.42	129.52	124.68
37	r	606	CHL	CMB-C2B-C3B	2.42	129.52	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	607	CHL	OMC-CMC-C2C	-2.42	120.92	125.12
37	s	607	CHL	CMB-C2B-C3B	2.42	129.51	124.68
27	B	610	CLA	CAA-CBA-CGA	-2.42	106.34	113.21
27	Y	610	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
27	y	610	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
27	c	505	CLA	CHB-C4A-NA	2.42	127.89	124.40
32	c	520	DGD	O3G-C1D-C2D	-2.42	104.60	108.27
38	R	620	LUT	C30-C31-C32	-2.42	116.20	123.20
31	A	413	LMG	O7-C10-O9	-2.42	118.06	123.70
37	S	607	CHL	CMB-C2B-C3B	2.42	129.51	124.68
31	A	413	LMG	C1-O6-C5	2.42	118.44	113.72
31	a	413	LMG	C1-O6-C5	2.42	118.44	113.72
27	c	513	CLA	C3B-C4B-NB	-2.42	108.37	110.53
37	G	605	CHL	CMB-C2B-C3B	2.42	129.51	124.68
37	g	605	CHL	CMB-C2B-C3B	2.42	129.51	124.68
29	a	411	BCR	C10-C11-C12	-2.41	116.20	123.20
32	c	518	DGD	O2D-C2D-C1D	-2.41	104.32	110.08
37	G	607	CHL	O2D-CGD-O1D	-2.41	119.15	123.85
38	Y	1620	LUT	C15-C35-C34	-2.41	118.58	123.52
38	y	1620	LUT	C15-C35-C34	-2.41	118.58	123.52
27	N	602	CLA	CHB-C4A-NA	2.41	127.88	124.40
38	r	620	LUT	C30-C31-C32	-2.41	116.21	123.20
37	y	601	CHL	O2D-CGD-O1D	-2.41	119.15	123.85
27	r	601	CLA	CHB-C4A-NA	2.41	127.88	124.40
29	H	101	BCR	C11-C10-C9	-2.41	123.90	127.28
29	C	514	BCR	C23-C24-C25	-2.41	120.56	127.00
40	S	1623	NEX	C30-C31-C32	-2.41	116.22	123.20
37	n	608	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
34	D	405	PL9	C22-C23-C24	-2.41	122.11	127.62
34	d	405	PL9	C22-C23-C24	-2.41	122.11	127.62
37	N	601	CHL	CMB-C2B-C3B	2.41	129.50	124.68
40	r	623	NEX	C17-C1-C6	-2.41	108.32	110.47
27	B	610	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
37	n	606	CHL	OMC-CMC-C2C	-2.41	120.94	125.12
31	C	521	LMG	C40-C39-C38	-2.41	102.21	114.37
37	g	606	CHL	CMA-C3A-C4A	-2.41	109.43	114.61
27	S	603	CLA	CHB-C4A-NA	2.40	127.87	124.40
30	A	412	SQD	O8-S-C6	2.40	110.61	105.97
27	Y	611	CLA	CHB-C4A-NA	2.40	127.87	124.40
27	c	512	CLA	C1-C2-C3	-2.40	122.26	126.20
37	y	607	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
31	c	521	LMG	C40-C39-C38	-2.40	102.22	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	S	601	CHL	CMB-C2B-C3B	2.40	129.48	124.68
37	y	608	CHL	CMB-C2B-C3B	2.40	129.48	124.68
37	n	607	CHL	OMC-CMC-C2C	-2.40	120.95	125.12
39	r	622	XAT	C18-C5-C4	2.40	116.94	114.24
38	R	620	LUT	C27-C28-C29	-2.40	121.16	126.32
29	c	514	BCR	C23-C24-C25	-2.40	120.59	127.00
40	Y	1623	NEX	C39-C29-C30	-2.40	118.93	122.82
29	b	619	BCR	C21-C20-C19	-2.40	116.25	123.20
40	s	1623	NEX	C30-C31-C32	-2.40	116.25	123.20
29	A	411	BCR	C10-C11-C12	-2.40	116.25	123.20
27	C	505	CLA	CHB-C4A-NA	2.40	127.86	124.40
35	D	409	LHG	C18-C17-C16	-2.40	102.25	114.37
37	R	608	CHL	C4C-CHD-C1D	2.40	124.65	116.07
35	d	409	LHG	C18-C17-C16	-2.40	102.25	114.37
37	Y	601	CHL	O2D-CGD-O1D	-2.39	119.19	123.85
37	g	606	CHL	CAC-C3C-C4C	2.39	130.18	124.03
27	N	614	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
38	S	1620	LUT	C8-C7-C6	-2.39	120.61	127.00
38	r	620	LUT	C27-C28-C29	-2.39	121.19	126.32
37	r	608	CHL	C4C-CHD-C1D	2.39	124.61	116.07
37	N	608	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
37	G	606	CHL	CMA-C3A-C4A	-2.39	109.47	114.61
27	g	602	CLA	CHB-C4A-NA	2.39	127.84	124.40
27	Y	610	CLA	CHB-C4A-NA	2.39	127.84	124.40
27	n	602	CLA	CHB-C4A-NA	2.39	127.84	124.40
32	C	518	DGD	O2D-C2D-C1D	-2.39	104.39	110.08
29	b	618	BCR	C8-C7-C6	-2.39	120.62	127.00
29	B	619	BCR	C21-C20-C19	-2.39	116.29	123.20
32	C	519	DGD	O2D-C2D-C1D	-2.38	104.39	110.08
32	c	519	DGD	O2D-C2D-C1D	-2.38	104.39	110.08
29	c	514	BCR	C34-C9-C8	2.38	121.73	118.09
29	h	101	BCR	C11-C10-C9	-2.38	123.94	127.28
39	r	622	XAT	C19-C9-C8	2.38	121.73	118.09
37	y	607	CHL	CAC-C3C-C4C	2.38	130.15	124.03
29	C	517	BCR	C3-C4-C5	-2.38	109.81	114.06
29	A	411	BCR	C28-C27-C26	-2.38	109.81	114.06
29	c	517	BCR	C3-C4-C5	-2.38	109.81	114.06
37	N	606	CHL	OMC-CMC-C2C	-2.38	120.98	125.12
27	y	611	CLA	CHB-C4A-NA	2.38	127.84	124.40
38	N	1620	LUT	C39-C29-C28	2.38	121.72	118.09
27	G	602	CLA	CHB-C4A-NA	2.38	127.83	124.40
37	Y	607	CHL	CAC-C3C-C4C	2.38	130.15	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	516	BCR	C33-C5-C4	2.38	118.67	113.60
40	y	1623	NEX	C39-C29-C30	-2.38	118.96	122.82
35	D	408	LHG	C27-C26-C25	-2.38	102.35	114.37
27	n	614	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
39	R	622	XAT	C19-C9-C8	2.38	121.72	118.09
27	C	512	CLA	C1-C2-C3	-2.38	122.30	126.20
35	d	408	LHG	C27-C26-C25	-2.38	102.36	114.37
29	C	514	BCR	C34-C9-C8	2.38	121.72	118.09
32	c	518	DGD	O6D-C5D-C6D	-2.38	101.99	106.69
31	B	622	LMG	C1-C2-C3	-2.37	105.01	110.01
29	c	516	BCR	C33-C5-C4	2.37	118.66	113.60
29	a	411	BCR	C28-C27-C26	-2.37	109.82	114.06
27	B	614	CLA	CHB-C4A-NA	2.37	127.83	124.40
28	A	409	PHO	O2D-CGD-O1D	-2.37	119.23	123.85
38	s	1620	LUT	C8-C7-C6	-2.37	120.66	127.00
27	C	512	CLA	CHB-C4A-NA	2.37	127.82	124.40
37	Y	609	CHL	O2D-CGD-O1D	-2.37	119.23	123.85
27	N	611	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
37	s	601	CHL	CMB-C2B-C3B	2.37	129.42	124.68
27	b	614	CLA	CHB-C4A-NA	2.37	127.82	124.40
27	B	610	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
37	G	606	CHL	CAC-C3C-C4C	2.37	130.11	124.03
37	y	601	CHL	CMA-C3A-C4A	-2.37	109.51	114.61
31	b	622	LMG	C1-C2-C3	-2.36	105.04	110.01
27	R	612	CLA	CHB-C4A-NA	2.36	127.81	124.40
27	b	605	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
32	C	520	DGD	C3D-C4D-C5D	-2.36	105.95	110.23
37	Y	601	CHL	CMA-C3A-C4A	-2.36	109.52	114.61
35	r	2630	LHG	C11-C10-C9	-2.36	102.43	114.37
29	c	514	BCR	C37-C22-C23	2.36	121.69	118.09
38	n	1620	LUT	C39-C29-C28	2.36	121.69	118.09
35	d	409	LHG	O8-C23-C24	2.36	119.03	111.83
32	C	518	DGD	O6D-C5D-C6D	-2.36	102.02	106.69
35	R	2630	LHG	C11-C10-C9	-2.36	102.45	114.37
35	R	2630	LHG	C20-C19-C18	-2.36	102.45	114.37
35	r	2630	LHG	C20-C19-C18	-2.36	102.45	114.37
27	B	605	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
27	n	611	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
27	d	402	CLA	CHB-C4A-NA	2.36	127.80	124.40
27	c	503	CLA	CHB-C4A-NA	2.36	127.80	124.40
37	N	606	CHL	CMB-C2B-C3B	2.36	129.39	124.68
27	C	510	CLA	CMB-C2B-C1B	-2.36	121.83	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	r	611	CLA	CHB-C4A-NA	2.35	127.80	124.40
29	B	618	BCR	C8-C7-C6	-2.35	120.71	127.00
31	C	521	LMG	C38-C37-C36	-2.35	102.47	114.37
37	S	606	CHL	OMC-CMC-C2C	-2.35	121.04	125.12
37	s	606	CHL	OMC-CMC-C2C	-2.35	121.04	125.12
38	g	1620	LUT	C20-C13-C12	2.35	121.68	118.09
27	b	610	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
35	D	409	LHG	O8-C23-C24	2.35	119.00	111.83
27	s	612	CLA	C3B-C4B-NB	-2.35	108.43	110.53
37	N	607	CHL	O2D-CGD-O1D	-2.35	119.28	123.85
35	g	2630	LHG	O8-C23-C24	2.35	118.99	111.83
29	C	515	BCR	C33-C5-C6	-2.35	121.92	124.48
29	a	411	BCR	C15-C16-C17	-2.35	118.72	123.52
29	c	515	BCR	C38-C26-C25	-2.35	121.92	124.48
37	n	607	CHL	O2D-CGD-O1D	-2.34	119.28	123.85
32	c	520	DGD	C3D-C4D-C5D	-2.34	105.98	110.23
31	c	521	LMG	C38-C37-C36	-2.34	102.52	114.37
29	C	515	BCR	C23-C24-C25	-2.34	120.74	127.00
37	S	601	CHL	CMA-C3A-C4A	-2.34	109.56	114.61
27	R	611	CLA	CHB-C4A-NA	2.34	127.78	124.40
37	s	601	CHL	CMA-C3A-C4A	-2.34	109.56	114.61
37	n	606	CHL	CMB-C2B-C3B	2.34	129.36	124.68
31	B	622	LMG	O3-C3-C2	-2.34	104.86	110.38
29	C	517	BCR	C16-C15-C14	-2.34	118.73	123.52
29	c	517	BCR	C16-C15-C14	-2.34	118.73	123.52
27	C	501	CLA	CHB-C4A-NA	2.34	127.78	124.40
27	c	512	CLA	CHB-C4A-NA	2.34	127.77	124.40
29	A	411	BCR	C15-C16-C17	-2.34	118.74	123.52
27	D	403	CLA	CHB-C4A-NA	2.34	127.77	124.40
27	B	606	CLA	CHB-C1B-NB	2.34	127.56	124.05
27	c	506	CLA	CHB-C4A-NA	2.34	127.77	124.40
27	y	610	CLA	CHB-C4A-NA	2.34	127.77	124.40
37	S	606	CHL	O2D-CGD-O1D	-2.34	119.30	123.85
27	c	501	CLA	CHB-C4A-NA	2.34	127.77	124.40
27	B	603	CLA	C3B-C4B-NB	-2.34	108.44	110.53
27	b	603	CLA	CHB-C4A-NA	2.34	127.77	124.40
35	G	2630	LHG	O8-C23-C24	2.33	118.95	111.83
31	b	622	LMG	O3-C3-C2	-2.33	104.88	110.38
37	N	601	CHL	CBC-CAC-C3C	-2.33	109.53	112.87
29	b	620	BCR	C10-C11-C12	-2.33	116.44	123.20
38	S	1621	LUT	C19-C9-C8	2.33	121.65	118.09
27	B	603	CLA	CHB-C4A-NA	2.33	127.76	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	411	BCR	C33-C5-C4	2.33	118.57	113.60
37	y	609	CHL	O2D-CGD-O1D	-2.33	119.31	123.85
29	b	619	BCR	C23-C24-C25	-2.33	120.77	127.00
29	c	515	BCR	C23-C24-C25	-2.33	120.78	127.00
38	Y	1621	LUT	C39-C29-C28	2.33	121.65	118.09
27	b	606	CLA	CHB-C1B-NB	2.33	127.54	124.05
27	g	604	CLA	CHB-C4A-NA	2.33	127.76	124.40
38	S	1621	LUT	C15-C35-C34	-2.33	118.75	123.52
27	y	613	CLA	CHB-C4A-NA	2.33	127.76	124.40
29	B	619	BCR	C23-C24-C25	-2.33	120.78	127.00
27	r	612	CLA	CHB-C4A-NA	2.33	127.76	124.40
29	C	515	BCR	C38-C26-C25	-2.33	121.94	124.48
29	C	515	BCR	C8-C7-C6	-2.33	120.78	127.00
29	c	515	BCR	C8-C7-C6	-2.33	120.78	127.00
37	n	601	CHL	CBC-CAC-C3C	-2.33	109.54	112.87
27	S	612	CLA	C3B-C4B-NB	-2.33	108.45	110.53
27	b	603	CLA	C3B-C4B-NB	-2.32	108.45	110.53
29	C	514	BCR	C37-C22-C23	2.32	121.64	118.09
27	B	612	CLA	CHB-C4A-NA	2.32	127.75	124.40
27	b	607	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
29	B	620	BCR	C10-C11-C12	-2.32	116.47	123.20
37	n	608	CHL	CMB-C2B-C3B	2.32	129.32	124.68
27	C	503	CLA	CHB-C4A-NA	2.32	127.75	124.40
32	c	518	DGD	O3E-C3E-C2E	-2.32	104.91	110.38
38	G	1620	LUT	C20-C13-C12	2.32	121.63	118.09
38	s	1621	LUT	C19-C9-C8	2.32	121.63	118.09
27	c	510	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
27	B	617	CLA	CHB-C4A-NA	2.32	127.74	124.40
27	b	617	CLA	CHB-C4A-NA	2.32	127.74	124.40
37	Y	607	CHL	CMA-C3A-C4A	-2.32	109.62	114.61
32	C	518	DGD	O3E-C3E-C2E	-2.32	104.92	110.38
38	s	1621	LUT	C15-C35-C34	-2.32	118.78	123.52
37	N	607	CHL	C4-C3-C5	2.32	119.25	115.23
37	n	607	CHL	C4-C3-C5	2.32	119.25	115.23
27	C	506	CLA	CHB-C4A-NA	2.32	127.74	124.40
27	D	402	CLA	CHB-C4A-NA	2.32	127.74	124.40
27	d	403	CLA	CMB-C2B-C3B	2.32	132.00	126.55
27	B	607	CLA	O2A-CGA-O1A	-2.32	117.84	123.63
29	H	101	BCR	C39-C30-C25	-2.31	106.61	110.24
29	A	411	BCR	C33-C5-C4	2.31	118.53	113.60
34	d	405	PL9	O2-C1-C6	2.31	124.16	120.48
35	L	101	LHG	C18-C17-C16	-2.31	102.68	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	s	1620	LUT	C39-C29-C28	2.31	121.62	118.09
27	S	613	CLA	CHB-C4A-NA	2.31	127.73	124.40
27	s	613	CLA	CHB-C4A-NA	2.31	127.73	124.40
39	g	1622	XAT	C10-C11-C12	-2.31	116.50	123.20
37	R	608	CHL	CMB-C2B-C3B	2.31	129.30	124.68
38	G	1621	LUT	C15-C35-C34	-2.31	118.79	123.52
38	g	1621	LUT	C15-C35-C34	-2.31	118.79	123.52
27	B	611	CLA	CHB-C4A-NA	2.31	127.73	124.40
27	b	611	CLA	CHB-C4A-NA	2.31	127.73	124.40
37	y	607	CHL	CMA-C3A-C4A	-2.31	109.64	114.61
30	a	412	SQD	O48-C23-C24	2.31	118.88	111.83
27	Y	612	CLA	CHB-C4A-NA	2.31	127.73	124.40
29	c	515	BCR	C33-C5-C6	-2.31	121.97	124.48
30	A	412	SQD	O48-C23-C24	2.31	118.87	111.83
37	N	608	CHL	CMB-C2B-C3B	2.31	129.29	124.68
28	a	408	PHO	O2D-CGD-O1D	-2.31	119.36	123.85
39	G	1622	XAT	C10-C11-C12	-2.31	116.52	123.20
27	B	606	CLA	CHB-C4A-NA	2.31	127.73	124.40
27	b	606	CLA	CHB-C4A-NA	2.31	127.73	124.40
37	G	607	CHL	CAC-C3C-C4C	2.31	129.96	124.03
38	G	1621	LUT	C35-C15-C14	-2.30	118.80	123.52
38	g	1621	LUT	C35-C15-C14	-2.30	118.80	123.52
27	d	403	CLA	CHB-C4A-NA	2.30	127.72	124.40
38	S	1620	LUT	C39-C29-C28	2.30	121.61	118.09
39	r	622	XAT	C20-C13-C12	2.30	121.61	118.09
27	b	612	CLA	CHB-C4A-NA	2.30	127.72	124.40
37	r	607	CHL	CMA-C3A-C4A	-2.30	109.65	114.61
27	G	604	CLA	CHB-C4A-NA	2.30	127.72	124.40
27	R	601	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
31	Z	101	LMG	C40-C39-C38	-2.30	102.74	114.37
37	g	606	CHL	O2D-CGD-O1D	-2.30	119.37	123.85
35	l	101	LHG	C18-C17-C16	-2.30	102.74	114.37
27	G	610	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
37	g	607	CHL	CAC-C3C-C4C	2.30	129.94	124.03
38	y	1621	LUT	C30-C31-C32	-2.30	116.54	123.20
27	A	405	CLA	C1-C2-C3	-2.30	122.44	126.20
40	G	1623	NEX	C38-C25-C24	2.30	116.82	114.24
27	c	513	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
27	Y	613	CLA	CHB-C4A-NA	2.29	127.71	124.40
37	G	606	CHL	O2D-CGD-O1D	-2.29	119.39	123.85
29	d	404	BCR	C21-C20-C19	-2.29	116.56	123.20
27	C	503	CLA	O2A-CGA-O1A	-2.29	117.89	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	S	608	CHL	OMC-CMC-C2C	-2.29	121.14	125.12
27	r	601	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
27	B	604	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
37	s	606	CHL	O2D-CGD-O1D	-2.29	119.39	123.85
37	g	601	CHL	O2D-CGD-O1D	-2.29	119.39	123.85
31	z	101	LMG	C40-C39-C38	-2.29	102.79	114.37
34	d	405	PL9	C37-C38-C39	-2.29	122.38	127.62
38	R	620	LUT	C16-C1-C6	-2.29	106.65	110.24
37	G	607	CHL	CBC-CAC-C3C	-2.29	109.59	112.87
28	A	408	PHO	O2D-CGD-O1D	-2.29	119.39	123.85
37	G	601	CHL	O2D-CGD-O1D	-2.29	119.40	123.85
38	Y	1621	LUT	C30-C31-C32	-2.29	116.57	123.20
34	D	405	PL9	O2-C1-C6	2.29	124.12	120.48
35	s	2630	LHG	C18-C17-C16	-2.28	102.82	114.37
27	D	403	CLA	CMB-C2B-C3B	2.28	131.92	126.55
38	Y	1620	LUT	C8-C7-C6	-2.28	120.89	127.00
38	y	1620	LUT	C8-C7-C6	-2.28	120.89	127.00
37	r	608	CHL	CMB-C2B-C3B	2.28	129.25	124.68
27	C	509	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
27	b	604	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
29	D	404	BCR	C21-C20-C19	-2.28	116.59	123.20
27	b	612	CLA	CHB-C1B-NB	2.28	127.47	124.05
27	B	617	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
27	b	617	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
29	h	101	BCR	C39-C30-C25	-2.28	106.67	110.24
29	C	516	BCR	C10-C11-C12	-2.28	116.60	123.20
37	S	608	CHL	CMA-C3A-C4A	-2.28	109.70	114.61
35	S	2630	LHG	C18-C17-C16	-2.28	102.85	114.37
37	s	608	CHL	CMA-C3A-C4A	-2.28	109.70	114.61
38	y	1621	LUT	C39-C29-C28	2.28	121.57	118.09
37	r	607	CHL	CAC-C3C-C4C	2.28	129.88	124.03
34	D	405	PL9	C37-C38-C39	-2.28	122.41	127.62
38	n	1620	LUT	C31-C30-C29	-2.28	124.08	127.28
35	l	101	LHG	C27-C26-C25	-2.28	102.86	114.37
27	B	612	CLA	CHB-C1B-NB	2.28	127.46	124.05
37	g	607	CHL	CBC-CAC-C3C	-2.28	109.61	112.87
27	b	604	CLA	CHB-C1B-NB	2.28	127.46	124.05
38	r	620	LUT	C15-C35-C34	-2.28	118.86	123.52
39	R	622	XAT	C20-C13-C12	2.27	121.56	118.09
35	n	2630	LHG	C20-C19-C18	-2.27	102.87	114.37
37	R	607	CHL	CAC-C3C-C4C	2.27	129.88	124.03
27	c	508	CLA	CHC-C1C-NC	2.27	127.74	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	G	1621	LUT	C40-C33-C32	2.27	121.56	118.09
27	c	503	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
35	L	101	LHG	C27-C26-C25	-2.27	102.88	114.37
27	C	513	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
29	c	516	BCR	C10-C11-C12	-2.27	116.61	123.20
35	N	2630	LHG	C27-C26-C25	-2.27	102.89	114.37
37	G	601	CHL	OMC-CMC-C2C	-2.27	121.18	125.12
37	g	601	CHL	OMC-CMC-C2C	-2.27	121.18	125.12
38	r	620	LUT	C16-C1-C6	-2.27	106.68	110.24
35	n	2630	LHG	C27-C26-C25	-2.27	102.89	114.37
40	g	1623	NEX	C38-C25-C24	2.27	116.79	114.24
35	D	409	LHG	C27-C26-C25	-2.27	102.90	114.37
35	d	409	LHG	C27-C26-C25	-2.27	102.90	114.37
37	r	606	CHL	O2D-CGD-O1D	-2.27	119.43	123.85
27	B	604	CLA	CHB-C1B-NB	2.27	127.45	124.05
37	s	606	CHL	CMB-C2B-C3B	2.27	129.22	124.68
37	y	601	CHL	OMC-CMC-C2C	-2.27	121.18	125.12
38	S	1621	LUT	C39-C29-C28	2.27	121.55	118.09
37	N	601	CHL	O2D-CGD-O1D	-2.27	119.43	123.85
27	a	405	CLA	C1-C2-C3	-2.27	122.48	126.20
37	s	608	CHL	OMC-CMC-C2C	-2.27	121.18	125.12
37	g	601	CHL	CMB-C2B-C3B	2.27	129.21	124.68
37	s	607	CHL	O2D-CGD-O1D	-2.27	119.44	123.85
27	y	612	CLA	CHB-C4A-NA	2.27	127.67	124.40
38	Y	1620	LUT	C16-C1-C6	-2.27	106.69	110.24
38	y	1620	LUT	C16-C1-C6	-2.27	106.69	110.24
35	N	2630	LHG	C20-C19-C18	-2.27	102.92	114.37
38	R	620	LUT	C15-C35-C34	-2.27	118.88	123.52
37	R	607	CHL	CMA-C3A-C4A	-2.27	109.73	114.61
30	A	418	SQD	O8-S-C6	2.27	110.35	105.97
30	a	418	SQD	O8-S-C6	2.27	110.35	105.97
38	s	1621	LUT	C3-C4-C5	-2.27	106.54	112.18
27	c	509	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
29	b	618	BCR	C33-C5-C4	2.26	118.42	113.60
27	C	509	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
31	Z	101	LMG	O3-C3-C2	-2.26	105.04	110.38
40	r	623	NEX	C11-C12-C13	-2.26	120.16	126.36
38	S	1621	LUT	C3-C4-C5	-2.26	106.54	112.18
40	R	623	NEX	C11-C12-C13	-2.26	120.16	126.36
30	A	418	SQD	C1-C2-C3	2.26	114.77	110.01
31	z	101	LMG	O3-C3-C2	-2.26	105.05	110.38
39	N	1622	XAT	C19-C9-C8	2.26	121.54	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	618	BCR	C38-C26-C27	2.26	118.42	113.60
37	N	605	CHL	CMB-C2B-C3B	2.26	129.20	124.68
37	y	606	CHL	OMC-CMC-C2C	-2.26	121.20	125.12
27	N	610	CLA	O2D-CGD-CBD	2.26	115.18	111.23
38	g	1621	LUT	C40-C33-C32	2.26	121.54	118.09
27	g	610	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
37	G	609	CHL	OMC-CMC-C2C	-2.26	121.20	125.12
37	S	607	CHL	O2D-CGD-O1D	-2.26	119.45	123.85
37	n	605	CHL	CMB-C2B-C3B	2.26	129.19	124.68
37	Y	609	CHL	OMC-CMC-C2C	-2.26	121.20	125.12
37	R	606	CHL	CAC-C3C-C4C	2.25	129.83	124.03
37	r	606	CHL	CAC-C3C-C4C	2.25	129.83	124.03
37	Y	606	CHL	OMC-CMC-C2C	-2.25	121.20	125.12
37	g	607	CHL	OMC-CMC-C2C	-2.25	121.21	125.12
27	C	508	CLA	CHC-C1C-NC	2.25	127.70	124.31
31	c	521	LMG	O3-C3-C2	-2.25	105.07	110.38
37	G	609	CHL	CED-O2D-CGD	2.25	121.02	115.92
32	C	518	DGD	O3G-C1D-C2D	-2.25	104.85	108.27
37	G	607	CHL	OMC-CMC-C2C	-2.25	121.21	125.12
37	g	605	CHL	OMC-CMC-C2C	-2.25	121.21	125.12
27	D	402	CLA	C1-C2-C3	-2.25	122.51	126.20
38	s	1621	LUT	C39-C29-C28	2.25	121.53	118.09
37	n	601	CHL	O2D-CGD-O1D	-2.25	119.47	123.85
38	Y	1621	LUT	C16-C1-C6	-2.25	106.71	110.24
38	y	1621	LUT	C16-C1-C6	-2.25	106.71	110.24
38	g	1621	LUT	C38-C25-C24	-2.25	118.03	123.36
27	G	613	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
27	g	613	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
37	S	606	CHL	CMB-C2B-C3B	2.25	129.18	124.68
30	a	418	SQD	C1-C2-C3	2.25	114.74	110.01
27	B	602	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
27	B	604	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
37	n	607	CHL	CAC-C3C-C4C	2.25	129.81	124.03
37	n	601	CHL	CMA-C3A-C4A	-2.25	109.77	114.61
27	b	602	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
31	c	521	LMG	O2-C2-C1	-2.25	104.72	110.08
37	R	606	CHL	O2D-CGD-O1D	-2.25	119.47	123.85
37	Y	601	CHL	OMC-CMC-C2C	-2.25	121.22	125.12
29	B	620	BCR	C37-C22-C23	2.25	121.52	118.09
37	N	608	CHL	CMD-C2D-C3D	-2.24	120.20	124.68
37	n	608	CHL	CMD-C2D-C3D	-2.24	120.20	124.68
29	B	618	BCR	C33-C5-C4	2.24	118.38	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	605	CHL	OMC-CMC-C2C	-2.24	121.22	125.12
27	b	604	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
39	g	1622	XAT	C24-C23-C22	-2.24	106.59	110.79
37	N	607	CHL	CAC-C3C-C4C	2.24	129.79	124.03
37	n	607	CHL	CBC-CAC-C3C	-2.24	109.66	112.87
31	C	521	LMG	O2-C2-C1	-2.24	104.73	110.08
27	b	613	CLA	CAA-CBA-CGA	-2.24	106.84	113.21
38	y	1620	LUT	C19-C9-C8	2.24	121.51	118.09
37	G	608	CHL	O2D-CGD-O1D	-2.24	119.49	123.85
37	g	608	CHL	O2D-CGD-O1D	-2.24	119.49	123.85
32	c	518	DGD	O3G-C1D-C2D	-2.24	104.87	108.27
29	H	101	BCR	C33-C5-C6	-2.24	122.04	124.48
38	N	1620	LUT	C31-C30-C29	-2.24	124.14	127.28
37	g	609	CHL	OMC-CMC-C2C	-2.24	121.23	125.12
29	b	618	BCR	C38-C26-C27	2.24	118.37	113.60
38	G	1621	LUT	C38-C25-C24	-2.24	118.06	123.36
27	d	402	CLA	C1-C2-C3	-2.24	122.53	126.20
38	n	1621	LUT	C38-C25-C24	-2.24	118.07	123.36
39	G	1622	XAT	C19-C9-C8	2.24	121.50	118.09
37	g	609	CHL	CED-O2D-CGD	2.24	120.99	115.92
37	G	601	CHL	CMB-C2B-C3B	2.23	129.15	124.68
31	C	521	LMG	O3-C3-C2	-2.23	105.11	110.38
34	D	405	PL9	C36-C34-C33	-2.23	116.15	121.17
34	d	405	PL9	C36-C34-C33	-2.23	116.15	121.17
37	N	601	CHL	CMA-C3A-C4A	-2.23	109.80	114.61
27	C	502	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
35	r	2630	LHG	C27-C26-C25	-2.23	103.09	114.37
27	n	610	CLA	O2D-CGD-CBD	2.23	115.13	111.23
39	Y	1622	XAT	O4-C5-C18	2.23	117.54	115.05
39	y	1622	XAT	O4-C5-C18	2.23	117.54	115.05
37	y	609	CHL	OMC-CMC-C2C	-2.23	121.25	125.12
31	Z	101	LMG	O2-C2-C1	-2.23	104.76	110.08
27	R	603	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
27	g	610	CLA	C1-C2-C3	-2.23	122.54	126.20
37	Y	606	CHL	CAC-C3C-C4C	2.23	129.76	124.03
37	y	606	CHL	CAC-C3C-C4C	2.23	129.76	124.03
27	R	611	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
27	A	406	CLA	C1-C2-C3	-2.23	122.55	126.20
39	g	1622	XAT	C19-C9-C8	2.23	121.49	118.09
29	H	101	BCR	C3-C4-C5	-2.23	110.08	114.06
29	h	101	BCR	C3-C4-C5	-2.23	110.08	114.06
27	r	603	CLA	O2A-CGA-O1A	-2.23	118.05	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	R	2630	LHG	C27-C26-C25	-2.23	103.10	114.37
27	S	603	CLA	C3B-C4B-NB	-2.23	108.54	110.53
28	a	409	PHO	C2B-C1B-NB	-2.22	107.82	109.43
27	B	613	CLA	CAA-CBA-CGA	-2.22	106.89	113.21
27	s	610	CLA	CMB-C2B-C3B	2.22	131.78	126.55
37	Y	605	CHL	CMB-C2B-C3B	2.22	129.13	124.68
27	c	509	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
27	C	510	CLA	CHB-C4A-NA	2.22	127.61	124.40
39	G	1622	XAT	C24-C23-C22	-2.22	106.63	110.79
38	N	1621	LUT	C38-C25-C24	-2.22	118.10	123.36
38	R	620	LUT	C19-C9-C8	2.22	121.48	118.09
38	r	620	LUT	C19-C9-C8	2.22	121.48	118.09
27	c	510	CLA	CHB-C4A-NA	2.22	127.61	124.40
31	z	101	LMG	O6-C1-O1	-2.22	104.80	110.04
27	c	507	CLA	C1-C2-C3	-2.22	122.56	126.20
27	C	501	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
32	C	520	DGD	O6E-C1E-O5D	-2.22	104.80	110.04
37	s	601	CHL	CAC-C3C-C4C	2.22	129.73	124.03
32	c	520	DGD	O6E-C1E-O5D	-2.22	104.80	110.04
38	s	1620	LUT	C20-C13-C12	2.22	121.47	118.09
27	c	502	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
27	c	501	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
31	C	521	LMG	O1-C1-C2	-2.22	104.91	108.27
31	c	521	LMG	O1-C1-C2	-2.22	104.91	108.27
37	r	606	CHL	C4C-CHD-C1D	2.21	123.99	116.07
27	C	507	CLA	C1-C2-C3	-2.21	122.57	126.20
29	b	618	BCR	C29-C30-C25	2.21	113.65	110.44
27	a	406	CLA	C1-C2-C3	-2.21	122.57	126.20
31	Z	101	LMG	O6-C1-O1	-2.21	104.82	110.04
39	n	1622	XAT	C19-C9-C8	2.21	121.47	118.09
38	n	1620	LUT	C11-C10-C9	-2.21	124.18	127.28
32	c	518	DGD	CBB-CAB-C9B	-2.21	103.19	114.37
35	g	2630	LHG	O8-C23-O10	-2.21	118.10	123.63
29	b	620	BCR	C37-C22-C23	2.21	121.47	118.09
38	n	1621	LUT	C19-C9-C8	2.21	121.47	118.09
32	C	519	DGD	C5B-C4B-C3B	-2.21	103.19	114.37
37	y	605	CHL	CMB-C2B-C3B	2.21	129.10	124.68
32	c	519	DGD	C5B-C4B-C3B	-2.21	103.20	114.37
32	C	518	DGD	CBB-CAB-C9B	-2.21	103.21	114.37
37	N	607	CHL	CBC-CAC-C3C	-2.21	109.71	112.87
37	y	609	CHL	C11-C10-C8	-2.21	108.63	115.97
38	S	1620	LUT	C20-C13-C12	2.21	121.46	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	S	601	CHL	CAC-C3C-C4C	2.21	129.70	124.03
29	d	404	BCR	C15-C14-C13	-2.21	124.18	127.28
31	z	101	LMG	O2-C2-C1	-2.21	104.82	110.08
40	r	623	NEX	C39-C29-C30	-2.21	119.24	122.82
27	S	610	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
40	Y	1623	NEX	C15-C35-C34	-2.21	119.01	123.52
40	y	1623	NEX	C15-C35-C34	-2.21	119.01	123.52
38	Y	1620	LUT	C39-C29-C28	2.20	121.46	118.09
29	C	516	BCR	C21-C20-C19	-2.20	116.81	123.20
36	F	101	HEM	CHC-C1C-NC	2.20	126.85	124.45
36	f	101	HEM	CHC-C1C-NC	2.20	126.85	124.45
29	B	618	BCR	C29-C30-C25	2.20	113.64	110.44
38	Y	1620	LUT	C19-C9-C8	2.20	121.45	118.09
27	s	614	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
27	r	611	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
31	a	413	LMG	O6-C1-C2	2.20	114.89	110.37
37	Y	609	CHL	C11-C10-C8	-2.20	108.66	115.97
29	c	516	BCR	C35-C13-C12	2.20	121.45	118.09
40	g	1623	NEX	C20-C13-C14	-2.20	119.25	122.82
27	s	610	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
29	h	101	BCR	C33-C5-C6	-2.20	122.09	124.48
35	D	410	LHG	C27-C26-C25	-2.20	103.27	114.37
35	G	2630	LHG	O8-C23-O10	-2.20	118.14	123.63
37	R	606	CHL	C4C-CHD-C1D	2.20	123.92	116.07
27	N	610	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
29	c	516	BCR	C21-C20-C19	-2.19	116.84	123.20
35	d	410	LHG	C27-C26-C25	-2.19	103.28	114.37
35	y	2630	LHG	C18-C17-C16	-2.19	103.28	114.37
27	C	502	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
37	R	606	CHL	CMA-C3A-C4A	-2.19	109.89	114.61
35	Y	2630	LHG	C18-C17-C16	-2.19	103.28	114.37
39	y	1622	XAT	C10-C11-C12	-2.19	116.84	123.20
27	y	612	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
38	n	1621	LUT	C15-C35-C34	-2.19	119.03	123.52
27	Y	612	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
37	G	601	CHL	CMD-C2D-C3D	-2.19	120.31	124.68
27	n	612	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
27	A	405	CLA	CAA-CBA-CGA	-2.19	106.99	113.21
28	A	409	PHO	C2B-C1B-NB	-2.19	107.85	109.43
31	A	413	LMG	O6-C1-C2	2.19	114.87	110.37
27	S	610	CLA	CMB-C2B-C3B	2.19	131.70	126.55
27	G	610	CLA	C1-C2-C3	-2.19	122.61	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	y	1621	LUT	C38-C25-C24	-2.19	118.18	123.36
35	y	2630	LHG	C5-O7-C7	-2.19	112.56	117.80
35	Y	2630	LHG	C5-O7-C7	-2.19	112.56	117.80
27	S	614	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
27	Y	614	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
29	c	515	BCR	C37-C22-C23	2.19	121.43	118.09
27	n	610	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
29	C	516	BCR	C38-C26-C27	2.19	118.26	113.60
40	R	623	NEX	C39-C29-C30	-2.19	119.28	122.82
27	a	405	CLA	CAA-CBA-CGA	-2.18	107.00	113.21
38	N	1620	LUT	C11-C10-C9	-2.18	124.21	127.28
37	r	606	CHL	CMA-C3A-C4A	-2.18	109.90	114.61
29	C	516	BCR	C35-C13-C12	2.18	121.42	118.09
38	N	1621	LUT	C15-C35-C34	-2.18	119.05	123.52
40	N	1623	NEX	C38-C25-C24	2.18	116.69	114.24
38	N	1621	LUT	C39-C29-C28	2.18	121.42	118.09
38	n	1621	LUT	C39-C29-C28	2.18	121.42	118.09
38	y	1620	LUT	C39-C29-C28	2.18	121.42	118.09
27	c	509	CLA	CAA-CBA-CGA	-2.18	107.01	113.21
27	C	509	CLA	CAA-CBA-CGA	-2.18	107.01	113.21
37	R	606	CHL	C4D-ND-C1D	-2.18	103.56	105.22
38	N	1621	LUT	C19-C9-C8	2.18	121.42	118.09
27	N	612	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
27	s	603	CLA	C3B-C4B-NB	-2.18	108.58	110.53
39	Y	1622	XAT	C10-C11-C12	-2.18	116.88	123.20
38	Y	1621	LUT	C38-C25-C24	-2.18	118.20	123.36
29	C	514	BCR	C11-C12-C13	-2.18	120.39	126.36
37	y	605	CHL	C4D-ND-C1D	-2.18	103.57	105.22
39	n	1622	XAT	C39-C29-C30	-2.18	119.29	122.82
37	y	608	CHL	OMC-CMC-C2C	-2.18	121.34	125.12
27	n	611	CLA	C3B-C4B-NB	-2.18	108.59	110.53
37	n	605	CHL	C4C-CHD-C1D	2.17	123.85	116.07
29	D	404	BCR	C15-C14-C13	-2.17	124.23	127.28
27	c	502	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
27	b	612	CLA	CAC-C3C-C4C	2.17	127.62	124.79
27	c	513	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
38	n	1620	LUT	C16-C1-C6	-2.17	106.84	110.24
32	c	518	DGD	CAB-C9B-C8B	-2.17	103.40	114.37
31	D	411	LMG	O3-C3-C2	-2.17	105.26	110.38
29	c	514	BCR	C16-C15-C14	-2.17	119.08	123.52
35	S	2630	LHG	C27-C26-C25	-2.17	103.40	114.37
35	s	2630	LHG	C27-C26-C25	-2.17	103.40	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	y	614	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
37	N	605	CHL	C4C-CHD-C1D	2.17	123.83	116.07
29	c	515	BCR	C2-C1-C6	2.17	113.59	110.44
27	g	612	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
37	G	608	CHL	CMD-C2D-C3D	-2.17	120.35	124.68
37	Y	608	CHL	OMC-CMC-C2C	-2.17	121.36	125.12
39	N	1622	XAT	C39-C29-C30	-2.16	119.31	122.82
32	C	518	DGD	CAB-C9B-C8B	-2.16	103.43	114.37
31	d	411	LMG	O3-C3-C2	-2.16	105.28	110.38
39	y	1622	XAT	C40-C33-C34	-2.16	119.31	122.82
27	c	513	CLA	CMB-C2B-C3B	2.16	131.63	126.55
38	N	1620	LUT	C16-C1-C6	-2.16	106.85	110.24
38	S	1621	LUT	C7-C8-C9	-2.16	123.04	126.23
27	S	604	CLA	C3B-C4B-NB	-2.16	108.60	110.53
27	B	611	CLA	O1D-CGD-CBD	2.16	128.78	124.52
35	g	2630	LHG	C27-C26-C25	-2.16	103.45	114.37
37	g	601	CHL	CMD-C2D-C3D	-2.16	120.37	124.68
34	D	405	PL9	C12-C13-C14	-2.16	122.68	127.62
34	d	405	PL9	C12-C13-C14	-2.16	122.68	127.62
29	c	516	BCR	C38-C26-C27	2.16	118.20	113.60
37	n	609	CHL	C1-O2A-CGA	2.16	121.88	116.65
40	G	1623	NEX	C20-C13-C14	-2.16	119.32	122.82
29	c	514	BCR	C11-C12-C13	-2.16	120.45	126.36
27	C	513	CLA	CMB-C2B-C3B	2.16	131.62	126.55
35	G	2630	LHG	C18-C17-C16	-2.16	103.47	114.37
35	g	2630	LHG	C18-C17-C16	-2.16	103.47	114.37
37	N	606	CHL	CMA-C3A-C4A	-2.16	109.97	114.61
37	n	606	CHL	CMA-C3A-C4A	-2.16	109.97	114.61
35	G	2630	LHG	C27-C26-C25	-2.16	103.47	114.37
29	C	514	BCR	C16-C15-C14	-2.15	119.11	123.52
27	R	610	CLA	C1-C2-C3	-2.15	122.67	126.20
29	h	101	BCR	C29-C30-C25	2.15	113.57	110.44
29	c	515	BCR	C11-C12-C13	-2.15	120.46	126.36
38	n	1620	LUT	C15-C35-C34	-2.15	119.11	123.52
29	C	515	BCR	C37-C22-C23	2.15	121.38	118.09
29	C	515	BCR	C11-C12-C13	-2.15	120.47	126.36
37	N	601	CHL	CMD-C2D-C3D	-2.15	120.39	124.68
27	y	602	CLA	C16-C15-C13	-2.15	108.82	115.97
27	C	513	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
37	Y	605	CHL	C4D-ND-C1D	-2.15	103.59	105.22
40	Y	1623	NEX	C30-C31-C32	-2.15	116.98	123.20
27	G	612	CLA	O2A-CGA-O1A	-2.14	118.26	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	612	CLA	CAC-C3C-C4C	2.14	127.58	124.79
37	g	608	CHL	CMD-C2D-C3D	-2.14	120.40	124.68
27	B	610	CLA	C1-C2-C3	-2.14	122.68	126.20
29	b	619	BCR	C38-C26-C27	2.14	118.17	113.60
40	n	1623	NEX	C38-C25-C24	2.14	116.65	114.24
37	n	601	CHL	CMD-C2D-C3D	-2.14	120.40	124.68
38	R	620	LUT	C11-C10-C9	-2.14	124.27	127.28
38	r	620	LUT	C11-C10-C9	-2.14	124.27	127.28
37	N	609	CHL	C1-O2A-CGA	2.14	121.84	116.65
29	H	101	BCR	C29-C30-C25	2.14	113.55	110.44
31	A	413	LMG	O2-C2-C1	-2.14	104.97	110.08
27	R	616	CLA	O2D-CGD-CBD	2.14	114.97	111.23
27	r	616	CLA	O2D-CGD-CBD	2.14	114.97	111.23
27	r	610	CLA	C1-C2-C3	-2.14	122.69	126.20
27	A	410	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
27	a	410	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
27	s	612	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
27	c	507	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
29	A	411	BCR	C37-C22-C23	2.14	121.36	118.09
40	r	623	NEX	C40-C33-C32	2.14	121.36	118.09
27	s	604	CLA	C3B-C4B-NB	-2.14	108.62	110.53
27	S	612	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
39	Y	1622	XAT	C6-C7-C8	-2.14	121.47	125.99
27	b	611	CLA	O1D-CGD-CBD	2.14	128.73	124.52
39	Y	1622	XAT	C40-C33-C34	-2.14	119.35	122.82
38	S	1621	LUT	C40-C33-C32	2.14	121.35	118.09
31	Z	101	LMG	C38-C37-C36	-2.14	103.57	114.37
38	N	1620	LUT	C15-C35-C34	-2.14	119.15	123.52
27	b	613	CLA	CMB-C2B-C3B	2.14	131.57	126.55
37	R	608	CHL	OBD-CAD-C3D	-2.14	124.56	127.89
27	C	506	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
31	z	101	LMG	C38-C37-C36	-2.13	103.58	114.37
38	s	1621	LUT	C7-C8-C9	-2.13	123.08	126.23
27	a	407	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
37	g	605	CHL	C4C-CHD-C1D	2.13	123.70	116.07
35	n	2630	LHG	C18-C17-C16	-2.13	103.59	114.37
27	g	610	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
27	Y	613	CLA	C1-C2-C3	-2.13	122.70	126.20
32	H	102	DGD	O3E-C3E-C2E	-2.13	105.35	110.38
40	y	1623	NEX	C30-C31-C32	-2.13	117.03	123.20
27	Y	602	CLA	C16-C15-C13	-2.13	108.88	115.97
35	N	2630	LHG	C18-C17-C16	-2.13	103.60	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	610	CLA	CHB-C1B-NB	2.13	127.24	124.05
37	n	607	CHL	C6-C5-C3	-2.13	108.28	113.47
37	r	606	CHL	C4D-ND-C1D	-2.13	103.60	105.22
31	a	413	LMG	O2-C2-C1	-2.13	105.00	110.08
38	N	1620	LUT	C18-C5-C4	2.13	118.33	114.42
30	a	412	SQD	O5-C5-C4	2.13	113.53	109.70
27	S	602	CLA	O1D-CGD-CBD	2.13	128.71	124.52
39	y	1622	XAT	C6-C7-C8	-2.13	121.50	125.99
27	s	602	CLA	O1D-CGD-CBD	2.13	128.71	124.52
27	a	405	CLA	CHB-C4A-NA	2.13	127.47	124.40
38	s	1621	LUT	C40-C33-C32	2.12	121.33	118.09
38	y	1620	LUT	C40-C33-C32	2.12	121.33	118.09
37	N	607	CHL	C6-C5-C3	-2.12	108.29	113.47
27	G	610	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
27	a	406	CLA	CMB-C2B-C1B	-2.12	122.18	125.42
31	c	521	LMG	O1-C7-C8	-2.12	105.65	110.82
37	N	605	CHL	CAC-C3C-C4C	2.12	129.49	124.03
30	B	621	SQD	O48-C23-O10	-2.12	118.32	123.63
27	b	609	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
27	b	610	CLA	C1-C2-C3	-2.12	122.72	126.20
29	B	619	BCR	C38-C26-C27	2.12	118.12	113.60
27	d	403	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
27	A	407	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
29	C	515	BCR	C2-C1-C6	2.12	113.52	110.44
27	B	609	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
32	h	102	DGD	O3E-C3E-C2E	-2.12	105.39	110.38
32	c	518	DGD	C5B-C4B-C3B	-2.12	103.67	114.37
27	B	607	CLA	O2D-CGD-CBD	2.12	114.93	111.23
38	G	1621	LUT	C20-C13-C12	2.12	121.32	118.09
27	C	507	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
27	A	406	CLA	CMB-C2B-C1B	-2.12	122.20	125.42
27	b	613	CLA	CMB-C2B-C1B	-2.12	122.20	125.42
38	Y	1620	LUT	C40-C33-C32	2.12	121.32	118.09
38	g	1621	LUT	C20-C13-C12	2.12	121.32	118.09
27	a	407	CLA	CMB-C2B-C3B	2.11	131.52	126.55
27	c	506	CLA	CMB-C2B-C3B	2.11	131.52	126.55
37	G	605	CHL	C4C-CHD-C1D	2.11	123.63	116.07
27	c	506	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
30	A	412	SQD	O5-C5-C4	2.11	113.51	109.70
29	C	515	BCR	C33-C5-C4	2.11	118.10	113.60
27	N	611	CLA	C3B-C4B-NB	-2.11	108.64	110.53
32	C	518	DGD	C5B-C4B-C3B	-2.11	103.69	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	r	602	CLA	O1D-CGD-CBD	2.11	128.68	124.52
29	c	515	BCR	C33-C5-C4	2.11	118.10	113.60
31	z	101	LMG	C1-C2-C3	-2.11	105.57	110.01
38	n	1620	LUT	C18-C5-C4	2.11	118.30	114.42
27	c	503	CLA	CAA-CBA-CGA	-2.11	107.22	113.21
30	a	412	SQD	C1-O5-C5	2.11	117.83	113.72
29	a	411	BCR	C37-C22-C23	2.11	121.31	118.09
27	g	602	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
29	D	404	BCR	C28-C27-C26	-2.11	110.30	114.06
30	a	418	SQD	O5-C5-C4	2.11	113.49	109.70
37	n	605	CHL	CAC-C3C-C4C	2.11	129.44	124.03
32	c	518	DGD	O5E-C6E-C5E	-2.11	104.16	111.33
40	R	623	NEX	C40-C33-C32	2.11	121.30	118.09
27	Y	610	CLA	CMB-C2B-C3B	2.10	131.50	126.55
40	s	1623	NEX	C39-C29-C30	-2.10	119.41	122.82
27	s	613	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
27	b	607	CLA	O2D-CGD-CBD	2.10	114.91	111.23
32	C	519	DGD	C3D-C4D-C5D	-2.10	106.42	110.23
32	c	519	DGD	C3D-C4D-C5D	-2.10	106.42	110.23
37	Y	605	CHL	C4C-CHD-C1D	2.10	123.59	116.07
27	D	403	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
38	S	1621	LUT	C18-C5-C4	2.10	118.28	114.42
39	R	622	XAT	C39-C29-C28	2.10	121.30	118.09
27	n	610	CLA	CHB-C1B-NB	2.10	127.20	124.05
30	b	621	SQD	O48-C23-O10	-2.10	118.38	123.63
39	Y	1622	XAT	C27-C28-C29	-2.10	122.27	125.53
30	b	621	SQD	C44-O6-C1	2.10	118.30	113.80
39	g	1622	XAT	C11-C10-C9	-2.10	124.33	127.28
37	y	605	CHL	C4C-CHD-C1D	2.10	123.58	116.07
30	A	412	SQD	C1-O5-C5	2.10	117.82	113.72
27	A	407	CLA	CMB-C2B-C3B	2.10	131.48	126.55
32	C	518	DGD	O5E-C6E-C5E	-2.10	104.19	111.33
31	C	521	LMG	O1-C7-C8	-2.10	105.72	110.82
31	D	411	LMG	C1-O6-C5	-2.10	109.63	113.72
31	d	411	LMG	C1-O6-C5	-2.10	109.63	113.72
27	B	609	CLA	O2D-CGD-CBD	2.10	114.89	111.23
37	S	601	CHL	C4C-CHD-C1D	2.09	123.56	116.07
37	R	608	CHL	CMA-C3A-C4A	-2.09	110.10	114.61
40	R	623	NEX	C2-C1-C6	2.09	111.25	109.21
27	c	503	CLA	CHC-C4B-NB	2.09	127.19	124.05
32	c	519	DGD	O6E-C1E-O5D	-2.09	105.10	110.04
27	B	613	CLA	CMB-C2B-C3B	2.09	131.47	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	609	CLA	O2D-CGD-CBD	2.09	114.89	111.23
27	C	511	CLA	CMB-C2B-C3B	2.09	131.47	126.55
31	Z	101	LMG	C1-C2-C3	-2.09	105.61	110.01
27	r	609	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
37	r	608	CHL	OBD-CAD-C3D	-2.09	124.63	127.89
37	N	609	CHL	CAC-C3C-C4C	2.09	129.40	124.03
27	R	612	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
40	r	623	NEX	C2-C1-C6	2.09	111.24	109.21
35	d	409	LHG	O8-C6-C5	-2.09	102.38	108.40
37	n	609	CHL	CAC-C3C-C4C	2.09	129.40	124.03
30	B	621	SQD	C44-O6-C1	2.09	118.27	113.80
38	g	1620	LUT	C18-C5-C4	2.09	118.26	114.42
27	G	602	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
27	C	506	CLA	CMB-C2B-C3B	2.09	131.46	126.55
37	s	601	CHL	C4C-CHD-C1D	2.09	123.53	116.07
37	r	608	CHL	CMA-C3A-C4A	-2.09	110.12	114.61
40	S	1623	NEX	C39-C29-C30	-2.09	119.44	122.82
27	B	608	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
27	g	611	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
35	D	409	LHG	O8-C6-C5	-2.08	102.39	108.40
27	g	613	CLA	CHB-C1B-NB	2.08	127.18	124.05
31	A	413	LMG	C9-C8-C7	-2.08	106.92	111.78
27	C	503	CLA	CAA-CBA-CGA	-2.08	107.29	113.21
27	g	611	CLA	O2D-CGD-CBD	2.08	114.87	111.23
30	A	412	SQD	O5-C1-C2	2.08	114.65	110.37
27	S	613	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
27	C	506	CLA	CHB-C1B-NB	2.08	127.17	124.05
27	c	506	CLA	CHB-C1B-NB	2.08	127.17	124.05
27	R	602	CLA	O1D-CGD-CBD	2.08	128.62	124.52
37	Y	606	CHL	O2D-CGD-O1D	-2.08	119.80	123.85
27	R	609	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
32	C	519	DGD	O6E-C1E-O5D	-2.08	105.13	110.04
27	C	510	CLA	CMB-C2B-C3B	2.08	131.44	126.55
27	A	406	CLA	CMB-C2B-C3B	2.08	131.44	126.55
31	a	413	LMG	O6-C1-O1	-2.08	105.14	110.04
29	c	516	BCR	C39-C30-C25	-2.08	106.99	110.24
27	S	611	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
27	s	611	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
27	c	510	CLA	CMB-C2B-C3B	2.08	131.44	126.55
29	C	515	BCR	C36-C18-C19	2.08	121.26	118.09
37	N	609	CHL	O2D-CGD-O1D	-2.08	119.81	123.85
37	n	609	CHL	O2D-CGD-O1D	-2.08	119.81	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	404	BCR	C28-C27-C26	-2.08	110.35	114.06
27	g	613	CLA	CHB-C4A-NA	2.08	127.39	124.40
31	A	413	LMG	O6-C1-O1	-2.07	105.14	110.04
27	a	405	CLA	CMB-C2B-C3B	2.07	131.43	126.55
27	y	610	CLA	CMB-C2B-C3B	2.07	131.43	126.55
39	G	1622	XAT	C7-C8-C9	-2.07	122.31	125.53
40	n	1623	NEX	O24-C25-C26	-2.07	57.29	58.93
35	D	408	LHG	O8-C6-C5	-2.07	102.42	108.40
37	y	606	CHL	O2D-CGD-O1D	-2.07	119.81	123.85
27	A	405	CLA	CMB-C2B-C3B	2.07	131.43	126.55
27	A	405	CLA	CHB-C4A-NA	2.07	127.39	124.40
27	B	609	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
27	r	612	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
38	S	1621	LUT	C11-C10-C9	-2.07	124.37	127.28
37	y	609	CHL	C4C-CHD-C1D	2.07	123.48	116.07
27	c	511	CLA	CMB-C2B-C3B	2.07	131.42	126.55
27	b	613	CLA	C11-C12-C13	-2.07	109.09	115.97
27	y	613	CLA	C1-C2-C3	-2.07	122.81	126.20
31	a	413	LMG	C9-C8-C7	-2.07	106.96	111.78
38	g	1620	LUT	C39-C29-C28	2.07	121.25	118.09
37	Y	609	CHL	CAC-C3C-C4C	2.07	129.34	124.03
27	B	608	CLA	CMB-C2B-C3B	2.07	131.41	126.55
30	A	418	SQD	O5-C5-C4	2.07	113.42	109.70
38	G	1620	LUT	C18-C5-C4	2.07	118.22	114.42
27	C	503	CLA	CHC-C4B-NB	2.07	127.15	124.05
27	G	611	CLA	O2D-CGD-CBD	2.07	114.84	111.23
27	B	613	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
27	G	613	CLA	CHB-C1B-NB	2.07	127.15	124.05
37	R	607	CHL	C4C-CHD-C1D	2.07	123.46	116.07
39	g	1622	XAT	C7-C8-C9	-2.06	122.33	125.53
27	Y	604	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
27	G	613	CLA	CHB-C4A-NA	2.06	127.38	124.40
29	B	618	BCR	C10-C11-C12	-2.06	117.22	123.20
38	s	1621	LUT	C18-C5-C4	2.06	118.22	114.42
37	Y	609	CHL	C4C-CHD-C1D	2.06	123.45	116.07
27	r	613	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
35	R	2630	LHG	C18-C17-C16	-2.06	103.94	114.37
37	N	606	CHL	C4C-CHD-C1D	2.06	123.45	116.07
37	n	606	CHL	C4C-CHD-C1D	2.06	123.45	116.07
38	N	1621	LUT	C31-C30-C29	-2.06	124.39	127.28
38	n	1621	LUT	C31-C30-C29	-2.06	124.39	127.28
27	b	608	CLA	O1D-CGD-CBD	2.06	128.59	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Y	1623	NEX	C28-C29-C30	2.06	122.25	119.01
39	y	1622	XAT	C27-C28-C29	-2.06	122.33	125.53
27	G	611	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
27	S	604	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
27	b	605	CLA	O1D-CGD-CBD	2.06	128.58	124.52
27	a	406	CLA	CMB-C2B-C3B	2.06	131.39	126.55
27	r	611	CLA	O1D-CGD-CBD	2.06	128.58	124.52
27	b	609	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
37	G	608	CHL	C4C-CHD-C1D	2.06	123.43	116.07
38	s	1621	LUT	C11-C10-C9	-2.06	124.39	127.28
27	y	604	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
29	b	619	BCR	C11-C12-C13	-2.06	120.72	126.36
40	N	1623	NEX	C15-C35-C34	-2.06	119.31	123.52
37	g	607	CHL	C4C-CHD-C1D	2.06	123.42	116.07
32	c	519	DGD	C7B-C6B-C5B	-2.06	103.98	114.37
37	G	609	CHL	CAC-C3C-C4C	2.06	129.31	124.03
37	g	609	CHL	CAC-C3C-C4C	2.06	129.31	124.03
37	g	608	CHL	C4C-CHD-C1D	2.06	123.42	116.07
29	c	515	BCR	C36-C18-C19	2.06	121.23	118.09
37	r	607	CHL	C4C-CHD-C1D	2.05	123.42	116.07
29	B	619	BCR	C11-C12-C13	-2.05	120.73	126.36
29	b	618	BCR	C10-C11-C12	-2.05	117.25	123.20
39	r	622	XAT	C39-C29-C28	2.05	121.22	118.09
27	B	613	CLA	C11-C12-C13	-2.05	109.14	115.97
37	G	607	CHL	C4C-CHD-C1D	2.05	123.41	116.07
32	C	519	DGD	C7B-C6B-C5B	-2.05	104.00	114.37
35	r	2630	LHG	C18-C17-C16	-2.05	104.00	114.37
27	D	402	CLA	O2D-CGD-CBD	2.05	114.82	111.23
40	N	1623	NEX	O24-C25-C26	-2.05	57.30	58.93
38	g	1621	LUT	C39-C29-C28	2.05	121.22	118.09
27	B	608	CLA	O1D-CGD-CBD	2.05	128.56	124.52
34	D	405	PL9	O2-C1-C2	-2.05	117.17	121.83
27	b	610	CLA	O1D-CGD-CBD	2.05	128.56	124.52
37	y	609	CHL	CAC-C3C-C4C	2.05	129.30	124.03
27	Y	610	CLA	CHB-C1B-NB	2.05	127.12	124.05
39	G	1622	XAT	C11-C10-C9	-2.05	124.41	127.28
37	N	605	CHL	CBC-CAC-C3C	-2.05	109.94	112.87
27	B	613	CLA	O1D-CGD-CBD	2.05	128.56	124.52
31	d	411	LMG	O8-C28-O10	-2.05	118.51	123.63
35	d	408	LHG	O8-C6-C5	-2.05	102.49	108.40
29	c	515	BCR	C4-C5-C6	-2.05	119.94	122.70
27	R	611	CLA	O1D-CGD-CBD	2.05	128.56	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	n	608	CHL	CMA-C3A-C4A	-2.05	110.20	114.61
29	C	516	BCR	C39-C30-C25	-2.05	107.03	110.24
38	G	1620	LUT	C39-C29-C28	2.05	121.21	118.09
27	B	605	CLA	O1D-CGD-CBD	2.05	128.55	124.52
32	c	519	DGD	C8B-C7B-C6B	-2.04	104.03	114.37
27	y	604	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
32	h	102	DGD	C5B-C4B-C3B	-2.04	104.03	114.37
40	y	1623	NEX	C28-C29-C30	2.04	122.22	119.01
30	a	412	SQD	O5-C1-C2	2.04	114.57	110.37
27	b	612	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
32	C	519	DGD	C8B-C7B-C6B	-2.04	104.04	114.37
39	n	1622	XAT	O24-C25-C26	-2.04	57.31	58.93
37	n	605	CHL	CBC-CAC-C3C	-2.04	109.95	112.87
37	n	606	CHL	C4D-ND-C1D	-2.04	103.67	105.22
27	N	614	CLA	O2D-CGD-CBD	2.04	114.80	111.23
27	b	607	CLA	CHB-C1B-NB	2.04	127.11	124.05
34	d	405	PL9	O2-C1-C2	-2.04	117.19	121.83
32	h	102	DGD	O3D-C3D-C4D	-2.04	105.57	110.38
37	G	608	CHL	O1D-CGD-CBD	-2.04	121.63	124.72
37	g	608	CHL	O1D-CGD-CBD	-2.04	121.63	124.72
27	b	614	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
39	N	1622	XAT	O24-C25-C26	-2.04	57.31	58.93
37	s	607	CHL	CAC-C3C-C4C	2.04	129.27	124.03
27	R	613	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
37	S	601	CHL	O2D-CGD-O1D	-2.04	119.88	123.85
37	s	601	CHL	O2D-CGD-O1D	-2.04	119.88	123.85
27	b	608	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
32	H	102	DGD	C5B-C4B-C3B	-2.04	104.08	114.37
27	B	612	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
37	R	608	CHL	O2D-CGD-O1D	-2.04	119.89	123.85
27	C	509	CLA	CMB-C2B-C3B	2.04	131.34	126.55
27	n	614	CLA	O2D-CGD-CBD	2.03	114.79	111.23
31	A	413	LMG	O1-C7-C8	-2.03	105.87	110.82
27	s	604	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
27	N	603	CLA	C3B-C4B-NB	-2.03	108.72	110.53
31	D	411	LMG	O2-C2-C1	-2.03	105.23	110.08
31	a	413	LMG	O1-C7-C8	-2.03	105.88	110.82
27	c	509	CLA	CMB-C2B-C3B	2.03	131.33	126.55
31	D	411	LMG	O8-C28-O10	-2.03	118.55	123.63
27	g	614	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
27	y	602	CLA	O1D-CGD-CBD	2.03	128.52	124.52
27	G	614	CLA	O2A-CGA-O1A	-2.03	118.55	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Y	613	CLA	CHB-C1B-NB	2.03	127.09	124.05
27	y	613	CLA	CHB-C1B-NB	2.03	127.09	124.05
37	g	605	CHL	CMA-C3A-C4A	-2.03	110.24	114.61
27	B	614	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
27	d	402	CLA	O2D-CGD-CBD	2.03	114.78	111.23
37	y	605	CHL	CMA-C3A-C4A	-2.03	110.24	114.61
27	y	611	CLA	C3B-C4B-NB	-2.03	108.72	110.53
38	G	1621	LUT	C39-C29-C28	2.03	121.19	118.09
32	C	520	DGD	C5B-C4B-C3B	-2.03	104.12	114.37
31	D	411	LMG	C4-C3-C2	-2.03	107.27	110.83
38	r	620	LUT	C20-C13-C12	2.03	121.18	118.09
29	B	619	BCR	C33-C5-C4	2.03	117.92	113.60
40	n	1623	NEX	C15-C35-C34	-2.03	119.38	123.52
27	B	610	CLA	O1D-CGD-CBD	2.02	128.51	124.52
35	D	409	LHG	O8-C23-O10	-2.02	118.56	123.63
27	b	608	CLA	CMB-C2B-C3B	2.02	131.31	126.55
27	Y	602	CLA	O1D-CGD-CBD	2.02	128.51	124.52
29	b	619	BCR	C33-C5-C4	2.02	117.91	113.60
32	c	520	DGD	C5B-C4B-C3B	-2.02	104.14	114.37
37	N	608	CHL	CMA-C3A-C4A	-2.02	110.25	114.61
27	N	604	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
27	s	603	CLA	O1D-CGD-CBD	2.02	128.50	124.52
29	C	515	BCR	C4-C5-C6	-2.02	119.97	122.70
27	s	610	CLA	CHB-C1B-NB	2.02	127.08	124.05
27	S	603	CLA	O1D-CGD-CBD	2.02	128.50	124.52
27	b	617	CLA	C1-C2-C3	-2.02	122.89	126.20
27	B	607	CLA	CHB-C1B-NB	2.02	127.08	124.05
35	d	409	LHG	O8-C23-O10	-2.02	118.58	123.63
27	g	604	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
37	y	601	CHL	C4C-CHD-C1D	2.02	123.29	116.07
31	D	411	LMG	O7-C10-O9	-2.02	118.99	123.70
31	d	411	LMG	O7-C10-O9	-2.02	118.99	123.70
27	C	509	CLA	C11-C10-C8	-2.02	109.26	115.97
37	S	607	CHL	CAC-C3C-C4C	2.02	129.21	124.03
27	b	613	CLA	O1D-CGD-CBD	2.02	128.49	124.52
37	Y	601	CHL	C4C-CHD-C1D	2.01	123.28	116.07
38	R	620	LUT	C20-C13-C12	2.01	121.17	118.09
27	B	612	CLA	C1-C2-C3	-2.01	122.90	126.20
27	b	612	CLA	C1-C2-C3	-2.01	122.90	126.20
27	b	611	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
31	d	411	LMG	O2-C2-C1	-2.01	105.28	110.08
27	n	604	CLA	O2A-CGA-O1A	-2.01	118.60	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	502	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
27	c	502	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
27	y	610	CLA	CHB-C1B-NB	2.01	127.06	124.05
37	G	605	CHL	CMA-C3A-C4A	-2.01	110.28	114.61
27	S	610	CLA	CHB-C1B-NB	2.01	127.06	124.05
27	B	611	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
31	d	411	LMG	C4-C3-C2	-2.01	107.30	110.83
27	c	509	CLA	C11-C10-C8	-2.01	109.29	115.97
29	a	411	BCR	C20-C19-C18	-2.01	120.86	126.36
27	n	603	CLA	C3B-C4B-NB	-2.01	108.74	110.53
27	c	501	CLA	O2D-CGD-CBD	2.01	114.74	111.23
27	Y	604	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
27	r	601	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
32	H	102	DGD	O3D-C3D-C4D	-2.01	105.65	110.38
29	A	411	BCR	C35-C13-C12	2.01	121.15	118.09
29	a	411	BCR	C35-C13-C12	2.01	121.15	118.09
37	Y	608	CHL	CMA-C3A-C4A	-2.01	110.29	114.61
27	Y	603	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
27	G	604	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
27	b	616	CLA	C1-C2-C3	-2.00	122.91	126.20
29	A	411	BCR	C20-C19-C18	-2.00	120.87	126.36
27	B	617	CLA	O2D-CGD-CBD	2.00	114.73	111.23
27	b	617	CLA	O2D-CGD-CBD	2.00	114.73	111.23
27	C	502	CLA	CMB-C2B-C3B	2.00	131.26	126.55
27	R	601	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
27	c	503	CLA	C1-C2-C3	-2.00	122.92	126.20
37	Y	605	CHL	CMA-C3A-C4A	-2.00	110.30	114.61
27	A	406	CLA	O2D-CGD-CBD	2.00	114.73	111.23
29	D	404	BCR	C23-C24-C25	-2.00	121.65	127.00
29	d	404	BCR	C23-C24-C25	-2.00	121.65	127.00
27	C	501	CLA	O2D-CGD-CBD	2.00	114.73	111.23

All (312) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	405	CLA	ND
27	A	406	CLA	ND
27	A	407	CLA	ND
27	A	410	CLA	ND
27	B	602	CLA	ND
27	B	603	CLA	ND
27	B	604	CLA	ND

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Mol	Chain	Res	Type	Atom
27	B	605	CLA	ND
27	B	606	CLA	ND
27	B	607	CLA	ND
27	B	608	CLA	ND
27	B	609	CLA	ND
27	B	610	CLA	ND
27	B	611	CLA	ND
27	B	612	CLA	ND
27	B	613	CLA	ND
27	B	614	CLA	ND
27	B	615	CLA	ND
27	B	616	CLA	ND
27	B	617	CLA	ND
27	C	502	CLA	ND
27	C	503	CLA	ND
27	C	501	CLA	ND
27	C	504	CLA	ND
27	C	505	CLA	ND
27	C	506	CLA	ND
27	C	507	CLA	ND
27	C	508	CLA	ND
27	C	509	CLA	ND
27	C	510	CLA	ND
27	C	511	CLA	ND
27	C	512	CLA	ND
27	C	513	CLA	ND
27	D	402	CLA	ND
27	D	403	CLA	ND
27	G	602	CLA	ND
27	G	603	CLA	ND
27	G	604	CLA	ND
27	G	610	CLA	ND
27	G	611	CLA	ND
27	G	612	CLA	ND
27	G	613	CLA	ND
27	G	614	CLA	ND
27	N	602	CLA	ND
27	N	603	CLA	ND
27	N	604	CLA	ND
27	N	610	CLA	ND
27	N	611	CLA	ND
27	N	612	CLA	ND

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Mol	Chain	Res	Type	Atom
27	N	613	CLA	ND
27	N	614	CLA	ND
27	R	601	CLA	ND
27	R	602	CLA	ND
27	R	603	CLA	ND
27	R	604	CLA	ND
27	R	609	CLA	ND
27	R	610	CLA	ND
27	R	611	CLA	ND
27	R	612	CLA	ND
27	R	613	CLA	ND
27	R	616	CLA	ND
27	S	602	CLA	ND
27	S	604	CLA	ND
27	S	609	CLA	ND
27	S	610	CLA	ND
27	S	611	CLA	ND
27	S	612	CLA	ND
27	S	613	CLA	ND
27	S	614	CLA	ND
27	Y	602	CLA	ND
27	Y	603	CLA	ND
27	Y	604	CLA	ND
27	Y	610	CLA	ND
27	Y	611	CLA	ND
27	Y	612	CLA	ND
27	Y	613	CLA	ND
27	Y	614	CLA	ND
27	a	405	CLA	ND
27	a	406	CLA	ND
27	a	407	CLA	ND
27	a	410	CLA	ND
27	b	602	CLA	ND
27	b	603	CLA	ND
27	b	604	CLA	ND
27	b	605	CLA	ND
27	b	606	CLA	ND
27	b	607	CLA	ND
27	b	608	CLA	ND
27	b	609	CLA	ND
27	b	610	CLA	ND
27	b	611	CLA	ND

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Mol	Chain	Res	Type	Atom
27	b	612	CLA	ND
27	b	613	CLA	ND
27	b	614	CLA	ND
27	b	615	CLA	ND
27	b	616	CLA	ND
27	b	617	CLA	ND
27	c	502	CLA	ND
27	c	503	CLA	ND
27	c	501	CLA	ND
27	c	504	CLA	ND
27	c	505	CLA	ND
27	c	506	CLA	ND
27	c	507	CLA	ND
27	c	508	CLA	ND
27	c	509	CLA	ND
27	c	510	CLA	ND
27	c	511	CLA	ND
27	c	512	CLA	ND
27	c	513	CLA	ND
27	d	402	CLA	ND
27	d	403	CLA	ND
27	g	602	CLA	ND
27	g	603	CLA	ND
27	g	604	CLA	ND
27	g	610	CLA	ND
27	g	611	CLA	ND
27	g	612	CLA	ND
27	g	613	CLA	ND
27	g	614	CLA	ND
27	n	602	CLA	ND
27	n	603	CLA	ND
27	n	604	CLA	ND
27	n	610	CLA	ND
27	n	611	CLA	ND
27	n	612	CLA	ND
27	n	613	CLA	ND
27	n	614	CLA	ND
27	r	601	CLA	ND
27	r	602	CLA	ND
27	r	603	CLA	ND
27	r	604	CLA	ND
27	r	609	CLA	ND

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Mol	Chain	Res	Type	Atom
27	r	610	CLA	ND
27	r	611	CLA	ND
27	r	612	CLA	ND
27	r	613	CLA	ND
27	r	616	CLA	ND
27	s	602	CLA	ND
27	s	604	CLA	ND
27	s	609	CLA	ND
27	s	610	CLA	ND
27	s	611	CLA	ND
27	s	612	CLA	ND
27	s	613	CLA	ND
27	s	614	CLA	ND
27	y	602	CLA	ND
27	y	603	CLA	ND
27	y	604	CLA	ND
27	y	610	CLA	ND
27	y	611	CLA	ND
27	y	612	CLA	ND
27	y	613	CLA	ND
27	y	614	CLA	ND
37	G	601	CHL	ND
37	G	601	CHL	C8
37	G	601	CHL	NC
37	G	601	CHL	NA
37	G	605	CHL	ND
37	G	605	CHL	NC
37	G	605	CHL	NA
37	G	606	CHL	ND
37	G	606	CHL	NC
37	G	606	CHL	NA
37	G	607	CHL	ND
37	G	607	CHL	NC
37	G	607	CHL	NA
37	G	608	CHL	ND
37	G	608	CHL	NC
37	G	608	CHL	NA
37	G	609	CHL	ND
37	G	609	CHL	NC
37	G	609	CHL	NA
37	N	601	CHL	ND
37	N	601	CHL	NC

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Mol	Chain	Res	Type	Atom
37	N	601	CHL	NA
37	N	605	CHL	ND
37	N	605	CHL	NC
37	N	605	CHL	NA
37	N	606	CHL	ND
37	N	606	CHL	NC
37	N	606	CHL	NA
37	N	607	CHL	ND
37	N	607	CHL	C8
37	N	607	CHL	NC
37	N	607	CHL	NA
37	N	608	CHL	ND
37	N	608	CHL	NC
37	N	608	CHL	NA
37	N	609	CHL	ND
37	N	609	CHL	NC
37	N	609	CHL	NA
37	R	606	CHL	ND
37	R	606	CHL	NC
37	R	606	CHL	NA
37	R	607	CHL	ND
37	R	607	CHL	NC
37	R	607	CHL	NA
37	R	608	CHL	ND
37	R	608	CHL	NC
37	R	608	CHL	NA
37	S	601	CHL	ND
37	S	601	CHL	NC
37	S	601	CHL	NA
37	S	606	CHL	ND
37	S	606	CHL	NC
37	S	606	CHL	NA
37	S	607	CHL	ND
37	S	607	CHL	NC
37	S	607	CHL	NA
37	S	608	CHL	ND
37	S	608	CHL	NC
37	S	608	CHL	NA
37	Y	601	CHL	ND
37	Y	601	CHL	C8
37	Y	601	CHL	NC
37	Y	601	CHL	NA

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

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Mol	Chain	Res	Type	Atom
37	n	606	CHL	NC
37	n	606	CHL	NA
37	n	607	CHL	ND
37	n	607	CHL	C8
37	n	607	CHL	NC
37	n	607	CHL	NA
37	n	608	CHL	ND
37	n	608	CHL	NC
37	n	608	CHL	NA
37	n	609	CHL	ND
37	n	609	CHL	NC
37	n	609	CHL	NA
37	r	606	CHL	ND
37	r	606	CHL	NC
37	r	606	CHL	NA
37	r	607	CHL	ND
37	r	607	CHL	NC
37	r	607	CHL	NA
37	r	608	CHL	ND
37	r	608	CHL	NC
37	r	608	CHL	NA
37	s	601	CHL	ND
37	s	601	CHL	NC
37	s	601	CHL	NA
37	s	606	CHL	ND
37	s	606	CHL	NC
37	s	606	CHL	NA
37	s	607	CHL	ND
37	s	607	CHL	NC
37	s	607	CHL	NA
37	s	608	CHL	ND
37	s	608	CHL	NC
37	s	608	CHL	NA
37	y	601	CHL	ND
37	y	601	CHL	C8
37	y	601	CHL	NC
37	y	601	CHL	NA
37	y	605	CHL	ND
37	y	605	CHL	NC
37	y	605	CHL	NA
37	y	606	CHL	ND
37	y	606	CHL	NC

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Mol	Chain	Res	Type	Atom
37	y	606	CHL	NA
37	y	607	CHL	ND
37	y	607	CHL	NC
37	y	607	CHL	NA
37	y	608	CHL	ND
37	y	608	CHL	NC
37	y	608	CHL	NA
37	y	609	CHL	ND
37	y	609	CHL	C8
37	y	609	CHL	NC
37	y	609	CHL	NA

