



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 06:58 PM EDT

PDB ID : 5E79 / pdb_00005e79
Title : Macromolecular diffractive imaging using imperfect crystals
Authors : Ayer, K.; Yefanov, O.; Oberthur, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffer, A.; Dorner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.
Deposited on : 2015-10-12
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>
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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12

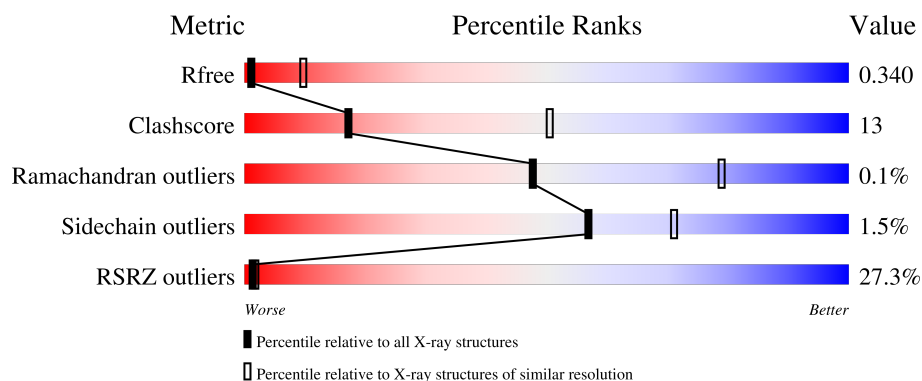
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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
22	CL	U	201	-	-	-	X
22	CL	a	604	-	-	-	X
22	CL	u	201	-	-	-	X
23	BCT	A	605	-	X	-	-
23	BCT	a	605	-	X	-	-
24	CLA	A	606	X	-	-	-
24	CLA	A	607	X	-	-	-
24	CLA	A	609	X	-	-	-
24	CLA	B	602	X	-	-	-

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607[A]	X	-	-	-
24	CLA	B	607[B]	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	606	X	-	-	-
24	CLA	a	607	X	-	-	-
24	CLA	a	609	X	-	-	-
24	CLA	a	615	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608[A]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	b	608[B]	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	A	610	-	X	-	-
26	BCR	B	618	-	X	X	-
26	BCR	B	619	-	X	-	-
26	BCR	B	620	-	X	-	-
26	BCR	C	514	-	X	-	-
26	BCR	F	101	-	X	-	-
26	BCR	H	101	-	X	-	-
26	BCR	I	101	-	X	-	-
26	BCR	K	101	-	X	-	-
26	BCR	K	102	-	X	-	-
26	BCR	T	101	-	X	X	-
26	BCR	a	610	-	X	-	-
26	BCR	b	619	-	X	X	-
26	BCR	b	620	-	X	-	-
26	BCR	b	621	-	X	-	-
26	BCR	c	514	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	BCR	c	515	-	X	-	-
26	BCR	c	521	-	X	-	-
26	BCR	f	101	-	X	X	-
26	BCR	h	101	-	X	-	-
26	BCR	k	101	-	X	-	-
26	BCR	t	101	-	X	X	-
27	PL9	D	405	-	X	-	-
27	PL9	a	611	-	-	-	X
27	PL9	d	404	-	X	-	-
29	LMG	Z	101	-	-	-	X
29	LMG	c	520	-	-	-	X
30	LHG	E	102	-	-	-	X
31	CA	b	602	-	-	-	X

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	250.80Å 250.80Å 250.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 29.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.98-3.50) 99.8 (29.98-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.324 , 0.331 0.344 , 0.340	Depositor DCC
R_{free} test set	45921 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.7	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	50074	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality ⓘ

3.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.75	0/2734	0.99	1/3727 (0.0%)
1	a	0.64	0/2734	0.99	7/3727 (0.2%)
2	B	0.66	1/4194 (0.0%)	0.96	7/5713 (0.1%)
2	b	0.63	0/4194	0.96	13/5713 (0.2%)
3	C	0.64	0/3634	1.00	4/4947 (0.1%)
3	c	0.61	0/3634	0.95	5/4947 (0.1%)
4	D	0.67	0/2821	0.98	9/3844 (0.2%)
4	d	0.61	0/2821	0.93	6/3844 (0.2%)
5	E	0.62	0/693	0.94	0/944
5	e	0.60	0/693	0.93	0/944
6	F	0.76	1/284 (0.4%)	0.95	0/387
6	f	0.60	0/284	0.92	0/387
7	H	0.63	0/544	0.94	1/739 (0.1%)
7	h	0.64	0/544	0.91	1/739 (0.1%)
8	I	0.71	0/327	0.96	0/439
8	i	0.61	0/327	0.89	0/439
9	J	0.67	0/278	0.89	0/376
9	j	0.56	0/278	0.93	0/376
10	K	0.65	0/303	1.03	2/416 (0.5%)
10	k	0.77	0/303	1.41	4/416 (1.0%)
11	L	0.72	0/319	0.94	0/433
11	l	0.62	0/319	0.89	2/433 (0.5%)
12	M	0.69	0/278	1.18	1/378 (0.3%)
12	m	0.66	0/278	1.10	4/378 (1.1%)
13	O	0.59	0/1926	0.92	1/2611 (0.0%)
13	o	0.54	0/1926	0.88	2/2611 (0.1%)
14	T	0.81	0/282	0.90	0/382
14	t	0.65	0/282	0.92	0/382
15	U	0.63	0/785	0.87	0/1064
15	u	0.61	0/785	0.88	0/1064
16	V	0.64	0/1096	0.97	0/1487
16	v	0.56	0/1096	0.92	1/1487 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.61	0/216	0.96	1/289 (0.3%)
17	y	0.62	0/216	0.97	0/289
18	X	0.64	0/298	0.91	0/403
18	x	0.65	0/298	0.96	0/403
19	Z	0.61	0/490	1.00	0/669
19	z	0.68	1/490 (0.2%)	1.01	1/669 (0.1%)
All	All	0.64	3/43004 (0.0%)	0.96	73/58496 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	z	23	VAL	CA-CB	6.75	1.57	1.54
6	F	28	VAL	CA-CB	5.67	1.57	1.54
2	B	381	ILE	CA-CB	-5.42	1.48	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	k	11	LEU	CA-C-N	-8.17	109.63	119.84
10	k	11	LEU	C-N-CA	-8.17	109.63	119.84
4	d	170	ALA	CA-C-N	-8.03	111.73	119.76
4	d	170	ALA	C-N-CA	-8.03	111.73	119.76
4	D	170	ALA	CA-C-N	-7.58	112.18	119.76
4	D	170	ALA	C-N-CA	-7.58	112.18	119.76
3	c	336	GLY	N-CA-C	-7.23	105.26	114.37
1	a	83	VAL	CA-C-N	7.22	127.26	119.89
1	a	83	VAL	C-N-CA	7.22	127.26	119.89
7	H	52	THR	N-CA-C	-6.91	103.85	112.90
2	b	478	VAL	N-CA-C	6.88	118.70	112.17
2	b	328	GLY	CA-C-N	6.63	126.54	119.85
2	b	328	GLY	C-N-CA	6.63	126.54	119.85
4	D	308	ASP	CA-C-N	6.57	127.41	120.12
4	D	308	ASP	C-N-CA	6.57	127.41	120.12
3	c	100	GLY	CA-C-N	6.45	126.48	119.90
3	c	100	GLY	C-N-CA	6.45	126.48	119.90
4	d	308	ASP	CA-C-N	6.31	127.12	120.12
4	d	308	ASP	C-N-CA	6.31	127.12	120.12
3	C	38	GLY	N-CA-C	6.28	120.49	112.83
2	b	87	ASP	CA-C-N	6.27	126.81	120.04
2	b	87	ASP	C-N-CA	6.27	126.81	120.04
13	O	11	VAL	N-CA-C	6.11	117.17	108.93
4	d	94	GLY	CA-C-N	6.08	126.19	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	94	GLY	C-N-CA	6.08	126.19	119.87
19	z	53	VAL	N-CA-C	6.07	116.25	110.42
2	b	48	SER	CA-C-N	-5.83	117.15	122.28
2	b	48	SER	C-N-CA	-5.83	117.15	122.28
2	b	220	ARG	CA-C-N	5.83	123.92	119.66
2	b	220	ARG	C-N-CA	5.83	123.92	119.66
17	Y	31	ALA	N-CA-C	5.75	118.02	111.11
12	m	17	VAL	CA-C-N	-5.67	113.18	119.19
12	m	17	VAL	C-N-CA	-5.67	113.18	119.19
12	m	3	VAL	N-CA-C	5.59	116.14	110.05
4	D	37	LEU	N-CA-C	5.57	117.04	110.97
1	a	202	VAL	N-CA-C	5.55	115.75	110.42
4	D	94	GLY	CA-C-N	5.51	125.60	119.87
4	D	94	GLY	C-N-CA	5.51	125.60	119.87
2	B	194	ASN	CA-C-N	5.50	125.16	119.05
2	B	194	ASN	C-N-CA	5.50	125.16	119.05
12	m	3	VAL	CB-CA-C	-5.50	105.54	111.59
7	h	52	THR	N-CA-C	-5.46	105.74	112.90
2	B	48	SER	CA-C-N	-5.46	117.48	122.28
2	B	48	SER	C-N-CA	-5.46	117.48	122.28
4	D	80	THR	CA-C-N	-5.45	114.63	120.03
4	D	80	THR	C-N-CA	-5.45	114.63	120.03
16	v	105	ARG	N-CA-C	5.43	117.96	111.71
10	K	25	LEU	CA-C-N	-5.41	114.05	119.56
10	K	25	LEU	C-N-CA	-5.41	114.05	119.56
2	b	399	VAL	N-CA-C	5.37	115.85	108.12
2	b	196	GLY	N-CA-C	-5.37	106.21	113.24
2	B	49	ASP	CA-C-N	5.36	125.03	119.56
2	B	49	ASP	C-N-CA	5.36	125.03	119.56
10	k	18	PHE	N-CA-C	5.34	122.17	110.80
10	k	25	LEU	N-CA-C	5.32	121.56	109.81
2	B	221	PRO	O-C-N	5.25	123.73	121.31
3	C	221	GLU	N-CA-C	-5.25	105.09	112.12
3	C	60	ILE	N-CA-C	5.23	115.44	110.42
3	C	291	TRP	N-CA-C	5.23	117.06	111.36
1	a	204	GLY	N-CA-C	5.16	118.49	112.50
1	a	83	VAL	N-CA-C	5.14	113.05	108.63
1	a	142	TRP	N-CA-C	5.12	119.22	112.92
13	o	55	GLU	CA-C-N	5.12	125.36	119.83
13	o	55	GLU	C-N-CA	5.12	125.36	119.83
3	c	421	SER	CA-C-N	5.11	125.40	119.47
3	c	421	SER	C-N-CA	5.11	125.40	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	l	4	ASN	CA-C-N	5.10	125.55	120.04
11	l	4	ASN	C-N-CA	5.10	125.55	120.04
1	A	83	VAL	N-CA-C	5.05	112.97	108.63
12	M	7	GLY	N-CA-C	-5.02	106.66	113.24
1	a	77	ILE	N-CA-C	5.02	115.74	110.62
2	b	194	ASN	CA-C-N	5.01	124.61	119.05
2	b	194	ASN	C-N-CA	5.01	124.61	119.05

There are no chirality outliers.

There are no planarity outliers.

3.2 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	2637	0	2551	68	0
1	a	2637	0	2551	59	0
2	B	4024	0	3901	100	0
2	b	4024	0	3901	99	0
3	C	3506	0	3439	67	0
3	c	3506	0	3439	61	0
4	D	2726	0	2627	76	0
4	d	2726	0	2627	65	0
5	E	668	0	658	16	0
5	e	668	0	658	7	0
6	F	275	0	282	17	0
6	f	275	0	282	11	0
7	H	525	0	558	20	0
7	h	525	0	558	18	0
8	I	320	0	339	7	0
8	i	320	0	339	4	0
9	J	272	0	279	2	0
9	j	272	0	279	5	0
10	K	293	0	305	10	0
10	k	293	0	305	15	0
11	L	309	0	327	14	0
11	l	309	0	327	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	M	272	0	300	10	0
12	m	272	0	300	11	0
13	O	1883	0	1865	28	0
13	o	1883	0	1865	26	0
14	T	270	0	278	15	0
14	t	270	0	278	13	0
15	U	774	0	773	9	0
15	u	774	0	773	8	0
16	V	1072	0	1088	13	0
16	v	1072	0	1088	9	0
17	Y	215	0	246	2	0
17	y	215	0	246	6	0
18	X	292	0	328	8	0
18	x	292	0	328	9	0
19	Z	479	0	516	2	0
19	z	479	0	516	2	0
20	A	10	0	0	0	0
20	a	10	0	0	1	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	1	0
22	U	1	0	0	0	0
22	a	2	0	0	0	0
22	u	1	0	0	0	0
23	A	4	0	1	0	0
23	a	4	0	1	0	0
24	A	195	0	216	19	0
24	B	1105	0	1224	67	0
24	C	845	0	936	53	0
24	D	195	0	216	13	0
24	a	260	0	288	16	0
24	b	1105	0	1224	59	0
24	c	845	0	936	40	0
24	d	130	0	144	7	0
25	A	64	0	74	3	0
25	D	64	0	74	10	0
25	a	64	0	74	2	0
25	d	64	0	74	4	0
26	A	40	0	55	14	0
26	B	120	0	165	58	0
26	C	40	0	55	14	0
26	F	40	0	55	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	H	40	0	55	16	0
26	I	40	0	55	18	0
26	K	80	0	110	29	0
26	T	40	0	55	22	0
26	a	40	0	55	13	0
26	b	120	0	166	59	0
26	c	120	0	165	53	0
26	f	40	0	55	21	0
26	h	40	0	55	17	0
26	k	40	0	55	18	0
26	t	40	0	55	23	0
27	A	55	0	80	11	0
27	D	55	0	80	13	0
27	a	55	0	80	12	0
27	d	55	0	80	7	0
28	A	108	0	156	7	0
28	B	54	0	30	8	0
28	L	54	0	26	12	0
28	X	43	0	53	3	0
28	a	108	0	156	3	0
28	b	54	0	30	12	0
28	l	54	0	29	5	0
28	x	43	0	53	4	0
29	A	51	0	72	2	0
29	B	51	0	72	2	0
29	C	102	0	144	4	0
29	D	51	0	72	7	0
29	Z	37	0	44	0	0
29	a	51	0	72	1	0
29	b	51	0	72	4	0
29	c	102	0	144	2	0
29	j	51	0	72	6	0
29	z	37	0	44	1	0
30	A	49	0	74	10	0
30	D	98	0	148	8	0
30	E	42	0	57	0	0
30	L	49	0	74	6	0
30	a	49	0	74	10	0
30	d	98	0	148	4	0
30	e	42	0	57	2	0
30	l	49	0	74	6	0
31	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	F	1	0	0	0	0
31	O	1	0	0	0	0
31	b	1	0	0	0	0
31	f	1	0	0	0	0
31	o	1	0	0	0	0
32	C	186	0	246	5	0
32	E	62	0	82	1	0
32	H	62	0	82	6	0
32	c	186	0	246	8	0
32	d	62	0	82	4	0
32	h	62	0	82	6	0
33	E	43	0	30	6	0
33	V	43	0	30	7	0
33	e	43	0	30	2	0
33	v	43	0	30	4	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	50074	0	51320	1280	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 13.

