



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:08 PM UTC

PDB ID : 4FBY / pdb_00004fby
Title : fs X-ray diffraction of Photosystem II
Authors : Kern, J.; Alonso-Mori, R.; Hellmich, J.; Tran, R.; Hattne, J.; Laksmono, H.; Gloeckner, C.; Echols, N.; Sierra, R.G.; Sellberg, J.; Lassalle-Kaiser, B.; Gildea, R.J.; Glatzel, P.; Grosse-Kunstleve, R.W.; Latimer, M.J.; McQueen, T.A.; Difiore, D.; Fry, A.R.; Messerschmidt, M.M.; Miahnahri, A.; Schafer, D.W.; Seibert, M.M.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; White, W.E.; Adams, P.D.; Bogan, M.J.; Boutet, S.; Williams, G.J.; Messinger, J.; Sauter, N.K.; Zouni, A.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : 2012-05-23
Resolution : 6.56 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)

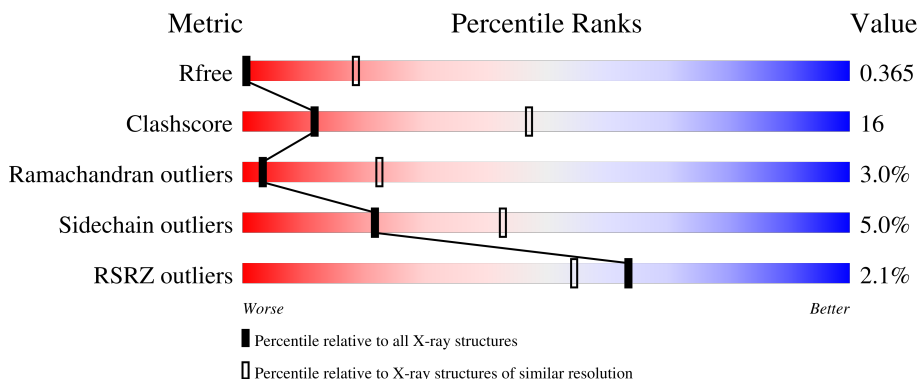
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.56 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	1162 (9.00-4.00)
Clashscore	190562	1000 (9.00-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	% 60% 34% ...
1	G	344	4% 59% 35% ..

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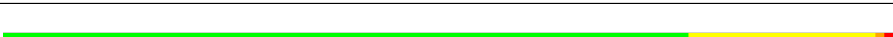
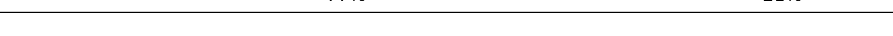
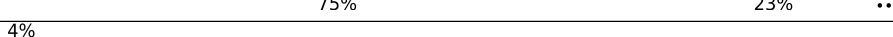
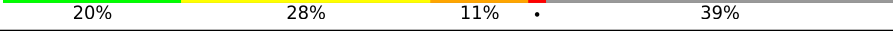
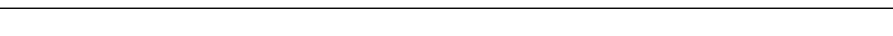
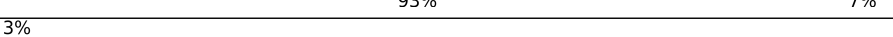
Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	B	510	
2	N	510	
3	C	461	
3	P	461	
4	D	352	
4	Q	352	
5	E	83	
5	R	83	
6	F	44	
6	S	44	
7	H	65	
7	W	65	
8	I	38	
8	a	38	
9	J	39	
9	b	39	
10	K	37	
10	c	37	
11	L	37	
11	d	37	
12	M	36	
12	e	36	
13	O	246	
13	f	246	
14	T	32	

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Mol	Chain	Length	Quality of chain
14	g	32	
15	U	104	
15	h	104	
16	V	137	
16	i	137	
17	m	46	
17	y	46	
18	X	40	
18	j	40	
19	Y	28	
19	k	28	
20	Z	62	
20	l	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	401	X	-	-	-
21	CLA	A	402	X	-	-	-
21	CLA	A	403	X	-	-	-
21	CLA	A	405	X	-	-	-
21	CLA	B	601	X	-	-	-
21	CLA	B	602	X	-	-	-
21	CLA	B	603	X	-	-	-
21	CLA	B	604	X	-	-	-
21	CLA	B	605	X	-	-	-
21	CLA	B	606	X	-	-	-
21	CLA	B	607	X	-	-	-
21	CLA	B	608	X	-	-	-
21	CLA	B	609	X	-	-	-
21	CLA	B	610	X	-	-	-
21	CLA	B	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	612	X	-	-	-
21	CLA	B	613	X	-	-	-
21	CLA	B	614	X	-	-	-
21	CLA	B	615	X	-	-	-
21	CLA	B	616	X	-	-	-
21	CLA	C	501	X	-	-	-
21	CLA	C	502	X	-	-	-
21	CLA	C	503	X	-	-	-
21	CLA	C	504	X	-	-	-
21	CLA	C	505	X	-	-	-
21	CLA	C	506	X	-	-	-
21	CLA	C	507	X	-	-	-
21	CLA	C	508	X	-	-	-
21	CLA	C	509	X	-	-	-
21	CLA	C	510	X	-	-	-
21	CLA	C	511	X	-	-	-
21	CLA	C	512	X	-	-	-
21	CLA	C	513	X	-	-	-
21	CLA	D	401	X	-	-	-
21	CLA	D	403	X	-	-	-
21	CLA	G	402	X	-	-	-
21	CLA	G	403	X	-	-	-
21	CLA	G	404	X	-	-	-
21	CLA	G	406	X	-	-	-
21	CLA	N	605	X	-	-	-
21	CLA	N	606	X	-	-	-
21	CLA	N	607	X	-	-	-
21	CLA	N	608	X	-	-	-
21	CLA	N	609	X	-	-	-
21	CLA	N	610	X	-	-	-
21	CLA	N	611	X	-	-	-
21	CLA	N	612	X	-	-	-
21	CLA	N	613	X	-	-	-
21	CLA	N	614	X	-	-	-
21	CLA	N	615	X	-	-	-
21	CLA	N	616	X	-	-	-
21	CLA	N	617	X	-	-	-
21	CLA	N	618	X	-	-	-
21	CLA	N	619	X	-	-	-
21	CLA	N	620	X	-	-	-
21	CLA	P	501	X	-	-	-
21	CLA	P	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	P	503	X	-	-	-
21	CLA	P	504	X	-	-	-
21	CLA	P	505	X	-	-	-
21	CLA	P	506	X	-	-	-
21	CLA	P	507	X	-	-	-
21	CLA	P	508	X	-	-	-
21	CLA	P	509	X	-	-	-
21	CLA	P	510	X	-	-	-
21	CLA	P	511	X	-	-	-
21	CLA	P	512	X	-	-	-
21	CLA	P	513	X	-	-	-
21	CLA	Q	402	X	-	-	-
21	CLA	Q	404	X	-	-	-
24	DGD	A	407	X	-	-	-
24	DGD	B	621	X	-	-	-
24	DGD	B	628	X	-	-	-
24	DGD	C	516	X	-	-	-
24	DGD	C	517	X	-	-	-
24	DGD	C	518	X	-	-	-
24	DGD	D	408	X	-	-	-
24	DGD	G	408	X	-	-	-
24	DGD	N	602	X	-	-	-
24	DGD	P	517	X	-	-	-
24	DGD	P	518	X	-	-	-
24	DGD	P	519	X	-	-	-
24	DGD	Q	409	X	-	-	-
24	DGD	W	102	X	-	-	-
27	LMG	A	410	X	-	-	-
27	LMG	B	622	X	-	-	-
27	LMG	B	623	X	-	-	-
27	LMG	C	519	X	-	-	-
27	LMG	C	520	X	-	-	-
27	LMG	D	406	X	-	-	-
27	LMG	D	407	X	-	-	-
27	LMG	D	412	X	-	-	-
27	LMG	E	102	X	-	-	-
27	LMG	G	411	X	-	-	-
27	LMG	I	102	X	-	-	-
27	LMG	M	101	X	-	-	-
27	LMG	N	622	X	-	-	-
27	LMG	N	623	X	-	-	-
27	LMG	P	520	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	P	521	X	-	-	-
27	LMG	Q	401	X	-	-	-
27	LMG	Q	406	X	-	-	-
27	LMG	Q	407	X	-	-	-
27	LMG	R	102	X	-	-	-
27	LMG	a	102	X	-	-	-
27	LMG	e	102	X	-	-	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	G	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	N	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	P	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	Q	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	R	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	S	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	W	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	a	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	b	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	c	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	d	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	e	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	f	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	g	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	h	97	Total	C	N	O	0	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	i	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	m	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O		0	0	0
			270	182	41	47				
18	j	37	Total	C	N	O		0	0	0
			270	182	41	47				

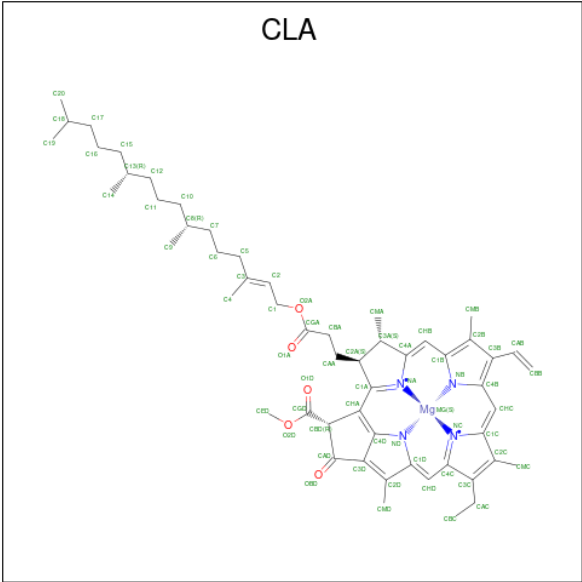
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	k	28	Total	C	N	O		0	0	0
			140	84	28	28				

- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	l	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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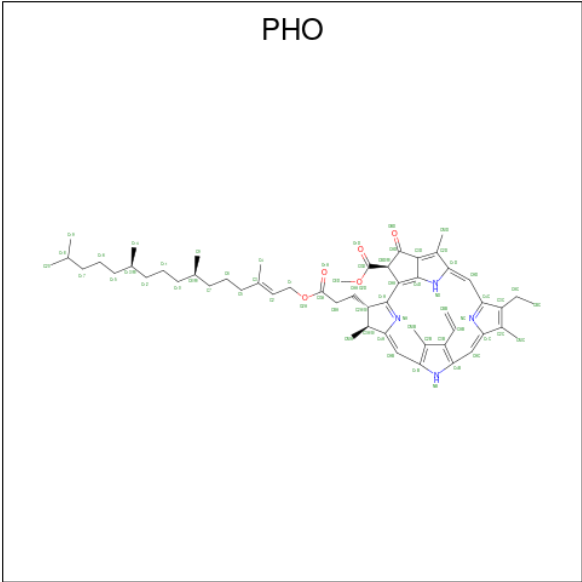
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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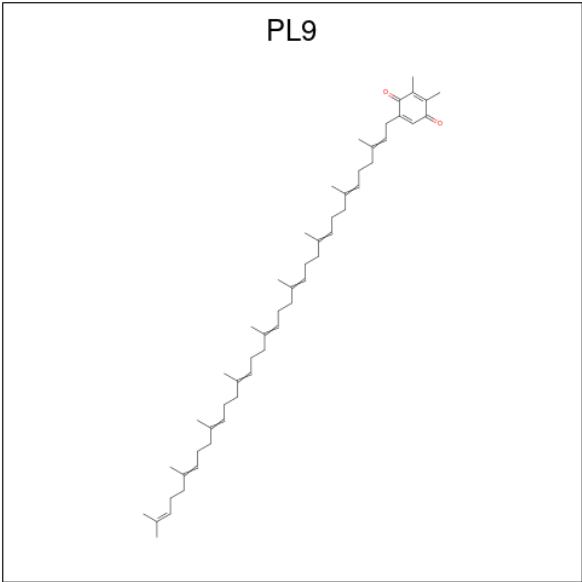
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

- Molecule 22 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



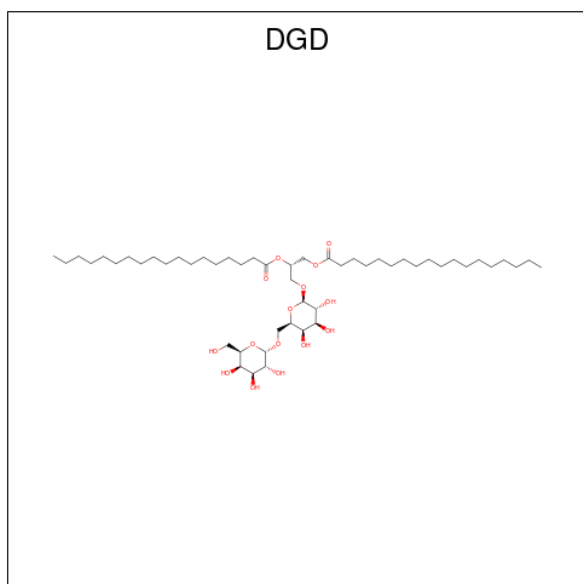
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			64	55	4	5		
22	D	1	Total	C	N	O	0	0
			64	55	4	5		
22	G	1	Total	C	N	O	0	0
			64	55	4	5		
22	Q	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 23 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	G	1	Total	C	O	0	0
			45	43	2		
23	Q	1	Total	C	O	0	0
			55	53	2		
23	b	1	Total	C	O	0	0
			35	33	2		

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



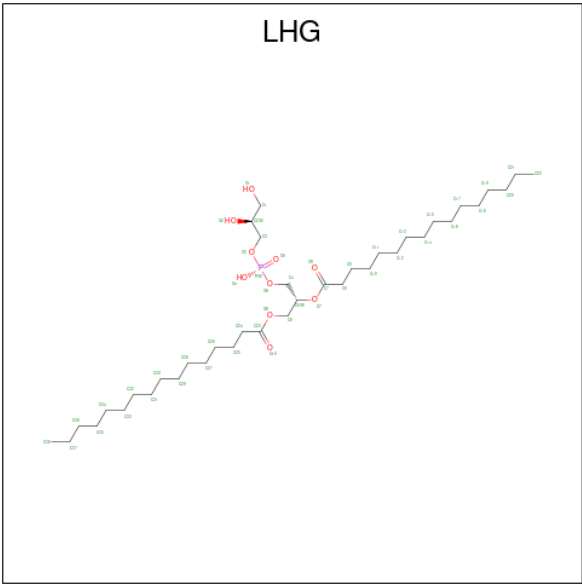
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	O	0	0
			56	41	15		
24	B	1	Total	C	O	0	0
			58	43	15		
24	B	1	Total	C	O	0	0
			52	37	15		
24	C	1	Total	C	O	0	0
			53	38	15		
24	C	1	Total	C	O	0	0
			62	47	15		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			66	51	15		
24	D	1	Total	C	O	0	0
			63	48	15		
24	G	1	Total	C	O	0	0
			56	41	15		
24	N	1	Total	C	O	0	0
			52	37	15		
24	P	1	Total	C	O	0	0
			53	38	15		
24	P	1	Total	C	O	0	0
			62	47	15		
24	P	1	Total	C	O	0	0
			66	51	15		
24	Q	1	Total	C	O	0	0
			63	48	15		
24	W	1	Total	C	O	0	0
			58	43	15		