All (3150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	405	CLA	CBD-CGD-O2D-CED
27	A	407	CLA	CHA-CBD-CGD-O1D
27	A	407	CLA	CHA-CBD-CGD-O2D
27	A	407	CLA	CBD-CGD-O2D-CED
27	B	602	CLA	C1A-C2A-CAA-CBA
27	B	602	CLA	C3A-C2A-CAA-CBA
27	B	603	CLA	C4-C3-C5-C6
27	B	608	CLA	CBD-CGD-O2D-CED
27	B	610	CLA	CAD-CBD-CGD-O1D
27	B	610	CLA	CAD-CBD-CGD-O2D
27	B	610	CLA	C6-C7-C8-C9
27	B	613	CLA	C1A-C2A-CAA-CBA
27	B	613	CLA	C3A-C2A-CAA-CBA
27	B	614	CLA	CBD-CGD-O2D-CED
27	B	617	CLA	CHA-CBD-CGD-O1D
27	B	617	CLA	CHA-CBD-CGD-O2D
27	C	503	CLA	CHA-CBD-CGD-O1D
27	C	503	CLA	CHA-CBD-CGD-O2D
27	C	504	CLA	CHA-CBD-CGD-O1D
27	C	504	CLA	CHA-CBD-CGD-O2D
27	C	506	CLA	CAD-CBD-CGD-O1D
27	C	506	CLA	CAD-CBD-CGD-O2D
27	C	507	CLA	CHA-CBD-CGD-O1D
27	C	507	CLA	CHA-CBD-CGD-O2D
27	C	508	CLA	CHA-CBD-CGD-O1D
27	C	508	CLA	CHA-CBD-CGD-O2D
27	C	510	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	C	512	CLA	C1A-C2A-CAA-CBA
27	C	512	CLA	C3A-C2A-CAA-CBA
27	G	603	CLA	CHA-CBD-CGD-O2D
27	G	604	CLA	CHA-CBD-CGD-O2D
27	G	604	CLA	CBD-CGD-O2D-CED
27	G	610	CLA	C1A-C2A-CAA-CBA
27	G	610	CLA	C4-C3-C5-C6
27	G	611	CLA	C1A-C2A-CAA-CBA
27	G	611	CLA	C3A-C2A-CAA-CBA
27	G	612	CLA	CHA-CBD-CGD-O1D
27	G	612	CLA	CHA-CBD-CGD-O2D
27	G	612	CLA	CBD-CGD-O2D-CED
27	N	604	CLA	CHA-CBD-CGD-O2D
27	N	610	CLA	C2B-C3B-CAB-CBB
27	N	610	CLA	C4B-C3B-CAB-CBB
27	N	611	CLA	CAD-CBD-CGD-O1D
27	N	611	CLA	CAD-CBD-CGD-O2D
27	N	612	CLA	CHA-CBD-CGD-O1D
27	N	612	CLA	CHA-CBD-CGD-O2D
27	N	613	CLA	CBD-CGD-O2D-CED
27	N	614	CLA	CAD-CBD-CGD-O1D
27	N	614	CLA	CAD-CBD-CGD-O2D
27	R	601	CLA	C1A-C2A-CAA-CBA
27	R	601	CLA	C3A-C2A-CAA-CBA
27	R	603	CLA	CHA-CBD-CGD-O1D
27	R	603	CLA	CHA-CBD-CGD-O2D
27	R	604	CLA	C1A-C2A-CAA-CBA
27	R	604	CLA	CHA-CBD-CGD-O1D
27	R	604	CLA	CHA-CBD-CGD-O2D
27	R	609	CLA	C1A-C2A-CAA-CBA
27	R	609	CLA	C3A-C2A-CAA-CBA
27	R	610	CLA	C2-C3-C5-C6
27	R	610	CLA	C4-C3-C5-C6
27	R	611	CLA	C1A-C2A-CAA-CBA
27	R	611	CLA	C3A-C2A-CAA-CBA
27	R	612	CLA	CBD-CGD-O2D-CED
27	R	616	CLA	CBA-CGA-O2A-C1
27	R	616	CLA	O1A-CGA-O2A-C1
27	S	602	CLA	CHA-CBD-CGD-O1D
27	S	602	CLA	CHA-CBD-CGD-O2D
27	S	604	CLA	C1A-C2A-CAA-CBA
27	S	604	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	S	604	CLA	CAD-CBD-CGD-O2D
27	S	609	CLA	C1A-C2A-CAA-CBA
27	S	609	CLA	C3A-C2A-CAA-CBA
27	S	609	CLA	CBD-CGD-O2D-CED
27	S	612	CLA	CBD-CGD-O2D-CED
27	Y	602	CLA	CHA-CBD-CGD-O1D
27	Y	602	CLA	CHA-CBD-CGD-O2D
27	Y	613	CLA	C2B-C3B-CAB-CBB
27	Y	613	CLA	C4B-C3B-CAB-CBB
27	a	405	CLA	CBD-CGD-O2D-CED
27	a	407	CLA	CHA-CBD-CGD-O1D
27	a	407	CLA	CHA-CBD-CGD-O2D
27	a	407	CLA	CBD-CGD-O2D-CED
27	b	602	CLA	C1A-C2A-CAA-CBA
27	b	602	CLA	C3A-C2A-CAA-CBA
27	b	608	CLA	CBD-CGD-O2D-CED
27	b	610	CLA	CAD-CBD-CGD-O1D
27	b	610	CLA	CAD-CBD-CGD-O2D
27	b	610	CLA	C6-C7-C8-C9
27	b	613	CLA	C1A-C2A-CAA-CBA
27	b	613	CLA	C3A-C2A-CAA-CBA
27	b	614	CLA	CBD-CGD-O2D-CED
27	b	617	CLA	CHA-CBD-CGD-O1D
27	b	617	CLA	CHA-CBD-CGD-O2D
27	c	503	CLA	CHA-CBD-CGD-O1D
27	c	503	CLA	CHA-CBD-CGD-O2D
27	c	504	CLA	CHA-CBD-CGD-O1D
27	c	504	CLA	CHA-CBD-CGD-O2D
27	c	506	CLA	CAD-CBD-CGD-O1D
27	c	506	CLA	CAD-CBD-CGD-O2D
27	c	507	CLA	CHA-CBD-CGD-O1D
27	c	507	CLA	CHA-CBD-CGD-O2D
27	c	508	CLA	CHA-CBD-CGD-O1D
27	c	508	CLA	CHA-CBD-CGD-O2D
27	c	510	CLA	CBD-CGD-O2D-CED
27	c	512	CLA	C1A-C2A-CAA-CBA
27	c	512	CLA	C3A-C2A-CAA-CBA
27	g	603	CLA	CHA-CBD-CGD-O2D
27	g	604	CLA	CHA-CBD-CGD-O2D
27	g	604	CLA	CBD-CGD-O2D-CED
27	g	610	CLA	C1A-C2A-CAA-CBA
27	g	610	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	g	611	CLA	C1A-C2A-CAA-CBA
27	g	611	CLA	C3A-C2A-CAA-CBA
27	g	612	CLA	CHA-CBD-CGD-O1D
27	g	612	CLA	CHA-CBD-CGD-O2D
27	g	612	CLA	CBD-CGD-O2D-CED
27	n	604	CLA	CHA-CBD-CGD-O2D
27	n	610	CLA	C2B-C3B-CAB-CBB
27	n	610	CLA	C4B-C3B-CAB-CBB
27	n	611	CLA	CAD-CBD-CGD-O1D
27	n	611	CLA	CAD-CBD-CGD-O2D
27	n	612	CLA	CHA-CBD-CGD-O1D
27	n	612	CLA	CHA-CBD-CGD-O2D
27	n	613	CLA	CBD-CGD-O2D-CED
27	n	614	CLA	CAD-CBD-CGD-O1D
27	n	614	CLA	CAD-CBD-CGD-O2D
27	r	601	CLA	C1A-C2A-CAA-CBA
27	r	601	CLA	C3A-C2A-CAA-CBA
27	r	603	CLA	CHA-CBD-CGD-O1D
27	r	603	CLA	CHA-CBD-CGD-O2D
27	r	604	CLA	C1A-C2A-CAA-CBA
27	r	604	CLA	CHA-CBD-CGD-O1D
27	r	604	CLA	CHA-CBD-CGD-O2D
27	r	609	CLA	C1A-C2A-CAA-CBA
27	r	609	CLA	C3A-C2A-CAA-CBA
27	r	610	CLA	C2-C3-C5-C6
27	r	610	CLA	C4-C3-C5-C6
27	r	611	CLA	C1A-C2A-CAA-CBA
27	r	611	CLA	C3A-C2A-CAA-CBA
27	r	612	CLA	CBD-CGD-O2D-CED
27	r	616	CLA	CBA-CGA-O2A-C1
27	r	616	CLA	O1A-CGA-O2A-C1
27	s	602	CLA	CHA-CBD-CGD-O1D
27	s	602	CLA	CHA-CBD-CGD-O2D
27	s	604	CLA	C1A-C2A-CAA-CBA
27	s	604	CLA	CAD-CBD-CGD-O1D
27	s	604	CLA	CAD-CBD-CGD-O2D
27	s	609	CLA	C1A-C2A-CAA-CBA
27	s	609	CLA	C3A-C2A-CAA-CBA
27	s	609	CLA	CBD-CGD-O2D-CED
27	s	612	CLA	CBD-CGD-O2D-CED
27	y	602	CLA	CHA-CBD-CGD-O1D
27	y	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	y	613	CLA	C2B-C3B-CAB-CBB
27	y	613	CLA	C4B-C3B-CAB-CBB
28	A	409	PHO	C1A-C2A-CAA-CBA
28	a	409	PHO	C1A-C2A-CAA-CBA
29	B	620	BCR	C7-C8-C9-C10
29	B	620	BCR	C7-C8-C9-C34
29	C	516	BCR	C7-C8-C9-C10
29	C	516	BCR	C7-C8-C9-C34
29	C	516	BCR	C19-C20-C21-C22
29	D	404	BCR	C7-C8-C9-C10
29	D	404	BCR	C21-C22-C23-C24
29	D	404	BCR	C37-C22-C23-C24
29	b	620	BCR	C7-C8-C9-C10
29	b	620	BCR	C7-C8-C9-C34
29	c	516	BCR	C7-C8-C9-C10
29	c	516	BCR	C7-C8-C9-C34
29	c	516	BCR	C19-C20-C21-C22
29	d	404	BCR	C7-C8-C9-C10
29	d	404	BCR	C21-C22-C23-C24
29	d	404	BCR	C37-C22-C23-C24
30	A	412	SQD	O5-C1-O6-C44
30	A	412	SQD	O5-C5-C6-S
30	A	418	SQD	C2-C1-O6-C44
30	A	418	SQD	O5-C1-O6-C44
30	A	418	SQD	C24-C23-O48-C46
30	B	621	SQD	C2-C1-O6-C44
30	B	621	SQD	O5-C1-O6-C44
30	B	621	SQD	O5-C5-C6-S
30	a	412	SQD	O5-C1-O6-C44
30	a	412	SQD	O5-C5-C6-S
30	a	418	SQD	C2-C1-O6-C44
30	a	418	SQD	O5-C1-O6-C44
30	a	418	SQD	C24-C23-O48-C46
30	b	621	SQD	C2-C1-O6-C44
30	b	621	SQD	O5-C1-O6-C44
30	b	621	SQD	O5-C5-C6-S
31	A	413	LMG	C2-C1-O1-C7
31	A	413	LMG	O6-C1-O1-C7
31	C	521	LMG	C11-C10-O7-C8
31	a	413	LMG	C2-C1-O1-C7
31	a	413	LMG	O6-C1-O1-C7
31	c	521	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	D	405	PL9	C7-C8-C9-C11
34	D	405	PL9	C12-C11-C9-C10
34	D	405	PL9	C42-C43-C44-C46
34	d	405	PL9	C7-C8-C9-C11
34	d	405	PL9	C12-C11-C9-C10
34	d	405	PL9	C42-C43-C44-C46
35	D	408	LHG	O1-C1-C2-O2
35	D	408	LHG	O1-C1-C2-C3
35	D	408	LHG	C3-O3-P-O6
35	D	408	LHG	C4-O6-P-O3
35	D	408	LHG	C4-O6-P-O4
35	D	409	LHG	C3-O3-P-O5
35	D	409	LHG	C4-O6-P-O3
35	D	409	LHG	C4-O6-P-O4
35	D	410	LHG	C3-O3-P-O5
35	D	410	LHG	C3-O3-P-O6
35	G	2630	LHG	C4-O6-P-O5
35	G	2630	LHG	O7-C5-C6-O8
35	L	101	LHG	O1-C1-C2-O2
35	L	101	LHG	O1-C1-C2-C3
35	L	101	LHG	C4-O6-P-O5
35	L	101	LHG	O6-C4-C5-O7
35	N	2630	LHG	O1-C1-C2-C3
35	N	2630	LHG	C3-O3-P-O4
35	N	2630	LHG	C3-O3-P-O6
35	N	2630	LHG	C4-O6-P-O3
35	N	2630	LHG	C4-O6-P-O4
35	R	2630	LHG	C8-C7-O7-C5
35	S	2630	LHG	C3-O3-P-O4
35	Y	2630	LHG	O1-C1-C2-C3
35	Y	2630	LHG	O7-C5-C6-O8
35	d	408	LHG	O1-C1-C2-O2
35	d	408	LHG	O1-C1-C2-C3
35	d	408	LHG	C3-O3-P-O6
35	d	408	LHG	C4-O6-P-O3
35	d	408	LHG	C4-O6-P-O4
35	d	409	LHG	C3-O3-P-O5
35	d	409	LHG	C4-O6-P-O3
35	d	409	LHG	C4-O6-P-O4
35	d	410	LHG	C3-O3-P-O5
35	d	410	LHG	C3-O3-P-O6
35	g	2630	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
35	g	2630	LHG	O7-C5-C6-O8
35	l	101	LHG	O1-C1-C2-O2
35	l	101	LHG	O1-C1-C2-C3
35	l	101	LHG	C4-O6-P-O5
35	l	101	LHG	O6-C4-C5-O7
35	n	2630	LHG	O1-C1-C2-C3
35	n	2630	LHG	C3-O3-P-O4
35	n	2630	LHG	C3-O3-P-O6
35	n	2630	LHG	C4-O6-P-O3
35	n	2630	LHG	C4-O6-P-O4
35	r	2630	LHG	C8-C7-O7-C5
35	s	2630	LHG	C3-O3-P-O4
35	y	2630	LHG	O1-C1-C2-C3
35	y	2630	LHG	O7-C5-C6-O8
37	G	607	CHL	C1C-C2C-CMC-OMC
37	G	607	CHL	C4C-C3C-CAC-CBC
37	G	608	CHL	C1C-C2C-CMC-OMC
37	G	608	CHL	C3C-C2C-CMC-OMC
37	G	608	CHL	CBD-CGD-O2D-CED
37	G	609	CHL	C1C-C2C-CMC-OMC
37	G	609	CHL	C4C-C3C-CAC-CBC
37	N	605	CHL	C1C-C2C-CMC-OMC
37	N	605	CHL	C3C-C2C-CMC-OMC
37	N	607	CHL	C11-C12-C13-C15
37	N	608	CHL	CBD-CGD-O2D-CED
37	R	606	CHL	C1C-C2C-CMC-OMC
37	R	606	CHL	C3C-C2C-CMC-OMC
37	R	608	CHL	CBD-CGD-O2D-CED
37	S	601	CHL	C1C-C2C-CMC-OMC
37	S	601	CHL	C3C-C2C-CMC-OMC
37	S	606	CHL	CAD-CBD-CGD-O1D
37	S	606	CHL	CAD-CBD-CGD-O2D
37	S	607	CHL	C1C-C2C-CMC-OMC
37	S	607	CHL	C3C-C2C-CMC-OMC
37	S	608	CHL	CBD-CGD-O2D-CED
37	Y	605	CHL	C1A-C2A-CAA-CBA
37	Y	605	CHL	C1C-C2C-CMC-OMC
37	Y	605	CHL	C3C-C2C-CMC-OMC
37	Y	608	CHL	CBD-CGD-O2D-CED
37	g	607	CHL	C1C-C2C-CMC-OMC
37	g	607	CHL	C4C-C3C-CAC-CBC
37	g	608	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
37	g	608	CHL	C3C-C2C-CMC-OMC
37	g	608	CHL	CBD-CGD-O2D-CED
37	g	609	CHL	C1C-C2C-CMC-OMC
37	g	609	CHL	C4C-C3C-CAC-CBC
37	n	605	CHL	C1C-C2C-CMC-OMC
37	n	605	CHL	C3C-C2C-CMC-OMC
37	n	607	CHL	C11-C12-C13-C15
37	n	608	CHL	CBD-CGD-O2D-CED
37	r	606	CHL	C1C-C2C-CMC-OMC
37	r	606	CHL	C3C-C2C-CMC-OMC
37	r	608	CHL	CBD-CGD-O2D-CED
37	s	601	CHL	C1C-C2C-CMC-OMC
37	s	601	CHL	C3C-C2C-CMC-OMC
37	s	606	CHL	CAD-CBD-CGD-O1D
37	s	606	CHL	CAD-CBD-CGD-O2D
37	s	607	CHL	C1C-C2C-CMC-OMC
37	s	607	CHL	C3C-C2C-CMC-OMC
37	s	608	CHL	CBD-CGD-O2D-CED
37	y	605	CHL	C1A-C2A-CAA-CBA
37	y	605	CHL	C1C-C2C-CMC-OMC
37	y	605	CHL	C3C-C2C-CMC-OMC
37	y	608	CHL	CBD-CGD-O2D-CED
40	G	1623	NEX	C7-C8-C9-C10
40	G	1623	NEX	O24-C26-C27-C28
40	S	1623	NEX	O24-C26-C27-C28
40	g	1623	NEX	C7-C8-C9-C10
40	g	1623	NEX	O24-C26-C27-C28
40	s	1623	NEX	O24-C26-C27-C28
27	A	405	CLA	O1D-CGD-O2D-CED
27	C	504	CLA	O1D-CGD-O2D-CED
27	N	612	CLA	O1D-CGD-O2D-CED
27	N	613	CLA	O1D-CGD-O2D-CED
27	R	602	CLA	O1D-CGD-O2D-CED
27	R	612	CLA	O1D-CGD-O2D-CED
27	S	614	CLA	O1D-CGD-O2D-CED
27	a	405	CLA	O1D-CGD-O2D-CED
27	c	504	CLA	O1D-CGD-O2D-CED
27	n	612	CLA	O1D-CGD-O2D-CED
27	n	613	CLA	O1D-CGD-O2D-CED
27	r	602	CLA	O1D-CGD-O2D-CED
27	r	612	CLA	O1D-CGD-O2D-CED
27	s	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	A	407	CLA	O1D-CGD-O2D-CED
27	B	612	CLA	O1D-CGD-O2D-CED
27	B	614	CLA	O1D-CGD-O2D-CED
27	G	604	CLA	O1D-CGD-O2D-CED
27	G	612	CLA	O1D-CGD-O2D-CED
27	S	604	CLA	O1D-CGD-O2D-CED
27	a	407	CLA	O1D-CGD-O2D-CED
27	b	612	CLA	O1D-CGD-O2D-CED
27	b	614	CLA	O1D-CGD-O2D-CED
27	g	604	CLA	O1D-CGD-O2D-CED
27	g	612	CLA	O1D-CGD-O2D-CED
27	s	604	CLA	O1D-CGD-O2D-CED
27	B	606	CLA	CBD-CGD-O2D-CED
27	B	610	CLA	CBD-CGD-O2D-CED
27	B	612	CLA	CBD-CGD-O2D-CED
27	B	615	CLA	CBD-CGD-O2D-CED
27	C	503	CLA	CBD-CGD-O2D-CED
27	C	504	CLA	CBD-CGD-O2D-CED
27	C	511	CLA	CBD-CGD-O2D-CED
27	G	610	CLA	CBD-CGD-O2D-CED
27	G	614	CLA	CBD-CGD-O2D-CED
27	N	612	CLA	CBD-CGD-O2D-CED
27	N	614	CLA	CBD-CGD-O2D-CED
27	R	601	CLA	CBD-CGD-O2D-CED
27	R	602	CLA	CBD-CGD-O2D-CED
27	R	609	CLA	CBD-CGD-O2D-CED
27	R	611	CLA	CBD-CGD-O2D-CED
27	S	603	CLA	CBD-CGD-O2D-CED
27	S	604	CLA	CBD-CGD-O2D-CED
27	S	614	CLA	CBD-CGD-O2D-CED
27	Y	604	CLA	CBD-CGD-O2D-CED
27	b	606	CLA	CBD-CGD-O2D-CED
27	b	610	CLA	CBD-CGD-O2D-CED
27	b	612	CLA	CBD-CGD-O2D-CED
27	b	615	CLA	CBD-CGD-O2D-CED
27	c	503	CLA	CBD-CGD-O2D-CED
27	c	504	CLA	CBD-CGD-O2D-CED
27	c	511	CLA	CBD-CGD-O2D-CED
27	g	610	CLA	CBD-CGD-O2D-CED
27	g	614	CLA	CBD-CGD-O2D-CED
27	n	612	CLA	CBD-CGD-O2D-CED
27	n	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	r	601	CLA	CBD-CGD-O2D-CED
27	r	602	CLA	CBD-CGD-O2D-CED
27	r	609	CLA	CBD-CGD-O2D-CED
27	r	611	CLA	CBD-CGD-O2D-CED
27	s	603	CLA	CBD-CGD-O2D-CED
27	s	604	CLA	CBD-CGD-O2D-CED
27	s	614	CLA	CBD-CGD-O2D-CED
27	y	604	CLA	CBD-CGD-O2D-CED
37	S	606	CHL	CBD-CGD-O2D-CED
37	s	606	CHL	CBD-CGD-O2D-CED
27	B	615	CLA	O1A-CGA-O2A-C1
27	R	611	CLA	O1A-CGA-O2A-C1
27	b	615	CLA	O1A-CGA-O2A-C1
27	r	611	CLA	O1A-CGA-O2A-C1
30	A	418	SQD	O10-C23-O48-C46
30	a	418	SQD	O10-C23-O48-C46
34	D	405	PL9	C47-C48-C49-C50
34	D	405	PL9	C47-C48-C49-C51
34	d	405	PL9	C47-C48-C49-C50
34	d	405	PL9	C47-C48-C49-C51
27	B	610	CLA	O1D-CGD-O2D-CED
27	N	614	CLA	O1D-CGD-O2D-CED
27	b	610	CLA	O1D-CGD-O2D-CED
27	n	614	CLA	O1D-CGD-O2D-CED
27	B	615	CLA	CBA-CGA-O2A-C1
27	R	611	CLA	CBA-CGA-O2A-C1
27	b	615	CLA	CBA-CGA-O2A-C1
27	r	611	CLA	CBA-CGA-O2A-C1
27	N	602	CLA	CBD-CGD-O2D-CED
27	n	602	CLA	CBD-CGD-O2D-CED
27	G	604	CLA	O1A-CGA-O2A-C1
27	G	613	CLA	O1A-CGA-O2A-C1
27	G	614	CLA	O1A-CGA-O2A-C1
27	N	611	CLA	O1A-CGA-O2A-C1
27	R	601	CLA	O1A-CGA-O2A-C1
27	g	604	CLA	O1A-CGA-O2A-C1
27	g	613	CLA	O1A-CGA-O2A-C1
27	g	614	CLA	O1A-CGA-O2A-C1
27	n	611	CLA	O1A-CGA-O2A-C1
27	r	601	CLA	O1A-CGA-O2A-C1
31	B	622	LMG	O10-C28-O8-C9
31	Z	101	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
31	b	622	LMG	O10-C28-O8-C9
31	z	101	LMG	O10-C28-O8-C9
35	N	2630	LHG	O10-C23-O8-C6
35	S	2630	LHG	O10-C23-O8-C6
35	n	2630	LHG	O10-C23-O8-C6
35	s	2630	LHG	O10-C23-O8-C6
27	G	614	CLA	O1D-CGD-O2D-CED
27	R	601	CLA	O1D-CGD-O2D-CED
27	S	609	CLA	O1D-CGD-O2D-CED
27	g	614	CLA	O1D-CGD-O2D-CED
27	r	601	CLA	O1D-CGD-O2D-CED
27	s	609	CLA	O1D-CGD-O2D-CED
37	Y	608	CHL	O1D-CGD-O2D-CED
37	y	608	CHL	O1D-CGD-O2D-CED
27	C	510	CLA	O1D-CGD-O2D-CED
27	S	612	CLA	O1D-CGD-O2D-CED
27	c	510	CLA	O1D-CGD-O2D-CED
27	s	612	CLA	O1D-CGD-O2D-CED
37	G	608	CHL	O1D-CGD-O2D-CED
37	N	608	CHL	O1D-CGD-O2D-CED
37	S	608	CHL	O1D-CGD-O2D-CED
37	g	608	CHL	O1D-CGD-O2D-CED
37	n	608	CHL	O1D-CGD-O2D-CED
37	s	608	CHL	O1D-CGD-O2D-CED
27	C	501	CLA	CBD-CGD-O2D-CED
27	Y	610	CLA	CBD-CGD-O2D-CED
27	c	501	CLA	CBD-CGD-O2D-CED
27	y	610	CLA	CBD-CGD-O2D-CED
30	A	412	SQD	O49-C7-O47-C45
30	B	621	SQD	O49-C7-O47-C45
30	a	412	SQD	O49-C7-O47-C45
30	b	621	SQD	O49-C7-O47-C45
31	C	521	LMG	O9-C10-O7-C8
31	c	521	LMG	O9-C10-O7-C8
35	R	2630	LHG	O9-C7-O7-C5
35	r	2630	LHG	O9-C7-O7-C5
37	R	608	CHL	O1D-CGD-O2D-CED
37	r	608	CHL	O1D-CGD-O2D-CED
27	C	512	CLA	C3-C5-C6-C7
27	Y	613	CLA	C3-C5-C6-C7
27	c	512	CLA	C3-C5-C6-C7
27	y	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	A	408	PHO	C3-C5-C6-C7
28	A	409	PHO	C3-C5-C6-C7
28	a	408	PHO	C3-C5-C6-C7
28	a	409	PHO	C3-C5-C6-C7
27	B	608	CLA	O1D-CGD-O2D-CED
27	G	604	CLA	CBA-CGA-O2A-C1
27	g	604	CLA	CBA-CGA-O2A-C1
31	B	622	LMG	C29-C28-O8-C9
31	Z	101	LMG	C29-C28-O8-C9
31	b	622	LMG	C29-C28-O8-C9
31	z	101	LMG	C29-C28-O8-C9
35	S	2630	LHG	C24-C23-O8-C6
35	s	2630	LHG	C24-C23-O8-C6
27	B	602	CLA	CBD-CGD-O2D-CED
27	C	506	CLA	CBD-CGD-O2D-CED
27	C	513	CLA	CBD-CGD-O2D-CED
27	D	402	CLA	CBD-CGD-O2D-CED
27	D	403	CLA	CBD-CGD-O2D-CED
27	G	602	CLA	CBD-CGD-O2D-CED
27	N	610	CLA	CBD-CGD-O2D-CED
27	R	610	CLA	CBD-CGD-O2D-CED
27	S	602	CLA	CBD-CGD-O2D-CED
27	S	613	CLA	CBD-CGD-O2D-CED
27	Y	602	CLA	CBD-CGD-O2D-CED
27	Y	603	CLA	CBD-CGD-O2D-CED
27	Y	611	CLA	CBD-CGD-O2D-CED
27	Y	613	CLA	CBD-CGD-O2D-CED
27	b	602	CLA	CBD-CGD-O2D-CED
27	c	506	CLA	CBD-CGD-O2D-CED
27	c	513	CLA	CBD-CGD-O2D-CED
27	d	402	CLA	CBD-CGD-O2D-CED
27	d	403	CLA	CBD-CGD-O2D-CED
27	g	602	CLA	CBD-CGD-O2D-CED
27	n	610	CLA	CBD-CGD-O2D-CED
27	r	610	CLA	CBD-CGD-O2D-CED
27	s	602	CLA	CBD-CGD-O2D-CED
27	s	613	CLA	CBD-CGD-O2D-CED
27	y	602	CLA	CBD-CGD-O2D-CED
27	y	603	CLA	CBD-CGD-O2D-CED
27	y	611	CLA	CBD-CGD-O2D-CED
27	y	613	CLA	CBD-CGD-O2D-CED
28	A	409	PHO	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	a	409	PHO	CBD-CGD-O2D-CED
37	Y	607	CHL	CBD-CGD-O2D-CED
37	y	607	CHL	CBD-CGD-O2D-CED
30	A	412	SQD	C8-C7-O47-C45
30	a	412	SQD	C8-C7-O47-C45
31	B	622	LMG	C11-C10-O7-C8
31	b	622	LMG	C11-C10-O7-C8
27	B	606	CLA	O1D-CGD-O2D-CED
27	b	606	CLA	O1D-CGD-O2D-CED
27	b	608	CLA	O1D-CGD-O2D-CED
27	R	601	CLA	C2C-C3C-CAC-CBC
27	r	601	CLA	C2C-C3C-CAC-CBC
27	B	604	CLA	C4-C3-C5-C6
27	B	609	CLA	C4-C3-C5-C6
27	b	603	CLA	C4-C3-C5-C6
27	b	604	CLA	C4-C3-C5-C6
27	b	609	CLA	C4-C3-C5-C6
34	D	405	PL9	C40-C39-C41-C42
34	d	405	PL9	C40-C39-C41-C42
27	B	603	CLA	C2-C3-C5-C6
27	B	609	CLA	C2-C3-C5-C6
27	G	610	CLA	C2-C3-C5-C6
27	b	603	CLA	C2-C3-C5-C6
27	b	609	CLA	C2-C3-C5-C6
27	g	610	CLA	C2-C3-C5-C6
27	C	502	CLA	CBD-CGD-O2D-CED
27	c	502	CLA	CBD-CGD-O2D-CED
27	R	609	CLA	O1D-CGD-O2D-CED
27	r	609	CLA	O1D-CGD-O2D-CED
32	C	519	DGD	O6E-C5E-C6E-O5E
32	C	520	DGD	O6E-C5E-C6E-O5E
32	c	519	DGD	O6E-C5E-C6E-O5E
32	c	520	DGD	O6E-C5E-C6E-O5E
27	B	605	CLA	C2A-CAA-CBA-CGA
27	B	615	CLA	C2A-CAA-CBA-CGA
27	C	507	CLA	C2A-CAA-CBA-CGA
27	b	605	CLA	C2A-CAA-CBA-CGA
27	b	615	CLA	C2A-CAA-CBA-CGA
27	c	507	CLA	C2A-CAA-CBA-CGA
27	G	602	CLA	C3-C5-C6-C7
27	g	602	CLA	C3-C5-C6-C7
27	B	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	C	510	CLA	CBA-CGA-O2A-C1
27	G	613	CLA	CBA-CGA-O2A-C1
27	G	614	CLA	CBA-CGA-O2A-C1
27	N	611	CLA	CBA-CGA-O2A-C1
27	R	601	CLA	CBA-CGA-O2A-C1
27	S	614	CLA	CBA-CGA-O2A-C1
27	b	603	CLA	CBA-CGA-O2A-C1
27	c	510	CLA	CBA-CGA-O2A-C1
27	g	613	CLA	CBA-CGA-O2A-C1
27	g	614	CLA	CBA-CGA-O2A-C1
27	n	611	CLA	CBA-CGA-O2A-C1
27	r	601	CLA	CBA-CGA-O2A-C1
27	s	614	CLA	CBA-CGA-O2A-C1
35	G	2630	LHG	C24-C23-O8-C6
35	N	2630	LHG	C24-C23-O8-C6
35	g	2630	LHG	C24-C23-O8-C6
35	n	2630	LHG	C24-C23-O8-C6
27	B	603	CLA	O1A-CGA-O2A-C1
27	R	604	CLA	O1A-CGA-O2A-C1
27	S	614	CLA	O1A-CGA-O2A-C1
27	b	603	CLA	O1A-CGA-O2A-C1
27	r	604	CLA	O1A-CGA-O2A-C1
27	s	614	CLA	O1A-CGA-O2A-C1
35	R	2630	LHG	O10-C23-O8-C6
35	r	2630	LHG	O10-C23-O8-C6
27	S	603	CLA	O1D-CGD-O2D-CED
27	s	603	CLA	O1D-CGD-O2D-CED
27	C	503	CLA	O1D-CGD-O2D-CED
27	C	511	CLA	O1D-CGD-O2D-CED
27	R	611	CLA	O1D-CGD-O2D-CED
27	c	503	CLA	O1D-CGD-O2D-CED
27	c	511	CLA	O1D-CGD-O2D-CED
27	r	611	CLA	O1D-CGD-O2D-CED
37	Y	601	CHL	C3-C5-C6-C7
37	y	601	CHL	C3-C5-C6-C7
37	R	606	CHL	CBD-CGD-O2D-CED
37	r	606	CHL	CBD-CGD-O2D-CED
35	D	409	LHG	O2-C2-C3-O3
35	G	2630	LHG	O2-C2-C3-O3
35	d	409	LHG	O2-C2-C3-O3
35	g	2630	LHG	O2-C2-C3-O3
27	B	615	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	b	615	CLA	O1D-CGD-O2D-CED
37	S	606	CHL	O1D-CGD-O2D-CED
37	s	606	CHL	O1D-CGD-O2D-CED
27	S	611	CLA	CBA-CGA-O2A-C1
27	s	611	CLA	CBA-CGA-O2A-C1
31	Z	101	LMG	O6-C5-C6-O5
31	z	101	LMG	O6-C5-C6-O5
27	C	510	CLA	O1A-CGA-O2A-C1
27	c	510	CLA	O1A-CGA-O2A-C1
27	B	611	CLA	CBD-CGD-O2D-CED
27	R	613	CLA	CBD-CGD-O2D-CED
27	b	611	CLA	CBD-CGD-O2D-CED
27	r	613	CLA	CBD-CGD-O2D-CED
37	Y	605	CHL	CBD-CGD-O2D-CED
37	y	605	CHL	CBD-CGD-O2D-CED
30	B	621	SQD	C8-C7-O47-C45
30	b	621	SQD	C8-C7-O47-C45
27	C	506	CLA	C3-C5-C6-C7
27	c	506	CLA	C3-C5-C6-C7
37	N	605	CHL	CBD-CGD-O2D-CED
37	n	605	CHL	CBD-CGD-O2D-CED
32	C	520	DGD	C4E-C5E-C6E-O5E
32	c	520	DGD	C4E-C5E-C6E-O5E
27	Y	604	CLA	O1D-CGD-O2D-CED
27	y	604	CLA	O1D-CGD-O2D-CED
27	R	604	CLA	CBA-CGA-O2A-C1
27	r	604	CLA	CBA-CGA-O2A-C1
27	G	602	CLA	C4-C3-C5-C6
27	g	602	CLA	C4-C3-C5-C6
27	B	604	CLA	C2-C3-C5-C6
27	b	604	CLA	C2-C3-C5-C6
34	D	405	PL9	C38-C39-C41-C42
34	d	405	PL9	C38-C39-C41-C42
27	S	611	CLA	O1A-CGA-O2A-C1
27	s	611	CLA	O1A-CGA-O2A-C1
35	Y	2630	LHG	O10-C23-O8-C6
35	y	2630	LHG	O10-C23-O8-C6
31	Z	101	LMG	C4-C5-C6-O5
31	z	101	LMG	C4-C5-C6-O5
27	G	610	CLA	O1D-CGD-O2D-CED
27	g	610	CLA	O1D-CGD-O2D-CED
27	C	502	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	c	502	CLA	O1A-CGA-O2A-C1
32	C	519	DGD	O6E-C1E-O5D-C6D
32	c	519	DGD	O6E-C1E-O5D-C6D
32	C	519	DGD	C4E-C5E-C6E-O5E
32	c	519	DGD	C4E-C5E-C6E-O5E
27	C	502	CLA	CBA-CGA-O2A-C1
27	c	502	CLA	CBA-CGA-O2A-C1
27	Y	614	CLA	CBD-CGD-O2D-CED
27	y	614	CLA	CBD-CGD-O2D-CED
37	G	607	CHL	CBD-CGD-O2D-CED
37	G	609	CHL	CBD-CGD-O2D-CED
37	g	607	CHL	CBD-CGD-O2D-CED
37	g	609	CHL	CBD-CGD-O2D-CED
32	H	102	DGD	O6E-C5E-C6E-O5E
32	h	102	DGD	O6E-C5E-C6E-O5E
27	N	602	CLA	O1D-CGD-O2D-CED
27	n	602	CLA	O1D-CGD-O2D-CED
27	C	508	CLA	CBD-CGD-O2D-CED
27	c	508	CLA	CBD-CGD-O2D-CED
35	D	408	LHG	C1-C2-C3-O3
35	d	408	LHG	C1-C2-C3-O3
27	A	410	CLA	CBA-CGA-O2A-C1
27	C	505	CLA	CBA-CGA-O2A-C1
27	G	611	CLA	CBA-CGA-O2A-C1
27	S	603	CLA	CBA-CGA-O2A-C1
27	S	609	CLA	CBA-CGA-O2A-C1
27	Y	612	CLA	CBA-CGA-O2A-C1
27	a	410	CLA	CBA-CGA-O2A-C1
27	c	505	CLA	CBA-CGA-O2A-C1
27	g	611	CLA	CBA-CGA-O2A-C1
27	s	603	CLA	CBA-CGA-O2A-C1
27	s	609	CLA	CBA-CGA-O2A-C1
27	y	612	CLA	CBA-CGA-O2A-C1
35	R	2630	LHG	C24-C23-O8-C6
35	Y	2630	LHG	C24-C23-O8-C6
35	r	2630	LHG	C24-C23-O8-C6
35	y	2630	LHG	C24-C23-O8-C6
37	N	607	CHL	CBA-CGA-O2A-C1
37	n	607	CHL	CBA-CGA-O2A-C1
37	R	607	CHL	CBD-CGD-O2D-CED
37	r	607	CHL	CBD-CGD-O2D-CED
27	C	501	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	D	402	CLA	O1D-CGD-O2D-CED
27	N	610	CLA	O1D-CGD-O2D-CED
27	Y	610	CLA	O1D-CGD-O2D-CED
27	c	501	CLA	O1D-CGD-O2D-CED
27	d	402	CLA	O1D-CGD-O2D-CED
27	n	610	CLA	O1D-CGD-O2D-CED
27	y	610	CLA	O1D-CGD-O2D-CED
27	Y	612	CLA	CBD-CGD-O2D-CED
27	y	612	CLA	CBD-CGD-O2D-CED
27	A	405	CLA	C11-C12-C13-C14
27	A	410	CLA	C11-C10-C8-C9
27	B	602	CLA	C14-C13-C15-C16
27	B	603	CLA	C6-C7-C8-C9
27	B	605	CLA	C6-C7-C8-C9
27	B	606	CLA	C14-C13-C15-C16
27	B	609	CLA	C11-C10-C8-C9
27	B	609	CLA	C14-C13-C15-C16
27	B	611	CLA	C11-C12-C13-C14
27	B	615	CLA	C11-C10-C8-C9
27	C	502	CLA	C11-C10-C8-C9
27	C	507	CLA	C11-C12-C13-C14
27	C	509	CLA	C6-C7-C8-C9
27	a	405	CLA	C11-C12-C13-C14
27	a	410	CLA	C11-C10-C8-C9
27	b	602	CLA	C14-C13-C15-C16
27	b	603	CLA	C6-C7-C8-C9
27	b	605	CLA	C6-C7-C8-C9
27	b	606	CLA	C14-C13-C15-C16
27	b	609	CLA	C11-C10-C8-C9
27	b	609	CLA	C14-C13-C15-C16
27	b	611	CLA	C11-C12-C13-C14
27	b	615	CLA	C11-C10-C8-C9
27	c	502	CLA	C11-C10-C8-C9
27	c	507	CLA	C11-C12-C13-C14
27	c	509	CLA	C6-C7-C8-C9
28	A	409	PHO	C11-C12-C13-C14
28	a	409	PHO	C11-C12-C13-C14
37	G	601	CHL	C11-C12-C13-C14
37	Y	601	CHL	C11-C10-C8-C9
37	g	601	CHL	C11-C12-C13-C14
37	y	601	CHL	C11-C10-C8-C9
32	H	102	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
32	h	102	DGD	C4E-C5E-C6E-O5E
28	A	409	PHO	O1D-CGD-O2D-CED
28	a	409	PHO	O1D-CGD-O2D-CED
32	C	519	DGD	C2E-C1E-O5D-C6D
32	c	519	DGD	C2E-C1E-O5D-C6D
35	D	408	LHG	O2-C2-C3-O3
35	d	408	LHG	O2-C2-C3-O3
27	Y	611	CLA	O1D-CGD-O2D-CED
27	y	611	CLA	O1D-CGD-O2D-CED
27	A	410	CLA	O1A-CGA-O2A-C1
27	a	410	CLA	O1A-CGA-O2A-C1
27	B	602	CLA	O1D-CGD-O2D-CED
27	C	513	CLA	O1D-CGD-O2D-CED
27	Y	603	CLA	O1D-CGD-O2D-CED
27	b	602	CLA	O1D-CGD-O2D-CED
27	c	513	CLA	O1D-CGD-O2D-CED
27	y	603	CLA	O1D-CGD-O2D-CED
37	Y	607	CHL	O1D-CGD-O2D-CED
37	y	607	CHL	O1D-CGD-O2D-CED
29	B	618	BCR	C36-C18-C19-C20
29	C	516	BCR	C37-C22-C23-C24
29	C	514	BCR	C37-C22-C23-C24
29	D	404	BCR	C7-C8-C9-C34
29	b	618	BCR	C36-C18-C19-C20
29	c	516	BCR	C37-C22-C23-C24
29	c	514	BCR	C37-C22-C23-C24
29	d	404	BCR	C7-C8-C9-C34
40	N	1623	NEX	C11-C12-C13-C20
40	n	1623	NEX	C11-C12-C13-C20
29	C	516	BCR	C21-C22-C23-C24
29	c	516	BCR	C21-C22-C23-C24
35	L	101	LHG	C7-C8-C9-C10
35	l	101	LHG	C7-C8-C9-C10
27	G	602	CLA	O1D-CGD-O2D-CED
27	g	602	CLA	O1D-CGD-O2D-CED
27	r	610	CLA	O1D-CGD-O2D-CED
27	S	603	CLA	O1A-CGA-O2A-C1
27	Y	612	CLA	O1A-CGA-O2A-C1
27	s	603	CLA	O1A-CGA-O2A-C1
27	y	612	CLA	O1A-CGA-O2A-C1
27	D	403	CLA	O1D-CGD-O2D-CED
27	R	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	d	403	CLA	O1D-CGD-O2D-CED
28	a	409	PHO	CBA-CGA-O2A-C1
27	Y	612	CLA	C8-C10-C11-C12
27	y	612	CLA	C8-C10-C11-C12
37	Y	601	CHL	C5-C6-C7-C8
37	y	601	CHL	C5-C6-C7-C8
27	S	602	CLA	O1D-CGD-O2D-CED
27	S	613	CLA	O1D-CGD-O2D-CED
27	s	602	CLA	O1D-CGD-O2D-CED
37	R	608	CHL	C2C-C3C-CAC-CBC
37	r	608	CHL	C2C-C3C-CAC-CBC
27	Y	611	CLA	C10-C11-C12-C13
27	y	611	CLA	C10-C11-C12-C13
37	Y	609	CHL	C13-C15-C16-C17
37	y	609	CHL	C13-C15-C16-C17
27	s	613	CLA	O1D-CGD-O2D-CED
35	Y	2630	LHG	O1-C1-C2-O2
35	y	2630	LHG	O1-C1-C2-O2
27	Y	613	CLA	O1D-CGD-O2D-CED
27	y	613	CLA	O1D-CGD-O2D-CED
27	B	615	CLA	C10-C11-C12-C13
27	b	615	CLA	C10-C11-C12-C13
27	B	605	CLA	CBD-CGD-O2D-CED
27	b	605	CLA	CBD-CGD-O2D-CED
27	B	603	CLA	C11-C12-C13-C15
27	B	612	CLA	C12-C13-C15-C16
27	B	616	CLA	C11-C12-C13-C15
27	G	610	CLA	C11-C12-C13-C15
27	b	603	CLA	C11-C12-C13-C15
27	b	612	CLA	C12-C13-C15-C16
27	b	616	CLA	C11-C12-C13-C15
27	g	610	CLA	C11-C12-C13-C15
37	Y	609	CHL	C11-C12-C13-C15
37	y	609	CHL	C11-C12-C13-C15
28	A	409	PHO	CBA-CGA-O2A-C1
35	D	409	LHG	C32-C33-C34-C35
35	d	409	LHG	C32-C33-C34-C35
27	C	508	CLA	C4-C3-C5-C6
27	c	508	CLA	C4-C3-C5-C6
31	B	622	LMG	O6-C5-C6-O5
31	b	622	LMG	O6-C5-C6-O5
37	Y	609	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
37	y	609	CHL	C15-C16-C17-C18
27	Y	602	CLA	O1D-CGD-O2D-CED
35	S	2630	LHG	C23-C24-C25-C26
35	s	2630	LHG	C23-C24-C25-C26
39	N	1622	XAT	C29-C30-C31-C32
39	n	1622	XAT	C29-C30-C31-C32
27	y	602	CLA	O1D-CGD-O2D-CED
27	g	602	CLA	C8-C10-C11-C12
30	A	412	SQD	C7-C8-C9-C10
30	a	412	SQD	C7-C8-C9-C10
35	D	408	LHG	C23-C24-C25-C26
35	G	2630	LHG	C7-C8-C9-C10
35	d	408	LHG	C23-C24-C25-C26
27	C	505	CLA	O1A-CGA-O2A-C1
27	S	609	CLA	O1A-CGA-O2A-C1
27	c	505	CLA	O1A-CGA-O2A-C1
27	s	609	CLA	O1A-CGA-O2A-C1
27	A	405	CLA	C13-C15-C16-C17
27	G	602	CLA	C8-C10-C11-C12
27	N	602	CLA	C10-C11-C12-C13
27	R	602	CLA	C8-C10-C11-C12
27	Y	610	CLA	C5-C6-C7-C8
27	a	405	CLA	C13-C15-C16-C17
27	b	605	CLA	C15-C16-C17-C18
27	n	602	CLA	C10-C11-C12-C13
27	r	602	CLA	C8-C10-C11-C12
27	y	610	CLA	C5-C6-C7-C8
27	A	406	CLA	C2A-CAA-CBA-CGA
27	A	407	CLA	C2A-CAA-CBA-CGA
27	B	602	CLA	C2A-CAA-CBA-CGA
27	B	607	CLA	C2A-CAA-CBA-CGA
27	B	608	CLA	C2A-CAA-CBA-CGA
27	B	611	CLA	C2A-CAA-CBA-CGA
27	C	504	CLA	C2A-CAA-CBA-CGA
27	Y	604	CLA	C2A-CAA-CBA-CGA
27	Y	614	CLA	C2A-CAA-CBA-CGA
27	a	406	CLA	C2A-CAA-CBA-CGA
27	a	407	CLA	C2A-CAA-CBA-CGA
27	b	602	CLA	C2A-CAA-CBA-CGA
27	b	607	CLA	C2A-CAA-CBA-CGA
27	b	608	CLA	C2A-CAA-CBA-CGA
27	b	611	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	c	504	CLA	C2A-CAA-CBA-CGA
27	y	604	CLA	C2A-CAA-CBA-CGA
27	y	614	CLA	C2A-CAA-CBA-CGA
37	N	608	CHL	C2A-CAA-CBA-CGA
37	Y	606	CHL	C2A-CAA-CBA-CGA
37	Y	608	CHL	C2A-CAA-CBA-CGA
37	n	608	CHL	C2A-CAA-CBA-CGA
37	y	606	CHL	C2A-CAA-CBA-CGA
37	y	608	CHL	C2A-CAA-CBA-CGA
27	B	603	CLA	C5-C6-C7-C8
27	B	605	CLA	C15-C16-C17-C18
27	C	506	CLA	C15-C16-C17-C18
27	b	603	CLA	C5-C6-C7-C8
35	D	410	LHG	C7-C8-C9-C10
35	Y	2630	LHG	C23-C24-C25-C26
35	d	410	LHG	C7-C8-C9-C10
35	g	2630	LHG	C7-C8-C9-C10
35	y	2630	LHG	C23-C24-C25-C26
27	G	611	CLA	O1A-CGA-O2A-C1
27	g	611	CLA	O1A-CGA-O2A-C1
37	N	607	CHL	O1A-CGA-O2A-C1
37	n	607	CHL	O1A-CGA-O2A-C1
27	G	613	CLA	CBD-CGD-O2D-CED
27	g	613	CLA	CBD-CGD-O2D-CED
32	C	519	DGD	O6D-C1D-O3G-C3G
32	c	519	DGD	O6D-C1D-O3G-C3G
35	Y	2630	LHG	C24-C25-C26-C27
35	y	2630	LHG	C24-C25-C26-C27
27	A	410	CLA	C10-C11-C12-C13
27	B	606	CLA	C5-C6-C7-C8
27	B	610	CLA	C15-C16-C17-C18
27	B	614	CLA	C10-C11-C12-C13
27	C	510	CLA	C13-C15-C16-C17
27	G	602	CLA	C5-C6-C7-C8
27	a	410	CLA	C10-C11-C12-C13
27	b	606	CLA	C5-C6-C7-C8
27	b	610	CLA	C15-C16-C17-C18
27	b	614	CLA	C10-C11-C12-C13
27	c	506	CLA	C15-C16-C17-C18
27	c	510	CLA	C13-C15-C16-C17
27	g	602	CLA	C5-C6-C7-C8
37	G	601	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
37	G	601	CHL	C8-C10-C11-C12
37	Y	601	CHL	C13-C15-C16-C17
37	g	601	CHL	C5-C6-C7-C8
37	g	601	CHL	C8-C10-C11-C12
37	y	601	CHL	C13-C15-C16-C17
35	D	408	LHG	C7-C8-C9-C10
35	d	408	LHG	C7-C8-C9-C10
27	C	503	CLA	C15-C16-C17-C18
27	c	503	CLA	C15-C16-C17-C18
37	G	601	CHL	C13-C15-C16-C17
37	g	601	CHL	C13-C15-C16-C17
27	C	502	CLA	O1D-CGD-O2D-CED
31	B	622	LMG	C4-C5-C6-O5
31	b	622	LMG	C4-C5-C6-O5
27	C	506	CLA	O1D-CGD-O2D-CED
27	c	502	CLA	O1D-CGD-O2D-CED
27	c	506	CLA	O1D-CGD-O2D-CED
27	A	405	CLA	C15-C16-C17-C18
27	R	603	CLA	CBD-CGD-O2D-CED
27	r	603	CLA	CBD-CGD-O2D-CED
35	G	2630	LHG	O10-C23-O8-C6
35	g	2630	LHG	O10-C23-O8-C6
27	G	602	CLA	C2-C3-C5-C6
27	g	602	CLA	C2-C3-C5-C6
27	a	405	CLA	C15-C16-C17-C18
37	N	607	CHL	C15-C16-C17-C18
37	n	607	CHL	C15-C16-C17-C18
27	B	613	CLA	CBA-CGA-O2A-C1
27	C	511	CLA	CBA-CGA-O2A-C1
27	N	603	CLA	CBA-CGA-O2A-C1
27	b	613	CLA	CBA-CGA-O2A-C1
27	c	511	CLA	CBA-CGA-O2A-C1
27	n	603	CLA	CBA-CGA-O2A-C1
27	R	601	CLA	C4C-C3C-CAC-CBC
27	r	601	CLA	C4C-C3C-CAC-CBC
27	B	612	CLA	C8-C10-C11-C12
27	b	612	CLA	C8-C10-C11-C12
27	B	609	CLA	C3-C5-C6-C7
27	B	617	CLA	C3-C5-C6-C7
27	b	617	CLA	C3-C5-C6-C7
37	s	607	CHL	CBD-CGD-O2D-CED
28	a	409	PHO	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
35	D	409	LHG	C1-C2-C3-O3
35	d	409	LHG	C1-C2-C3-O3
37	G	608	CHL	C2A-CAA-CBA-CGA
37	R	607	CHL	C2A-CAA-CBA-CGA
37	Y	607	CHL	C2A-CAA-CBA-CGA
37	g	608	CHL	C2A-CAA-CBA-CGA
37	r	607	CHL	C2A-CAA-CBA-CGA
37	y	607	CHL	C2A-CAA-CBA-CGA
37	y	605	CHL	O1D-CGD-O2D-CED
27	B	617	CLA	CBA-CGA-O2A-C1
27	C	504	CLA	CBA-CGA-O2A-C1
27	C	512	CLA	CBA-CGA-O2A-C1
27	C	513	CLA	CBA-CGA-O2A-C1
27	N	604	CLA	CBA-CGA-O2A-C1
27	b	617	CLA	CBA-CGA-O2A-C1
27	c	504	CLA	CBA-CGA-O2A-C1
27	c	512	CLA	CBA-CGA-O2A-C1
27	c	513	CLA	CBA-CGA-O2A-C1
27	n	604	CLA	CBA-CGA-O2A-C1
27	C	503	CLA	C8-C10-C11-C12
27	C	510	CLA	C15-C16-C17-C18
27	Y	602	CLA	C10-C11-C12-C13
27	c	503	CLA	C8-C10-C11-C12
27	c	510	CLA	C15-C16-C17-C18
27	y	602	CLA	C10-C11-C12-C13
37	Y	609	CHL	C8-C10-C11-C12
37	S	607	CHL	CBD-CGD-O2D-CED
28	A	409	PHO	O1A-CGA-O2A-C1
27	b	609	CLA	C3-C5-C6-C7
37	R	606	CHL	O1D-CGD-O2D-CED
37	Y	605	CHL	O1D-CGD-O2D-CED
37	r	606	CHL	O1D-CGD-O2D-CED
37	y	609	CHL	C8-C10-C11-C12
27	Y	604	CLA	CBA-CGA-O2A-C1
27	y	604	CLA	CBA-CGA-O2A-C1
27	C	512	CLA	C4-C3-C5-C6
27	c	512	CLA	C4-C3-C5-C6
28	A	409	PHO	C8-C10-C11-C12
28	a	409	PHO	C8-C10-C11-C12
37	Y	609	CHL	C10-C11-C12-C13
37	y	609	CHL	C10-C11-C12-C13
27	D	403	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	d	403	CLA	C3-C5-C6-C7
35	L	101	LHG	C8-C7-O7-C5
35	l	101	LHG	C8-C7-O7-C5
30	A	412	SQD	C2-C1-O6-C44
30	a	412	SQD	C2-C1-O6-C44
32	C	519	DGD	C2D-C1D-O3G-C3G
32	c	519	DGD	C2D-C1D-O3G-C3G
27	B	613	CLA	C10-C11-C12-C13
27	b	613	CLA	C10-C11-C12-C13
27	R	613	CLA	O1D-CGD-O2D-CED
27	r	613	CLA	O1D-CGD-O2D-CED
37	N	605	CHL	O1D-CGD-O2D-CED
37	n	605	CHL	O1D-CGD-O2D-CED
27	Y	610	CLA	C16-C17-C18-C20
27	y	610	CLA	C16-C17-C18-C20
31	C	521	LMG	C28-C29-C30-C31
31	c	521	LMG	C28-C29-C30-C31
37	s	601	CHL	CBD-CGD-O2D-CED
40	N	1623	NEX	C11-C12-C13-C14
40	n	1623	NEX	C11-C12-C13-C14
27	C	511	CLA	O1A-CGA-O2A-C1
27	N	603	CLA	O1A-CGA-O2A-C1
27	A	405	CLA	C2A-CAA-CBA-CGA
27	B	613	CLA	C2A-CAA-CBA-CGA
27	C	505	CLA	C2A-CAA-CBA-CGA
27	a	405	CLA	C2A-CAA-CBA-CGA
27	b	613	CLA	C2A-CAA-CBA-CGA
27	c	505	CLA	C2A-CAA-CBA-CGA
37	G	606	CHL	C2A-CAA-CBA-CGA
37	N	605	CHL	C2A-CAA-CBA-CGA
37	S	607	CHL	C2A-CAA-CBA-CGA
37	g	606	CHL	C2A-CAA-CBA-CGA
37	n	605	CHL	C2A-CAA-CBA-CGA
37	s	607	CHL	C2A-CAA-CBA-CGA
30	A	412	SQD	C46-C45-O47-C7
30	a	412	SQD	C46-C45-O47-C7
27	N	610	CLA	C16-C17-C18-C20
27	n	610	CLA	C16-C17-C18-C20
27	C	504	CLA	O1A-CGA-O2A-C1
27	c	511	CLA	O1A-CGA-O2A-C1
27	n	603	CLA	O1A-CGA-O2A-C1
35	r	2630	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
31	B	622	LMG	O6-C1-O1-C7
31	b	622	LMG	O6-C1-O1-C7
35	R	2630	LHG	C28-C29-C30-C31
35	S	2630	LHG	C28-C29-C30-C31
35	s	2630	LHG	C28-C29-C30-C31
27	B	611	CLA	O1D-CGD-O2D-CED
27	b	611	CLA	O1D-CGD-O2D-CED
27	c	504	CLA	O1A-CGA-O2A-C1
30	A	412	SQD	O6-C44-C45-O47
30	a	412	SQD	O6-C44-C45-O47
37	G	608	CHL	CBA-CGA-O2A-C1
37	g	608	CHL	CBA-CGA-O2A-C1
27	B	612	CLA	C10-C11-C12-C13
27	C	509	CLA	C13-C15-C16-C17
27	b	607	CLA	C5-C6-C7-C8
27	b	612	CLA	C10-C11-C12-C13
27	c	509	CLA	C13-C15-C16-C17
37	S	601	CHL	CBD-CGD-O2D-CED
37	S	608	CHL	O2A-C1-C2-C3
37	s	608	CHL	O2A-C1-C2-C3
27	A	405	CLA	C16-C17-C18-C20
27	C	508	CLA	C16-C17-C18-C20
27	a	405	CLA	C16-C17-C18-C20
27	c	508	CLA	C16-C17-C18-C20
37	G	601	CHL	C16-C17-C18-C19
37	N	607	CHL	C16-C17-C18-C19
37	g	601	CHL	C16-C17-C18-C19
37	n	607	CHL	C16-C17-C18-C19
27	N	604	CLA	O1A-CGA-O2A-C1
27	n	604	CLA	O1A-CGA-O2A-C1
27	B	607	CLA	C5-C6-C7-C8
37	Y	601	CHL	C8-C10-C11-C12
37	y	601	CHL	C8-C10-C11-C12
35	G	2630	LHG	C12-C13-C14-C15
35	g	2630	LHG	C12-C13-C14-C15
31	Z	101	LMG	C18-C19-C20-C21
31	z	101	LMG	C18-C19-C20-C21
35	D	408	LHG	C27-C28-C29-C30
35	R	2630	LHG	C25-C26-C27-C28
35	d	408	LHG	C27-C28-C29-C30
35	r	2630	LHG	C25-C26-C27-C28
27	N	610	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	n	610	CLA	C13-C15-C16-C17
31	B	622	LMG	C31-C32-C33-C34
31	b	622	LMG	C31-C32-C33-C34
35	D	408	LHG	C29-C30-C31-C32
35	d	408	LHG	C29-C30-C31-C32
27	A	405	CLA	CBA-CGA-O2A-C1
27	a	405	CLA	CBA-CGA-O2A-C1
32	C	520	DGD	C6A-C7A-C8A-C9A
32	c	520	DGD	C6A-C7A-C8A-C9A
35	G	2630	LHG	O9-C7-O7-C5
35	g	2630	LHG	O9-C7-O7-C5
35	N	2630	LHG	O1-C1-C2-O2
35	n	2630	LHG	O1-C1-C2-O2
31	B	622	LMG	C19-C20-C21-C22
31	b	622	LMG	C19-C20-C21-C22
32	C	519	DGD	C5B-C6B-C7B-C8B
32	c	519	DGD	C5B-C6B-C7B-C8B
37	G	609	CHL	O1D-CGD-O2D-CED
37	g	609	CHL	O1D-CGD-O2D-CED
37	Y	601	CHL	C15-C16-C17-C18
37	y	601	CHL	C15-C16-C17-C18
27	B	604	CLA	C4B-C3B-CAB-CBB
27	B	615	CLA	C4B-C3B-CAB-CBB
27	D	402	CLA	C4B-C3B-CAB-CBB
27	G	612	CLA	C4B-C3B-CAB-CBB
27	G	613	CLA	C4B-C3B-CAB-CBB
27	G	614	CLA	C4B-C3B-CAB-CBB
27	N	612	CLA	C4B-C3B-CAB-CBB
27	b	604	CLA	C4B-C3B-CAB-CBB
27	b	615	CLA	C4B-C3B-CAB-CBB
27	d	402	CLA	C4B-C3B-CAB-CBB
27	g	612	CLA	C4B-C3B-CAB-CBB
27	g	613	CLA	C4B-C3B-CAB-CBB
27	g	614	CLA	C4B-C3B-CAB-CBB
27	n	612	CLA	C4B-C3B-CAB-CBB
31	c	521	LMG	C33-C34-C35-C36
27	C	508	CLA	C16-C17-C18-C19
27	c	508	CLA	C16-C17-C18-C19
28	A	408	PHO	C16-C17-C18-C20
28	a	408	PHO	C16-C17-C18-C20
37	Y	609	CHL	C16-C17-C18-C19
37	Y	609	CHL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
37	y	609	CHL	C16-C17-C18-C19
27	B	613	CLA	O1A-CGA-O2A-C1
27	b	613	CLA	O1A-CGA-O2A-C1
31	A	413	LMG	C31-C32-C33-C34
31	C	521	LMG	C33-C34-C35-C36
31	a	413	LMG	C31-C32-C33-C34
35	G	2630	LHG	C32-C33-C34-C35
35	g	2630	LHG	C32-C33-C34-C35
27	D	402	CLA	C10-C11-C12-C13
27	d	402	CLA	C10-C11-C12-C13
35	N	2630	LHG	C8-C7-O7-C5
35	n	2630	LHG	C8-C7-O7-C5
30	A	412	SQD	C16-C17-C18-C19
30	B	621	SQD	C11-C10-C9-C8
32	C	520	DGD	C8A-C9A-CAA-CBA
32	c	520	DGD	C8A-C9A-CAA-CBA
37	g	607	CHL	C2C-C3C-CAC-CBC
27	B	613	CLA	C12-C13-C15-C16
27	C	509	CLA	C6-C7-C8-C10
27	C	512	CLA	C11-C10-C8-C7
27	b	613	CLA	C12-C13-C15-C16
27	c	509	CLA	C6-C7-C8-C10
27	c	512	CLA	C11-C10-C8-C7
37	G	601	CHL	C12-C13-C15-C16
37	g	601	CHL	C12-C13-C15-C16
30	a	412	SQD	C16-C17-C18-C19
31	C	521	LMG	C31-C32-C33-C34
31	c	521	LMG	C31-C32-C33-C34
32	C	520	DGD	C5B-C6B-C7B-C8B
35	G	2630	LHG	C33-C34-C35-C36
35	L	101	LHG	C27-C28-C29-C30
35	l	101	LHG	C27-C28-C29-C30
35	Y	2630	LHG	O2-C2-C3-O3
35	y	2630	LHG	O2-C2-C3-O3
37	G	607	CHL	C2C-C3C-CAC-CBC
27	C	506	CLA	C8-C10-C11-C12
27	Y	602	CLA	C8-C10-C11-C12
27	c	506	CLA	C8-C10-C11-C12
27	y	602	CLA	C8-C10-C11-C12
30	A	418	SQD	C11-C12-C13-C14
30	a	418	SQD	C11-C12-C13-C14
30	b	621	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
35	D	409	LHG	C16-C17-C18-C19
35	d	409	LHG	C16-C17-C18-C19
35	g	2630	LHG	C33-C34-C35-C36
32	H	102	DGD	C4D-C5D-C6D-O5D
32	h	102	DGD	C4D-C5D-C6D-O5D
27	C	513	CLA	O1A-CGA-O2A-C1
27	c	513	CLA	O1A-CGA-O2A-C1
27	B	605	CLA	C3A-C2A-CAA-CBA
27	D	402	CLA	C3A-C2A-CAA-CBA
27	G	603	CLA	C3A-C2A-CAA-CBA
27	G	610	CLA	C3A-C2A-CAA-CBA
27	N	603	CLA	C3A-C2A-CAA-CBA
27	S	604	CLA	C3A-C2A-CAA-CBA
27	b	605	CLA	C3A-C2A-CAA-CBA
27	d	402	CLA	C3A-C2A-CAA-CBA
27	g	603	CLA	C3A-C2A-CAA-CBA
27	g	610	CLA	C3A-C2A-CAA-CBA
27	n	603	CLA	C3A-C2A-CAA-CBA
27	s	604	CLA	C3A-C2A-CAA-CBA
28	A	409	PHO	C3A-C2A-CAA-CBA
28	a	409	PHO	C3A-C2A-CAA-CBA
37	R	606	CHL	C3A-C2A-CAA-CBA
37	S	607	CHL	C3A-C2A-CAA-CBA
37	r	606	CHL	C3A-C2A-CAA-CBA
37	s	607	CHL	C3A-C2A-CAA-CBA
32	c	520	DGD	C5B-C6B-C7B-C8B
35	D	408	LHG	C26-C27-C28-C29
35	d	408	LHG	C26-C27-C28-C29
27	B	609	CLA	C13-C15-C16-C17
27	C	502	CLA	C13-C15-C16-C17
27	C	503	CLA	C13-C15-C16-C17
27	C	507	CLA	C15-C16-C17-C18
27	b	609	CLA	C13-C15-C16-C17
27	c	502	CLA	C13-C15-C16-C17
27	c	503	CLA	C13-C15-C16-C17
27	c	507	CLA	C15-C16-C17-C18
27	N	610	CLA	C16-C17-C18-C19
27	n	610	CLA	C16-C17-C18-C19
37	y	609	CHL	C16-C17-C18-C20
27	B	617	CLA	O1A-CGA-O2A-C1
27	b	617	CLA	O1A-CGA-O2A-C1
35	d	410	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
30	a	412	SQD	C29-C30-C31-C32
31	B	622	LMG	C32-C33-C34-C35
31	b	622	LMG	C32-C33-C34-C35
32	c	520	DGD	C4A-C5A-C6A-C7A
35	D	410	LHG	C27-C28-C29-C30
30	A	412	SQD	C29-C30-C31-C32
32	C	520	DGD	C4A-C5A-C6A-C7A
32	H	102	DGD	CCA-CDA-CEA-CFA
30	B	621	SQD	C17-C18-C19-C20
30	B	621	SQD	C33-C34-C35-C36
30	b	621	SQD	C17-C18-C19-C20
30	b	621	SQD	C33-C34-C35-C36
31	C	521	LMG	C32-C33-C34-C35
31	c	521	LMG	C32-C33-C34-C35
32	C	519	DGD	C7B-C8B-C9B-CAB
32	c	519	DGD	C6B-C7B-C8B-C9B
32	c	519	DGD	C7B-C8B-C9B-CAB
32	h	102	DGD	CCA-CDA-CEA-CFA
35	D	410	LHG	C25-C26-C27-C28
35	N	2630	LHG	C32-C33-C34-C35
35	Y	2630	LHG	C29-C30-C31-C32
35	d	410	LHG	C25-C26-C27-C28
35	y	2630	LHG	C29-C30-C31-C32
27	C	512	CLA	O1A-CGA-O2A-C1
27	Y	604	CLA	O1A-CGA-O2A-C1
27	c	512	CLA	O1A-CGA-O2A-C1
27	y	604	CLA	O1A-CGA-O2A-C1
32	C	519	DGD	C6B-C7B-C8B-C9B
35	G	2630	LHG	C24-C25-C26-C27
35	g	2630	LHG	C24-C25-C26-C27
35	n	2630	LHG	C32-C33-C34-C35
37	G	607	CHL	O1D-CGD-O2D-CED
37	g	607	CHL	O1D-CGD-O2D-CED
27	A	405	CLA	C16-C17-C18-C19
27	a	405	CLA	C16-C17-C18-C19
27	B	602	CLA	C2B-C3B-CAB-CBB
27	B	607	CLA	C2B-C3B-CAB-CBB
27	G	612	CLA	C2B-C3B-CAB-CBB
27	G	613	CLA	C2B-C3B-CAB-CBB
27	G	614	CLA	C2B-C3B-CAB-CBB
27	S	611	CLA	C2B-C3B-CAB-CBB
27	b	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	b	607	CLA	C2B-C3B-CAB-CBB
27	g	612	CLA	C2B-C3B-CAB-CBB
27	g	613	CLA	C2B-C3B-CAB-CBB
27	g	614	CLA	C2B-C3B-CAB-CBB
27	s	611	CLA	C2B-C3B-CAB-CBB
29	B	618	BCR	C1-C6-C7-C8
29	B	618	BCR	C5-C6-C7-C8
29	B	620	BCR	C5-C6-C7-C8
29	D	404	BCR	C1-C6-C7-C8
29	D	404	BCR	C5-C6-C7-C8
29	b	618	BCR	C1-C6-C7-C8
29	b	618	BCR	C5-C6-C7-C8
29	b	620	BCR	C5-C6-C7-C8
29	d	404	BCR	C1-C6-C7-C8
29	d	404	BCR	C5-C6-C7-C8
31	B	622	LMG	C38-C39-C40-C41
35	G	2630	LHG	C8-C7-O7-C5
35	g	2630	LHG	C8-C7-O7-C5
30	B	621	SQD	C24-C23-O48-C46
30	b	621	SQD	C24-C23-O48-C46
30	B	621	SQD	C31-C32-C33-C34
30	b	621	SQD	C31-C32-C33-C34
31	b	622	LMG	C38-C39-C40-C41
32	H	102	DGD	CBA-CCA-CDA-CEA
32	h	102	DGD	CBA-CCA-CDA-CEA
27	C	508	CLA	O1D-CGD-O2D-CED
30	A	412	SQD	C13-C14-C15-C16
30	a	412	SQD	C13-C14-C15-C16
31	A	413	LMG	C36-C37-C38-C39
31	C	521	LMG	C11-C12-C13-C14
31	a	413	LMG	C36-C37-C38-C39
31	c	521	LMG	C11-C12-C13-C14
35	R	2630	LHG	C32-C33-C34-C35
35	r	2630	LHG	C32-C33-C34-C35
27	R	610	CLA	C2A-CAA-CBA-CGA
27	r	610	CLA	C2A-CAA-CBA-CGA
37	G	607	CHL	C2A-CAA-CBA-CGA
37	S	601	CHL	C2A-CAA-CBA-CGA
37	g	607	CHL	C2A-CAA-CBA-CGA
37	s	601	CHL	C2A-CAA-CBA-CGA
35	L	101	LHG	C23-C24-C25-C26
35	l	101	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
31	C	521	LMG	C17-C18-C19-C20
31	c	521	LMG	C17-C18-C19-C20
35	Y	2630	LHG	C15-C16-C17-C18
27	A	405	CLA	O1A-CGA-O2A-C1
27	a	405	CLA	O1A-CGA-O2A-C1
37	G	608	CHL	O1A-CGA-O2A-C1
37	g	608	CHL	O1A-CGA-O2A-C1
30	A	412	SQD	C26-C27-C28-C29
30	a	412	SQD	C26-C27-C28-C29
35	y	2630	LHG	C15-C16-C17-C18
35	N	2630	LHG	C14-C15-C16-C17
35	n	2630	LHG	C14-C15-C16-C17
27	C	508	CLA	C2-C3-C5-C6
27	C	512	CLA	C2-C3-C5-C6
27	c	508	CLA	C2-C3-C5-C6
27	c	512	CLA	C2-C3-C5-C6
37	N	607	CHL	C16-C17-C18-C20
37	n	607	CHL	C16-C17-C18-C20
32	C	520	DGD	C5A-C6A-C7A-C8A
32	H	102	DGD	C5B-C6B-C7B-C8B
32	c	520	DGD	C5A-C6A-C7A-C8A
32	h	102	DGD	C5B-C6B-C7B-C8B
35	R	2630	LHG	C29-C30-C31-C32
27	c	508	CLA	O1D-CGD-O2D-CED
35	L	101	LHG	C32-C33-C34-C35
35	l	101	LHG	C32-C33-C34-C35
35	r	2630	LHG	C29-C30-C31-C32
31	D	411	LMG	C18-C19-C20-C21
31	d	411	LMG	C18-C19-C20-C21
35	S	2630	LHG	C25-C26-C27-C28
35	s	2630	LHG	C25-C26-C27-C28
27	C	507	CLA	C13-C15-C16-C17
27	c	507	CLA	C13-C15-C16-C17
32	C	518	DGD	CBB-CCB-CDB-CEB
32	c	518	DGD	CBB-CCB-CDB-CEB
35	L	101	LHG	C24-C25-C26-C27
35	l	101	LHG	C24-C25-C26-C27
27	N	613	CLA	CBA-CGA-O2A-C1
27	n	613	CLA	CBA-CGA-O2A-C1
37	R	607	CHL	CBA-CGA-O2A-C1
37	r	607	CHL	CBA-CGA-O2A-C1
27	Y	610	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	y	610	CLA	C16-C17-C18-C19
35	S	2630	LHG	C8-C7-O7-C5
35	s	2630	LHG	C8-C7-O7-C5
35	S	2630	LHG	C32-C33-C34-C35
27	C	502	CLA	C5-C6-C7-C8
27	N	602	CLA	C8-C10-C11-C12
27	c	502	CLA	C5-C6-C7-C8
27	n	602	CLA	C8-C10-C11-C12
31	B	622	LMG	O9-C10-O7-C8
31	b	622	LMG	O9-C10-O7-C8
35	s	2630	LHG	C32-C33-C34-C35
35	g	2630	LHG	C27-C28-C29-C30
29	B	620	BCR	C37-C22-C23-C24
29	b	620	BCR	C37-C22-C23-C24
39	g	1622	XAT	C31-C32-C33-C40
35	G	2630	LHG	C27-C28-C29-C30
29	B	618	BCR	C17-C18-C19-C20
29	b	618	BCR	C17-C18-C19-C20
35	G	2630	LHG	C30-C31-C32-C33
35	g	2630	LHG	C30-C31-C32-C33
27	r	602	CLA	C10-C11-C12-C13
27	C	512	CLA	C2A-CAA-CBA-CGA
27	c	512	CLA	C2A-CAA-CBA-CGA
27	B	616	CLA	C16-C17-C18-C19
27	C	504	CLA	C16-C17-C18-C20
27	Y	613	CLA	C16-C17-C18-C19
27	b	616	CLA	C16-C17-C18-C19
27	c	504	CLA	C16-C17-C18-C20
27	y	613	CLA	C16-C17-C18-C19
37	Y	601	CHL	C16-C17-C18-C19
37	y	601	CHL	C16-C17-C18-C19
35	L	101	LHG	C13-C14-C15-C16
35	S	2630	LHG	C31-C32-C33-C34
35	s	2630	LHG	C31-C32-C33-C34
28	A	408	PHO	C4-C3-C5-C6
28	a	408	PHO	C4-C3-C5-C6
35	l	101	LHG	C13-C14-C15-C16
27	R	602	CLA	C10-C11-C12-C13
32	C	518	DGD	C7B-C8B-C9B-CAB
32	c	518	DGD	C7B-C8B-C9B-CAB
35	L	101	LHG	C14-C15-C16-C17
35	g	2630	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
35	l	101	LHG	C14-C15-C16-C17
35	G	2630	LHG	C28-C29-C30-C31
27	A	405	CLA	C5-C6-C7-C8
27	A	406	CLA	C15-C16-C17-C18
27	a	405	CLA	C5-C6-C7-C8
27	a	406	CLA	C15-C16-C17-C18
35	Y	2630	LHG	C14-C15-C16-C17
35	y	2630	LHG	C14-C15-C16-C17
30	A	412	SQD	C14-C15-C16-C17
30	a	412	SQD	C14-C15-C16-C17
31	a	413	LMG	C13-C14-C15-C16
31	c	521	LMG	C37-C38-C39-C40
31	A	413	LMG	C13-C14-C15-C16
31	C	521	LMG	C37-C38-C39-C40
27	y	614	CLA	O1D-CGD-O2D-CED
27	Y	614	CLA	O1D-CGD-O2D-CED
31	a	413	LMG	C11-C12-C13-C14
31	A	413	LMG	C11-C12-C13-C14
30	A	412	SQD	C30-C31-C32-C33
30	a	412	SQD	C30-C31-C32-C33
32	C	518	DGD	C4A-C5A-C6A-C7A
32	c	518	DGD	C4A-C5A-C6A-C7A
31	A	413	LMG	C16-C17-C18-C19
31	a	413	LMG	C16-C17-C18-C19
27	n	603	CLA	CBD-CGD-O2D-CED
31	a	413	LMG	C37-C38-C39-C40
35	Y	2630	LHG	C34-C35-C36-C37
31	A	413	LMG	C37-C38-C39-C40
32	c	520	DGD	CBA-CCA-CDA-CEA
35	y	2630	LHG	C34-C35-C36-C37
32	C	518	DGD	C2A-C3A-C4A-C5A
32	C	520	DGD	CBA-CCA-CDA-CEA
32	c	518	DGD	C2A-C3A-C4A-C5A
27	Y	613	CLA	C4-C3-C5-C6
27	y	613	CLA	C4-C3-C5-C6
28	A	408	PHO	C2-C3-C5-C6
28	a	408	PHO	C2-C3-C5-C6
30	a	412	SQD	C12-C13-C14-C15
31	D	411	LMG	C30-C31-C32-C33
31	b	622	LMG	C29-C30-C31-C32
27	C	501	CLA	C2A-CAA-CBA-CGA
27	G	610	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	G	613	CLA	C2A-CAA-CBA-CGA
27	N	611	CLA	C2A-CAA-CBA-CGA
27	N	614	CLA	C2A-CAA-CBA-CGA
27	c	501	CLA	C2A-CAA-CBA-CGA
27	g	610	CLA	C2A-CAA-CBA-CGA
27	g	613	CLA	C2A-CAA-CBA-CGA
27	n	611	CLA	C2A-CAA-CBA-CGA
27	n	614	CLA	C2A-CAA-CBA-CGA
37	R	608	CHL	C2A-CAA-CBA-CGA
37	r	608	CHL	C2A-CAA-CBA-CGA
27	N	603	CLA	CBD-CGD-O2D-CED
37	N	607	CHL	CBD-CGD-O2D-CED
37	Y	609	CHL	CBD-CGD-O2D-CED
37	n	607	CHL	CBD-CGD-O2D-CED
37	y	609	CHL	CBD-CGD-O2D-CED
30	A	412	SQD	C12-C13-C14-C15
31	B	622	LMG	C29-C30-C31-C32
31	d	411	LMG	C30-C31-C32-C33
35	D	409	LHG	C24-C25-C26-C27
35	d	409	LHG	C24-C25-C26-C27
31	B	622	LMG	C13-C14-C15-C16
31	b	622	LMG	C13-C14-C15-C16
27	Y	612	CLA	C15-C16-C17-C18
27	y	612	CLA	C15-C16-C17-C18
32	C	518	DGD	C2B-C3B-C4B-C5B
27	B	612	CLA	C16-C17-C18-C19
27	b	612	CLA	C16-C17-C18-C19
37	r	607	CHL	O1D-CGD-O2D-CED
30	A	412	SQD	C15-C16-C17-C18
30	a	412	SQD	C15-C16-C17-C18
32	c	518	DGD	C2B-C3B-C4B-C5B
30	b	621	SQD	C26-C27-C28-C29
27	A	406	CLA	C1A-C2A-CAA-CBA
27	B	605	CLA	C1A-C2A-CAA-CBA
27	B	615	CLA	C1A-C2A-CAA-CBA
27	C	501	CLA	C1A-C2A-CAA-CBA
27	G	603	CLA	C1A-C2A-CAA-CBA
27	G	604	CLA	C1A-C2A-CAA-CBA
27	N	603	CLA	C1A-C2A-CAA-CBA
27	N	610	CLA	C1A-C2A-CAA-CBA
27	R	610	CLA	C1A-C2A-CAA-CBA
27	S	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	a	406	CLA	C1A-C2A-CAA-CBA
27	b	605	CLA	C1A-C2A-CAA-CBA
27	b	615	CLA	C1A-C2A-CAA-CBA
27	c	501	CLA	C1A-C2A-CAA-CBA
27	g	603	CLA	C1A-C2A-CAA-CBA
27	g	604	CLA	C1A-C2A-CAA-CBA
27	n	603	CLA	C1A-C2A-CAA-CBA
27	n	610	CLA	C1A-C2A-CAA-CBA
27	r	610	CLA	C1A-C2A-CAA-CBA
27	s	610	CLA	C1A-C2A-CAA-CBA
27	C	501	CLA	C8-C10-C11-C12
27	c	501	CLA	C8-C10-C11-C12
30	B	621	SQD	C26-C27-C28-C29
35	y	2630	LHG	C32-C33-C34-C35
31	A	413	LMG	C35-C36-C37-C38
35	L	101	LHG	C30-C31-C32-C33
35	Y	2630	LHG	C32-C33-C34-C35
37	r	607	CHL	O1A-CGA-O2A-C1
31	a	413	LMG	C35-C36-C37-C38
35	G	2630	LHG	C17-C18-C19-C20
35	g	2630	LHG	C17-C18-C19-C20
35	l	101	LHG	C30-C31-C32-C33
35	L	101	LHG	O6-C4-C5-C6
35	N	2630	LHG	O6-C4-C5-C6
35	l	101	LHG	O6-C4-C5-C6
35	n	2630	LHG	O6-C4-C5-C6
35	S	2630	LHG	O9-C7-O7-C5
35	s	2630	LHG	O9-C7-O7-C5
30	b	621	SQD	C27-C28-C29-C30
37	R	607	CHL	O1D-CGD-O2D-CED
27	B	604	CLA	C11-C10-C8-C7
27	B	605	CLA	C11-C10-C8-C7
27	B	606	CLA	C11-C12-C13-C15
27	B	609	CLA	C6-C7-C8-C10
27	B	614	CLA	C12-C13-C15-C16
27	B	617	CLA	C12-C13-C15-C16
27	C	507	CLA	C12-C13-C15-C16
27	C	511	CLA	C11-C12-C13-C15
27	D	403	CLA	C11-C10-C8-C7
27	Y	602	CLA	C6-C7-C8-C10
27	Y	612	CLA	C11-C12-C13-C15
27	b	604	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
27	b	605	CLA	C11-C10-C8-C7
27	b	606	CLA	C11-C12-C13-C15
27	b	609	CLA	C6-C7-C8-C10
27	b	614	CLA	C12-C13-C15-C16
27	b	617	CLA	C12-C13-C15-C16
27	c	507	CLA	C12-C13-C15-C16
27	c	511	CLA	C11-C12-C13-C15
27	d	403	CLA	C11-C10-C8-C7
27	y	602	CLA	C6-C7-C8-C10
27	y	612	CLA	C11-C12-C13-C15
37	G	601	CHL	C6-C7-C8-C10
37	G	601	CHL	C11-C12-C13-C15
37	Y	601	CHL	C6-C7-C8-C10
37	Y	601	CHL	C11-C12-C13-C15
37	g	601	CHL	C6-C7-C8-C10
37	g	601	CHL	C11-C12-C13-C15
37	y	601	CHL	C6-C7-C8-C10
37	y	601	CHL	C11-C12-C13-C15
30	B	621	SQD	C27-C28-C29-C30
27	B	616	CLA	C16-C17-C18-C20
27	b	616	CLA	C16-C17-C18-C20
27	B	605	CLA	C13-C15-C16-C17
27	b	605	CLA	C13-C15-C16-C17
27	y	613	CLA	C5-C6-C7-C8
37	R	607	CHL	O1A-CGA-O2A-C1
27	Y	613	CLA	C5-C6-C7-C8
35	s	2630	LHG	C7-C8-C9-C10
32	H	102	DGD	C4A-C5A-C6A-C7A
32	h	102	DGD	C4A-C5A-C6A-C7A
27	B	610	CLA	C2-C3-C5-C6
30	B	621	SQD	C32-C33-C34-C35
27	B	602	CLA	C13-C15-C16-C17
27	b	602	CLA	C13-C15-C16-C17
27	Y	612	CLA	O1D-CGD-O2D-CED
27	y	612	CLA	O1D-CGD-O2D-CED
27	B	604	CLA	C2A-CAA-CBA-CGA
27	G	604	CLA	C2A-CAA-CBA-CGA
27	S	611	CLA	C2A-CAA-CBA-CGA
27	S	614	CLA	C2A-CAA-CBA-CGA
27	Y	602	CLA	C2A-CAA-CBA-CGA
27	b	604	CLA	C2A-CAA-CBA-CGA
27	g	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	s	611	CLA	C2A-CAA-CBA-CGA
27	s	614	CLA	C2A-CAA-CBA-CGA
27	y	602	CLA	C2A-CAA-CBA-CGA
27	A	410	CLA	C6-C7-C8-C9
27	B	604	CLA	C6-C7-C8-C9
27	B	604	CLA	C11-C10-C8-C9
27	B	605	CLA	C11-C10-C8-C9
27	B	608	CLA	C14-C13-C15-C16
27	B	609	CLA	C6-C7-C8-C9
27	B	612	CLA	C14-C13-C15-C16
27	C	512	CLA	C11-C10-C8-C9
27	G	602	CLA	C11-C10-C8-C9
27	a	410	CLA	C6-C7-C8-C9
27	b	604	CLA	C6-C7-C8-C9
27	b	604	CLA	C11-C10-C8-C9
27	b	605	CLA	C11-C10-C8-C9
27	b	608	CLA	C14-C13-C15-C16
27	b	609	CLA	C6-C7-C8-C9
27	b	612	CLA	C14-C13-C15-C16
27	c	512	CLA	C11-C10-C8-C9
27	g	602	CLA	C11-C10-C8-C9
30	b	621	SQD	C32-C33-C34-C35
35	S	2630	LHG	C7-C8-C9-C10
37	N	601	CHL	CBA-CGA-O2A-C1
37	Y	605	CHL	CBA-CGA-O2A-C1
37	n	601	CHL	CBA-CGA-O2A-C1
37	y	605	CHL	CBA-CGA-O2A-C1
31	A	413	LMG	C34-C35-C36-C37
31	a	413	LMG	C34-C35-C36-C37
30	A	412	SQD	O6-C44-C45-C46
30	a	412	SQD	O6-C44-C45-C46
31	B	622	LMG	C7-C8-C9-O8
31	Z	101	LMG	O1-C7-C8-C9
31	b	622	LMG	C7-C8-C9-O8
31	z	101	LMG	O1-C7-C8-C9
35	D	410	LHG	C4-C5-C6-O8
35	G	2630	LHG	C4-C5-C6-O8
35	d	410	LHG	C4-C5-C6-O8
35	g	2630	LHG	C4-C5-C6-O8
35	D	408	LHG	C34-C35-C36-C37
35	d	408	LHG	C34-C35-C36-C37
27	B	615	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	b	615	CLA	C5-C6-C7-C8
37	G	609	CHL	C2C-C3C-CAC-CBC
37	g	609	CHL	C2C-C3C-CAC-CBC
27	C	510	CLA	C16-C17-C18-C20
27	c	510	CLA	C16-C17-C18-C20
37	Y	601	CHL	C16-C17-C18-C20
37	y	601	CHL	C16-C17-C18-C20
32	C	520	DGD	C9B-CAB-CBB-CCB
32	c	520	DGD	C9B-CAB-CBB-CCB
35	n	2630	LHG	C15-C16-C17-C18
35	N	2630	LHG	C15-C16-C17-C18
37	N	609	CHL	CHA-CBD-CGD-O1D
37	N	609	CHL	CHA-CBD-CGD-O2D
37	Y	609	CHL	CHA-CBD-CGD-O1D
37	Y	609	CHL	CHA-CBD-CGD-O2D
37	n	609	CHL	CHA-CBD-CGD-O1D
37	n	609	CHL	CHA-CBD-CGD-O2D
37	y	609	CHL	CHA-CBD-CGD-O1D
37	y	609	CHL	CHA-CBD-CGD-O2D
27	N	613	CLA	O1A-CGA-O2A-C1
27	n	613	CLA	O1A-CGA-O2A-C1
27	B	610	CLA	C4-C3-C5-C6
27	b	610	CLA	C4-C3-C5-C6
27	B	612	CLA	C2-C3-C5-C6
27	Y	613	CLA	C2-C3-C5-C6
27	b	610	CLA	C2-C3-C5-C6
27	b	612	CLA	C2-C3-C5-C6
27	y	613	CLA	C2-C3-C5-C6
39	G	1622	XAT	C31-C32-C33-C40
30	B	621	SQD	C11-C12-C13-C14
30	b	621	SQD	C11-C12-C13-C14
32	C	520	DGD	C7A-C8A-C9A-CAA
32	c	519	DGD	C9A-CAA-CBA-CCA
35	Y	2630	LHG	C28-C29-C30-C31
35	y	2630	LHG	C28-C29-C30-C31
29	C	514	BCR	C21-C22-C23-C24
29	c	514	BCR	C21-C22-C23-C24
32	C	519	DGD	C9A-CAA-CBA-CCA
32	c	520	DGD	C7A-C8A-C9A-CAA
27	B	609	CLA	C15-C16-C17-C18
27	b	609	CLA	C15-C16-C17-C18
31	D	411	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	d	411	LMG	C32-C33-C34-C35
30	b	621	SQD	C24-C25-C26-C27
35	N	2630	LHG	C13-C14-C15-C16
30	B	621	SQD	C24-C25-C26-C27
30	b	621	SQD	C9-C10-C11-C12
31	B	622	LMG	C14-C15-C16-C17
31	Z	101	LMG	C15-C16-C17-C18
31	b	622	LMG	C14-C15-C16-C17
31	z	101	LMG	C15-C16-C17-C18
35	n	2630	LHG	C13-C14-C15-C16
37	G	607	CHL	C3C-C2C-CMC-OMC
37	G	609	CHL	C3C-C2C-CMC-OMC
37	g	607	CHL	C3C-C2C-CMC-OMC
37	g	609	CHL	C3C-C2C-CMC-OMC
30	B	621	SQD	C9-C10-C11-C12
35	d	409	LHG	C17-C18-C19-C20
35	n	2630	LHG	C24-C25-C26-C27
35	D	409	LHG	C17-C18-C19-C20
27	Y	611	CLA	CBA-CGA-O2A-C1
27	y	611	CLA	CBA-CGA-O2A-C1
37	N	605	CHL	CBA-CGA-O2A-C1
37	n	605	CHL	CBA-CGA-O2A-C1
35	N	2630	LHG	C24-C25-C26-C27
27	Y	610	CLA	C15-C16-C17-C18
27	y	610	CLA	C15-C16-C17-C18
35	D	410	LHG	C9-C10-C11-C12
35	d	410	LHG	C9-C10-C11-C12
37	y	606	CHL	CBD-CGD-O2D-CED
35	Y	2630	LHG	C13-C14-C15-C16
35	y	2630	LHG	C13-C14-C15-C16
30	A	412	SQD	C28-C29-C30-C31
30	a	412	SQD	C28-C29-C30-C31
31	A	413	LMG	C30-C31-C32-C33
31	Z	101	LMG	C11-C12-C13-C14
31	a	413	LMG	C30-C31-C32-C33
31	z	101	LMG	C11-C12-C13-C14
35	D	410	LHG	O7-C5-C6-O8
35	d	410	LHG	O7-C5-C6-O8
35	D	410	LHG	C32-C33-C34-C35
35	d	410	LHG	C32-C33-C34-C35
32	c	518	DGD	CCB-CDB-CEB-CFB
35	N	2630	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
35	n	2630	LHG	C28-C29-C30-C31
32	C	518	DGD	CCB-CDB-CEB-CFB
31	C	521	LMG	C14-C15-C16-C17
31	c	521	LMG	C14-C15-C16-C17
37	Y	606	CHL	CBD-CGD-O2D-CED
31	D	411	LMG	C17-C18-C19-C20
31	d	411	LMG	C17-C18-C19-C20
35	L	101	LHG	C11-C10-C9-C8
27	R	603	CLA	O1D-CGD-O2D-CED
27	D	403	CLA	CBA-CGA-O2A-C1
27	S	604	CLA	CBA-CGA-O2A-C1
27	d	403	CLA	CBA-CGA-O2A-C1
27	s	604	CLA	CBA-CGA-O2A-C1
35	L	101	LHG	C24-C23-O8-C6
35	l	101	LHG	C24-C23-O8-C6
32	c	519	DGD	C2B-C3B-C4B-C5B
32	C	519	DGD	C2B-C3B-C4B-C5B
35	l	101	LHG	C11-C10-C9-C8
35	G	2630	LHG	C31-C32-C33-C34
35	g	2630	LHG	C31-C32-C33-C34
27	r	603	CLA	O1D-CGD-O2D-CED
27	G	613	CLA	O1D-CGD-O2D-CED
27	g	613	CLA	O1D-CGD-O2D-CED
27	B	612	CLA	C4-C3-C5-C6
27	b	612	CLA	C4-C3-C5-C6
30	a	412	SQD	C23-C24-C25-C26
37	S	607	CHL	O1D-CGD-O2D-CED
31	B	622	LMG	C30-C31-C32-C33
31	b	622	LMG	C30-C31-C32-C33
35	Y	2630	LHG	C11-C10-C9-C8
35	y	2630	LHG	C11-C10-C9-C8
27	A	406	CLA	C14-C13-C15-C16
27	B	602	CLA	C11-C12-C13-C14
27	B	603	CLA	C11-C12-C13-C14
27	B	606	CLA	C11-C12-C13-C14
27	B	608	CLA	C6-C7-C8-C9
27	B	614	CLA	C14-C13-C15-C16
27	B	617	CLA	C14-C13-C15-C16
27	C	507	CLA	C14-C13-C15-C16
27	C	508	CLA	C11-C10-C8-C9
27	C	510	CLA	C6-C7-C8-C9
27	G	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	N	602	CLA	C6-C7-C8-C9
27	R	602	CLA	C6-C7-C8-C9
27	Y	602	CLA	C6-C7-C8-C9
27	Y	610	CLA	C6-C7-C8-C9
27	Y	610	CLA	C11-C12-C13-C14
27	Y	612	CLA	C11-C12-C13-C14
27	a	406	CLA	C14-C13-C15-C16
27	b	602	CLA	C11-C12-C13-C14
27	b	603	CLA	C11-C12-C13-C14
27	b	606	CLA	C11-C12-C13-C14
27	b	608	CLA	C6-C7-C8-C9
27	b	614	CLA	C14-C13-C15-C16
27	b	617	CLA	C14-C13-C15-C16
27	c	507	CLA	C14-C13-C15-C16
27	c	508	CLA	C11-C10-C8-C9
27	c	510	CLA	C6-C7-C8-C9
27	g	602	CLA	C6-C7-C8-C9
27	n	602	CLA	C6-C7-C8-C9
27	r	602	CLA	C6-C7-C8-C9
27	y	602	CLA	C6-C7-C8-C9
27	y	610	CLA	C6-C7-C8-C9
27	y	610	CLA	C11-C12-C13-C14
27	y	612	CLA	C11-C12-C13-C14
28	A	408	PHO	C6-C7-C8-C9
28	A	409	PHO	C6-C7-C8-C9
28	a	408	PHO	C6-C7-C8-C9
28	a	409	PHO	C6-C7-C8-C9
37	G	601	CHL	C6-C7-C8-C9
37	G	601	CHL	C14-C13-C15-C16
37	Y	601	CHL	C11-C12-C13-C14
37	g	601	CHL	C6-C7-C8-C9
37	g	601	CHL	C14-C13-C15-C16
37	y	601	CHL	C11-C12-C13-C14
30	A	412	SQD	C34-C35-C36-C37
27	B	605	CLA	O1D-CGD-O2D-CED
27	b	605	CLA	O1D-CGD-O2D-CED
37	s	607	CHL	O1D-CGD-O2D-CED
27	B	602	CLA	C4B-C3B-CAB-CBB
27	B	607	CLA	C4B-C3B-CAB-CBB
27	C	503	CLA	C4B-C3B-CAB-CBB
27	G	604	CLA	C4B-C3B-CAB-CBB
27	S	611	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	Y	602	CLA	C4B-C3B-CAB-CBB
27	Y	614	CLA	C4B-C3B-CAB-CBB
27	b	602	CLA	C4B-C3B-CAB-CBB
27	b	607	CLA	C4B-C3B-CAB-CBB
27	c	503	CLA	C4B-C3B-CAB-CBB
27	g	604	CLA	C4B-C3B-CAB-CBB
27	s	611	CLA	C4B-C3B-CAB-CBB
27	y	602	CLA	C4B-C3B-CAB-CBB
27	y	614	CLA	C4B-C3B-CAB-CBB
30	a	412	SQD	C34-C35-C36-C37
27	B	605	CLA	C5-C6-C7-C8
27	C	512	CLA	C10-C11-C12-C13
27	b	605	CLA	C5-C6-C7-C8
27	c	512	CLA	C10-C11-C12-C13
27	R	610	CLA	C16-C17-C18-C20
27	R	604	CLA	C2A-CAA-CBA-CGA
27	r	604	CLA	C2A-CAA-CBA-CGA
27	B	616	CLA	C15-C16-C17-C18
27	C	502	CLA	C10-C11-C12-C13
31	Z	101	LMG	C31-C32-C33-C34
30	A	412	SQD	C23-C24-C25-C26
35	G	2630	LHG	O6-C4-C5-C6
35	g	2630	LHG	O6-C4-C5-C6
31	z	101	LMG	C31-C32-C33-C34
27	A	410	CLA	C6-C7-C8-C10
27	B	602	CLA	C11-C12-C13-C15
27	B	604	CLA	C6-C7-C8-C10
27	B	608	CLA	C12-C13-C15-C16
27	B	610	CLA	C6-C7-C8-C10
27	C	504	CLA	C12-C13-C15-C16
27	C	508	CLA	C11-C10-C8-C7
27	C	509	CLA	C11-C12-C13-C15
27	C	510	CLA	C6-C7-C8-C10
27	N	602	CLA	C6-C7-C8-C10
27	N	610	CLA	C12-C13-C15-C16
27	R	602	CLA	C6-C7-C8-C10
27	R	602	CLA	C11-C12-C13-C15
27	a	410	CLA	C6-C7-C8-C10
27	b	602	CLA	C11-C12-C13-C15
27	b	604	CLA	C6-C7-C8-C10
27	b	608	CLA	C12-C13-C15-C16
27	b	610	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
27	b	612	CLA	C6-C7-C8-C10
27	c	504	CLA	C12-C13-C15-C16
27	c	508	CLA	C11-C10-C8-C7
27	c	509	CLA	C11-C12-C13-C15
27	c	510	CLA	C6-C7-C8-C10
27	n	602	CLA	C6-C7-C8-C10
27	n	610	CLA	C12-C13-C15-C16
27	r	602	CLA	C6-C7-C8-C10
27	r	602	CLA	C11-C12-C13-C15
28	A	409	PHO	C6-C7-C8-C10
28	a	409	PHO	C6-C7-C8-C10
27	b	616	CLA	C15-C16-C17-C18
27	c	502	CLA	C10-C11-C12-C13
37	Y	605	CHL	O1A-CGA-O2A-C1
37	y	605	CHL	O1A-CGA-O2A-C1
31	A	413	LMG	C19-C20-C21-C22
31	a	413	LMG	C19-C20-C21-C22
27	r	610	CLA	C16-C17-C18-C20
30	a	412	SQD	C19-C20-C21-C22
31	a	413	LMG	C40-C41-C42-C43
30	A	412	SQD	C19-C20-C21-C22
31	A	413	LMG	C40-C41-C42-C43
27	C	510	CLA	C4-C3-C5-C6
37	N	606	CHL	C3A-C2A-CAA-CBA
37	R	608	CHL	C3A-C2A-CAA-CBA
37	Y	608	CHL	C3A-C2A-CAA-CBA
37	n	606	CHL	C3A-C2A-CAA-CBA
37	r	608	CHL	C3A-C2A-CAA-CBA
37	y	608	CHL	C3A-C2A-CAA-CBA
37	N	601	CHL	O1A-CGA-O2A-C1
37	n	601	CHL	O1A-CGA-O2A-C1
27	a	406	CLA	CBA-CGA-O2A-C1
37	Y	601	CHL	CBA-CGA-O2A-C1
37	y	601	CHL	CBA-CGA-O2A-C1
29	H	101	BCR	C9-C10-C11-C12
29	h	101	BCR	C9-C10-C11-C12
39	Y	1622	XAT	C31-C32-C33-C40
39	y	1622	XAT	C31-C32-C33-C40
27	Y	611	CLA	O1A-CGA-O2A-C1
27	y	611	CLA	O1A-CGA-O2A-C1
37	N	605	CHL	O1A-CGA-O2A-C1
37	n	605	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	B	605	CLA	C8-C10-C11-C12
27	b	605	CLA	C8-C10-C11-C12
27	b	615	CLA	C15-C16-C17-C18
30	A	418	SQD	C25-C26-C27-C28
30	a	418	SQD	C25-C26-C27-C28
27	S	603	CLA	O2A-C1-C2-C3
27	s	603	CLA	O2A-C1-C2-C3
27	A	406	CLA	CBA-CGA-O2A-C1
27	B	615	CLA	C15-C16-C17-C18
31	Z	101	LMG	C7-C8-C9-O8
31	z	101	LMG	C7-C8-C9-O8
35	Y	2630	LHG	C4-C5-C6-O8
35	y	2630	LHG	C4-C5-C6-O8
35	G	2630	LHG	C23-C24-C25-C26
35	g	2630	LHG	C23-C24-C25-C26
32	c	519	DGD	CBA-CCA-CDA-CEA
32	h	102	DGD	C6A-C7A-C8A-C9A
37	s	601	CHL	O1D-CGD-O2D-CED
37	R	606	CHL	C1A-C2A-CAA-CBA
37	S	607	CHL	C1A-C2A-CAA-CBA
37	r	606	CHL	C1A-C2A-CAA-CBA
37	s	607	CHL	C1A-C2A-CAA-CBA
31	d	411	LMG	C33-C34-C35-C36
32	H	102	DGD	C6A-C7A-C8A-C9A
27	C	506	CLA	C4-C3-C5-C6
27	c	506	CLA	C4-C3-C5-C6
27	c	510	CLA	C4-C3-C5-C6
34	D	405	PL9	C45-C44-C46-C47
34	d	405	PL9	C45-C44-C46-C47
31	D	411	LMG	C33-C34-C35-C36
32	C	519	DGD	CBA-CCA-CDA-CEA
35	G	2630	LHG	C25-C26-C27-C28
35	g	2630	LHG	C25-C26-C27-C28
27	C	510	CLA	C2-C3-C5-C6
27	c	510	CLA	C2-C3-C5-C6
37	S	601	CHL	O1D-CGD-O2D-CED
35	G	2630	LHG	C9-C10-C11-C12
27	B	612	CLA	C16-C17-C18-C20
27	C	502	CLA	C16-C17-C18-C20
27	b	612	CLA	C16-C17-C18-C20
27	c	502	CLA	C16-C17-C18-C20
30	A	418	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	a	418	SQD	C9-C10-C11-C12
35	g	2630	LHG	C9-C10-C11-C12
27	b	611	CLA	C2B-C3B-CAB-CBB
38	N	1620	LUT	C1-C6-C7-C8
38	N	1621	LUT	C1-C6-C7-C8
38	n	1620	LUT	C1-C6-C7-C8
38	n	1621	LUT	C1-C6-C7-C8
37	N	607	CHL	O1D-CGD-O2D-CED
35	D	410	LHG	C2-C3-O3-P
35	d	410	LHG	C2-C3-O3-P
35	D	410	LHG	C11-C10-C9-C8
35	d	410	LHG	C11-C10-C9-C8
31	B	622	LMG	C37-C38-C39-C40
27	B	606	CLA	C13-C15-C16-C17
27	C	506	CLA	C5-C6-C7-C8
27	Y	611	CLA	C8-C10-C11-C12
27	b	606	CLA	C13-C15-C16-C17
27	c	506	CLA	C5-C6-C7-C8
27	y	602	CLA	C15-C16-C17-C18
27	y	611	CLA	C8-C10-C11-C12
37	N	609	CHL	CBD-CGD-O2D-CED
37	n	609	CHL	CBD-CGD-O2D-CED
31	b	622	LMG	C37-C38-C39-C40
37	G	601	CHL	C16-C17-C18-C20
37	g	601	CHL	C16-C17-C18-C20
37	n	607	CHL	O1D-CGD-O2D-CED
27	Y	602	CLA	C15-C16-C17-C18
37	N	607	CHL	C13-C15-C16-C17
31	B	622	LMG	O7-C8-C9-O8
31	Z	101	LMG	O1-C7-C8-O7
31	b	622	LMG	O7-C8-C9-O8
31	z	101	LMG	O1-C7-C8-O7
35	S	2630	LHG	O7-C5-C6-O8
35	s	2630	LHG	O7-C5-C6-O8
31	Z	101	LMG	C33-C34-C35-C36
31	C	521	LMG	C39-C40-C41-C42
35	D	410	LHG	C10-C11-C12-C13
31	c	521	LMG	C39-C40-C41-C42
31	z	101	LMG	C33-C34-C35-C36
37	n	607	CHL	C13-C15-C16-C17
35	d	410	LHG	C10-C11-C12-C13
27	R	610	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	r	610	CLA	C16-C17-C18-C19
32	C	520	DGD	CCA-CDA-CEA-CFA
32	c	520	DGD	CCA-CDA-CEA-CFA
32	C	520	DGD	C1A-C2A-C3A-C4A
32	c	520	DGD	C1A-C2A-C3A-C4A
27	B	605	CLA	CBA-CGA-O2A-C1
27	b	605	CLA	CBA-CGA-O2A-C1
27	B	602	CLA	C11-C10-C8-C9
27	C	504	CLA	C6-C7-C8-C9
27	C	509	CLA	C11-C10-C8-C9
27	D	403	CLA	C11-C10-C8-C9
27	N	610	CLA	C14-C13-C15-C16
27	b	602	CLA	C11-C10-C8-C9
27	c	504	CLA	C6-C7-C8-C9
27	c	509	CLA	C11-C10-C8-C9
27	d	403	CLA	C11-C10-C8-C9
27	n	610	CLA	C14-C13-C15-C16
30	A	418	SQD	C16-C17-C18-C19
30	a	418	SQD	C16-C17-C18-C19
32	C	518	DGD	O6E-C1E-O5D-C6D
32	c	518	DGD	O6E-C1E-O5D-C6D
27	Y	613	CLA	C16-C17-C18-C20
27	y	613	CLA	C16-C17-C18-C20
28	A	408	PHO	C16-C17-C18-C19
28	a	408	PHO	C16-C17-C18-C19
27	G	611	CLA	O2A-C1-C2-C3
27	R	604	CLA	O2A-C1-C2-C3
27	R	613	CLA	O2A-C1-C2-C3
27	S	613	CLA	O2A-C1-C2-C3
27	g	611	CLA	O2A-C1-C2-C3
27	r	604	CLA	O2A-C1-C2-C3
27	r	613	CLA	O2A-C1-C2-C3
27	s	613	CLA	O2A-C1-C2-C3
27	R	603	CLA	C2A-CAA-CBA-CGA
27	r	603	CLA	C2A-CAA-CBA-CGA
30	A	418	SQD	C10-C11-C12-C13
35	G	2630	LHG	C35-C36-C37-C38
35	g	2630	LHG	C35-C36-C37-C38
30	a	418	SQD	C10-C11-C12-C13
29	C	517	BCR	C9-C10-C11-C12
29	c	517	BCR	C9-C10-C11-C12
27	C	502	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	c	502	CLA	C16-C17-C18-C19
32	h	102	DGD	CCB-CDB-CEB-CFB
32	C	520	DGD	C3A-C4A-C5A-C6A
32	H	102	DGD	CCB-CDB-CEB-CFB
32	c	520	DGD	C3A-C4A-C5A-C6A
35	S	2630	LHG	C26-C27-C28-C29
35	s	2630	LHG	C26-C27-C28-C29
27	n	603	CLA	O1D-CGD-O2D-CED
32	C	519	DGD	CCA-CDA-CEA-CFA
32	c	519	DGD	CCA-CDA-CEA-CFA
27	B	612	CLA	C6-C7-C8-C10
27	B	613	CLA	C11-C10-C8-C7
27	C	509	CLA	C11-C10-C8-C7
27	b	613	CLA	C11-C10-C8-C7
27	c	509	CLA	C11-C10-C8-C7
37	G	601	CHL	C11-C10-C8-C7
37	N	607	CHL	C12-C13-C15-C16
37	Y	609	CHL	C11-C10-C8-C7
37	g	601	CHL	C11-C10-C8-C7
37	n	607	CHL	C12-C13-C15-C16
37	y	609	CHL	C11-C10-C8-C7
30	A	418	SQD	C23-C24-C25-C26
30	a	418	SQD	C23-C24-C25-C26
35	n	2630	LHG	C11-C10-C9-C8
35	N	2630	LHG	C11-C10-C9-C8
35	R	2630	LHG	C10-C11-C12-C13
35	r	2630	LHG	C10-C11-C12-C13
27	B	604	CLA	CBD-CGD-O2D-CED
27	B	616	CLA	CBD-CGD-O2D-CED
27	b	616	CLA	CBD-CGD-O2D-CED
35	D	409	LHG	C24-C23-O8-C6
37	N	609	CHL	CBA-CGA-O2A-C1
37	n	609	CHL	CBA-CGA-O2A-C1
35	d	410	LHG	C30-C31-C32-C33
31	Z	101	LMG	C8-C7-O1-C1
31	z	101	LMG	C8-C7-O1-C1
31	d	411	LMG	C19-C20-C21-C22
27	G	602	CLA	C2A-CAA-CBA-CGA
27	N	602	CLA	C2A-CAA-CBA-CGA
27	g	602	CLA	C2A-CAA-CBA-CGA
27	n	602	CLA	C2A-CAA-CBA-CGA
31	D	411	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
35	D	410	LHG	C30-C31-C32-C33
27	C	504	CLA	C16-C17-C18-C19
27	c	504	CLA	C16-C17-C18-C19
27	b	604	CLA	CBD-CGD-O2D-CED
27	N	603	CLA	O1D-CGD-O2D-CED
32	h	102	DGD	O2G-C1B-C2B-C3B
27	D	403	CLA	O1A-CGA-O2A-C1
27	a	406	CLA	O1A-CGA-O2A-C1
27	b	605	CLA	O1A-CGA-O2A-C1
27	d	403	CLA	O1A-CGA-O2A-C1
37	y	601	CHL	O1A-CGA-O2A-C1
37	G	601	CHL	C3-C5-C6-C7
37	g	601	CHL	C3-C5-C6-C7
35	d	409	LHG	C24-C23-O8-C6
27	b	607	CLA	C8-C10-C11-C12
27	A	406	CLA	O1A-CGA-O2A-C1
37	Y	601	CHL	O1A-CGA-O2A-C1
31	Z	101	LMG	C39-C40-C41-C42
32	C	518	DGD	CAB-CBB-CCB-CDB
32	c	518	DGD	CAB-CBB-CCB-CDB
27	B	607	CLA	C8-C10-C11-C12
31	z	101	LMG	C39-C40-C41-C42
27	A	406	CLA	C16-C17-C18-C19
27	C	510	CLA	C16-C17-C18-C19
27	a	406	CLA	C16-C17-C18-C19
27	c	510	CLA	C16-C17-C18-C19
27	B	605	CLA	O1A-CGA-O2A-C1
27	S	604	CLA	O1A-CGA-O2A-C1
27	s	604	CLA	O1A-CGA-O2A-C1
37	y	606	CHL	O1D-CGD-O2D-CED
32	H	102	DGD	O2G-C1B-C2B-C3B
35	D	408	LHG	O6-C4-C5-O7
35	G	2630	LHG	O6-C4-C5-O7
35	d	408	LHG	O6-C4-C5-O7
35	g	2630	LHG	O6-C4-C5-O7
27	N	612	CLA	O2A-C1-C2-C3
27	N	613	CLA	O2A-C1-C2-C3
27	S	602	CLA	O2A-C1-C2-C3
27	n	612	CLA	O2A-C1-C2-C3
27	n	613	CLA	O2A-C1-C2-C3
27	s	602	CLA	O2A-C1-C2-C3
37	Y	606	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	H	102	DGD	CBB-CCB-CDB-CEB
30	A	412	SQD	C44-C45-C46-O48
30	a	412	SQD	C44-C45-C46-O48
35	S	2630	LHG	C4-C5-C6-O8
35	s	2630	LHG	C4-C5-C6-O8
35	R	2630	LHG	C23-C24-C25-C26
35	r	2630	LHG	C23-C24-C25-C26
32	h	102	DGD	CBB-CCB-CDB-CEB
32	C	519	DGD	C6A-C7A-C8A-C9A
32	c	519	DGD	C6A-C7A-C8A-C9A
37	Y	605	CHL	C2A-CAA-CBA-CGA
37	y	605	CHL	C2A-CAA-CBA-CGA
35	y	2630	LHG	C33-C34-C35-C36
40	S	1623	NEX	C7-C8-C9-C19
40	s	1623	NEX	C7-C8-C9-C19
35	D	408	LHG	C12-C13-C14-C15
35	Y	2630	LHG	C33-C34-C35-C36
35	d	408	LHG	C12-C13-C14-C15
30	A	418	SQD	C32-C33-C34-C35
30	a	418	SQD	C32-C33-C34-C35
31	B	622	LMG	C17-C18-C19-C20
31	Z	101	LMG	O7-C8-C9-O8
31	z	101	LMG	O7-C8-C9-O8
37	G	601	CHL	C11-C10-C8-C9
37	N	607	CHL	C14-C13-C15-C16
37	g	601	CHL	C11-C10-C8-C9
37	n	607	CHL	C14-C13-C15-C16
27	A	406	CLA	C16-C17-C18-C20
27	a	406	CLA	C16-C17-C18-C20
31	b	622	LMG	C17-C18-C19-C20
32	C	518	DGD	C4B-C5B-C6B-C7B
32	c	518	DGD	C4B-C5B-C6B-C7B
31	D	411	LMG	C16-C17-C18-C19
31	d	411	LMG	C16-C17-C18-C19
27	B	602	CLA	C5-C6-C7-C8
27	b	602	CLA	C5-C6-C7-C8
37	G	601	CHL	C15-C16-C17-C18
37	g	601	CHL	C15-C16-C17-C18
37	n	607	CHL	C8-C10-C11-C12
35	N	2630	LHG	C30-C31-C32-C33
35	n	2630	LHG	C30-C31-C32-C33
27	C	507	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	c	507	CLA	C10-C11-C12-C13
32	C	518	DGD	C4D-C5D-C6D-O5D
32	c	518	DGD	C4D-C5D-C6D-O5D
37	Y	609	CHL	O1D-CGD-O2D-CED
31	A	413	LMG	C32-C33-C34-C35
37	R	608	CHL	CBA-CGA-O2A-C1
37	r	608	CHL	CBA-CGA-O2A-C1
37	N	607	CHL	C8-C10-C11-C12
31	a	413	LMG	C32-C33-C34-C35
37	y	609	CHL	O1D-CGD-O2D-CED
27	Y	613	CLA	C8-C10-C11-C12
27	y	613	CLA	C8-C10-C11-C12
27	b	603	CLA	C2A-CAA-CBA-CGA
32	c	518	DGD	C5B-C6B-C7B-C8B
35	D	409	LHG	C14-C15-C16-C17
35	d	409	LHG	C14-C15-C16-C17
27	B	602	CLA	C3-C5-C6-C7
27	b	602	CLA	C3-C5-C6-C7
37	G	605	CHL	C4C-C3C-CAC-CBC
37	N	601	CHL	C4C-C3C-CAC-CBC
37	N	609	CHL	C4C-C3C-CAC-CBC
37	S	606	CHL	C4C-C3C-CAC-CBC
37	g	605	CHL	C4C-C3C-CAC-CBC
37	n	601	CHL	C4C-C3C-CAC-CBC
37	n	609	CHL	C4C-C3C-CAC-CBC
37	s	606	CHL	C4C-C3C-CAC-CBC
31	z	101	LMG	C34-C35-C36-C37
32	C	518	DGD	C5B-C6B-C7B-C8B
31	Z	101	LMG	C34-C35-C36-C37
35	D	408	LHG	C25-C26-C27-C28
35	d	408	LHG	C25-C26-C27-C28
27	B	611	CLA	C4B-C3B-CAB-CBB
27	C	503	CLA	C1A-C2A-CAA-CBA
27	C	504	CLA	C4B-C3B-CAB-CBB
27	N	602	CLA	C1A-C2A-CAA-CBA
27	N	611	CLA	C4B-C3B-CAB-CBB
27	N	614	CLA	C4B-C3B-CAB-CBB
27	R	616	CLA	C4B-C3B-CAB-CBB
27	S	609	CLA	C4B-C3B-CAB-CBB
27	b	611	CLA	C4B-C3B-CAB-CBB
27	c	503	CLA	C1A-C2A-CAA-CBA
27	c	504	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	n	602	CLA	C1A-C2A-CAA-CBA
27	n	611	CLA	C4B-C3B-CAB-CBB
27	n	614	CLA	C4B-C3B-CAB-CBB
27	r	616	CLA	C4B-C3B-CAB-CBB
27	s	609	CLA	C4B-C3B-CAB-CBB
27	D	403	CLA	C4-C3-C5-C6
27	b	606	CLA	C4-C3-C5-C6
27	d	403	CLA	C4-C3-C5-C6
39	G	1622	XAT	C31-C32-C33-C34
39	g	1622	XAT	C31-C32-C33-C34
30	A	412	SQD	C17-C18-C19-C20
30	a	412	SQD	C17-C18-C19-C20
35	l	101	LHG	C11-C12-C13-C14
37	n	609	CHL	O1A-CGA-O2A-C1
27	B	603	CLA	C2A-CAA-CBA-CGA
27	Y	613	CLA	C2A-CAA-CBA-CGA
27	y	613	CLA	C2A-CAA-CBA-CGA
35	L	101	LHG	C11-C12-C13-C14
35	D	408	LHG	O6-C4-C5-C6
35	d	408	LHG	O6-C4-C5-C6
32	C	519	DGD	C8B-C9B-CAB-CBB
30	A	418	SQD	C5-C6-S-O9
30	B	621	SQD	C5-C6-S-O9
30	a	418	SQD	C5-C6-S-O9
30	b	621	SQD	C5-C6-S-O9
35	D	410	LHG	C29-C30-C31-C32
37	Y	609	CHL	C3-C5-C6-C7
27	B	613	CLA	C11-C12-C13-C15
27	C	507	CLA	C11-C12-C13-C15
27	C	512	CLA	C11-C12-C13-C15
27	Y	610	CLA	C11-C10-C8-C7
27	b	613	CLA	C11-C12-C13-C15
27	c	507	CLA	C11-C12-C13-C15
27	c	512	CLA	C11-C12-C13-C15
27	y	610	CLA	C11-C10-C8-C7
31	C	521	LMG	C12-C13-C14-C15
31	c	521	LMG	C12-C13-C14-C15
35	d	410	LHG	C29-C30-C31-C32
27	B	617	CLA	C16-C17-C18-C20
27	b	617	CLA	C16-C17-C18-C20
32	c	519	DGD	C8B-C9B-CAB-CBB
37	Y	601	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
37	y	601	CHL	O1D-CGD-O2D-CED
37	N	609	CHL	O1A-CGA-O2A-C1
35	D	410	LHG	C23-C24-C25-C26
35	d	410	LHG	C23-C24-C25-C26
37	Y	609	CHL	CBA-CGA-O2A-C1
37	y	609	CHL	CBA-CGA-O2A-C1
37	y	609	CHL	C3-C5-C6-C7
27	C	508	CLA	C5-C6-C7-C8
27	c	508	CLA	C5-C6-C7-C8
27	B	606	CLA	C4-C3-C5-C6
35	N	2630	LHG	O6-C4-C5-O7
35	S	2630	LHG	O6-C4-C5-O7
35	n	2630	LHG	O6-C4-C5-O7
35	s	2630	LHG	O6-C4-C5-O7
27	Y	603	CLA	C2A-CAA-CBA-CGA
27	y	603	CLA	C2A-CAA-CBA-CGA
27	B	612	CLA	C6-C7-C8-C9
27	B	613	CLA	C11-C10-C8-C9
27	B	614	CLA	C6-C7-C8-C9
27	b	612	CLA	C6-C7-C8-C9
27	b	613	CLA	C11-C10-C8-C9
27	b	614	CLA	C6-C7-C8-C9
37	r	608	CHL	O1A-CGA-O2A-C1
35	S	2630	LHG	C13-C14-C15-C16
27	A	407	CLA	C1-C2-C3-C4
27	C	513	CLA	C1-C2-C3-C4
27	G	603	CLA	C1-C2-C3-C4
27	G	604	CLA	C1-C2-C3-C4
27	G	611	CLA	C1-C2-C3-C4
27	G	612	CLA	C1-C2-C3-C4
27	G	613	CLA	C1-C2-C3-C4
27	G	614	CLA	C1-C2-C3-C4
27	N	603	CLA	C1-C2-C3-C4
27	N	604	CLA	C1-C2-C3-C4
27	N	611	CLA	C1-C2-C3-C4
27	N	612	CLA	C1-C2-C3-C4
27	N	613	CLA	C1-C2-C3-C4
27	N	614	CLA	C1-C2-C3-C4
27	R	601	CLA	C1-C2-C3-C4
27	R	603	CLA	C1-C2-C3-C4
27	R	604	CLA	C1-C2-C3-C4
27	R	609	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
27	R	611	CLA	C1-C2-C3-C4
27	R	612	CLA	C1-C2-C3-C4
27	R	613	CLA	C1-C2-C3-C4
27	R	616	CLA	C1-C2-C3-C4
27	S	602	CLA	C1-C2-C3-C4
27	S	603	CLA	C1-C2-C3-C4
27	S	604	CLA	C1-C2-C3-C4
27	S	609	CLA	C1-C2-C3-C4
27	S	610	CLA	C1-C2-C3-C4
27	S	611	CLA	C1-C2-C3-C4
27	S	612	CLA	C1-C2-C3-C4
27	S	613	CLA	C1-C2-C3-C4
27	S	614	CLA	C1-C2-C3-C4
27	Y	603	CLA	C1-C2-C3-C4
27	Y	604	CLA	C1-C2-C3-C4
27	Y	614	CLA	C1-C2-C3-C4
27	a	407	CLA	C1-C2-C3-C4
27	c	513	CLA	C1-C2-C3-C4
27	g	603	CLA	C1-C2-C3-C4
27	g	604	CLA	C1-C2-C3-C4
27	g	611	CLA	C1-C2-C3-C4
27	g	612	CLA	C1-C2-C3-C4
27	g	613	CLA	C1-C2-C3-C4
27	g	614	CLA	C1-C2-C3-C4
27	n	603	CLA	C1-C2-C3-C4
27	n	604	CLA	C1-C2-C3-C4
27	n	611	CLA	C1-C2-C3-C4
27	n	612	CLA	C1-C2-C3-C4
27	n	613	CLA	C1-C2-C3-C4
27	n	614	CLA	C1-C2-C3-C4
27	r	601	CLA	C1-C2-C3-C4
27	r	603	CLA	C1-C2-C3-C4
27	r	604	CLA	C1-C2-C3-C4
27	r	609	CLA	C1-C2-C3-C4
27	r	611	CLA	C1-C2-C3-C4
27	r	612	CLA	C1-C2-C3-C4
27	r	613	CLA	C1-C2-C3-C4
27	r	616	CLA	C1-C2-C3-C4
27	s	602	CLA	C1-C2-C3-C4
27	s	603	CLA	C1-C2-C3-C4
27	s	604	CLA	C1-C2-C3-C4
27	s	609	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
27	s	610	CLA	C1-C2-C3-C4
27	s	611	CLA	C1-C2-C3-C4
27	s	612	CLA	C1-C2-C3-C4
27	s	613	CLA	C1-C2-C3-C4
27	s	614	CLA	C1-C2-C3-C4
27	y	603	CLA	C1-C2-C3-C4
27	y	604	CLA	C1-C2-C3-C4
27	y	614	CLA	C1-C2-C3-C4
37	G	606	CHL	C1-C2-C3-C4
37	G	607	CHL	C1-C2-C3-C4
37	G	608	CHL	C1-C2-C3-C4
37	G	609	CHL	C1-C2-C3-C4
37	N	601	CHL	C1-C2-C3-C4
37	N	606	CHL	C1-C2-C3-C4
37	N	608	CHL	C1-C2-C3-C4
37	N	609	CHL	C1-C2-C3-C4
37	R	606	CHL	C1-C2-C3-C4
37	R	607	CHL	C1-C2-C3-C4
37	R	608	CHL	C1-C2-C3-C4
37	S	606	CHL	C1-C2-C3-C4
37	S	607	CHL	C1-C2-C3-C4
37	Y	606	CHL	C1-C2-C3-C4
37	Y	607	CHL	C1-C2-C3-C4
37	Y	608	CHL	C1-C2-C3-C4
37	g	606	CHL	C1-C2-C3-C4
37	g	607	CHL	C1-C2-C3-C4
37	g	608	CHL	C1-C2-C3-C4
37	g	609	CHL	C1-C2-C3-C4
37	n	601	CHL	C1-C2-C3-C4
37	n	606	CHL	C1-C2-C3-C4
37	n	608	CHL	C1-C2-C3-C4
37	n	609	CHL	C1-C2-C3-C4
37	r	606	CHL	C1-C2-C3-C4
37	r	607	CHL	C1-C2-C3-C4
37	r	608	CHL	C1-C2-C3-C4
37	s	606	CHL	C1-C2-C3-C4
37	s	607	CHL	C1-C2-C3-C4
37	y	606	CHL	C1-C2-C3-C4
37	y	607	CHL	C1-C2-C3-C4
37	y	608	CHL	C1-C2-C3-C4
40	S	1623	NEX	C7-C8-C9-C10
40	s	1623	NEX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
35	s	2630	LHG	C13-C14-C15-C16
31	z	101	LMG	C37-C38-C39-C40
27	b	616	CLA	O1D-CGD-O2D-CED
27	r	609	CLA	C2C-C3C-CAC-CBC
31	Z	101	LMG	C37-C38-C39-C40
37	R	608	CHL	O1A-CGA-O2A-C1
30	A	412	SQD	O47-C45-C46-O48
30	a	412	SQD	O47-C45-C46-O48
32	H	102	DGD	C2E-C1E-O5D-C6D
32	h	102	DGD	C2E-C1E-O5D-C6D
32	C	519	DGD	C1G-C2G-C3G-O3G
32	c	519	DGD	C1G-C2G-C3G-O3G
32	H	102	DGD	C8A-C9A-CAA-CBA
27	B	615	CLA	CAD-CBD-CGD-O2D
27	C	505	CLA	CAD-CBD-CGD-O2D
27	b	615	CLA	CAD-CBD-CGD-O2D
27	c	505	CLA	CAD-CBD-CGD-O2D
32	H	102	DGD	C3A-C4A-C5A-C6A
32	h	102	DGD	C3A-C4A-C5A-C6A
37	G	605	CHL	O1D-CGD-O2D-CED
37	N	609	CHL	O1D-CGD-O2D-CED
37	n	609	CHL	O1D-CGD-O2D-CED
27	R	609	CLA	C2C-C3C-CAC-CBC
32	h	102	DGD	C8A-C9A-CAA-CBA
37	g	605	CHL	O1D-CGD-O2D-CED
27	c	505	CLA	C3-C5-C6-C7
31	C	521	LMG	C29-C30-C31-C32
35	D	408	LHG	C32-C33-C34-C35
31	c	521	LMG	C29-C30-C31-C32
35	d	408	LHG	C32-C33-C34-C35
27	B	613	CLA	CAD-CBD-CGD-O1D
27	B	615	CLA	CAD-CBD-CGD-O1D
27	C	505	CLA	CAD-CBD-CGD-O1D
27	G	603	CLA	CHA-CBD-CGD-O1D
27	G	604	CLA	CHA-CBD-CGD-O1D
27	G	610	CLA	CHA-CBD-CGD-O1D
27	N	604	CLA	CHA-CBD-CGD-O1D
27	R	602	CLA	CHA-CBD-CGD-O1D
27	R	602	CLA	CHA-CBD-CGD-O2D
27	Y	603	CLA	CHA-CBD-CGD-O2D
27	Y	610	CLA	CHA-CBD-CGD-O1D
27	b	613	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	b	615	CLA	CAD-CBD-CGD-O1D
27	c	505	CLA	CAD-CBD-CGD-O1D
27	g	603	CLA	CHA-CBD-CGD-O1D
27	g	604	CLA	CHA-CBD-CGD-O1D
27	g	610	CLA	CHA-CBD-CGD-O1D
27	n	604	CLA	CHA-CBD-CGD-O1D
27	r	602	CLA	CHA-CBD-CGD-O1D
27	r	602	CLA	CHA-CBD-CGD-O2D
27	y	603	CLA	CHA-CBD-CGD-O2D
27	y	610	CLA	CHA-CBD-CGD-O1D
35	D	408	LHG	C3-O3-P-O5
35	D	410	LHG	C3-O3-P-O4
35	G	2630	LHG	C4-O6-P-O3
35	L	101	LHG	C3-O3-P-O5
35	L	101	LHG	C4-O6-P-O3
35	S	2630	LHG	C3-O3-P-O6
35	d	408	LHG	C3-O3-P-O5
35	d	410	LHG	C3-O3-P-O4
35	g	2630	LHG	C4-O6-P-O3
35	l	101	LHG	C3-O3-P-O5
35	l	101	LHG	C4-O6-P-O3
35	s	2630	LHG	C3-O3-P-O6
39	Y	1622	XAT	C13-C14-C15-C35
39	y	1622	XAT	C13-C14-C15-C35
27	B	616	CLA	C13-C15-C16-C17
27	B	616	CLA	O1D-CGD-O2D-CED
31	A	413	LMG	C12-C13-C14-C15
31	a	413	LMG	C12-C13-C14-C15
32	C	518	DGD	C5A-C6A-C7A-C8A
32	c	518	DGD	C5A-C6A-C7A-C8A
27	b	616	CLA	C13-C15-C16-C17
27	B	604	CLA	C2B-C3B-CAB-CBB
27	B	611	CLA	C2B-C3B-CAB-CBB
27	B	615	CLA	C2B-C3B-CAB-CBB
27	C	504	CLA	C2B-C3B-CAB-CBB
27	D	402	CLA	C2B-C3B-CAB-CBB
27	G	611	CLA	C2B-C3B-CAB-CBB
27	N	612	CLA	C2B-C3B-CAB-CBB
27	N	614	CLA	C2B-C3B-CAB-CBB
27	b	604	CLA	C2B-C3B-CAB-CBB
27	b	615	CLA	C2B-C3B-CAB-CBB
27	c	504	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	d	402	CLA	C2B-C3B-CAB-CBB
27	g	611	CLA	C2B-C3B-CAB-CBB
27	n	612	CLA	C2B-C3B-CAB-CBB
27	n	614	CLA	C2B-C3B-CAB-CBB
29	B	620	BCR	C1-C6-C7-C8
29	b	620	BCR	C1-C6-C7-C8
38	S	1621	LUT	C1-C6-C7-C8
38	s	1621	LUT	C1-C6-C7-C8
35	S	2630	LHG	C2-C3-O3-P
35	s	2630	LHG	C2-C3-O3-P
27	C	505	CLA	C3-C5-C6-C7
37	g	605	CHL	CBD-CGD-O2D-CED
30	a	412	SQD	C11-C12-C13-C14
31	c	521	LMG	C16-C17-C18-C19
30	A	412	SQD	C11-C12-C13-C14
31	C	521	LMG	C16-C17-C18-C19
27	B	612	CLA	O1A-CGA-O2A-C1
34	D	405	PL9	C4-C3-C7-C8
34	d	405	PL9	C4-C3-C7-C8
27	b	612	CLA	O1A-CGA-O2A-C1
27	C	507	CLA	C8-C10-C11-C12
27	c	507	CLA	C8-C10-C11-C12
30	B	621	SQD	C46-C45-O47-C7
30	b	621	SQD	C46-C45-O47-C7
27	N	610	CLA	C15-C16-C17-C18
27	n	610	CLA	C15-C16-C17-C18
34	D	405	PL9	C7-C8-C9-C10
34	d	405	PL9	C7-C8-C9-C10
32	H	102	DGD	CDB-CEB-CFB-CGB
35	R	2630	LHG	C34-C35-C36-C37
35	r	2630	LHG	C34-C35-C36-C37
29	D	404	BCR	C9-C10-C11-C12
29	d	404	BCR	C9-C10-C11-C12
39	r	622	XAT	C33-C34-C35-C15
27	C	507	CLA	C5-C6-C7-C8
27	c	507	CLA	C5-C6-C7-C8
32	h	102	DGD	CDB-CEB-CFB-CGB
35	S	2630	LHG	O6-C4-C5-C6
35	s	2630	LHG	O6-C4-C5-C6
31	B	622	LMG	C34-C35-C36-C37
31	b	622	LMG	C34-C35-C36-C37
37	Y	609	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	y	609	CHL	O1A-CGA-O2A-C1
27	B	616	CLA	C11-C10-C8-C9
27	B	617	CLA	C11-C10-C8-C9
27	C	509	CLA	C11-C12-C13-C14
27	C	512	CLA	C6-C7-C8-C9
27	R	602	CLA	C11-C12-C13-C14
27	b	616	CLA	C11-C10-C8-C9
27	b	617	CLA	C11-C10-C8-C9
27	c	509	CLA	C11-C12-C13-C14
27	c	512	CLA	C6-C7-C8-C9
27	r	602	CLA	C11-C12-C13-C14
27	A	410	CLA	C11-C10-C8-C7
27	B	609	CLA	C11-C10-C8-C7
27	C	505	CLA	C11-C10-C8-C7
27	Y	611	CLA	C11-C10-C8-C7
27	a	410	CLA	C11-C10-C8-C7
27	b	609	CLA	C11-C10-C8-C7
27	c	505	CLA	C11-C10-C8-C7
27	y	611	CLA	C11-C10-C8-C7
35	G	2630	LHG	C1-C2-C3-O3
35	g	2630	LHG	C1-C2-C3-O3
32	H	102	DGD	O6E-C1E-O5D-C6D
32	h	102	DGD	O6E-C1E-O5D-C6D
27	N	610	CLA	C5-C6-C7-C8
37	G	605	CHL	CBD-CGD-O2D-CED
27	n	610	CLA	C5-C6-C7-C8
27	R	602	CLA	C4-C3-C5-C6
27	r	602	CLA	C4-C3-C5-C6
30	A	418	SQD	C26-C27-C28-C29
30	a	418	SQD	C26-C27-C28-C29
37	N	605	CHL	CAA-CBA-CGA-O2A
37	n	605	CHL	CAA-CBA-CGA-O2A
27	B	612	CLA	CBA-CGA-O2A-C1
27	b	612	CLA	CBA-CGA-O2A-C1
27	B	604	CLA	C16-C17-C18-C19
27	G	610	CLA	C16-C17-C18-C20
35	N	2630	LHG	O9-C7-O7-C5
35	n	2630	LHG	O9-C7-O7-C5
35	N	2630	LHG	C33-C34-C35-C36
35	L	101	LHG	O7-C5-C6-O8
35	l	101	LHG	O7-C5-C6-O8
35	n	2630	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
39	R	622	XAT	C33-C34-C35-C15
27	b	604	CLA	C16-C17-C18-C19
27	g	610	CLA	C16-C17-C18-C20
37	Y	601	CHL	CBD-CGD-O2D-CED
27	Y	613	CLA	CBA-CGA-O2A-C1
27	y	613	CLA	CBA-CGA-O2A-C1
35	d	410	LHG	C28-C29-C30-C31
27	S	604	CLA	C2-C1-O2A-CGA
27	s	604	CLA	C2-C1-O2A-CGA
27	A	410	CLA	C4-C3-C5-C6
27	a	410	CLA	C4-C3-C5-C6
27	R	616	CLA	O2A-C1-C2-C3
27	r	616	CLA	O2A-C1-C2-C3
37	R	608	CHL	O2A-C1-C2-C3
37	r	608	CHL	O2A-C1-C2-C3
35	D	410	LHG	C28-C29-C30-C31
30	B	621	SQD	C23-C24-C25-C26
31	D	411	LMG	C10-C11-C12-C13
31	d	411	LMG	C10-C11-C12-C13
37	y	601	CHL	CBD-CGD-O2D-CED
30	b	621	SQD	C23-C24-C25-C26
30	A	412	SQD	C9-C10-C11-C12
30	a	412	SQD	C9-C10-C11-C12
37	G	605	CHL	C2A-CAA-CBA-CGA
37	g	605	CHL	C2A-CAA-CBA-CGA
38	N	1621	LUT	C29-C30-C31-C32
38	n	1621	LUT	C29-C30-C31-C32
32	C	518	DGD	C3A-C4A-C5A-C6A
32	c	518	DGD	C3A-C4A-C5A-C6A
27	A	406	CLA	C13-C15-C16-C17
27	C	512	CLA	C16-C17-C18-C20
27	c	512	CLA	C16-C17-C18-C20
27	B	613	CLA	C14-C13-C15-C16
27	C	504	CLA	C14-C13-C15-C16
27	Y	610	CLA	C11-C10-C8-C9
27	b	613	CLA	C14-C13-C15-C16
27	c	504	CLA	C14-C13-C15-C16
27	r	610	CLA	C11-C12-C13-C14
27	y	610	CLA	C11-C10-C8-C9
27	b	604	CLA	O1D-CGD-O2D-CED
27	C	503	CLA	CBA-CGA-O2A-C1
27	c	503	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	a	408	PHO	C2C-C3C-CAC-CBC
28	A	408	PHO	C2C-C3C-CAC-CBC
27	B	603	CLA	C4B-C3B-CAB-CBB
27	G	611	CLA	C4B-C3B-CAB-CBB
27	N	602	CLA	C4B-C3B-CAB-CBB
27	R	611	CLA	C4B-C3B-CAB-CBB
27	Y	612	CLA	C4B-C3B-CAB-CBB
27	b	603	CLA	C4B-C3B-CAB-CBB
27	b	606	CLA	C4B-C3B-CAB-CBB
27	g	611	CLA	C4B-C3B-CAB-CBB
27	n	602	CLA	C4B-C3B-CAB-CBB
27	n	603	CLA	C4B-C3B-CAB-CBB
27	r	611	CLA	C4B-C3B-CAB-CBB
27	y	612	CLA	C4B-C3B-CAB-CBB
27	B	604	CLA	C5-C6-C7-C8
31	C	521	LMG	C29-C28-O8-C9
31	c	521	LMG	C29-C28-O8-C9
27	R	610	CLA	C5-C6-C7-C8
27	a	406	CLA	C13-C15-C16-C17
27	b	604	CLA	C5-C6-C7-C8
27	r	610	CLA	C5-C6-C7-C8
27	B	604	CLA	O1D-CGD-O2D-CED
27	A	410	CLA	C2-C3-C5-C6
27	a	410	CLA	C2-C3-C5-C6
27	N	603	CLA	O2A-C1-C2-C3
27	n	603	CLA	O2A-C1-C2-C3
32	C	518	DGD	O6D-C5D-C6D-O5D
32	c	518	DGD	O6D-C5D-C6D-O5D
30	A	418	SQD	C33-C34-C35-C36
30	a	418	SQD	C33-C34-C35-C36
31	z	101	LMG	C16-C17-C18-C19
31	Z	101	LMG	C16-C17-C18-C19
37	G	601	CHL	C10-C11-C12-C13
37	g	601	CHL	C10-C11-C12-C13
35	L	101	LHG	C33-C34-C35-C36
27	C	502	CLA	C11-C10-C8-C7
27	C	503	CLA	C12-C13-C15-C16
27	c	502	CLA	C11-C10-C8-C7
27	c	503	CLA	C12-C13-C15-C16
27	Y	613	CLA	C13-C15-C16-C17
27	y	613	CLA	C13-C15-C16-C17
35	l	101	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
27	b	613	CLA	C15-C16-C17-C18
31	B	622	LMG	C18-C19-C20-C21
27	y	613	CLA	O1A-CGA-O2A-C1
31	b	622	LMG	C18-C19-C20-C21
27	Y	614	CLA	CBA-CGA-O2A-C1
27	y	614	CLA	CBA-CGA-O2A-C1
37	G	609	CHL	CBA-CGA-O2A-C1
37	g	609	CHL	CBA-CGA-O2A-C1
27	B	613	CLA	C15-C16-C17-C18
27	Y	610	CLA	O1A-CGA-O2A-C1
27	Y	613	CLA	O1A-CGA-O2A-C1
27	y	610	CLA	O1A-CGA-O2A-C1
30	a	418	SQD	O6-C44-C45-O47
37	S	606	CHL	C3A-C2A-CAA-CBA
37	s	606	CHL	C3A-C2A-CAA-CBA
27	b	617	CLA	C13-C15-C16-C17
32	C	518	DGD	C6A-C7A-C8A-C9A
32	c	518	DGD	C6A-C7A-C8A-C9A
27	B	617	CLA	C13-C15-C16-C17
40	G	1623	NEX	C39-C29-C30-C31
40	N	1623	NEX	C39-C29-C30-C31
40	R	623	NEX	C39-C29-C30-C31
40	S	1623	NEX	C39-C29-C30-C31
40	Y	1623	NEX	C39-C29-C30-C31
40	g	1623	NEX	C39-C29-C30-C31
40	n	1623	NEX	C39-C29-C30-C31
40	r	623	NEX	C39-C29-C30-C31
40	s	1623	NEX	C39-C29-C30-C31
40	y	1623	NEX	C39-C29-C30-C31
27	B	602	CLA	C15-C16-C17-C18
27	b	602	CLA	C15-C16-C17-C18
30	A	412	SQD	C35-C36-C37-C38
27	R	609	CLA	C4C-C3C-CAC-CBC
27	r	609	CLA	C4C-C3C-CAC-CBC
35	N	2630	LHG	C5-C4-O6-P
35	n	2630	LHG	C5-C4-O6-P
30	a	412	SQD	C35-C36-C37-C38
29	B	620	BCR	C21-C22-C23-C24
29	b	620	BCR	C21-C22-C23-C24
31	c	521	LMG	C30-C31-C32-C33
32	C	519	DGD	O6D-C5D-C6D-O5D
32	c	519	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
31	C	521	LMG	C30-C31-C32-C33
34	D	405	PL9	C34-C36-C37-C38
34	d	405	PL9	C34-C36-C37-C38
35	L	101	LHG	C4-C5-C6-O8
35	l	101	LHG	C4-C5-C6-O8
27	B	611	CLA	C15-C16-C17-C18
27	r	602	CLA	C15-C16-C17-C18
27	B	603	CLA	C14-C13-C15-C16
27	B	613	CLA	C11-C12-C13-C14
27	C	503	CLA	C14-C13-C15-C16
27	C	501	CLA	C14-C13-C15-C16
27	C	504	CLA	C11-C12-C13-C14
27	R	610	CLA	C11-C12-C13-C14
27	b	603	CLA	C14-C13-C15-C16
27	b	613	CLA	C11-C12-C13-C14
27	c	503	CLA	C14-C13-C15-C16
27	c	501	CLA	C14-C13-C15-C16
27	c	504	CLA	C11-C12-C13-C14
32	C	519	DGD	C1G-C2G-O2G-C1B
32	c	519	DGD	C1G-C2G-O2G-C1B
27	b	611	CLA	C15-C16-C17-C18
37	R	607	CHL	C1A-C2A-CAA-CBA
37	r	607	CHL	C1A-C2A-CAA-CBA
27	R	602	CLA	C15-C16-C17-C18
37	Y	609	CHL	C4-C3-C5-C6
37	y	609	CHL	C4-C3-C5-C6
31	D	411	LMG	C12-C13-C14-C15
31	d	411	LMG	C12-C13-C14-C15
35	G	2630	LHG	C11-C10-C9-C8
27	C	503	CLA	O1A-CGA-O2A-C1
27	B	604	CLA	C1A-C2A-CAA-CBA
27	B	612	CLA	C1A-C2A-CAA-CBA
27	C	511	CLA	C1A-C2A-CAA-CBA
27	D	402	CLA	C1A-C2A-CAA-CBA
27	S	603	CLA	C1A-C2A-CAA-CBA
27	Y	610	CLA	C1A-C2A-CAA-CBA
27	b	604	CLA	C1A-C2A-CAA-CBA
27	b	612	CLA	C1A-C2A-CAA-CBA
27	c	511	CLA	C1A-C2A-CAA-CBA
27	d	402	CLA	C1A-C2A-CAA-CBA
27	s	603	CLA	C1A-C2A-CAA-CBA
27	y	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
40	G	1623	NEX	C28-C29-C30-C31
40	N	1623	NEX	C28-C29-C30-C31
40	R	623	NEX	C28-C29-C30-C31
40	S	1623	NEX	C28-C29-C30-C31
40	Y	1623	NEX	C28-C29-C30-C31
40	g	1623	NEX	C28-C29-C30-C31
40	n	1623	NEX	C28-C29-C30-C31
40	r	623	NEX	C28-C29-C30-C31
40	s	1623	NEX	C28-C29-C30-C31
40	y	1623	NEX	C28-C29-C30-C31
35	g	2630	LHG	C11-C10-C9-C8
27	B	603	CLA	C2B-C3B-CAB-CBB
27	C	503	CLA	C2B-C3B-CAB-CBB
27	G	604	CLA	C2B-C3B-CAB-CBB
27	N	611	CLA	C2B-C3B-CAB-CBB
27	R	616	CLA	C2B-C3B-CAB-CBB
27	S	609	CLA	C2B-C3B-CAB-CBB
27	Y	614	CLA	C2B-C3B-CAB-CBB
27	b	603	CLA	C2B-C3B-CAB-CBB
27	c	503	CLA	C2B-C3B-CAB-CBB
27	g	604	CLA	C2B-C3B-CAB-CBB
27	n	611	CLA	C2B-C3B-CAB-CBB
27	r	616	CLA	C2B-C3B-CAB-CBB
27	s	609	CLA	C2B-C3B-CAB-CBB
27	y	614	CLA	C2B-C3B-CAB-CBB
29	H	101	BCR	C23-C24-C25-C30
29	h	101	BCR	C23-C24-C25-C30
38	G	1620	LUT	C1-C6-C7-C8
38	R	620	LUT	C1-C6-C7-C8
38	S	1620	LUT	C1-C6-C7-C8
38	g	1620	LUT	C1-C6-C7-C8
38	r	620	LUT	C1-C6-C7-C8
38	s	1620	LUT	C1-C6-C7-C8
30	b	621	SQD	C12-C13-C14-C15
27	Y	610	CLA	CBA-CGA-O2A-C1
27	y	610	CLA	CBA-CGA-O2A-C1
30	B	621	SQD	C12-C13-C14-C15
31	B	622	LMG	C36-C37-C38-C39
31	b	622	LMG	C36-C37-C38-C39
27	Y	614	CLA	O1A-CGA-O2A-C1
27	c	503	CLA	O1A-CGA-O2A-C1
27	G	612	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
27	R	609	CLA	O2A-C1-C2-C3
27	R	612	CLA	O2A-C1-C2-C3
27	g	612	CLA	O2A-C1-C2-C3
27	r	609	CLA	O2A-C1-C2-C3
27	r	612	CLA	O2A-C1-C2-C3
37	G	606	CHL	O2A-C1-C2-C3
37	G	609	CHL	O2A-C1-C2-C3
37	N	606	CHL	O2A-C1-C2-C3
37	N	608	CHL	O2A-C1-C2-C3
37	N	609	CHL	O2A-C1-C2-C3
37	S	607	CHL	O2A-C1-C2-C3
37	Y	608	CHL	O2A-C1-C2-C3
37	g	606	CHL	O2A-C1-C2-C3
37	g	608	CHL	O2A-C1-C2-C3
37	g	609	CHL	O2A-C1-C2-C3
37	n	606	CHL	O2A-C1-C2-C3
37	n	608	CHL	O2A-C1-C2-C3
37	n	609	CHL	O2A-C1-C2-C3
37	y	608	CHL	O2A-C1-C2-C3
27	B	603	CLA	C6-C7-C8-C10
27	B	606	CLA	C12-C13-C15-C16
27	B	614	CLA	C11-C10-C8-C7
27	B	615	CLA	C11-C10-C8-C7
27	b	603	CLA	C6-C7-C8-C10
27	b	606	CLA	C12-C13-C15-C16
27	b	614	CLA	C11-C10-C8-C7
27	b	615	CLA	C11-C10-C8-C7
27	B	605	CLA	C16-C17-C18-C19
27	b	605	CLA	C16-C17-C18-C19
30	A	418	SQD	O6-C44-C45-O47
37	g	609	CHL	O1A-CGA-O2A-C1
35	g	2630	LHG	C14-C15-C16-C17
35	G	2630	LHG	C14-C15-C16-C17
35	r	2630	LHG	C26-C27-C28-C29
35	R	2630	LHG	C26-C27-C28-C29
27	Y	612	CLA	C4-C3-C5-C6
27	y	612	CLA	C4-C3-C5-C6
27	y	614	CLA	O1A-CGA-O2A-C1
37	G	609	CHL	O1A-CGA-O2A-C1
37	S	606	CHL	C2-C1-O2A-CGA
37	s	606	CHL	C2-C1-O2A-CGA
39	Y	1622	XAT	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
39	y	1622	XAT	C31-C32-C33-C34
27	A	406	CLA	C2C-C3C-CAC-CBC
31	Z	101	LMG	C32-C33-C34-C35
27	C	506	CLA	C11-C12-C13-C14
27	c	506	CLA	C11-C12-C13-C14
37	N	607	CHL	C11-C12-C13-C14
37	n	607	CHL	C11-C12-C13-C14
31	z	101	LMG	C32-C33-C34-C35
27	B	617	CLA	C15-C16-C17-C18
27	b	617	CLA	C15-C16-C17-C18
27	A	410	CLA	C8-C10-C11-C12
27	C	506	CLA	C2-C3-C5-C6
27	c	506	CLA	C2-C3-C5-C6
34	D	405	PL9	C43-C44-C46-C47
34	d	405	PL9	C43-C44-C46-C47
32	h	102	DGD	C9B-CAB-CBB-CCB
27	a	410	CLA	C8-C10-C11-C12
27	G	610	CLA	C16-C17-C18-C19
27	g	610	CLA	C16-C17-C18-C19
35	l	101	LHG	O9-C7-O7-C5
32	H	102	DGD	C9B-CAB-CBB-CCB
27	S	609	CLA	O2A-C1-C2-C3
27	s	609	CLA	O2A-C1-C2-C3
37	G	608	CHL	O2A-C1-C2-C3
37	Y	607	CHL	O2A-C1-C2-C3
37	s	607	CHL	O2A-C1-C2-C3
37	y	607	CHL	O2A-C1-C2-C3
27	C	510	CLA	C8-C10-C11-C12
30	A	418	SQD	C44-C45-C46-O48
30	a	418	SQD	C44-C45-C46-O48
27	c	510	CLA	C8-C10-C11-C12
27	a	406	CLA	C2C-C3C-CAC-CBC
27	b	611	CLA	C13-C15-C16-C17
35	L	101	LHG	O9-C7-O7-C5
27	B	611	CLA	C13-C15-C16-C17
30	B	621	SQD	C13-C14-C15-C16
30	b	621	SQD	C13-C14-C15-C16
30	A	418	SQD	O47-C7-C8-C9
30	a	418	SQD	O47-C7-C8-C9
27	c	507	CLA	C16-C17-C18-C20
27	B	605	CLA	C10-C11-C12-C13
27	b	605	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	B	606	CLA	C4B-C3B-CAB-CBB
27	N	603	CLA	C4B-C3B-CAB-CBB
27	r	602	CLA	C4B-C3B-CAB-CBB
27	C	507	CLA	C16-C17-C18-C20
35	D	410	LHG	C1-C2-C3-O3
35	L	101	LHG	C1-C2-C3-O3
35	d	410	LHG	C1-C2-C3-O3
35	l	101	LHG	C1-C2-C3-O3
37	N	601	CHL	CHA-CBD-CGD-O1D
37	N	601	CHL	CHA-CBD-CGD-O2D
37	N	606	CHL	CHA-CBD-CGD-O1D
37	N	606	CHL	CHA-CBD-CGD-O2D
37	S	608	CHL	CHA-CBD-CGD-O1D
37	S	608	CHL	CHA-CBD-CGD-O2D
37	n	601	CHL	CHA-CBD-CGD-O1D
37	n	601	CHL	CHA-CBD-CGD-O2D
37	n	606	CHL	CHA-CBD-CGD-O1D
37	n	606	CHL	CHA-CBD-CGD-O2D
37	s	608	CHL	CHA-CBD-CGD-O1D
37	s	608	CHL	CHA-CBD-CGD-O2D
35	D	409	LHG	C12-C13-C14-C15
35	d	409	LHG	C12-C13-C14-C15
32	C	519	DGD	O2G-C2G-C3G-O3G
32	c	519	DGD	O2G-C2G-C3G-O3G
37	R	607	CHL	CAA-CBA-CGA-O2A
27	S	611	CLA	O2A-C1-C2-C3
27	S	614	CLA	O2A-C1-C2-C3
27	Y	614	CLA	O2A-C1-C2-C3
27	s	614	CLA	O2A-C1-C2-C3
27	y	614	CLA	O2A-C1-C2-C3
37	G	607	CHL	O2A-C1-C2-C3
37	R	606	CHL	O2A-C1-C2-C3
37	g	607	CHL	O2A-C1-C2-C3
37	r	606	CHL	O2A-C1-C2-C3
37	r	607	CHL	CAA-CBA-CGA-O2A
27	B	617	CLA	C6-C7-C8-C9
27	C	501	CLA	C11-C10-C8-C9
27	C	512	CLA	C11-C12-C13-C14
27	b	617	CLA	C6-C7-C8-C9
27	c	501	CLA	C11-C10-C8-C9
27	c	512	CLA	C11-C12-C13-C14
27	S	604	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	s	604	CLA	CAA-CBA-CGA-O2A
27	B	613	CLA	C8-C10-C11-C12
27	b	613	CLA	C8-C10-C11-C12
27	R	602	CLA	C2A-CAA-CBA-CGA
27	r	602	CLA	C2A-CAA-CBA-CGA
37	R	606	CHL	C2A-CAA-CBA-CGA
37	r	606	CHL	C2A-CAA-CBA-CGA
27	G	602	CLA	C2-C1-O2A-CGA
27	g	602	CLA	C2-C1-O2A-CGA
37	Y	609	CHL	C2-C1-O2A-CGA
37	y	609	CHL	C2-C1-O2A-CGA
27	B	609	CLA	C3A-C2A-CAA-CBA
27	C	504	CLA	C3A-C2A-CAA-CBA
27	S	603	CLA	C3A-C2A-CAA-CBA
27	b	609	CLA	C3A-C2A-CAA-CBA
27	c	504	CLA	C3A-C2A-CAA-CBA
27	s	603	CLA	C3A-C2A-CAA-CBA
37	N	608	CHL	C3A-C2A-CAA-CBA
37	n	608	CHL	C3A-C2A-CAA-CBA
27	d	403	CLA	C2-C3-C5-C6
32	h	102	DGD	C1B-C2B-C3B-C4B
32	H	102	DGD	C1B-C2B-C3B-C4B
37	R	608	CHL	C3C-C2C-CMC-OMC
37	r	608	CHL	C3C-C2C-CMC-OMC
27	B	606	CLA	C2-C3-C5-C6
27	D	403	CLA	C2-C3-C5-C6
27	b	606	CLA	C2-C3-C5-C6
27	B	606	CLA	CBA-CGA-O2A-C1
27	b	606	CLA	CBA-CGA-O2A-C1
27	C	505	CLA	C5-C6-C7-C8
27	c	505	CLA	C5-C6-C7-C8
39	G	1622	XAT	O4-C6-C7-C8
39	R	622	XAT	O24-C26-C27-C28
39	g	1622	XAT	O4-C6-C7-C8
39	r	622	XAT	O24-C26-C27-C28
40	N	1623	NEX	O24-C26-C27-C28
40	R	623	NEX	O24-C26-C27-C28
40	Y	1623	NEX	O24-C26-C27-C28
40	n	1623	NEX	O24-C26-C27-C28
40	r	623	NEX	O24-C26-C27-C28
40	y	1623	NEX	O24-C26-C27-C28
27	G	603	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
27	G	614	CLA	O2A-C1-C2-C3
27	N	604	CLA	O2A-C1-C2-C3
27	N	614	CLA	O2A-C1-C2-C3
27	g	614	CLA	O2A-C1-C2-C3
27	n	604	CLA	O2A-C1-C2-C3
27	n	614	CLA	O2A-C1-C2-C3
27	s	611	CLA	O2A-C1-C2-C3
31	D	411	LMG	C29-C28-O8-C9
31	d	411	LMG	C29-C28-O8-C9
32	H	102	DGD	O1B-C1B-C2B-C3B
27	R	602	CLA	C2-C3-C5-C6
27	r	602	CLA	C2-C3-C5-C6
40	G	1623	NEX	C7-C8-C9-C19
40	g	1623	NEX	C7-C8-C9-C19
27	a	410	CLA	C11-C12-C13-C15
32	h	102	DGD	O1B-C1B-C2B-C3B
27	r	602	CLA	C13-C15-C16-C17
27	R	610	CLA	CAA-CBA-CGA-O2A
27	r	610	CLA	CAA-CBA-CGA-O2A
35	g	2630	LHG	O8-C23-C24-C25
35	N	2630	LHG	O7-C5-C6-O8
35	n	2630	LHG	O7-C5-C6-O8
27	R	602	CLA	C13-C15-C16-C17
27	Y	611	CLA	C6-C7-C8-C9
27	y	611	CLA	C6-C7-C8-C9
27	A	410	CLA	C11-C12-C13-C15
28	A	409	PHO	CAA-CBA-CGA-O2A
28	a	409	PHO	CAA-CBA-CGA-O2A
35	G	2630	LHG	O8-C23-C24-C25
35	S	2630	LHG	O8-C23-C24-C25
35	s	2630	LHG	O8-C23-C24-C25
27	G	610	CLA	CAA-CBA-CGA-O2A
27	N	613	CLA	C2A-CAA-CBA-CGA
27	n	613	CLA	C2A-CAA-CBA-CGA
27	A	405	CLA	C11-C12-C13-C15
27	B	602	CLA	C12-C13-C15-C16
27	B	607	CLA	C6-C7-C8-C10
27	B	610	CLA	C11-C12-C13-C15
27	B	617	CLA	C6-C7-C8-C10
27	C	506	CLA	C11-C12-C13-C15
27	a	405	CLA	C11-C12-C13-C15
27	b	602	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
27	b	607	CLA	C6-C7-C8-C10
27	b	610	CLA	C11-C12-C13-C15
27	b	617	CLA	C6-C7-C8-C10
27	c	506	CLA	C11-C12-C13-C15
37	Y	609	CHL	C12-C13-C15-C16
37	y	609	CHL	C12-C13-C15-C16
35	S	2630	LHG	C33-C34-C35-C36
27	N	602	CLA	C2B-C3B-CAB-CBB
27	S	614	CLA	C2B-C3B-CAB-CBB
27	Y	602	CLA	C2B-C3B-CAB-CBB
27	Y	612	CLA	C2B-C3B-CAB-CBB
27	n	602	CLA	C2B-C3B-CAB-CBB
27	s	614	CLA	C2B-C3B-CAB-CBB
27	y	602	CLA	C2B-C3B-CAB-CBB
27	y	612	CLA	C2B-C3B-CAB-CBB
29	D	404	BCR	C23-C24-C25-C26
29	D	404	BCR	C23-C24-C25-C30
29	H	101	BCR	C23-C24-C25-C26
29	d	404	BCR	C23-C24-C25-C26
29	d	404	BCR	C23-C24-C25-C30
29	h	101	BCR	C23-C24-C25-C26
38	G	1620	LUT	C5-C6-C7-C8
38	N	1621	LUT	C5-C6-C7-C8
38	R	620	LUT	C5-C6-C7-C8
38	S	1620	LUT	C5-C6-C7-C8
38	S	1621	LUT	C5-C6-C7-C8
38	g	1620	LUT	C5-C6-C7-C8
38	n	1621	LUT	C5-C6-C7-C8
38	r	620	LUT	C5-C6-C7-C8
38	s	1620	LUT	C5-C6-C7-C8
38	s	1621	LUT	C5-C6-C7-C8
35	s	2630	LHG	C33-C34-C35-C36
27	R	601	CLA	CAA-CBA-CGA-O2A
27	r	601	CLA	CAA-CBA-CGA-O2A
30	B	621	SQD	C10-C11-C12-C13
30	b	621	SQD	C10-C11-C12-C13
35	s	2630	LHG	C16-C17-C18-C19
27	B	611	CLA	C2-C1-O2A-CGA
27	C	502	CLA	C2-C1-O2A-CGA
27	C	511	CLA	C2-C1-O2A-CGA
27	b	611	CLA	C2-C1-O2A-CGA
27	c	502	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
27	c	511	CLA	C2-C1-O2A-CGA
37	N	607	CHL	C2-C1-O2A-CGA
37	N	609	CHL	C2-C1-O2A-CGA
37	n	607	CHL	C2-C1-O2A-CGA
37	n	609	CHL	C2-C1-O2A-CGA
35	S	2630	LHG	C16-C17-C18-C19
27	G	604	CLA	O2A-C1-C2-C3
27	S	610	CLA	O2A-C1-C2-C3
27	g	603	CLA	O2A-C1-C2-C3
27	g	604	CLA	O2A-C1-C2-C3
27	s	610	CLA	O2A-C1-C2-C3
27	N	603	CLA	CAA-CBA-CGA-O2A
27	g	610	CLA	CAA-CBA-CGA-O2A
27	n	603	CLA	CAA-CBA-CGA-O2A
31	D	411	LMG	O9-C10-O7-C8
31	d	411	LMG	O9-C10-O7-C8
32	C	519	DGD	O1B-C1B-O2G-C2G
32	c	519	DGD	O1B-C1B-O2G-C2G
35	l	101	LHG	O2-C2-C3-O3
27	R	611	CLA	C2A-CAA-CBA-CGA
27	r	611	CLA	C2A-CAA-CBA-CGA
27	B	606	CLA	O1A-CGA-O2A-C1
27	b	606	CLA	O1A-CGA-O2A-C1
27	B	617	CLA	CAA-CBA-CGA-O2A
27	b	617	CLA	CAA-CBA-CGA-O2A
27	g	603	CLA	CAA-CBA-CGA-O2A
32	c	520	DGD	O2G-C1B-C2B-C3B
37	S	601	CHL	CAA-CBA-CGA-O2A
37	s	601	CHL	CAA-CBA-CGA-O2A
32	C	518	DGD	CDB-CEB-CFB-CGB
32	c	518	DGD	CDB-CEB-CFB-CGB
27	C	501	CLA	CAA-CBA-CGA-O2A
27	N	612	CLA	CAA-CBA-CGA-O2A
27	c	501	CLA	CAA-CBA-CGA-O2A
27	n	612	CLA	CAA-CBA-CGA-O2A
32	C	520	DGD	O2G-C1B-C2B-C3B
27	N	602	CLA	CAA-CBA-CGA-O2A
27	n	602	CLA	CAA-CBA-CGA-O2A
27	a	405	CLA	C8-C10-C11-C12
28	a	408	PHO	O1D-CGD-O2D-CED
27	C	507	CLA	C11-C10-C8-C9
27	c	507	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
32	C	519	DGD	C8A-C9A-CAA-CBA
32	c	519	DGD	C8A-C9A-CAA-CBA
27	G	603	CLA	CAA-CBA-CGA-O2A
27	S	603	CLA	CAA-CBA-CGA-O2A
35	L	101	LHG	O2-C2-C3-O3
30	A	418	SQD	O6-C44-C45-C46
30	a	418	SQD	O6-C44-C45-C46
32	C	519	DGD	O1G-C1G-C2G-C3G
32	c	519	DGD	O1G-C1G-C2G-C3G
28	A	408	PHO	O1D-CGD-O2D-CED
27	A	405	CLA	C8-C10-C11-C12
27	B	607	CLA	C1A-C2A-CAA-CBA
27	N	612	CLA	C1A-C2A-CAA-CBA
27	R	602	CLA	C4B-C3B-CAB-CBB
27	S	602	CLA	C1A-C2A-CAA-CBA
27	S	614	CLA	C4B-C3B-CAB-CBB
27	n	612	CLA	C1A-C2A-CAA-CBA
27	s	602	CLA	C1A-C2A-CAA-CBA
27	s	614	CLA	C4B-C3B-CAB-CBB
27	C	506	CLA	C10-C11-C12-C13
27	c	506	CLA	C10-C11-C12-C13
35	l	101	LHG	C35-C36-C37-C38
27	B	609	CLA	CAA-CBA-CGA-O2A
27	G	602	CLA	CAA-CBA-CGA-O2A
27	b	609	CLA	CAA-CBA-CGA-O2A
27	g	602	CLA	CAA-CBA-CGA-O2A
31	C	521	LMG	O7-C10-C11-C12
31	c	521	LMG	O7-C10-C11-C12
31	C	521	LMG	O7-C8-C9-O8
31	c	521	LMG	O7-C8-C9-O8
38	S	1621	LUT	C29-C30-C31-C32
38	s	1621	LUT	C29-C30-C31-C32
35	L	101	LHG	C35-C36-C37-C38
27	b	602	CLA	O1A-CGA-O2A-C1
27	Y	602	CLA	CAA-CBA-CGA-O2A
27	s	603	CLA	CAA-CBA-CGA-O2A
27	y	602	CLA	CAA-CBA-CGA-O2A
31	C	521	LMG	O8-C28-C29-C30
31	c	521	LMG	O8-C28-C29-C30
35	R	2630	LHG	C11-C12-C13-C14
35	r	2630	LHG	C11-C12-C13-C14
37	N	607	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
37	n	607	CHL	C2A-CAA-CBA-CGA
27	B	602	CLA	O1A-CGA-O2A-C1
27	G	610	CLA	O1A-CGA-O2A-C1
27	g	610	CLA	O1A-CGA-O2A-C1
35	D	408	LHG	C11-C10-C9-C8
30	a	418	SQD	O48-C23-C24-C25
35	d	408	LHG	C11-C10-C9-C8
27	R	610	CLA	C2-C1-O2A-CGA
27	R	616	CLA	C2-C1-O2A-CGA
27	r	610	CLA	C2-C1-O2A-CGA
27	r	616	CLA	C2-C1-O2A-CGA
37	R	607	CHL	C2-C1-O2A-CGA
37	Y	606	CHL	C2-C1-O2A-CGA
37	Y	607	CHL	C2-C1-O2A-CGA
37	r	607	CHL	C2-C1-O2A-CGA
37	s	601	CHL	C2-C1-O2A-CGA
37	y	606	CHL	C2-C1-O2A-CGA
37	y	607	CHL	C2-C1-O2A-CGA
27	R	616	CLA	CAA-CBA-CGA-O2A
27	r	616	CLA	CAA-CBA-CGA-O2A
30	A	418	SQD	O48-C23-C24-C25
27	B	605	CLA	C6-C7-C8-C10
27	B	611	CLA	C11-C12-C13-C15
27	C	501	CLA	C11-C10-C8-C7
27	C	506	CLA	C11-C10-C8-C7
27	C	510	CLA	C11-C10-C8-C7
27	b	605	CLA	C6-C7-C8-C10
27	b	611	CLA	C11-C12-C13-C15
27	c	501	CLA	C11-C10-C8-C7
27	c	506	CLA	C11-C10-C8-C7
27	c	510	CLA	C11-C10-C8-C7
28	A	409	PHO	C11-C12-C13-C15
28	a	409	PHO	C11-C12-C13-C15
37	Y	601	CHL	C11-C10-C8-C7
37	y	601	CHL	C11-C10-C8-C7
27	B	602	CLA	CBA-CGA-O2A-C1
27	B	608	CLA	CBA-CGA-O2A-C1
27	b	602	CLA	CBA-CGA-O2A-C1
27	b	608	CLA	CBA-CGA-O2A-C1
27	D	402	CLA	C16-C17-C18-C19
27	d	402	CLA	C16-C17-C18-C19
28	A	408	PHO	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
28	a	408	PHO	O2A-C1-C2-C3
31	Z	101	LMG	C21-C22-C23-C24
35	D	410	LHG	O2-C2-C3-O3
35	d	410	LHG	O2-C2-C3-O3
31	z	101	LMG	C21-C22-C23-C24
27	B	609	CLA	C5-C6-C7-C8
27	b	609	CLA	C5-C6-C7-C8
27	C	510	CLA	C2A-CAA-CBA-CGA
27	R	613	CLA	C2A-CAA-CBA-CGA
27	c	510	CLA	C2A-CAA-CBA-CGA
27	r	613	CLA	C2A-CAA-CBA-CGA
34	D	405	PL9	C3-C7-C8-C9
34	d	405	PL9	C3-C7-C8-C9
35	Y	2630	LHG	C5-C4-O6-P
35	y	2630	LHG	C5-C4-O6-P
27	B	603	CLA	C3A-C2A-CAA-CBA
27	R	604	CLA	C3A-C2A-CAA-CBA
27	b	603	CLA	C3A-C2A-CAA-CBA
27	r	604	CLA	C3A-C2A-CAA-CBA
35	N	2630	LHG	O10-C23-C24-C25
31	Z	101	LMG	C14-C15-C16-C17
31	z	101	LMG	C14-C15-C16-C17
35	D	409	LHG	C23-C24-C25-C26
35	d	409	LHG	C23-C24-C25-C26
31	B	622	LMG	C15-C16-C17-C18
31	b	622	LMG	C15-C16-C17-C18
37	G	605	CHL	C2-C1-O2A-CGA
37	g	605	CHL	C2-C1-O2A-CGA
27	R	601	CLA	CAA-CBA-CGA-O1A
27	r	601	CLA	CAA-CBA-CGA-O1A
35	n	2630	LHG	O10-C23-C24-C25
27	C	501	CLA	O1A-CGA-O2A-C1
27	c	501	CLA	O1A-CGA-O2A-C1
27	b	617	CLA	CAA-CBA-CGA-O1A
28	A	409	PHO	CAA-CBA-CGA-O1A
28	a	409	PHO	CAA-CBA-CGA-O1A
27	B	609	CLA	C2A-CAA-CBA-CGA
27	S	613	CLA	C2A-CAA-CBA-CGA
27	b	609	CLA	C2A-CAA-CBA-CGA
27	s	613	CLA	C2A-CAA-CBA-CGA
27	C	506	CLA	C11-C10-C8-C9
27	C	510	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
27	c	506	CLA	C11-C10-C8-C9
27	c	510	CLA	C11-C10-C8-C9
37	Y	609	CHL	C11-C10-C8-C9
37	Y	609	CHL	C14-C13-C15-C16
37	y	609	CHL	C11-C10-C8-C9
37	y	609	CHL	C14-C13-C15-C16
35	D	410	LHG	C24-C25-C26-C27
35	d	410	LHG	C24-C25-C26-C27
27	B	617	CLA	CAA-CBA-CGA-O1A
27	R	610	CLA	CAA-CBA-CGA-O1A
27	N	602	CLA	CAA-CBA-CGA-O1A
27	r	610	CLA	CAA-CBA-CGA-O1A
31	c	521	LMG	O9-C10-C11-C12
27	b	603	CLA	O1D-CGD-O2D-CED
27	N	614	CLA	CBA-CGA-O2A-C1
27	G	603	CLA	CAA-CBA-CGA-O1A
27	G	610	CLA	CAA-CBA-CGA-O1A
27	N	603	CLA	CAA-CBA-CGA-O1A
27	g	603	CLA	CAA-CBA-CGA-O1A
27	g	610	CLA	CAA-CBA-CGA-O1A
27	n	602	CLA	CAA-CBA-CGA-O1A
27	n	603	CLA	CAA-CBA-CGA-O1A
31	C	521	LMG	O9-C10-C11-C12
31	D	411	LMG	O9-C10-C11-C12
31	d	411	LMG	O9-C10-C11-C12
35	Y	2630	LHG	O10-C23-C24-C25
35	y	2630	LHG	O10-C23-C24-C25
32	C	518	DGD	C5D-C6D-O5D-C1E
32	c	518	DGD	C5D-C6D-O5D-C1E
27	N	611	CLA	O2A-C1-C2-C3
27	R	601	CLA	O2A-C1-C2-C3
27	n	611	CLA	O2A-C1-C2-C3
27	r	601	CLA	O2A-C1-C2-C3
27	G	602	CLA	CAA-CBA-CGA-O1A
27	g	602	CLA	CAA-CBA-CGA-O1A
30	A	412	SQD	C33-C34-C35-C36
30	a	412	SQD	C33-C34-C35-C36
27	N	612	CLA	CAA-CBA-CGA-O1A
27	y	602	CLA	CAA-CBA-CGA-O1A
27	C	502	CLA	C15-C16-C17-C18
27	c	502	CLA	C15-C16-C17-C18
37	N	605	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
37	Y	609	CHL	C2-C3-C5-C6
37	n	605	CHL	C2-C1-O2A-CGA
37	y	609	CHL	C2-C3-C5-C6
27	Y	602	CLA	CAA-CBA-CGA-O1A
27	n	612	CLA	CAA-CBA-CGA-O1A
27	r	616	CLA	CAA-CBA-CGA-O1A
37	S	601	CHL	CAA-CBA-CGA-O1A
37	s	601	CHL	CAA-CBA-CGA-O1A
27	B	606	CLA	CAD-CBD-CGD-O2D
27	B	611	CLA	CAD-CBD-CGD-O2D
27	B	613	CLA	CAD-CBD-CGD-O2D
27	C	502	CLA	CAD-CBD-CGD-O2D
27	Y	612	CLA	CAD-CBD-CGD-O2D
27	Y	614	CLA	CAD-CBD-CGD-O2D
27	b	606	CLA	CAD-CBD-CGD-O2D
27	b	611	CLA	CAD-CBD-CGD-O2D
27	b	613	CLA	CAD-CBD-CGD-O2D
27	c	502	CLA	CAD-CBD-CGD-O2D
27	y	612	CLA	CAD-CBD-CGD-O2D
27	y	614	CLA	CAD-CBD-CGD-O2D
27	B	610	CLA	C3-C5-C6-C7
27	b	610	CLA	C3-C5-C6-C7
27	R	616	CLA	CAA-CBA-CGA-O1A
30	a	412	SQD	C18-C19-C20-C21
30	A	412	SQD	C18-C19-C20-C21
27	n	614	CLA	CBA-CGA-O2A-C1
27	C	505	CLA	C2-C1-O2A-CGA
27	c	505	CLA	C2-C1-O2A-CGA
37	N	601	CHL	C2-C1-O2A-CGA
37	S	601	CHL	C2-C1-O2A-CGA
37	n	601	CHL	C2-C1-O2A-CGA
35	g	2630	LHG	C34-C35-C36-C37
27	C	501	CLA	CAA-CBA-CGA-O1A
27	B	603	CLA	O1D-CGD-O2D-CED
27	N	614	CLA	O1A-CGA-O2A-C1
35	G	2630	LHG	C34-C35-C36-C37
32	H	102	DGD	C6B-C7B-C8B-C9B
27	B	609	CLA	CAA-CBA-CGA-O1A
27	B	608	CLA	O1A-CGA-O2A-C1
32	h	102	DGD	C6B-C7B-C8B-C9B
27	c	501	CLA	CAA-CBA-CGA-O1A
27	B	614	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	R	613	CLA	CAA-CBA-CGA-O2A
27	b	614	CLA	CAA-CBA-CGA-O2A
27	r	613	CLA	CAA-CBA-CGA-O2A
31	D	411	LMG	O7-C10-C11-C12
31	d	411	LMG	O7-C10-C11-C12
37	Y	601	CHL	CAA-CBA-CGA-O2A
37	Y	607	CHL	CAA-CBA-CGA-O2A
37	y	601	CHL	CAA-CBA-CGA-O2A
37	y	607	CHL	CAA-CBA-CGA-O2A
27	b	608	CLA	O1A-CGA-O2A-C1
27	n	614	CLA	O1A-CGA-O2A-C1
34	D	405	PL9	C22-C23-C24-C26
34	d	405	PL9	C22-C23-C24-C26
27	S	603	CLA	CAA-CBA-CGA-O1A
27	s	603	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

307 monomers are involved in 1441 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	c	516	BCR	10	0
38	S	1621	LUT	8	0
27	S	604	CLA	6	0
39	r	622	XAT	7	0
27	y	604	CLA	4	0
37	S	608	CHL	4	0
27	n	613	CLA	1	0
27	r	611	CLA	4	0
29	b	618	BCR	9	0
29	b	620	BCR	1	0
38	g	1620	LUT	7	0
27	N	602	CLA	9	0
27	c	509	CLA	5	0
29	a	411	BCR	4	0
37	R	608	CHL	10	0
27	d	403	CLA	6	0
37	g	608	CHL	7	0
29	C	514	BCR	7	0
29	B	618	BCR	7	0
28	A	408	PHO	6	0
35	l	101	LHG	7	0
27	C	506	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	s	2630	LHG	3	0
38	s	1620	LUT	9	0
28	a	409	PHO	4	0
27	C	508	CLA	5	0
27	S	613	CLA	2	0
27	B	609	CLA	8	0
27	y	613	CLA	6	0
27	B	607	CLA	5	0
37	y	605	CHL	5	0
27	c	511	CLA	6	0
37	r	607	CHL	3	0
27	C	502	CLA	10	0
27	A	405	CLA	8	0
27	N	610	CLA	8	0
37	n	609	CHL	5	0
31	z	101	LMG	4	0
27	b	604	CLA	10	0
27	b	607	CLA	7	0
27	b	602	CLA	6	0
27	Y	603	CLA	5	0
27	s	604	CLA	6	0
27	N	613	CLA	1	0
37	r	608	CHL	8	0
37	g	601	CHL	13	0
31	b	622	LMG	9	0
27	C	504	CLA	7	0
27	c	501	CLA	3	0
27	s	602	CLA	5	0
31	A	413	LMG	7	0
38	N	1621	LUT	6	0
27	B	605	CLA	5	0
35	L	101	LHG	6	0
27	G	613	CLA	4	0
27	a	406	CLA	5	0
27	Y	614	CLA	2	0
33	d	401	BCT	4	0
37	N	606	CHL	3	0
31	D	411	LMG	4	0
30	A	418	SQD	3	0
37	g	607	CHL	5	0
37	R	607	CHL	4	0
33	D	401	BCT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	Y	602	CLA	7	0
27	b	613	CLA	9	0
38	R	620	LUT	11	0
27	n	603	CLA	1	0
27	C	512	CLA	3	0
27	n	602	CLA	9	0
24	A	401	OEX	2	0
27	S	614	CLA	2	0
27	Y	612	CLA	4	0
29	d	404	BCR	5	0
37	s	601	CHL	2	0
27	n	610	CLA	10	0
38	S	1620	LUT	9	0
27	C	505	CLA	8	0
37	N	605	CHL	6	0
27	G	610	CLA	12	0
29	c	515	BCR	6	0
27	y	603	CLA	5	0
27	D	403	CLA	7	0
28	a	408	PHO	5	0
27	S	602	CLA	5	0
27	y	614	CLA	2	0
29	B	620	BCR	2	0
38	G	1621	LUT	6	0
37	s	606	CHL	4	0
29	B	619	BCR	6	0
35	D	410	LHG	5	0
27	a	407	CLA	8	0
27	B	611	CLA	3	0
35	r	2630	LHG	3	0
27	R	616	CLA	4	0
31	c	521	LMG	5	0
27	D	402	CLA	8	0
35	g	2630	LHG	13	0
30	B	621	SQD	3	0
27	N	603	CLA	1	0
27	c	508	CLA	5	0
27	G	614	CLA	1	0
27	R	610	CLA	10	0
27	b	616	CLA	6	0
27	c	502	CLA	10	0
32	c	519	DGD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	608	CLA	2	0
40	g	1623	NEX	3	0
27	c	513	CLA	3	0
27	B	617	CLA	3	0
37	N	607	CHL	8	0
27	r	612	CLA	1	0
27	B	604	CLA	7	0
27	N	614	CLA	2	0
37	Y	608	CHL	3	0
38	r	620	LUT	10	0
27	C	503	CLA	9	0
27	R	604	CLA	5	0
27	S	610	CLA	8	0
27	B	614	CLA	3	0
27	R	602	CLA	11	0
27	c	504	CLA	8	0
29	A	411	BCR	6	0
37	S	601	CHL	2	0
40	G	1623	NEX	3	0
29	D	404	BCR	5	0
27	b	606	CLA	2	0
34	D	405	PL9	7	0
37	Y	607	CHL	6	0
29	c	514	BCR	6	0
27	y	611	CLA	5	0
27	b	609	CLA	8	0
27	a	405	CLA	7	0
40	s	1623	NEX	4	0
27	r	610	CLA	9	0
32	h	102	DGD	9	0
27	B	606	CLA	5	0
35	d	410	LHG	3	0
28	A	409	PHO	4	0
37	G	607	CHL	5	0
39	y	1622	XAT	9	0
35	y	2630	LHG	8	0
37	s	608	CHL	4	0
35	D	408	LHG	5	0
37	n	605	CHL	6	0
27	G	612	CLA	1	0
27	g	610	CLA	11	0
27	G	603	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	G	602	CLA	8	0
27	c	512	CLA	2	0
27	r	602	CLA	13	0
30	a	418	SQD	3	0
37	G	609	CHL	4	0
27	g	613	CLA	4	0
27	g	612	CLA	1	0
32	C	519	DGD	6	0
37	n	601	CHL	7	0
37	g	609	CHL	4	0
27	N	611	CLA	2	0
27	g	611	CLA	6	0
27	r	604	CLA	5	0
27	r	613	CLA	6	0
27	b	612	CLA	3	0
27	C	513	CLA	3	0
37	y	607	CHL	6	0
39	Y	1622	XAT	9	0
27	A	406	CLA	6	0
27	b	615	CLA	6	0
29	C	516	BCR	10	0
37	R	606	CHL	5	0
32	c	518	DGD	5	0
35	S	2630	LHG	2	0
27	A	410	CLA	4	0
27	C	509	CLA	5	0
30	a	412	SQD	3	0
38	g	1621	LUT	6	0
27	g	604	CLA	2	0
37	n	607	CHL	9	0
38	y	1620	LUT	7	0
31	a	413	LMG	8	0
27	s	611	CLA	1	0
27	n	614	CLA	2	0
27	s	610	CLA	8	0
29	c	517	BCR	7	0
27	a	410	CLA	3	0
27	C	511	CLA	6	0
31	B	622	LMG	10	0
34	d	405	PL9	9	0
27	b	617	CLA	2	0
37	S	607	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	c	520	DGD	18	0
31	d	411	LMG	4	0
37	y	608	CHL	3	0
32	H	102	DGD	10	0
27	r	616	CLA	4	0
35	N	2630	LHG	7	0
29	H	101	BCR	6	0
27	B	603	CLA	10	0
27	s	613	CLA	2	0
27	s	612	CLA	2	0
27	b	605	CLA	6	0
27	b	611	CLA	3	0
38	Y	1620	LUT	6	0
27	y	612	CLA	4	0
35	d	409	LHG	4	0
35	Y	2630	LHG	7	0
40	R	623	NEX	6	0
38	y	1621	LUT	10	0
31	Z	101	LMG	6	0
40	N	1623	NEX	3	0
38	N	1620	LUT	10	0
29	C	517	BCR	7	0
27	Y	611	CLA	5	0
38	G	1620	LUT	9	0
37	r	606	CHL	5	0
35	G	2630	LHG	14	0
27	b	614	CLA	3	0
27	g	603	CLA	2	0
36	F	101	HEM	5	0
35	D	409	LHG	3	0
27	g	602	CLA	7	0
27	c	507	CLA	5	0
27	G	611	CLA	7	0
27	c	510	CLA	5	0
30	b	621	SQD	3	0
40	Y	1623	NEX	4	0
38	s	1621	LUT	8	0
27	n	611	CLA	2	0
37	y	601	CHL	7	0
27	g	614	CLA	3	0
27	c	505	CLA	8	0
27	S	609	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	612	CLA	3	0
37	N	608	CHL	5	0
27	S	611	CLA	1	0
27	s	614	CLA	2	0
36	f	101	HEM	5	0
27	r	601	CLA	5	0
27	Y	604	CLA	3	0
40	r	623	NEX	6	0
29	C	515	BCR	6	0
27	Y	610	CLA	8	0
29	h	101	BCR	6	0
27	G	604	CLA	2	0
37	y	609	CHL	5	0
27	b	610	CLA	12	0
27	c	503	CLA	7	0
32	C	520	DGD	19	0
27	R	612	CLA	1	0
27	b	608	CLA	2	0
27	B	602	CLA	6	0
31	C	521	LMG	4	0
27	R	601	CLA	5	0
27	R	609	CLA	3	0
37	Y	601	CHL	9	0
37	Y	609	CHL	6	0
39	n	1622	XAT	6	0
27	R	613	CLA	5	0
27	B	610	CLA	10	0
27	d	402	CLA	9	0
37	G	608	CHL	6	0
32	C	518	DGD	5	0
27	b	603	CLA	8	0
27	A	407	CLA	8	0
27	C	501	CLA	3	0
37	N	609	CHL	5	0
27	s	609	CLA	2	0
37	G	601	CHL	12	0
30	A	412	SQD	3	0
39	g	1622	XAT	6	0
37	g	606	CHL	2	0
37	G	605	CHL	6	0
35	n	2630	LHG	7	0
27	c	506	CLA	6	0