All (1280) 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)
26:T:101:BCR:C22	26:T:101:BCR:C37	1.74	1.65
26:B:619:BCR:C19	26:B:619:BCR:C20	1.76	1.64
26:B:620:BCR:C37	26:B:620:BCR:C22	1.76	1.64
26:c:514:BCR:C20	26:c:514:BCR:C19	1.74	1.62
26:b:619:BCR:C22	26:b:619:BCR:C37	1.75	1.62
26:t:101:BCR:C20	26:t:101:BCR:C19	1.76	1.62
26:b:619:BCR:C19	26:b:619:BCR:C20	1.75	1.62
26:B:618:BCR:C18	26:B:618:BCR:C36	1.77	1.61
26:B:619:BCR:C18	26:B:619:BCR:C36	1.76	1.61
26:f:101:BCR:C37	26:f:101:BCR:C22	1.75	1.61
26:C:514:BCR:C20	26:C:514:BCR:C21	1.78	1.61
26:T:101:BCR:C20	26:T:101:BCR:C21	1.78	1.61
26:t:101:BCR:C18	26:t:101:BCR:C36	1.78	1.61
26:T:101:BCR:C20	26:T:101:BCR:C19	1.75	1.61
26:k:101:BCR:C37	26:k:101:BCR:C22	1.75	1.61
26:B:618:BCR:C20	26:B:618:BCR:C19	1.75	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:621:BCR:C18	26:b:621:BCR:C36	1.78	1.60
26:c:515:BCR:C20	26:c:515:BCR:C21	1.78	1.60
26:H:101:BCR:C18	26:H:101:BCR:C36	1.79	1.60
26:K:102:BCR:C20	26:K:102:BCR:C21	1.79	1.59
26:b:620:BCR:C36	26:b:620:BCR:C18	1.79	1.59
26:B:618:BCR:C37	26:B:618:BCR:C22	1.75	1.59
26:A:610:BCR:C18	26:A:610:BCR:C36	1.79	1.59
26:F:101:BCR:C20	26:F:101:BCR:C21	1.80	1.59
26:b:621:BCR:C37	26:b:621:BCR:C22	1.77	1.59
26:h:101:BCR:C18	26:h:101:BCR:C36	1.81	1.59
26:F:101:BCR:C18	26:F:101:BCR:C36	1.77	1.59
26:a:610:BCR:C18	26:a:610:BCR:C36	1.78	1.59
26:c:515:BCR:C20	26:c:515:BCR:C19	1.74	1.59
26:k:101:BCR:C21	26:k:101:BCR:C20	1.78	1.59
26:C:514:BCR:C18	26:C:514:BCR:C36	1.80	1.58
26:b:619:BCR:C20	26:b:619:BCR:C21	1.79	1.58
26:C:514:BCR:C37	26:C:514:BCR:C22	1.76	1.58
26:f:101:BCR:C18	26:f:101:BCR:C36	1.78	1.58
26:F:101:BCR:C20	26:F:101:BCR:C19	1.74	1.57
26:T:101:BCR:C18	26:T:101:BCR:C36	1.79	1.57
26:a:610:BCR:C21	26:a:610:BCR:C20	1.77	1.57
26:t:101:BCR:C37	26:t:101:BCR:C22	1.75	1.57
26:c:515:BCR:C18	26:c:515:BCR:C36	1.80	1.57
26:c:521:BCR:C19	26:c:521:BCR:C20	1.80	1.57
26:B:618:BCR:C20	26:B:618:BCR:C21	1.80	1.57
26:h:101:BCR:C20	26:h:101:BCR:C19	1.75	1.57
26:A:610:BCR:C21	26:A:610:BCR:C20	1.77	1.56
26:A:610:BCR:C37	26:A:610:BCR:C22	1.75	1.56
26:c:514:BCR:C20	26:c:514:BCR:C21	1.76	1.56
26:B:620:BCR:C18	26:B:620:BCR:C36	1.80	1.56
26:I:101:BCR:C21	26:I:101:BCR:C20	1.78	1.56
26:K:102:BCR:C22	26:K:102:BCR:C37	1.76	1.56
26:b:620:BCR:C20	26:b:620:BCR:C21	1.77	1.56
26:K:102:BCR:C18	26:K:102:BCR:C36	1.80	1.56
26:H:101:BCR:C20	26:H:101:BCR:C21	1.76	1.55
26:k:101:BCR:C18	26:k:101:BCR:C36	1.80	1.55
26:K:101:BCR:C37	26:K:101:BCR:C22	1.75	1.55
26:B:620:BCR:C20	26:B:620:BCR:C21	1.78	1.55
26:h:101:BCR:C20	26:h:101:BCR:C21	1.78	1.55
26:b:619:BCR:C18	26:b:619:BCR:C36	1.79	1.54
26:K:101:BCR:C21	26:K:101:BCR:C20	1.78	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:521:BCR:C22	26:c:521:BCR:C37	1.83	1.54
26:a:610:BCR:C37	26:a:610:BCR:C22	1.75	1.54
26:b:621:BCR:C20	26:b:621:BCR:C19	1.82	1.54
26:t:101:BCR:C20	26:t:101:BCR:C21	1.79	1.54
26:c:521:BCR:C18	26:c:521:BCR:C36	1.82	1.54
26:B:619:BCR:C20	26:B:619:BCR:C21	1.80	1.53
26:I:101:BCR:C18	26:I:101:BCR:C36	1.79	1.53
26:f:101:BCR:C21	26:f:101:BCR:C20	1.78	1.53
26:K:101:BCR:C18	26:K:101:BCR:C36	1.78	1.52
26:c:514:BCR:C18	26:c:514:BCR:C36	1.80	1.52
26:c:521:BCR:C20	26:c:521:BCR:C21	1.83	1.52
26:b:621:BCR:C20	26:b:621:BCR:C21	1.90	1.48
2:b:113:TRP:HB2	26:b:621:BCR:H21C	1.32	1.12
3:c:165:LEU:HD21	24:c:506:CLA:HAB	1.41	1.01
24:b:609:CLA:HMC2	26:b:620:BCR:HC8	1.44	1.00
26:B:618:BCR:C37	26:B:618:BCR:C21	2.42	0.97
26:T:101:BCR:C37	26:T:101:BCR:C21	2.43	0.96
26:b:621:BCR:C36	26:b:621:BCR:C19	2.44	0.96
28:b:601:SQD:H121	24:b:616:CLA:H43	1.44	0.95
26:B:618:BCR:H12C	26:B:619:BCR:H10C	1.48	0.94
2:B:106:LEU:HB3	26:B:620:BCR:H15C	1.49	0.94
26:k:101:BCR:C37	26:k:101:BCR:C21	2.45	0.93
26:c:521:BCR:C20	26:c:521:BCR:C22	2.45	0.93
26:B:619:BCR:C19	26:B:619:BCR:C36	2.47	0.93
26:c:514:BCR:C20	26:c:514:BCR:C22	2.45	0.93
26:K:102:BCR:C20	26:K:102:BCR:C22	2.46	0.92
26:b:619:BCR:C37	26:b:619:BCR:C21	2.43	0.92
3:C:124:VAL:HG11	26:C:514:BCR:H17C	1.48	0.92
26:b:619:BCR:C19	26:b:619:BCR:H20C	2.01	0.90
26:A:610:BCR:C21	26:A:610:BCR:C37	2.48	0.90
26:h:101:BCR:C19	26:h:101:BCR:H20C	2.02	0.89
24:B:615:CLA:H43	28:B:622:SQD:H121	1.54	0.89
26:K:101:BCR:C37	26:K:101:BCR:C21	2.45	0.89
26:K:102:BCR:C21	26:K:102:BCR:C37	2.49	0.89
26:c:514:BCR:C19	26:c:514:BCR:H20C	2.01	0.88
26:B:620:BCR:C37	26:B:620:BCR:C21	2.46	0.88
26:C:514:BCR:C20	26:C:514:BCR:C22	2.47	0.88
26:T:101:BCR:C19	26:T:101:BCR:H20C	2.01	0.87
26:b:620:BCR:C20	26:b:620:BCR:C22	2.46	0.87
26:c:515:BCR:C19	26:c:515:BCR:H20C	2.02	0.87
26:b:619:BCR:C21	26:b:619:BCR:H20C	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:101:BCR:C22	26:T:101:BCR:C20	2.50	0.87
26:c:514:BCR:C21	26:c:514:BCR:H20C	2.03	0.86
26:A:610:BCR:C21	26:A:610:BCR:H20C	2.05	0.86
26:B:618:BCR:C19	26:B:618:BCR:H20C	2.03	0.86
26:b:621:BCR:C37	26:b:621:BCR:C21	2.50	0.86
26:B:619:BCR:C20	26:B:619:BCR:C18	2.51	0.86
26:T:101:BCR:C21	26:T:101:BCR:H20C	2.04	0.86
26:a:610:BCR:C21	26:a:610:BCR:H20C	2.03	0.86
26:B:620:BCR:C22	26:B:620:BCR:C20	2.51	0.85
26:t:101:BCR:C21	26:t:101:BCR:H20C	2.06	0.85
26:h:101:BCR:C21	26:h:101:BCR:H20C	2.05	0.85
26:F:101:BCR:C19	26:F:101:BCR:H20C	2.03	0.85
26:a:610:BCR:C20	26:a:610:BCR:C22	2.48	0.85
26:h:101:BCR:C20	26:h:101:BCR:C22	2.48	0.84
18:x:24:THR:HA	28:x:101:SQD:H331	1.59	0.84
26:I:101:BCR:C21	26:I:101:BCR:H20C	2.04	0.84
26:b:621:BCR:C22	26:b:621:BCR:C20	2.55	0.84
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.39	0.84
26:t:101:BCR:C37	26:t:101:BCR:C21	2.49	0.84
26:b:619:BCR:C22	26:b:619:BCR:C20	2.50	0.83
26:k:101:BCR:C21	26:k:101:BCR:H20C	2.08	0.83
26:C:514:BCR:C21	26:C:514:BCR:C37	2.48	0.83
26:a:610:BCR:C21	26:a:610:BCR:C37	2.49	0.83
26:f:101:BCR:C37	26:f:101:BCR:C21	2.50	0.83
26:K:101:BCR:C36	26:K:101:BCR:C19	2.55	0.83
26:B:618:BCR:C20	26:B:618:BCR:C22	2.50	0.83
26:K:102:BCR:C21	26:K:102:BCR:H20C	2.06	0.83
26:c:515:BCR:C21	26:c:515:BCR:H20C	2.05	0.82
26:h:101:BCR:C18	26:h:101:BCR:C20	2.54	0.82
26:F:101:BCR:C36	26:F:101:BCR:C17	2.58	0.82
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.60	0.82
2:b:127:ARG:HH11	2:b:127:ARG:HG3	1.44	0.82
2:b:432:PHE:O	13:o:178:LYS:NZ	2.12	0.82
26:t:101:BCR:C19	26:t:101:BCR:H20C	2.03	0.82
26:B:620:BCR:C21	26:B:620:BCR:H20C	2.09	0.82
26:k:101:BCR:C22	26:k:101:BCR:C20	2.53	0.82
26:I:101:BCR:C20	26:I:101:BCR:C22	2.49	0.81
26:b:620:BCR:C21	26:b:620:BCR:H20C	2.05	0.81
26:B:619:BCR:C21	26:B:619:BCR:H20C	2.09	0.81
24:a:609:CLA:HAC1	26:a:610:BCR:H15C	1.63	0.81
26:c:514:BCR:C20	26:c:514:BCR:C18	2.51	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:514:BCR:C36	26:C:514:BCR:C19	2.57	0.81
26:f:101:BCR:C21	26:f:101:BCR:H20C	2.08	0.81
30:A:615:LHG:H382	30:A:615:LHG:H112	1.63	0.80
7:H:38:PHE:HB2	26:H:101:BCR:H10C	1.62	0.80
26:B:619:BCR:C19	26:B:619:BCR:H20C	2.05	0.80
3:c:124:VAL:HG11	26:c:514:BCR:H17C	1.64	0.80
26:b:621:BCR:C19	26:b:621:BCR:H20C	2.10	0.79
26:c:521:BCR:C19	26:c:521:BCR:H20C	2.08	0.79
4:d:24:ARG:HD3	18:x:37:VAL:HG22	1.63	0.79
26:c:521:BCR:C19	26:c:521:BCR:C36	2.58	0.79
26:B:618:BCR:C21	26:B:618:BCR:H20C	2.07	0.78
30:a:616:LHG:H151	30:a:616:LHG:H352	1.64	0.78
26:c:521:BCR:C21	26:c:521:BCR:H20C	2.11	0.78
24:c:501:CLA:H193	24:c:507:CLA:HBB1	1.64	0.78
26:C:514:BCR:C21	26:C:514:BCR:H20C	2.06	0.78
26:K:101:BCR:C21	26:K:101:BCR:H20C	2.08	0.77
26:A:610:BCR:C36	26:A:610:BCR:C19	2.57	0.77
26:F:101:BCR:C21	26:F:101:BCR:H20C	2.08	0.76
26:T:101:BCR:C19	26:T:101:BCR:C36	2.59	0.76
26:c:515:BCR:C19	26:c:515:BCR:C36	2.56	0.76
26:H:101:BCR:C20	26:H:101:BCR:C22	2.53	0.75
11:L:14:ARG:HD3	28:L:102:SQD:H241	1.68	0.75
3:C:339:LYS:NZ	15:U:99:ASN:O	2.18	0.75
26:A:610:BCR:C20	26:A:610:BCR:C22	2.54	0.75
26:b:620:BCR:C36	26:b:620:BCR:C19	2.58	0.75
4:D:193:LEU:O	11:L:34:TYR:OH	2.02	0.75
26:K:101:BCR:H16C	17:Y:33:PRO:HD3	1.68	0.75
24:b:603:CLA:H152	26:h:101:BCR:H17C	1.68	0.75
24:B:602:CLA:HHC	24:B:602:CLA:HBB1	1.68	0.74
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.68	0.74
5:e:56:TYR:O	16:v:1:ALA:N	2.16	0.74
24:c:510:CLA:HBC3	24:c:510:CLA:H192	1.70	0.74
32:d:405:DGD:HA91	26:f:101:BCR:H322	1.70	0.74
2:B:479:PHE:O	4:D:139:ARG:NH2	2.21	0.74
26:H:101:BCR:C21	26:H:101:BCR:H20C	2.10	0.73
4:D:87:HIS:ND1	32:H:102:DGD:O2D	2.15	0.73
26:a:610:BCR:C36	26:a:610:BCR:C19	2.59	0.73
26:c:515:BCR:C20	26:c:515:BCR:C22	2.53	0.73
26:t:101:BCR:C19	26:t:101:BCR:C36	2.59	0.73
28:L:102:SQD:O49	28:b:601:SQD:C46	2.29	0.73
24:a:607:CLA:H152	27:a:611:PL9:H262	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:33:TRP:N	26:b:620:BCR:H15C	2.04	0.73
26:c:515:BCR:C20	26:c:515:BCR:C18	2.58	0.73
26:I:101:BCR:C20	26:I:101:BCR:C37	2.67	0.72
1:A:214:MET:HG2	27:A:611:PL9:H102	1.71	0.72
3:C:213[B]:LEU:HD21	26:I:101:BCR:H20C	1.71	0.72
26:T:101:BCR:C20	26:T:101:BCR:C18	2.57	0.72
26:B:618:BCR:H402	28:B:622:SQD:H82	1.71	0.72
1:A:50:ILE:HG22	26:A:610:BCR:H271	1.72	0.72
26:k:101:BCR:C36	26:k:101:BCR:C19	2.57	0.71
26:t:101:BCR:C20	26:t:101:BCR:C22	2.54	0.71
3:C:124:VAL:HG11	26:C:514:BCR:C17	2.18	0.71
1:a:106:LEU:HD21	26:a:610:BCR:H383	1.71	0.71
28:b:601:SQD:H62	11:l:7:ARG:HH21	1.53	0.71
10:k:34:ALA:HB1	26:k:101:BCR:C20	2.21	0.71
26:f:101:BCR:C36	26:f:101:BCR:C17	2.66	0.70
24:C:501:CLA:C1D	24:C:503:CLA:H2	2.21	0.70
4:D:279:LEU:HD22	25:D:401:PHO:HBC3	1.73	0.70
27:D:405:PL9:H411	11:L:29:LEU:HD23	1.74	0.70
10:K:17:ILE:H	10:K:17:ILE:HD13	1.56	0.70
26:B:620:BCR:C36	26:B:620:BCR:C19	2.63	0.69
3:c:213[B]:LEU:HD11	26:c:515:BCR:C22	2.22	0.69
26:F:101:BCR:C20	26:F:101:BCR:C22	2.57	0.69
7:h:38:PHE:HB2	26:h:101:BCR:H10C	1.73	0.69
28:A:614:SQD:H272	26:b:621:BCR:H19C	1.74	0.69
26:b:621:BCR:C21	26:b:621:BCR:H20C	2.16	0.68
26:B:619:BCR:H381	26:t:101:BCR:H341	1.75	0.68
1:a:214:MET:HG2	27:a:611:PL9:H102	1.74	0.68
26:c:521:BCR:C20	26:c:521:BCR:C18	2.63	0.68
28:A:614:SQD:C27	26:b:621:BCR:H19C	2.24	0.68
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.74	0.68
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.73	0.68
26:K:101:BCR:C22	26:K:101:BCR:C20	2.55	0.68
26:I:101:BCR:C36	26:I:101:BCR:C19	2.59	0.67
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.76	0.67
24:b:616:CLA:H18	29:b:622:LMG:H421	1.77	0.67
24:C:501:CLA:H192	24:C:506:CLA:C1B	2.24	0.67
26:H:101:BCR:C36	26:H:101:BCR:C19	2.61	0.67
26:c:514:BCR:C19	26:c:514:BCR:C36	2.62	0.67
5:E:23:HIS:NE2	33:E:103:HEM:ND	2.44	0.66
24:C:501:CLA:C2D	24:C:503:CLA:H2	2.25	0.66
24:C:513:CLA:HBB1	24:C:513:CLA:HMB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:x:31:ILE:HG23	28:x:101:SQD:H462	1.78	0.66
24:b:616:CLA:HMB1	24:b:616:CLA:HBB1	1.78	0.66
1:A:310:LYS:NZ	5:E:58:GLN:O	2.29	0.66
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.31	0.66
26:c:521:BCR:H391	10:k:36:ALA:HB2	1.78	0.66
28:L:102:SQD:O49	28:b:601:SQD:H461	1.94	0.65
30:a:616:LHG:H223	32:c:518:DGD:HBH2	1.79	0.65
26:b:619:BCR:C37	26:b:619:BCR:C20	2.74	0.65
26:F:101:BCR:H20C	26:F:101:BCR:C37	2.27	0.65
26:B:618:BCR:C36	26:B:618:BCR:C17	2.70	0.65
16:V:3:LEU:HD23	16:V:23:GLU:HG3	1.78	0.65
4:D:192:THR:HG23	24:D:403:CLA:HBC2	1.78	0.65
11:l:21:LEU:HD13	28:l:101:SQD:H312	1.78	0.65
26:B:618:BCR:C18	26:B:618:BCR:C20	2.59	0.65
24:b:612:CLA:OBD	24:b:612:CLA:H152	1.97	0.65
28:A:612:SQD:O7	3:C:28:GLN:NE2	2.24	0.65
2:b:113:TRP:CB	26:b:621:BCR:H21C	2.18	0.65
24:B:616:CLA:H51	26:B:620:BCR:H11C	1.77	0.64
2:B:450:TRP:CD1	24:B:608:CLA:HBA1	2.32	0.64
26:b:621:BCR:C18	26:b:621:BCR:C20	2.65	0.64
4:d:186:GLN:HB2	24:d:402:CLA:HBC1	1.80	0.64
26:K:102:BCR:C36	26:K:102:BCR:C19	2.62	0.64
4:d:315:TYR:CZ	4:d:319:LEU:HD11	2.33	0.64
2:B:383:PHE:O	13:O:166:SER:HA	1.97	0.64
26:h:101:BCR:C36	26:h:101:BCR:C17	2.71	0.64
3:C:213[B]:LEU:HD11	26:I:101:BCR:C22	2.27	0.64
24:a:607:CLA:H122	27:a:611:PL9:H23	1.79	0.64
3:C:406:SER:HA	3:C:420:VAL:HG23	1.79	0.64
4:d:87:HIS:ND1	32:h:102:DGD:O2D	2.27	0.64
26:F:101:BCR:C20	26:F:101:BCR:C18	2.61	0.63
2:B:464:PHE:HD2	24:B:612:CLA:HAC2	1.63	0.63
26:B:619:BCR:H17C	26:t:101:BCR:C17	2.28	0.63
3:C:71:GLU:HB3	3:C:86:LEU:HD22	1.79	0.63
4:D:141:TYR:OH	30:D:406:LHG:O4	2.16	0.63
26:h:101:BCR:C36	26:h:101:BCR:C19	2.64	0.63
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.78	0.63
26:f:101:BCR:C36	26:f:101:BCR:C19	2.63	0.63
28:L:102:SQD:H45	14:T:23:PHE:CD1	2.33	0.63
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.79	0.63
2:B:29:LEU:HD21	26:B:618:BCR:H19C	1.80	0.63
26:B:618:BCR:C36	26:B:618:BCR:C19	2.60	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:507:CLA:OBD	24:C:509:CLA:H122	1.99	0.62
1:a:308:ASP:HB2	5:e:52:PRO:O	1.98	0.62
24:A:609:CLA:HAC2	26:A:610:BCR:H362	1.82	0.62
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.81	0.62
14:T:1[B]:MET:HB3	14:T:4:ILE:HD12	1.81	0.62
26:c:521:BCR:H15C	26:k:101:BCR:H342	1.81	0.62
24:C:501:CLA:H193	24:C:507:CLA:HBB1	1.80	0.62
3:c:83:GLU:OE2	3:c:398:HIS:NE2	2.32	0.62
13:o:57:LYS:O	13:o:58:ASN:HB2	1.99	0.62
26:b:619:BCR:C36	26:b:619:BCR:C17	2.70	0.62
26:c:521:BCR:C37	26:c:521:BCR:C21	2.60	0.62
13:o:58:ASN:HA	13:o:60:ARG:NH2	2.15	0.62
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.82	0.62
26:c:515:BCR:H20C	26:c:515:BCR:C37	2.28	0.62
26:f:101:BCR:C22	26:f:101:BCR:C20	2.58	0.62
28:l:101:SQD:H342	14:t:12:CYS:HB3	1.81	0.62
24:C:506:CLA:HMB3	24:C:506:CLA:HBB1	1.80	0.62
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.81	0.62
30:l:102:LHG:H271	12:m:22:LEU:HD11	1.82	0.62
26:b:619:BCR:C37	26:b:619:BCR:H20C	2.30	0.61
3:C:443:TRP:CE2	24:C:508:CLA:HMD2	2.35	0.61
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.82	0.61
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.82	0.61
28:B:622:SQD:H442	28:l:101:SQD:O7	2.00	0.61
4:d:214:HIS:ND1	27:d:404:PL9:O2	2.28	0.61
26:C:514:BCR:H15C	29:C:519:LMG:H401	1.83	0.61
30:d:406:LHG:HC91	30:l:102:LHG:HC81	1.82	0.61
28:A:614:SQD:H132	26:T:101:BCR:HC41	1.82	0.61
30:A:615:LHG:H371	24:C:508:CLA:H92	1.82	0.61
24:B:614:CLA:H193	26:B:619:BCR:C5	2.31	0.61
26:B:618:BCR:H15C	26:B:619:BCR:H352	1.83	0.61
10:K:36:ALA:HB2	26:K:102:BCR:H391	1.83	0.61
1:a:132:GLU:O	1:a:136:ARG:HG2	2.00	0.61
24:C:501:CLA:C1C	24:C:503:CLA:H71	2.30	0.61
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.83	0.61
1:a:172:MET:HE1	24:a:615:CLA:CHC	2.31	0.61
13:o:58:ASN:HA	13:o:60:ARG:HH21	1.66	0.60
33:E:103:HEM:HBB2	33:E:103:HEM:HMB2	1.81	0.60
8:i:1[C]:MET:HE3	8:i:4:LEU:HB2	1.83	0.60
2:B:32:GLY:HA3	26:B:619:BCR:H19C	1.82	0.60
33:V:201:HEM:HMB1	33:V:201:HEM:HBB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:619:BCR:H333	12:m:13:LEU:HD12	1.83	0.60
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.02	0.60
6:F:20:TRP:CE2	6:F:24:HIS:CE1	2.90	0.60
1:A:42:LEU:HD13	26:A:610:BCR:H353	1.83	0.60
11:L:22:LEU:HD23	30:L:101:LHG:H162	1.84	0.60
24:b:614:CLA:H91	24:b:615:CLA:HBB1	1.84	0.59
33:v:201:HEM:HMC1	33:v:201:HEM:HBC2	1.84	0.59
24:B:612:CLA:H162	26:B:619:BCR:H342	1.84	0.59
26:B:619:BCR:C20	26:B:619:BCR:C22	2.60	0.59
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.85	0.59
3:C:324:LEU:HB3	15:U:32:ILE:HD13	1.84	0.59
24:D:404:CLA:H2	18:X:14:LEU:HA	1.83	0.59
26:c:514:BCR:C36	26:c:514:BCR:C17	2.74	0.59
1:A:84:PRO:HA	1:A:112:TYR:CG	2.37	0.59
24:A:607:CLA:H152	27:A:611:PL9:H262	1.83	0.59
14:T:8:PHE:CE1	24:b:616:CLA:H171	2.37	0.59
2:b:18:ARG:NH2	28:b:601:SQD:O9	2.36	0.59
26:T:101:BCR:C17	26:b:620:BCR:H17C	2.33	0.59
1:A:126:TYR:CZ	25:A:608:PHO:HBA1	2.38	0.59
24:C:511:CLA:HBB1	24:C:511:CLA:HMB3	1.84	0.59
29:D:408:LMG:H411	6:F:30:THR:HG21	1.85	0.59
1:A:269:ARG:NH1	4:D:222:LEU:HD13	2.18	0.59
1:A:308:ASP:HB2	5:E:52:PRO:O	2.02	0.59
2:B:30:VAL:HG22	24:B:614:CLA:C3C	2.33	0.58
3:C:165:LEU:HD21	24:C:506:CLA:HAB	1.85	0.58
24:b:616:CLA:H101	26:b:619:BCR:H362	1.84	0.58
3:c:213[B]:LEU:HD11	26:c:515:BCR:C21	2.32	0.58
33:e:102:HEM:HMB1	33:e:102:HEM:HBB2	1.84	0.58
3:c:210:PHE:HD2	3:c:213[B]:LEU:HD22	1.68	0.58
3:c:124:VAL:HG11	26:c:514:BCR:C17	2.33	0.58
4:d:123:ILE:HD11	32:h:102:DGD:HAH2	1.86	0.58
26:T:101:BCR:C37	26:T:101:BCR:H20C	2.32	0.58
1:a:323:ARG:HB3	4:d:329:MET:HA	1.84	0.58
15:U:27:LEU:HD21	15:U:82:PHE:CG	2.39	0.58
30:a:616:LHG:H132	30:a:616:LHG:H372	1.86	0.58
26:T:101:BCR:C37	26:T:101:BCR:C20	2.81	0.58
26:f:101:BCR:C37	26:f:101:BCR:C23	2.75	0.58
13:o:142:PHE:HB2	13:o:199:LEU:HB2	1.86	0.58
3:C:206:PRO:HG3	3:C:239:TRP:HZ2	1.69	0.58
26:K:102:BCR:C36	26:K:102:BCR:C16	2.82	0.58
24:a:615:CLA:H41	27:d:404:PL9:H202	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:t:101:BCR:C20	26:t:101:BCR:C18	2.65	0.58
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.86	0.57
24:C:501:CLA:C3D	24:C:503:CLA:H2	2.34	0.57
26:b:619:BCR:C19	26:b:619:BCR:C36	2.63	0.57
2:B:339:ALA:HB2	13:o:58:ASN:HB3	1.85	0.57
3:C:418:ASN:HB2	32:C:517:DGD:O4E	2.03	0.57
24:c:506:CLA:H162	26:c:515:BCR:H15C	1.84	0.57
26:F:101:BCR:C36	26:F:101:BCR:C19	2.65	0.57
30:a:616:LHG:H112	30:a:616:LHG:H382	1.85	0.57
5:E:56:TYR:O	16:V:1:ALA:N	2.23	0.57
24:b:606:CLA:H12	24:b:607:CLA:ND	2.19	0.57
1:a:215:HIS:HA	27:a:611:PL9:O1	2.05	0.57
26:B:620:BCR:C36	26:B:620:BCR:C17	2.72	0.57
6:F:34:LEU:HD21	26:F:101:BCR:H373	1.87	0.57
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.40	0.57
1:A:153:SER:HB2	24:A:606:CLA:H43	1.86	0.57
2:B:126:PRO:HB3	7:H:12[B]:ARG:NH1	2.19	0.57
2:B:467:ILE:HG13	4:D:126:MET:HE1	1.87	0.57
8:I:20:VAL:HG13	26:I:101:BCR:HC41	1.86	0.57
13:O:57:LYS:O	13:O:58:ASN:HB2	2.03	0.57
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.86	0.57
3:C:334:PRO:HA	13:O:153:THR:OG1	2.05	0.57
4:d:257:PHE:O	30:d:407:LHG:H351	2.04	0.57
3:C:400:PRO:C	3:C:401:LEU:HD12	2.30	0.57
13:O:58:ASN:HA	13:O:60:ARG:HH21	1.70	0.57
26:t:101:BCR:C37	26:t:101:BCR:H20C	2.35	0.57
16:v:41:HIS:CD2	33:v:201:HEM:NB	2.73	0.57
2:B:28:ALA:HB1	28:B:622:SQD:H221	1.87	0.57
32:E:101:DGD:O1B	32:E:101:DGD:O2D	2.21	0.57
4:d:67:TYR:O	29:j:101:LMG:O5	2.20	0.56
2:B:72:THR:HG22	2:B:80:ILE:HD11	1.86	0.56
26:B:619:BCR:C36	26:B:619:BCR:C17	2.75	0.56
8:I:1[C]:MET:HE3	8:I:4:LEU:HB2	1.86	0.56
26:H:101:BCR:C36	26:H:101:BCR:C17	2.72	0.56
26:a:610:BCR:C36	26:a:610:BCR:C17	2.73	0.56
3:c:178:LYS:HB2	24:c:502:CLA:H141	1.88	0.56
24:B:605:CLA:H12	24:B:606:CLA:ND	2.21	0.56
10:K:35:LEU:HB2	26:K:101:BCR:H15C	1.85	0.56
1:a:129:ARG:NH2	4:d:255:GLN:O	2.39	0.56
2:b:475:PHE:CD2	4:d:140:PRO:HG3	2.41	0.56
3:c:429:SER:HA	32:c:517:DGD:HBE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:501:CLA:C2D	24:c:503:CLA:H2	2.36	0.56
1:A:332:HIS:HA	22:A:603:CL:CL	2.43	0.56
27:a:611:PL9:H221	25:d:401:PHO:HMA2	1.87	0.56
2:b:127:ARG:HG3	2:b:127:ARG:NH1	2.18	0.56
2:b:383:PHE:O	13:o:166:SER:HA	2.05	0.56
26:I:101:BCR:C36	26:I:101:BCR:C17	2.74	0.56
10:K:34:ALA:HB1	26:K:101:BCR:C20	2.35	0.56
28:L:102:SQD:H181	26:T:101:BCR:H351	1.88	0.56
2:b:479:PHE:O	4:d:139:ARG:NH2	2.33	0.56
24:b:613:CLA:HBB1	24:b:613:CLA:HMB1	1.88	0.56
24:c:508:CLA:HBC3	24:c:510:CLA:H71	1.88	0.56
1:A:74:GLY:O	4:D:301:GLN:NE2	2.39	0.55
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.21	0.55
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.36	0.55
3:c:406:SER:HA	3:c:420:VAL:HG23	1.87	0.55
7:h:65:LEU:HD12	7:h:66:GLY:H	1.72	0.55
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.89	0.55
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.40	0.55
3:C:216:SER:HB3	3:C:221:GLU:HG3	1.89	0.55
16:V:122:GLU:HG3	16:V:126:LEU:HD12	1.88	0.55
24:C:506:CLA:H162	26:I:101:BCR:H15C	1.89	0.55
7:H:35:MET:CG	26:H:101:BCR:HC42	2.37	0.55
10:K:25:LEU:HD21	26:K:101:BCR:HC41	1.89	0.55
1:A:195:HIS:CE1	1:A:197:PHE:HB2	2.41	0.55
24:A:607:CLA:H122	27:A:611:PL9:H23	1.88	0.55
14:T:8:PHE:HD1	26:T:101:BCR:H373	1.72	0.55
16:V:40:CYS:SG	33:V:201:HEM:CAC	2.95	0.55
4:d:149:PRO:HA	24:d:402:CLA:H41	1.88	0.55
11:l:14:ARG:HD3	28:l:101:SQD:H241	1.89	0.55
24:c:501:CLA:C1D	24:c:503:CLA:H2	2.36	0.55
26:K:102:BCR:C36	26:K:102:BCR:C17	2.73	0.55
28:L:102:SQD:H311	28:b:601:SQD:H292	1.84	0.55
16:V:41:HIS:CD2	33:V:201:HEM:NB	2.75	0.55
2:b:25:MET:HG2	26:b:619:BCR:C21	2.37	0.55
9:j:9:PRO:HD2	9:j:12:ILE:HD12	1.89	0.54
26:t:101:BCR:C36	26:t:101:BCR:C17	2.75	0.54
7:h:36:GLY:O	7:h:40:VAL:HG23	2.08	0.54
1:A:308:ASP:HB3	1:A:314:ILE:HD11	1.88	0.54
2:B:457:VAL:HG11	29:B:621:LMG:H211	1.89	0.54
15:U:76:ARG:HA	15:U:79:LEU:HG	1.89	0.54
4:D:269:PHE:CD2	30:D:406:LHG:HC11	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:58:ASN:HA	13:O:60:ARG:NH2	2.23	0.54
24:b:606:CLA:H2	24:b:607:CLA:C4C	2.37	0.54
26:k:101:BCR:H17C	17:y:33:PRO:HD3	1.88	0.54
15:u:27:LEU:HD21	15:u:82:PHE:CG	2.43	0.54
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.88	0.54
14:t:22:PHE:CE2	26:t:101:BCR:H333	2.43	0.54
30:A:615:LHG:H352	30:A:615:LHG:H151	1.90	0.54
2:b:460:LEU:O	2:b:463:PHE:HB3	2.08	0.54
4:d:193:LEU:O	11:l:34:TYR:OH	2.19	0.54
1:A:225:ARG:HA	2:B:480:SER:O	2.08	0.54
24:A:609:CLA:HMA2	29:A:613:LMG:H132	1.90	0.54
7:H:35:MET:HG2	26:H:101:BCR:HC42	1.90	0.54
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.88	0.54
1:A:276:ALA:HB1	30:A:615:LHG:H262	1.90	0.53
2:B:432:PHE:O	13:O:178:LYS:NZ	2.35	0.53
24:B:604:CLA:O1A	24:B:604:CLA:H3A	2.08	0.53
26:K:101:BCR:HC8	19:Z:20:VAL:HG21	1.90	0.53
24:c:509:CLA:HMB1	24:c:509:CLA:HBB1	1.90	0.53
1:A:105:TRP:HZ3	26:A:610:BCR:H24C	1.72	0.53
26:A:610:BCR:C36	26:A:610:BCR:C17	2.74	0.53
2:B:190:PHE:HB3	7:H:45:ILE:HG22	1.90	0.53
26:c:521:BCR:H24C	26:c:521:BCR:H371	1.91	0.53
26:f:101:BCR:H372	29:j:101:LMG:H292	1.90	0.53
1:A:132:GLU:O	1:A:136:ARG:HG2	2.07	0.53
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.88	0.53
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.89	0.53
1:a:210:LEU:HG	25:d:401:PHO:NC	2.22	0.53
26:I:101:BCR:H20C	26:I:101:BCR:C37	2.37	0.53
1:a:153:SER:HB3	24:a:606:CLA:HED1	1.90	0.53
24:C:510:CLA:HMB1	24:C:510:CLA:HBB1	1.88	0.53
5:E:8:ARG:O	6:F:19:ARG:NH2	2.34	0.53
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.89	0.53
1:A:24:THR:O	4:D:255:GLN:NE2	2.41	0.53
24:C:510:CLA:HBC3	24:C:510:CLA:H192	1.90	0.53
24:b:609:CLA:H102	29:b:622:LMG:H221	1.91	0.53
24:c:501:CLA:C1C	24:c:503:CLA:H71	2.39	0.53
2:B:274:GLN:HB3	2:B:280:PHE:CE2	2.43	0.53
24:B:616:CLA:H2	24:B:617:CLA:HBB2	1.91	0.53
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.91	0.53
4:D:303:ILE:HG21	12:M:2:GLU:HG3	1.89	0.53
20:a:601:OEX:O2	3:c:357:ARG:NH2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:601:SQD:H82	26:b:619:BCR:H402	1.91	0.53
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.44	0.53
4:D:48:TRP:CD1	25:D:401:PHO:H162	2.43	0.53
5:E:51:ARG:N	5:E:54[B]:SER:OG	2.42	0.53
26:b:619:BCR:C20	26:b:619:BCR:C18	2.64	0.53
1:A:206:PHE:CZ	24:D:403:CLA:HAA1	2.44	0.52
6:F:37:ILE:HA	6:F:40:MET:SD	2.48	0.52
14:t:8:PHE:HD1	26:t:101:BCR:H373	1.74	0.52
2:B:127:ARG:HG3	2:B:127:ARG:NH1	2.13	0.52
1:a:201:GLY:HA3	1:a:286:ALA:HB2	1.91	0.52
3:c:223:TRP:CG	3:c:224:ILE:H	2.27	0.52
2:B:172:TYR:CE1	2:B:283:GLU:HB2	2.44	0.52
24:C:506:CLA:C2C	24:C:507:CLA:H122	2.39	0.52
2:b:101:ILE:HG23	26:b:620:BCR:C21	2.40	0.52
18:x:35:ASP:OD1	28:x:101:SQD:H1	2.09	0.52
24:c:506:CLA:CBB	24:c:507:CLA:HMA3	2.39	0.52
26:c:515:BCR:C20	26:c:515:BCR:C17	2.88	0.52
24:B:615:CLA:C12	26:B:618:BCR:H17C	2.40	0.52
28:L:102:SQD:H92	28:b:601:SQD:H251	1.91	0.52
30:a:616:LHG:H382	30:a:616:LHG:C11	2.40	0.52
2:b:137:LYS:NZ	7:h:17:GLU:OE2	2.31	0.52
3:c:327:ASN:HB3	13:o:99:ASP:OD2	2.09	0.52
11:L:21:LEU:HD22	28:L:102:SQD:H361	1.91	0.52
1:a:206:PHE:CZ	24:d:402:CLA:HAA1	2.43	0.52
1:A:176:ILE:O	1:A:179:THR:HB	2.09	0.52
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.92	0.52
24:B:617:CLA:H3A	26:B:620:BCR:H17C	1.91	0.52
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.45	0.52
14:t:8:PHE:CD1	26:t:101:BCR:H373	2.45	0.52
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.92	0.52
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.75	0.52
29:D:408:LMG:H172	26:F:101:BCR:H383	1.90	0.52
3:C:213[B]:LEU:HD11	26:I:101:BCR:C21	2.40	0.52
14:T:1[B]:MET:HE1	14:T:3:THR:HB	1.91	0.52
26:f:101:BCR:C37	26:f:101:BCR:C24	2.88	0.52
26:A:610:BCR:H392	26:A:610:BCR:H23C	1.92	0.52
3:c:233:VAL:O	3:c:237:HIS:ND1	2.38	0.52
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.92	0.52
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.45	0.51
24:C:506:CLA:HMC1	24:C:507:CLA:H102	1.92	0.51
4:D:49:LEU:HD22	26:F:101:BCR:H362	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:614:SQD:H132	26:t:101:BCR:HC41	1.92	0.51
24:b:612:CLA:H162	24:b:617:CLA:CAD	2.40	0.51
2:B:42:LEU:HD11	2:B:93:PHE:HB3	1.93	0.51
4:D:72:ASN:HA	29:D:408:LMG:HC1	1.92	0.51
29:D:408:LMG:H231	26:F:101:BCR:H381	1.91	0.51
10:k:21:LEU:O	10:k:25:LEU:HG	2.10	0.51
30:A:615:LHG:H223	32:C:517:DGD:HBH2	1.92	0.51
2:B:393:GLU:HB3	15:U:18:GLY:CA	2.40	0.51
28:B:622:SQD:C1	28:B:622:SQD:H462	2.41	0.51
30:a:616:LHG:H371	24:c:508:CLA:H92	1.91	0.51
2:b:24:LEU:HD21	24:b:618:CLA:CAB	2.40	0.51
2:b:384:ARG:HD3	15:u:102:LEU:HG	1.92	0.51
24:B:602:CLA:HAC1	26:H:101:BCR:H23C	1.93	0.51
32:d:405:DGD:HA72	26:f:101:BCR:C2	2.41	0.51
11:L:18:TYR:CE2	14:T:20:ALA:HA	2.45	0.51
1:a:191:ASN:HB2	3:c:411:ALA:HB1	1.92	0.51
28:b:601:SQD:H121	24:b:616:CLA:C4	2.29	0.51
2:B:139:PHE:CZ	2:B:143:LEU:HD22	2.46	0.51
3:C:170:ILE:HD13	24:C:512:CLA:H111	1.92	0.51
4:D:261:PHE:CE1	4:D:267:LEU:HA	2.45	0.51
7:H:38:PHE:CB	26:H:101:BCR:H10C	2.37	0.51
2:b:63:LEU:HA	2:b:66:MET:HE3	1.93	0.51
4:d:192:THR:HG23	24:d:402:CLA:HBC2	1.93	0.51
10:k:21:LEU:HD21	26:k:101:BCR:HC31	1.93	0.51
3:C:213[B]:LEU:HD21	26:I:101:BCR:C20	2.40	0.51
3:C:223:TRP:CG	3:C:224:ILE:H	2.28	0.51
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.92	0.51
24:a:607:CLA:HMB1	24:a:607:CLA:HBB1	1.93	0.51
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.46	0.51
2:B:200:ALA:HB3	24:B:603:CLA:HMB1	1.93	0.51
26:K:101:BCR:HC21	19:Z:13:VAL:HG13	1.93	0.51
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.93	0.51
24:c:501:CLA:C3D	24:c:503:CLA:H2	2.40	0.51
24:B:604:CLA:C1C	24:B:606:CLA:H71	2.40	0.51
4:D:23:LYS:HD3	4:D:135:LEU:HD21	1.92	0.51
26:C:514:BCR:C36	26:C:514:BCR:C17	2.77	0.50
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.41	0.50
16:V:37:CYS:SG	33:V:201:HEM:CAB	2.99	0.50
3:c:119:LEU:HG	26:c:521:BCR:H10C	1.91	0.50
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.93	0.50
1:A:131:TRP:CH2	24:C:505:CLA:HAA2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:53:THR:HA	4:D:67:TYR:HD2	1.75	0.50
27:A:611:PL9:H403	6:F:22:ALA:HB2	1.92	0.50
2:B:29:LEU:HD21	28:B:622:SQD:H191	1.92	0.50
4:D:43:LEU:HD11	24:D:404:CLA:C3C	2.41	0.50
12:M:20:VAL:HG11	12:m:20:VAL:HG21	1.93	0.50
26:T:101:BCR:C37	26:T:101:BCR:C23	2.80	0.50
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.50
3:c:213[B]:LEU:HD21	26:c:515:BCR:C20	2.42	0.50
10:k:17:ILE:HD13	10:k:17:ILE:H	1.76	0.50
24:C:504:CLA:C4B	32:C:516:DGD:HB71	2.42	0.50
24:C:508:CLA:HMB3	24:C:508:CLA:HBB1	1.94	0.50
4:D:214:HIS:HA	27:D:405:PL9:O2	2.12	0.50
33:E:103:HEM:HMC2	33:E:103:HEM:HBC2	1.92	0.50
25:A:608:PHO:HBB1	25:A:608:PHO:HMB3	1.94	0.50
3:C:323:LYS:NZ	3:C:389:GLU:OE2	2.32	0.50
4:D:129:GLN:NE2	25:D:401:PHO:OBD	2.44	0.50
3:c:182:PHE:CE2	24:c:502:CLA:H201	2.46	0.50
3:C:116:VAL:HG11	26:C:514:BCR:C5	2.41	0.50
32:C:516:DGD:HB51	29:C:518:LMG:H392	1.93	0.50
14:T:8:PHE:CD1	26:T:101:BCR:H373	2.46	0.50
1:a:269:ARG:NH1	4:d:231:THR:HB	2.26	0.50
3:c:339:LYS:NZ	15:u:99:ASN:O	2.40	0.50
3:C:178:LYS:HB2	24:C:502:CLA:H141	1.94	0.50
2:b:472:ARG:HA	2:b:479:PHE:CE1	2.47	0.50
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.94	0.50
24:C:507:CLA:H142	26:I:101:BCR:H362	1.93	0.50
2:b:12:LEU:HB2	24:b:614:CLA:HMC2	1.93	0.50
6:f:30:THR:OG1	29:j:101:LMG:H392	2.11	0.50
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.94	0.50
26:B:618:BCR:C37	26:B:618:BCR:C23	2.82	0.50
26:H:101:BCR:C20	26:H:101:BCR:C37	2.90	0.50
2:b:226:TYR:OH	7:h:19:GLY:HA2	2.12	0.50
2:b:262:THR:C	2:b:264:PRO:HD3	2.37	0.50
1:A:24:THR:C	4:D:255:GLN:HE22	2.19	0.49
2:b:103:LEU:HD21	24:b:607:CLA:HMC3	1.93	0.49
24:B:609:CLA:HBC3	24:B:609:CLA:HHD	1.94	0.49
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.94	0.49
3:c:49:LEU:HD23	3:c:149:TYR:OH	2.12	0.49
4:D:283:ALA:O	4:D:287:VAL:HG23	2.11	0.49
2:b:393:GLU:HB3	15:u:18:GLY:CA	2.42	0.49
2:B:61:PHE:CZ	24:B:608:CLA:HBB1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.47	0.49
3:C:212:TYR:OH	3:C:232:ASP:OD2	2.24	0.49
1:a:326:LEU:HD22	16:v:134:LYS:HB2	1.93	0.49
2:b:442:ILE:HG12	13:o:173:ALA:O	2.13	0.49
1:a:139:MET:HG2	4:d:221:THR:HG22	1.95	0.49
2:b:208:VAL:HG21	24:b:604:CLA:HMC1	1.93	0.49
32:c:517:DGD:HAT1	32:c:518:DGD:HBH1	1.94	0.49
11:l:12:LEU:HD12	30:l:102:LHG:O1	2.12	0.49
13:o:222:ASP:CG	13:o:224:ASP:H	2.20	0.49
3:C:206:PRO:HG3	3:C:239:TRP:CZ2	2.46	0.49
1:a:153:SER:CB	24:a:606:CLA:HED1	2.43	0.49
24:c:507:CLA:OBD	24:c:509:CLA:H122	2.12	0.49
1:A:340:PRO:HD3	15:U:103:TYR:CZ	2.48	0.49
26:C:514:BCR:C37	26:C:514:BCR:C23	2.82	0.49
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.95	0.49
2:b:220:ARG:HG3	7:h:20:LYS:HD3	1.94	0.49
2:b:422:ARG:HH21	13:o:169:ASP:CG	2.19	0.49
2:B:347[B]:ARG:NH1	2:B:351:GLY:O	2.43	0.49
24:a:615:CLA:HED2	4:d:198:MET:SD	2.52	0.49
24:b:608[A]:CLA:H72	26:b:621:BCR:C8	2.43	0.49
2:B:181:VAL:HG11	2:B:195:PRO:HB2	1.94	0.49
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.41	0.49
10:K:10:LYS:HD2	10:K:10:LYS:N	2.28	0.49
24:B:607[B]:CLA:H93	26:B:620:BCR:H10C	1.95	0.48
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.48	0.48
2:b:464:PHE:HD2	24:b:613:CLA:HAC2	1.78	0.48
24:b:605:CLA:HAB	24:b:607:CLA:H171	1.94	0.48
30:A:615:LHG:H382	30:A:615:LHG:C11	2.40	0.48
24:B:604:CLA:H3A	24:B:604:CLA:CGA	2.43	0.48
24:D:404:CLA:C2	18:X:14:LEU:HA	2.43	0.48
5:E:69:ARG:NH2	7:H:50:ASN:O	2.29	0.48
26:F:101:BCR:C20	26:F:101:BCR:C37	2.89	0.48
26:K:102:BCR:H24C	26:K:102:BCR:H371	1.95	0.48
26:f:101:BCR:C24	26:f:101:BCR:H371	2.43	0.48
9:j:32:ALA:HA	29:j:101:LMG:O3	2.13	0.48
3:C:165:LEU:HD21	24:C:506:CLA:CAB	2.43	0.48
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.96	0.48
4:d:261:PHE:CE1	4:d:267:LEU:HA	2.47	0.48
4:d:279:LEU:O	4:d:282:SER:OG	2.26	0.48
1:A:217:SER:HB2	4:D:142:ASN:HA	1.95	0.48
2:B:102:VAL:HA	26:B:619:BCR:H401	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:TRP:NE1	24:B:608:CLA:HBA1	2.27	0.48
7:H:65:LEU:HD12	7:H:66:GLY:H	1.78	0.48
26:H:101:BCR:H20C	26:H:101:BCR:C37	2.43	0.48
1:a:131:TRP:CH2	24:c:505:CLA:HAA2	2.47	0.48
24:b:603:CLA:H152	26:h:101:BCR:C17	2.39	0.48
3:c:29:GLU:CD	3:c:29:GLU:H	2.22	0.48
10:k:28:ILE:O	10:k:31:LEU:HB2	2.12	0.48
16:v:129:LYS:HG2	16:v:136:TYR:O	2.13	0.48
1:A:323:ARG:HB3	4:D:329:MET:HA	1.95	0.48
2:B:29:LEU:HD11	26:B:618:BCR:C20	2.44	0.48
4:D:37:LEU:HD22	4:D:128:ARG:HD2	1.96	0.48
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.13	0.48
3:c:212:TYR:CD2	26:c:515:BCR:H401	2.48	0.48
24:c:501:CLA:C4D	24:c:503:CLA:H2	2.43	0.48
26:k:101:BCR:C36	26:k:101:BCR:C17	2.78	0.48
24:b:617:CLA:HED3	24:b:618:CLA:HAB	1.95	0.48
3:c:123:ALA:HB2	26:c:521:BCR:C12	2.44	0.48
26:c:515:BCR:H20C	26:c:515:BCR:H372	1.95	0.48
2:B:103:LEU:HD21	24:B:606:CLA:HMC3	1.96	0.48
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.49	0.48
24:c:501:CLA:CBB	24:c:501:CLA:H71	2.43	0.48
1:A:64:ARG:NH1	13:O:105:PRO:O	2.47	0.48
1:A:133:LEU:HD23	4:D:256:ILE:HG12	1.96	0.48
1:A:306:VAL:HG12	1:A:314:ILE:HB	1.96	0.48
24:b:608[B]:CLA:H102	24:b:608[B]:CLA:H61	1.62	0.48
24:b:617:CLA:HBA1	24:b:617:CLA:H3A	1.68	0.48
4:D:39:PRO:HG2	24:D:404:CLA:HAB	1.95	0.48
4:D:53:THR:HA	4:D:67:TYR:CD2	2.49	0.48
13:O:137:THR:C	13:O:139:SER:H	2.22	0.48
1:a:106:LEU:CD2	26:a:610:BCR:H383	2.40	0.48
1:a:300:PHE:HB3	1:a:302:PHE:CE1	2.49	0.48
3:c:223:TRP:CE3	3:c:224:ILE:HG12	2.49	0.48
11:l:20:GLY:HA3	12:m:22:LEU:HD13	1.96	0.48
2:B:471:ALA:HB1	4:D:140:PRO:HG2	1.96	0.48
2:B:479:PHE:HA	4:D:139:ARG:HE	1.79	0.48
3:C:464:GLU:OE2	4:D:245:SER:OG	2.20	0.48
6:F:21:VAL:O	6:F:25:THR:HG23	2.14	0.48
6:F:37:ILE:O	6:F:40:MET:HB2	2.14	0.48
14:t:1[B]:MET:HE1	14:t:3:THR:HB	1.95	0.48
28:A:614:SQD:H271	26:b:621:BCR:H19C	1.94	0.47
2:B:462:PHE:HA	24:B:612:CLA:HMC2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:323:LYS:O	15:U:47:LYS:HD2	2.14	0.47
6:F:20:TRP:NE1	6:F:24:HIS:CE1	2.82	0.47
2:b:200:ALA:HB3	24:b:604:CLA:HMB1	1.94	0.47
24:b:605:CLA:C4D	24:b:607:CLA:H43	2.44	0.47
4:d:123:ILE:HD11	32:h:102:DGD:HAE1	1.95	0.47
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.48	0.47
27:a:611:PL9:H103	27:a:611:PL9:HC2	1.97	0.47
30:e:101:LHG:H152	6:f:22:ALA:HB1	1.96	0.47
2:B:25:MET:HE3	26:B:618:BCR:C25	2.44	0.47
29:c:519:LMG:H171	10:k:27:VAL:HG11	1.96	0.47
4:d:274:VAL:HG22	27:d:404:PL9:H222	1.96	0.47
7:h:41:PHE:HB2	26:h:101:BCR:C15	2.44	0.47
1:A:267:ASN:HB3	1:A:270[B]:SER:OG	2.14	0.47
11:L:10:VAL:O	12:M:28:GLN:NE2	2.36	0.47
1:a:176:ILE:O	1:a:179:THR:HB	2.13	0.47
1:a:328:MET:HE1	4:d:183:LEU:HD13	1.95	0.47
24:c:513:CLA:HAB	26:c:514:BCR:H371	1.96	0.47
13:o:193:THR:HG21	13:o:220:LEU:HD12	1.97	0.47
2:B:33:TRP:CD1	26:t:101:BCR:H381	2.50	0.47
4:D:209:LEU:HD22	27:D:405:PL9:H161	1.96	0.47
26:T:101:BCR:C36	26:T:101:BCR:C17	2.77	0.47
1:a:215:HIS:ND1	27:a:611:PL9:O1	2.42	0.47
2:b:154:GLY:HA2	2:b:158:LEU:HD12	1.96	0.47
2:b:311:PHE:O	2:b:317:ASN:ND2	2.47	0.47
24:b:605:CLA:CGA	24:b:605:CLA:H3A	2.44	0.47
32:d:405:DGD:HA72	26:f:101:BCR:HC22	1.96	0.47
10:k:31:LEU:HB3	26:k:101:BCR:C15	2.44	0.47
26:k:101:BCR:C17	17:y:33:PRO:HD3	2.44	0.47
2:B:58:GLN:O	24:B:608:CLA:HED2	2.15	0.47
24:B:605:CLA:HBA1	24:B:605:CLA:H3A	1.69	0.47
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.96	0.47
1:a:296:ASN:HB3	3:c:401:LEU:HG	1.96	0.47
2:b:58:GLN:C	2:b:329:PRO:HB3	2.39	0.47
24:b:605:CLA:HMB1	24:b:605:CLA:HBB1	1.96	0.47
24:b:615:CLA:H193	26:b:620:BCR:C5	2.44	0.47
26:b:619:BCR:H20C	26:b:619:BCR:H372	1.95	0.47
30:e:101:LHG:H241	30:e:101:LHG:HC61	1.62	0.47
11:l:23:LEU:HA	30:l:102:LHG:H181	1.97	0.47
15:u:59:GLU:H	15:u:59:GLU:CD	2.22	0.47
24:A:606:CLA:HBD	24:D:402:CLA:HAC2	1.97	0.47
4:D:186:GLN:HB2	24:D:403:CLA:HBC1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:17:ILE:HD13	10:K:17:ILE:N	2.28	0.47
2:b:334:ASP:OD2	2:b:334:ASP:N	2.45	0.47
26:c:515:BCR:C36	26:c:515:BCR:C17	2.77	0.47
10:k:25:LEU:HB2	10:k:26:PRO:HD3	1.96	0.47
11:l:18:TYR:CE2	14:t:20:ALA:HA	2.50	0.47
26:c:521:BCR:C20	26:c:521:BCR:C37	2.93	0.47
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.50	0.47
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.50	0.47
29:B:621:LMG:H411	30:L:101:LHG:H383	1.96	0.47
12:M:16[C]:LEU:HD21	12:m:16[C]:LEU:HD22	1.96	0.47
2:b:115:TRP:HB2	26:b:619:BCR:H292	1.96	0.47
4:d:43:LEU:HD11	24:d:403:CLA:C2C	2.45	0.47
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.97	0.47
14:t:22:PHE:CZ	26:t:101:BCR:H333	2.49	0.47
2:B:274:GLN:HB3	2:B:280:PHE:HE2	1.79	0.47
2:B:422:ARG:HH21	13:O:169:ASP:CG	2.23	0.47
26:B:618:BCR:H381	14:t:19:PHE:CZ	2.48	0.47
4:D:43:LEU:HD11	24:D:404:CLA:C2C	2.44	0.47
27:D:405:PL9:H362	11:L:30:LEU:HD13	1.97	0.47
10:K:28:ILE:O	10:K:31:LEU:HB2	2.15	0.47
26:K:102:BCR:C20	26:K:102:BCR:C37	2.93	0.47
29:a:613:LMG:H382	32:c:516:DGD:HB42	1.97	0.47
11:l:22:LEU:HD23	30:l:102:LHG:H162	1.95	0.47
2:b:311:PHE:HA	2:b:430:PHE:CZ	2.51	0.46
3:c:158:THR:O	3:c:251:HIS:HB3	2.15	0.46
13:o:40:ILE:HG12	13:o:243:ILE:HD13	1.97	0.46
14:t:1[B]:MET:HB3	14:t:4:ILE:HD12	1.96	0.46
1:A:89:ILE:HG12	13:O:73:ARG:HH22	1.80	0.46
3:C:55:ALA:HB1	26:K:102:BCR:H373	1.98	0.46
3:C:330:SER:O	13:O:123:LYS:NZ	2.47	0.46
26:T:101:BCR:H20C	26:T:101:BCR:H373	1.96	0.46
30:a:616:LHG:H342	24:c:504:CLA:H201	1.96	0.46
24:A:606:CLA:HMB1	24:A:606:CLA:HBB1	1.97	0.46
24:B:611:CLA:H152	24:B:611:CLA:OBD	2.15	0.46
3:C:140:LEU:HD13	3:C:147:PHE:HB3	1.96	0.46
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.98	0.46
26:b:619:BCR:HC42	12:m:10:ALA:HA	1.98	0.46
24:c:501:CLA:HHB	26:c:515:BCR:H271	1.98	0.46
1:A:271:LEU:HD11	27:A:611:PL9:HC8	1.97	0.46
2:B:193:TYR:OH	32:H:102:DGD:HE1	2.16	0.46
24:B:604:CLA:C4D	24:B:606:CLA:H43	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:615:CLA:H101	26:B:618:BCR:C17	2.45	0.46
26:K:101:BCR:C36	26:K:101:BCR:C17	2.79	0.46
16:V:26:TYR:OH	16:V:122:GLU:OE2	2.25	0.46
1:a:214:MET:HG2	27:a:611:PL9:C10	2.43	0.46
26:b:619:BCR:C37	26:b:619:BCR:C23	2.84	0.46
26:c:514:BCR:C18	26:c:514:BCR:H20C	2.36	0.46
2:B:30:VAL:HG13	24:B:614:CLA:HMC3	1.98	0.46
2:B:460:LEU:O	2:B:463:PHE:HB3	2.15	0.46
2:b:389:LYS:HE3	2:b:390:TYR:CE1	2.51	0.46
2:B:334:ASP:OD2	2:B:334:ASP:N	2.44	0.46
3:C:321:ASP:OD2	3:C:340:TYR:OH	2.28	0.46
4:D:342:PRO:O	4:D:345:VAL:HG22	2.15	0.46
1:a:193:LEU:HD13	4:d:179:PHE:HB3	1.97	0.46
2:b:442:ILE:HD12	4:d:299:ILE:HG12	1.97	0.46
3:c:179:ALA:O	3:c:184:GLY:HA2	2.14	0.46
4:d:126:MET:HA	4:d:129:GLN:OE1	2.16	0.46
1:A:91:LEU:HD21	1:A:163:ILE:HA	1.97	0.46
24:B:607[B]:CLA:H61	24:B:607[B]:CLA:H102	1.62	0.46
24:B:615:CLA:HBB1	24:B:615:CLA:HMB1	1.98	0.46
26:T:101:BCR:H311	26:T:101:BCR:HC8	1.98	0.46
2:b:66:MET:HE2	24:b:607:CLA:HED3	1.98	0.46
4:d:342:PRO:O	4:d:345:VAL:HG22	2.16	0.46
13:o:110[B]:MET:HE3	13:o:110[B]:MET:HB3	1.84	0.46
2:B:383:PHE:CE1	13:O:167:GLY:HA2	2.51	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.97	0.46
4:D:199:MET:HG2	27:D:405:PL9:H321	1.96	0.46
1:a:58:VAL:HB	1:a:83:VAL:HB	1.97	0.46
1:a:129:ARG:NH2	4:d:256:ILE:HA	2.30	0.46
30:l:102:LHG:H142	30:l:102:LHG:H171	1.74	0.46
3:C:393:ALA:HB1	16:V:48:THR:HG21	1.97	0.46
1:a:296:ASN:HB2	3:c:400:PRO:O	2.15	0.46
2:b:440:ASP:O	13:o:174:LEU:HD22	2.16	0.46
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.98	0.46
26:t:101:BCR:C37	26:t:101:BCR:C23	2.81	0.46
1:A:112:TYR:O	1:A:116:ILE:HG12	2.15	0.46
30:A:615:LHG:H342	24:C:504:CLA:H201	1.97	0.46
26:B:618:BCR:H381	14:t:19:PHE:HZ	1.79	0.46
4:D:136:VAL:HG12	4:D:138:VAL:HG13	1.98	0.46
5:E:20:TRP:HZ2	9:J:13:VAL:HG13	1.81	0.46
1:a:139:MET:HE1	1:a:143:ILE:HD12	1.96	0.46
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:30:THR:HG21	29:j:101:LMG:H411	1.97	0.46
26:k:101:BCR:H17C	17:y:33:PRO:HG3	1.98	0.46
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.98	0.45
27:A:611:PL9:H102	27:A:611:PL9:HC72	1.65	0.45
2:B:149:LEU:HD23	24:B:604:CLA:HBC1	1.98	0.45
8:I:24:LEU:HG	26:I:101:BCR:HC31	1.97	0.45
26:K:102:BCR:C22	26:K:102:BCR:H20C	2.35	0.45
25:a:608:PHO:HED1	27:d:404:PL9:H153	1.98	0.45
26:h:101:BCR:HC8	26:h:101:BCR:H331	1.97	0.45
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.51	0.45
3:C:286:ALA:HB2	24:C:502:CLA:HMD2	1.98	0.45
25:D:401:PHO:HMB3	25:D:401:PHO:HBB1	1.98	0.45
1:a:212:CYS:HB2	4:d:211:CYS:HB2	1.98	0.45
2:b:150:CYS:HB2	24:b:605:CLA:CMC	2.46	0.45
24:A:606:CLA:HAA1	24:D:403:CLA:HBB2	1.98	0.45
2:B:201:HIS:HB2	24:B:603:CLA:C4A	2.46	0.45
3:C:158:THR:O	3:C:251:HIS:HB3	2.15	0.45
27:D:405:PL9:H43	27:D:405:PL9:H471	1.63	0.45
29:D:408:LMG:H352	26:F:101:BCR:H17C	1.99	0.45
26:b:619:BCR:H10C	29:b:622:LMG:H412	1.97	0.45
1:A:269:ARG:CZ	4:D:222:LEU:HD13	2.46	0.45
4:D:129:GLN:NE2	4:D:142:ASN:OD1	2.50	0.45
28:L:102:SQD:H321	14:T:16:LEU:HB2	1.98	0.45
13:O:158:ASP:OD1	13:O:158:ASP:C	2.59	0.45
28:a:612:SQD:H132	30:a:616:LHG:H142	1.98	0.45
13:o:97:GLU:HB2	13:o:125:LEU:HB3	1.99	0.45
2:B:246:PHE:CD1	2:B:246:PHE:C	2.94	0.45
24:B:614:CLA:HBC3	26:B:619:BCR:H11C	1.98	0.45
4:d:315:TYR:O	4:d:319:LEU:HG	2.16	0.45
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.52	0.45
24:B:606:CLA:H143	24:B:611:CLA:HED2	1.98	0.45
30:D:407:LHG:H141	30:D:407:LHG:H171	1.79	0.45
16:V:12:LEU:O	16:V:70:GLU:HG2	2.16	0.45
1:a:288:LEU:O	1:a:292:THR:HG23	2.16	0.45
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.52	0.45
2:B:33:TRP:NE1	24:B:608:CLA:HMC2	2.32	0.45
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.51	0.45
24:B:607[A]:CLA:H72	26:B:620:BCR:C9	2.47	0.45
26:B:620:BCR:C37	26:B:620:BCR:C23	2.84	0.45
7:H:28:THR:HB	7:H:29:PRO:HD3	1.99	0.45
18:X:31:ILE:HG23	28:X:101:SQD:H462	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:609:CLA:H42	29:b:622:LMG:H301	1.98	0.45
3:c:123:ALA:HB2	26:c:521:BCR:C13	2.47	0.45
1:A:153:SER:CB	24:A:606:CLA:H43	2.47	0.45
12:M:20:VAL:HG22	12:m:20:VAL:HG11	1.99	0.45
4:d:283:ALA:O	4:d:287:VAL:HG23	2.17	0.45
1:A:77:ILE:HB	11:L:33:SER:OG	2.16	0.45
2:B:102:VAL:HA	26:B:619:BCR:C40	2.47	0.45
2:B:324:LEU:HD21	4:D:196:PHE:HE2	1.81	0.45
4:D:155:SER:HA	4:D:159:ILE:HD12	1.99	0.45
30:L:101:LHG:H241	30:L:101:LHG:H111	1.99	0.45
2:b:224:ARG:NH1	4:d:16:ASP:OD2	2.41	0.45
26:b:619:BCR:H12C	26:b:620:BCR:C10	2.46	0.45
26:b:621:BCR:H24C	26:b:621:BCR:H371	1.99	0.45
3:C:274:TYR:CD1	24:C:505:CLA:HMD2	2.51	0.45
6:F:29:PRO:HB3	26:F:101:BCR:H12C	1.99	0.45
12:M:20:VAL:CG2	12:m:20:VAL:HG11	2.46	0.45
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.52	0.45
24:c:504:CLA:HED3	29:c:519:LMG:O3	2.17	0.45
24:A:609:CLA:H11	8:I:9:TYR:CE1	2.52	0.44
24:B:607[B]:CLA:H192	24:B:607[B]:CLA:H161	1.68	0.44
24:B:616:CLA:HBA1	24:B:616:CLA:H3A	1.62	0.44
1:a:127:MET:CE	24:c:505:CLA:HBB1	2.47	0.44
2:b:195:PRO:O	2:b:198:VAL:N	2.50	0.44
2:b:366:PHE:CD1	2:b:367:PRO:HD2	2.52	0.44
24:b:606:CLA:HBB1	24:b:609:CLA:HAB	1.98	0.44
4:d:49:LEU:HD22	26:f:101:BCR:H362	1.98	0.44
26:f:101:BCR:H403	9:j:25:VAL:HG21	1.98	0.44
29:A:613:LMG:H231	29:A:613:LMG:H201	1.72	0.44
3:C:307:PRO:HG3	3:C:358:PHE:CE1	2.52	0.44
3:C:424:SER:O	3:C:428:THR:HG23	2.17	0.44
3:c:297:TYR:HD1	3:c:302:TYR:CZ	2.35	0.44
24:c:501:CLA:HMB1	24:c:501:CLA:HBB1	1.99	0.44
15:u:69:GLU:OE2	15:u:72:LYS:NZ	2.32	0.44
16:v:12:LEU:O	16:v:70:GLU:HG2	2.18	0.44
24:A:609:CLA:HBA1	24:A:609:CLA:H3A	1.78	0.44
13:O:222:ASP:CG	13:O:224:ASP:H	2.25	0.44
1:a:129:ARG:HH22	4:d:256:ILE:HA	1.81	0.44
1:a:223:LEU:HD22	4:d:265:ARG:HG2	1.98	0.44
26:b:620:BCR:H11C	26:b:620:BCR:H341	1.82	0.44
29:z:101:LMG:O2	29:z:101:LMG:HC71	2.17	0.44
1:A:131:TRP:CZ3	24:C:505:CLA:HBA1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:610:BCR:C37	26:A:610:BCR:H20C	2.47	0.44
2:B:29:LEU:HD11	26:B:618:BCR:C19	2.47	0.44
24:C:506:CLA:H162	24:C:506:CLA:H122	1.72	0.44
27:D:405:PL9:C34	11:L:30:LEU:HD22	2.47	0.44
7:H:46:LEU:HD11	32:H:102:DGD:HA31	1.99	0.44
6:f:30:THR:HA	26:f:101:BCR:C16	2.48	0.44
26:f:101:BCR:H383	29:j:101:LMG:H172	1.98	0.44
10:k:10:LYS:HD2	10:k:10:LYS:N	2.33	0.44
1:A:202:VAL:HG11	24:A:607:CLA:C3D	2.47	0.44
27:A:611:PL9:H252	27:A:611:PL9:H272	1.74	0.44
2:B:249:ALA:HA	2:B:252:VAL:HG22	1.98	0.44
2:B:446:SER:HB2	2:B:447:PRO:HD2	2.00	0.44
24:B:606:CLA:C14	24:B:611:CLA:HED2	2.48	0.44
24:B:615:CLA:H122	26:B:618:BCR:H16C	1.99	0.44
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.44
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	1.99	0.44
5:E:19:TYR:CE2	5:E:23:HIS:CE1	3.05	0.44
16:V:93:PRO:HG2	33:V:201:HEM:HMC3	1.99	0.44
1:a:136:ARG:HH12	8:i:27:ASP:CG	2.25	0.44
2:b:18:ARG:HD3	2:b:115:TRP:CH2	2.53	0.44
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.52	0.44
24:b:610:CLA:HBC3	24:b:610:CLA:HHD	1.99	0.44
24:B:610:CLA:HAC1	7:H:34:PHE:CE1	2.53	0.44
3:C:347:GLY:HA3	13:O:17:ASN:HB2	1.99	0.44
4:D:37:LEU:CD2	4:D:128:ARG:HD2	2.48	0.44
26:I:101:BCR:H20C	26:I:101:BCR:H373	1.98	0.44
11:L:21:LEU:HD13	28:L:102:SQD:H312	1.99	0.44
3:c:42:LEU:HD21	24:c:511:CLA:H2A	2.00	0.44
7:h:49:TYR:CG	32:h:102:DGD:HB22	2.53	0.44
26:k:101:BCR:H17C	17:y:33:PRO:CG	2.47	0.44
27:A:611:PL9:H103	27:A:611:PL9:H121	1.79	0.44
24:B:606:CLA:H62	24:B:606:CLA:H41	1.77	0.44
32:H:102:DGD:HB62	32:H:102:DGD:HB91	1.81	0.44
33:V:201:HEM:HBA1	33:V:201:HEM:HHA	2.00	0.44
1:a:267:ASN:HB3	1:a:270[B]:SER:OG	2.17	0.44
2:b:382:PRO:HG2	2:b:385:ARG:HD2	2.00	0.44
27:D:405:PL9:H203	30:D:407:LHG:H122	2.00	0.44
30:D:406:LHG:HC91	30:L:101:LHG:HC81	1.99	0.44
5:E:23:HIS:HA	5:E:26:THR:OG1	2.16	0.44
2:b:69:LEU:HD12	24:b:607:CLA:HAA2	2.00	0.44
3:c:210:PHE:HA	3:c:213[B]:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:e:102:HEM:HBD1	6:f:20:TRP:CD1	2.53	0.44
6:f:20:TRP:CE2	6:f:24:HIS:CE1	3.05	0.44
24:A:607:CLA:HMB2	25:D:401:PHO:H172	2.00	0.44
2:B:41:GLU:HB3	2:B:60:MET:SD	2.58	0.44
24:B:607[B]:CLA:H111	24:B:607[B]:CLA:H142	1.76	0.44
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.53	0.44
24:C:510:CLA:HBA1	24:C:510:CLA:H3A	1.85	0.44
24:C:512:CLA:HMB3	24:C:512:CLA:H202	2.00	0.44
7:H:12[A]:ARG:NH1	7:H:15:ASN:O	2.47	0.44
14:T:18:PHE:HB2	26:T:101:BCR:HC8	1.99	0.44
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.00	0.44
2:B:133:LEU:HB3	2:B:138:MET:SD	2.58	0.43
3:C:182:PHE:CE2	24:C:502:CLA:H201	2.53	0.43
26:K:102:BCR:C37	26:K:102:BCR:C23	2.82	0.43
1:a:116:ILE:HG13	1:a:117:PHE:N	2.32	0.43
2:b:32:GLY:C	26:b:620:BCR:H15C	2.42	0.43
2:b:72:THR:HG22	2:b:80:ILE:HD11	1.99	0.43
26:b:620:BCR:C36	26:b:620:BCR:C17	2.77	0.43
3:c:54:VAL:HG12	3:c:125:LEU:O	2.18	0.43
1:A:334:ARG:HB2	13:O:157:LEU:HD12	1.99	0.43
24:A:609:CLA:H192	24:C:505:CLA:H142	2.00	0.43
2:B:63:LEU:HA	2:B:66:MET:HE3	2.01	0.43
3:C:86:LEU:O	3:C:90:PRO:HG2	2.18	0.43
3:C:87:ILE:C	3:C:90:PRO:HD2	2.43	0.43
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.89	0.43
2:b:102:VAL:HA	26:b:620:BCR:C40	2.48	0.43
4:d:303:ILE:HG21	12:m:2:GLU:HG3	2.00	0.43
26:h:101:BCR:H393	18:x:7:LEU:HD21	1.99	0.43
10:k:17:ILE:H	10:k:17:ILE:CD1	2.31	0.43
24:A:607:CLA:H142	29:D:408:LMG:H232	2.00	0.43
26:C:514:BCR:C15	29:C:519:LMG:H401	2.47	0.43
4:D:191:TRP:CE2	4:D:197:HIS:HB2	2.53	0.43
8:I:11:VAL:HG13	8:I:15:PHE:HE1	1.83	0.43
26:a:610:BCR:C36	26:a:610:BCR:C16	2.95	0.43
2:b:25:MET:HE1	2:b:108:PHE:CD1	2.53	0.43
24:b:612:CLA:HHC	24:b:612:CLA:HBB1	1.98	0.43
3:c:75:PHE:CZ	3:c:77:PRO:HA	2.54	0.43
3:c:168:LEU:HD21	24:c:509:CLA:H61	2.00	0.43
1:A:307:ILE:CG2	1:A:311:GLY:HA2	2.48	0.43
27:A:611:PL9:H203	27:A:611:PL9:H172	1.80	0.43
4:D:266:TRP:CZ2	11:L:19:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:298:PHE:O	4:D:301:GLN:HB2	2.18	0.43
1:a:304:HIS:CE1	3:c:414:ILE:HG21	2.53	0.43
1:A:288:LEU:HD22	3:C:432:VAL:HA	2.00	0.43
2:b:392:PHE:HA	2:b:397:VAL:HG23	2.00	0.43
18:x:27:VAL:HG21	28:x:101:SQD:H321	1.99	0.43
24:B:605:CLA:H2	24:B:606:CLA:C4C	2.48	0.43
24:C:501:CLA:ND	24:C:503:CLA:H2	2.33	0.43
4:D:53:THR:HG22	6:F:40:MET:HE1	1.99	0.43
27:D:405:PL9:H102	27:D:405:PL9:HC72	1.58	0.43
27:D:405:PL9:H252	27:D:405:PL9:H302	2.01	0.43
1:a:172:MET:SD	24:a:615:CLA:HMC2	2.58	0.43
24:a:609:CLA:HBB1	24:a:609:CLA:HMB3	2.01	0.43
3:c:185:LEU:HD13	24:c:501:CLA:HED2	2.01	0.43
7:h:56:ASP:OD2	18:x:2:THR:HB	2.19	0.43
16:v:122:GLU:HG3	16:v:126:LEU:HD12	1.99	0.43
2:B:33:TRP:HD1	26:t:101:BCR:H381	1.84	0.43
3:C:34:ALA:HB3	3:C:36:TRP:CE2	2.53	0.43
3:C:344:SER:OG	3:C:348:GLU:OE2	2.36	0.43
27:a:611:PL9:H531	27:a:611:PL9:H523	1.83	0.43
2:b:57:ARG:HH22	2:b:334:ASP:CG	2.26	0.43
2:b:149:LEU:HD22	24:b:606:CLA:H152	2.01	0.43
3:C:269:GLU:OE2	3:C:447:ARG:HD3	2.18	0.43
33:E:103:HEM:HBC2	6:F:31:ILE:HG13	1.99	0.43
30:L:101:LHG:H171	30:L:101:LHG:H142	1.87	0.43
18:X:27:VAL:HG21	28:X:101:SQD:H321	2.00	0.43
1:a:164:GLY:HA3	1:a:294:ALA:O	2.19	0.43
1:a:249:VAL:HG12	2:b:491:VAL:HG21	2.01	0.43
2:b:30:VAL:HG12	24:b:607:CLA:HMD3	2.01	0.43
2:b:118:TRP:CD1	11:l:4:ASN:HD22	2.37	0.43
26:c:521:BCR:C22	26:c:521:BCR:H20C	2.40	0.43
1:A:183:MET:HA	24:A:606:CLA:HMD2	2.01	0.43
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.54	0.43
2:B:321:LYS:NZ	2:B:363:PHE:O	2.52	0.43
24:C:504:CLA:HBC1	10:K:27:VAL:HA	2.01	0.43
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.43
5:E:34:GLY:HA3	6:F:32:PHE:O	2.19	0.43
18:X:21:LEU:O	18:X:25:PHE:HD1	2.01	0.43
1:a:76:ASN:OD1	1:a:79:THR:HG23	2.18	0.43
1:a:237:TYR:CE1	1:a:241:GLN:HG2	2.54	0.43
24:a:609:CLA:H192	24:c:505:CLA:H142	2.00	0.43
24:a:609:CLA:H92	8:i:13:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:615:CLA:HMA2	27:d:404:PL9:C38	2.49	0.43
3:c:170:ILE:HD13	24:c:512:CLA:H111	2.01	0.43
13:o:49[A]:THR:OG1	13:o:236:GLN:HB2	2.19	0.43
2:B:149:LEU:HD22	24:B:605:CLA:H152	2.00	0.43
30:D:406:LHG:O9	30:L:101:LHG:HC81	2.19	0.43
27:a:611:PL9:C22	25:d:401:PHO:HMA2	2.47	0.43
2:b:118:TRP:CE2	11:l:4:ASN:ND2	2.87	0.43
2:b:204:ALA:HB3	24:b:604:CLA:HAB	2.00	0.43
2:b:461:LEU:HD22	30:d:406:LHG:H301	2.01	0.43
7:h:49:TYR:CD2	32:h:102:DGD:HB22	2.54	0.43
10:k:15:TYR:CZ	19:z:5:PHE:HZ	2.36	0.43
2:B:256:MET:HA	2:B:263:THR:HG21	2.00	0.42
24:B:602:CLA:H152	26:H:101:BCR:H17C	2.01	0.42
3:C:223:TRP:CG	3:C:224:ILE:N	2.87	0.42
24:C:504:CLA:HED3	29:C:518:LMG:O3	2.19	0.42
4:D:87:HIS:HA	4:D:167:TRP:CD1	2.53	0.42
1:a:112:TYR:O	1:a:116:ILE:HG12	2.19	0.42
2:B:61:PHE:CE2	24:B:608:CLA:HBB1	2.55	0.42
24:C:502:CLA:H51	24:C:503:CLA:NC	2.33	0.42
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.54	0.42
27:D:405:PL9:H302	27:D:405:PL9:H271	1.55	0.42
28:L:102:SQD:C7	28:b:601:SQD:O48	2.66	0.42
4:d:136:VAL:HG12	4:d:138:VAL:HG13	2.01	0.42
16:v:100:ILE:HG13	16:v:101:PHE:CD2	2.54	0.42
2:B:124:ARG:O	7:H:12[A]:ARG:NH1	2.51	0.42
32:C:517:DGD:HA41	29:D:408:LMG:H121	2.00	0.42
26:F:101:BCR:H11C	26:F:101:BCR:H341	1.69	0.42
1:a:141:PRO:HG3	3:c:446:GLY:C	2.44	0.42
13:o:92:SER:HB3	13:o:131:PRO:HA	2.00	0.42
1:A:279:PRO:O	1:A:283:VAL:HG23	2.19	0.42
4:D:65:SER:HB2	4:D:77:ALA:O	2.20	0.42
4:D:125:PHE:CE1	25:D:401:PHO:HBD	2.54	0.42
27:D:405:PL9:H453	27:D:405:PL9:H421	1.68	0.42
1:a:278:TRP:HB3	1:a:279:PRO:CD	2.49	0.42
2:b:204:ALA:CB	24:b:604:CLA:HAB	2.49	0.42
2:b:422:ARG:O	2:b:425:ILE:HG12	2.19	0.42
3:c:274:TYR:CD1	24:c:505:CLA:HMD2	2.54	0.42
26:c:521:BCR:HC42	10:k:15:TYR:CE1	2.54	0.42
4:d:17:ILE:O	4:d:20:ASP:HB2	2.20	0.42
24:d:403:CLA:HBB1	18:x:21:LEU:HD21	2.01	0.42
26:t:101:BCR:C20	26:t:101:BCR:C37	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:HB2	2:B:466:HIS:ND1	2.34	0.42
2:B:458:PHE:HB3	24:B:605:CLA:HBC2	2.01	0.42
3:C:185:LEU:HB2	3:C:230:LEU:HD13	2.02	0.42
4:D:154:VAL:HG21	32:H:102:DGD:HAN1	2.02	0.42
25:D:401:PHO:H72	25:D:401:PHO:H112	1.88	0.42
14:T:25[A]:GLU:HA	14:T:26:PRO:HD3	1.89	0.42
2:b:136:PRO:O	2:b:139:PHE:HB3	2.19	0.42
2:b:138:MET:HE3	24:b:617:CLA:CHD	2.50	0.42
4:d:141:TYR:OH	30:d:406:LHG:O4	2.18	0.42
13:o:137:THR:C	13:o:139:SER:H	2.28	0.42
24:A:606:CLA:CB D	24:D:402:CLA:HAC2	2.49	0.42
24:B:610:CLA:HBA1	24:B:610:CLA:H3A	1.86	0.42
24:C:508:CLA:HBB2	24:C:509:CLA:HMA3	2.01	0.42
4:D:233:ARG:C	4:D:235:PHE:H	2.28	0.42
13:O:81:ILE:HD11	13:O:102:ASP:HA	2.02	0.42
13:O:170:SER:HA	13:O:186:ASN:CG	2.45	0.42
18:X:24:THR:HA	28:X:101:SQD:H331	2.01	0.42
24:a:609:CLA:H162	24:a:609:CLA:H122	1.76	0.42
24:b:603:CLA:HMC1	26:h:101:BCR:H19C	2.02	0.42
3:c:95:LEU:CD1	24:c:503:CLA:HAA2	2.50	0.42
3:c:130:VAL:O	3:c:134:ILE:HG12	2.20	0.42
27:d:404:PL9:HC72	27:d:404:PL9:H102	1.74	0.42
24:B:613:CLA:H91	24:B:614:CLA:HBB1	2.02	0.42
4:D:72:ASN:O	4:D:76:VAL:HG13	2.20	0.42
24:b:608[A]:CLA:H91	24:b:608[A]:CLA:H112	1.88	0.42
24:b:608[B]:CLA:H142	24:b:608[B]:CLA:H111	1.76	0.42
3:c:182:PHE:CG	24:c:502:CLA:H191	2.54	0.42
1:A:89:ILE:HG23	1:A:92:HIS:HB2	2.02	0.42
2:B:18:ARG:NH2	28:B:622:SQD:O9	2.45	0.42
3:C:76:ILE:HA	3:C:77:PRO:HD3	1.91	0.42
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.54	0.42
27:D:405:PL9:H122	30:D:407:LHG:H111	2.02	0.42
5:E:30:LEU:HD12	33:E:103:HEM:HMC1	2.02	0.42
8:I:33:LYS:HB3	8:I:34:ARG:H	1.43	0.42
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.50	0.42
27:d:404:PL9:H472	27:d:404:PL9:H512	1.69	0.42
6:f:21:VAL:O	6:f:25:THR:HG23	2.19	0.42
1:A:330:VAL:HG21	4:D:328:TRP:CE2	2.55	0.42
24:A:609:CLA:H92	8:I:13:THR:HG23	2.02	0.42
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.55	0.42
24:C:508:CLA:HBB1	24:C:508:CLA:CMB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:18:TYR:CD2	14:T:20:ALA:HA	2.55	0.42
27:a:611:PL9:H252	27:a:611:PL9:H272	1.69	0.42
2:b:190:PHE:HB3	7:h:45:ILE:HG22	2.02	0.42
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.01	0.42
3:c:390:ARG:HD3	16:v:100:ILE:HD12	2.01	0.42
32:c:517:DGD:HE5	32:c:517:DGD:HD4	2.01	0.42
4:d:30:VAL:HA	4:d:38:PHE:HE1	1.85	0.42
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.19	0.42
28:A:614:SQD:H291	24:b:608[A]:CLA:H203	2.02	0.42
2:B:74:SER:OG	2:B:94:GLU:OE2	2.36	0.42
2:B:222:PRO:HB3	7:H:25:TRP:C	2.44	0.42
30:a:616:LHG:O3	30:a:616:LHG:O1	2.38	0.42
2:b:18:ARG:HD3	2:b:115:TRP:CZ3	2.55	0.42
2:b:246:PHE:CD1	2:b:246:PHE:C	2.97	0.42
3:c:171:GLY:O	3:c:174:LEU:HB2	2.20	0.42
3:c:315:MET:HG2	3:c:392:ALA:HB2	2.02	0.42
32:d:405:DGD:HA72	26:f:101:BCR:HC21	2.02	0.42
13:o:184:ARG:HA	15:u:9:LEU:CD1	2.50	0.42
2:B:413:ASP:HA	2:B:414:PRO:HD3	1.95	0.41
24:D:403:CLA:HBB1	24:D:403:CLA:HMB3	2.01	0.41
13:O:127:ALA:HA	13:O:144:GLY:HA3	2.02	0.41
13:O:162:ARG:HD2	13:O:186:ASN:HA	2.02	0.41
1:a:217:SER:HB2	4:d:142:ASN:HA	2.02	0.41
1:a:269:ARG:NH1	4:d:222:LEU:HD13	2.35	0.41
4:d:70:GLY:O	9:j:37:GLY:HA3	2.19	0.41
1:A:329:GLU:OE1	16:V:134:LYS:NZ	2.41	0.41
2:B:69:LEU:HD12	24:B:606:CLA:HAA2	2.02	0.41
3:C:38:GLY:HA3	24:C:511:CLA:HMD2	2.02	0.41
3:C:72:LEU:HD11	3:C:108:THR:HB	2.02	0.41
24:C:507:CLA:H92	24:C:507:CLA:H61	1.94	0.41
30:a:616:LHG:HC42	4:d:232:PHE:CE1	2.54	0.41
2:b:7:ARG:HG2	24:b:613:CLA:O2D	2.20	0.41
2:b:65:PHE:HE1	24:b:606:CLA:HED2	1.85	0.41
2:b:347[B]:ARG:NH1	2:b:351:GLY:O	2.51	0.41
2:b:366:PHE:CG	2:b:367:PRO:HD2	2.55	0.41
2:b:399:VAL:HG12	2:b:417:VAL:HG22	2.02	0.41
2:b:458:PHE:HB3	24:b:606:CLA:HMC2	2.02	0.41
1:A:340:PRO:HB3	15:U:103:TYR:CG	2.55	0.41
24:B:605:CLA:H43	24:B:606:CLA:H2	2.01	0.41
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.84	0.41
13:O:17:ASN:O	13:O:77:SER:OG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:609:CLA:HBA1	24:b:609:CLA:H3A	1.76	0.41
5:e:34:GLY:HA3	6:f:32:PHE:O	2.20	0.41
7:h:6:TRP:CE2	7:h:10:ILE:HD11	2.55	0.41
2:B:383:PHE:CG	4:D:347:PRO:HA	2.55	0.41
3:C:70:PHE:CD2	3:C:70:PHE:C	2.99	0.41
4:D:91:LEU:HB3	4:D:93:TRP:CE2	2.56	0.41
13:O:42:ARG:HG3	13:O:80:GLN:HA	2.02	0.41
2:b:385:ARG:HG2	13:o:165:ALA:O	2.21	0.41
24:b:608[A]:CLA:H102	26:b:621:BCR:HC8	2.02	0.41
3:c:433:LEU:HD22	24:c:510:CLA:H143	2.02	0.41
24:c:505:CLA:H141	8:i:16:VAL:HG22	2.01	0.41
4:d:317:LYS:O	4:d:321:LEU:HG	2.20	0.41
15:u:76:ARG:HA	15:u:79:LEU:HG	2.01	0.41
1:A:217:SER:HA	4:D:272:LEU:HD12	2.02	0.41
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.82	0.41
24:B:609:CLA:HBB2	4:D:123:ILE:HG12	2.02	0.41
26:a:610:BCR:C37	26:a:610:BCR:H20C	2.50	0.41
2:b:103:LEU:HD21	24:b:607:CLA:CMC	2.50	0.41
2:b:325:PHE:CD2	11:l:34:TYR:HB3	2.55	0.41
24:b:606:CLA:H43	24:b:607:CLA:H2	2.02	0.41
3:c:27:ASP:HB3	10:k:46:ARG:HD2	2.02	0.41
4:d:80:THR:HB	4:d:168:PHE:HA	2.02	0.41
4:d:101:PHE:HE1	26:f:101:BCR:HC42	1.86	0.41
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.55	0.41
2:B:458:PHE:HB3	24:B:605:CLA:HMC2	2.02	0.41
26:B:620:BCR:H383	28:a:614:SQD:H241	2.01	0.41
7:H:41:PHE:HB2	26:H:101:BCR:C15	2.51	0.41
1:a:297:LEU:HD23	32:c:517:DGD:HBf2	2.02	0.41
2:b:181:VAL:HG11	2:b:195:PRO:HB2	2.01	0.41
2:b:446:SER:HB2	2:b:447:PRO:HD2	2.03	0.41
28:b:601:SQD:H131	26:b:619:BCR:H23C	2.03	0.41
24:b:616:CLA:HAB	26:b:619:BCR:H19C	2.01	0.41
3:c:223:TRP:CG	3:c:224:ILE:N	2.88	0.41
24:d:403:CLA:H2	18:x:14:LEU:HA	2.02	0.41
1:A:141:PRO:HG3	3:C:446:GLY:C	2.46	0.41
1:A:217:SER:O	1:A:221[A]:SER:HB3	2.21	0.41
1:A:271:LEU:CD1	27:A:611:PL9:HC8	2.49	0.41
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.03	0.41
24:B:606:CLA:HHC	24:B:606:CLA:HBB1	2.01	0.41
24:B:613:CLA:HBB1	24:B:615:CLA:CMB	2.51	0.41
24:B:614:CLA:H151	30:D:406:LHG:H182	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:L:102:SQD:O7	28:b:601:SQD:O5	2.25	0.41
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.03	0.41
1:a:64:ARG:NH1	13:o:105:PRO:O	2.50	0.41
24:a:607:CLA:HMD3	4:d:182:LEU:HD11	2.02	0.41
2:b:222:PRO:HD2	2:b:225:LEU:HD12	2.02	0.41
2:b:270:PRO:HG2	2:b:317:ASN:O	2.20	0.41
24:b:616:CLA:H8	26:b:619:BCR:H362	2.03	0.41
26:c:515:BCR:C20	26:c:515:BCR:H17C	2.50	0.41
7:h:39:LEU:HD23	7:h:39:LEU:C	2.45	0.41
24:B:603:CLA:H172	32:H:102:DGD:HAW1	2.03	0.41
24:B:607[B]:CLA:H72	26:B:620:BCR:C9	2.51	0.41
24:C:501:CLA:H192	24:C:506:CLA:CHB	2.50	0.41
4:D:48:TRP:NE1	25:D:401:PHO:H162	2.36	0.41
6:F:36:ALA:O	6:F:40:MET:HG3	2.21	0.41
7:H:35:MET:HE2	7:H:35:MET:HB3	1.96	0.41
26:H:101:BCR:H20C	26:H:101:BCR:H373	2.02	0.41
2:b:258:TYR:CZ	32:h:102:DGD:HG12	2.56	0.41
3:c:95:LEU:HD11	24:c:503:CLA:HAA2	2.01	0.41
4:d:53:THR:HG22	6:f:40:MET:HE1	2.02	0.41
5:e:69:ARG:NH2	7:h:50:ASN:O	2.44	0.41
5:e:82:GLN:C	5:e:84:LYS:H	2.29	0.41
1:A:65:GLU:OE1	1:A:335:ASN:ND2	2.44	0.41
28:A:612:SQD:H291	24:C:508:CLA:H71	2.03	0.41
30:A:615:LHG:H251	30:A:615:LHG:H281	1.63	0.41
30:A:615:LHG:H332	30:A:615:LHG:H302	1.87	0.41
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	2.02	0.41
2:B:24:LEU:HD21	24:B:617:CLA:CAB	2.50	0.41
2:B:39:LEU:HD23	2:B:39:LEU:HA	1.76	0.41
2:B:223[A]:GLN:CD	2:B:227:LYS:HD2	2.46	0.41
2:B:458:PHE:CG	24:B:605:CLA:HMC2	2.55	0.41
24:B:613:CLA:HBB1	24:B:613:CLA:HMB1	2.03	0.41
24:C:505:CLA:HAA1	24:C:505:CLA:CBD	2.50	0.41
24:C:511:CLA:HBB1	24:C:511:CLA:CMB	2.48	0.41
24:D:404:CLA:C2	18:X:14:LEU:HD12	2.51	0.41
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.03	0.41
1:a:299:GLY:O	3:c:403:SER:HB2	2.21	0.41
2:b:325:PHE:CG	11:l:34:TYR:HB3	2.55	0.41
2:b:383:PHE:CE1	13:o:167:GLY:HA2	2.56	0.41
3:c:203:THR:O	3:c:235:GLY:HA3	2.21	0.41
3:c:297:TYR:HA	3:c:302:TYR:CE2	2.56	0.41
24:c:513:CLA:HAB	26:c:514:BCR:H24C	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:41:HIS:NE2	33:v:201:HEM:NB	2.69	0.41
24:A:609:CLA:H162	24:A:609:CLA:H122	1.76	0.41
1:a:133:LEU:HD23	4:d:256:ILE:HG12	2.01	0.41
2:b:357:ARG:NH2	4:d:337:GLU:HB3	2.36	0.41
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.56	0.41
33:v:201:HEM:HMB2	33:v:201:HEM:HBB2	2.03	0.41
1:A:215:HIS:HA	27:A:611:PL9:O1	2.20	0.40
13:O:110[B]:MET:HE3	13:O:110[B]:MET:HB3	1.90	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.88	0.40
24:c:504:CLA:C1D	32:c:517:DGD:HB21	2.51	0.40
26:c:515:BCR:H11C	26:c:515:BCR:H341	1.70	0.40
1:A:57:PRO:HA	1:A:68:SER:HA	2.03	0.40
1:A:213:ALA:HB2	4:D:275:PRO:HG2	2.03	0.40
30:A:615:LHG:H132	30:A:615:LHG:H372	2.03	0.40
24:B:614:CLA:H121	24:B:614:CLA:H162	1.88	0.40
28:B:622:SQD:H341	28:l:101:SQD:H311	1.28	0.40
3:C:416[A]:SER:HB2	16:V:42:VAL:HG23	2.02	0.40
4:D:293:LEU:HA	4:D:293:LEU:HD12	1.80	0.40
11:L:24[A]:ILE:HD13	11:L:24[A]:ILE:HA	1.91	0.40
16:V:37:CYS:HG	33:V:201:HEM:CAB	2.34	0.40
25:a:608:PHO:HAB	4:d:205:LEU:HD13	2.03	0.40
2:b:125:ASP:HA	2:b:126:PRO:HD3	1.93	0.40
2:b:260:SER:N	2:b:263:THR:OG1	2.53	0.40
24:b:606:CLA:H2	24:b:607:CLA:NC	2.36	0.40
26:k:101:BCR:HC21	19:z:13:VAL:HG13	2.04	0.40
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.57	0.40
3:C:51:GLY:HA2	3:C:132:HIS:HB2	2.03	0.40
3:C:61:VAL:HG12	3:C:118:HIS:O	2.22	0.40
3:C:221:GLU:O	3:C:226:SER:HB3	2.21	0.40
2:b:192:PRO:HB3	7:h:49:TYR:CE2	2.57	0.40
24:b:607:CLA:H41	24:b:607:CLA:H62	1.77	0.40
26:k:101:BCR:H17C	17:y:33:PRO:CD	2.51	0.40
25:A:608:PHO:H61	25:A:608:PHO:H2	1.85	0.40
2:B:189:GLY:O	2:B:197:GLY:HA3	2.21	0.40
2:B:256:MET:HG3	2:B:448:ARG:HG3	2.03	0.40
26:B:619:BCR:C20	26:B:619:BCR:C36	3.00	0.40
3:C:210:PHE:HD2	3:C:213[B]:LEU:HD22	1.86	0.40
24:C:502:CLA:H61	24:C:512:CLA:H42	2.03	0.40
25:D:401:PHO:H62	25:D:401:PHO:H41	1.79	0.40
13:O:180:GLU:CD	13:O:180:GLU:H	2.30	0.40
14:T:14:ILE:HD13	14:T:14:ILE:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:611:PL9:H222	27:a:611:PL9:H253	1.86	0.40
2:b:110:ALA:HB2	26:b:621:BCR:H16C	2.02	0.40
24:b:603:CLA:CMC	26:h:101:BCR:H19C	2.51	0.40
3:c:210:PHE:CD2	3:c:213[B]:LEU:HD22	2.53	0.40
3:c:334:PRO:HA	13:o:153:THR:OG1	2.22	0.40
3:c:344:SER:OG	3:c:348:GLU:OE2	2.33	0.40
3:c:443:TRP:CE2	24:c:508:CLA:HMD2	2.56	0.40
7:h:28:THR:HB	7:h:29:PRO:HD3	2.04	0.40
13:o:126:VAL:O	13:o:144:GLY:HA3	2.22	0.40
2:B:105:GLY:O	2:B:108:PHE:HB3	2.20	0.40
2:B:125:ASP:OD1	7:H:18:TYR:HB3	2.22	0.40
2:B:220:ARG:HG3	7:H:20:LYS:HD3	2.02	0.40
3:C:59:LEU:HD23	3:C:59:LEU:HA	1.77	0.40
24:C:501:CLA:CHB	26:I:101:BCR:H271	2.51	0.40
24:C:512:CLA:H101	24:C:513:CLA:H141	2.04	0.40
4:D:279:LEU:HD11	25:D:401:PHO:HMC3	2.04	0.40
5:E:22:ILE:HD13	33:E:103:HEM:HMA1	2.03	0.40
6:F:34:LEU:HG	26:F:101:BCR:H19C	2.03	0.40
26:F:101:BCR:H393	26:F:101:BCR:H281	1.80	0.40
12:M:23:ILE:O	12:M:27:VAL:HG23	2.21	0.40
1:a:269:ARG:CZ	4:d:222:LEU:HD13	2.51	0.40
1:a:330:VAL:HG21	4:d:328:TRP:CE2	2.56	0.40
2:b:477:ASP:OD1	2:b:478:VAL:N	2.54	0.40
3:c:114:VAL:HG11	24:c:503:CLA:HED2	2.04	0.40
3:c:418:ASN:HB2	32:c:518:DGD:O4E	2.21	0.40
24:c:502:CLA:H61	24:c:512:CLA:H42	2.03	0.40
4:d:65:SER:HB2	4:d:77:ALA:O	2.22	0.40
25:d:401:PHO:H112	25:d:401:PHO:H72	1.85	0.40

There are no symmetry-related clashes.

3.3 Torsion angles [i](#)

3.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	36	67
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	36	67
2	B	512/504 (102%)	506 (99%)	6 (1%)	0	100	100
2	b	512/504 (102%)	505 (99%)	7 (1%)	0	100	100
3	C	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	30	62
3	c	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	30	62
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	3	26
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	30	62
13	o	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	30	62
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5139 (98%)	104 (2%)	9 (0%)	48	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
10	k	11	LEU
1	A	259	ILE
1	a	259	ILE

3.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/269 (102%)	273 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	412/402 (102%)	406 (98%)	6 (2%)	57	71
2	b	412/402 (102%)	406 (98%)	6 (2%)	57	71
3	C	357/352 (101%)	349 (98%)	8 (2%)	45	65
3	c	357/352 (101%)	352 (99%)	5 (1%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	277/277 (100%)	275 (99%)	2 (1%)	76	78
4	d	277/277 (100%)	275 (99%)	2 (1%)	76	78
5	E	74/72 (103%)	73 (99%)	1 (1%)	59	71
5	e	74/72 (103%)	73 (99%)	1 (1%)	59	71
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	57
6	f	28/28 (100%)	27 (96%)	1 (4%)	31	57
7	H	56/54 (104%)	53 (95%)	3 (5%)	20	46
7	h	56/54 (104%)	53 (95%)	3 (5%)	20	46
8	I	36/35 (103%)	36 (100%)	0	100	100
8	i	36/35 (103%)	36 (100%)	0	100	100
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15	41
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	28
11	L	36/35 (103%)	35 (97%)	1 (3%)	38	61
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	61
12	M	32/31 (103%)	31 (97%)	1 (3%)	35	59
12	m	32/31 (103%)	30 (94%)	2 (6%)	16	42
13	O	210/206 (102%)	206 (98%)	4 (2%)	50	68
13	o	210/206 (102%)	206 (98%)	4 (2%)	50	68
14	T	29/27 (107%)	29 (100%)	0	100	100
14	t	29/27 (107%)	29 (100%)	0	100	100
15	U	84/84 (100%)	83 (99%)	1 (1%)	63	73
15	u	84/84 (100%)	83 (99%)	1 (1%)	63	73
16	V	118/117 (101%)	117 (99%)	1 (1%)	73	77
16	v	118/117 (101%)	117 (99%)	1 (1%)	73	77
17	Y	22/22 (100%)	21 (96%)	1 (4%)	24	50
17	y	22/22 (100%)	21 (96%)	1 (4%)	24	50
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	33 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	55
All	All	4370/4302 (102%)	4303 (98%)	67 (2%)	57	71

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	80	ILE
2	B	84	THR
2	B	86	ILE
2	B	127	ARG
2	B	467	ILE
2	B	472	ARG
3	C	24	THR
3	C	29	GLU
3	C	142	GLU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
3	C	416[A]	SER
3	C	416[B]	SER
4	D	11	GLU
4	D	90	LEU
5	E	71	GLU
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	65	LEU
10	K	13	GLU
10	K	17	ILE
11	L	1	MET
12	M	9	ILE
13	O	61	GLN
13	O	62	GLU
13	O	181	GLU
13	O	234	LYS
15	U	70	ARG
16	V	30	LYS
17	Y	27	MET
19	Z	4	LEU
19	Z	6	GLN
2	b	84	THR
2	b	86	ILE

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Mol	Chain	Res	Type
2	b	127	ARG
2	b	236	THR
2	b	467	ILE
2	b	472	ARG
3	c	24	THR
3	c	29	GLU
3	c	142	GLU
3	c	289	PHE
3	c	315	MET
4	d	11	GLU
4	d	90	LEU
5	e	71	GLU
6	f	44	GLN
7	h	12[A]	ARG
7	h	12[B]	ARG
7	h	65	LEU
10	k	13	GLU
10	k	17	ILE
10	k	26	PRO
11	l	1	MET
12	m	9	ILE
12	m	20	VAL
13	o	61	GLN
13	o	62	GLU
13	o	181	GLU
13	o	234	LYS
15	u	70	ARG
16	v	30	LYS
17	y	27	MET
19	z	4	LEU
19	z	6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
2	B	216	HIS
2	B	409	GLN
3	C	44	ASN
3	C	132	HIS
3	C	201	ASN

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Mol	Chain	Res	Type
4	D	255	GLN
10	K	40	GLN
11	L	6	ASN
12	M	5	GLN
12	M	33	GLN
1	a	75	ASN
1	a	165	GLN
1	a	198	HIS
1	a	296	ASN
1	a	338	ASN
2	b	26	HIS
2	b	331	ASN
2	b	409	GLN
3	c	44	ASN
3	c	53	HIS
4	d	142	ASN
4	d	186	GLN
4	d	197	HIS
10	k	40	GLN
15	u	73	GLN
19	z	58	ASN

3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.6 Ligand geometry [i](#)

Of 168 ligands modelled in this entry, 168 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

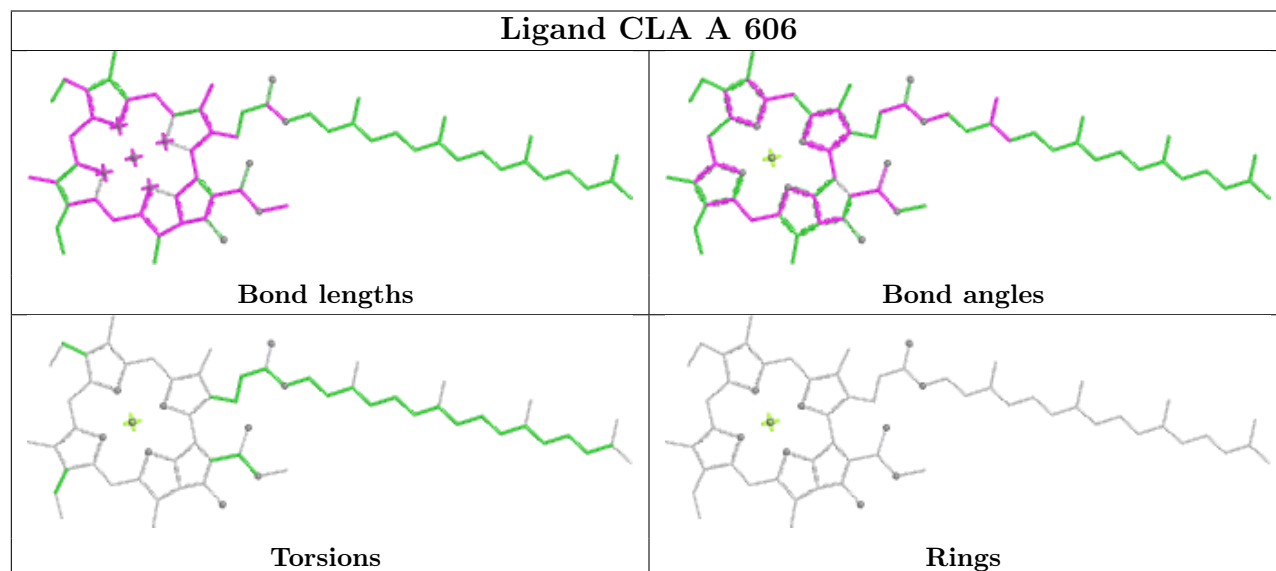
There are no chirality outliers.