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



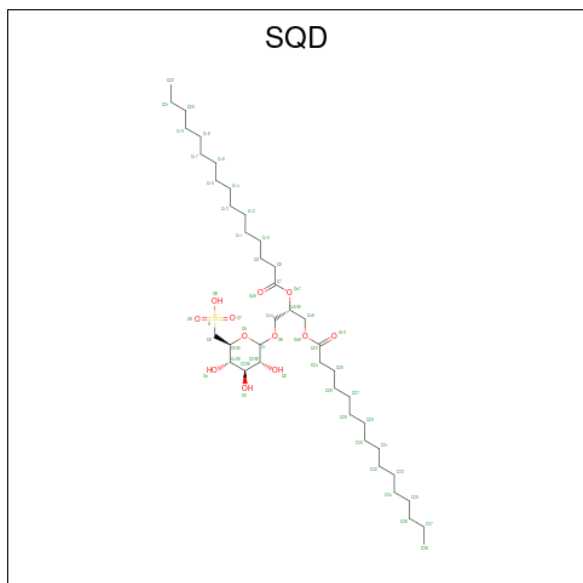
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	O	P	0	0
			39	28	10	1		
25	A	1	Total	C	O	P	0	0
			37	26	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	G	1	Total	C	O	P	0	0
			39	28	10	1		
25	G	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



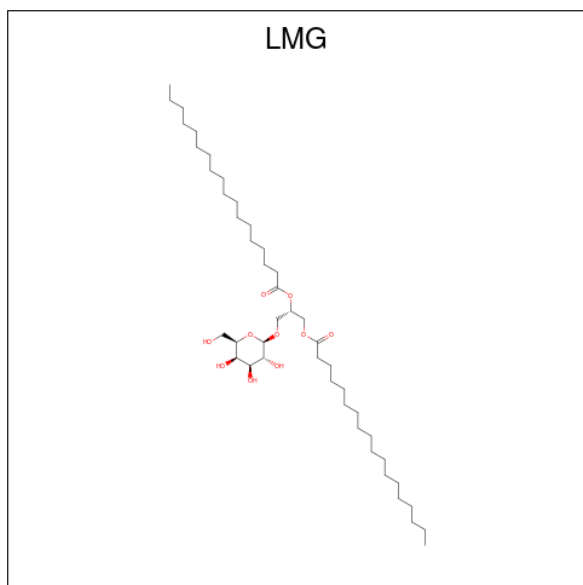
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			51	38	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			43	30	12	1		
26	B	1	Total	C	O	S	0	0
			47	34	12	1		
26	F	1	Total	C	O	S	0	0
			45	32	12	1		
26	G	1	Total	C	O	S	0	0
			54	41	12	1		
26	G	1	Total	C	O	S	0	0
			51	38	12	1		
26	N	1	Total	C	O	S	0	0
			47	34	12	1		
26	Q	1	Total	C	O	S	0	0
			43	30	12	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	S	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



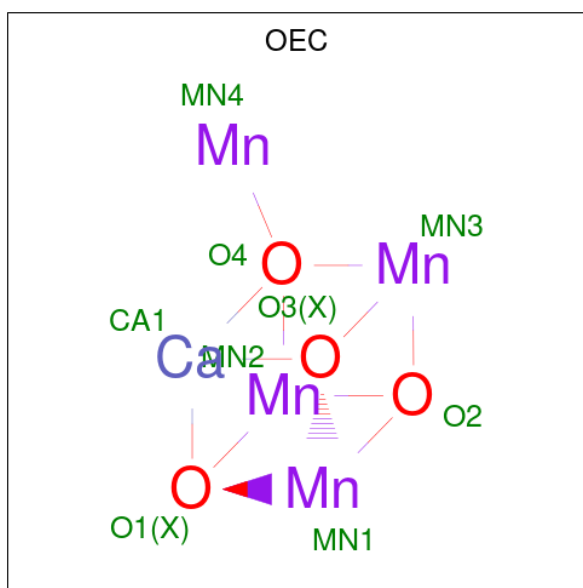
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O		0	0
			51	41	10			
27	B	1	Total	C	O		0	0
			49	39	10			
27	B	1	Total	C	O		0	0
			49	39	10			
27	C	1	Total	C	O		0	0
			48	38	10			
27	C	1	Total	C	O		0	0
			45	35	10			
27	D	1	Total	C	O		0	0
			46	36	10			
27	D	1	Total	C	O		0	0
			48	38	10			
27	D	1	Total	C	O		0	0
			42	32	10			
27	E	1	Total	C	O		0	0
			44	34	10			
27	I	1	Total	C	O		0	0
			43	33	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	M	1	Total	C	O	0	0
			42	32	10		
27	G	1	Total	C	O	0	0
			51	41	10		
27	N	1	Total	C	O	0	0
			49	39	10		
27	N	1	Total	C	O	0	0
			49	39	10		
27	P	1	Total	C	O	0	0
			48	38	10		
27	P	1	Total	C	O	0	0
			45	35	10		
27	Q	1	Total	C	O	0	0
			42	32	10		
27	Q	1	Total	C	O	0	0
			48	38	10		
27	Q	1	Total	C	O	0	0
			46	36	10		
27	R	1	Total	C	O	0	0
			44	34	10		
27	a	1	Total	C	O	0	0
			43	33	10		
27	e	1	Total	C	O	0	0
			42	32	10		

- Molecule 28 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: CaMn_4O_4).

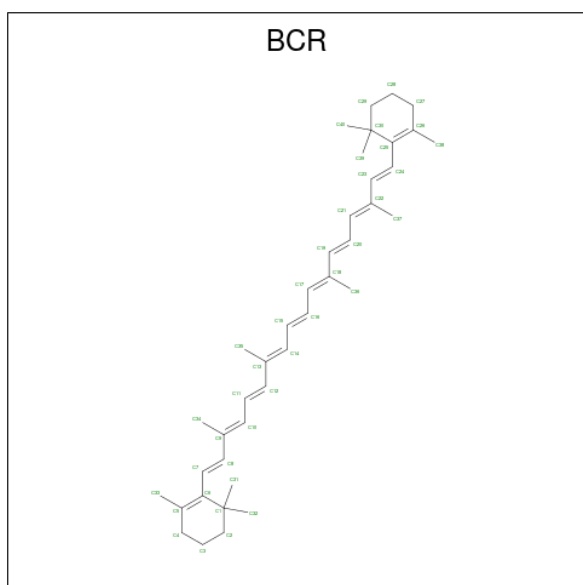


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	0	0
			5	1	4		
28	G	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	1	Total	Fe	0	0
			1	1		
29	G	1	Total	Fe	0	0
			1	1		

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



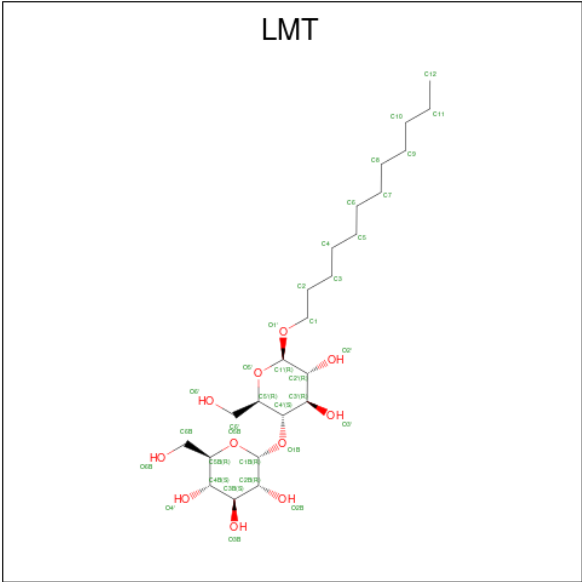
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	1	Total	C	0	0
			40	40		
30	B	1	Total	C	0	0
			40	40		
30	B	1	Total	C	0	0
			40	40		
30	B	1	Total	C	0	0
			40	40		
30	C	1	Total	C	0	0
			40	40		
30	C	1	Total	C	0	0
			40	40		

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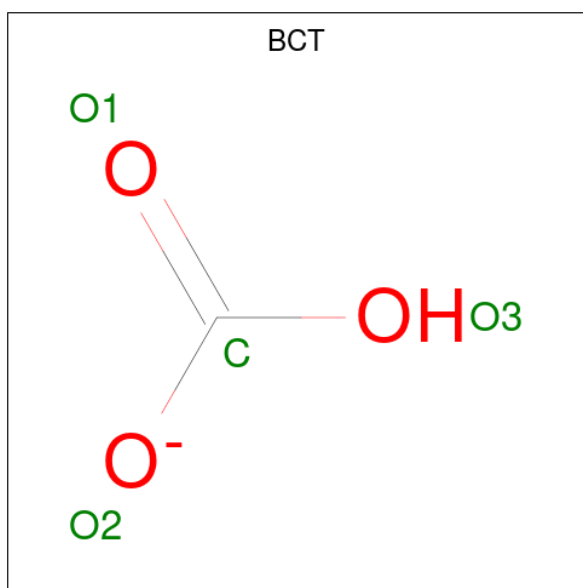
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	D	1	Total C 40 40	0	0
30	H	1	Total C 40 40	0	0
30	I	1	Total C 40 40	0	0
30	J	1	Total C 40 40	0	0
30	K	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	Z	1	Total C 40 40	0	0
30	N	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	S	1	Total C 40 40	0	0
30	W	1	Total C 40 40	0	0
30	a	1	Total C 40 40	0	0
30	b	1	Total C 40 40	0	0
30	c	1	Total C 40 40	0	0

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	D	1	Total	C	O	0	0
			31	20	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	Q	1	Total	C	O	0	0
			31	20	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	e	1	Total	C	O	0	0
			35	24	11		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	0
			4	1	3		
32	Q	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CHLORIDE ION (CCD ID: CL) (formula: Cl^-).

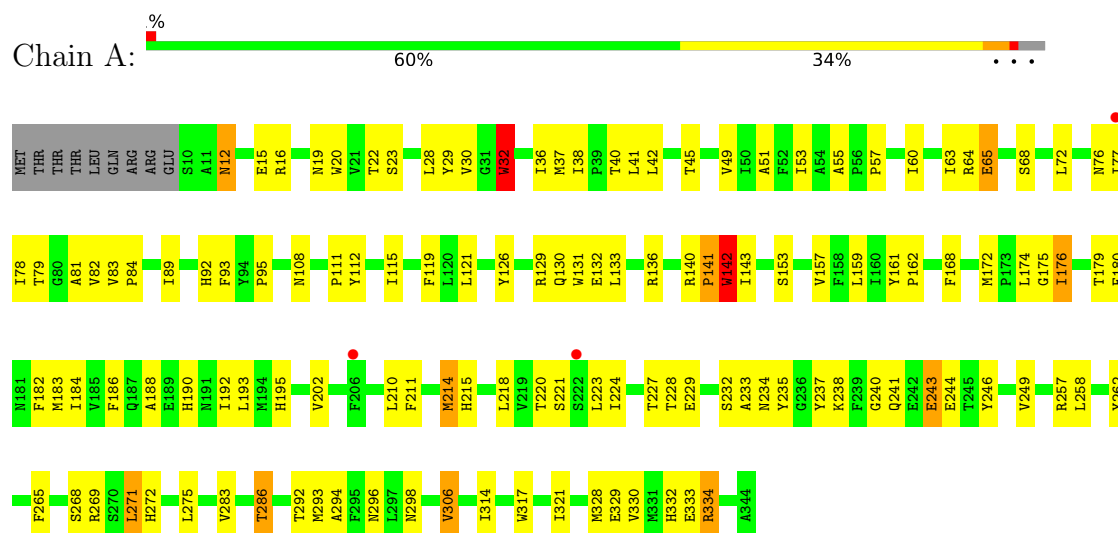
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	D	1	Total	Cl	0	0
			1	1		
33	G	1	Total	Cl	0	0
			1	1		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).