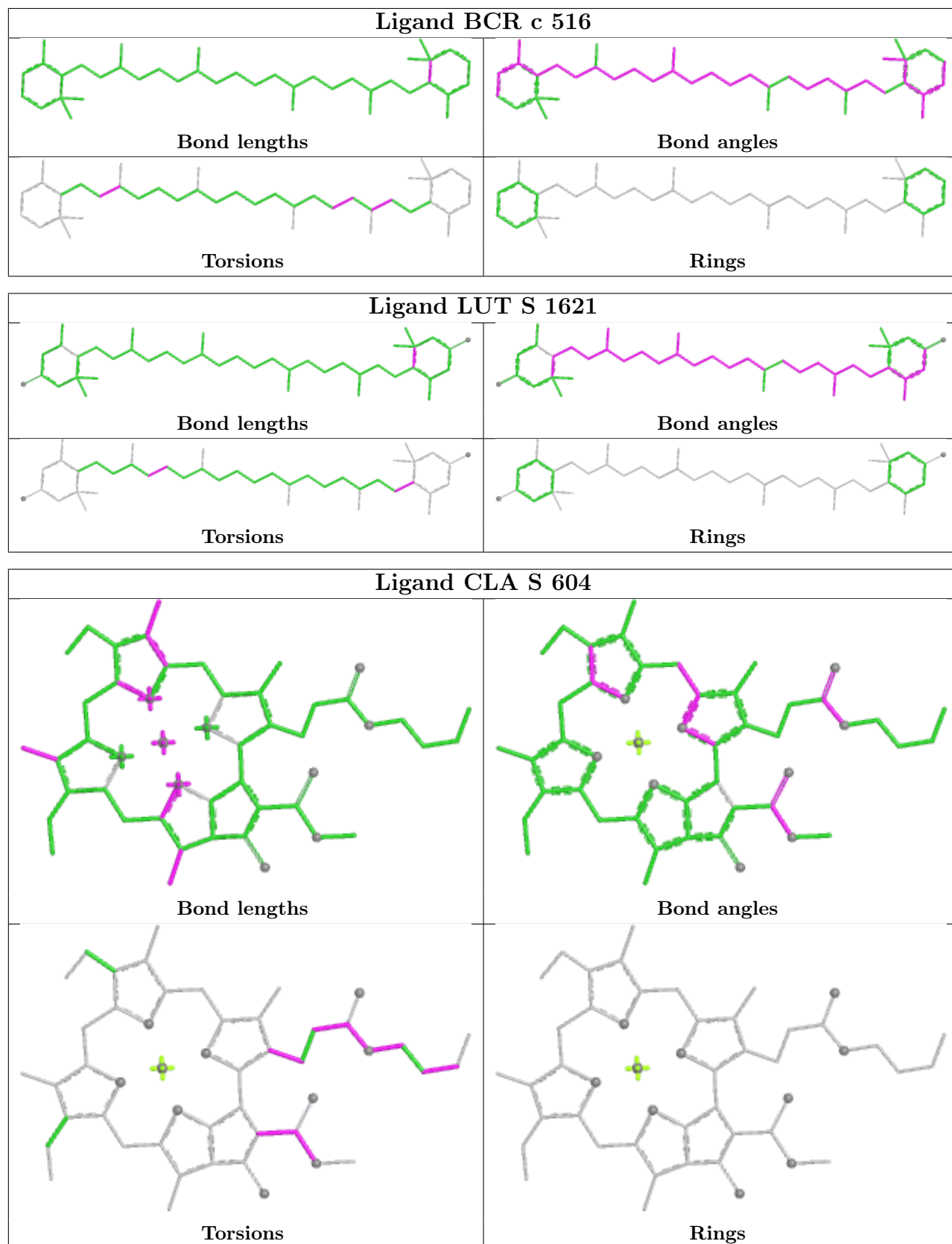
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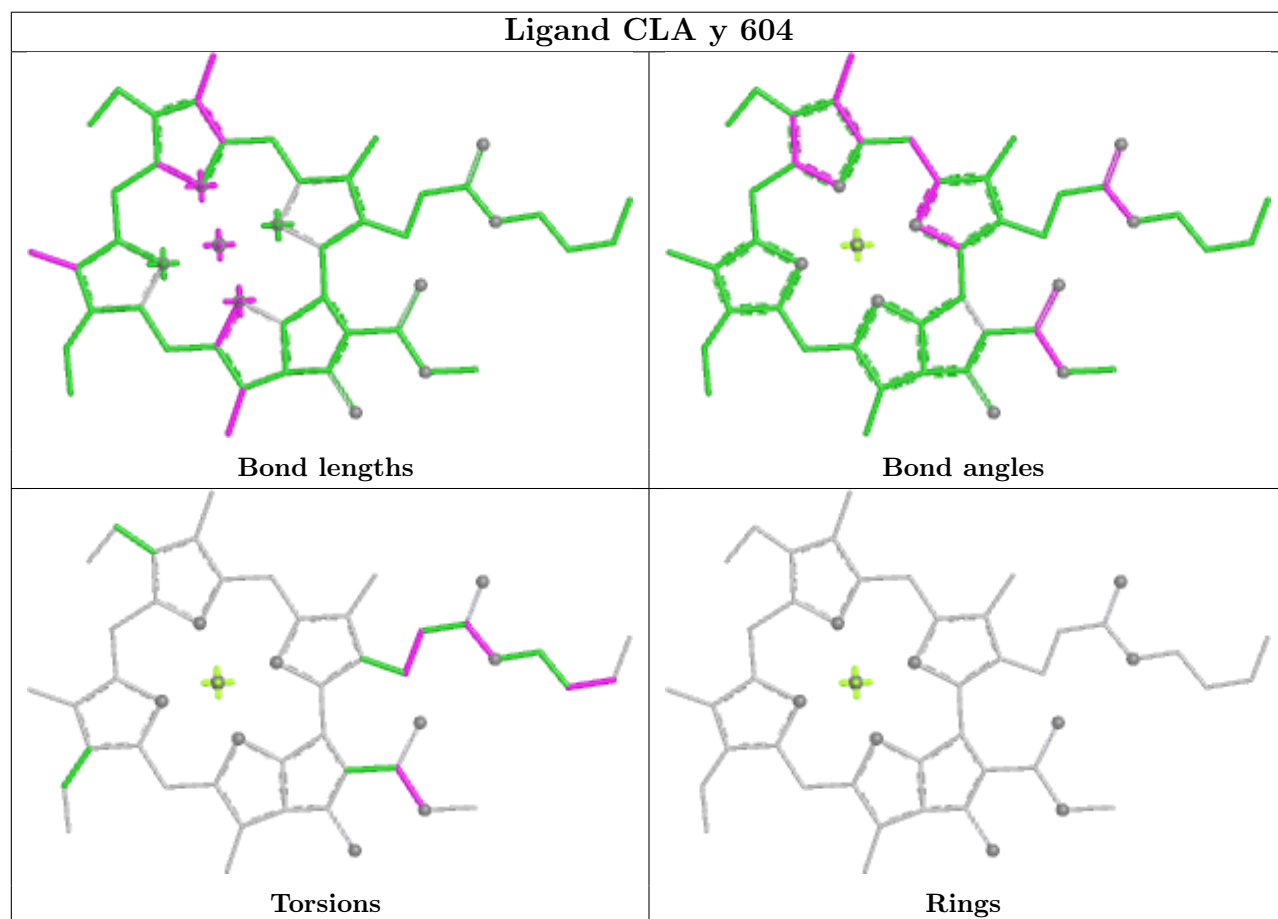
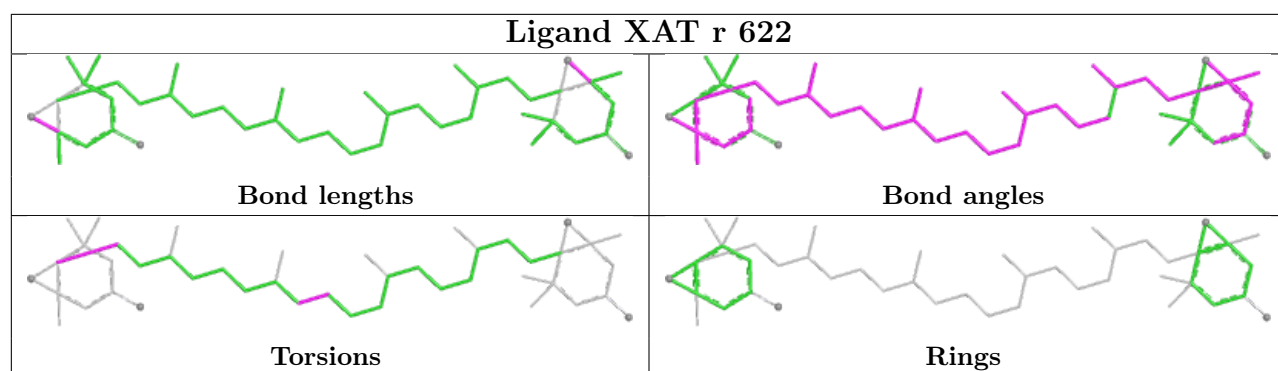
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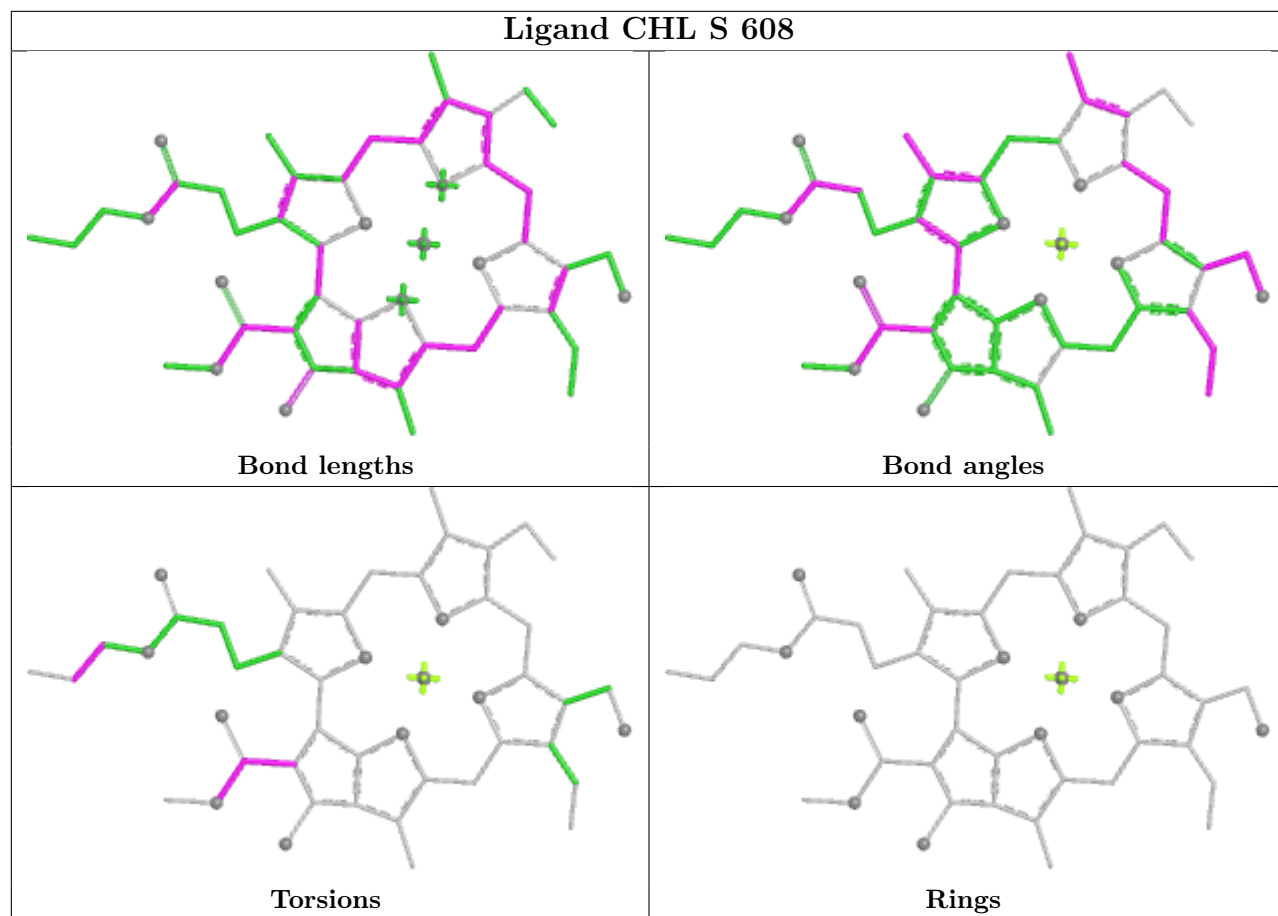
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	R	2630	LHG	3	0
39	R	622	XAT	7	0
27	C	510	CLA	6	0
38	n	1620	LUT	9	0
27	y	610	CLA	9	0
27	Y	613	CLA	7	0
27	R	611	CLA	3	0
37	Y	605	CHL	5	0
37	s	607	CHL	2	0
38	Y	1621	LUT	8	0
24	a	401	OEX	2	0
40	n	1623	NEX	3	0
37	N	601	CHL	8	0
27	r	609	CLA	3	0
37	G	606	CHL	2	0
27	B	613	CLA	10	0
39	N	1622	XAT	7	0
40	S	1623	NEX	4	0
37	n	606	CHL	3	0
27	B	616	CLA	5	0
27	B	615	CLA	5	0
37	g	605	CHL	6	0
27	n	612	CLA	1	0
27	y	602	CLA	8	0
27	C	507	CLA	5	0
29	b	619	BCR	5	0
38	n	1621	LUT	7	0
37	S	606	CHL	4	0
40	y	1623	NEX	3	0
35	d	408	LHG	5	0
37	n	608	CHL	5	0
39	G	1622	XAT	7	0
27	S	612	CLA	2	0

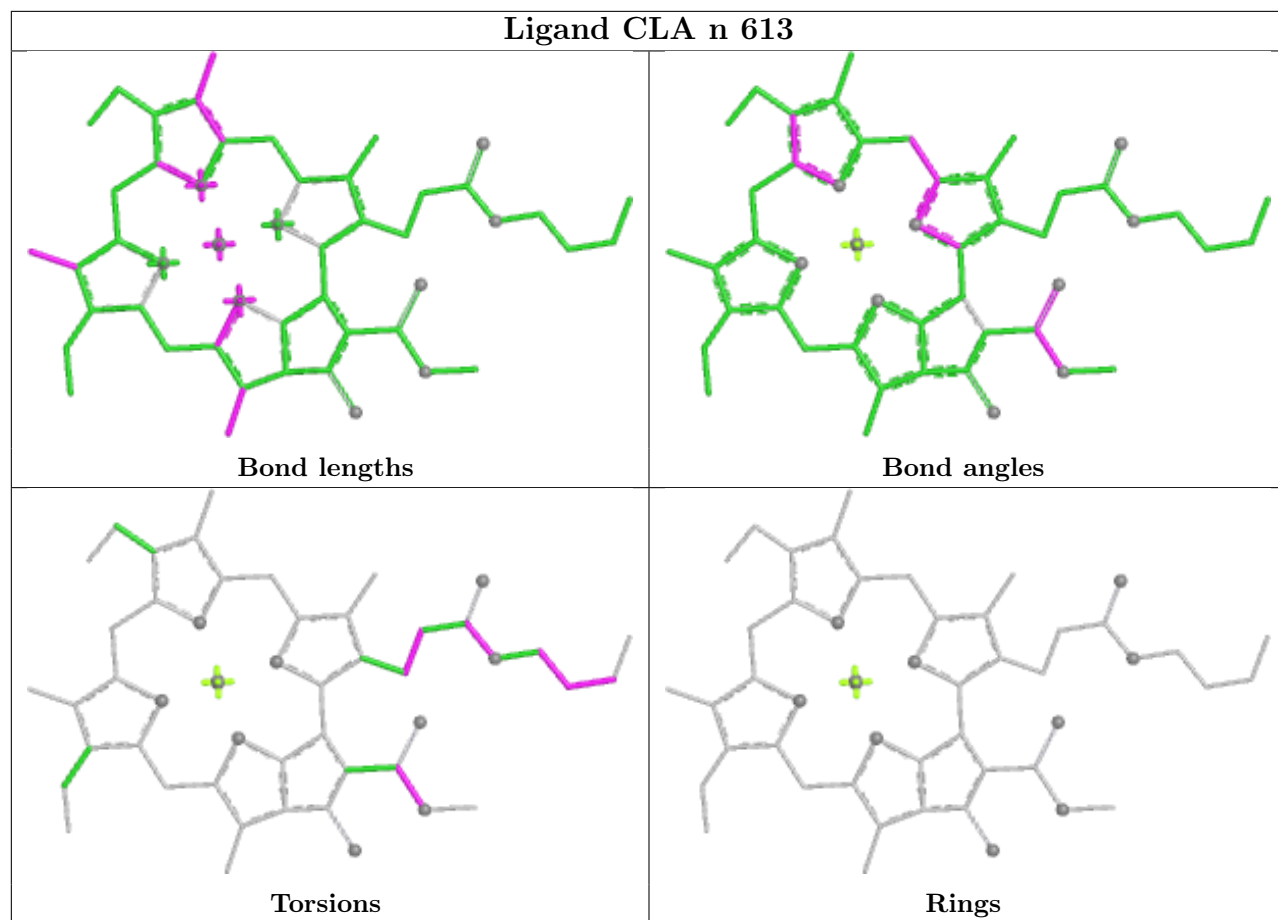
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

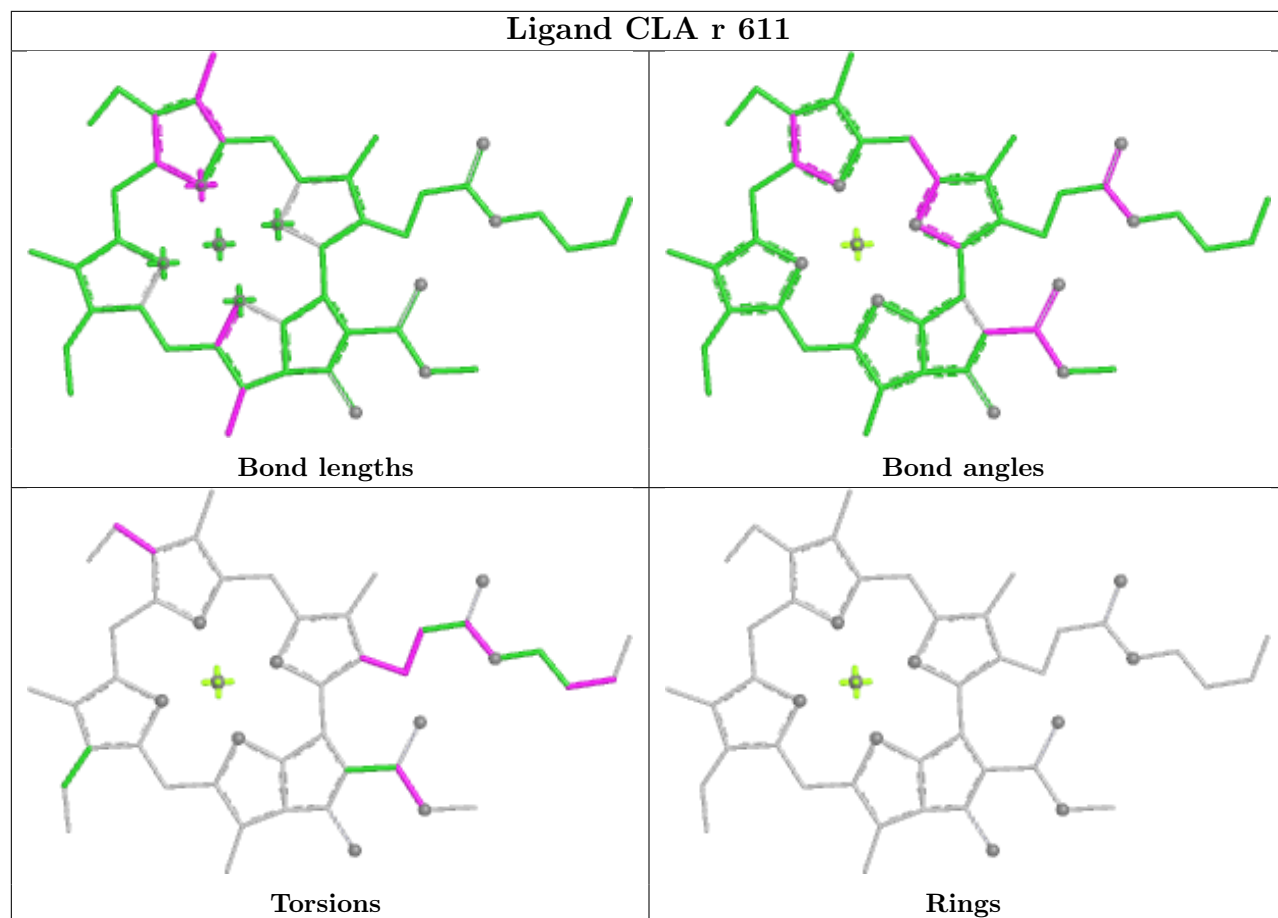




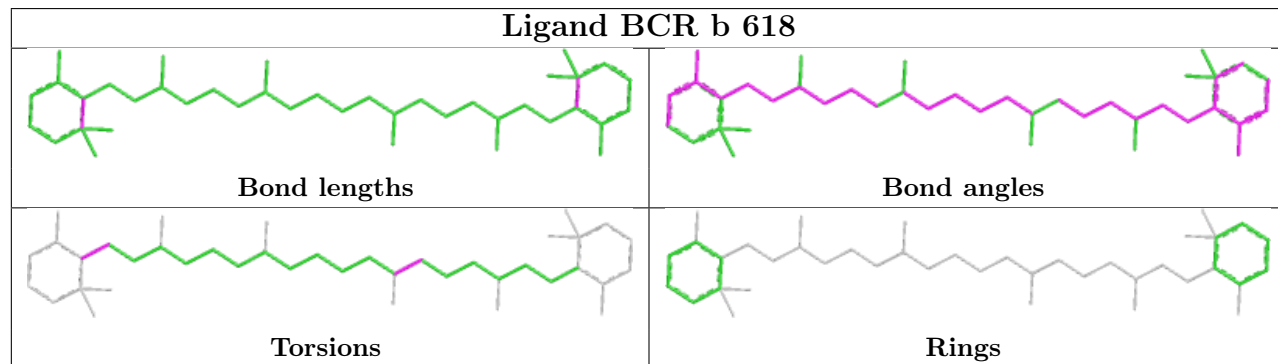




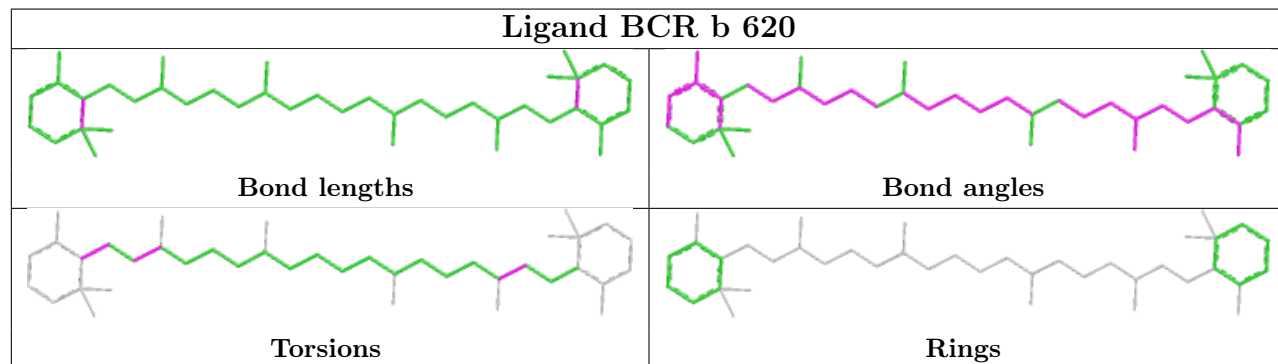
Ligand CLA r 611

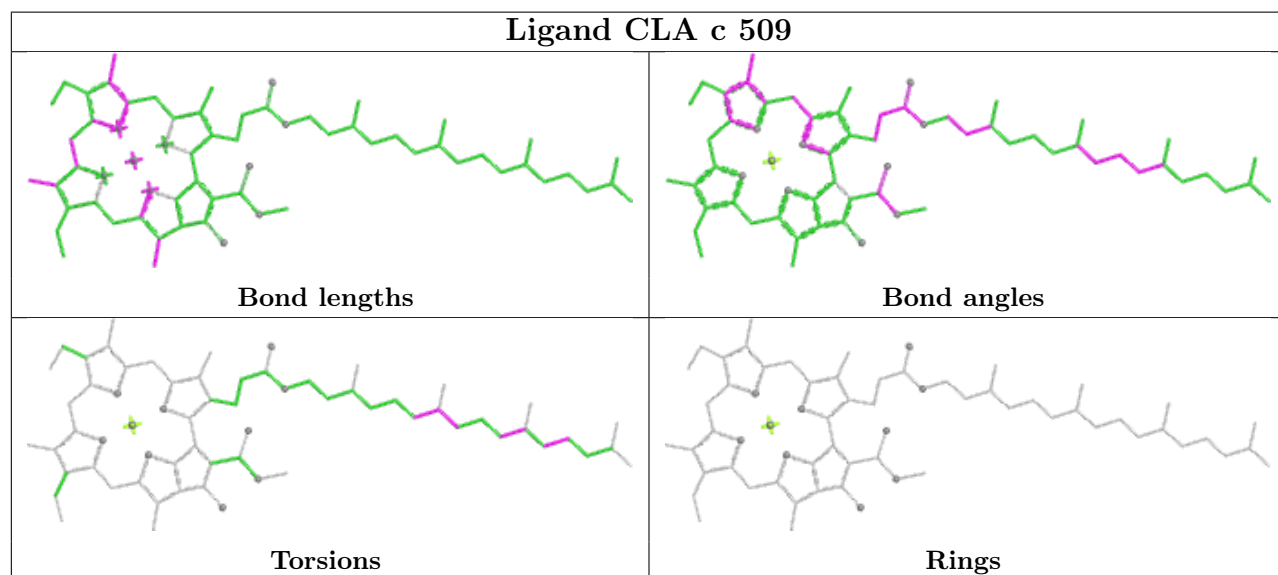
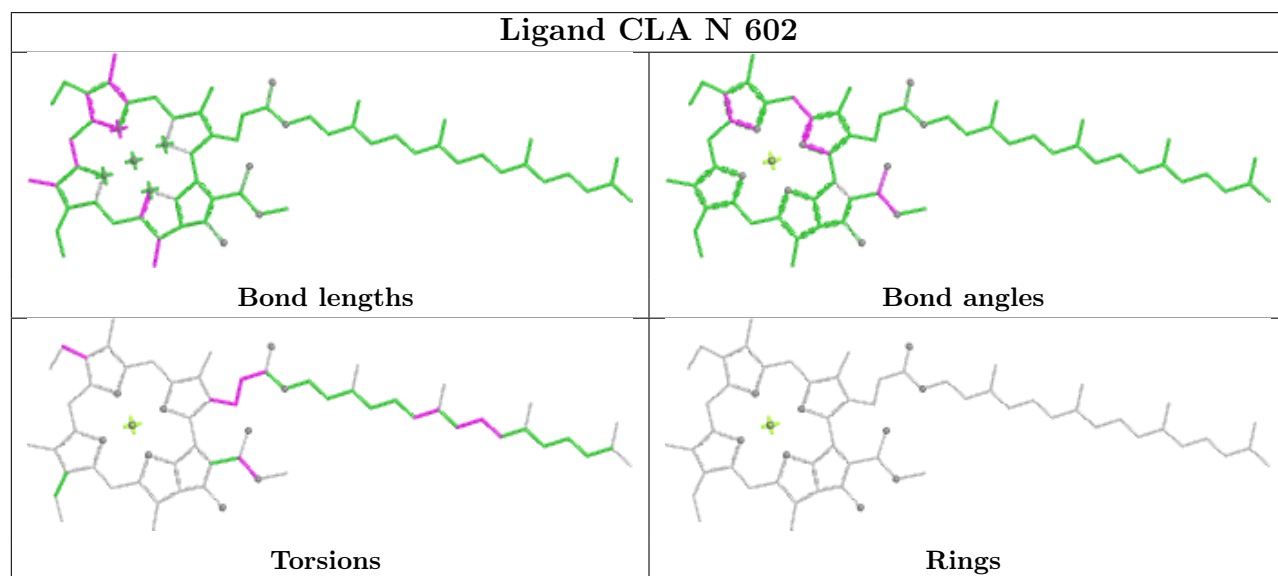
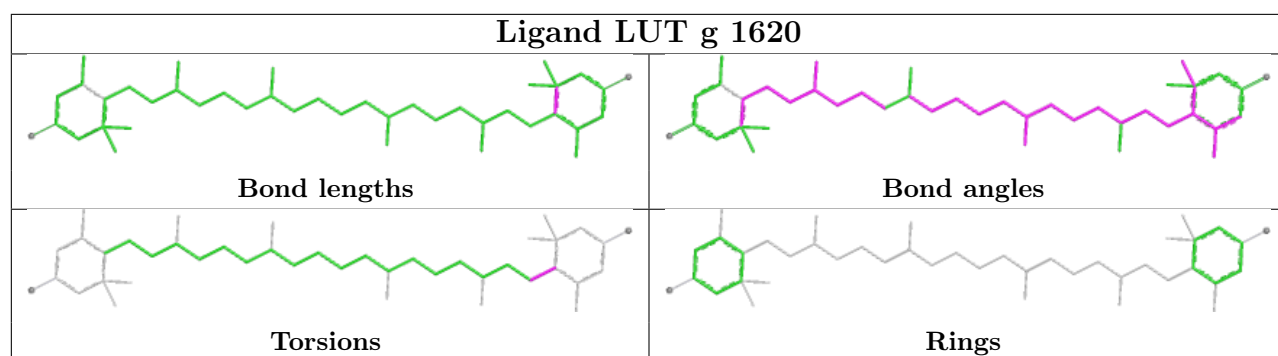


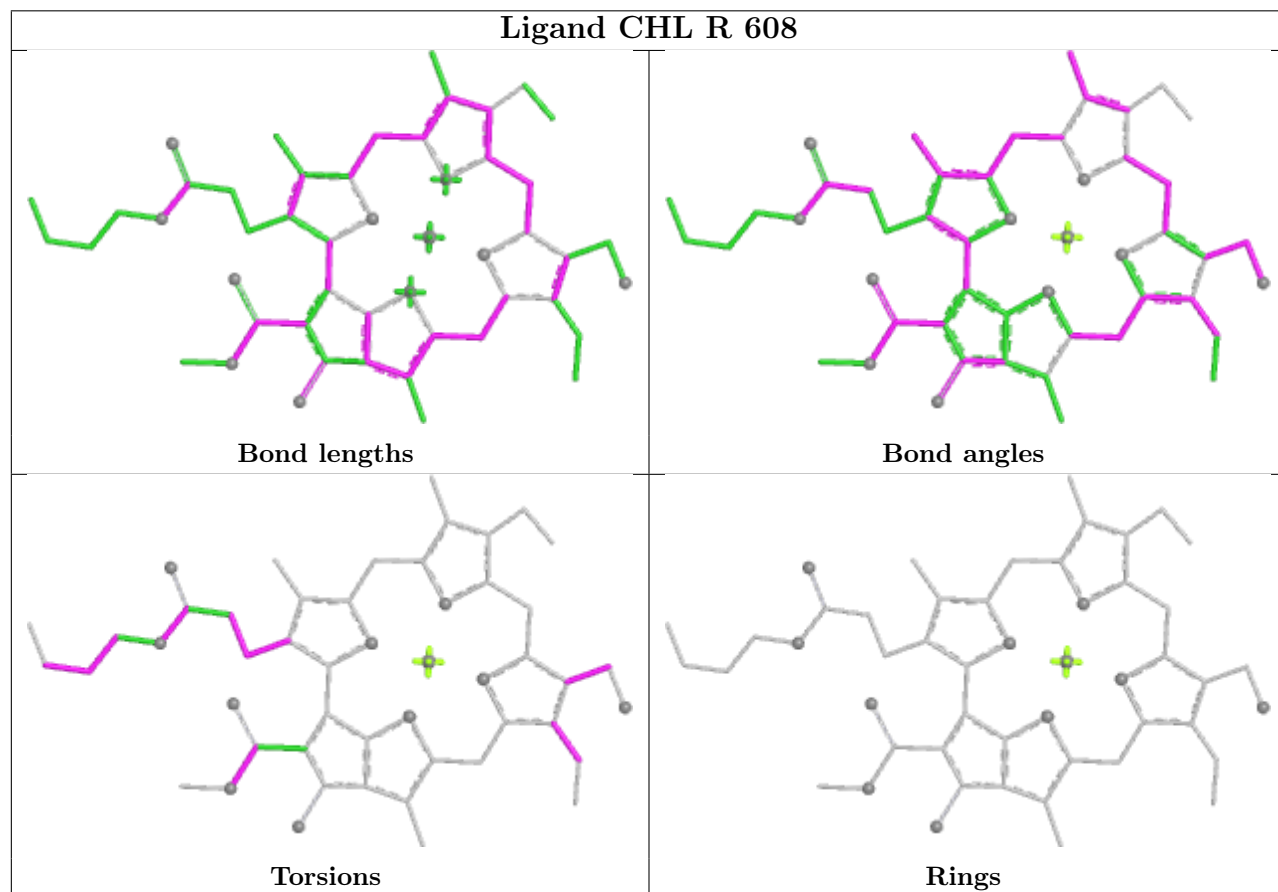
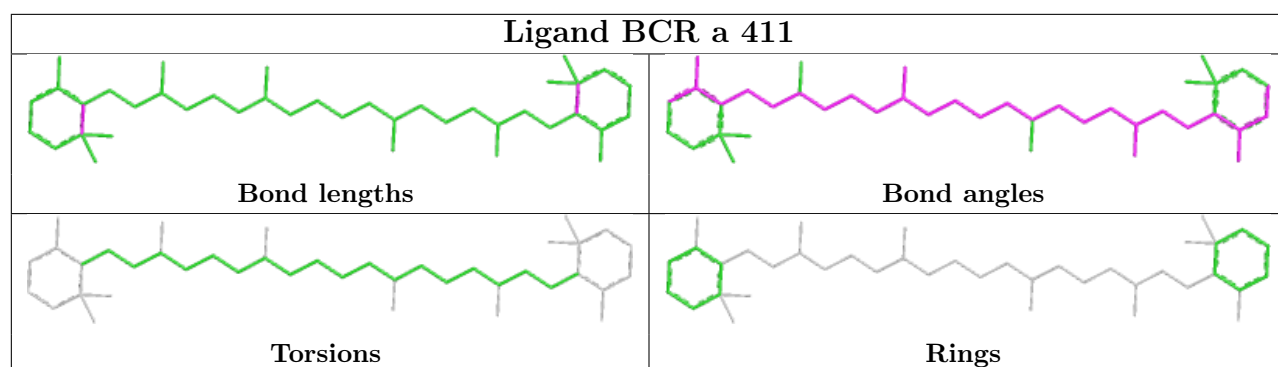
Ligand BCR b 618

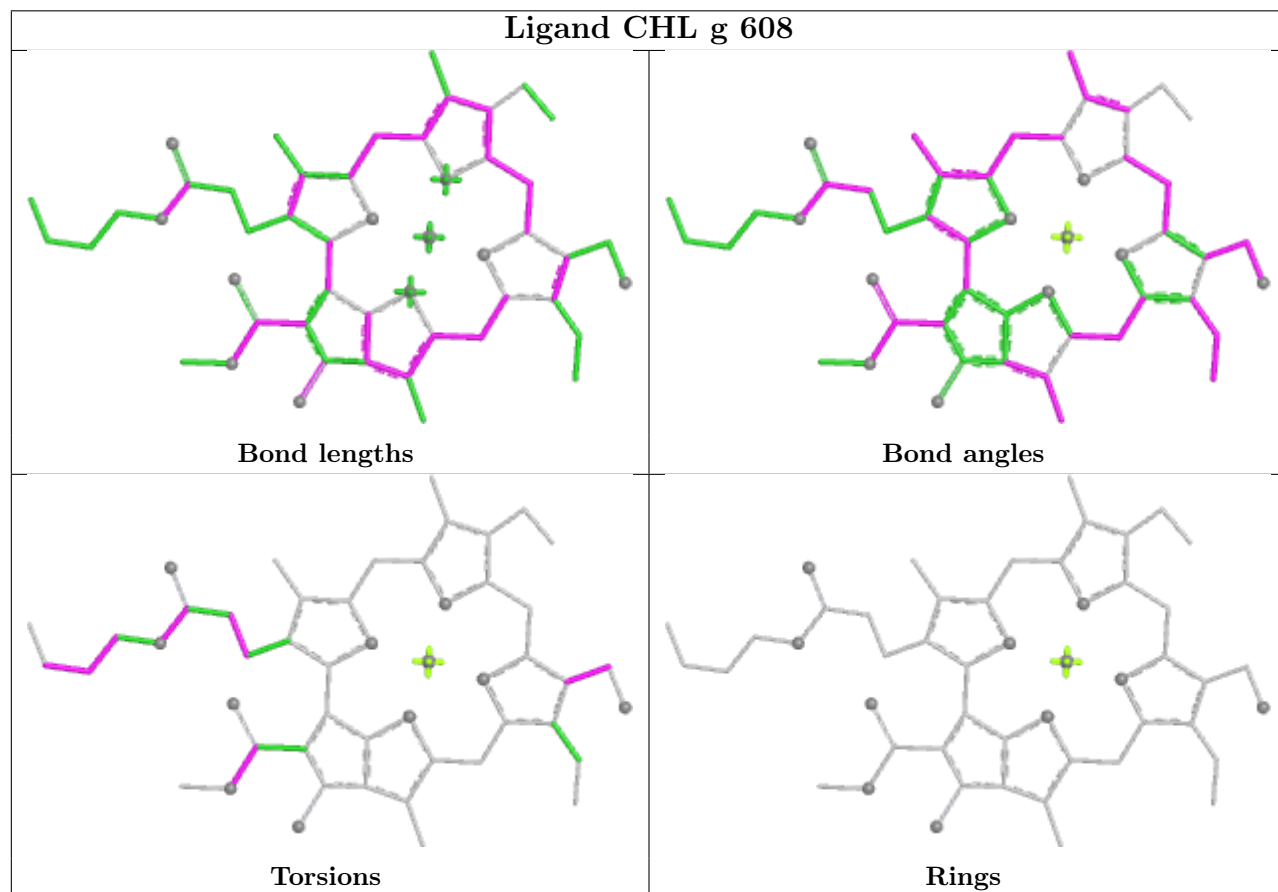
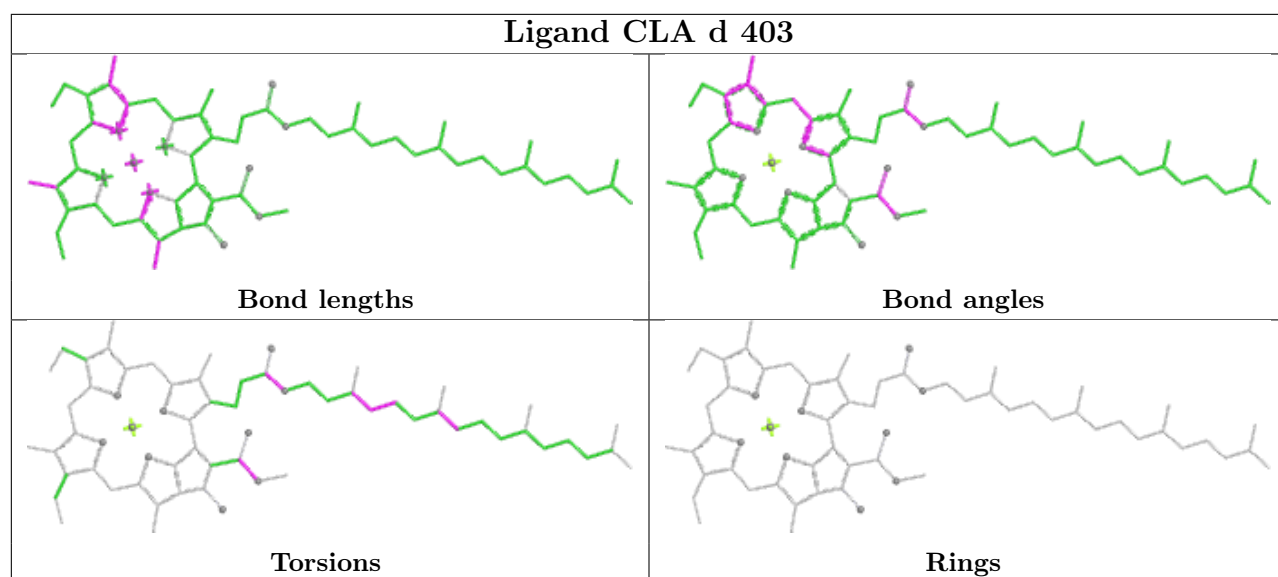


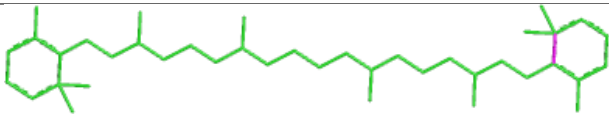
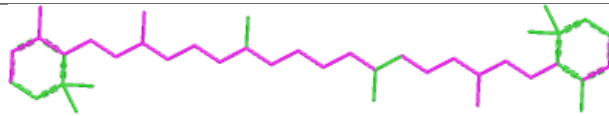
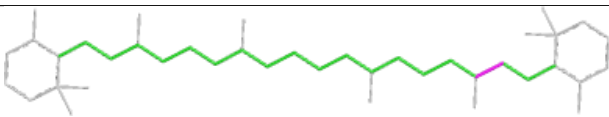
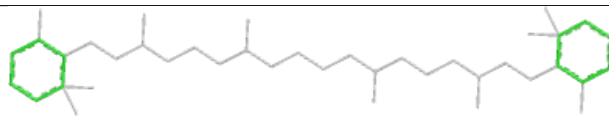
Ligand BCR b 620

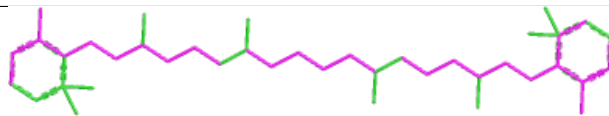
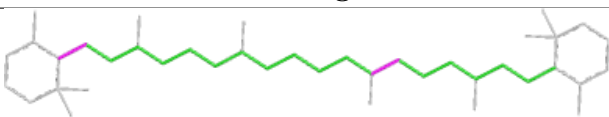
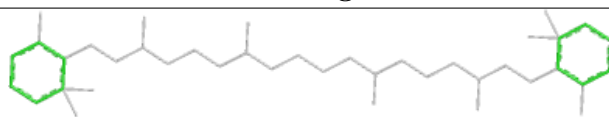


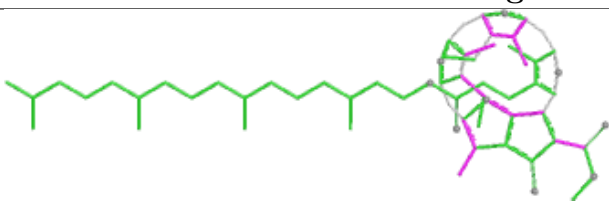
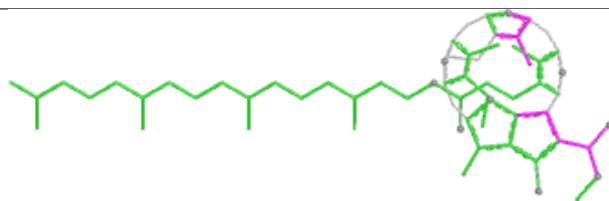
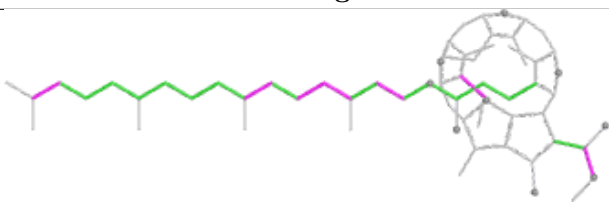
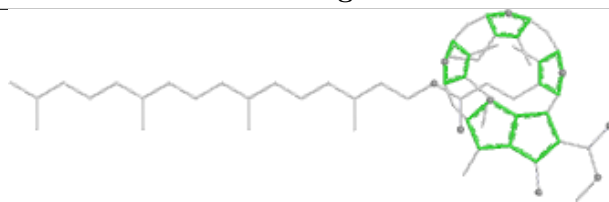


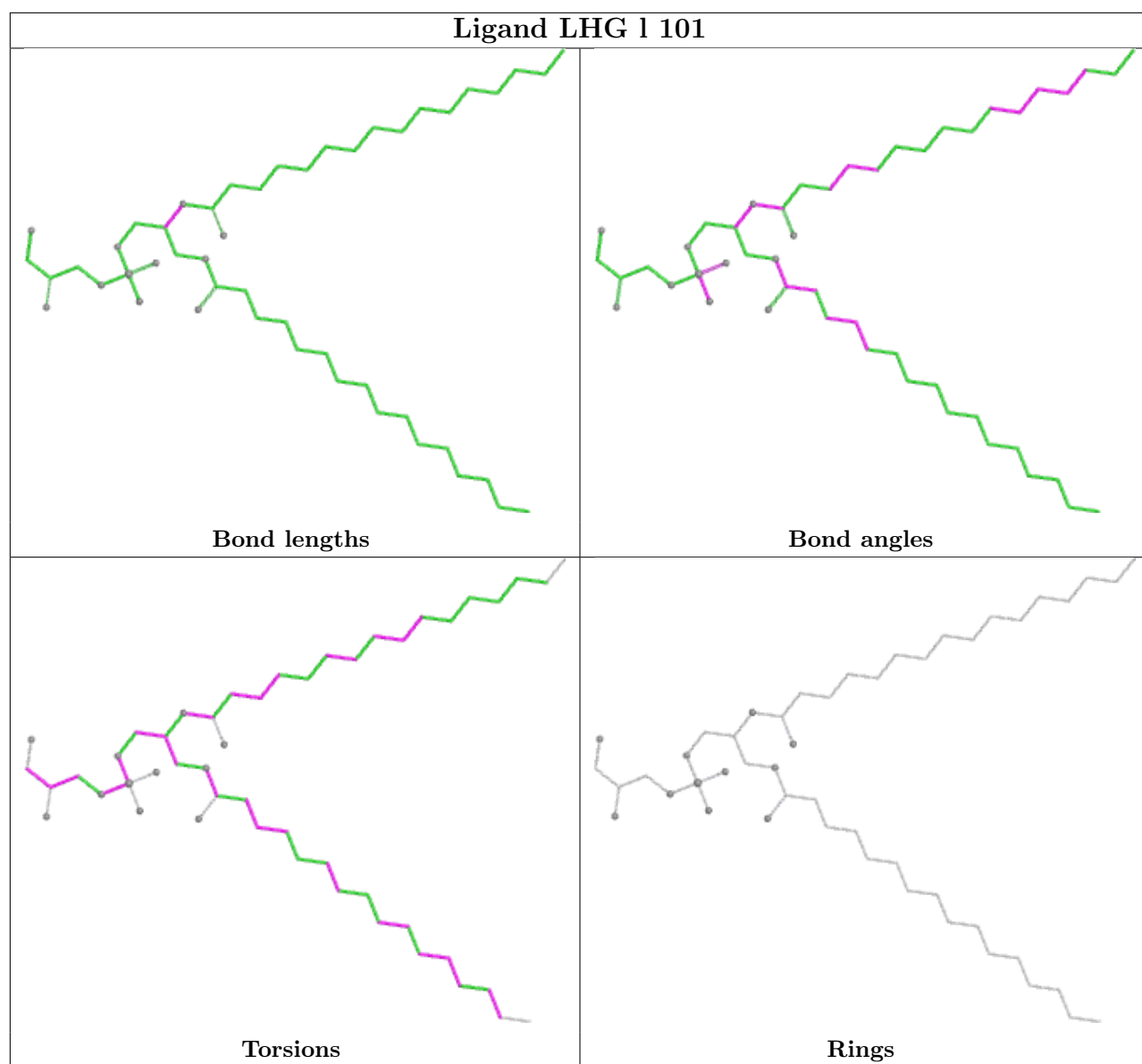




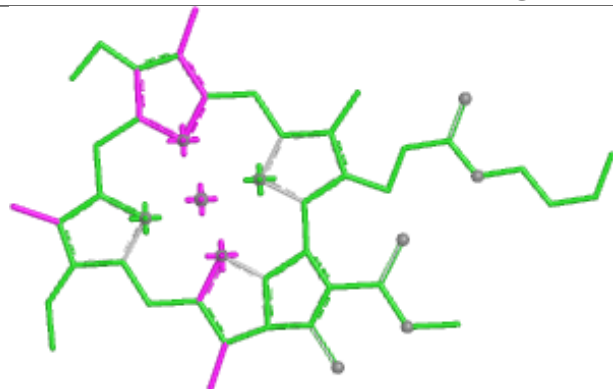
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

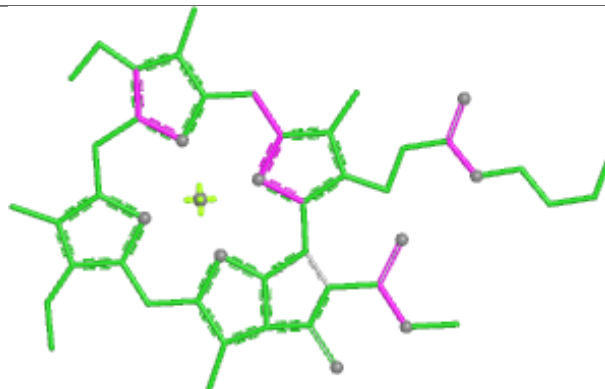
Ligand PHO A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings



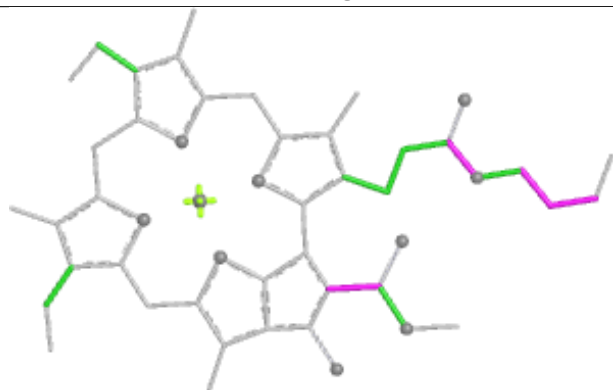
Ligand CLA N 604



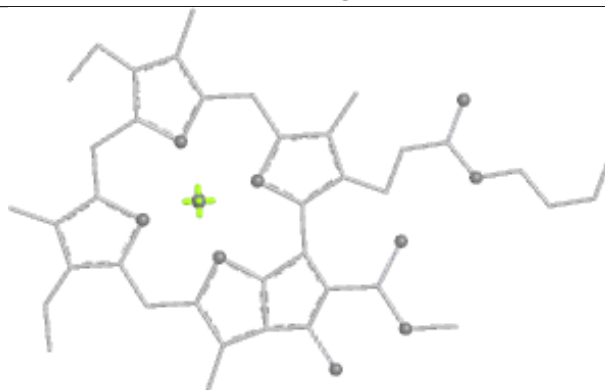
Bond lengths



Bond angles

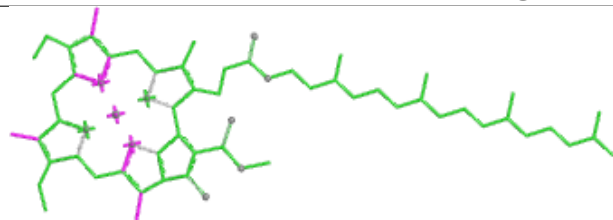


Torsions

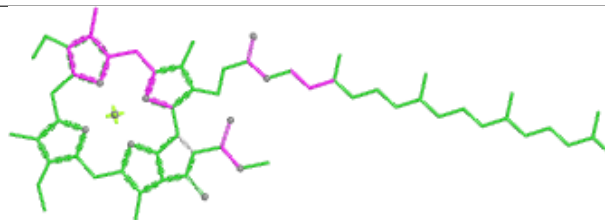


Rings

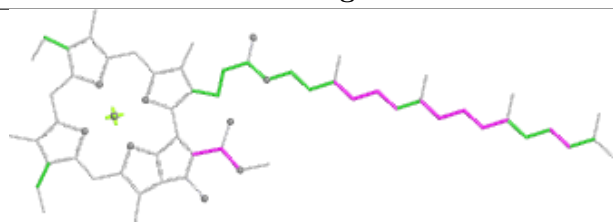
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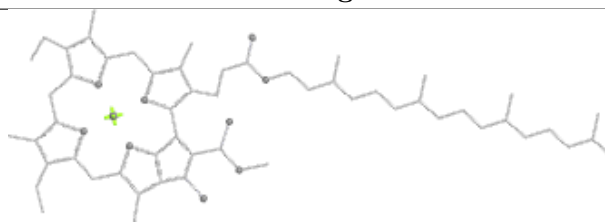
Bond lengths



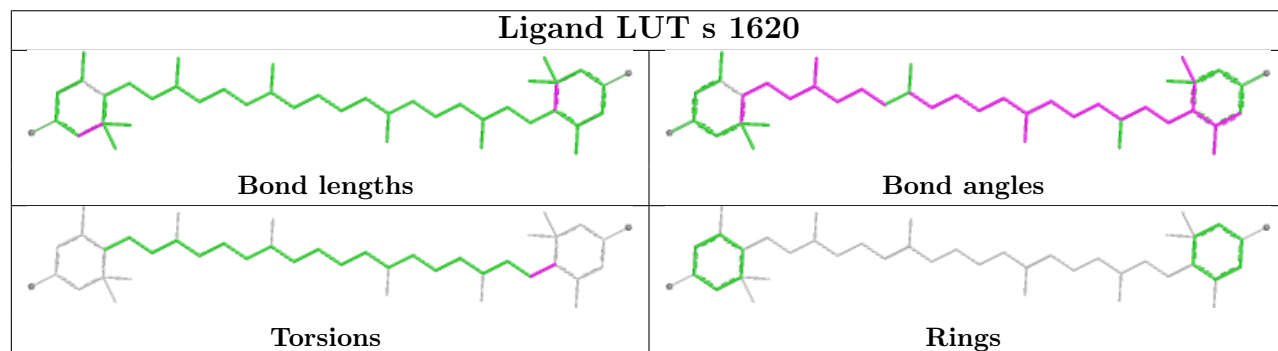
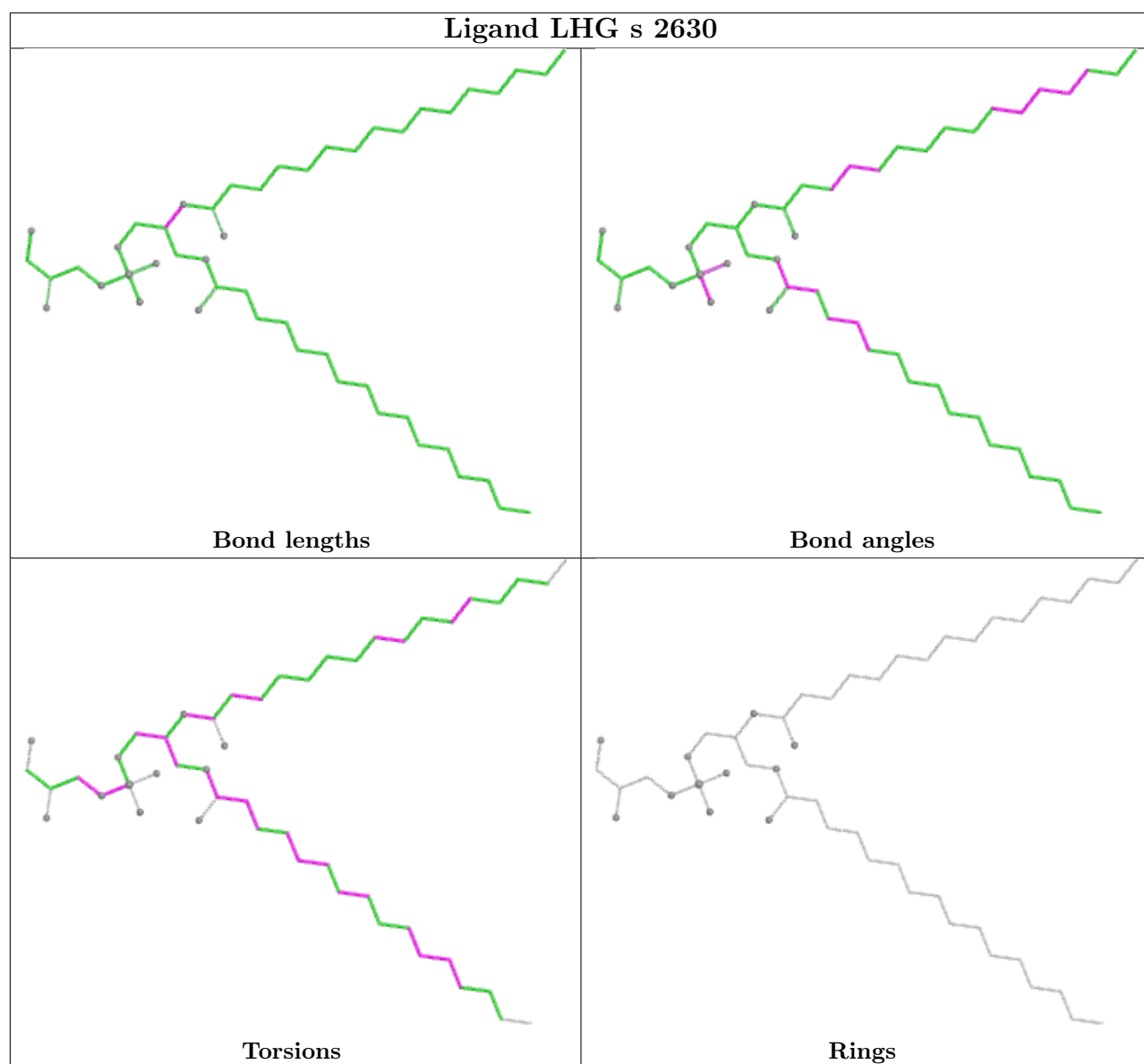
Bond angles

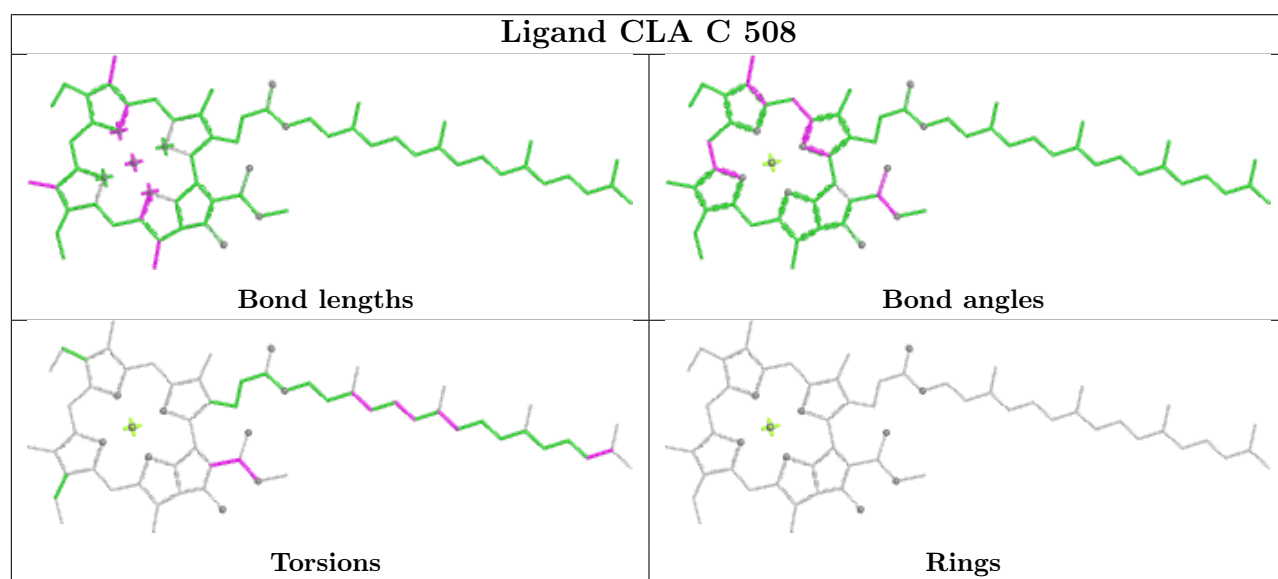
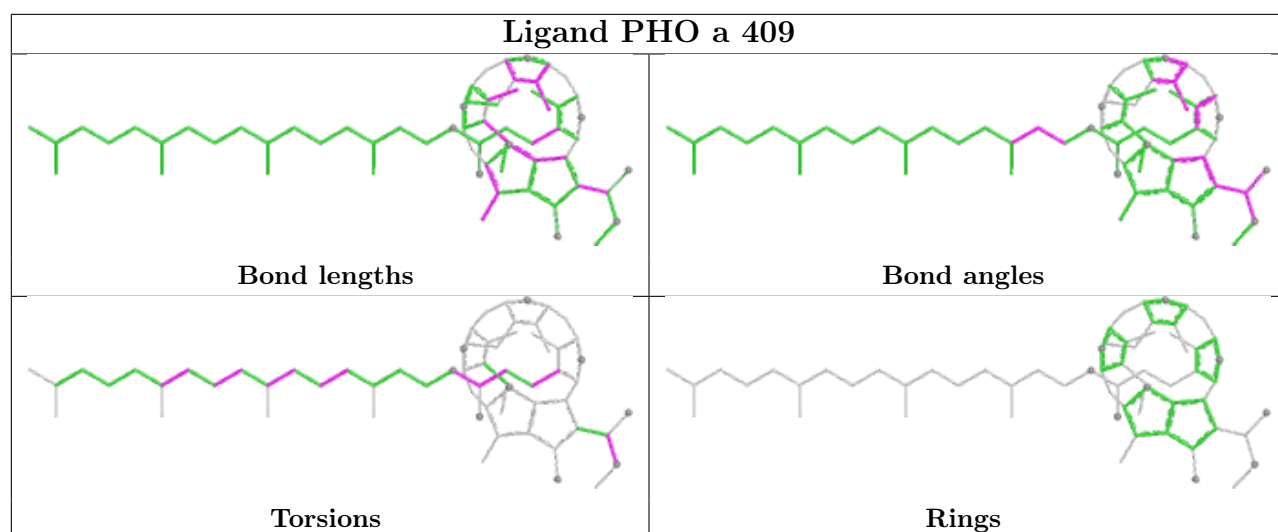


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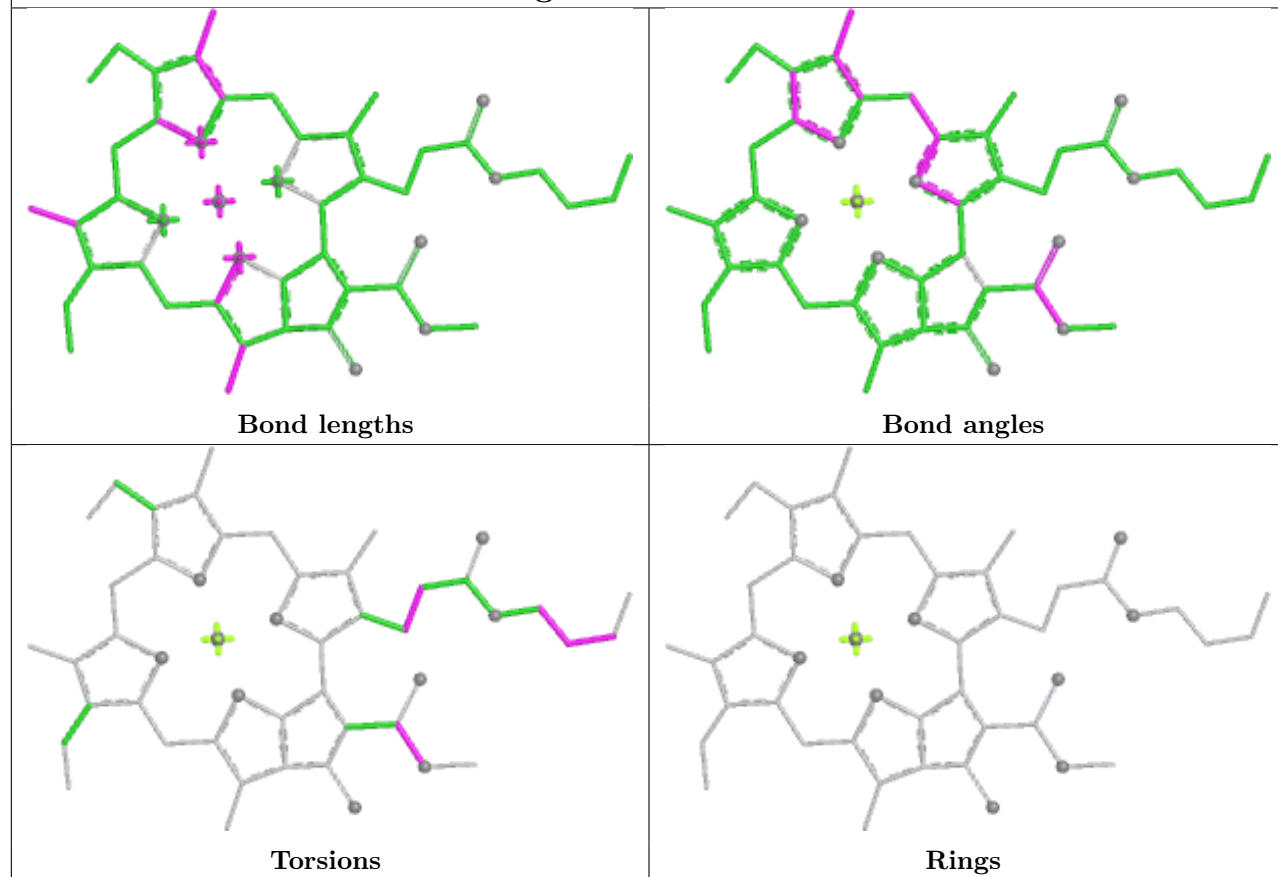


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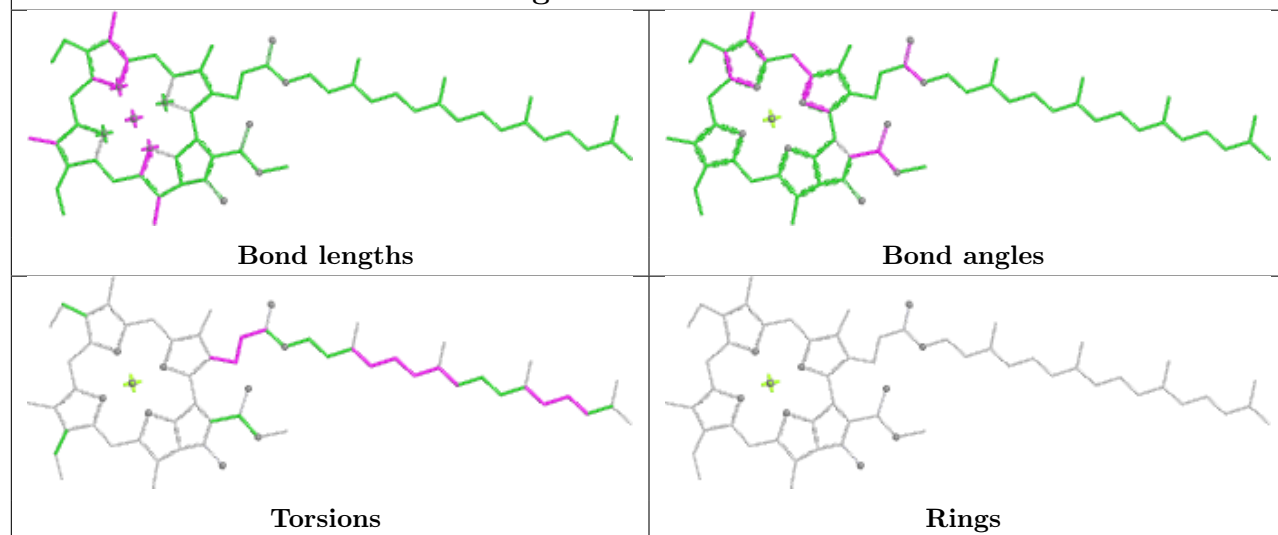


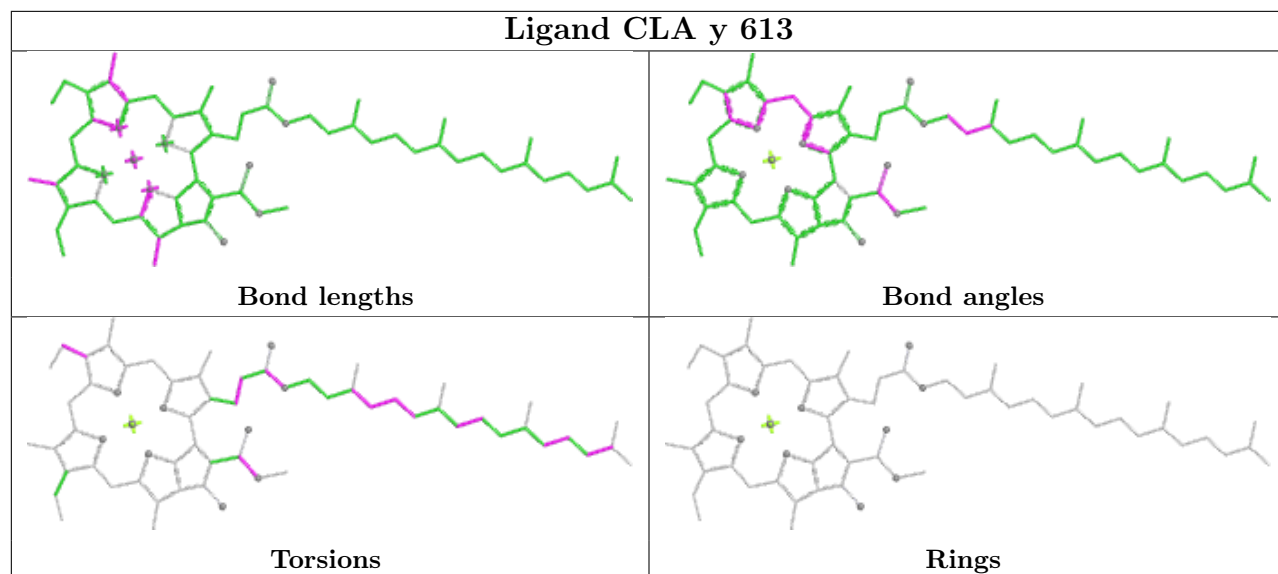
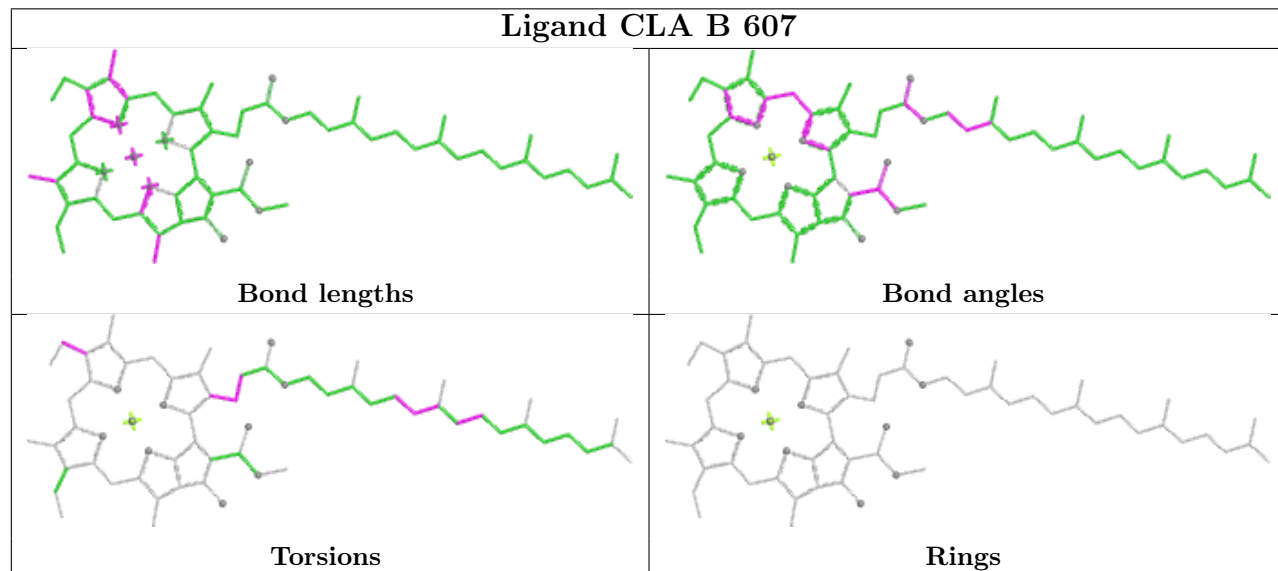


Ligand CLA S 613

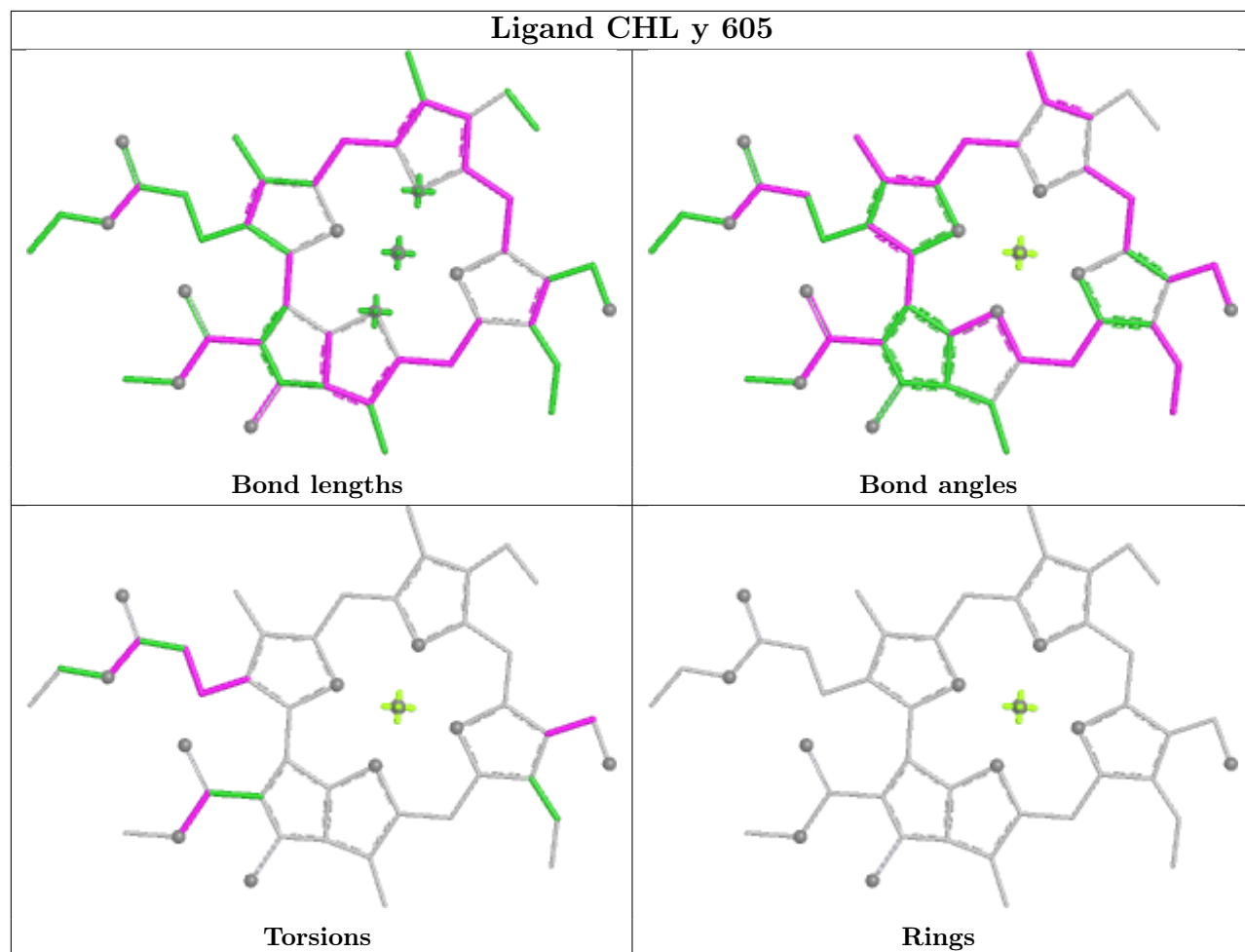


Ligand CLA B 609

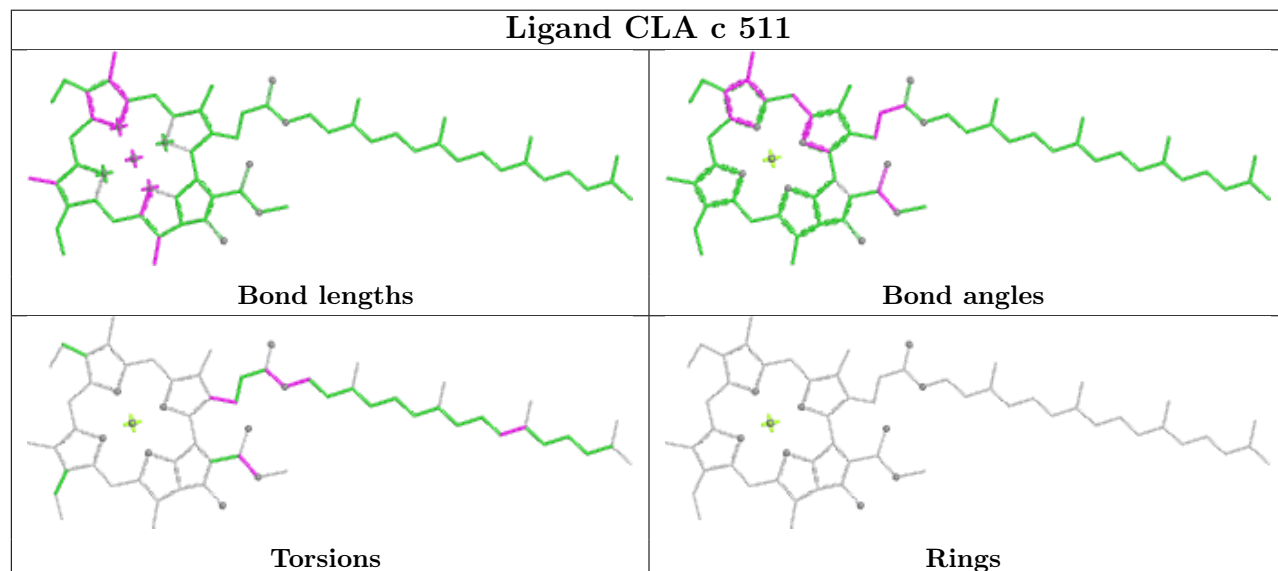


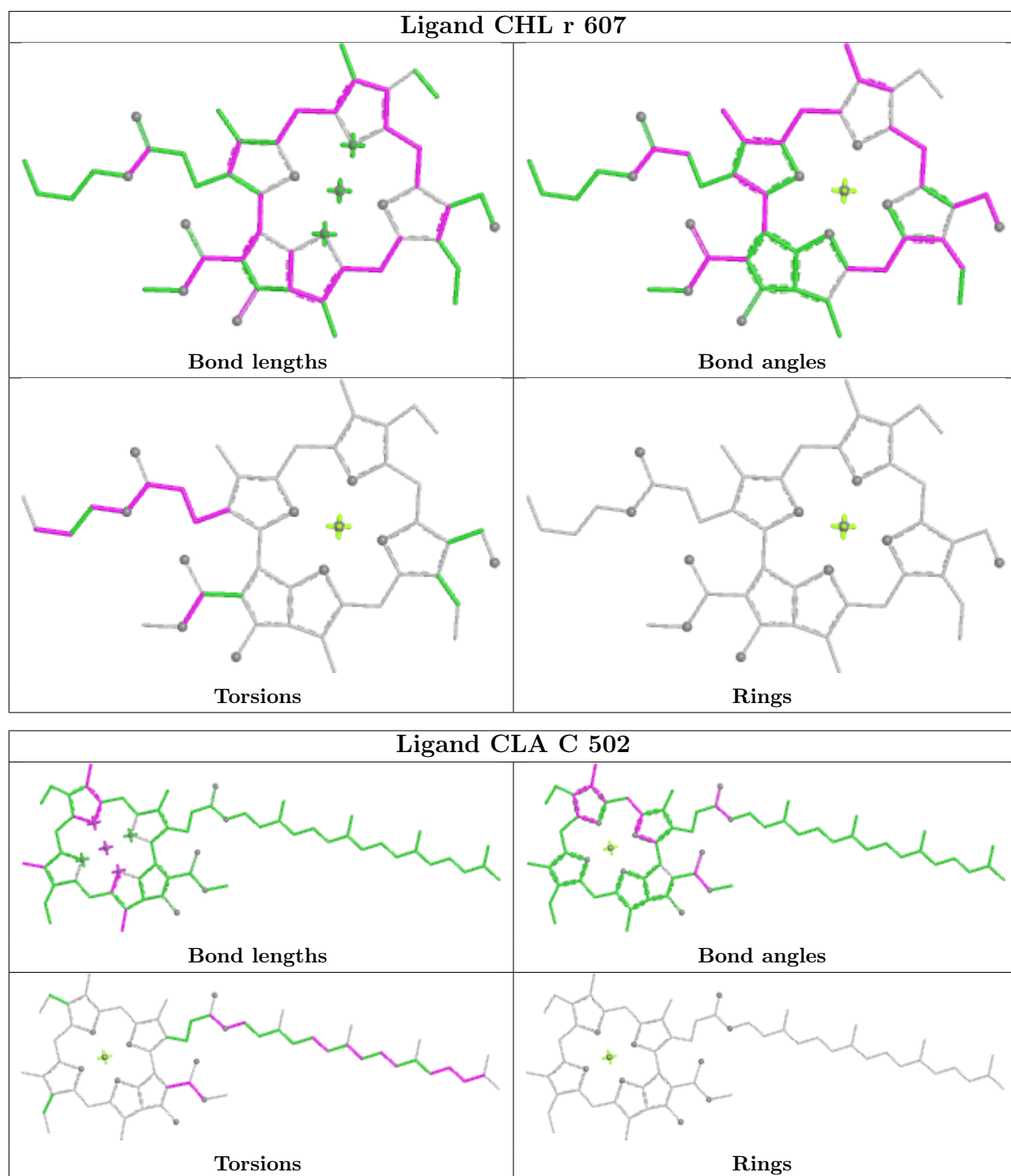
Ligand CLA y 613**Ligand CLA B 607**

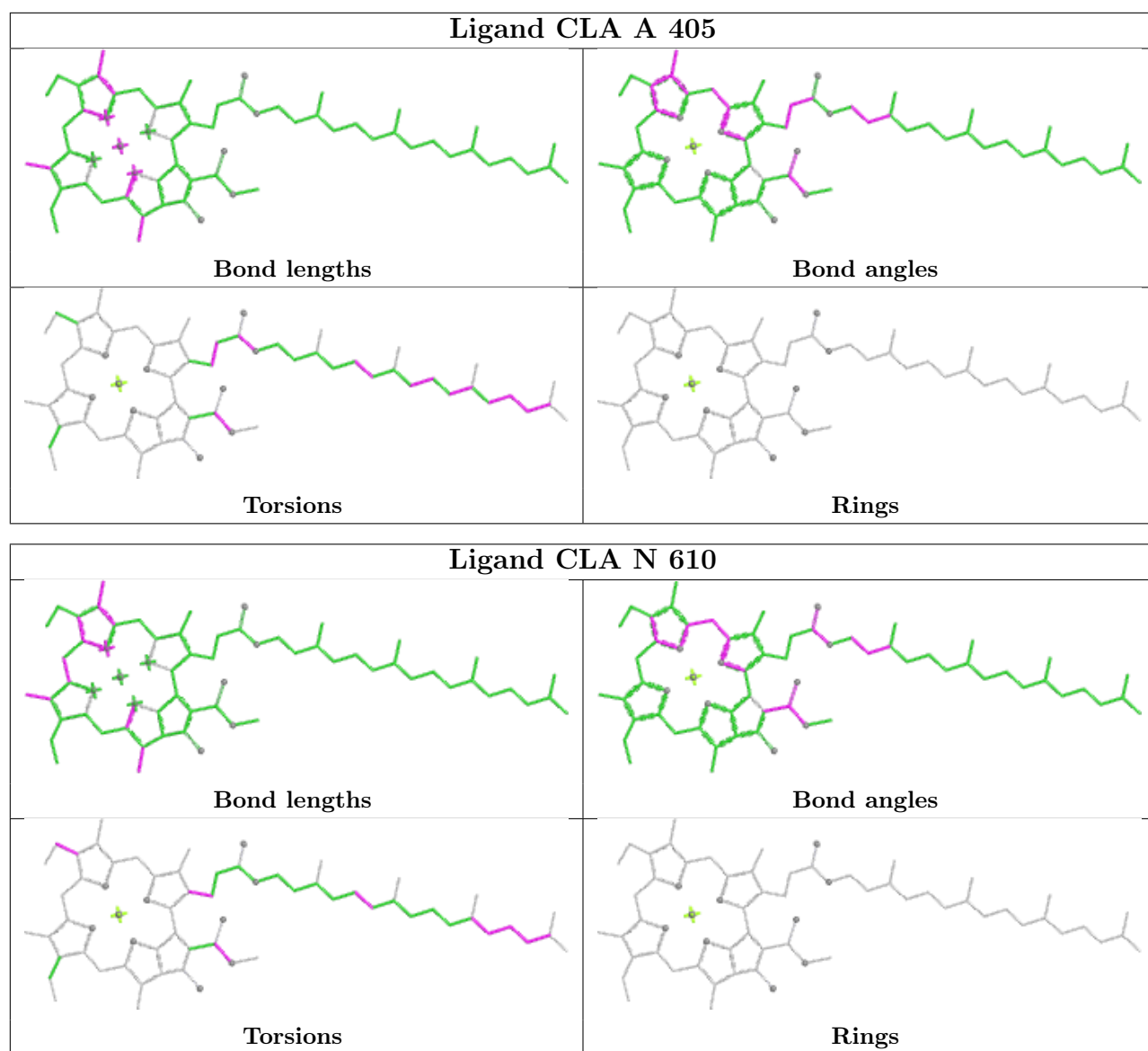
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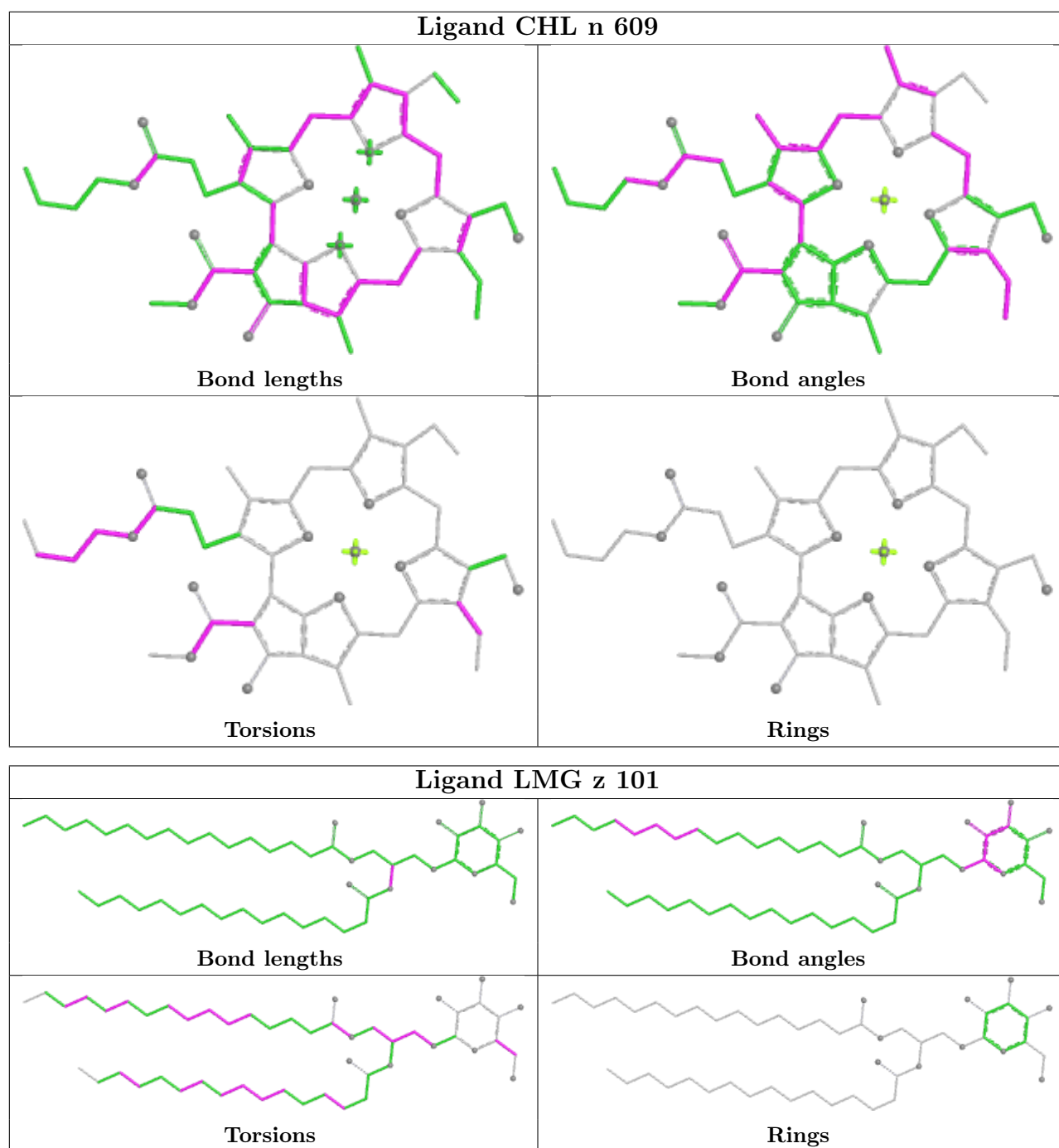


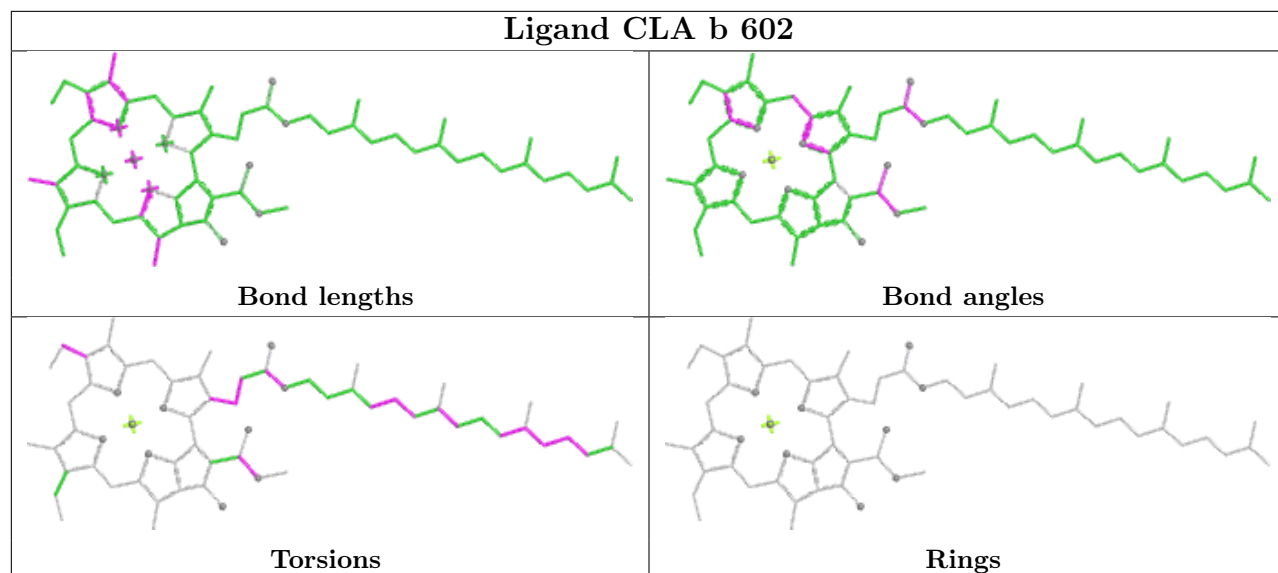
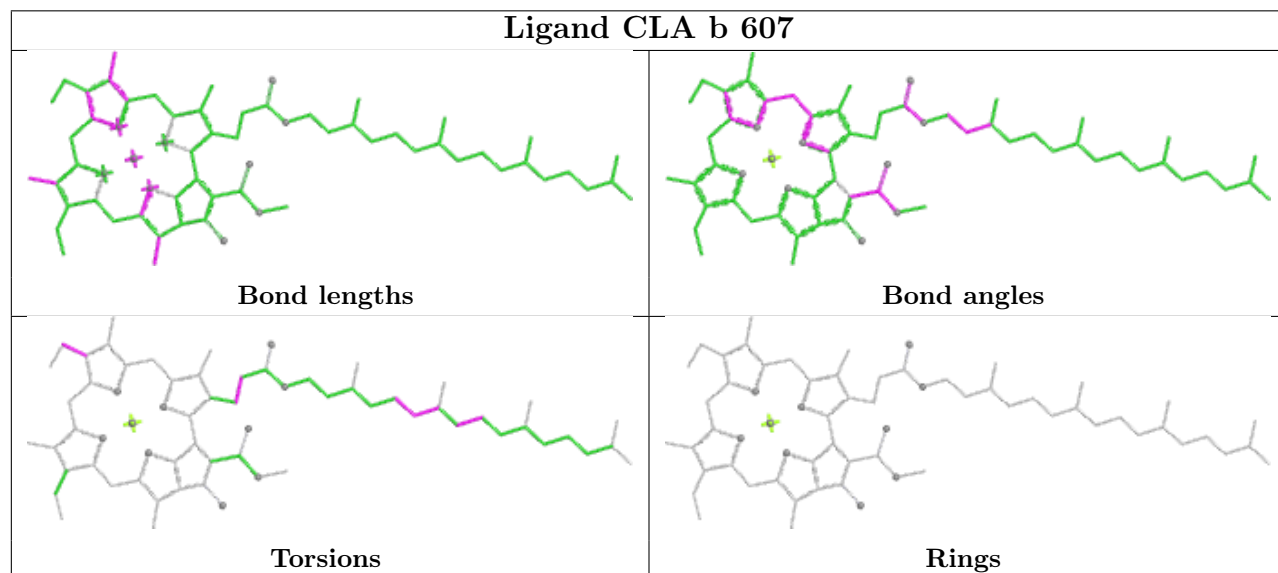
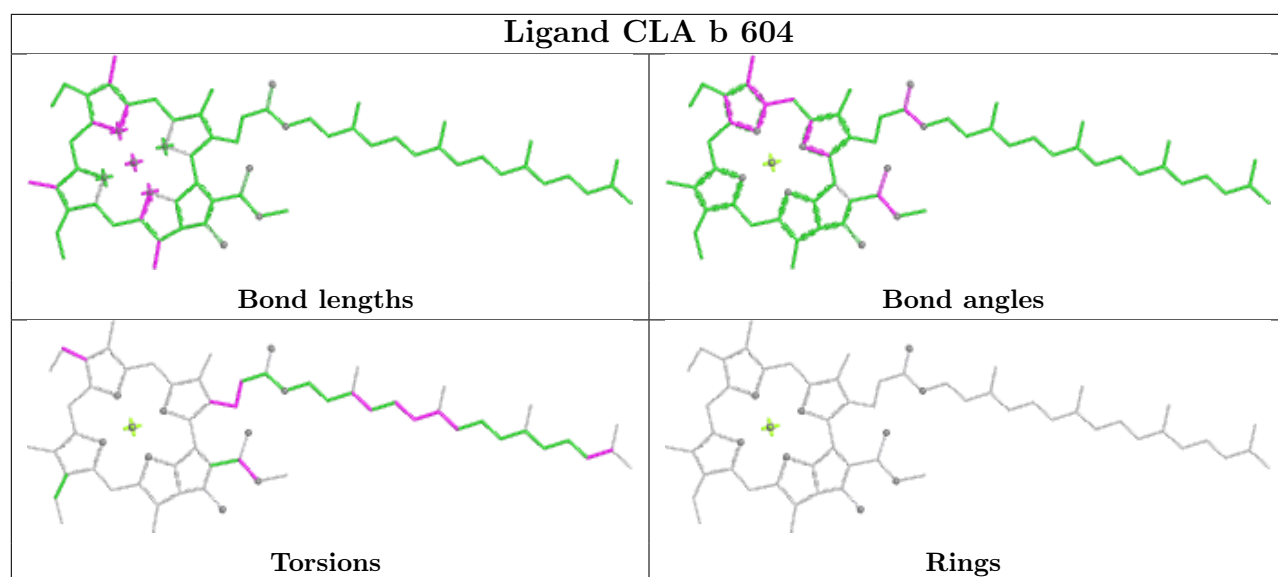
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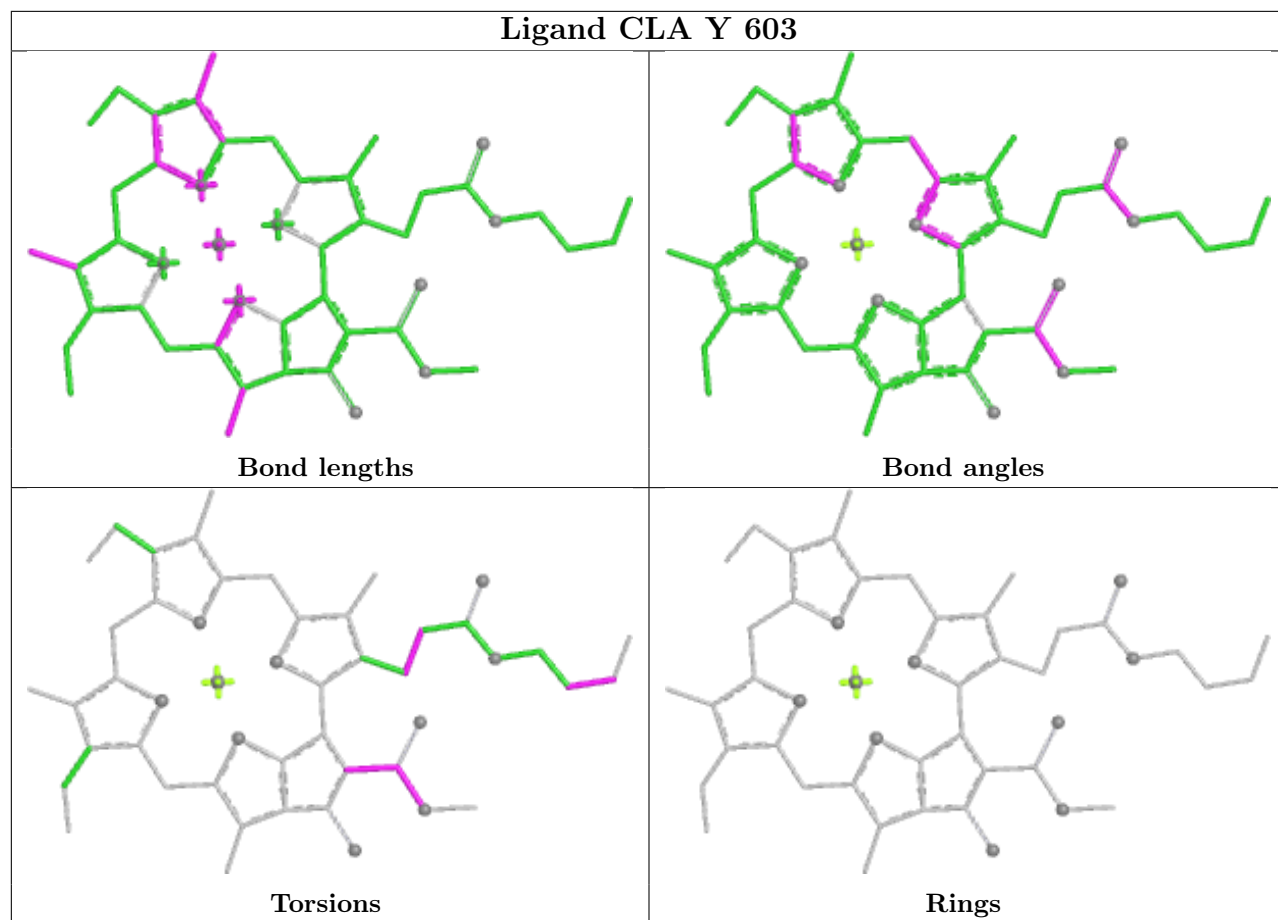


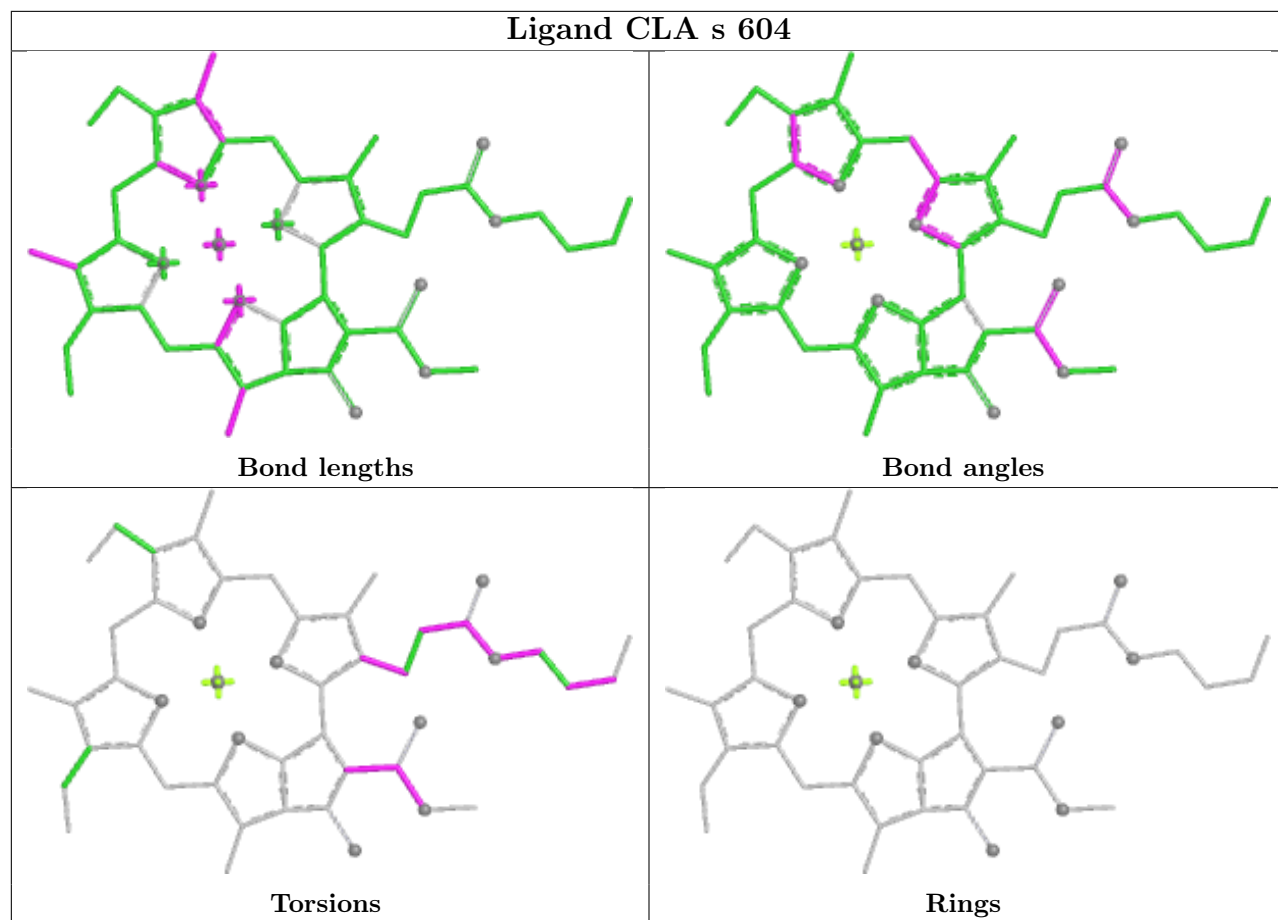


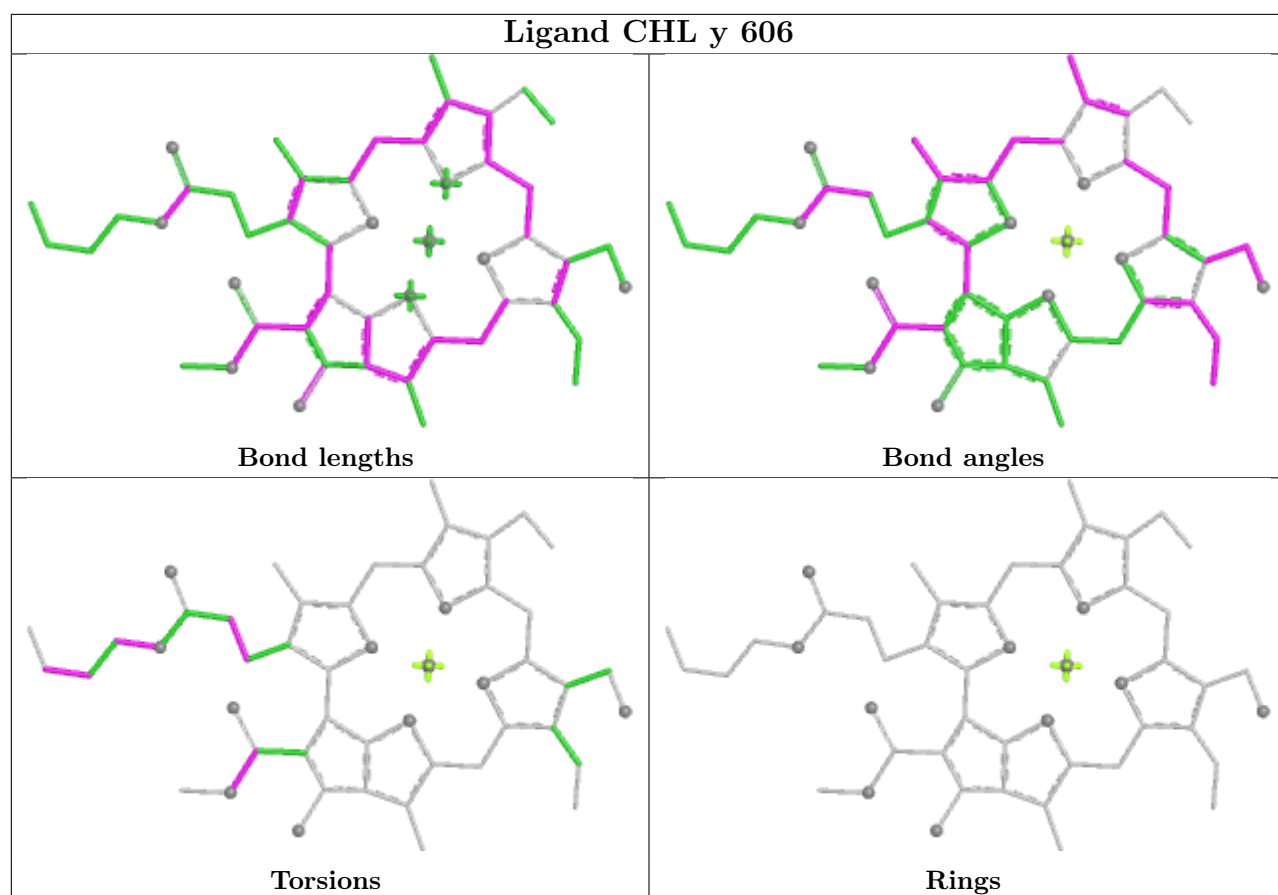


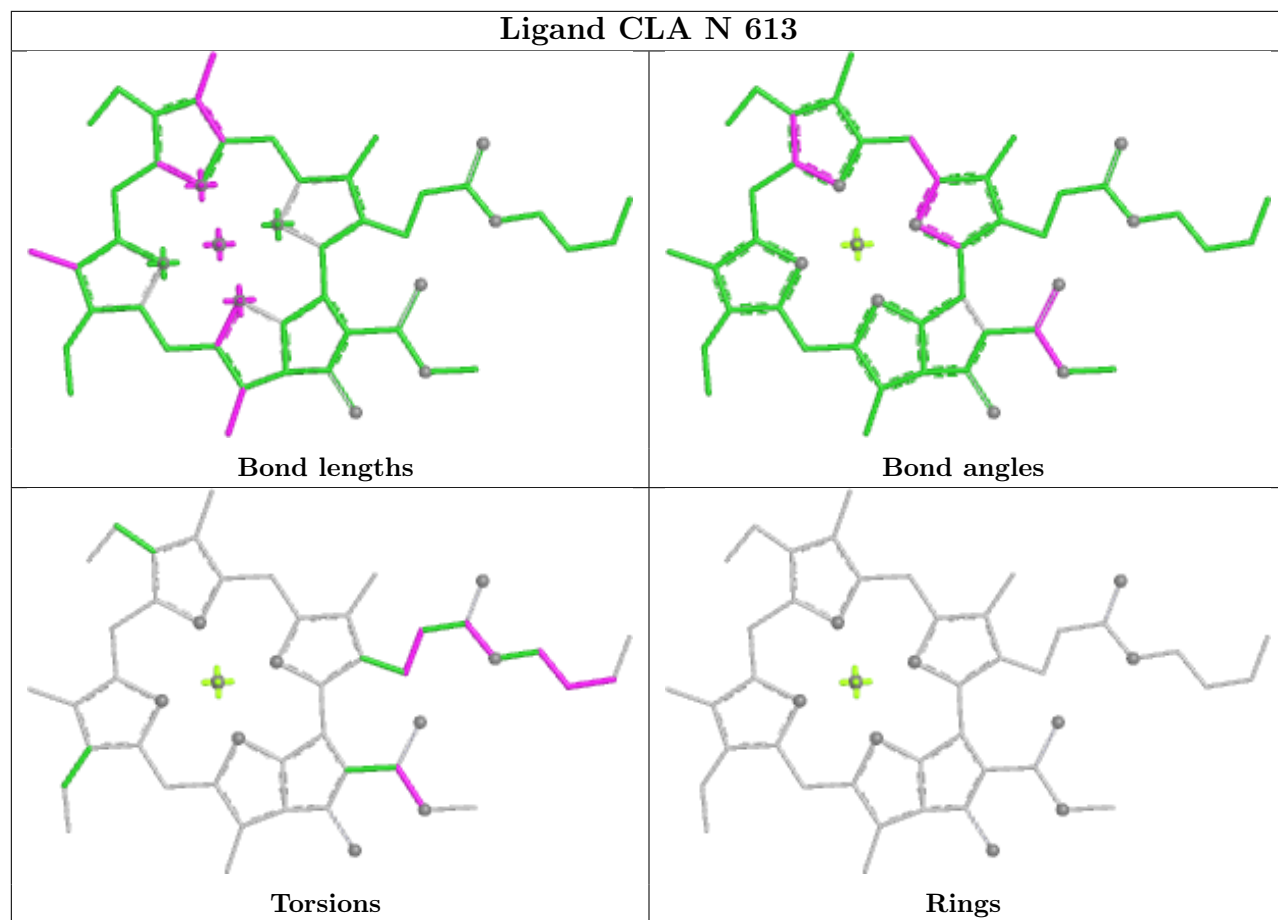


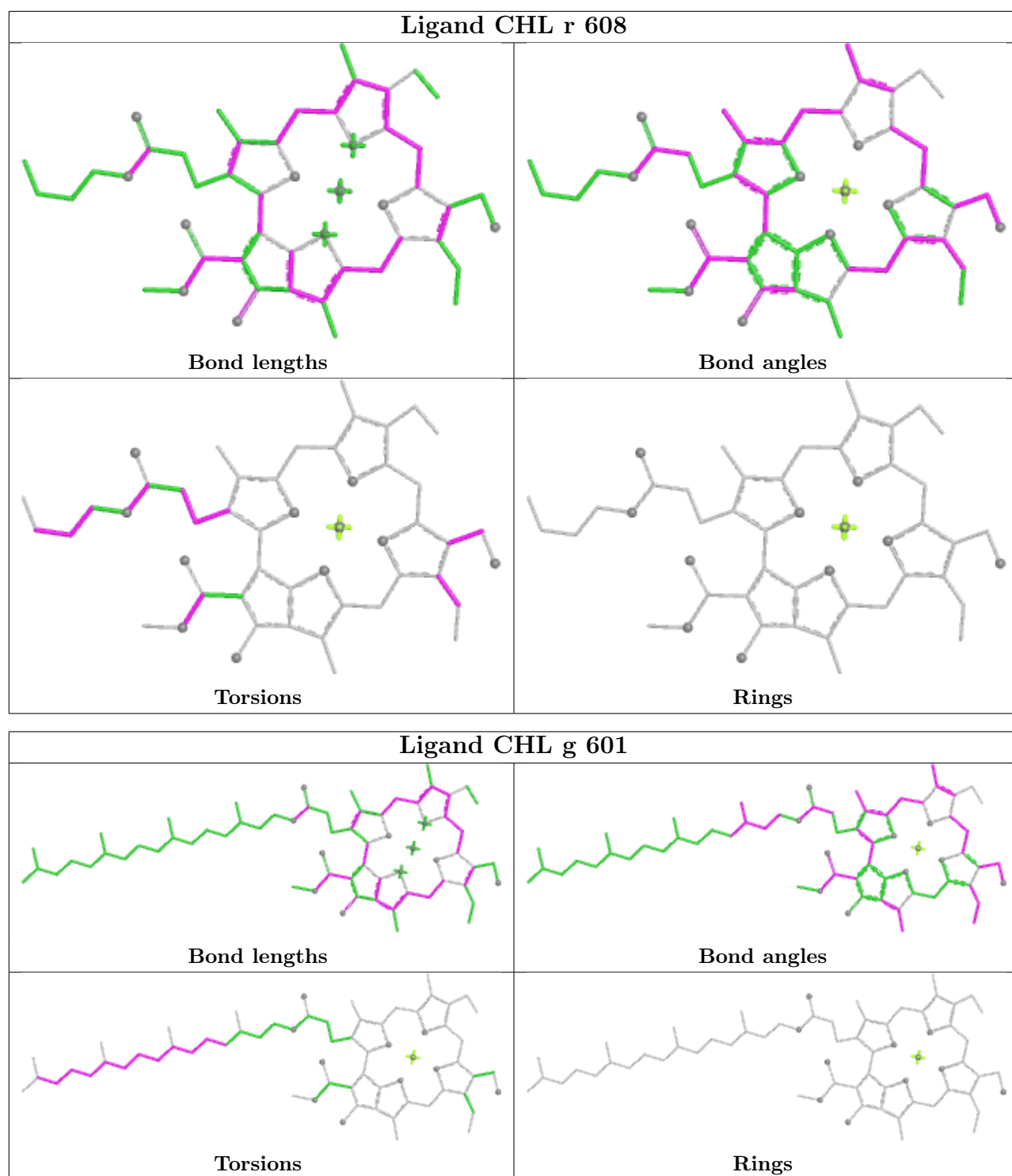


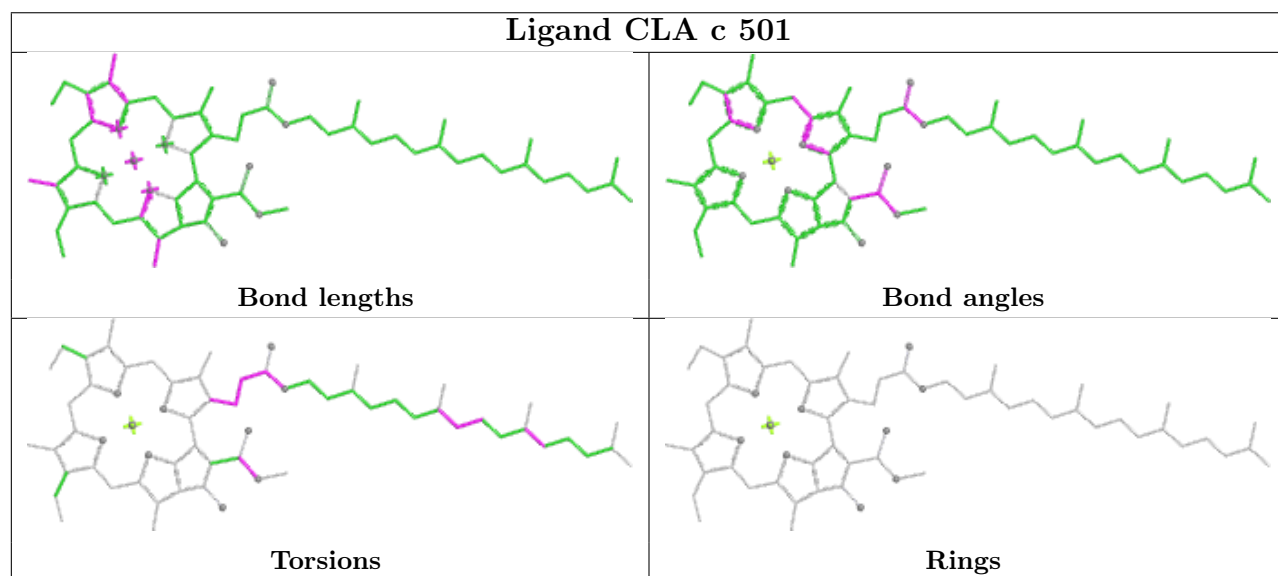
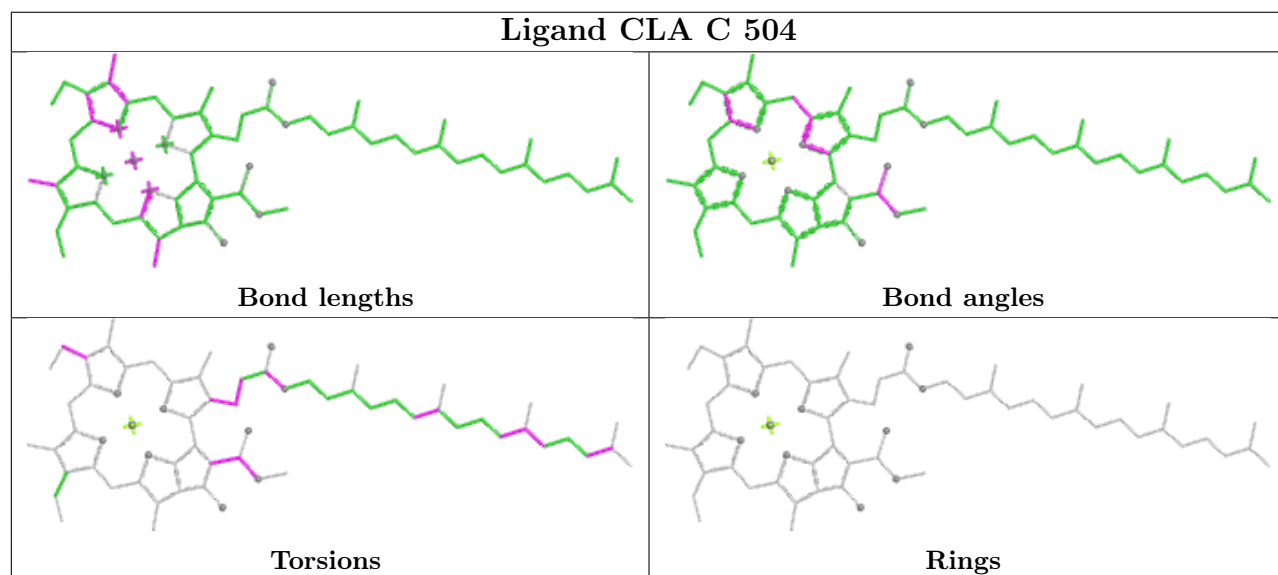
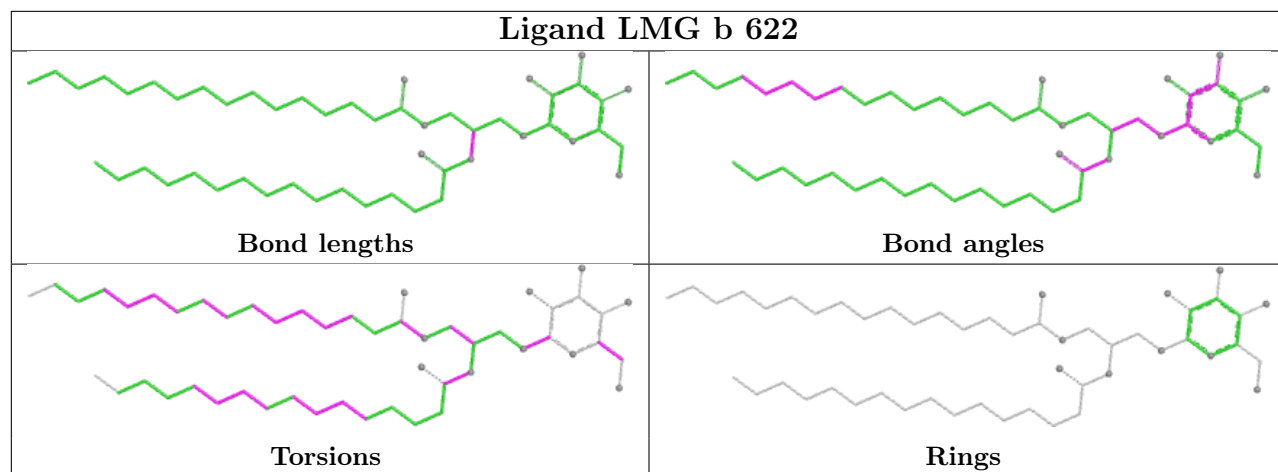




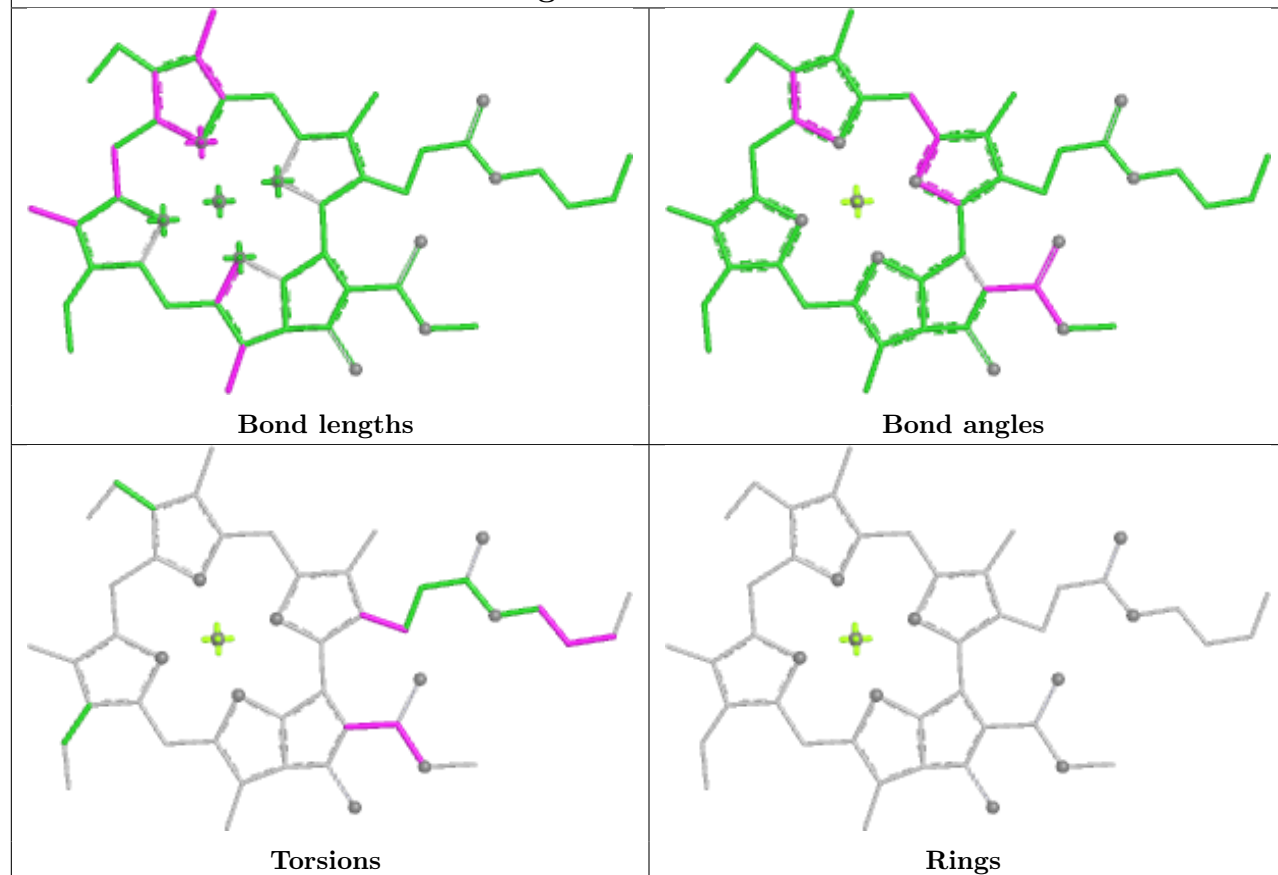




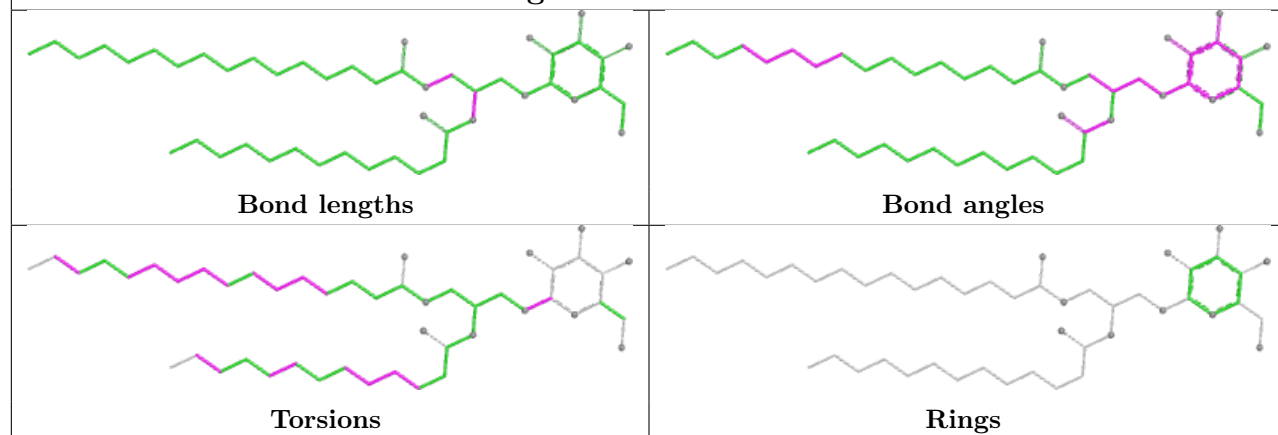




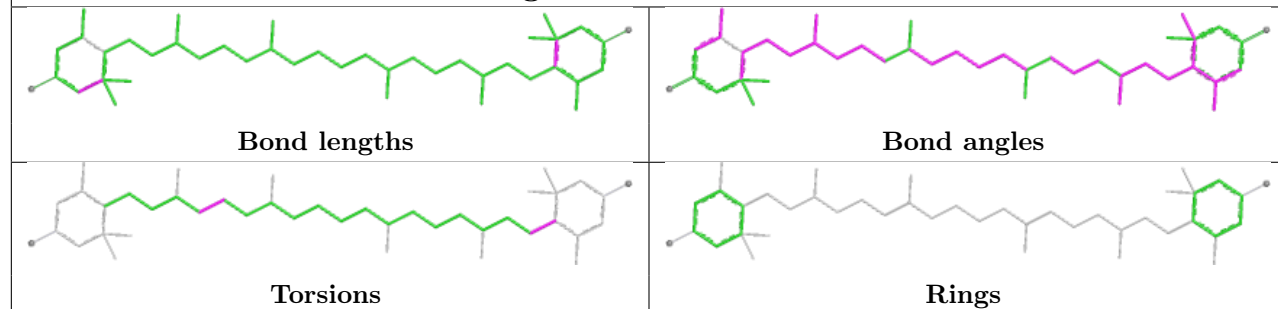
Ligand CLA s 602

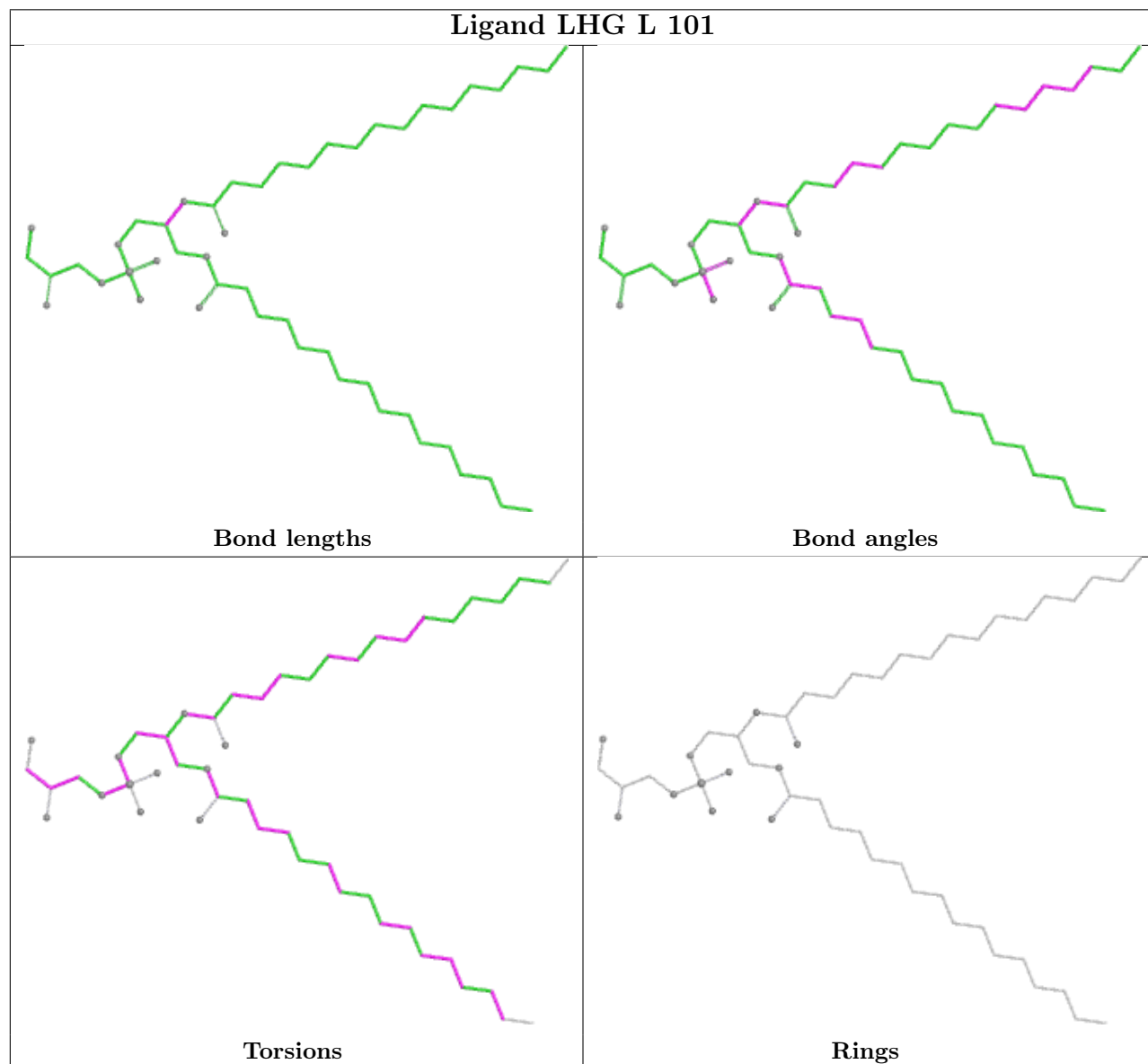
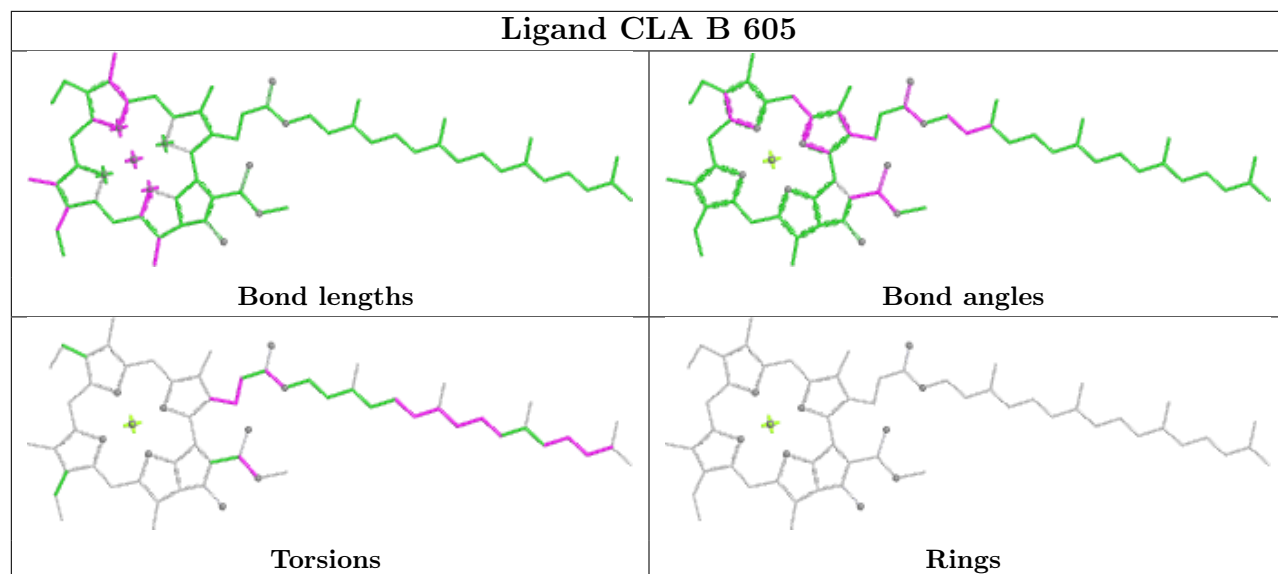