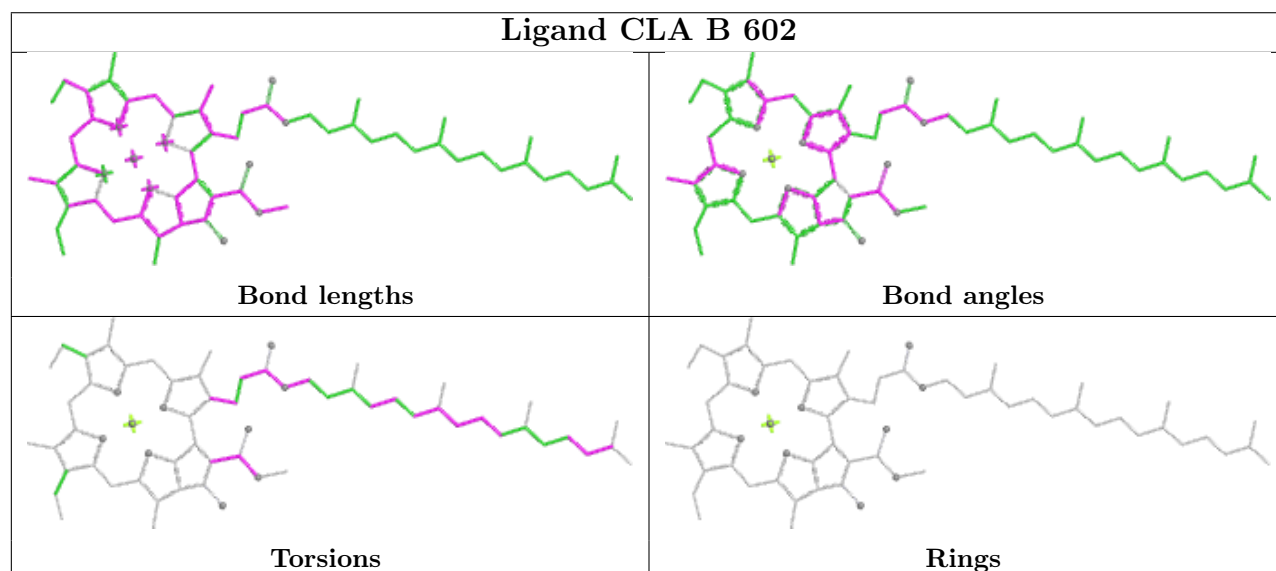
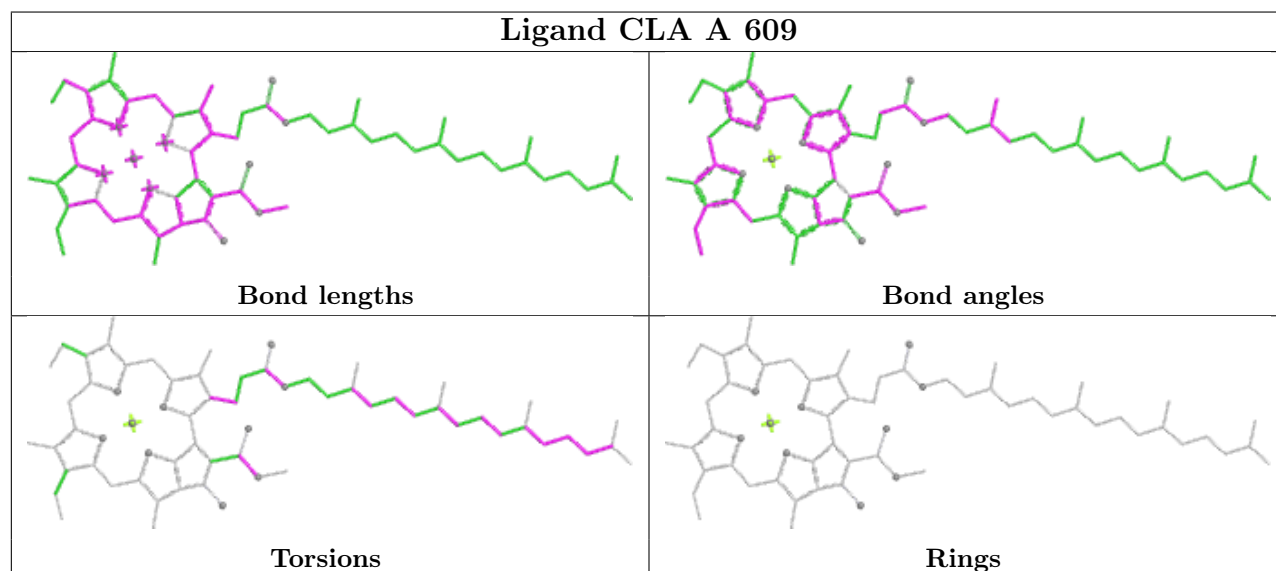
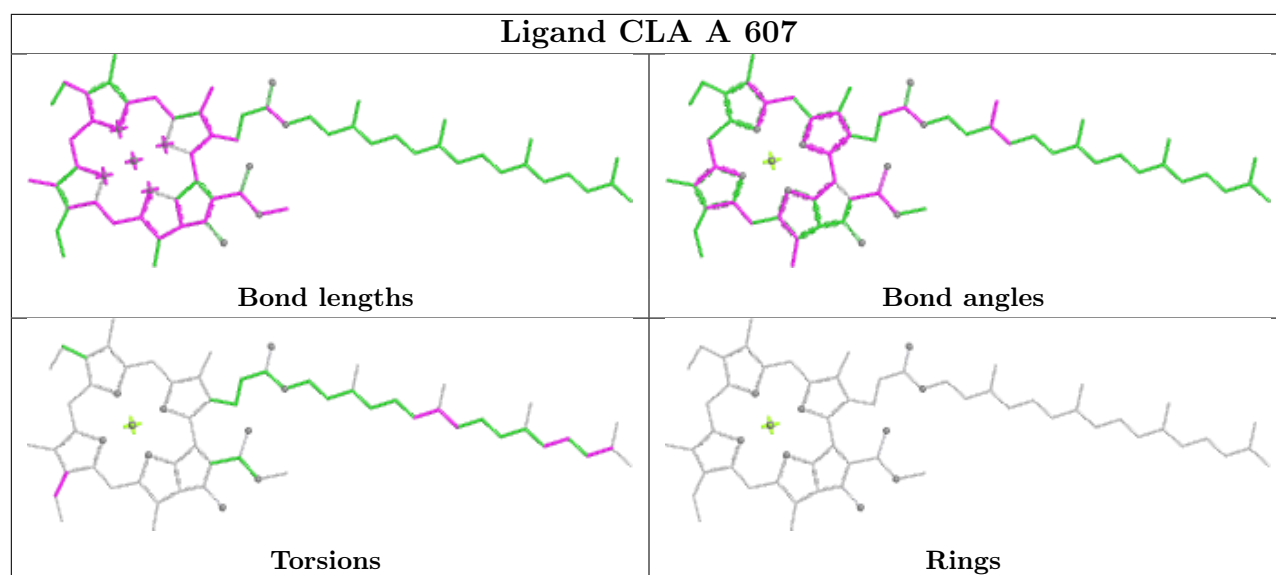
There are no torsion outliers.

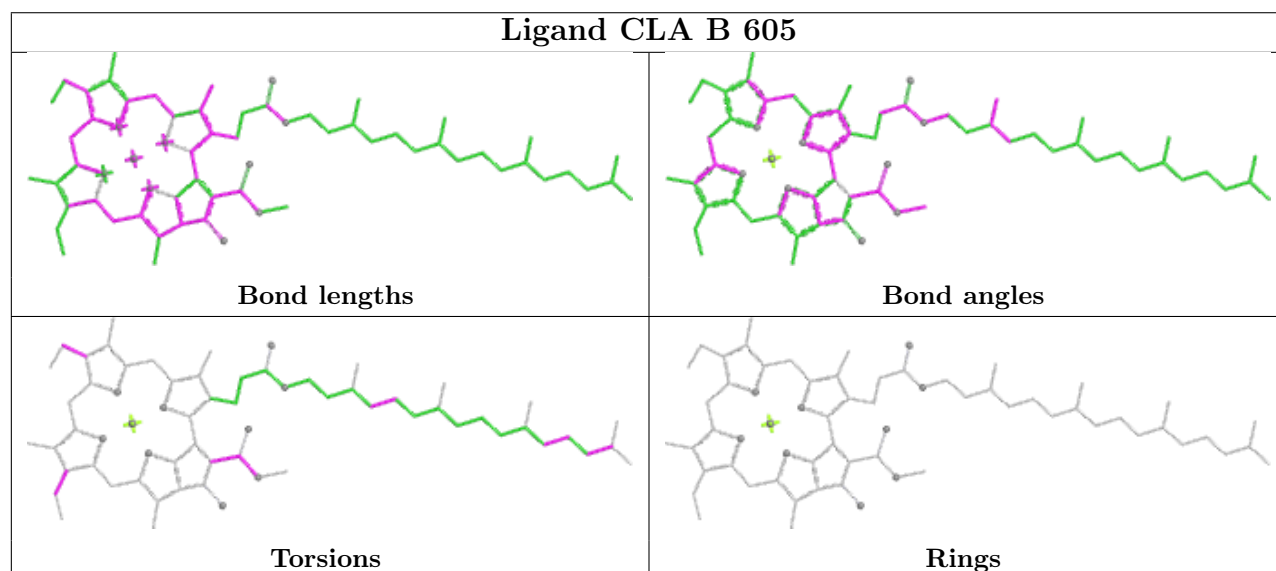
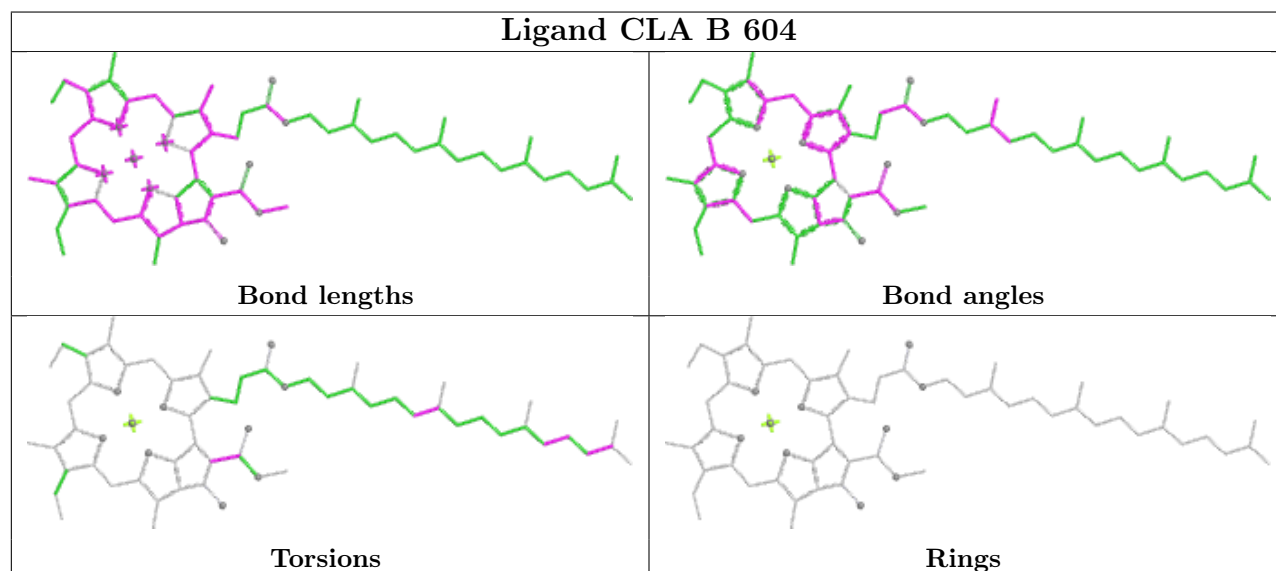
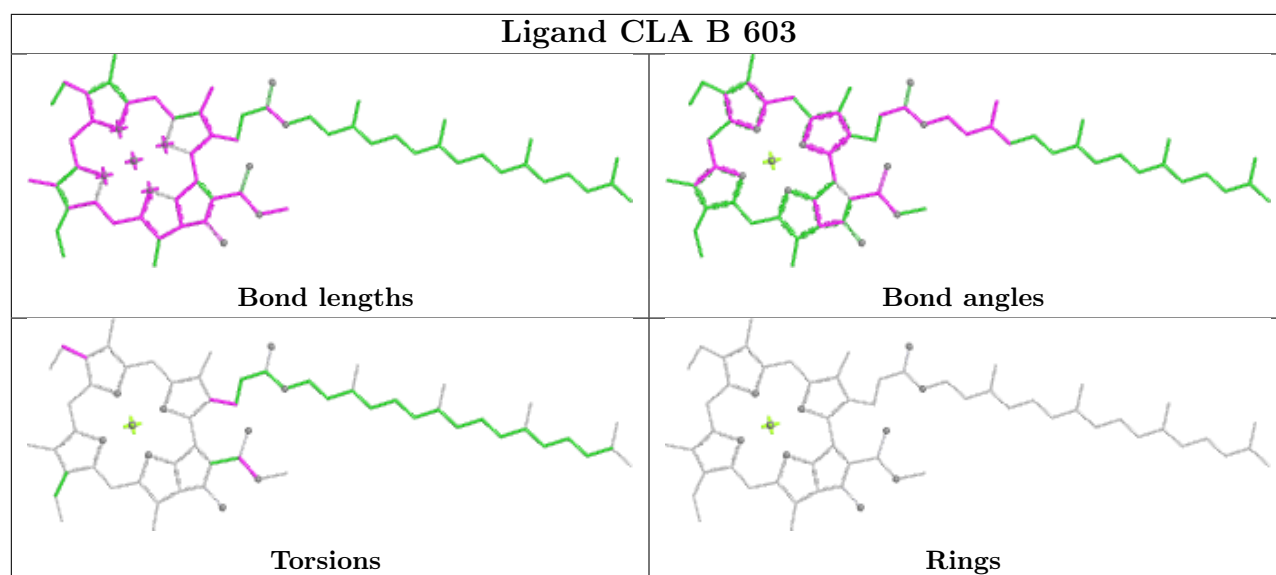
There are no ring outliers.

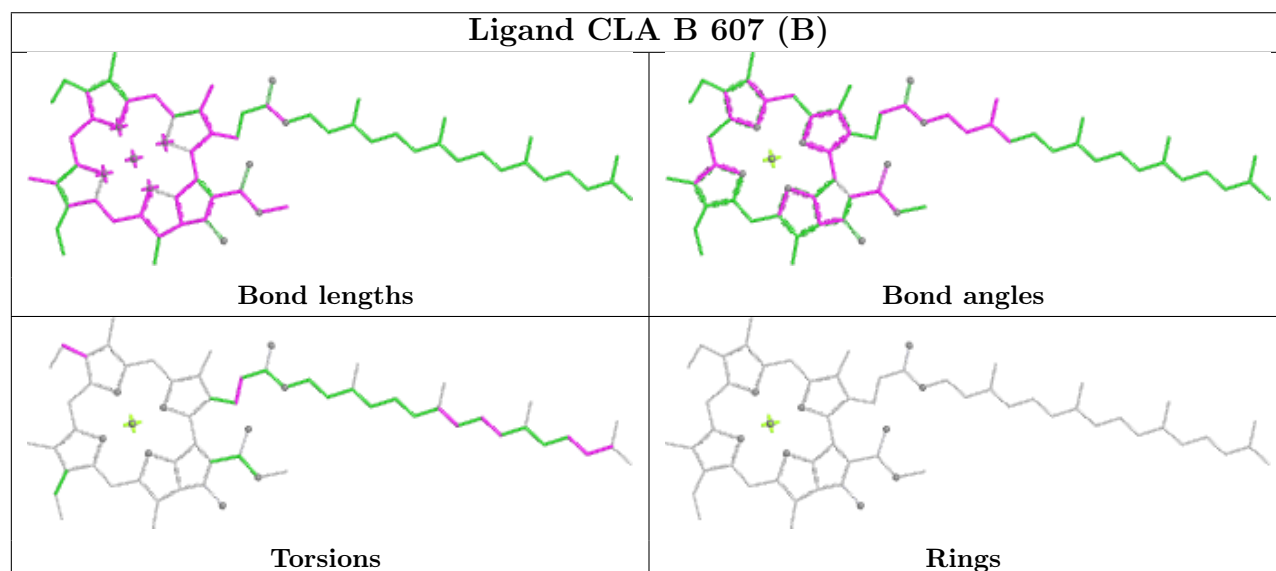
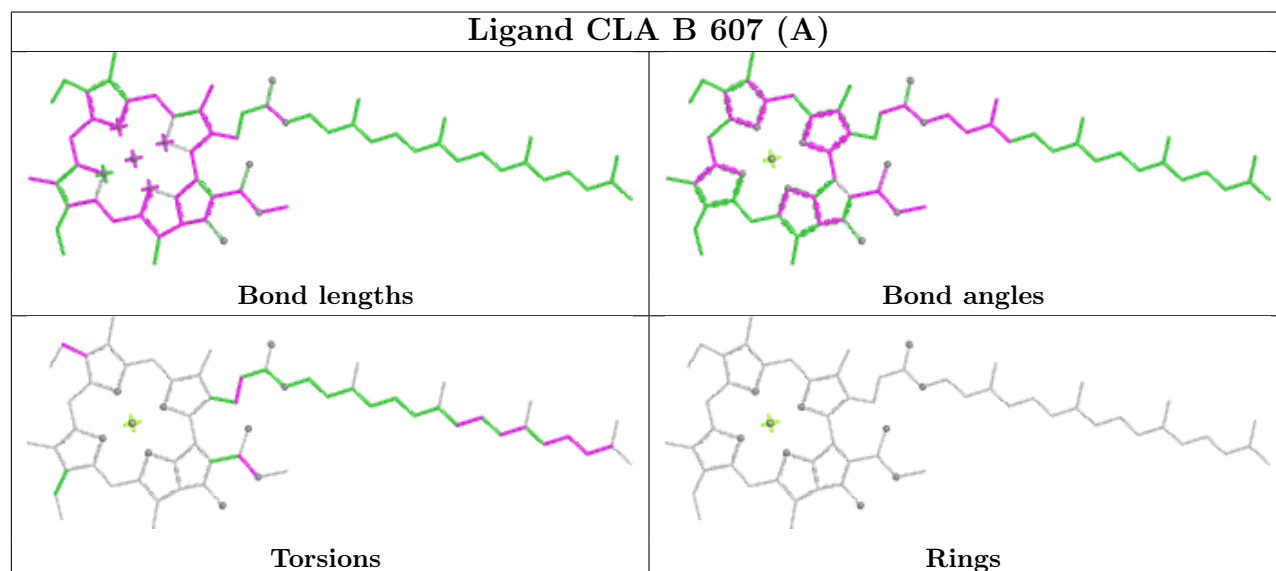
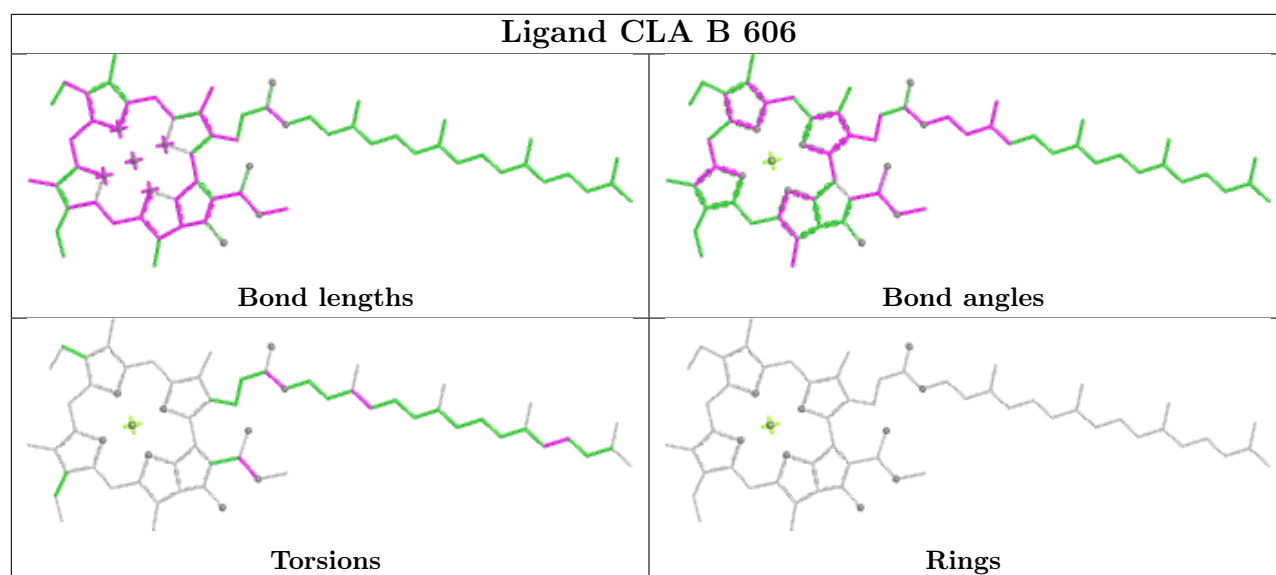
No monomer is involved in short contacts.

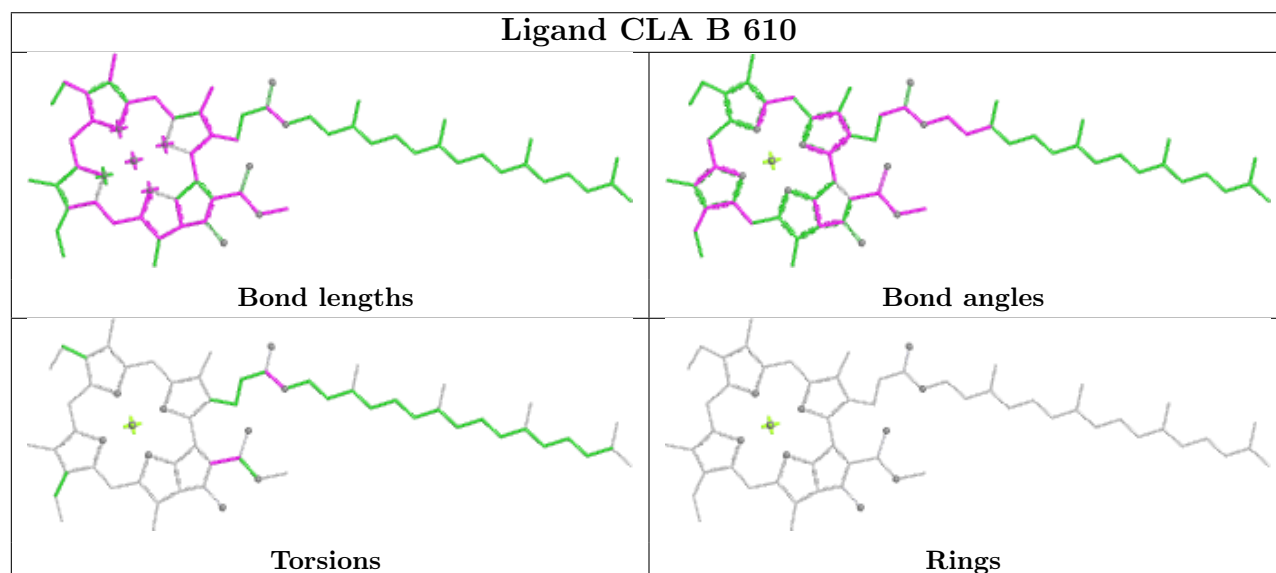
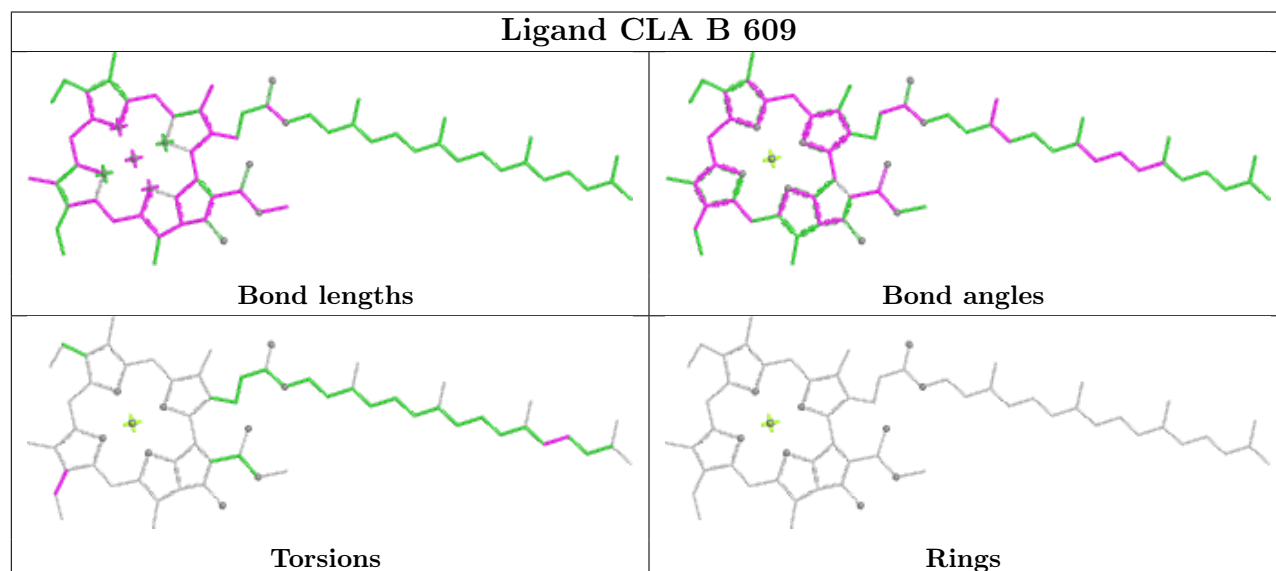
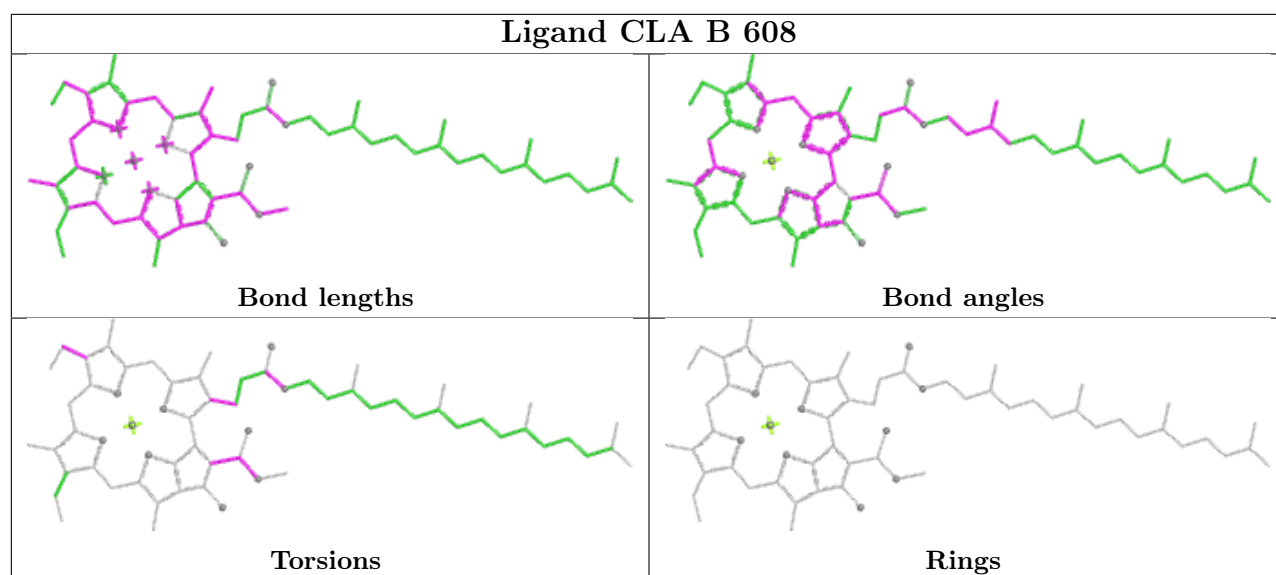
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

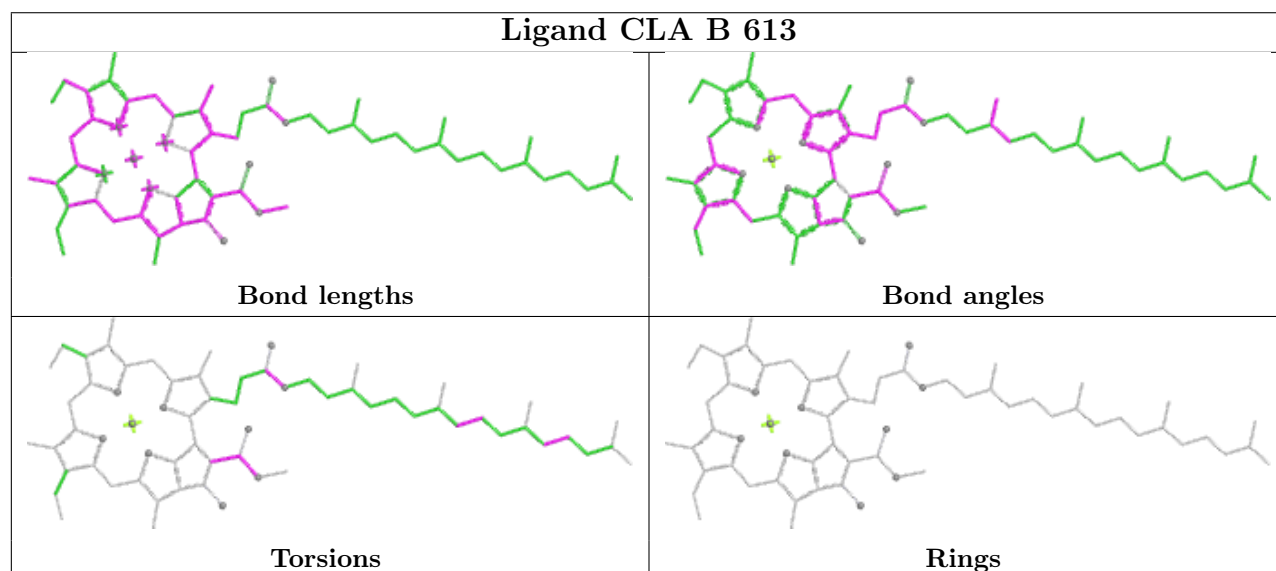
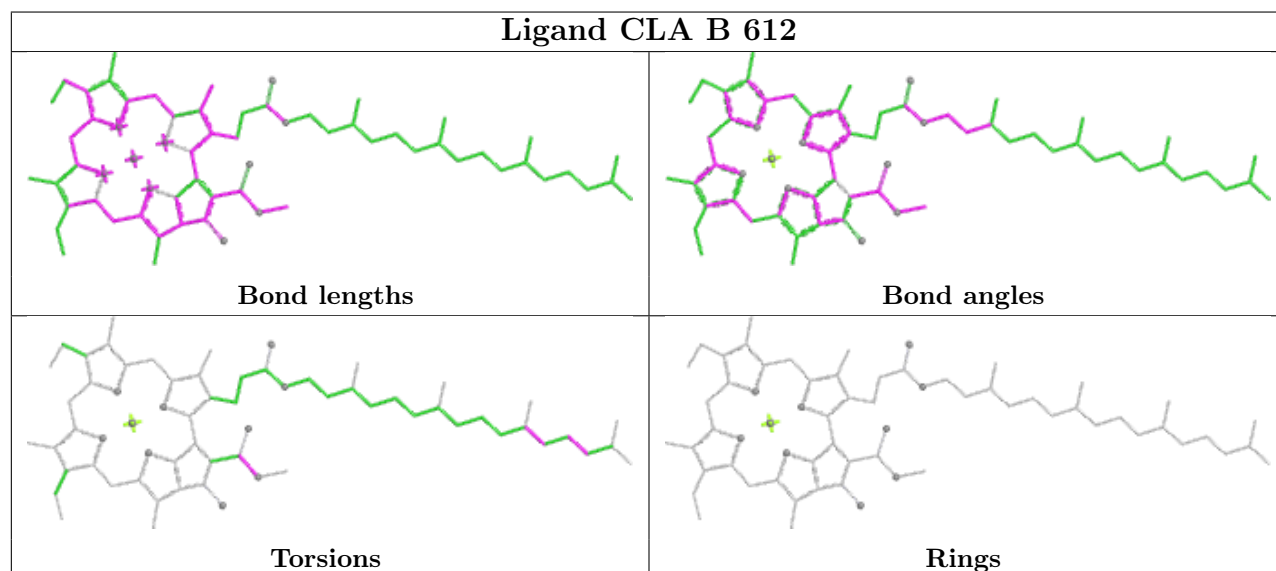
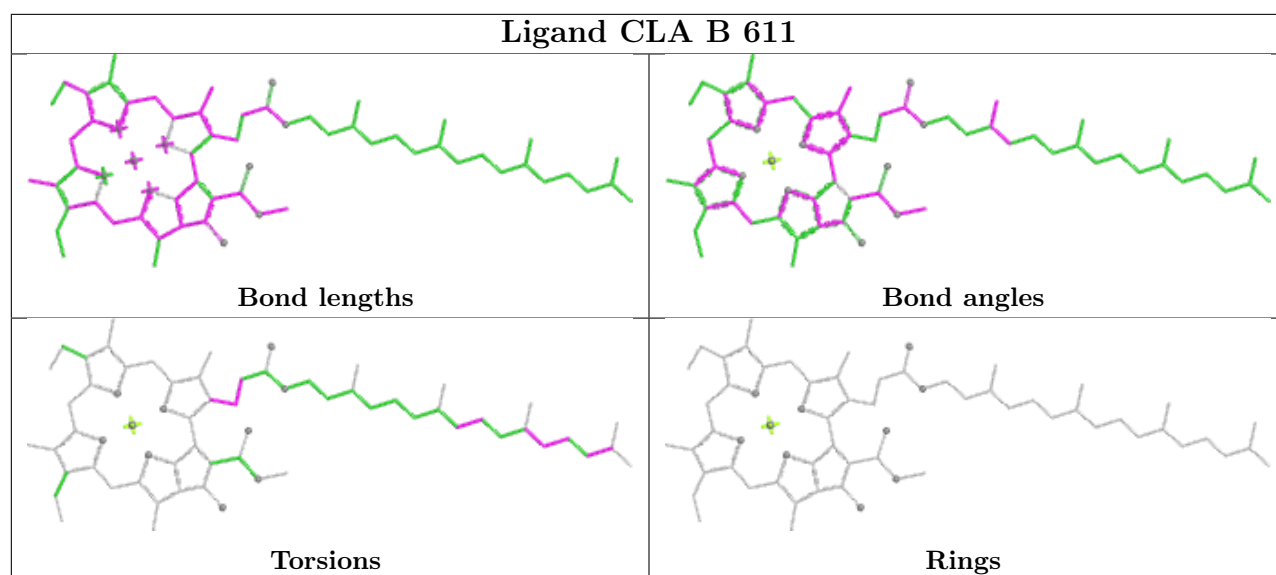


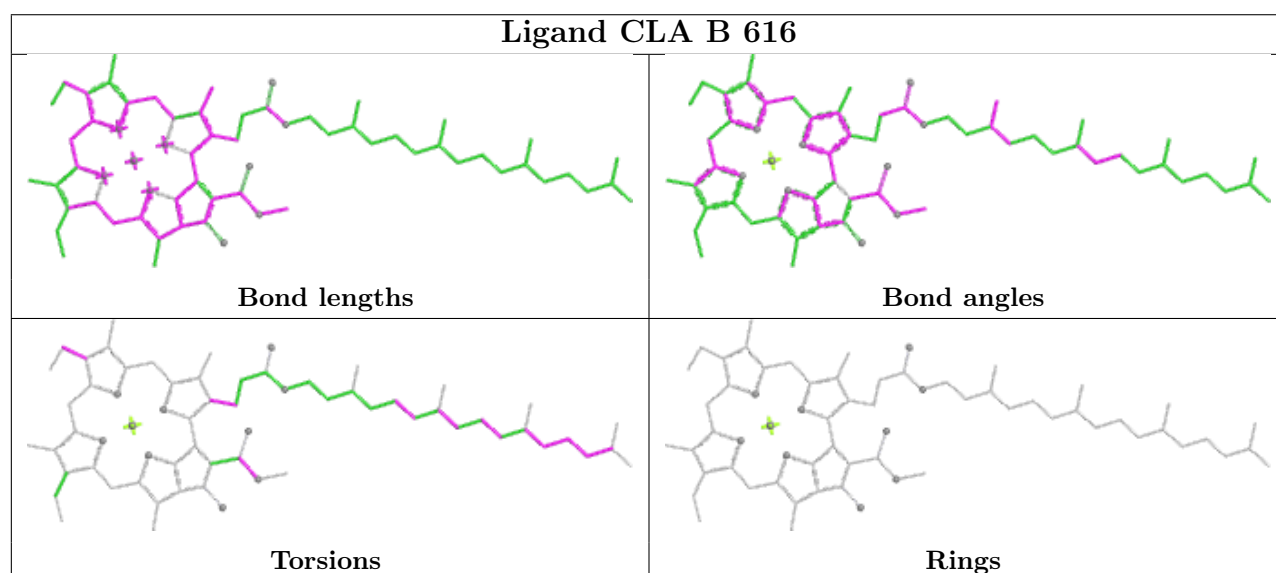
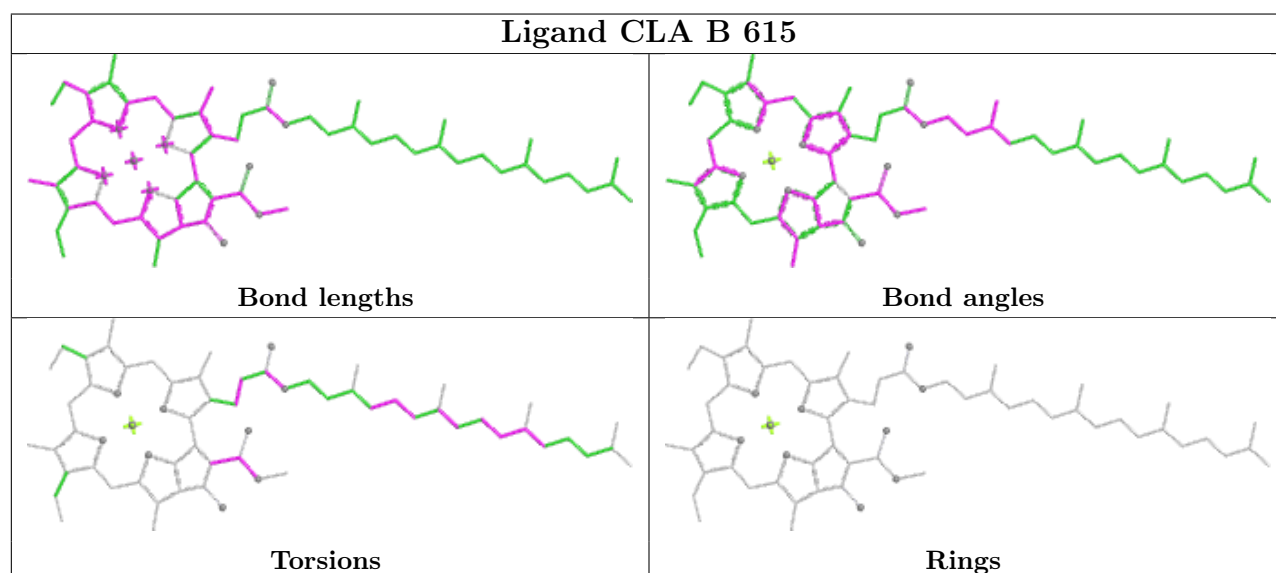
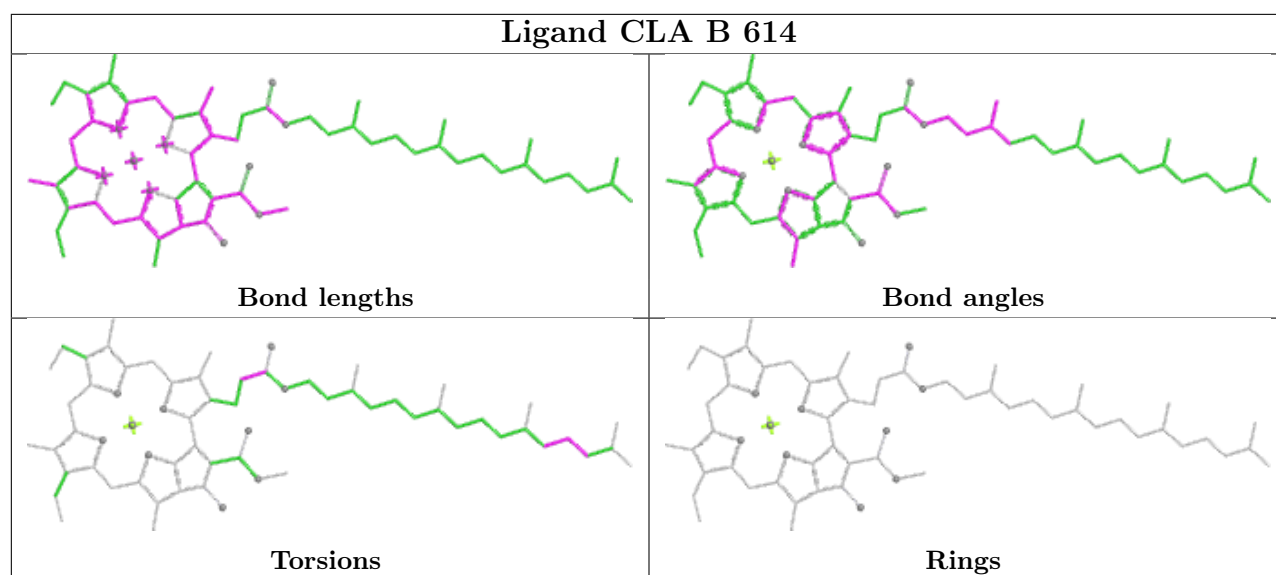


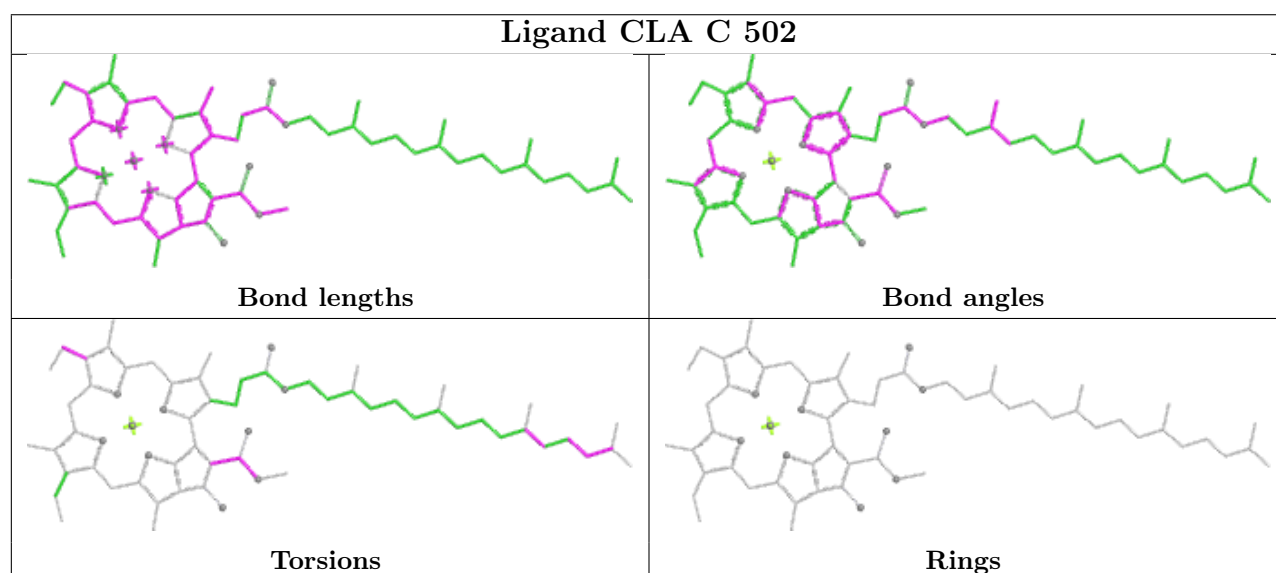
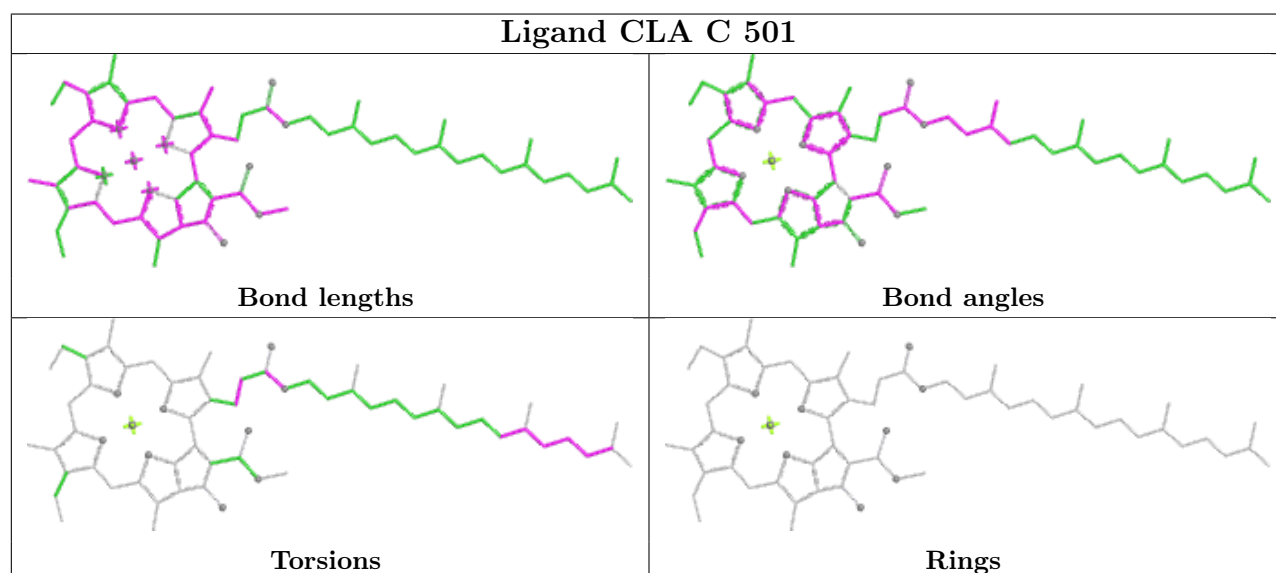
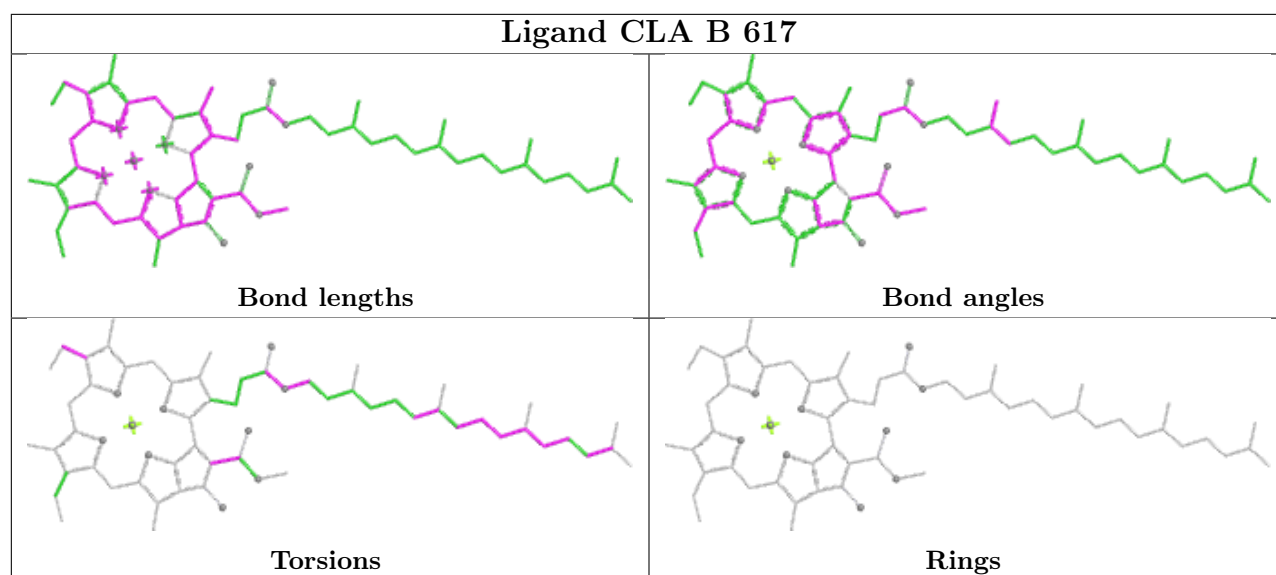


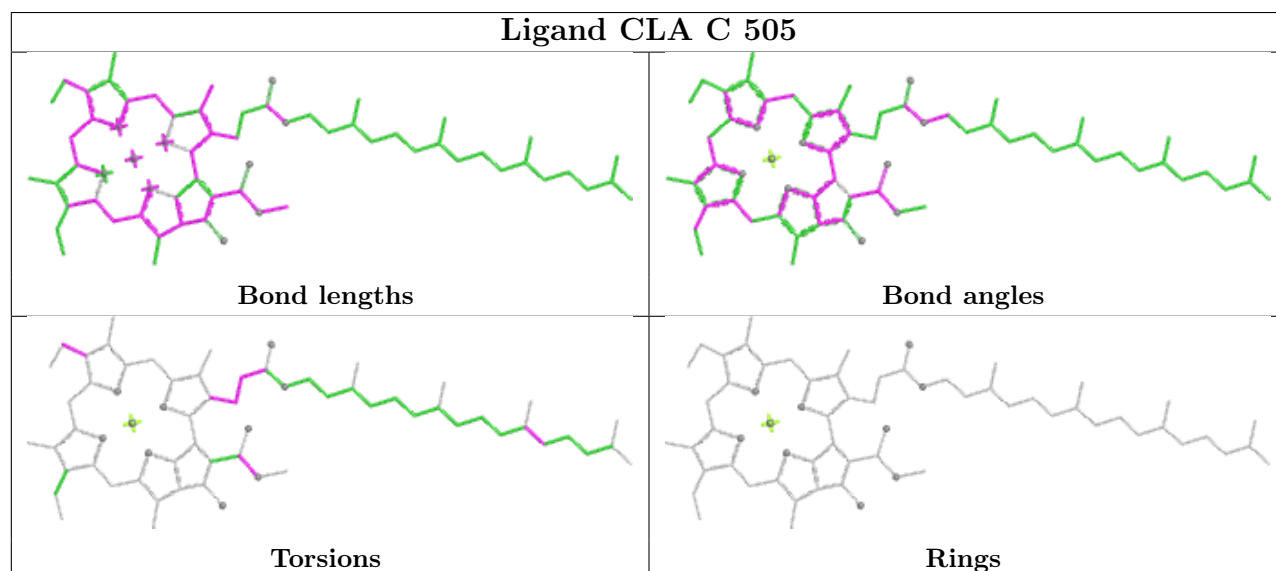
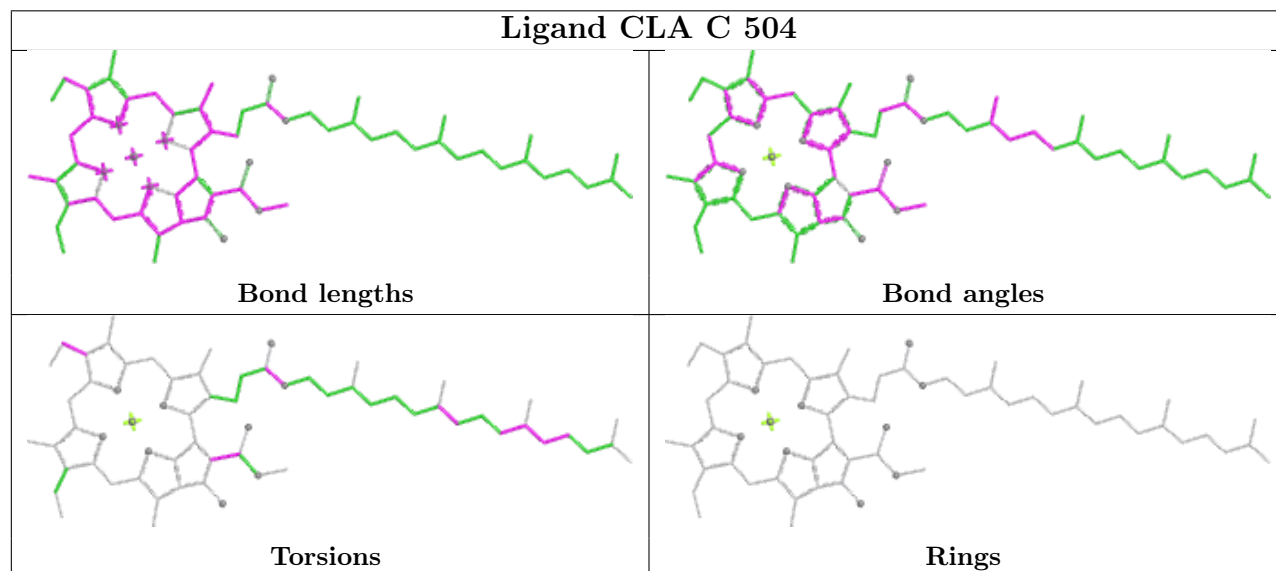
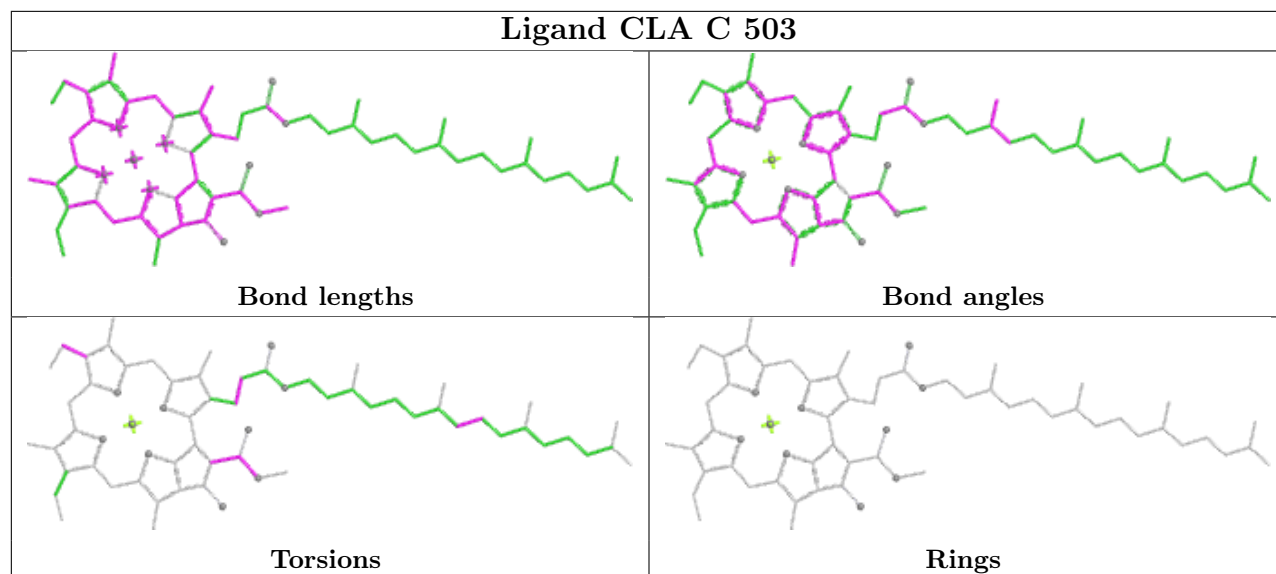


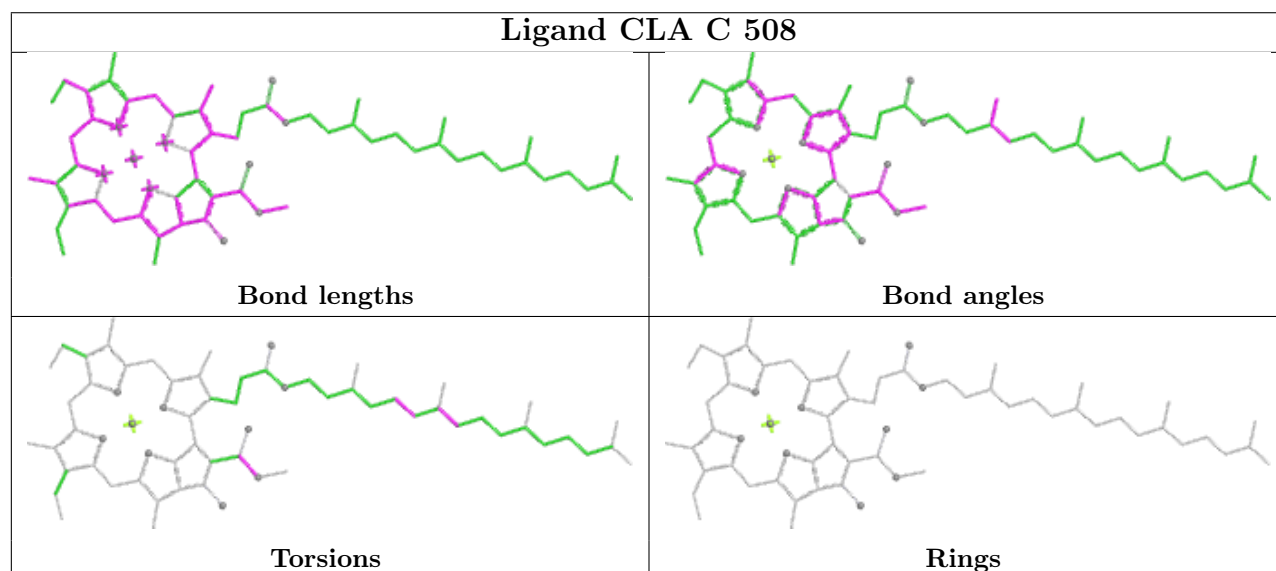
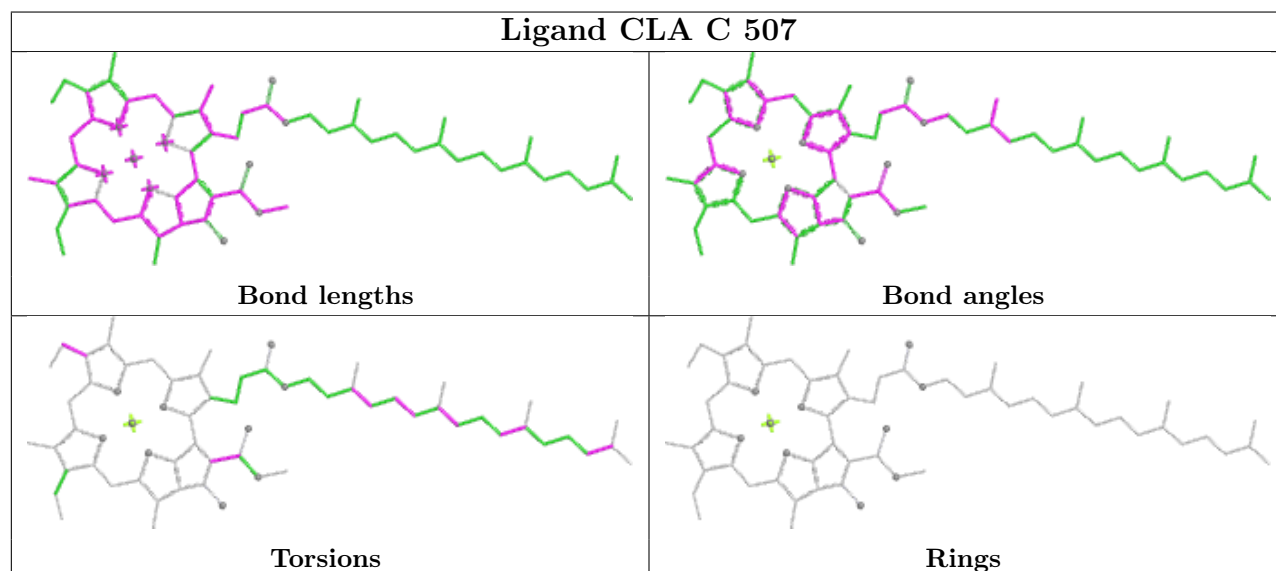
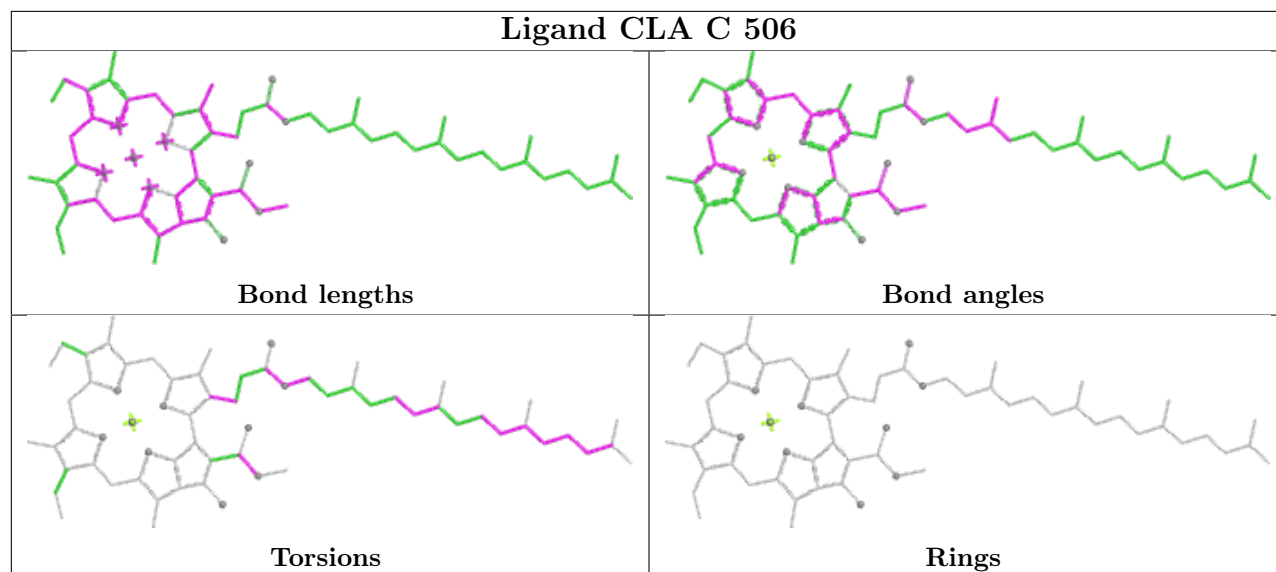