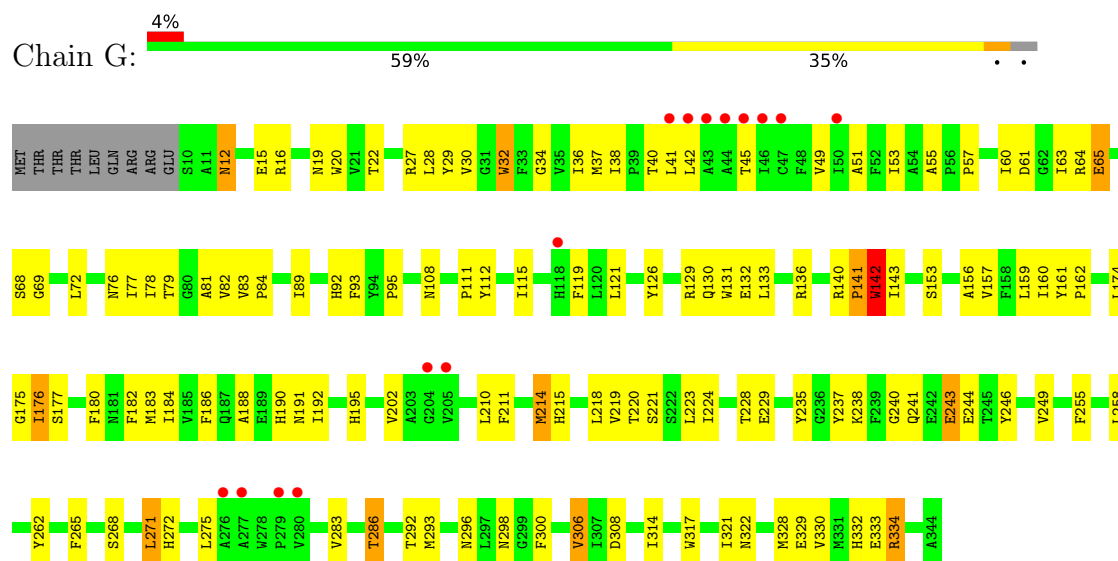
3 Residue-property plots

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

• Molecule 1: Photosystem Q(B) protein 1

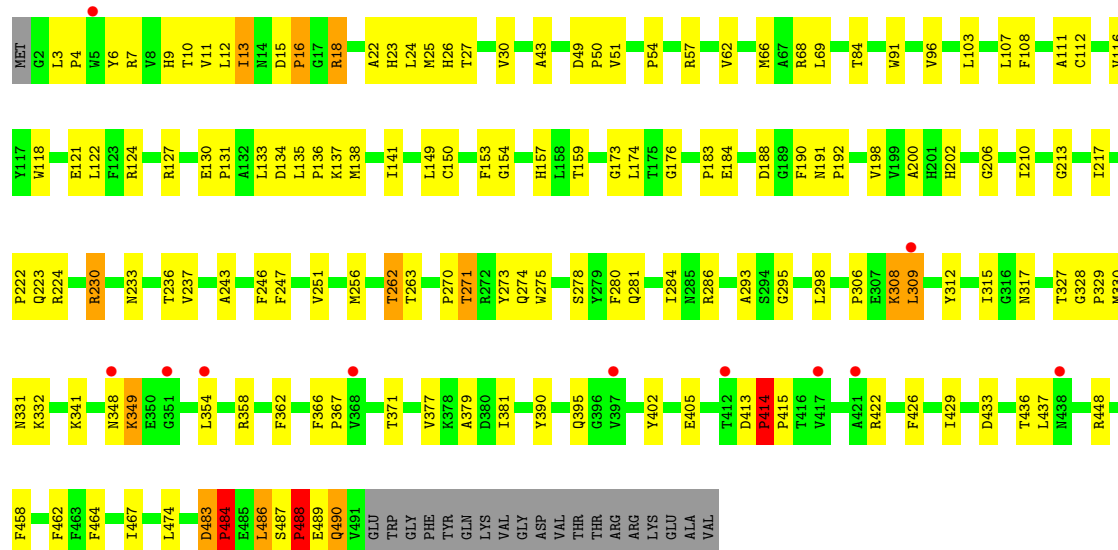


• Molecule 1: Photosystem Q(B) protein 1

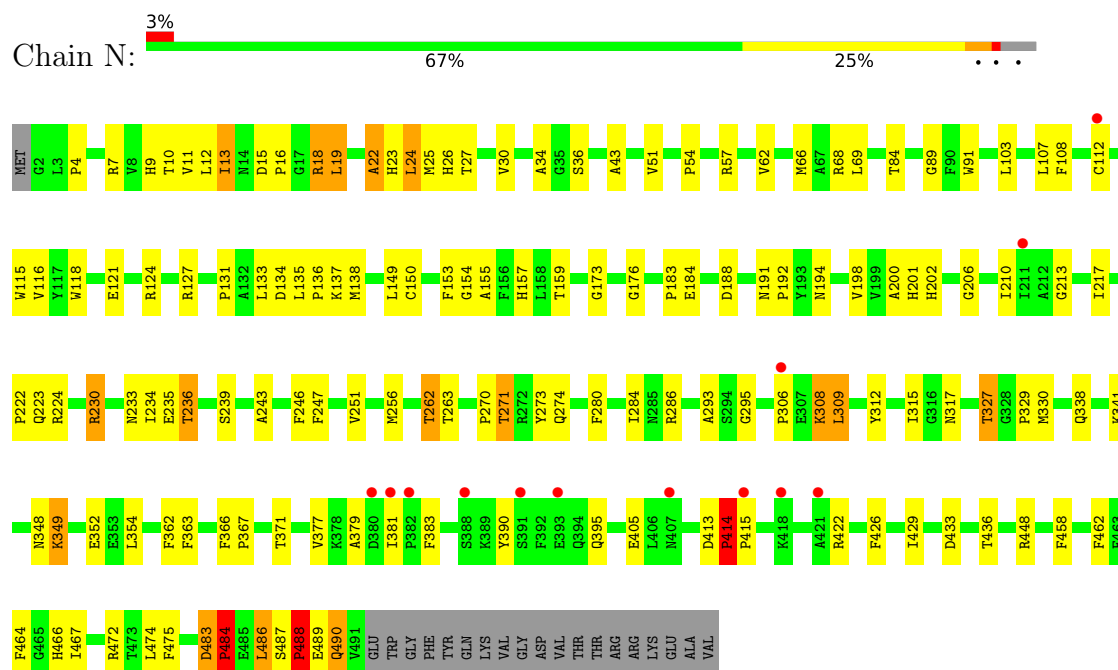


• Molecule 2: Photosystem II core light harvesting protein

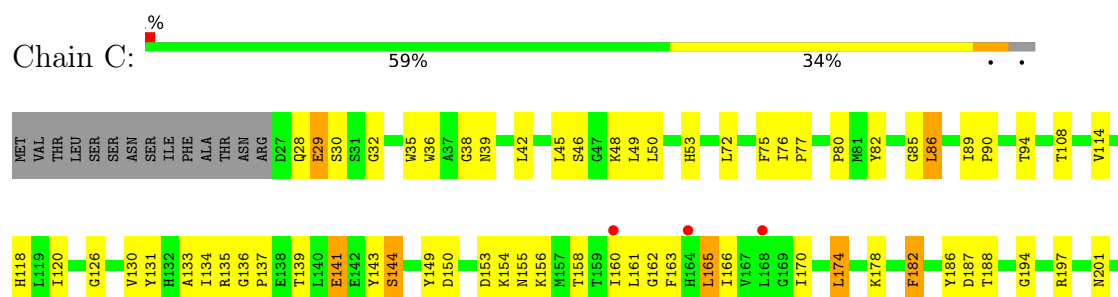


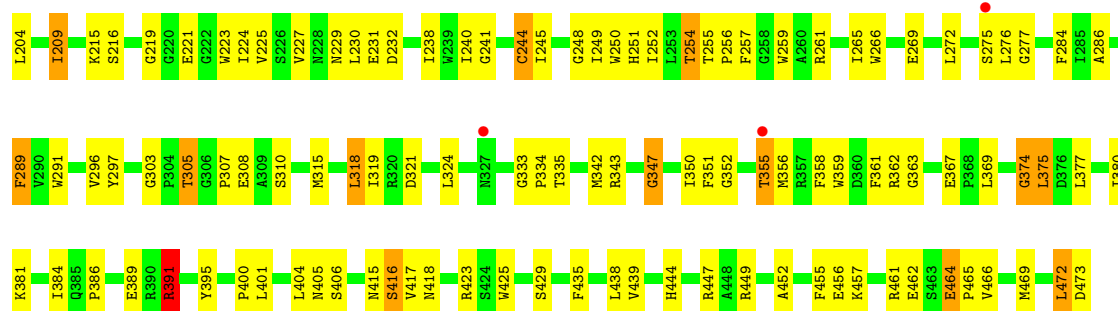


• Molecule 2: Photosystem II core light harvesting protein

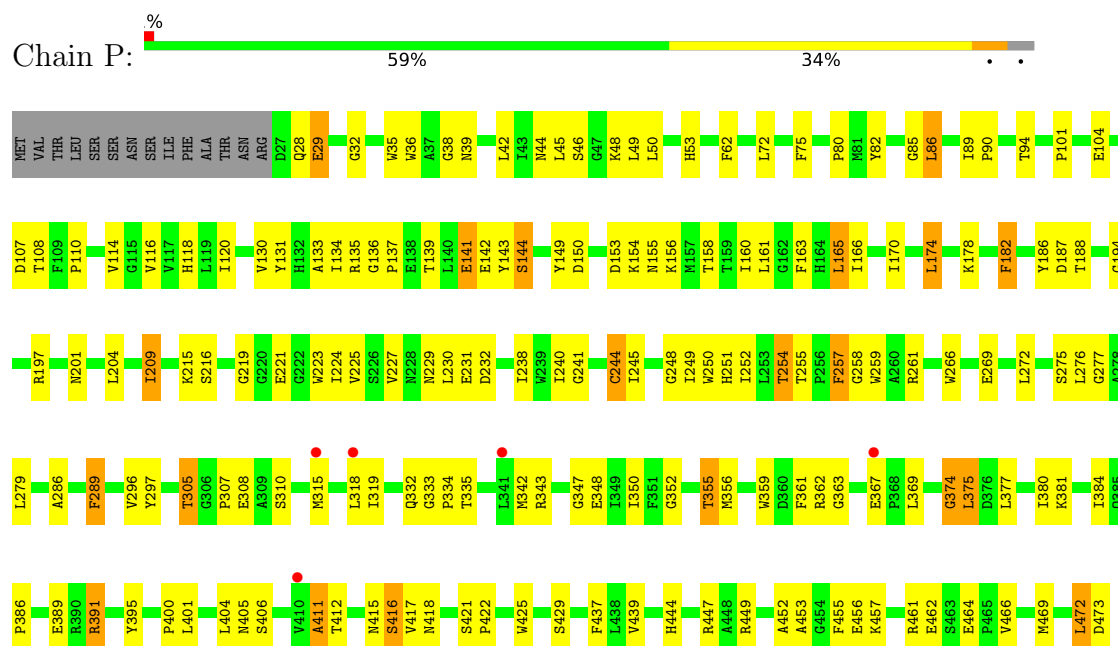


• Molecule 3: Photosystem II CP43 protein





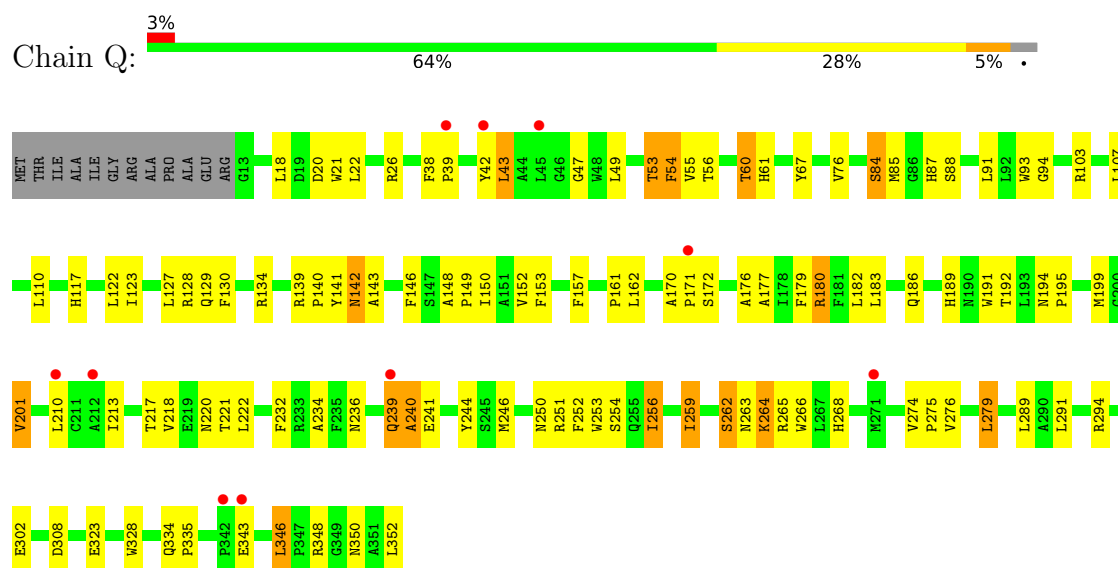
• Molecule 3: Photosystem II CP43 protein



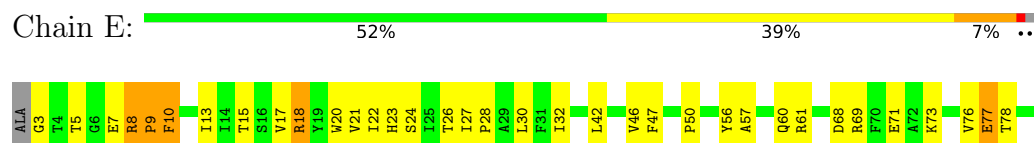
• Molecule 4: Photosystem II D2 protein



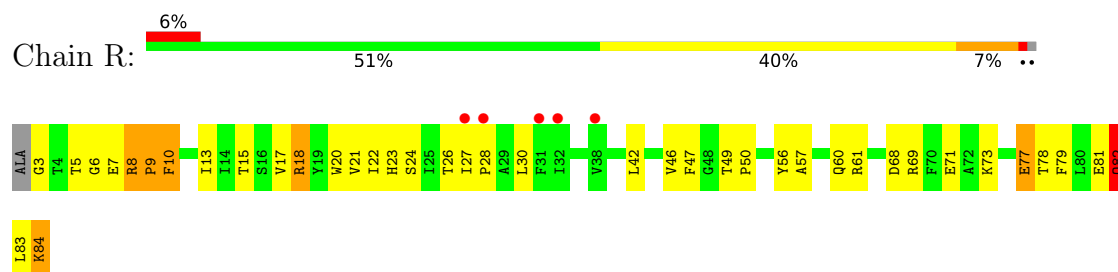
• Molecule 4: Photosystem II D2 protein



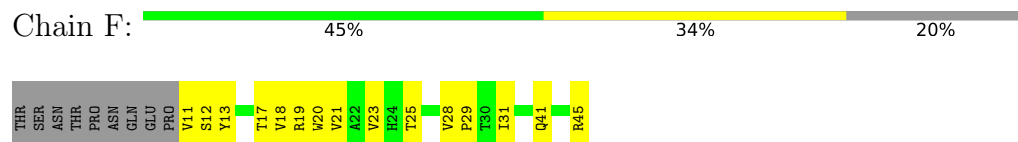
- Molecule 5: Cytochrome b559 subunit alpha



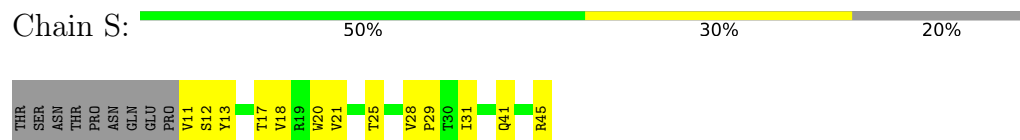
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



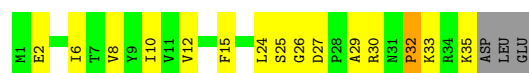
- Molecule 7: Photosystem II reaction center protein H



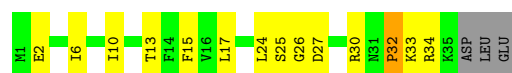
- Molecule 7: Photosystem II reaction center protein H



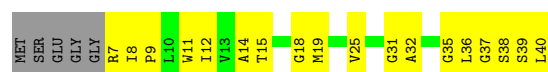
- Molecule 8: Photosystem II reaction center protein I



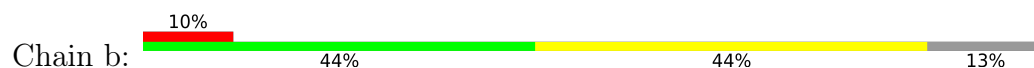
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



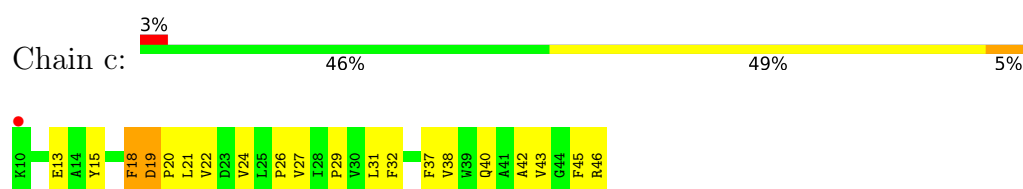
- Molecule 9: Photosystem II reaction center protein J