Ligand LMG A 413

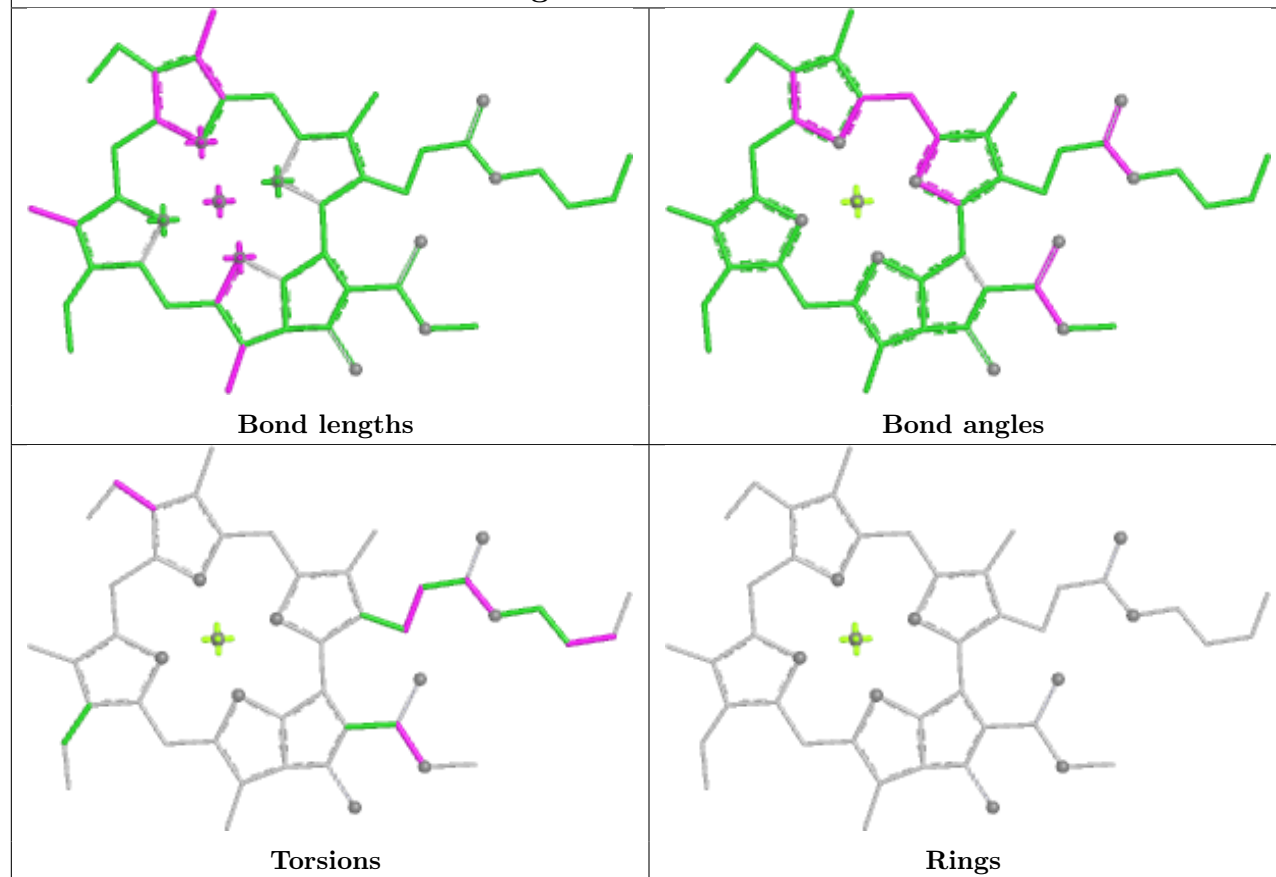


Ligand LUT N 1621

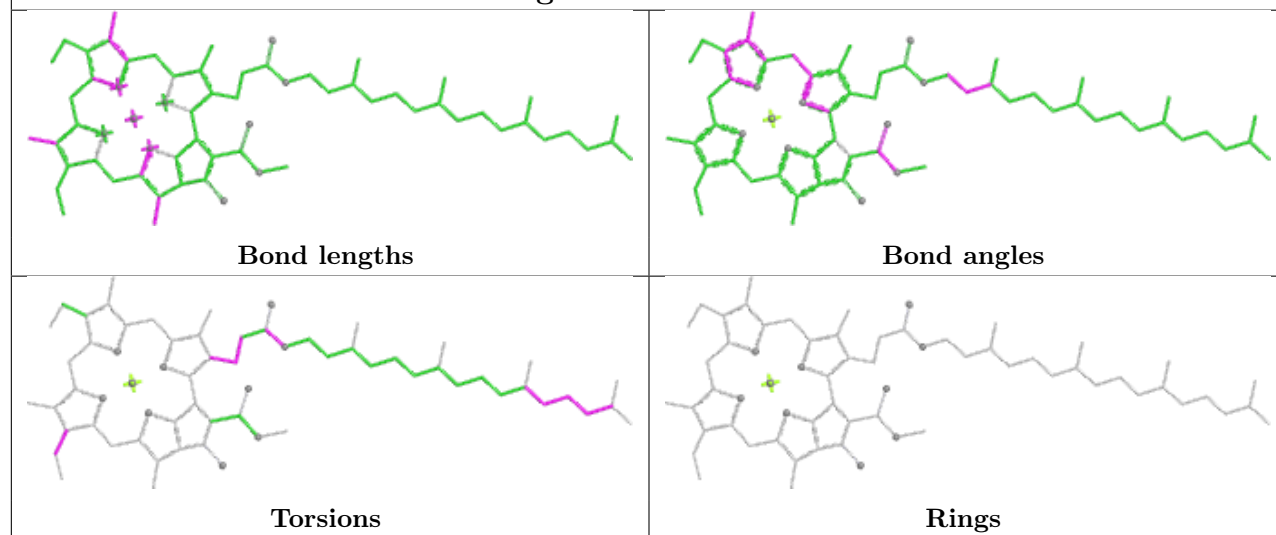


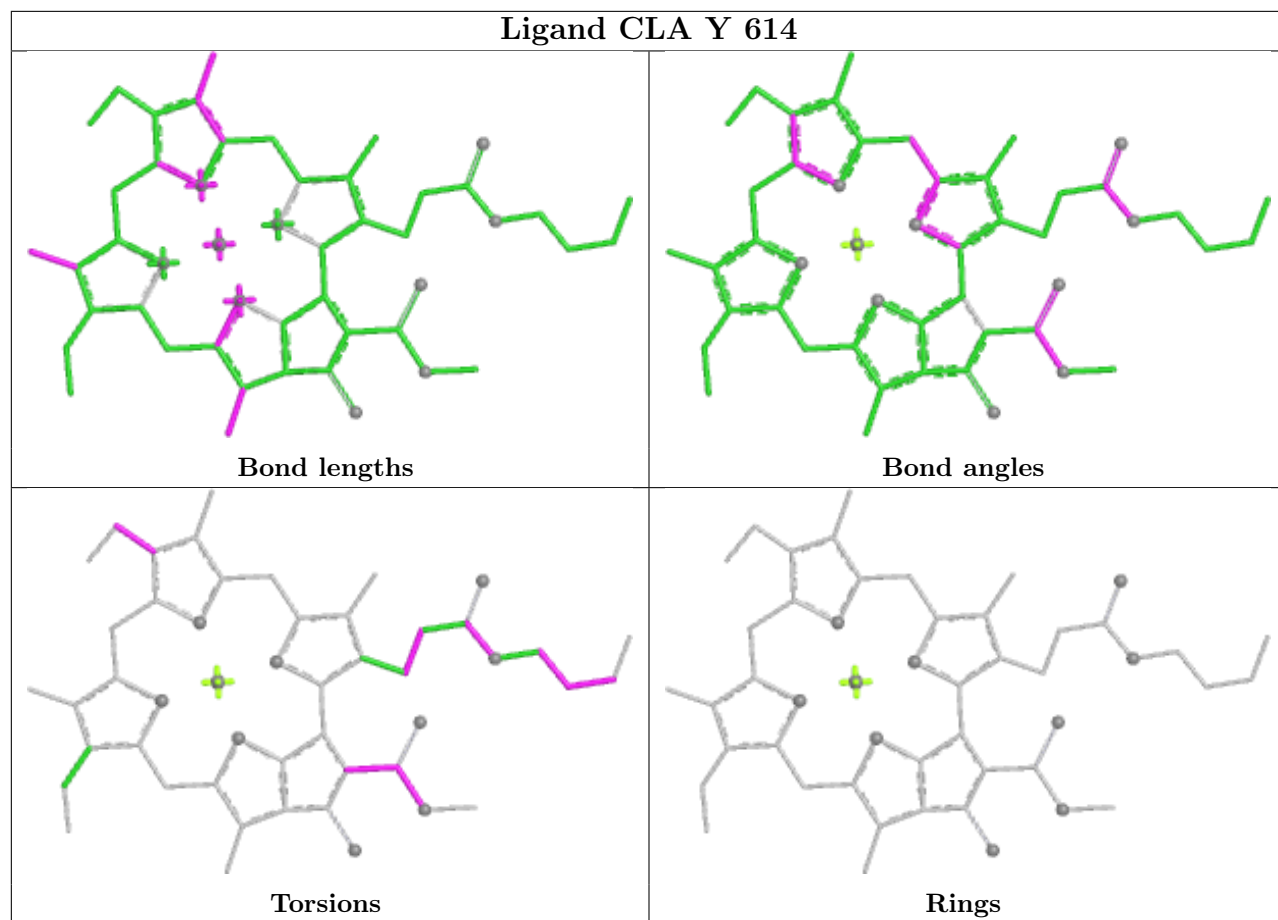


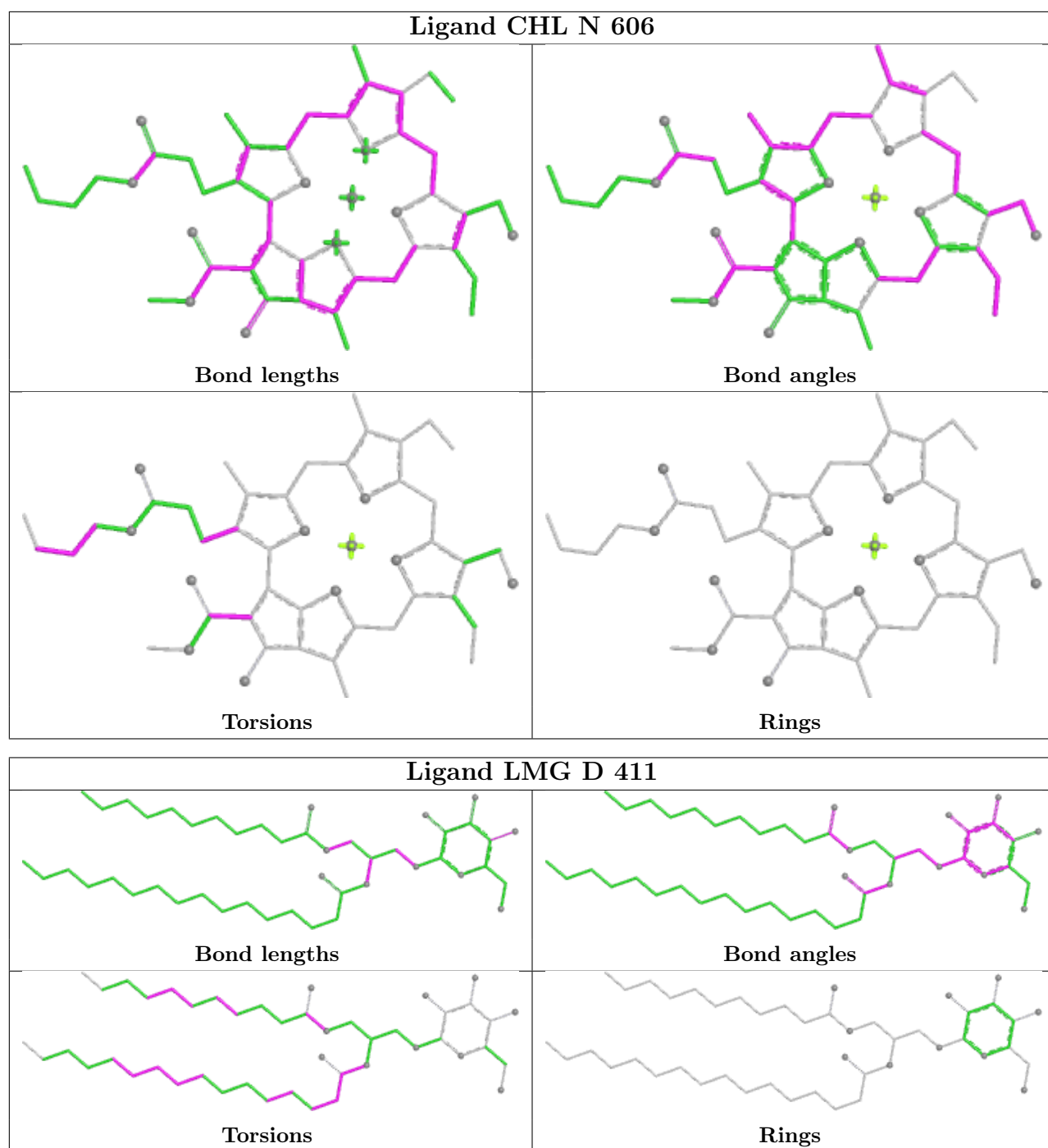
Ligand CLA G 613

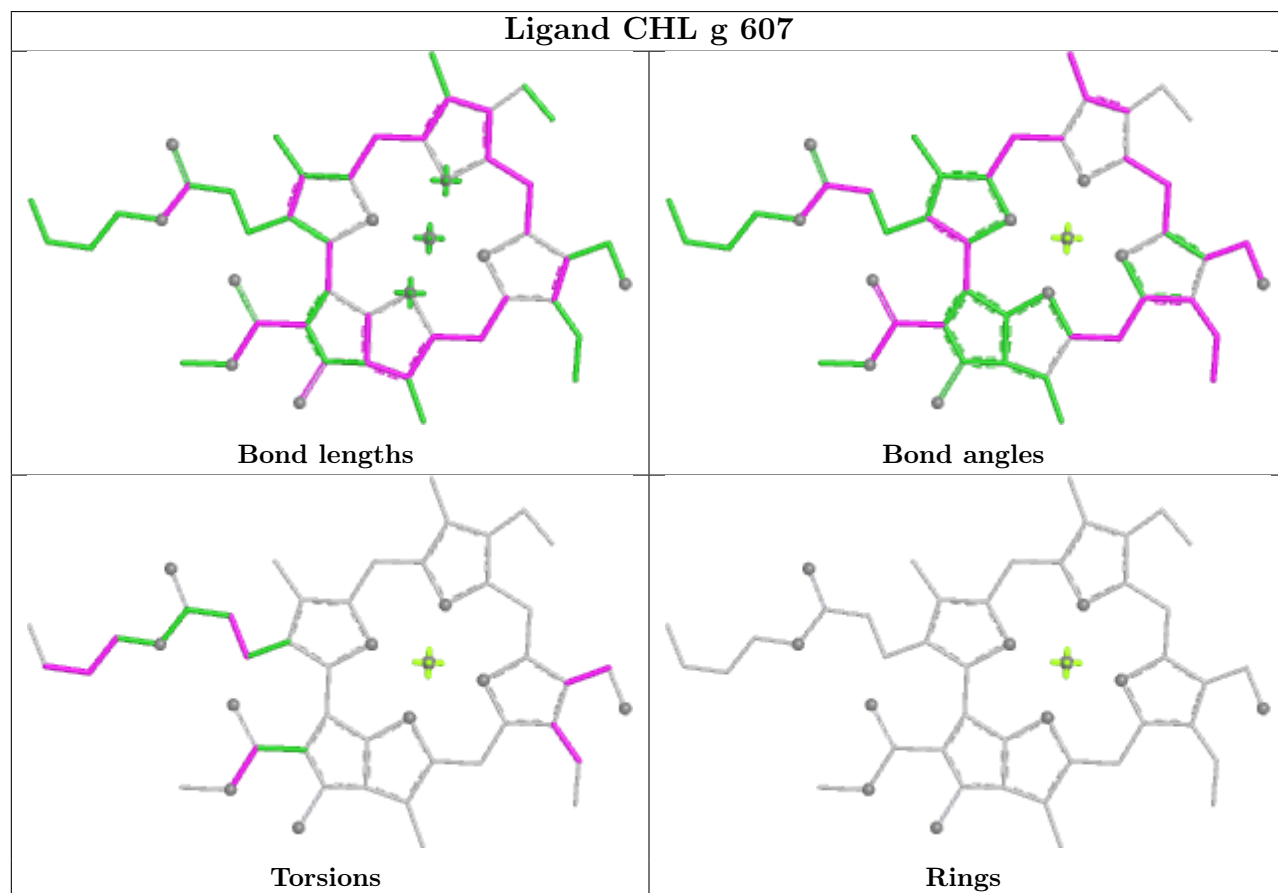
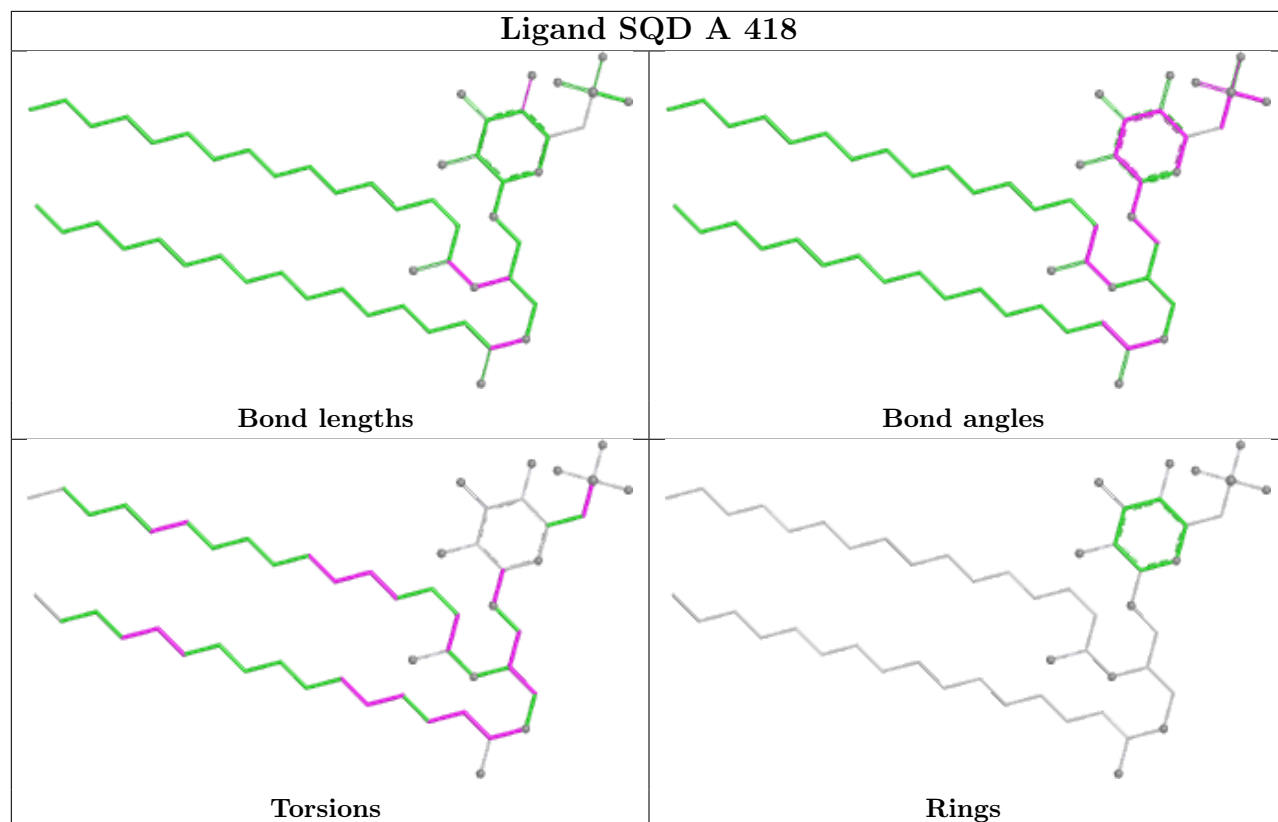


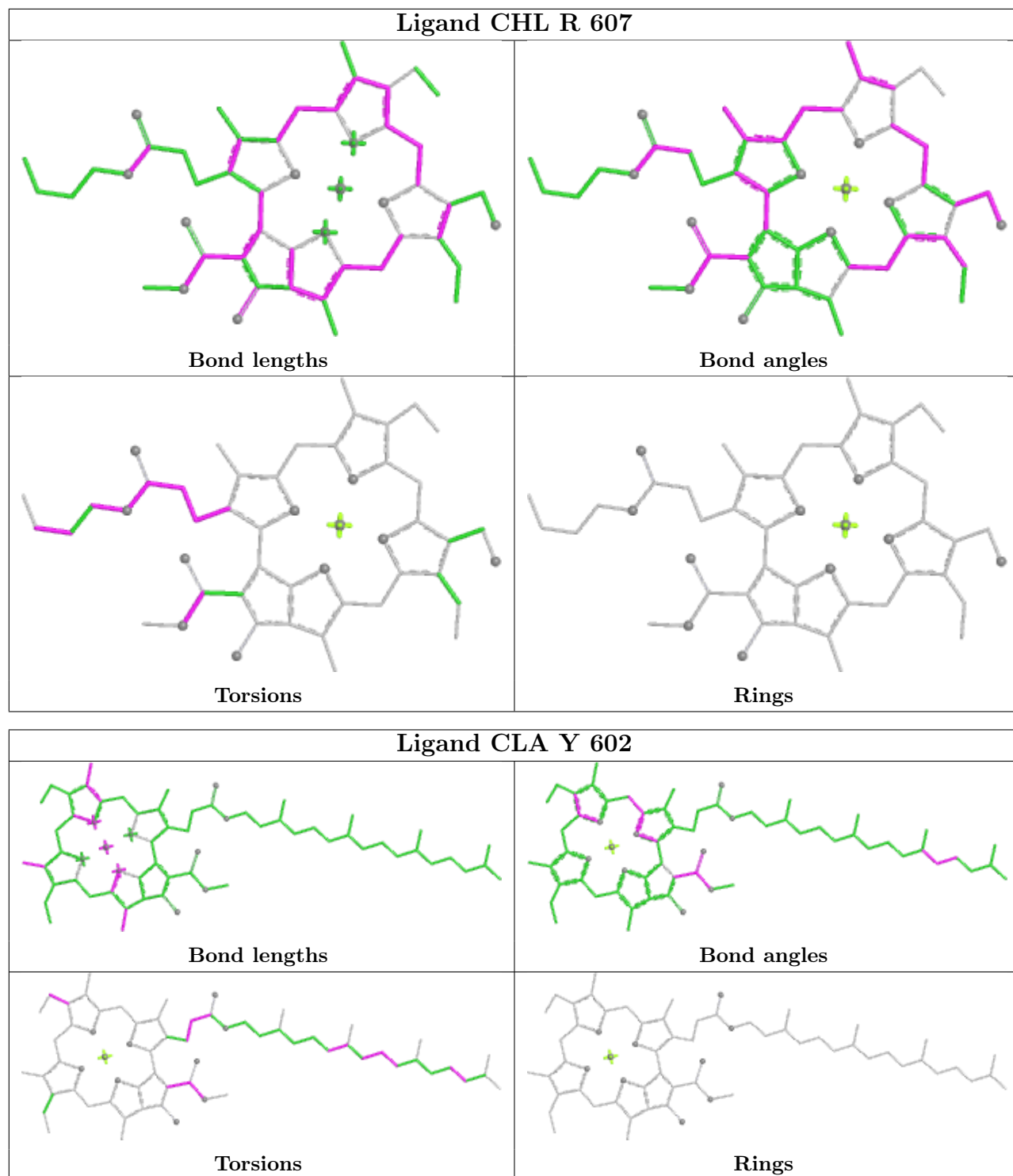
Ligand CLA a 406

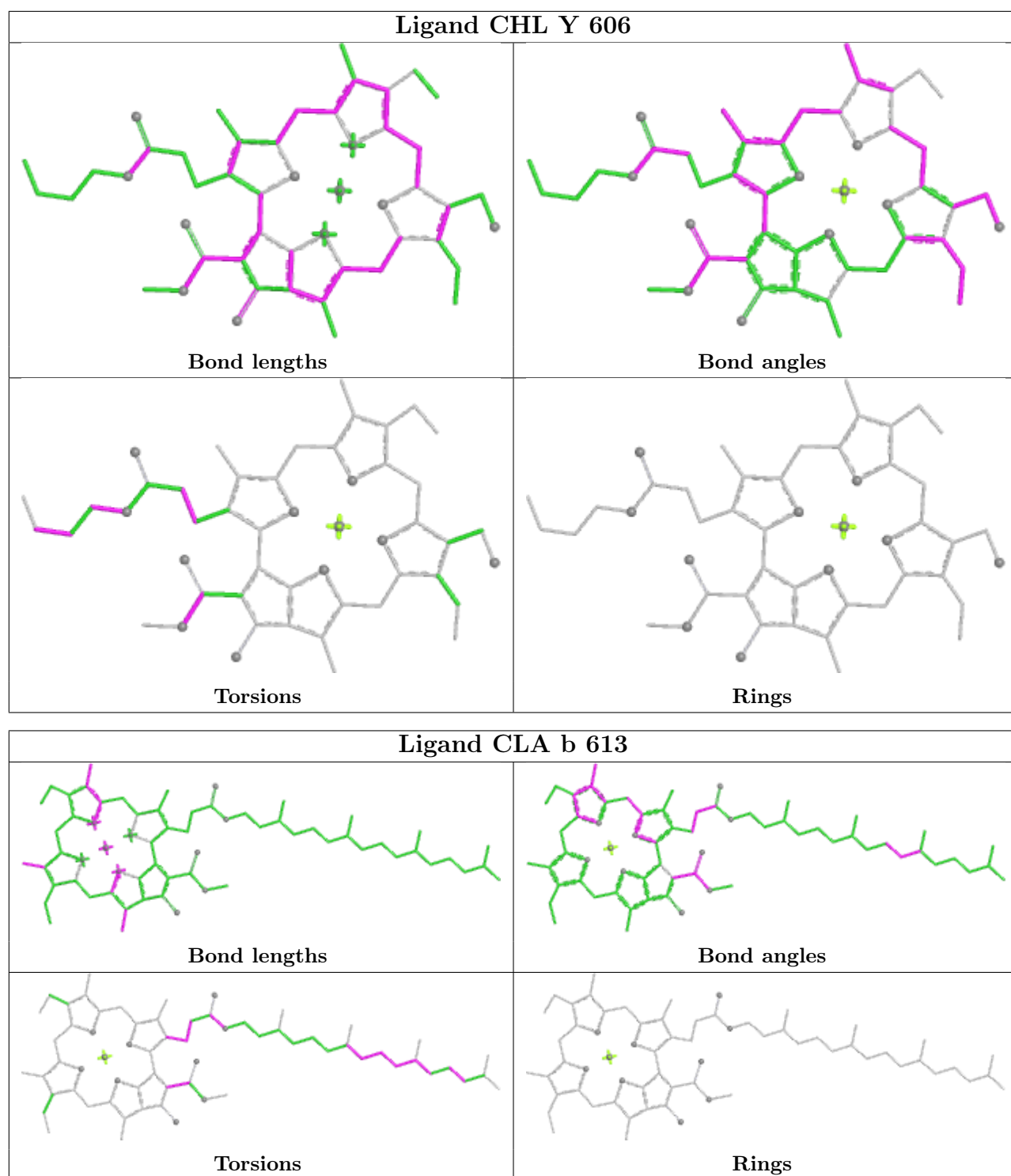


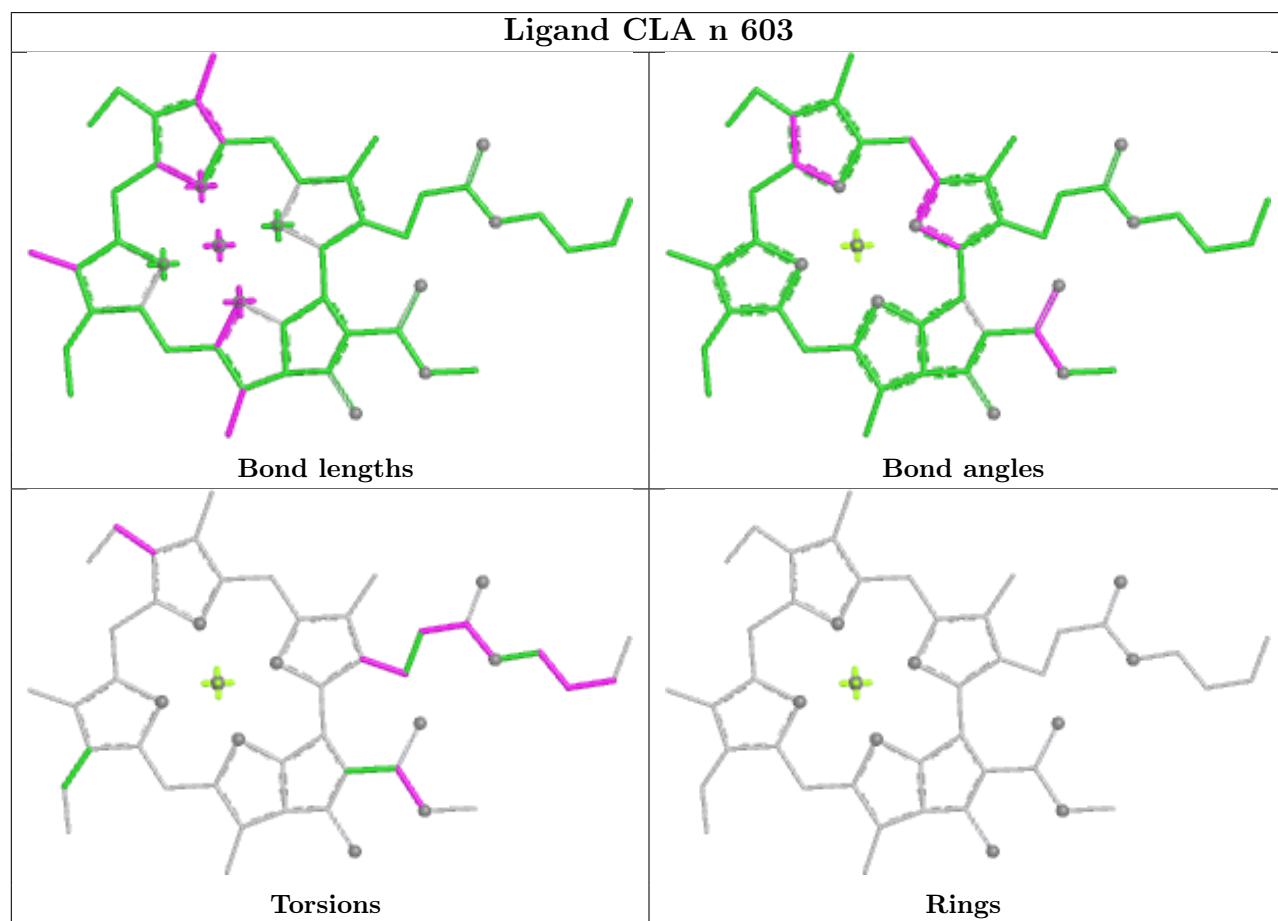
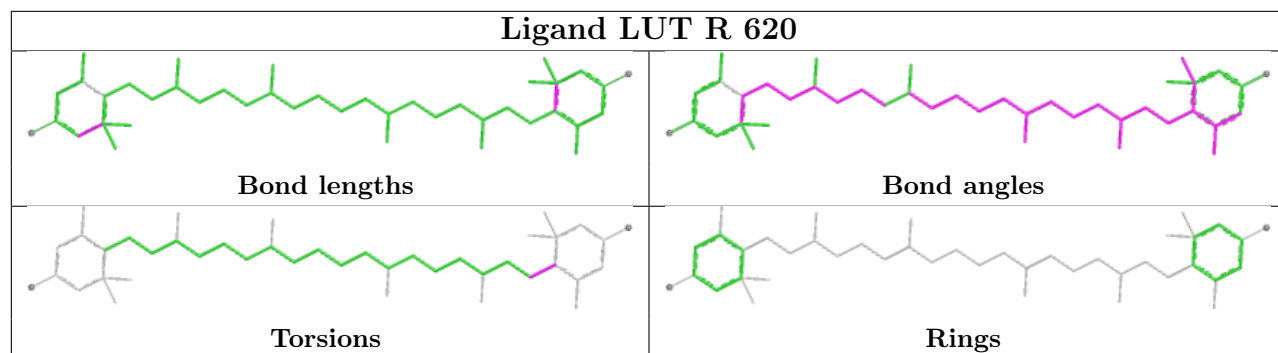


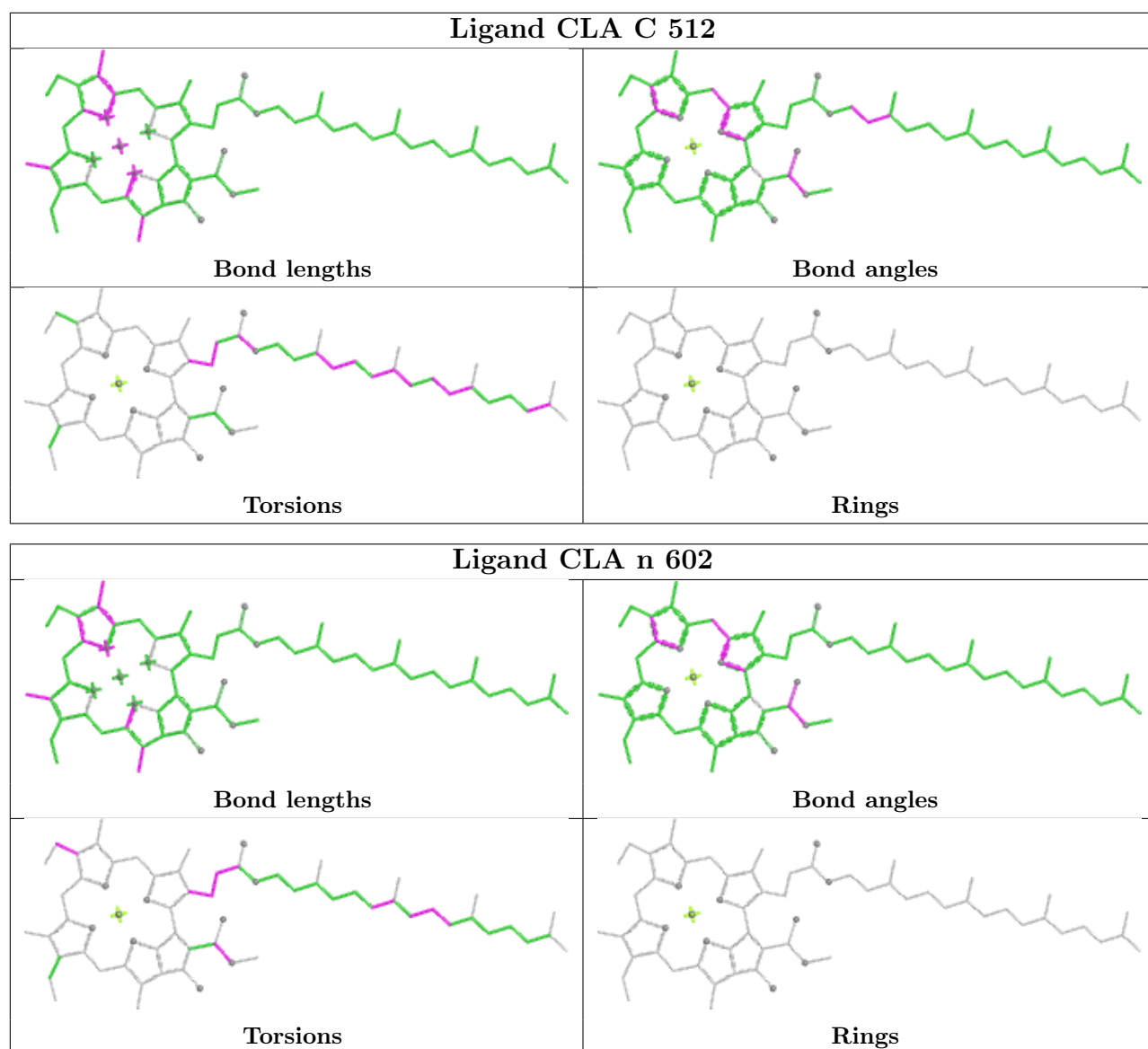




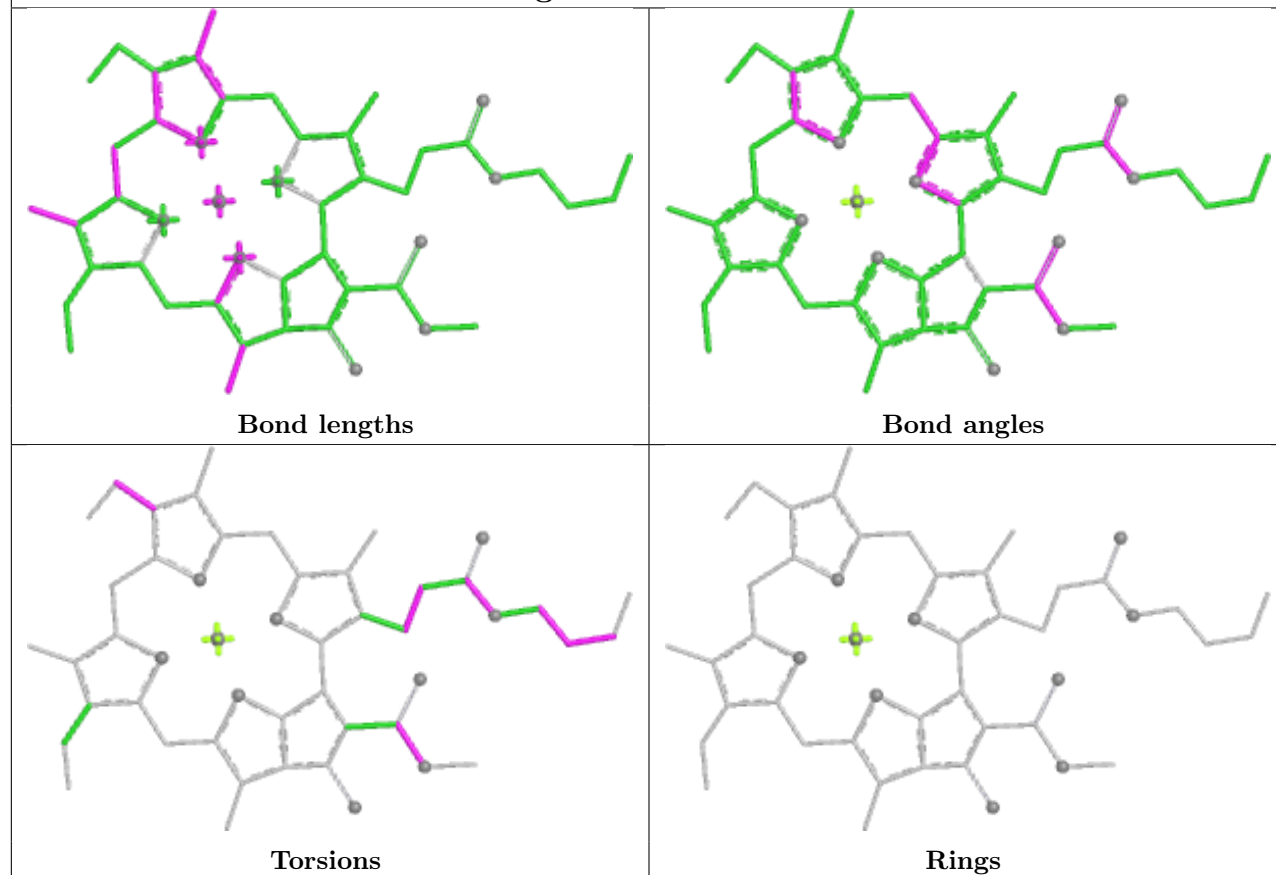




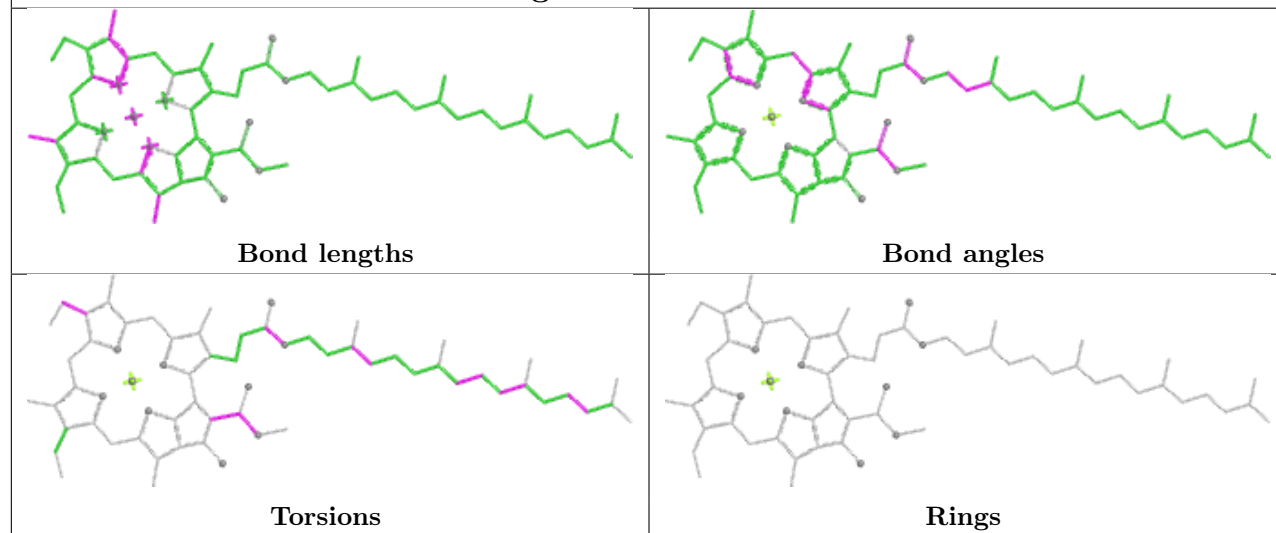


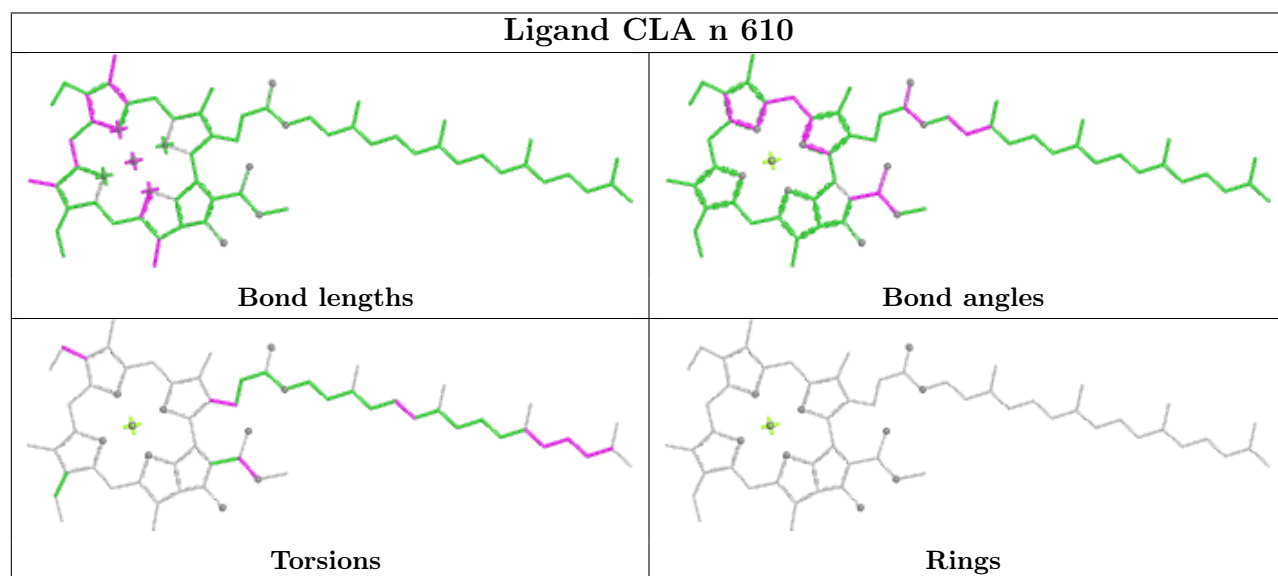
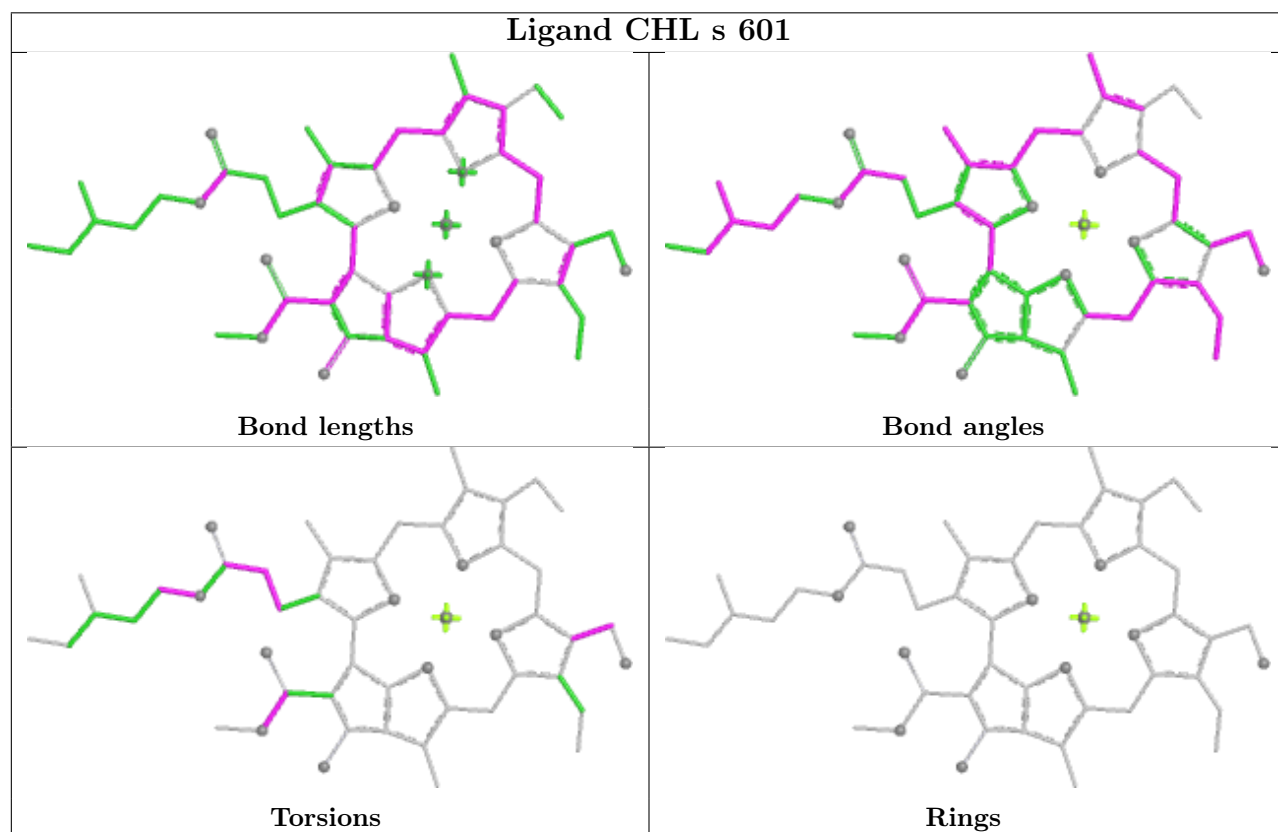
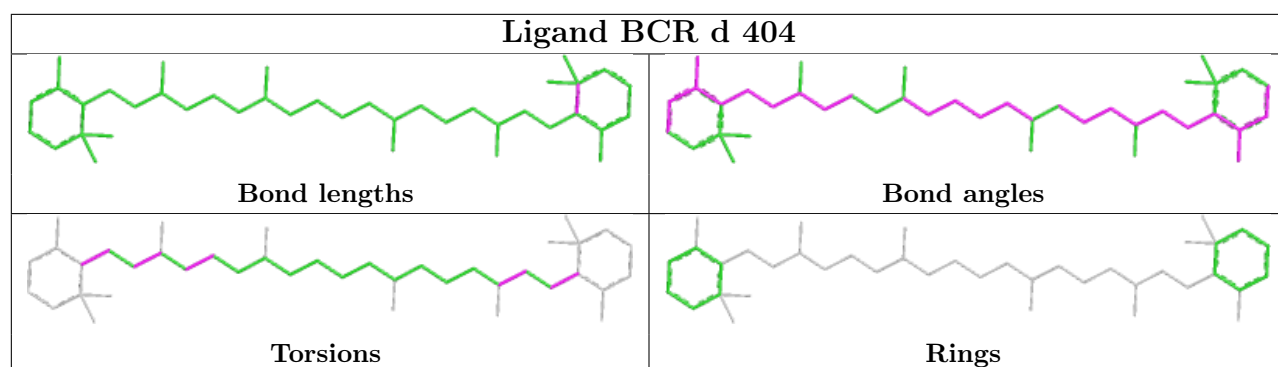


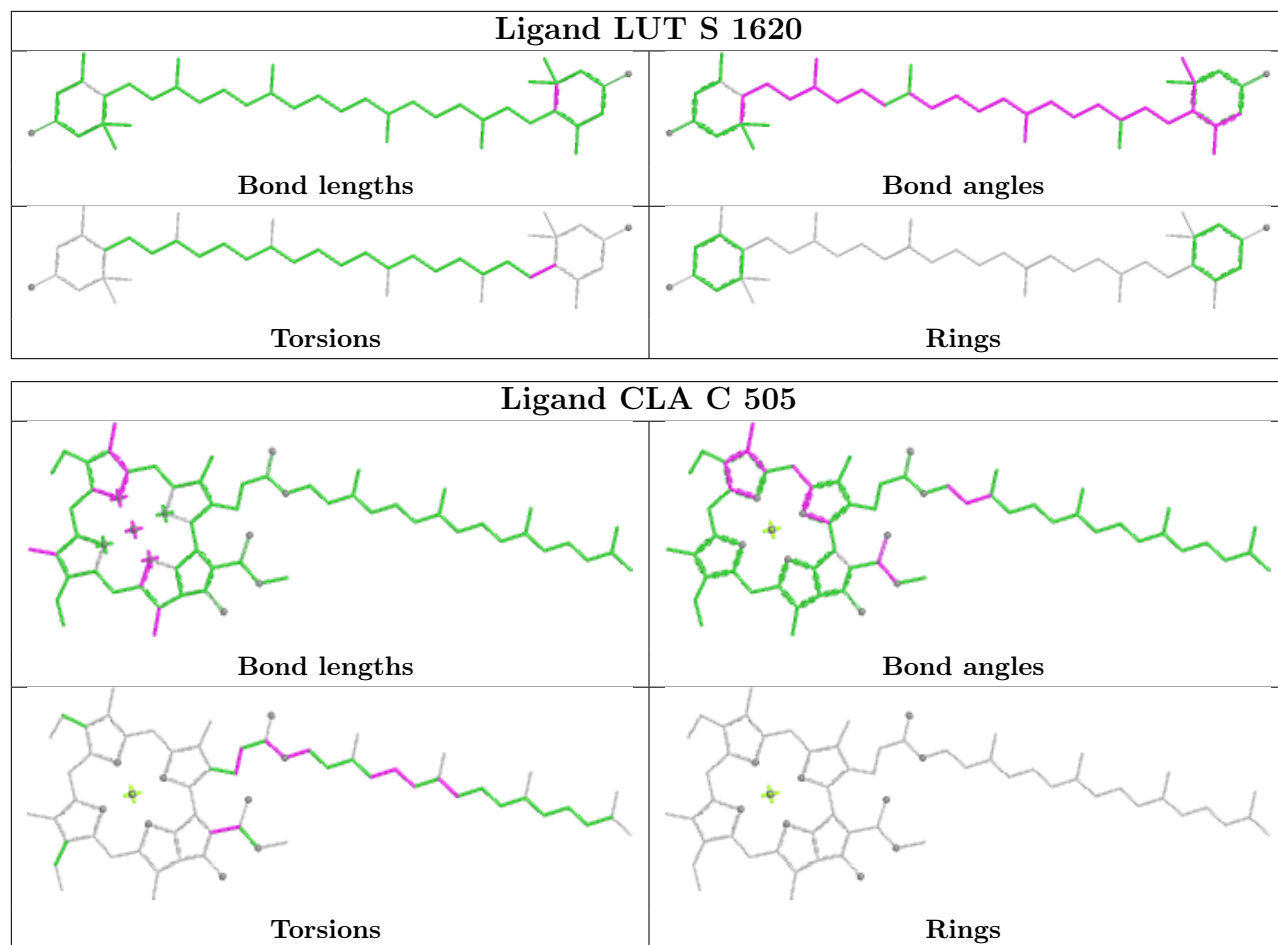
Ligand CLA S 614

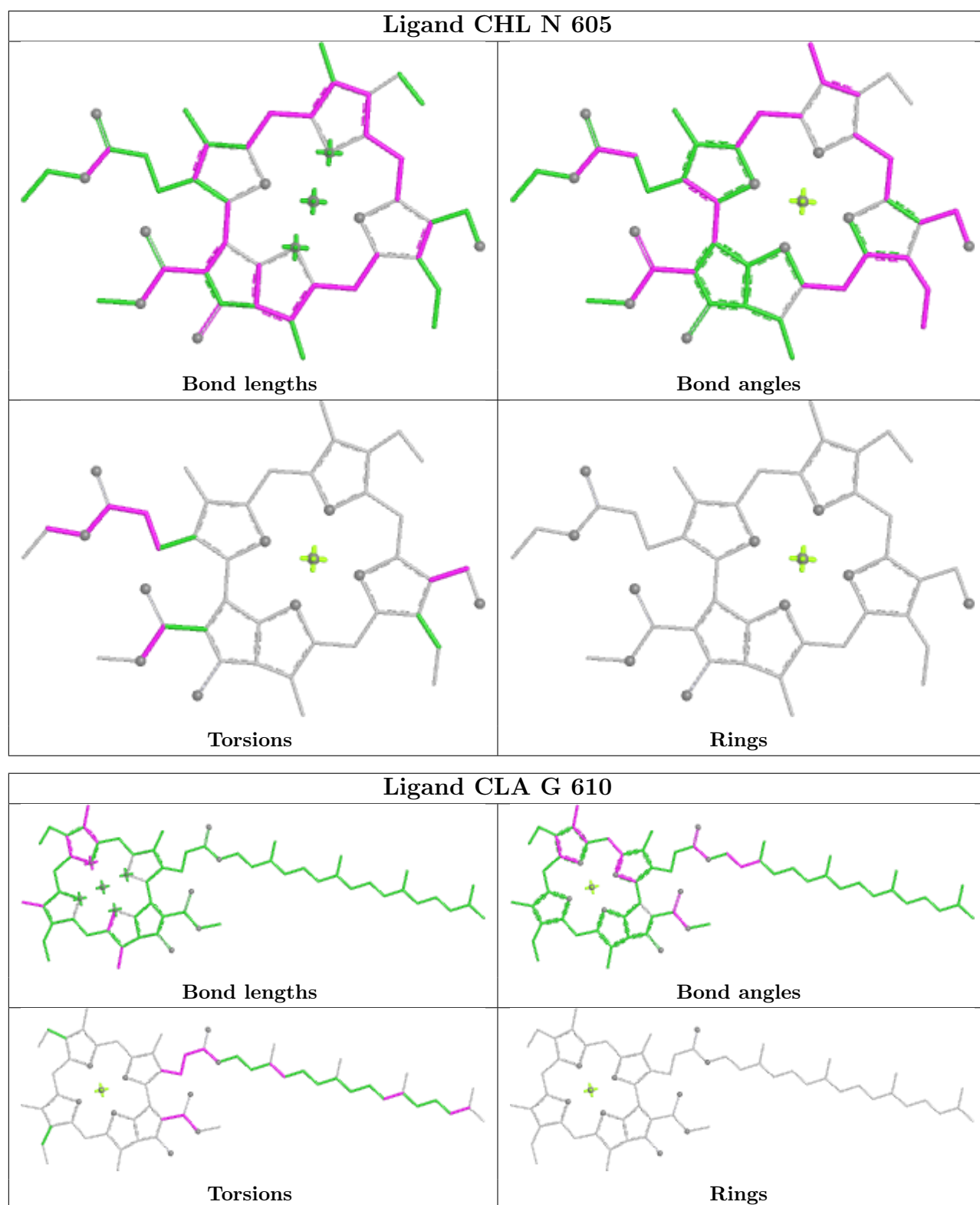


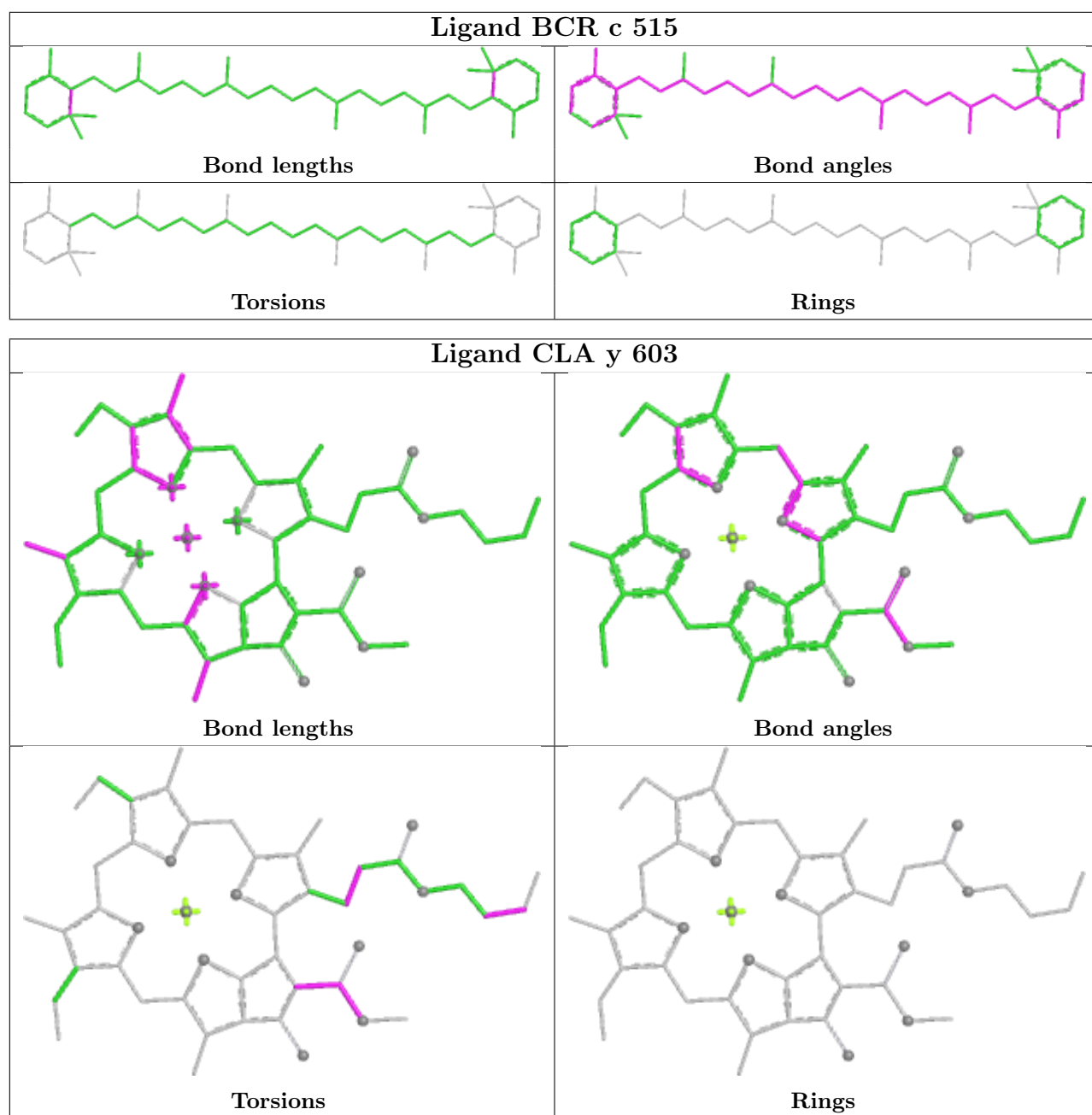
Ligand CLA Y 612

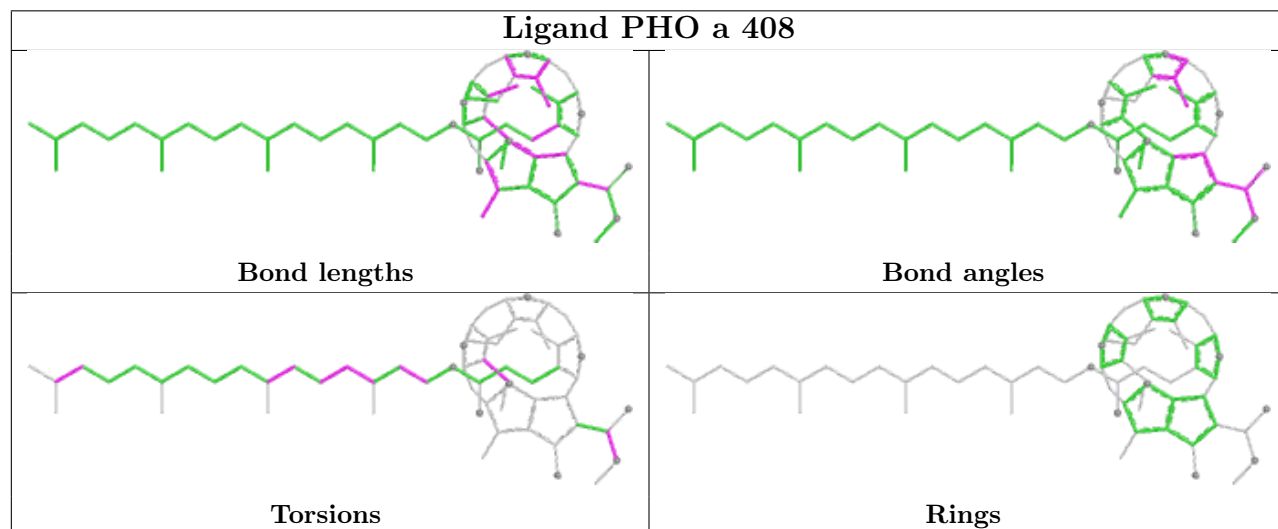
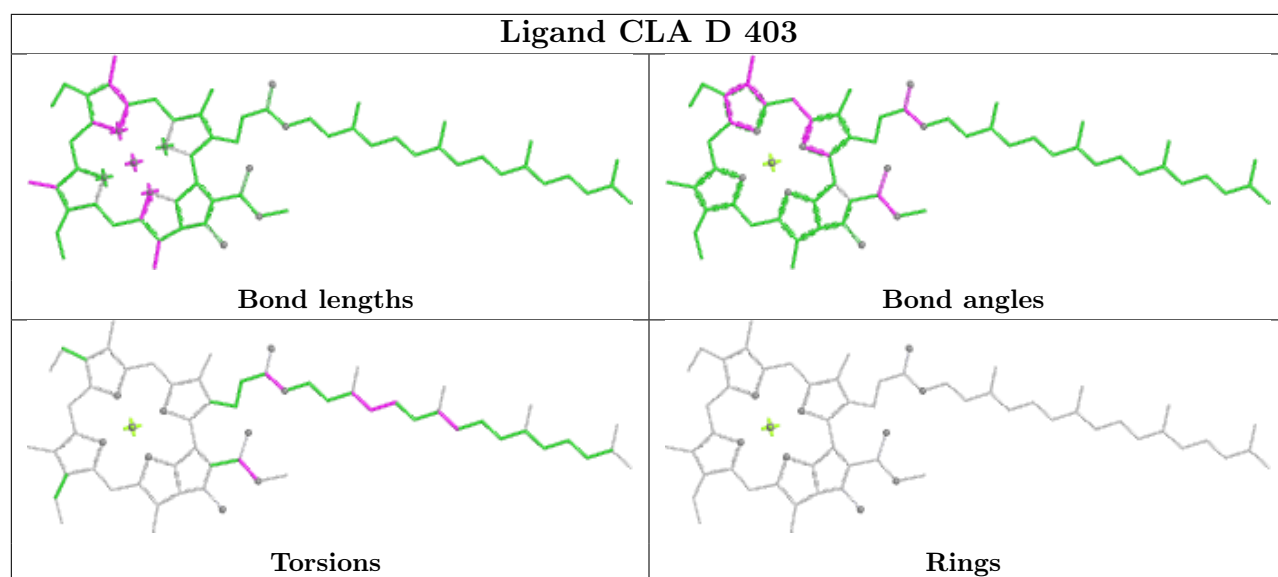


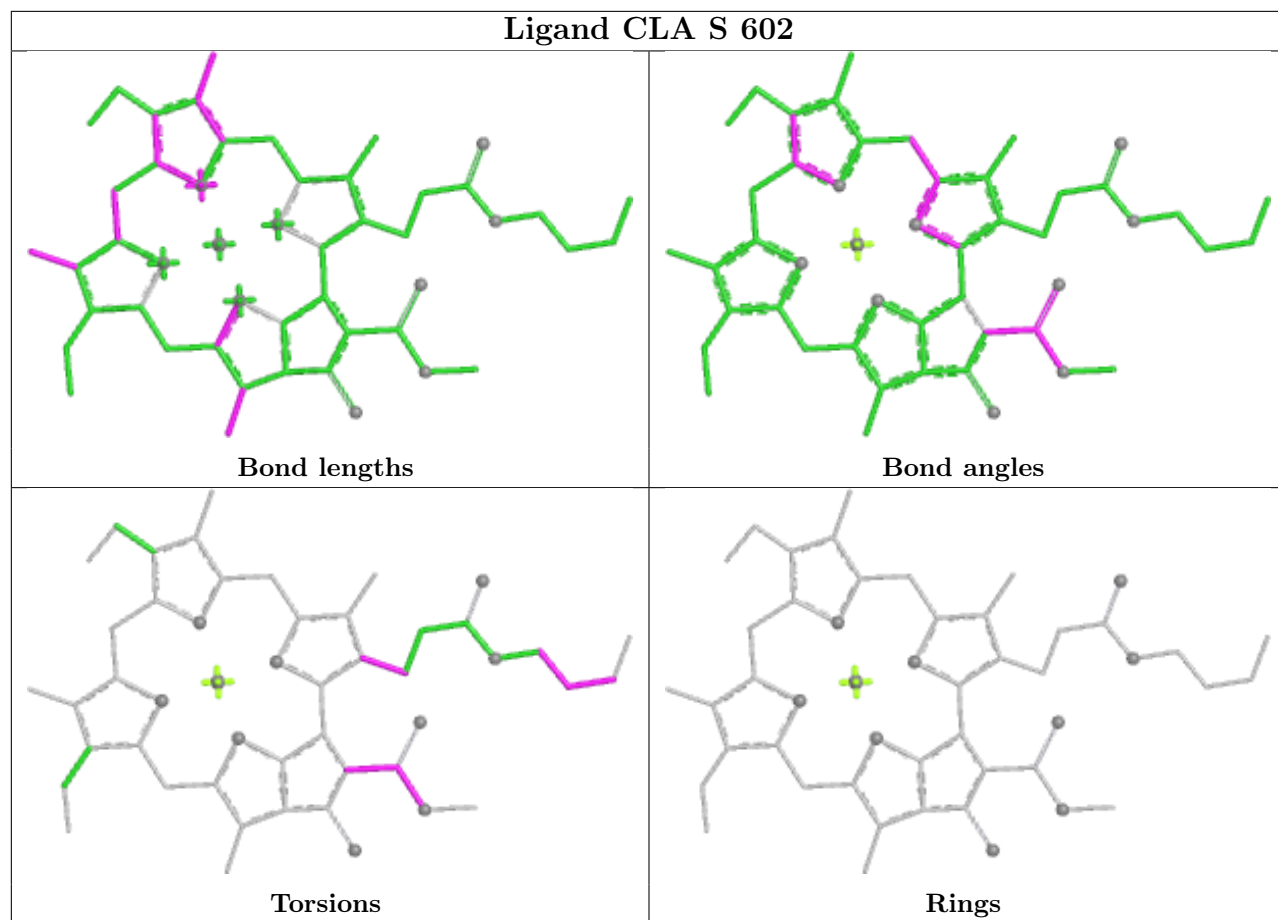


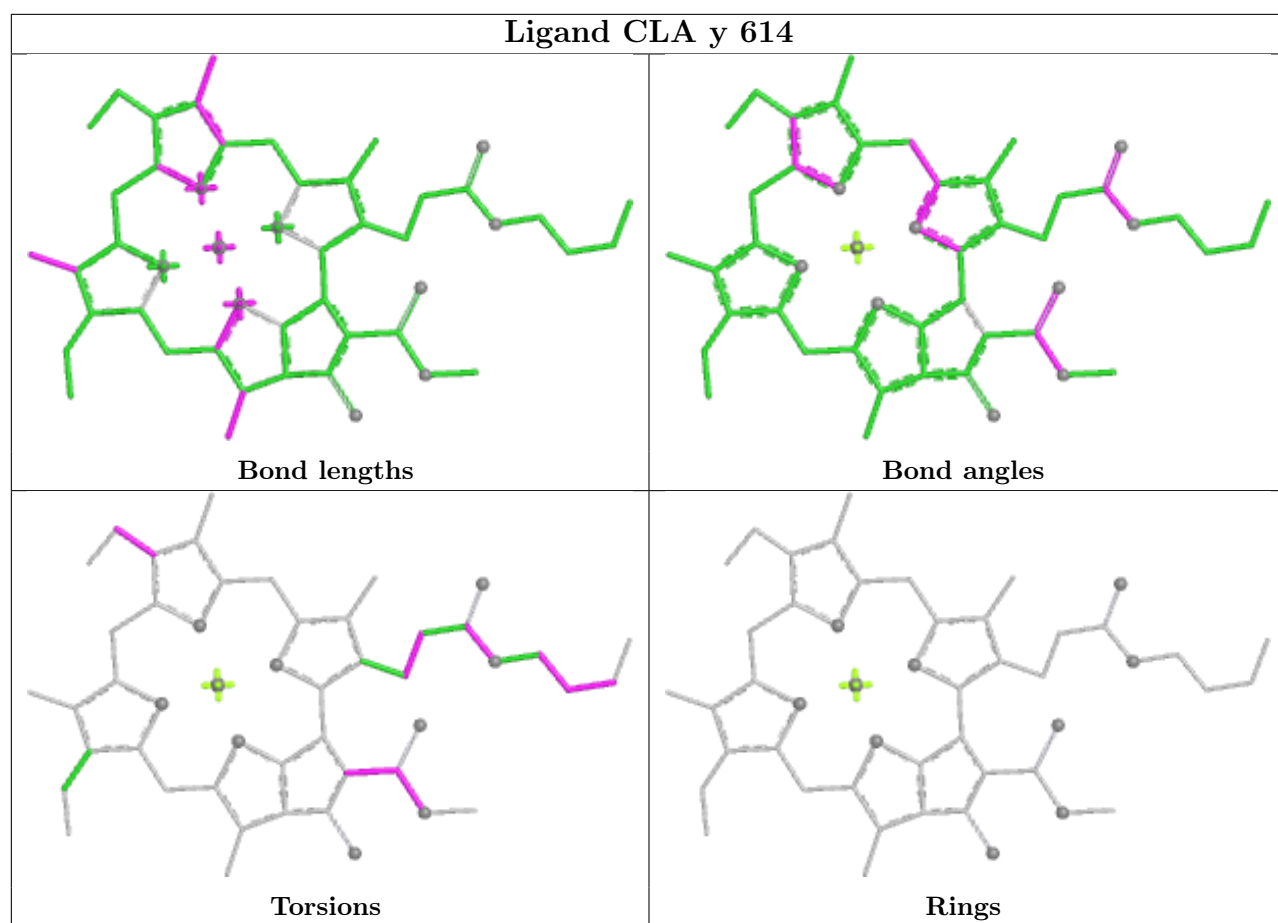


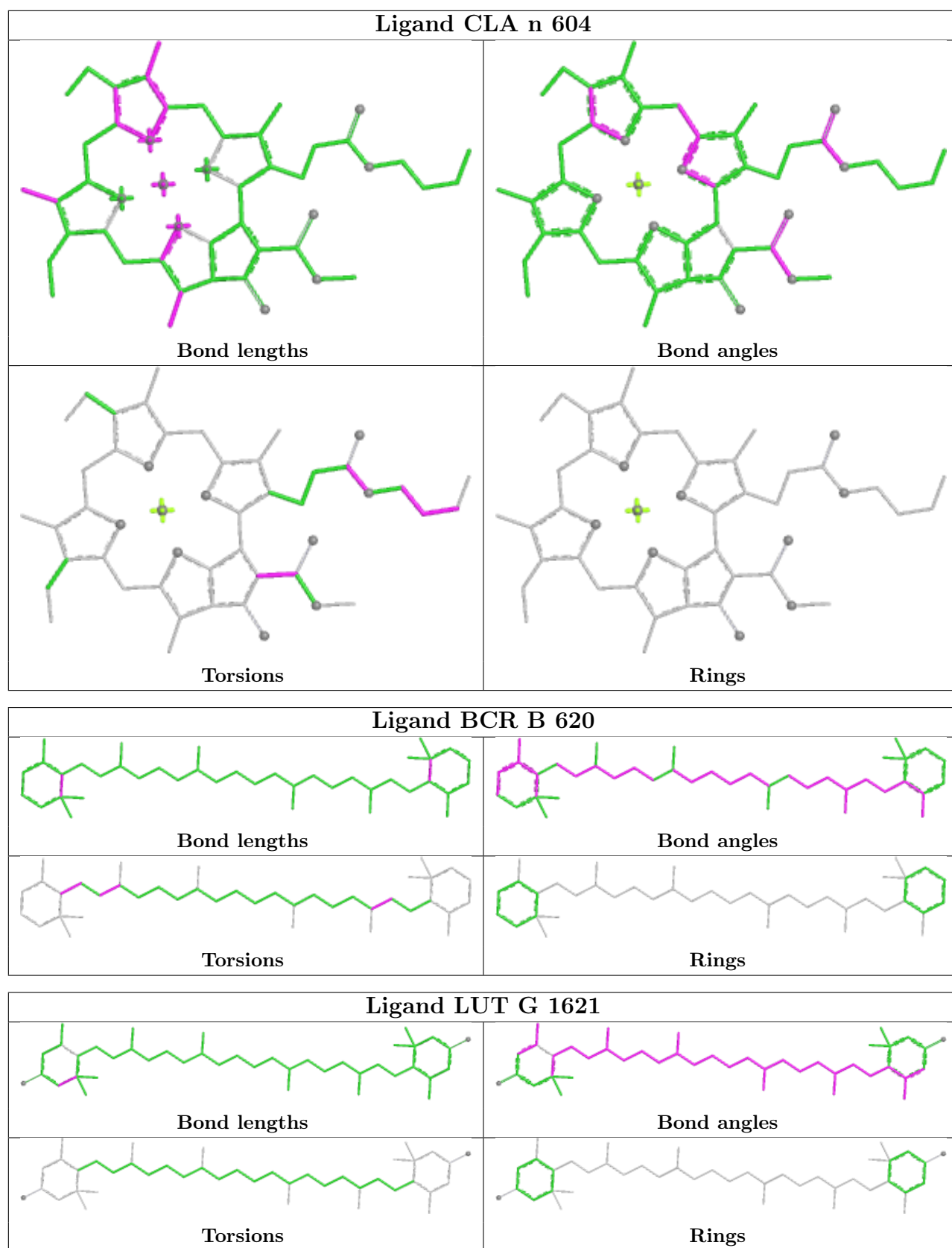


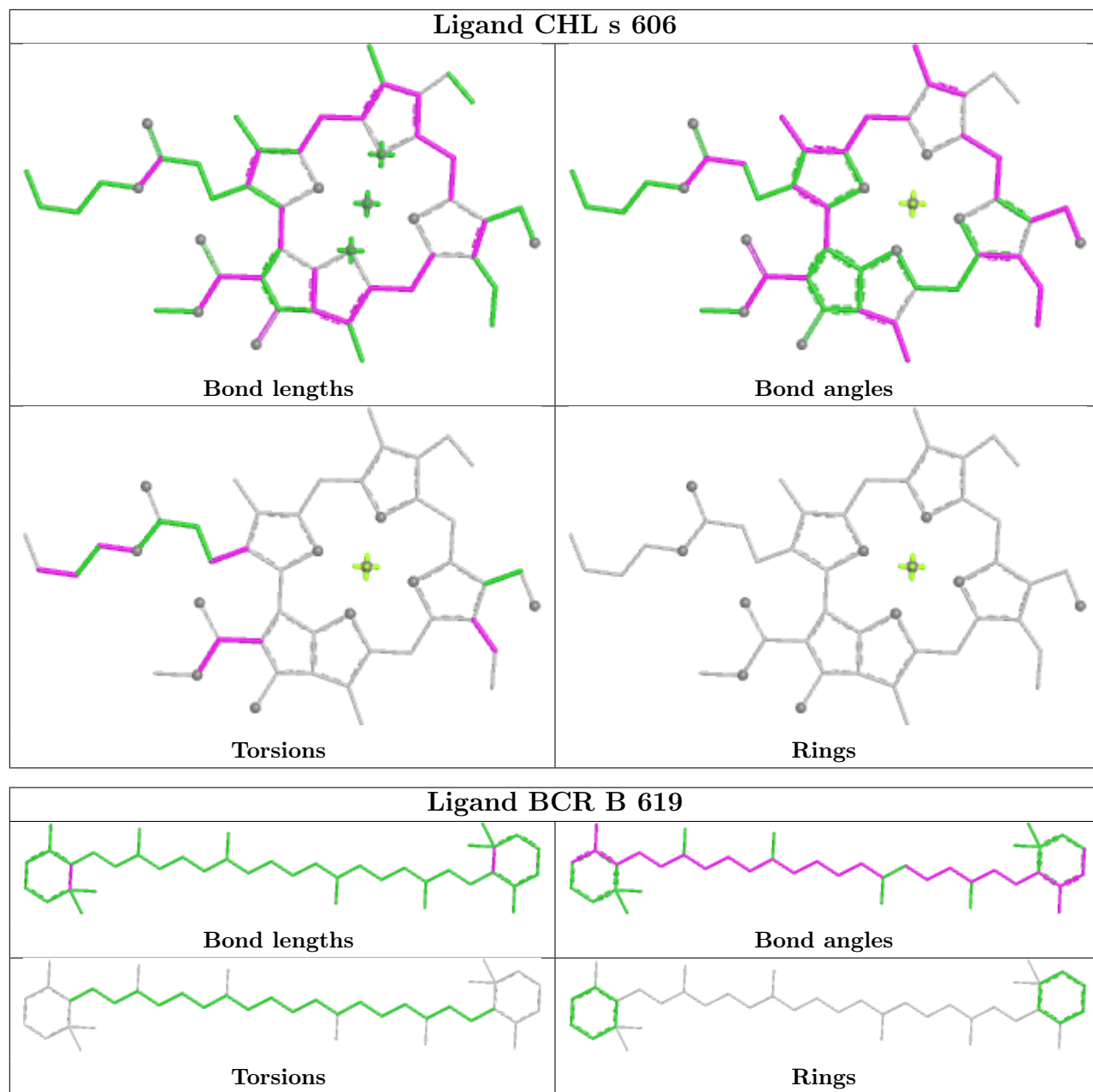


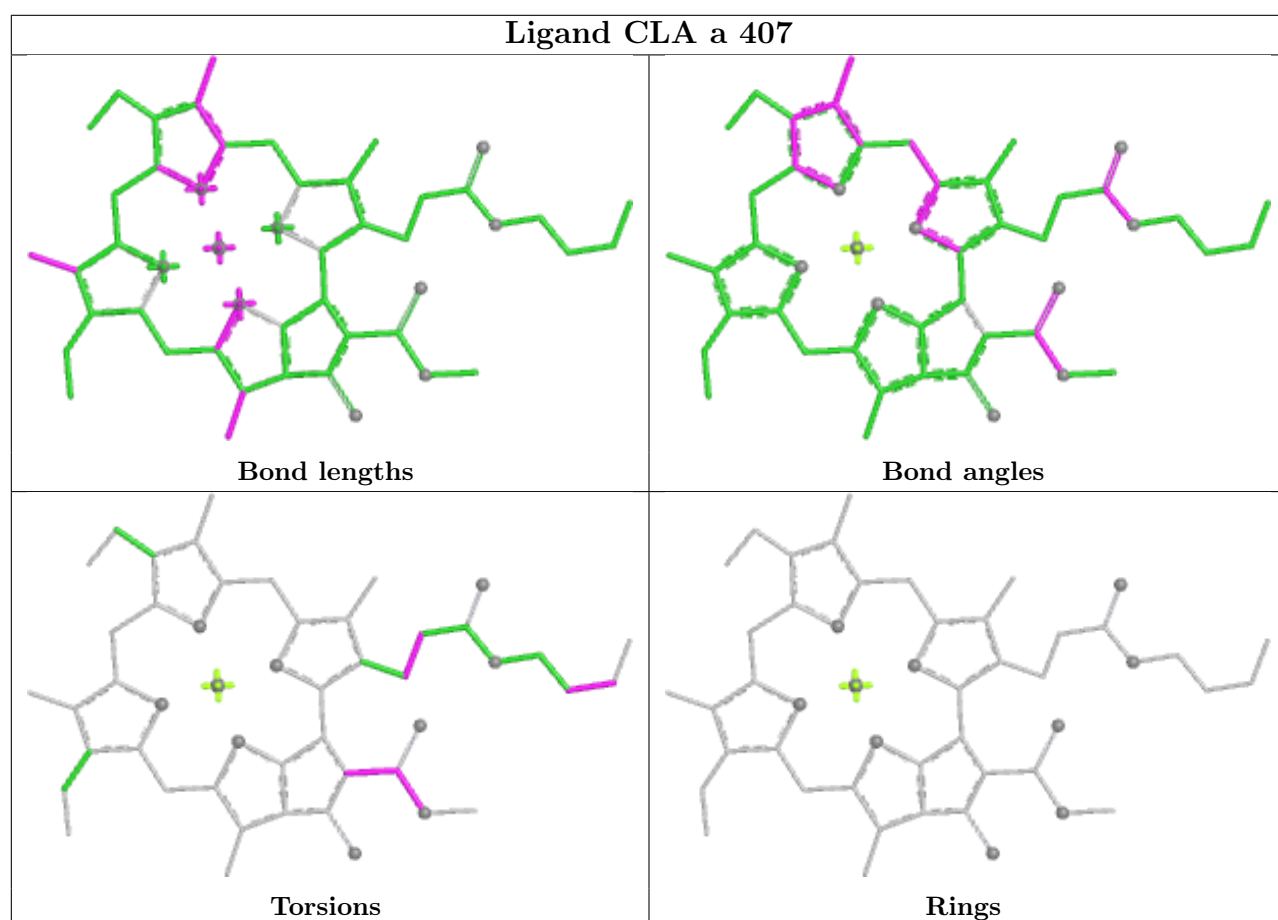
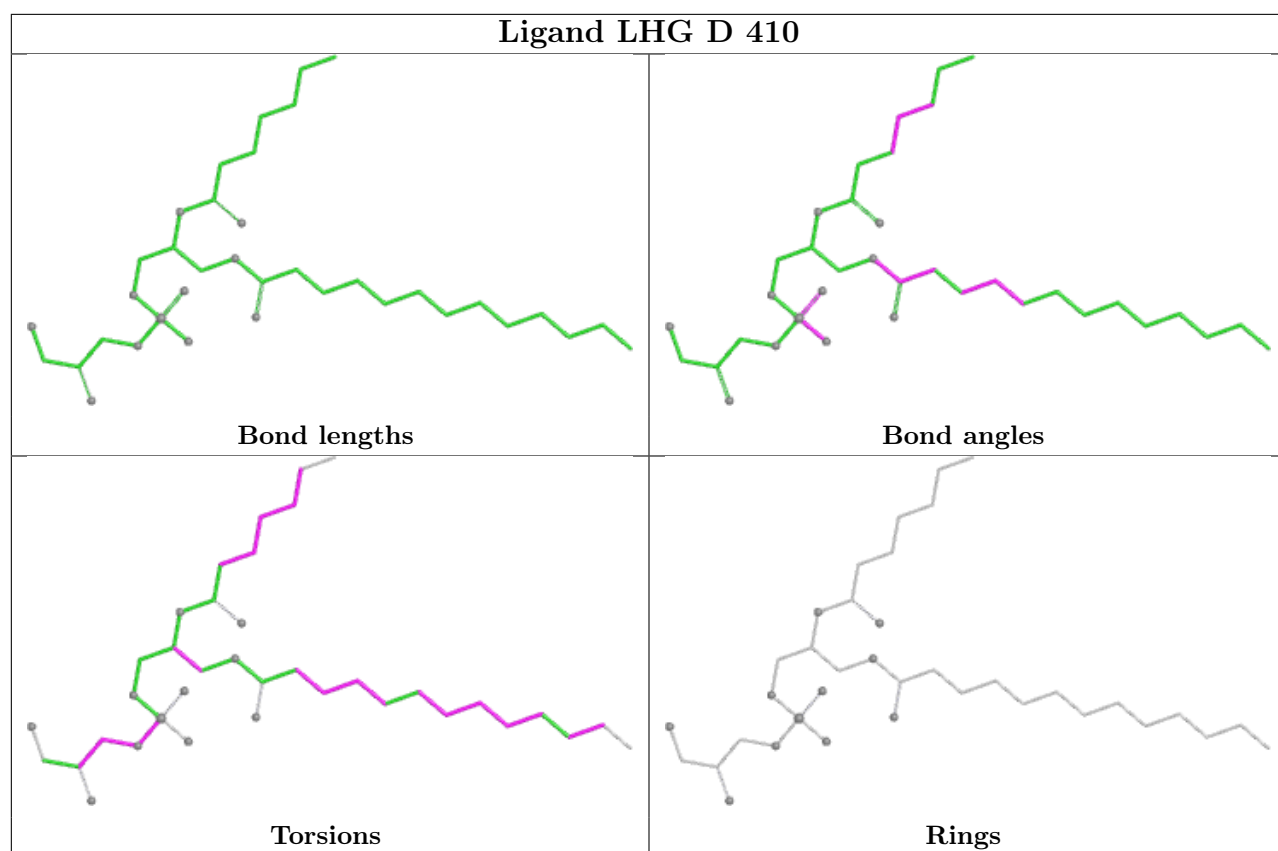


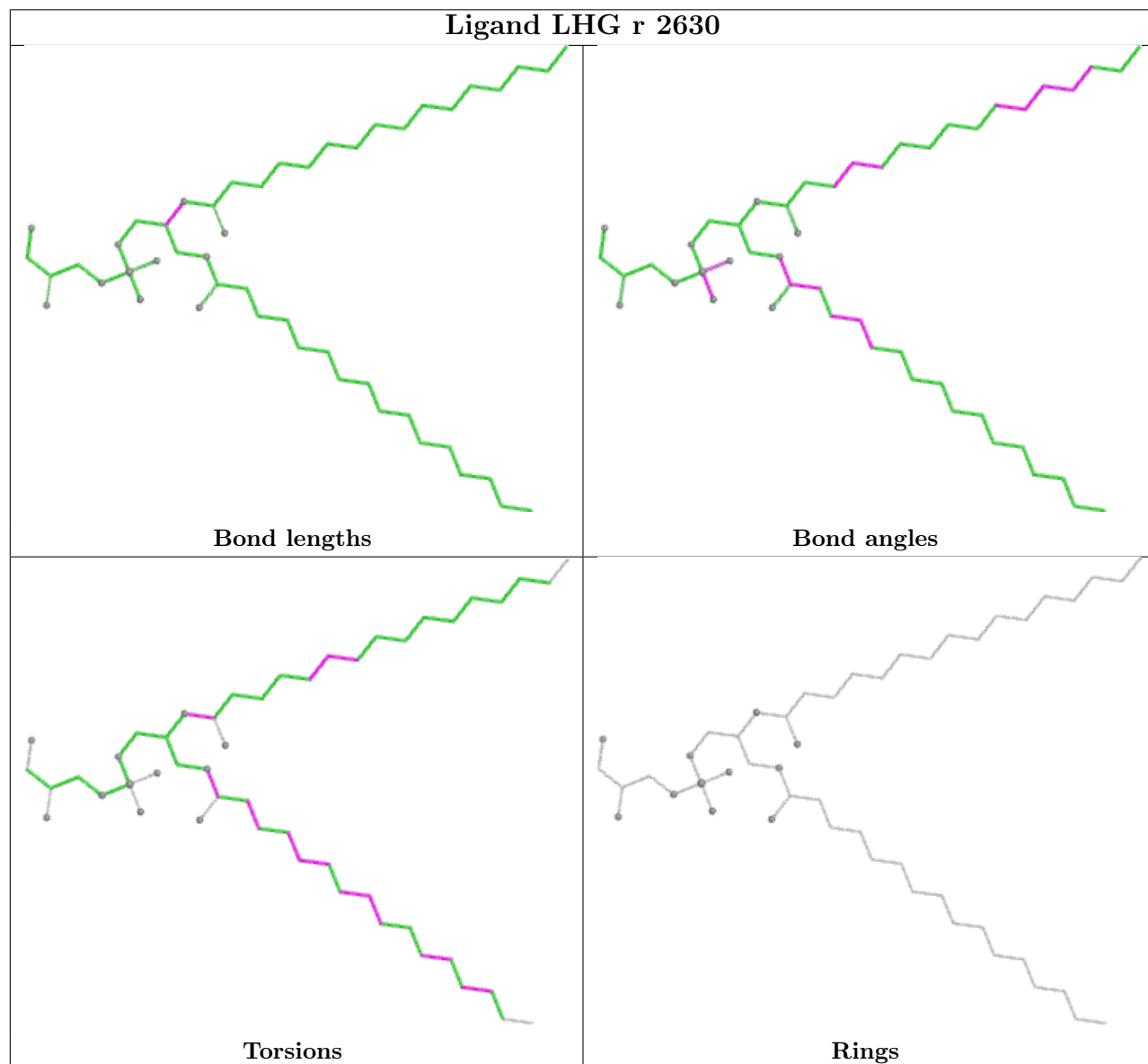
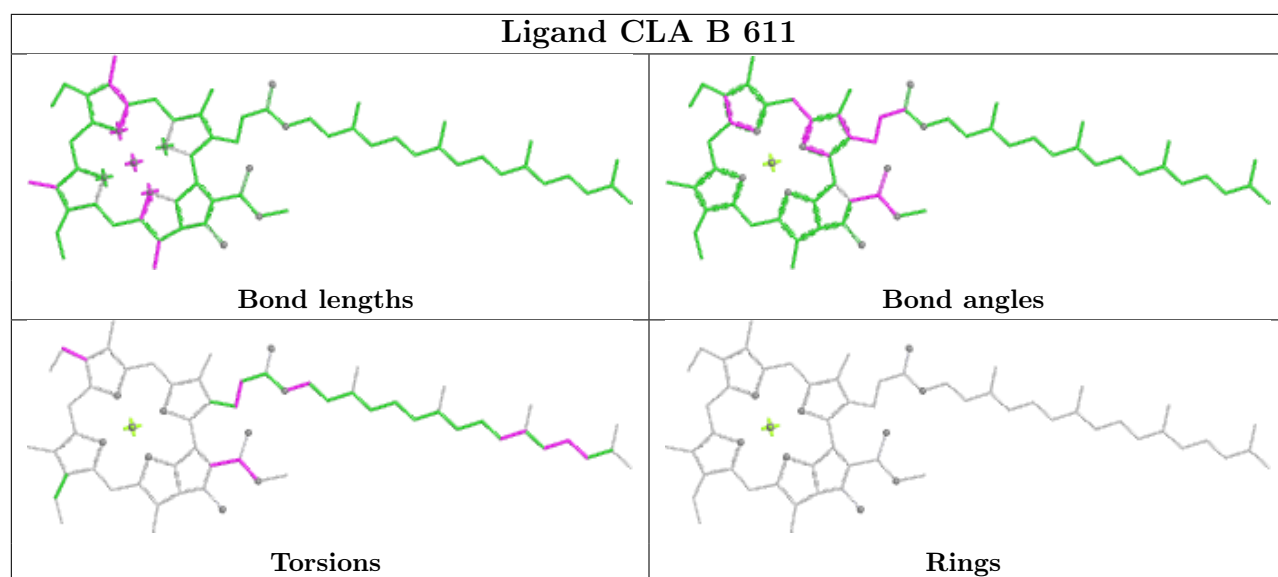


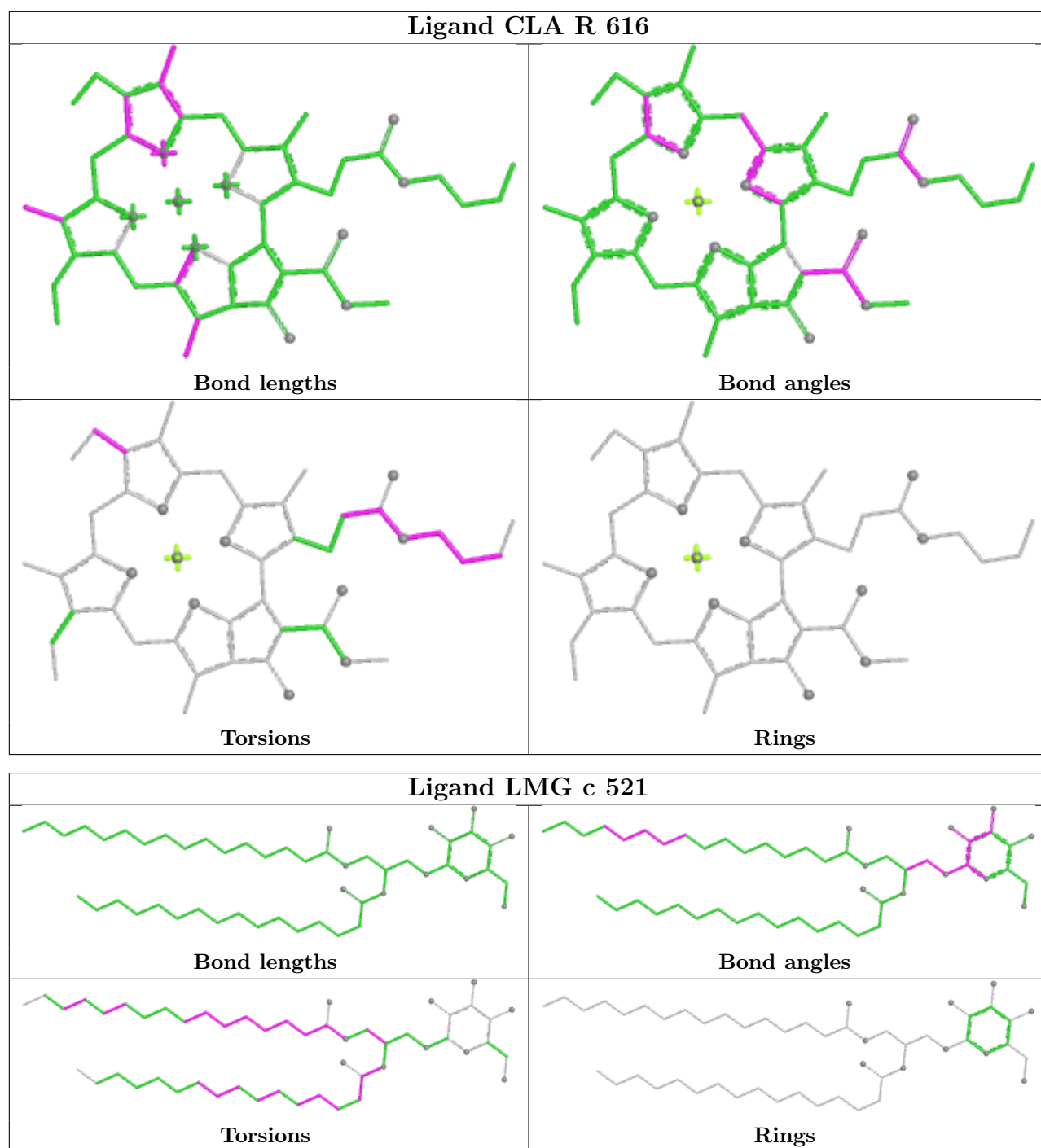


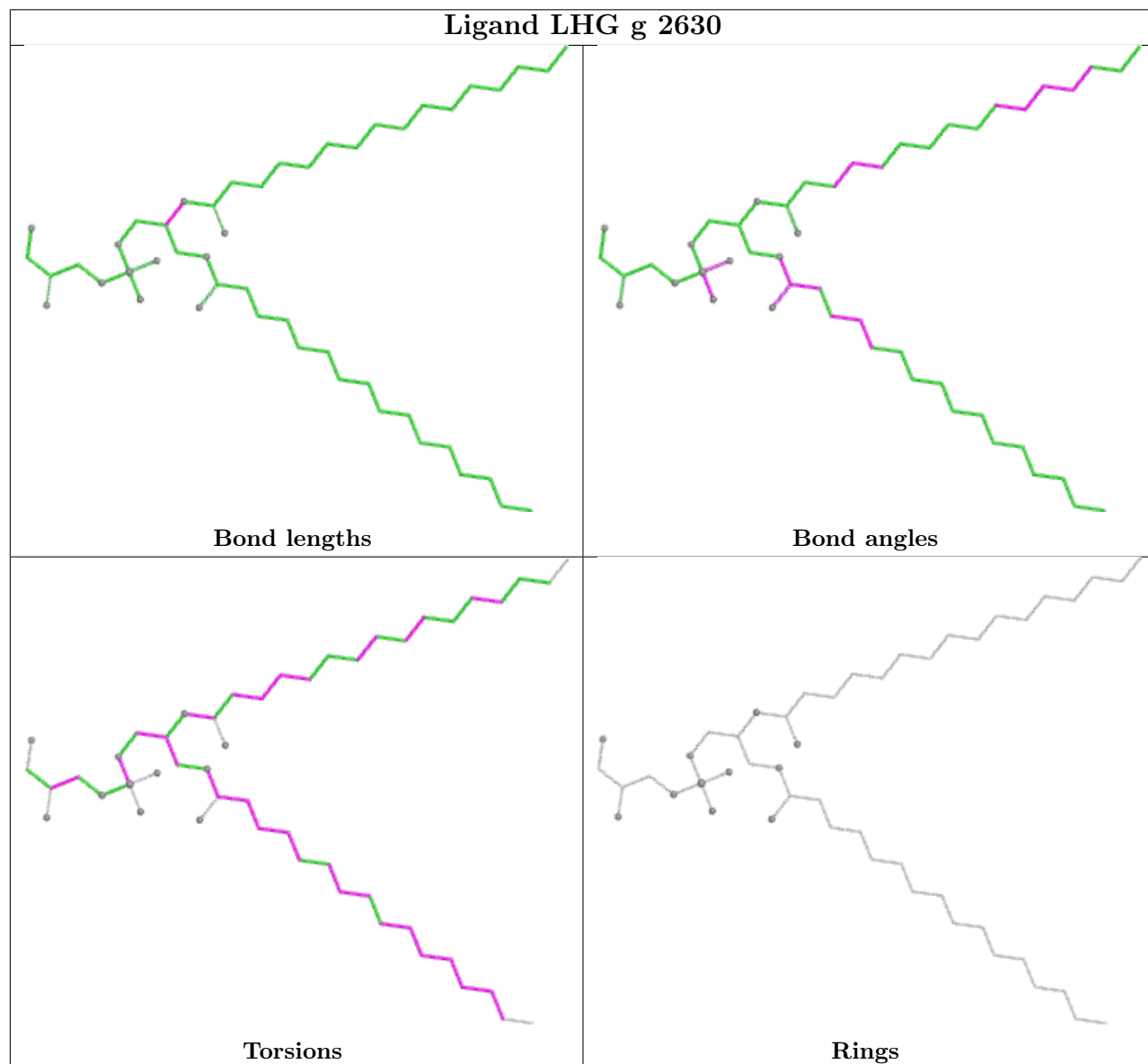
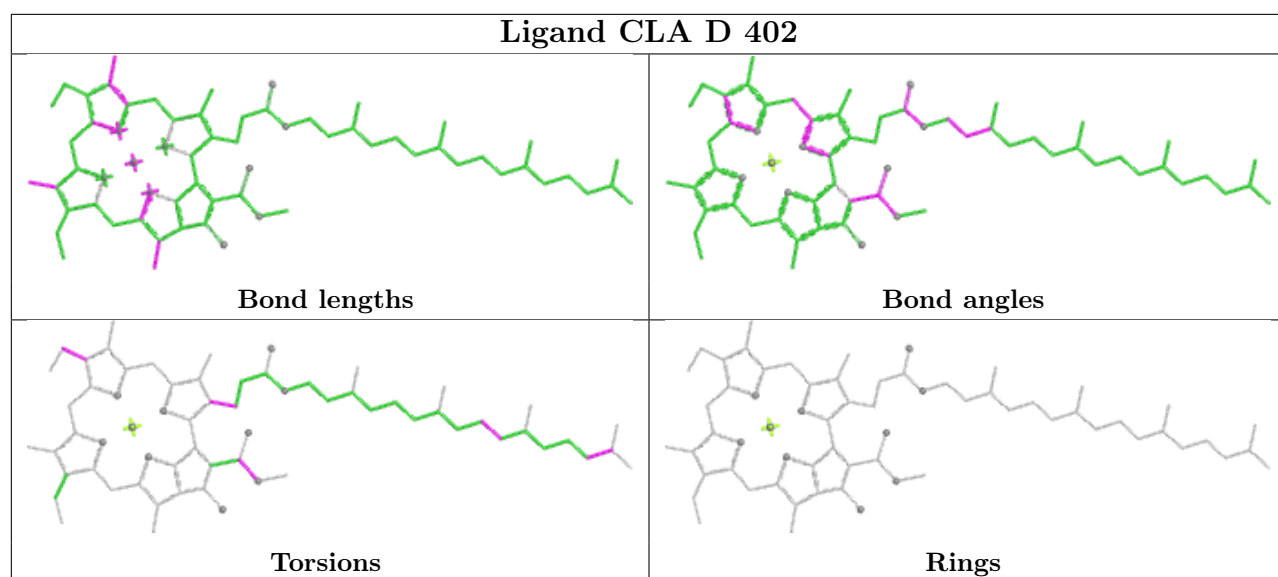


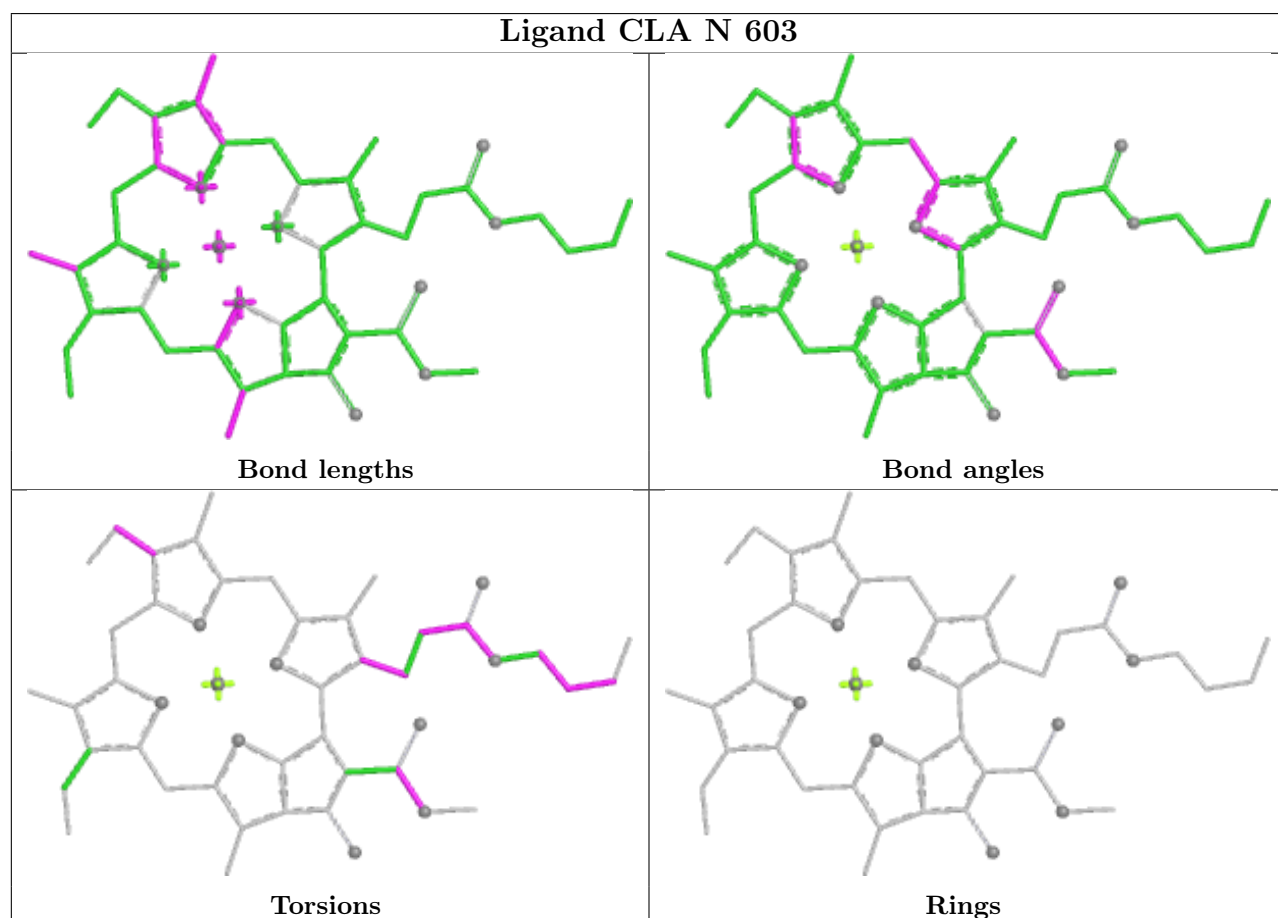
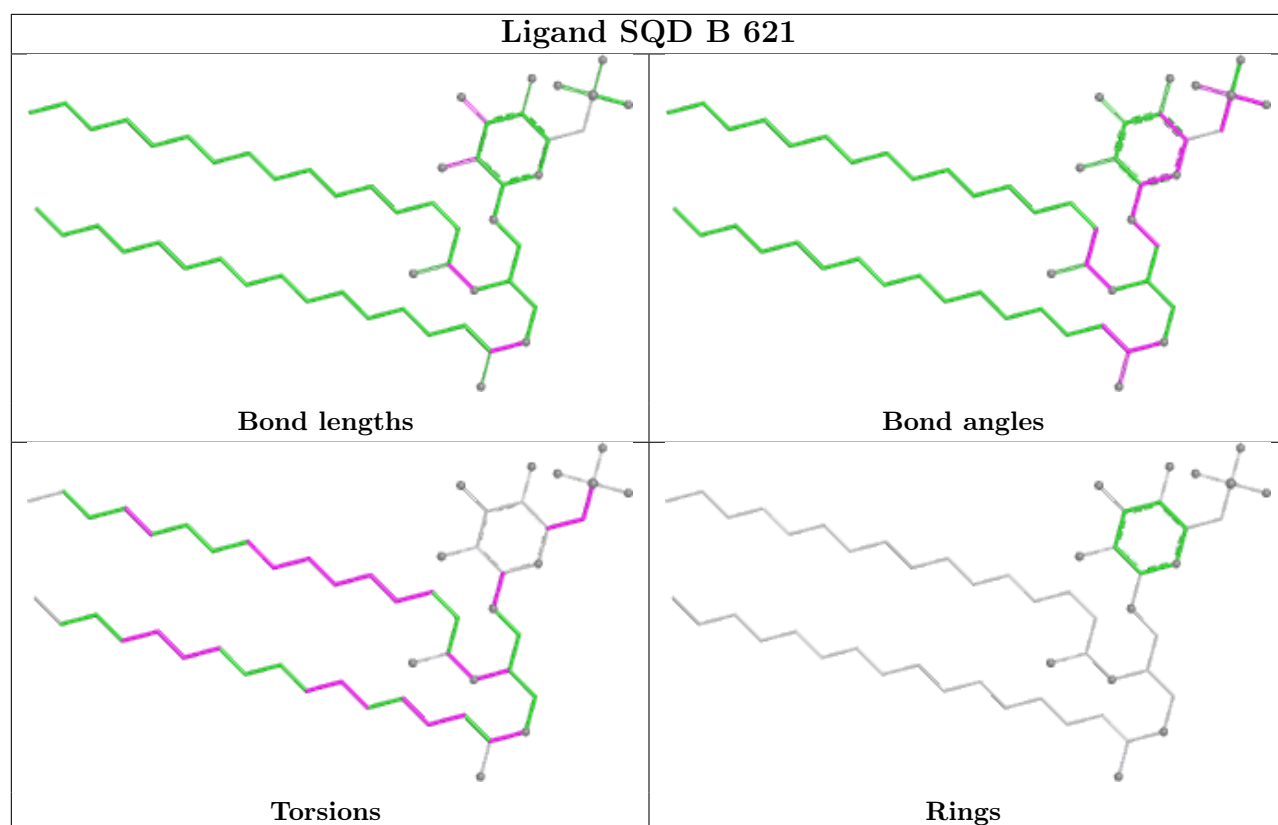




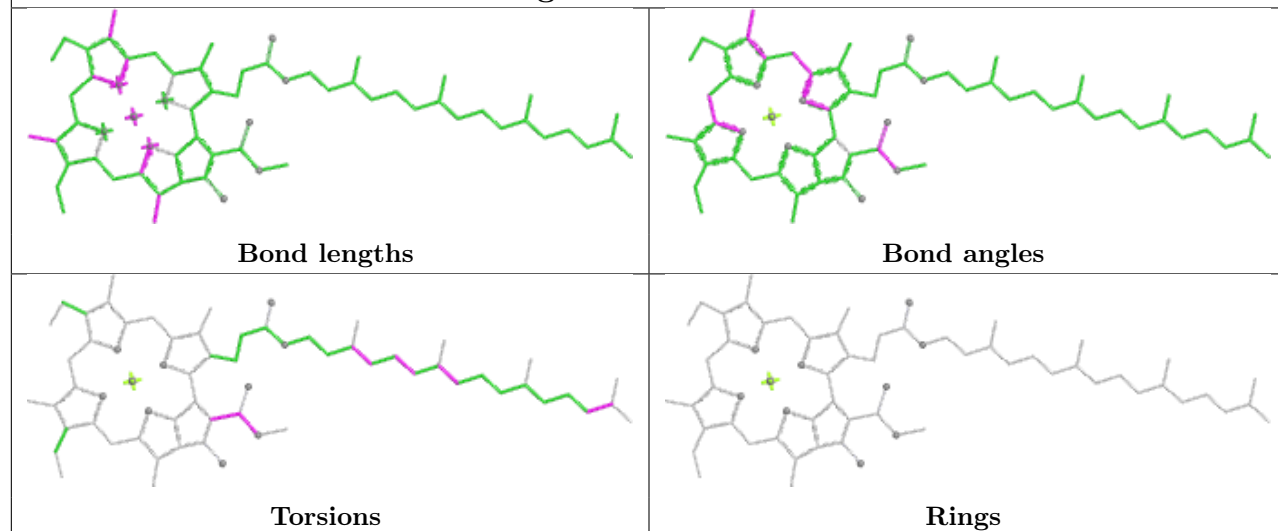




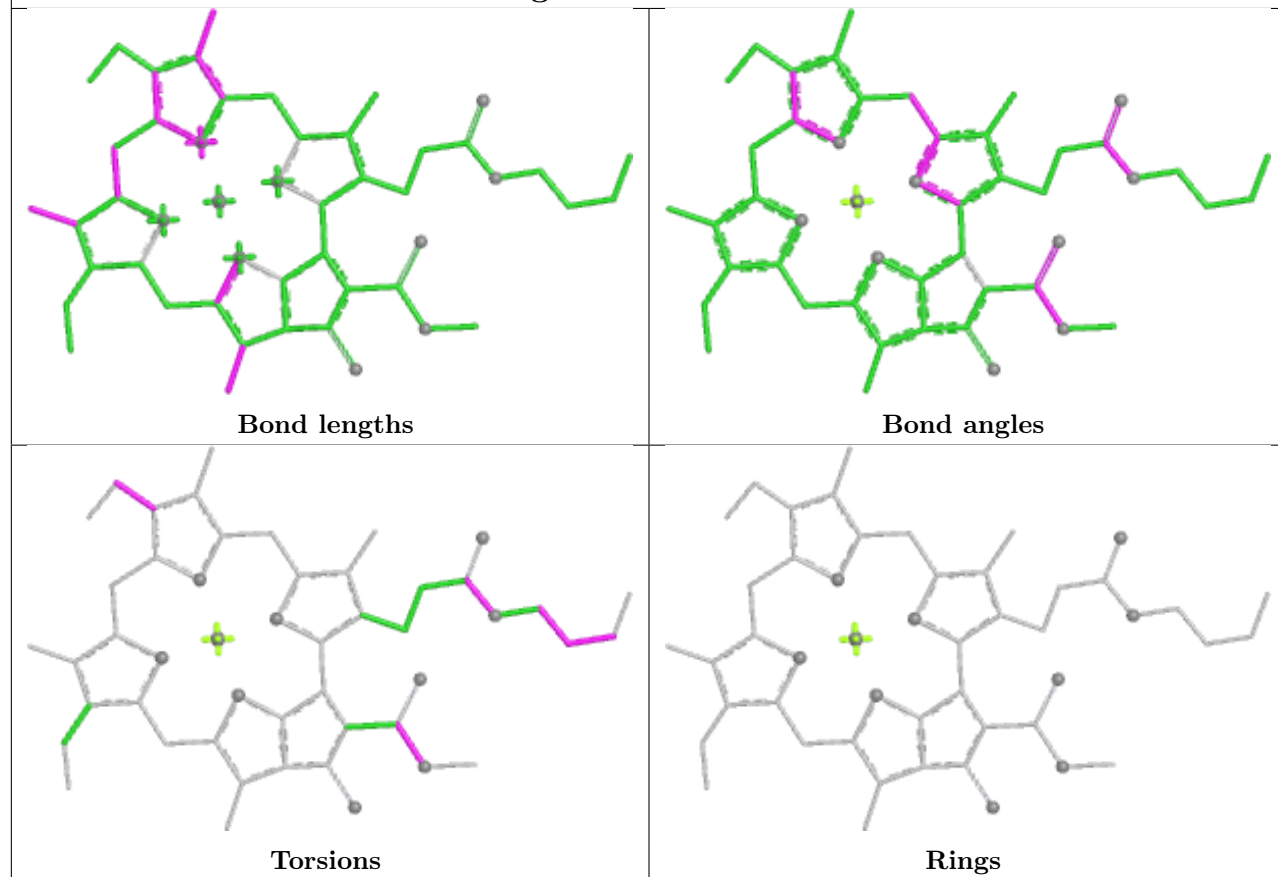


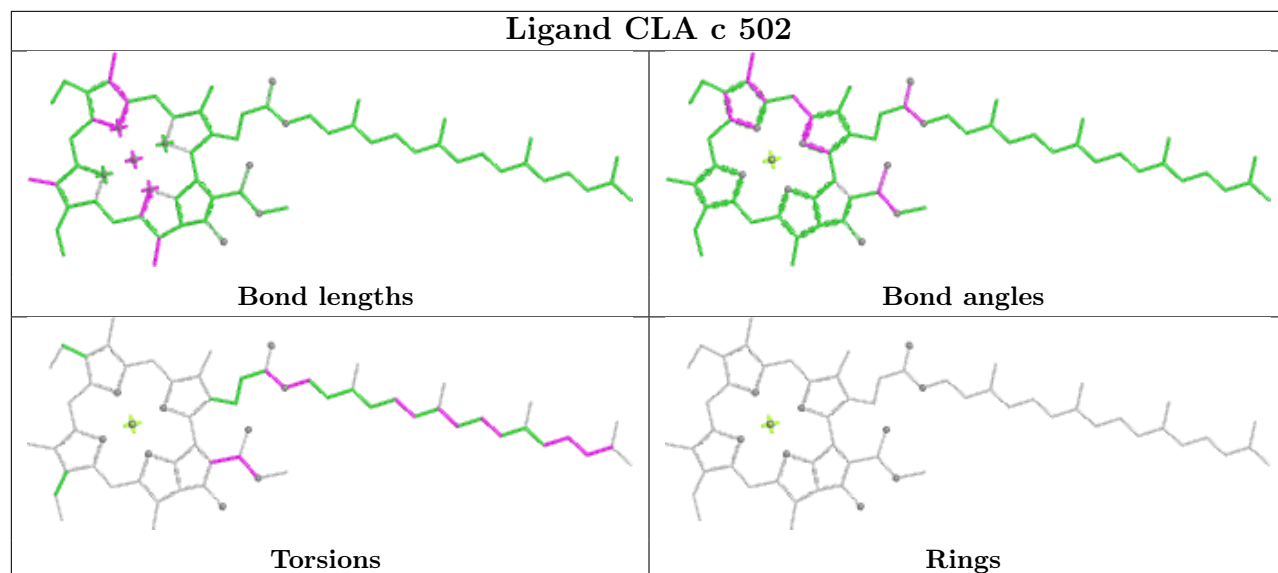
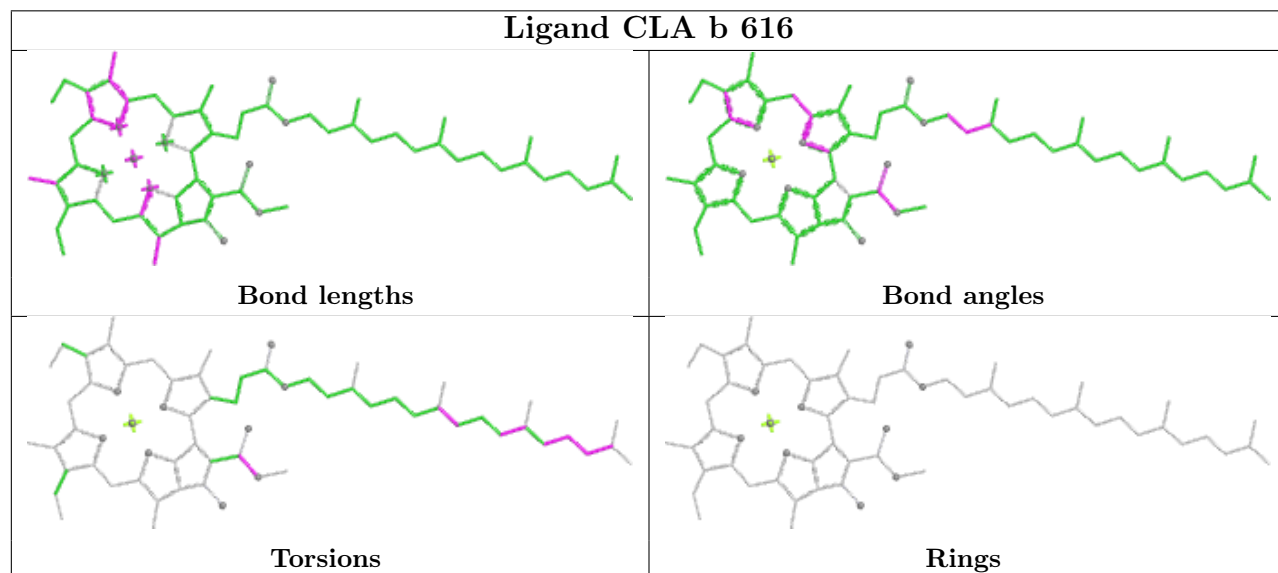
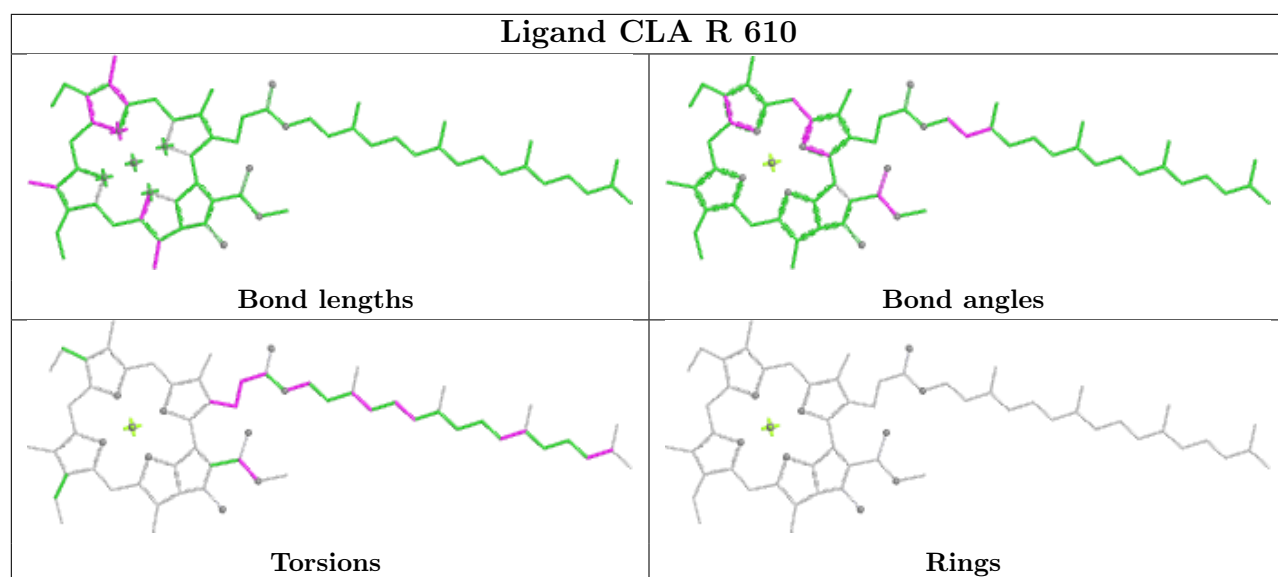


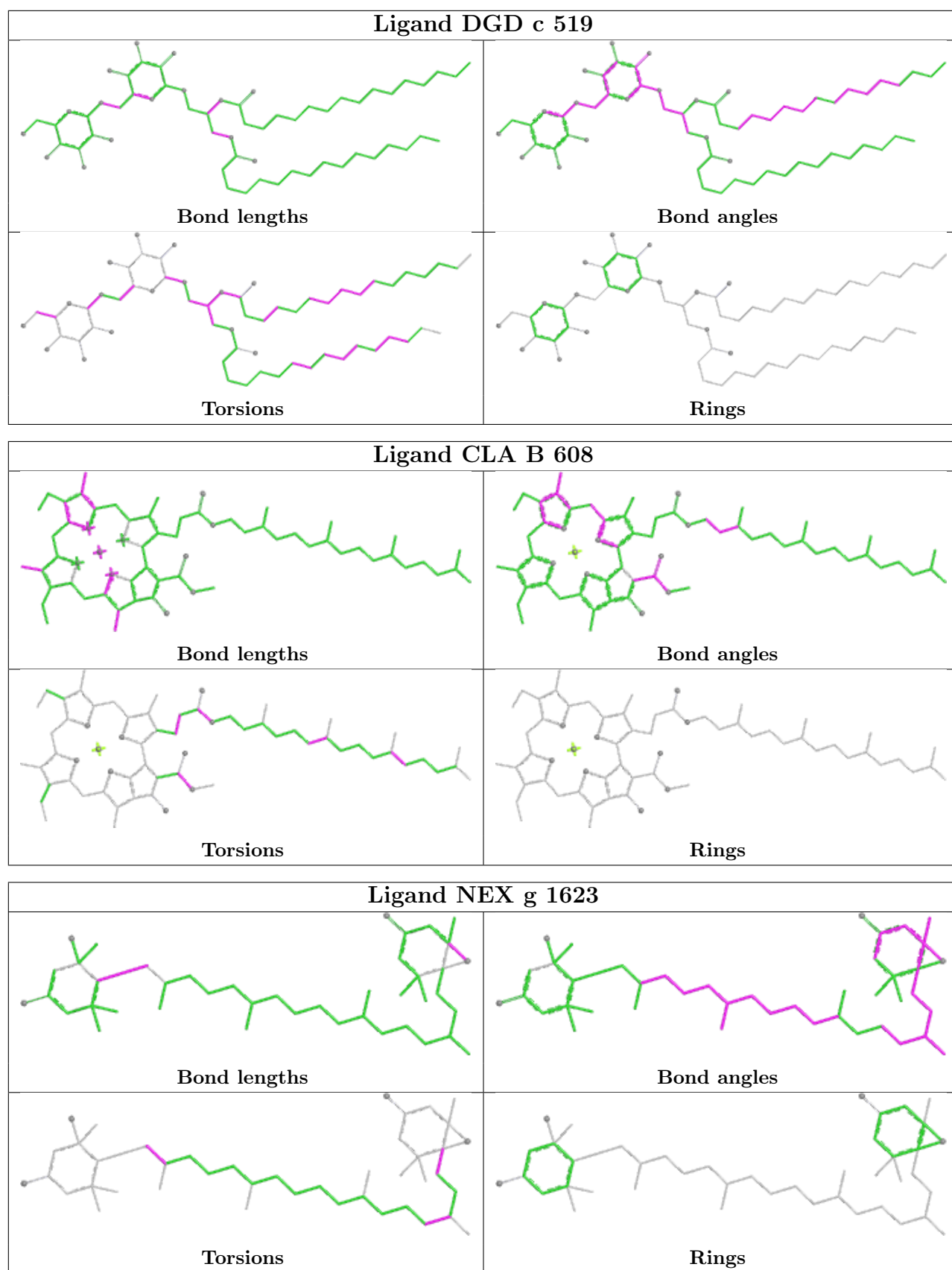
Ligand CLA c 508



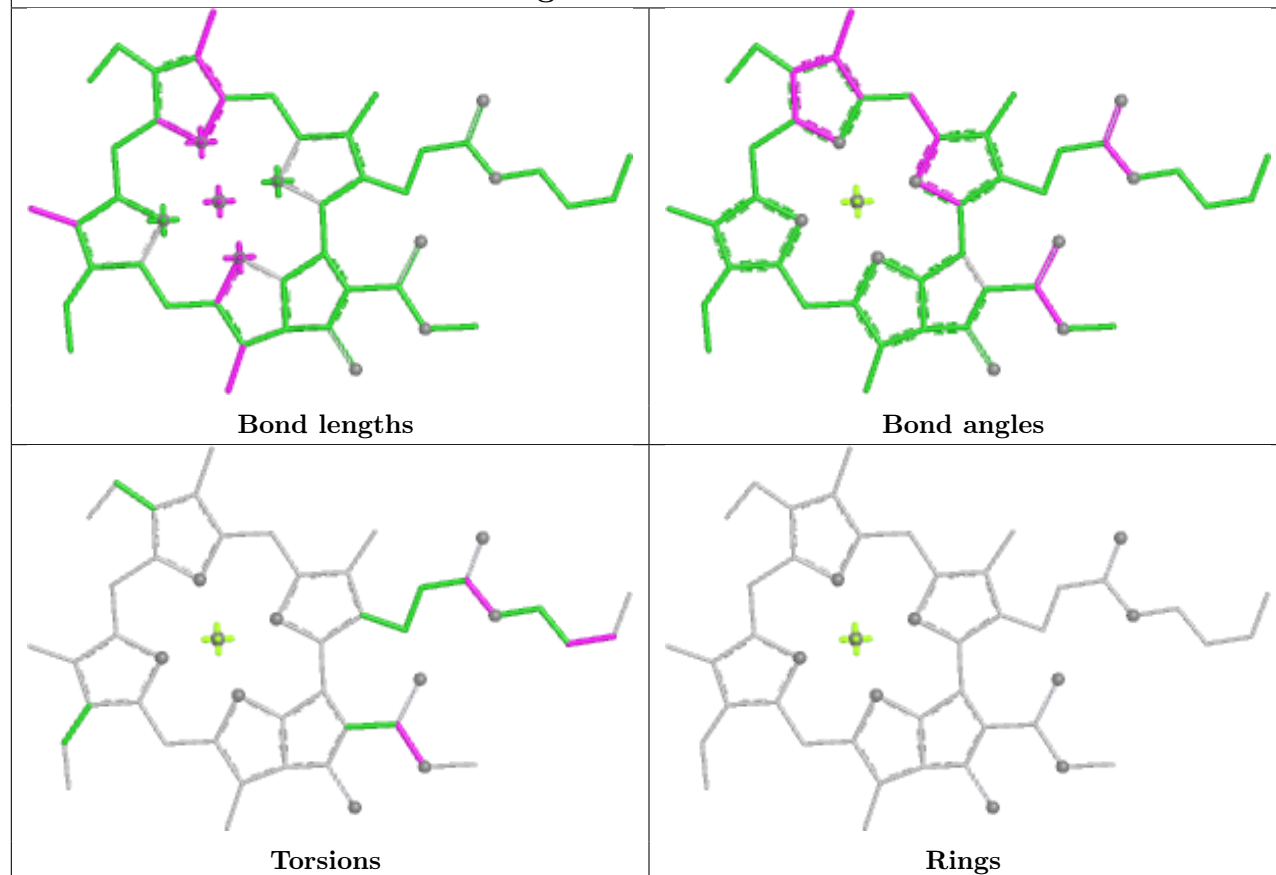
Ligand CLA G 614



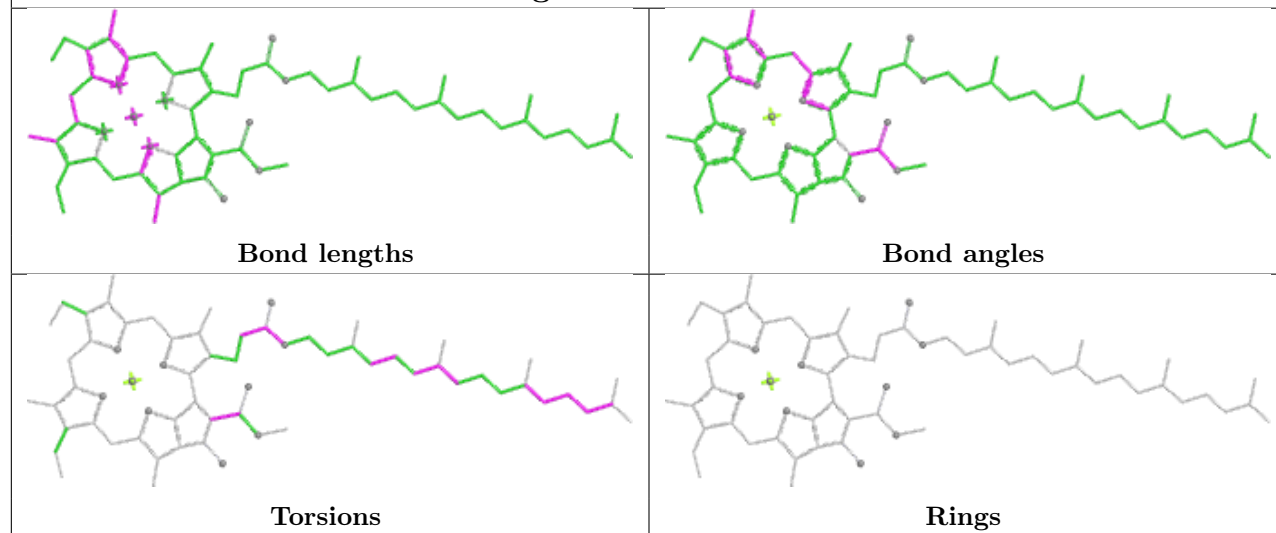


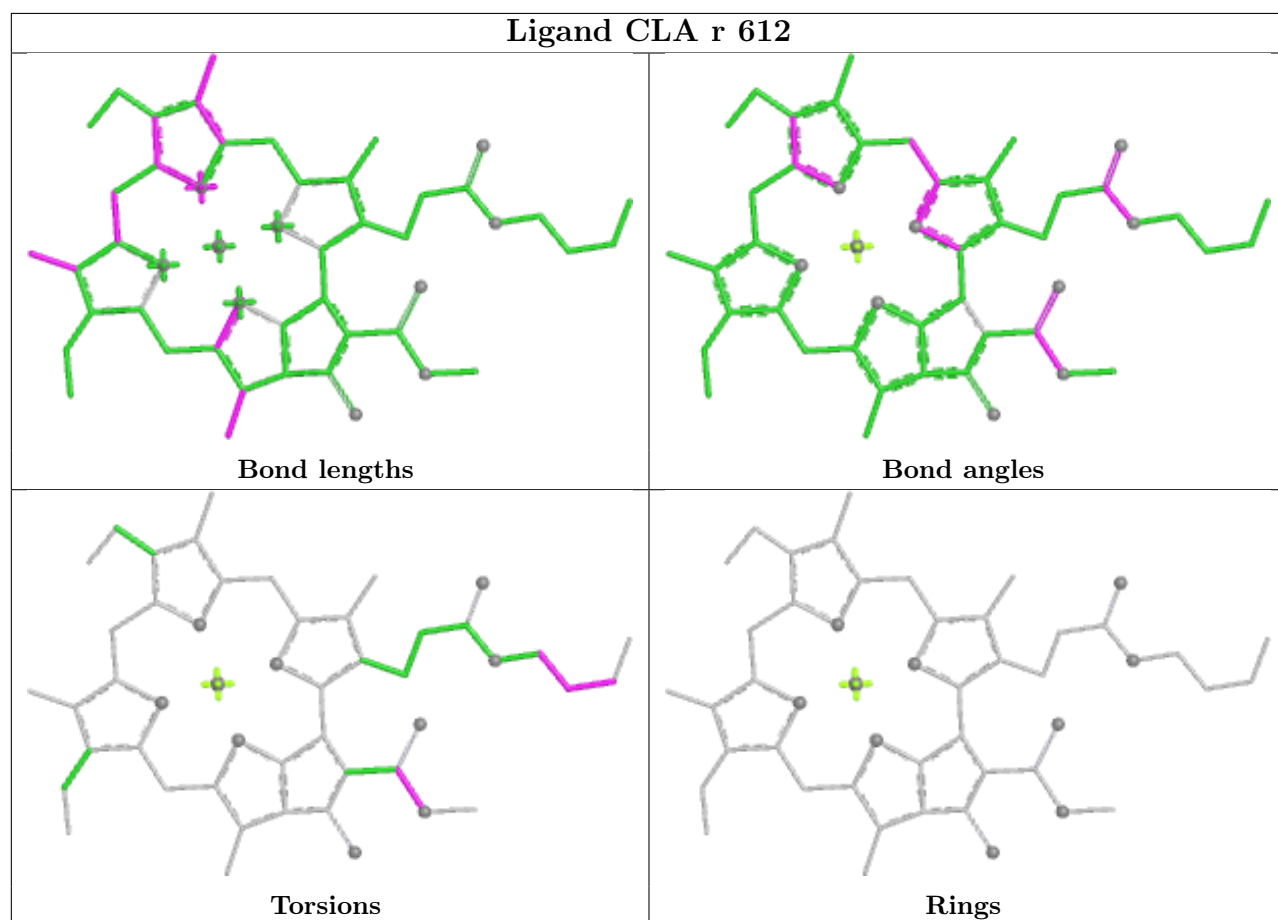
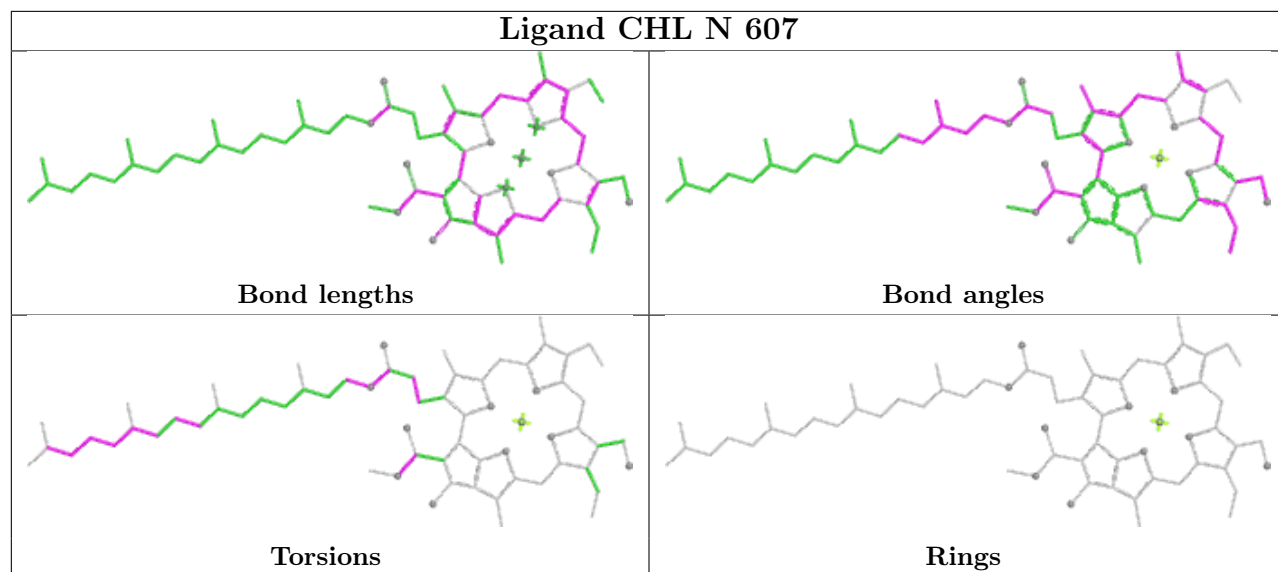