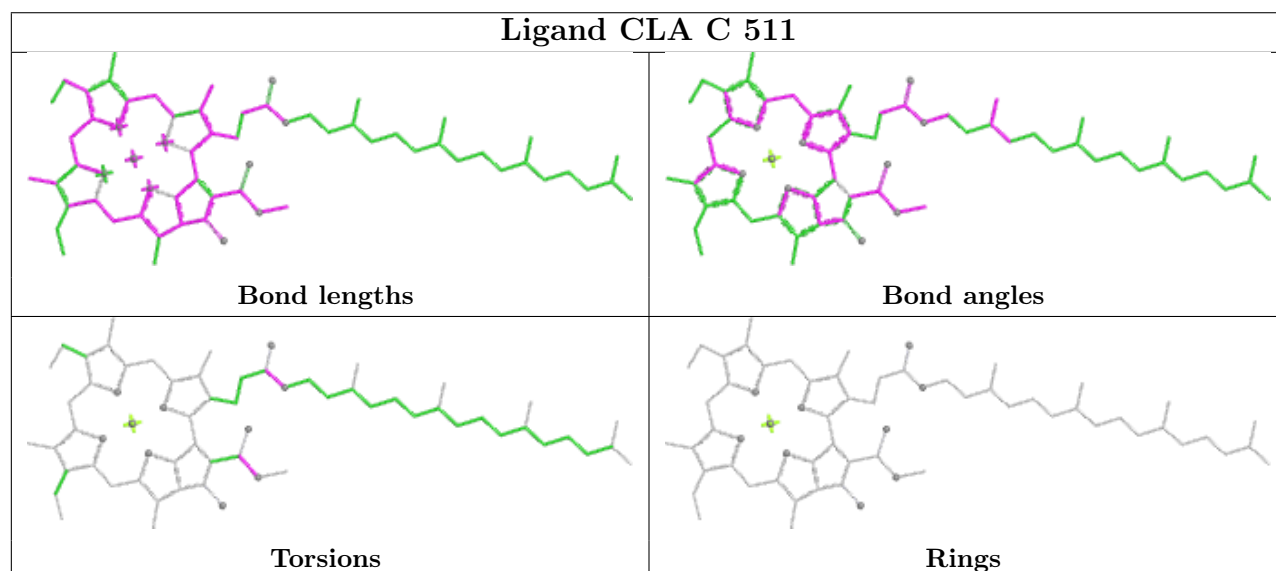
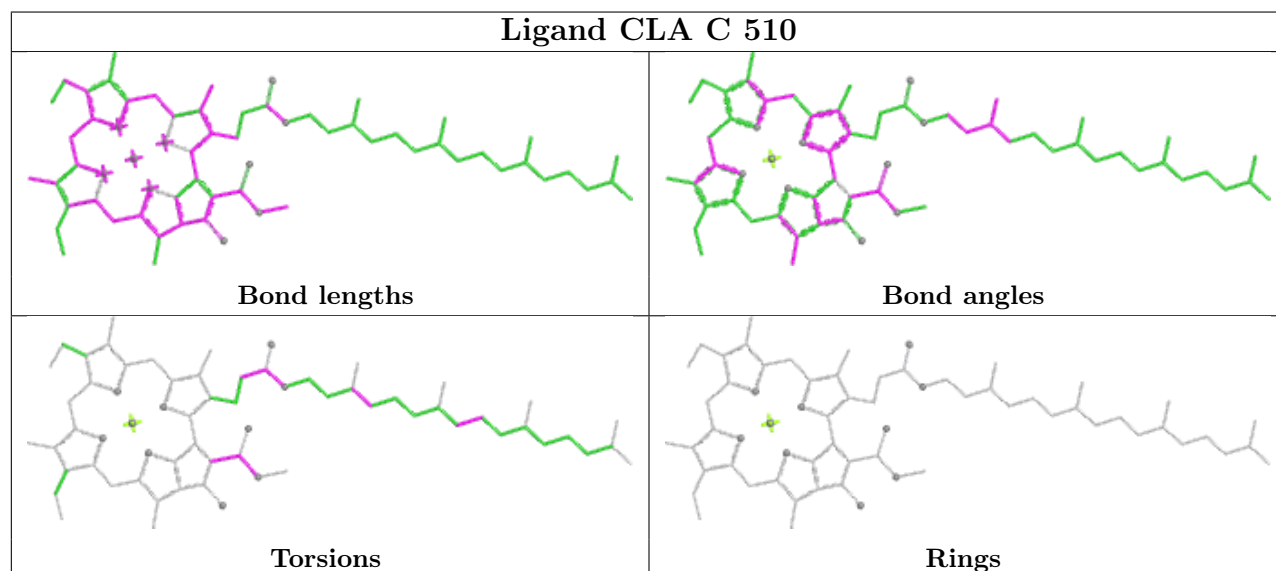
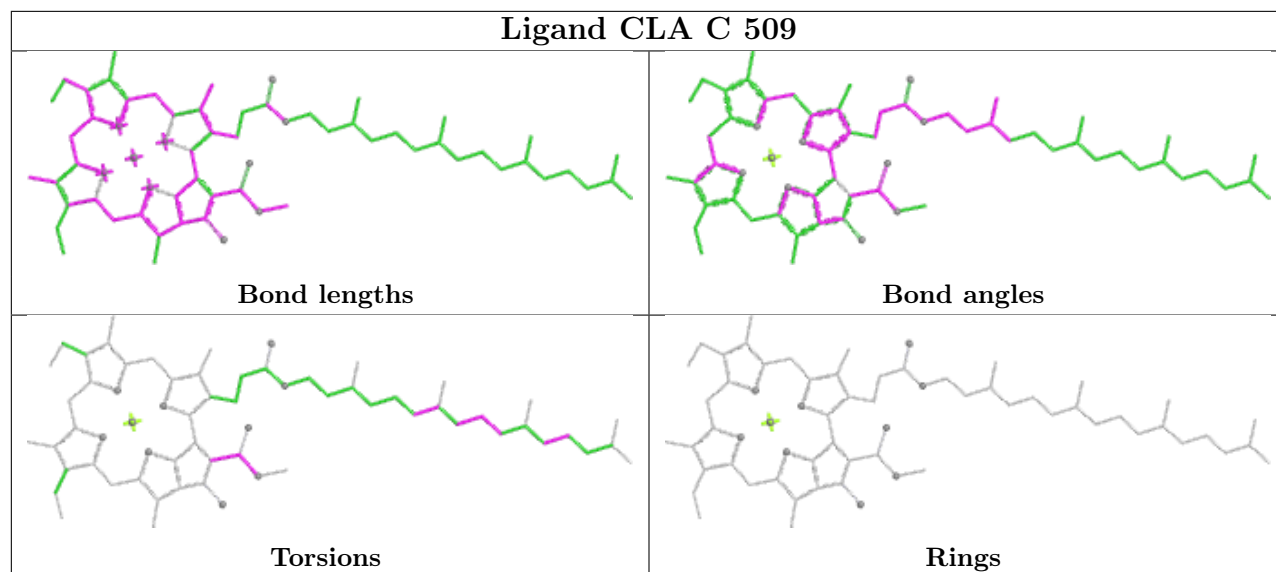


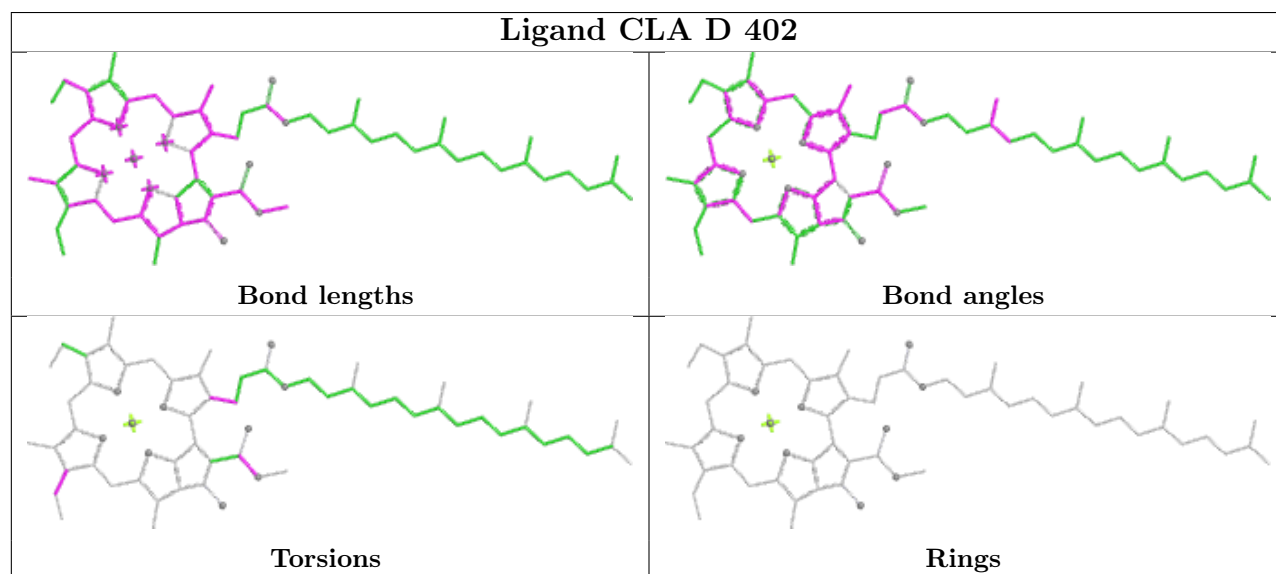
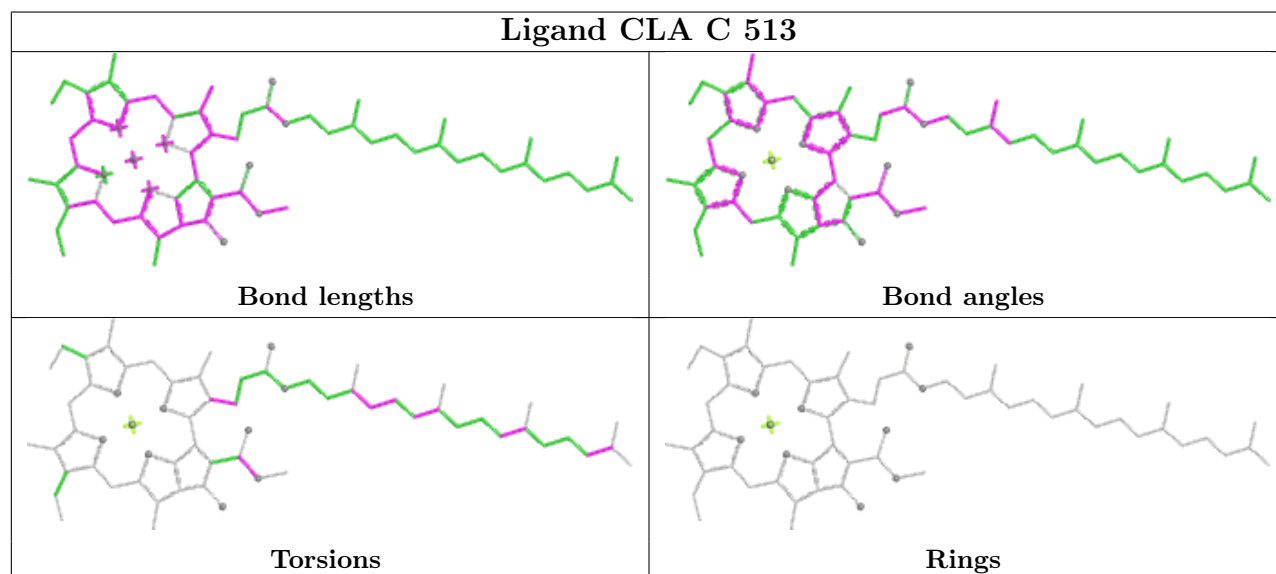
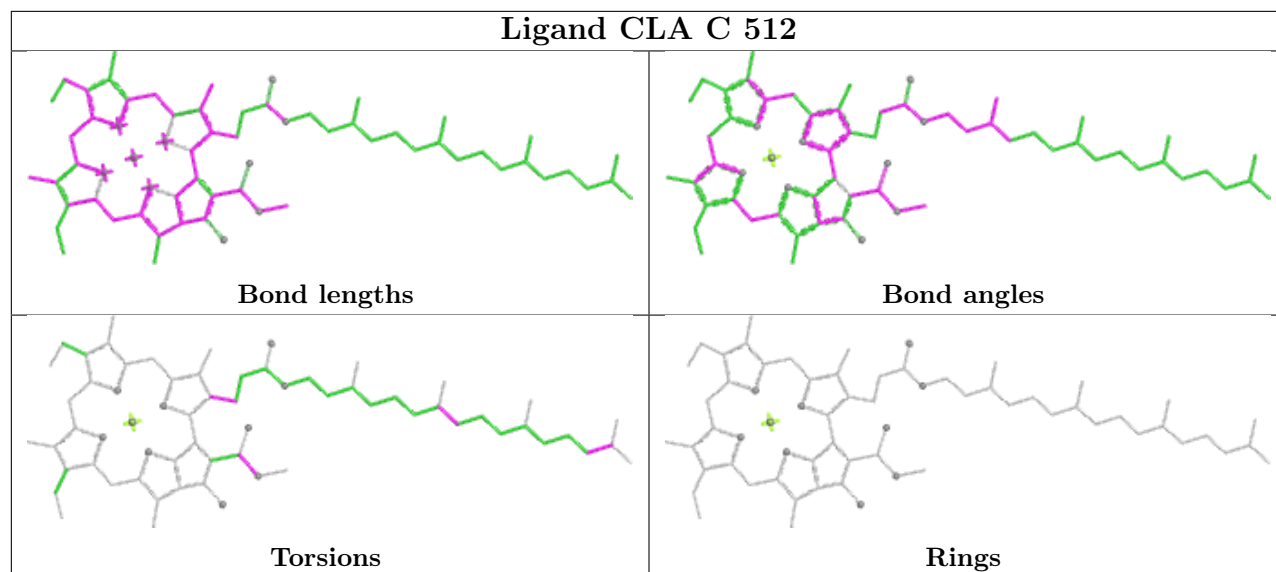


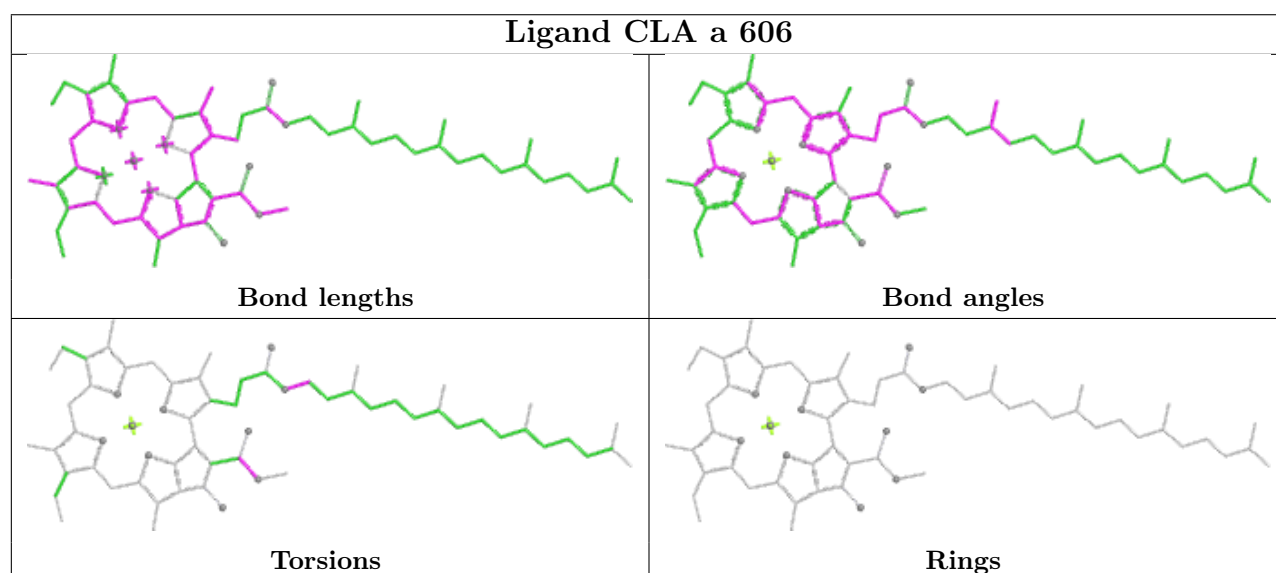
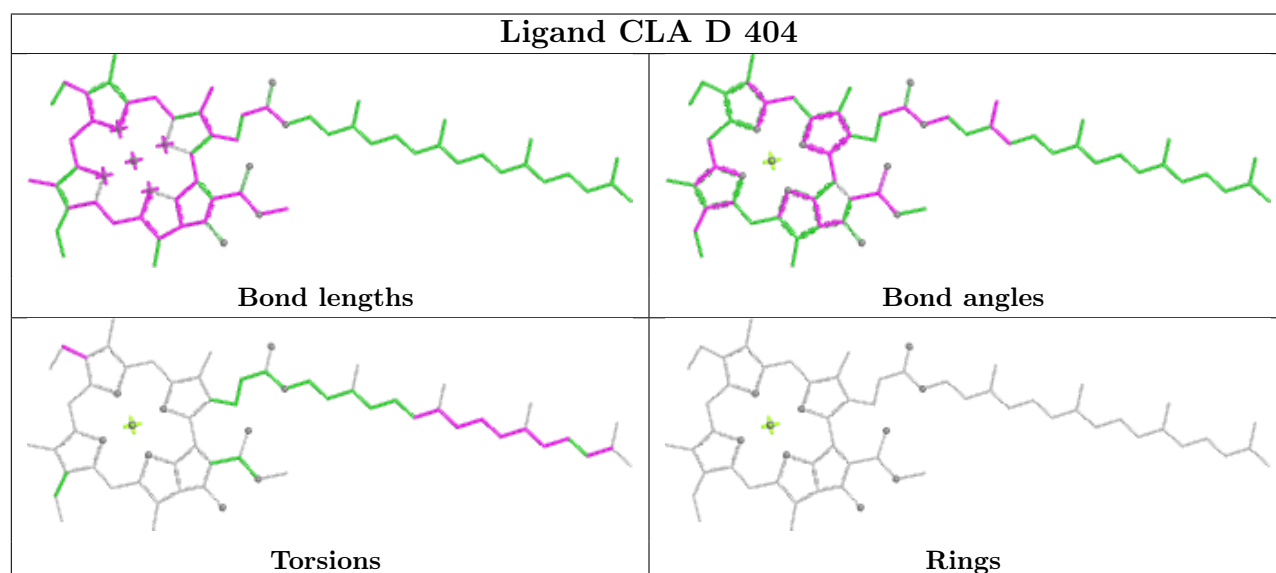
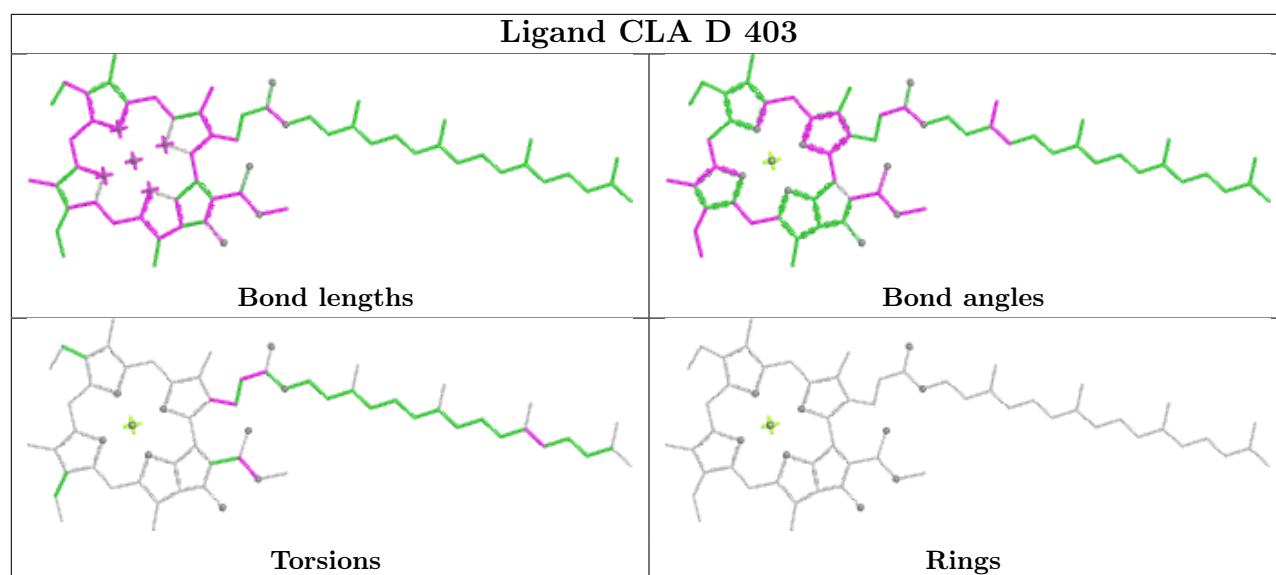




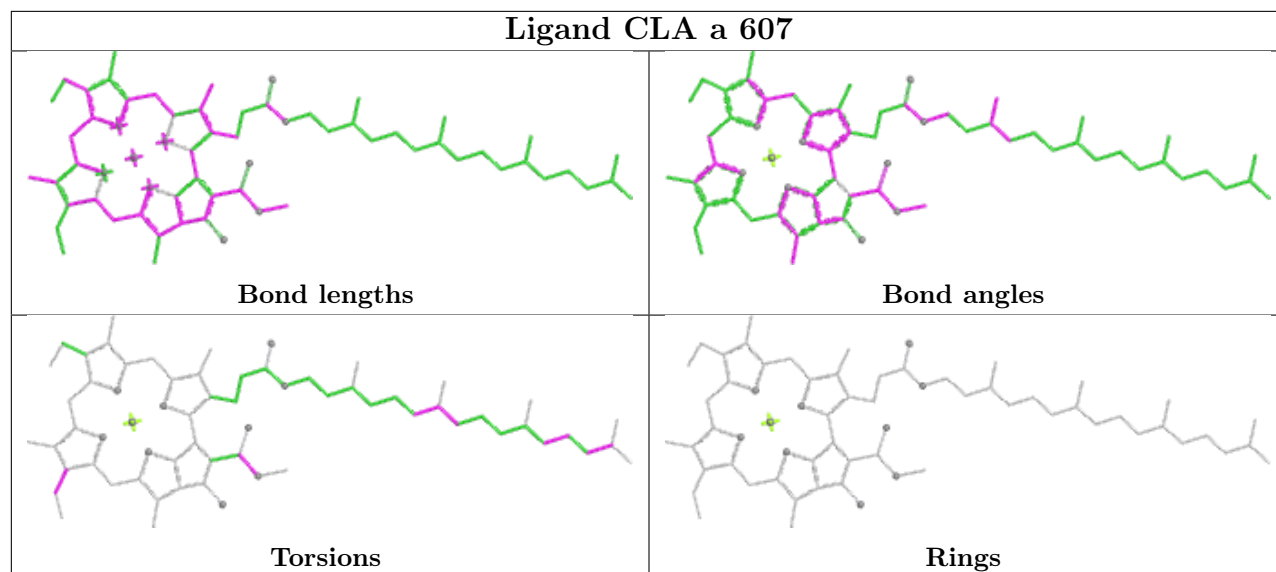




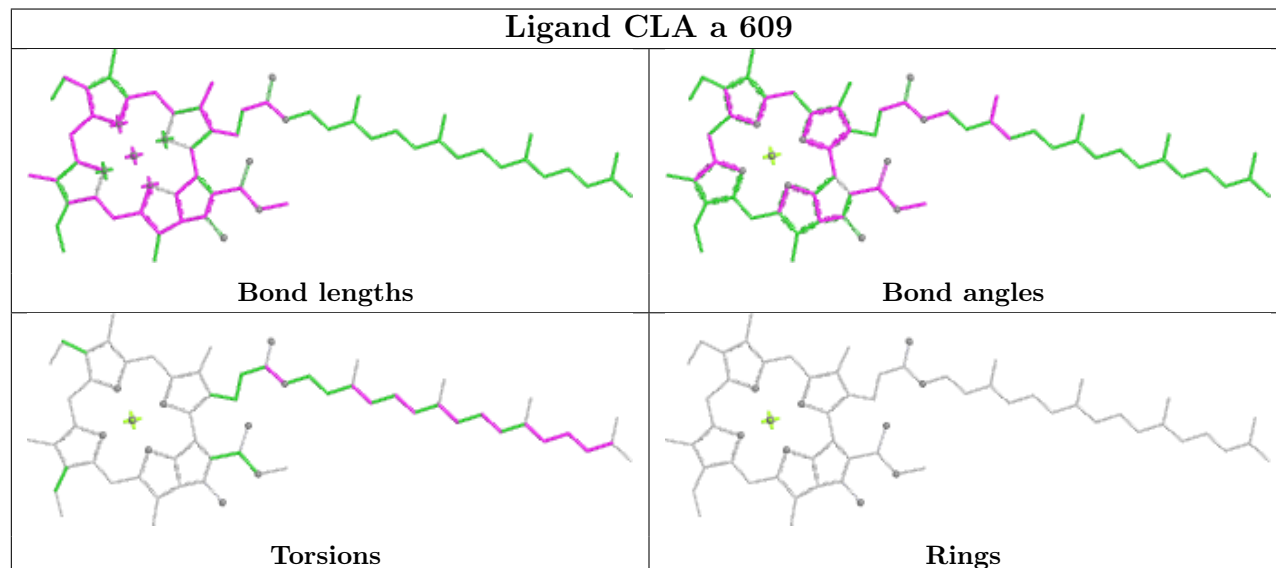




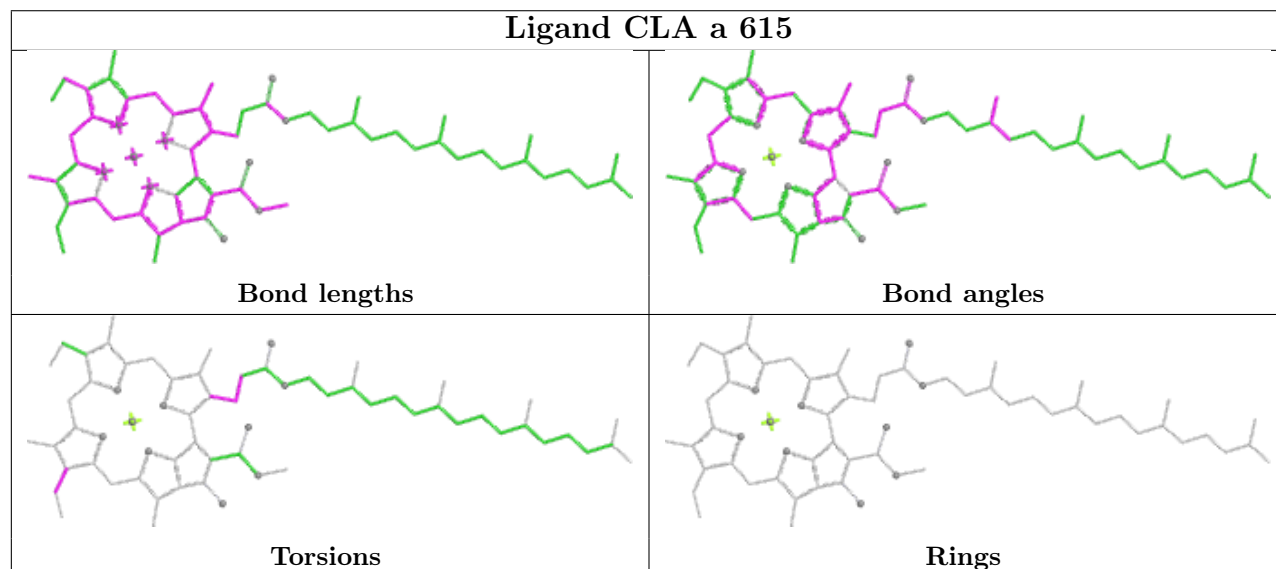
Ligand CLA a 607



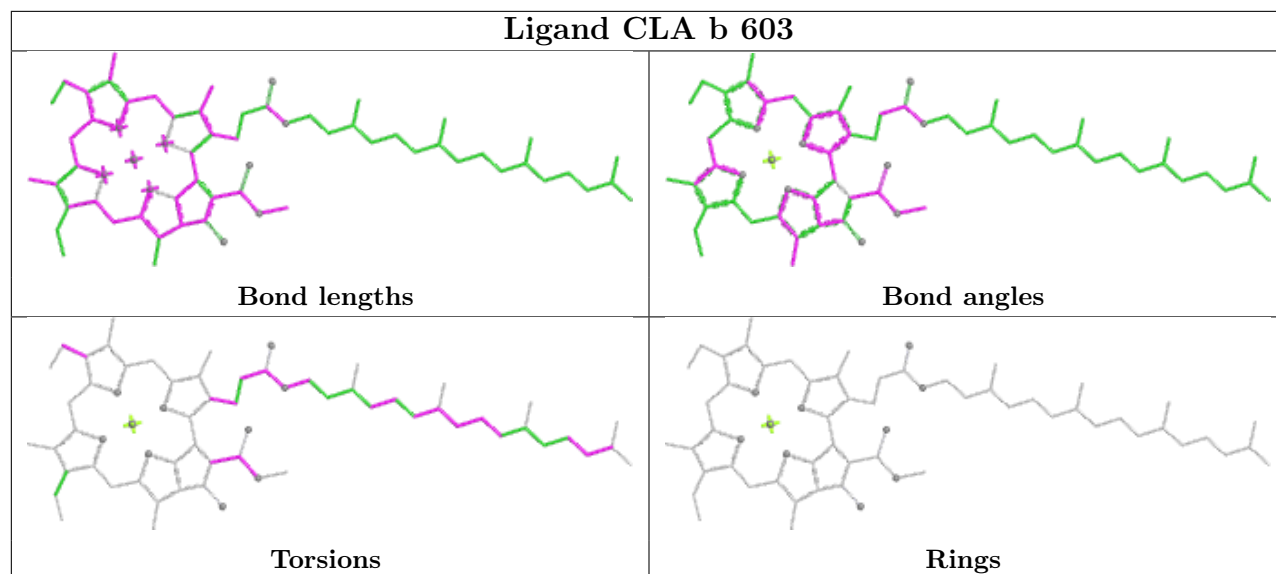
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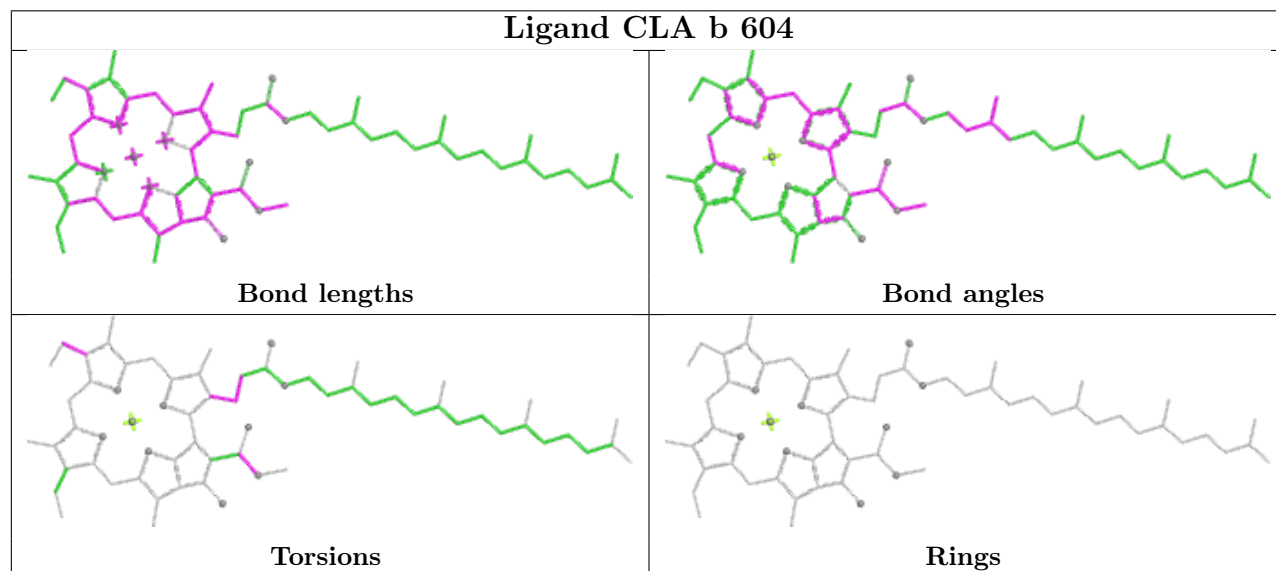
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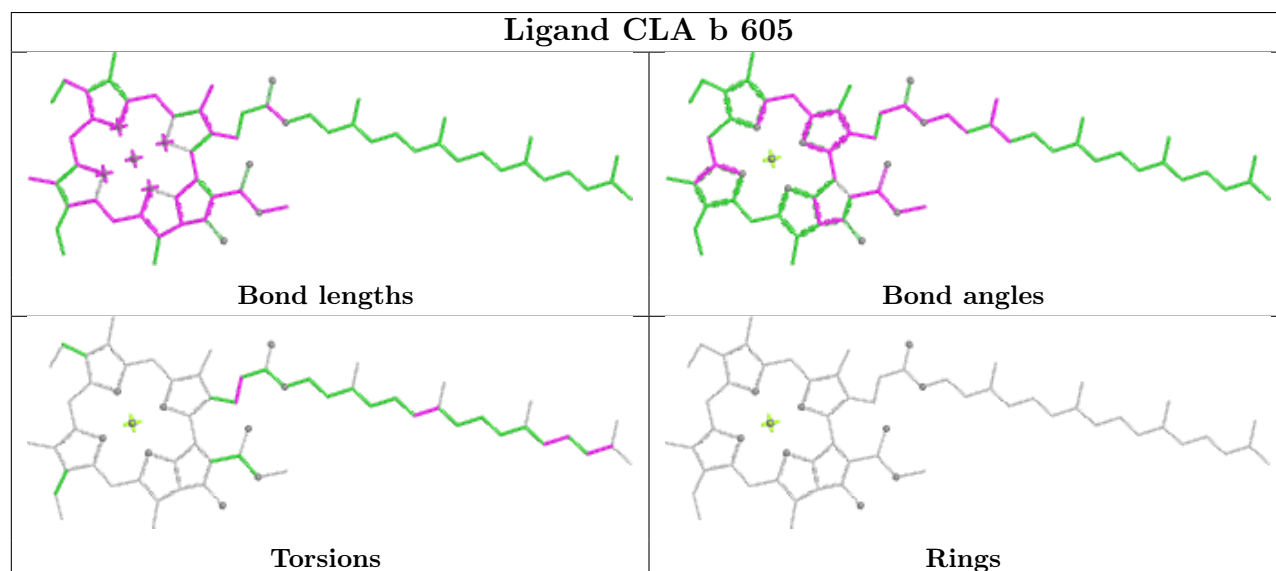
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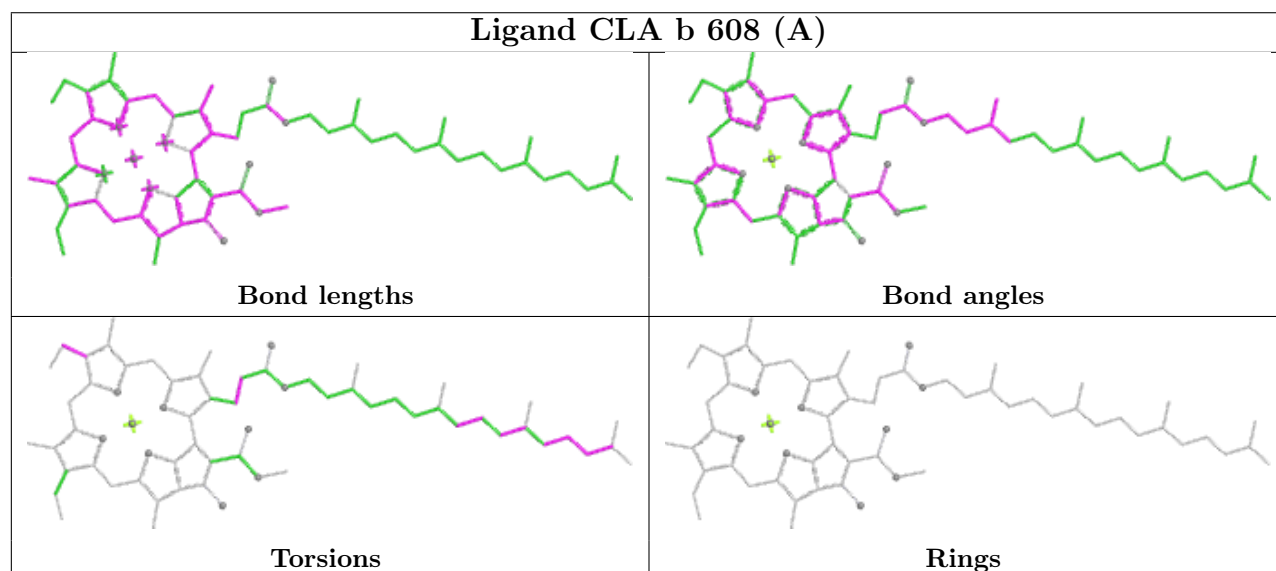
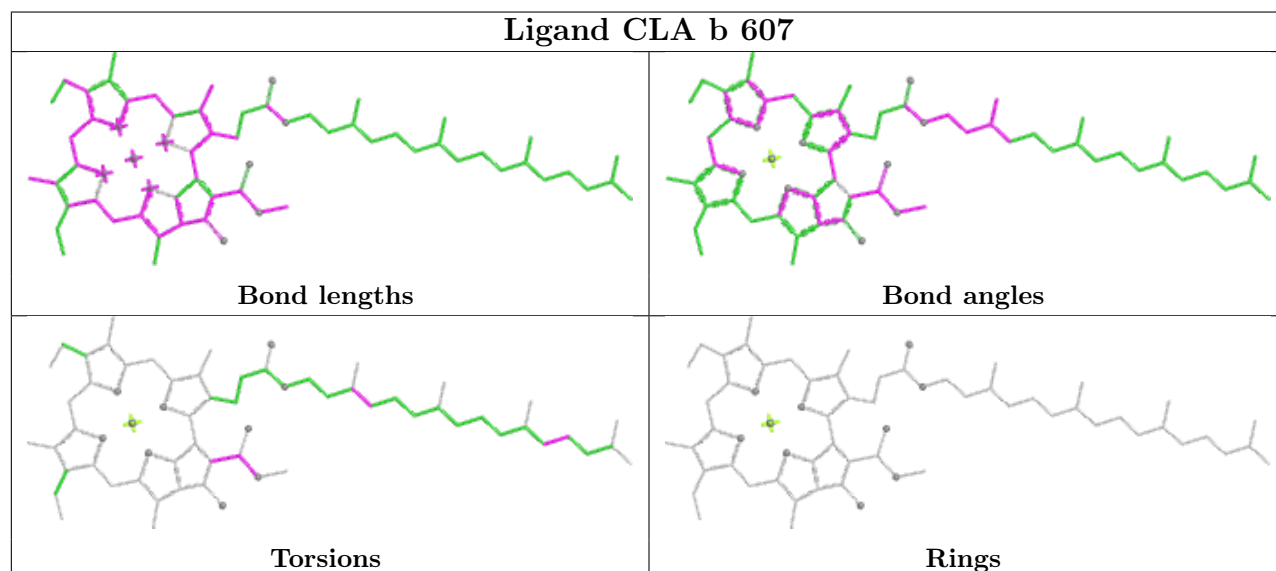
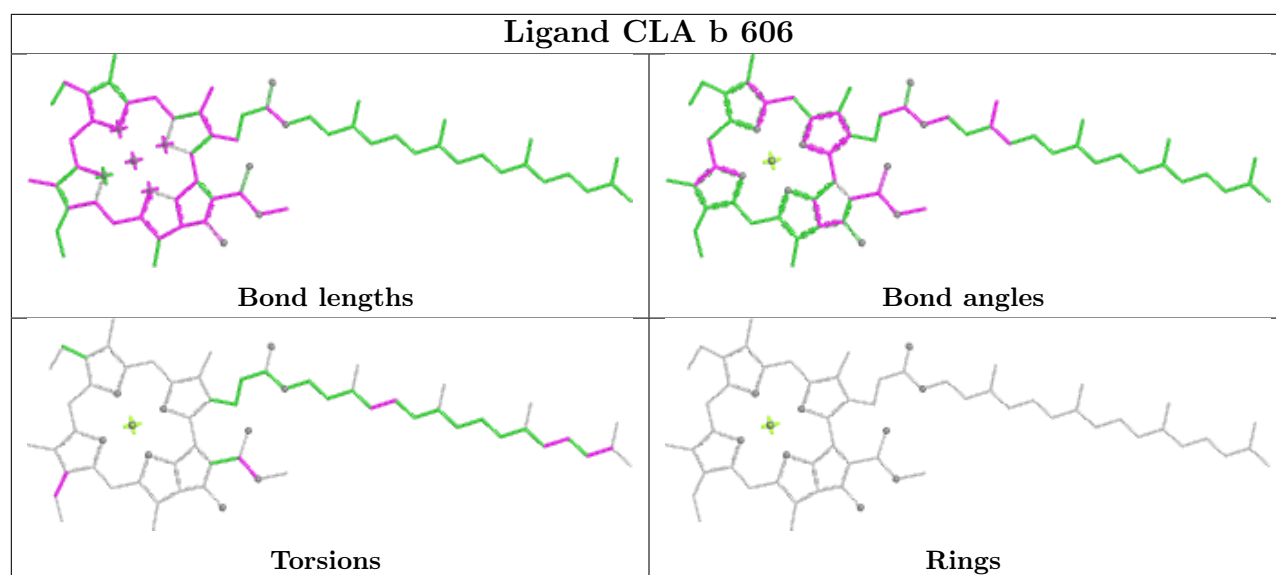


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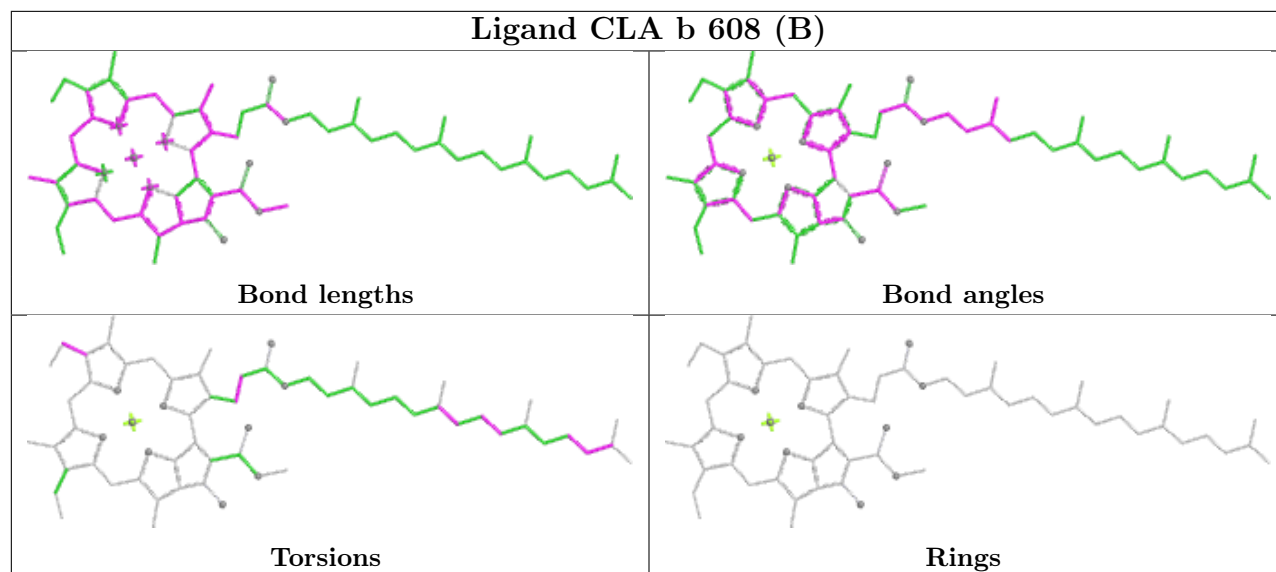


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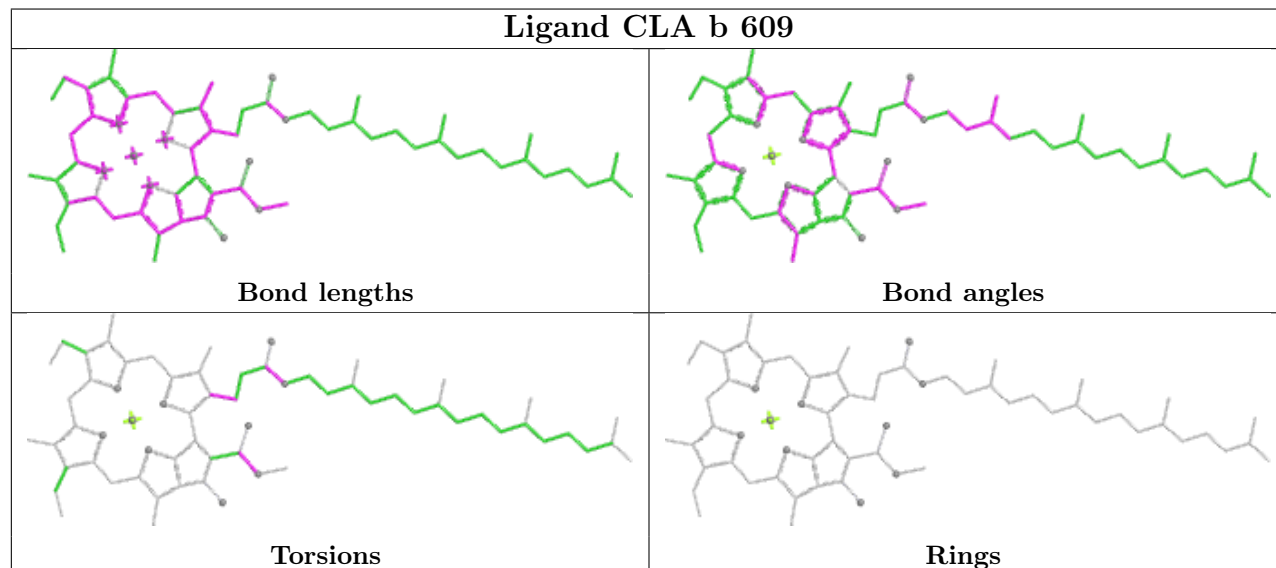




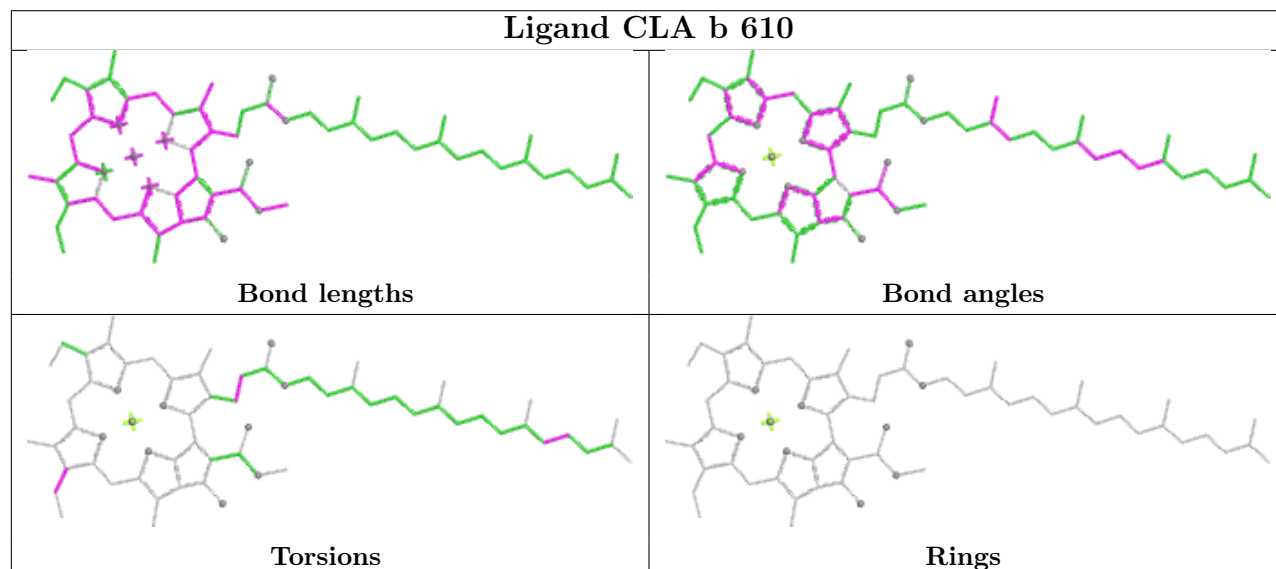
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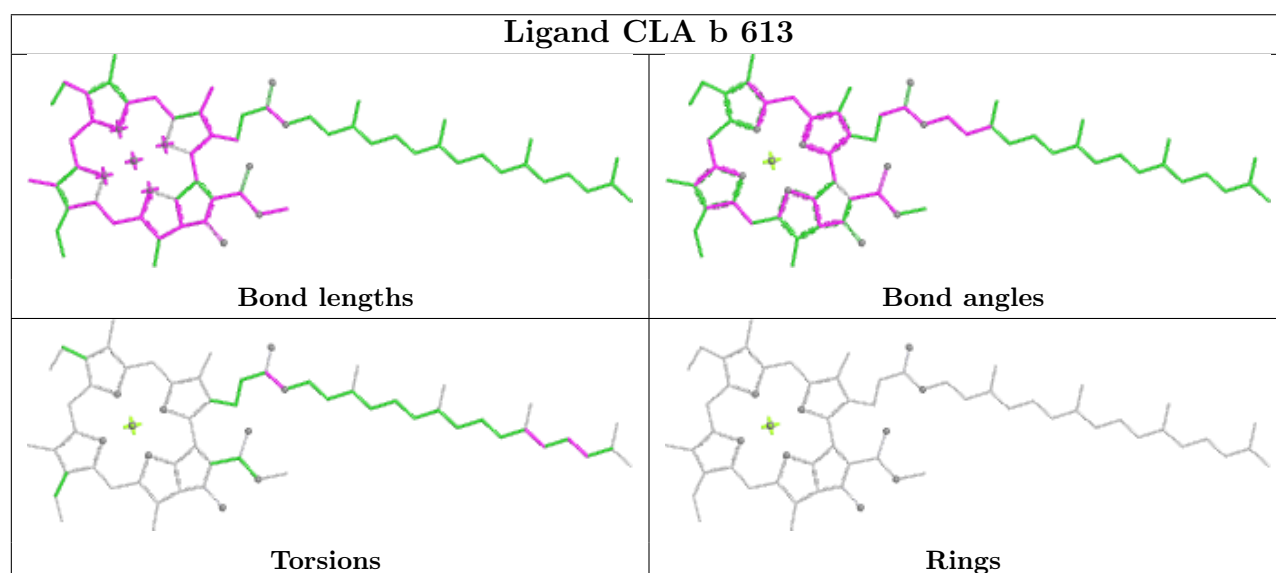
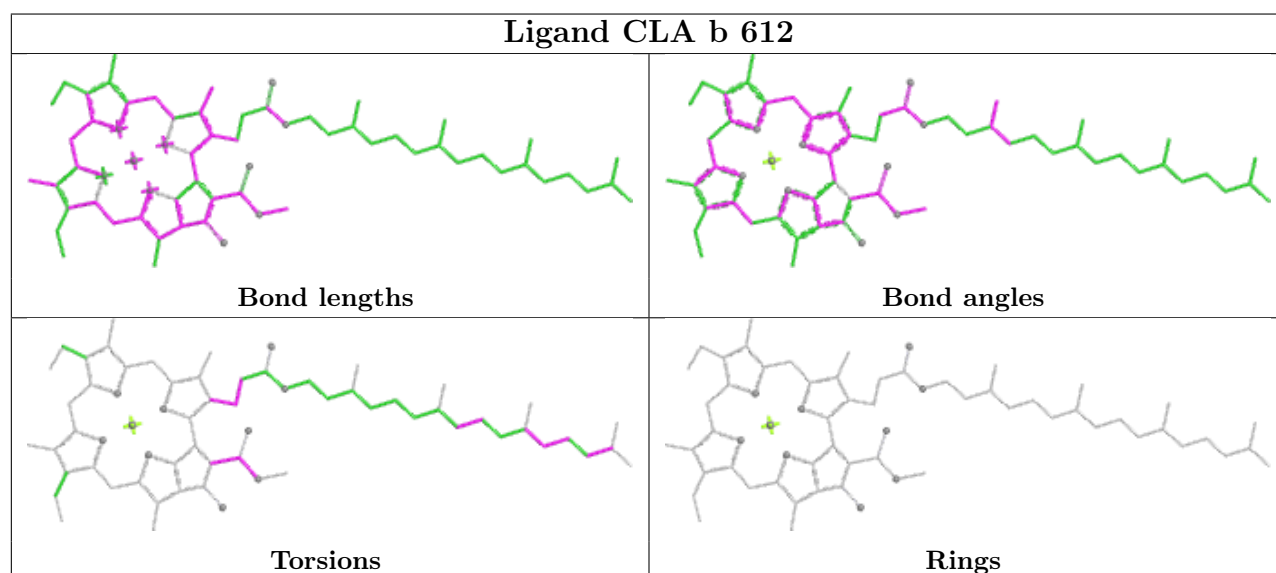
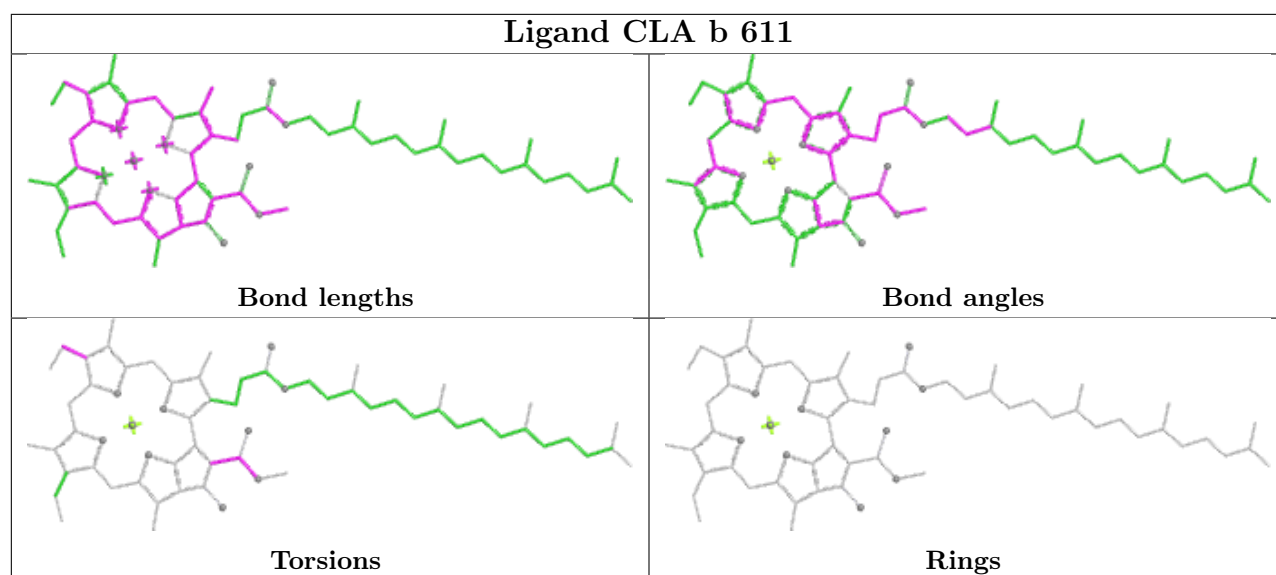


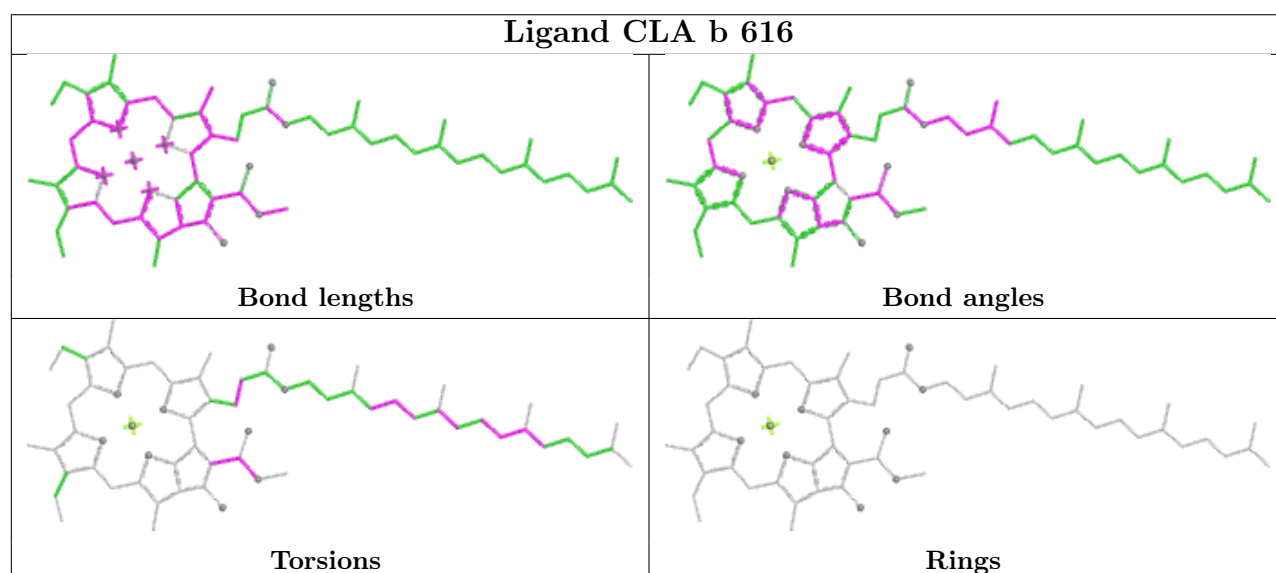
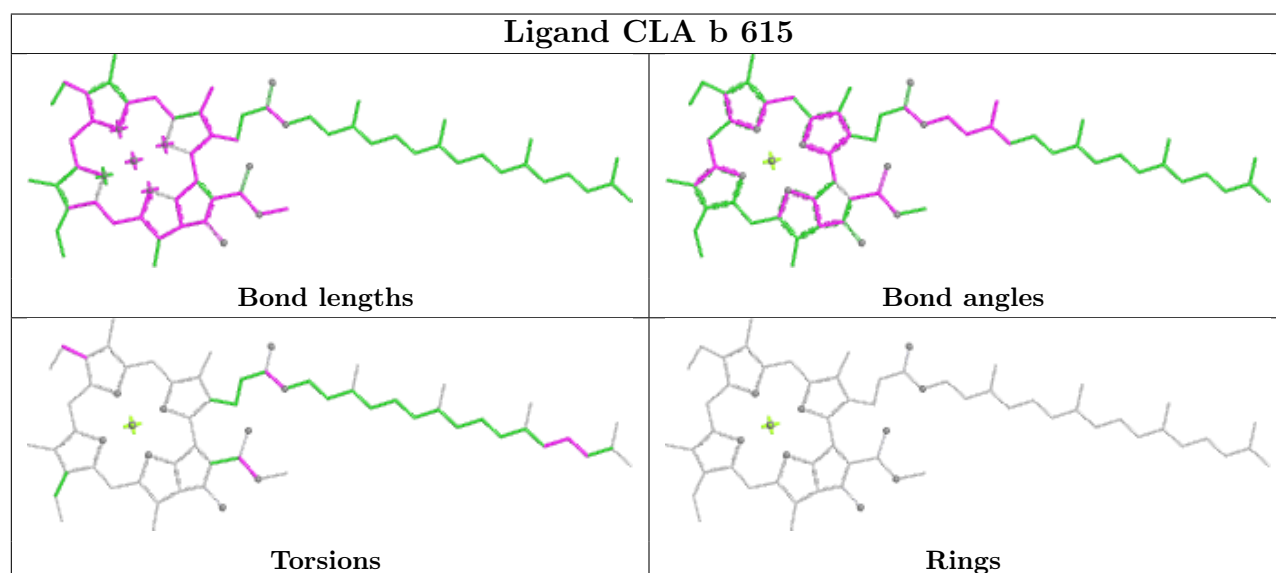
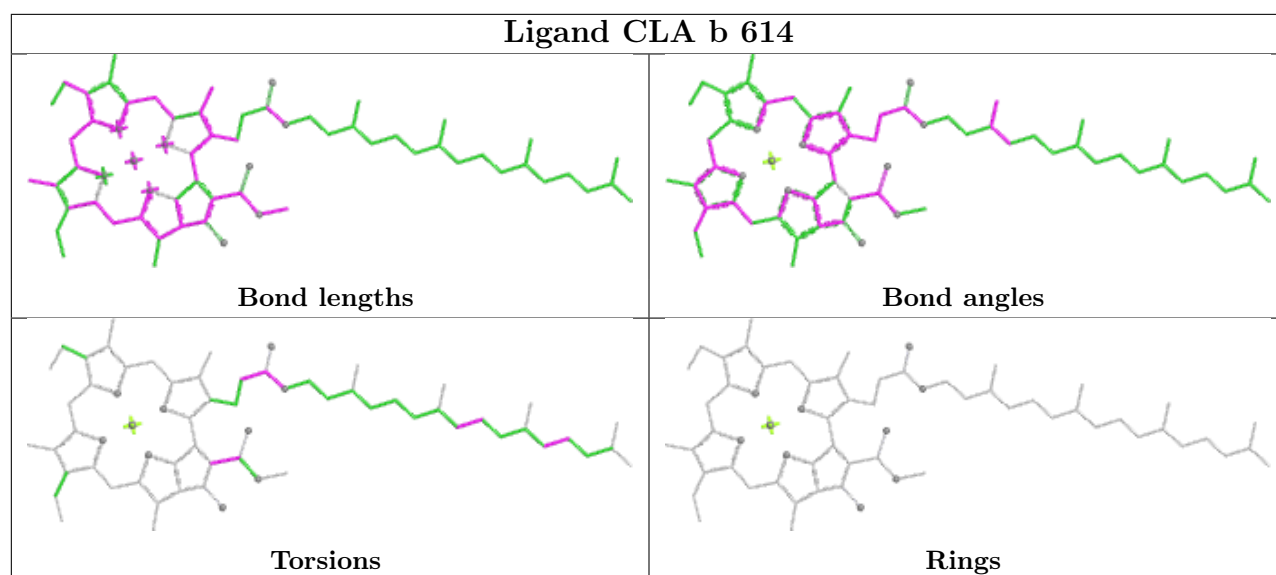
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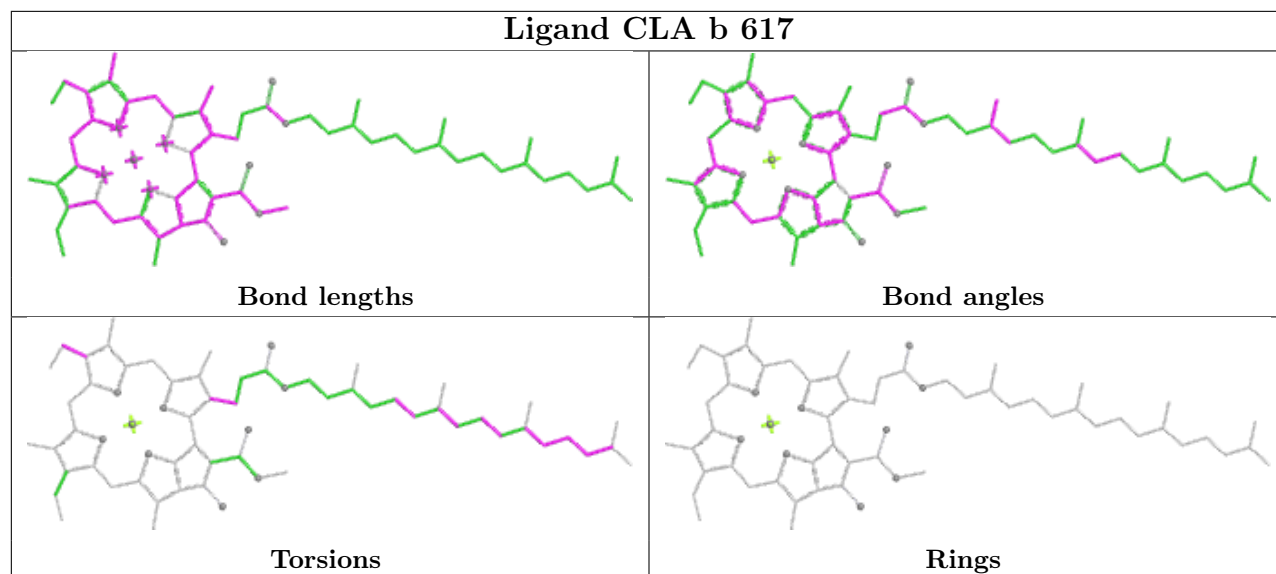
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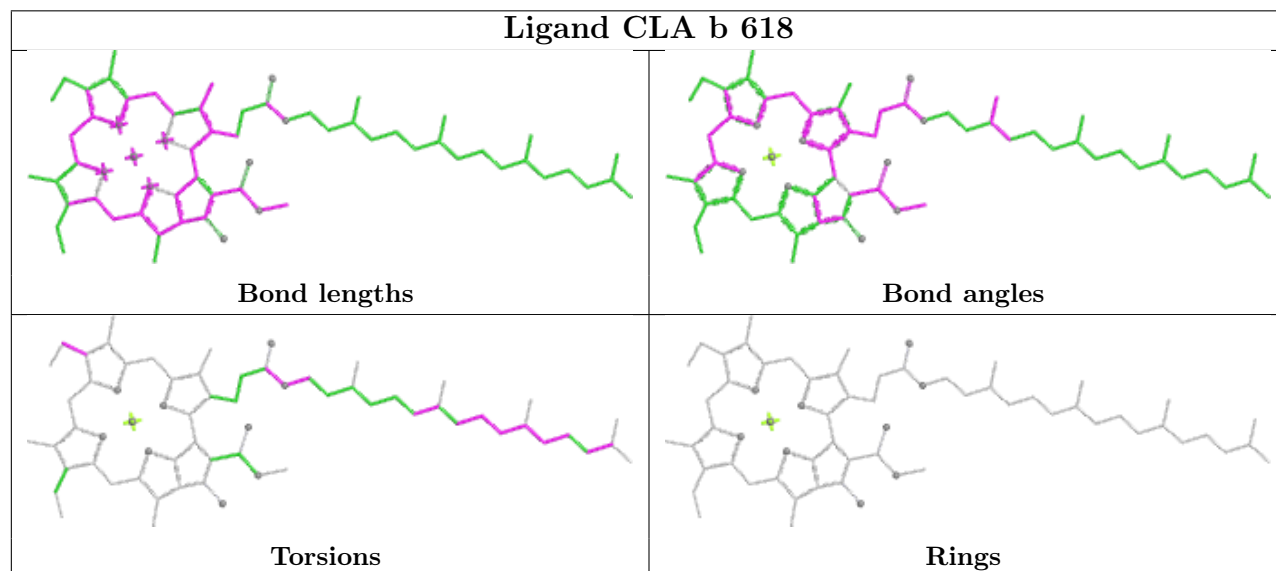