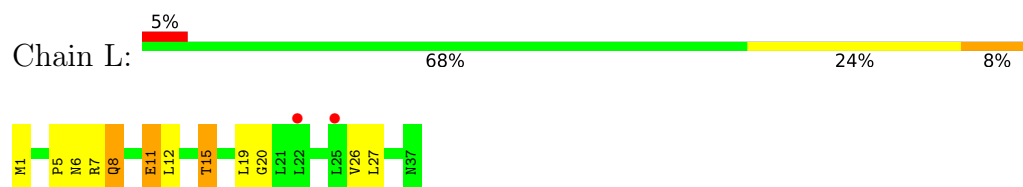
- Molecule 10: Photosystem II reaction center protein K



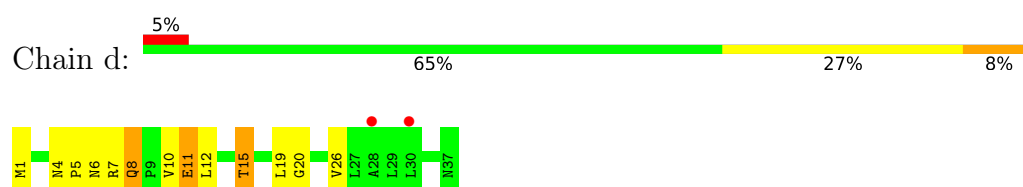
- Molecule 10: Photosystem II reaction center protein K



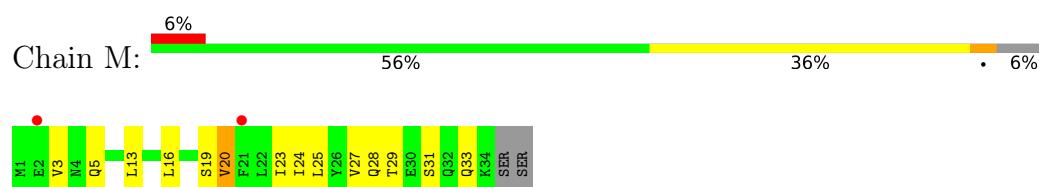
- Molecule 11: Photosystem II reaction center protein L



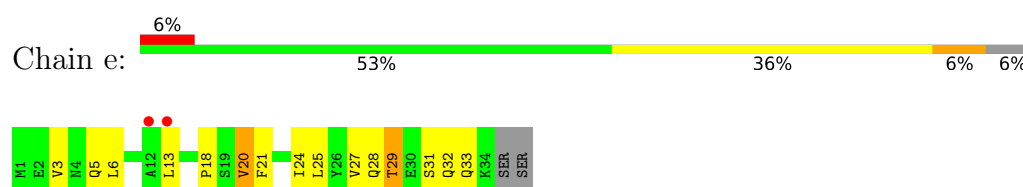
- Molecule 11: Photosystem II reaction center protein L



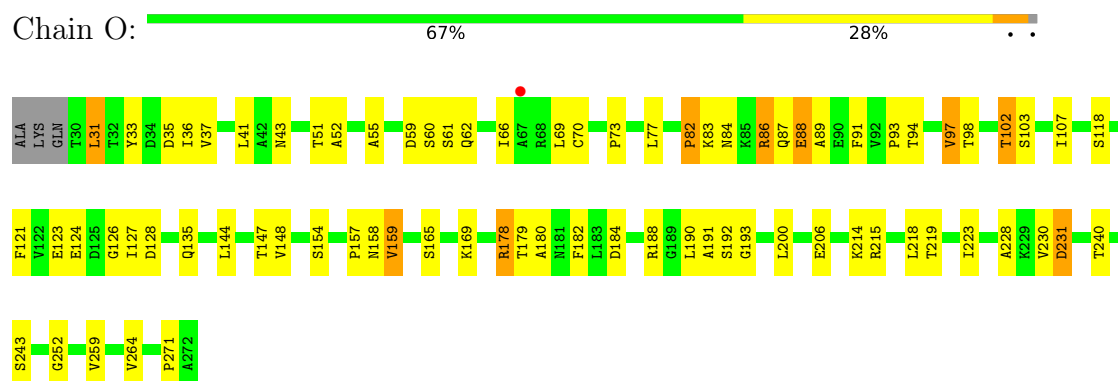
- Molecule 12: Photosystem II reaction center protein M



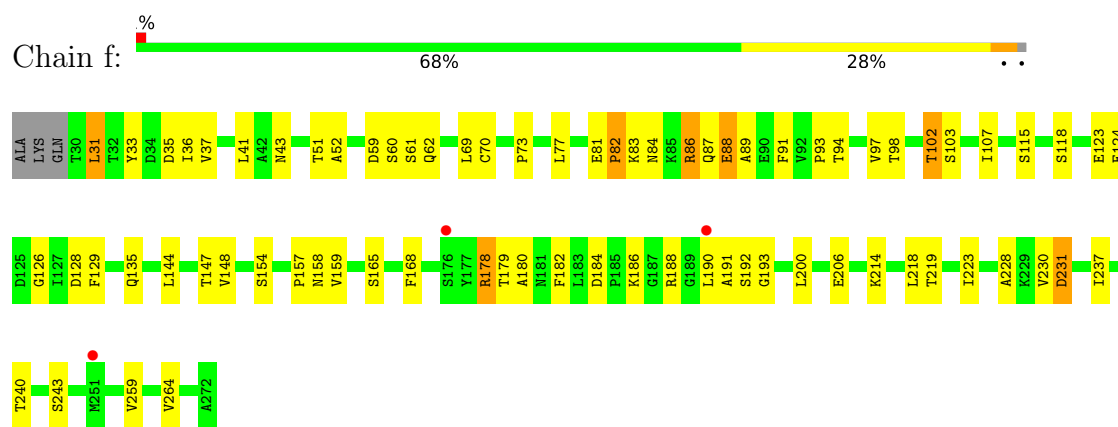
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



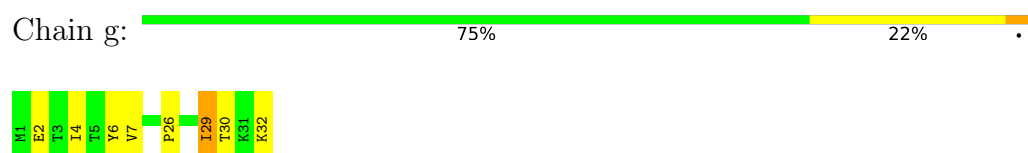
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



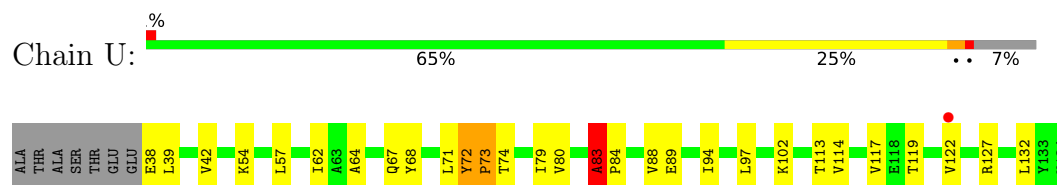
- Molecule 14: Photosystem II reaction center protein T



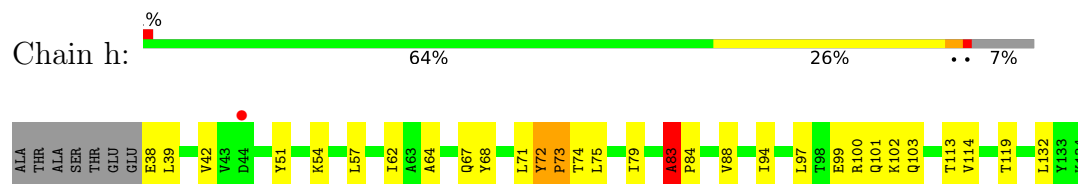
- Molecule 14: Photosystem II reaction center protein T



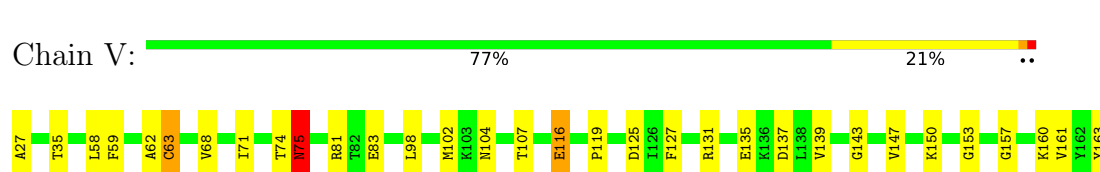
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550

Chain i:  75% 23% ..



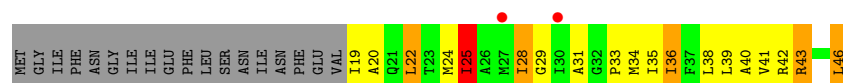
- Molecule 17: Photosystem II reaction center protein ycf12

Chain y:  20% 30% 9% . 39%

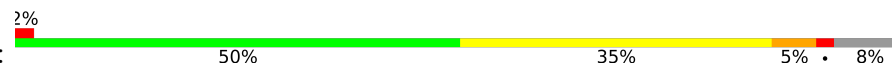


- Molecule 17: Photosystem II reaction center protein ycf12

Chain m:  4% 20% 28% 11% . 39%



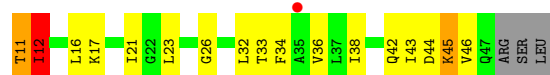
- Molecule 18: Photosystem II reaction center protein X

Chain X:  2% 50% 35% 5% . 8%

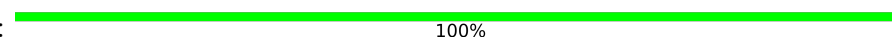


- Molecule 18: Photosystem II reaction center protein X

Chain j:  2% 50% 35% 5% . 8%

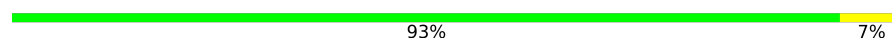


- Molecule 19: Photosystem II reaction center protein Y

Chain Y:  100%

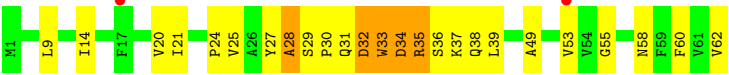
There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

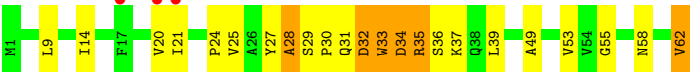
Chain k:  93% 7%



- Molecule 20: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.78Å 227.76Å 308.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.89 – 6.56 85.89 – 6.56	Depositor EDS
% Data completeness (in resolution range)	97.8 (85.89-6.56) 97.9 (85.89-6.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 6.72Å)	Xtriage
Refinement program	PHENIX 1.7.3	Depositor
R, R_{free}	0.366 , 0.385 0.343 , 0.365	Depositor DCC
R_{free} test set	897 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	6.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 106.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.66	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