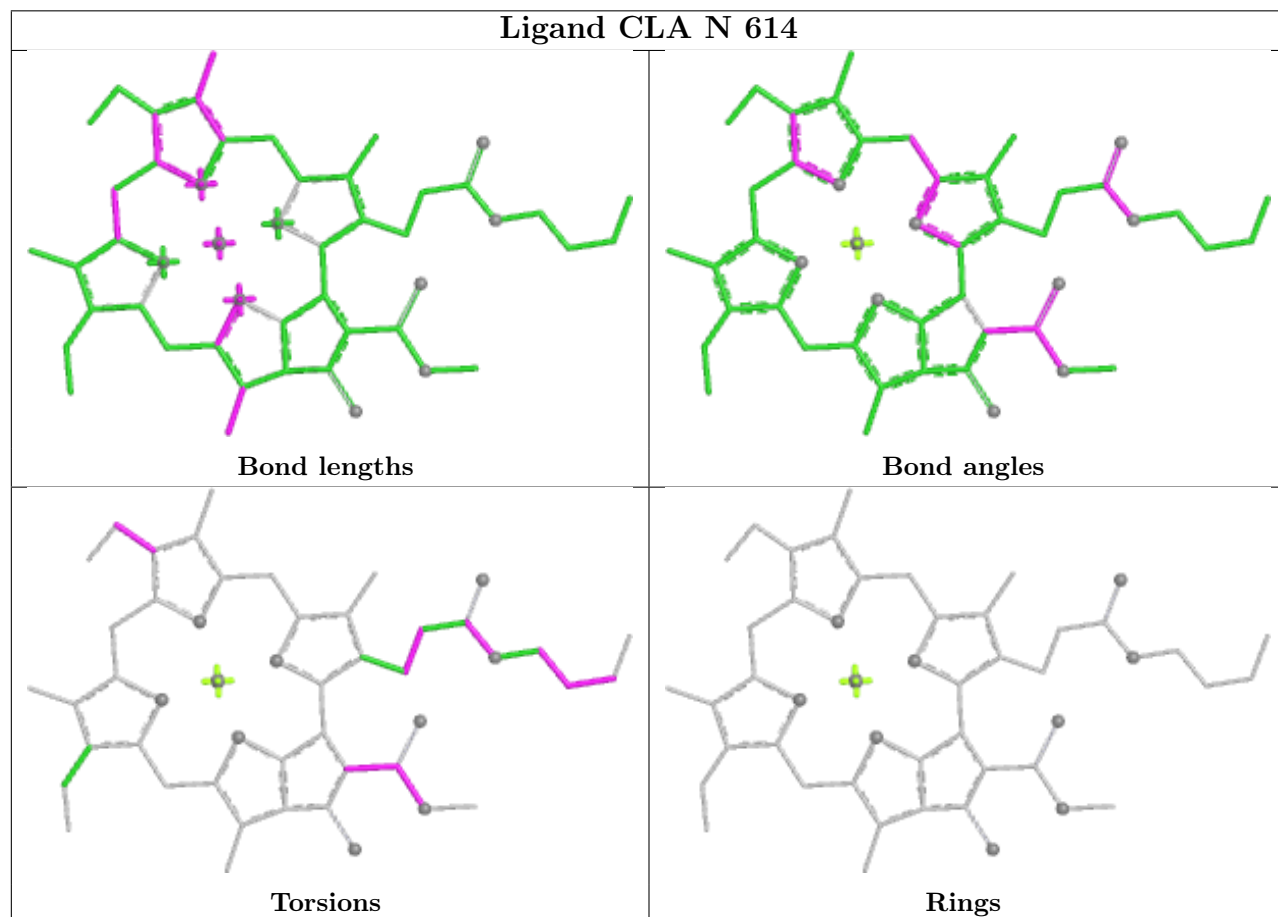
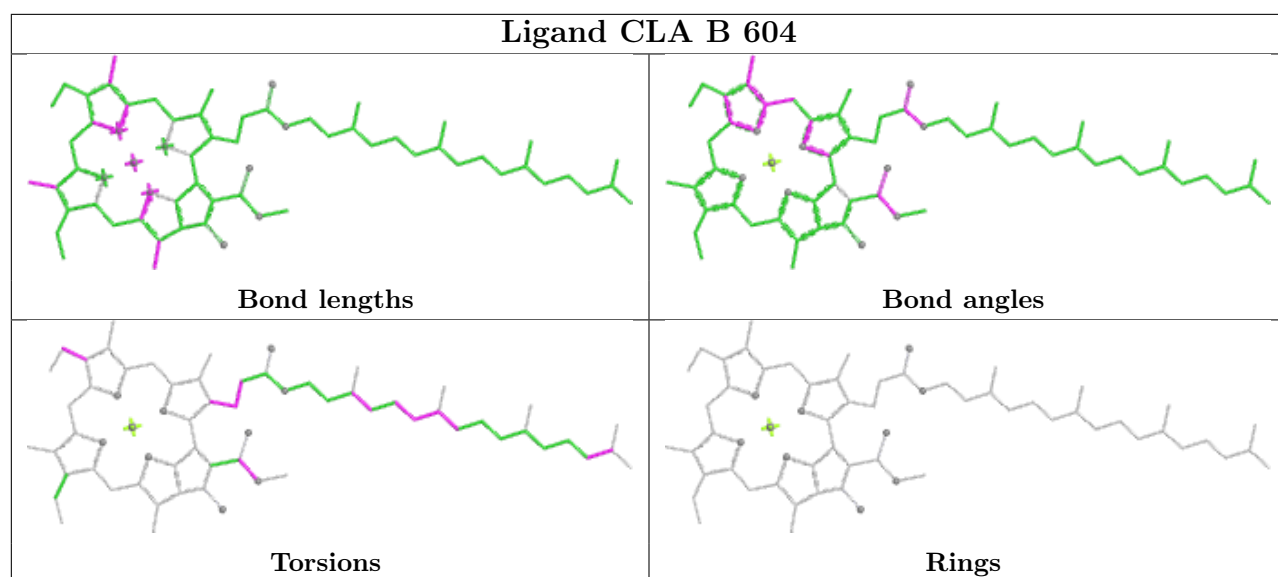
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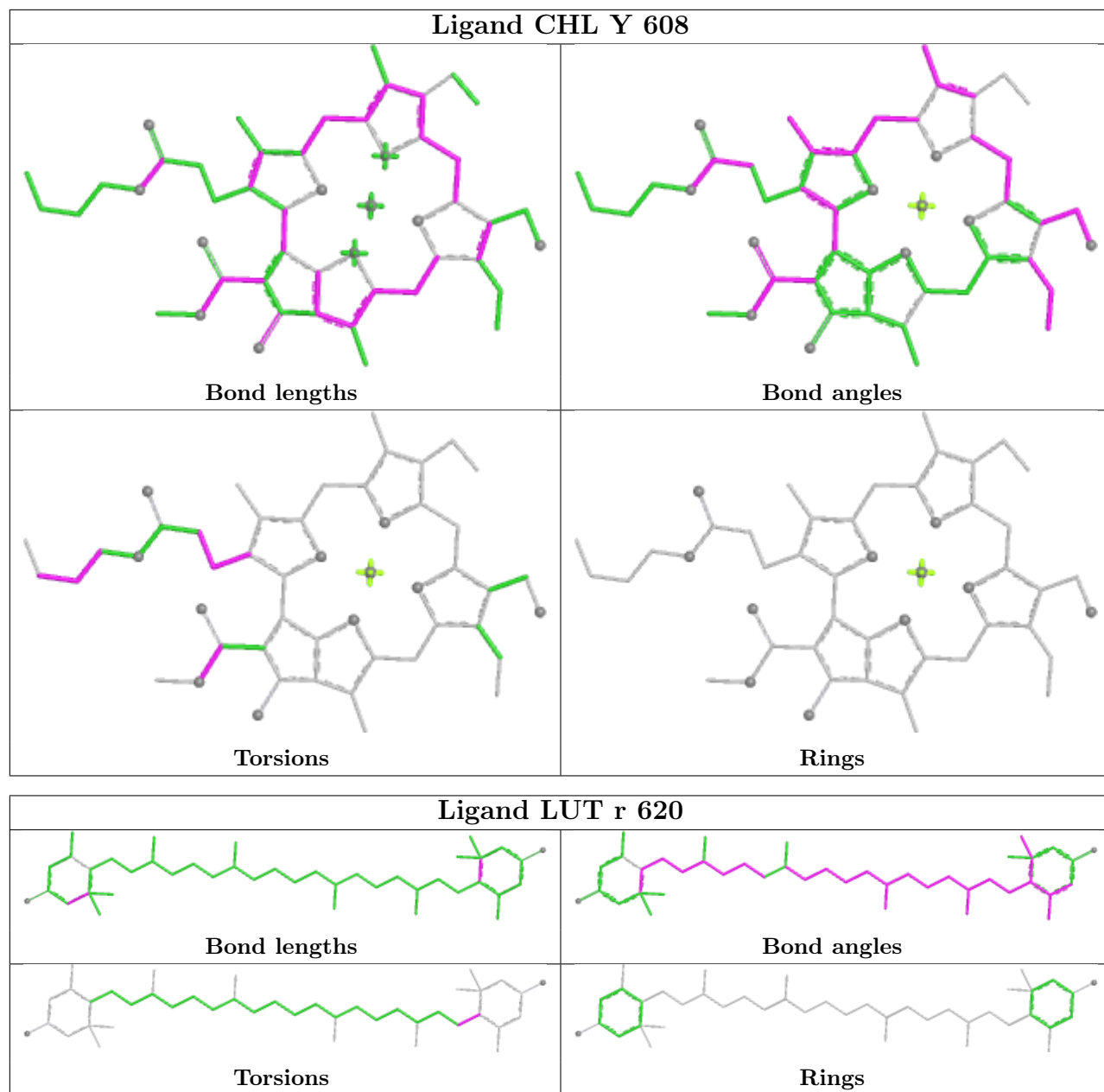


Ligand CLA B 617

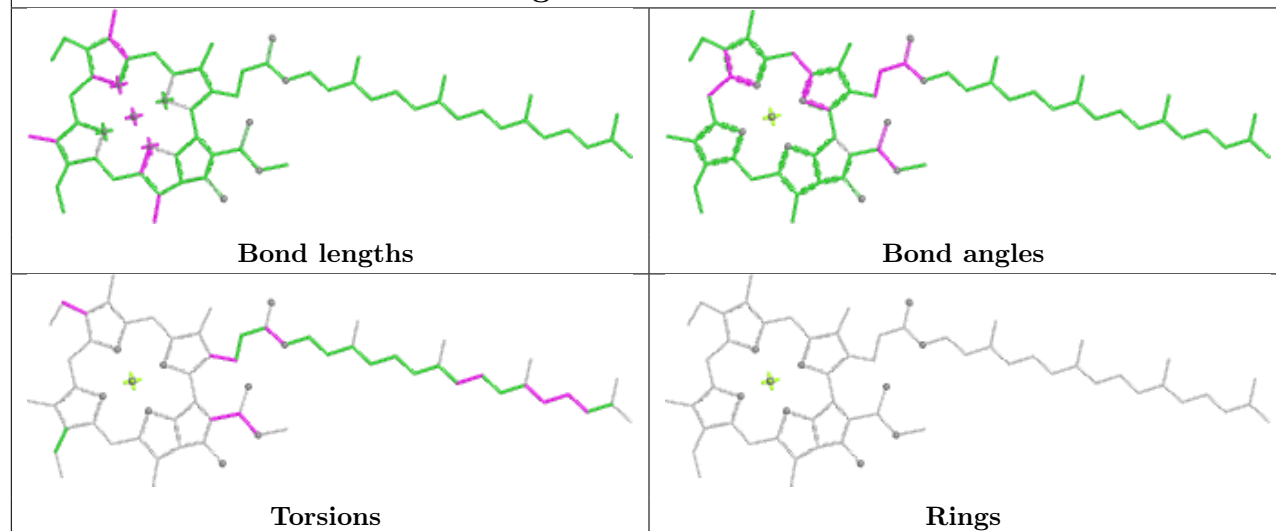




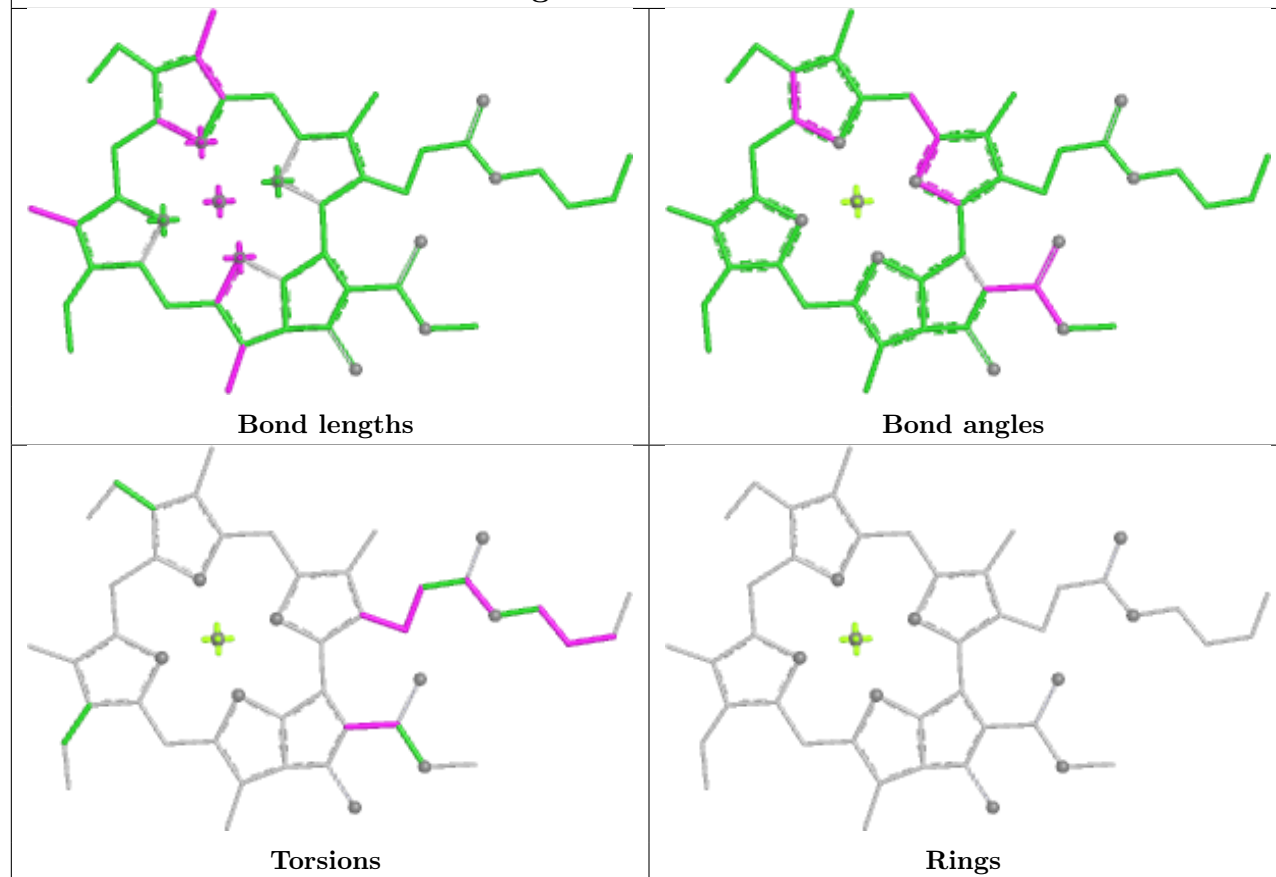




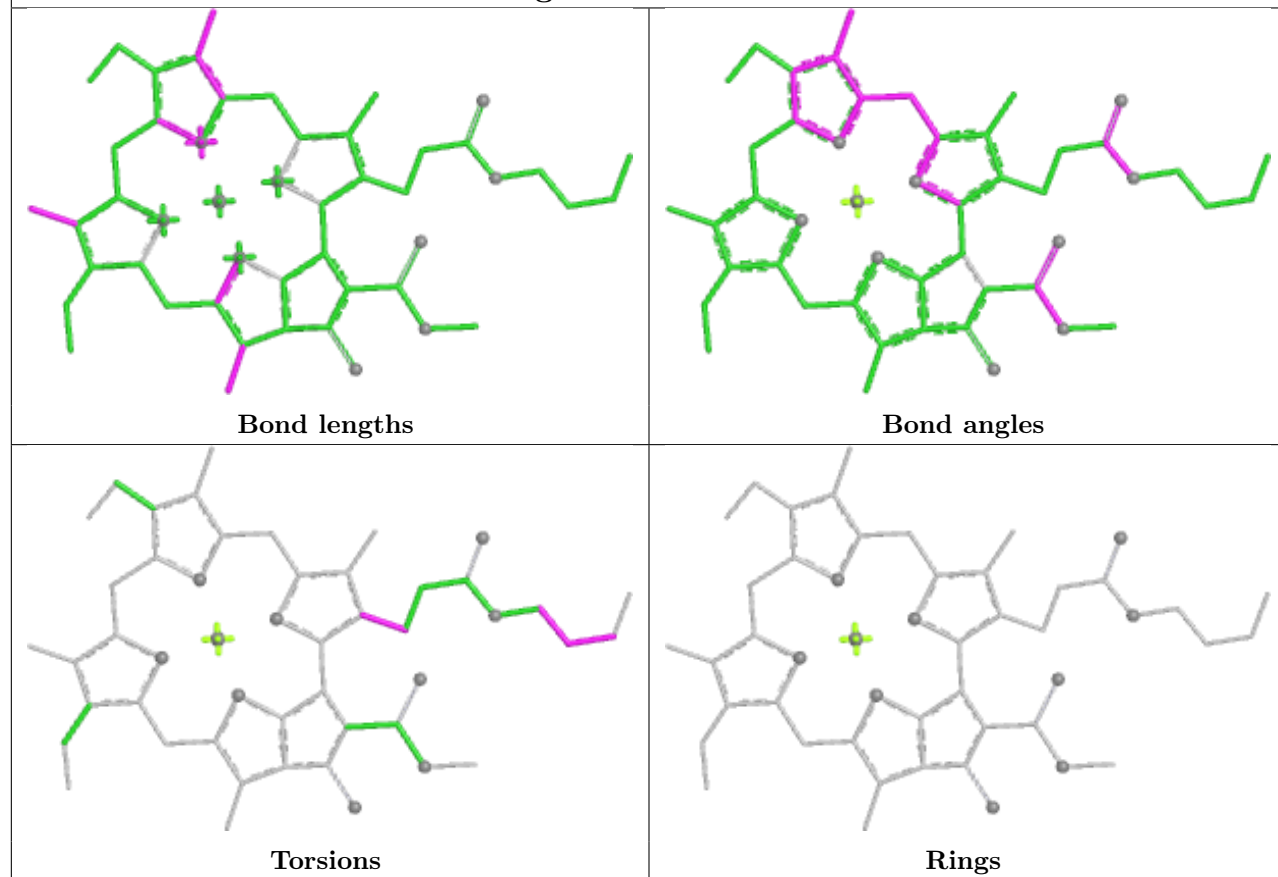
Ligand CLA C 503



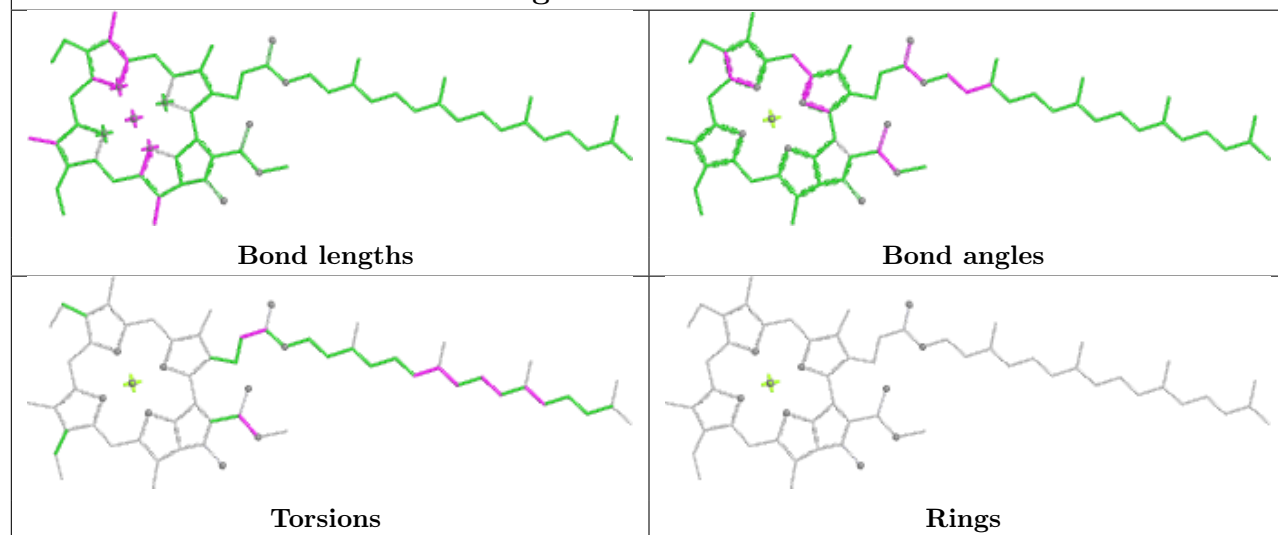
Ligand CLA R 604

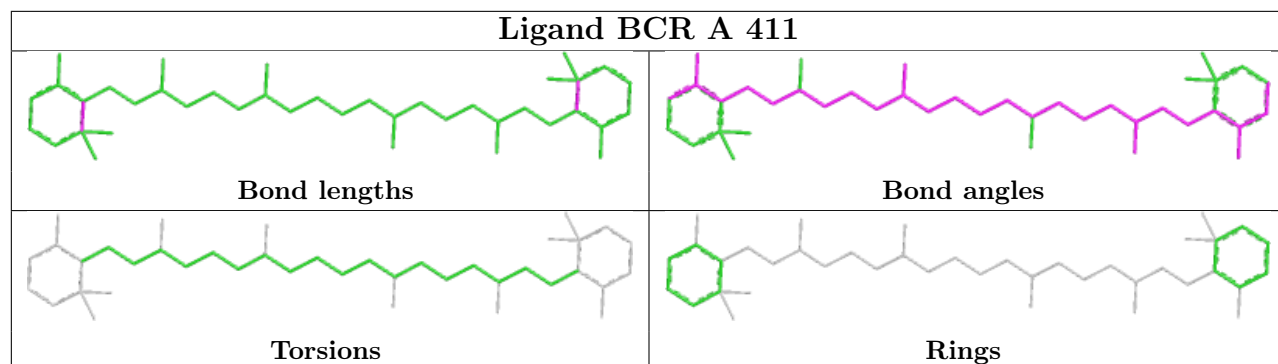
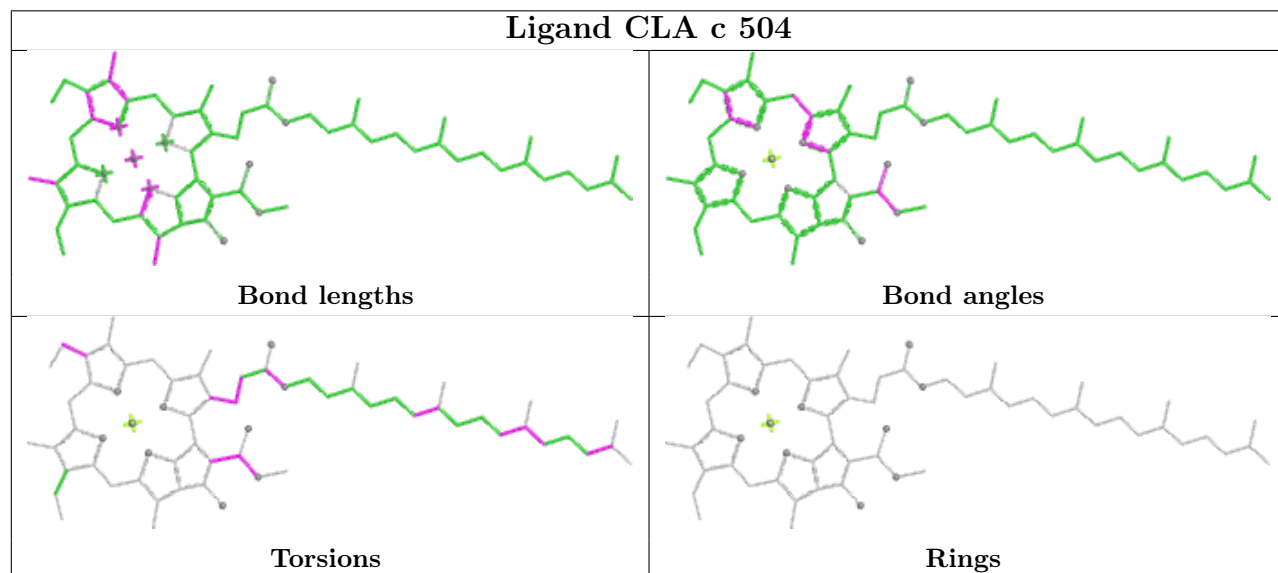
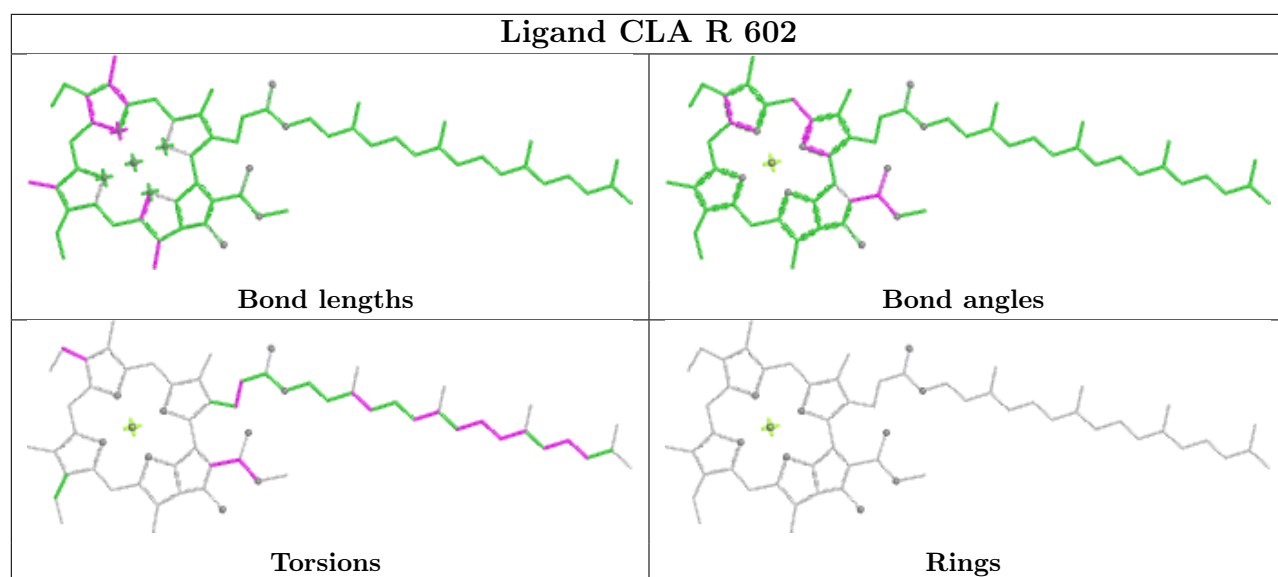


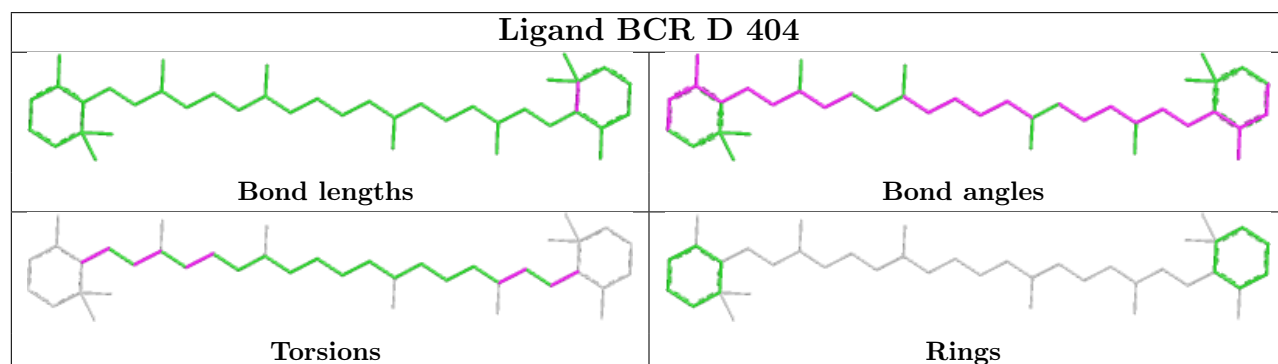
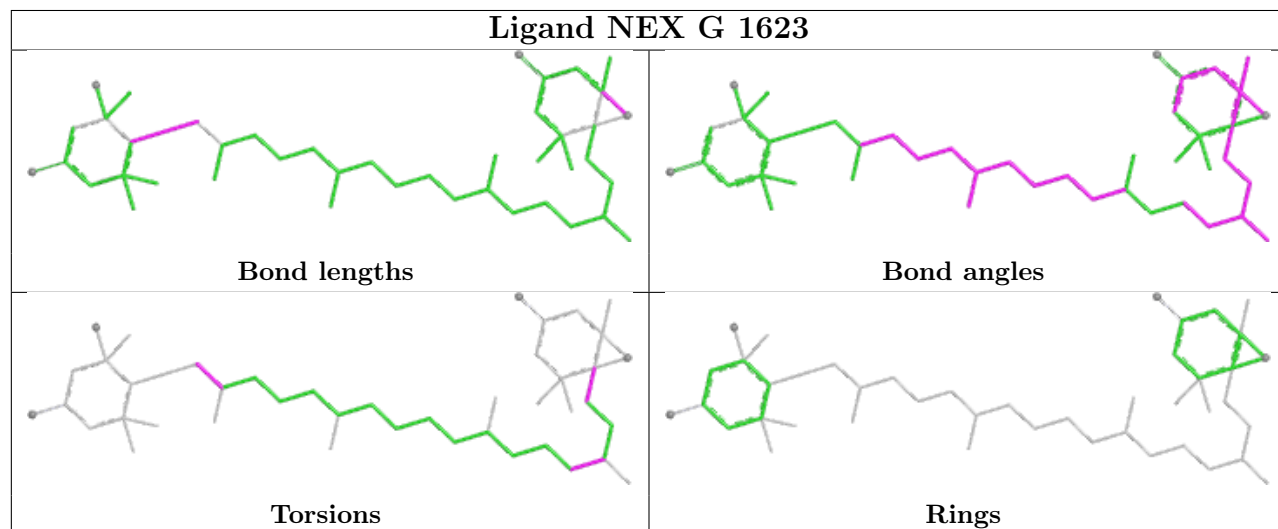
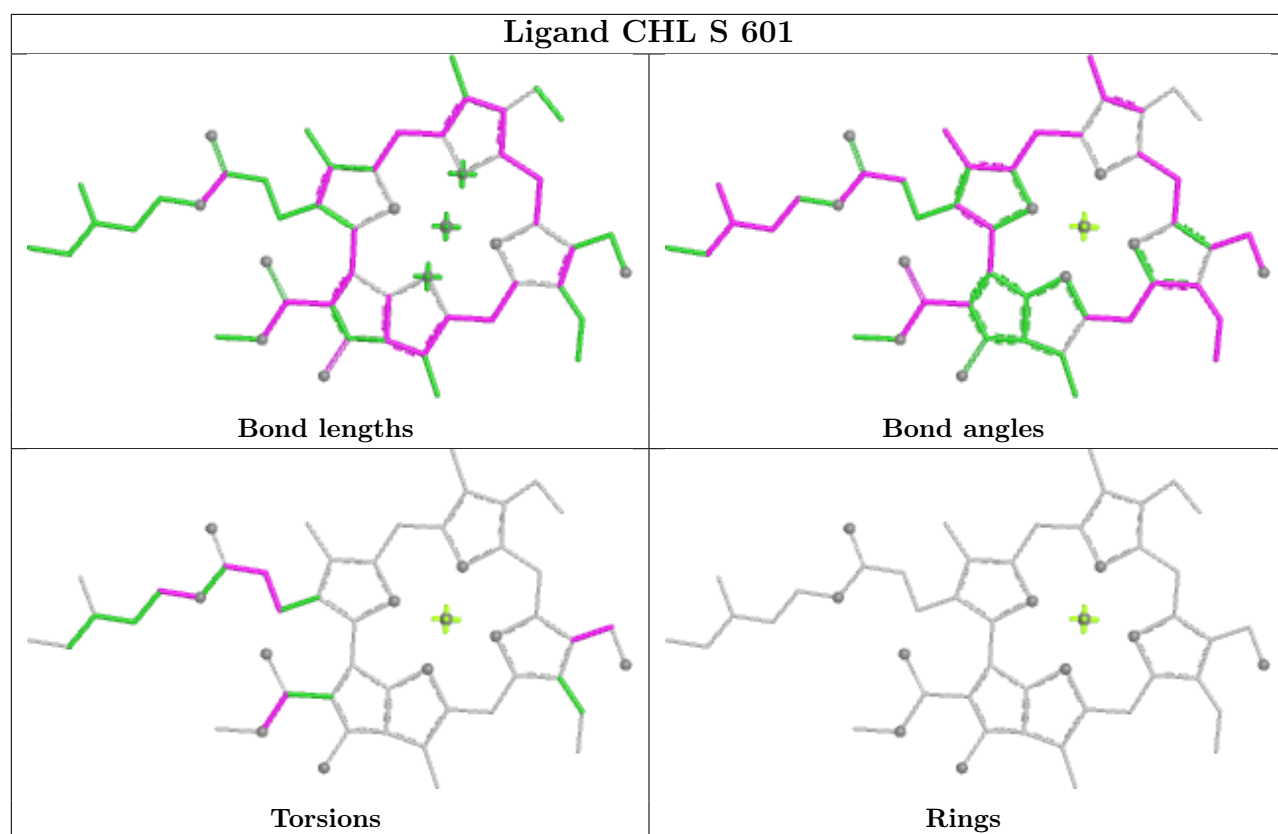
Ligand CLA S 610



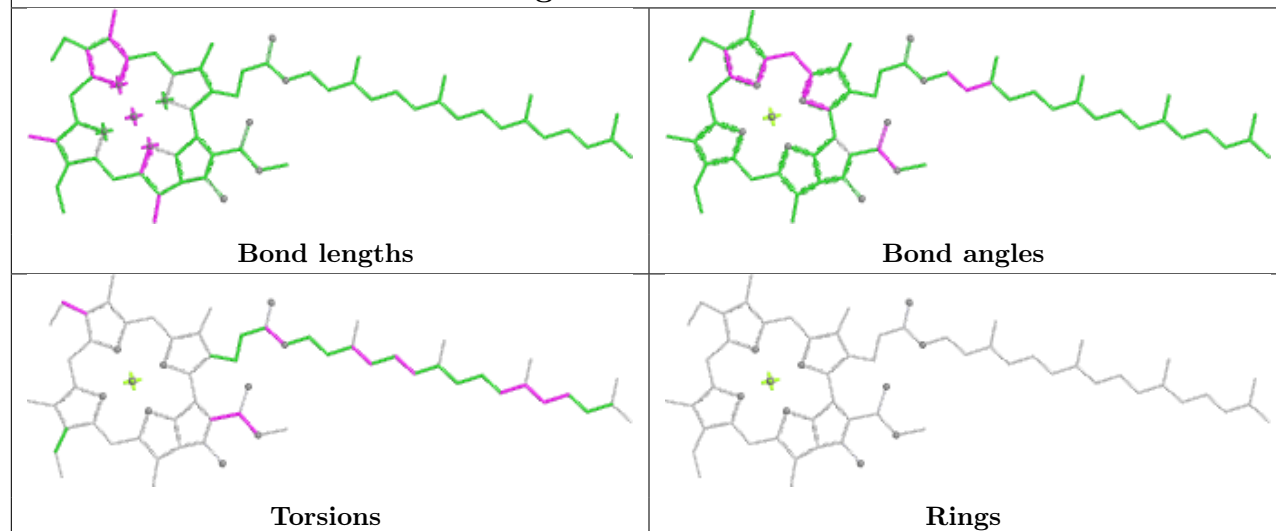
Ligand CLA B 614



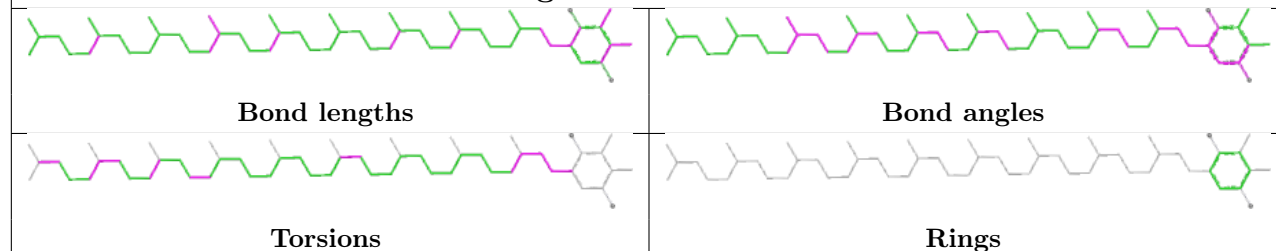




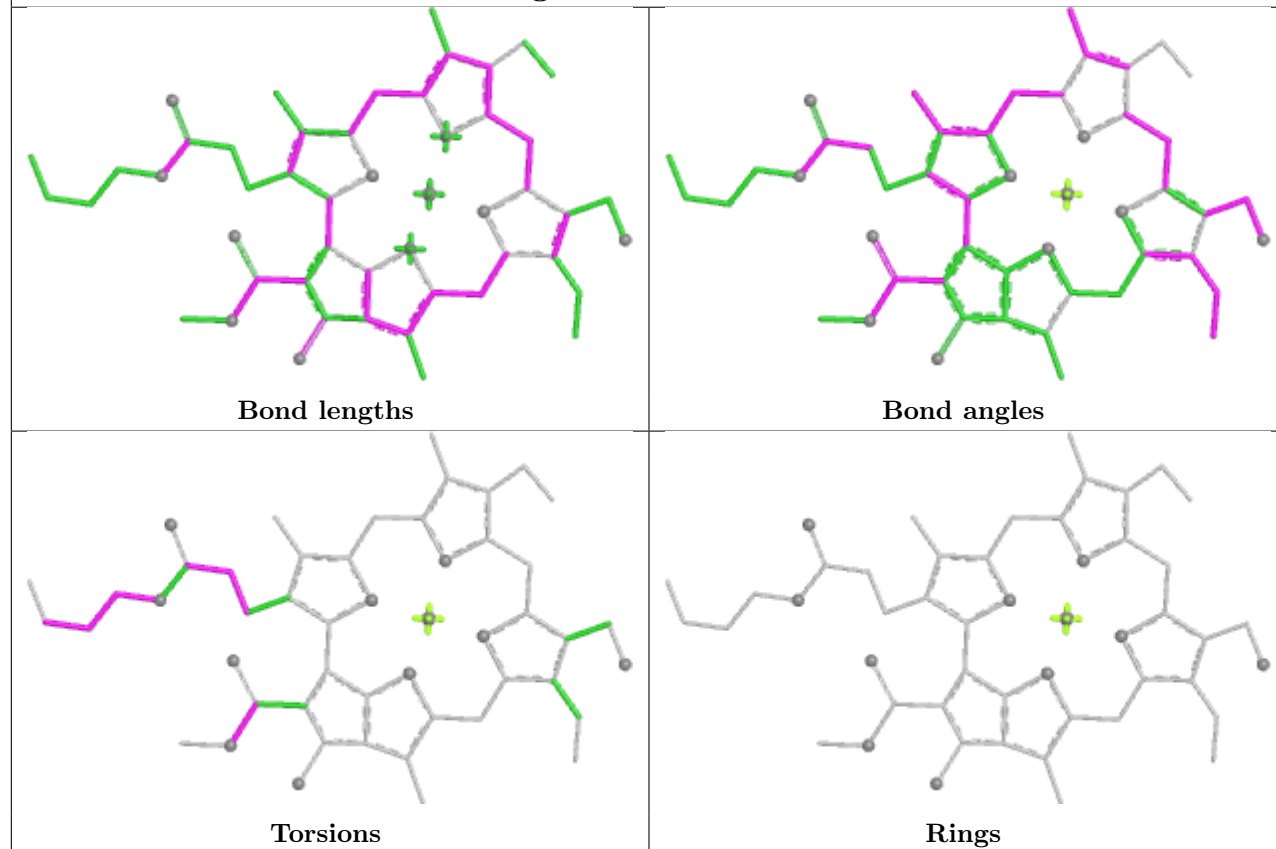
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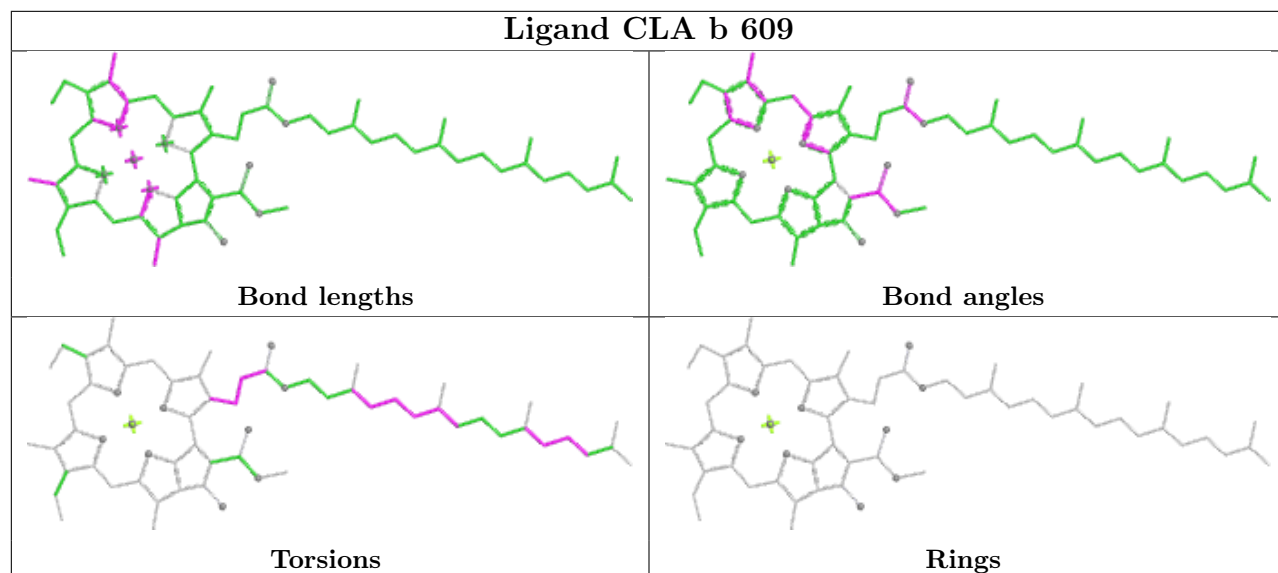
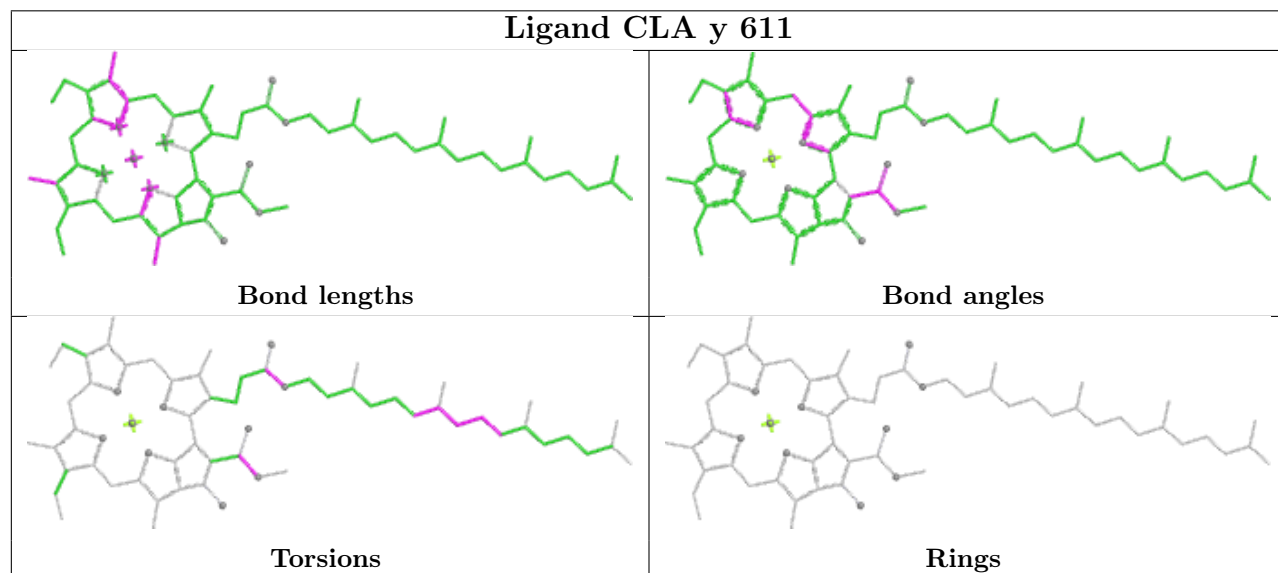
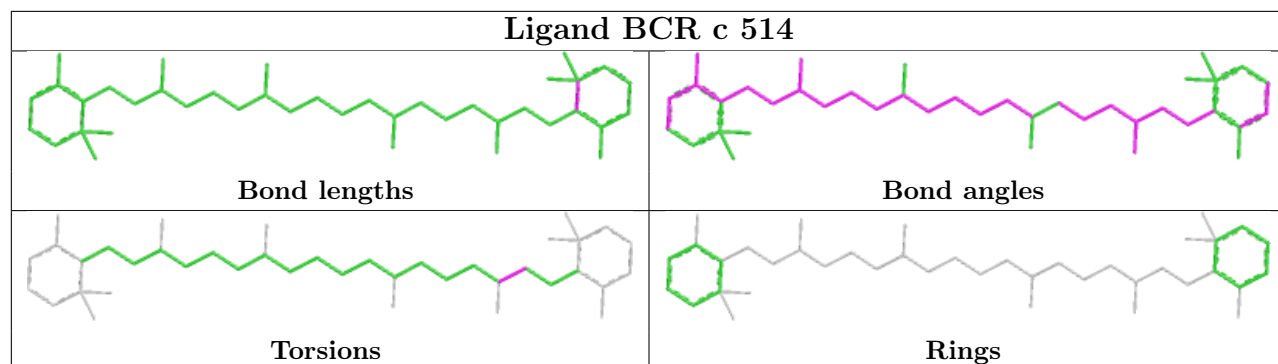


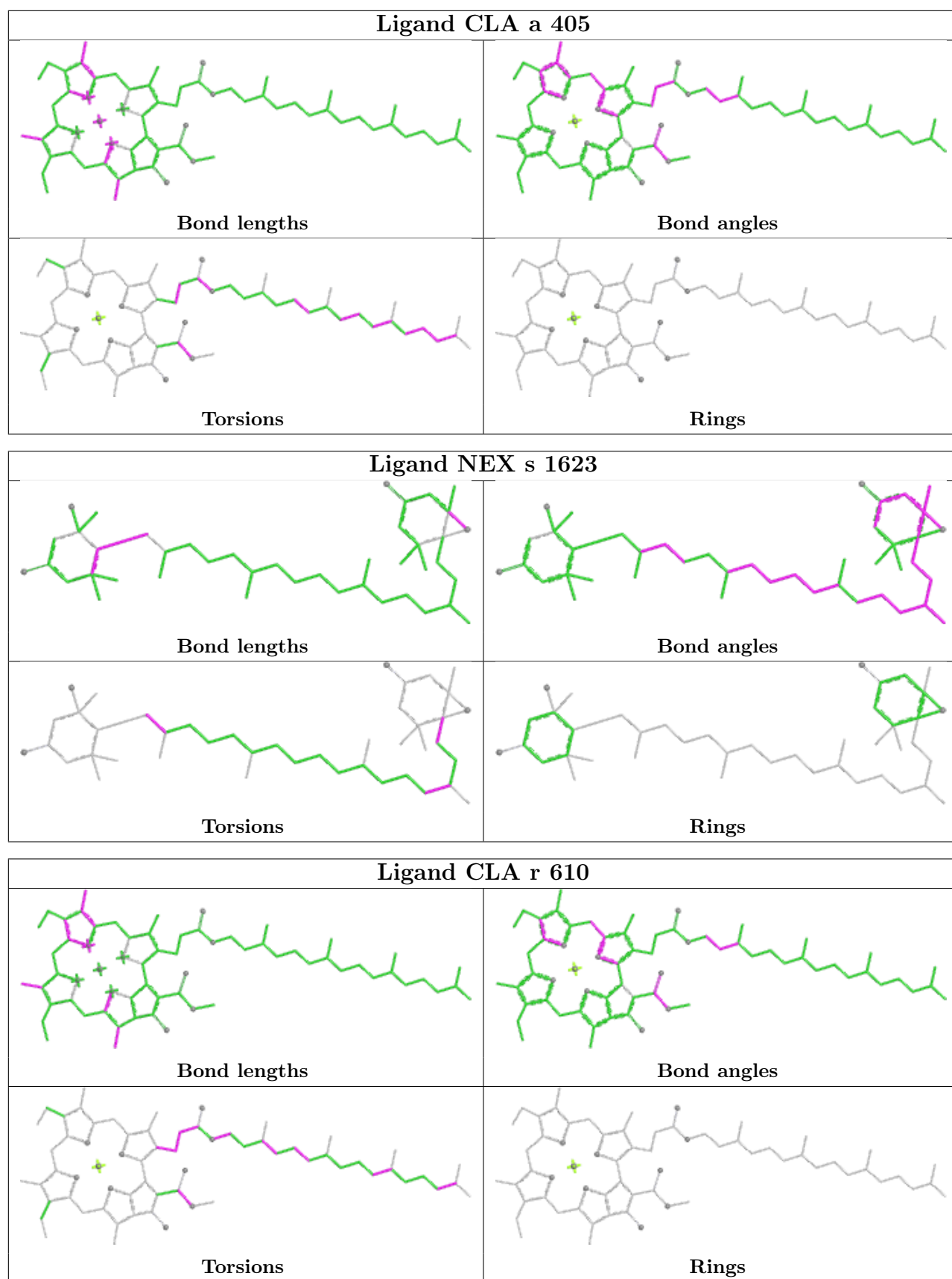
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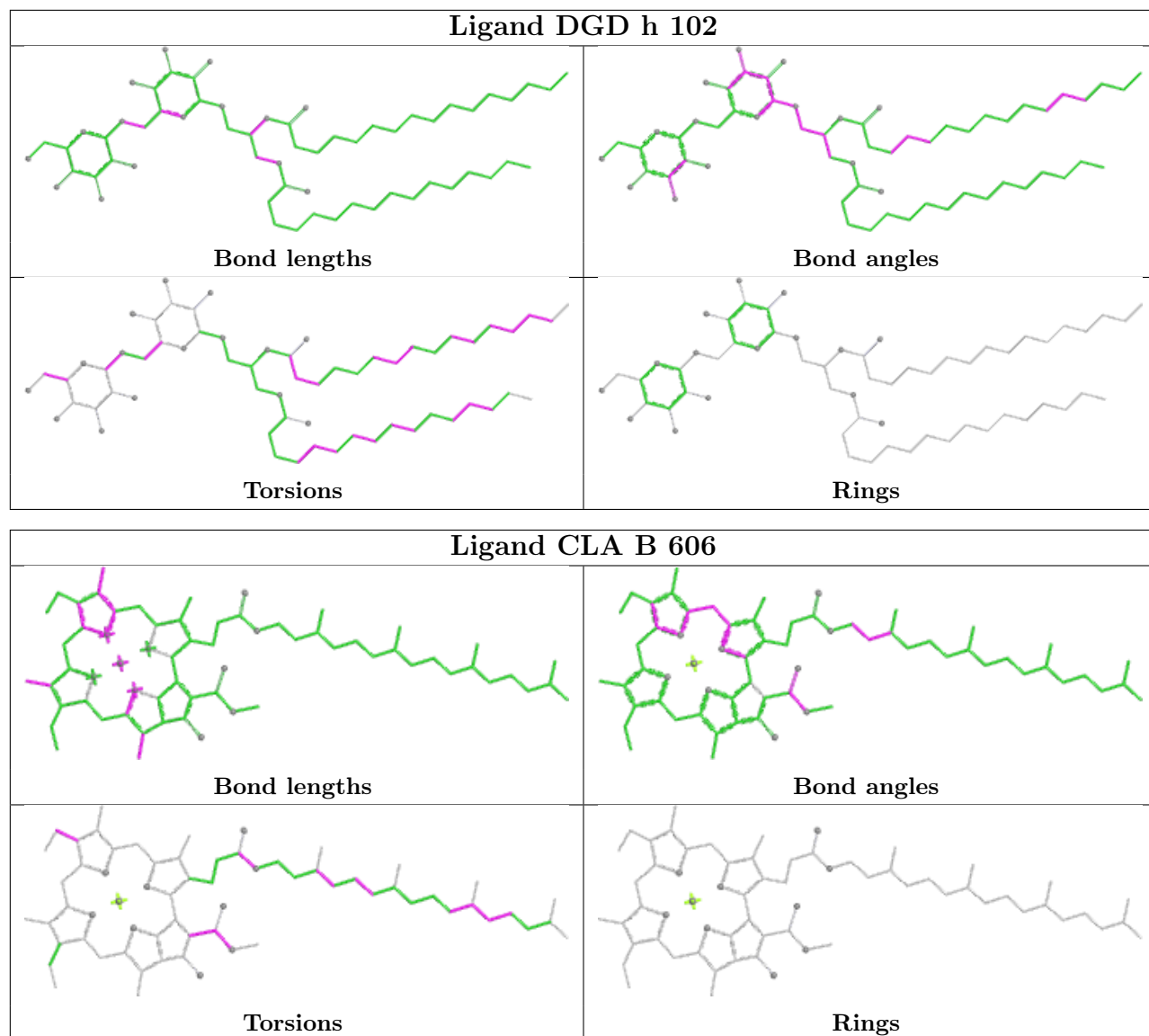


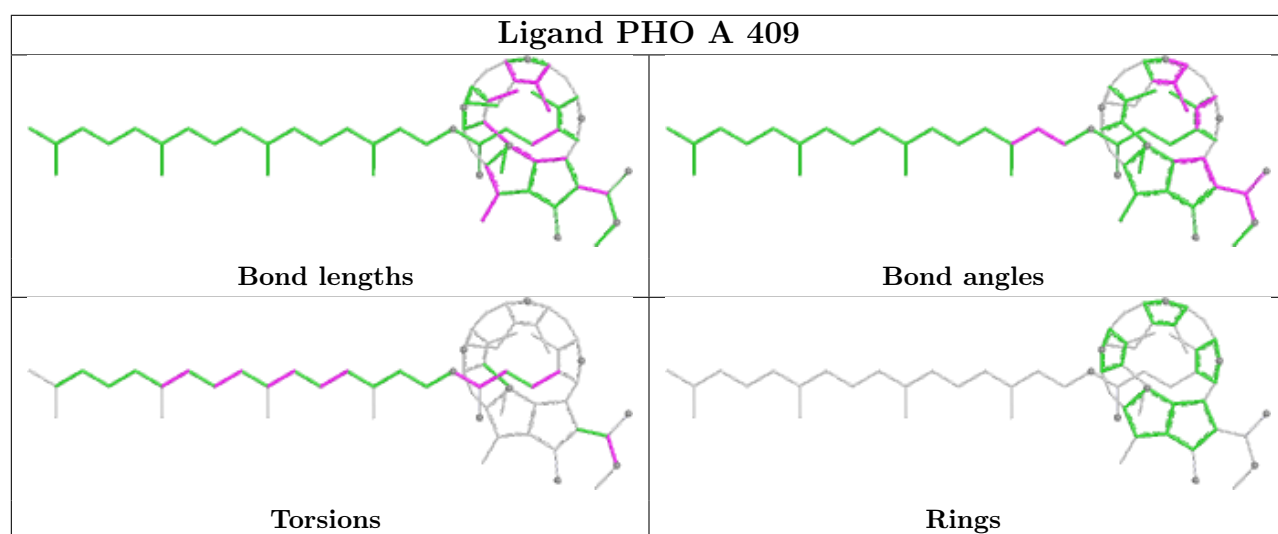
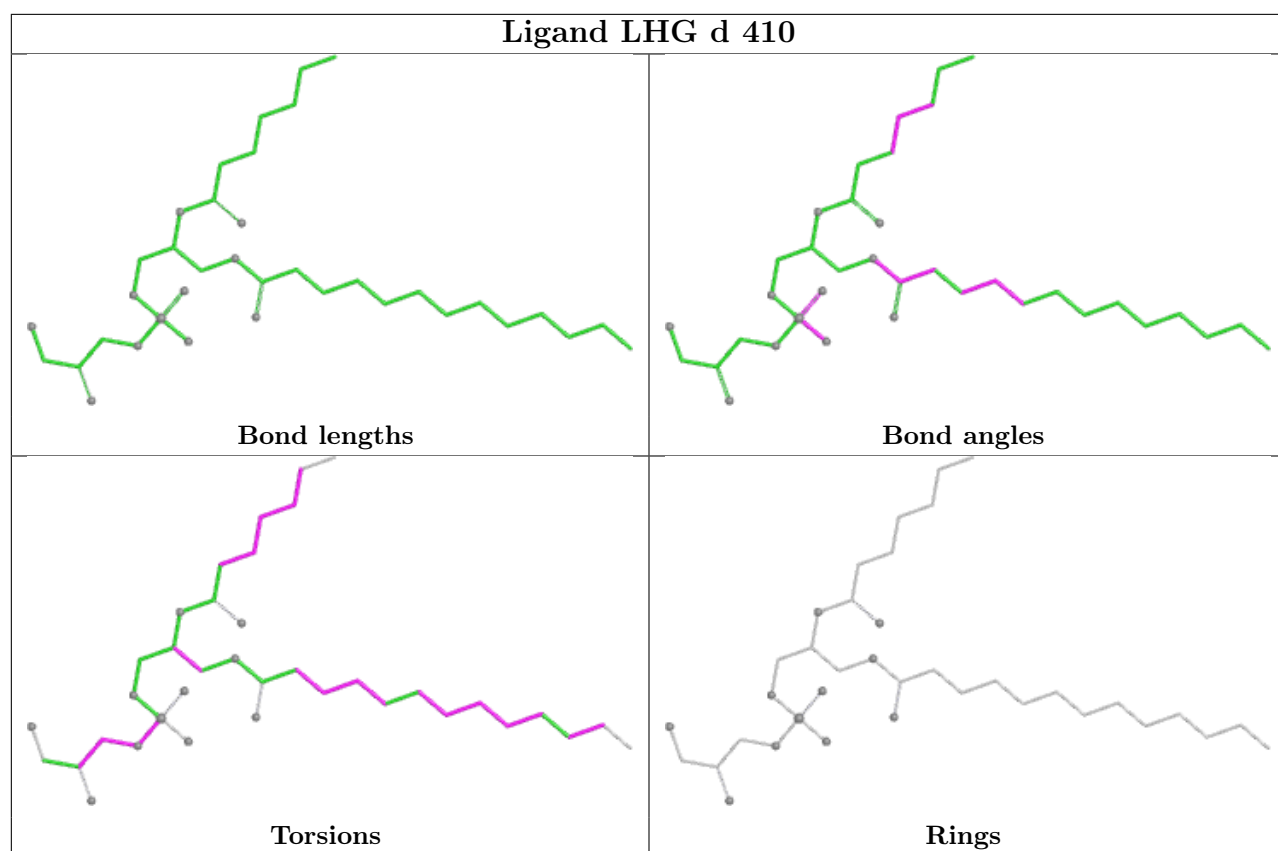
Ligand CHL Y 607

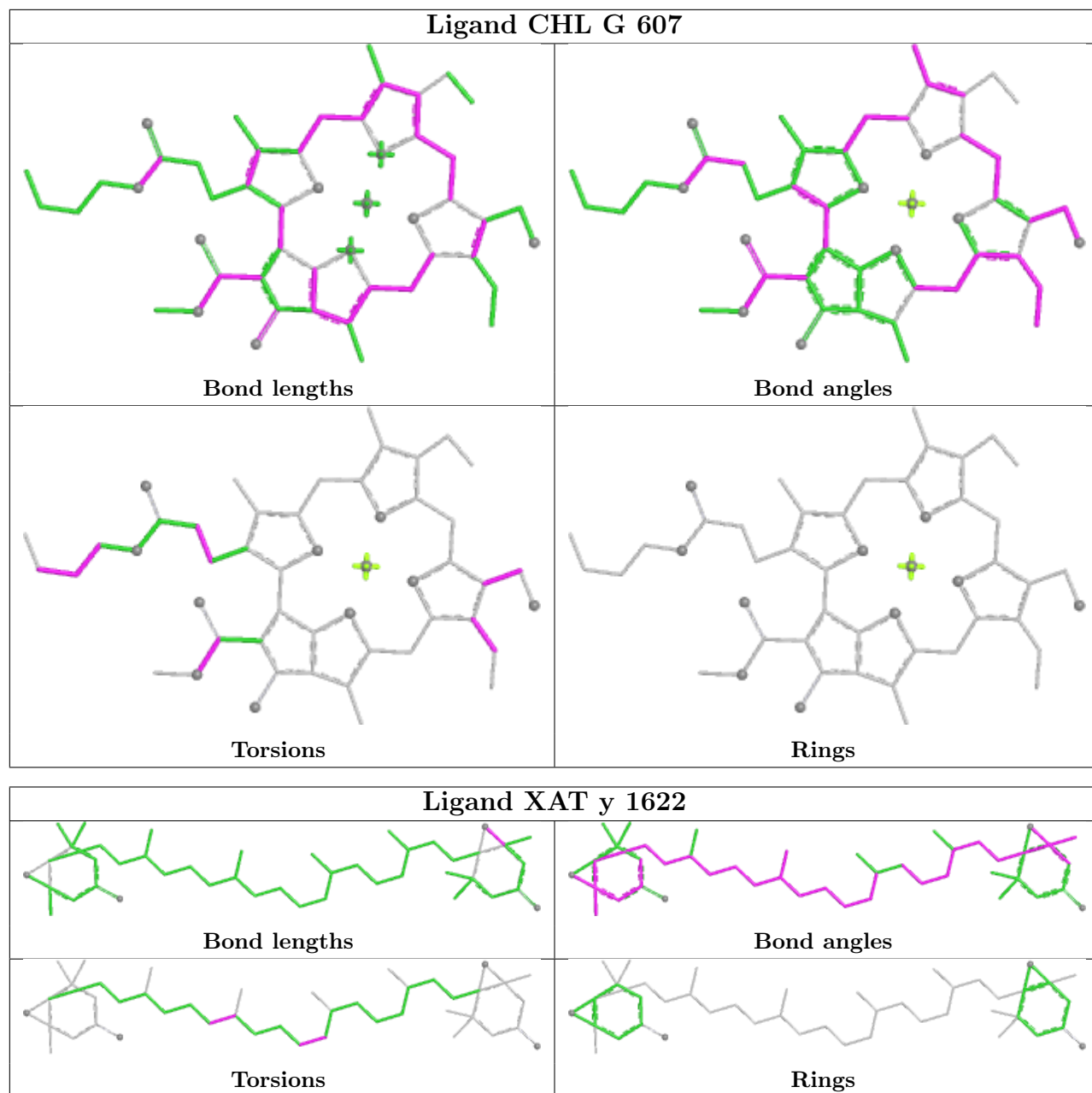


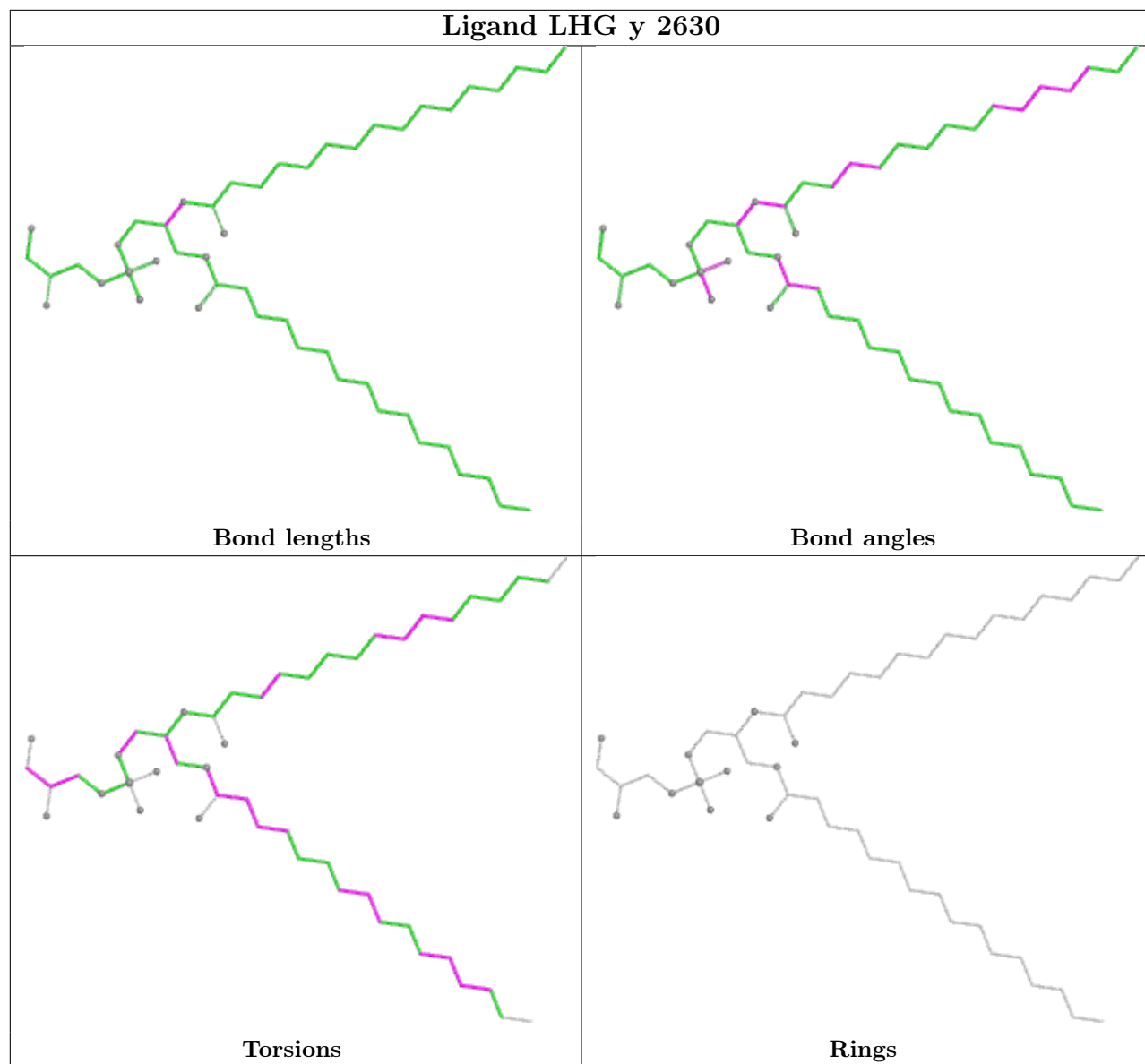


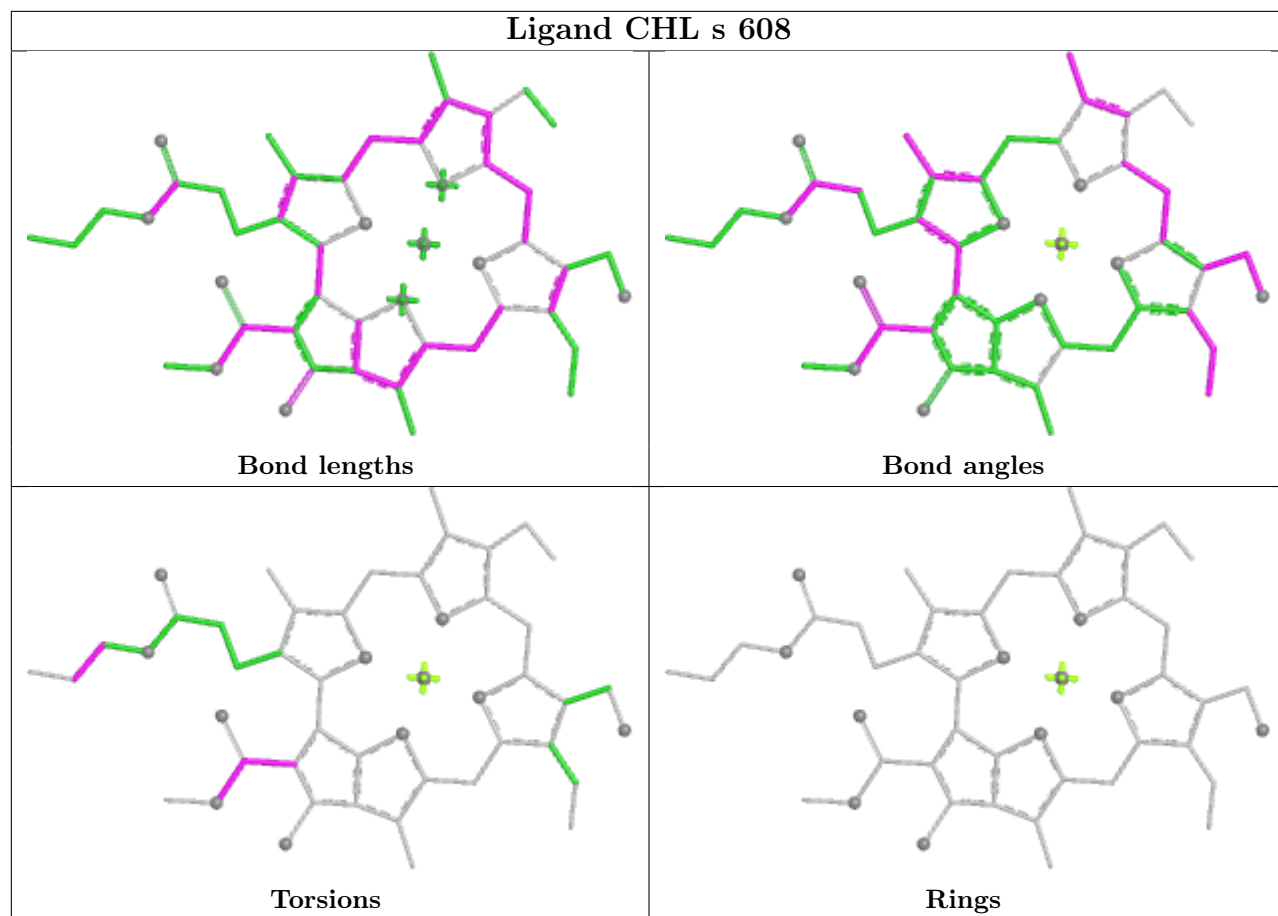


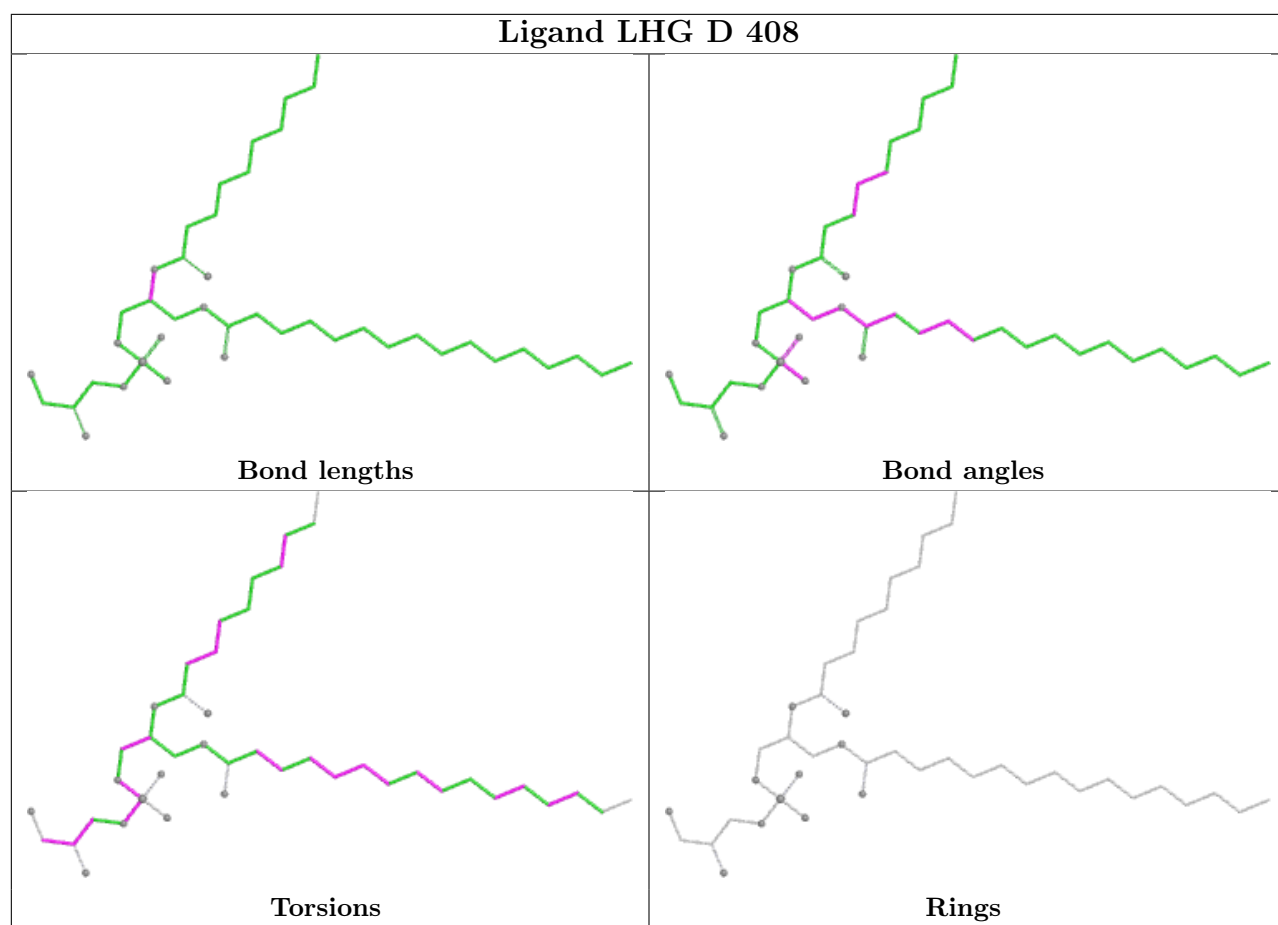


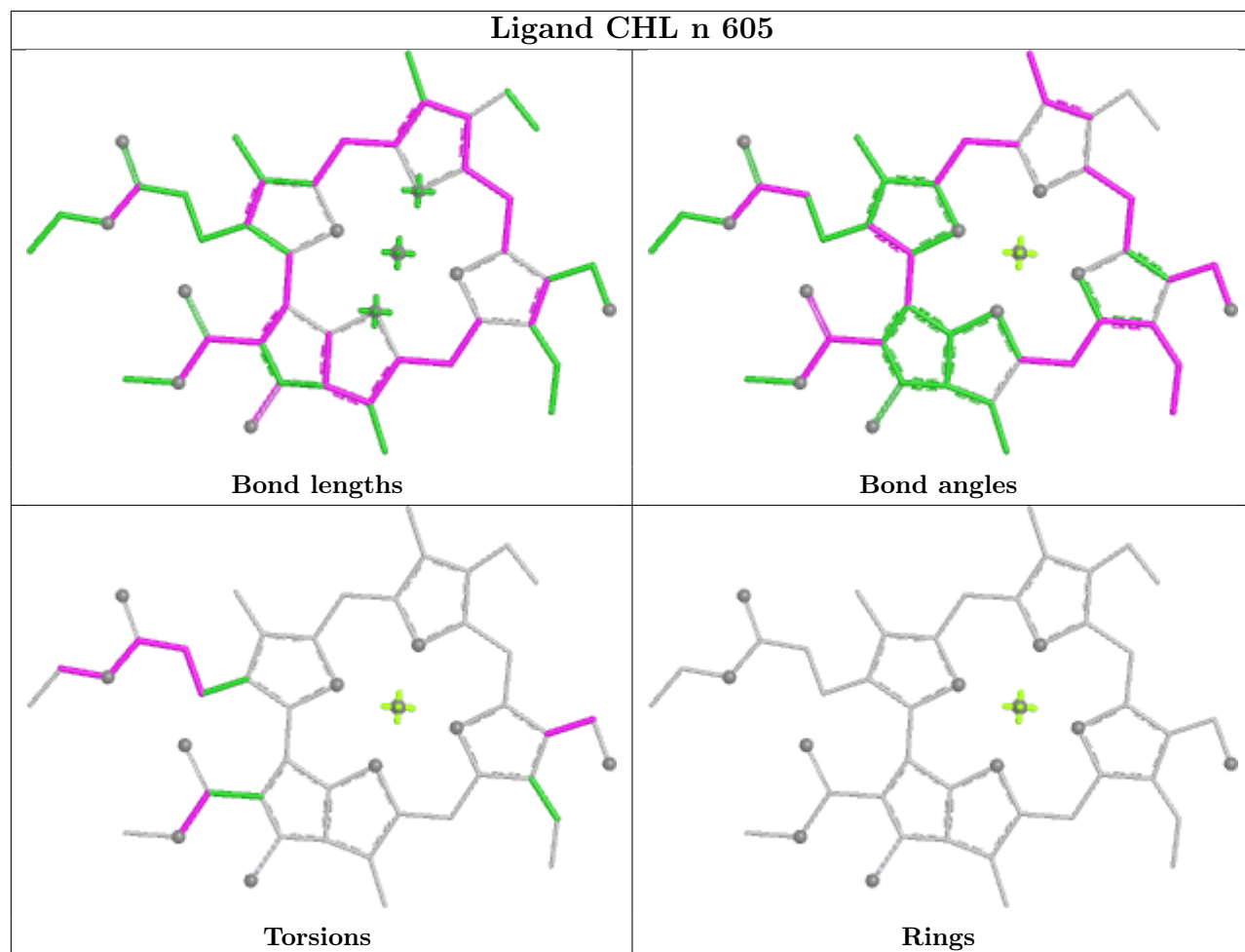




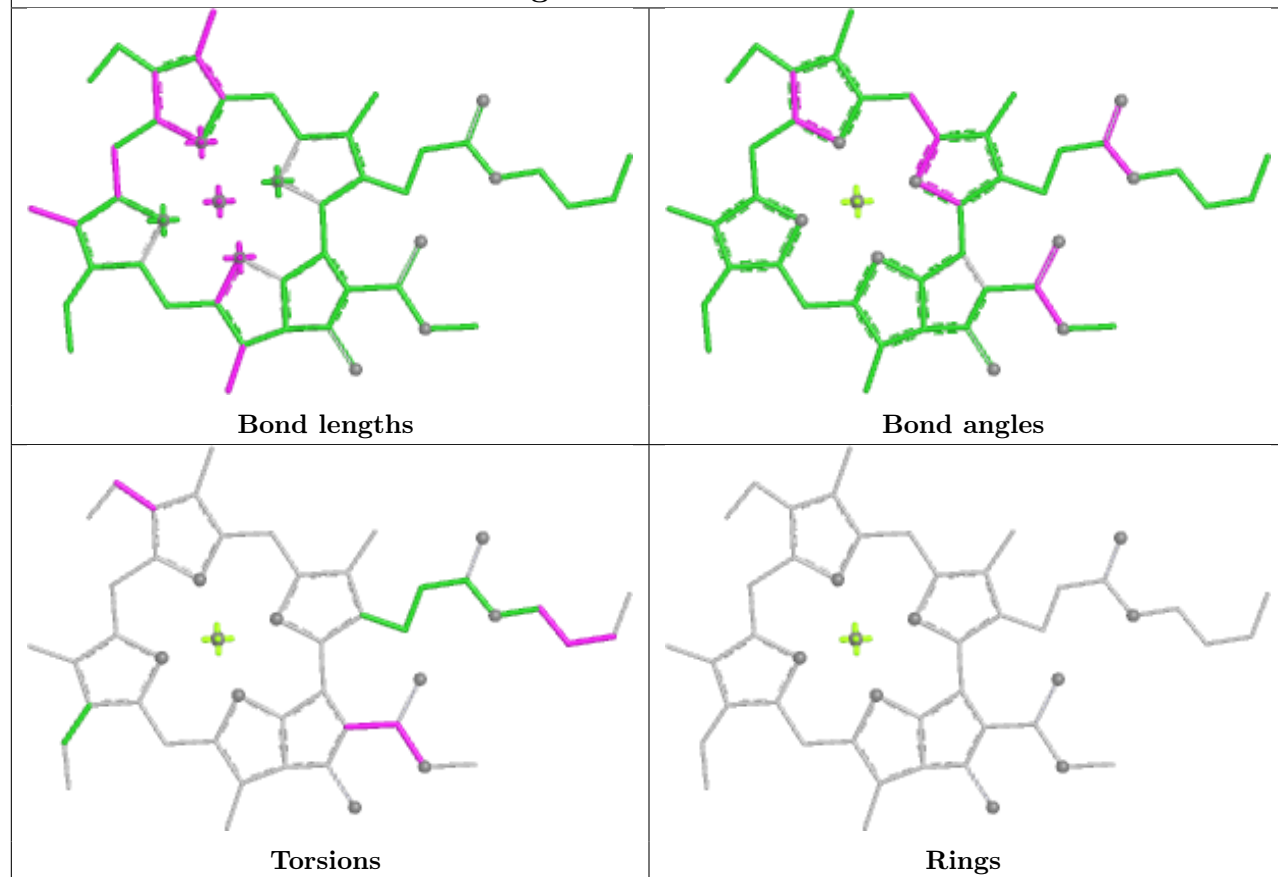




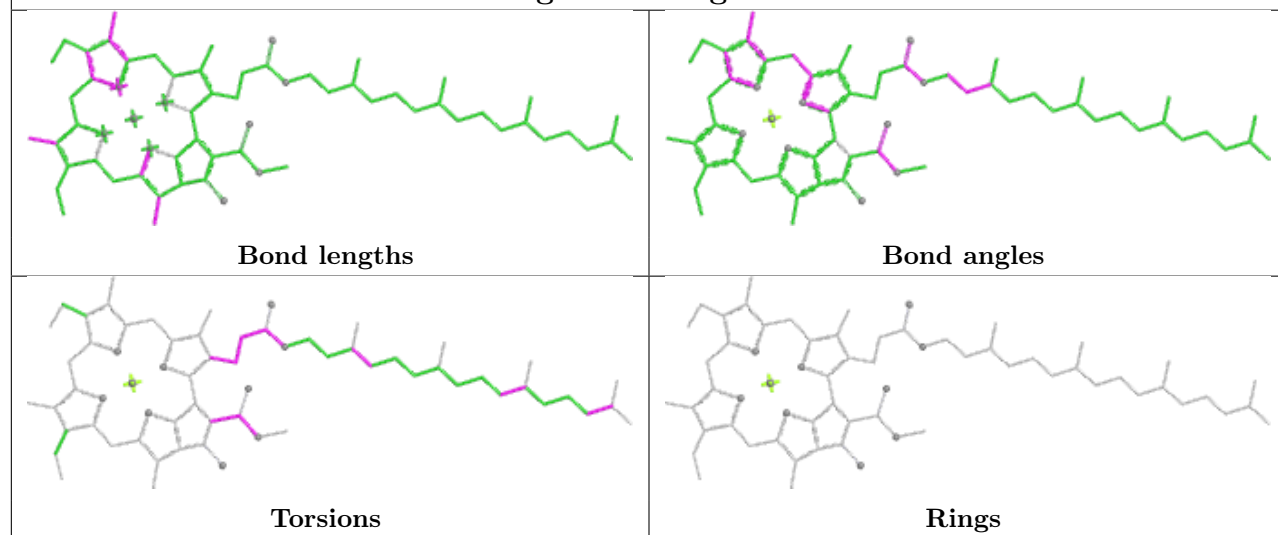




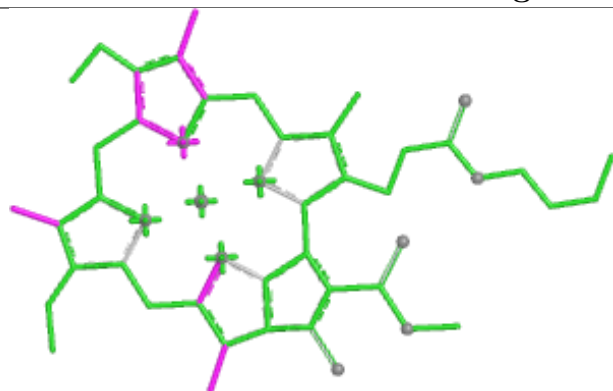
Ligand CLA G 612



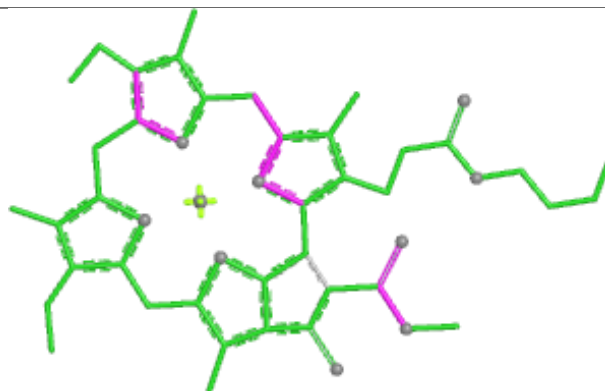
Ligand CLA g 610



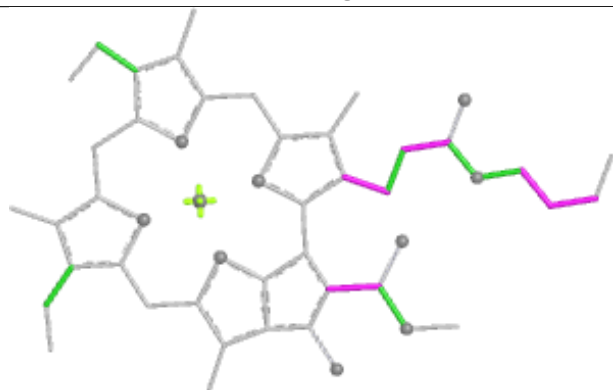
Ligand CLA G 603



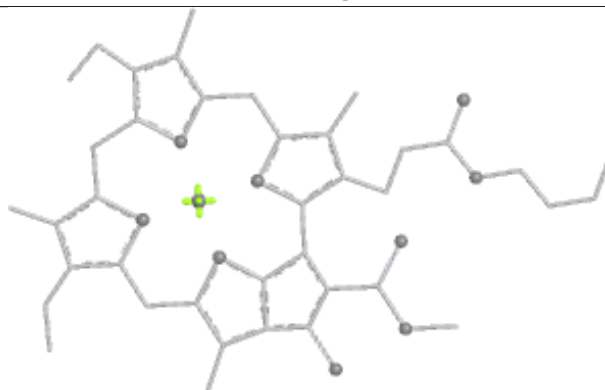
Bond lengths



Bond angles

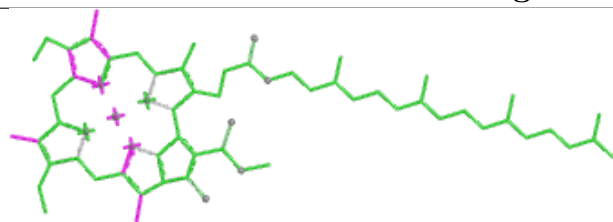


Torsions

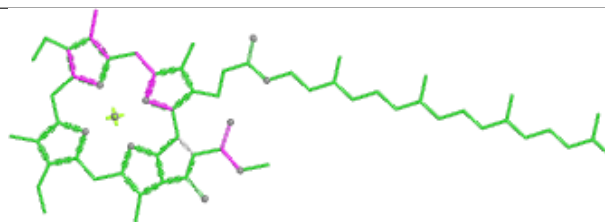


Rings

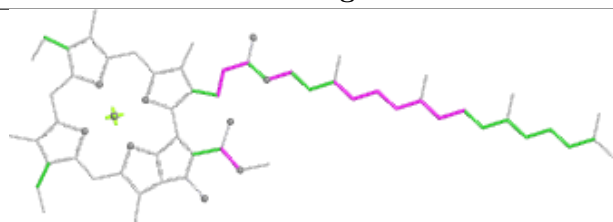
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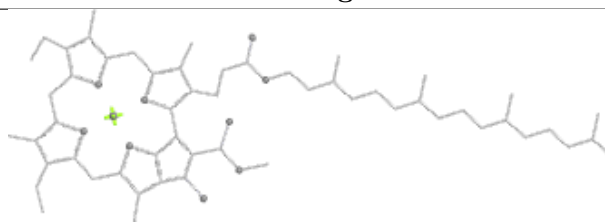
Bond lengths



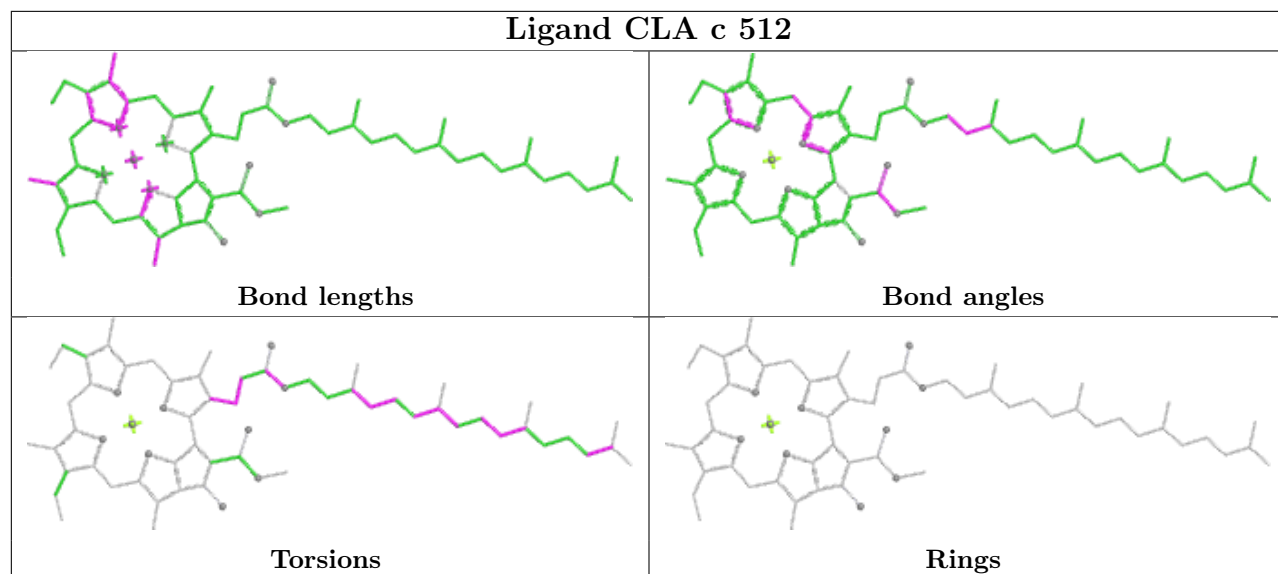
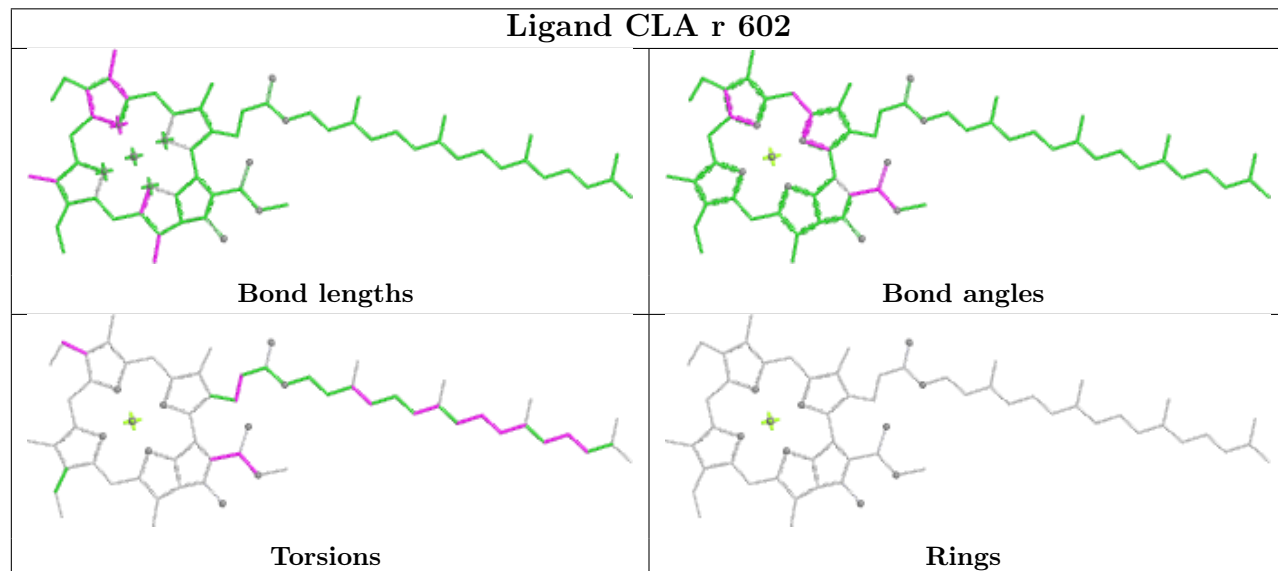
Bond angles

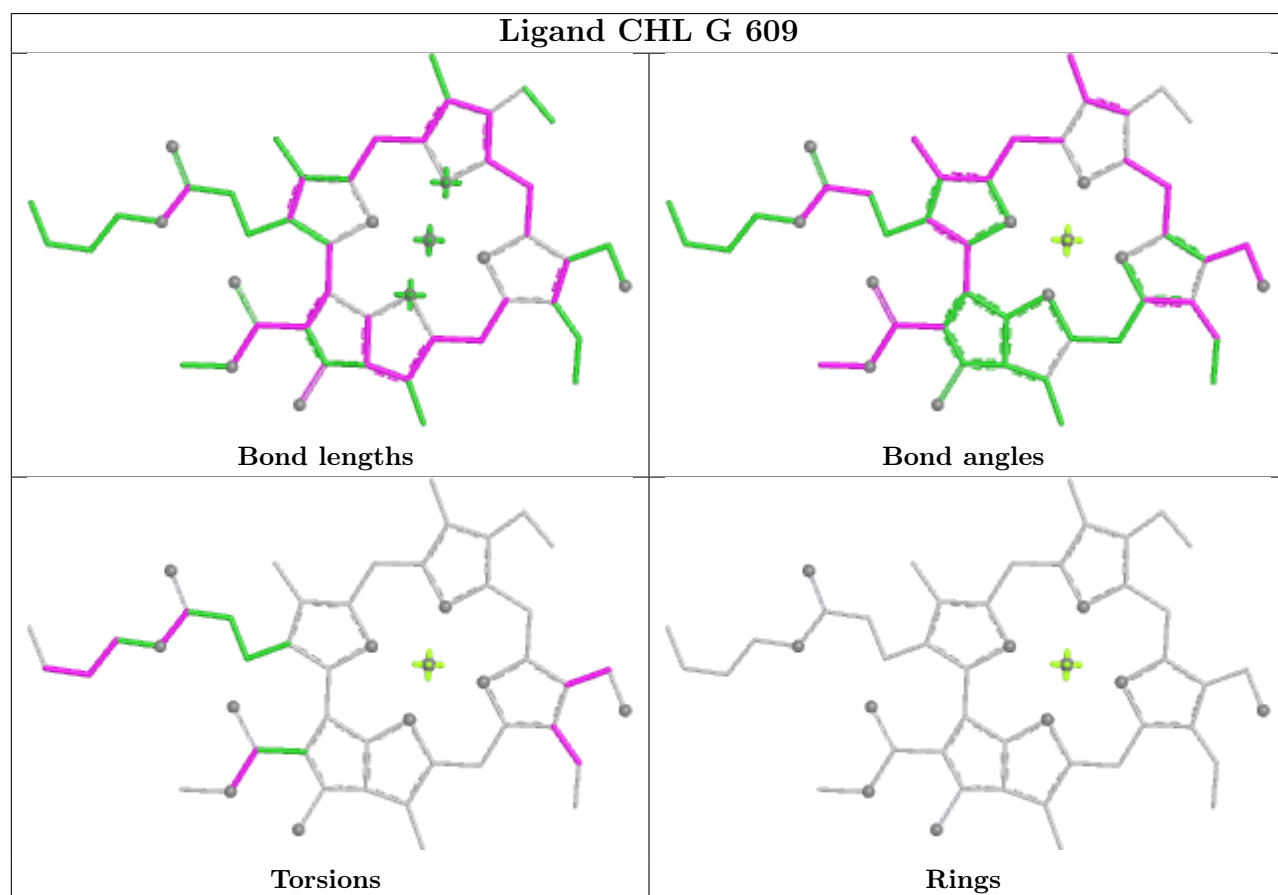
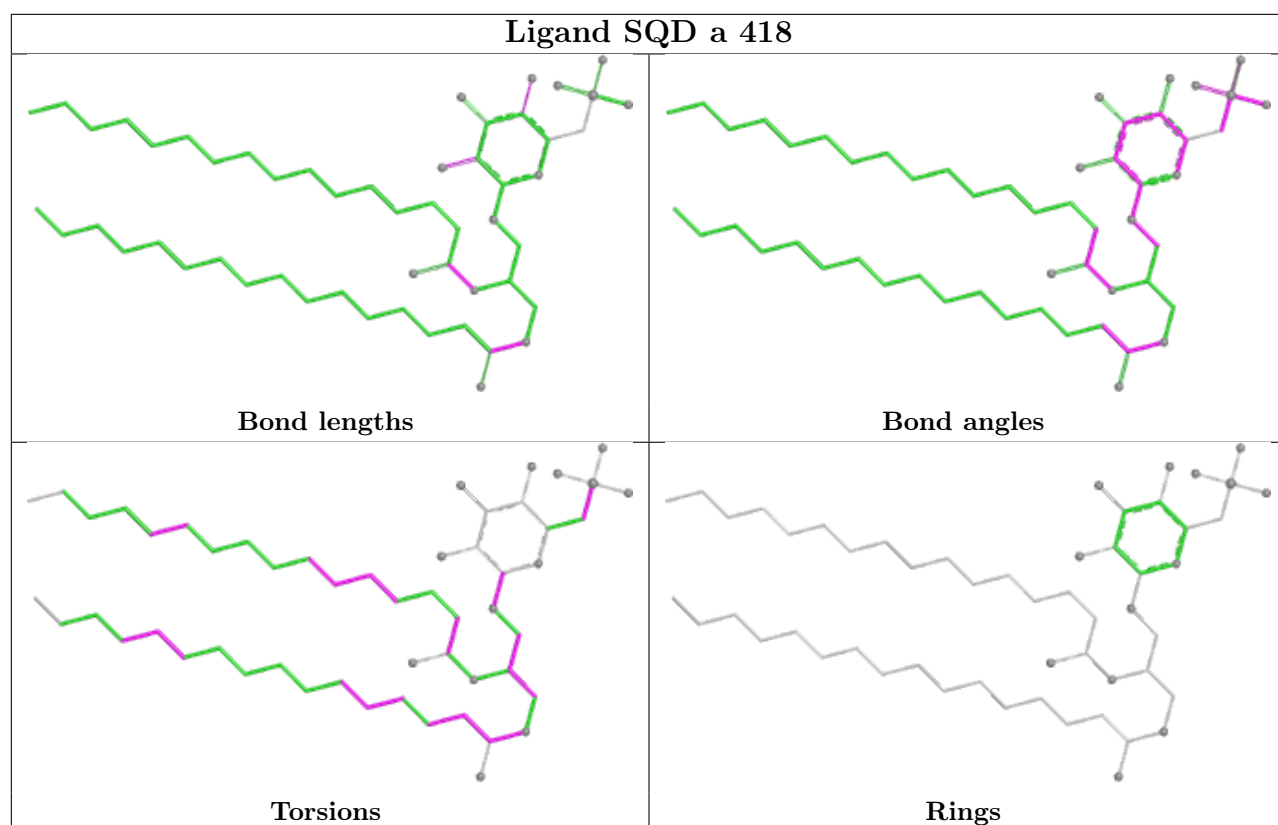


Torsions

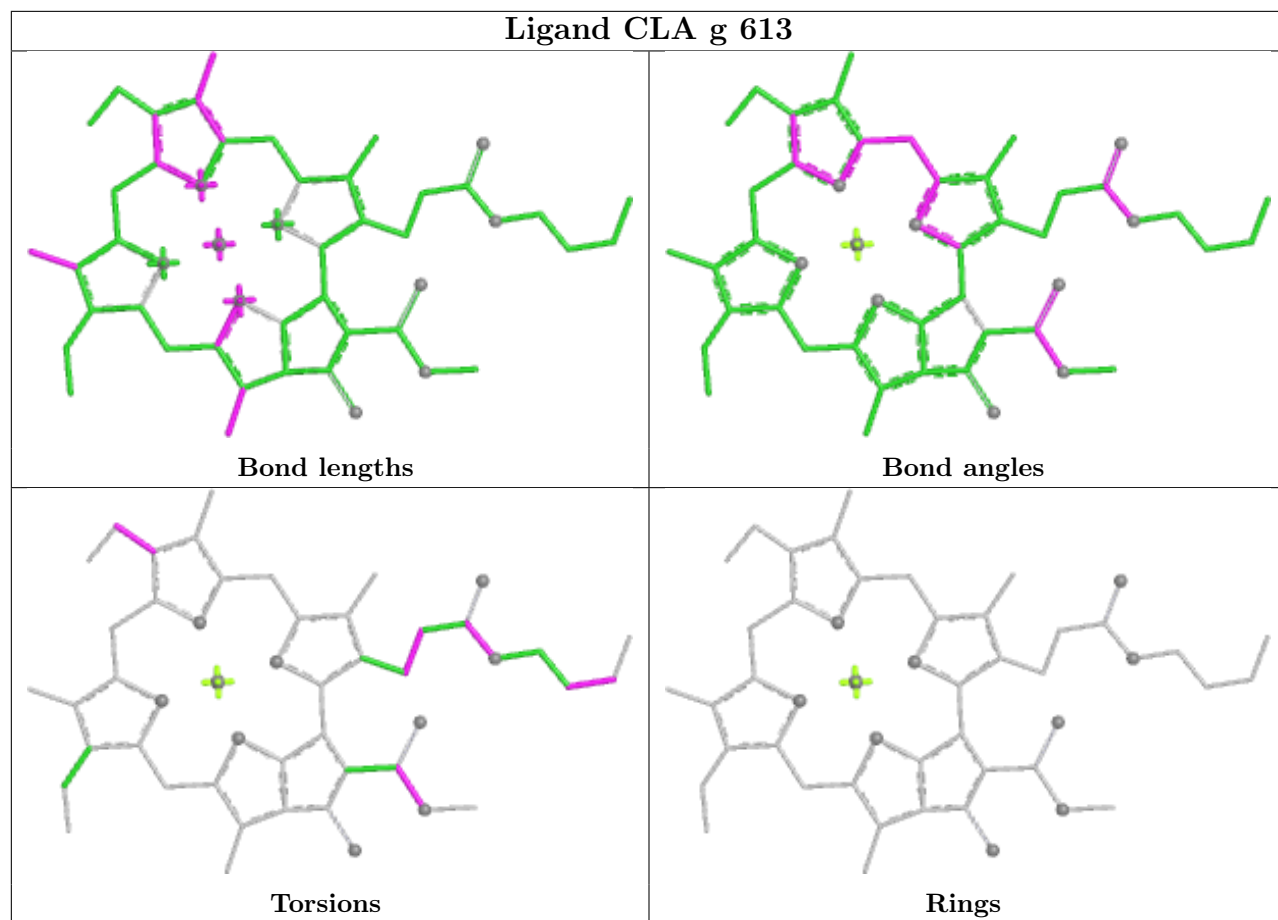


Rings

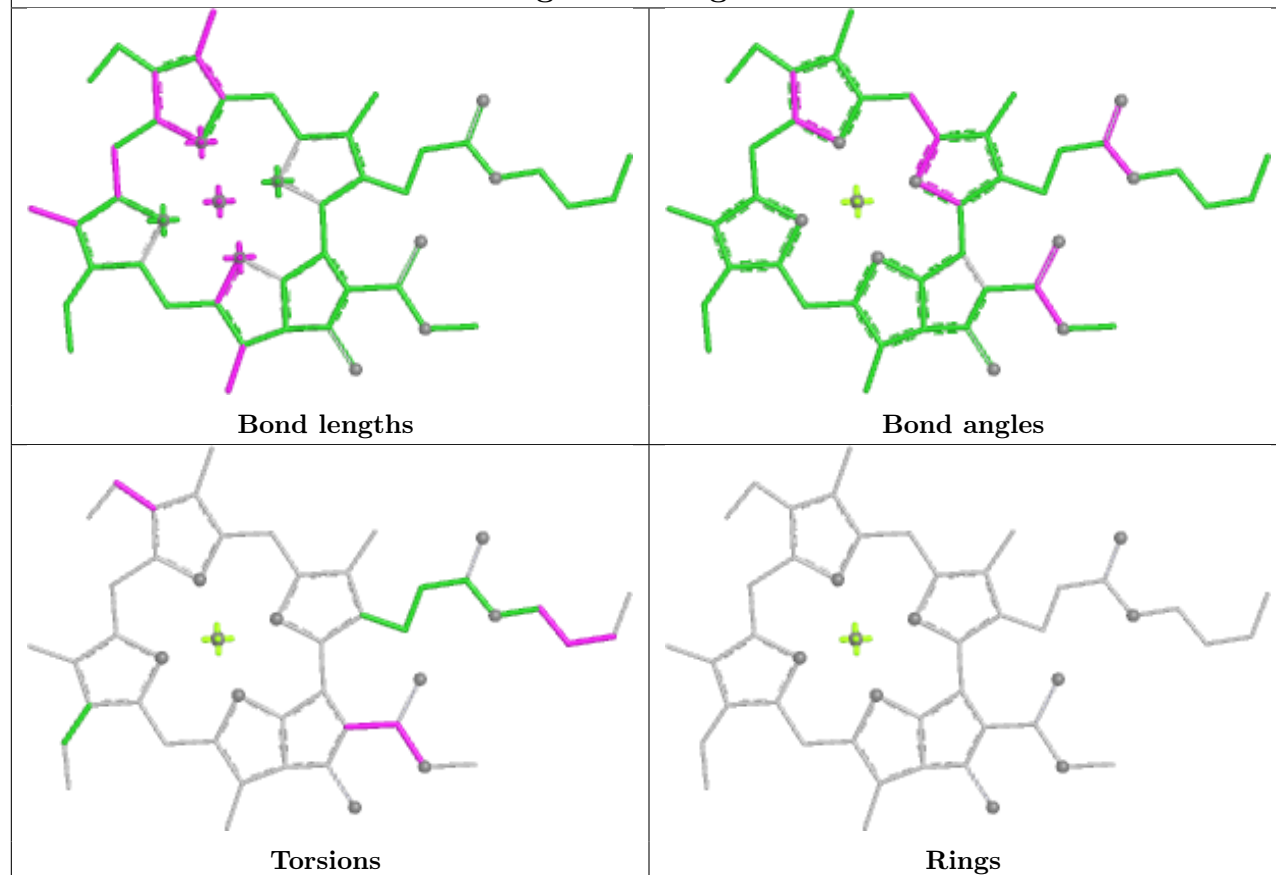
Ligand CLA c 512**Ligand CLA r 602**



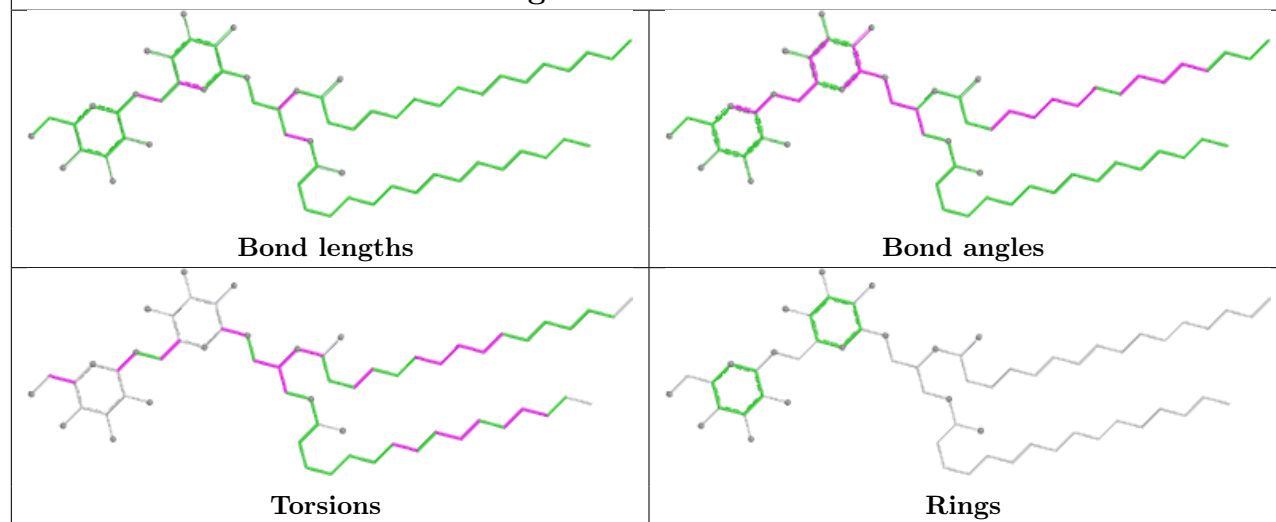
Ligand CLA g 613



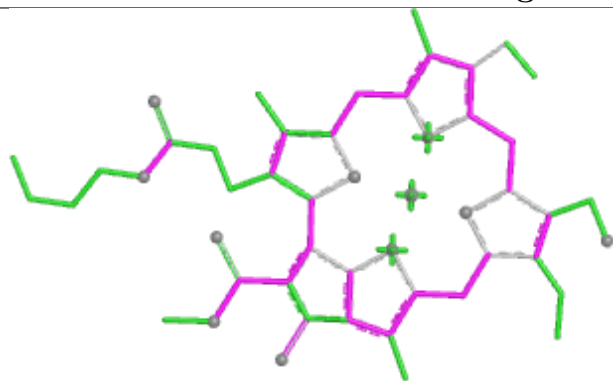
Ligand CLA g 612



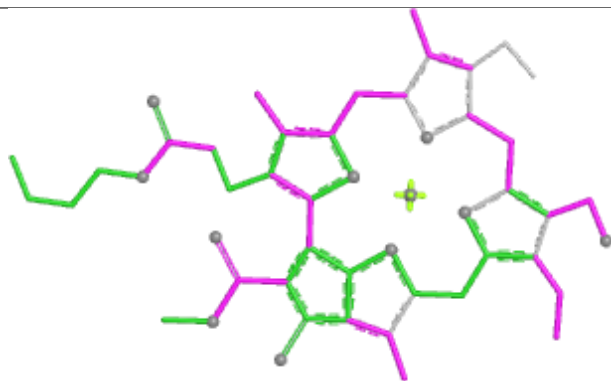
Ligand DGD C 519



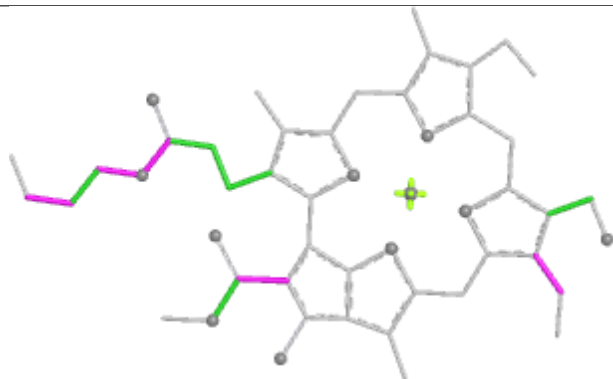
Ligand CHL n 601



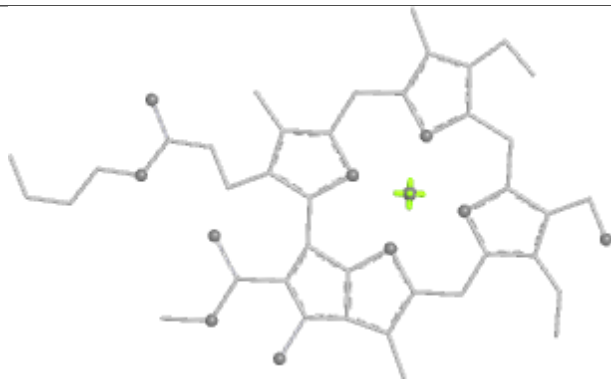
Bond lengths



Bond angles

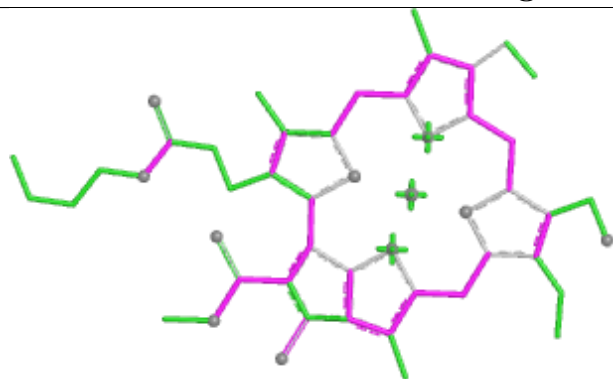


Torsions

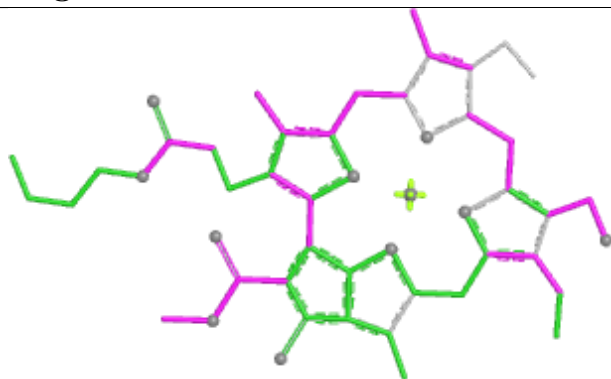


Rings

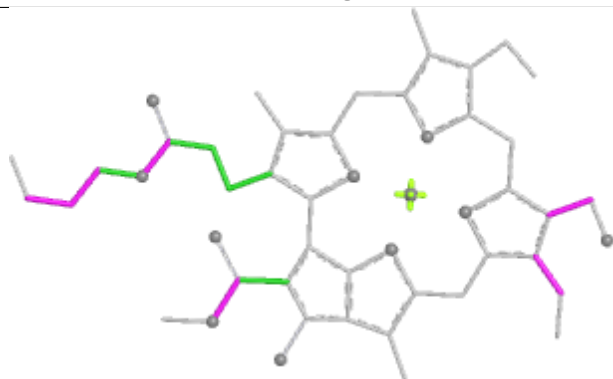
Ligand CHL g 609



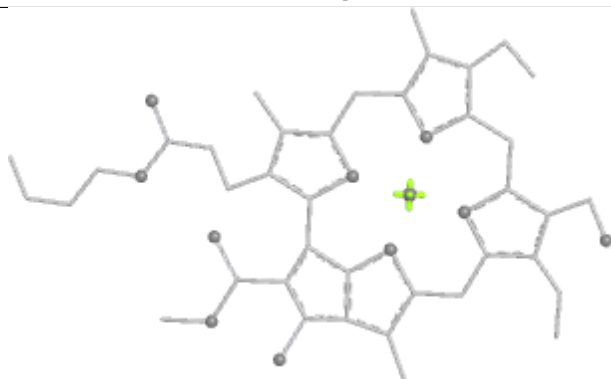
Bond lengths



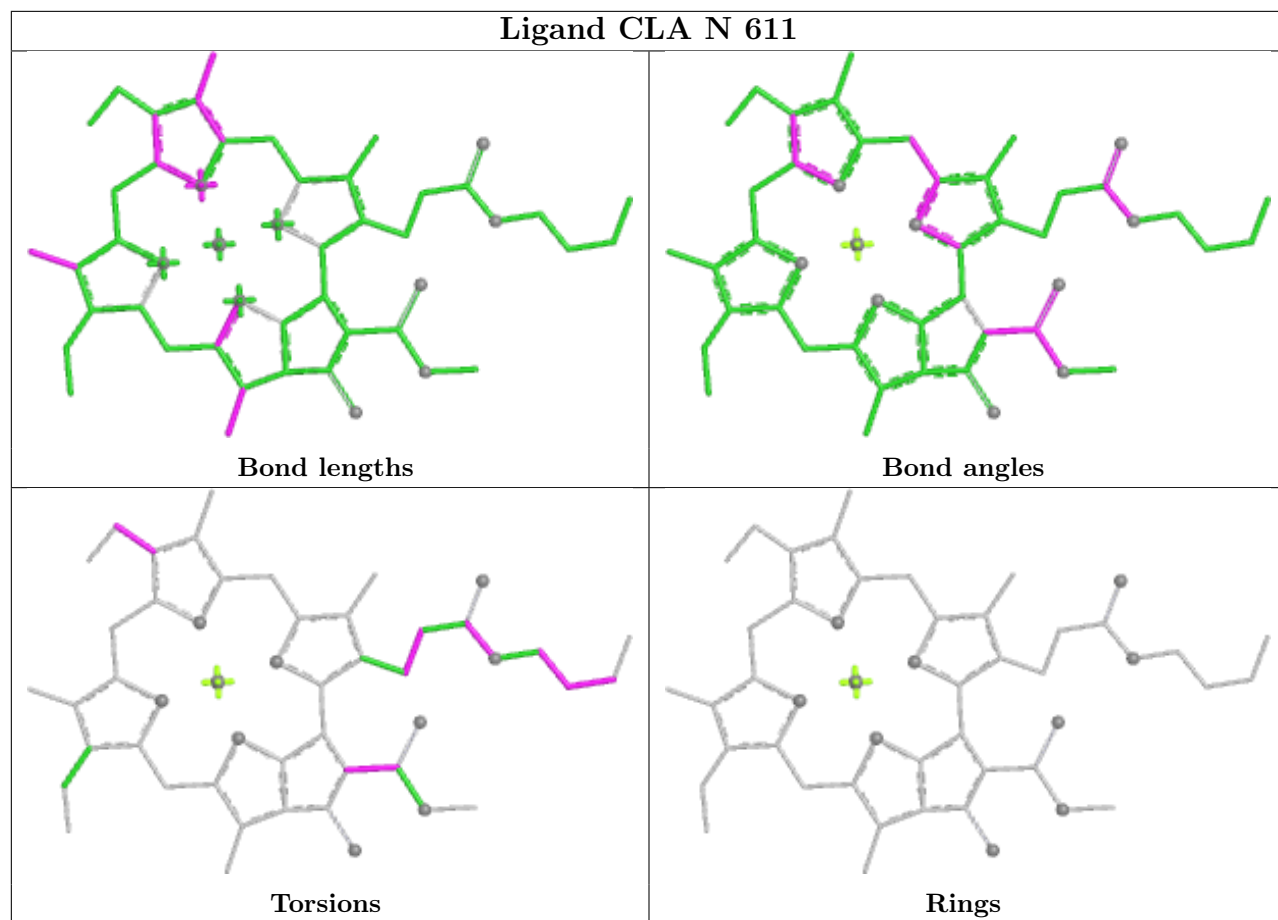
Bond angles



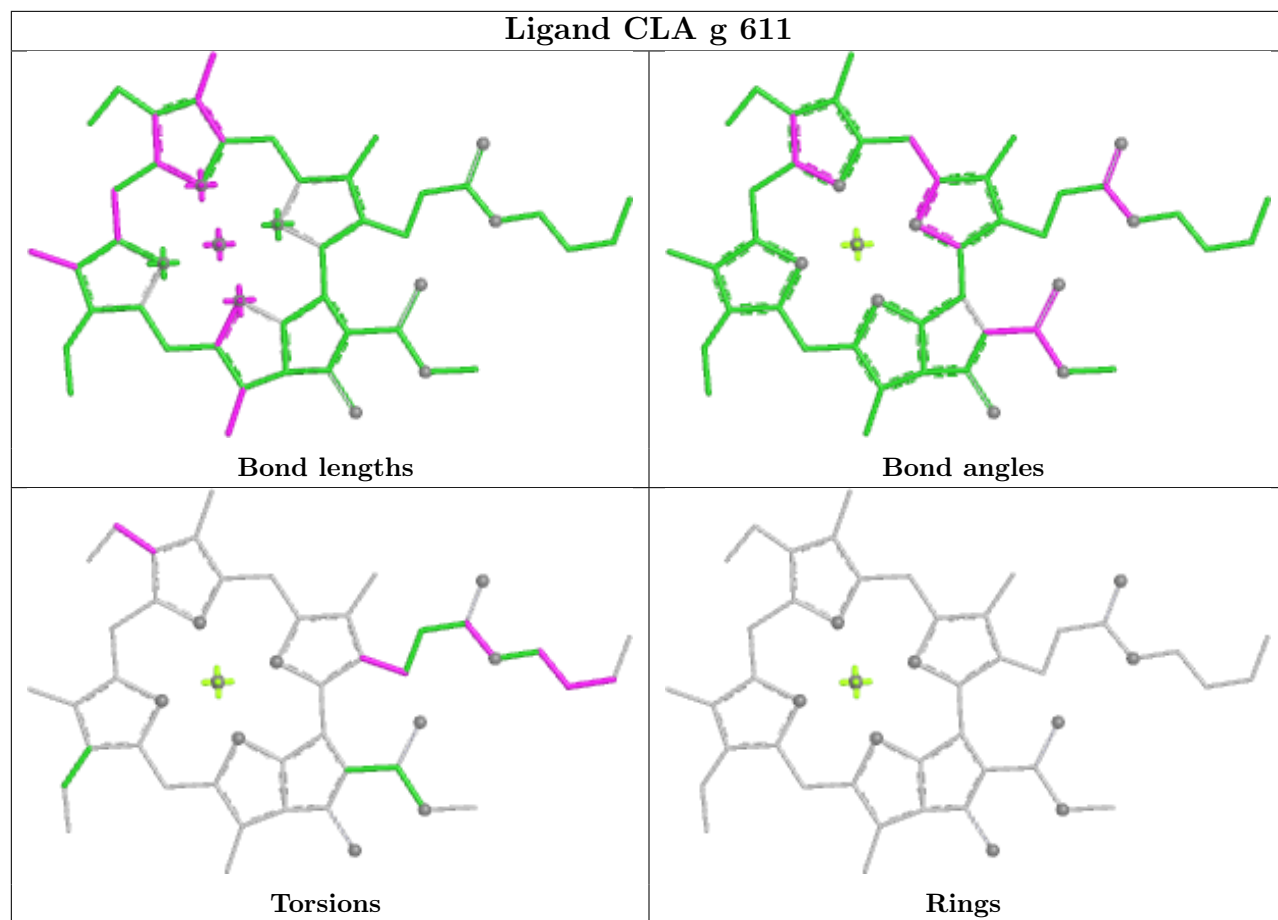
Torsions

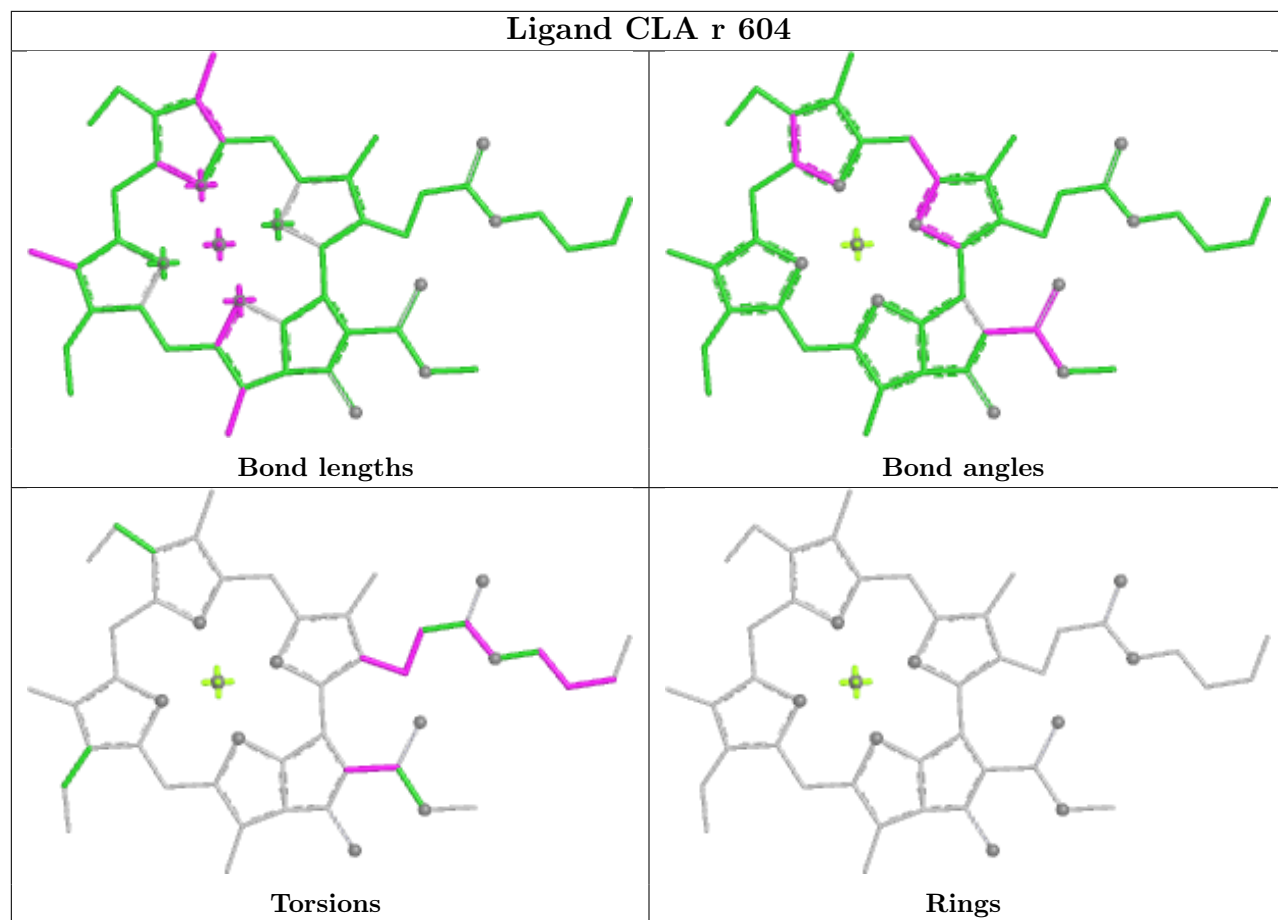


Rings

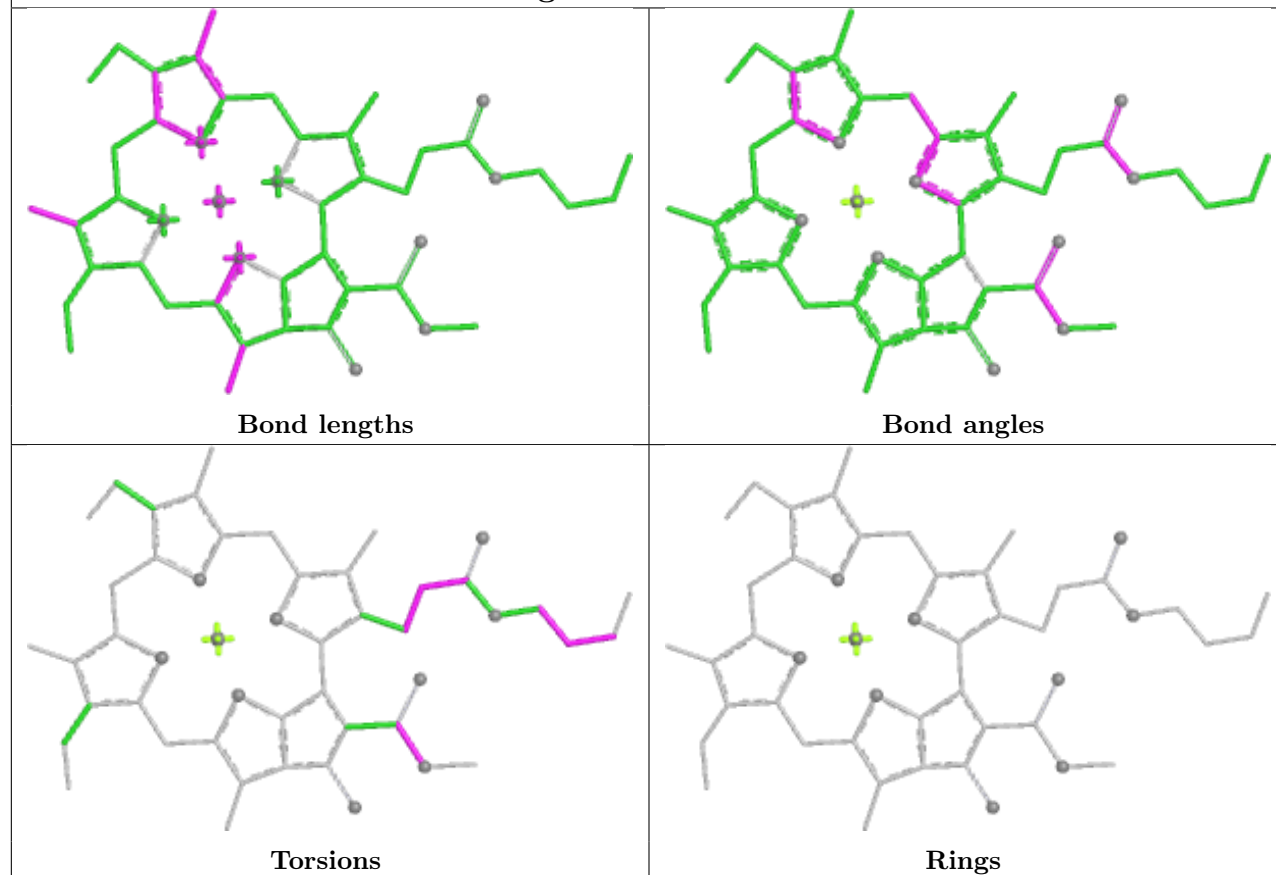


Ligand CLA g 611

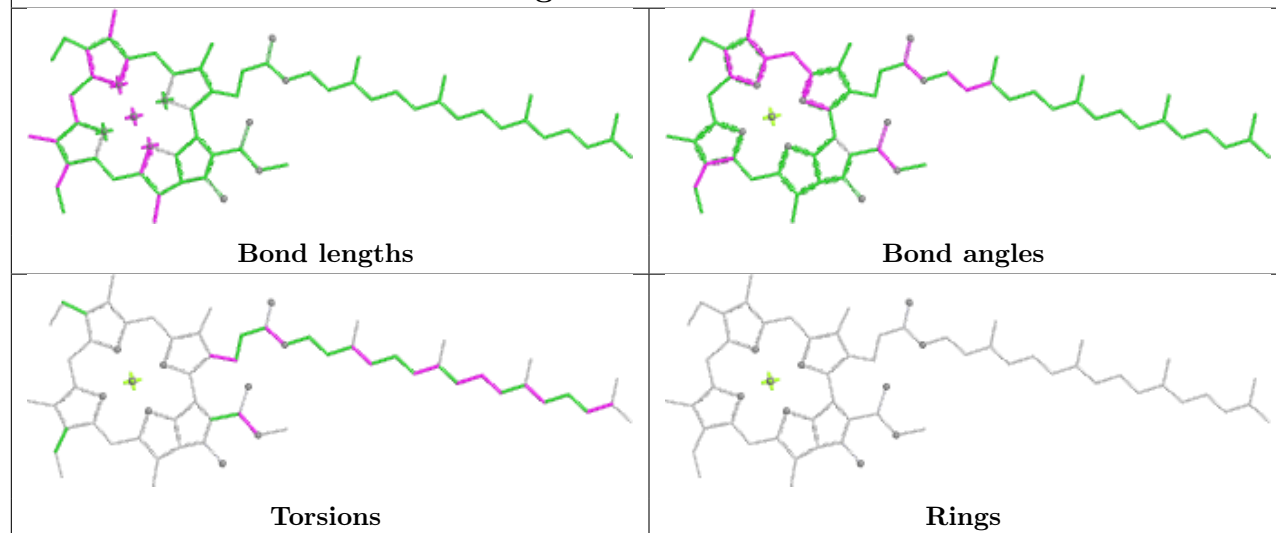


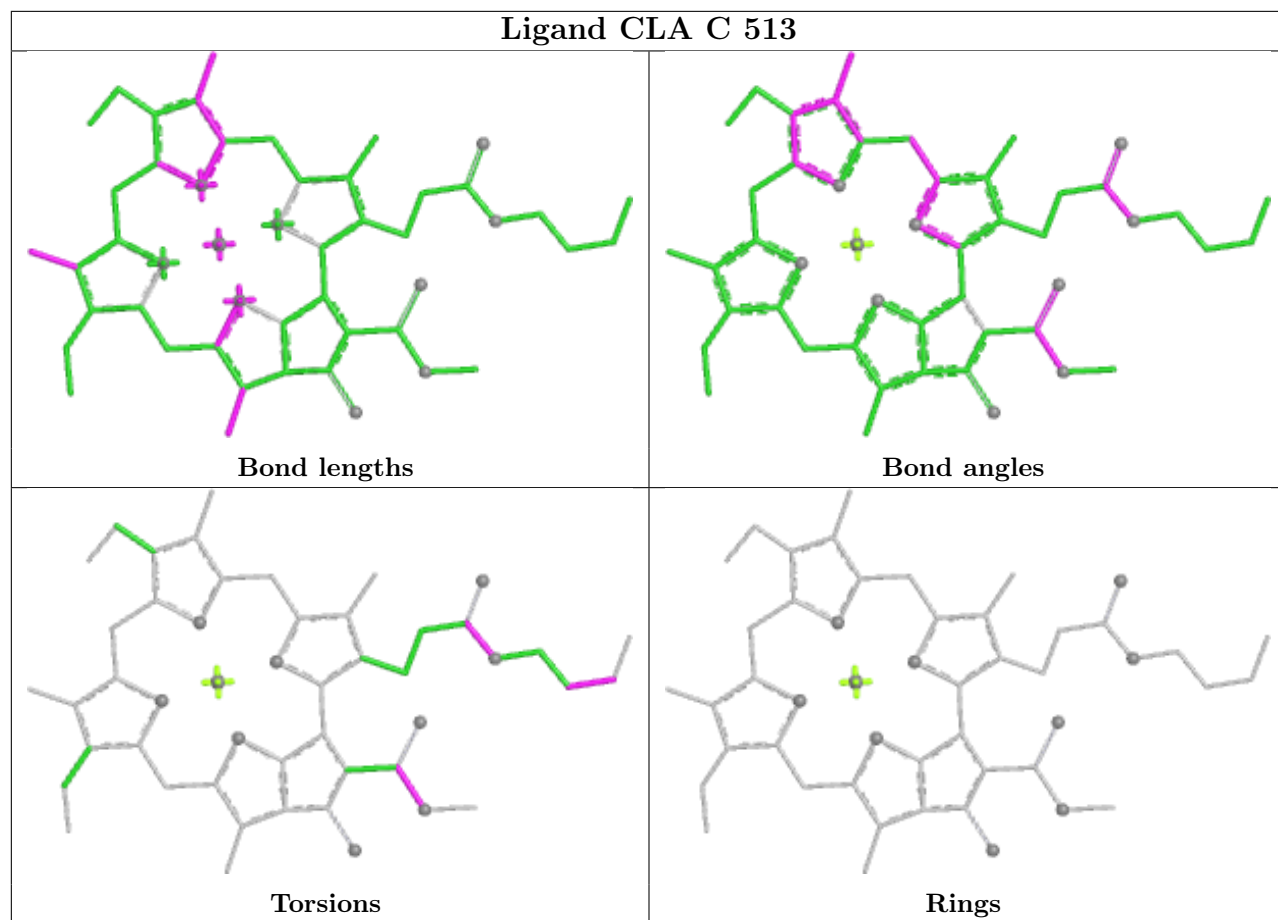


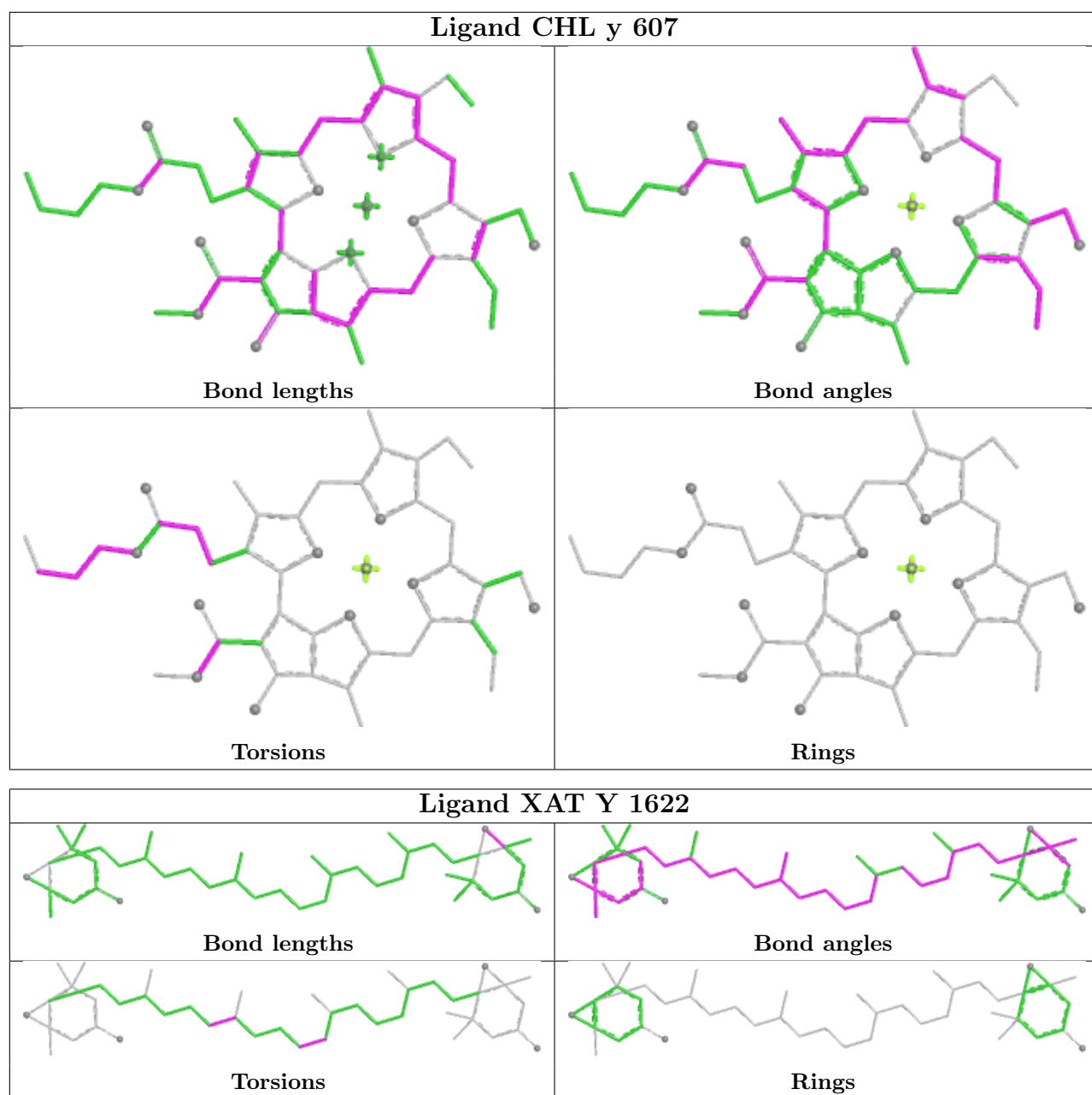
Ligand CLA r 613

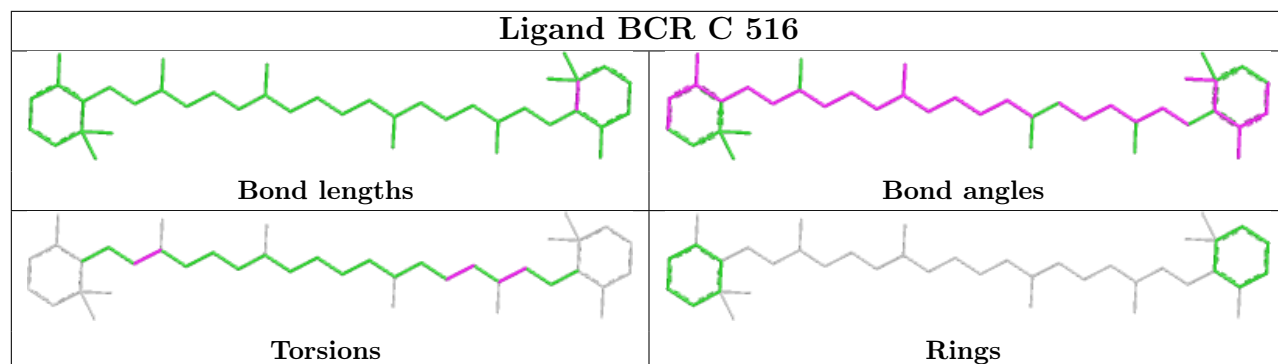
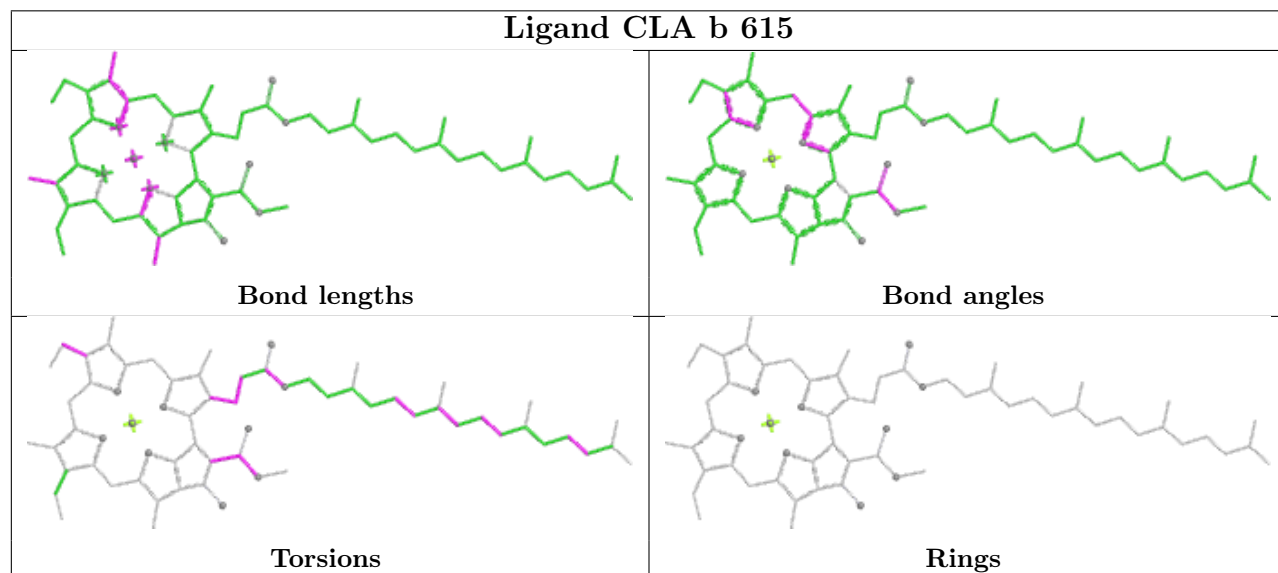
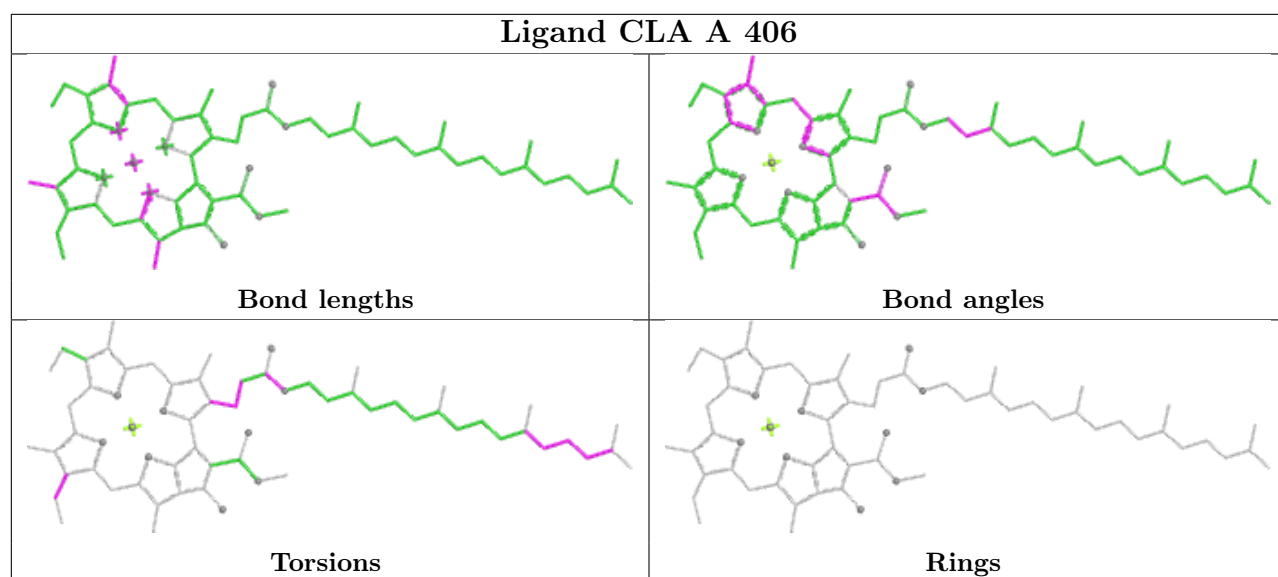