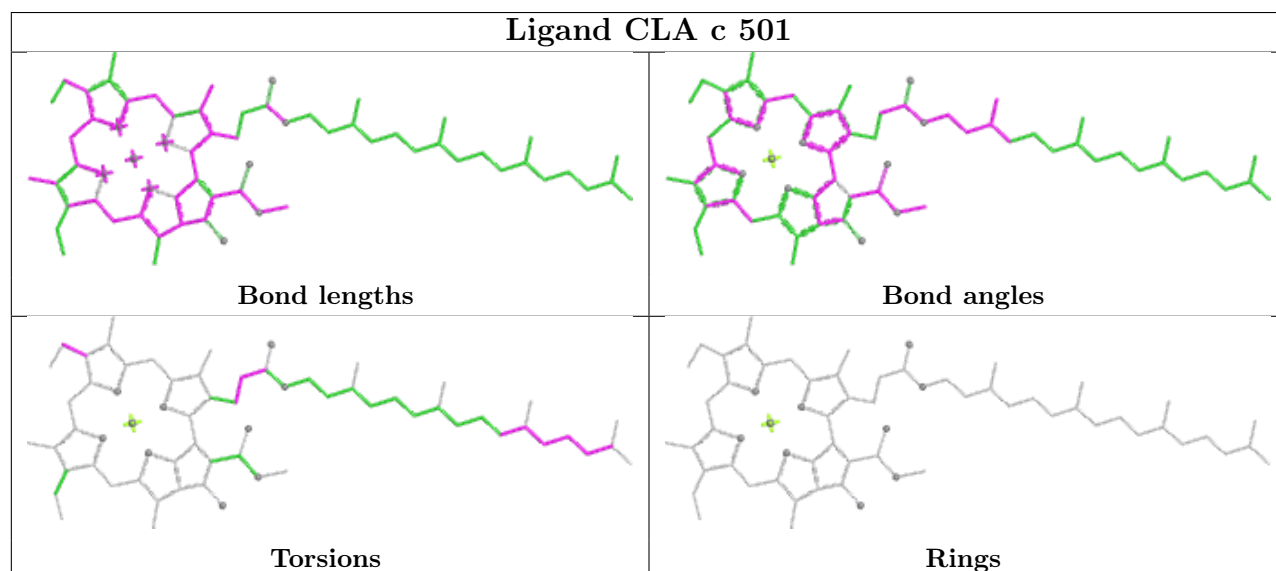
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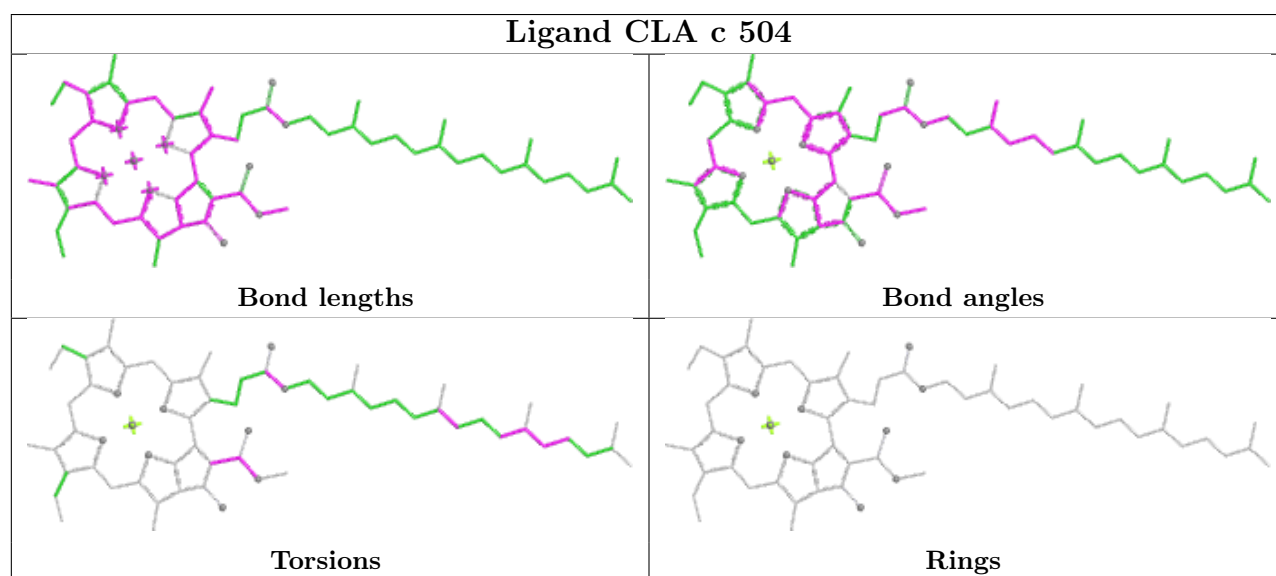
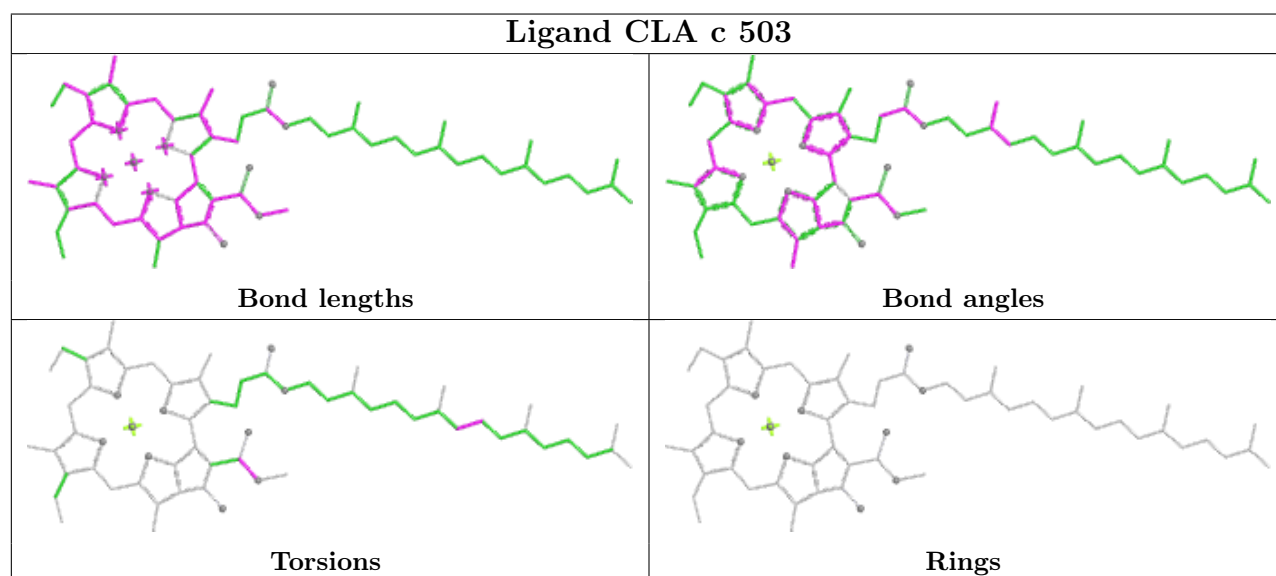
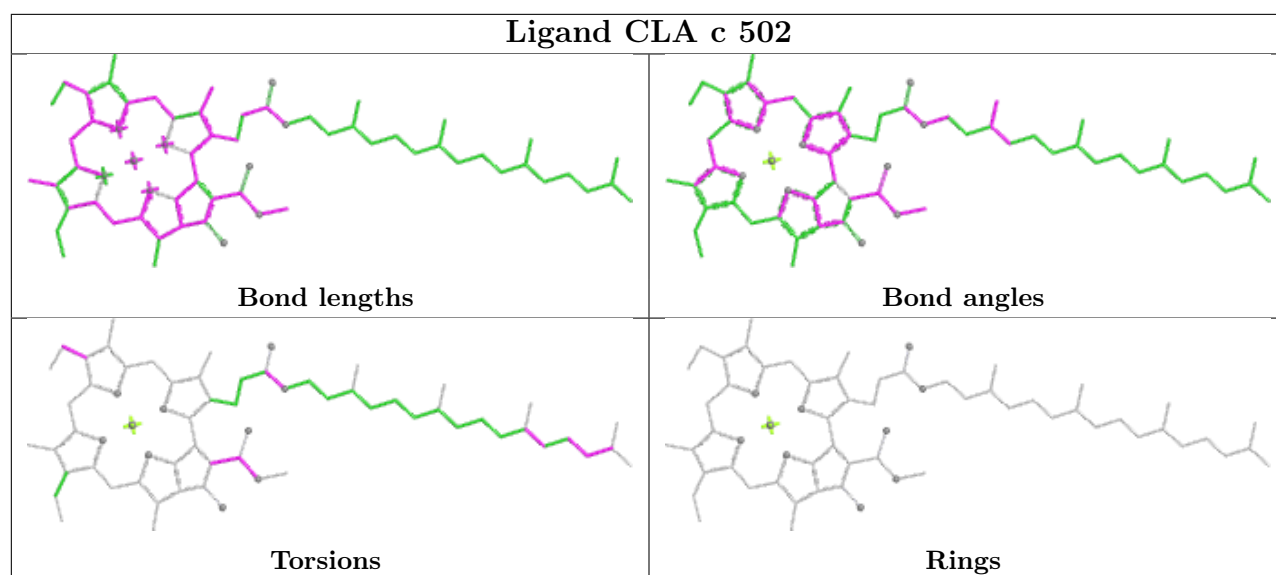


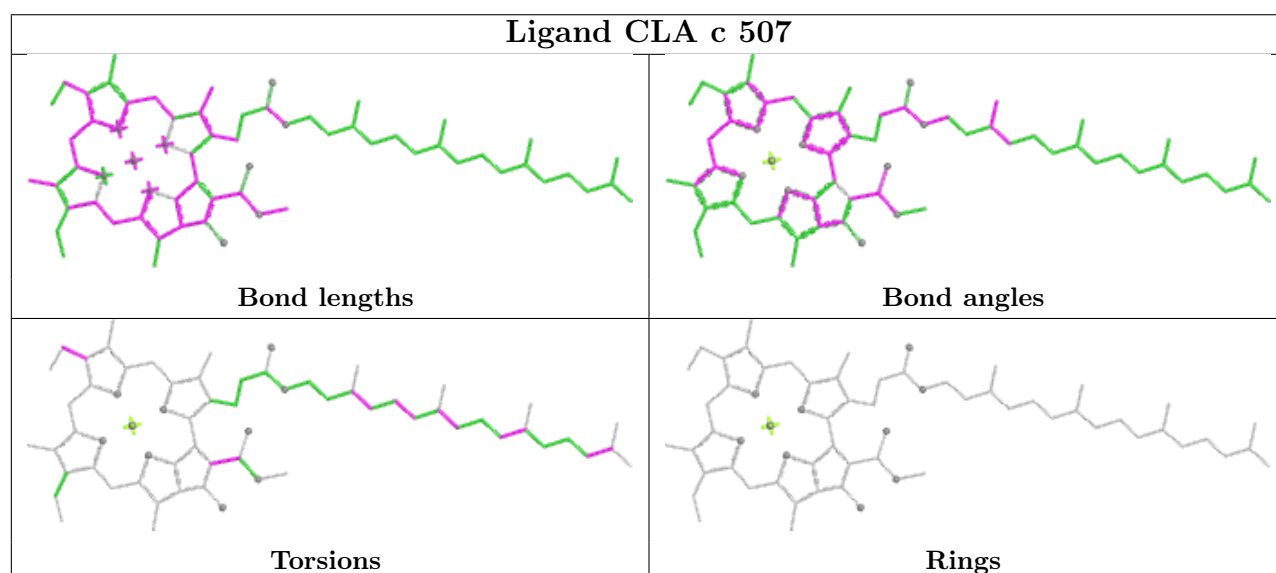
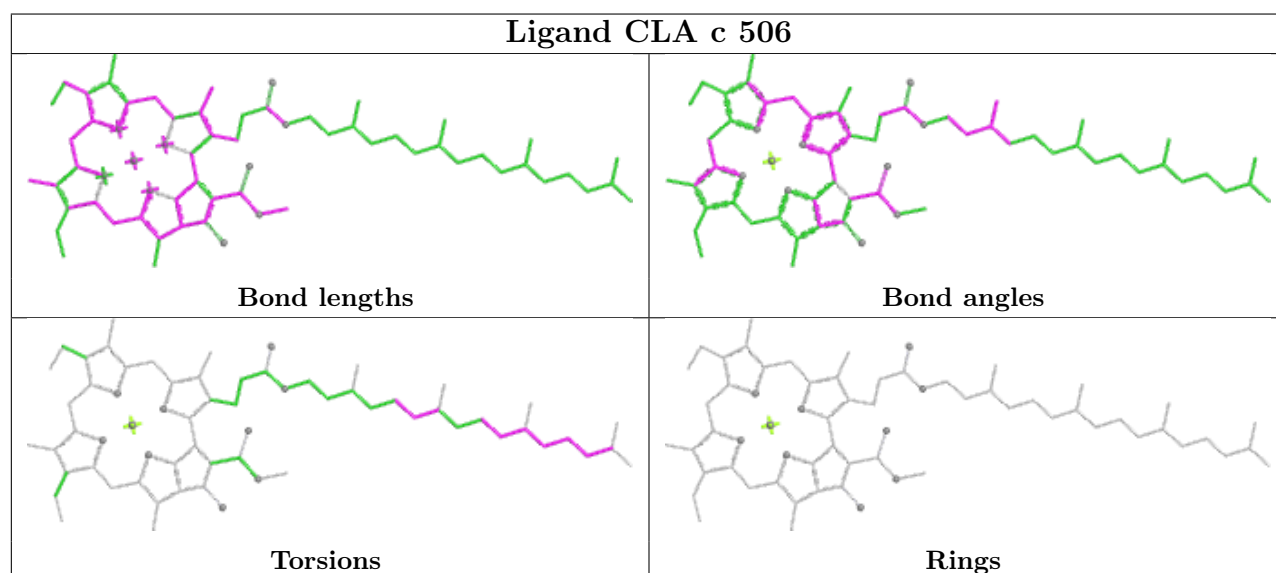
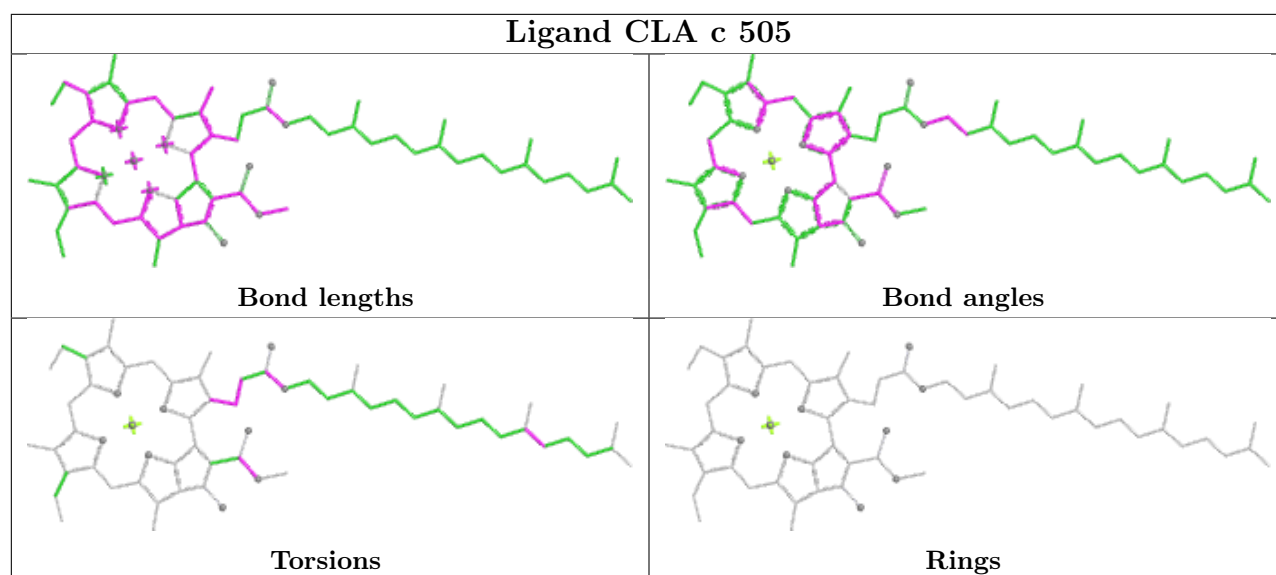
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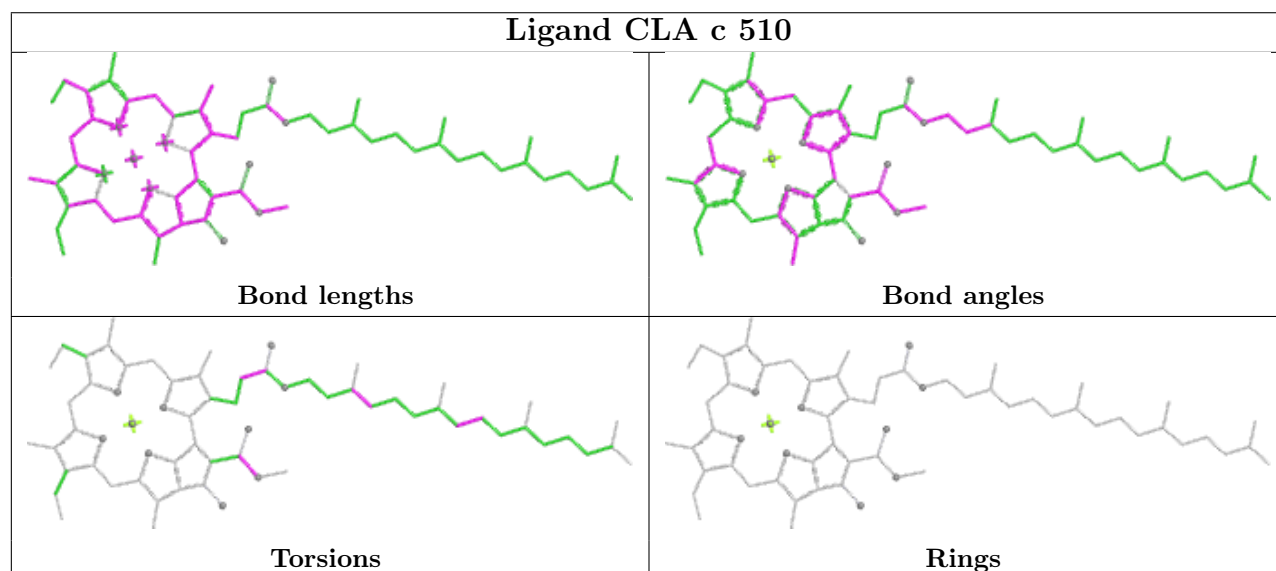
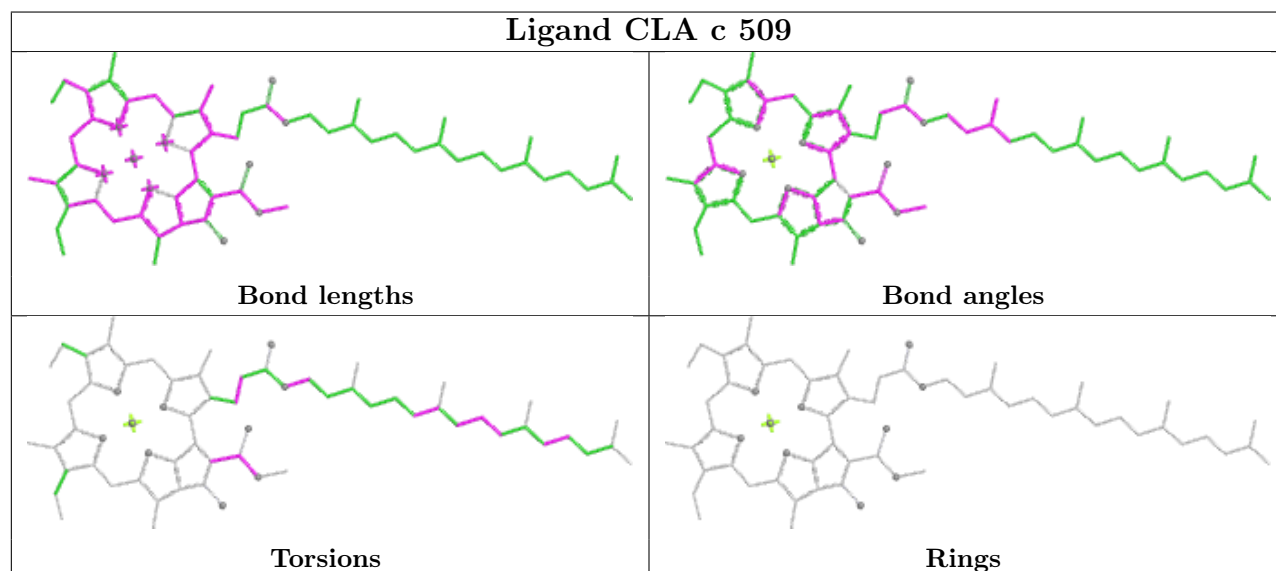
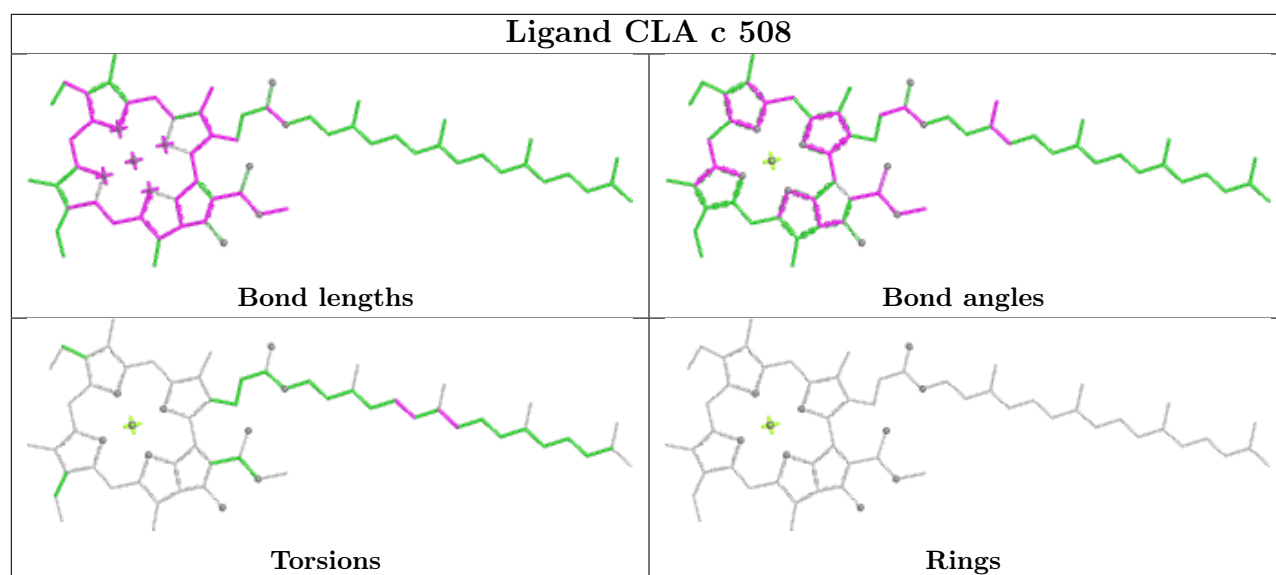


Ligand CLA c 501

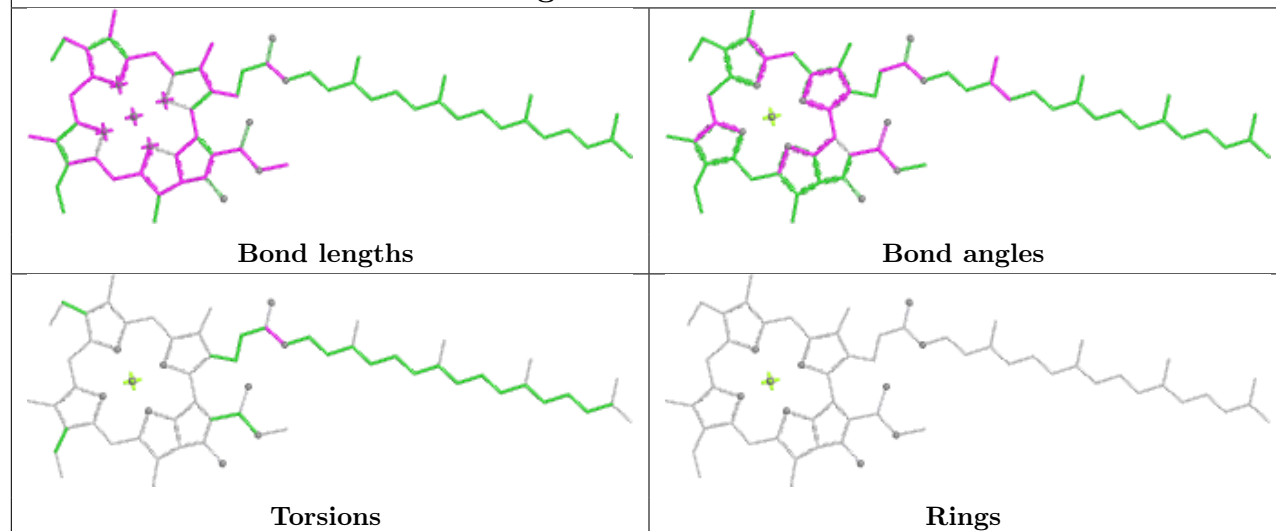




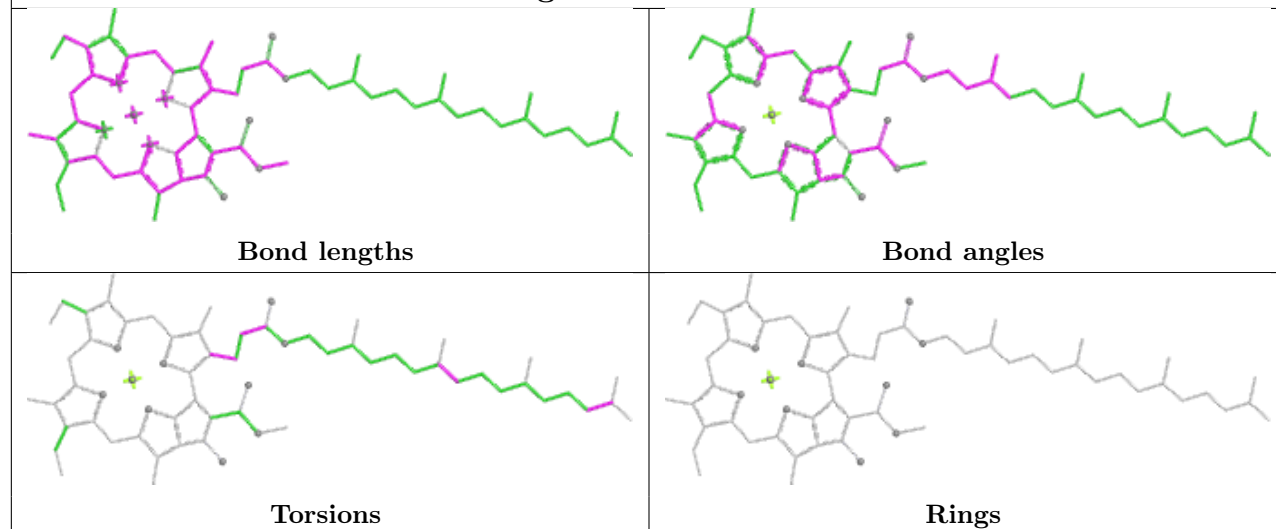




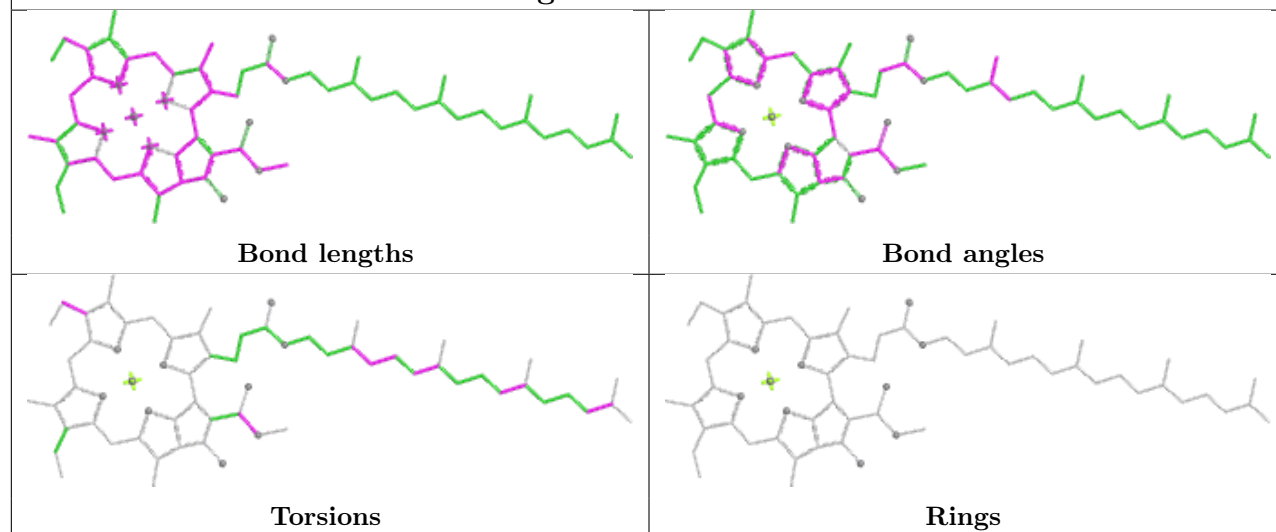
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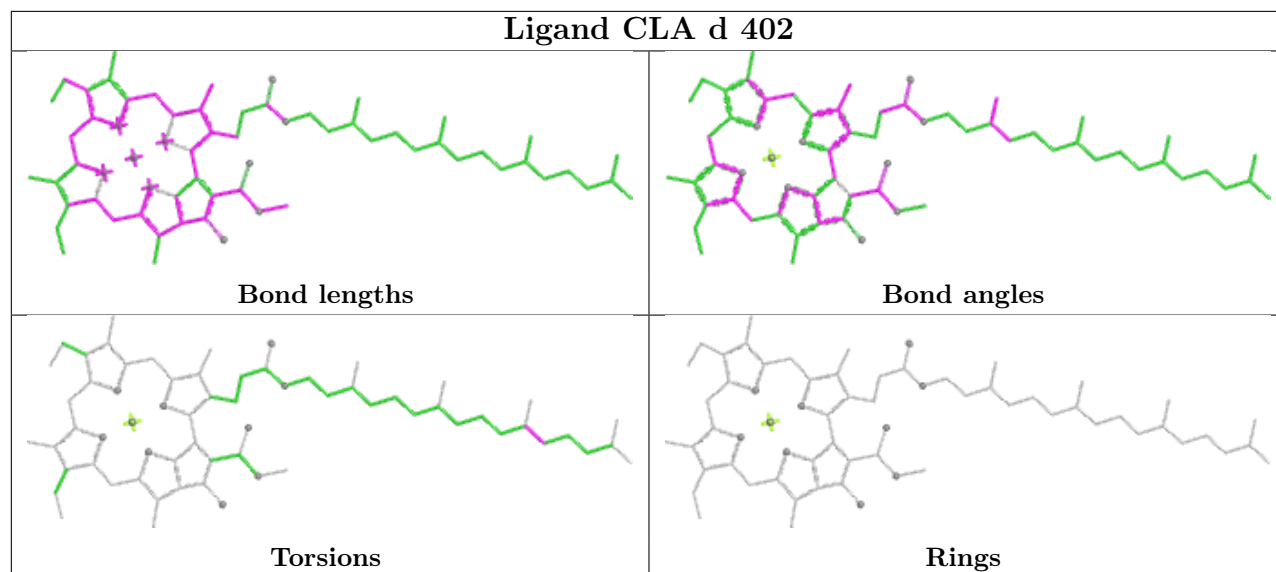
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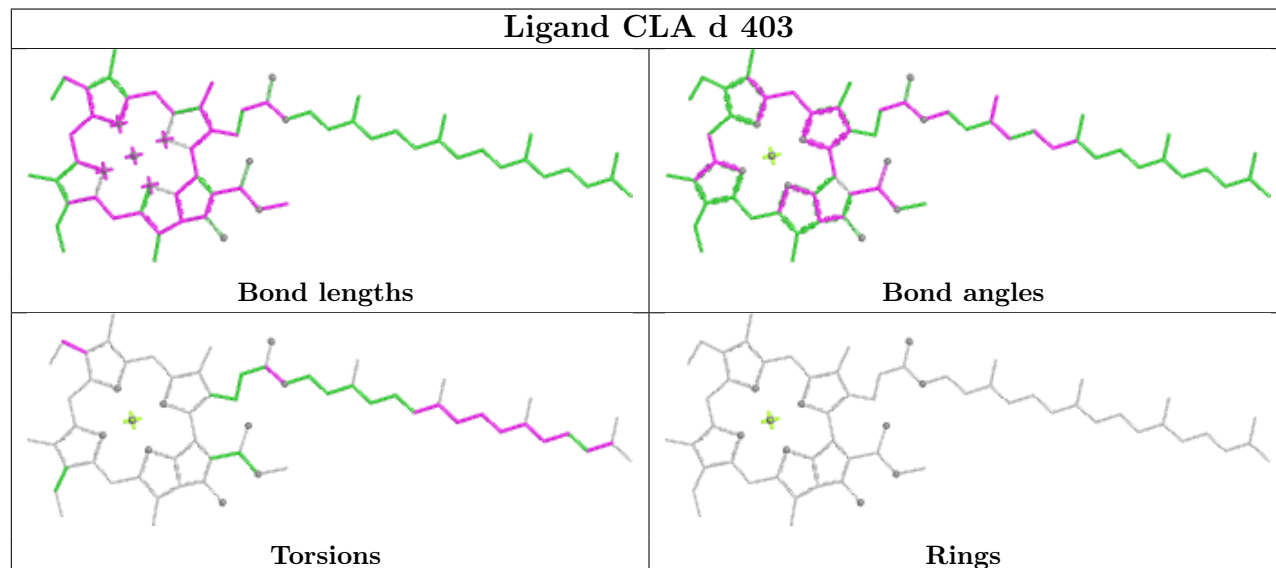
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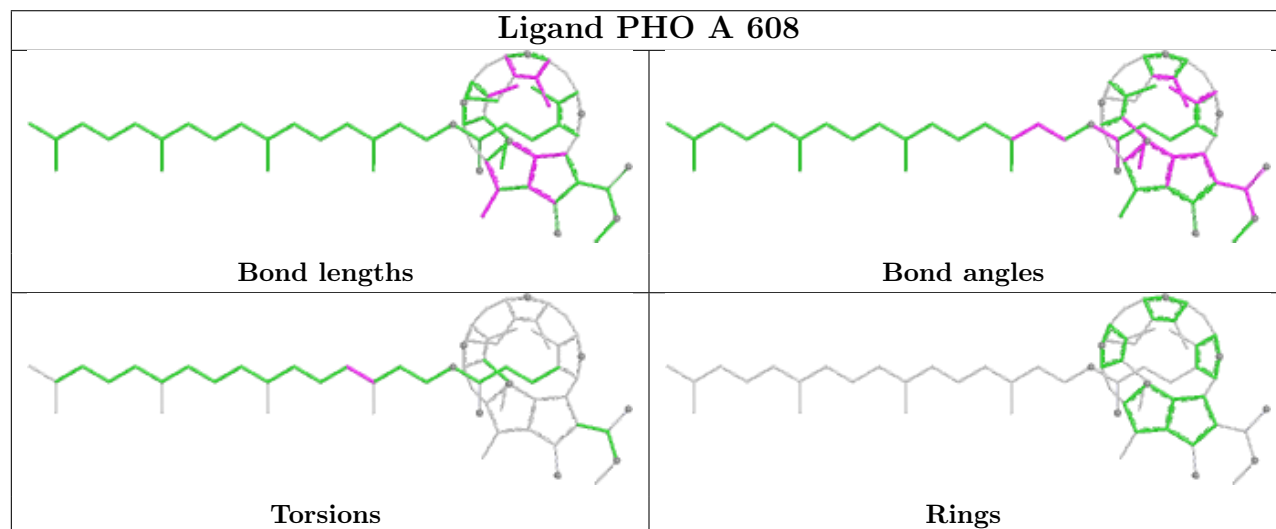
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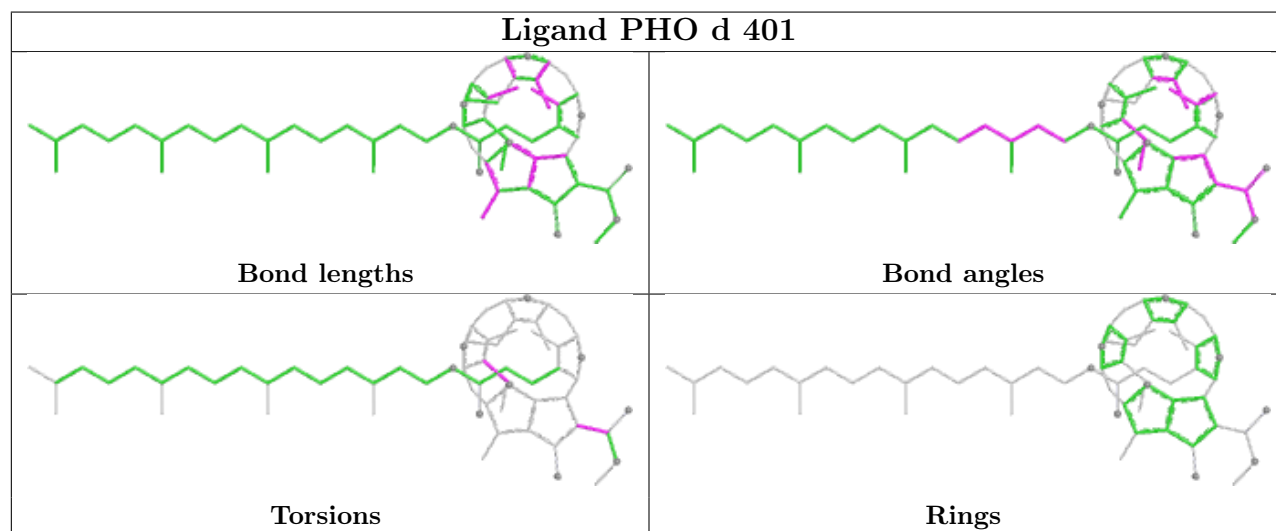
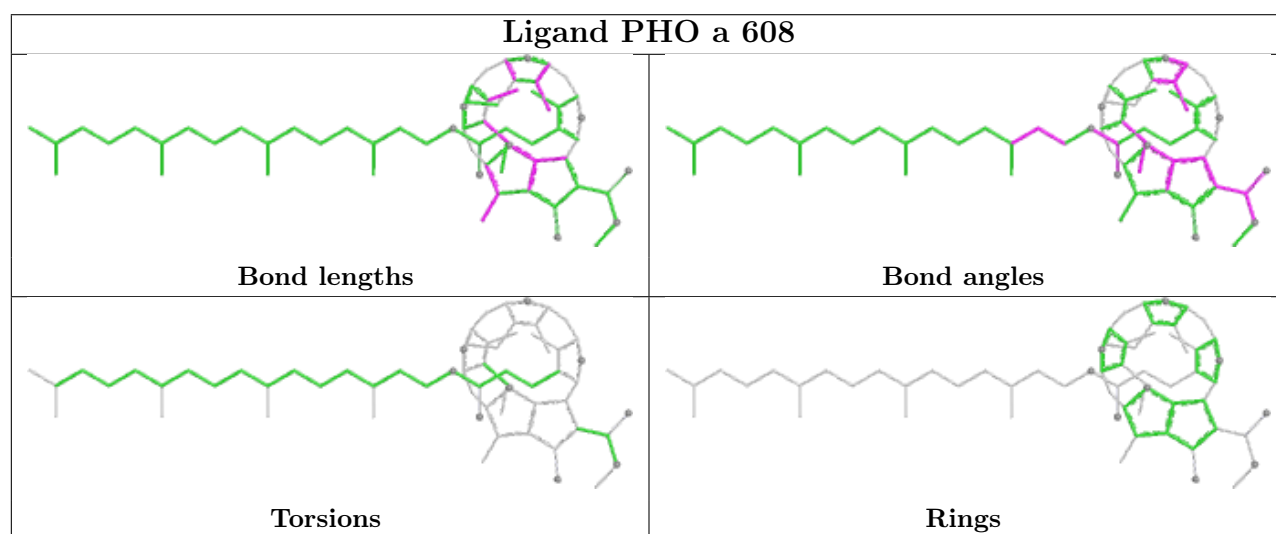
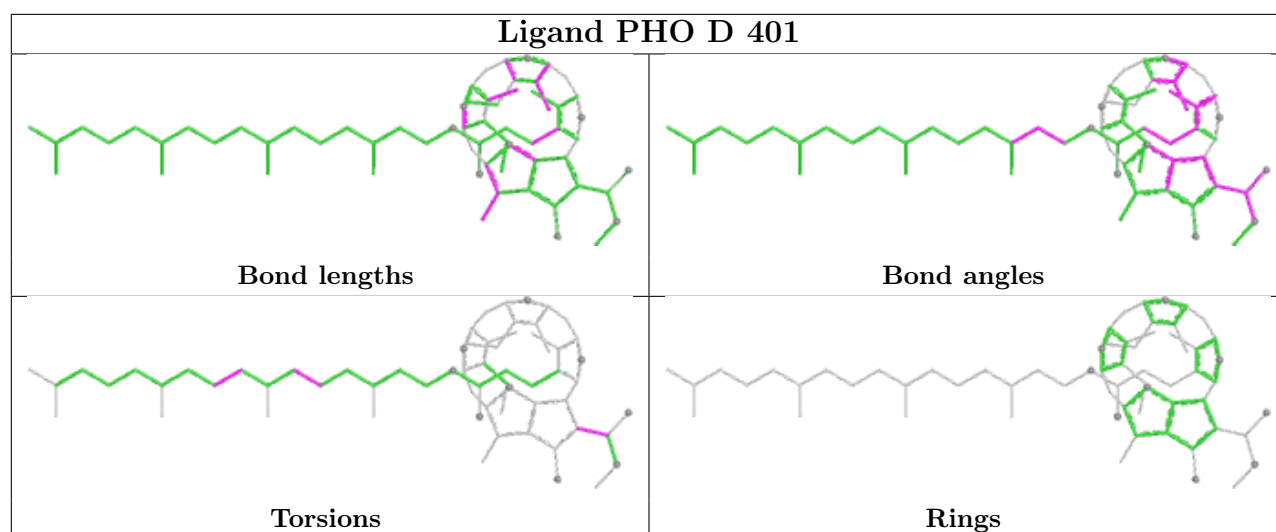


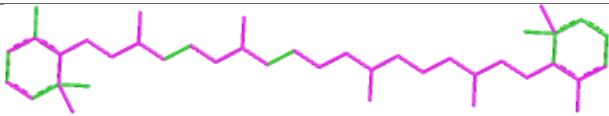
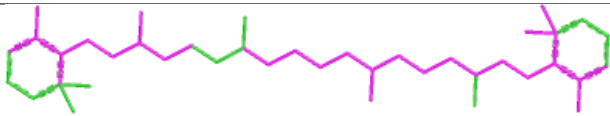
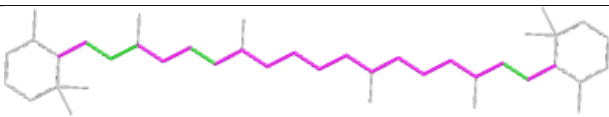
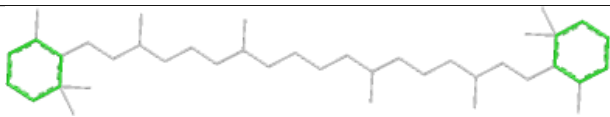
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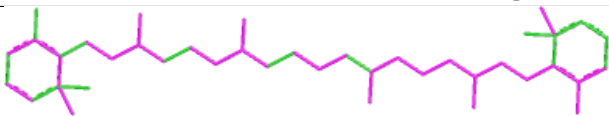
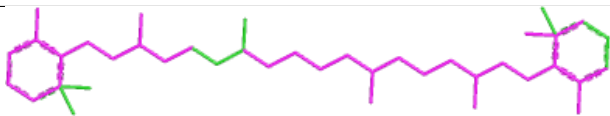
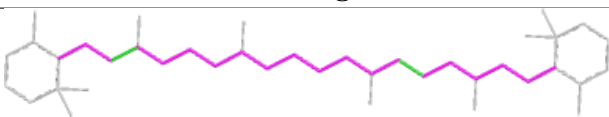
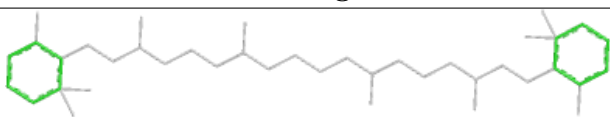


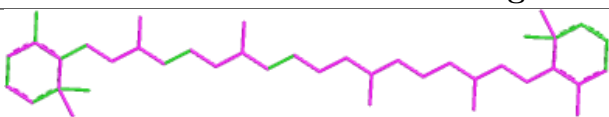
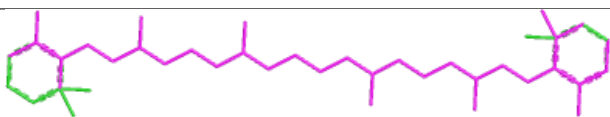
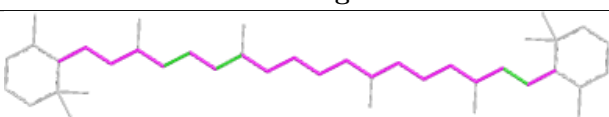
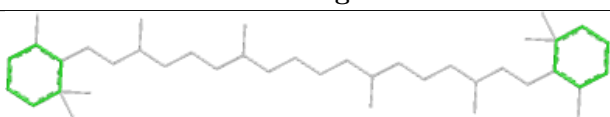
Ligand PHO A 608

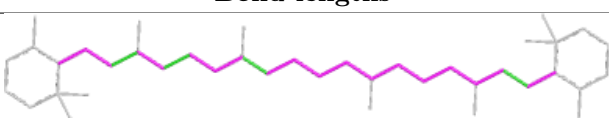
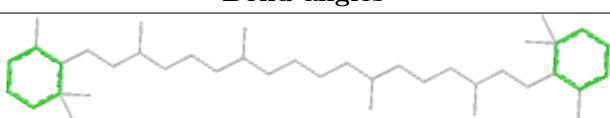


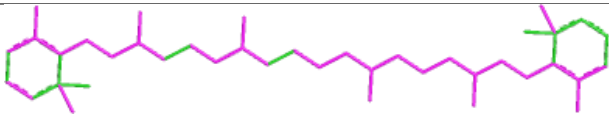
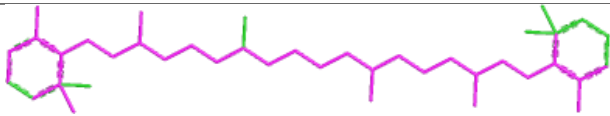
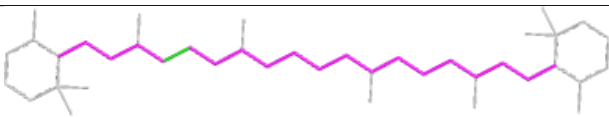
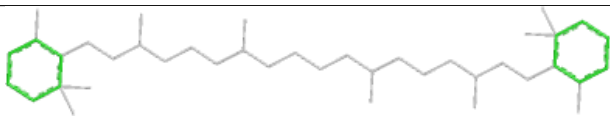


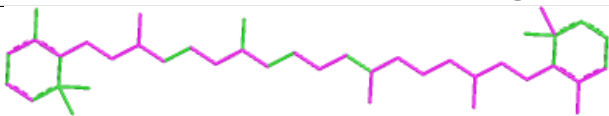
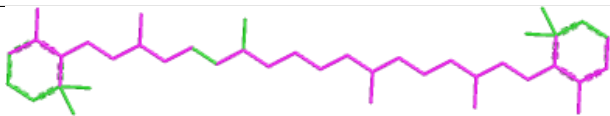
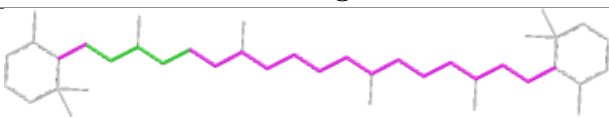
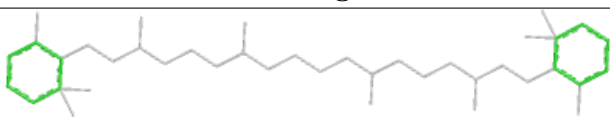
Ligand BCR A 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

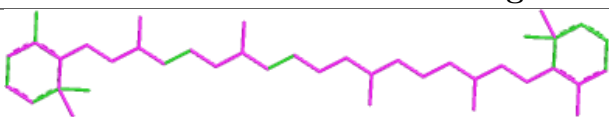
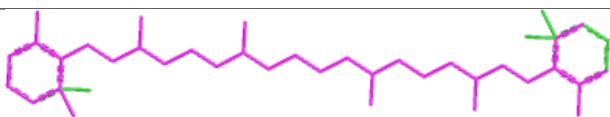
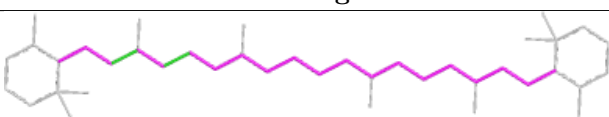
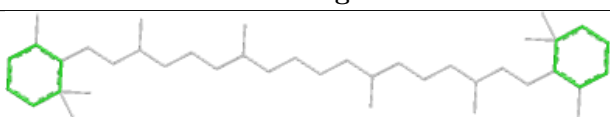
Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

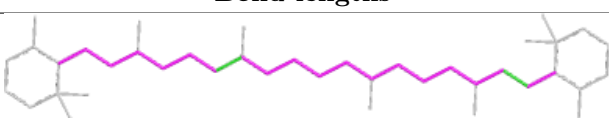
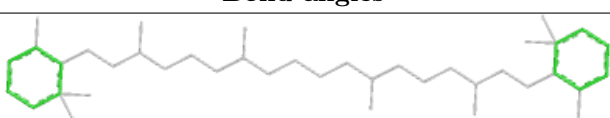
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

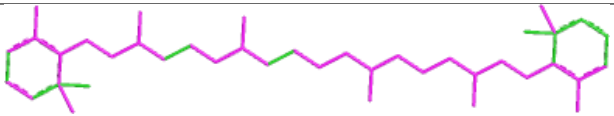
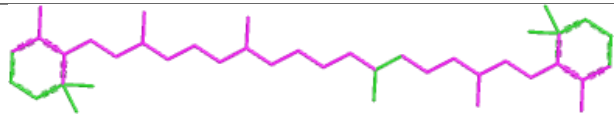
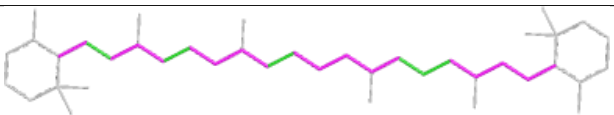
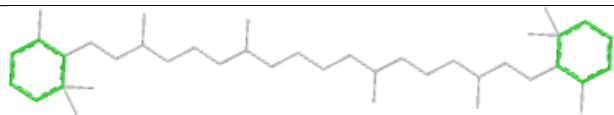
Ligand BCR B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

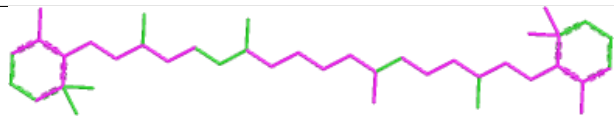
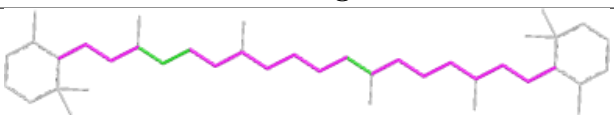
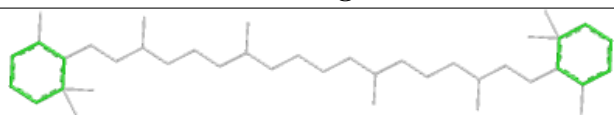
Ligand BCR C 514	
	Bond lengths
	Bond angles
	Torsions
	Rings

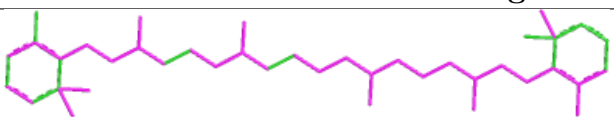
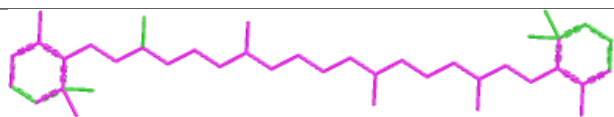
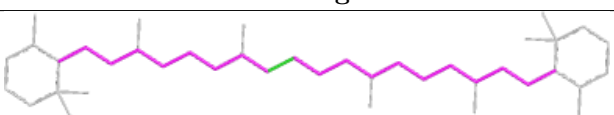
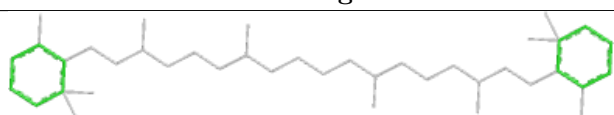
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	Bond angles
	Torsions
	Rings

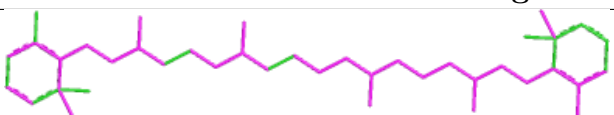
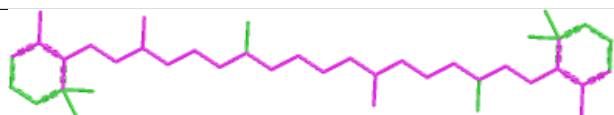
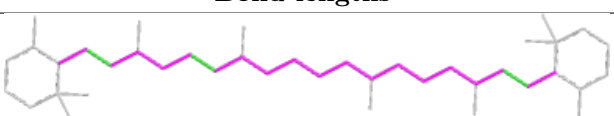
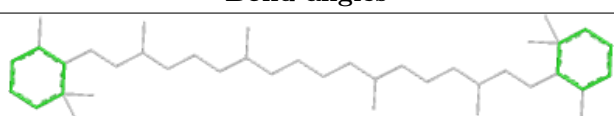
Ligand BCR H 101	
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	Bond angles
	Torsions
	Rings

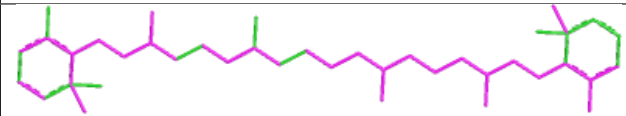
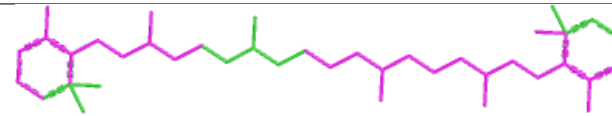
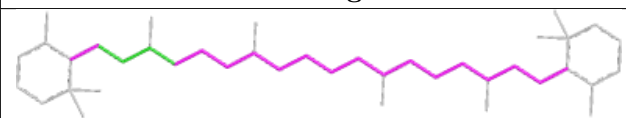
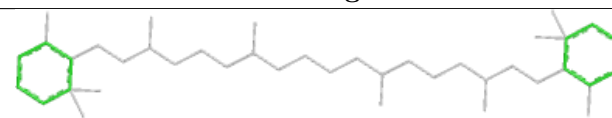
Ligand BCR I 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

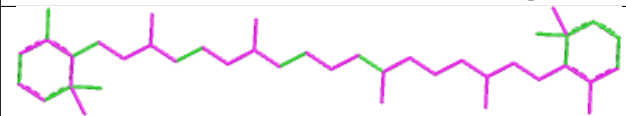
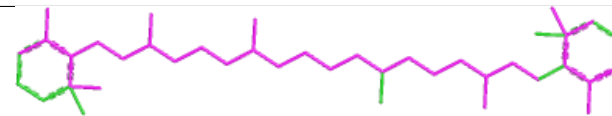
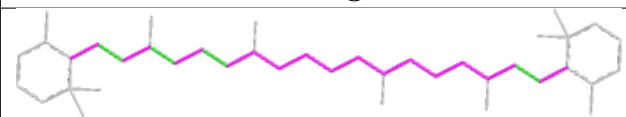
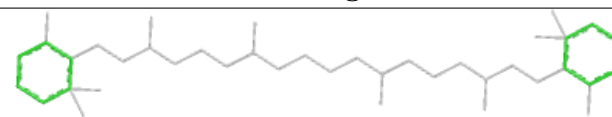
Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

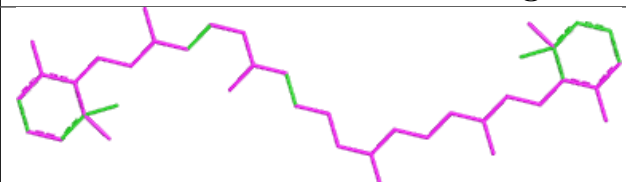
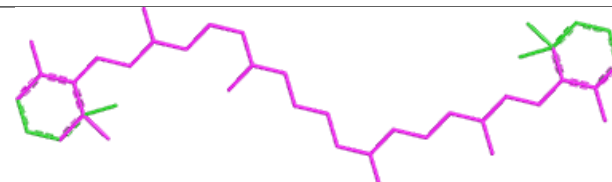
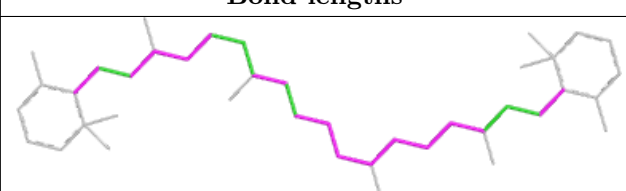
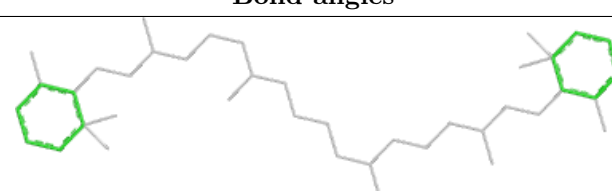
Ligand BCR K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