5 Model quality

5.1 Standard geometry

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

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	0.34	0/2713	0.95	8/3700 (0.2%)
1	G	0.35	0/2713	0.95	6/3700 (0.2%)
2	B	0.35	0/3986	0.95	14/5433 (0.3%)
2	N	0.36	0/3986	0.98	18/5433 (0.3%)
3	C	0.34	0/3556	0.94	10/4842 (0.2%)
3	P	0.34	0/3556	0.94	9/4842 (0.2%)
4	D	0.33	0/2801	0.92	8/3818 (0.2%)
4	Q	0.33	0/2801	0.92	6/3818 (0.2%)
5	E	0.38	0/685	1.01	4/933 (0.4%)
5	R	0.38	0/685	1.03	5/933 (0.5%)
6	F	0.41	0/291	0.80	0/397
6	S	0.37	0/291	0.79	0/397
7	H	0.40	0/520	0.91	0/709
7	W	0.41	0/520	0.91	0/709
8	I	0.34	0/293	0.92	1/395 (0.3%)
8	a	0.35	0/293	0.94	1/395 (0.3%)
9	J	0.36	0/255	1.07	2/346 (0.6%)
9	b	0.36	0/255	1.08	2/346 (0.6%)
10	K	0.46	0/303	0.88	0/416
10	c	0.46	0/303	0.89	0/416
11	L	0.32	0/311	0.90	0/422
11	d	0.32	0/311	0.92	2/422 (0.5%)
12	M	0.39	0/270	0.94	1/367 (0.3%)
12	e	0.40	0/270	0.93	1/367 (0.3%)
13	O	0.34	0/1876	0.87	5/2548 (0.2%)
13	f	0.33	0/1876	0.87	5/2548 (0.2%)
14	T	0.32	0/284	0.90	0/381
14	g	0.32	0/284	0.90	0/381
15	U	0.41	0/785	0.97	4/1064 (0.4%)
15	h	0.41	0/785	1.00	5/1064 (0.5%)
16	V	0.33	0/1081	0.89	6/1468 (0.4%)
16	i	0.33	0/1081	0.89	4/1468 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	m	0.42	0/202	1.03	2/272 (0.7%)
17	y	0.45	0/202	1.01	1/272 (0.4%)
18	X	0.50	0/273	0.91	1/370 (0.3%)
18	j	0.50	0/273	0.95	1/370 (0.3%)
20	Z	0.38	0/490	1.00	2/669 (0.3%)
20	l	0.38	0/490	1.00	2/669 (0.3%)
All	All	0.36	0/41950	0.94	136/57100 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	22	ALA	CA-C-N	9.36	134.04	120.38
2	N	22	ALA	C-N-CA	9.36	134.04	120.38
2	N	483	ASP	CA-C-N	8.80	130.84	119.84
2	N	483	ASP	C-N-CA	8.80	130.84	119.84
2	B	483	ASP	CA-C-N	8.59	130.58	119.84
2	B	483	ASP	C-N-CA	8.59	130.58	119.84
20	l	34	ASP	N-CA-C	-7.94	103.42	113.43
20	Z	34	ASP	N-CA-C	-7.93	103.43	113.43
9	J	36	LEU	N-CA-C	-7.47	104.31	113.50
9	b	36	LEU	N-CA-C	-7.31	104.51	113.50
5	R	57	ALA	N-CA-C	-7.16	101.29	110.53
2	B	381	ILE	CA-C-N	7.04	127.03	119.78
2	B	381	ILE	C-N-CA	7.04	127.03	119.78
5	E	57	ALA	N-CA-C	-7.00	101.50	110.53
15	h	83	ALA	CA-C-N	-6.89	113.69	120.52
15	h	83	ALA	C-N-CA	-6.89	113.69	120.52
13	f	102	THR	N-CA-C	6.86	118.83	111.36
3	C	318	LEU	N-CA-C	-6.84	103.91	111.36
17	m	22	LEU	N-CA-C	-6.75	104.30	112.54
1	G	36	ILE	N-CA-C	-6.72	106.03	111.81
2	N	381	ILE	CA-C-N	6.49	126.47	119.78
2	N	381	ILE	C-N-CA	6.49	126.47	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	102	THR	N-CA-C	6.49	118.43	111.36
15	U	83	ALA	CA-C-N	-6.47	114.12	120.52
15	U	83	ALA	C-N-CA	-6.47	114.12	120.52
2	N	413	ASP	CA-C-N	6.39	126.97	120.38
2	N	413	ASP	C-N-CA	6.39	126.97	120.38
12	M	29	THR	N-CA-C	-6.39	103.94	111.03
2	N	484	PRO	N-CA-C	6.33	125.51	112.47
2	N	24	LEU	N-CA-C	-6.30	104.50	111.36
2	B	413	ASP	CA-C-N	6.20	126.77	120.38
2	B	413	ASP	C-N-CA	6.20	126.77	120.38
2	B	484	PRO	N-CA-C	6.20	125.24	112.47
3	P	318	LEU	N-CA-C	-6.08	104.73	111.36
12	e	29	THR	N-CA-C	-6.03	104.33	111.03
20	l	35	ARG	N-CA-C	-6.02	104.64	112.23
2	B	236	THR	N-CA-C	-6.02	106.55	114.31
8	a	2	GLU	N-CA-C	-6.01	105.44	112.89
5	R	8	ARG	CA-C-N	5.99	127.32	119.84
5	R	8	ARG	C-N-CA	5.99	127.32	119.84
16	i	104	ASN	CA-C-N	5.94	125.85	119.85
16	i	104	ASN	C-N-CA	5.94	125.85	119.85
1	G	195	HIS	CA-C-N	5.93	125.41	119.24
1	G	195	HIS	C-N-CA	5.93	125.41	119.24
13	f	228	ALA	N-CA-C	-5.93	107.86	114.62
15	h	51	TYR	N-CA-C	-5.88	101.71	110.23
3	P	439	VAL	N-CA-C	-5.86	105.02	110.53
9	b	39	SER	N-CA-C	-5.85	105.50	114.16
4	D	308	ASP	CA-C-N	5.84	126.60	120.12
4	D	308	ASP	C-N-CA	5.84	126.60	120.12
2	N	15	ASP	CA-C-N	5.77	127.05	119.84
2	N	15	ASP	C-N-CA	5.77	127.05	119.84
4	Q	308	ASP	CA-C-N	5.74	126.49	120.12
4	Q	308	ASP	C-N-CA	5.74	126.49	120.12
9	J	39	SER	N-CA-C	-5.71	105.72	114.16
4	D	94	GLY	CA-C-N	5.70	126.08	119.47
4	D	94	GLY	C-N-CA	5.70	126.08	119.47
1	A	195	HIS	CA-C-N	5.70	125.16	119.24
1	A	195	HIS	C-N-CA	5.70	125.16	119.24
13	f	103	SER	N-CA-C	5.66	118.44	110.23
5	E	8	ARG	CA-C-N	5.66	126.91	119.84
5	E	8	ARG	C-N-CA	5.66	126.91	119.84
13	f	200	LEU	CA-C-N	5.64	126.89	119.84
13	f	200	LEU	C-N-CA	5.64	126.89	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ILE	N-CA-C	-5.63	106.97	111.81
15	h	74	THR	N-CA-C	5.60	117.08	110.97
2	N	236	THR	N-CA-C	-5.59	107.09	114.31
15	U	62	ILE	N-CA-C	5.59	116.99	110.62
18	X	46	VAL	N-CA-C	5.56	117.45	109.51
3	C	464	GLU	CA-C-N	5.55	126.78	119.84
3	C	464	GLU	C-N-CA	5.55	126.78	119.84
3	P	182	PHE	N-CA-C	5.54	119.91	113.20
13	O	103	SER	N-CA-C	5.51	118.22	110.23
1	G	65	GLU	CA-C-N	5.50	125.82	119.93
1	G	65	GLU	C-N-CA	5.50	125.82	119.93
17	y	22	LEU	N-CA-C	-5.49	105.84	112.54
2	B	15	ASP	CA-C-N	5.48	126.69	119.84
2	B	15	ASP	C-N-CA	5.48	126.69	119.84
2	B	328	GLY	CA-C-N	5.47	125.47	120.21
2	B	328	GLY	C-N-CA	5.47	125.47	120.21
3	P	464	GLU	CA-C-N	5.47	126.67	119.84
3	P	464	GLU	C-N-CA	5.47	126.67	119.84
16	V	104	ASN	CA-C-N	5.46	125.36	119.85
16	V	104	ASN	C-N-CA	5.46	125.36	119.85
8	I	2	GLU	N-CA-C	-5.44	106.15	112.89
4	Q	54	PHE	N-CA-C	5.42	119.66	112.72
18	j	46	VAL	N-CA-C	5.42	117.26	109.51
3	P	333	GLY	CA-C-N	5.42	126.61	119.84
3	P	333	GLY	C-N-CA	5.42	126.61	119.84
13	O	200	LEU	CA-C-N	5.38	126.56	119.84
13	O	200	LEU	C-N-CA	5.38	126.56	119.84
16	V	75	ASN	CA-C-N	5.38	125.09	119.82
16	V	75	ASN	C-N-CA	5.38	125.09	119.82
1	A	294	ALA	N-CA-C	-5.37	106.73	113.28
3	C	333	GLY	CA-C-N	5.35	126.53	119.84
3	C	333	GLY	C-N-CA	5.35	126.53	119.84
4	Q	94	GLY	CA-C-N	5.35	125.67	119.47
4	Q	94	GLY	C-N-CA	5.35	125.67	119.47
3	C	374	GLY	CA-C-O	-5.34	118.30	122.52
4	Q	142	ASN	N-CA-C	-5.33	106.61	113.23
3	C	439	VAL	N-CA-C	-5.33	105.52	110.53
3	C	391	ARG	N-CA-C	-5.33	105.39	111.14
5	R	24	SER	N-CA-C	-5.32	106.05	112.54
1	A	65	GLU	CA-C-N	5.31	126.48	119.84
1	A	65	GLU	C-N-CA	5.31	126.48	119.84
3	C	182	PHE	N-CA-C	5.30	119.62	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	228	ALA	N-CA-C	-5.30	108.58	114.62
15	h	62	ILE	N-CA-C	5.30	116.66	110.62
2	N	19	LEU	N-CA-C	-5.29	105.18	111.69
3	P	374	GLY	CA-C-O	-5.29	118.34	122.52
4	D	156	VAL	N-CA-C	5.27	115.93	110.82
1	A	32	TRP	N-CA-C	-5.20	105.30	111.69
3	P	374	GLY	N-CA-C	-5.19	106.05	112.33
11	d	4	ASN	CA-C-N	5.18	126.31	119.84
11	d	4	ASN	C-N-CA	5.18	126.31	119.84
4	D	297	ASP	N-CA-C	5.17	117.27	109.41
16	i	75	ASN	CA-C-N	5.17	124.88	119.82
16	i	75	ASN	C-N-CA	5.17	124.88	119.82
5	E	24	SER	N-CA-C	-5.16	106.25	112.54
1	A	142	TRP	N-CA-C	5.14	121.75	110.80
4	D	142	ASN	N-CA-C	-5.13	106.86	113.23
3	C	347	GLY	N-CA-C	5.12	120.79	114.69
2	B	332	LYS	N-CA-C	-5.10	107.01	113.18
5	R	6	GLY	N-CA-C	5.09	119.04	112.83
16	V	127	PHE	CA-C-N	5.09	126.20	119.84
16	V	127	PHE	C-N-CA	5.09	126.20	119.84
1	G	142	TRP	N-CA-C	5.09	121.63	110.80
15	U	74	THR	N-CA-C	5.08	116.51	110.97
2	N	327	THR	N-CA-C	5.06	116.64	110.41
17	m	40	ALA	N-CA-C	-5.06	106.62	112.89
20	Z	35	ARG	N-CA-C	-5.05	105.86	112.23
2	N	194	ASN	CA-C-N	5.03	125.06	119.32
2	N	194	ASN	C-N-CA	5.03	125.06	119.32
2	N	363	PHE	N-CA-C	5.01	116.92	108.96
2	B	237	VAL	N-CA-C	-5.01	104.83	111.09
4	D	54	PHE	N-CA-C	5.00	119.12	112.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	23	HIS	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	106	0
1	G	2628	0	2524	108	0
2	B	3850	0	3718	108	0
2	N	3850	0	3718	111	0
3	C	3444	0	3365	131	0
3	P	3444	0	3365	131	0
4	D	2706	0	2608	100	0
4	Q	2706	0	2608	103	0
5	E	666	0	651	39	0
5	R	666	0	651	38	0
6	F	282	0	291	13	0
6	S	282	0	291	12	0
7	H	507	0	521	26	0
7	W	507	0	521	26	0
8	I	286	0	308	8	0
8	a	286	0	308	8	0
9	J	249	0	262	18	0
9	b	249	0	262	18	0
10	K	293	0	305	18	0
10	c	293	0	305	21	0
11	L	304	0	316	15	0
11	d	304	0	316	14	0
12	M	267	0	289	17	0
12	e	267	0	289	18	0
13	O	1845	0	1801	48	0
13	f	1845	0	1801	49	1
14	T	275	0	288	13	0
14	g	275	0	288	9	0
15	U	774	0	773	16	0
15	h	774	0	773	16	0
16	V	1060	0	1068	22	0
16	i	1060	0	1068	23	0
17	m	201	0	226	18	0
17	y	201	0	226	17	0
18	X	270	0	299	10	0
18	j	270	0	299	10	0
19	Y	140	0	32	0	0
19	k	140	0	32	1	0
20	Z	479	0	516	21	1
20	l	479	0	516	21	0
21	A	260	0	288	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	1040	0	1152	66	0
21	C	845	0	936	49	0
21	D	130	0	144	11	0
21	G	260	0	288	26	0
21	N	1040	0	1152	65	0
21	P	845	0	936	45	0
21	Q	130	0	144	14	0
22	A	64	0	74	6	0
22	D	64	0	74	5	0
22	G	64	0	74	7	0
22	Q	64	0	74	5	0
23	A	45	0	61	5	0
23	D	55	0	80	6	0
23	G	45	0	61	5	0
23	J	35	0	45	1	0
23	Q	55	0	80	5	0
23	b	35	0	45	2	0
24	A	56	0	70	1	0
24	B	110	0	136	5	0
24	C	181	0	245	17	0
24	D	63	0	87	0	0
24	G	56	0	70	2	0
24	N	52	0	62	4	0
24	P	181	0	245	14	0
24	Q	63	0	87	1	0
24	W	58	0	74	3	0
25	A	76	0	95	4	0
25	G	76	0	95	4	0
26	A	105	0	147	13	0
26	B	90	0	111	10	0
26	F	45	0	54	2	0
26	G	105	0	147	16	0
26	N	47	0	61	7	0
26	Q	43	0	50	3	0
26	S	45	0	54	2	0
27	A	51	0	72	2	0
27	B	98	0	136	2	0
27	C	93	0	126	4	0
27	D	136	0	182	15	0
27	E	44	0	58	2	0
27	G	51	0	72	2	0
27	I	43	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	M	42	0	54	4	0
27	N	98	0	136	3	0
27	P	93	0	126	4	0
27	Q	136	0	182	15	0
27	R	44	0	58	2	0
27	a	43	0	56	2	0
27	e	42	0	54	3	0
28	A	5	0	0	0	0
28	G	5	0	0	0	0
29	A	1	0	0	0	0
29	G	1	0	0	0	0
30	B	160	0	224	16	0
30	C	80	0	112	16	0
30	D	40	0	56	3	0
30	H	40	0	56	2	0
30	I	40	0	56	5	0
30	J	40	0	56	4	0
30	K	40	0	56	11	0
30	N	40	0	56	4	0
30	P	120	0	168	20	0
30	S	40	0	56	5	0
30	T	120	0	168	17	0
30	W	40	0	56	3	0
30	Z	40	0	56	3	0
30	a	40	0	56	4	0
30	b	40	0	56	3	0
30	c	40	0	56	12	0
31	B	140	0	184	8	0
31	D	31	0	35	0	0
31	I	35	0	46	2	0
31	M	35	0	46	1	0
31	N	140	0	184	9	0
31	Q	31	0	35	0	0
31	a	35	0	46	1	0
31	e	35	0	46	1	0
32	D	4	0	1	0	0
32	Q	4	0	1	0	0
33	D	1	0	0	0	0
33	G	1	0	0	0	0
34	E	43	0	30	7	0
34	R	43	0	30	6	0
34	V	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	i	43	0	30	4	0
35	O	1	0	0	0	0
35	f	1	0	0	0	0
All	All	50232	0	51376	1600	1

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 16.