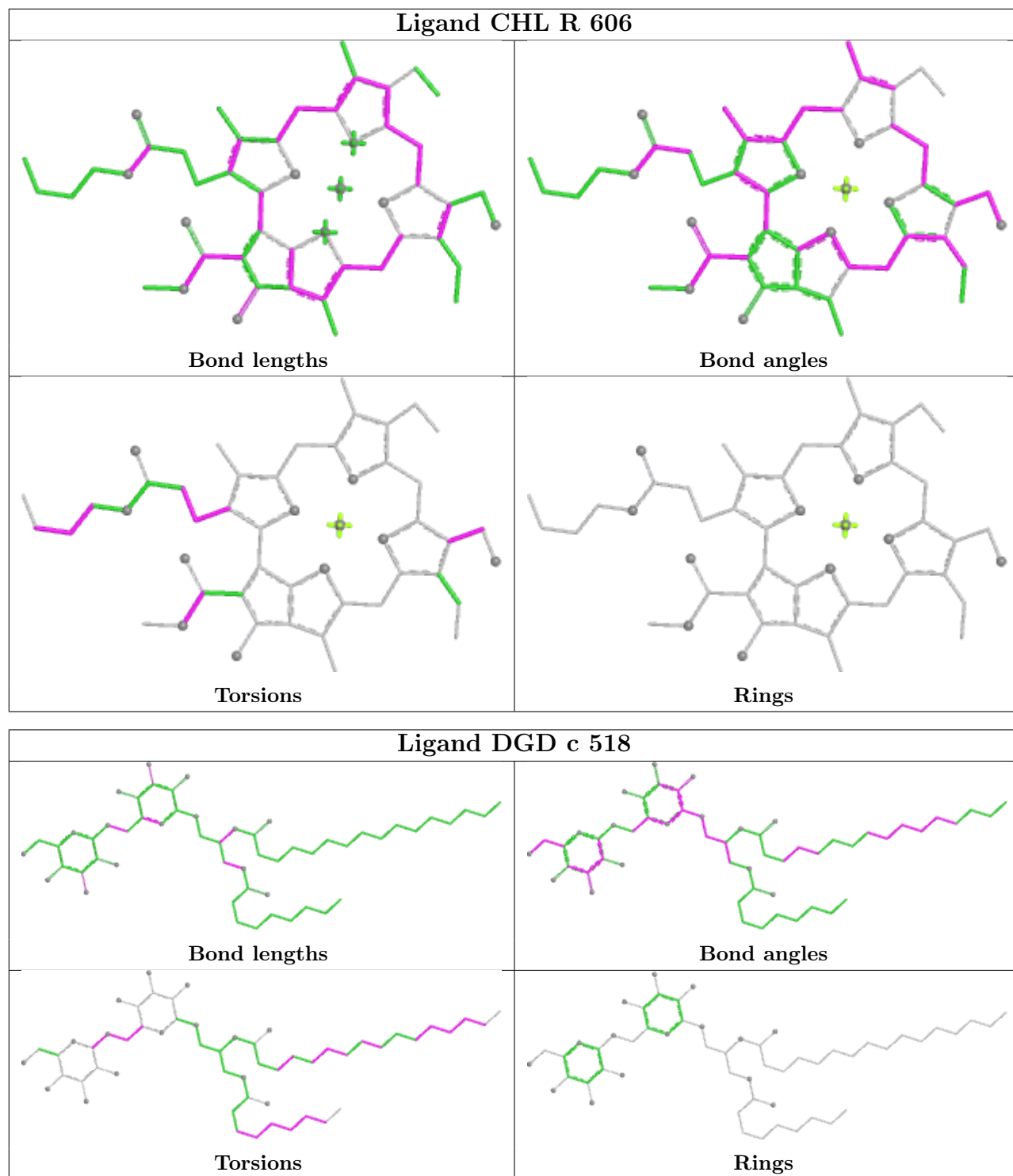
Ligand CLA b 612

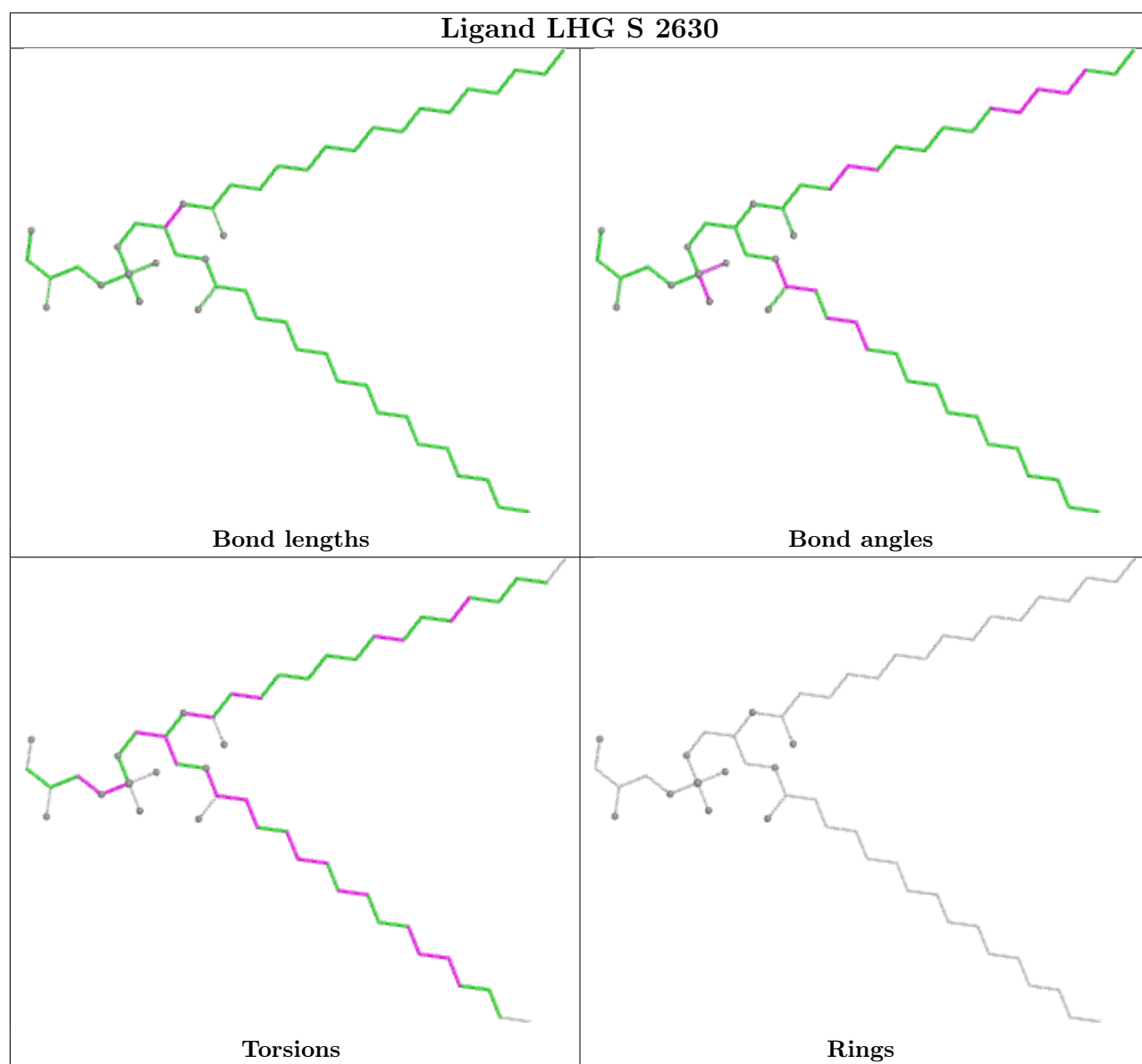


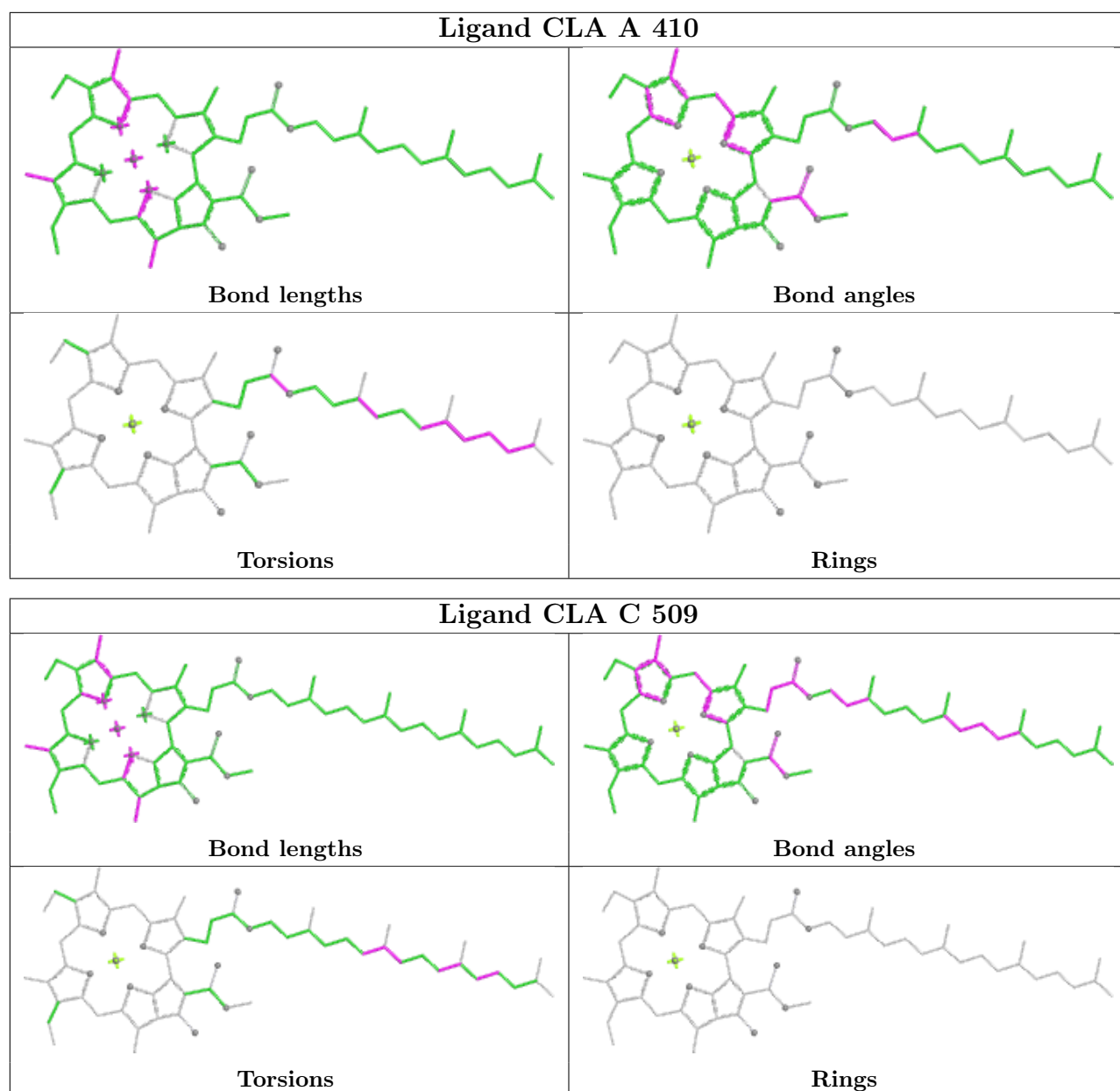


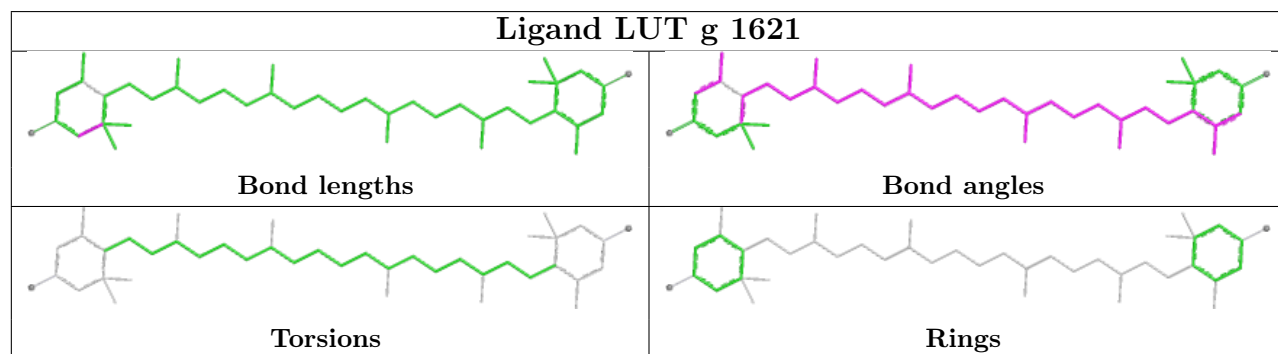
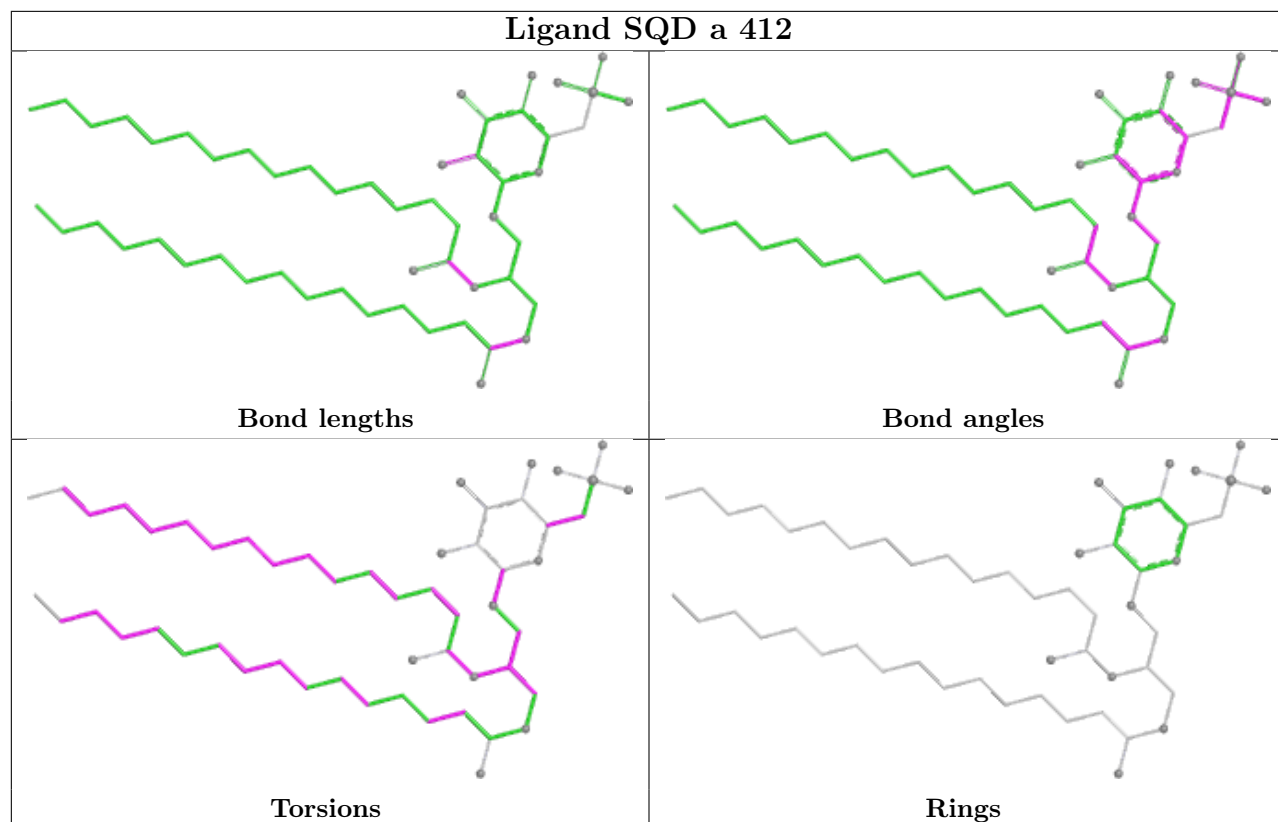


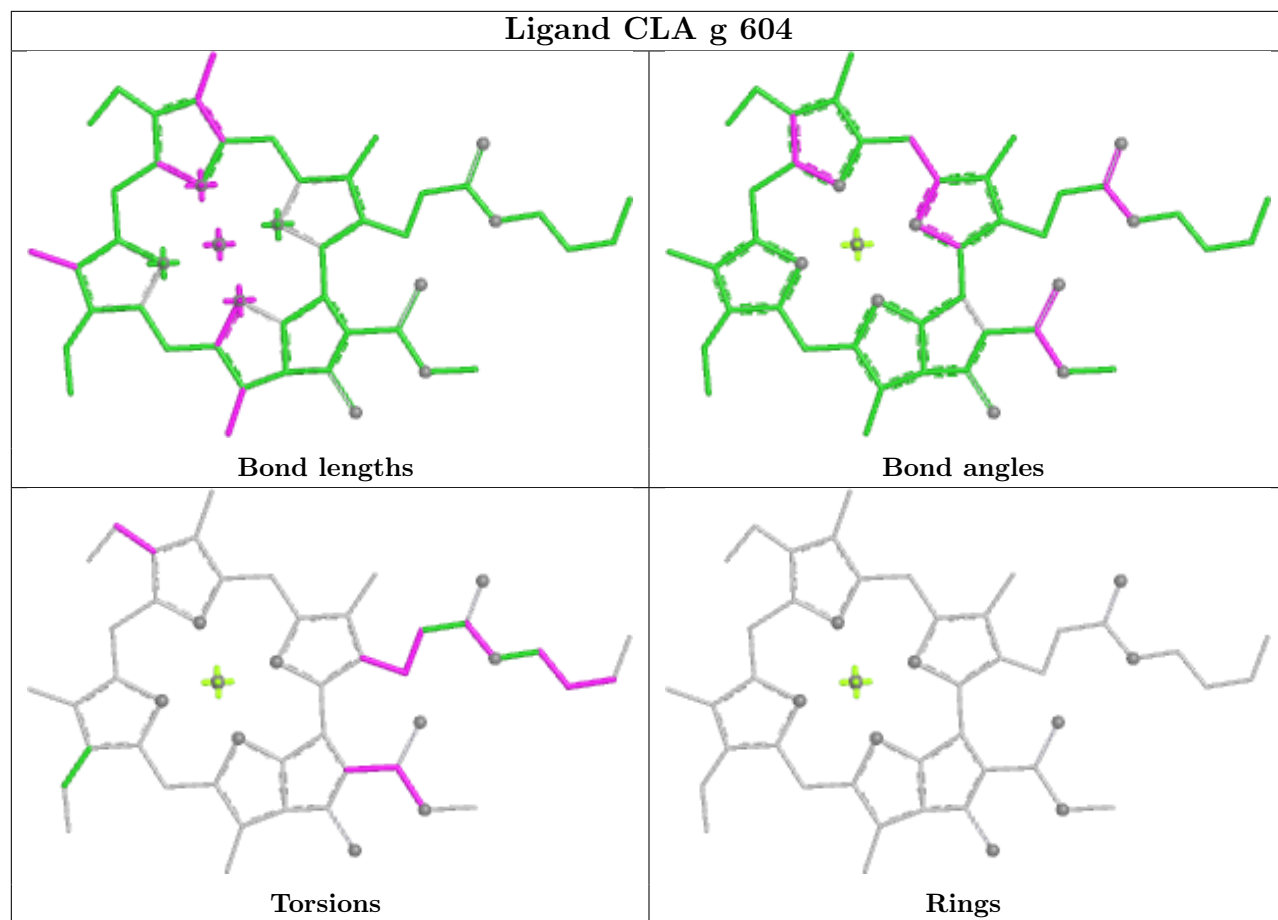




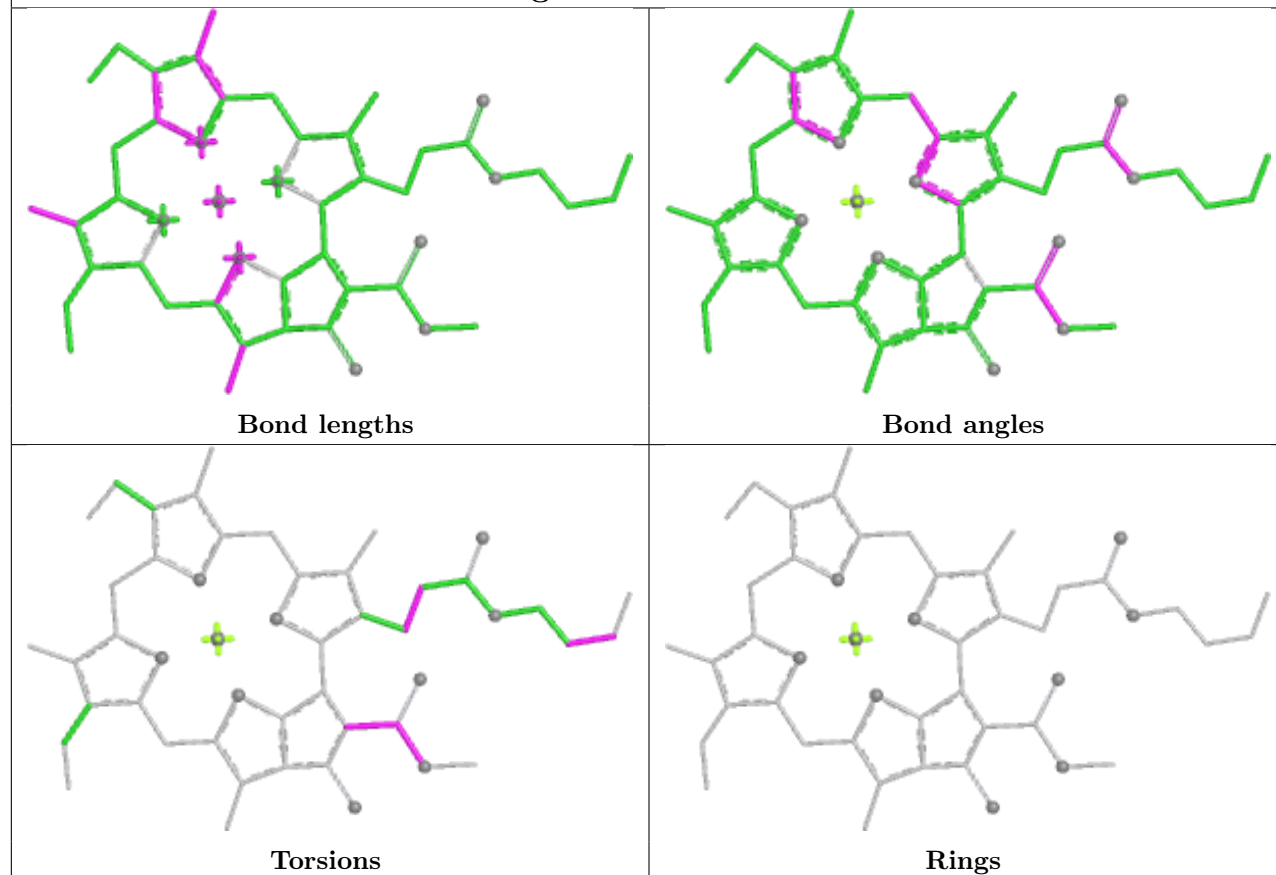




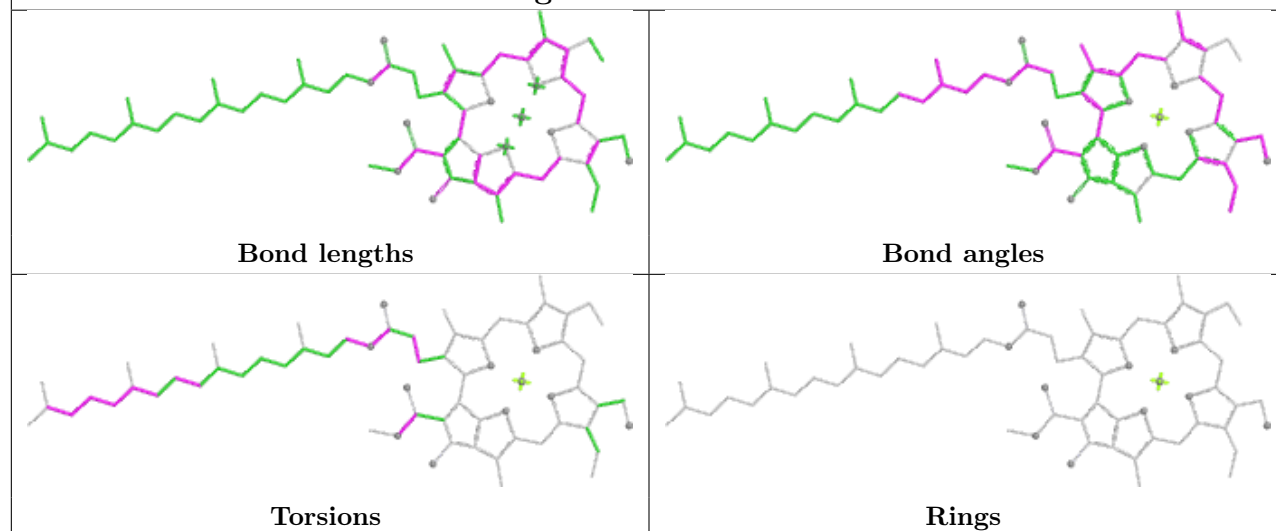


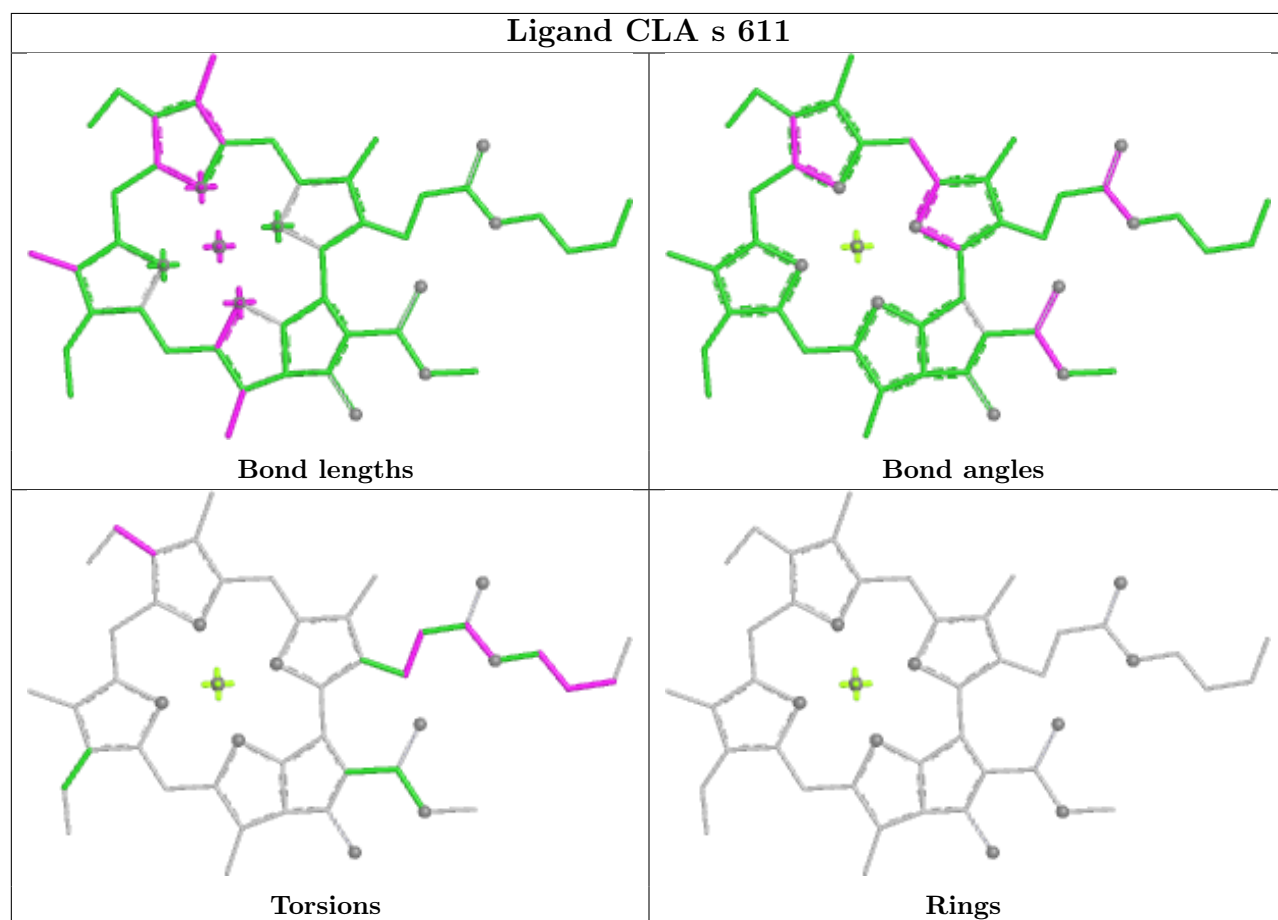
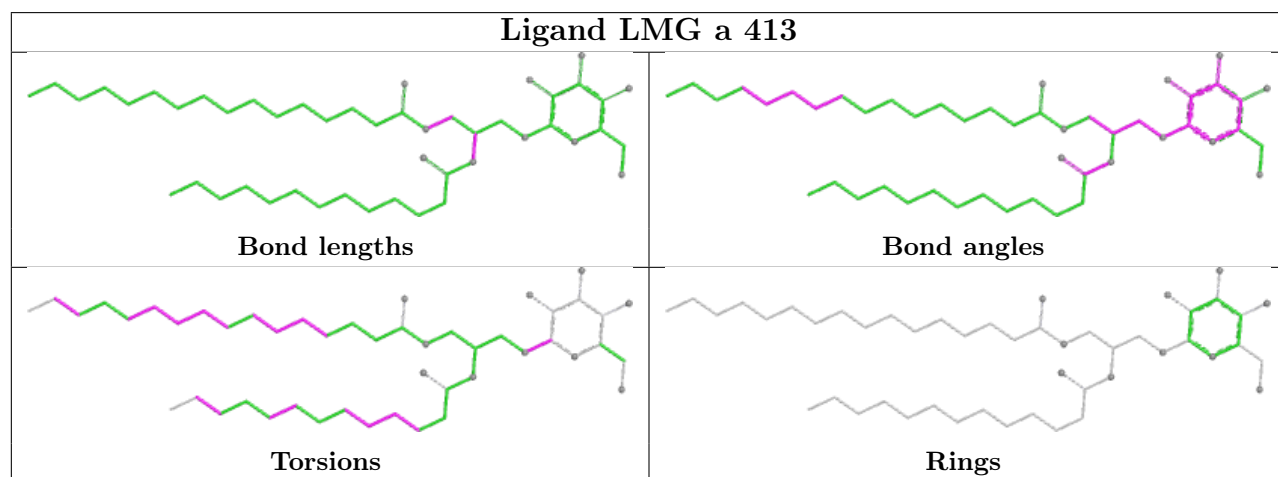
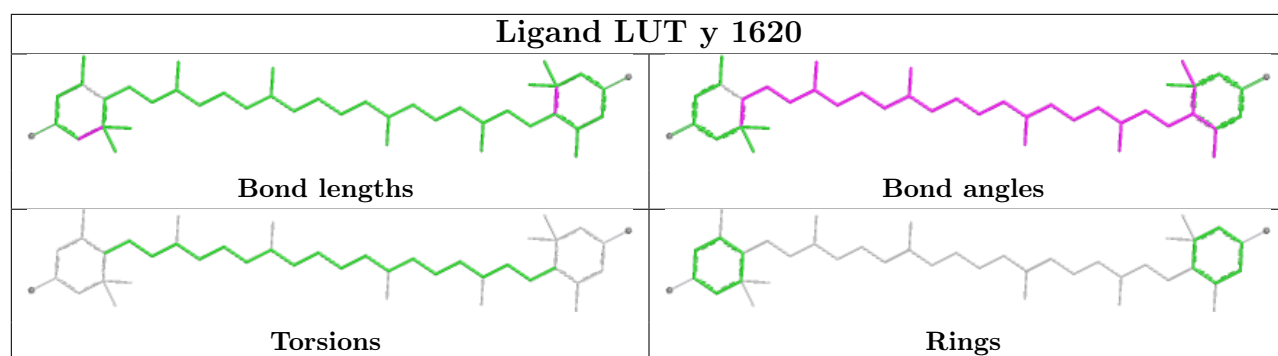


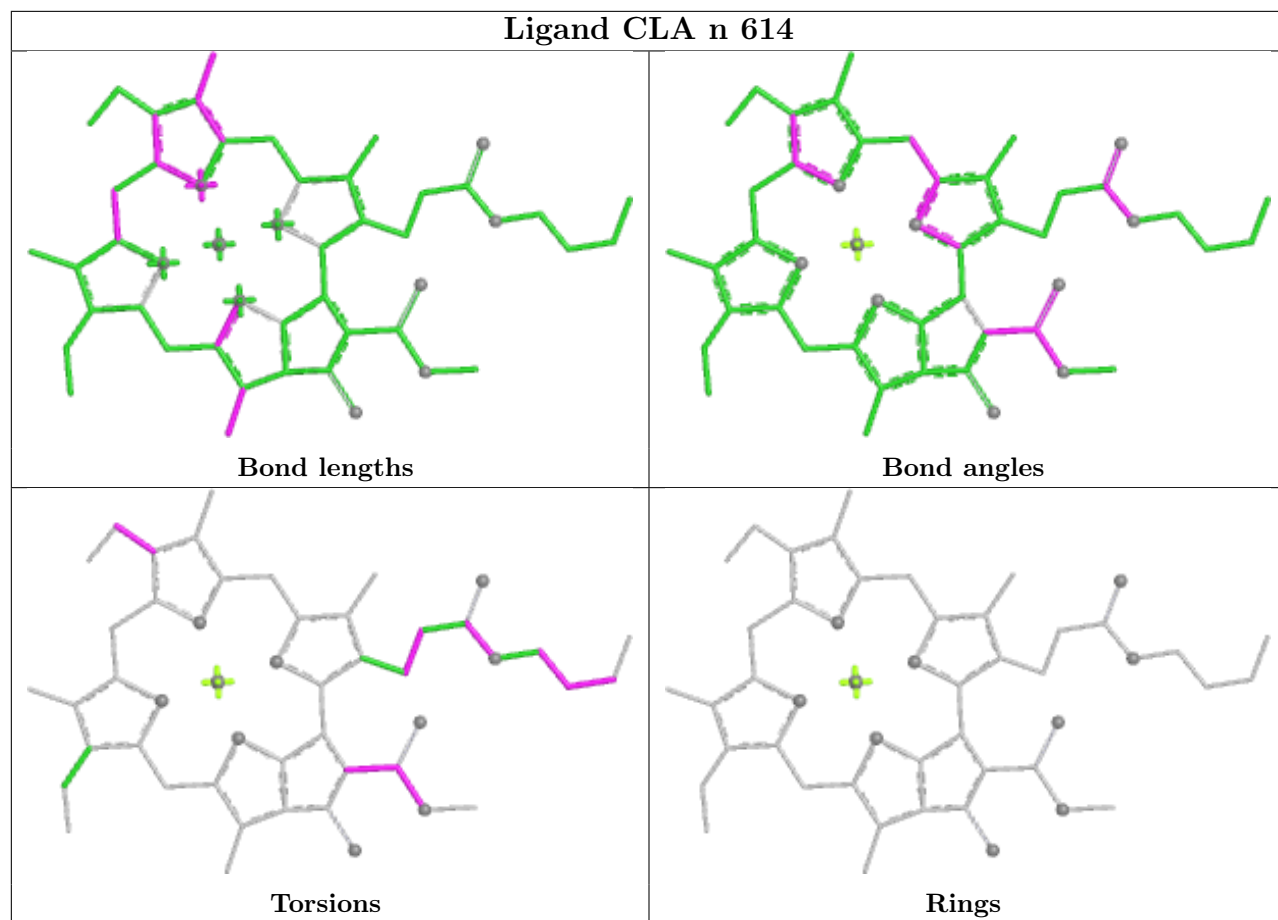
Ligand CLA R 603

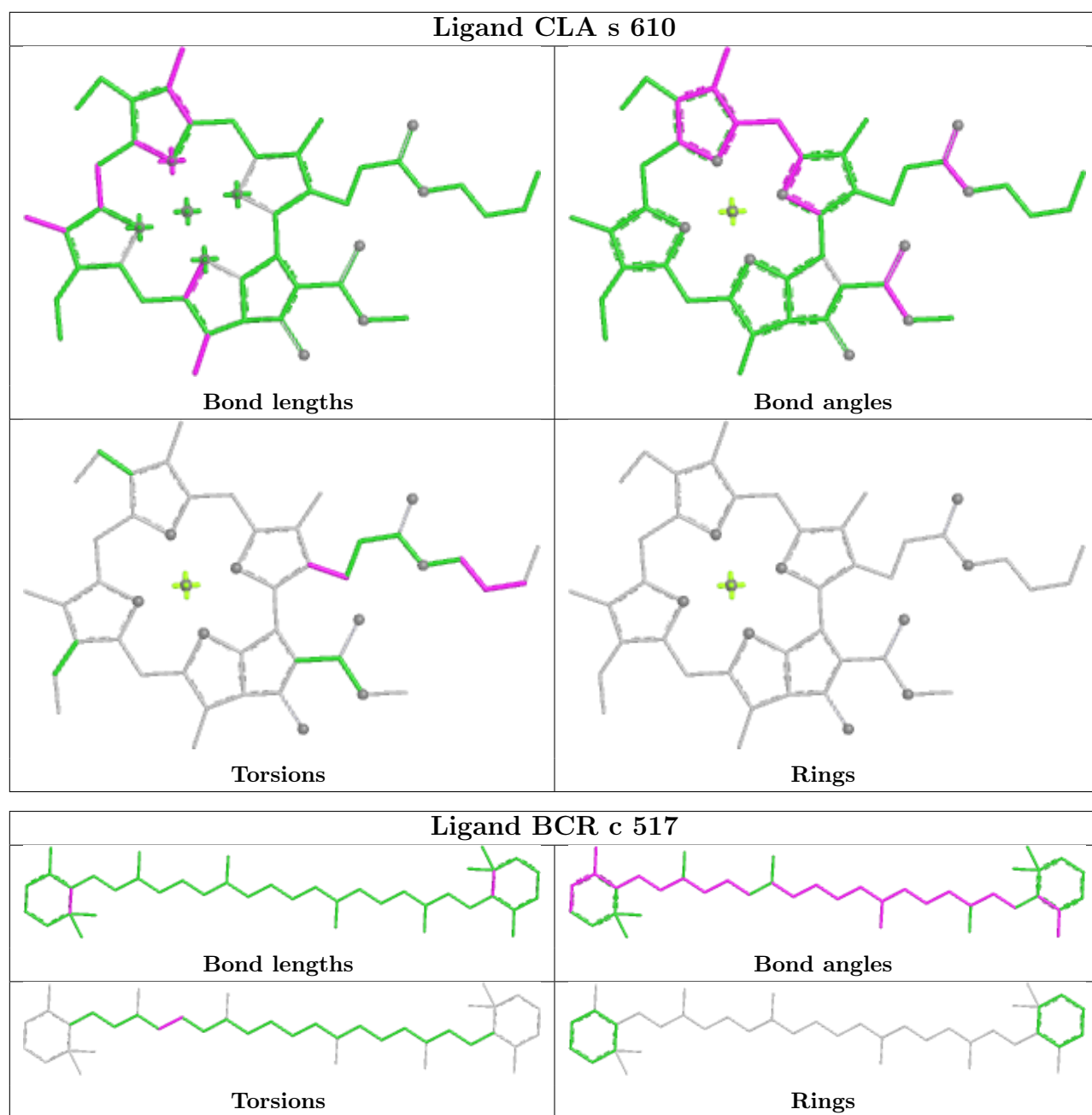


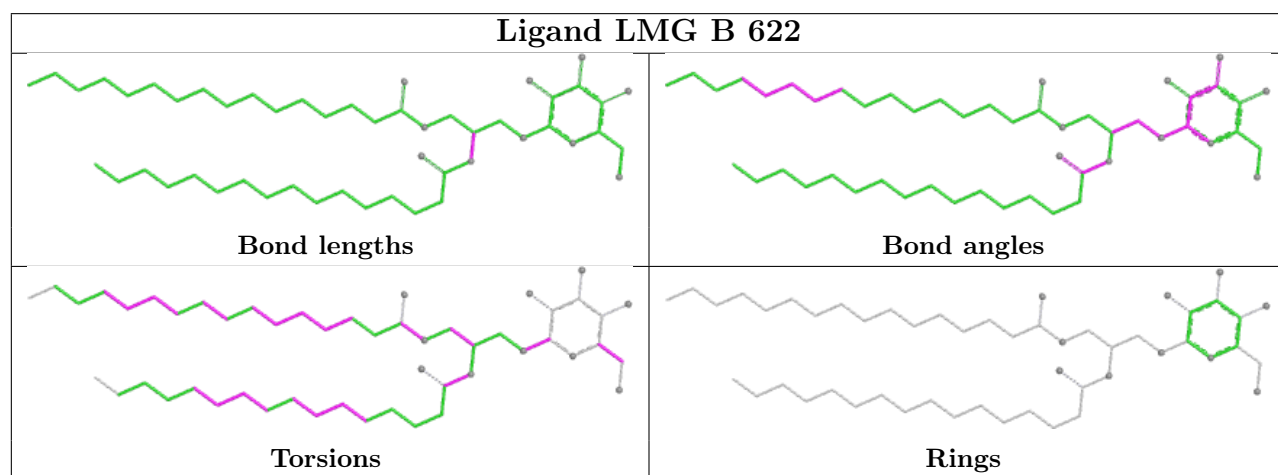
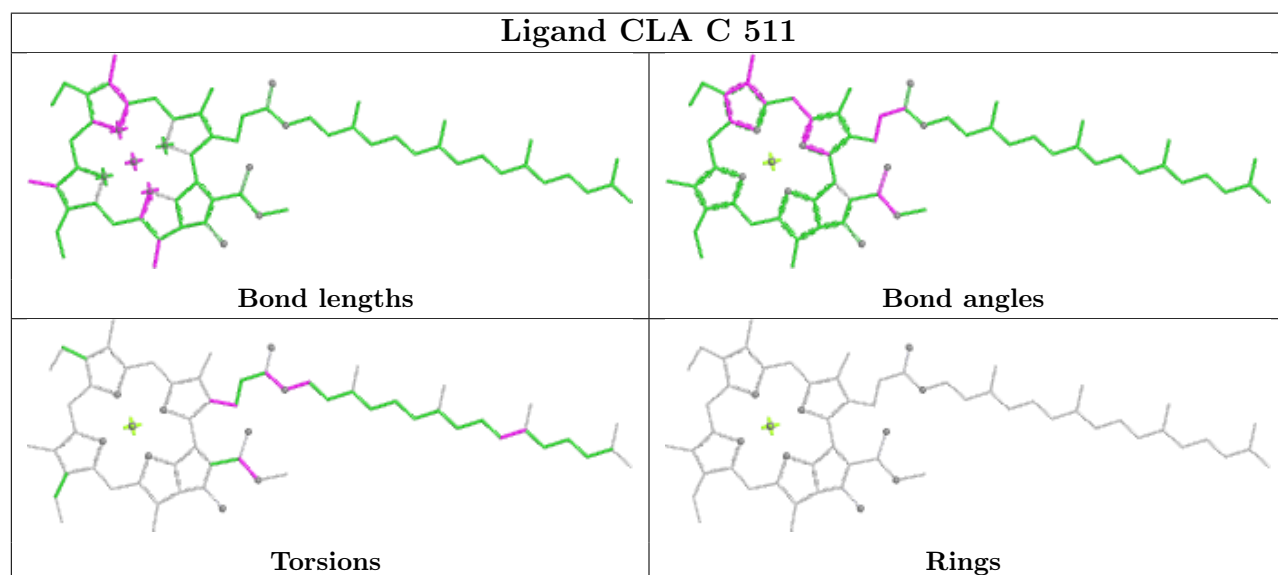
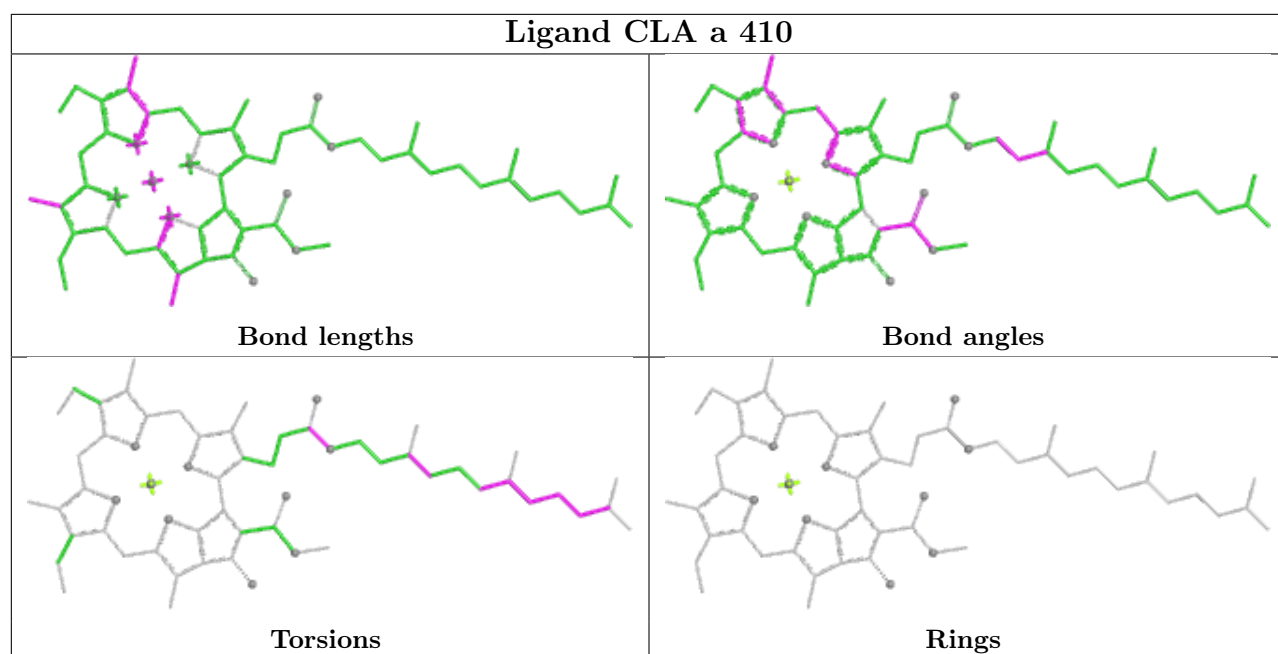
Ligand CHL n 607

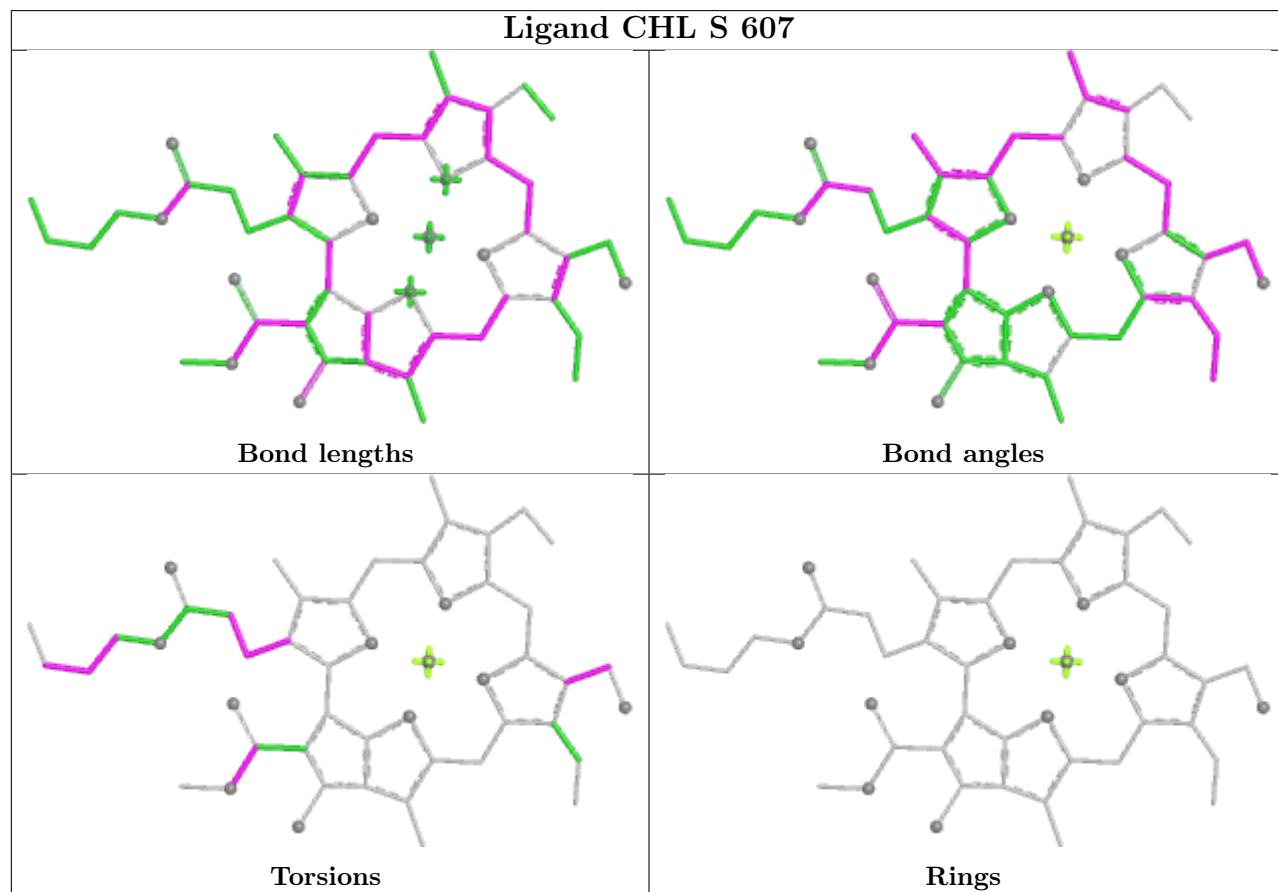
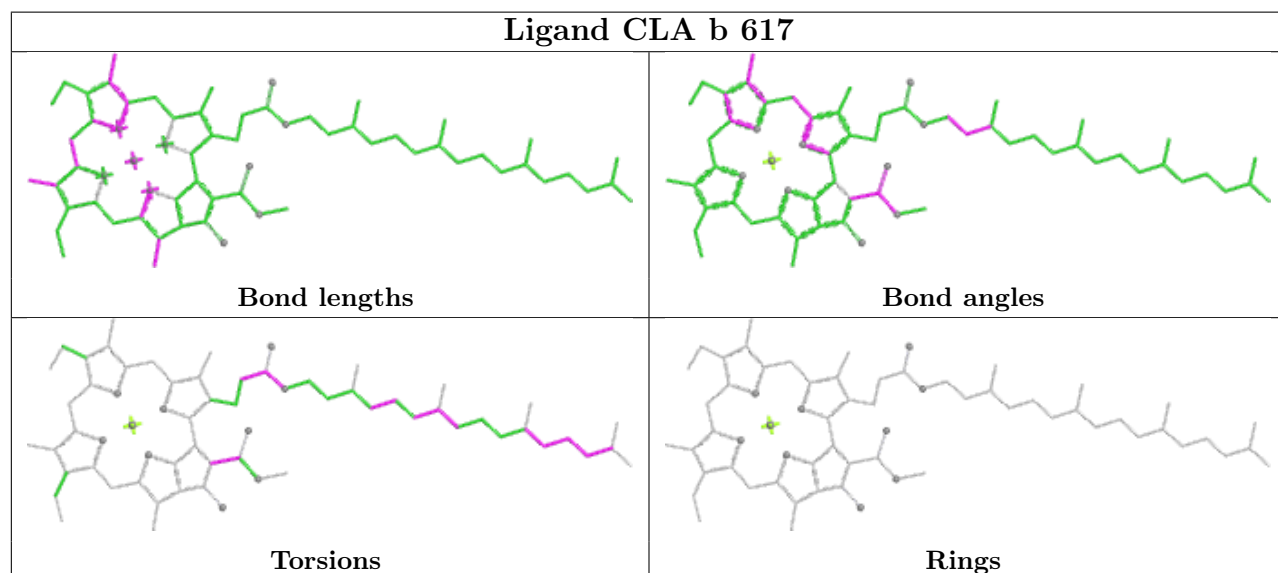
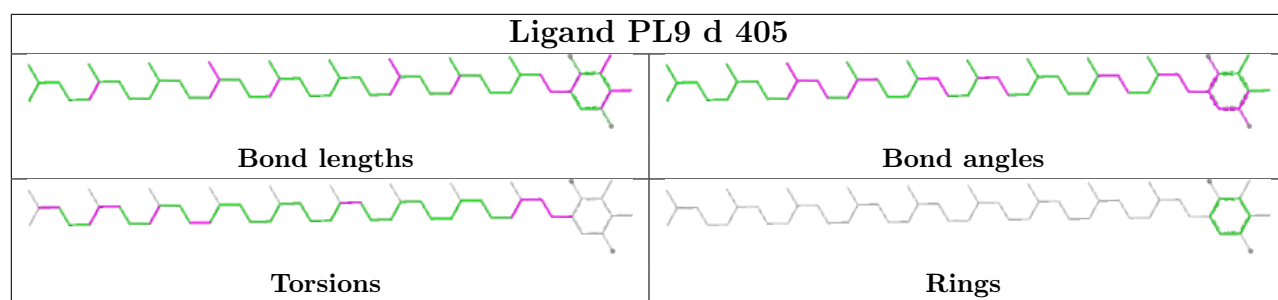


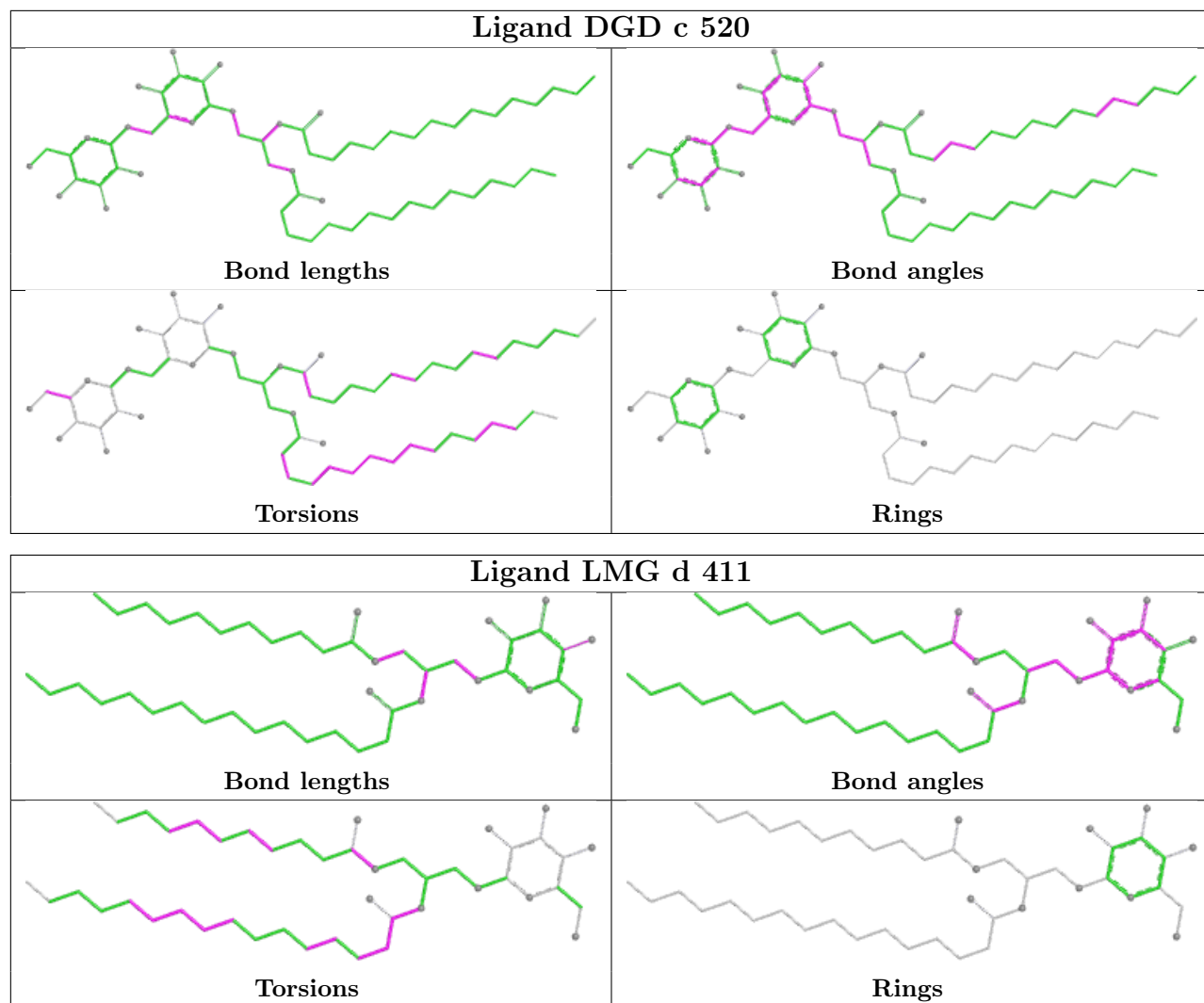


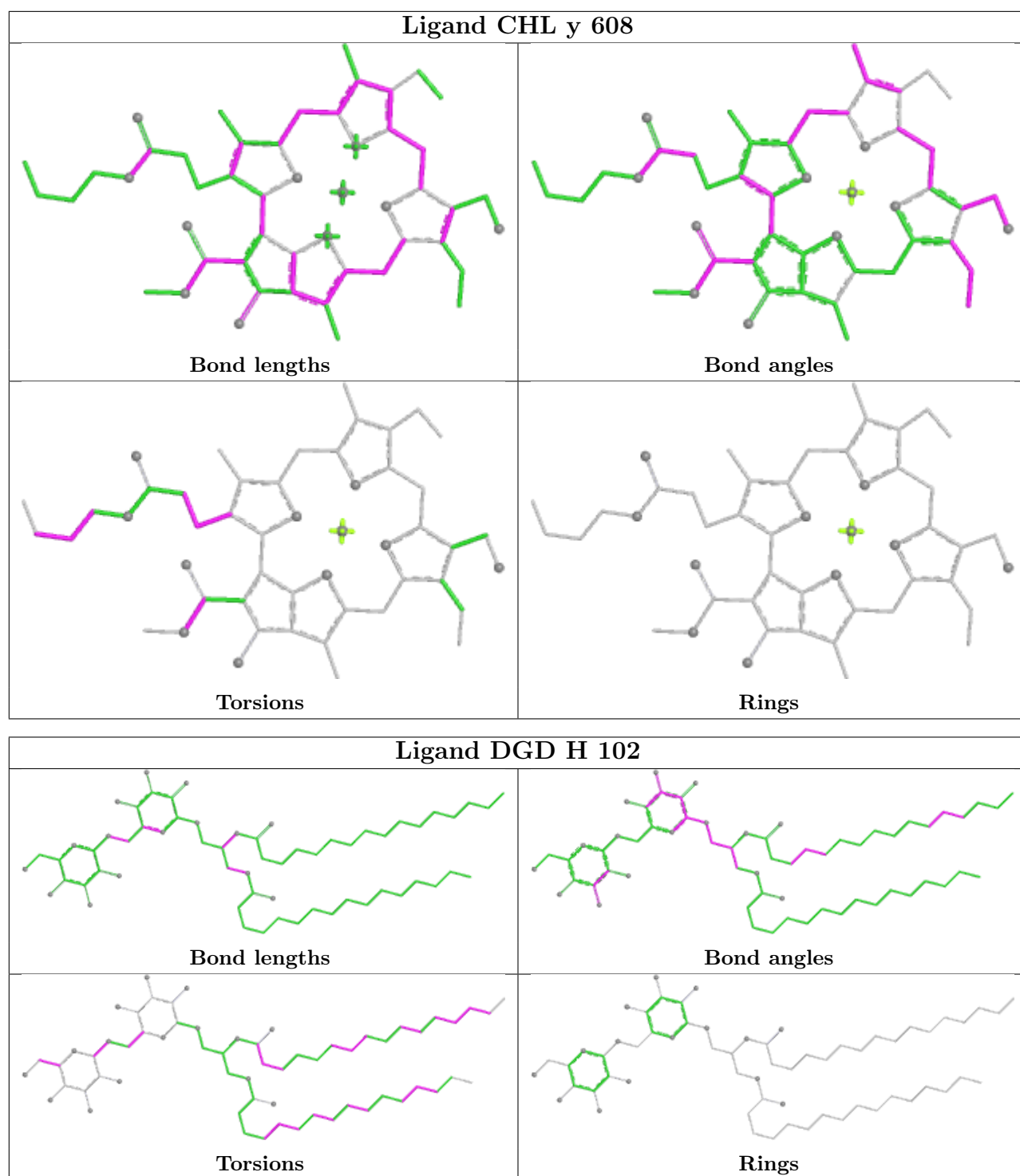




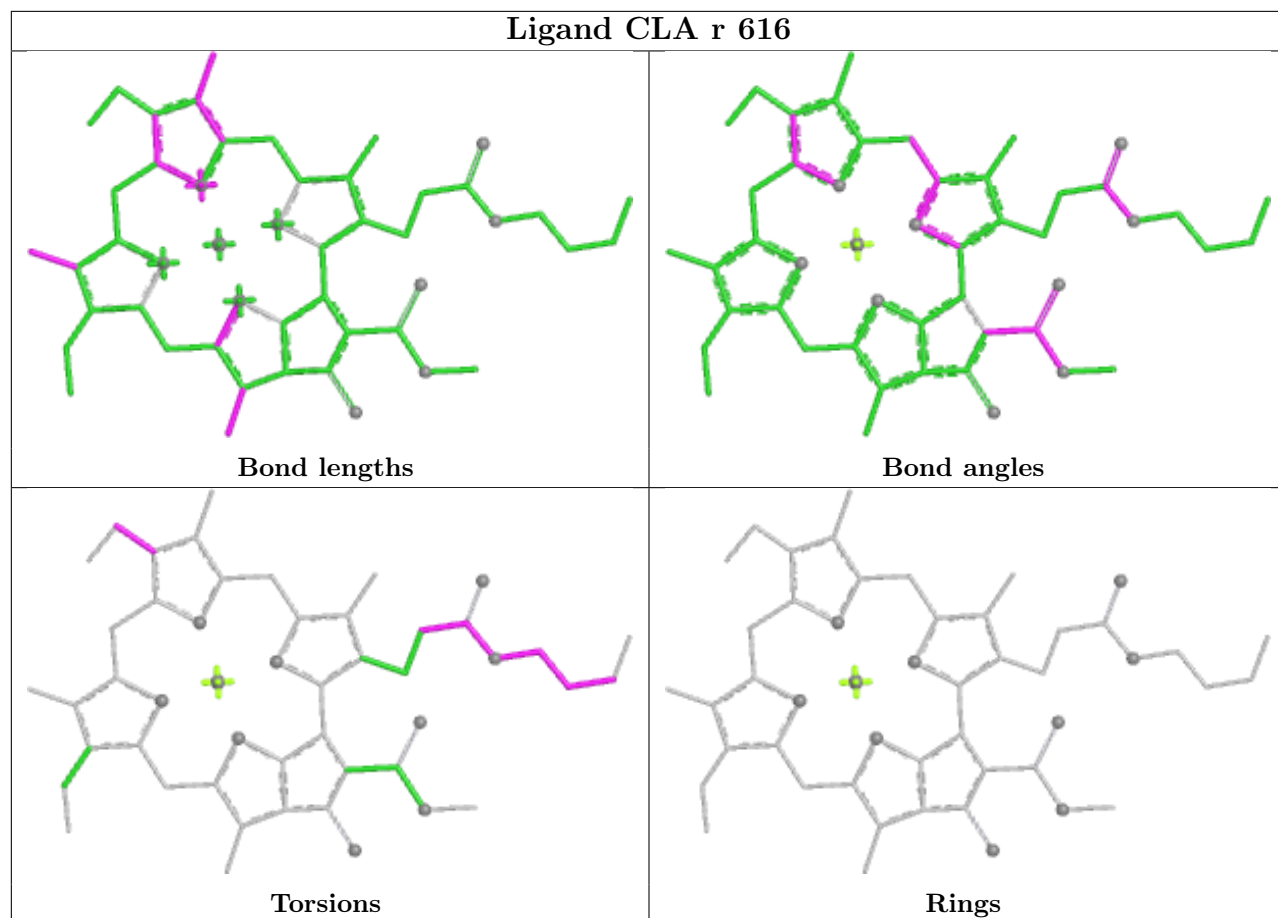


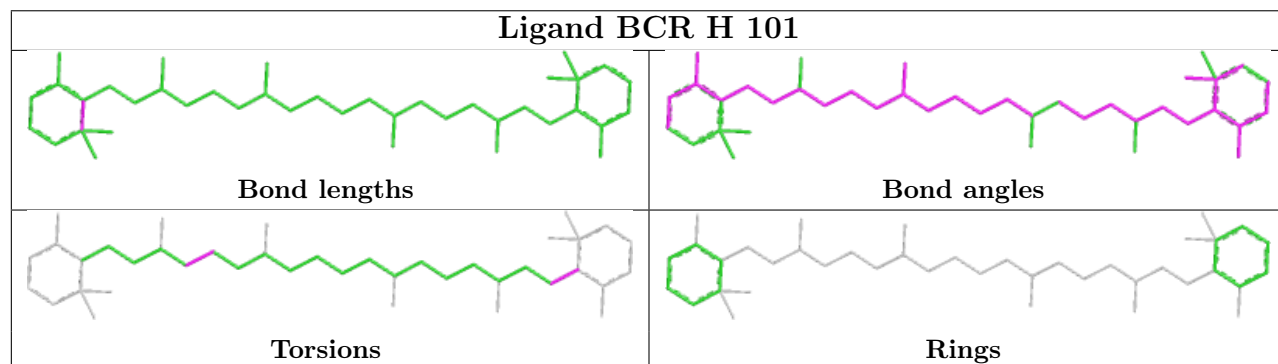
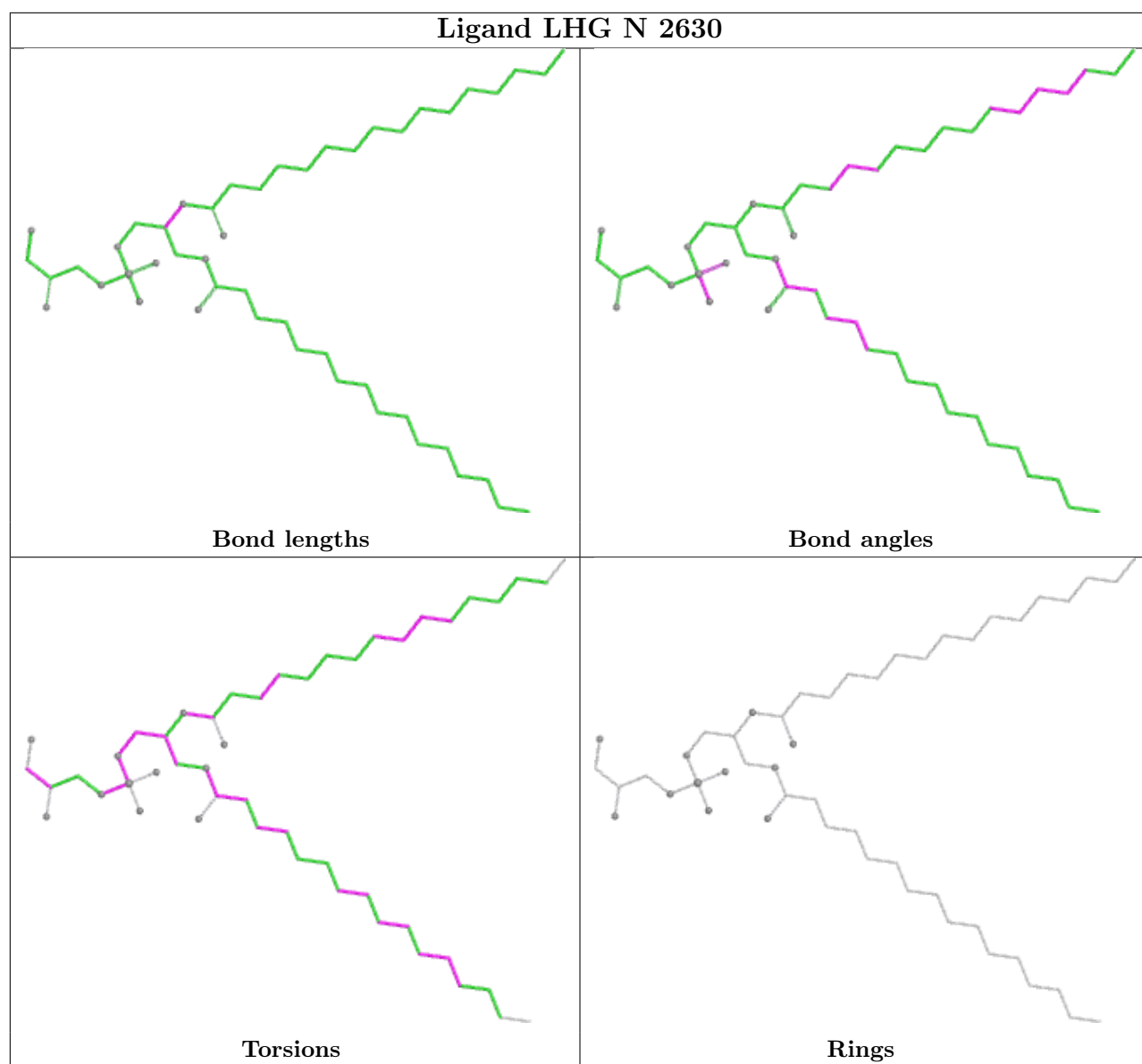


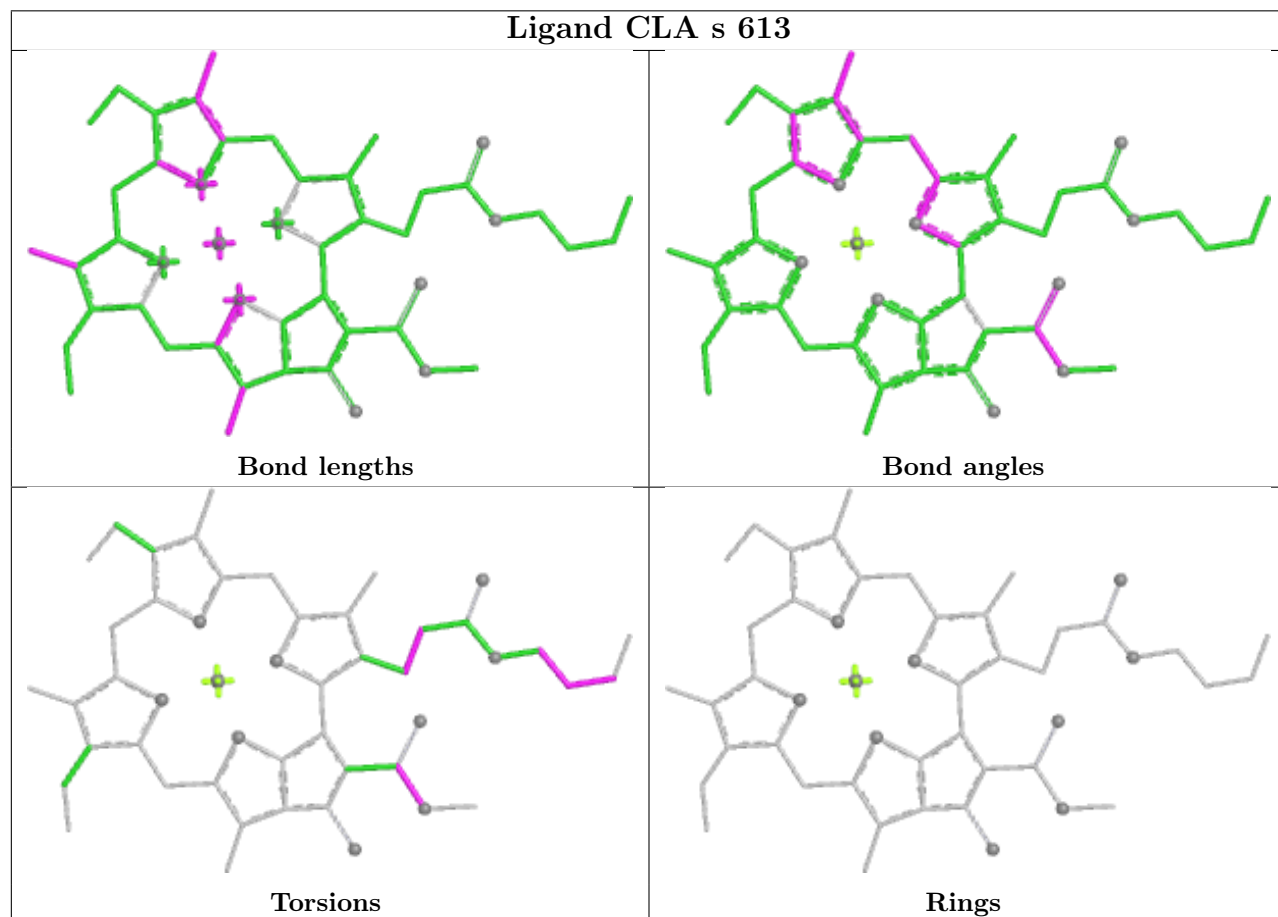
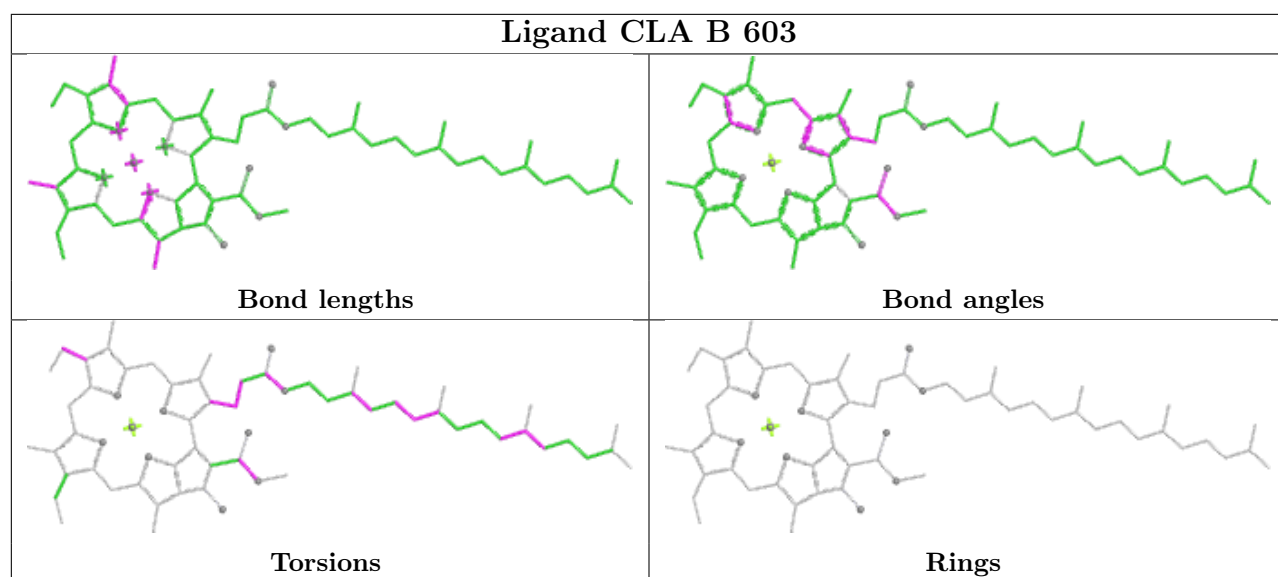




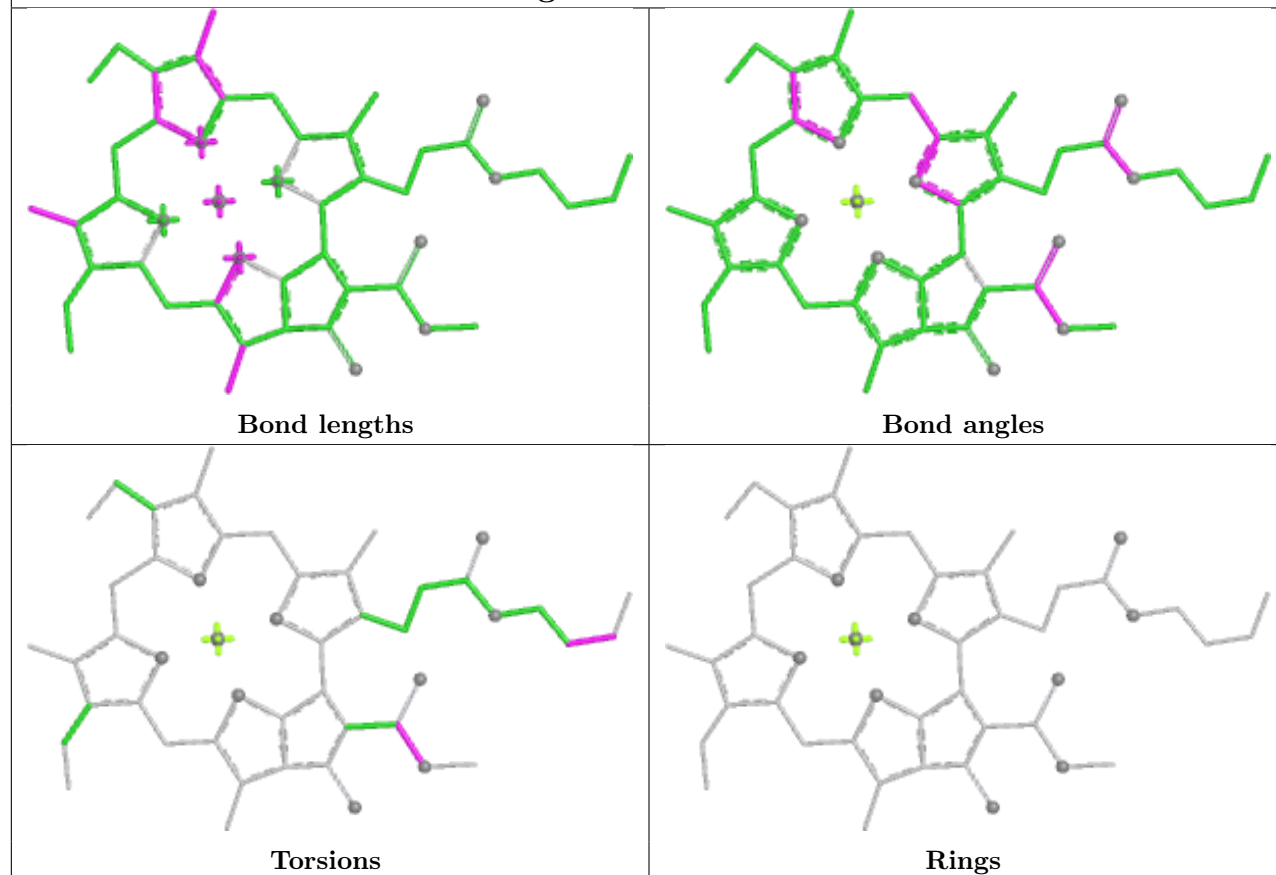
Ligand CLA r 616



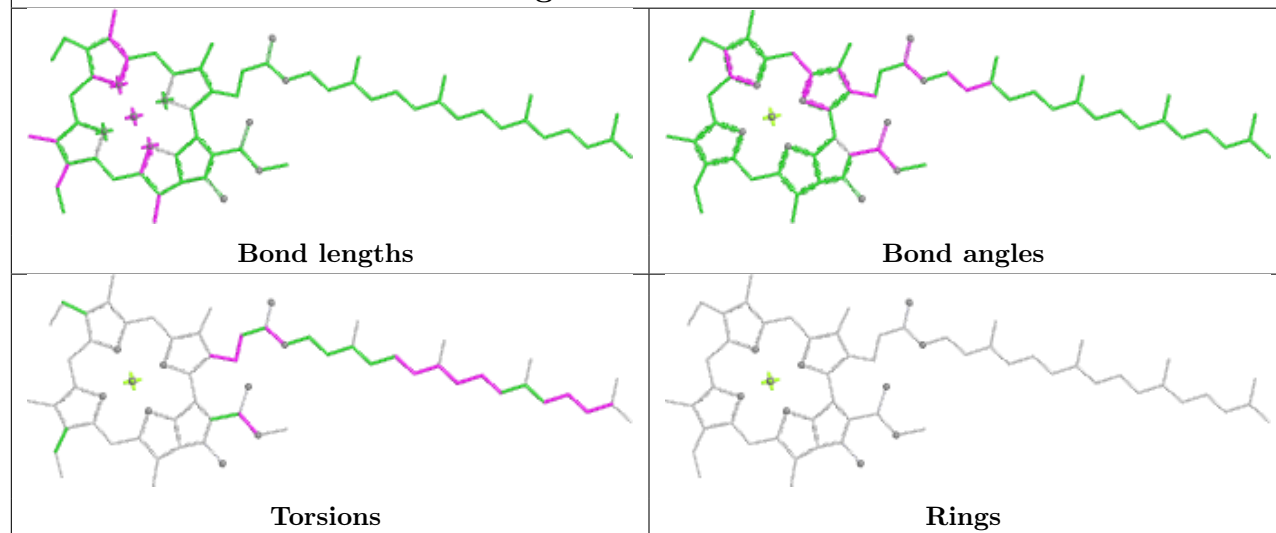


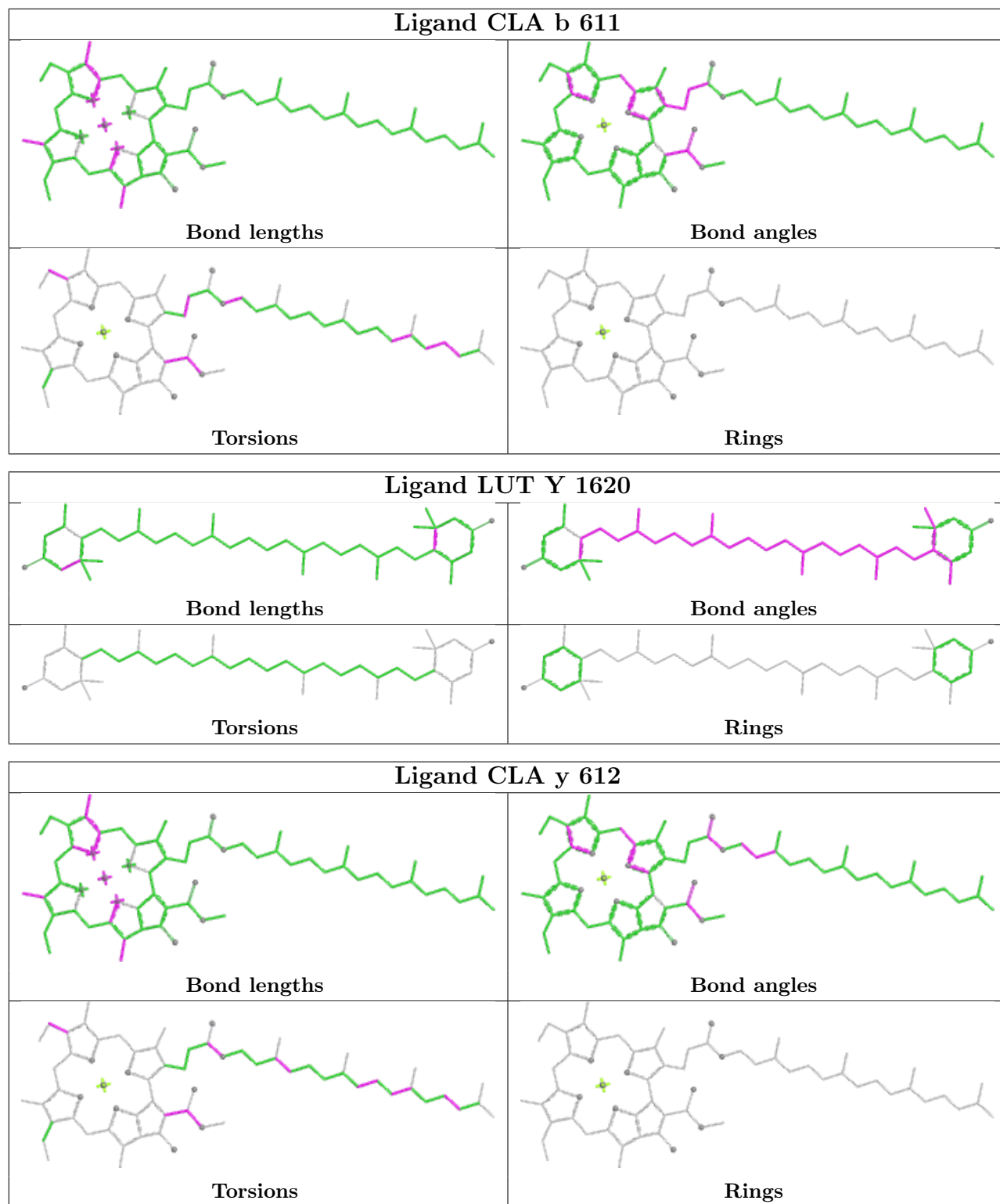


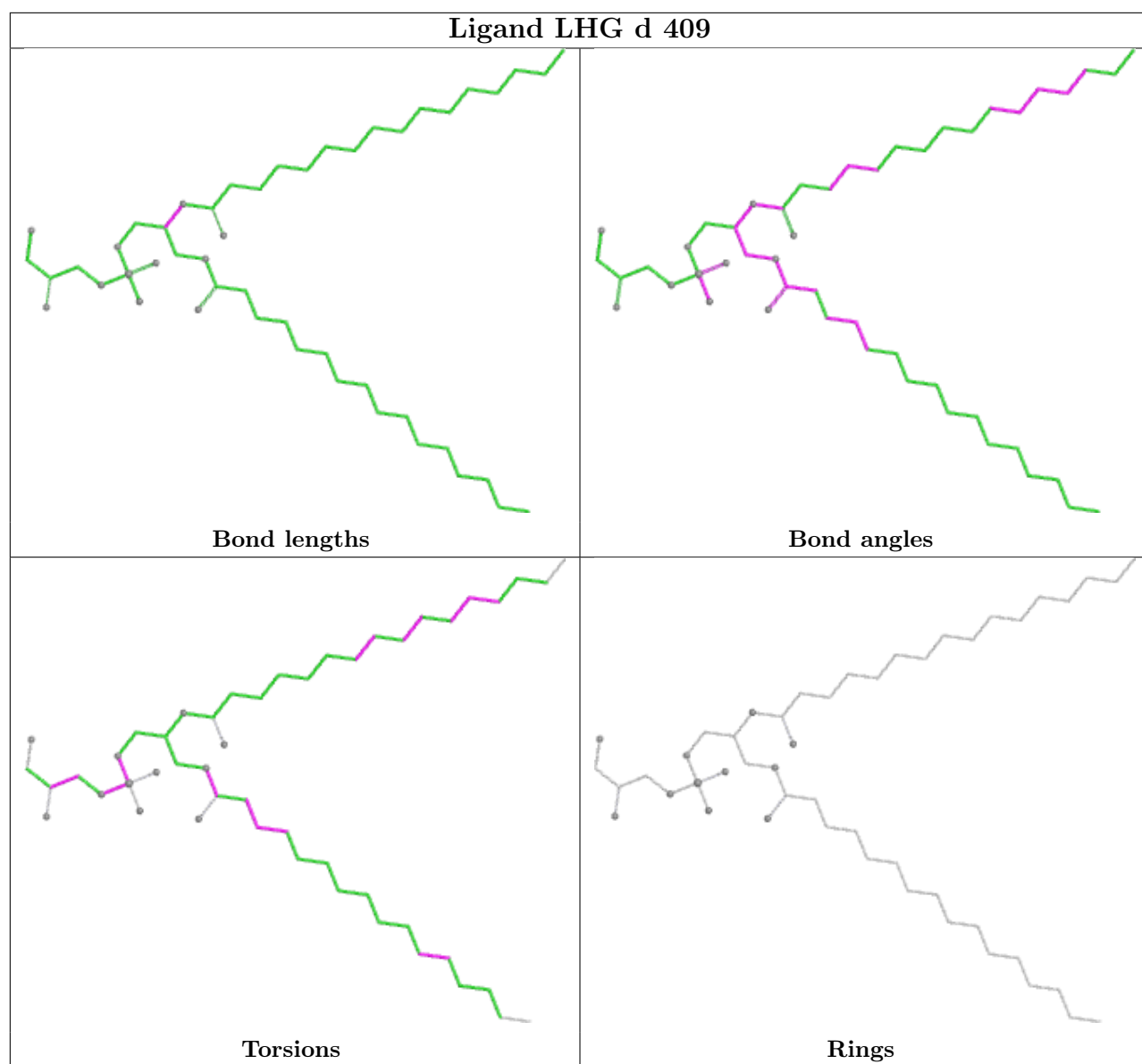
Ligand CLA s 612

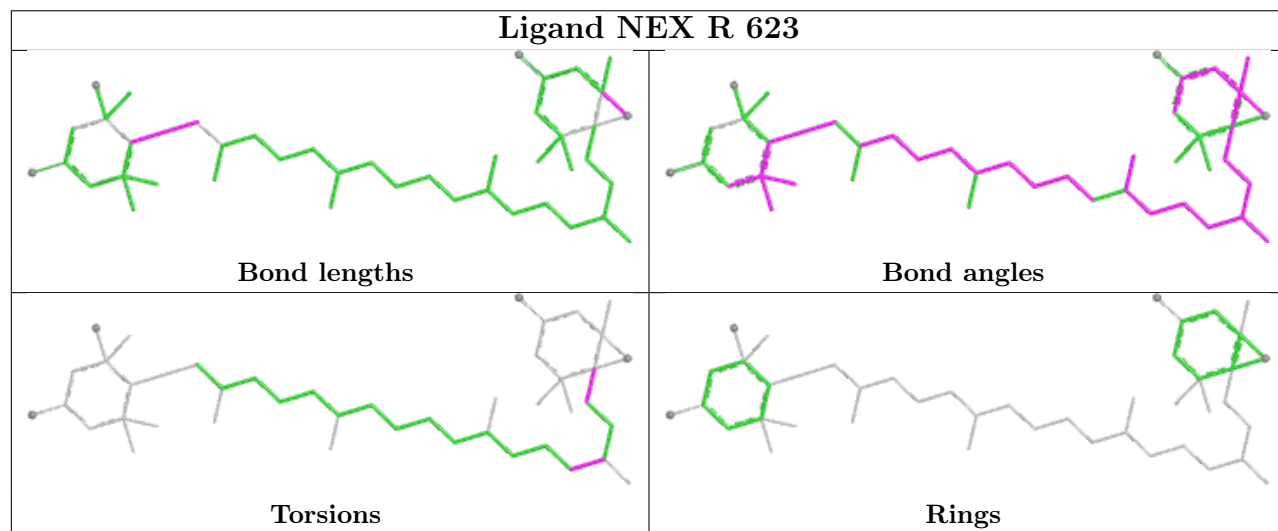
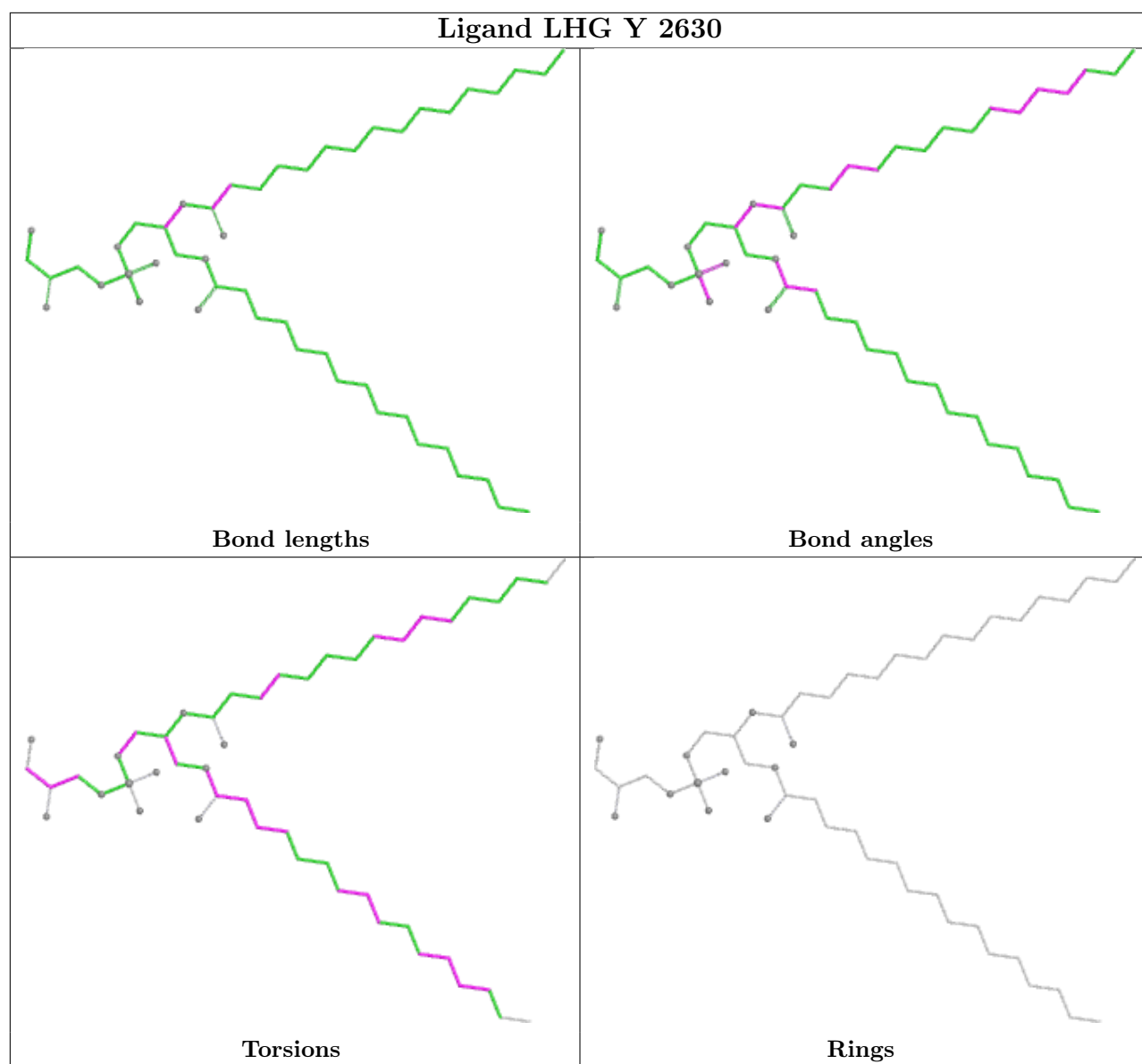


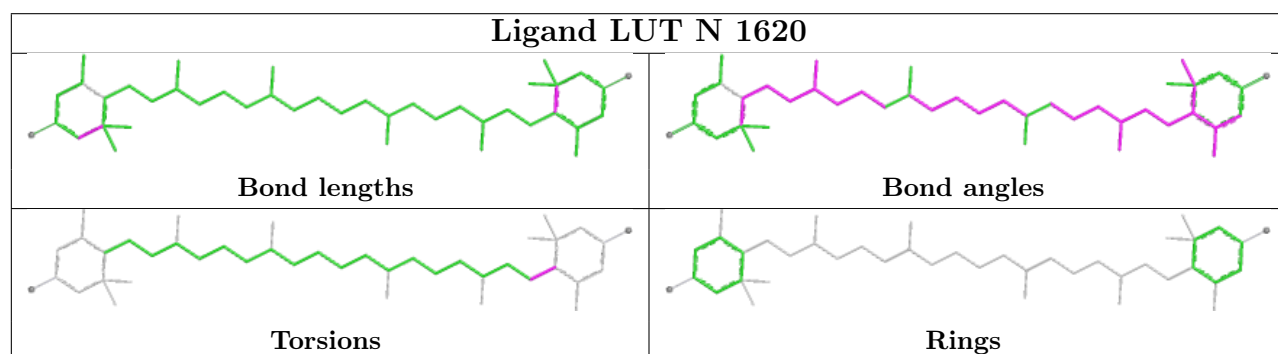
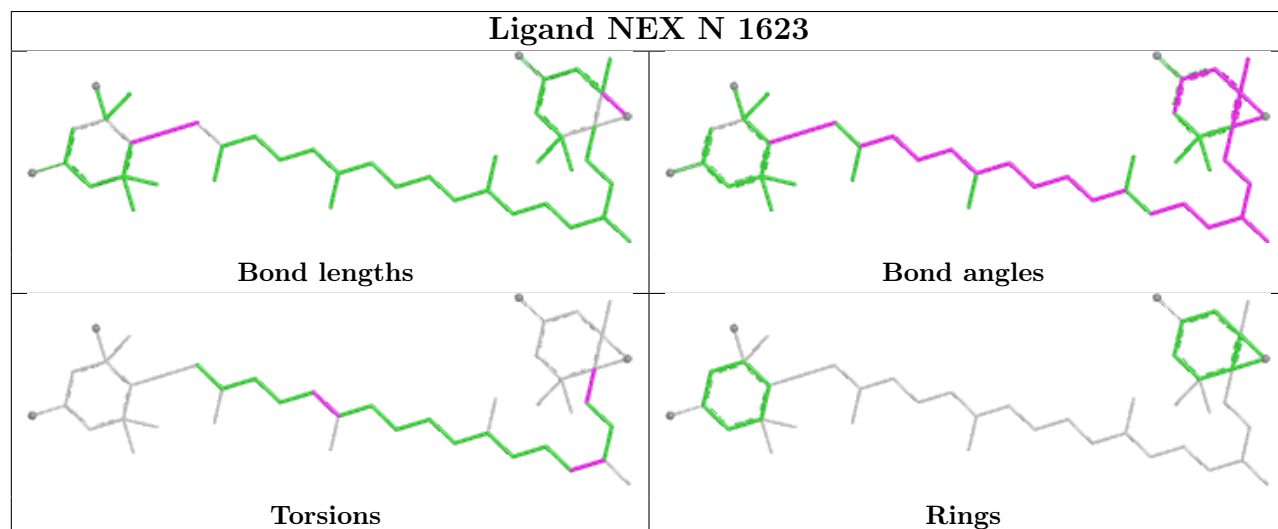
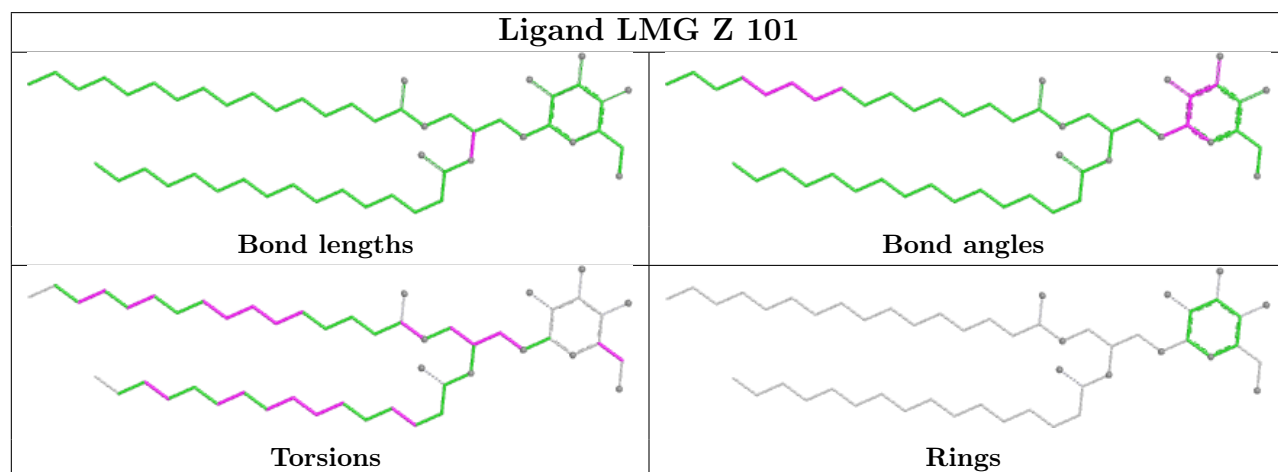
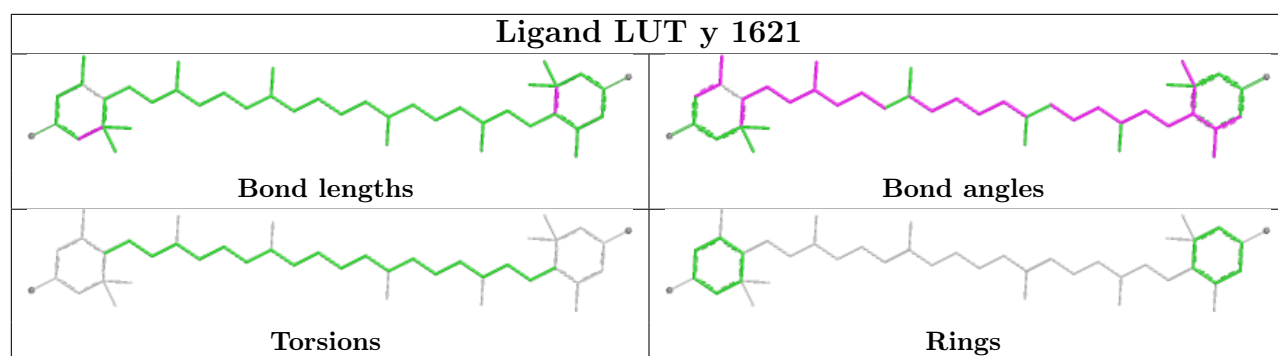
Ligand CLA b 605

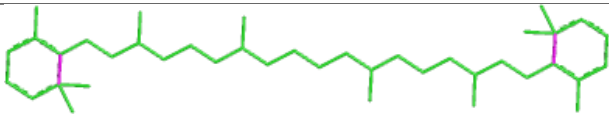
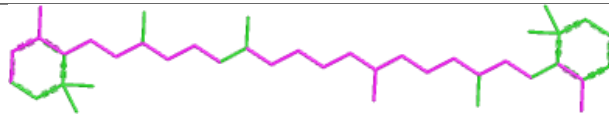
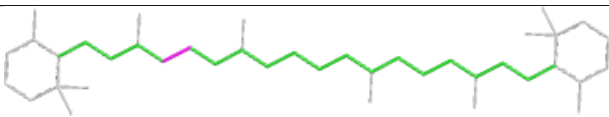
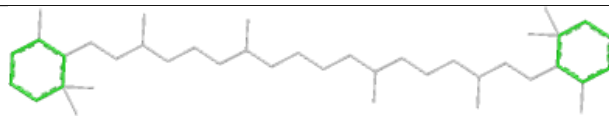


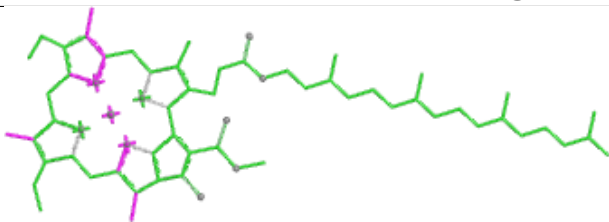
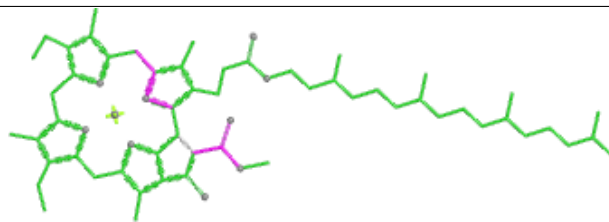
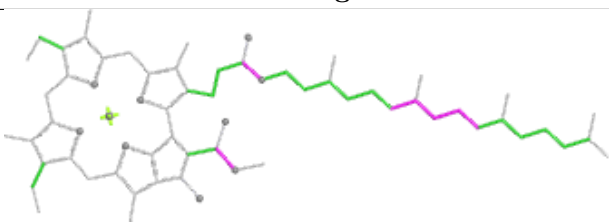
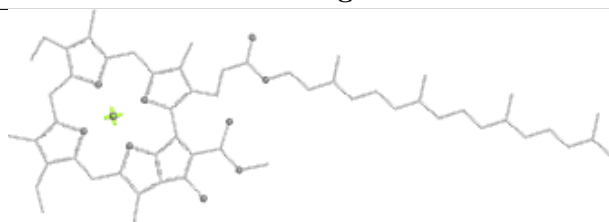


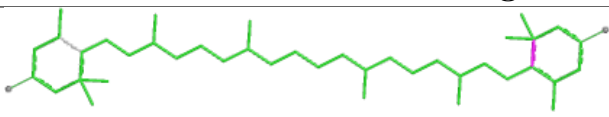
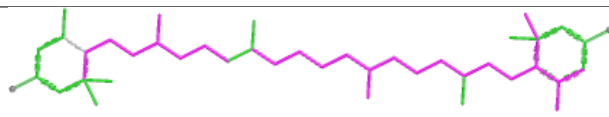
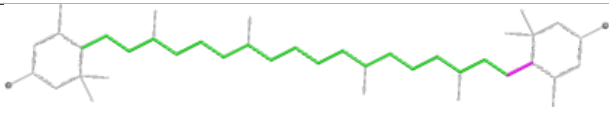
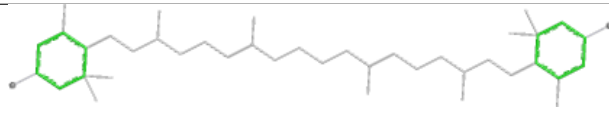


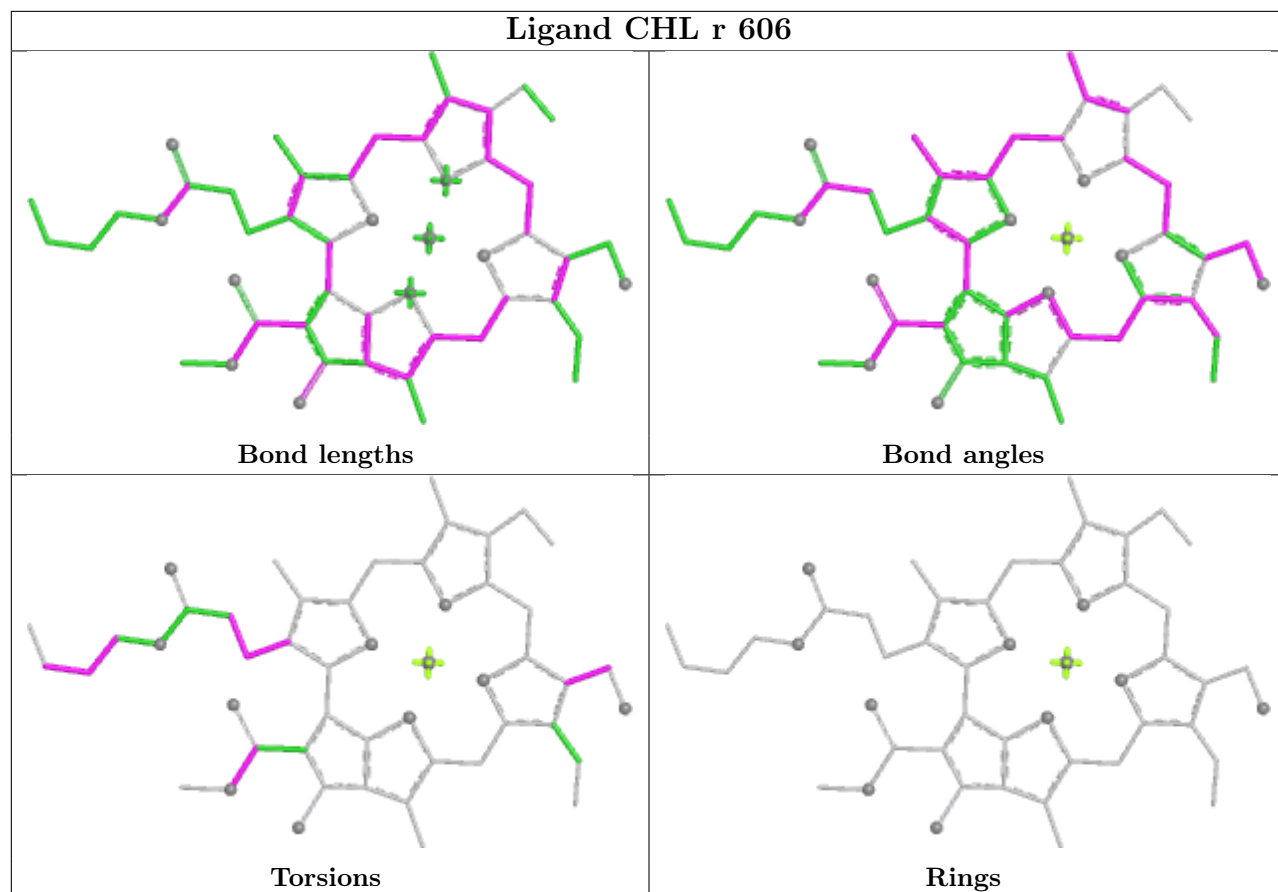


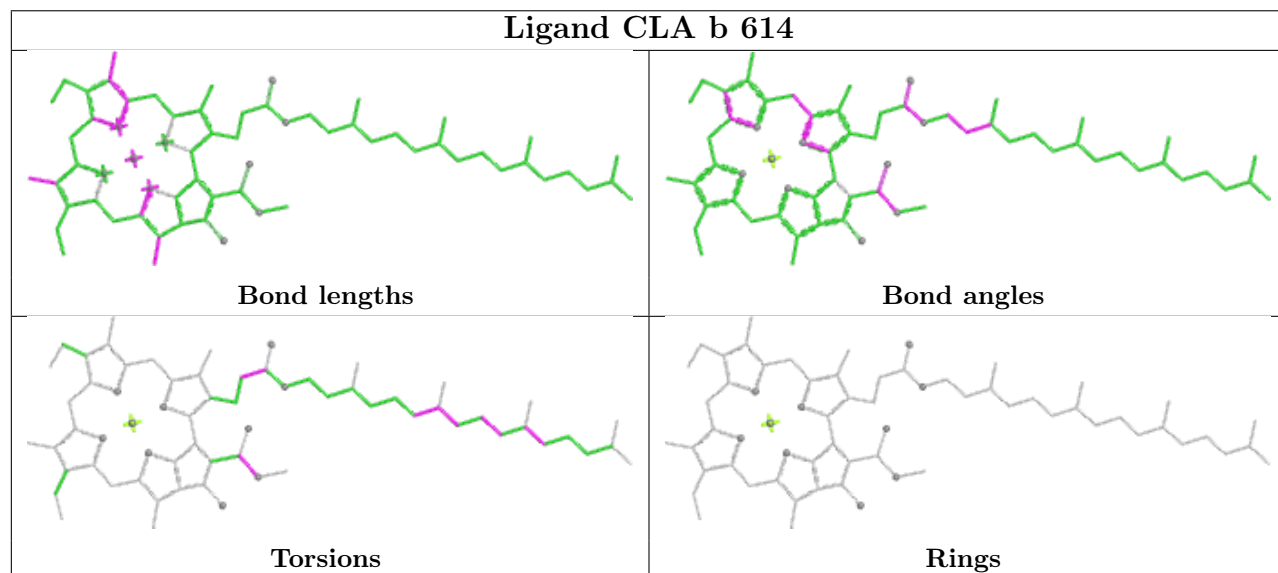
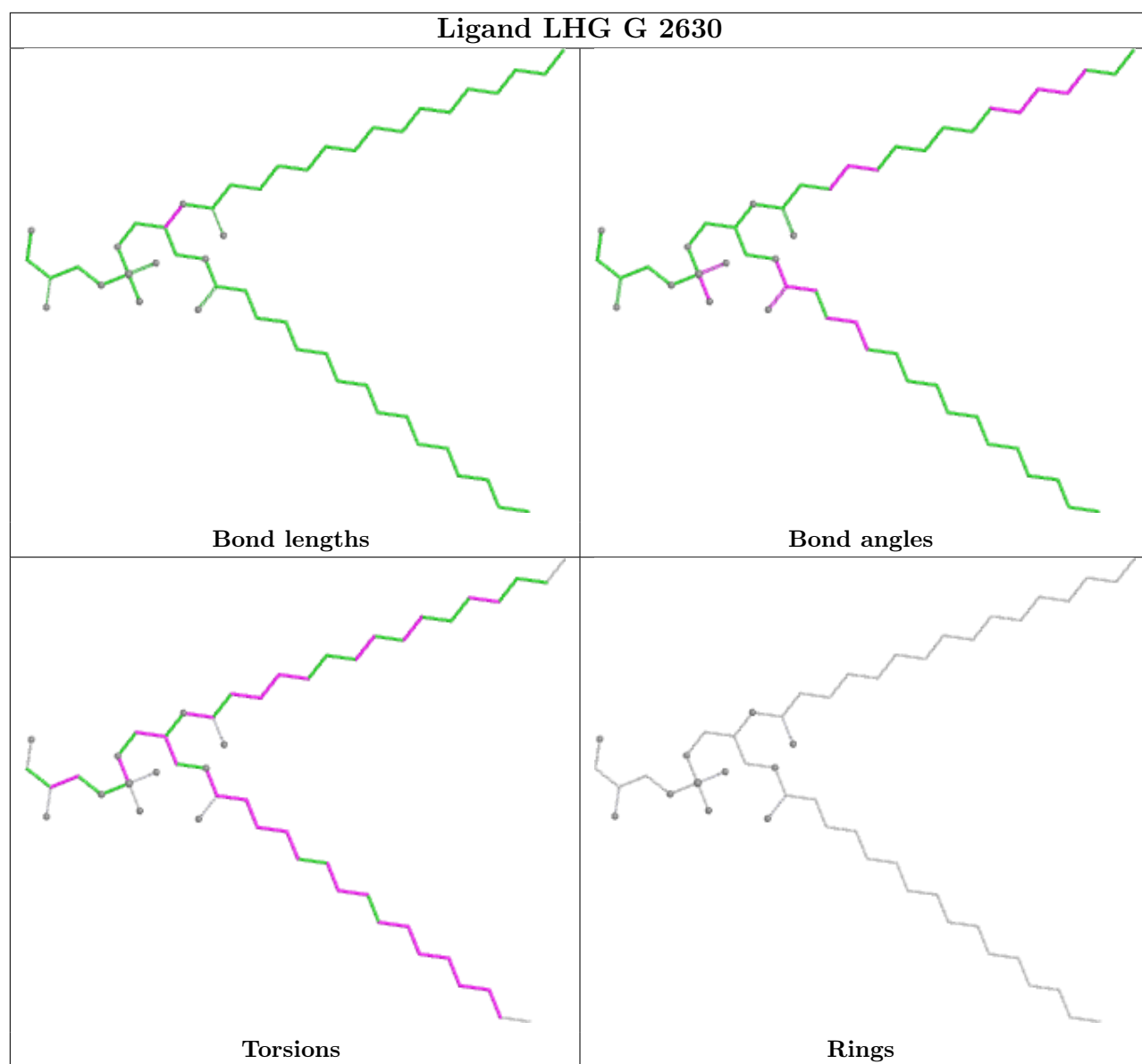


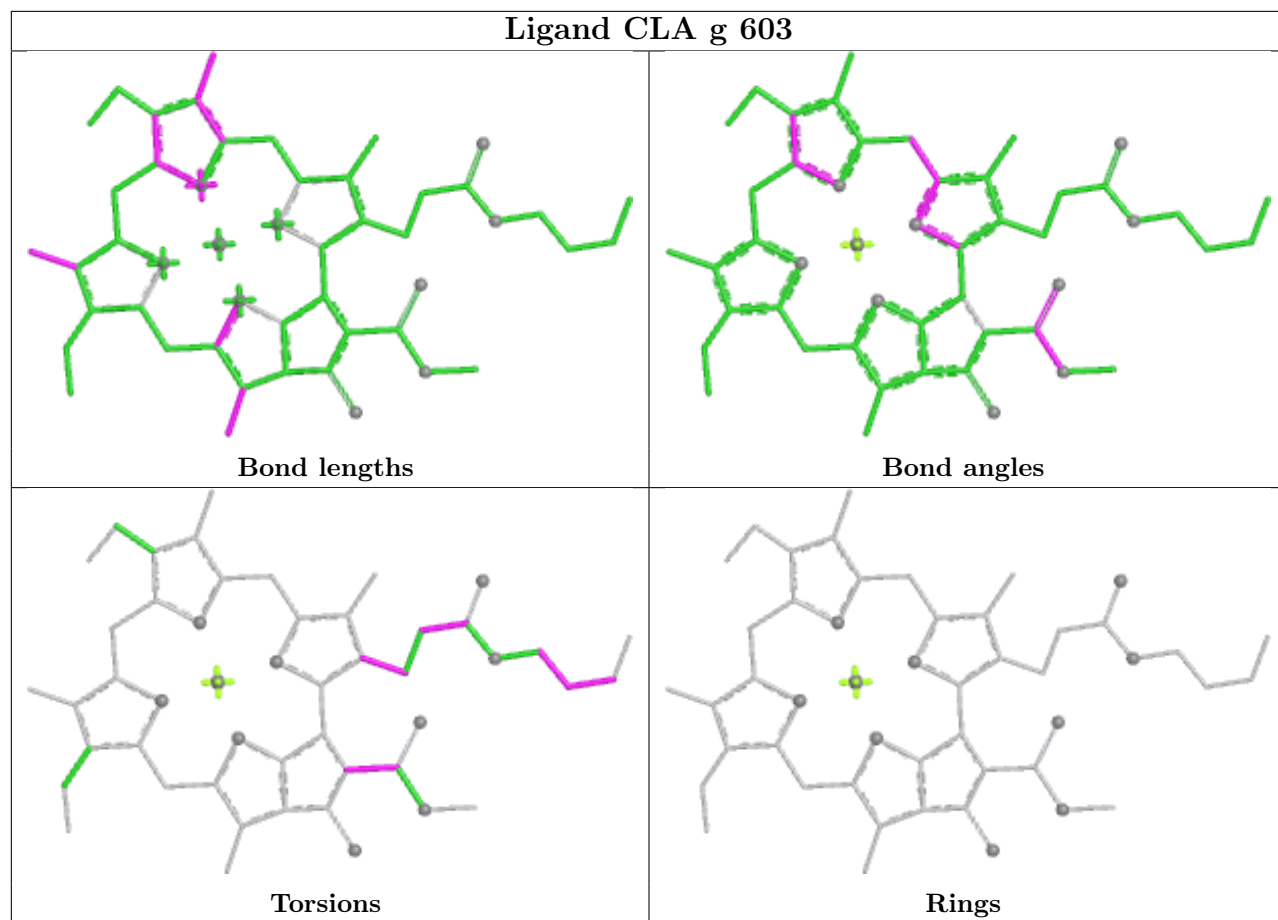
Ligand BCR C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