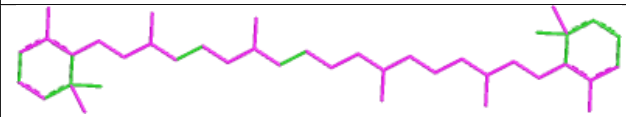
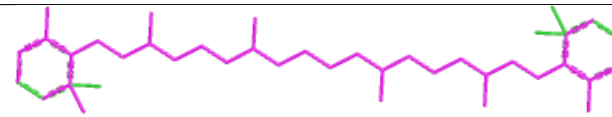
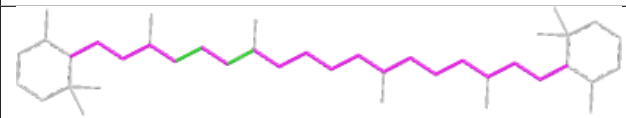
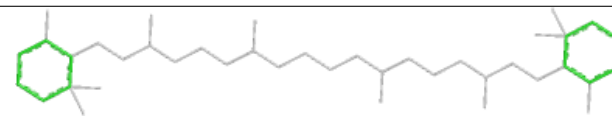
Ligand BCR T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

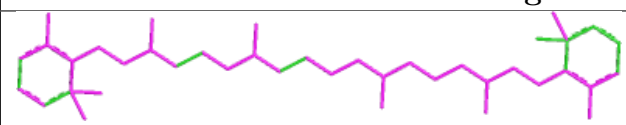
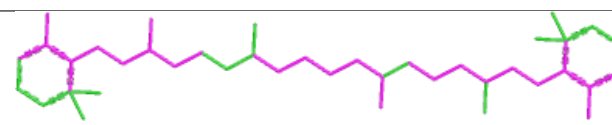
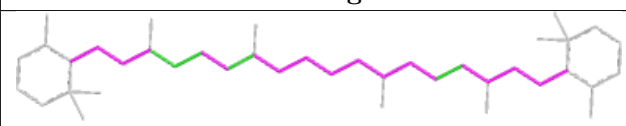
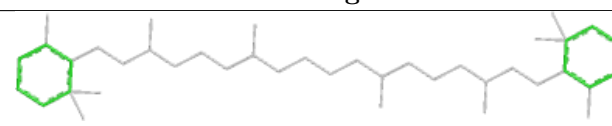
Ligand BCR a 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

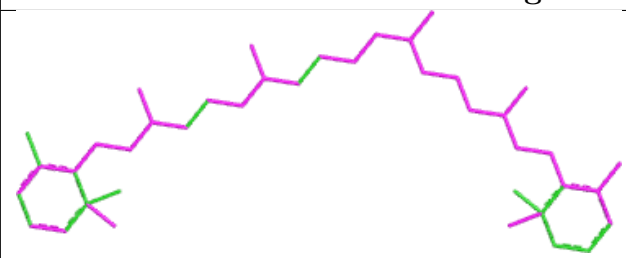
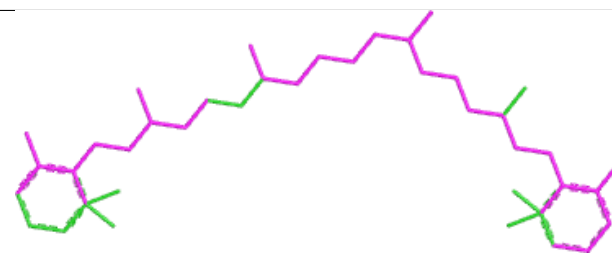
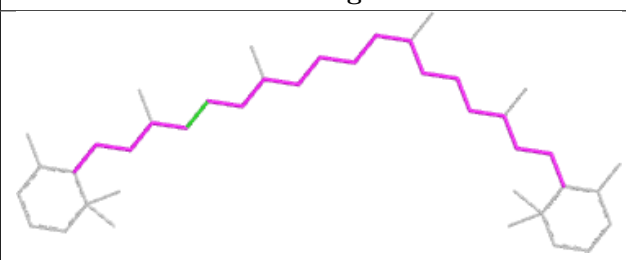
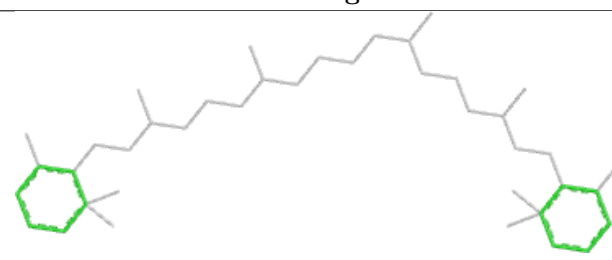
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Bond lengths	Bond angles
	
Torsions	Rings

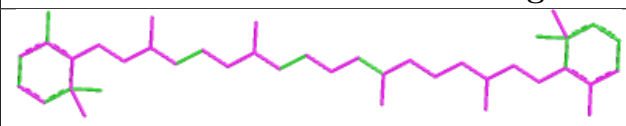
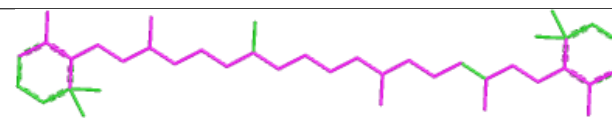
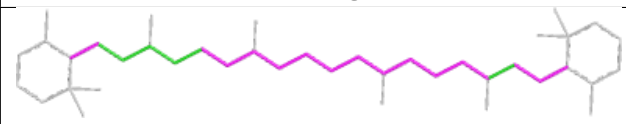
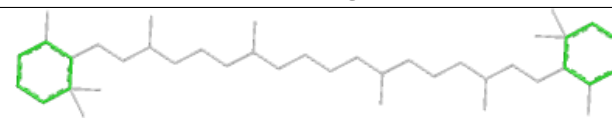
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Bond lengths	Bond angles
	
Torsions	Rings

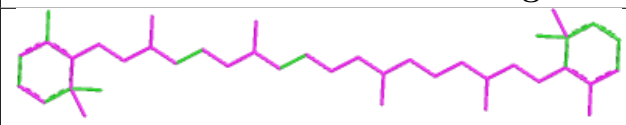
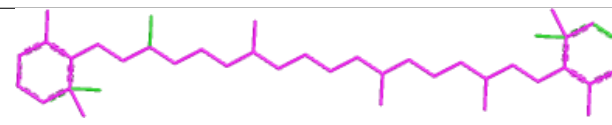
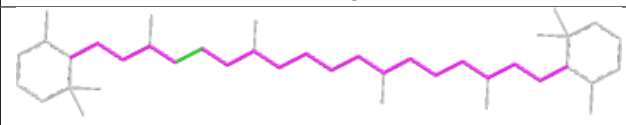
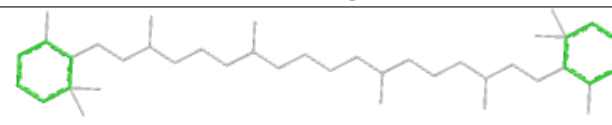
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Bond lengths	Bond angles
	
Torsions	Rings

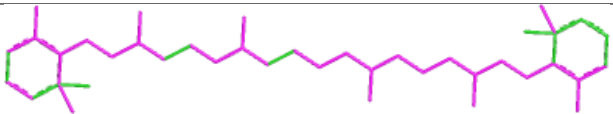
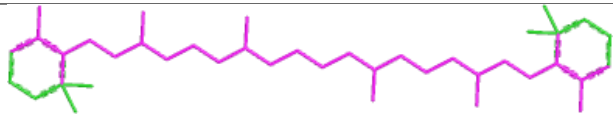
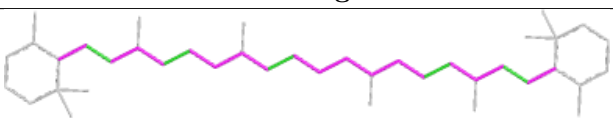
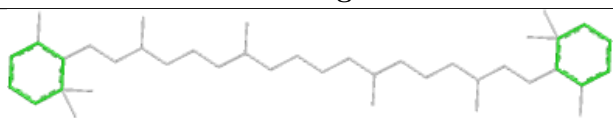
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Bond lengths	Bond angles
	
Torsions	Rings

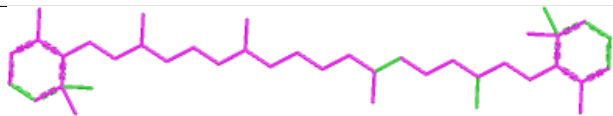
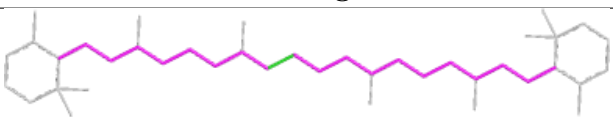
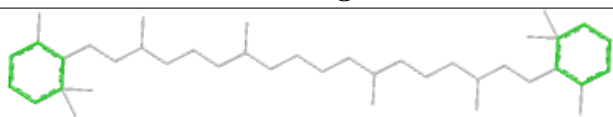
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Bond lengths	Bond angles
	
Torsions	Rings

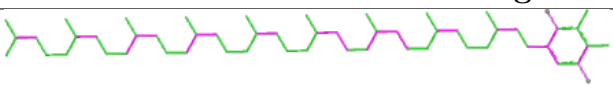
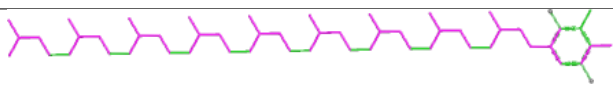
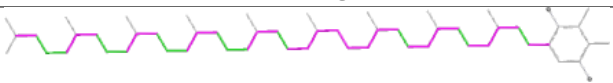
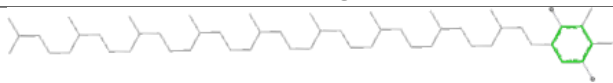
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Bond lengths	Bond angles
	
Torsions	Rings

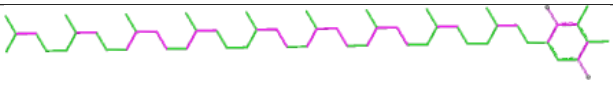
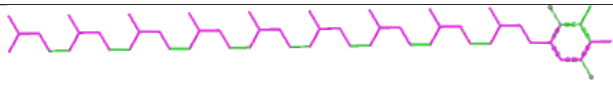
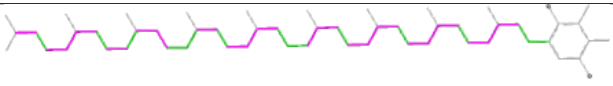
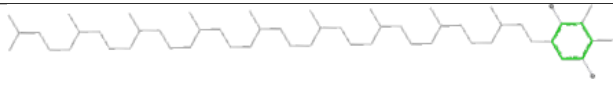
Ligand BCR f 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

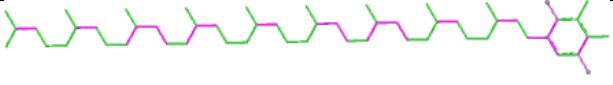
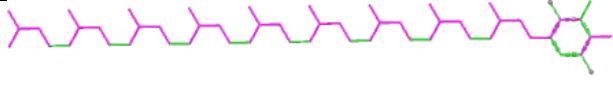
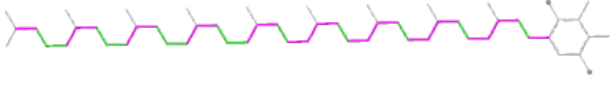
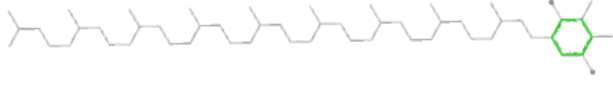
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Bond lengths	Bond angles
	
Torsions	Rings

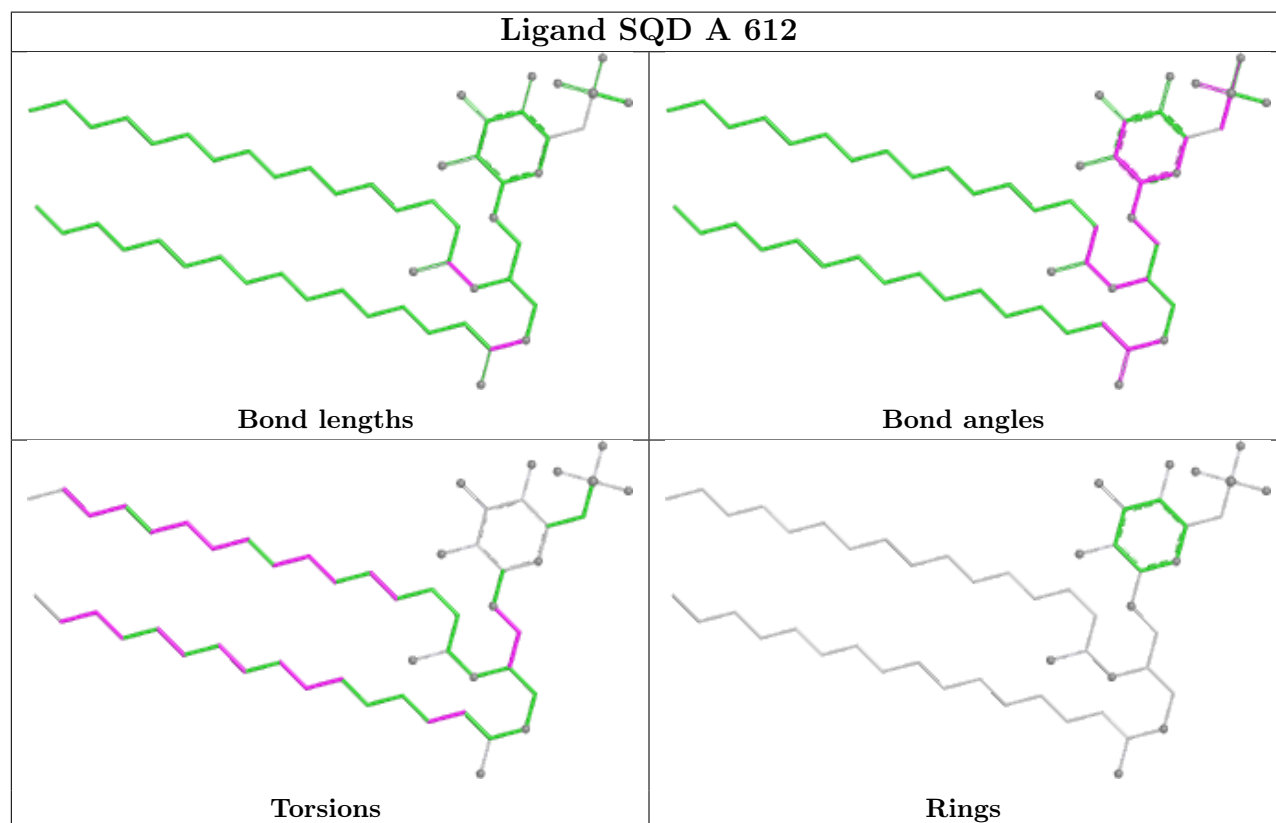
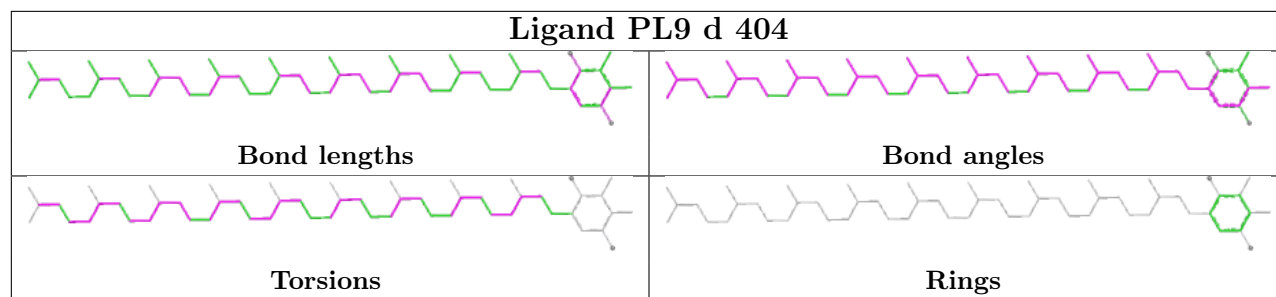
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Bond lengths	Bond angles
	
Torsions	Rings

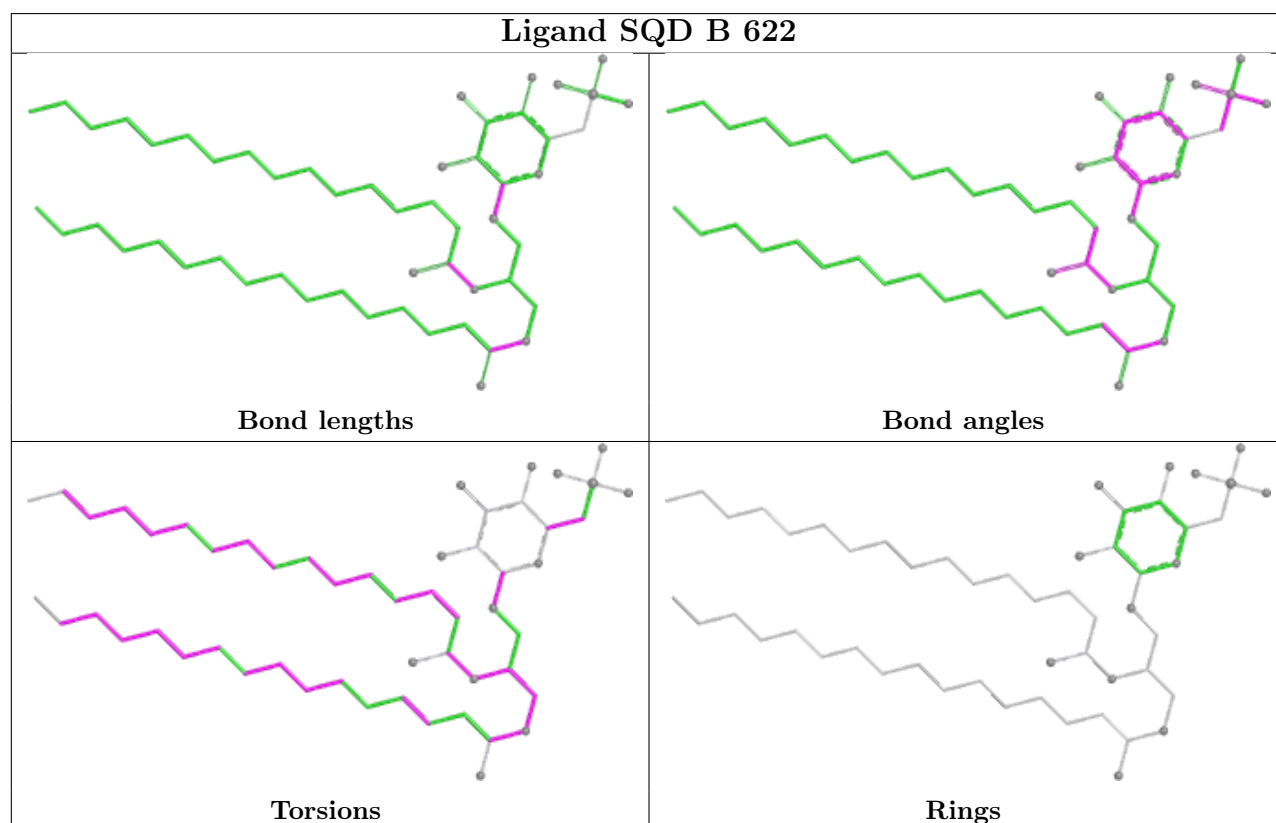
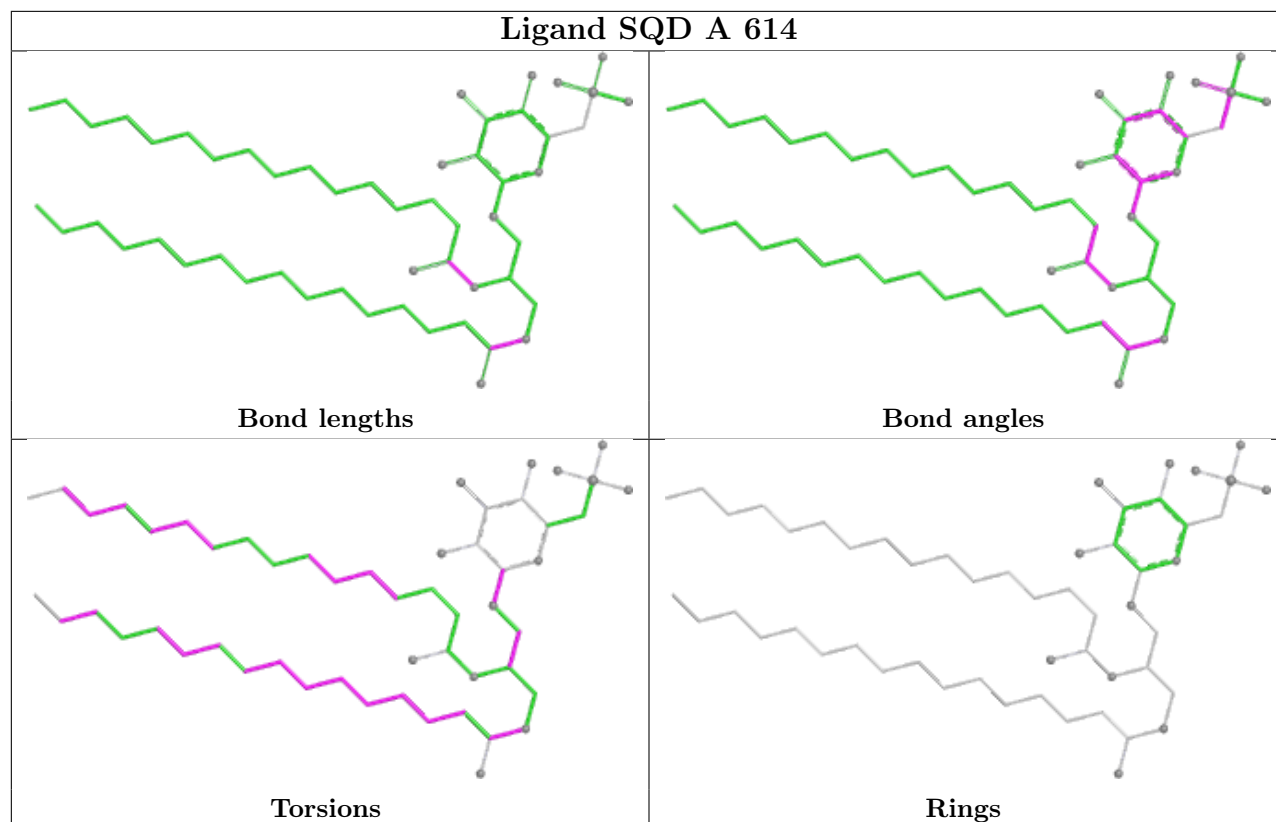
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Bond lengths	Bond angles
	
Torsions	Rings

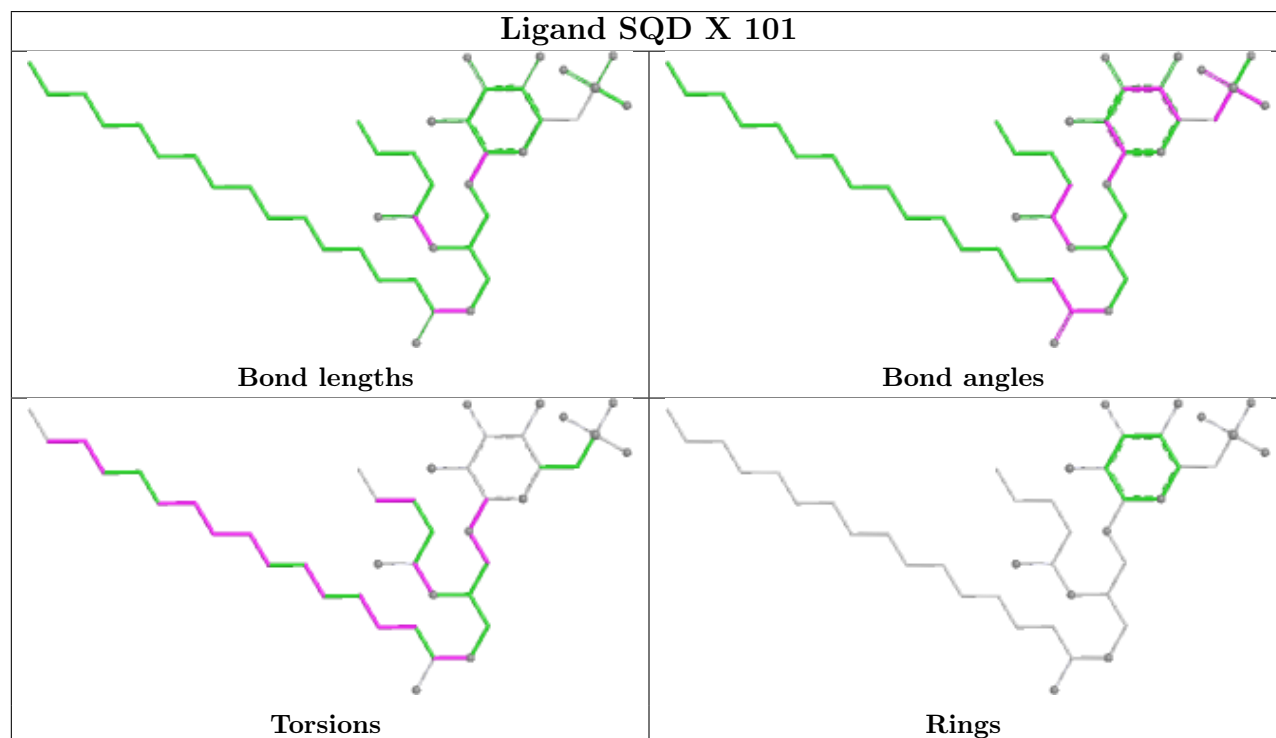
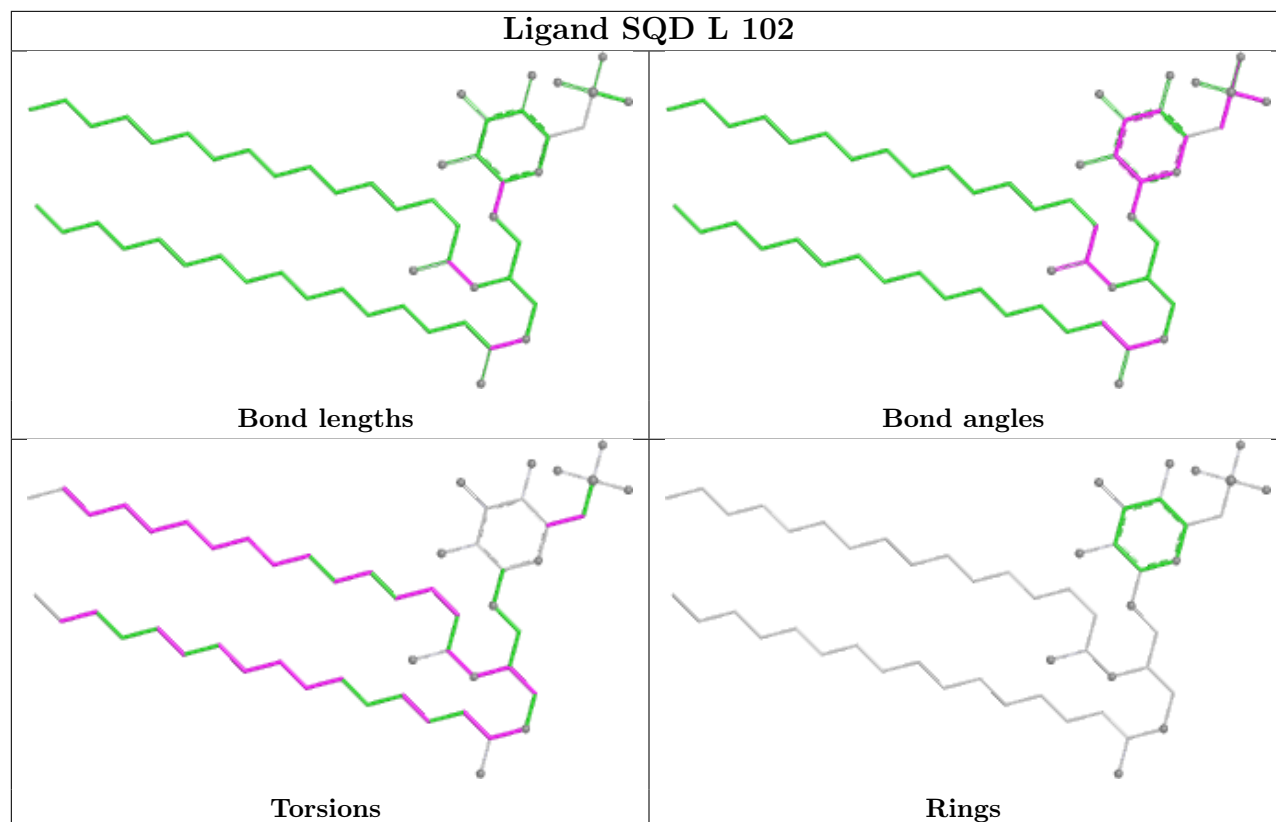
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Bond lengths	Bond angles
	
Torsions	Rings

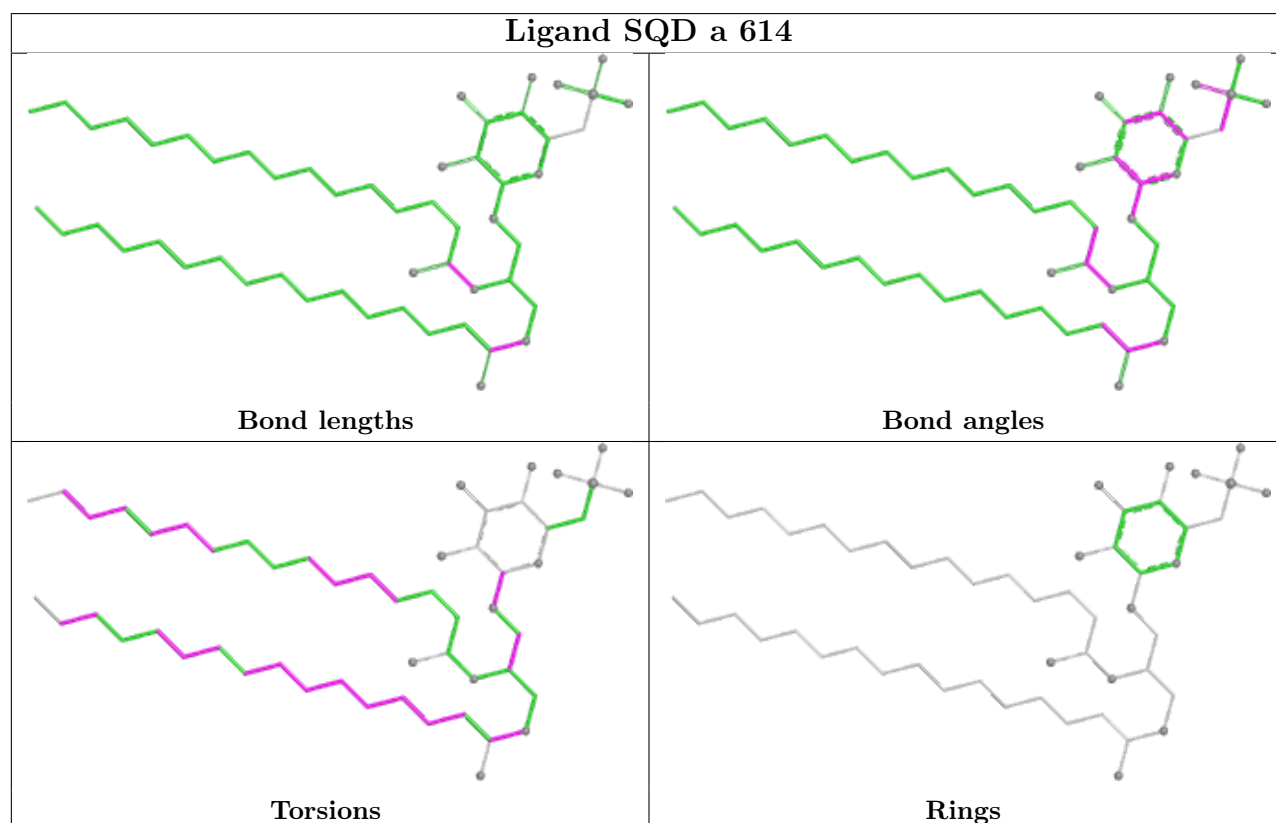
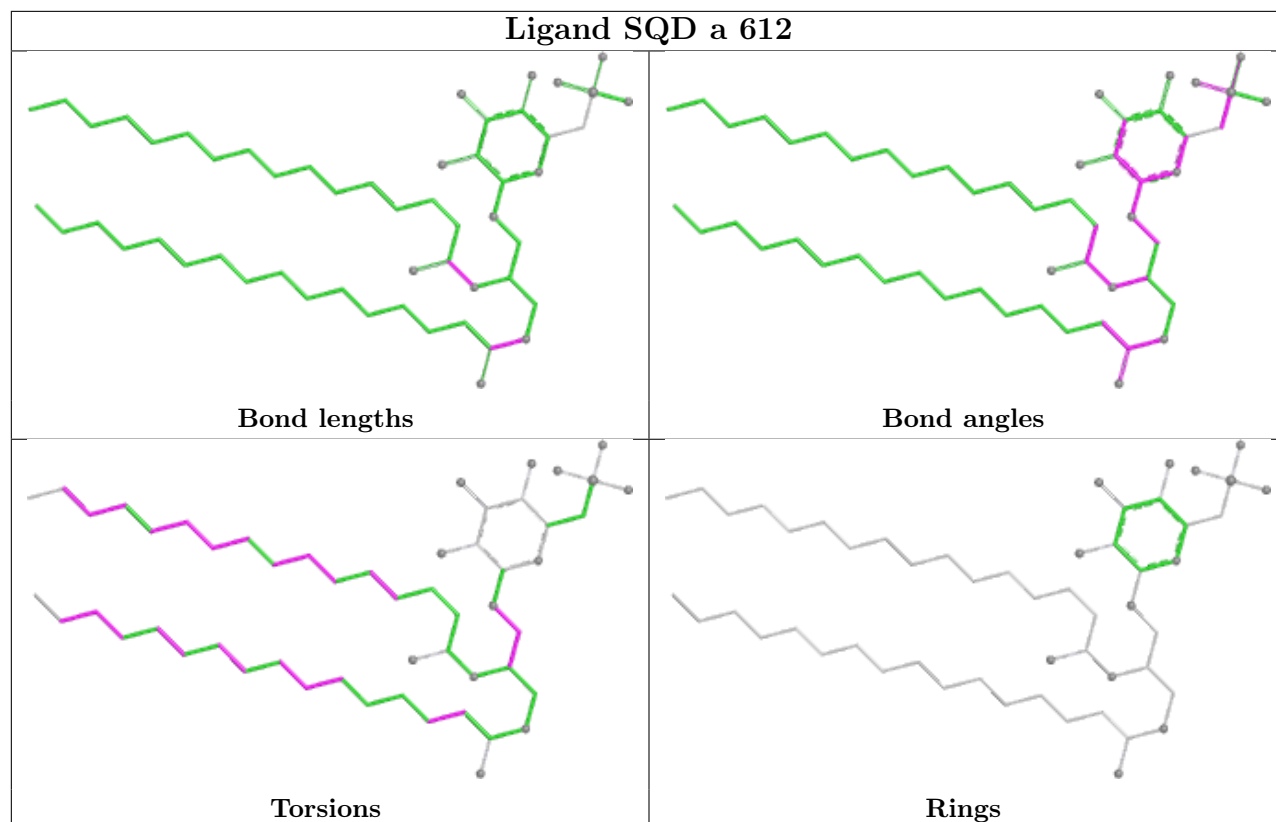
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Bond lengths	Bond angles
	
Torsions	Rings

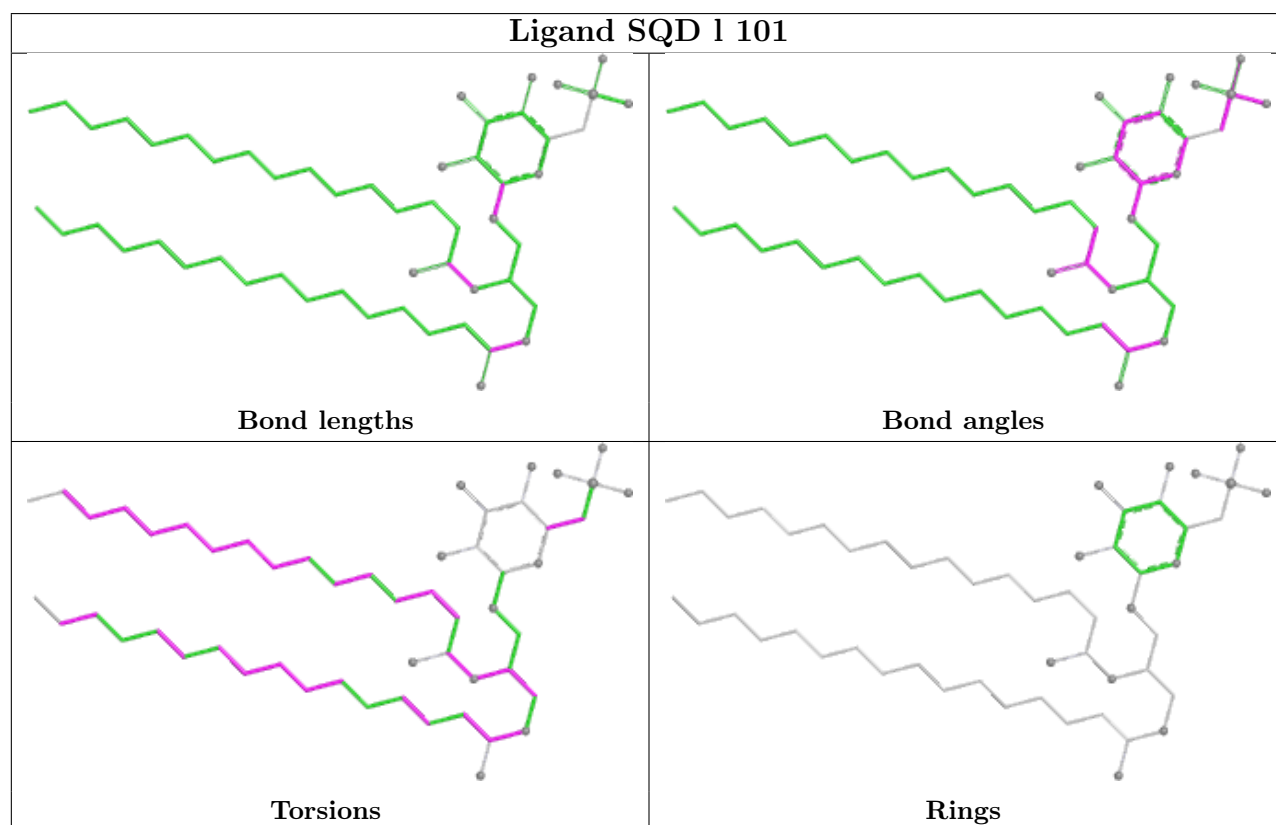
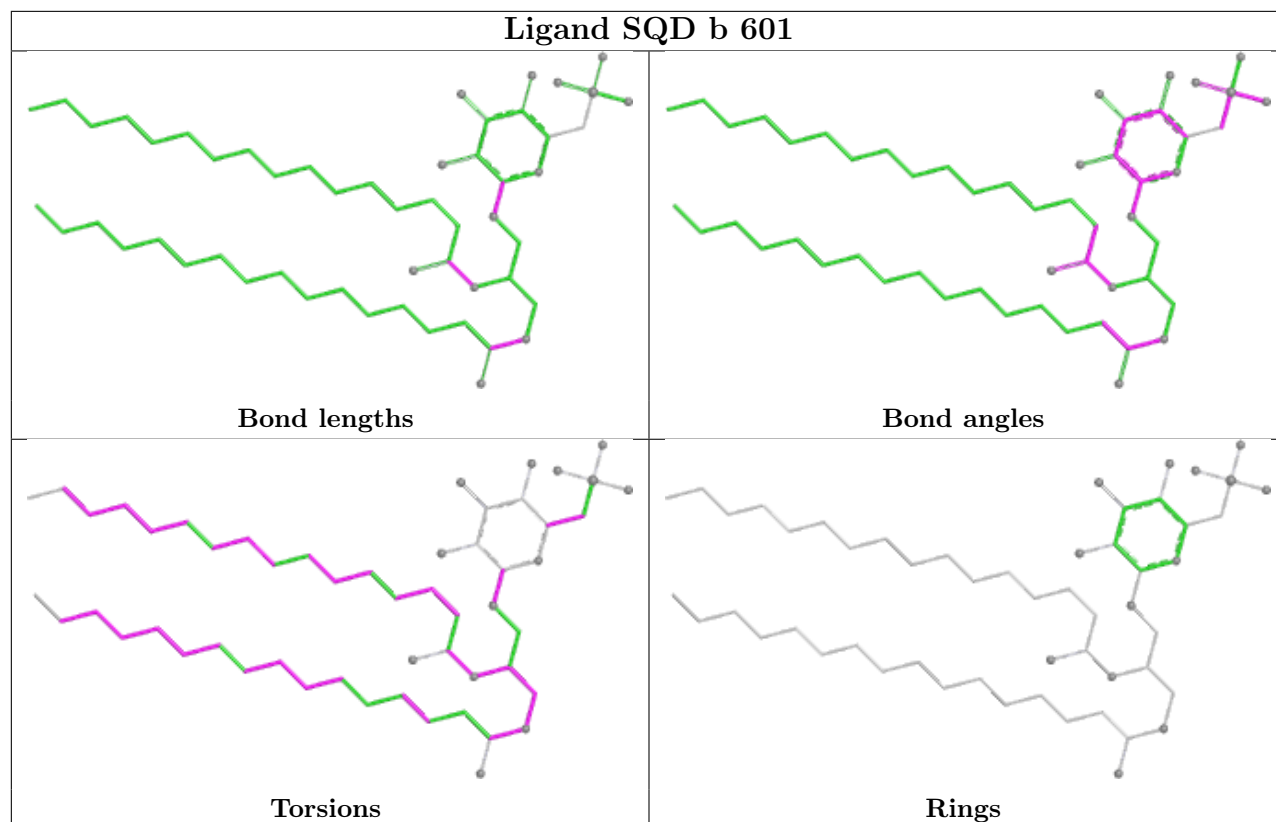
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Bond lengths	Bond angles
	
Torsions	Rings

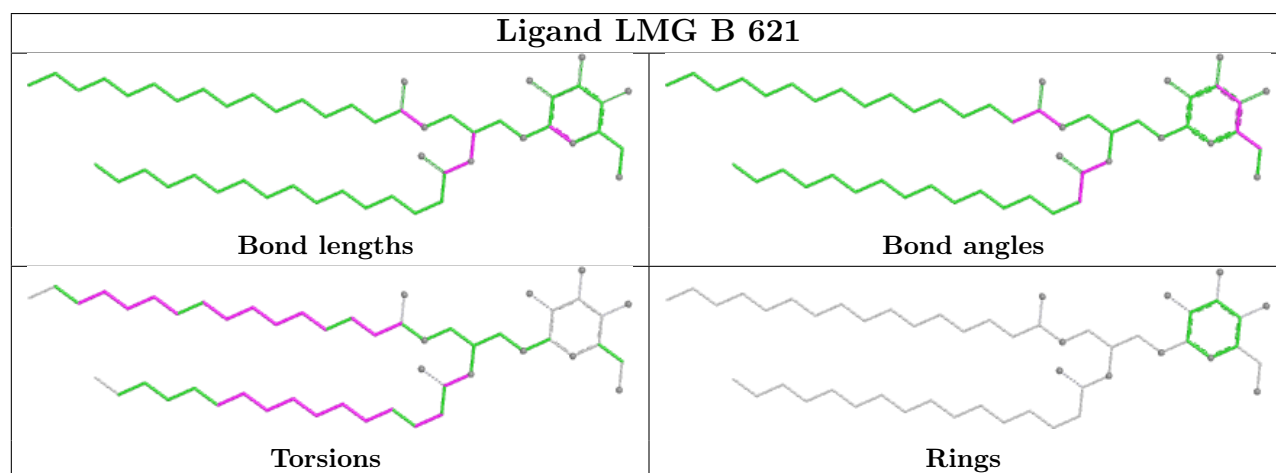
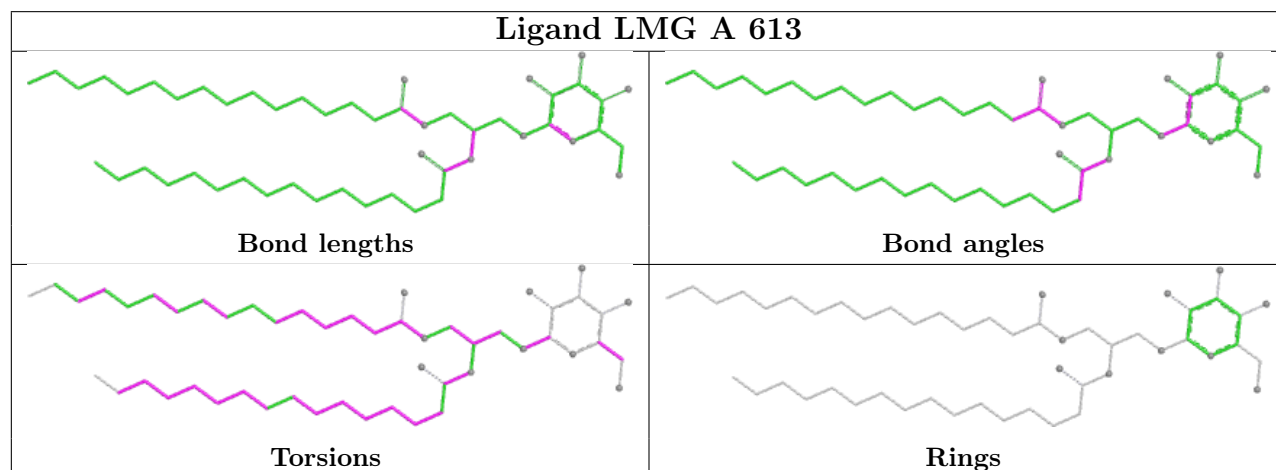
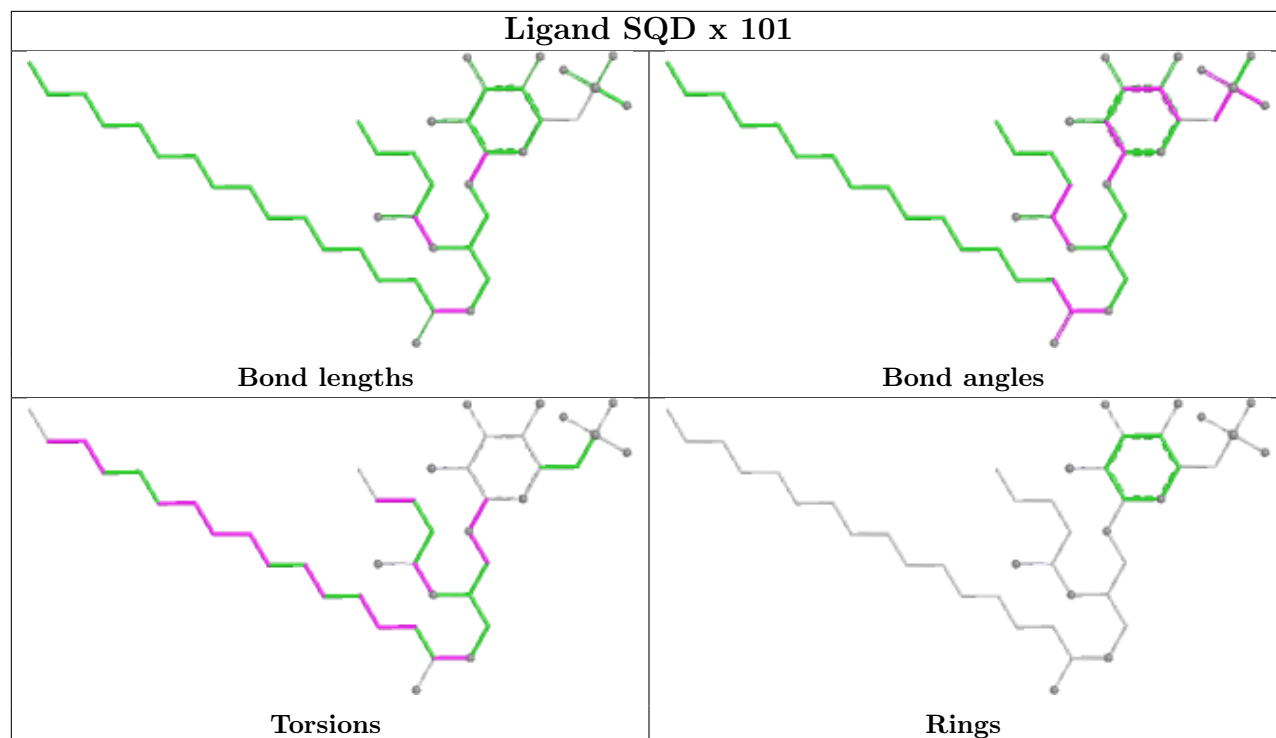


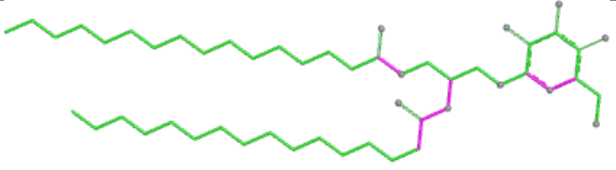
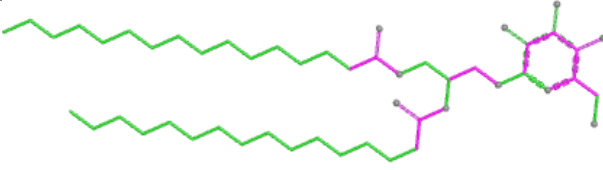
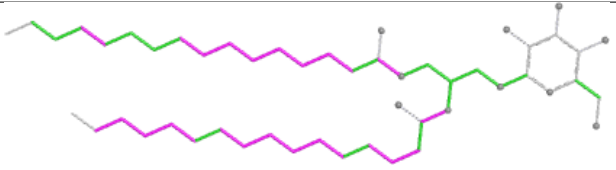
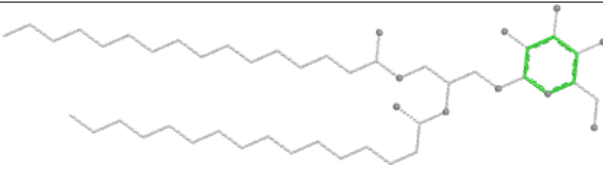


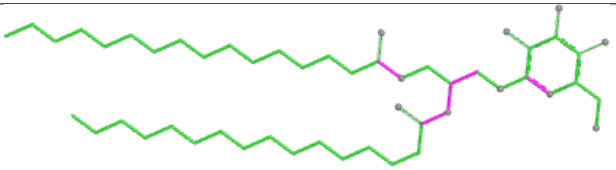
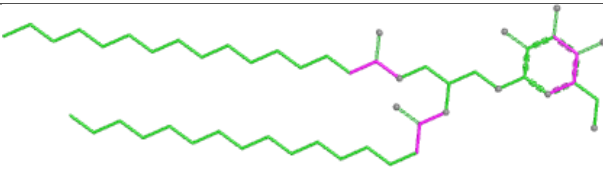
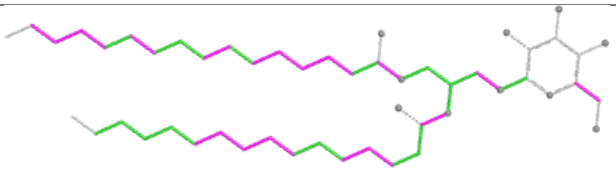
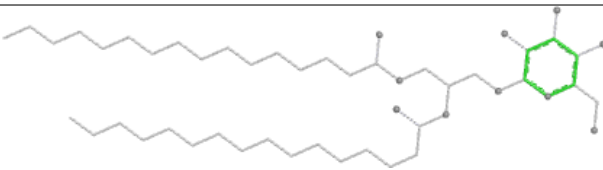


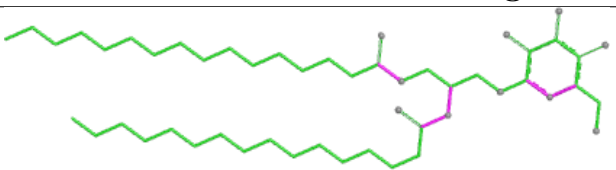
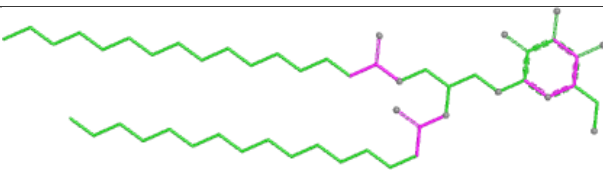
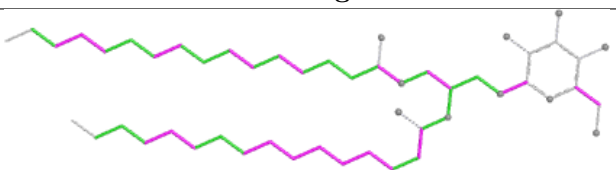
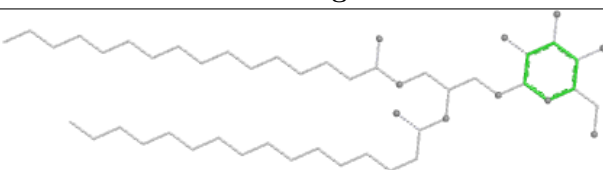


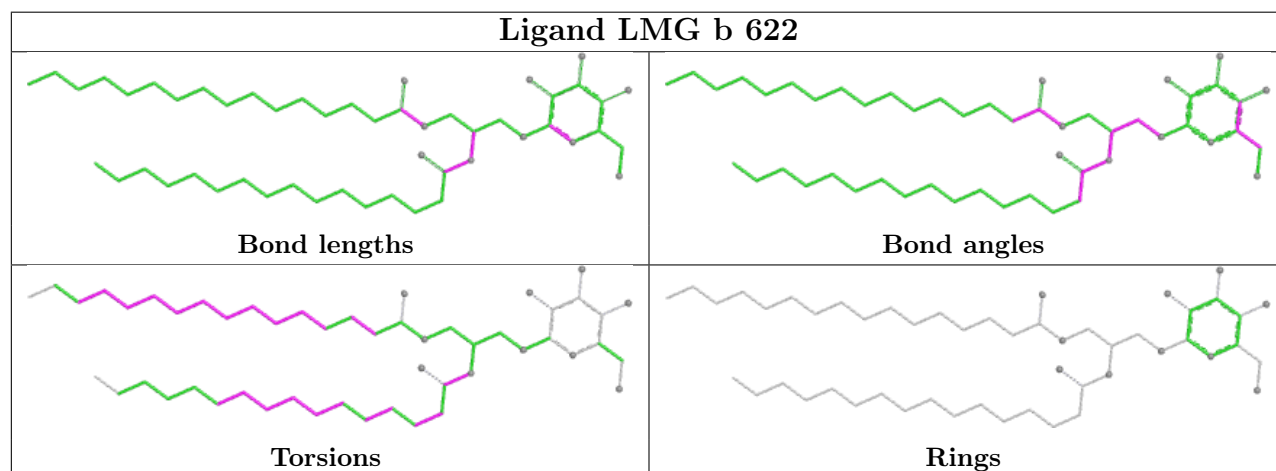
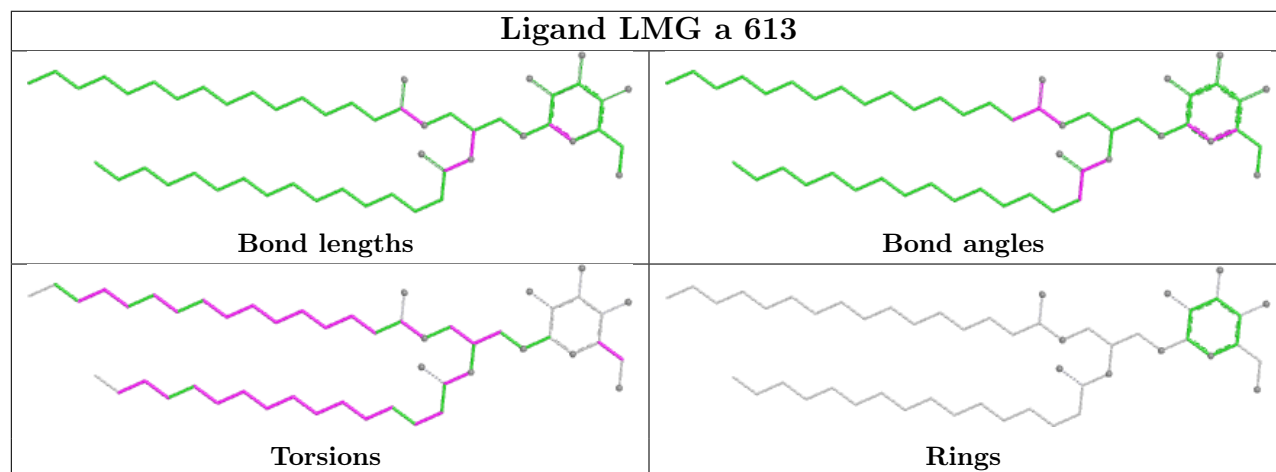
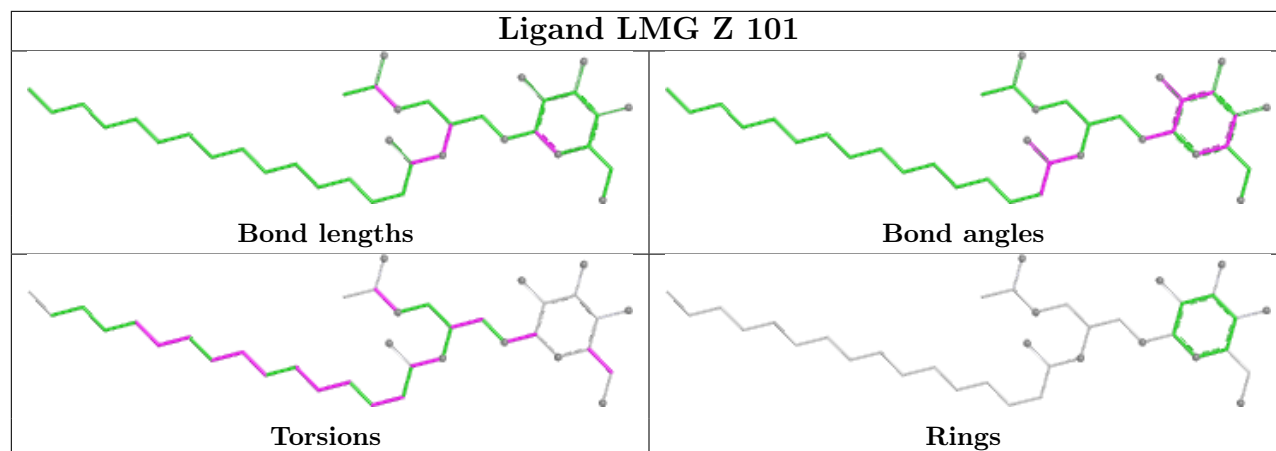


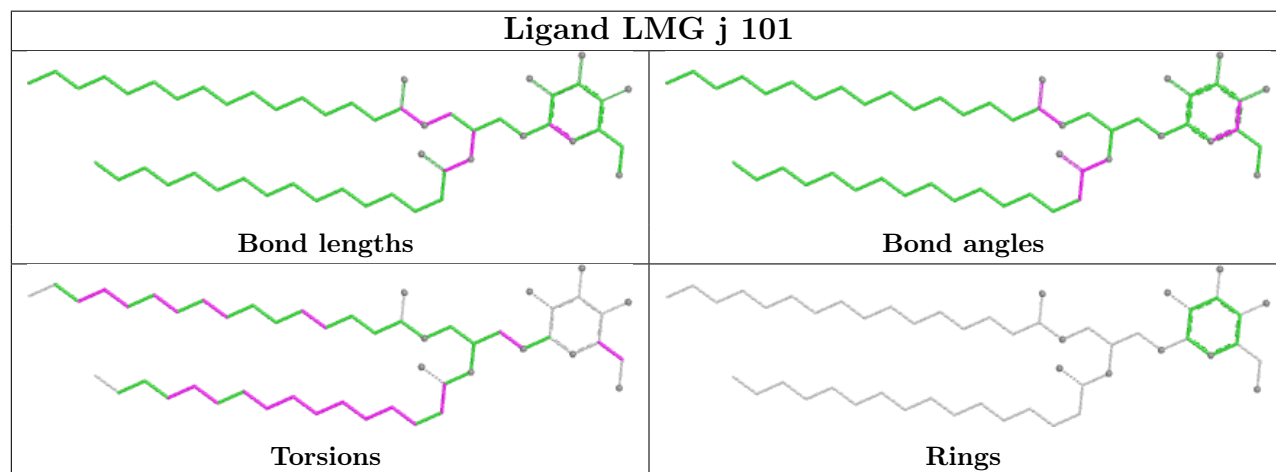
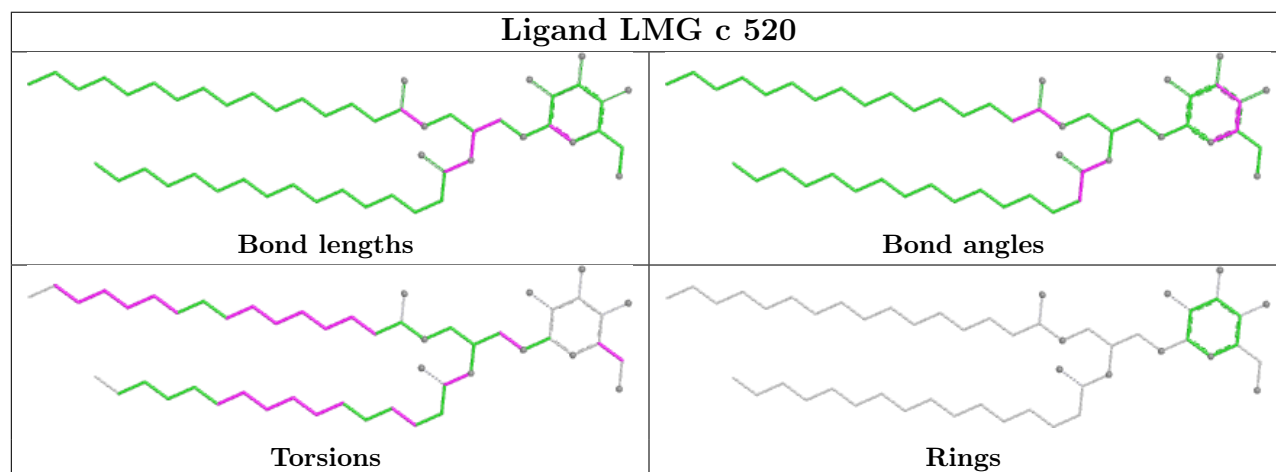
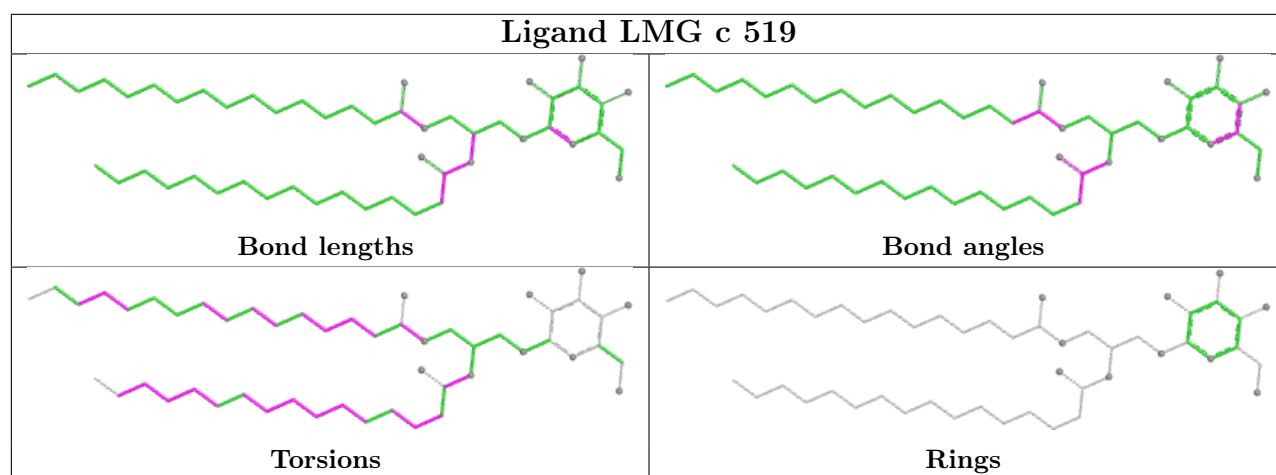