All (1600) 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)
12:M:33:GLN:HB3	12:e:33:GLN:HB3	1.41	1.02
2:N:121:GLU:HG2	7:W:4:ARG:HG2	1.49	0.94
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.50	0.93
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.52	0.92
4:Q:26:ARG:HD3	6:S:18:VAL:HG11	1.54	0.88
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.54	0.88
13:f:82:PRO:HG3	13:f:89:ALA:HB2	1.57	0.87
3:C:39:ASN:HB2	21:C:508:CLA:HBA1	1.59	0.83
21:P:505:CLA:HBD	21:P:505:CLA:HBA1	1.63	0.80
7:H:38:PHE:HB2	30:H:101:BCR:H10C	1.64	0.80
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.64	0.80
1:A:40:THR:HG23	21:A:405:CLA:HBB1	1.62	0.80
9:b:15:THR:HG21	10:c:38:VAL:HG13	1.62	0.79
21:N:612:CLA:H51	21:N:613:CLA:H101	1.64	0.79
7:W:38:PHE:HB2	30:W:101:BCR:H10C	1.63	0.79
2:B:25:MET:HE3	30:B:617:BCR:H23C	1.65	0.79
1:G:129:ARG:HH21	4:Q:256:ILE:HD12	1.48	0.78
17:m:35:ILE:HG22	20:l:21:ILE:HG23	1.66	0.77
13:f:69:LEU:HB3	13:f:107:ILE:HB	1.65	0.77
3:P:39:ASN:HB2	21:P:508:CLA:HBA1	1.64	0.77
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.66	0.76
1:G:174:LEU:HD22	22:G:405:PHO:H151	1.68	0.76
1:G:40:THR:HG23	21:G:406:CLA:HBB1	1.65	0.75
21:C:507:CLA:H112	30:C:515:BCR:H362	1.67	0.74
1:G:328:MET:HE1	4:Q:183:LEU:HD22	1.69	0.74
30:T:101:BCR:H23C	2:N:25:MET:HE3	1.69	0.74
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.50	0.74
1:G:192:ILE:HA	1:G:293:MET:HE1	1.69	0.74
3:P:305:THR:HG23	3:P:307:PRO:HD2	1.68	0.74
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.69	0.73
23:Q:405:PL9:H13	27:Q:407:LMG:H132	1.71	0.73
15:h:83:ALA:HB1	15:h:84:PRO:HD2	1.70	0.73
17:y:35:ILE:HG22	20:Z:21:ILE:HG23	1.71	0.72
21:C:505:CLA:HBA1	21:C:505:CLA:HBD	1.69	0.72
26:G:410:SQD:H311	21:P:508:CLA:H71	1.71	0.72
21:A:401:CLA:H152	22:A:404:PHO:H51	1.72	0.72
2:N:149:LEU:HG	21:N:607:CLA:HBC1	1.71	0.72
21:G:402:CLA:H152	22:G:405:PHO:H51	1.72	0.72
17:m:39:LEU:HB3	17:m:46:LEU:HD21	1.72	0.72
21:B:608:CLA:H51	21:B:609:CLA:H101	1.71	0.72
13:O:230:VAL:HG12	13:O:231:ASP:H	1.55	0.71
1:G:45:THR:HG21	26:G:401:SQD:H201	1.72	0.71
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.72	0.71
2:B:490:GLN:O	2:B:490:GLN:NE2	2.17	0.71
30:C:514:BCR:H353	30:K:101:BCR:H321	1.72	0.71
3:C:254:THR:HG22	3:C:255:THR:H	1.56	0.71
25:A:411:LHG:H271	25:A:411:LHG:H101	1.73	0.70
2:B:149:LEU:HG	21:B:603:CLA:HBC1	1.72	0.70
21:P:503:CLA:HBB1	27:P:521:LMG:H201	1.73	0.70
3:P:254:THR:HG22	3:P:255:THR:H	1.56	0.70
26:A:409:SQD:H311	21:C:508:CLA:H71	1.74	0.70
30:P:514:BCR:H353	30:c:101:BCR:H321	1.72	0.70
26:G:401:SQD:H311	30:a:101:BCR:H342	1.72	0.70
1:A:192:ILE:HA	1:A:293:MET:HE1	1.73	0.70
1:A:174:LEU:HD22	22:A:404:PHO:H151	1.74	0.69
26:A:414:SQD:H311	30:I:101:BCR:H342	1.73	0.69
30:C:514:BCR:H11C	30:K:101:BCR:H322	1.73	0.69
17:y:39:LEU:HB3	17:y:46:LEU:HD21	1.74	0.69
1:G:214:MET:HE2	1:G:214:MET:HA	1.74	0.69
21:P:507:CLA:H112	30:P:516:BCR:H362	1.74	0.69
13:f:230:VAL:HG12	13:f:231:ASP:H	1.56	0.69
3:P:473:ASP:HB2	14:g:26:PRO:HB3	1.74	0.69
21:C:503:CLA:HBB1	27:C:520:LMG:H201	1.72	0.69
3:C:166:ILE:HG23	3:C:245:ILE:HG23	1.74	0.69
30:T:101:BCR:H383	26:N:601:SQD:H92	1.75	0.69
30:S:101:BCR:H403	9:b:25:VAL:HG21	1.74	0.69
3:P:361:PHE:HA	24:P:517:DGD:HE61	1.75	0.69
1:A:72:LEU:HD13	27:D:412:LMG:H111	1.76	0.68
21:N:612:CLA:H151	21:N:613:CLA:H203	1.75	0.68
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:28:GLN:HA	12:e:28:GLN:HA	1.75	0.68
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.76	0.68
4:D:279:LEU:HG	22:D:402:PHO:HBC3	1.74	0.68
1:G:82:VAL:HB	1:G:174:LEU:HB2	1.73	0.68
4:Q:279:LEU:HG	22:Q:403:PHO:HBC3	1.74	0.68
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.57	0.68
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.76	0.68
3:P:166:ILE:HG23	3:P:245:ILE:HG23	1.76	0.68
30:B:617:BCR:H383	26:B:627:SQD:H92	1.76	0.68
12:e:25:LEU:O	12:e:28:GLN:HG3	1.93	0.67
13:f:83:LYS:HG2	13:f:84:ASN:H	1.59	0.67
1:A:28:LEU:HB2	26:A:414:SQD:H91	1.74	0.67
23:D:404:PL9:H13	27:D:407:LMG:H132	1.76	0.67
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.76	0.67
21:B:606:CLA:H72	30:B:620:BCR:H311	1.77	0.67
13:f:178:ARG:HH11	13:f:178:ARG:HG3	1.60	0.67
4:D:214:HIS:ND1	23:D:404:PL9:O2	2.25	0.67
21:D:403:CLA:H43	18:X:23:LEU:HA	1.76	0.67
2:B:271:THR:HG22	2:B:273:TYR:H	1.59	0.67
2:N:271:THR:HG22	2:N:273:TYR:H	1.59	0.67
30:D:405:BCR:H403	9:J:25:VAL:HG21	1.77	0.67
21:P:508:CLA:HBC3	21:P:510:CLA:H92	1.77	0.66
30:P:514:BCR:H11C	30:c:101:BCR:H322	1.77	0.66
30:K:101:BCR:HC8	30:K:101:BCR:H331	1.78	0.66
13:O:83:LYS:HG2	13:O:84:ASN:H	1.60	0.66
1:G:317:TRP:CZ3	4:Q:180:ARG:HD3	2.31	0.66
10:c:21:LEU:HD13	17:m:24:MET:HE2	1.78	0.66
12:M:25:LEU:O	12:M:28:GLN:HG3	1.96	0.66
1:G:77:ILE:HD11	14:g:6:TYR:HB3	1.78	0.66
4:D:60:THR:HG23	4:D:61:HIS:CD2	2.31	0.65
13:O:69:LEU:HD12	13:O:70:CYS:H	1.61	0.65
5:R:10:PHE:CE1	34:R:101:HEM:HBD2	2.31	0.65
21:B:612:CLA:H171	21:B:613:CLA:HBB2	1.79	0.65
26:N:601:SQD:H101	21:N:618:CLA:H2	1.77	0.65
6:S:17:THR:HG23	6:S:20:TRP:H	1.61	0.65
1:A:214:MET:HA	1:A:214:MET:HE2	1.79	0.65
3:P:49:LEU:O	3:P:53:HIS:ND1	2.29	0.65
5:E:10:PHE:CE1	34:E:101:HEM:HBD2	2.32	0.65
27:D:412:LMG:H112	2:N:43:ALA:HA	1.78	0.65
2:N:414:PRO:HB2	2:N:415:PRO:HD3	1.79	0.65
2:N:490:GLN:O	2:N:490:GLN:NE2	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:60:THR:HG23	4:Q:61:HIS:CD2	2.32	0.65
3:C:118:HIS:CE1	27:C:520:LMG:H192	2.32	0.64
2:N:24:LEU:HD21	21:N:620:CLA:HAB	1.80	0.64
2:N:379:ALA:HA	2:N:390:TYR:HB3	1.79	0.64
3:C:48:LYS:NZ	3:C:133:ALA:O	2.30	0.64
11:L:8:GLN:HE21	11:L:8:GLN:N	1.95	0.64
16:V:62:ALA:O	34:V:201:HEM:HAB	1.96	0.64
4:Q:129:GLN:NE2	4:Q:143:ALA:HA	2.13	0.64
30:T:102:BCR:H23C	30:T:102:BCR:H403	1.80	0.64
30:B:618:BCR:H403	30:B:618:BCR:H23C	1.79	0.64
21:C:508:CLA:HBC3	21:C:510:CLA:H92	1.79	0.64
3:P:150:ASP:HB3	3:P:153:ASP:HB2	1.79	0.64
13:f:69:LEU:HD12	13:f:70:CYS:H	1.63	0.64
2:N:135:LEU:HA	2:N:138:MET:HE3	1.80	0.64
2:B:43:ALA:HA	27:Q:401:LMG:H112	1.79	0.63
6:F:17:THR:HG23	6:F:20:TRP:H	1.63	0.63
21:D:403:CLA:H42	18:X:26:GLY:HA3	1.79	0.63
21:N:616:CLA:H171	21:N:617:CLA:HBB2	1.81	0.63
3:P:42:LEU:HD21	21:P:511:CLA:H2A	1.79	0.63
3:C:361:PHE:HA	24:C:516:DGD:HE61	1.80	0.63
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.79	0.63
1:G:89:ILE:HD11	1:G:108:ASN:HB3	1.80	0.63
21:G:403:CLA:HED1	23:Q:405:PL9:H372	1.80	0.63
3:P:118:HIS:CE1	27:P:521:LMG:H192	2.32	0.63
4:Q:201:VAL:HB	21:Q:402:CLA:HMB2	1.80	0.63
11:d:8:GLN:HE21	11:d:8:GLN:N	1.96	0.63
2:B:124:ARG:HE	2:B:131:PRO:HD3	1.63	0.63
5:R:10:PHE:HE1	34:R:101:HEM:HBD2	1.62	0.63
14:T:21:ILE:HD12	30:T:102:BCR:H332	1.81	0.63
3:C:224:ILE:O	3:C:227:VAL:HG23	1.98	0.63
21:B:603:CLA:H193	7:H:42:LEU:HD12	1.80	0.62
1:G:64:ARG:O	13:f:178:ARG:NH2	2.32	0.62
2:N:22:ALA:O	2:N:25:MET:HB3	2.00	0.62
30:B:618:BCR:H19C	30:B:619:BCR:H363	1.81	0.62
4:D:274:VAL:HA	23:D:404:PL9:H253	1.80	0.62
10:K:21:LEU:HD13	17:y:24:MET:HE2	1.81	0.62
21:Q:404:CLA:H43	18:j:23:LEU:HA	1.80	0.62
3:C:158:THR:O	3:C:251:HIS:HB3	1.99	0.62
2:N:327:THR:HG22	21:N:611:CLA:H12	1.81	0.62
2:B:188:ASP:HA	7:H:58:VAL:HG23	1.82	0.62
2:N:68:ARG:HH22	21:N:608:CLA:HED1	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:188:ASP:HA	7:W:58:VAL:HG23	1.81	0.62
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.81	0.62
21:N:607:CLA:H193	7:W:42:LEU:HD12	1.80	0.62
2:B:22:ALA:HB1	21:B:612:CLA:HBB1	1.81	0.62
2:B:458:PHE:HB3	21:B:604:CLA:HBC2	1.82	0.62
21:B:603:CLA:CGA	21:B:603:CLA:H3A	2.30	0.62
4:D:201:VAL:HB	21:D:401:CLA:HMB2	1.82	0.62
4:Q:274:VAL:HA	23:Q:405:PL9:H253	1.82	0.62
3:C:447:ARG:HG2	3:C:447:ARG:HH11	1.64	0.62
4:D:186:GLN:HB2	21:D:401:CLA:HBC1	1.81	0.62
2:B:327:THR:HG22	21:B:607:CLA:H12	1.82	0.62
3:C:42:LEU:HD21	21:C:511:CLA:H2A	1.81	0.62
30:T:103:BCR:H311	21:N:610:CLA:H72	1.81	0.62
16:i:62:ALA:O	34:i:201:HEM:HAB	2.00	0.62
2:B:68:ARG:HH22	21:B:604:CLA:HED1	1.65	0.61
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.65	0.61
1:G:190:HIS:HB3	1:G:293:MET:HE2	1.81	0.61
4:Q:148:ALA:HB2	4:Q:276:VAL:HG13	1.82	0.61
26:N:601:SQD:H1	26:N:601:SQD:H462	1.81	0.61
21:N:612:CLA:HAB	4:Q:123:ILE:HG23	1.80	0.61
27:Q:407:LMG:HC62	11:d:15:THR:HG21	1.83	0.61
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.82	0.61
2:N:4:PRO:HD2	2:N:7:ARG:HD2	1.82	0.61
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.83	0.61
21:B:605:CLA:HBB1	21:B:606:CLA:H51	1.81	0.61
3:P:406:SER:O	3:P:418:ASN:ND2	2.33	0.61
21:Q:404:CLA:H42	18:j:26:GLY:HA3	1.82	0.61
2:N:9:HIS:ND1	21:N:616:CLA:HAB	2.16	0.61
21:N:609:CLA:HBB1	21:N:610:CLA:H51	1.83	0.61
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.82	0.61
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.81	0.61
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.66	0.61
7:H:12:ARG:O	7:H:12:ARG:HD3	2.01	0.61
3:P:75:PHE:HD1	3:P:86:LEU:HD21	1.66	0.61
34:R:101:HEM:HBB2	34:R:101:HEM:HHC	1.81	0.61
13:f:180:ALA:HB1	13:f:191:ALA:HB2	1.83	0.61
26:A:414:SQD:H321	30:I:101:BCR:H321	1.82	0.60
14:T:29:ILE:H	14:T:29:ILE:HD12	1.66	0.60
3:P:224:ILE:O	3:P:227:VAL:HG23	2.01	0.60
1:G:221:SER:HB3	4:Q:141:TYR:HB2	1.82	0.60
20:l:32:ASP:CG	20:l:33:TRP:H	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:E:101:HEM:HHC	34:E:101:HEM:HBB2	1.83	0.60