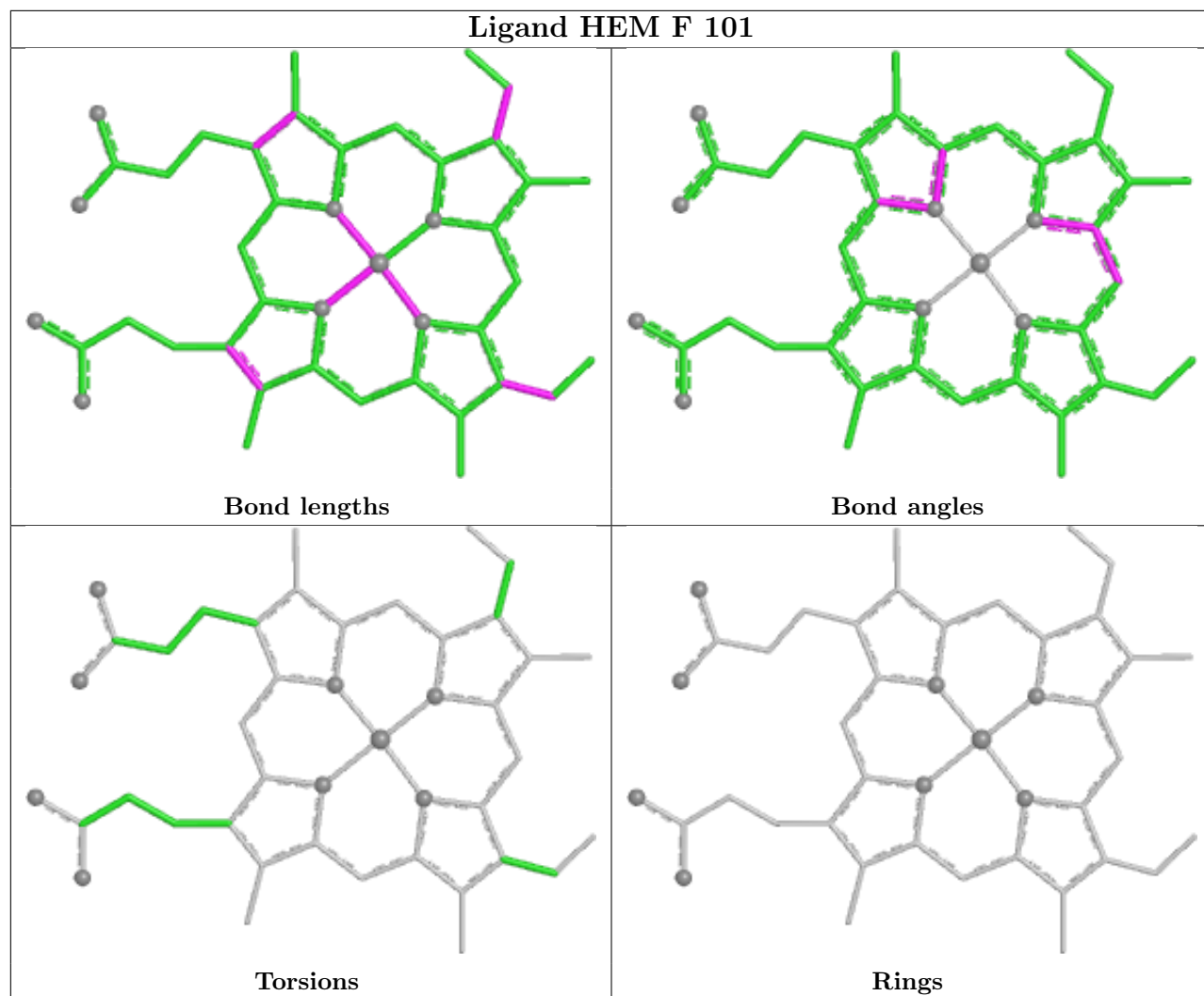
Ligand CLA Y 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

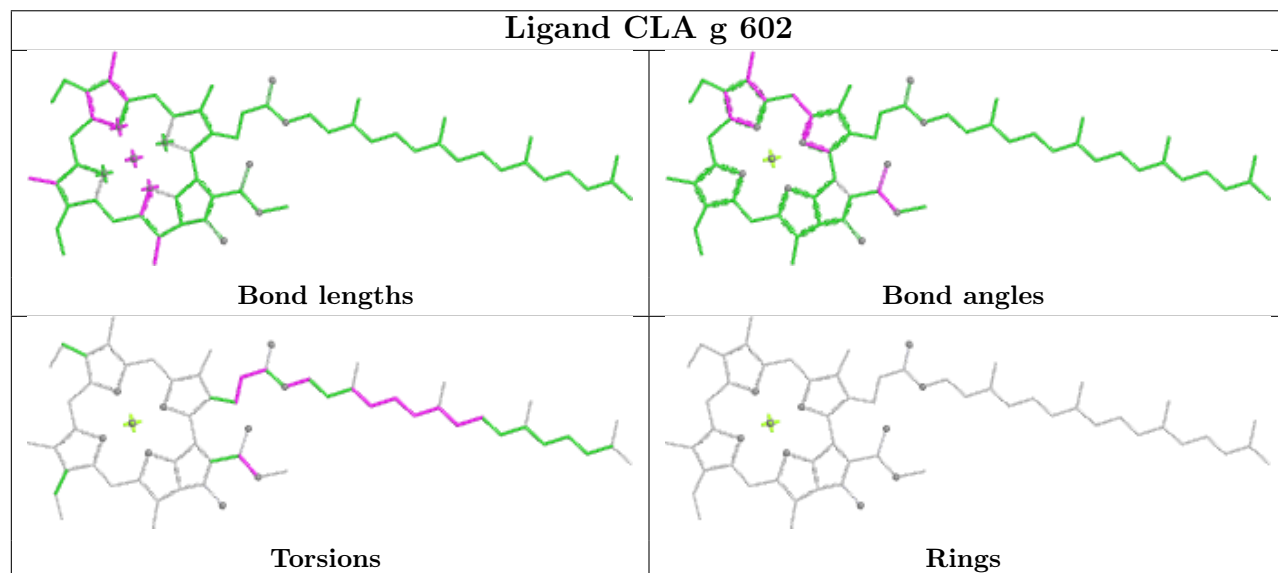
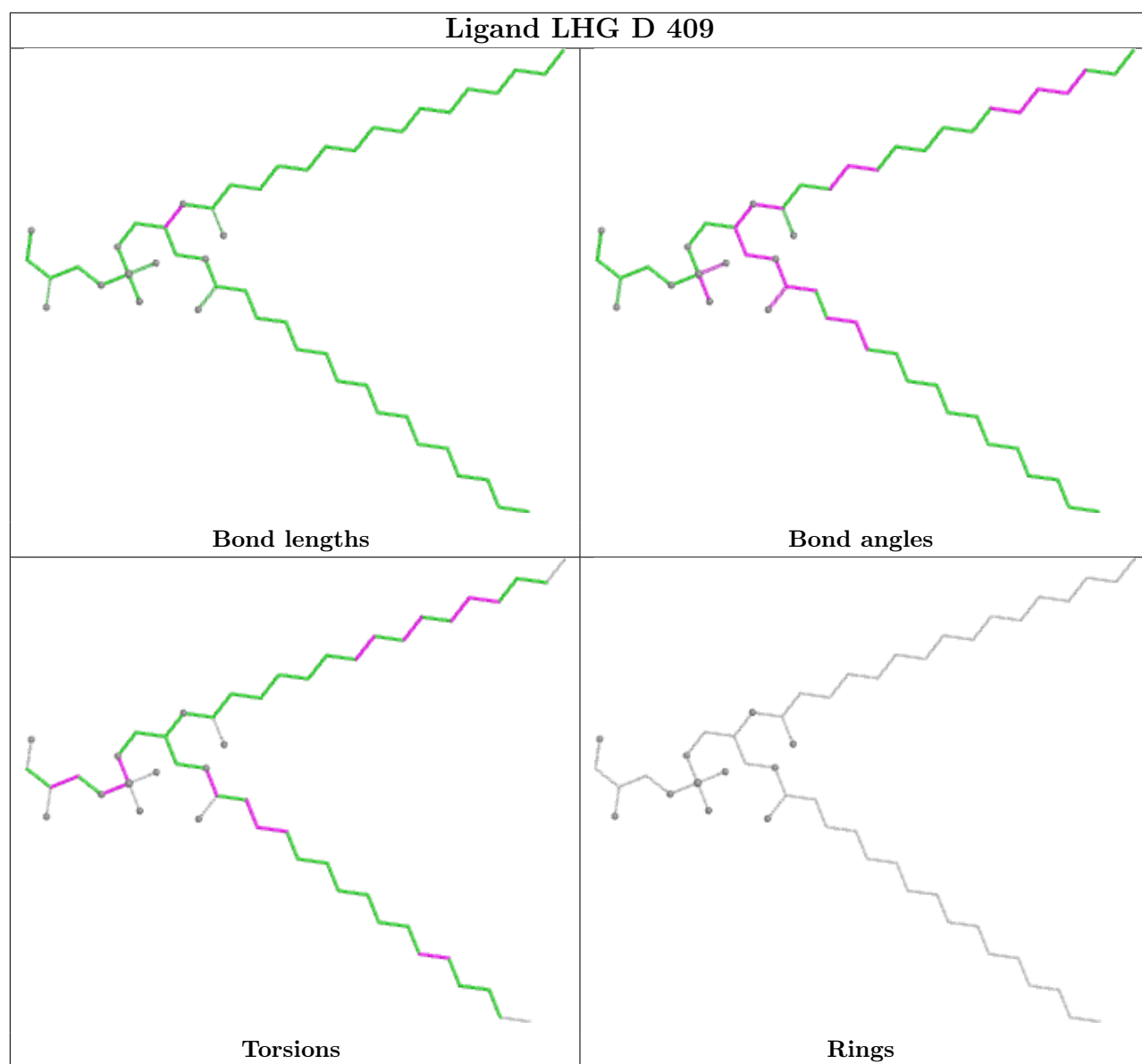
Ligand LUT G 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings



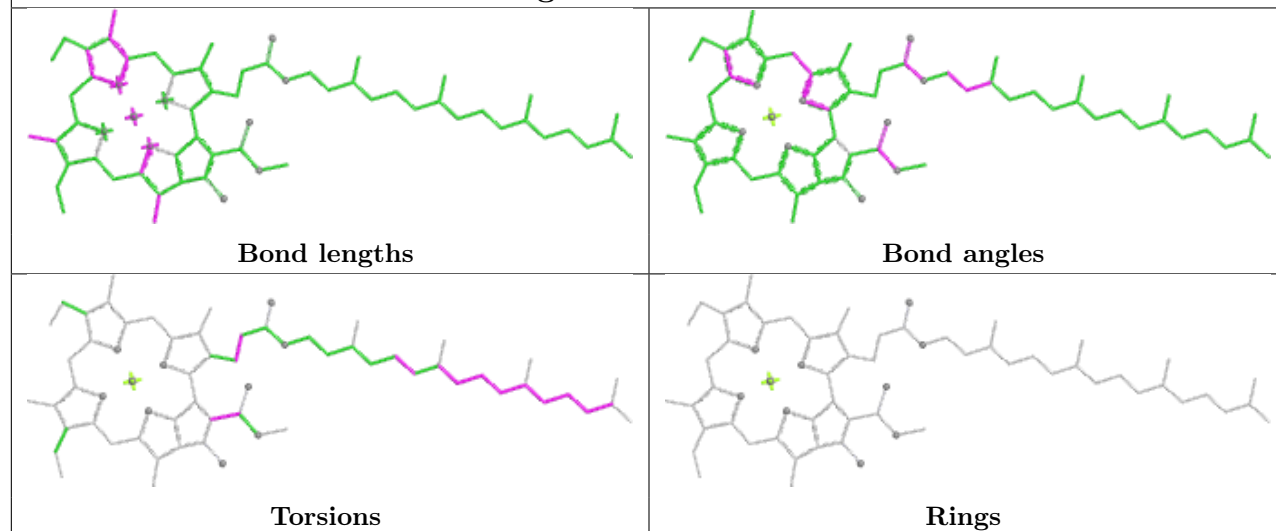




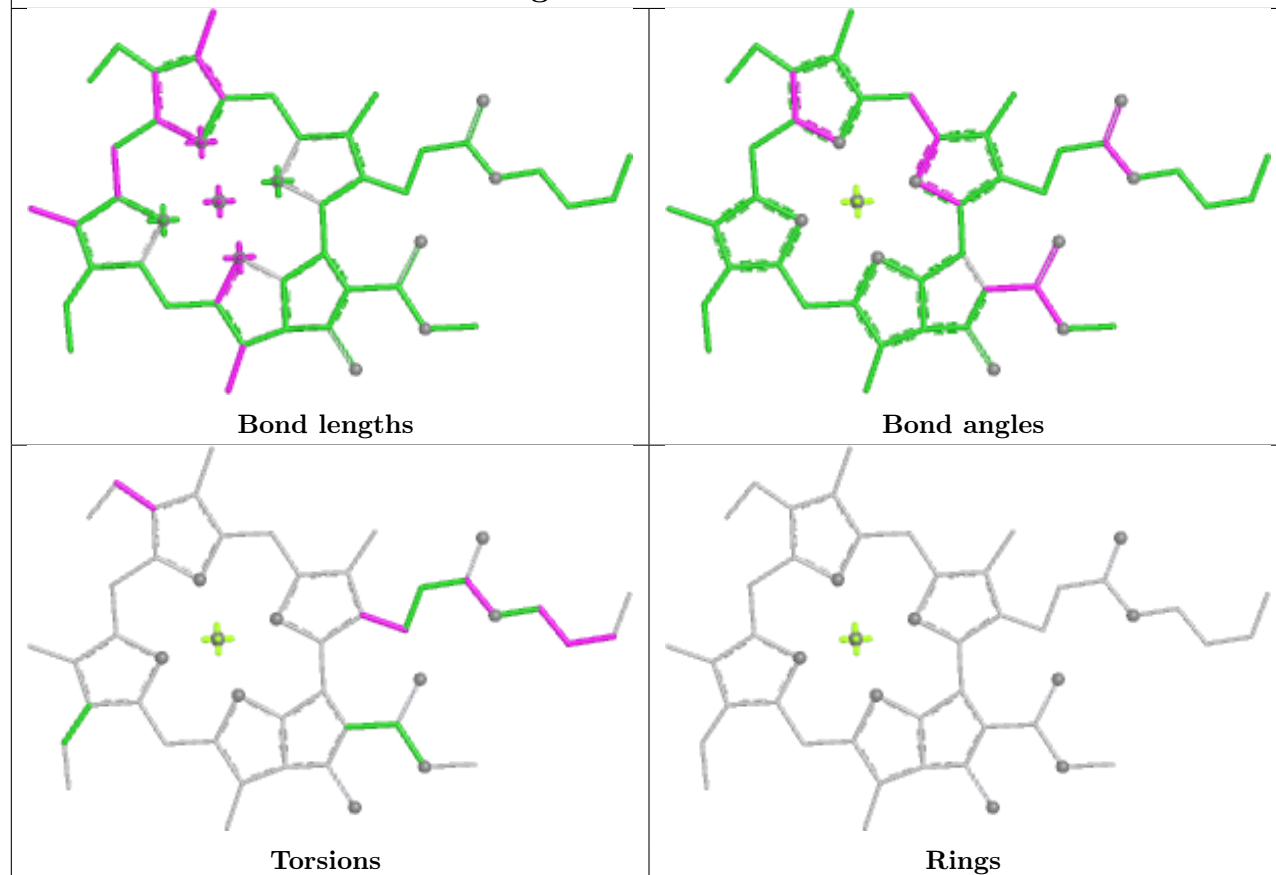


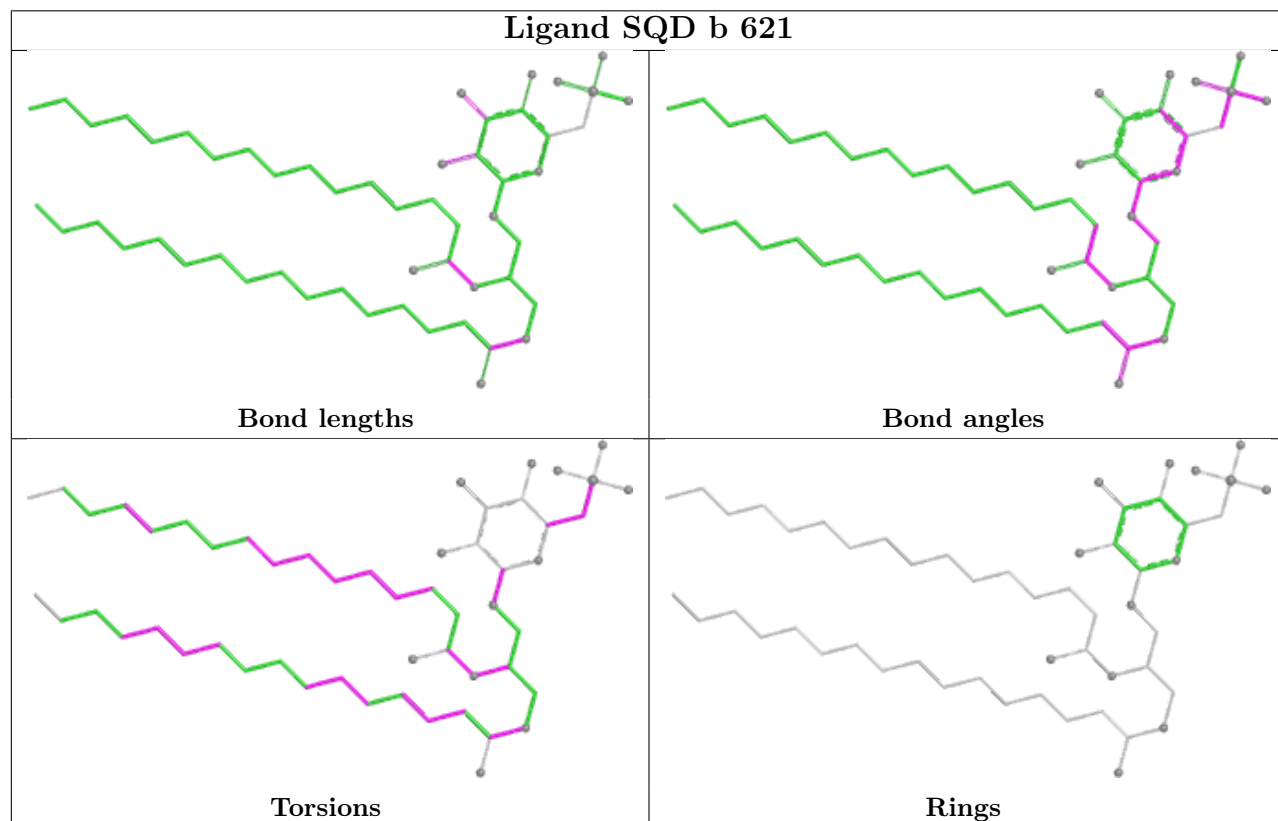
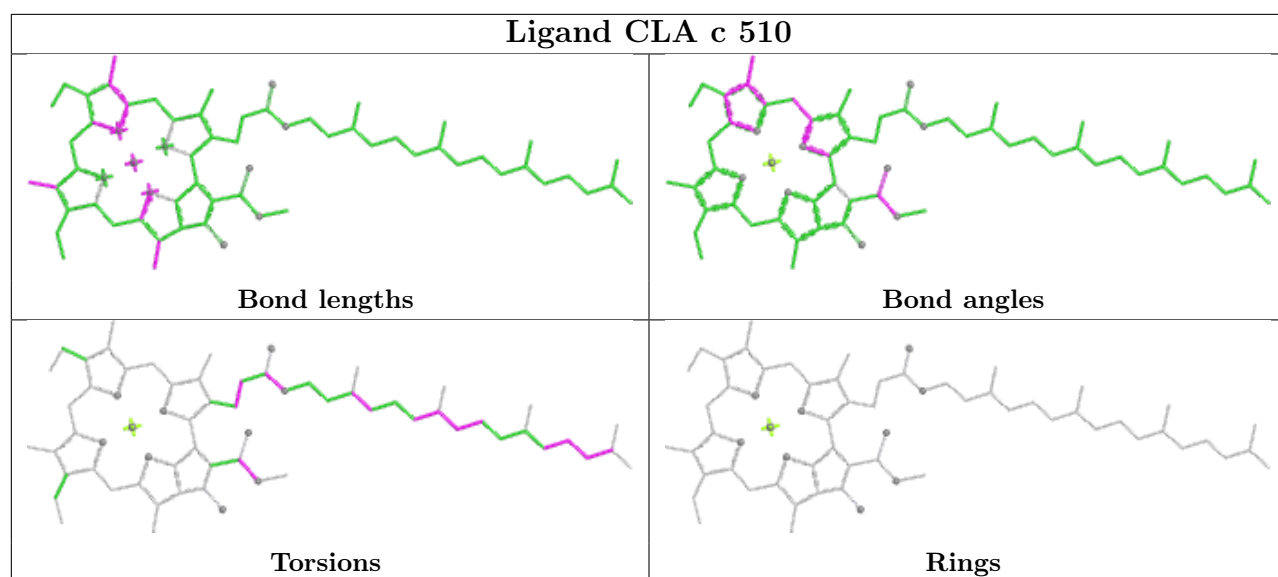


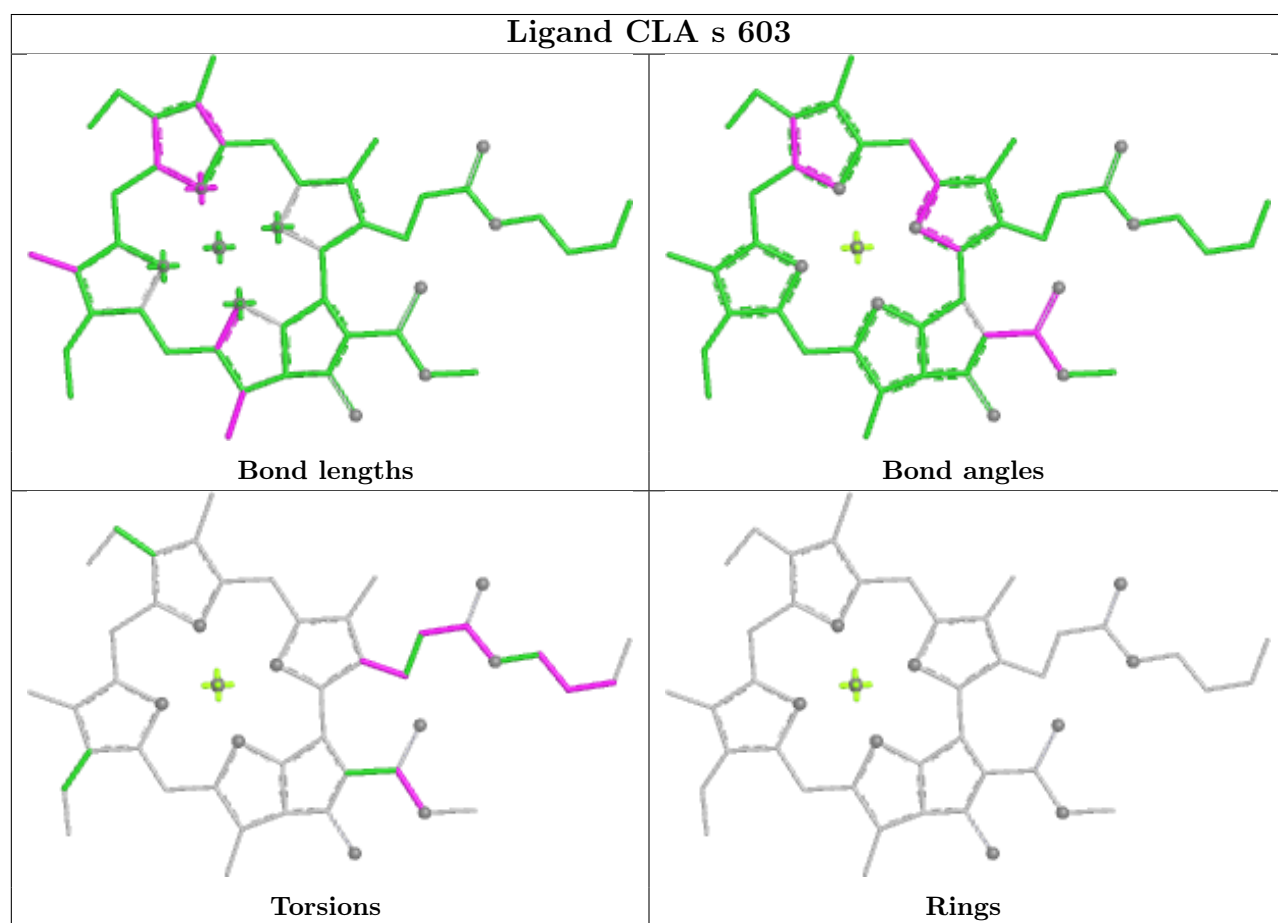
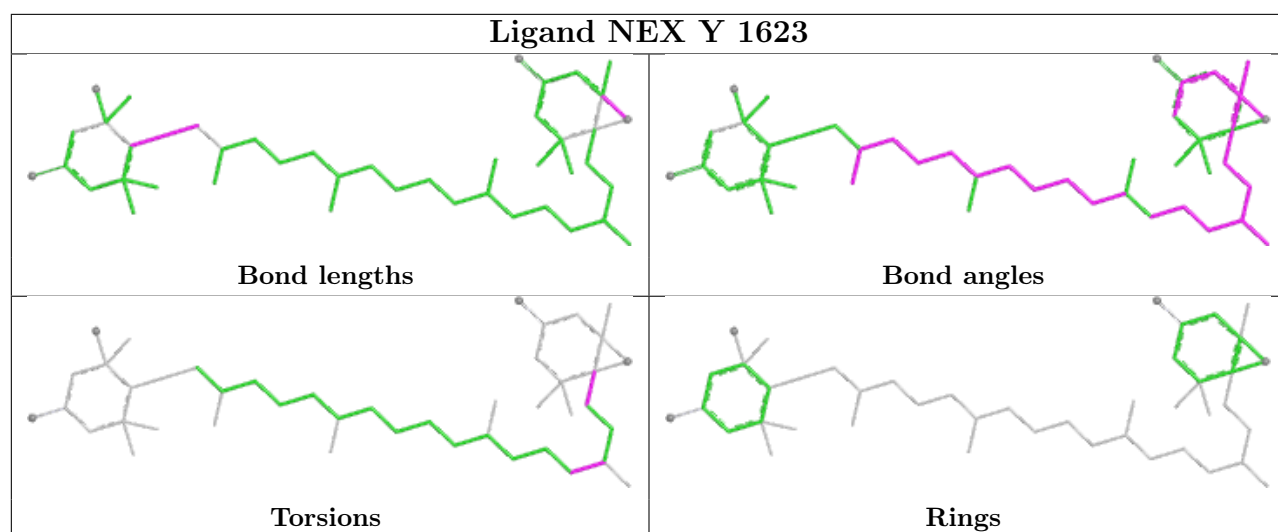
Ligand CLA c 507

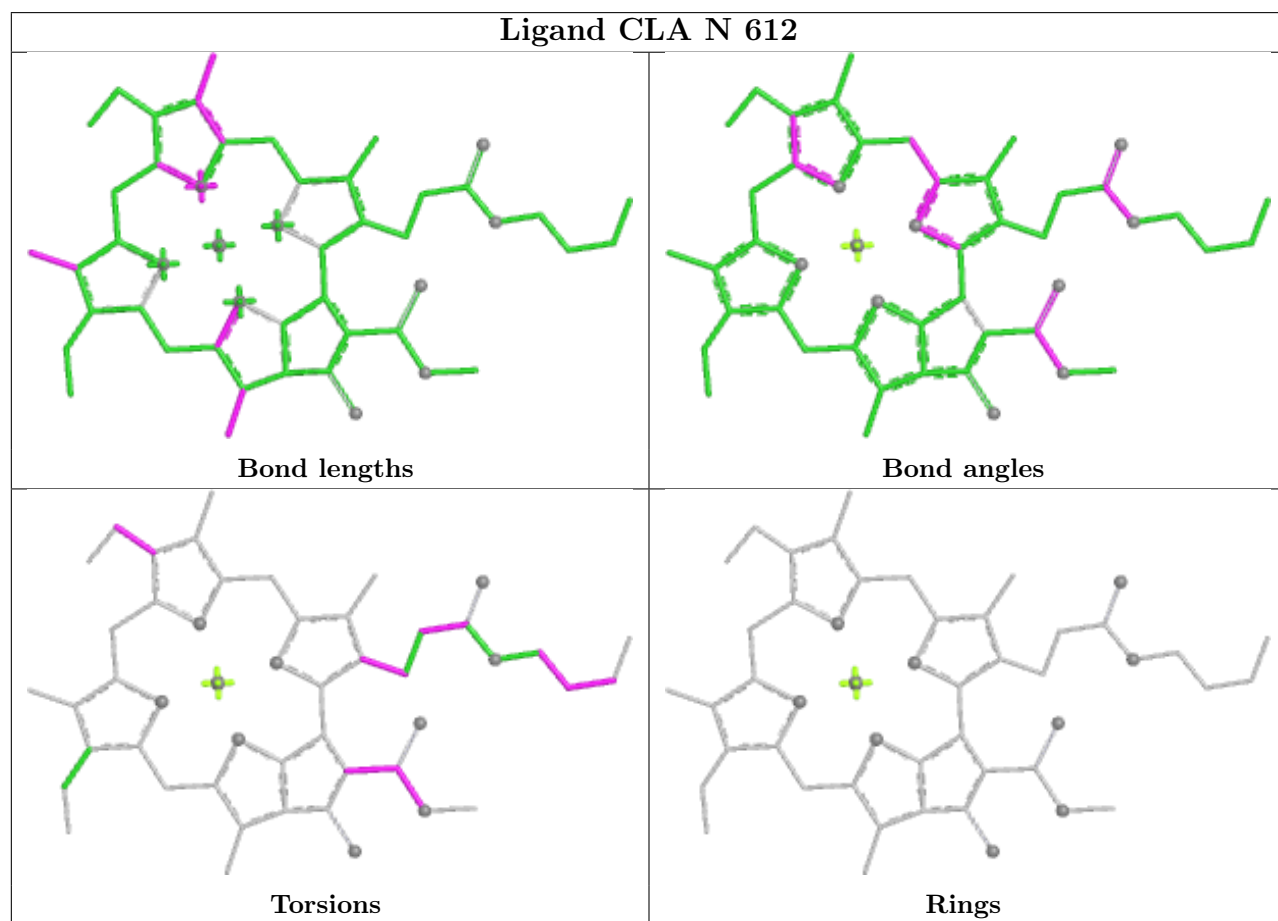
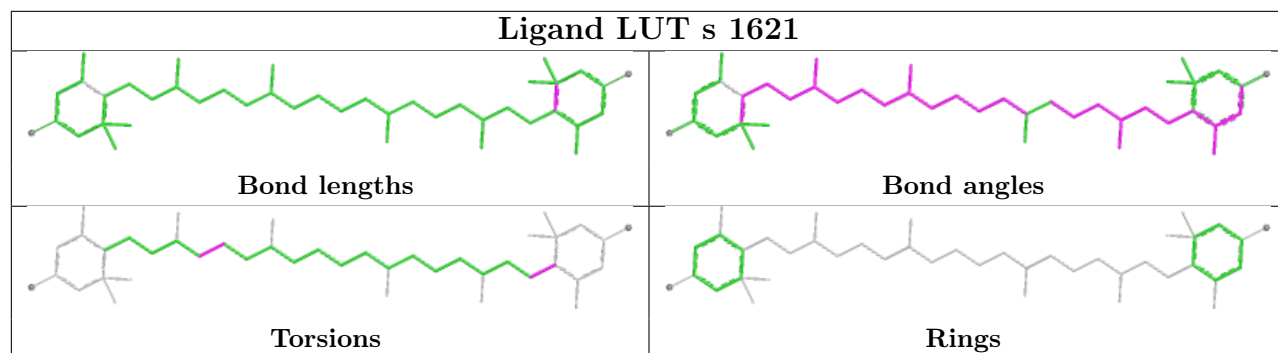


Ligand CLA G 611

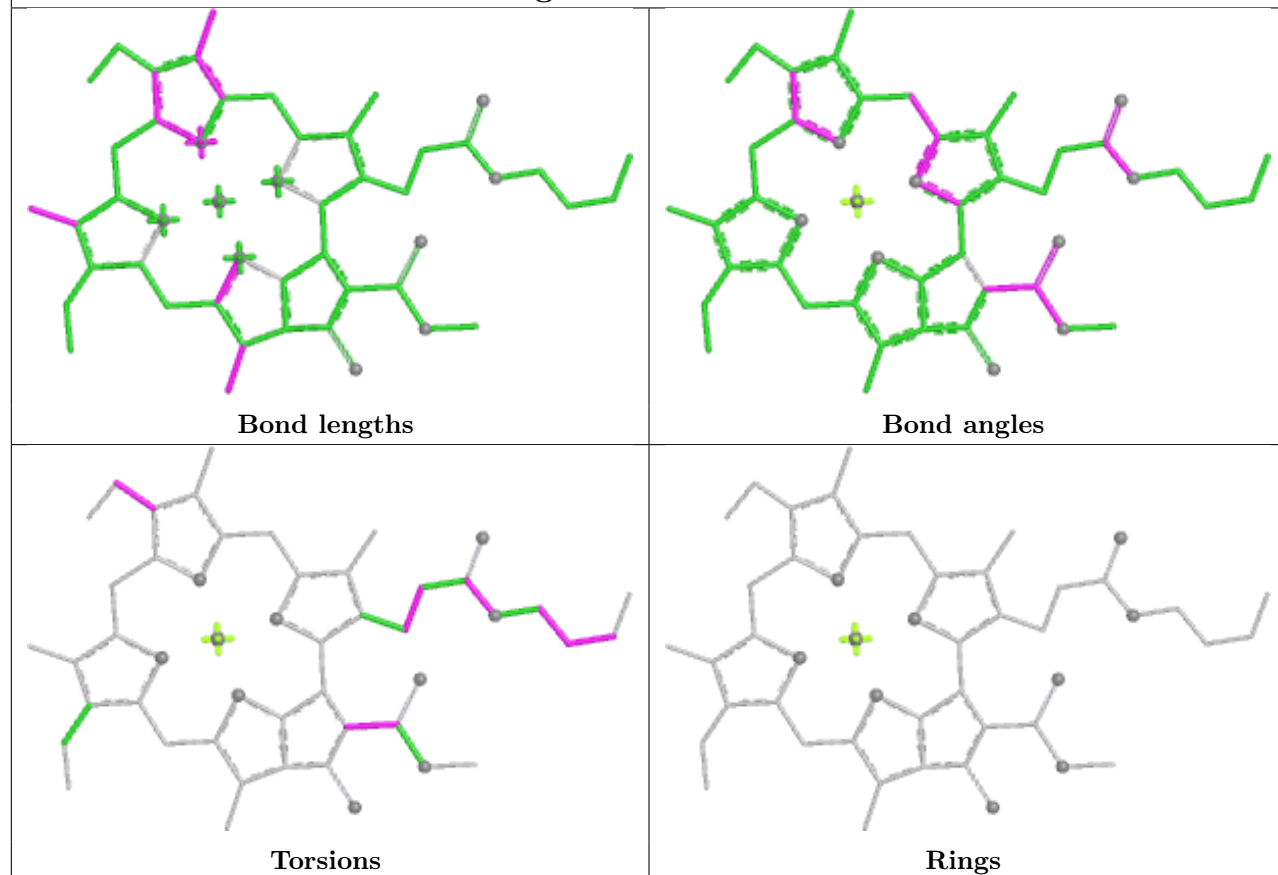




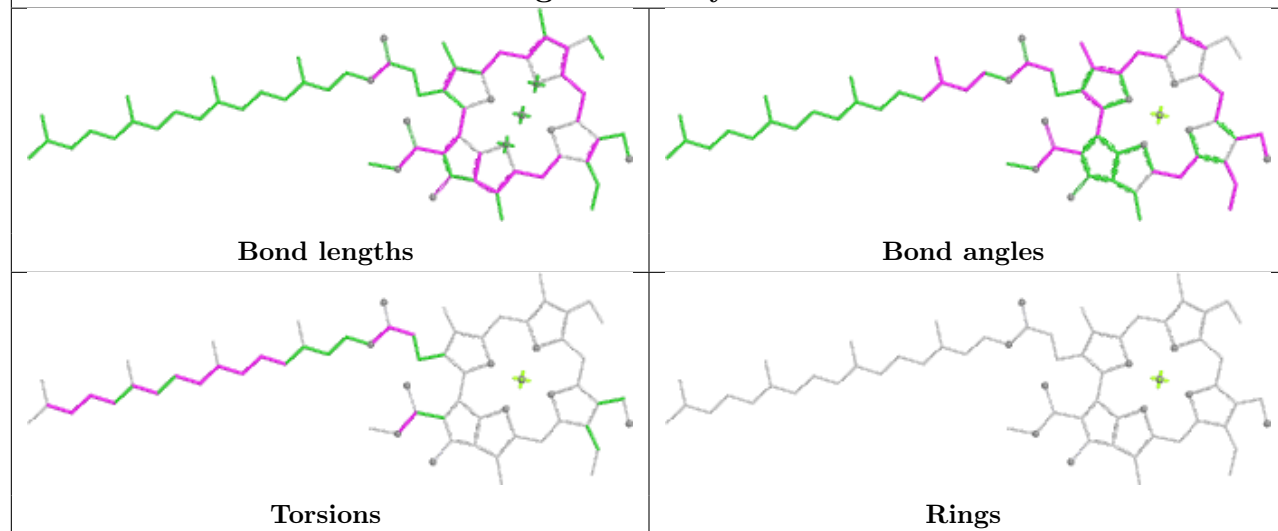




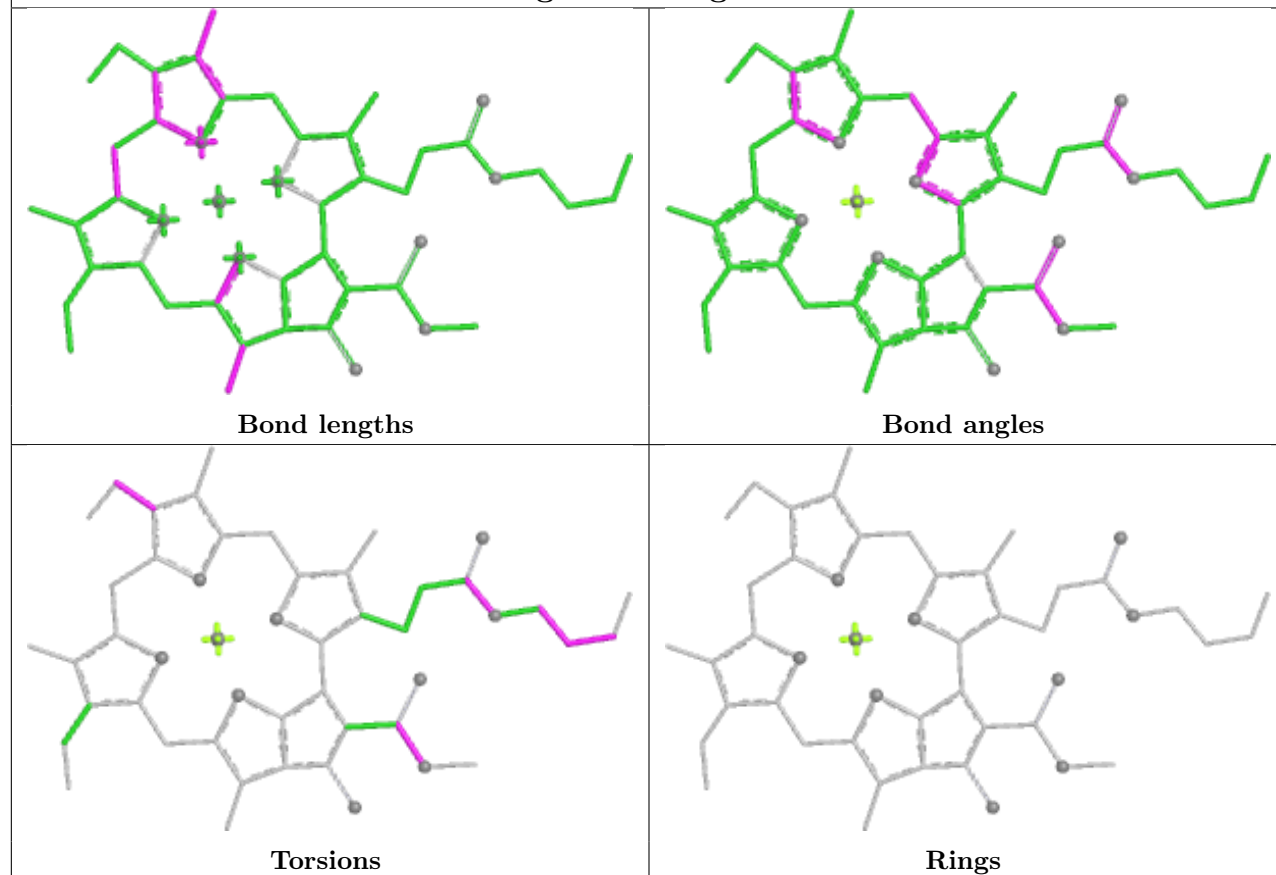
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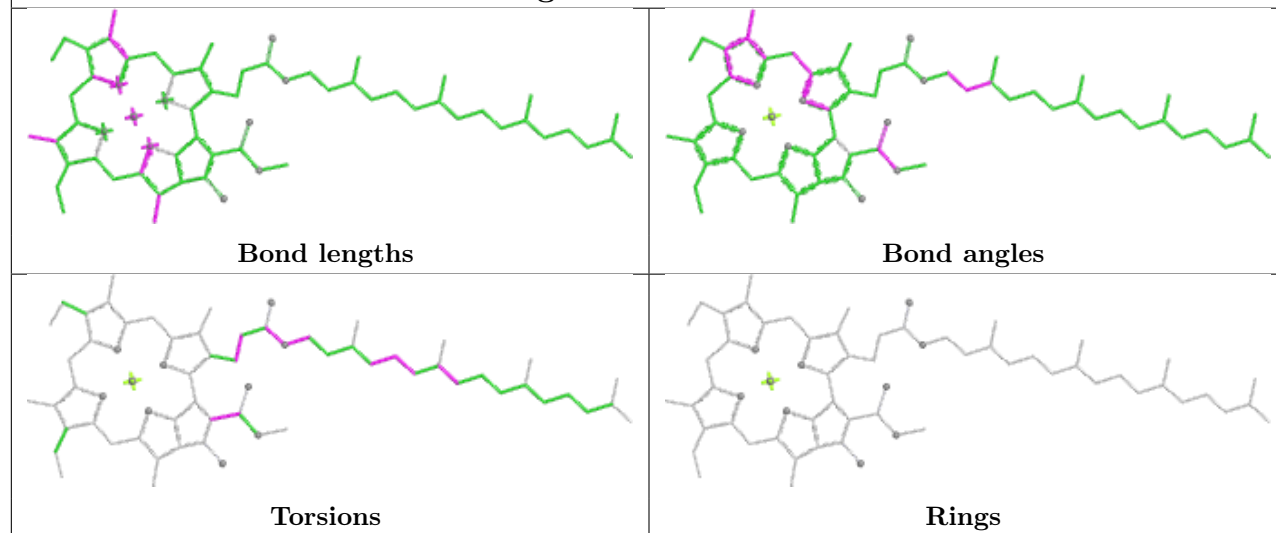
Ligand CHL y 601



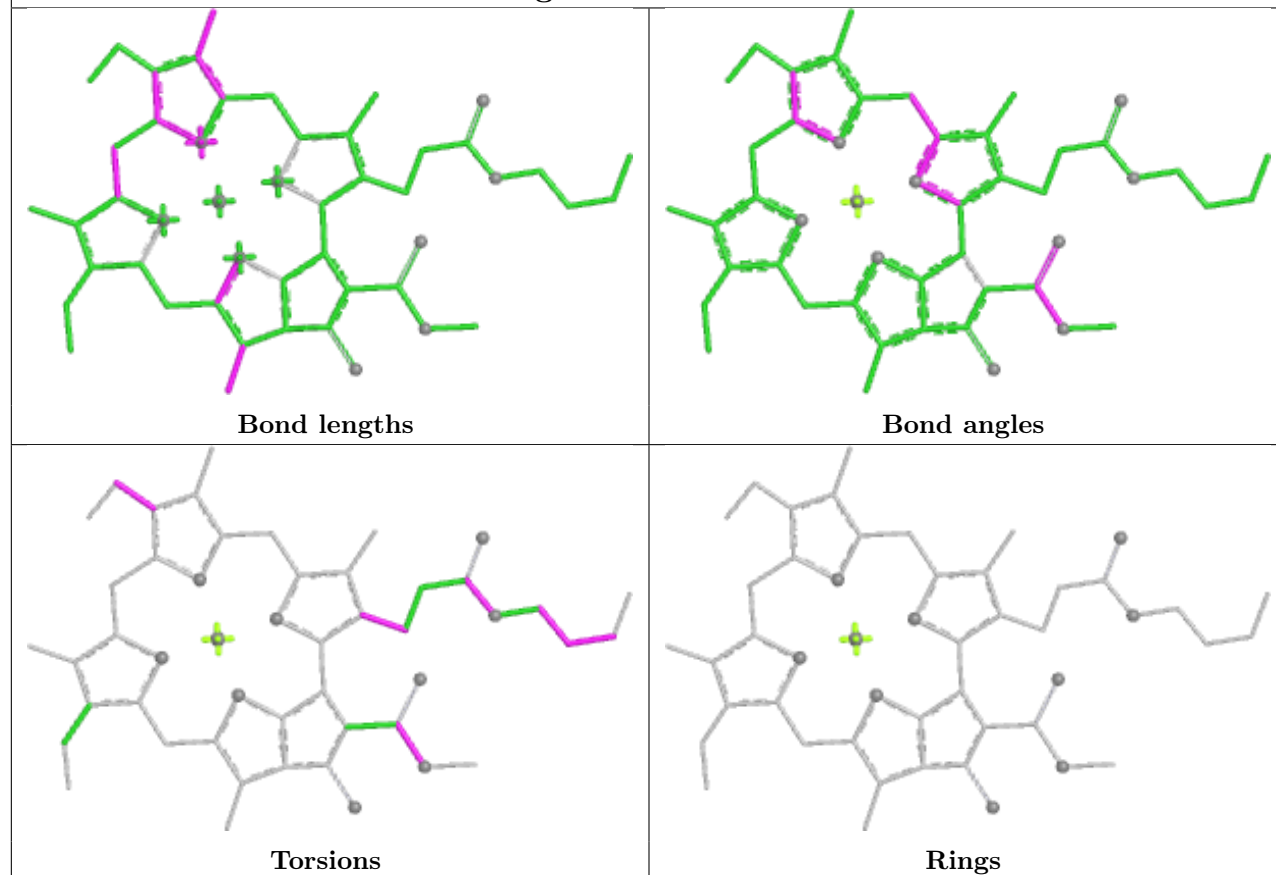
Ligand CLA g 614



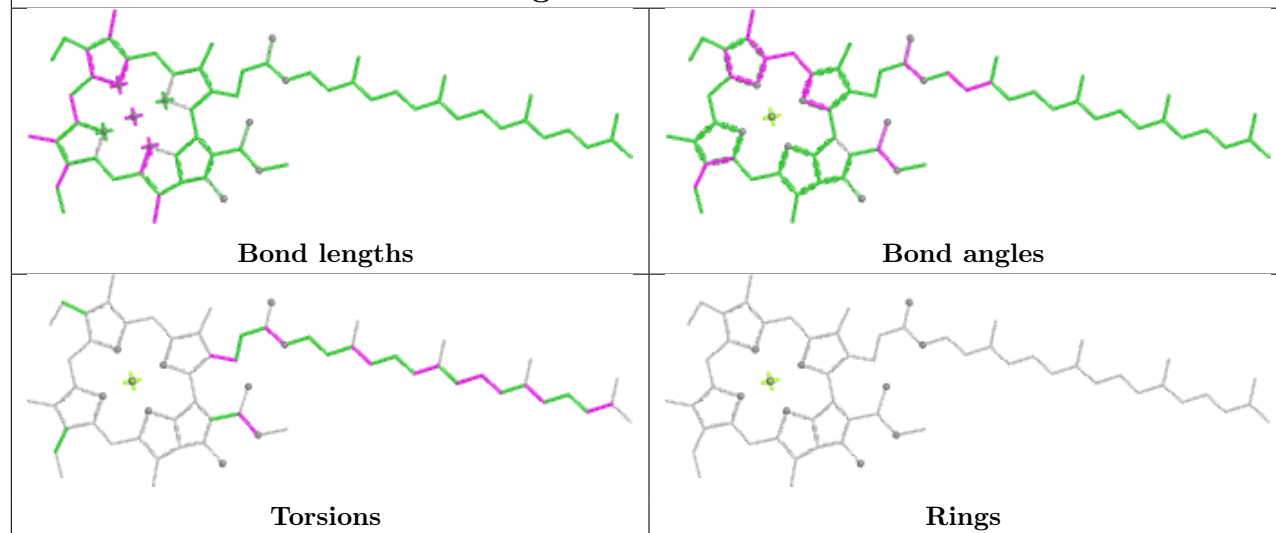
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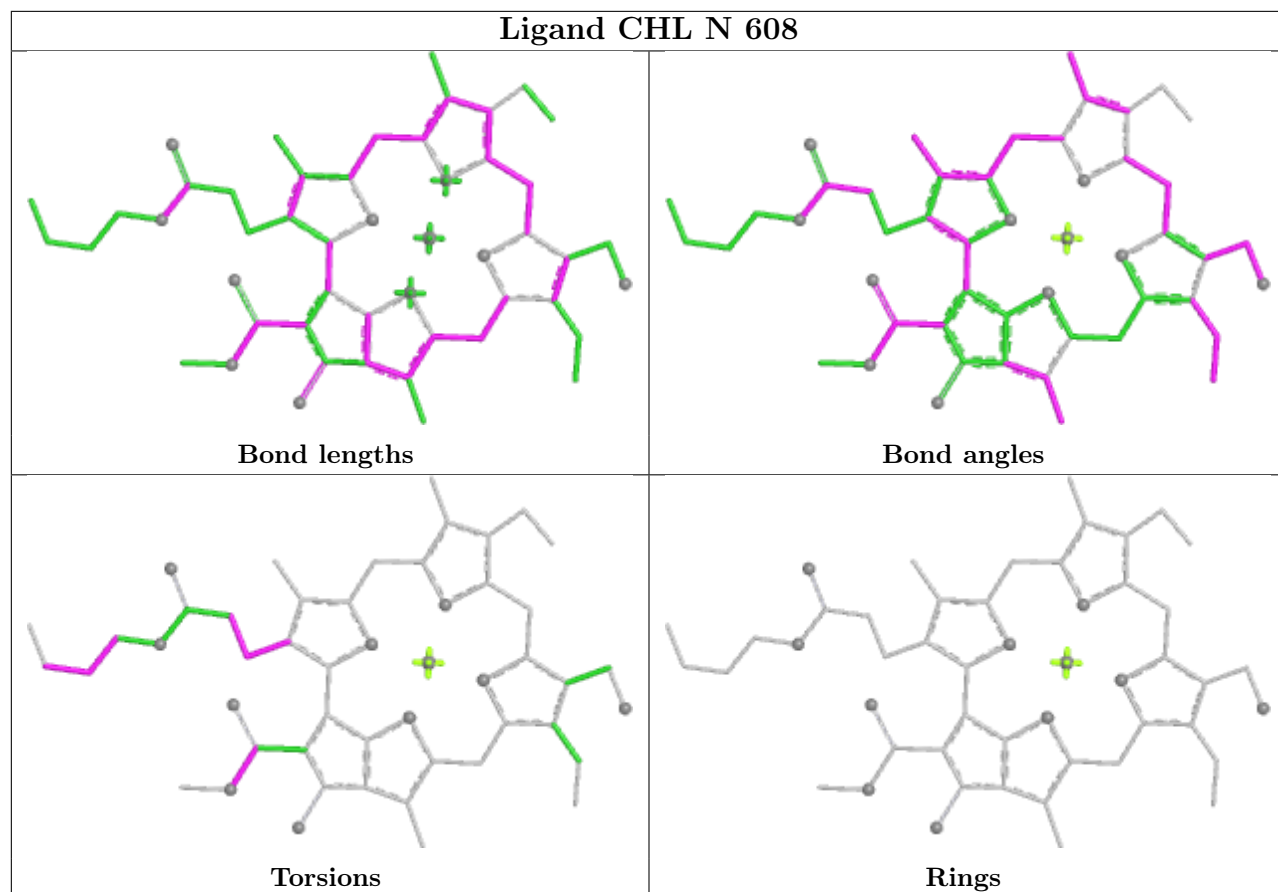


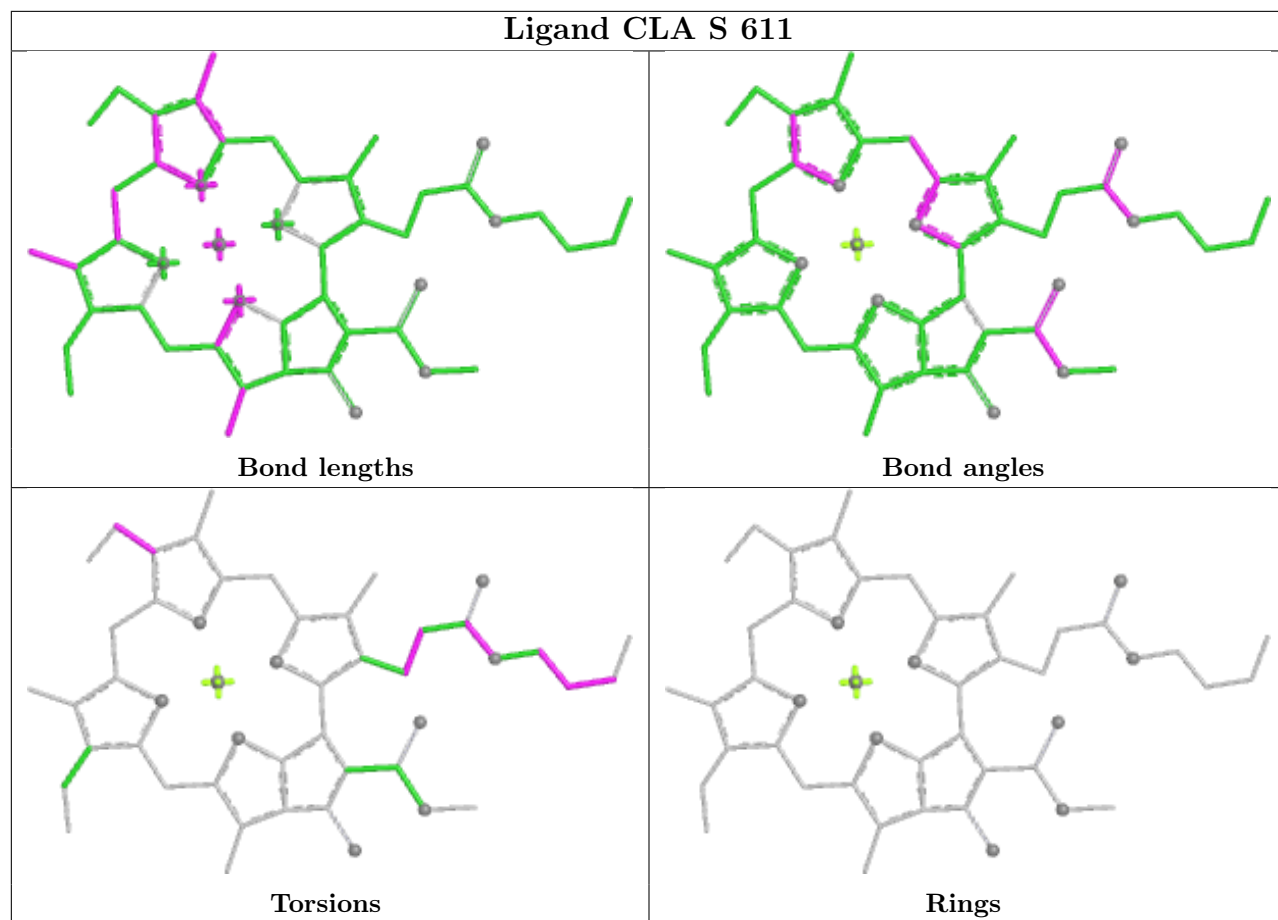
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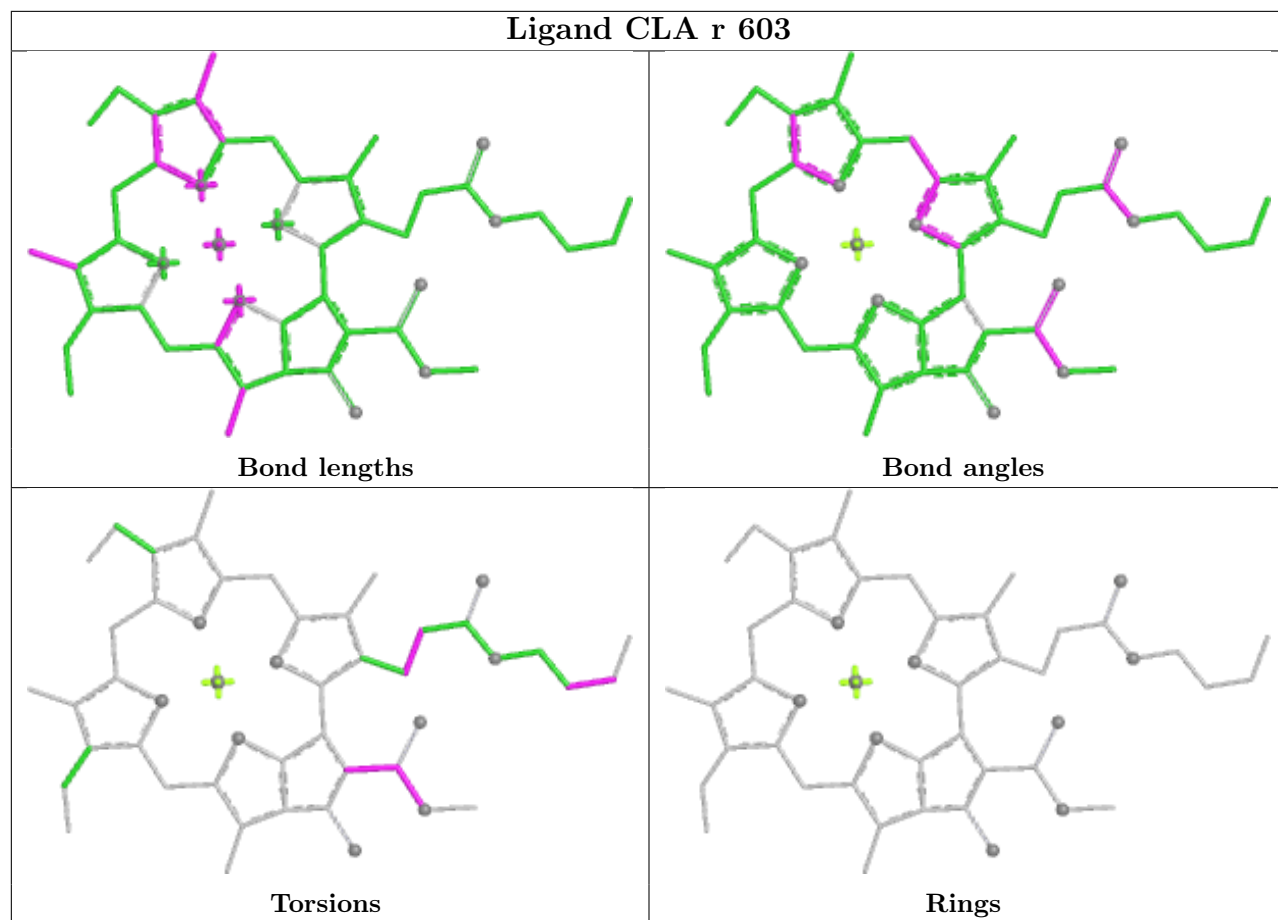


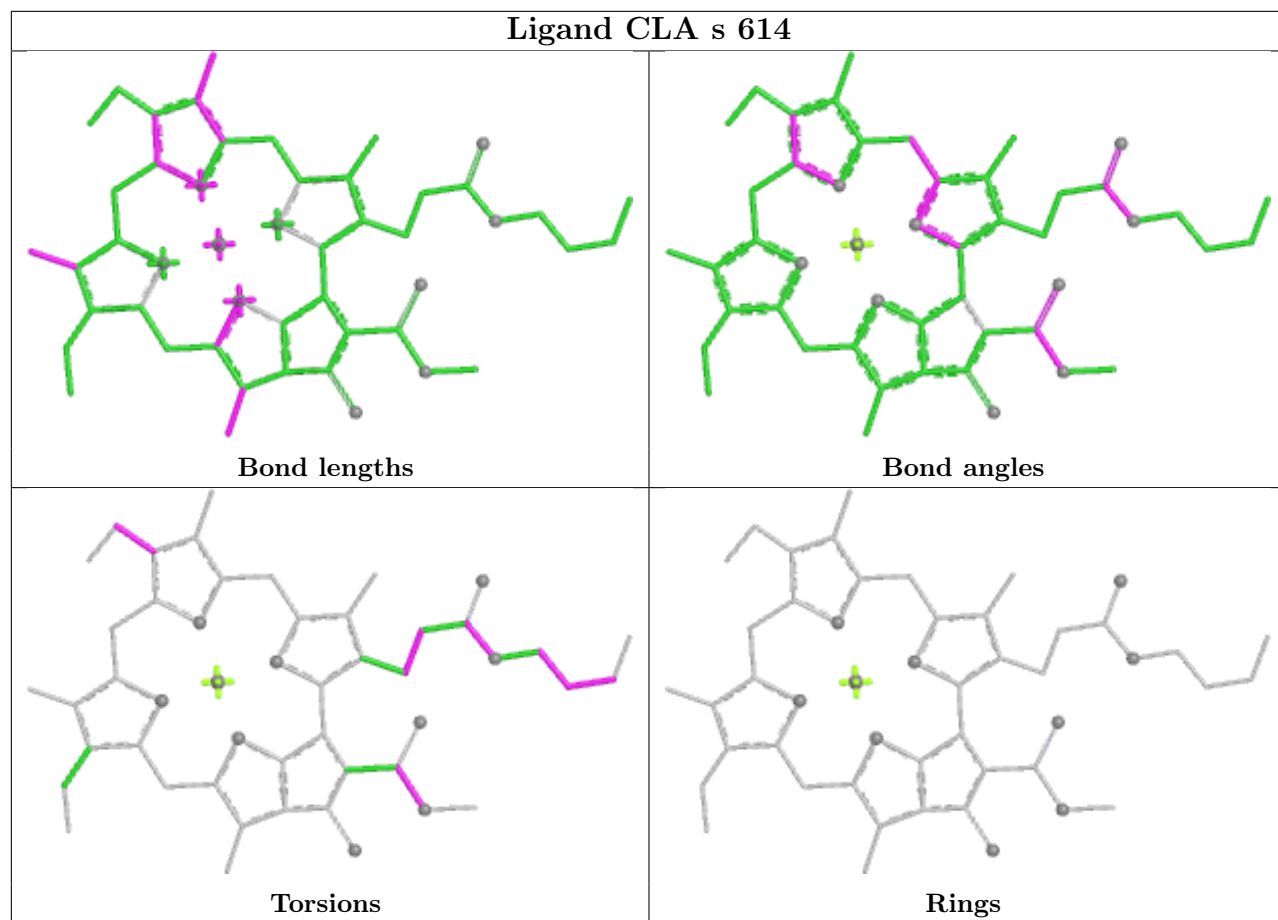
Ligand CLA B 612



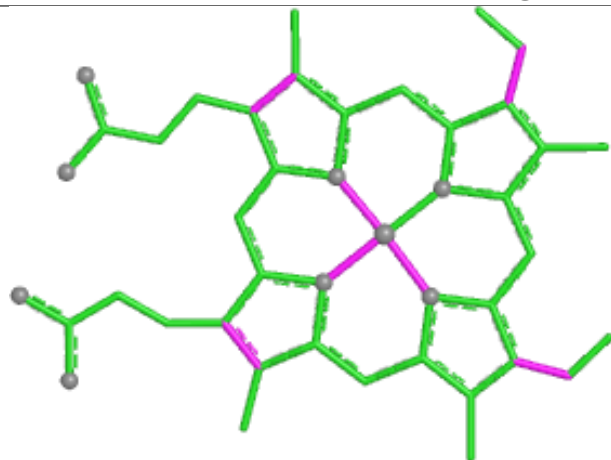




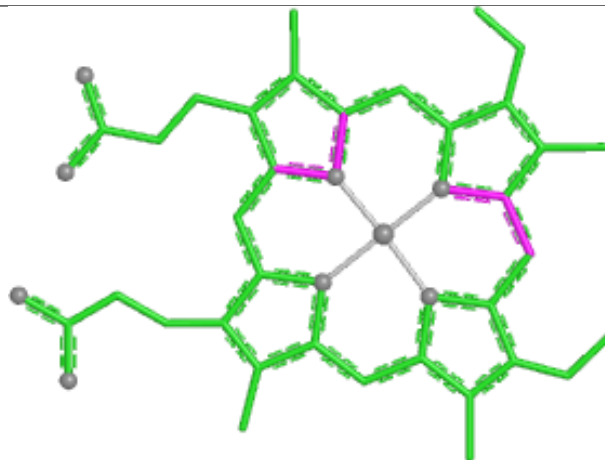




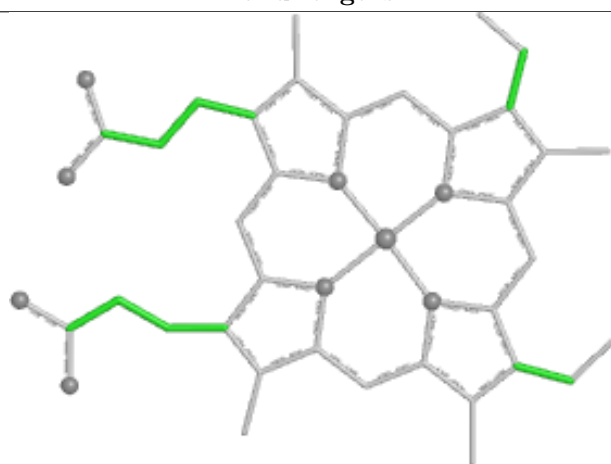
Ligand HEM f 101



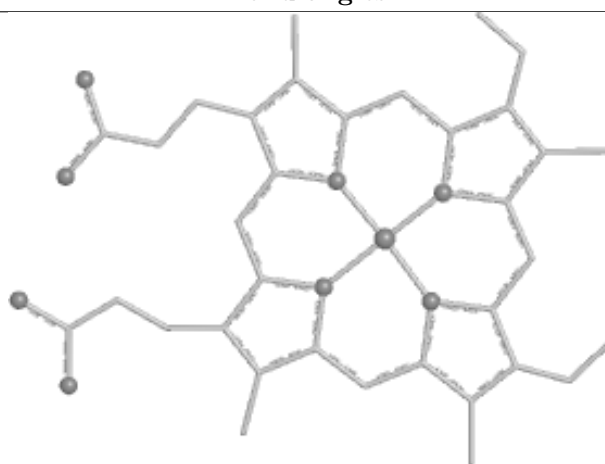
Bond lengths



Bond angles

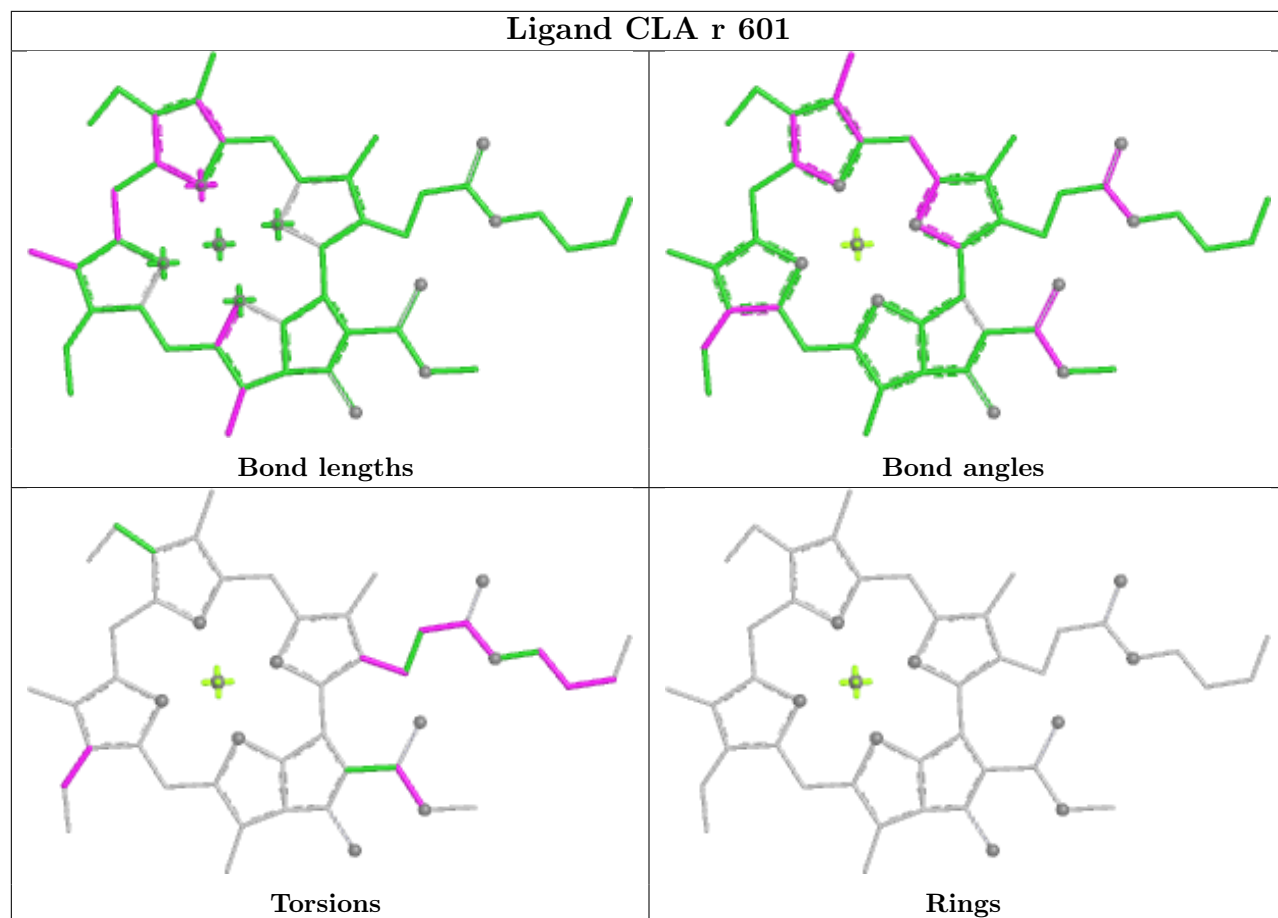


Torsions

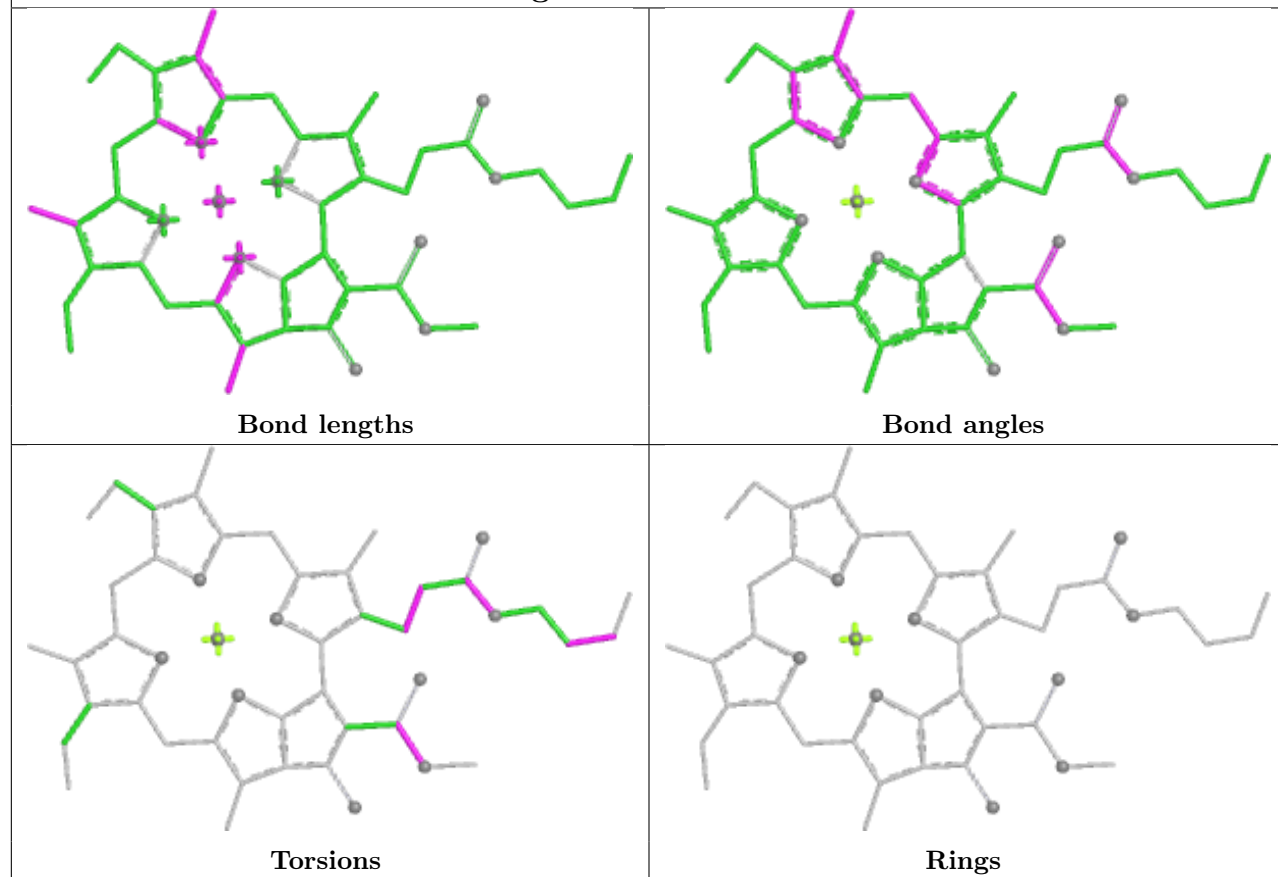


Rings

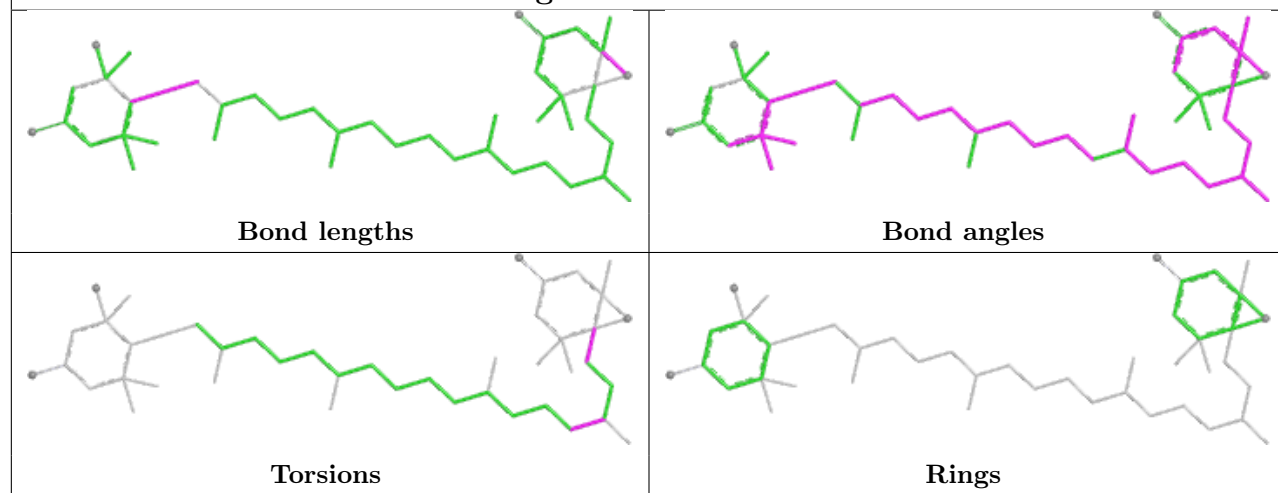
Ligand CLA r 601

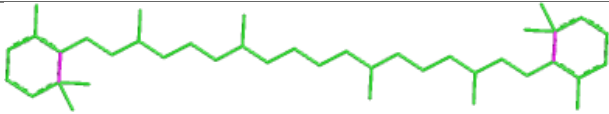
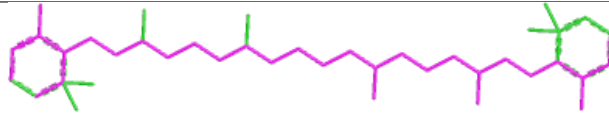
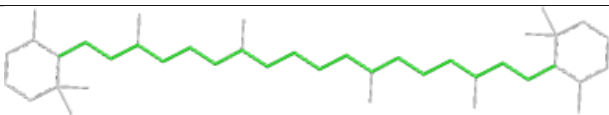
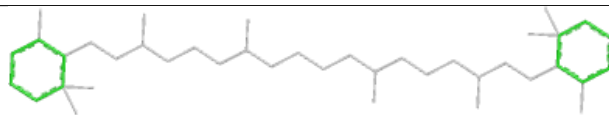


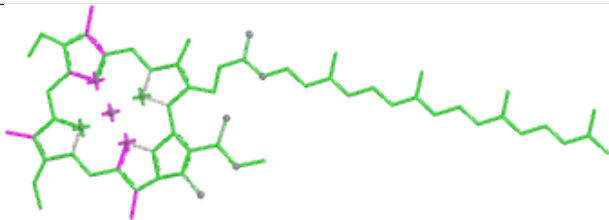
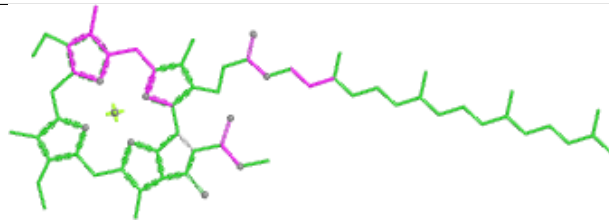
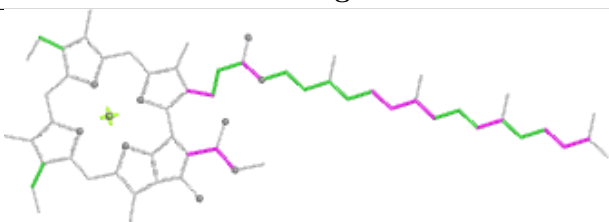
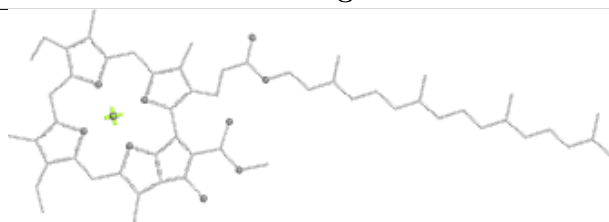
Ligand CLA Y 604

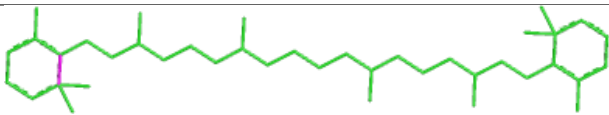
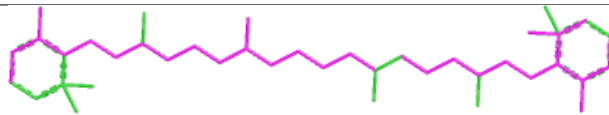
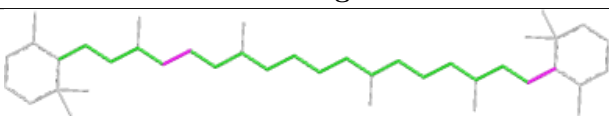
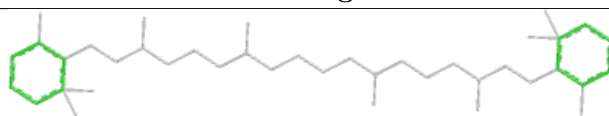


Ligand NEX r 623

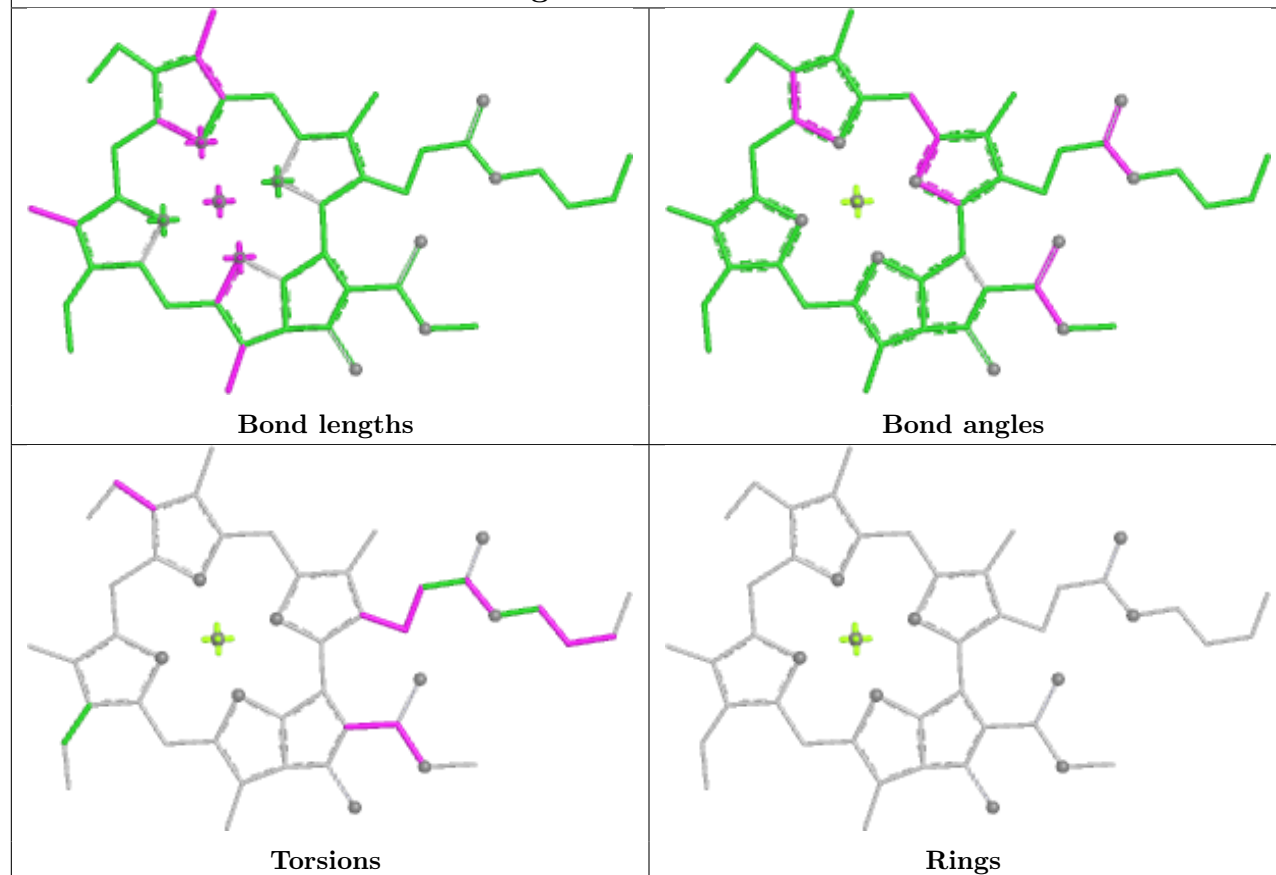


Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

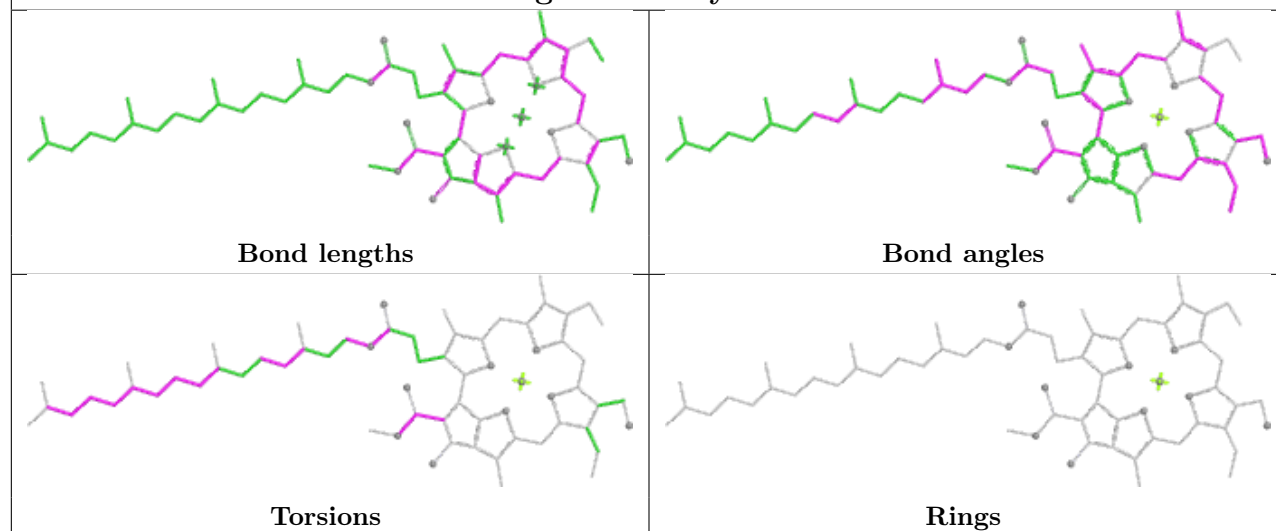
Ligand CLA Y 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

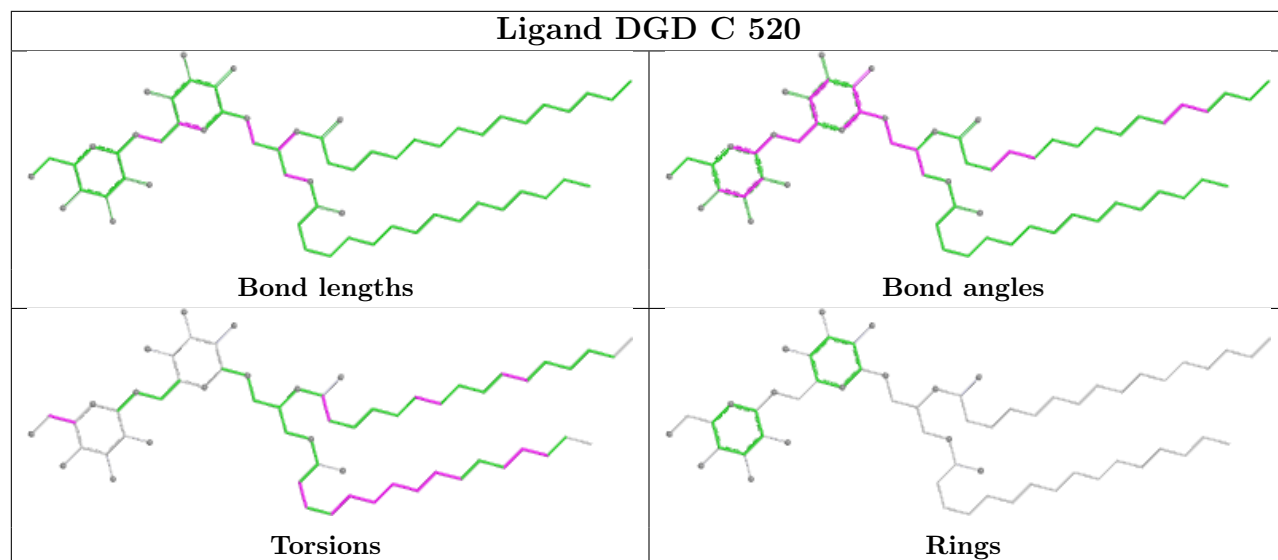
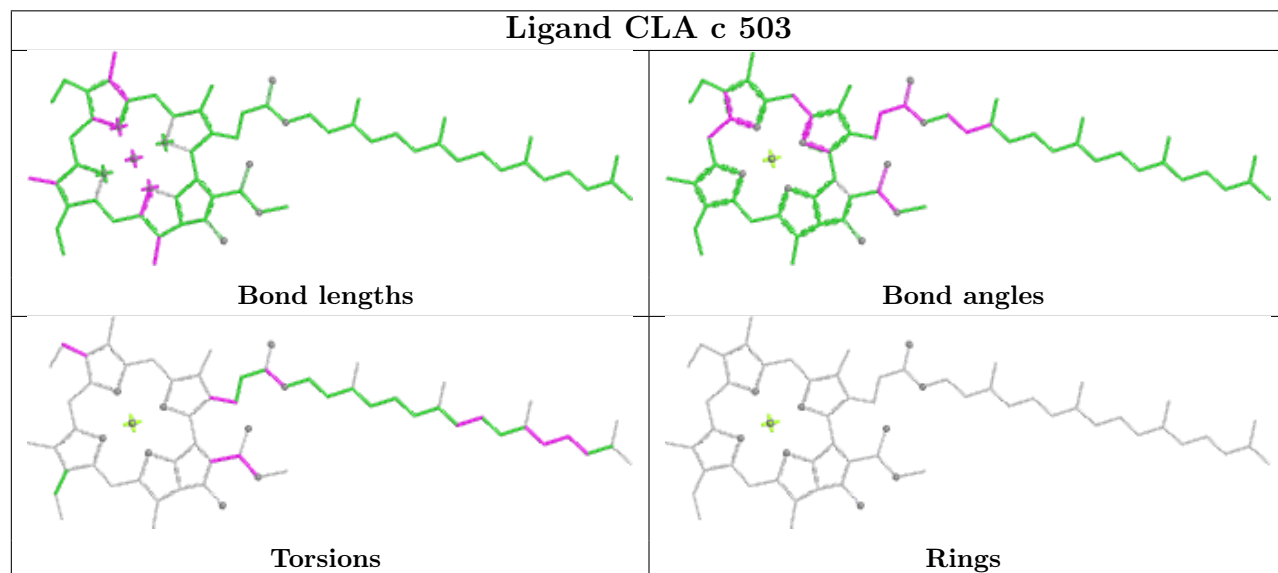
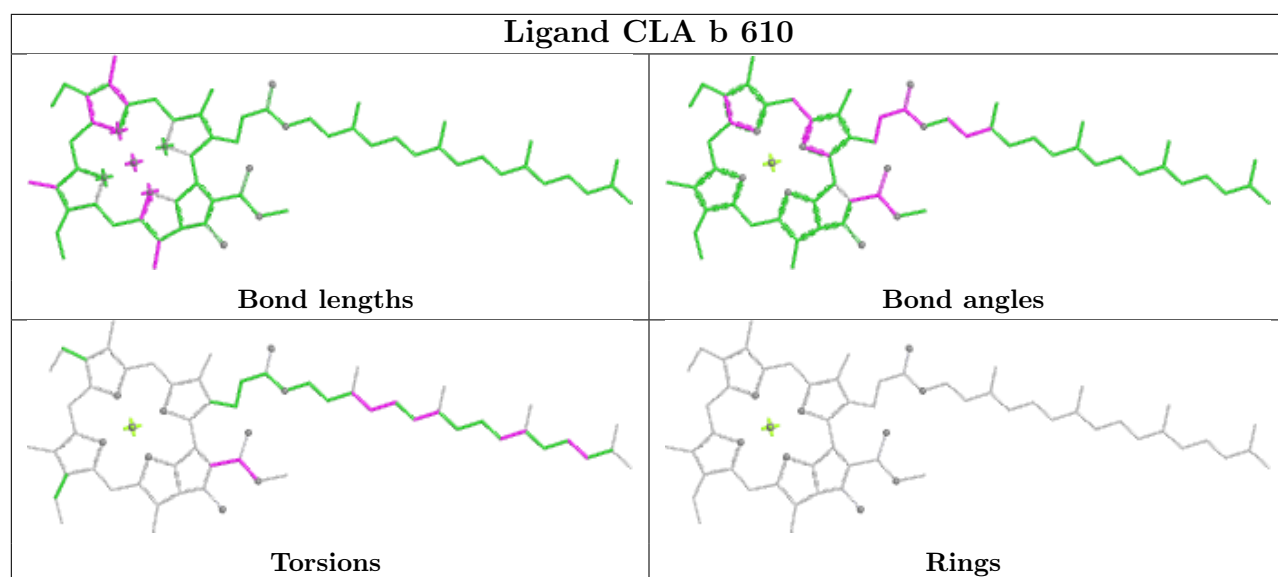
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 604

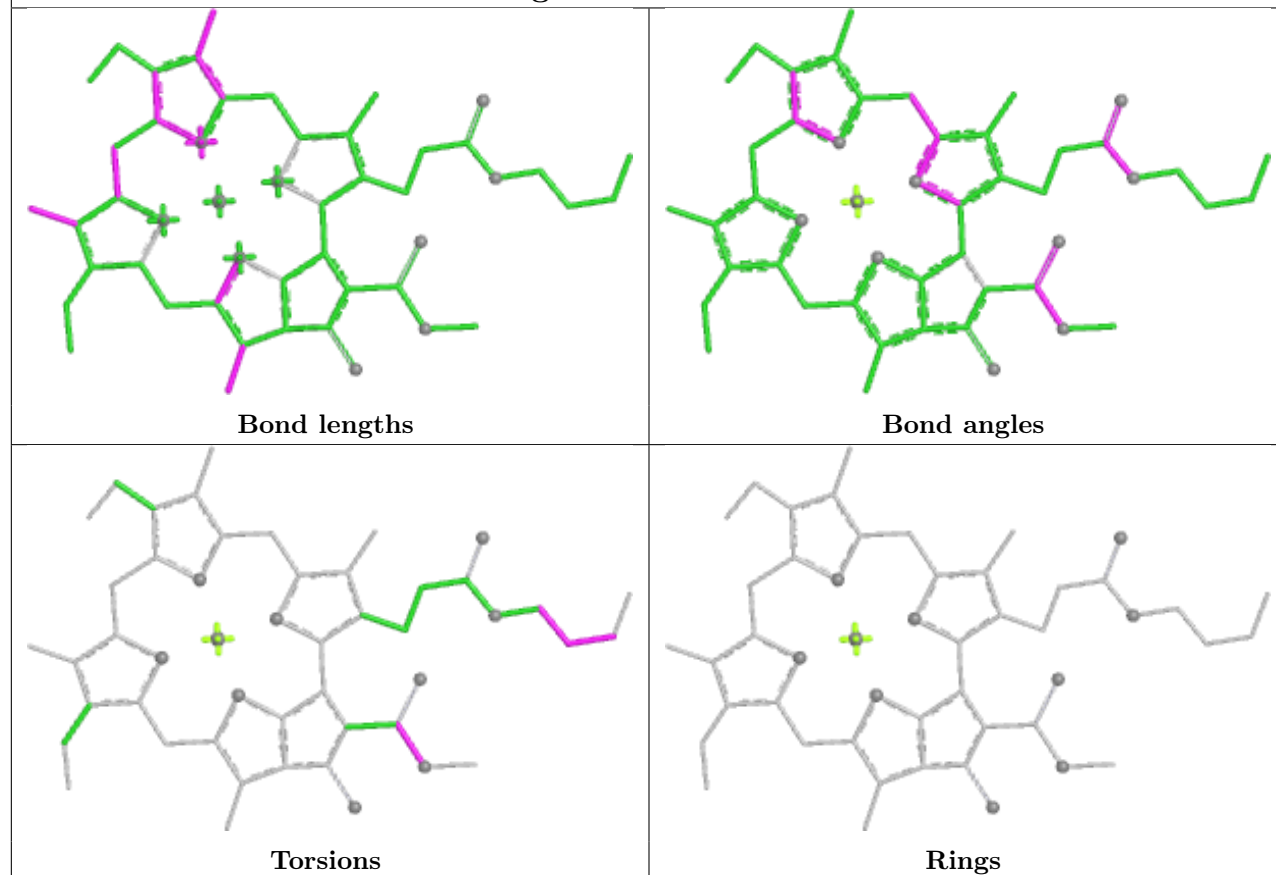


Ligand CHL y 609

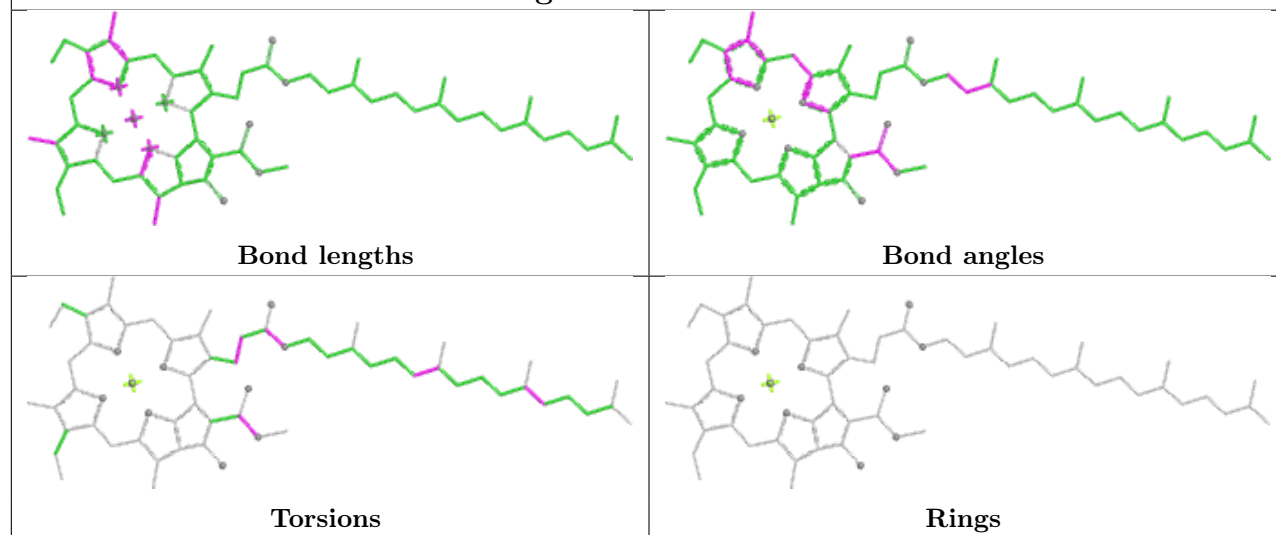


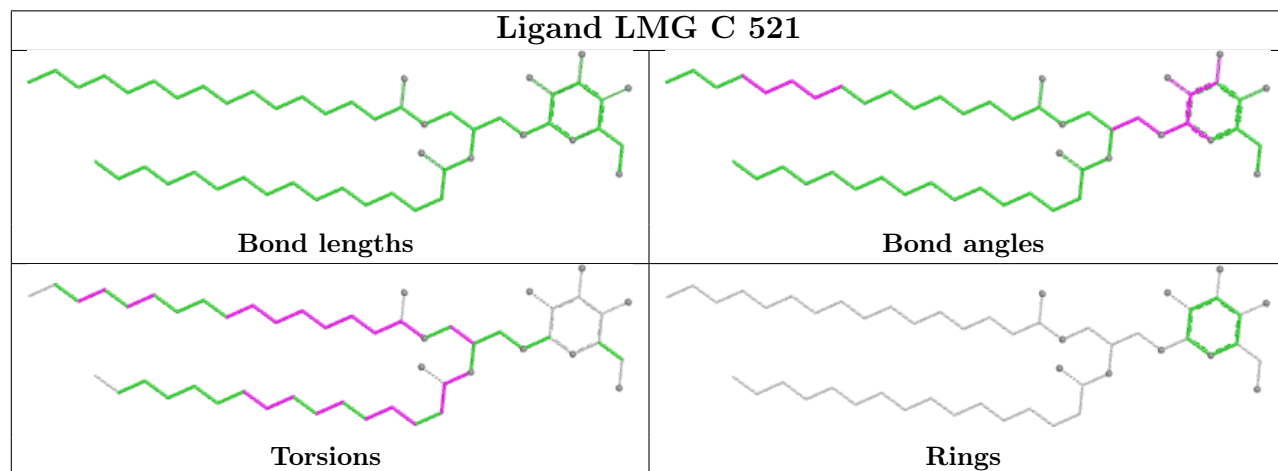
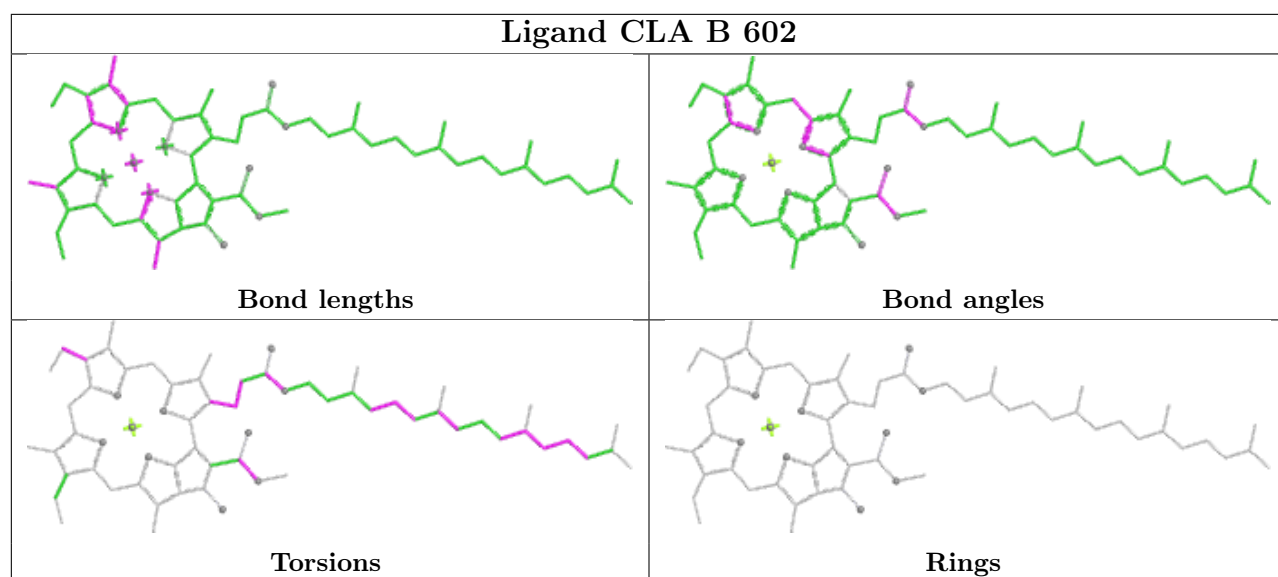


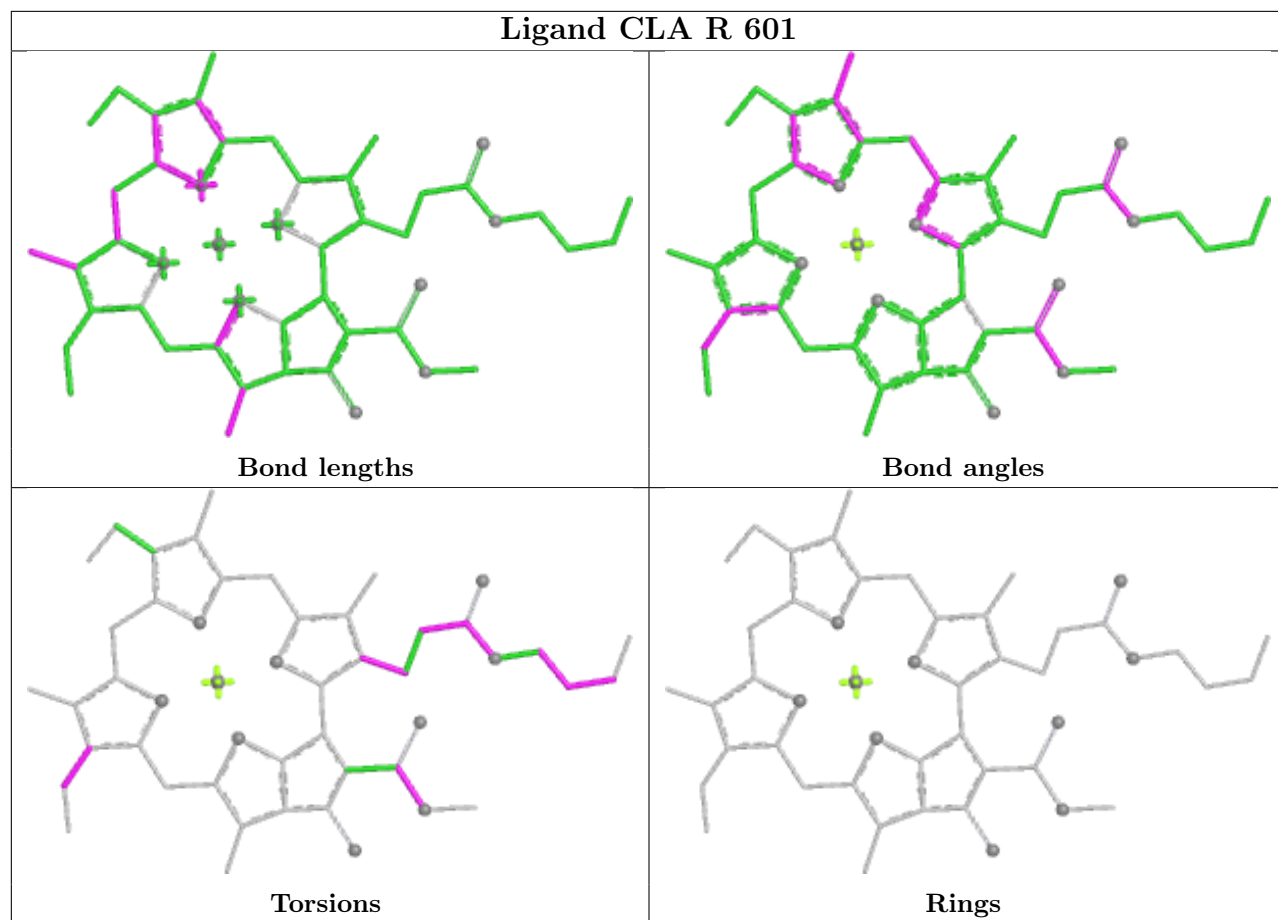
Ligand CLA R 612



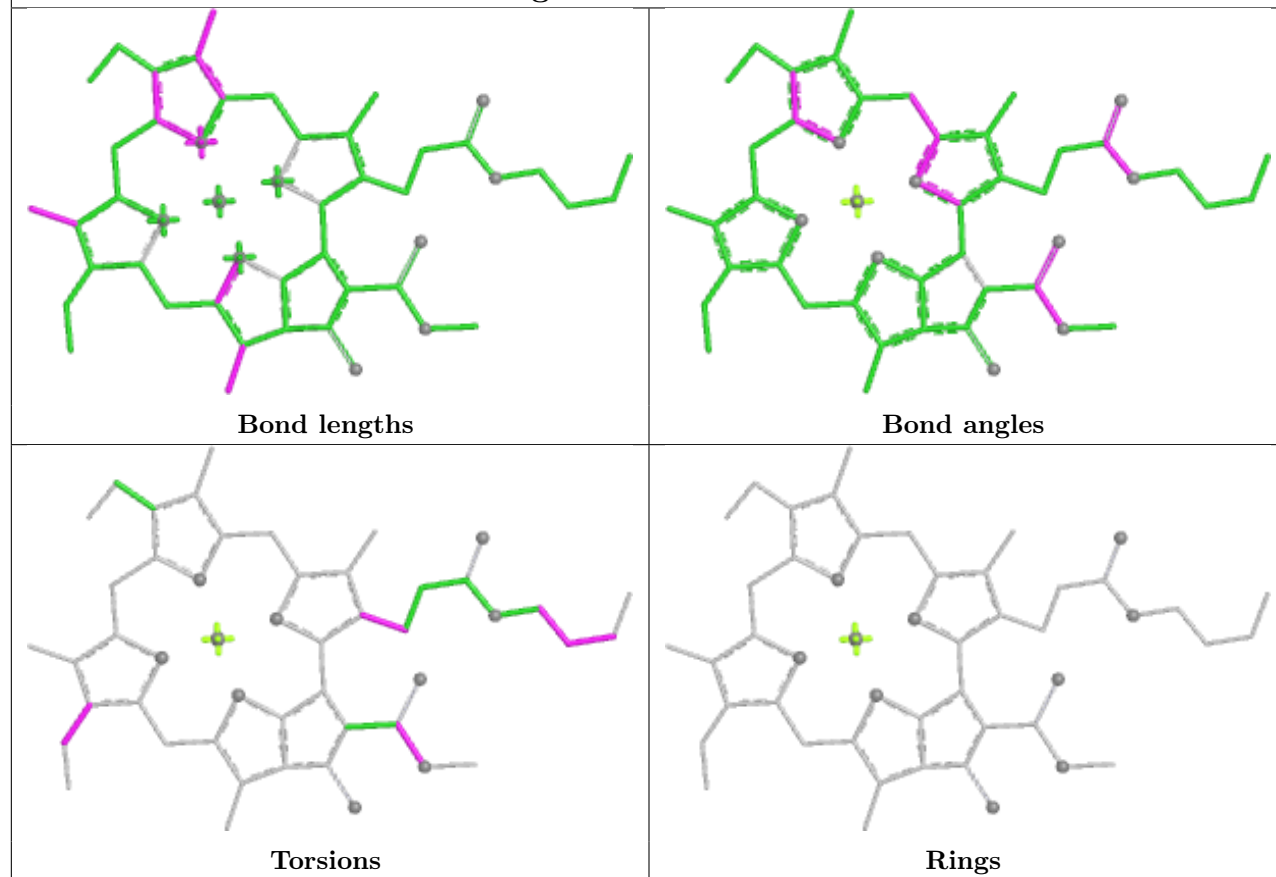
Ligand CLA b 608



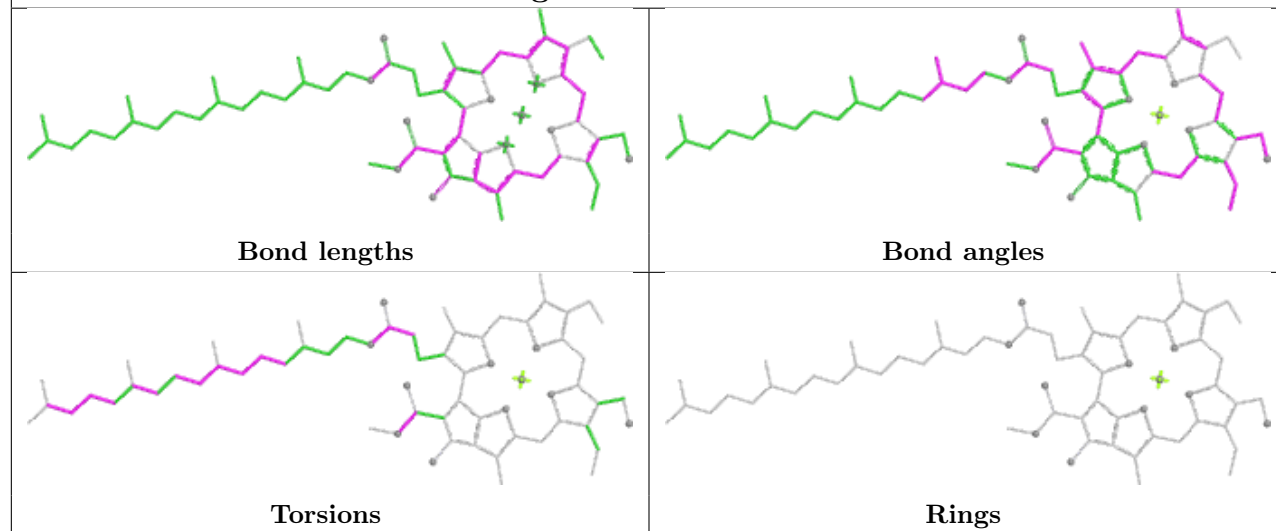


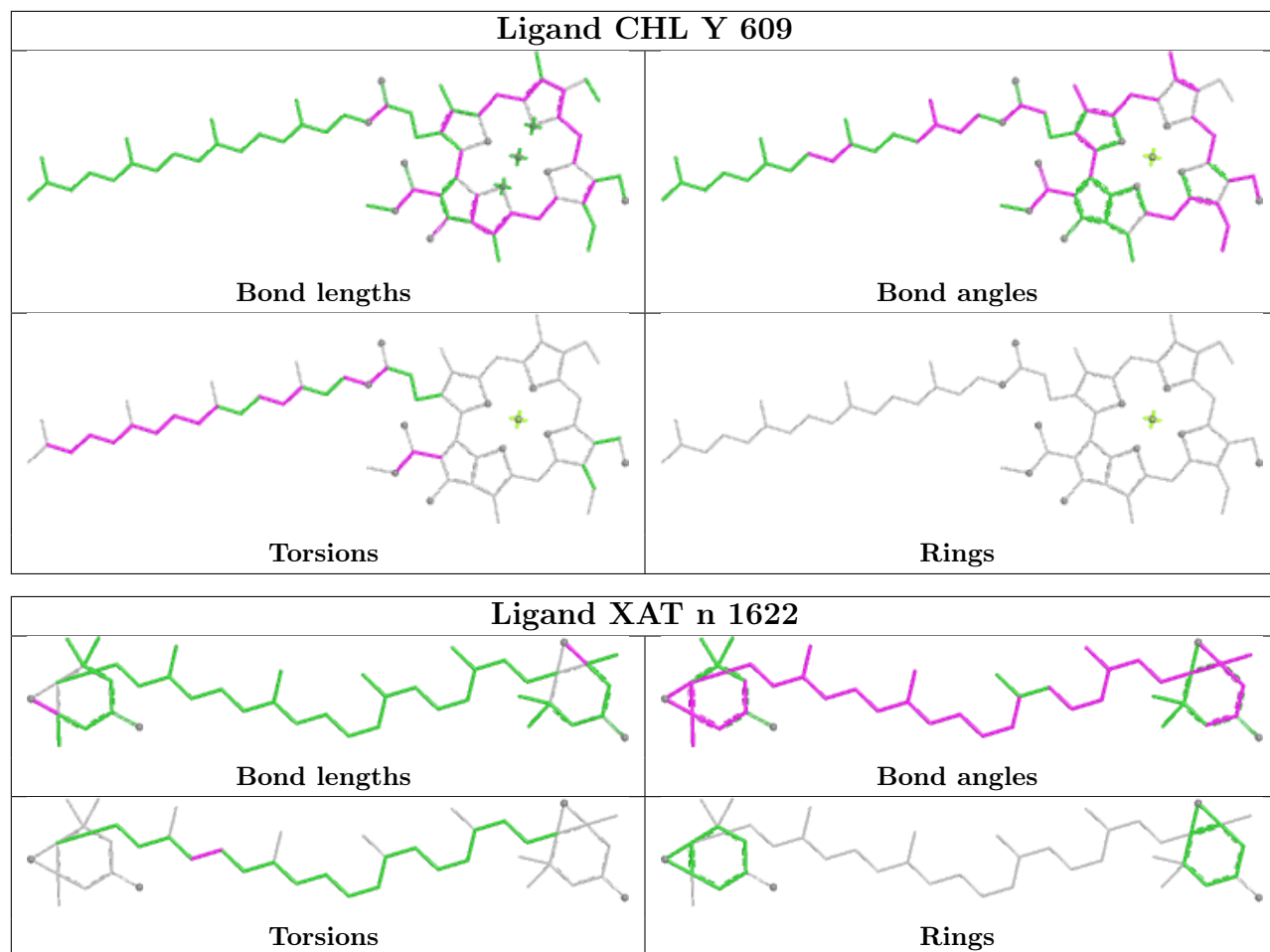


Ligand CLA R 609

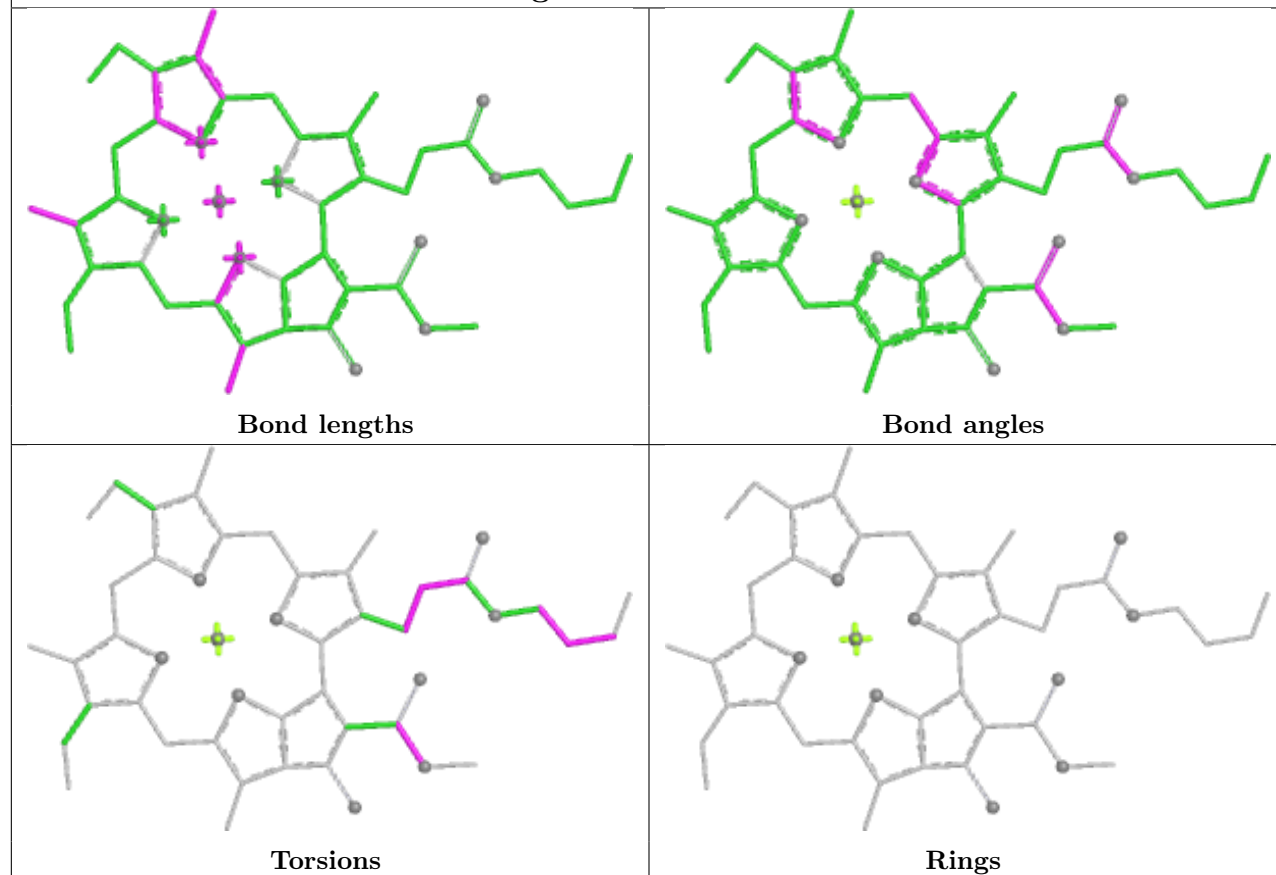


Ligand CHL Y 601

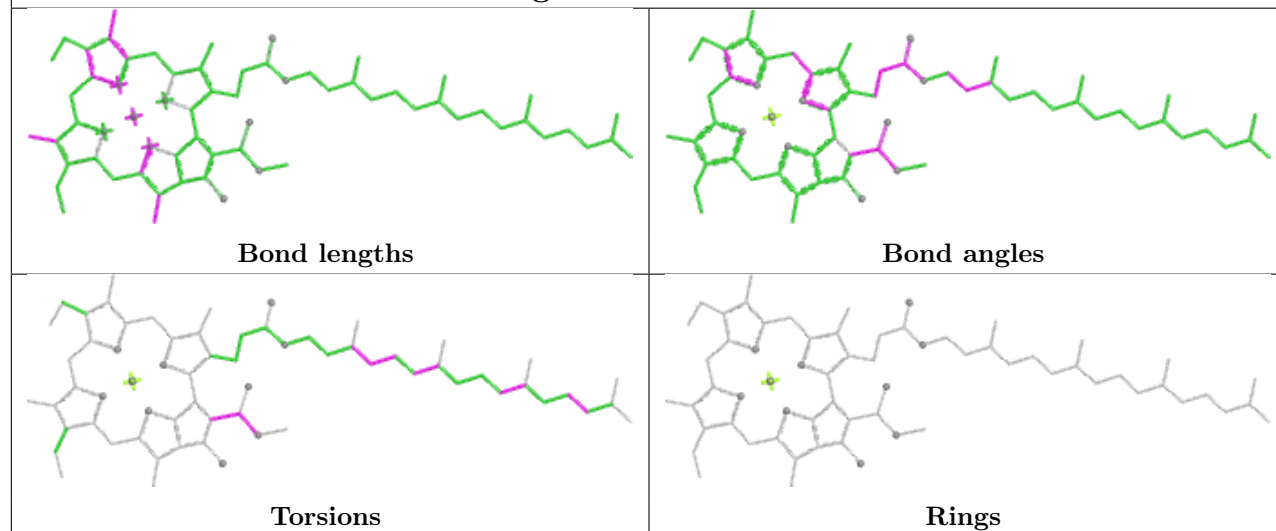


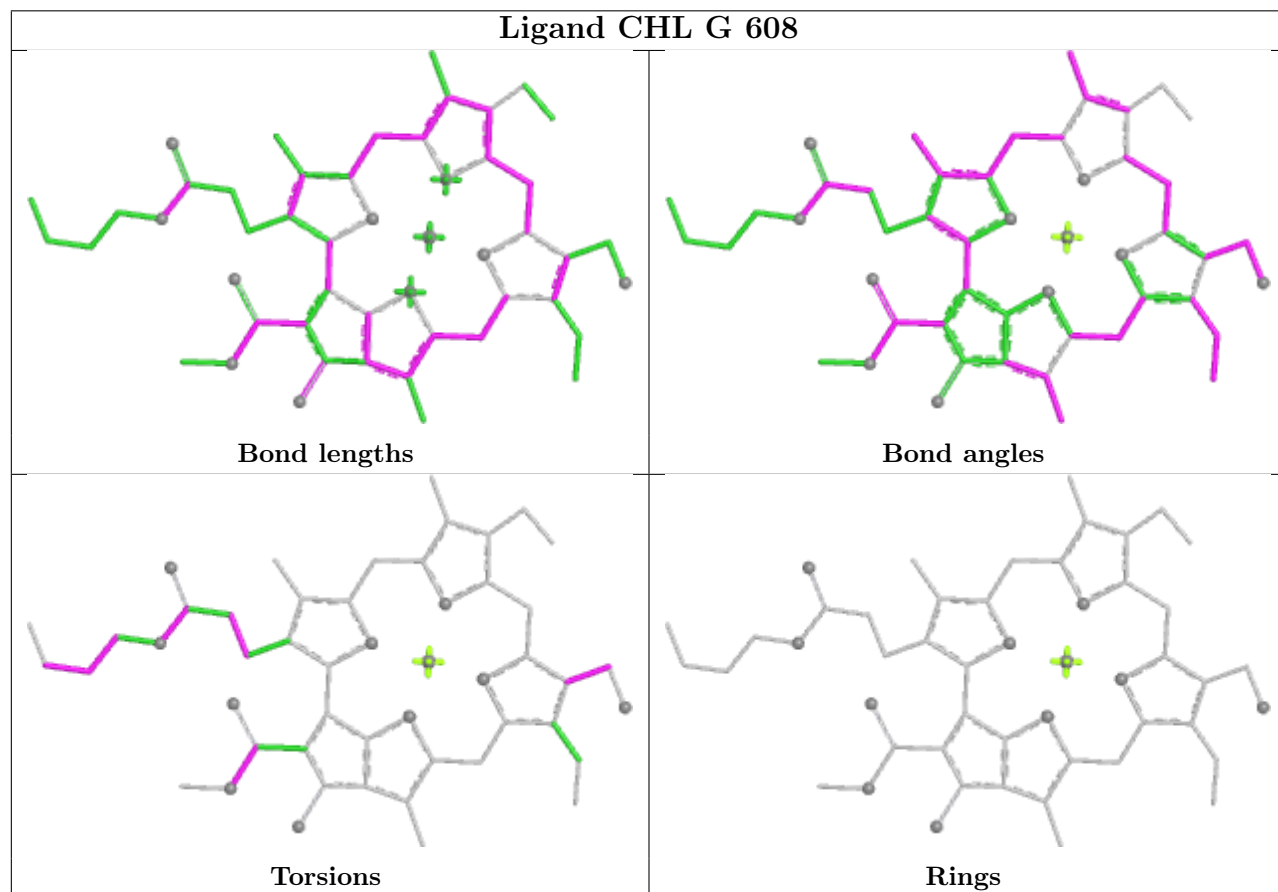
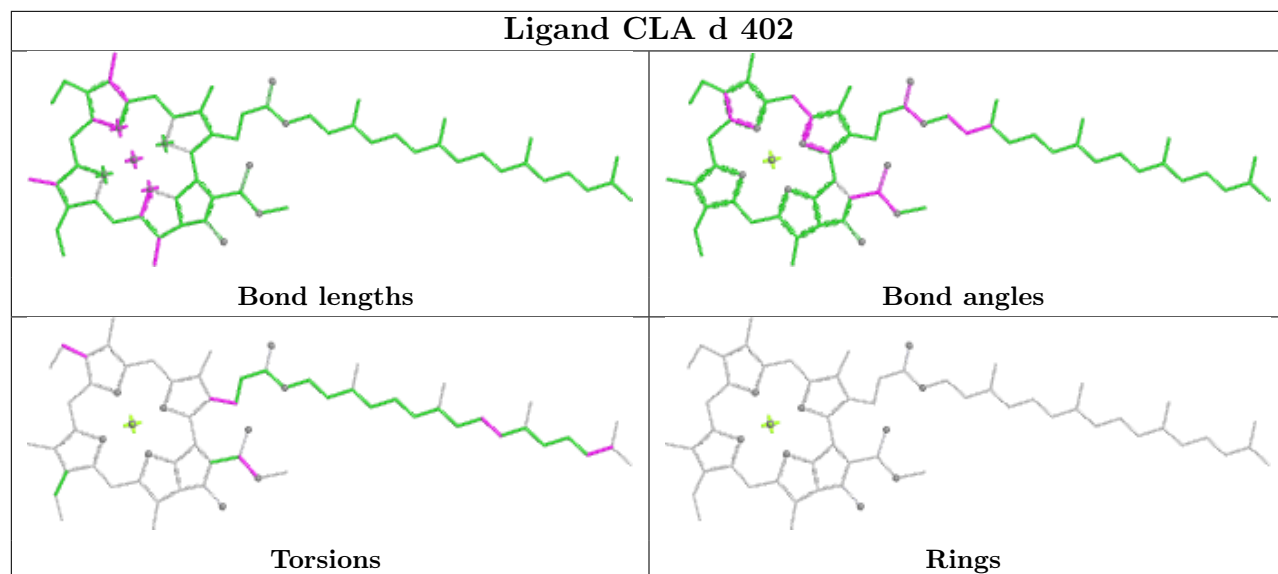