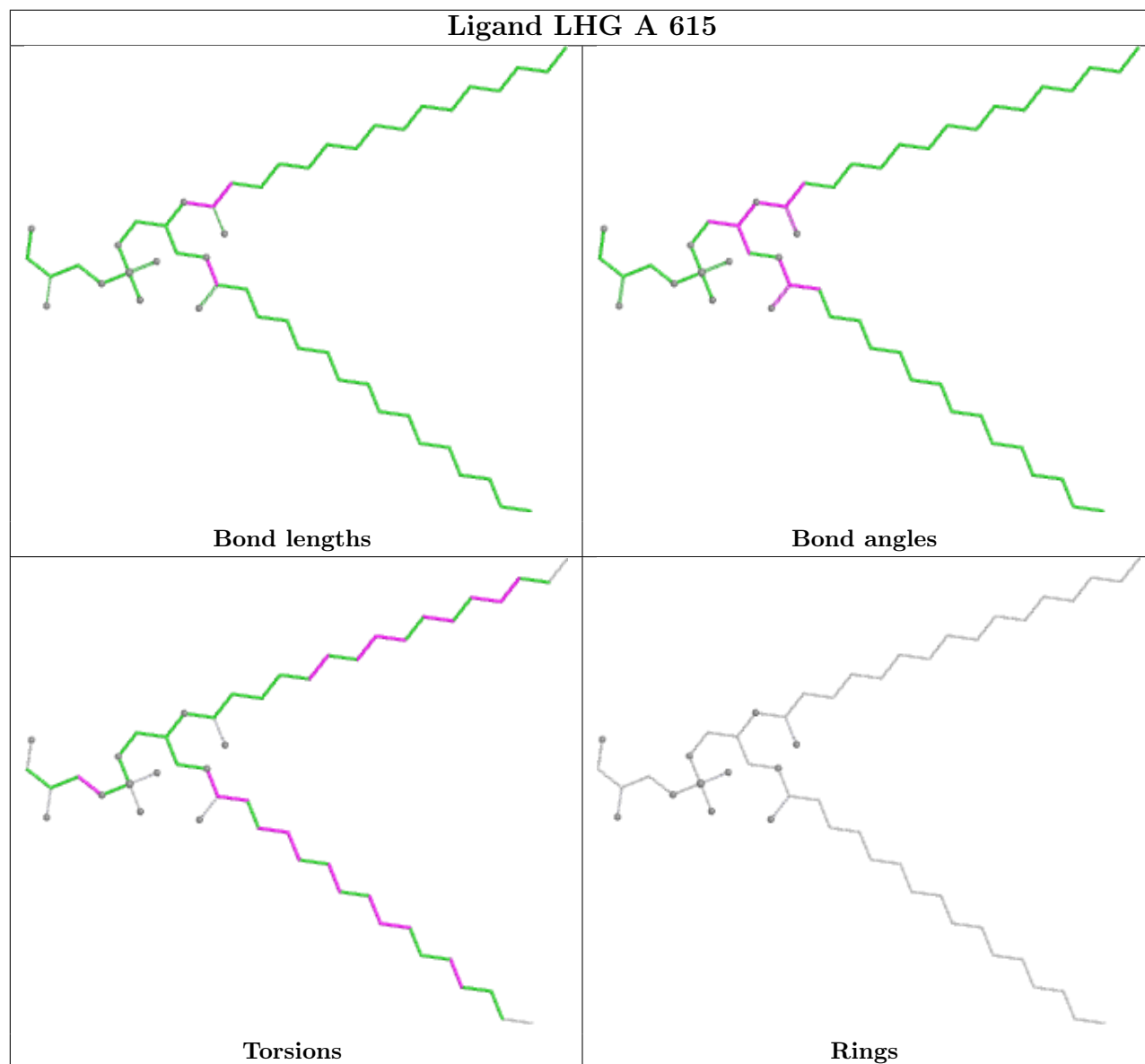
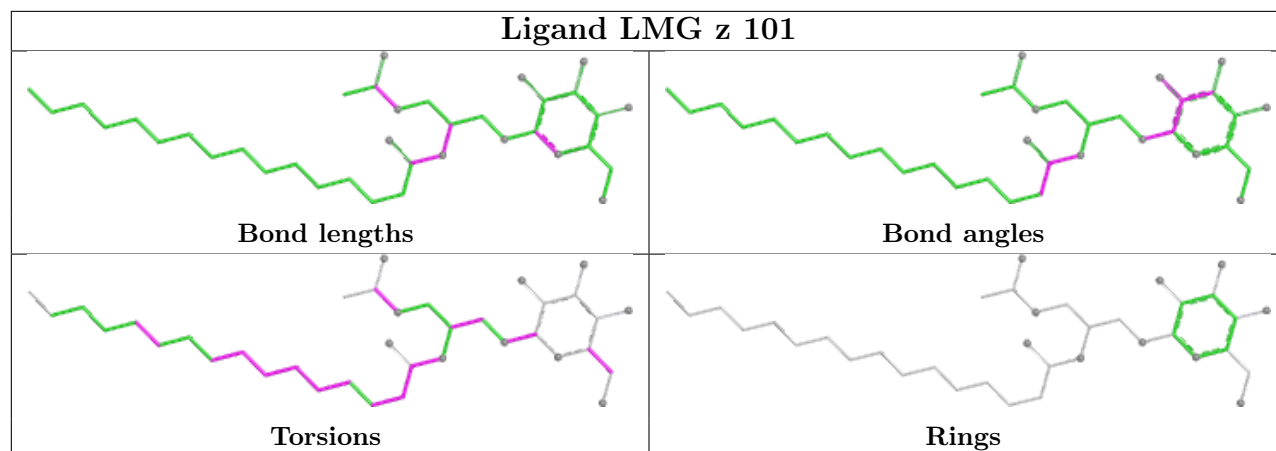
Ligand LMG C 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

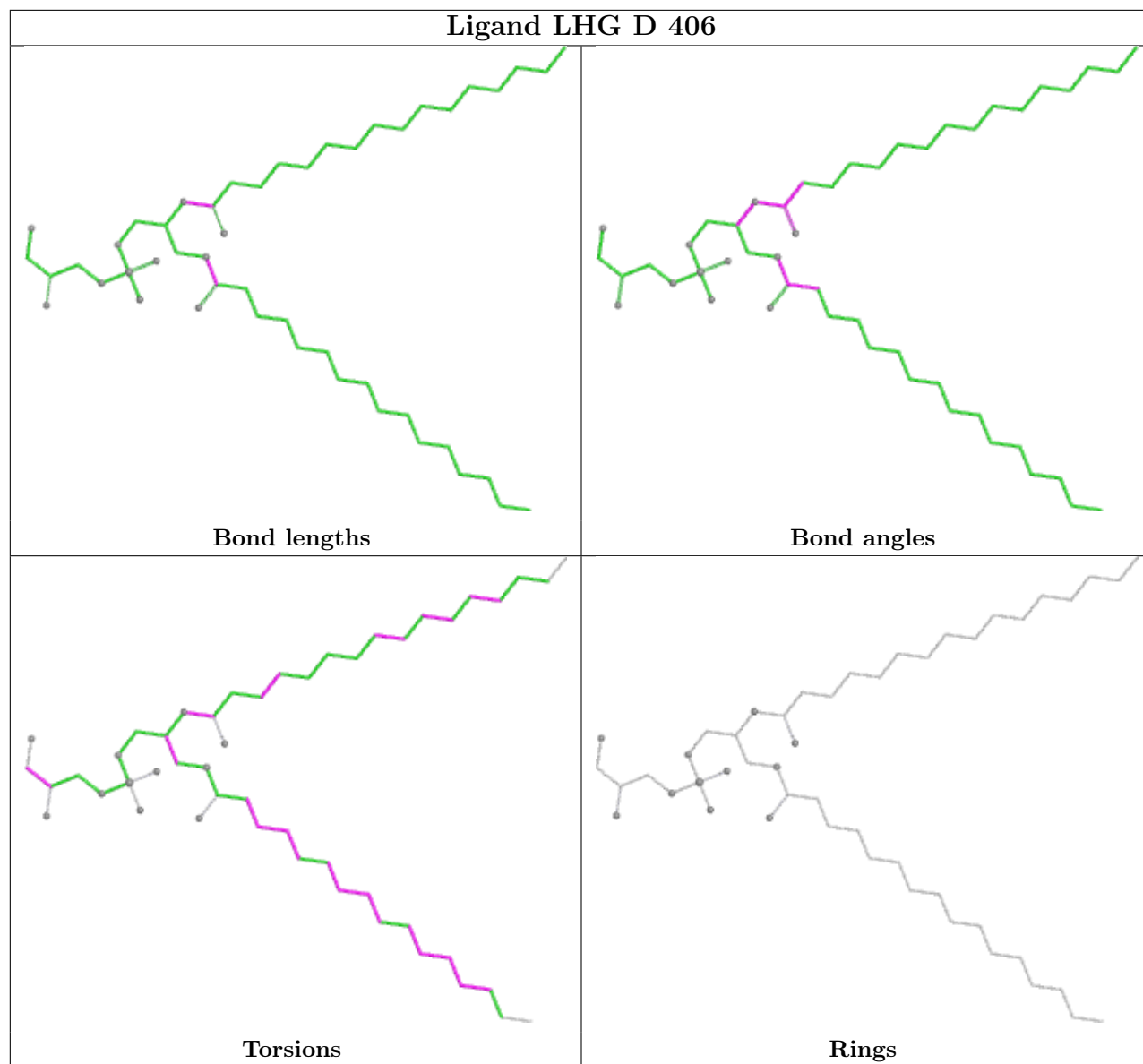
Ligand LMG C 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

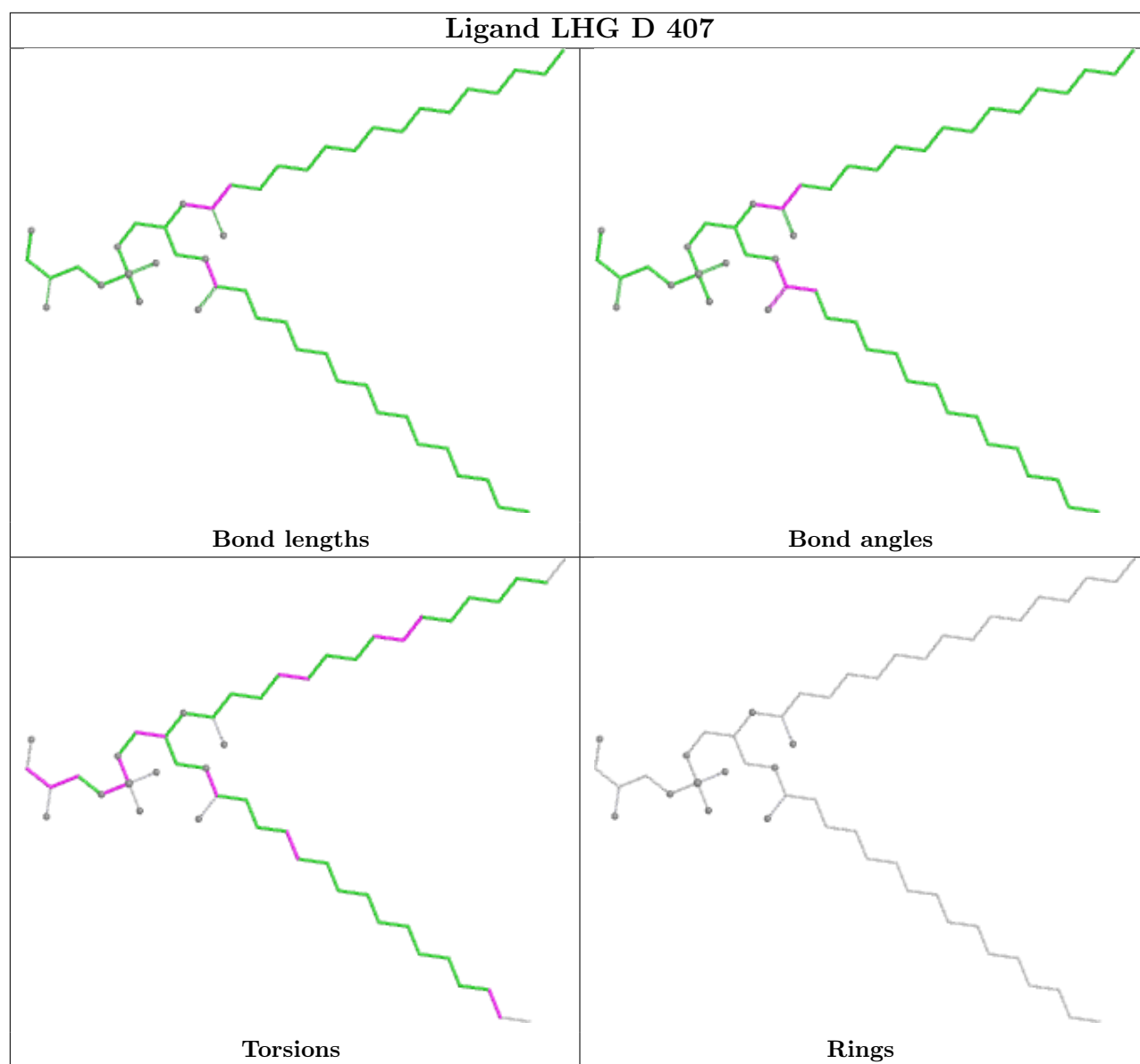
Ligand LMG D 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

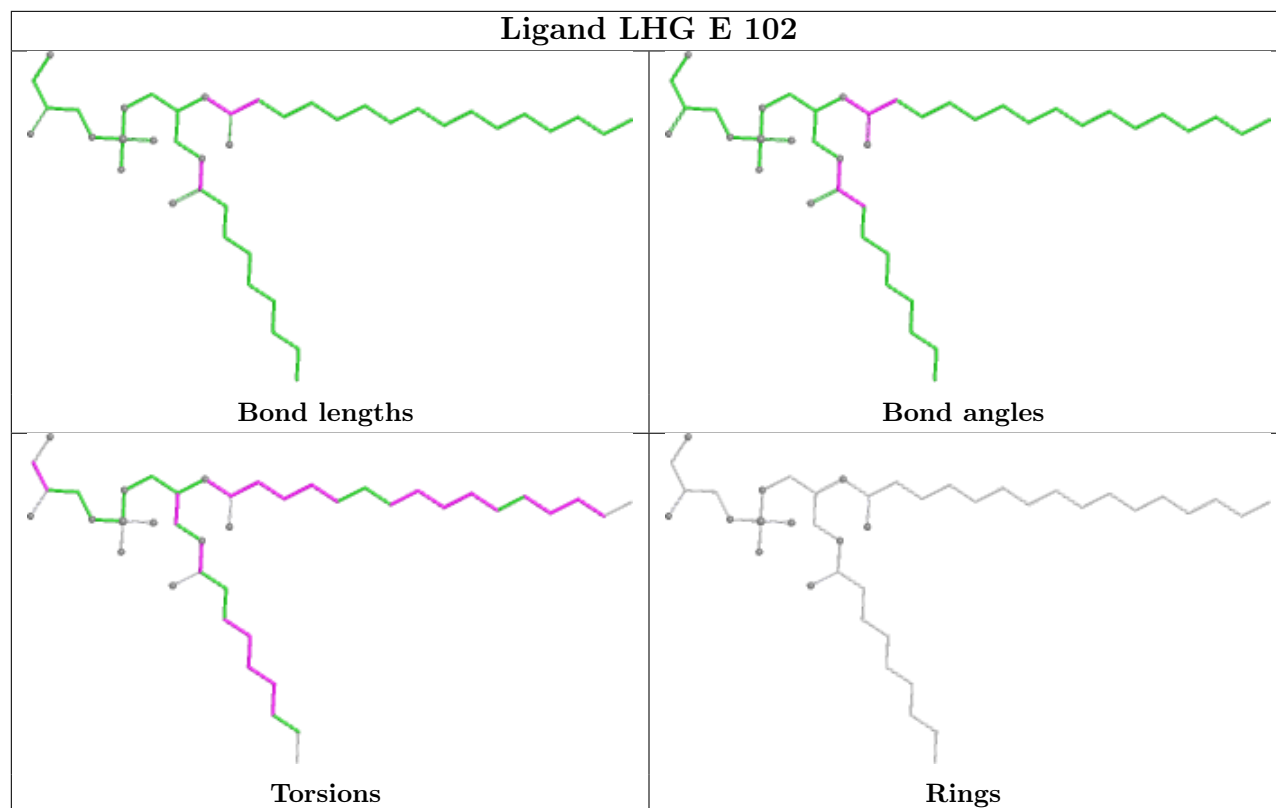


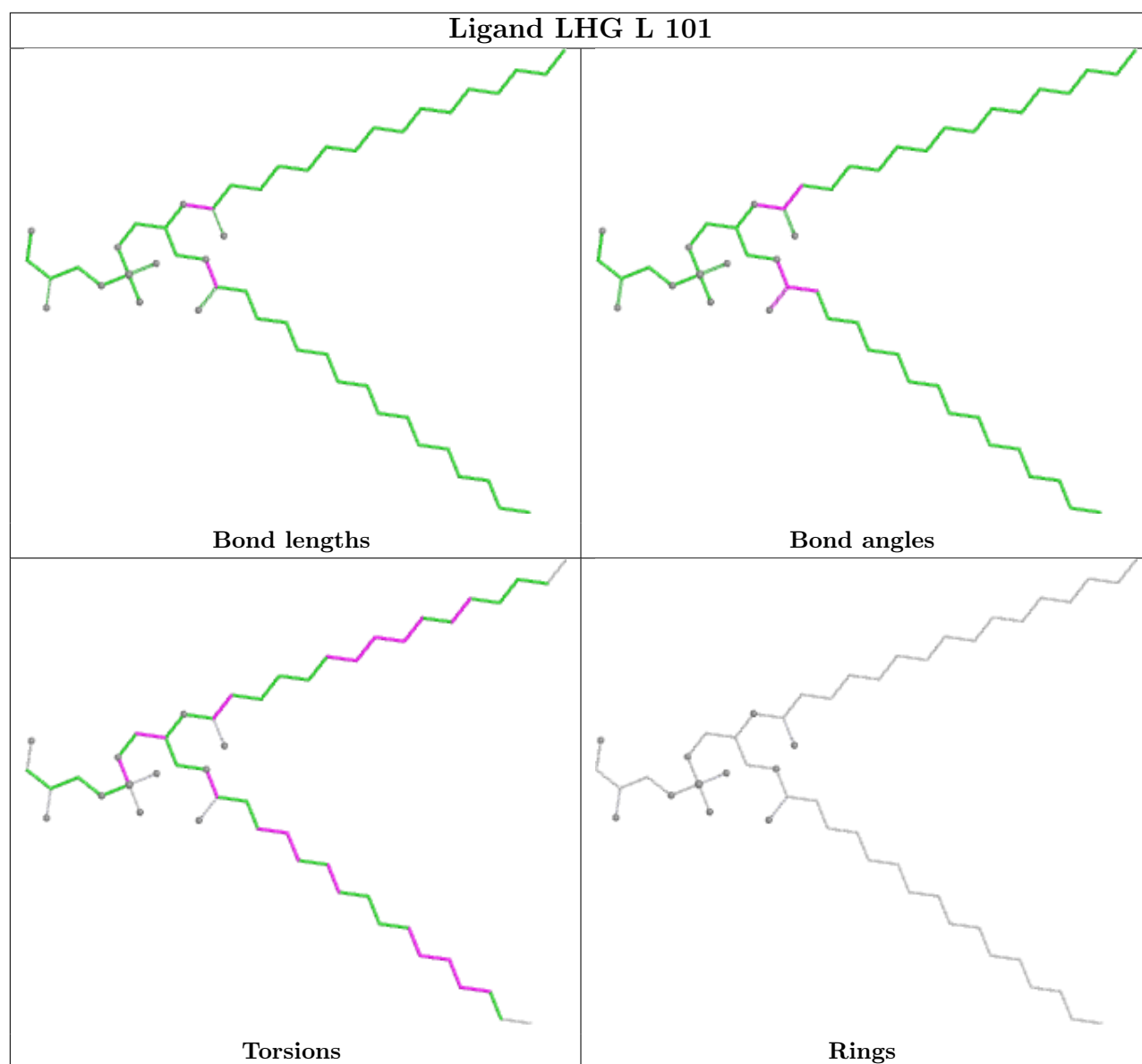


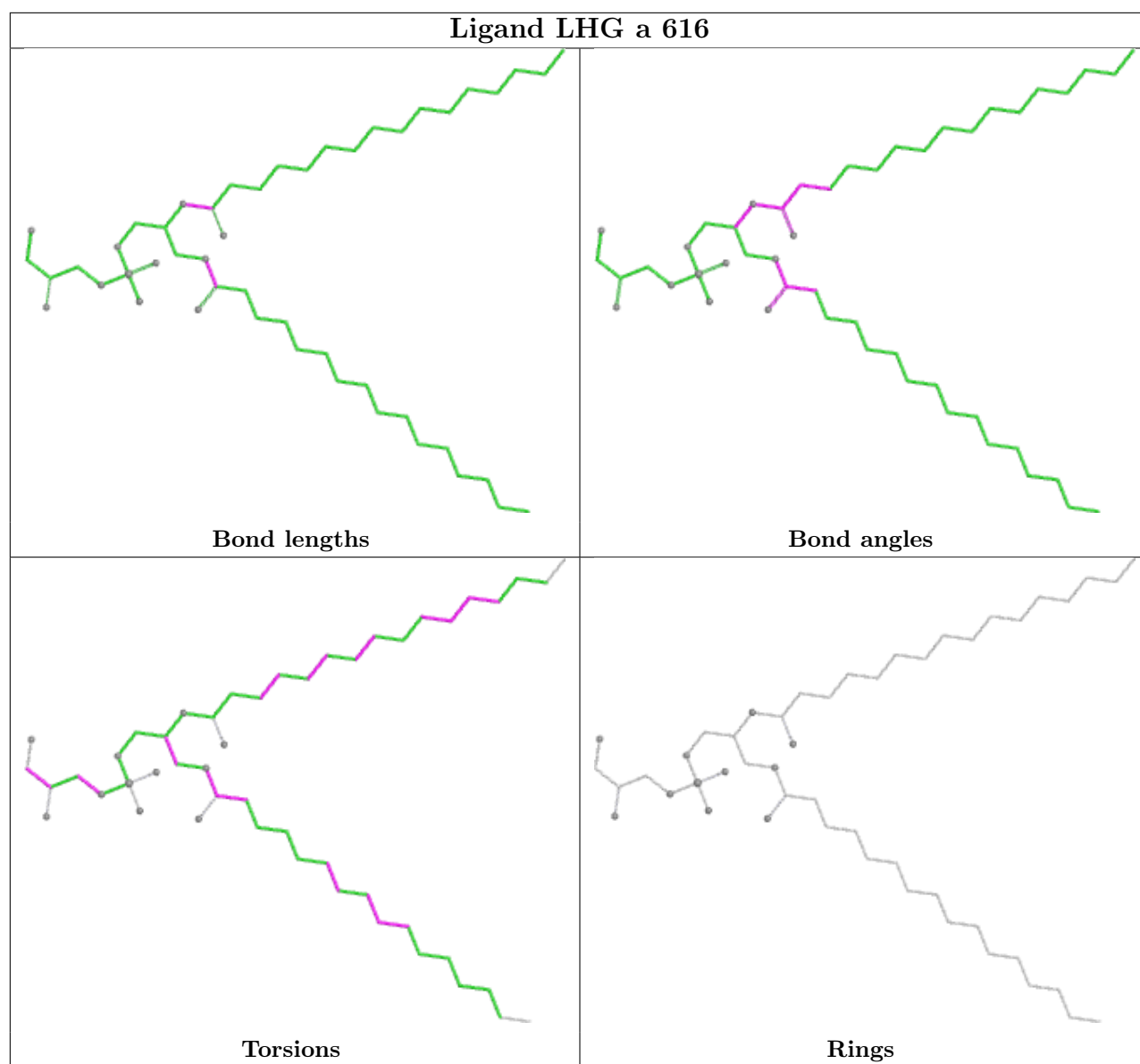


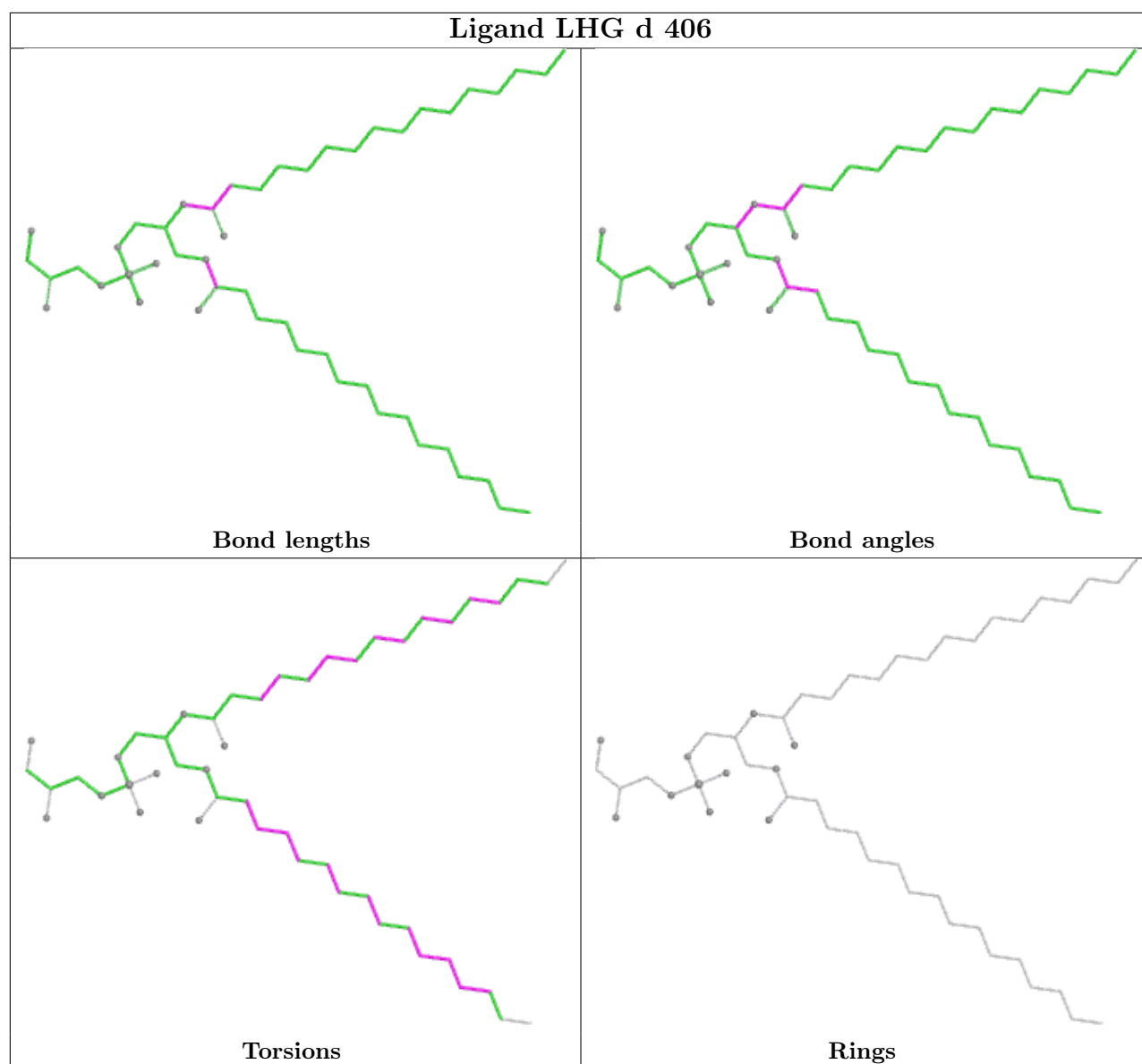


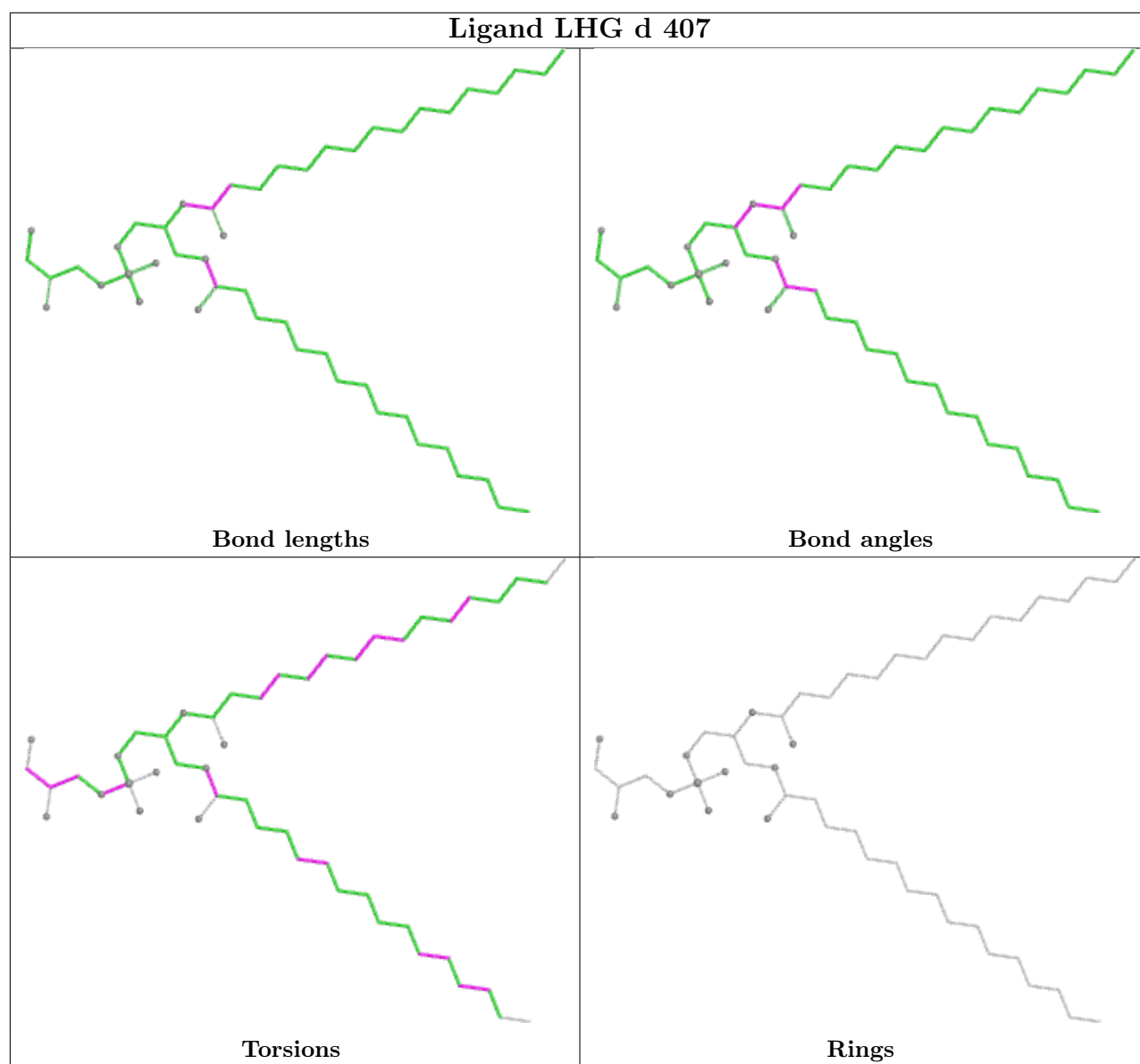


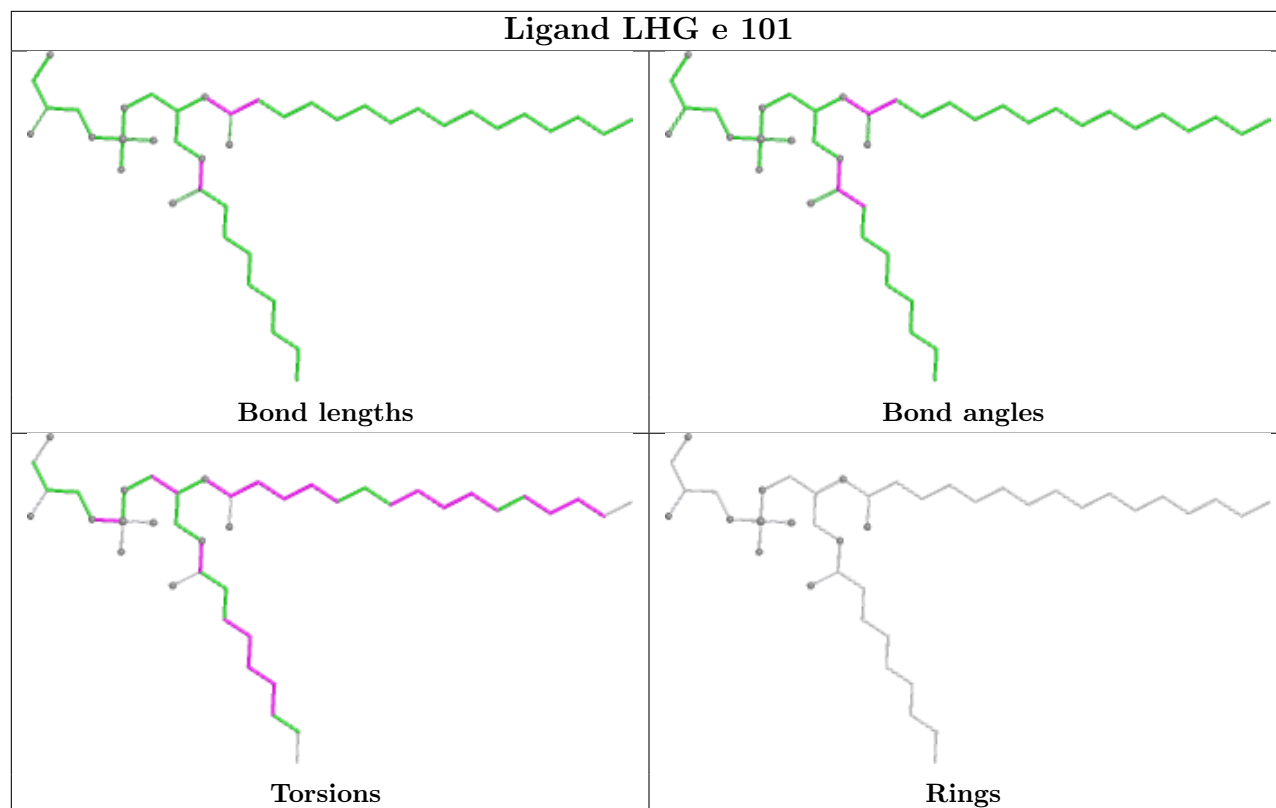


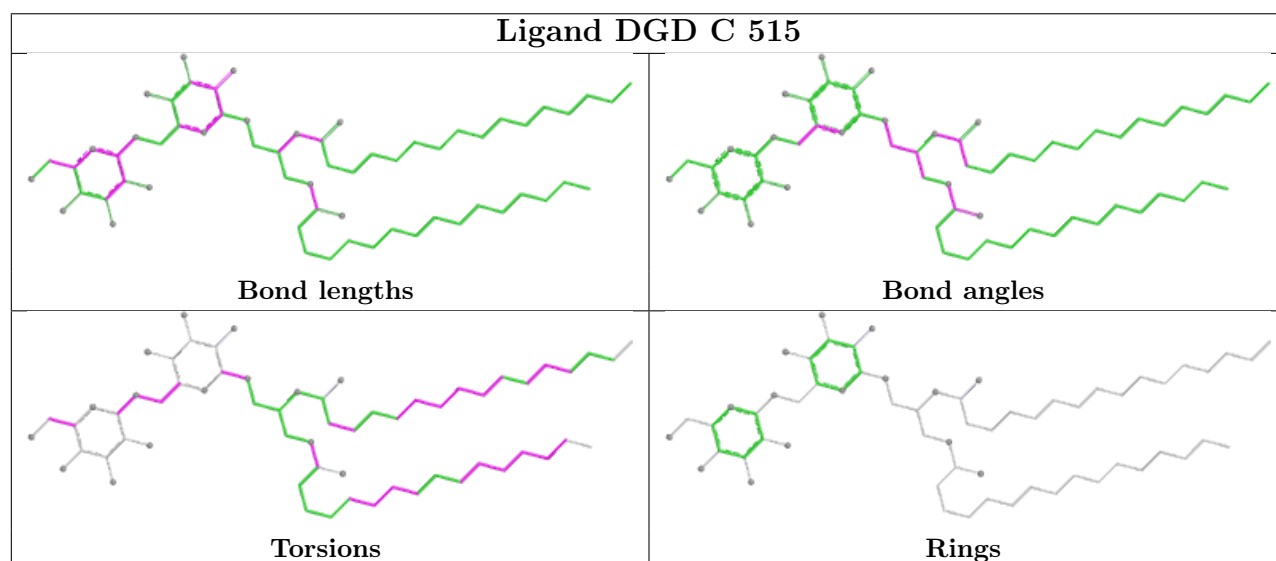
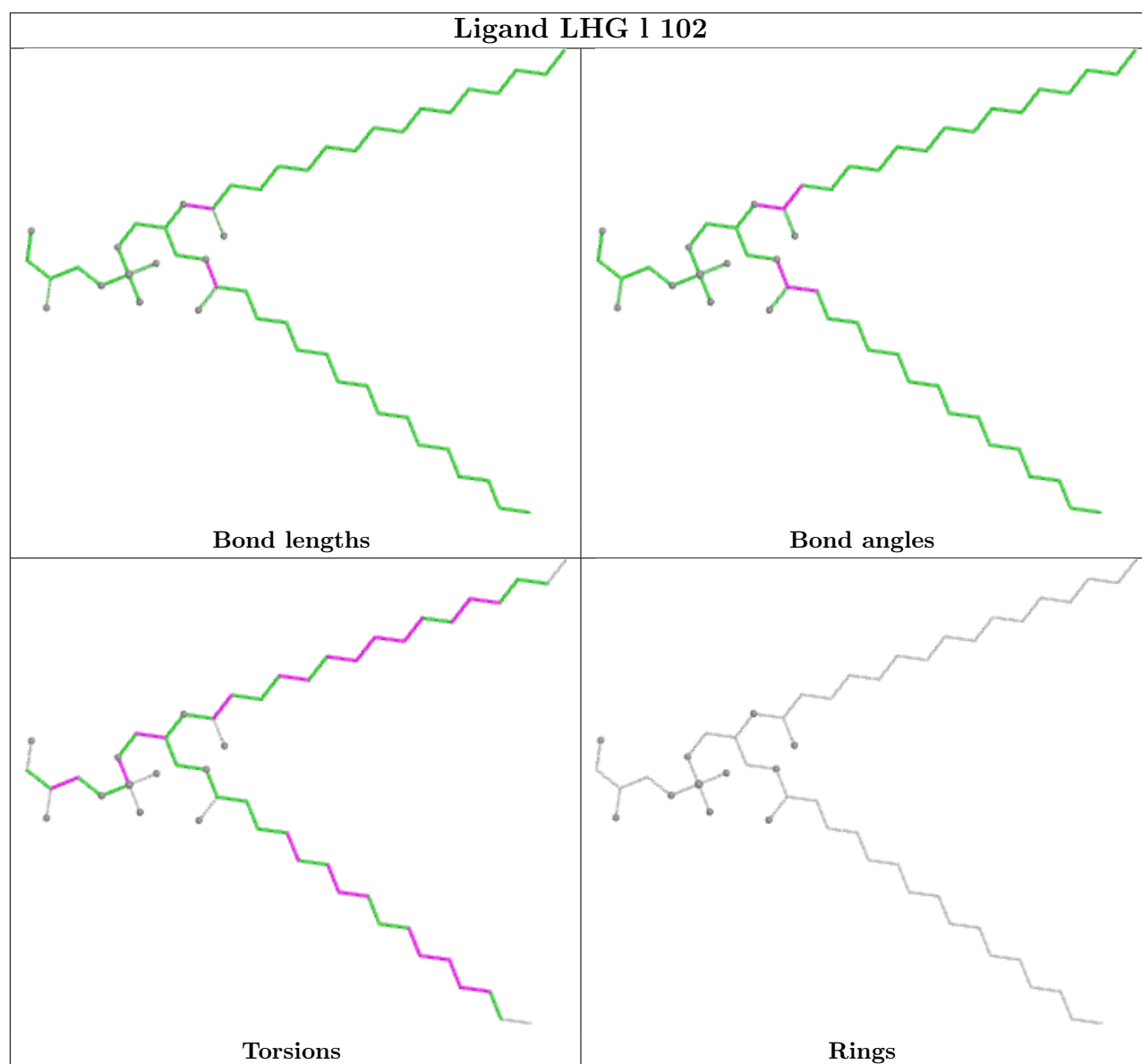


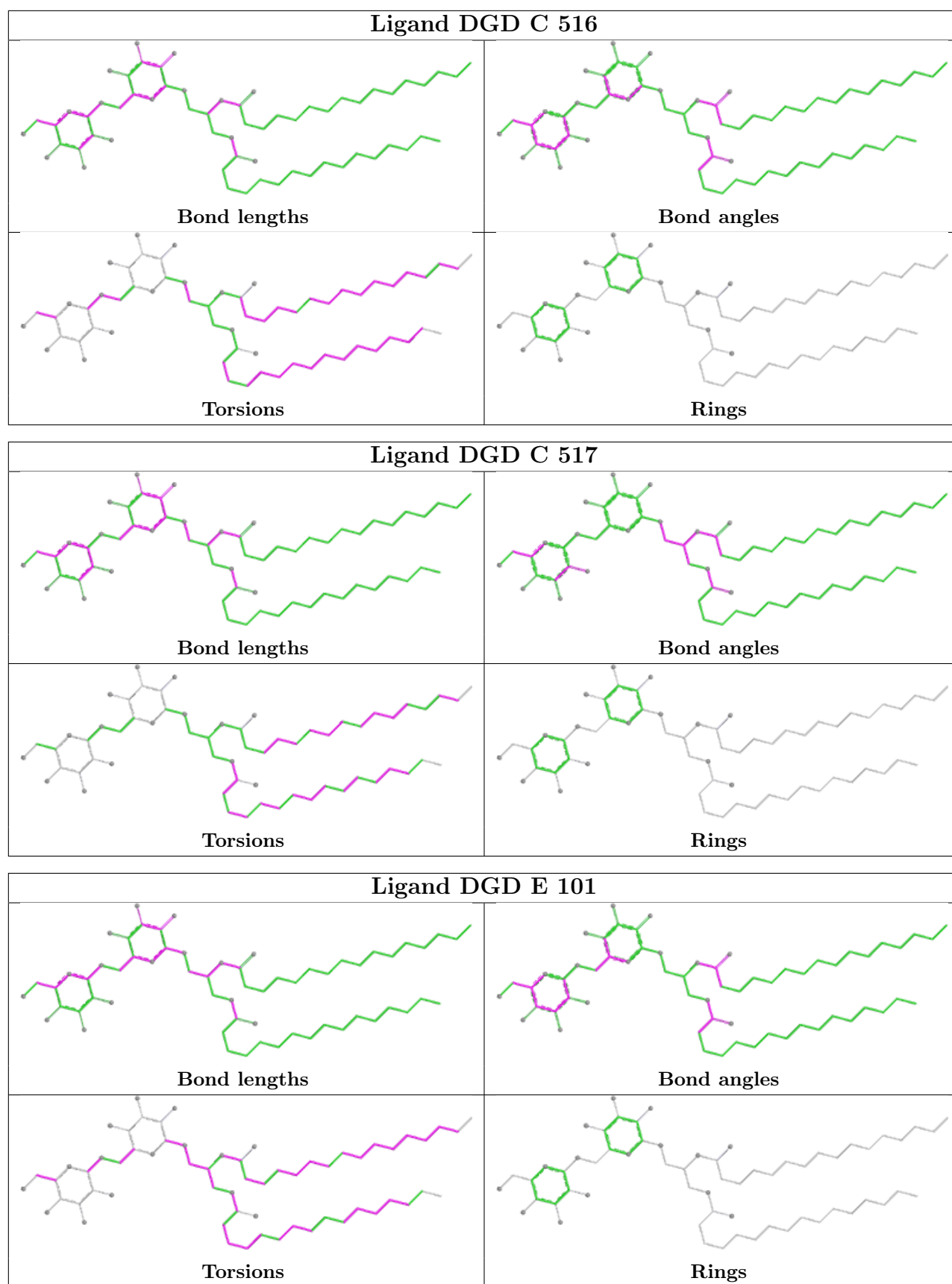


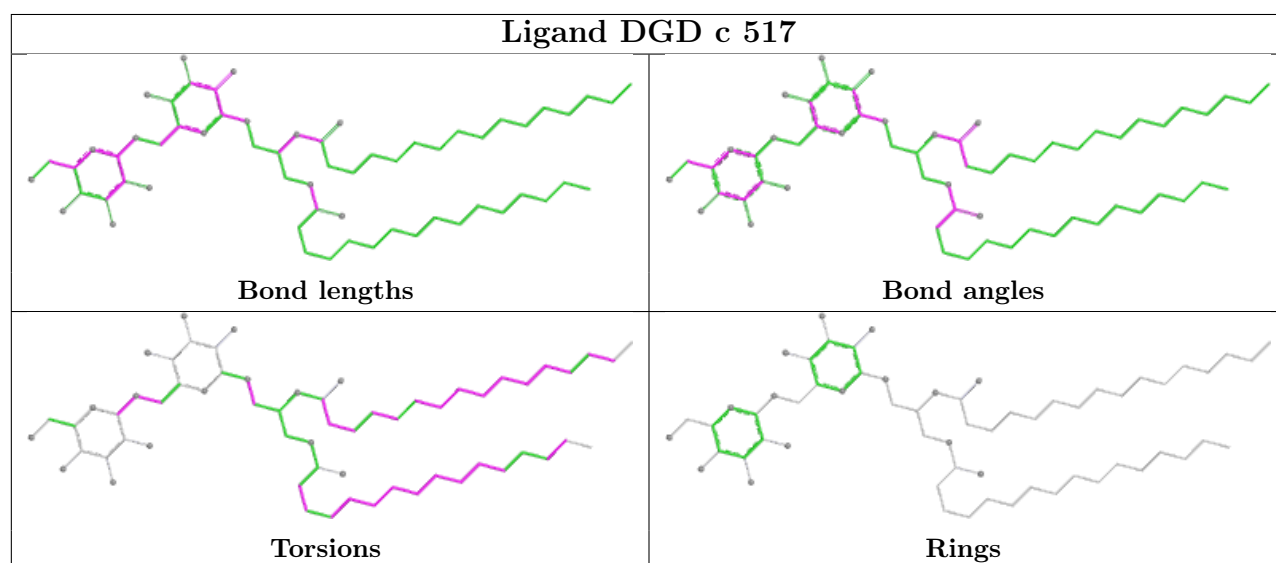
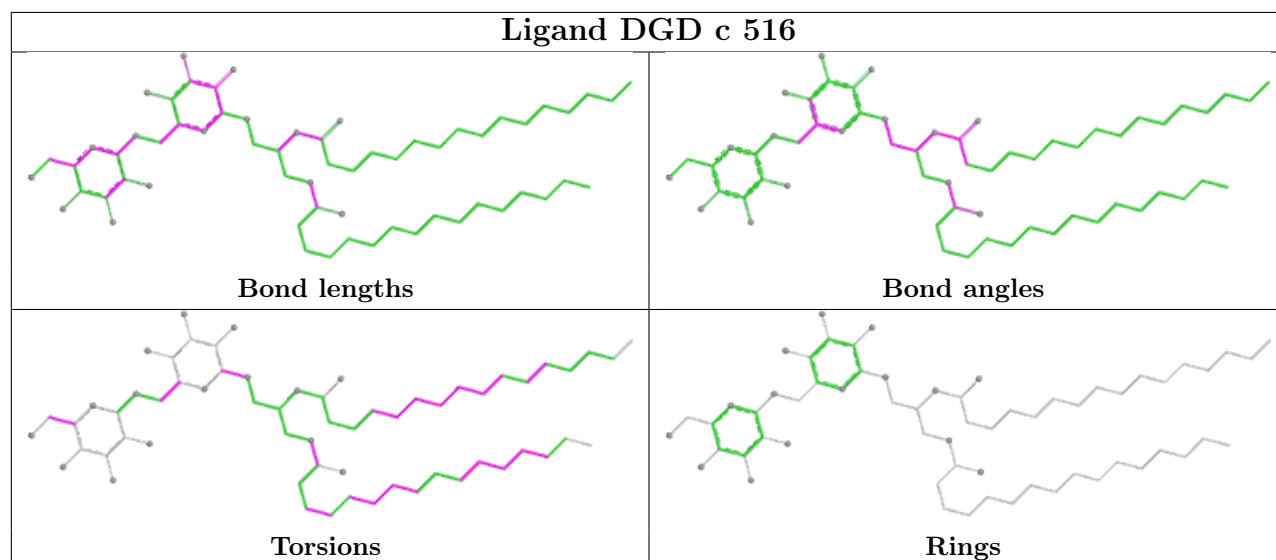
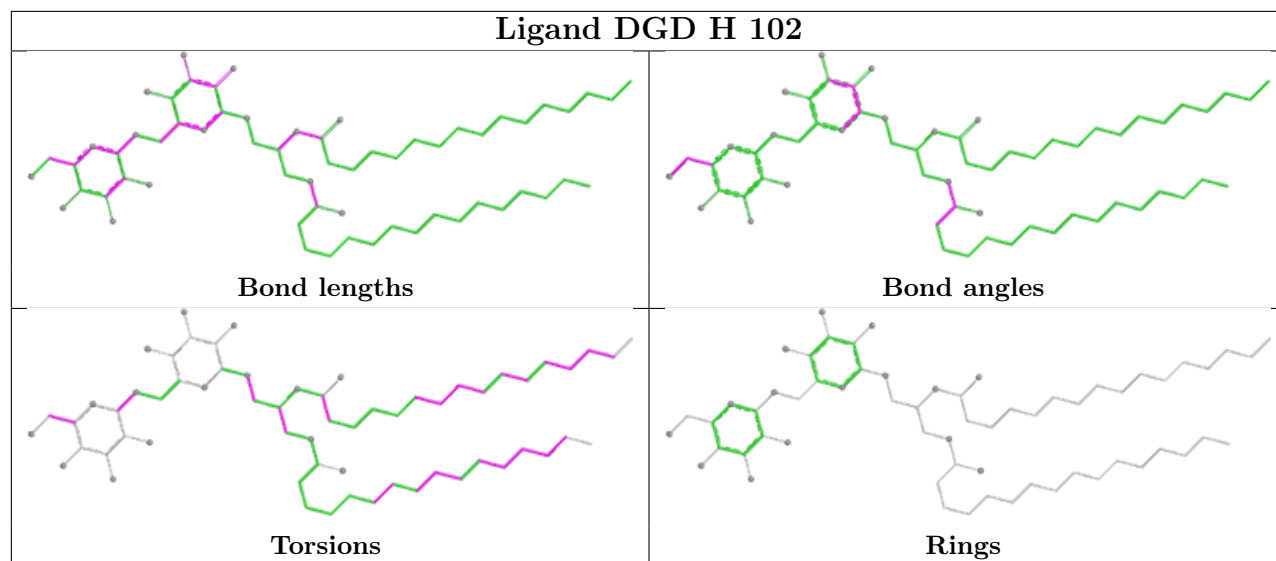