3:P:315:MET:HE1	3:P:369:LEU:HD12	1.83	0.60
2:N:270:PRO:HG3	2:N:312:TYR:HD2	1.67	0.60
7:W:12:ARG:O	7:W:12:ARG:HD3	2.02	0.60
20:l:32:ASP:HB2	20:l:35:ARG:HG2	1.84	0.60
3:P:48:LYS:NZ	3:P:133:ALA:O	2.35	0.60
14:g:29:ILE:HD12	14:g:29:ILE:H	1.66	0.60
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.67	0.60
21:B:608:CLA:H42	4:D:127:LEU:HD11	1.84	0.60
1:G:244:GLU:HG3	1:G:246:TYR:H	1.67	0.60
21:N:607:CLA:CGA	21:N:607:CLA:H3A	2.31	0.60
3:P:158:THR:O	3:P:251:HIS:HB3	2.02	0.60
5:E:18:ARG:HH11	5:E:18:ARG:HB3	1.65	0.60
13:f:77:LEU:HB3	13:f:91:PHE:HB3	1.84	0.60
30:c:101:BCR:HC8	30:c:101:BCR:H331	1.84	0.59
3:P:343:ARG:NH1	3:P:347:GLY:O	2.35	0.59
3:P:447:ARG:HG2	3:P:447:ARG:HH11	1.65	0.59
5:R:18:ARG:HH11	5:R:18:ARG:HB3	1.67	0.59
3:C:114:VAL:HG22	27:C:520:LMG:H152	1.84	0.59
27:D:407:LMG:HC62	11:L:15:THR:HG21	1.85	0.59
1:G:63:ILE:HB	3:P:335:THR:HG21	1.84	0.59
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.83	0.59
21:P:504:CLA:H151	24:P:518:DGD:HBW1	1.83	0.59
21:N:608:CLA:HBB1	21:N:611:CLA:CBB	2.33	0.59
3:P:466:VAL:HG13	4:Q:251:ARG:HD2	1.84	0.59
26:S:102:SQD:H162	18:j:33:THR:HA	1.84	0.59
2:B:247:PHE:HE1	21:B:602:CLA:H101	1.66	0.59
5:E:18:ARG:HD2	5:E:22:ILE:HD11	1.85	0.59
24:N:602:DGD:HA21	31:N:604:LMT:H121	1.83	0.59
21:C:511:CLA:H171	20:Z:20:VAL:HA	1.85	0.59
4:Q:186:GLN:HB2	21:Q:402:CLA:HBC1	1.82	0.59
1:A:15:GLU:O	1:A:19:ASN:ND2	2.35	0.59
2:B:135:LEU:HA	2:B:138:MET:HE3	1.83	0.59
3:C:49:LEU:O	3:C:53:HIS:ND1	2.32	0.59
3:C:315:MET:HE1	3:C:369:LEU:HD12	1.84	0.58
2:B:487:SER:N	2:B:488:PRO:HD2	2.18	0.58
26:B:627:SQD:H462	26:B:627:SQD:H1	1.83	0.58
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.84	0.58
4:Q:103:ARG:HG3	5:R:73:LYS:HG3	1.85	0.58
21:A:402:CLA:HED1	23:D:404:PL9:H372	1.85	0.58
5:E:81:GLU:C	5:E:83:LEU:H	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.85	0.58
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.03	0.58
1:G:84:PRO:HA	1:G:112:TYR:CG	2.39	0.58
3:P:131:TYR:HE1	3:P:135:ARG:HD2	1.69	0.58
3:P:166:ILE:O	3:P:170:ILE:HG13	2.03	0.58
4:Q:87:HIS:HD2	4:Q:162:LEU:HD23	1.67	0.58
5:R:81:GLU:C	5:R:83:LEU:H	2.11	0.58
20:Z:32:ASP:CG	20:Z:33:TRP:H	2.11	0.58
2:N:487:SER:N	2:N:488:PRO:HD2	2.18	0.58
27:Q:407:LMG:H111	11:d:19:LEU:HD21	1.84	0.58
21:B:614:CLA:H2	26:B:627:SQD:H101	1.85	0.58
4:D:279:LEU:HD11	22:D:402:PHO:HMC2	1.85	0.58
21:P:511:CLA:HMB1	30:P:514:BCR:H382	1.86	0.58
4:D:199:MET:HG2	23:D:404:PL9:H322	1.85	0.58
2:B:62:VAL:HG12	2:B:66:MET:HE2	1.86	0.58
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.85	0.58
3:C:343:ARG:NH1	3:C:347:GLY:O	2.37	0.58
20:l:33:TRP:O	20:l:37:LYS:HB2	2.03	0.57
3:C:377:LEU:O	3:C:381:LYS:HB2	2.04	0.57
21:C:503:CLA:H172	21:C:510:CLA:HBB2	1.86	0.57
5:E:10:PHE:HE1	34:E:101:HEM:HBD2	1.68	0.57
1:G:22:THR:HG21	8:a:30:ARG:HD3	1.86	0.57
1:A:244:GLU:HG3	1:A:246:TYR:H	1.69	0.57
21:B:608:CLA:HAB	4:D:123:ILE:HG23	1.85	0.57
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.04	0.57
1:G:317:TRP:HZ3	4:Q:180:ARG:HD3	1.67	0.57
3:C:137:PRO:HB2	3:C:139:THR:O	2.03	0.57
30:C:514:BCR:H341	30:K:101:BCR:H322	1.87	0.57
5:R:15:THR:HG23	9:b:8:ILE:O	2.03	0.57
5:E:81:GLU:O	5:E:83:LEU:N	2.35	0.57
2:N:341:LYS:HA	2:N:405:GLU:HB2	1.86	0.57
20:Z:32:ASP:HB2	20:Z:35:ARG:HG2	1.86	0.57
2:N:247:PHE:HE1	21:N:606:CLA:H101	1.68	0.57
4:Q:87:HIS:ND1	24:W:102:DGD:HD2	2.20	0.57
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.86	0.57
2:N:458:PHE:HB3	21:N:608:CLA:HBC2	1.85	0.57
3:P:429:SER:HB3	24:P:518:DGD:HA81	1.87	0.57
27:A:410:LMG:H211	11:L:26:VAL:HG21	1.87	0.57
2:N:213:GLY:O	2:N:217:ILE:HG13	2.04	0.57
7:W:3:ARG:NH2	11:d:1:MET:HE1	2.20	0.57
21:C:504:CLA:H202	24:C:518:DGD:HAF2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:GLU:O	1:G:19:ASN:ND2	2.37	0.57
21:P:503:CLA:H172	21:P:510:CLA:HBB2	1.85	0.57
7:W:3:ARG:HH21	11:d:1:MET:HE1	1.69	0.57
2:B:271:THR:HB	2:B:274:GLN:HG3	1.87	0.56
21:B:608:CLA:H151	21:B:609:CLA:H203	1.86	0.56
30:C:514:BCR:H382	21:C:511:CLA:HMB1	1.87	0.56
30:K:101:BCR:H331	30:K:101:BCR:C8	2.35	0.56
4:Q:259:ILE:HG12	27:Q:407:LMG:H292	1.86	0.56
1:A:111:PRO:O	1:A:115:ILE:HG13	2.04	0.56
1:A:193:LEU:HD11	21:A:401:CLA:HMC2	1.86	0.56
2:B:371:THR:HG22	2:B:377:VAL:HA	1.86	0.56
24:B:628:DGD:HD3	31:B:630:LMT:H12	1.87	0.56
4:D:87:HIS:HD2	4:D:162:LEU:HD23	1.70	0.56
1:G:153:SER:HB3	21:G:402:CLA:HED1	1.88	0.56
2:N:19:LEU:O	2:N:23:HIS:ND1	2.38	0.56
3:P:377:LEU:O	3:P:381:LYS:HB2	2.05	0.56
4:Q:21:TRP:O	4:Q:26:ARG:NH2	2.35	0.56
10:c:26:PRO:O	10:c:29:PRO:HD2	2.04	0.56
10:c:40:GLN:HA	10:c:43:VAL:HG12	1.86	0.56
13:f:223:ILE:HG13	13:f:243:SER:HB3	1.85	0.56
1:A:64:ARG:O	13:O:178:ARG:NH2	2.39	0.56
3:C:449:ARG:HE	21:C:505:CLA:HED1	1.70	0.56
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.87	0.56
21:A:403:CLA:H142	21:D:401:CLA:H151	1.87	0.56
2:B:213:GLY:O	2:B:217:ILE:HG13	2.06	0.56
21:B:603:CLA:HBA2	21:B:604:CLA:HED3	1.87	0.56
3:C:405:ASN:HD22	24:C:518:DGD:HD5	1.70	0.56
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.87	0.56
3:P:405:ASN:HD22	24:P:519:DGD:HD5	1.69	0.56
21:A:402:CLA:H203	22:A:404:PHO:H71	1.87	0.56
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.88	0.56
2:N:124:ARG:HE	2:N:131:PRO:HD3	1.71	0.56
3:P:114:VAL:HG22	27:P:521:LMG:H152	1.88	0.56
13:f:73:PRO:HG2	13:f:102:THR:HB	1.88	0.56
3:C:156:LYS:O	3:C:160:ILE:HG13	2.06	0.56
13:O:240:THR:HA	13:O:264:VAL:HA	1.86	0.56
16:i:81:ARG:CZ	16:i:157:GLY:HA3	2.36	0.56
1:A:240:GLY:HA3	14:T:29:ILE:HG22	1.88	0.56
1:G:28:LEU:HB2	26:G:401:SQD:H91	1.87	0.56
4:Q:148:ALA:HB3	4:Q:149:PRO:HD3	1.88	0.56
4:Q:192:THR:HG23	21:Q:402:CLA:HBC2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:84:LYS:HB2	5:R:84:LYS:NZ	2.21	0.56
16:i:59:PHE:HA	16:i:63:CYS:SG	2.46	0.56
4:D:259:ILE:HG12	27:D:407:LMG:H292	1.88	0.55
5:E:84:LYS:NZ	5:E:84:LYS:HB2	2.22	0.55
1:G:40:THR:HG21	1:G:121:LEU:HD23	1.88	0.55
21:P:511:CLA:H171	20:l:20:VAL:HA	1.87	0.55
4:Q:87:HIS:CD2	4:Q:162:LEU:HA	2.42	0.55
5:R:18:ARG:HD2	5:R:22:ILE:HD11	1.86	0.55
27:D:407:LMG:H111	11:L:19:LEU:HD21	1.89	0.55
1:G:32:TRP:HA	1:G:32:TRP:CE3	2.42	0.55
30:P:515:BCR:H24C	21:P:513:CLA:HAB	1.88	0.55
27:D:407:LMG:H392	30:T:102:BCR:HC32	1.89	0.55
21:N:612:CLA:H42	4:Q:127:LEU:HD11	1.88	0.55
4:Q:279:LEU:HD21	22:Q:403:PHO:HMC3	1.89	0.55
7:W:55:LEU:HB2	7:W:58:VAL:HG12	1.88	0.55
1:A:38:ILE:HG12	26:A:414:SQD:H142	1.88	0.55
21:B:604:CLA:HBB1	21:B:607:CLA:HBB2	1.89	0.55
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.87	0.55
2:N:348:ASN:HB3	2:N:354:LEU:HD21	1.87	0.55
2:N:371:THR:HG22	2:N:377:VAL:HA	1.87	0.55
4:D:266:TRP:CD1	27:D:407:LMG:HC3	2.42	0.55
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.39	0.55
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.88	0.55
20:Z:36:SER:HA	20:Z:39:LEU:HG	1.88	0.55
15:h:57:LEU:HD22	15:h:79:ILE:HG21	1.88	0.55
21:P:504:CLA:H202	24:P:519:DGD:HAF2	1.88	0.55
3:C:166:ILE:O	3:C:170:ILE:HG13	2.07	0.55
3:C:241:GLY:O	3:C:245:ILE:HG13	2.07	0.55
1:G:60:ILE:HD12	1:G:84:PRO:HD2	1.88	0.55
21:N:608:CLA:HBB1	21:N:611:CLA:HBB2	1.86	0.55
26:B:624:SQD:H241	26:B:624:SQD:H111	1.89	0.55
5:E:18:ARG:O	5:E:22:ILE:HG13	2.07	0.55
15:h:97:LEU:O	15:h:102:LYS:HE2	2.06	0.55
21:C:504:CLA:H151	24:C:517:DGD:HBW1	1.87	0.54
4:D:21:TRP:O	4:D:26:ARG:NH2	2.38	0.54
4:D:199:MET:HB3	23:D:404:PL9:H28	1.88	0.54
12:M:31:SER:HB3	27:M:101:LMG:HC71	1.88	0.54
2:N:89:GLY:HA2	24:N:602:DGD:HD5	1.88	0.54
3:P:137:PRO:HB2	3:P:139:THR:O	2.07	0.54
5:R:60:GLN:OE1	5:R:84:LYS:NZ	2.40	0.54
1:A:22:THR:HG21	8:I:30:ARG:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:O	1:A:241:GLN:HG3	2.07	0.54
16:i:102:MET:HE3	34:i:201:HEM:HBB2	1.89	0.54
21:G:403:CLA:HHC	21:G:403:CLA:HBB1	1.88	0.54
3:P:174:LEU:HD12	21:P:512:CLA:H71	1.89	0.54
21:A:402:CLA:HBB1	21:A:402:CLA:HHC	1.89	0.54
26:A:414:SQD:H332	21:N:610:CLA:H203	1.89	0.54
4:D:192:THR:HG23	21:D:401:CLA:HBC2	1.88	0.54
2:N:150:CYS:HA	21:N:607:CLA:HBC2	1.89	0.54
2:N:222:PRO:HG3	7:W:27:THR:H	1.73	0.54
24:P:519:DGD:HD2	9:b:32:ALA:O	2.08	0.54
30:c:101:BCR:H331	30:c:101:BCR:C8	2.36	0.54
3:C:429:SER:HB3	24:C:517:DGD:HA81	1.89	0.54
15:U:54:LYS:HB2	15:U:113:THR:HG23	1.88	0.54
5:R:56:TYR:O	16:i:27:ALA:HB2	2.07	0.54
5:E:15:THR:HG23	9:J:8:ILE:O	2.08	0.54
1:G:72:LEU:HD13	27:Q:401:LMG:H111	1.88	0.54
1:A:63:ILE:HB	3:C:335:THR:HG21	1.88	0.54
13:O:206:GLU:CD	13:O:206:GLU:H	2.16	0.54
3:P:215:LYS:HB3	3:P:223:TRP:HA	1.90	0.54
3:C:174:LEU:HD12	21:C:512:CLA:H71	1.89	0.54
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.43	0.54
7:H:35:MET:HE2	30:H:101:BCR:HC21	1.90	0.54
12:M:27:VAL:HG12	12:e:28:GLN:HB3	1.90	0.54
2:N:18:ARG:NH2	26:N:601:SQD:O9	2.41	0.54
21:B:614:CLA:H61	27:e:102:LMG:H181	1.90	0.54
24:C:518:DGD:HD2	9:J:32:ALA:O	2.08	0.54
16:V:59:PHE:HA	16:V:63:CYS:SG	2.48	0.54
20:l:36:SER:HA	20:l:39:LEU:HG	1.89	0.54
13:O:73:PRO:HG2	13:O:102:THR:HB	1.89	0.54
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.90	0.53
4:Q:122:LEU:HD11	22:Q:403:PHO:H92	1.90	0.53
1:A:32:TRP:CE3	1:A:32:TRP:HA	2.43	0.53
2:B:348:ASN:HB3	2:B:354:LEU:HD21	1.90	0.53
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.37	0.53
1:G:332:HIS:CD2	1:G:333:GLU:HG3	2.43	0.53
2:N:62:VAL:HG12	2:N:66:MET:HE2	1.90	0.53
1:A:45:THR:HG21	26:A:414:SQD:H201	1.91	0.53
3:C:466:VAL:HG13	4:D:251:ARG:HD2	1.89	0.53