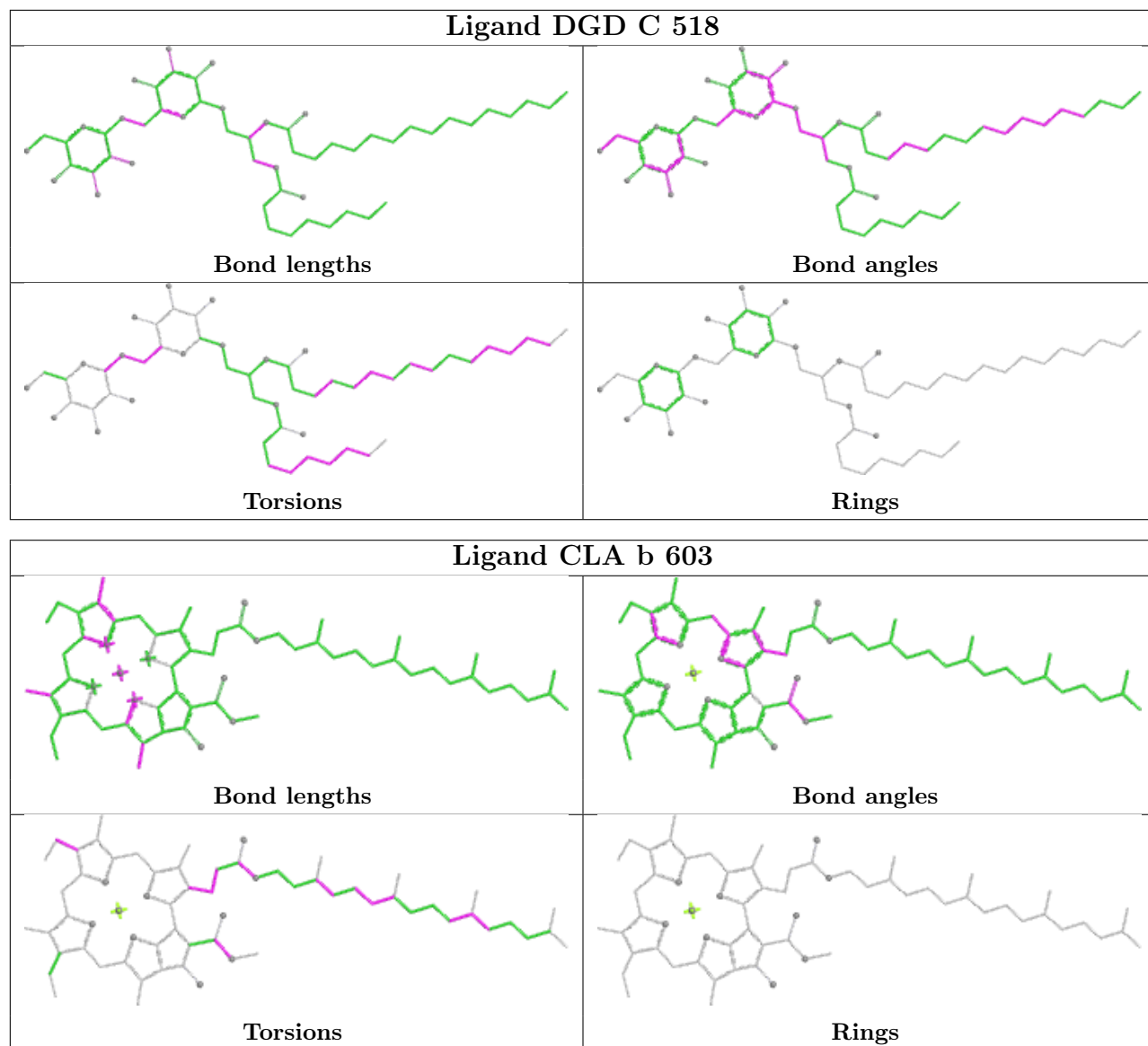
Ligand CLA R 613



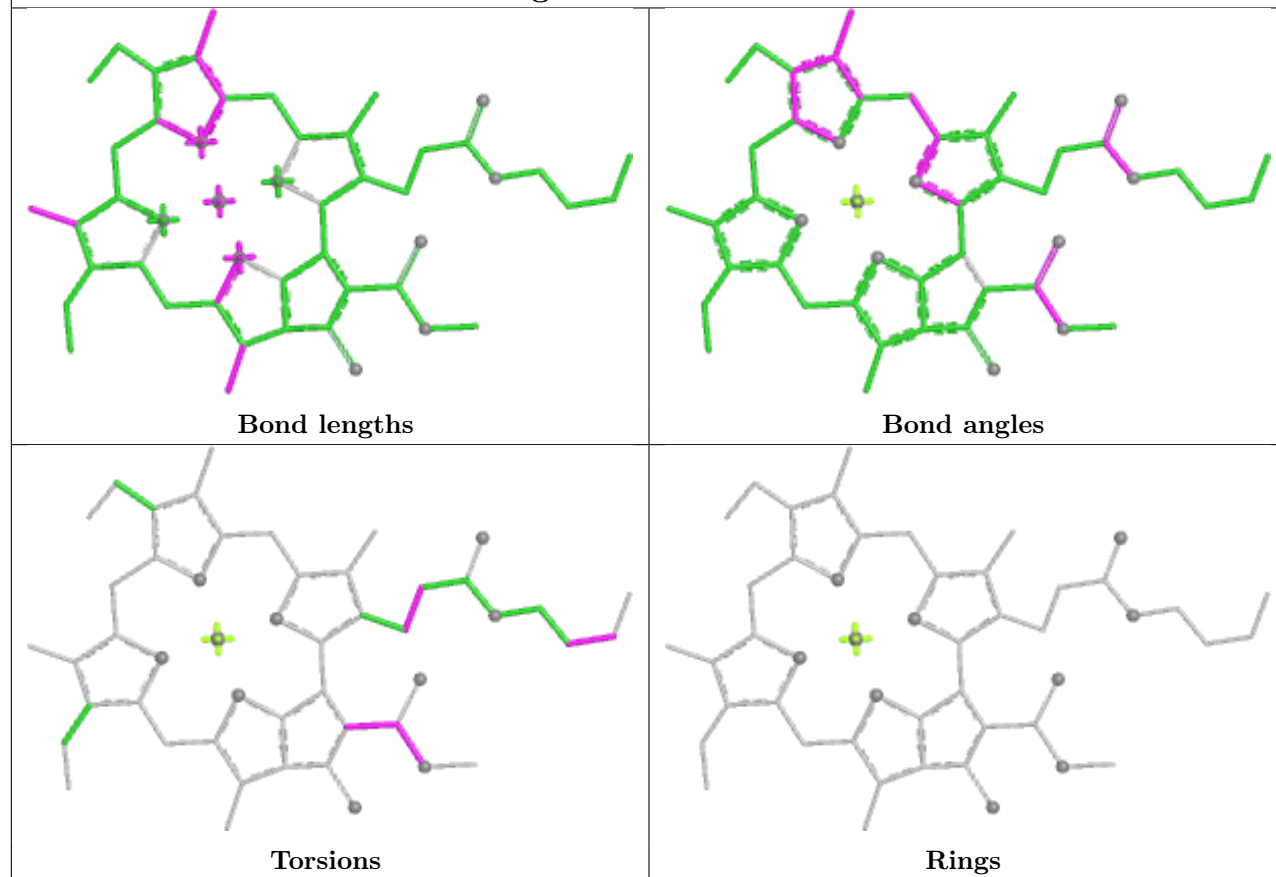
Ligand CLA B 610



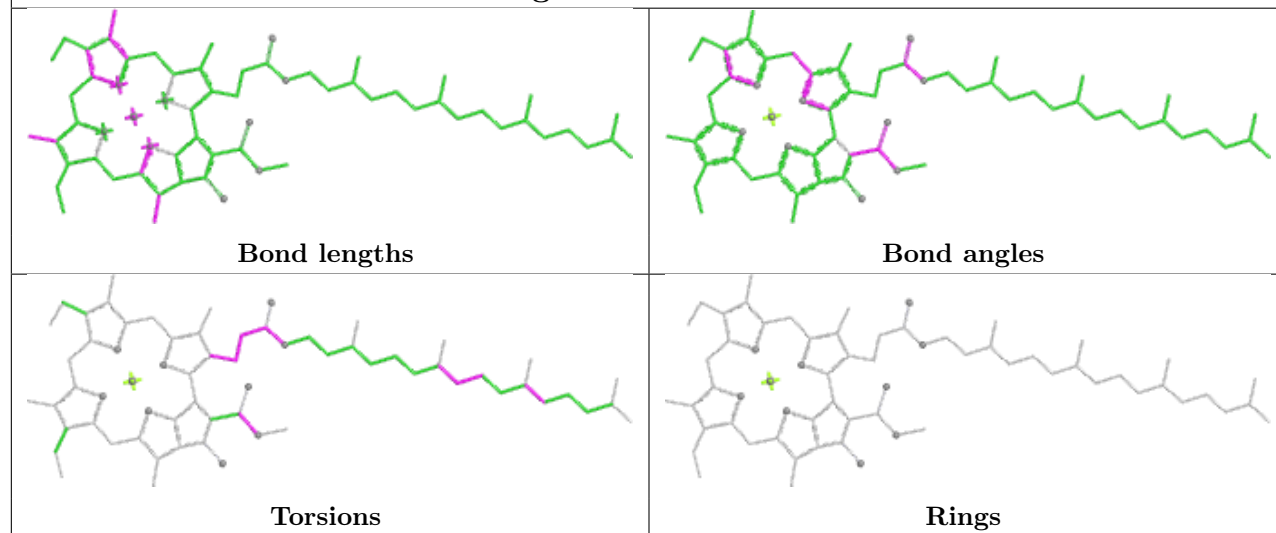


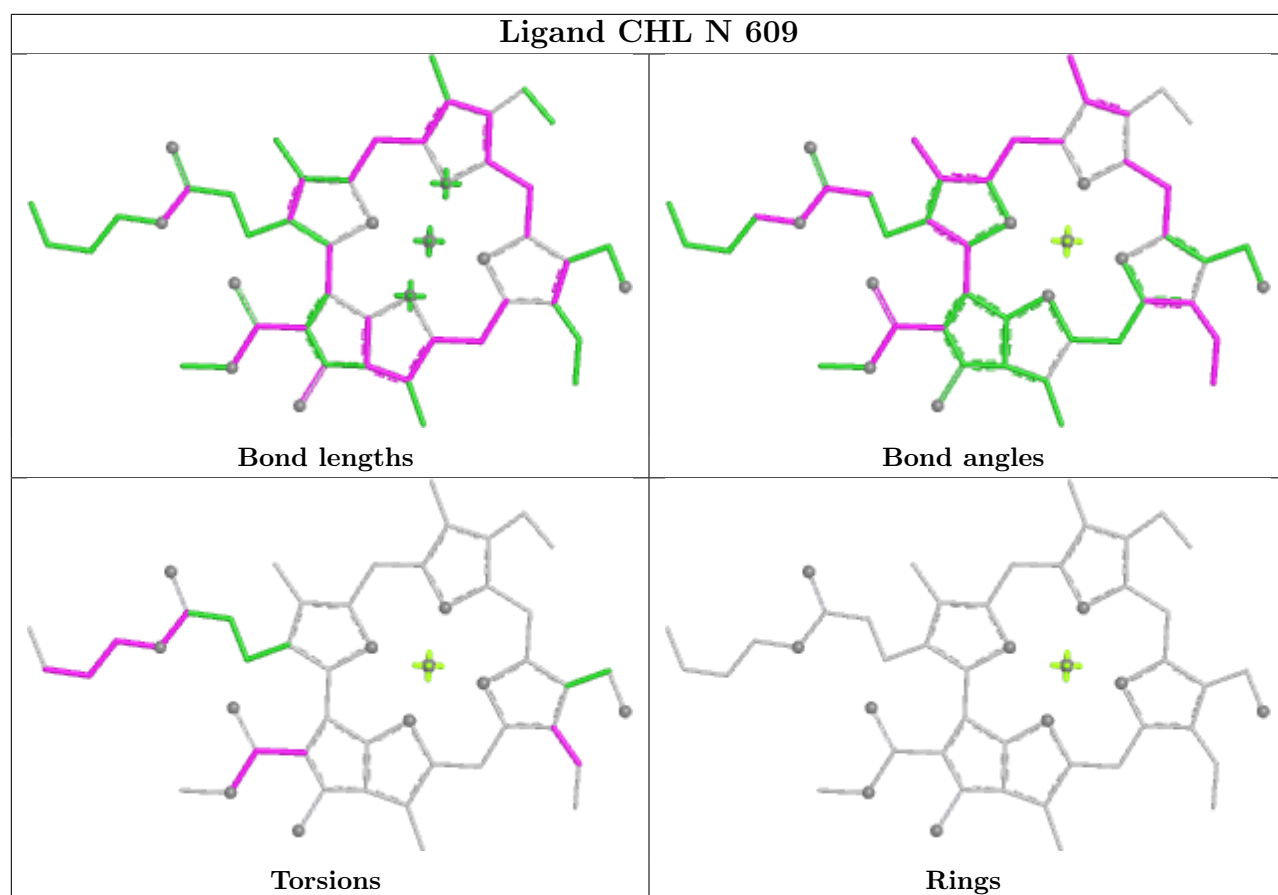


Ligand CLA A 407

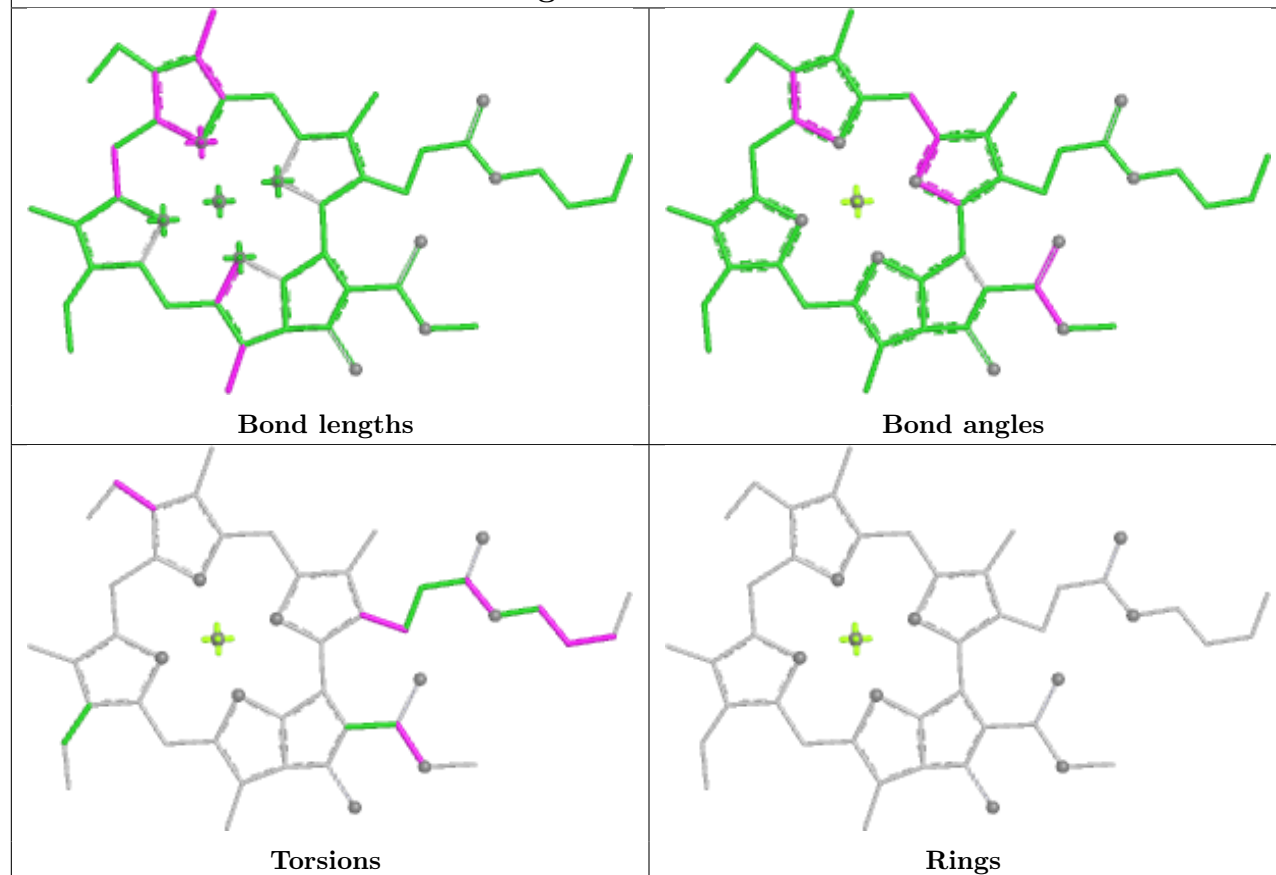


Ligand CLA C 501

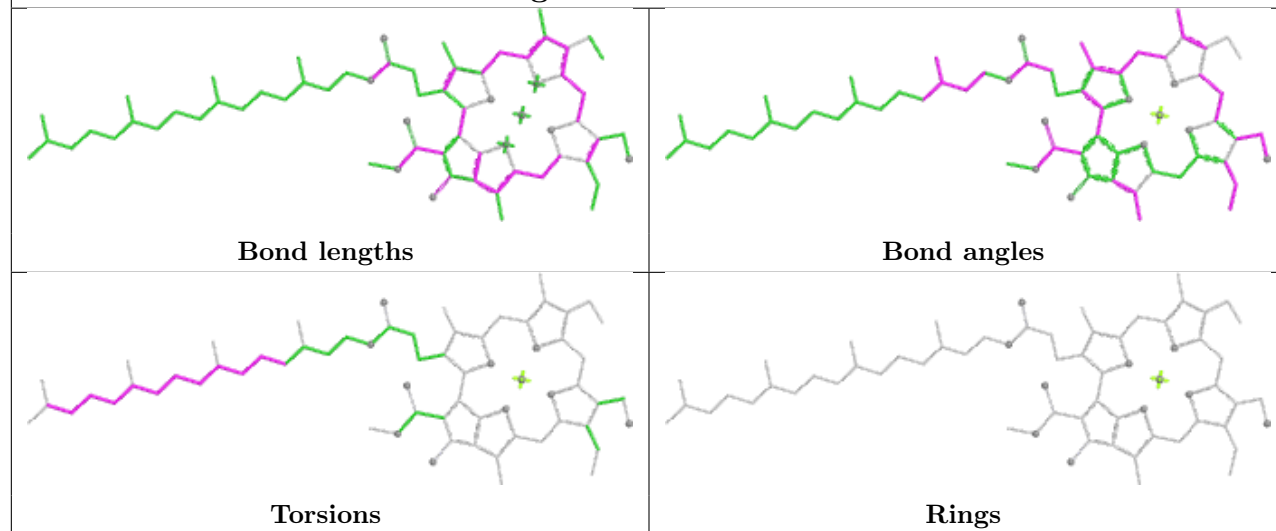


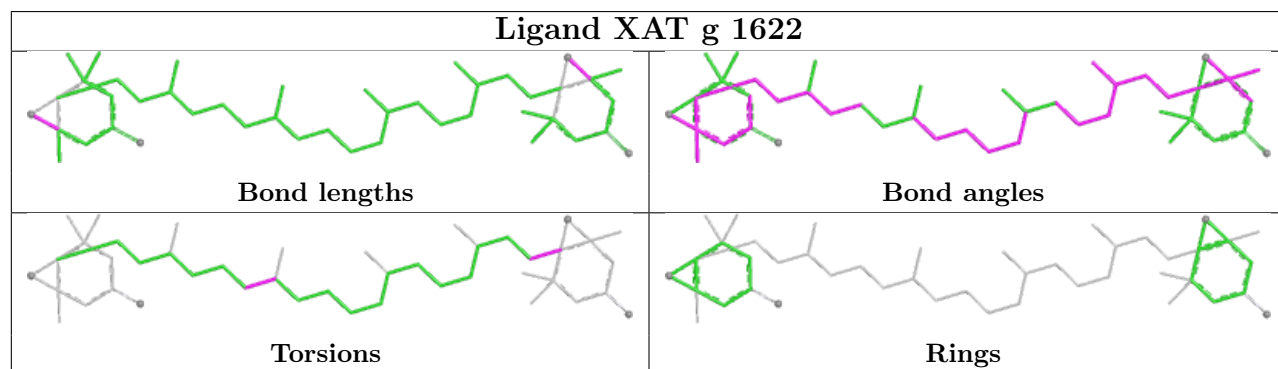
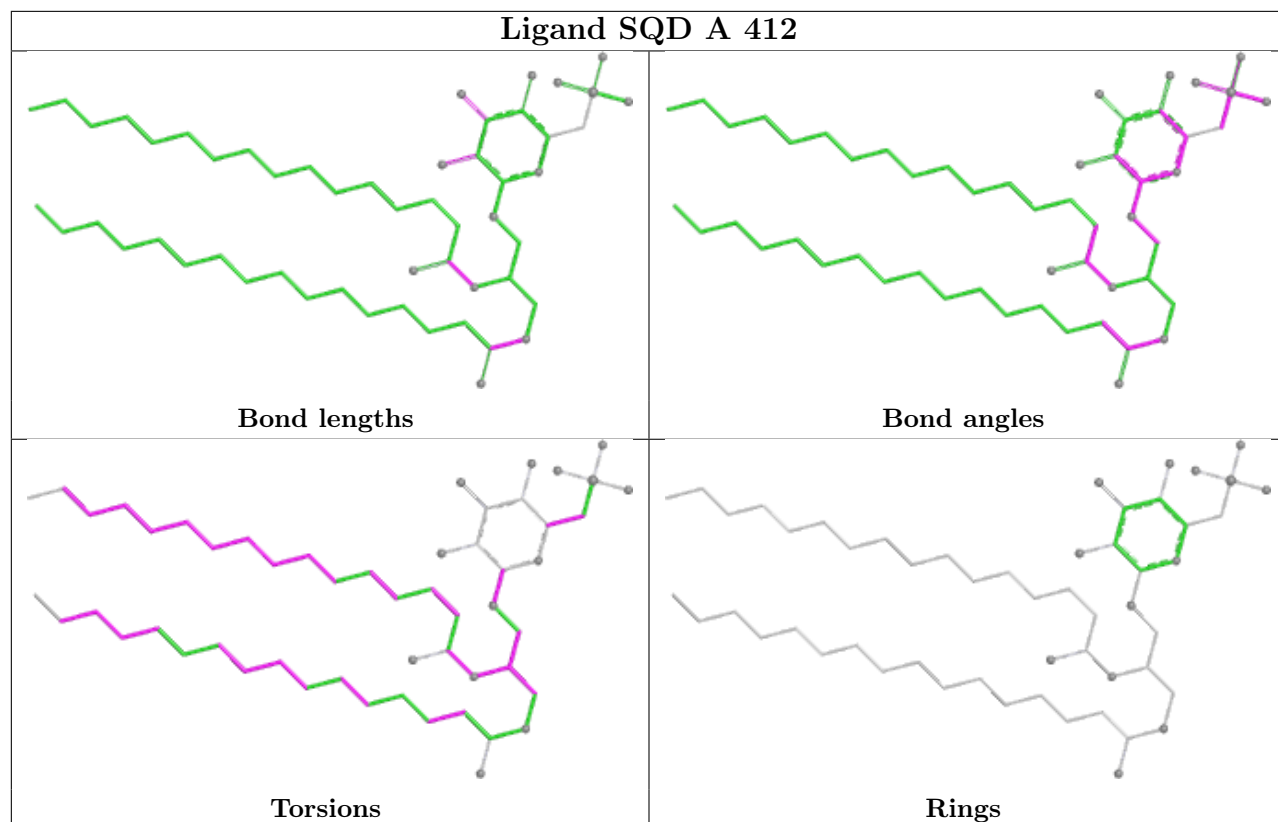


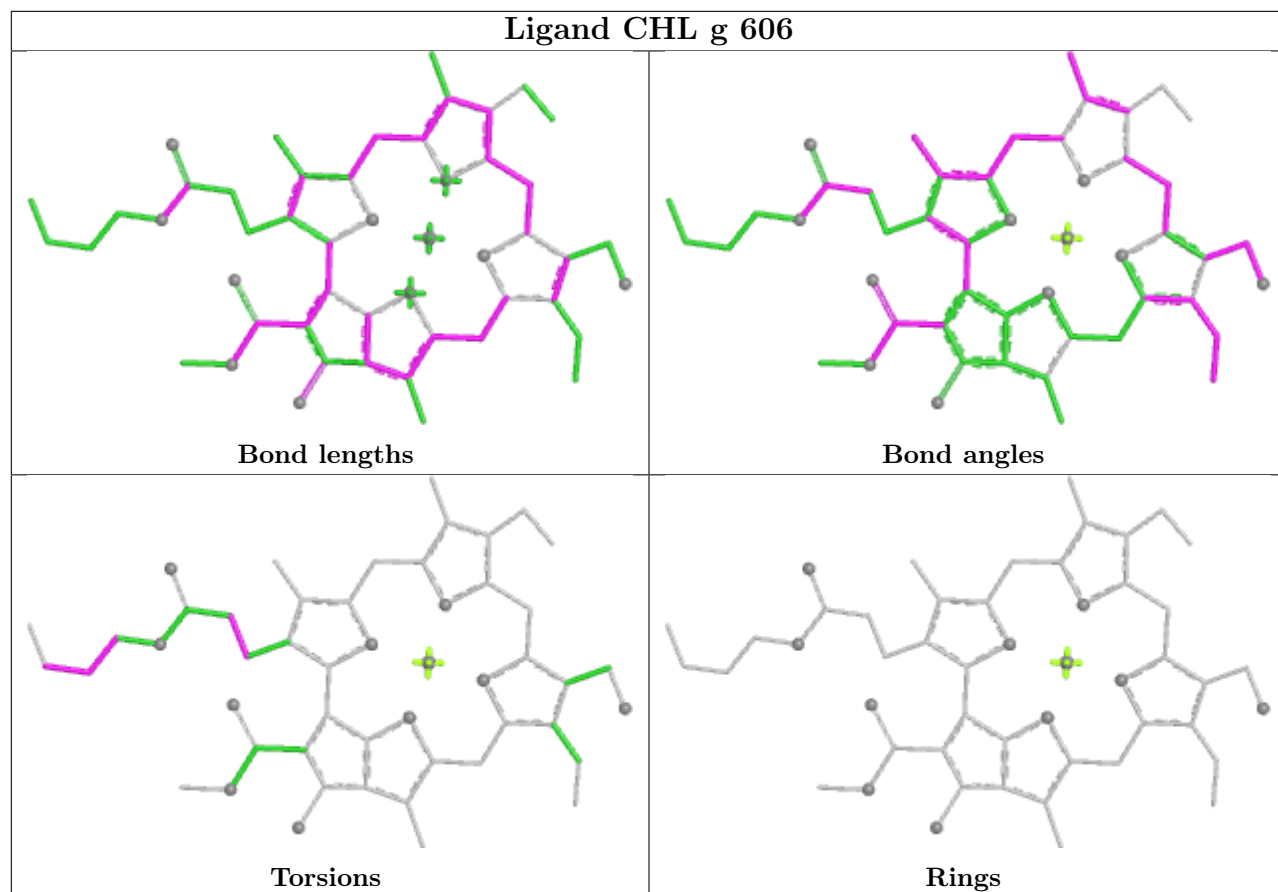
Ligand CLA s 609

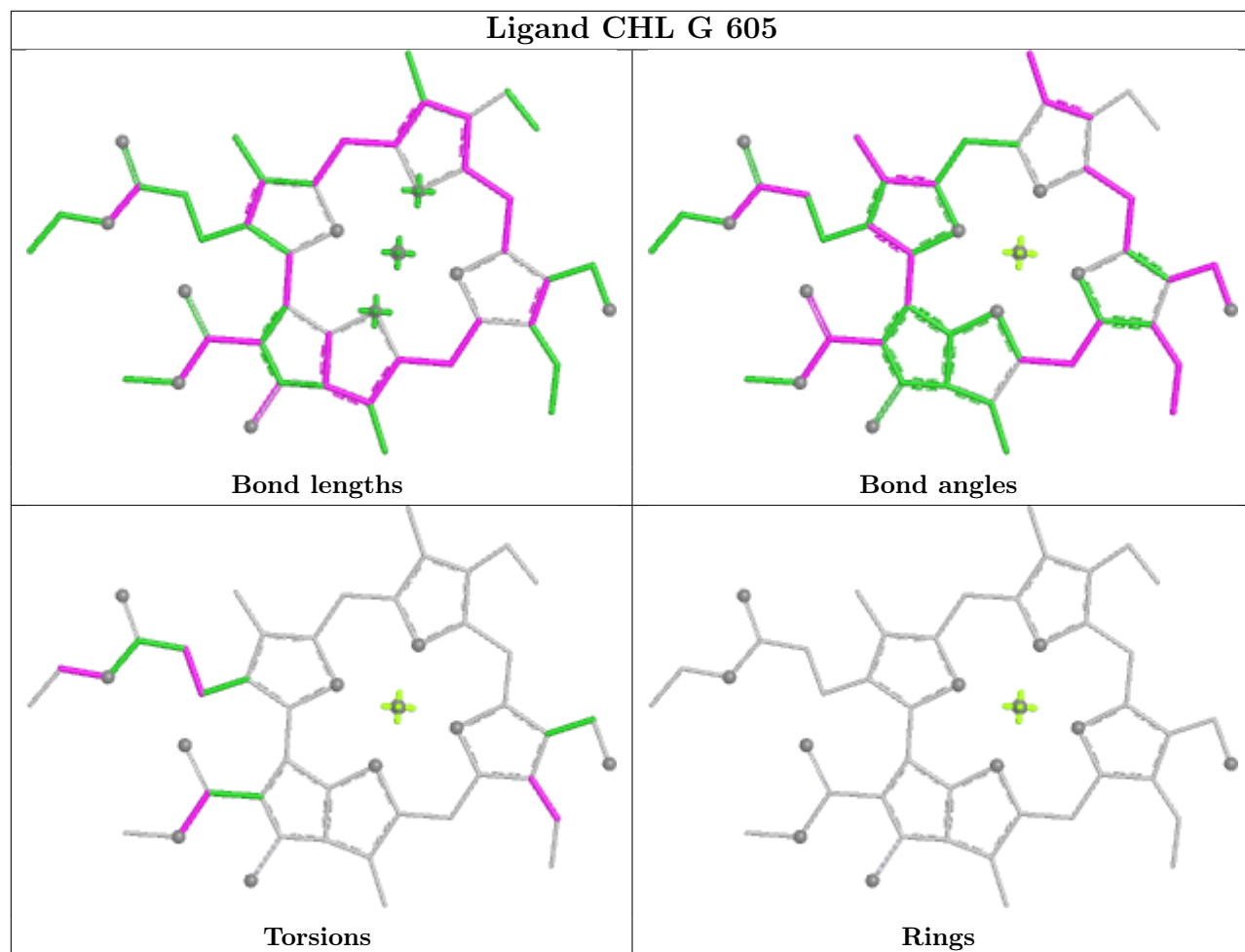


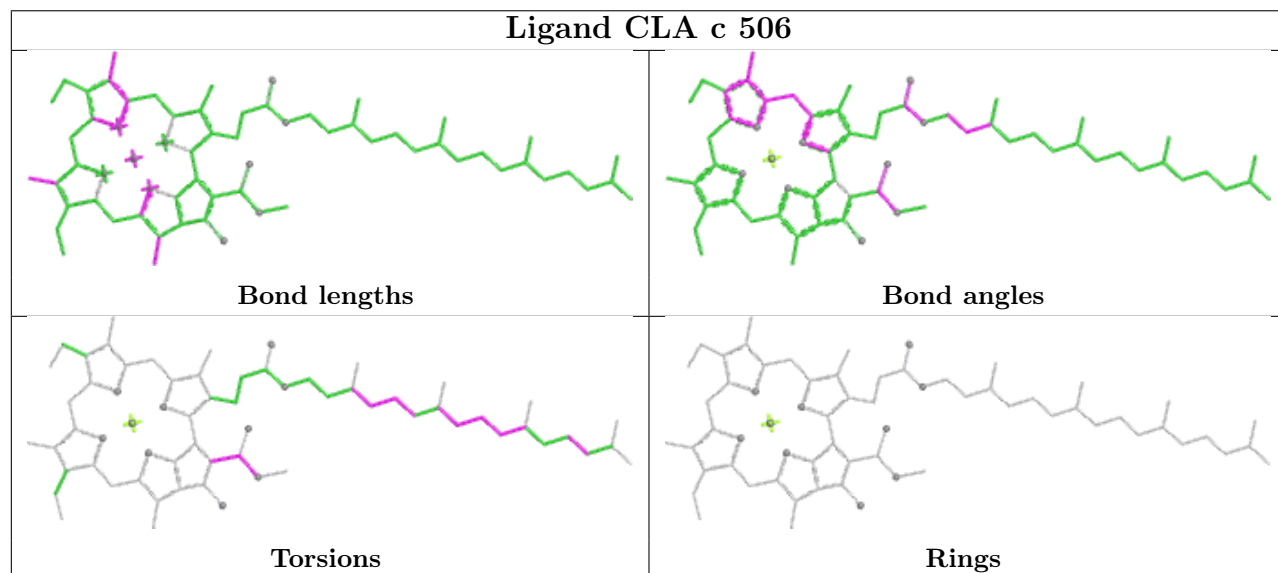
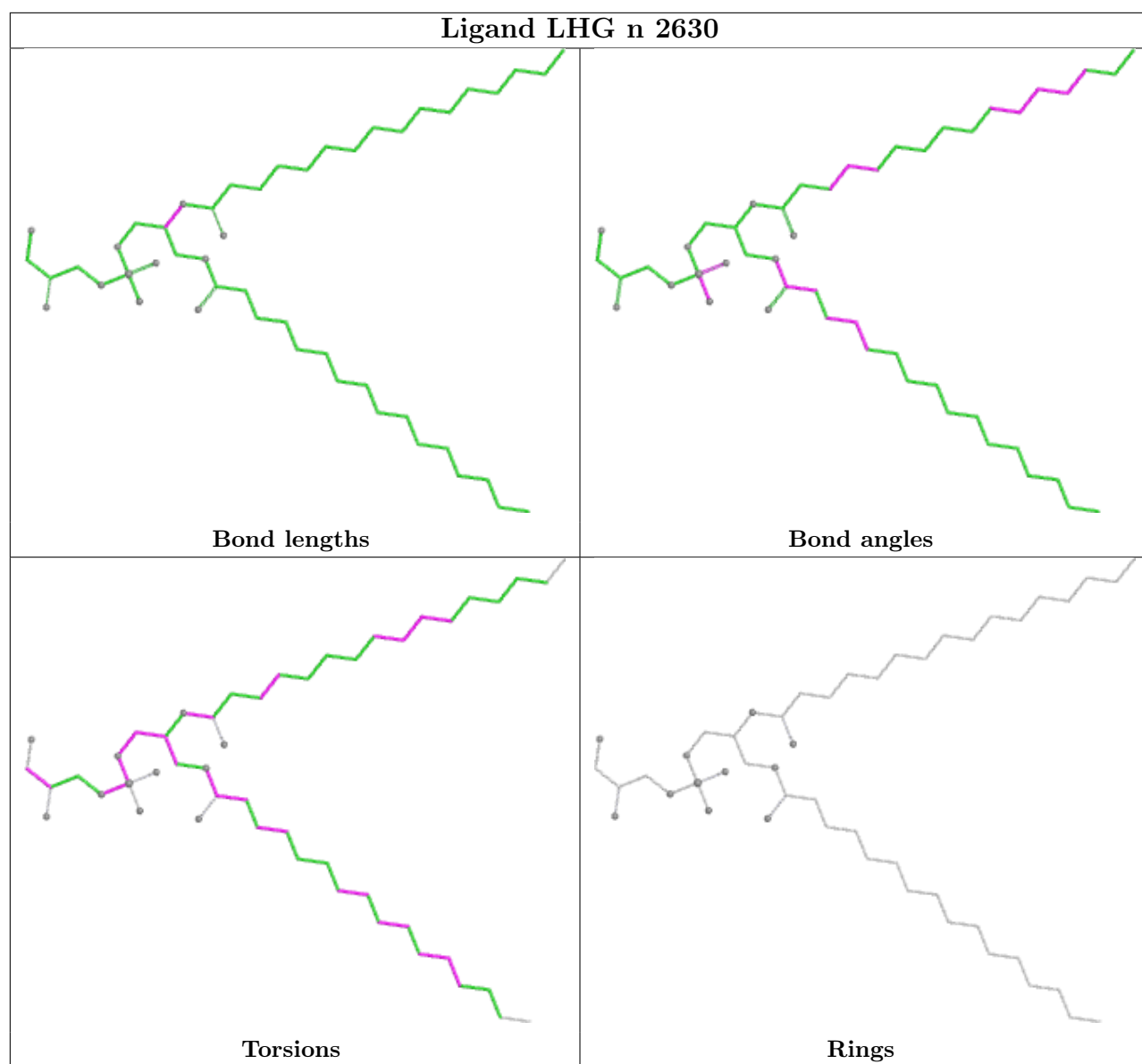
Ligand CHL G 601

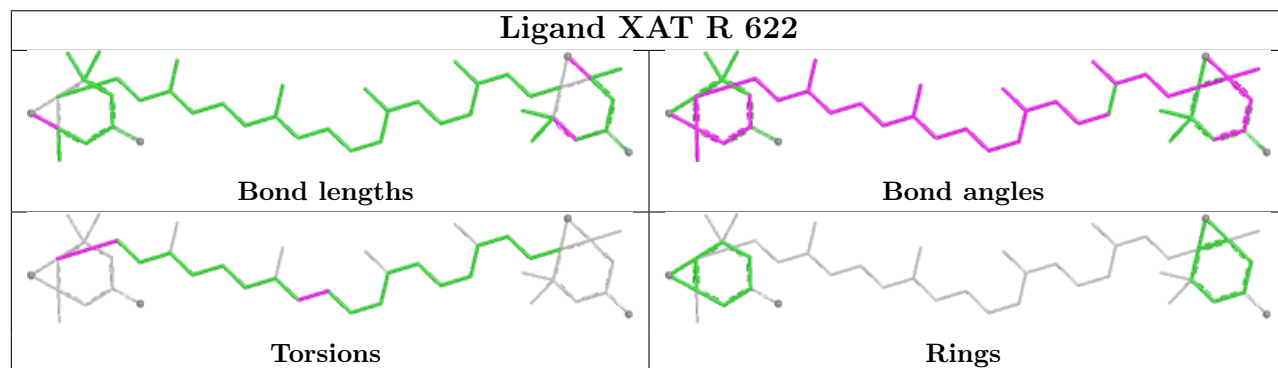
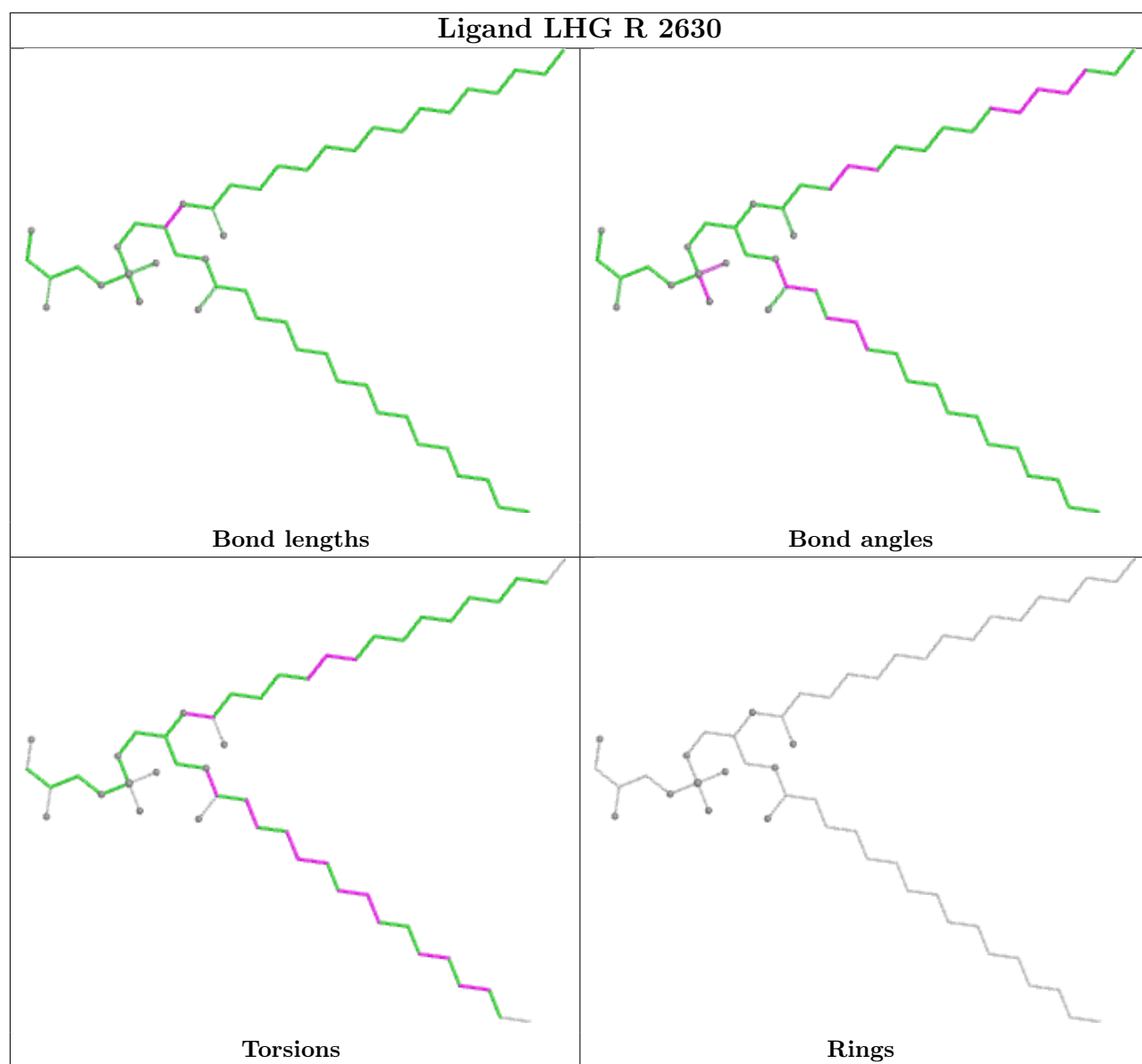


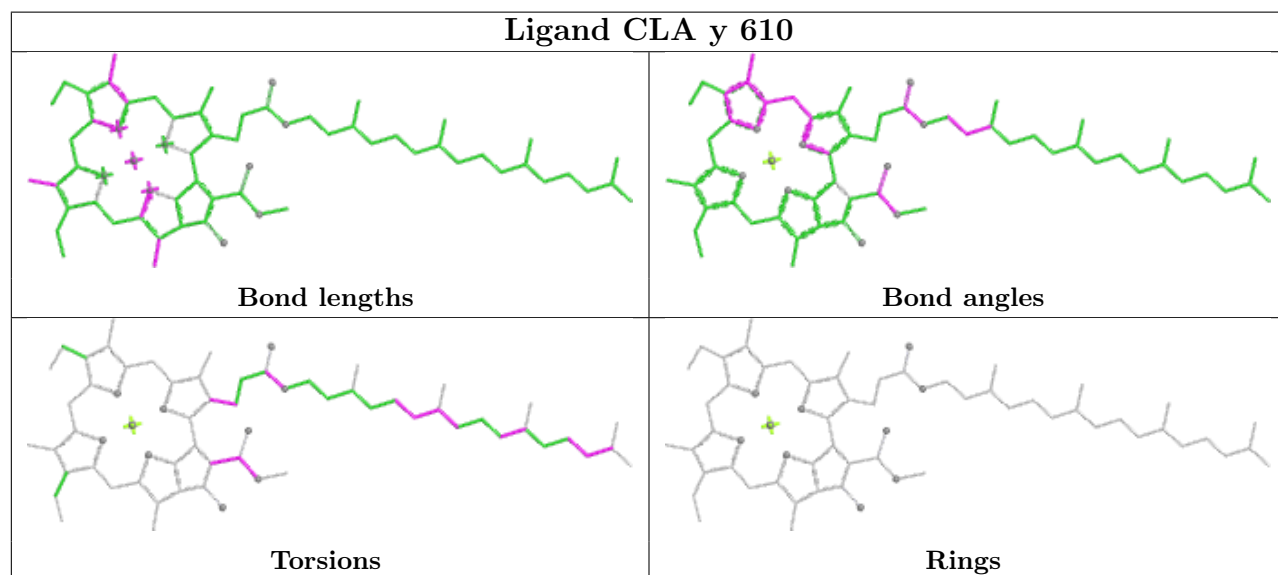
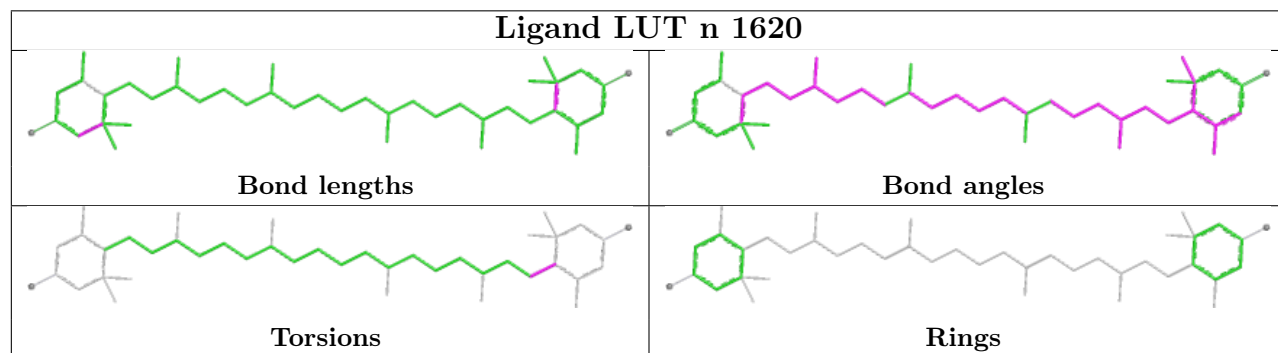
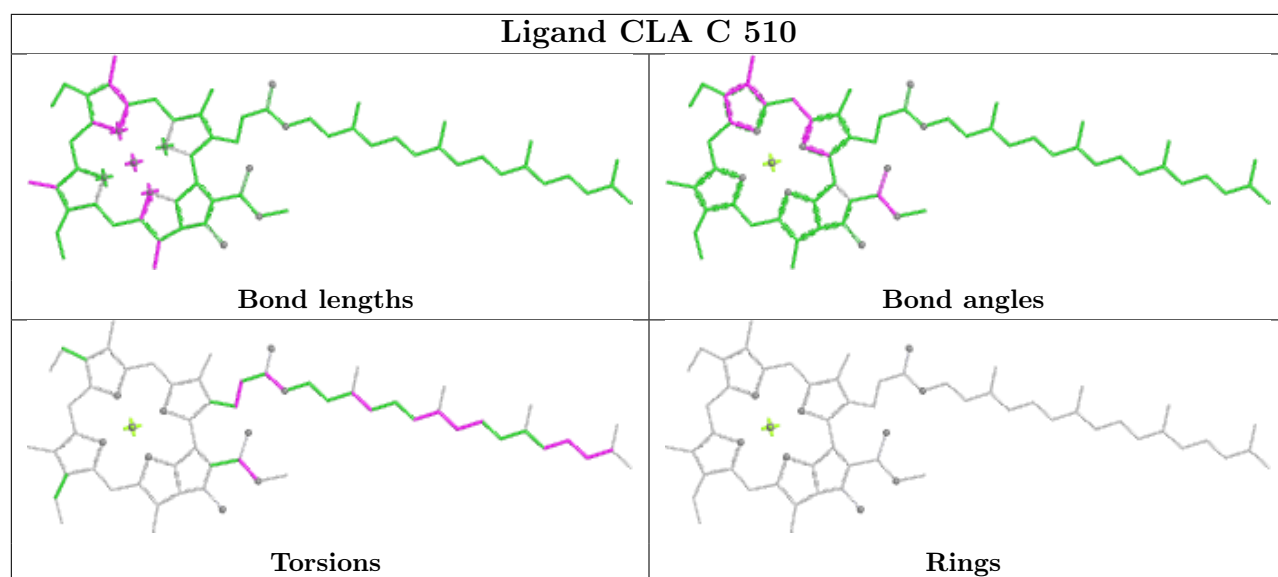




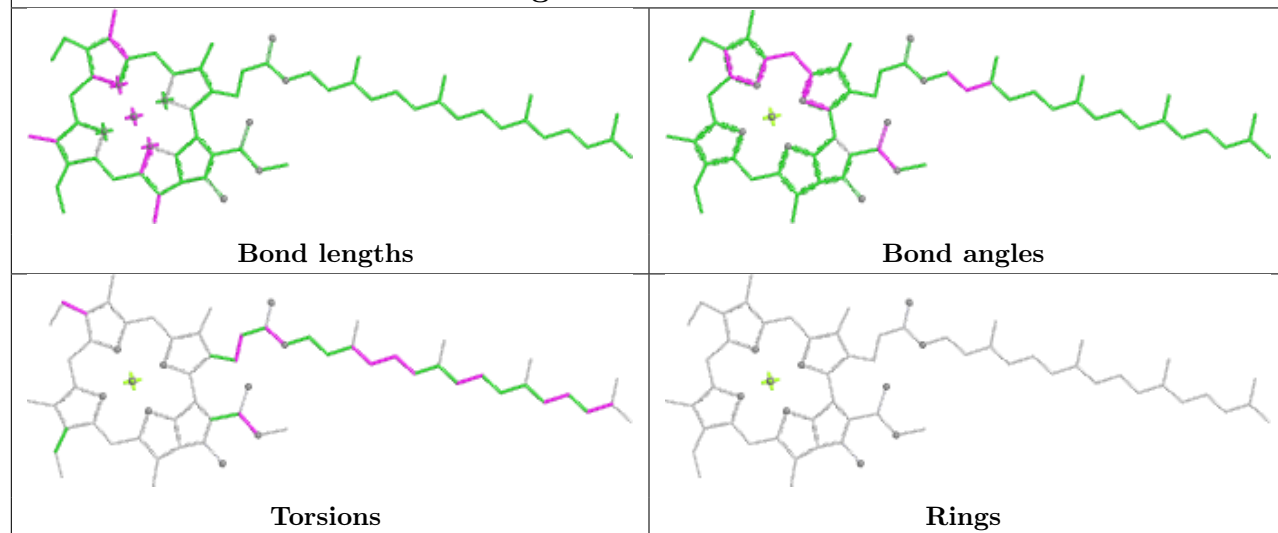




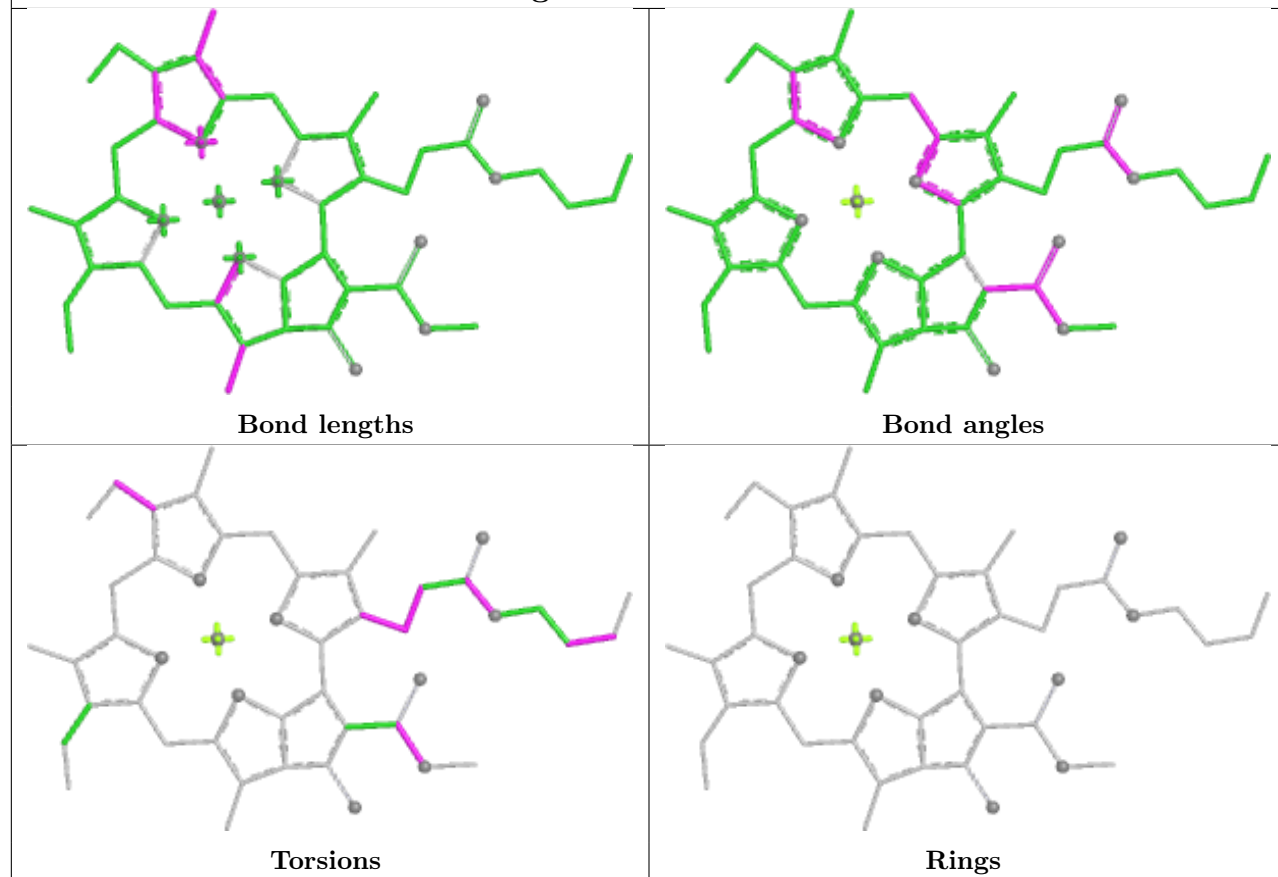


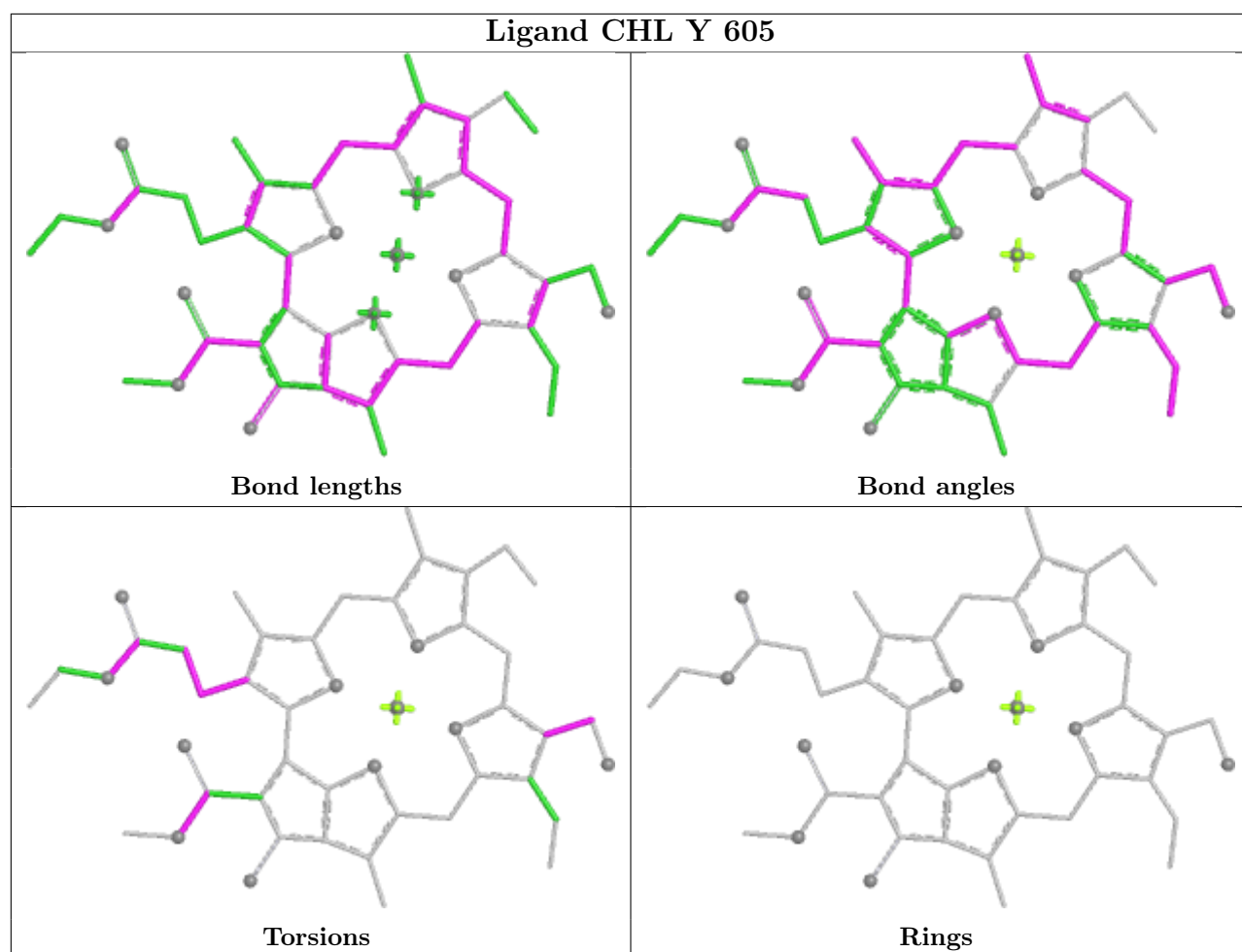


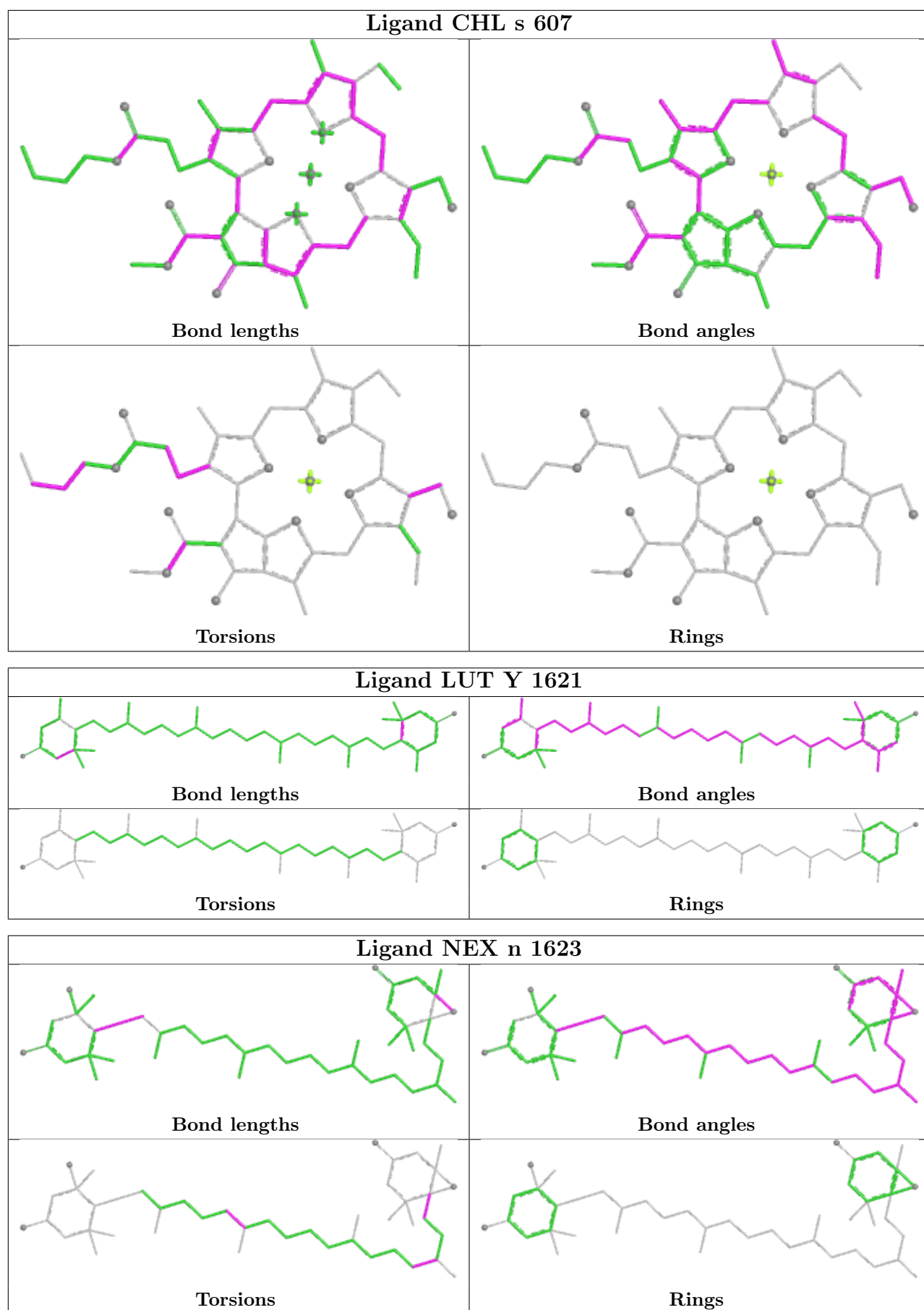
Ligand CLA Y 613

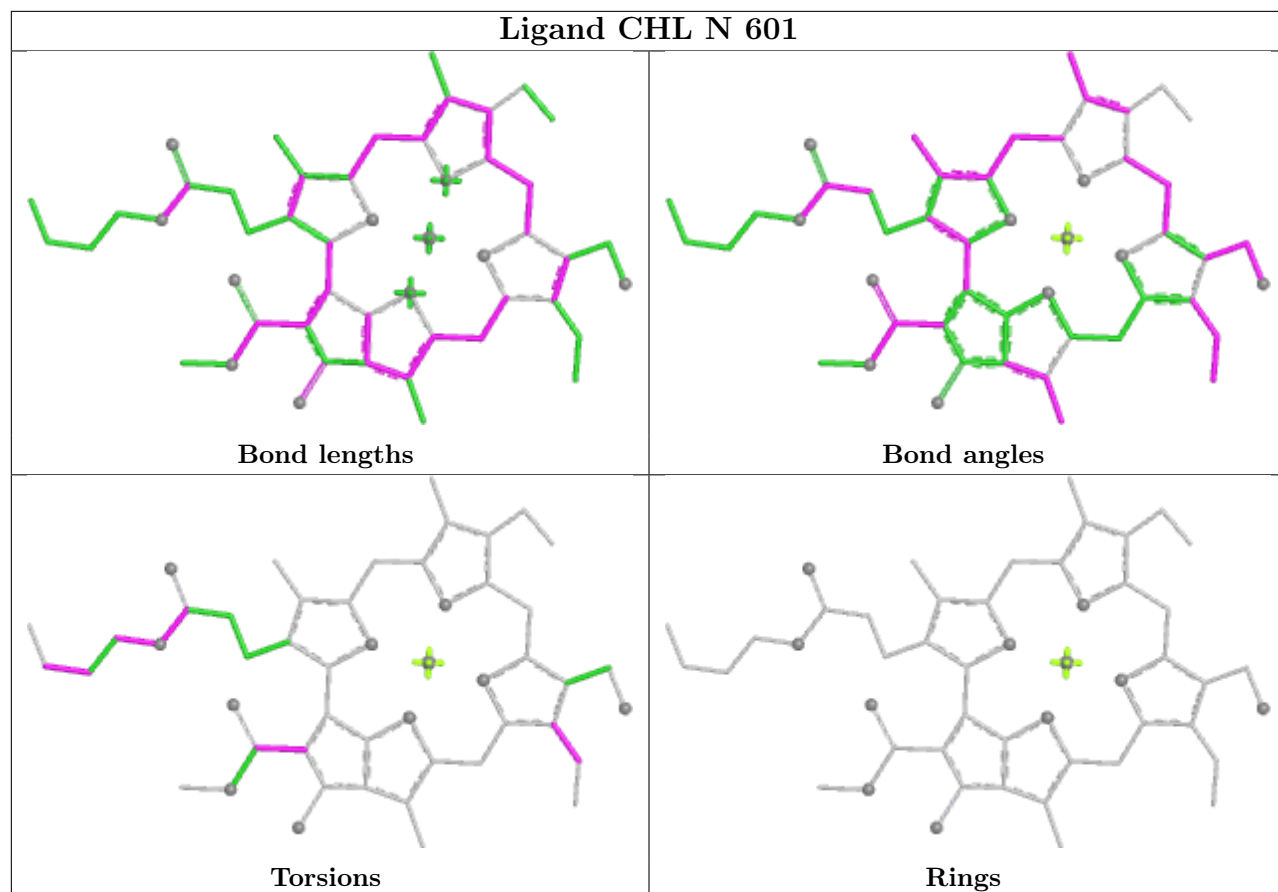


Ligand CLA R 611

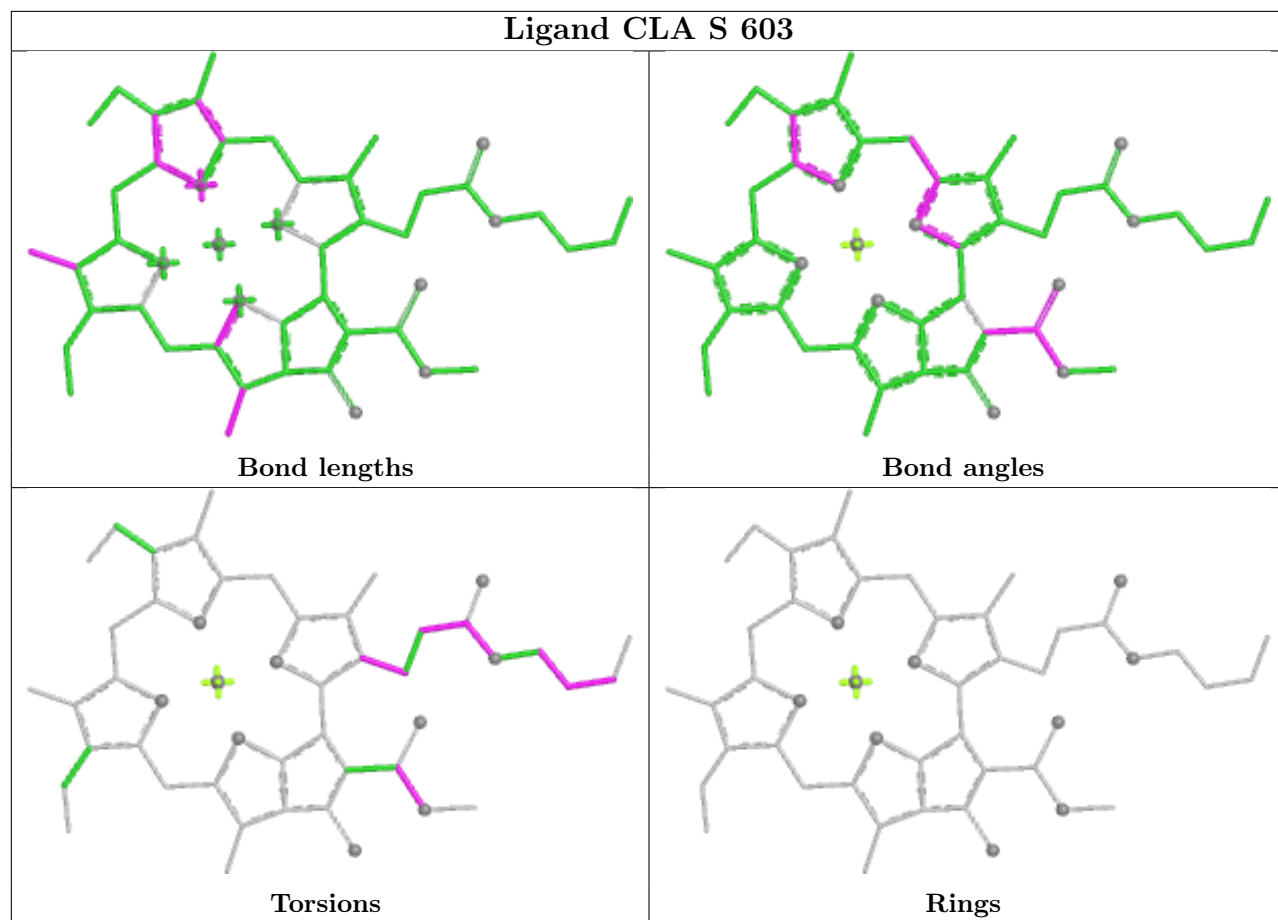


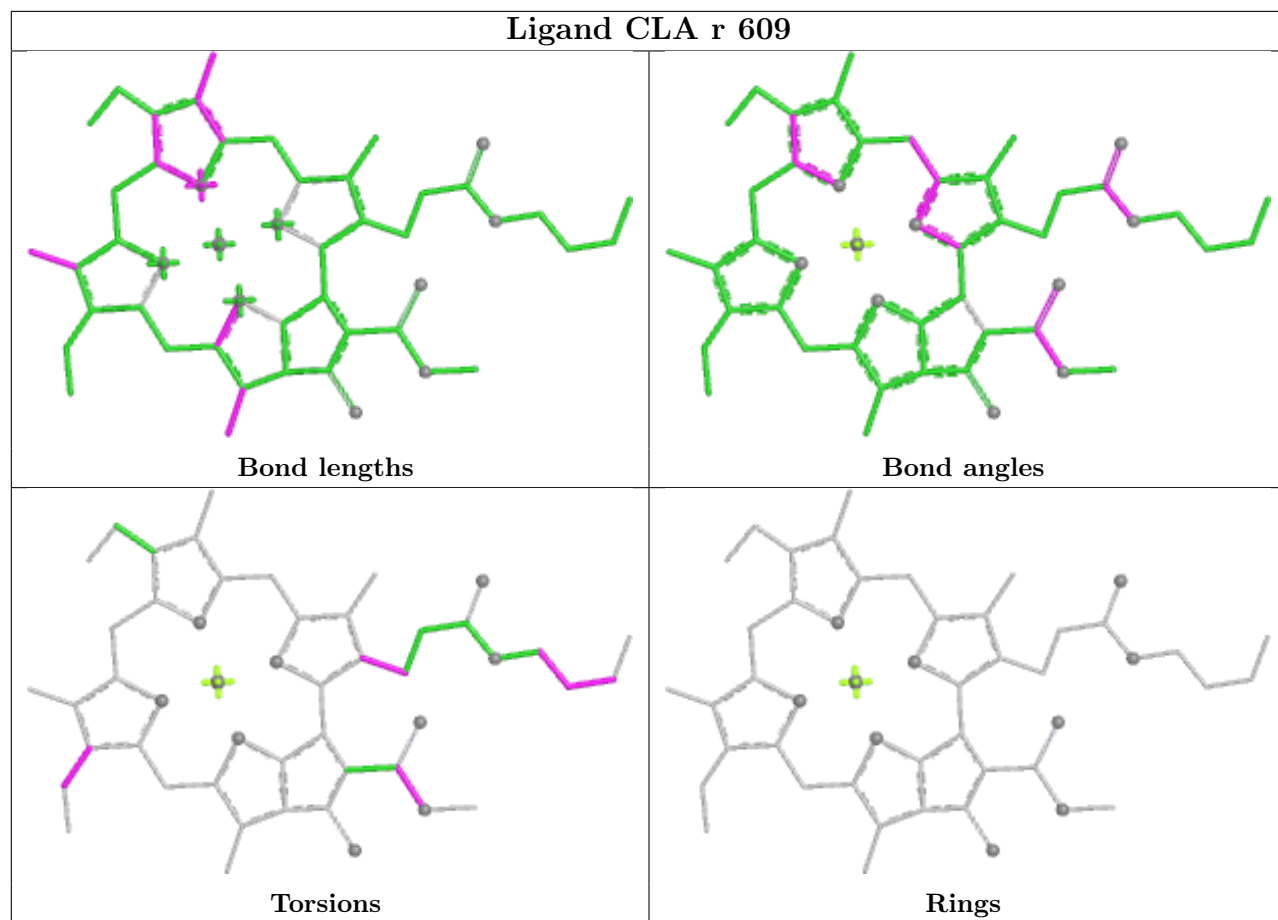


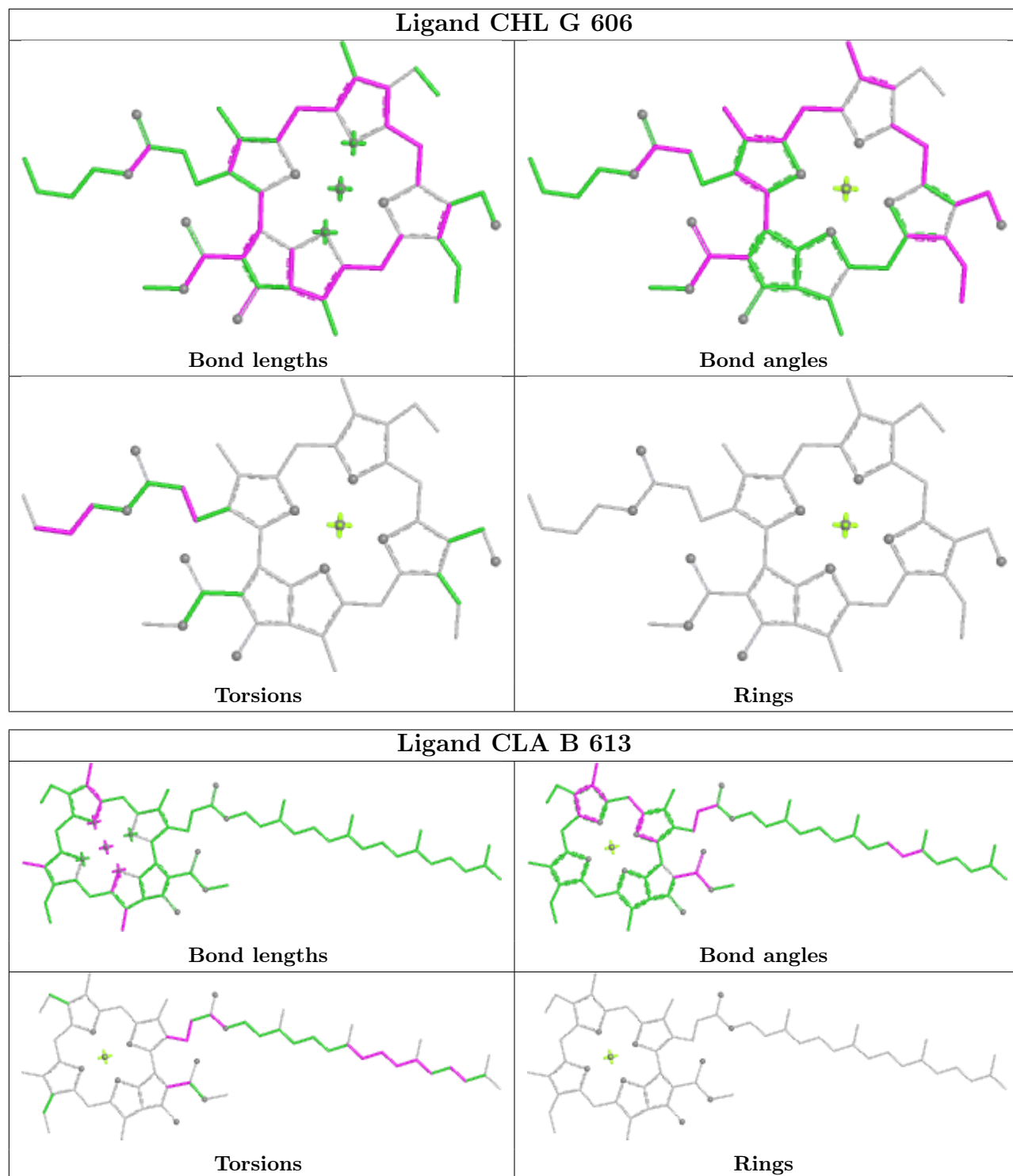


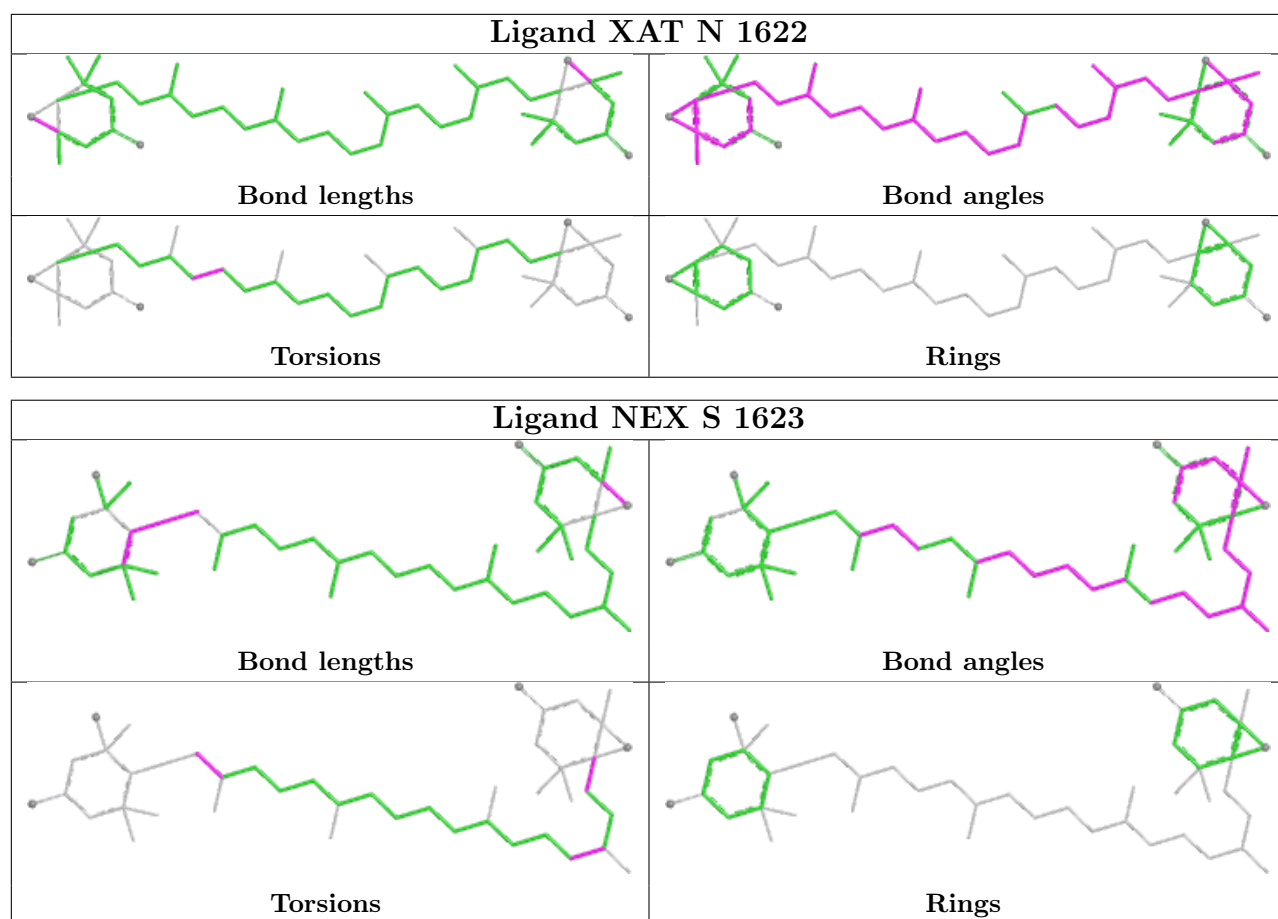


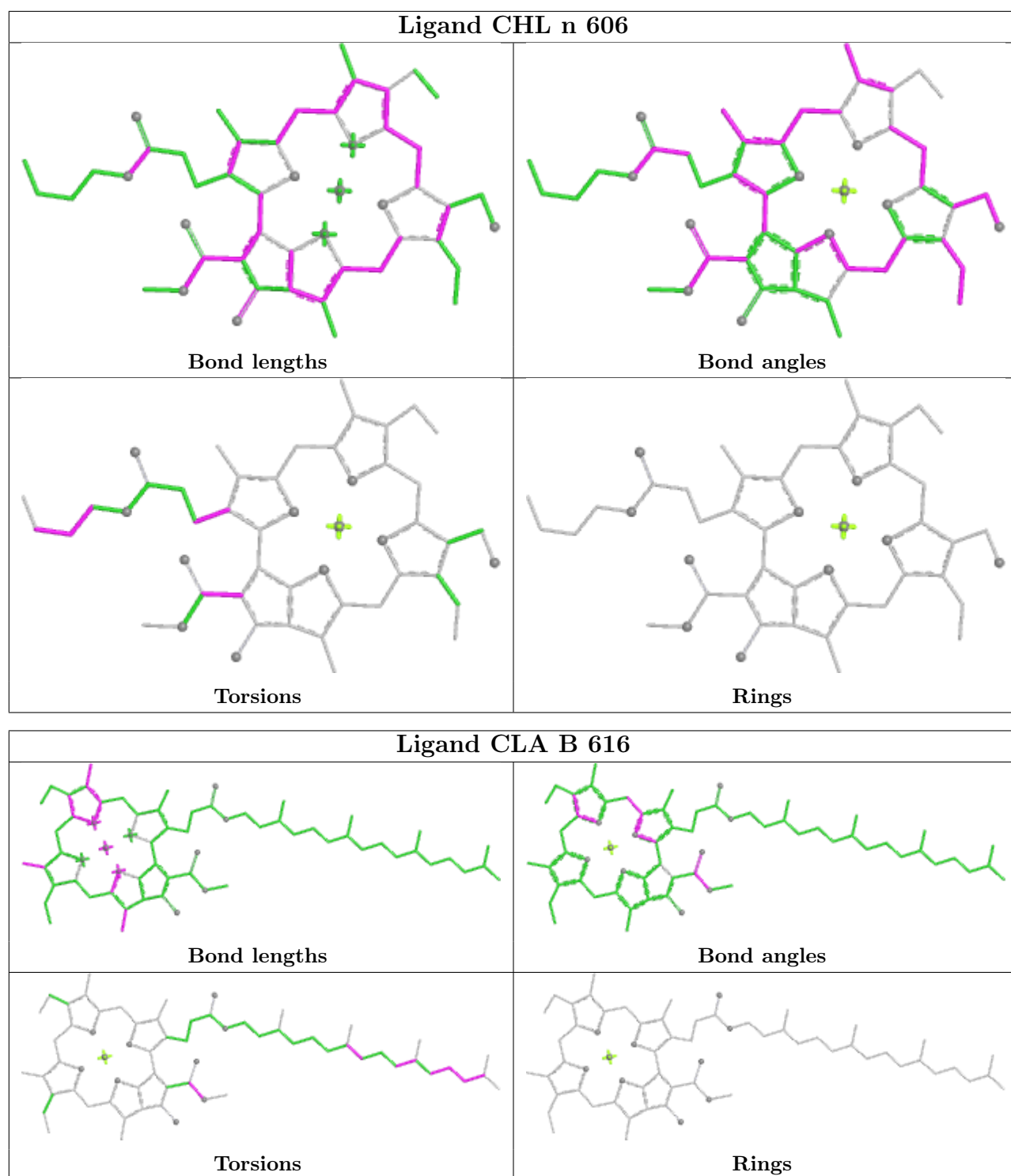
Ligand CLA S 603

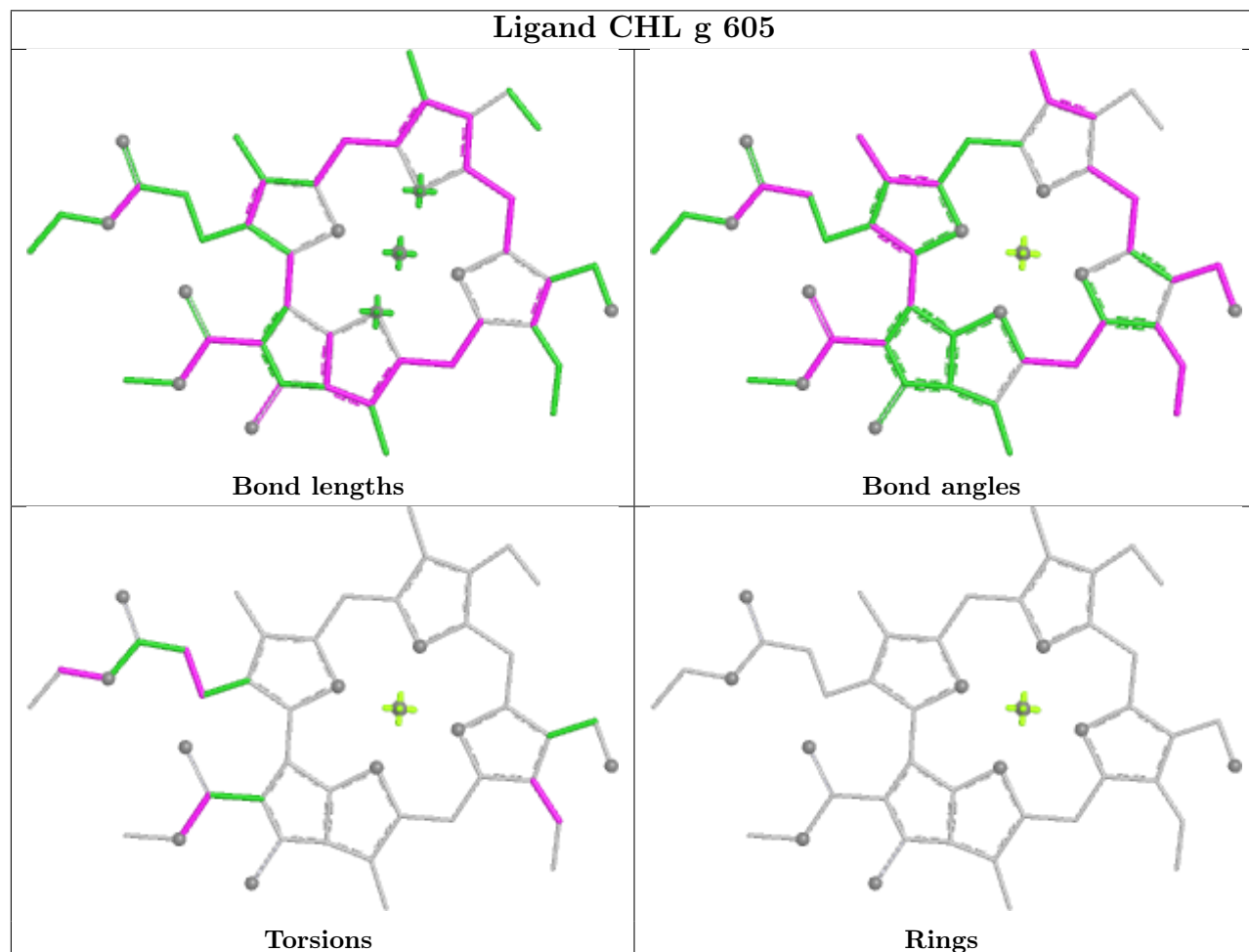
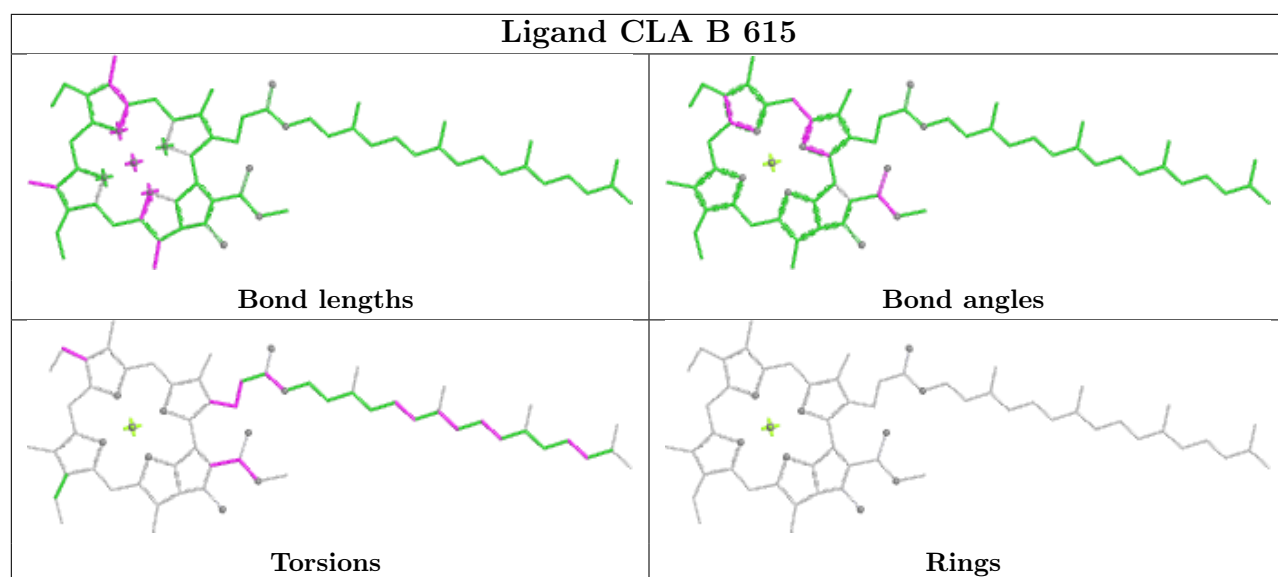




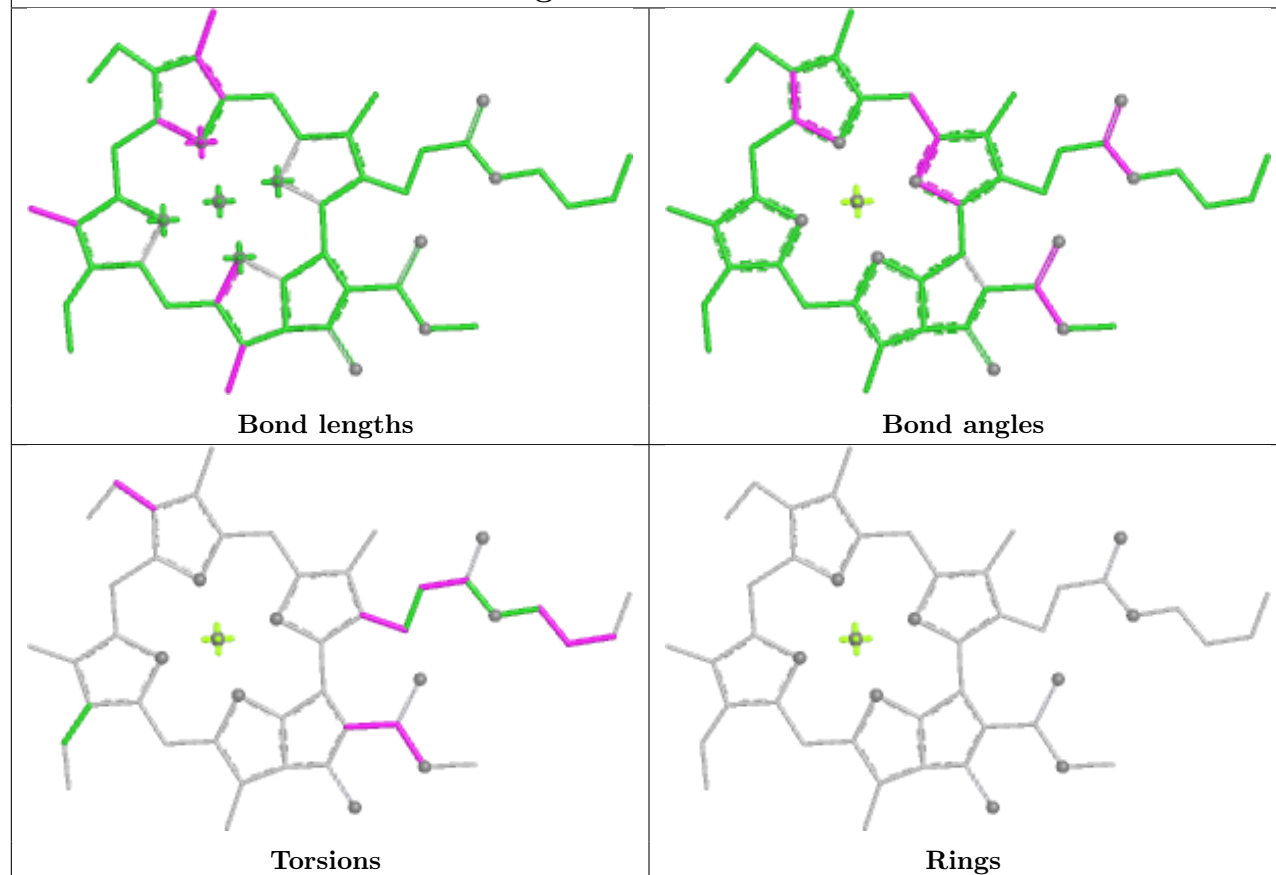




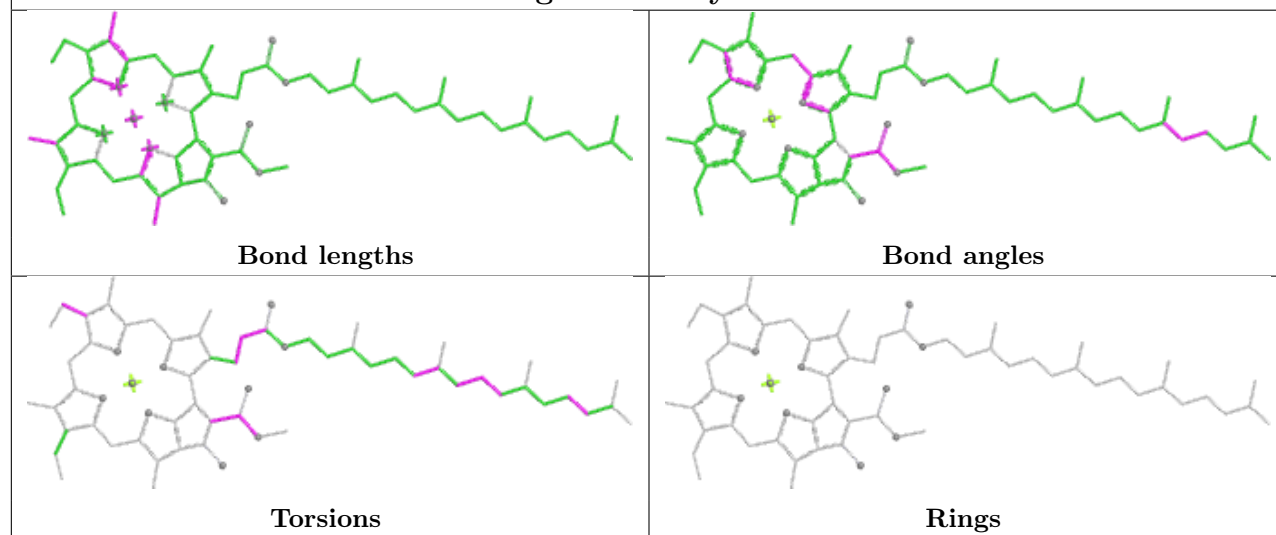


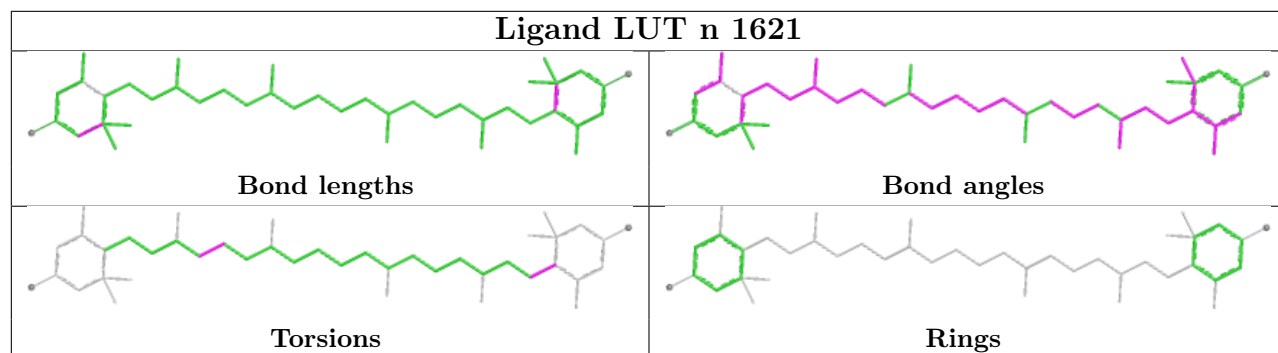
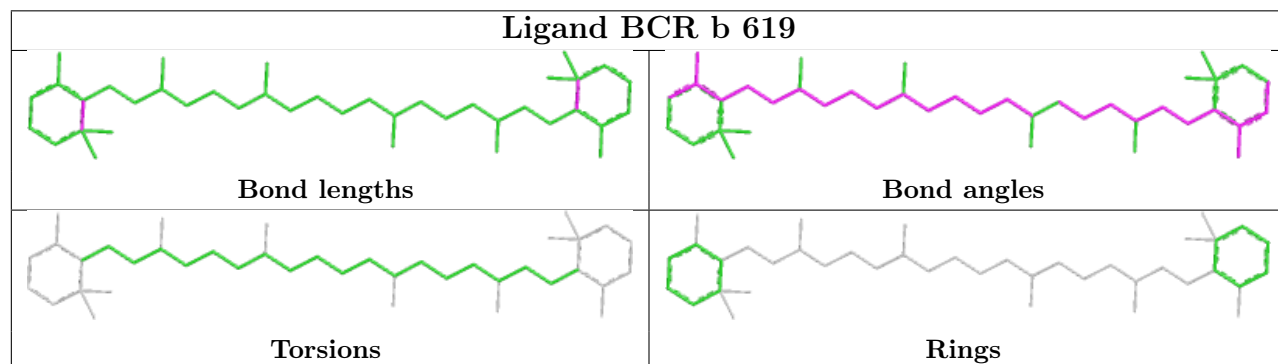
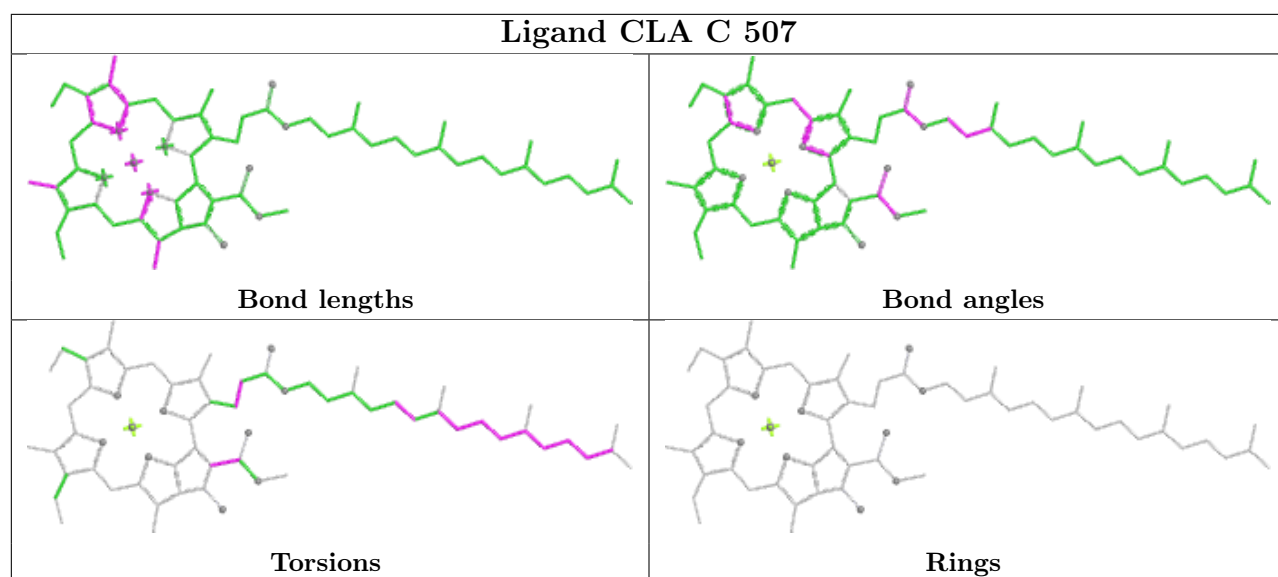


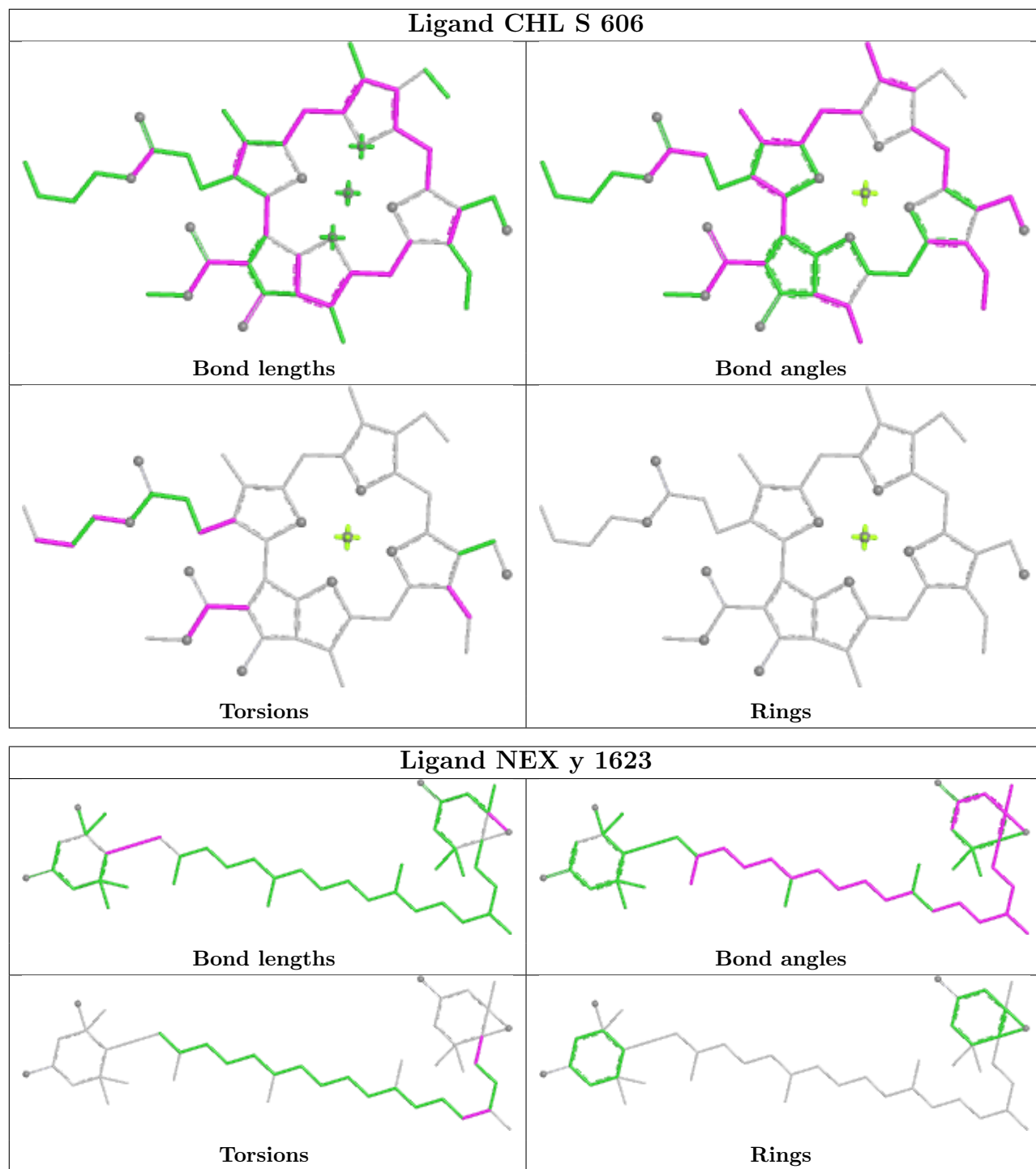
Ligand CLA n 612

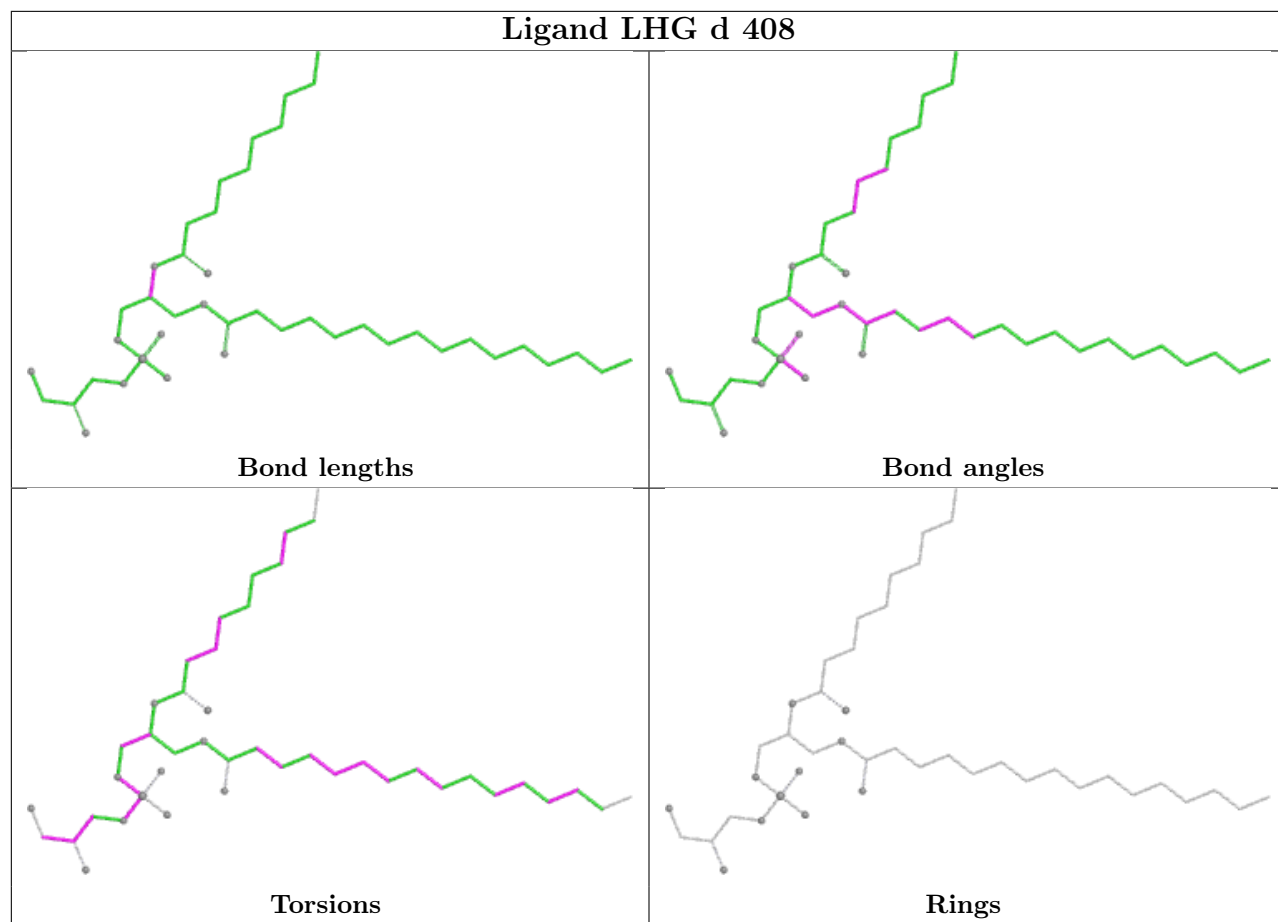


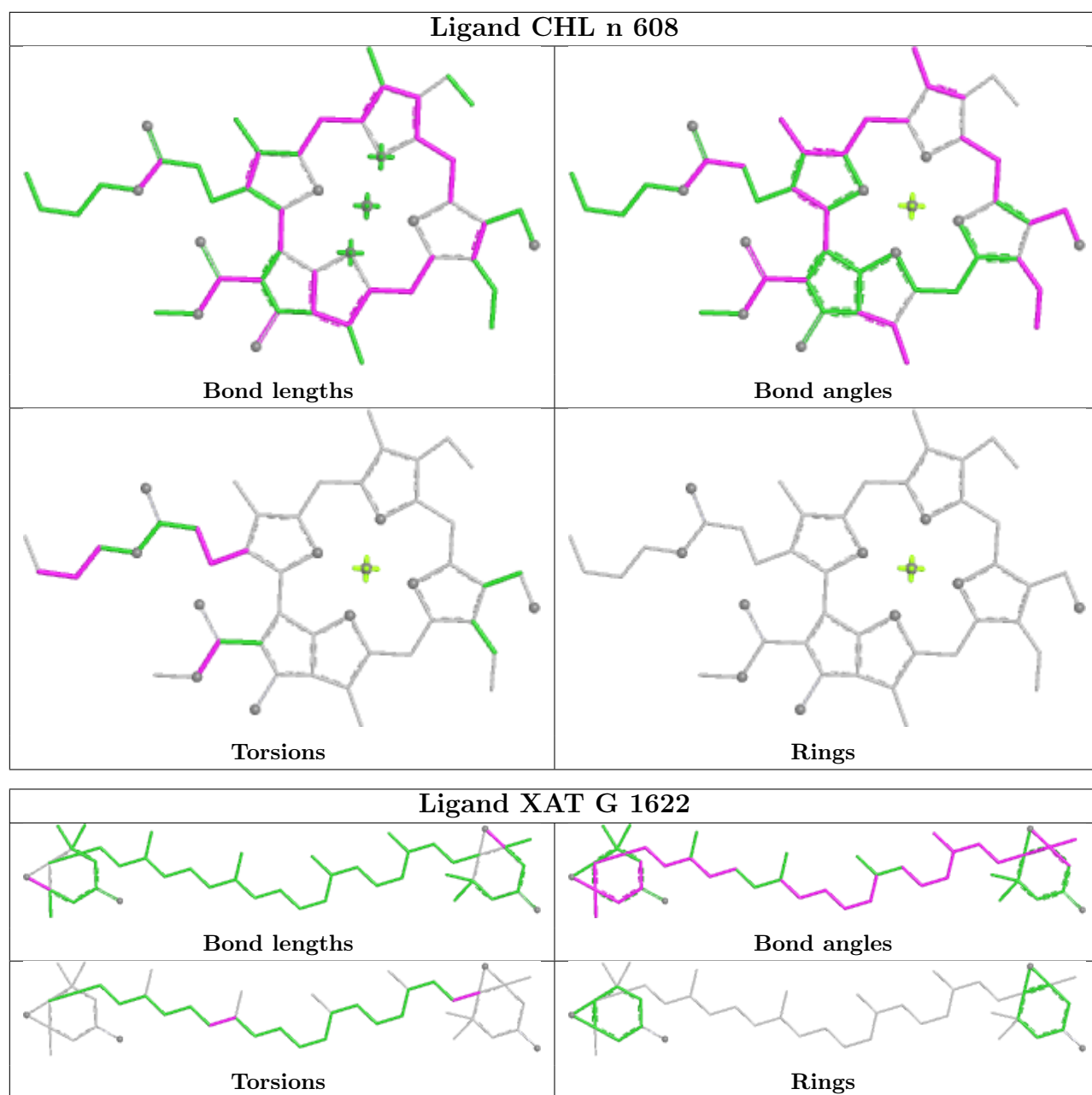
Ligand CLA y 602

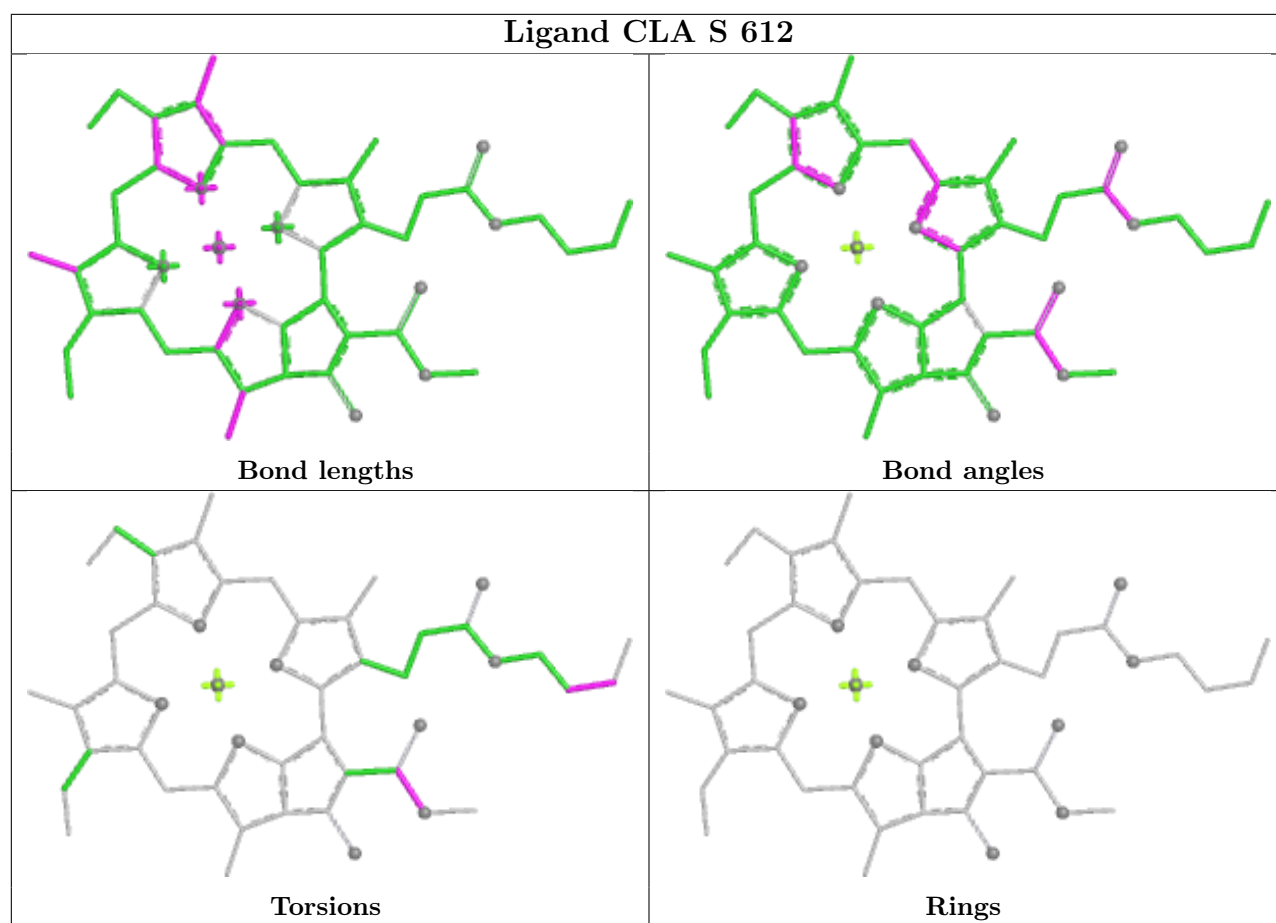












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

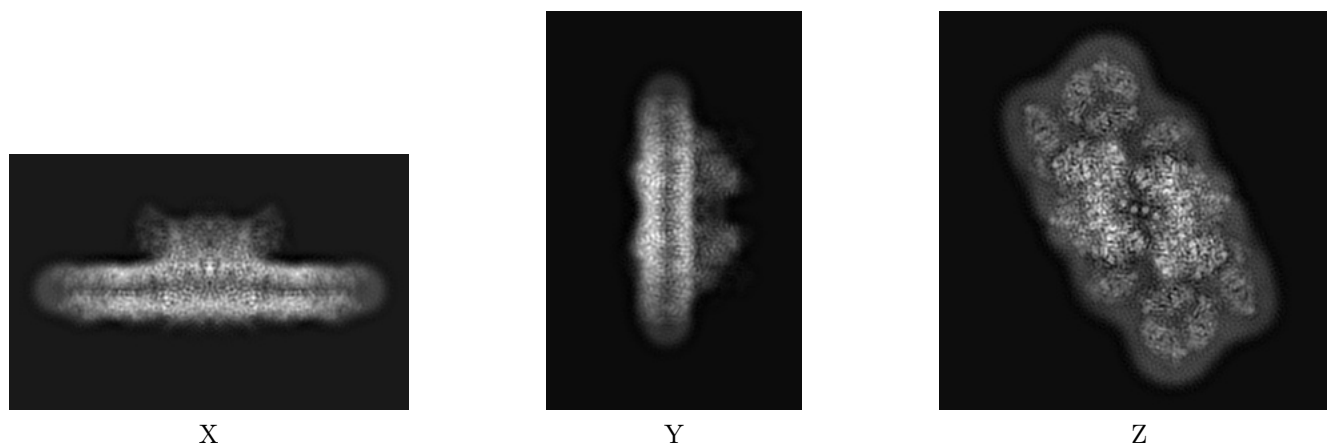
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6617. 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](#)

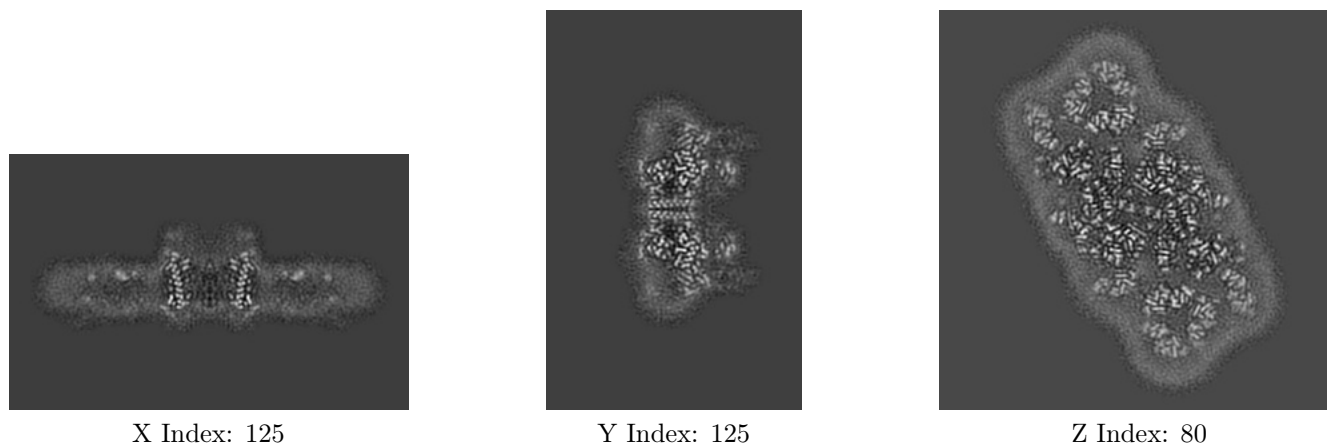
6.1.1 Primary map



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

6.2 Central slices [i](#)

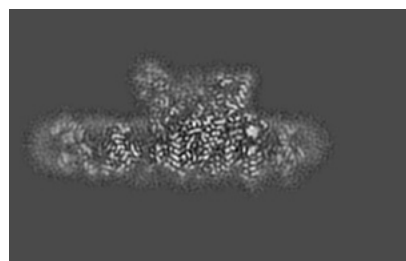
6.2.1 Primary map



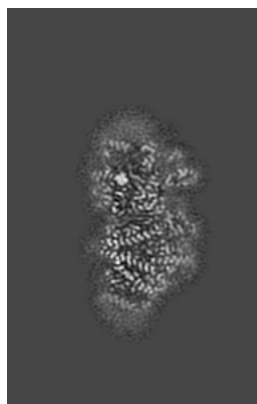
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

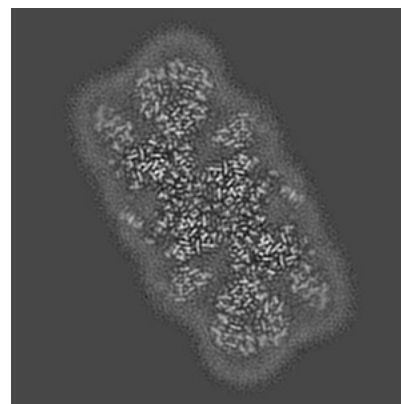
6.3.1 Primary map



X Index: 146



Y Index: 147

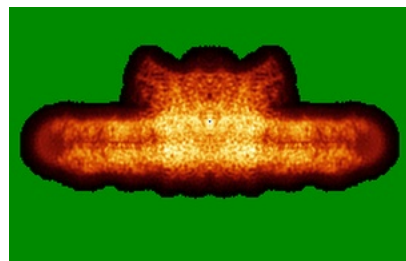


Z Index: 69

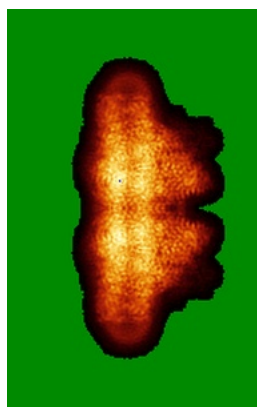
The images above show the largest variance slices of the map in three orthogonal directions.

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

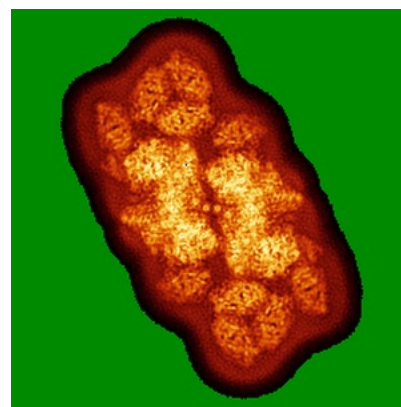
6.4.1 Primary map



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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

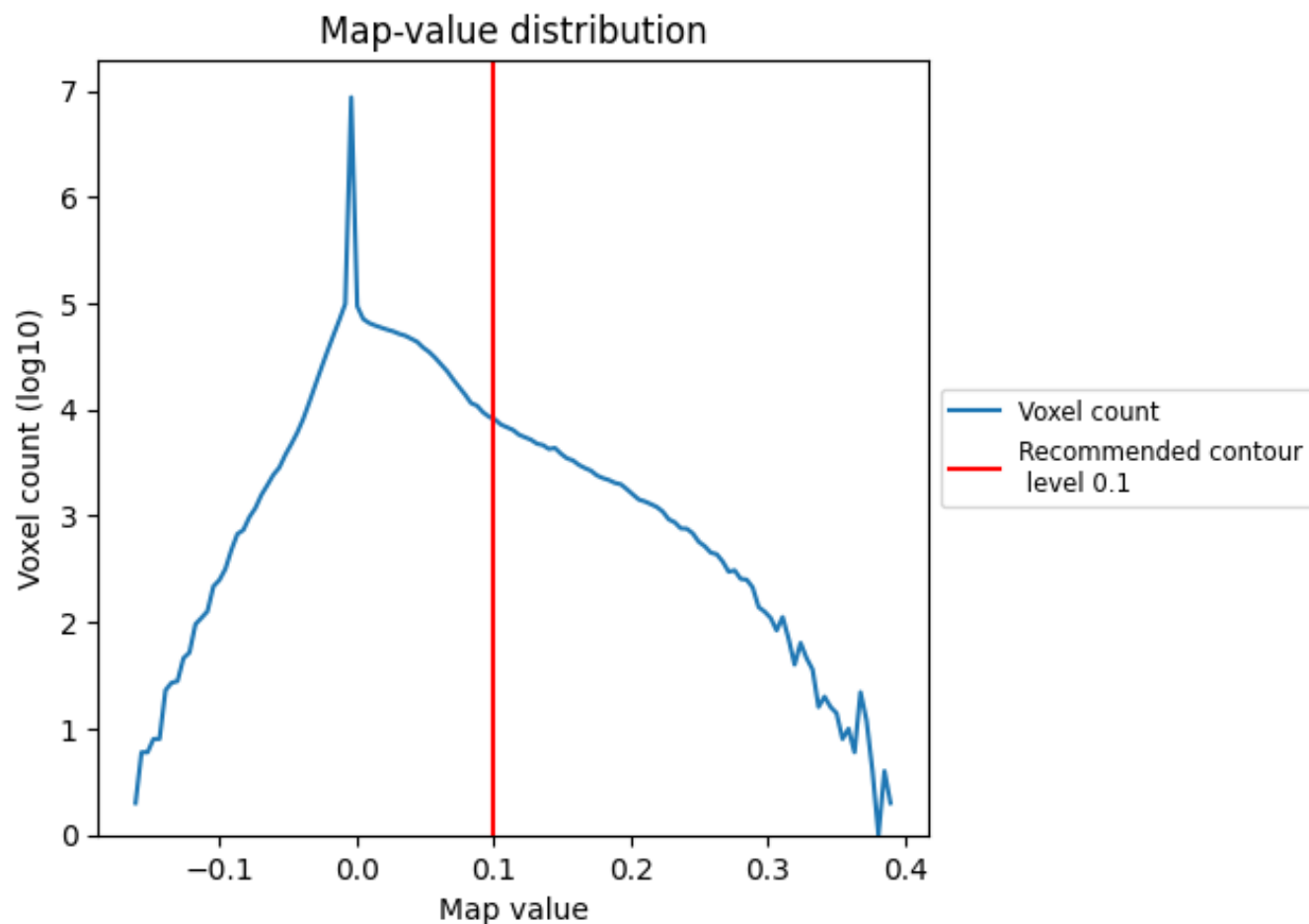
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

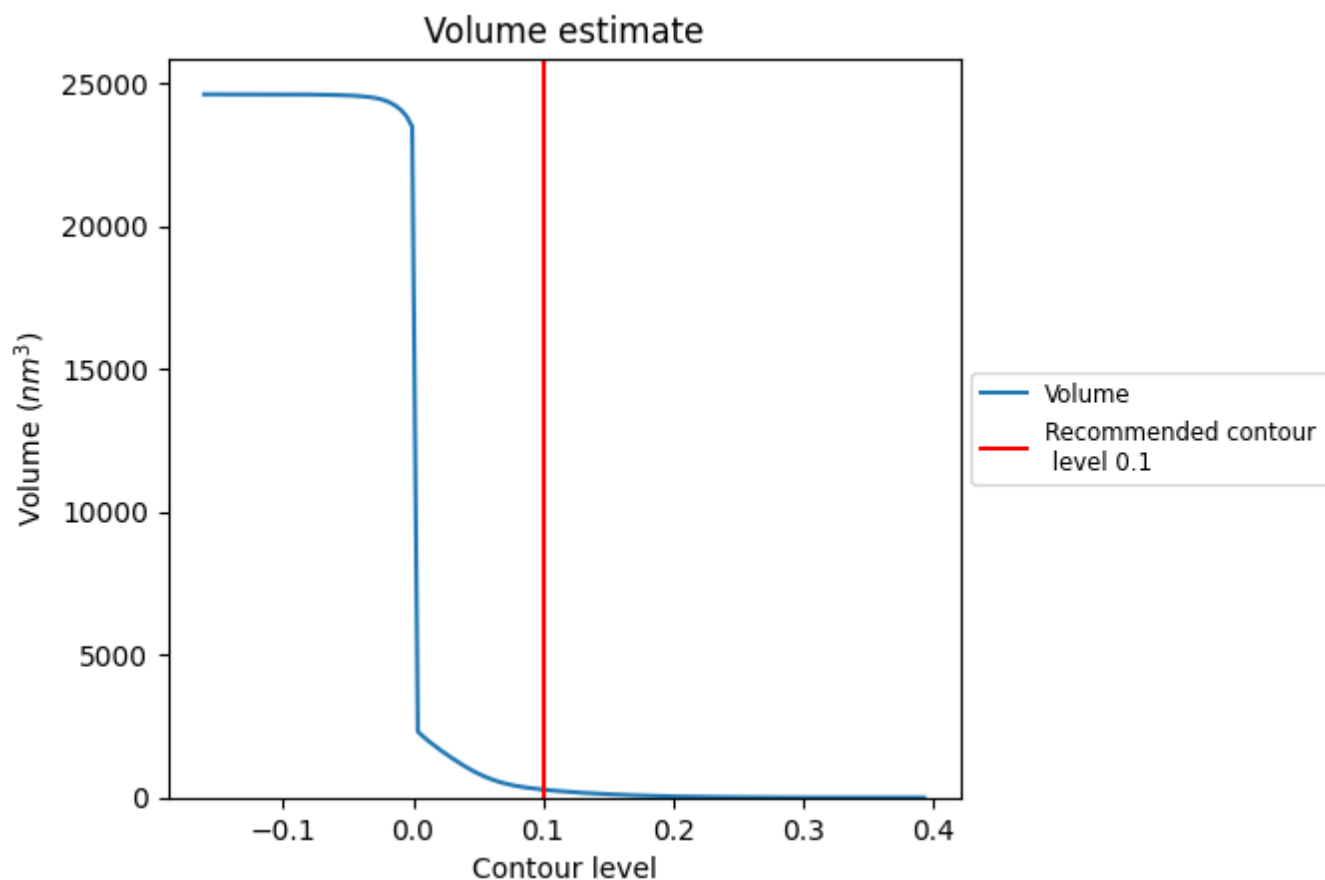
This section contains the results of statistical analysis of the map.

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 279 nm³; this corresponds to an approximate mass of 252 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

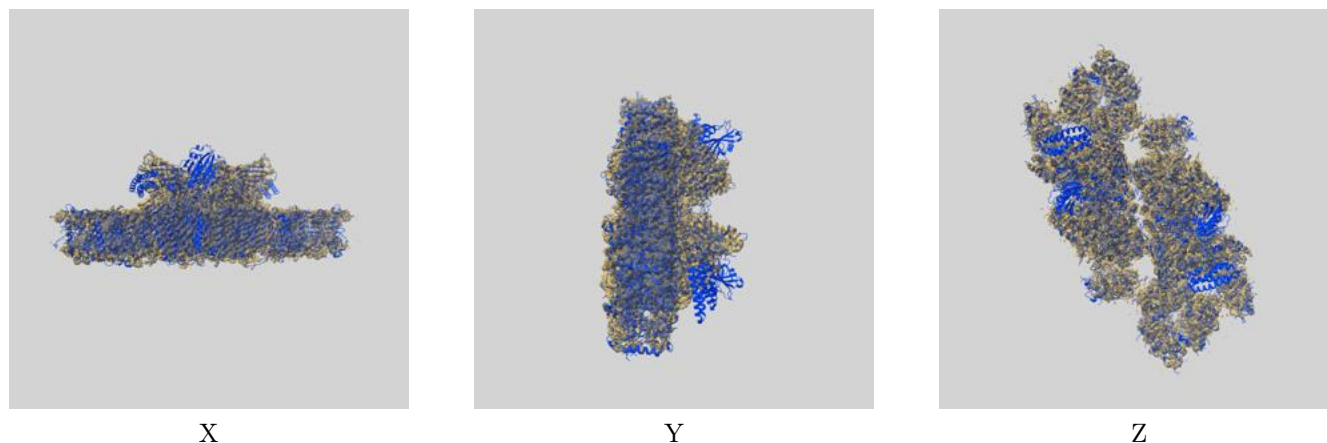
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

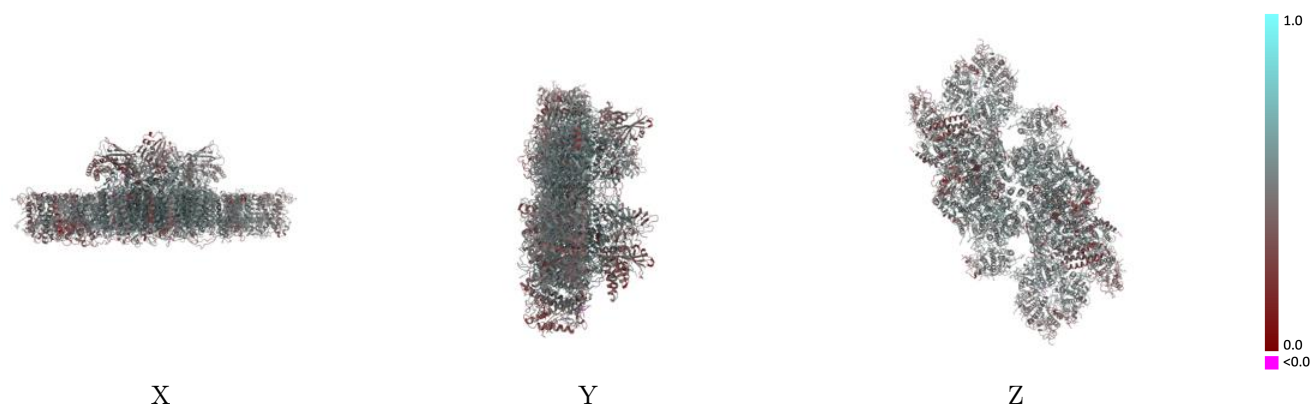
This section contains information regarding the fit between EMDB map EMD-6617 and PDB model 3JCU. Per-residue inclusion information can be found in section [3](#) on page [39](#).

9.1 Map-model overlay [i](#)



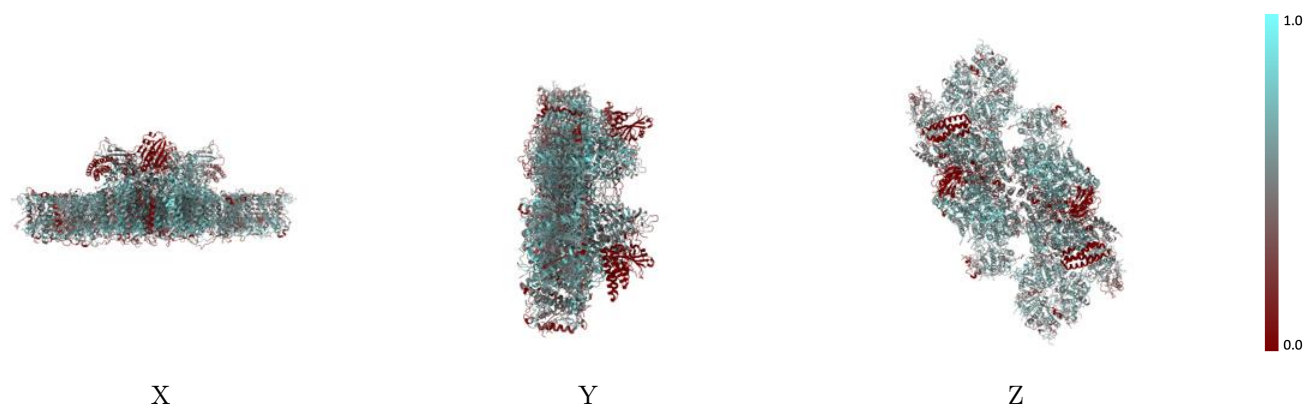
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



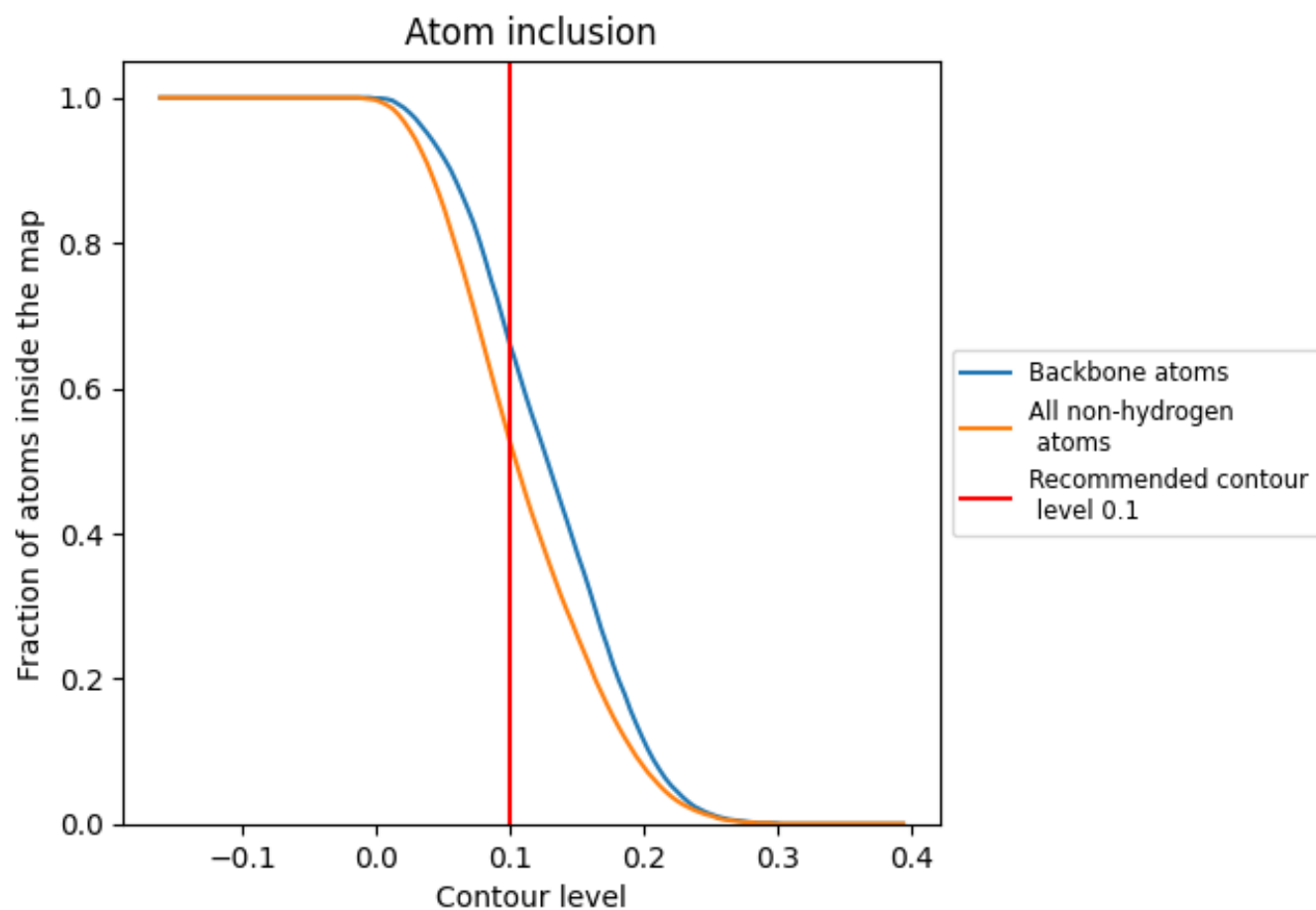
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 53% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5260	0.4830
A	0.6230	0.5310
B	0.6540	0.5350
C	0.6200	0.5220
D	0.6450	0.5370
E	0.5350	0.4210
F	0.5600	0.4540
G	0.5190	0.4420
H	0.5950	0.5320
I	0.6190	0.5090
J	0.1120	0.3960
K	0.5580	0.4630
L	0.5750	0.5270
M	0.4670	0.4960
N	0.5450	0.4720
O	0.3670	0.4340
P	0.0020	0.3960
Q	0.0040	0.3390
R	0.4520	0.4510
S	0.4440	0.3950
T	0.5580	0.5170
U	0.6310	0.4660
W	0.4910	0.4880
X	0.4960	0.4600
Y	0.6290	0.5190
Z	0.3900	0.4340
a	0.6240	0.5310
b	0.6540	0.5350
c	0.6190	0.5210
d	0.6450	0.5360
e	0.5360	0.4210
f	0.5600	0.4530
g	0.5170	0.4440
h	0.5950	0.5310
i	0.6190	0.5140



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Chain	Atom inclusion	Q-score
j	 0.1120	 0.3980
k	 0.5610	 0.4620
l	 0.5750	 0.5280
m	 0.4670	 0.4950
n	 0.5430	 0.4720
o	 0.3660	 0.4350
p	 0.0020	 0.3950
q	 0.0040	 0.3370
r	 0.4520	 0.4510
s	 0.4440	 0.3940
t	 0.5580	 0.5200
u	 0.6310	 0.4680
w	 0.4940	 0.4870
x	 0.4960	 0.4640
y	 0.6300	 0.5180
z	 0.3900	 0.4340