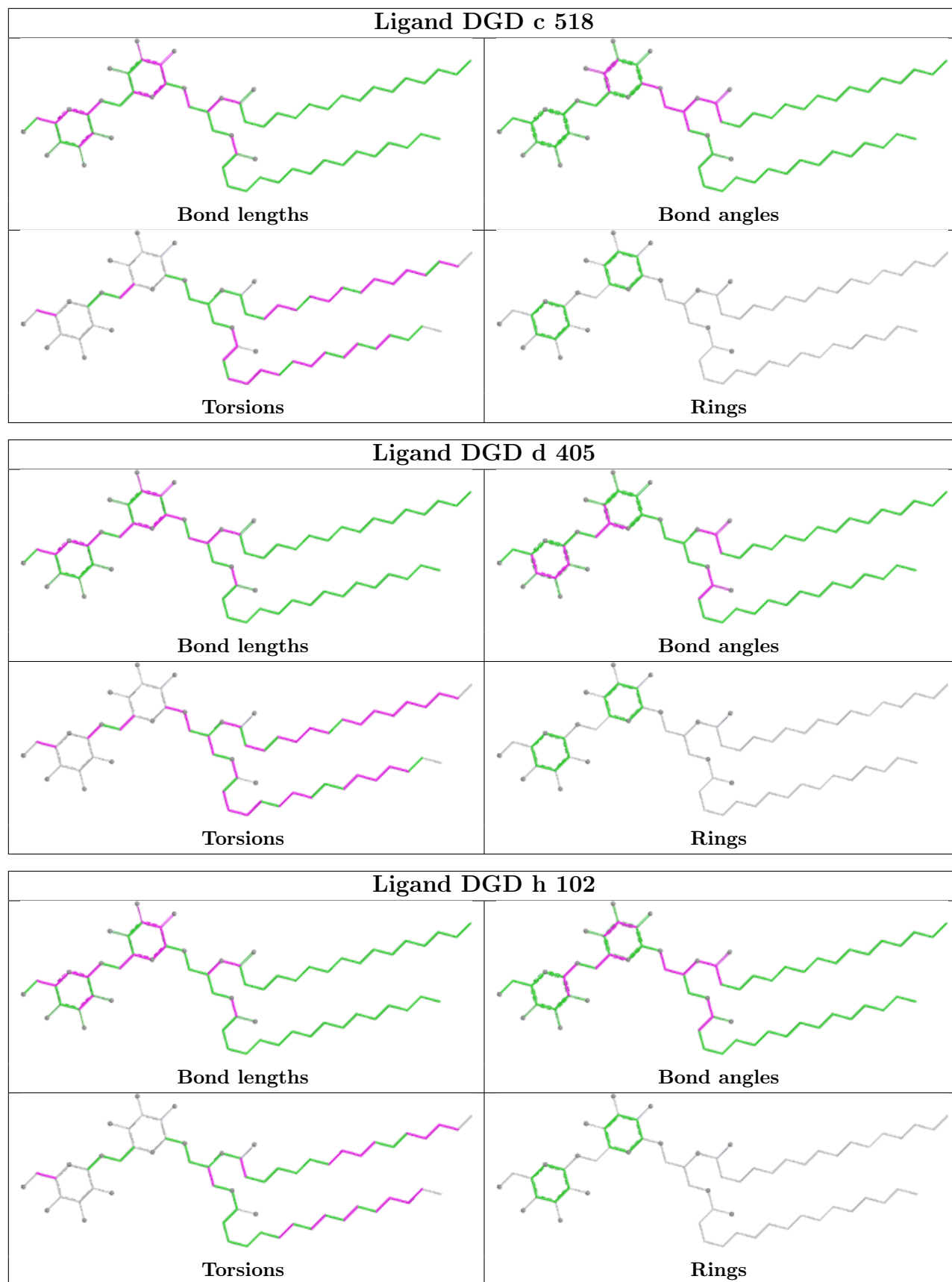


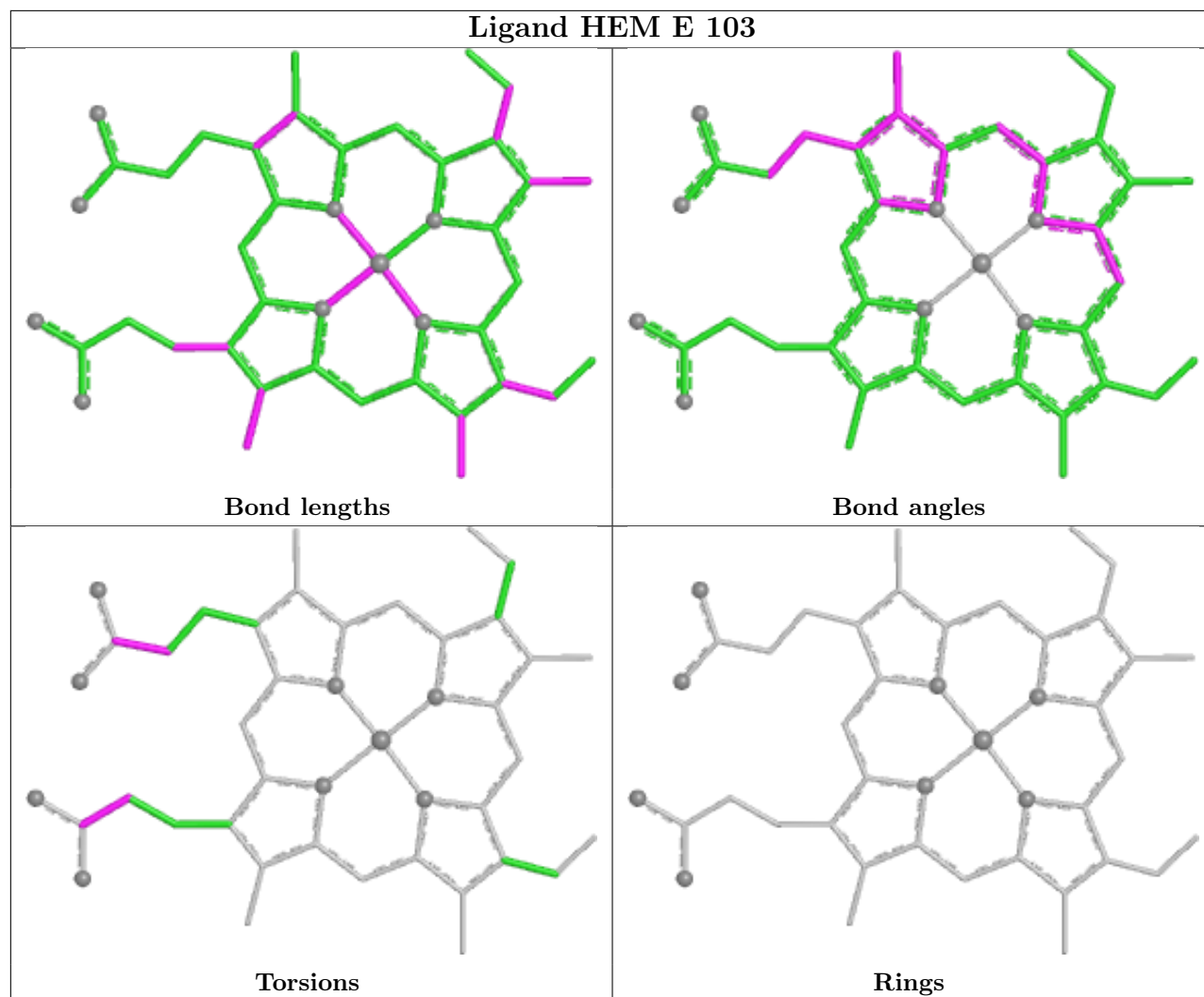


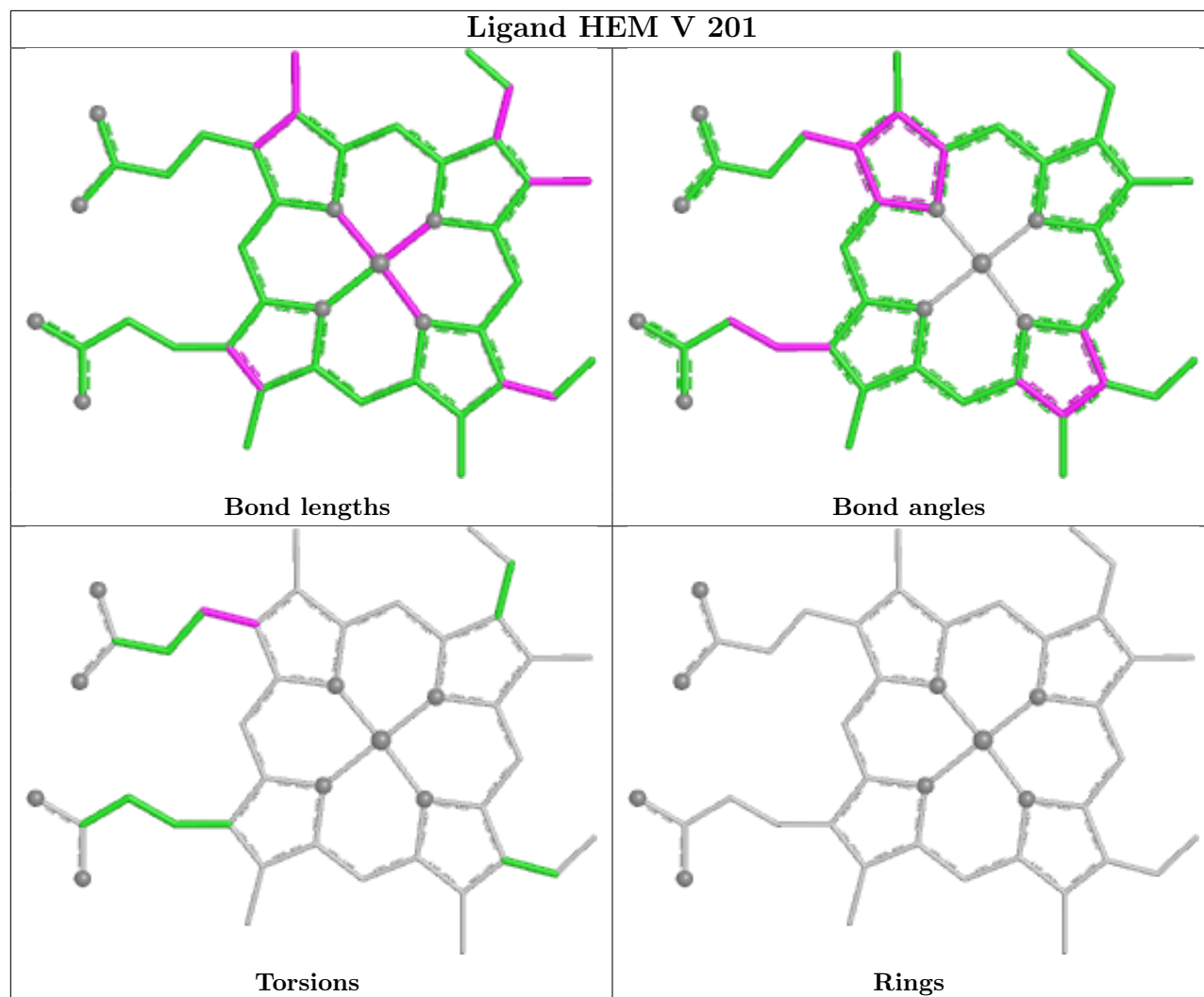


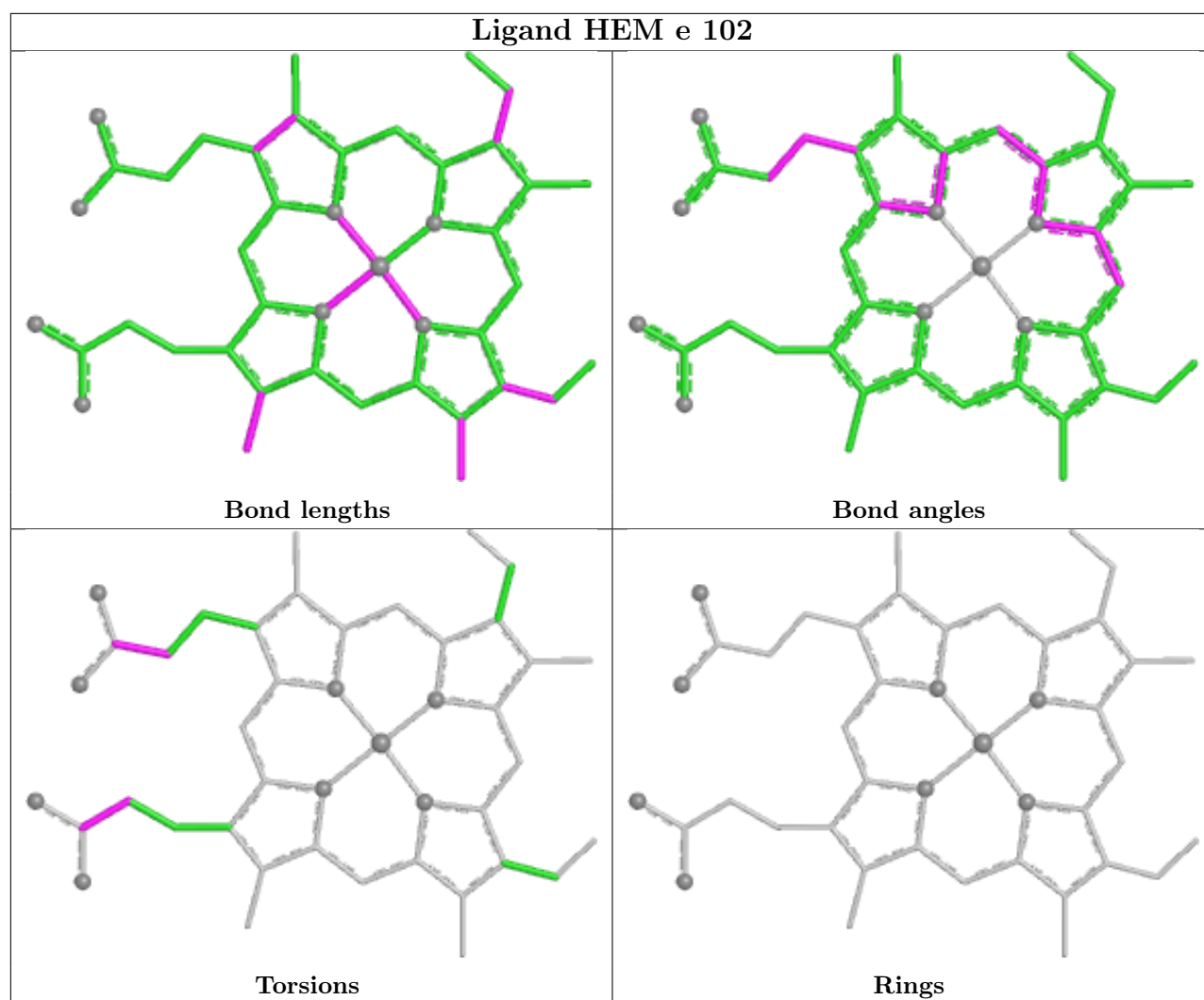


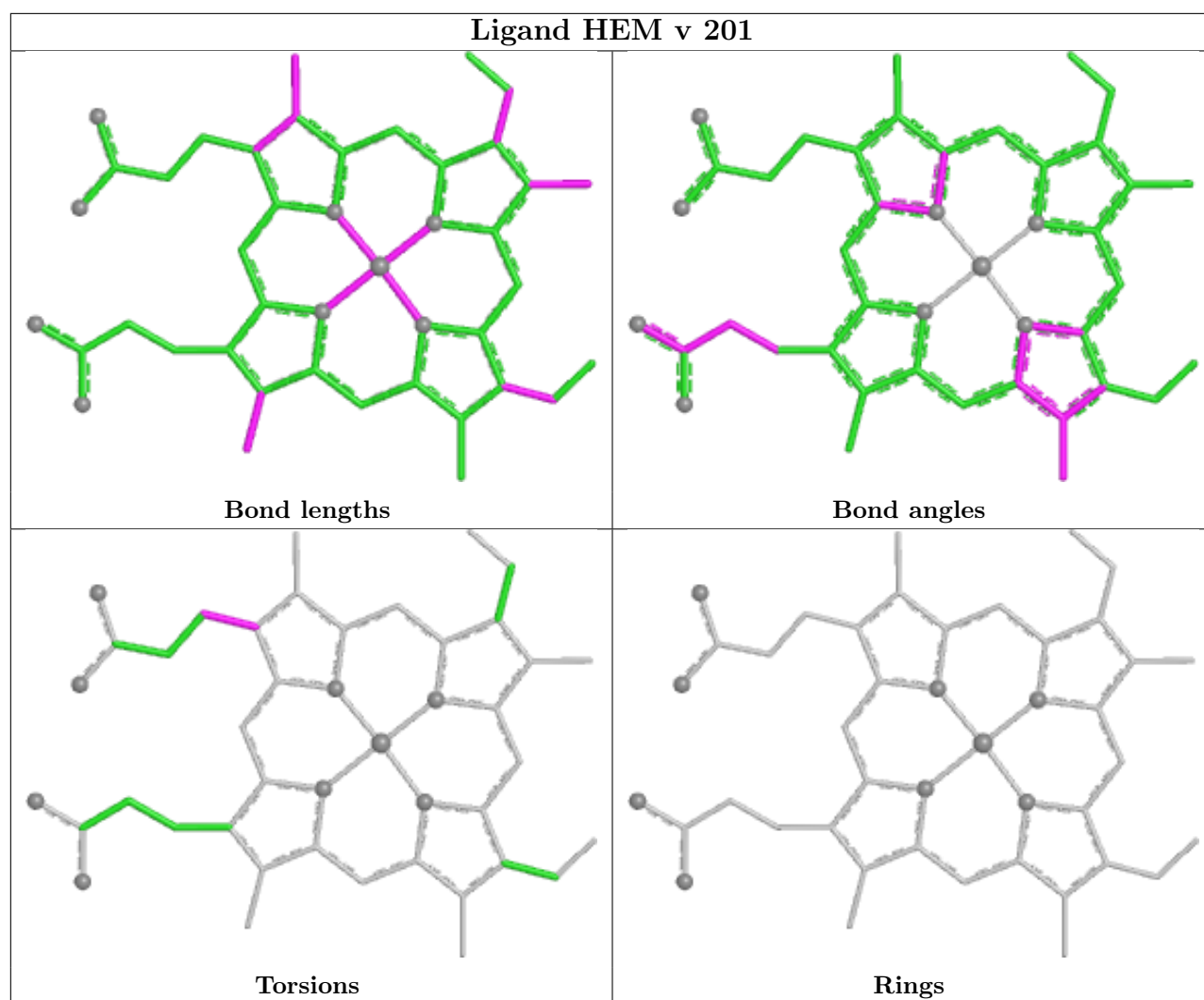












3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data [i](#)

4.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	1.45	69 (20%) 2 3	39, 63, 84, 93	4 (1%)
1	a	334/334 (100%)	1.74	110 (32%) 1 1	52, 84, 104, 114	4 (1%)
2	B	504/504 (100%)	1.29	96 (19%) 3 3	41, 68, 89, 111	10 (1%)
2	b	504/504 (100%)	1.73	160 (31%) 1 1	53, 88, 110, 131	10 (1%)
3	C	451/451 (100%)	1.31	89 (19%) 3 3	43, 72, 84, 97	5 (1%)
3	c	451/451 (100%)	1.74	154 (34%) 1 1	57, 92, 105, 118	5 (1%)
4	D	342/342 (100%)	1.32	71 (20%) 2 3	57, 64, 80, 102	0
4	d	342/342 (100%)	1.72	111 (32%) 1 1	78, 85, 101, 123	0
5	E	81/81 (100%)	1.53	20 (24%) 2 2	47, 80, 98, 104	2 (2%)
5	e	81/81 (100%)	1.93	37 (45%) 0 1	61, 101, 119, 125	2 (2%)
6	F	34/34 (100%)	1.39	6 (17%) 4 4	68, 74, 99, 102	0
6	f	34/34 (100%)	1.62	11 (32%) 1 1	89, 95, 120, 122	0
7	H	65/65 (100%)	1.43	16 (24%) 2 2	43, 74, 81, 99	2 (3%)
7	h	65/65 (100%)	1.99	25 (38%) 1 1	55, 95, 101, 120	2 (3%)
8	I	38/38 (100%)	1.76	13 (34%) 1 1	36, 74, 105, 109	1 (2%)
8	i	38/38 (100%)	2.13	16 (42%) 0 1	45, 95, 126, 130	1 (2%)
9	J	38/38 (100%)	1.65	9 (23%) 2 2	66, 78, 109, 112	0
9	j	38/38 (100%)	1.83	14 (36%) 1 1	87, 99, 129, 133	0
10	K	37/37 (100%)	1.06	3 (8%) 18 12	74, 79, 86, 88	0
10	k	37/37 (100%)	1.87	11 (29%) 1 1	94, 100, 107, 108	0
11	L	37/37 (100%)	1.34	8 (21%) 2 3	37, 62, 90, 99	1 (2%)
11	l	37/37 (100%)	1.76	12 (32%) 1 1	49, 83, 111, 120	1 (2%)
12	M	34/34 (100%)	1.66	10 (29%) 1 1	39, 64, 77, 93	1 (2%)
12	m	34/34 (100%)	2.36	12 (35%) 1 1	51, 84, 98, 114	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/243 (100%)	1.42	56 (23%) 2 2	40, 73, 95, 111	4 (1%)
13	o	243/243 (100%)	1.98	95 (39%) 1 1	53, 94, 116, 132	4 (1%)
14	T	30/30 (100%)	1.08	4 (13%) 7 6	32, 64, 85, 93	2 (6%)
14	t	30/30 (100%)	1.72	7 (23%) 2 2	43, 84, 105, 114	2 (6%)
15	U	97/97 (100%)	1.17	15 (15%) 5 5	64, 71, 89, 90	0
15	u	97/97 (100%)	1.64	30 (30%) 1 1	84, 92, 110, 111	0
16	V	137/137 (100%)	1.24	28 (20%) 3 3	39, 69, 80, 88	1 (0%)
16	v	137/137 (100%)	1.53	36 (26%) 1 2	51, 89, 101, 109	1 (0%)
17	Y	29/29 (100%)	1.43	7 (24%) 2 2	82, 89, 115, 118	0
17	y	29/29 (100%)	1.95	11 (37%) 1 1	103, 110, 136, 138	0
18	X	39/39 (100%)	1.32	6 (15%) 5 5	48, 80, 107, 108	1 (2%)
18	x	39/39 (100%)	1.71	11 (28%) 1 1	61, 101, 127, 129	1 (2%)
19	Z	62/62 (100%)	1.50	18 (29%) 1 1	80, 89, 109, 112	0
19	z	62/62 (100%)	2.04	29 (46%) 0 1	101, 110, 129, 133	0
All	All	5264/5264 (100%)	1.57	1436 (27%) 1 2	32, 83, 107, 138	68 (1%)

All (1436) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	d	11	GLU	12.1
12	m	5	GLN	11.3
8	i	38	GLU	10.2
2	b	485	GLU	10.0
9	j	3	SER	8.4
9	J	4	GLU	8.2
2	b	492	GLU	8.1
13	O	207	ARG	8.1
3	c	23	ALA	7.9
12	M	5	GLN	7.8
2	B	505	ARG	7.7
12	m	33	GLN	7.7
6	f	12	SER	7.6
13	o	55	GLU	7.6
18	x	40	SER	7.4
11	l	1	MET	7.3
3	c	201	ASN	7.3
1	A	13	LEU	7.2

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Mol	Chain	Res	Type	RSRZ
2	b	121	GLU	7.2
3	C	454	GLY	7.1
12	M	33	GLN	7.0
14	t	28	ARG	6.9
13	o	163	GLY	6.9
3	c	183	GLY	6.9
1	a	296	ASN	6.9
12	m	2	GLU	6.8
11	l	2	GLU	6.5
4	d	98	GLN	6.5
19	Z	35	ARG	6.4
3	c	135	ARG	6.3
15	u	101	GLY	6.3
7	H	2	ALA	6.3
4	D	11	GLU	6.2
9	j	7	ARG	6.2
3	c	293	ASN	6.2
3	c	44	ASN	6.2
10	k	46	ARG	6.2
9	J	3	SER	6.1
2	b	505	ARG	6.1
13	o	57	LYS	6.1
3	C	135	ARG	6.0
1	a	138	GLY	6.0
7	h	63[A]	LYS	5.9
12	m	30	GLU	5.9
3	C	266	TRP	5.9
2	b	83	GLU	5.9
3	c	153	ASP	5.9
13	o	62	GLU	5.7
13	o	98	GLU	5.7
10	k	10	LYS	5.7
13	o	64	GLU	5.7
7	h	26	GLY	5.5
2	b	387	GLU	5.5
18	x	38	GLN	5.5
17	y	42	ARG	5.5
6	F	12	SER	5.5
1	a	12	ASN	5.4
12	M	34	LYS	5.4
5	e	82	GLN	5.4
18	X	38	GLN	5.4

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Mol	Chain	Res	Type	RSRZ
11	L	2	GLU	5.4
7	h	66	GLY	5.4
1	A	19	ASN	5.3
19	z	2	THR	5.3
5	E	60	GLN	5.3
8	I	34	ARG	5.3
13	o	60	ARG	5.3
4	d	217	THR	5.3
15	u	70	ARG	5.2
3	C	267	SER	5.2
4	D	251	ARG	5.2
2	B	497	GLN	5.1
1	A	170	ASP	5.1
19	Z	34	ASP	5.1
13	O	163	GLY	5.1
2	b	130[A]	GLU	5.1
3	c	262	ARG	5.1
3	c	184	GLY	5.0
7	H	26	GLY	5.0
7	H	65	LEU	5.0
4	D	172	SER	5.0
5	e	54[A]	SER	5.0
3	c	338	GLY	4.9
1	a	337	HIS	4.9
8	i	27	ASP	4.9
16	v	77	LYS	4.9
19	z	30	PRO	4.9
2	b	124	ARG	4.9
17	y	41	VAL	4.9
4	d	141	TYR	4.9
3	C	417	VAL	4.8
5	E	12	ASP	4.8
2	b	490	GLN	4.8
13	O	64	GLU	4.8
2	b	443	PHE	4.8
12	m	32	GLN	4.8
3	C	201	ASN	4.8
2	b	70	GLY	4.8
1	A	242	GLU	4.8
18	x	39	ARG	4.7
4	D	227	GLU	4.7
16	v	6	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
10	K	10	LYS	4.7
13	o	4	THR	4.7
2	B	14	ASN	4.7
3	c	129	GLY	4.7
3	c	200	THR	4.7
3	c	128	GLY	4.7
1	A	266	ASN	4.7
17	y	19	ILE	4.7
5	e	61	ARG	4.6
4	d	318	ASN	4.6
1	a	229	GLU	4.6
2	b	226	TYR	4.6
16	V	34	GLN	4.6
13	o	161	GLY	4.6
3	C	23	ALA	4.6
3	c	458	GLY	4.6
13	o	222	ASP	4.6
1	a	19	ASN	4.6
1	a	266	ASN	4.6
12	m	31	SER	4.6
13	o	173	ALA	4.6
13	o	58	ASN	4.6
2	B	259	GLY	4.6
13	o	56	PRO	4.6
1	a	139	MET	4.6
13	o	54	GLU	4.5
1	a	105	TRP	4.5
2	b	322	GLY	4.5
5	e	6	GLY	4.5
19	z	3	ILE	4.5
8	i	35	LYS	4.5
4	d	234	ALA	4.5
4	d	332	GLN	4.5
2	b	129	GLY	4.5
3	C	131	TYR	4.5
2	B	387	GLU	4.5
13	O	57	LYS	4.5
11	l	7	ARG	4.5
2	B	328	GLY	4.4
1	A	243	GLU	4.4
2	B	495	PHE	4.4
2	b	167	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
2	b	224	ARG	4.4
2	b	302	TRP	4.4
15	u	37	GLN	4.4
3	c	74	HIS	4.4
5	e	41	GLY	4.4
9	J	5	GLY	4.4
1	A	191	ASN	4.4
19	Z	27	TYR	4.4
4	d	12	ARG	4.4
2	B	188	ASP	4.4
1	a	262	TYR	4.3
4	d	337	GLU	4.3
1	A	12	ASN	4.3
3	C	145[A]	SER	4.3
13	O	59	LYS	4.3
3	c	159	THR	4.3
1	a	243	GLU	4.3
7	h	57	GLY	4.3
3	c	53	HIS	4.3
2	B	485	GLU	4.3
8	i	2	GLU	4.3
1	a	140	ARG	4.3
6	F	44	GLN	4.2
2	B	127	ARG	4.2
14	T	28	ARG	4.2
3	c	102	GLY	4.2
2	b	476	ARG	4.2
13	o	207	ARG	4.2
4	D	71	CYS	4.2
4	d	295	SER	4.2
8	I	25	SER	4.2
2	b	87	ASP	4.2
11	l	4	ASN	4.2
19	z	34	ASP	4.2
13	o	84	GLU	4.2
9	j	4	GLU	4.2
2	B	393	GLU	4.2
2	b	497	GLN	4.2
16	V	6	GLU	4.2
1	a	221[A]	SER	4.1
3	C	451	ALA	4.1
3	c	302	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
2	b	171	PRO	4.1
3	c	292	PHE	4.1
11	L	1	MET	4.1
3	c	24	THR	4.1
13	o	39	ARG	4.1
1	a	302	PHE	4.1
10	k	43	VAL	4.1
13	o	139	SER	4.1
1	a	11	ALA	4.1
2	b	493	TRP	4.1
5	e	77	GLU	4.1
8	I	2	GLU	4.1
4	d	174	GLY	4.1
4	D	95	PRO	4.1
11	l	3	PRO	4.1
2	b	268	PHE	4.0
2	b	489	GLU	4.0
13	O	55	GLU	4.0
15	u	77	GLU	4.0
16	v	85	GLU	4.0
7	H	66	GLY	4.0
7	h	65	LEU	4.0
4	D	19	ASP	4.0
13	o	25	THR	4.0
13	o	132	ASN	4.0
5	E	18	ARG	4.0
7	h	4	ARG	4.0
4	d	54	PHE	4.0
4	d	71	CYS	4.0
7	h	2	ALA	4.0
13	O	29	ALA	4.0
13	o	27	ARG	4.0
1	a	236	GLY	3.9
1	A	296	ASN	3.9
3	c	163	PHE	3.9
3	c	194	GLY	3.9
5	e	59	GLU	3.9
16	v	90	GLU	3.9
2	b	386	ALA	3.9
4	d	27	PHE	3.9
4	d	172	SER	3.9
15	U	15	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
13	O	241	ALA	3.9
15	u	102	LEU	3.9
13	O	74[A]	GLU	3.9
5	e	84	LYS	3.9
7	H	63[A]	LYS	3.9
5	e	83	LEU	3.9
7	h	15	ASN	3.9
9	J	7	ARG	3.8
8	I	28	PRO	3.8
1	a	90	GLY	3.8
1	a	230	THR	3.8
3	c	297	TYR	3.8
8	I	38	GLU	3.8
1	A	61	ASP	3.8
2	b	59	GLY	3.8
3	c	261	ARG	3.8
1	a	190	HIS	3.8
3	c	342	MET	3.8
2	b	435[A]	GLU	3.8
3	c	473	ASP	3.8
15	u	8	GLU	3.8
2	b	218	LEU	3.8
3	c	373	ASN	3.8
13	o	155	ASN	3.8
2	B	357	ARG	3.8
17	y	43	ARG	3.8
19	z	35	ARG	3.8
2	B	134	ASP	3.8
4	D	131	GLU	3.8
13	o	86	LYS	3.8
5	e	18	ARG	3.8
13	o	189	ARG	3.8
2	b	330	MET	3.8
1	a	170	ASP	3.8
2	b	190	PHE	3.7
2	b	405[A]	GLU	3.7
8	I	32	PRO	3.7
16	v	118	HIS	3.7
2	b	137	LYS	3.7
2	b	373	LYS	3.7
13	o	53	LYS	3.7
14	t	30	THR	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	492	GLU	3.7
9	j	9	PRO	3.7
4	d	323	GLU	3.7
15	u	24	LYS	3.7
3	c	25	ASN	3.7
3	c	192	GLY	3.7
9	j	6	GLY	3.7
13	o	184	ARG	3.7
4	D	255	GLN	3.7
13	o	202	ALA	3.7
3	C	200	THR	3.7
3	c	347	GLY	3.7
2	b	144	PHE	3.7
3	c	456	GLU	3.7
13	o	21	THR	3.6
12	m	1	MET	3.6
19	z	4	LEU	3.6
3	c	417	VAL	3.6
4	d	233	ARG	3.6
16	V	31	ARG	3.6
13	o	69	LYS	3.6
2	B	282	GLN	3.6
3	c	34	ALA	3.6
4	d	64	ALA	3.6
4	d	297	ASP	3.6
13	o	191	SER	3.6
1	A	171	GLY	3.6
3	c	85	GLY	3.6
12	m	34	LYS	3.6
3	c	415	ASN	3.6
1	a	235	TYR	3.6
2	b	494	GLY	3.6
17	Y	19	ILE	3.6
2	B	226	TYR	3.6
5	E	55	TYR	3.6
13	o	181	GLU	3.6
8	I	24	LEU	3.6
2	b	232	GLY	3.6
13	O	213	GLY	3.6
5	e	60	GLN	3.5
13	o	59	LYS	3.5
1	a	242	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
13	o	97	GLU	3.5
13	o	151	TYR	3.5
15	U	86	GLU	3.5
2	b	333	GLY	3.5
1	A	304	HIS	3.5
3	C	229	ASN	3.5
7	h	20	LYS	3.5
1	A	262	TYR	3.5
3	c	186	TYR	3.5
4	D	59	TYR	3.5
19	z	26	ALA	3.5
4	d	206	GLY	3.5
1	A	108	ASN	3.5
16	v	24	LYS	3.5
4	d	186	GLN	3.5
3	c	193	GLY	3.5
4	d	237	PRO	3.5
3	C	70	PHE	3.5
2	b	111	ALA	3.5
2	b	279	TYR	3.5
7	H	64	ALA	3.5
2	B	2	GLY	3.5
2	B	396	GLY	3.5
4	d	338	ASN	3.5
1	A	17	PHE	3.5
3	C	29	GLU	3.5
2	b	480	SER	3.5
5	e	74	GLN	3.5
11	l	14	ARG	3.5
3	C	44	ASN	3.5
4	d	336	HIS	3.5
3	c	269	GLU	3.4
1	a	109	GLY	3.4
2	b	169	SER	3.4
13	O	209	GLY	3.4
2	B	7	ARG	3.4
3	c	357	ARG	3.4
1	a	335	ASN	3.4
4	d	223	PHE	3.4
17	Y	45	ASN	3.4
7	H	18	TYR	3.4
16	V	75	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
13	o	114	GLU	3.4
1	A	74	GLY	3.4
1	a	234	ASN	3.4
12	M	4	ASN	3.4
16	v	106	ASN	3.4
16	v	60	ALA	3.4
3	c	26	ARG	3.4
7	H	56	ASP	3.4
15	U	37	GLN	3.4
2	b	77	GLY	3.4
4	d	226	GLY	3.4
4	d	258	GLY	3.4
9	J	6	GLY	3.4
13	o	190	PHE	3.4
13	o	244	GLU	3.4
16	v	132	GLY	3.4
3	c	188	THR	3.4
3	c	294	ASN	3.4
14	t	22	PHE	3.4
1	A	240	GLY	3.3
2	b	350	GLU	3.3
13	o	46	GLN	3.3
13	o	61	GLN	3.3
4	D	252	PHE	3.3
7	h	51	SER	3.3
13	O	203	LYS	3.3
2	b	500	GLY	3.3
5	E	84	LYS	3.3
13	o	65	PHE	3.3
16	V	24	LYS	3.3
1	a	222	SER	3.3
3	c	155	ASN	3.3
5	E	61	ARG	3.3
2	b	441	GLY	3.3
2	B	83	GLU	3.3
1	a	61	ASP	3.3
2	b	212	ALA	3.3
1	a	320	ILE	3.3
16	v	100	ILE	3.3
2	b	193	TYR	3.3
5	e	55	TYR	3.3
3	C	300	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
19	z	1	MET	3.3
2	b	349	LYS	3.3
1	a	141	PRO	3.3
1	a	294	ALA	3.3
1	a	314	ILE	3.3
16	v	66	ARG	3.3
4	d	65	SER	3.3
1	A	166	GLY	3.3
13	O	237	GLY	3.3
13	o	112	GLY	3.3
2	B	114	HIS	3.3
3	c	359	TRP	3.3
7	h	21	VAL	3.3
13	O	61	GLN	3.3
16	v	34	GLN	3.3
17	Y	21	GLN	3.3
9	j	38	SER	3.2
13	o	34	SER	3.2
2	b	14	ASN	3.2
1	a	15	GLU	3.2
5	e	7	GLU	3.2
13	o	179	GLU	3.2
5	e	42	LEU	3.2
19	z	29	SER	3.2
3	c	126	GLY	3.2
18	X	2	THR	3.2
2	b	40	TYR	3.2
2	b	123	PHE	3.2
1	a	304	HIS	3.2
16	v	1	ALA	3.2
1	A	246	TYR	3.2
13	O	54	GLU	3.2
19	Z	4	LEU	3.2
4	D	70	GLY	3.2
2	b	363	PHE	3.2
3	C	87	ILE	3.2
13	o	186	ASN	3.2
1	A	257	ARG	3.2
3	C	271	TYR	3.2
3	c	138	GLU	3.2
5	E	17	VAL	3.2
10	k	42	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
13	O	139	SER	3.2
4	D	189	HIS	3.2
19	z	57	LEU	3.2
2	B	426	PHE	3.2
4	d	31	GLY	3.2
5	e	81	GLU	3.2
13	o	18	LYS	3.2
4	D	27	PHE	3.1
6	F	16	PHE	3.1
2	b	262	THR	3.1
17	y	45	ASN	3.1
3	c	215	LYS	3.1
16	v	110	LYS	3.1
2	B	266	GLU	3.1
4	d	25	ASP	3.1
7	h	64	ALA	3.1
19	z	8	ALA	3.1
5	E	9	PRO	3.1
1	A	182	PHE	3.1
3	C	134	ILE	3.1
3	c	132	HIS	3.1
8	i	30	ARG	3.1
13	O	82	GLN	3.1
3	C	418	ASN	3.1
16	V	26	TYR	3.1
19	Z	62	VAL	3.1
1	a	103	ASP	3.1
19	Z	32	ASP	3.1
2	b	425	ILE	3.1
4	D	24	ARG	3.1
15	u	76	ARG	3.1
13	o	130	GLN	3.1
17	y	21	GLN	3.1
1	a	317	TRP	3.1
2	B	493	TRP	3.1
1	A	11	ALA	3.1
3	C	142	GLU	3.1
2	b	46	ASP	3.1
3	c	288	CYS	3.1
13	o	8	ASP	3.1
19	z	14	ILE	3.1
2	b	264	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	73	PHE	3.1
1	a	74	GLY	3.1
19	Z	31	GLN	3.1
4	D	292	ASN	3.1
13	o	35	SER	3.1
2	b	64	PRO	3.1
5	e	12	ASP	3.1
8	i	34	ARG	3.1
10	k	19	ASP	3.1
3	c	398	HIS	3.1
1	a	306	VAL	3.1
2	B	130[A]	GLU	3.1
16	v	15	GLU	3.1
16	v	70	GLU	3.1
2	b	422	ARG	3.1
3	c	180	MET	3.1
19	z	52	LEU	3.1
1	A	190	HIS	3.1
2	b	282	GLN	3.0
1	A	222	SER	3.0
4	d	165	SER	3.0
13	o	221	SER	3.0
16	V	121	VAL	3.0
3	c	411	ALA	3.0
2	b	496	TYR	3.0
4	d	142	ASN	3.0
16	v	17	LYS	3.0
4	d	219	GLU	3.0
4	d	304	ARG	3.0
4	D	309	PRO	3.0
2	B	70	GLY	3.0
7	H	57	GLY	3.0
13	O	4	THR	3.0
4	d	87	HIS	3.0
1	A	87	ASN	3.0
1	a	191	ASN	3.0
2	b	18	ARG	3.0
13	O	60	ARG	3.0
4	d	242	GLU	3.0
6	F	14	PRO	3.0
1	A	256	GLY	3.0
1	A	299	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
3	c	360	ASP	3.0
19	Z	2	THR	3.0
1	a	257	ARG	3.0
2	B	476	ARG	3.0
1	a	254	TYR	3.0
7	h	18	TYR	3.0
1	a	65	GLU	3.0
4	d	171	PRO	3.0
8	i	33	LYS	3.0
1	a	13	LEU	3.0
3	C	263	ALA	3.0
3	C	26	ARG	3.0
1	a	247	ASN	3.0
3	C	186	TYR	3.0
4	d	59	TYR	3.0
4	d	350	ASN	3.0
13	o	200	ASN	3.0
3	C	389	GLU	3.0
4	d	312	GLU	3.0
14	t	2	GLU	3.0
4	D	140	PRO	3.0
8	i	28	PRO	3.0
2	B	341	LYS	3.0
14	t	29	ILE	3.0
10	k	44	GLY	3.0
2	b	483	ASP	3.0
3	c	107	ASP	3.0
3	C	151	TRP	3.0
13	o	178	LYS	3.0
17	y	25	ILE	3.0
3	C	268	GLY	3.0
2	b	84	THR	3.0
15	u	39	ARG	3.0
1	a	319	ASP	3.0
1	a	108	ASN	2.9
13	o	88	ASN	2.9
5	e	52	PRO	2.9
16	V	15	GLU	2.9
16	v	57	GLU	2.9
3	c	63	TRP	2.9
4	D	328	TRP	2.9
3	C	146	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
3	c	109	PHE	2.9
4	D	56	THR	2.9
13	o	166	SER	2.9
4	d	20	ASP	2.9
8	i	36	ASP	2.9
4	d	184	PHE	2.9
1	A	312	ASN	2.9
1	a	339	PHE	2.9
2	B	183	PRO	2.9
3	c	127	PHE	2.9
3	c	221	GLU	2.9
4	D	69	GLU	2.9
5	e	10	PHE	2.9
3	c	449	ARG	2.9
7	H	3	ARG	2.9
6	f	44	GLN	2.9
3	C	52	ALA	2.9
2	B	325	PHE	2.9
2	b	93	PHE	2.9
4	D	314	PHE	2.9
2	b	191	ASN	2.9
13	O	62	GLU	2.9
1	a	16	ARG	2.9
13	O	27	ARG	2.9
2	B	499	VAL	2.9
4	D	295	SER	2.9
13	o	11	VAL	2.9
13	O	26	ALA	2.9
1	A	125	CYS	2.9
2	b	267	LEU	2.9
1	a	303	ASN	2.9
2	B	488	PRO	2.9
3	c	149	TYR	2.9
9	J	9	PRO	2.9
11	L	5	PRO	2.9
2	b	307	GLU	2.9
4	D	241	GLU	2.9
4	d	307	GLU	2.9
16	v	31	ARG	2.9
1	A	86	SER	2.9
1	a	240	GLY	2.9
3	C	215	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	6	GLY	2.9
18	X	36	LYS	2.9
2	B	167	TRP	2.9
2	b	503	THR	2.9
1	A	344	ALA	2.9
1	A	16	ARG	2.9
19	z	27	TYR	2.9
15	u	63	ASN	2.9
3	C	347	GLY	2.8
18	X	33	GLN	2.8
2	b	5	TRP	2.8
13	O	127	ALA	2.8
3	C	149	TYR	2.8
4	d	42	TYR	2.8
1	a	241	GLN	2.8
3	c	306	GLY	2.8
13	o	28	GLY	2.8
15	u	18	GLY	2.8
16	v	84	GLY	2.8
4	D	234	ALA	2.8
3	C	423	ARG	2.8
3	c	340	TYR	2.8
15	u	54	PRO	2.8
2	B	121	GLU	2.8
3	c	353	GLY	2.8
4	d	40	CYS	2.8
16	V	86	GLN	2.8
1	a	233	ALA	2.8
8	I	36	ASP	2.8
1	a	274	PHE	2.8
2	b	392	PHE	2.8
4	d	314	PHE	2.8
2	b	357	ARG	2.8
13	o	172	ILE	2.8
3	c	296	VAL	2.8
1	a	199	GLN	2.8
2	b	323	GLY	2.8
4	d	86	GLY	2.8
12	m	4	ASN	2.8
1	a	212	CYS	2.8
1	a	293	MET	2.8
2	B	443	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	396	MET	2.8
13	o	203	LYS	2.8
8	I	30	ARG	2.8
13	o	152	ARG	2.8
2	b	12	LEU	2.8
2	b	52	LEU	2.8
3	c	253	LEU	2.8
4	D	135	LEU	2.8
3	C	25	ASN	2.8
3	c	29	GLU	2.8
19	Z	38	GLN	2.8
3	C	342	MET	2.8
2	B	227	LYS	2.8
11	L	7	ARG	2.8
3	c	46	SER	2.8
2	B	117	TYR	2.8
1	a	261	GLN	2.8
3	c	229	ASN	2.8
3	c	300	GLU	2.8
4	d	203	GLY	2.8
4	D	338	ASN	2.8
13	o	41	ALA	2.8
1	a	269	ARG	2.7
16	V	55[A]	ARG	2.7
1	A	25	ASP	2.7
4	d	218	VAL	2.7
3	c	381	LYS	2.7
11	l	8	GLN	2.7
15	u	47	LYS	2.7
3	c	409	GLY	2.7
1	a	344	ALA	2.7
5	E	77	GLU	2.7
13	O	210	GLU	2.7
2	B	255	THR	2.7
7	h	12[A]	ARG	2.7
3	c	266	TRP	2.7
13	o	135	SER	2.7
2	B	93	PHE	2.7
2	B	432	PHE	2.7
2	b	139	PHE	2.7
4	d	246	MET	2.7
17	y	27	MET	2.7

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Mol	Chain	Res	Type	RSRZ
19	z	60	PHE	2.7
4	d	334	GLN	2.7
13	O	130	GLN	2.7
15	u	38	TYR	2.7
1	a	226	GLU	2.7
3	c	69	LEU	2.7
7	h	14	LEU	2.7
13	o	164	LEU	2.7
1	a	198	HIS	2.7
2	b	341	LYS	2.7
3	C	46	SER	2.7
13	O	242	SER	2.7
13	o	24	ASP	2.7
4	d	153	PHE	2.7
8	i	32	PRO	2.7
2	B	320	ALA	2.7
3	c	352	GLY	2.7
4	d	224	GLN	2.7
16	V	37	CYS	2.7
2	b	57	ARG	2.7
3	c	343	ARG	2.7
13	o	74[A]	GLU	2.7
4	D	83	ASN	2.7
3	c	468	SER	2.7
13	o	150	SER	2.7
16	v	83	ASP	2.7
2	b	161	LEU	2.7
4	d	309	PRO	2.7
2	b	448	ARG	2.7
3	c	131	TYR	2.7
6	f	13	TYR	2.7
9	j	5	GLY	2.7
3	c	78	GLU	2.7
13	o	49[A]	THR	2.7
15	u	11	ASN	2.7
2	B	8	VAL	2.7
2	B	490	GLN	2.7
2	b	49	ASP	2.7
16	v	74	ASP	2.7
17	Y	42	ARG	2.7
1	a	166	GLY	2.7
2	b	140	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	b	320	ALA	2.7
4	D	244	TYR	2.7
13	o	177	ALA	2.7
2	b	393	GLU	2.7
13	O	97	GLU	2.7
15	U	8	GLU	2.7
16	v	109	GLU	2.7
16	v	124	LYS	2.7
2	b	362	PHE	2.7
16	V	14	SER	2.7
16	v	94	SER	2.7
18	x	37	VAL	2.6
5	e	51	ARG	2.6
10	k	12	PRO	2.6
19	z	24	PRO	2.6
3	c	84	GLN	2.6
2	b	146	ALA	2.6
3	C	326	ALA	2.6
4	d	108	GLY	2.6
9	j	37	GLY	2.6
16	V	43	GLY	2.6
16	v	75	TYR	2.6
3	C	457	LYS	2.6
3	c	231	GLU	2.6
1	A	139	MET	2.6
1	A	293	MET	2.6
3	C	293	ASN	2.6
1	A	197	PHE	2.6
3	c	242	LEU	2.6
1	a	68	SER	2.6
16	v	55[A]	ARG	2.6
1	a	340	PRO	2.6
1	a	100	ALA	2.6
13	O	80	GLN	2.6
3	C	325	GLY	2.6
3	c	151	TRP	2.6
3	c	454	GLY	2.6
2	B	431[A]	GLU	2.6
3	c	462[A]	GLU	2.6
4	D	219	GLU	2.6
3	c	140	LEU	2.6
11	l	6	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
13	O	35	SER	2.6
3	c	390	ARG	2.6
2	B	484	PRO	2.6
3	c	339	LYS	2.6
13	o	194	LYS	2.6
4	D	206	GLY	2.6
4	d	216	ALA	2.6
4	d	56	THR	2.6
13	o	118	LEU	2.6
1	A	98	GLU	2.6
1	A	189	GLU	2.6
4	D	242	GLU	2.6
13	o	145	GLU	2.6
5	E	24	SER	2.6
5	e	24	SER	2.6
2	b	499	VAL	2.6
3	c	167	VAL	2.6
2	b	230	ARG	2.6
2	b	321	LYS	2.6
2	b	50	PRO	2.6
4	D	336	HIS	2.6
5	e	58	GLN	2.6
13	O	196	GLN	2.6
16	V	25	GLN	2.6
4	D	137	GLY	2.6
4	D	228	GLY	2.6
5	E	41	GLY	2.6
19	z	15	LEU	2.6
1	a	197	PHE	2.6
4	d	185	PHE	2.6
6	F	13	TYR	2.6
9	j	33	TYR	2.6
2	b	266	GLU	2.6
2	b	353	GLU	2.6
4	D	16	ASP	2.6
13	O	169	ASP	2.6
13	o	218	GLU	2.6
8	i	25	SER	2.6
13	O	186	ASN	2.6
15	u	28	ASN	2.6
3	c	41	ARG	2.6
10	K	46	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
13	O	18	LYS	2.6
3	c	465	PRO	2.6
1	a	208	GLY	2.6
2	B	6	TYR	2.6
3	c	94	THR	2.6
1	a	333	GLU	2.6
2	b	127	ARG	2.6
3	c	195	ASP	2.6
2	b	194	ASN	2.6
3	C	294	ASN	2.6
4	d	83	ASN	2.6
4	d	139	ARG	2.6
1	A	241	GLN	2.6
11	L	8	GLN	2.6
2	b	295	GLY	2.6
3	c	112	PHE	2.6
8	i	26	GLY	2.6
2	B	203	ILE	2.5
3	c	143	TYR	2.5
13	O	7	TYR	2.5
19	Z	33	TRP	2.5
1	a	86	SER	2.5
2	B	448	ARG	2.5
2	b	300	GLU	2.5
3	c	104	GLU	2.5
3	c	216	SER	2.5
4	d	69	GLU	2.5
4	d	310	GLU	2.5
5	e	11	SER	2.5
1	A	306	VAL	2.5
3	C	155	ASN	2.5
3	C	187	ASP	2.5
2	B	218	LEU	2.5
3	C	411	ALA	2.5
15	u	73	GLN	2.5
1	a	92	HIS	2.5
1	a	228	THR	2.5
8	I	6	ILE	2.5
16	V	82	TYR	2.5
16	v	26	TYR	2.5
16	v	47	LYS	2.5
1	a	142	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
16	V	39	SER	2.5
13	O	58	ASN	2.5
13	o	23	ASP	2.5
2	b	182	ALA	2.5
15	u	40	GLY	2.5
1	A	73	TYR	2.5
1	A	305	SER	2.5
1	a	161	TYR	2.5
3	C	357	ARG	2.5
3	c	212	TYR	2.5
1	A	229	GLU	2.5
1	A	317	TRP	2.5
2	b	168	VAL	2.5
3	c	337	LEU	2.5
3	c	365	TRP	2.5
4	d	241	GLU	2.5
12	M	30	GLU	2.5
6	f	16	PHE	2.5
6	f	42	PHE	2.5
2	B	131	PRO	2.5
1	a	110	GLY	2.5
2	b	82	GLY	2.5
5	e	32	ILE	2.5
15	u	94	GLY	2.5
16	V	44	GLY	2.5
17	Y	25	ILE	2.5
2	B	286	ARG	2.5
7	h	11	LEU	2.5
12	m	8	LEU	2.5
2	b	491	VAL	2.5
4	d	78	VAL	2.5
3	c	291	TRP	2.5
13	O	180	GLU	2.5
4	D	98	GLN	2.5
4	D	170	ALA	2.5
4	d	239	GLN	2.5
4	d	275	PRO	2.5
4	d	303	ILE	2.5
18	x	3	ILE	2.5
19	Z	6	GLN	2.5
19	z	28	ALA	2.5
19	z	31	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
5	e	28	PRO	2.5
2	b	2	GLY	2.5
1	a	137	LEU	2.5
3	c	68	THR	2.5
8	I	3	THR	2.5
8	i	24	LEU	2.5
2	b	48	SER	2.5
2	b	294	SER	2.5
3	c	421	SER	2.5
2	B	299	GLU	2.5
2	b	299	GLU	2.5
2	b	428	GLU	2.5
1	a	315	ASN	2.5
2	B	418	LYS	2.5
2	b	337	ALA	2.5
3	c	134	ILE	2.5
13	o	147	ASN	2.5
2	b	338	GLN	2.5
2	B	375	GLY	2.5
3	C	222	GLY	2.5
3	c	336	GLY	2.5
3	c	408	GLY	2.5
4	d	99	GLY	2.5
7	h	24	GLY	2.5
10	k	23	ASP	2.5
2	B	503	THR	2.5
7	h	52	THR	2.5
1	a	82	VAL	2.5
13	o	204	VAL	2.5
1	A	107	TYR	2.5
1	a	73	TYR	2.5
3	C	340	TYR	2.5
2	B	26	HIS	2.4
2	B	321	LYS	2.4
2	B	435[A]	GLU	2.4
2	b	389	LYS	2.4
13	O	84	GLU	2.4
15	u	29	ASN	2.4
1	a	150	PRO	2.4
2	b	484	PRO	2.4
1	a	299	GLY	2.4
2	B	322	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	408	GLY	2.4
3	C	371	GLY	2.4
4	D	118	GLY	2.4
2	B	48	SER	2.4
2	b	487	SER	2.4
5	E	49	THR	2.4
1	a	17	PHE	2.4
1	a	135	TYR	2.4
2	b	495	PHE	2.4
1	a	244	GLU	2.4
1	a	290	ILE	2.4
3	C	221	GLU	2.4
3	c	389	GLU	2.4
5	E	81	GLU	2.4
1	a	223	LEU	2.4
2	b	185	TRP	2.4
7	h	62	TRP	2.4
3	c	39	ASN	2.4
4	D	260	ALA	2.4
16	v	36	ALA	2.4
3	C	80	PRO	2.4
2	b	465	GLY	2.4
3	c	220	GLY	2.4
3	c	258	GLY	2.4
3	c	268	GLY	2.4
9	j	35	GLY	2.4
2	b	440	ASP	2.4
8	i	3	THR	2.4
15	U	24	LYS	2.4
16	v	35	TYR	2.4
13	O	114	GLU	2.4
13	o	16	ALA	2.4
17	y	31	ALA	2.4
4	D	263	ASN	2.4
19	Z	1	MET	2.4
3	C	65	GLY	2.4
3	C	336	GLY	2.4
4	d	137	GLY	2.4
1	a	79	THR	2.4
1	a	305	SER	2.4
18	x	36	LYS	2.4
1	A	280	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
17	y	18	VAL	2.4
2	B	477	ASP	2.4
15	u	103	TYR	2.4
4	D	211	CYS	2.4
2	b	114	HIS	2.4
5	e	71	GLU	2.4
7	H	47	GLU	2.4
11	l	11	GLU	2.4
3	c	197	ARG	2.4
2	B	58	GLN	2.4
6	f	39	ALA	2.4
3	c	228	ASN	2.4
4	d	194	ASN	2.4
5	e	20	TRP	2.4
5	e	50	PRO	2.4
11	l	5	PRO	2.4
16	V	13	ASN	2.4
2	B	308	LYS	2.4
15	U	66	GLY	2.4
2	b	278	SER	2.4
2	b	65	PHE	2.4
3	C	24	THR	2.4
3	c	70	PHE	2.4
13	O	208	THR	2.4
2	b	134	ASP	2.4
7	H	49	TYR	2.4
5	e	8	ARG	2.4
1	a	328	MET	2.4
2	b	261	ALA	2.4
2	b	275	TRP	2.4
2	b	374	ASN	2.4
3	C	415	ASN	2.4
3	c	304	PRO	2.4
4	D	258	GLY	2.4
3	c	301	PHE	2.4
4	d	245	SER	2.4
13	o	242	SER	2.4
1	a	50	ILE	2.4
3	c	439	VAL	2.4
13	o	208	THR	2.4
19	z	39	LEU	2.4
3	c	354	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	290	ALA	2.4
19	Z	26	ALA	2.4
2	b	58	GLN	2.3
3	C	98	GLY	2.3
3	C	344	SER	2.3
4	D	14	TRP	2.3
4	d	38	PHE	2.3
5	e	31	PHE	2.3
19	Z	55	GLY	2.3
19	z	47	TRP	2.3
5	e	4	THR	2.3
13	o	134	THR	2.3
1	a	136	ARG	2.3
2	B	390	TYR	2.3
3	C	82	TYR	2.3
2	B	119	ASP	2.3
1	A	65	GLU	2.3
1	a	231	GLU	2.3
3	C	83	GLU	2.3
5	e	9	PRO	2.3
9	j	8	ILE	2.3
11	L	3	PRO	2.3
13	o	220	LEU	2.3
15	U	91	LEU	2.3
16	v	41	HIS	2.3
1	A	181	ASN	2.3
2	B	323	GLY	2.3
3	c	51	GLY	2.3
3	c	226	SER	2.3
1	a	220	THR	2.3
6	f	18	VAL	2.3
18	x	4	THR	2.3
2	b	7	ARG	2.3
1	a	88	ALA	2.3
4	d	240	ALA	2.3
2	b	280	PHE	2.3
3	c	431	PHE	2.3
4	d	298	PHE	2.3
5	e	79	PHE	2.3
9	J	36	LEU	2.3
1	a	177	SER	2.3
2	b	73	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	b	88	PRO	2.3
3	c	136	GLY	2.3
3	c	424	SER	2.3
3	c	463	SER	2.3
4	d	55	VAL	2.3
13	O	96	VAL	2.3
5	E	4	THR	2.3
13	O	37	THR	2.3
4	d	264	LYS	2.3
3	C	395	TYR	2.3
12	m	26	TYR	2.3
4	D	168	PHE	2.3
4	d	210	LEU	2.3
19	Z	3	ILE	2.3
4	d	16	ASP	2.3
2	B	126	PRO	2.3
4	d	335	PRO	2.3
13	O	175	PRO	2.3
13	o	206	GLY	2.3
16	v	65	PRO	2.3
19	Z	24	PRO	2.3
3	C	74	HIS	2.3
4	d	61	HIS	2.3
4	d	75	THR	2.3
4	d	190	ASN	2.3
4	d	243	THR	2.3
4	d	292	ASN	2.3
7	H	15	ASN	2.3
3	c	323	LYS	2.3
19	z	37	LYS	2.3
3	C	230	LEU	2.3
4	d	211	CYS	2.3
2	B	496	TYR	2.3
3	c	37	ALA	2.3
4	d	296	TYR	2.3
10	k	45	PHE	2.3
16	V	1	ALA	2.3
1	a	130	GLN	2.3
4	D	20	ASP	2.3
4	d	175	VAL	2.3
15	u	66	GLY	2.3
19	z	62	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	b	498	LYS	2.3
13	o	188	LYS	2.3
19	Z	37	LYS	2.3
1	A	179	THR	2.3
2	b	53	ASN	2.3
2	b	285	ASN	2.3
2	b	286	ARG	2.3
4	D	80	THR	2.3
13	O	94	THR	2.3
2	b	56	TRP	2.3
3	C	365	TRP	2.3
16	v	27	LEU	2.3
1	a	206	PHE	2.3
1	a	265	PHE	2.3
9	j	22	ILE	2.3
1	A	235	TYR	2.3
2	b	110	ALA	2.3
2	b	204	ALA	2.3
4	D	332	GLN	2.3
13	o	176	GLN	2.3
4	d	227	GLU	2.3
4	d	230	SER	2.3
13	o	180	GLU	2.3
15	U	56	GLU	2.3
1	a	111	PRO	2.3
3	C	235	GLY	2.3
9	J	13	VAL	2.3
13	O	100	GLY	2.3
13	o	67	PRO	2.3
15	U	51	LYS	2.3
15	U	54	PRO	2.3
15	u	65	PRO	2.3
1	A	328	MET	2.3
2	B	272	ARG	2.3
2	b	188	ASP	2.3
2	b	385	ARG	2.3
13	O	42	ARG	2.3
1	A	72	LEU	2.2
7	h	53	LEU	2.2
4	d	32	TRP	2.2
3	C	147	PHE	2.2
11	l	36	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
12	m	21	PHE	2.2
19	z	59	PHE	2.2
1	a	263	ALA	2.2
8	I	5	LYS	2.2
12	M	31	SER	2.2
3	C	104	GLU	2.2
15	U	59	GLU	2.2
4	D	203	GLY	2.2
13	o	225	MET	2.2
4	D	25	ASP	2.2
13	o	9	ASP	2.2
13	o	141	ASP	2.2
1	a	186	PHE	2.2
2	B	479	PHE	2.2
4	d	29	PHE	2.2
2	b	301	ALA	2.2
4	d	229	ALA	2.2
13	o	171	ALA	2.2
13	o	246	ALA	2.2
19	z	10	ALA	2.2
1	A	187	GLN	2.2
1	a	246	TYR	2.2
3	C	302	TYR	2.2
13	O	176	GLN	2.2
16	V	47	LYS	2.2
2	B	405[A]	GLU	2.2
1	a	164	GLY	2.2
3	c	423	ARG	2.2
3	c	461	ARG	2.2
4	D	76	VAL	2.2
4	d	265	ARG	2.2
19	z	18	VAL	2.2
2	B	128	THR	2.2
4	D	75	THR	2.2
4	d	263	ASN	2.2
18	X	34	ILE	2.2
3	c	91	HIS	2.2
13	O	16	ALA	2.2
15	u	72	LYS	2.2
3	C	311	GLN	2.2
3	c	144	SER	2.2
3	C	261	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
16	V	135	VAL	2.2
1	A	62	GLY	2.2
2	b	206	GLY	2.2
3	c	100	GLY	2.2
10	k	20	PRO	2.2
13	O	12	GLY	2.2
4	D	132	ILE	2.2
17	y	35	ILE	2.2
2	b	469	HIS	2.2
4	d	317	LYS	2.2
1	a	251	ALA	2.2
2	b	379	ALA	2.2
4	d	14	TRP	2.2
6	f	20	TRP	2.2
2	b	409	GLN	2.2
3	C	299	SER	2.2
3	c	230	LEU	2.2
3	c	404	LEU	2.2
4	D	57	SER	2.2
5	e	16	SER	2.2
12	M	32	GLN	2.2
6	f	19	ARG	2.2
13	o	125	LEU	2.2
16	V	105	ARG	2.2
2	B	178	VAL	2.2
3	c	227	VAL	2.2
3	C	71	GLU	2.2
2	b	482	ILE	2.2
3	c	256	PRO	2.2
4	D	307	GLU	2.2
6	f	35	GLY	2.2
7	H	17	GLU	2.2
13	o	213	GLY	2.2
16	V	65	PRO	2.2
5	e	78	THR	2.2
18	x	10	PHE	2.2
2	B	349	LYS	2.2
16	V	110	LYS	2.2
1	a	338	ASN	2.2
3	c	378	ASN	2.2
4	D	72	ASN	2.2
4	d	220	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	380	ASP	2.2
3	C	195	ASP	2.2
3	c	392	ALA	2.2
9	j	32	ALA	2.2
1	A	14	TRP	2.2
1	a	268	SER	2.2
2	b	340	TRP	2.2
3	c	45	LEU	2.2
2	b	358	ARG	2.2
6	f	41	GLN	2.2
15	u	71	GLN	2.2
2	b	314	TYR	2.2
1	a	189	GLU	2.2
2	b	16	PRO	2.2
4	D	54	PHE	2.2
4	d	73	PHE	2.2
15	u	23	GLU	2.2
15	u	80	GLU	2.2
15	u	86	GLU	2.2
2	b	72	THR	2.2
3	C	346	THR	2.2
14	T	30	THR	2.2
2	b	138	MET	2.2
4	D	318	ASN	2.2
8	i	1[A]	MET	2.2
12	M	1	MET	2.2
1	A	54	ALA	2.1
15	u	46	ALA	2.1
16	V	38	ALA	2.1
2	B	100	HIS	2.1
2	B	384	ARG	2.1
4	D	79	SER	2.1
5	E	82	GLN	2.1
6	F	45	ARG	2.1
7	h	56	ASP	2.1
15	U	60	ASP	2.1
2	B	113	TRP	2.1
5	E	56	TYR	2.1
17	Y	18	VAL	2.1
1	A	155	PHE	2.1
3	C	247	GLY	2.1
3	c	77	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	331	PRO	2.1
13	O	53	LYS	2.1
13	O	69	LYS	2.1
13	O	112	GLY	2.1
3	c	346	THR	2.1
2	b	225	LEU	2.1
1	A	294	ALA	2.1
1	a	54	ALA	2.1
4	d	249	ALA	2.1
2	b	472	ARG	2.1
2	b	223[A]	GLN	2.1
1	a	25	ASP	2.1
2	B	491	VAL	2.1
19	z	48	ILE	2.1
3	C	97	TRP	2.1
3	C	259	TRP	2.1
1	a	237	TYR	2.1
1	A	340	PRO	2.1
3	C	458	GLY	2.1
3	c	137	PRO	2.1
4	D	174	GLY	2.1
4	D	200	GLY	2.1
13	O	28	GLY	2.1
15	U	22	GLY	2.1
2	B	428	GLU	2.1
7	h	17	GLU	2.1
2	b	55	MET	2.1
3	C	180	MET	2.1
3	c	185	LEU	2.1
7	h	30	LEU	2.1
9	j	40	LEU	2.1
1	a	286	ALA	2.1
2	B	194	ASN	2.1
4	D	77	ALA	2.1
4	D	294	ARG	2.1
7	H	12[A]	ARG	2.1
11	L	14	ARG	2.1
2	B	76[A]	SER	2.1
3	C	310	SER	2.1
4	D	166	SER	2.1
18	x	33	GLN	2.1
1	A	310	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	106	VAL	2.1
10	K	30	VAL	2.1
10	k	18	PHE	2.1
2	B	258	TYR	2.1
2	B	273	TYR	2.1
7	h	49	TYR	2.1
3	c	219	GLY	2.1
3	C	138	GLU	2.1
13	O	153	THR	2.1
3	C	370	ARG	2.1
14	t	24	ARG	2.1
4	D	119	ALA	2.1
14	T	20	ALA	2.1
11	L	6	ASN	2.1
19	z	6	GLN	2.1
3	C	62	PHE	2.1
14	t	10	PHE	2.1
3	C	237	HIS	2.1
2	B	232	GLY	2.1
3	c	103	GLY	2.1
4	d	58	TRP	2.1
16	v	44	GLY	2.1
2	B	330	MET	2.1
2	B	415	PRO	2.1
3	c	71	GLU	2.1
3	c	254	THR	2.1
16	v	80	THR	2.1
1	A	225	ARG	2.1
15	U	70	ARG	2.1
1	A	88	ALA	2.1
3	c	349	ILE	2.1
17	Y	20	ALA	2.1
2	b	36[A]	SER	2.1
2	B	247	PHE	2.1
2	B	392	PHE	2.1
2	b	438	ASN	2.1
5	E	74	GLN	2.1
16	V	49	ASN	2.1
3	C	439	VAL	2.1
1	A	252	HIS	2.1
2	B	4	PRO	2.1
2	b	313	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	225	ASP	2.1
4	d	167	TRP	2.1
1	a	227	THR	2.1
7	h	47	GLU	2.1
13	o	210	GLU	2.1
4	D	12	ARG	2.1
1	A	70	SER	2.1
2	B	228	ALA	2.1
2	b	310	ALA	2.1
3	c	299	SER	2.1
3	c	330	SER	2.1
4	d	84	SER	2.1
3	c	351	PHE	2.1
3	C	405	ASN	2.1
4	d	322	ASN	2.1
4	d	340	VAL	2.1
9	J	33	TYR	2.0
12	M	7	GLY	2.0
2	b	54	PRO	2.0
2	b	183	PRO	2.0
1	A	15	GLU	2.0
2	B	398	THR	2.0
3	C	150	ASP	2.0
4	d	53	THR	2.0
4	d	221	THR	2.0
13	O	86	LYS	2.0
13	o	232	GLU	2.0
15	u	69	GLU	2.0
18	x	31	ILE	2.0
1	A	324	ALA	2.0
3	c	471[A]	SER	2.0
19	Z	60	PHE	2.0
2	b	309	LEU	2.0
19	z	7	LEU	2.0
13	o	87	VAL	2.0
2	b	481	GLY	2.0
15	U	40	GLY	2.0
1	A	92	HIS	2.0
3	C	262	ARG	2.0
3	c	400	PRO	2.0
13	O	56	PRO	2.0
13	O	178	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
16	V	41	HIS	2.0
5	e	49	THR	2.0
14	T	4	ILE	2.0
3	c	141	GLU	2.0
4	d	302	GLU	2.0
1	A	167	SER	2.0
1	A	186	PHE	2.0
2	b	155	ALA	2.0
4	d	166	SER	2.0
4	d	261	PHE	2.0
4	d	341	PHE	2.0
8	i	17	LEU	2.0
16	V	12	LEU	2.0
18	x	32	SER	2.0
7	H	59	ASN	2.0
2	B	17	GLY	2.0
2	B	449	GLY	2.0
2	B	164	PRO	2.0
2	B	414	PRO	2.0
3	C	447	ARG	2.0
3	c	271	TYR	2.0
4	D	141	TYR	2.0
5	e	56	TYR	2.0
11	l	15	THR	2.0
4	D	257	PHE	2.0
5	E	59	GLU	2.0
12	M	2	GLU	2.0
5	E	16	SER	2.0
8	I	27	ASP	2.0
18	X	10	PHE	2.0
13	o	63	ALA	2.0
13	o	111	ALA	2.0

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

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

4.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

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4.4 Other polymers [i](#)

There are no such residues in this entry.