21:C:511:CLA:H43	17:y:46:LEU:HD22	1.90	0.53
10:K:40:GLN:HA	10:K:43:VAL:HG12	1.91	0.53
20:Z:33:TRP:O	20:Z:33:TRP:CD1	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:256:MET:HA	2:N:263:THR:HG21	1.89	0.53
4:Q:43:LEU:HD23	4:Q:117:HIS:CE1	2.44	0.53
2:B:24:LEU:HD21	21:B:616:CLA:HAB	1.90	0.53
3:C:286:ALA:HB2	21:C:502:CLA:HMD1	1.90	0.53
1:G:190:HIS:O	1:G:298:ASN:HB3	2.09	0.53
15:h:72:TYR:HB3	15:h:73:PRO:HD3	1.90	0.53
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.44	0.53
5:E:8:ARG:HB2	6:F:13:TYR:HB3	1.89	0.53
20:Z:49:ALA:O	20:Z:53:VAL:HG23	2.09	0.53
2:N:19:LEU:HG	2:N:23:HIS:CE1	2.44	0.53
4:Q:199:MET:HG2	23:Q:405:PL9:H322	1.90	0.53
20:l:33:TRP:O	20:l:33:TRP:CD1	2.62	0.53
13:O:118:SER:HB3	13:O:157:PRO:HA	1.91	0.53
1:G:111:PRO:O	1:G:115:ILE:HG13	2.08	0.53
21:G:402:CLA:H122	22:G:405:PHO:H3A	1.90	0.53
26:G:410:SQD:H171	23:b:101:PL9:H522	1.90	0.53
3:P:350:ILE:HG21	3:P:359:TRP:HB2	1.91	0.53
4:Q:49:LEU:O	4:Q:53:THR:HG23	2.09	0.53
21:B:604:CLA:HBB1	21:B:607:CLA:CBB	2.38	0.53
3:C:45:LEU:HD23	3:C:48:LYS:HD2	1.91	0.53
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.91	0.53
1:G:183:MET:HE1	21:G:403:CLA:HMD2	1.91	0.53
2:N:69:LEU:HD12	21:N:609:CLA:HBA1	1.90	0.53
3:P:187:ASP:HB2	3:P:230:LEU:HD12	1.91	0.53
21:P:503:CLA:H152	21:P:509:CLA:H2	1.90	0.53
4:Q:103:ARG:NH1	5:R:77:GLU:OE2	2.42	0.53
15:h:83:ALA:HB1	15:h:84:PRO:CD	2.38	0.53
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.43	0.53
5:E:56:TYR:O	16:V:27:ALA:HB2	2.09	0.53
1:G:224:ILE:O	4:Q:265:ARG:NH2	2.40	0.53
3:P:449:ARG:HE	21:P:505:CLA:HED1	1.74	0.53
27:G:411:LMG:H211	11:d:26:VAL:HG21	1.90	0.52
23:A:406:PL9:H301	4:D:42:TYR:HA	1.91	0.52
5:E:61:ARG:HH22	16:V:153:GLY:HA3	1.74	0.52
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.74	0.52
5:R:8:ARG:NE	5:R:13:ILE:HG12	2.24	0.52
5:E:8:ARG:NE	5:E:13:ILE:HG12	2.24	0.52
1:G:93:PHE:CD2	1:G:95:PRO:HD3	2.44	0.52
6:S:21:VAL:O	6:S:25:THR:HG23	2.10	0.52
13:f:118:SER:HB3	13:f:157:PRO:HA	1.91	0.52
1:A:20:TRP:CD1	26:A:414:SQD:HO3	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:135:LEU:HB2	2:N:136:PRO:HD3	1.91	0.52
24:N:602:DGD:HD3	31:N:604:LMT:H12	1.92	0.52
21:N:620:CLA:H12	21:N:620:CLA:H72	1.92	0.52
3:P:149:TYR:HA	3:P:156:LYS:HD3	1.90	0.52
3:P:156:LYS:O	3:P:160:ILE:HG13	2.10	0.52
15:h:54:LYS:HB2	15:h:113:THR:HG23	1.91	0.52
20:l:49:ALA:O	20:l:53:VAL:HG23	2.09	0.52
27:D:406:LMG:O3	9:J:37:GLY:HA3	2.10	0.52
21:G:403:CLA:H203	22:G:405:PHO:H71	1.92	0.52
2:N:23:HIS:NE2	21:N:616:CLA:NB	2.58	0.52
1:A:140:ARG:HH22	25:A:408:LHG:P	2.32	0.52
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.90	0.52
2:B:329:PRO:HB3	21:B:607:CLA:HED1	1.92	0.52
4:D:266:TRP:HD1	27:D:407:LMG:HC3	1.75	0.52
10:K:26:PRO:O	10:K:29:PRO:HD2	2.10	0.52
12:M:28:GLN:HB3	12:e:27:VAL:HG12	1.91	0.52
30:T:101:BCR:H333	12:e:13:LEU:HD12	1.91	0.52
1:G:214:MET:HE1	4:Q:142:ASN:HD21	1.75	0.52
21:G:404:CLA:H142	21:Q:402:CLA:H151	1.90	0.52
2:N:9:HIS:HB2	21:N:615:CLA:HBA1	1.92	0.52
13:f:206:GLU:CD	13:f:206:GLU:H	2.17	0.52
1:A:190:HIS:O	1:A:298:ASN:HB3	2.10	0.52
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.74	0.52
5:E:7:GLU:H	5:E:7:GLU:CD	2.18	0.52
3:P:209:ILE:HG23	30:P:516:BCR:H382	1.91	0.52
3:P:240:ILE:O	3:P:244:CYS:HB2	2.10	0.52
4:Q:85:MET:HA	5:R:69:ARG:HB3	1.92	0.52
5:R:18:ARG:O	5:R:22:ILE:HG13	2.10	0.52
21:G:406:CLA:HBC1	27:a:102:LMG:H341	1.91	0.52
3:P:216:SER:HB3	3:P:221:GLU:HB2	1.92	0.52
4:Q:266:TRP:CD1	27:Q:407:LMG:HC3	2.45	0.52
5:R:7:GLU:CD	5:R:7:GLU:H	2.18	0.52
1:A:131:TRP:CH2	21:C:505:CLA:HAA2	2.45	0.52
1:A:329:GLU:O	1:A:332:HIS:ND1	2.38	0.52
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.43	0.52
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.92	0.52
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.91	0.52
27:G:411:LMG:H292	11:d:20:GLY:HA2	1.92	0.52
21:N:614:CLA:H152	21:N:619:CLA:HBD	1.92	0.52
5:R:8:ARG:HB2	6:S:13:TYR:HB3	1.91	0.52
10:c:37:PHE:HB3	30:c:101:BCR:C40	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:GLU:HB2	5:E:3:GLY:N	2.25	0.51
21:B:614:CLA:H2	26:B:627:SQD:H112	1.93	0.51
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.10	0.51
3:P:241:GLY:O	3:P:245:ILE:HG13	2.10	0.51
30:P:515:BCR:H312	20:l:55:GLY:HA2	1.91	0.51
5:R:81:GLU:O	5:R:83:LEU:N	2.36	0.51
27:I:102:LMG:H181	31:I:103:LMT:H42	1.91	0.51
12:M:28:GLN:CB	12:e:27:VAL:HG12	2.40	0.51
18:X:34:PHE:O	18:X:38:ILE:HG12	2.09	0.51
1:G:38:ILE:HG12	26:G:401:SQD:H142	1.93	0.51
1:G:238:LYS:O	1:G:241:GLN:HG3	2.10	0.51
3:P:130:VAL:O	3:P:134:ILE:HG12	2.10	0.51
12:e:31:SER:HB3	27:e:102:LMG:HC71	1.92	0.51
20:l:30:PRO:C	20:l:32:ASP:H	2.18	0.51
26:A:409:SQD:H241	25:A:411:LHG:HC81	1.91	0.51
21:B:616:CLA:H12	21:B:616:CLA:H72	1.91	0.51
15:U:57:LEU:HD22	15:U:79:ILE:HG21	1.92	0.51
15:h:38:GLU:HG2	15:h:39:LEU:N	2.26	0.51
3:C:347:GLY:HA3	13:O:43:ASN:HB2	1.93	0.51
20:Z:30:PRO:C	20:Z:32:ASP:H	2.19	0.51
1:G:119:PHE:HZ	21:G:402:CLA:H8	1.75	0.51
3:P:229:ASN:ND2	3:P:232:ASP:OD1	2.36	0.51
1:A:227:THR:HG21	1:A:233:ALA:HA	1.92	0.51
27:A:410:LMG:H292	11:L:20:GLY:HA2	1.93	0.51
2:B:9:HIS:HB2	21:B:611:CLA:HBA1	1.91	0.51
3:C:187:ASP:HB2	3:C:230:LEU:HD12	1.91	0.51
15:U:83:ALA:HB1	15:U:84:PRO:CD	2.38	0.51
3:P:45:LEU:HD23	3:P:48:LYS:HD2	1.93	0.51
3:P:120:ILE:HD11	30:P:514:BCR:HC8	1.93	0.51
2:B:256:MET:HA	2:B:263:THR:HG21	1.93	0.51
21:B:610:CLA:H152	21:B:615:CLA:HBD	1.93	0.51
1:G:140:ARG:HH22	25:G:409:LHG:P	2.33	0.51
26:A:409:SQD:H223	24:C:518:DGD:HAE1	1.93	0.51
2:B:280:PHE:O	2:B:284:ILE:HG13	2.11	0.51
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.93	0.51
3:P:248:GLY:O	3:P:252:ILE:HG12	2.11	0.51
1:A:159:LEU:C	1:A:162:PRO:HD2	2.36	0.51
2:N:315:ILE:HG22	2:N:426:PHE:HB3	1.93	0.51
18:j:34:PHE:O	18:j:38:ILE:HG12	2.10	0.51
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.92	0.51
3:C:240:ILE:O	3:C:244:CYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:ILE:HD11	30:C:515:BCR:H372	1.92	0.51
34:V:201:HEM:HBC2	34:V:201:HEM:HHD	1.93	0.51
21:G:402:CLA:H202	21:G:403:CLA:H93	1.93	0.51
2:N:26:HIS:CE1	21:N:616:CLA:HMA2	2.46	0.51
3:P:90:PRO:O	3:P:94:THR:HG23	2.11	0.51
13:f:184:ASP:OD2	13:f:188:ARG:HB2	2.11	0.51
13:f:190:LEU:HB2	13:f:214:LYS:HB2	1.93	0.51
2:B:230:ARG:O	2:B:233:ASN:HB3	2.11	0.51
10:K:37:PHE:HB3	30:K:101:BCR:C40	2.41	0.51
12:M:20:VAL:HG22	12:e:20:VAL:HG11	1.92	0.51
1:A:78:ILE:O	1:A:176:ILE:HB	2.11	0.50
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.46	0.50
26:A:409:SQD:H171	23:J:101:PL9:H522	1.92	0.50
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.92	0.50
1:G:57:PRO:HG3	1:G:68:SER:HB3	1.93	0.50
3:P:240:ILE:HD11	30:P:516:BCR:H372	1.93	0.50
4:Q:250:ASN:HD22	4:Q:262:SER:HB3	1.76	0.50
11:d:11:GLU:HG2	11:d:12:LEU:N	2.26	0.50
21:A:405:CLA:HBC1	27:I:102:LMG:H341	1.92	0.50
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.93	0.50
26:F:101:SQD:H162	18:X:33:THR:HA	1.92	0.50
1:G:136:ARG:NH2	8:a:27:ASP:OD1	2.42	0.50
12:e:3:VAL:HG11	14:g:2:GLU:HG2	1.92	0.50
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.92	0.50
3:P:72:LEU:HD11	3:P:108:THR:HB	1.92	0.50
13:f:87:GLN:O	13:f:88:GLU:HB3	2.11	0.50
1:A:183:MET:HE1	21:A:402:CLA:HMD2	1.92	0.50
2:B:133:LEU:HB3	2:B:138:MET:CE	2.41	0.50
24:B:628:DGD:HA21	31:B:630:LMT:H121	1.93	0.50
1:G:34:GLY:HA2	1:G:37:MET:HB3	1.92	0.50
4:Q:252:PHE:O	4:Q:256:ILE:HG22	2.11	0.50
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.93	0.50
1:A:235:TYR:C	1:A:237:TYR:H	2.20	0.50
1:A:332:HIS:CD2	1:A:333:GLU:HG3	2.46	0.50
1:G:188:ALA:HB2	1:G:328:MET:HB2	1.92	0.50
23:G:407:PL9:H301	4:Q:42:TYR:HA	1.94	0.50
21:A:403:CLA:HAB	21:D:401:CLA:H72	1.93	0.50
3:C:248:GLY:O	3:C:252:ILE:HG12	2.11	0.50
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.92	0.50
16:V:102:MET:HE3	34:V:201:HEM:HBB2	1.94	0.50
2:N:271:THR:HB	2:N:274:GLN:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:206:GLY:O	2:N:210:ILE:HG13	2.12	0.50
20:l:28:ALA:O	20:l:30:PRO:HD3	2.12	0.50
4:D:49:LEU:O	4:D:53:THR:HG23	2.11	0.50
13:f:144:LEU:HD13	13:f:259:VAL:HG11	1.93	0.50
1:A:224:ILE:O	4:D:265:ARG:NH2	2.41	0.49
3:C:90:PRO:O	3:C:94:THR:HG23	2.12	0.49
3:C:391:ARG:HB2	3:C:391:ARG:NH1	2.27	0.49
13:O:87:GLN:O	13:O:88:GLU:HB3	2.12	0.49
2:N:27:THR:HG22	2:N:107:LEU:HD13	1.94	0.49
3:P:347:GLY:HA3	13:f:43:ASN:HB2	1.93	0.49
4:Q:189:HIS:HA	4:Q:294:ARG:HD2	1.94	0.49
13:f:240:THR:HA	13:f:264:VAL:HA	1.94	0.49
1:G:258:LEU:HD12	4:Q:128:ARG:HD3	1.94	0.49
2:B:69:LEU:HD12	21:B:605:CLA:HBA1	1.93	0.49
2:B:222:PRO:HG3	7:H:27:THR:H	1.78	0.49
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.78	0.49
3:C:425:TRP:CE2	21:C:504:CLA:HBA1	2.46	0.49
21:C:507:CLA:OBD	21:C:509:CLA:H122	2.13	0.49
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.77	0.49
13:O:218:LEU:HD22	15:U:119:THR:HG21	1.93	0.49
2:N:486:LEU:HD13	2:N:486:LEU:O	2.12	0.49
3:P:29:GLU:HB3	10:c:46:ARG:HH11	1.78	0.49
3:C:165:LEU:HD21	21:C:506:CLA:HH11	1.94	0.49
21:C:513:CLA:HAB	30:Z:101:BCR:H24C	1.93	0.49
11:L:11:GLU:HG2	11:L:12:LEU:N	2.27	0.49
2:N:489:GLU:HB2	5:R:3:GLY:N	2.26	0.49
21:P:507:CLA:OBD	21:P:509:CLA:H122	2.12	0.49
7:W:35:MET:HE2	30:W:101:BCR:HC21	1.94	0.49
10:c:24:VAL:O	10:c:27:VAL:HG12	2.12	0.49
21:B:608:CLA:H12	4:D:127:LEU:HD21	1.93	0.49
1:G:235:TYR:C	1:G:237:TYR:H	2.20	0.49
4:Q:56:THR:HG21	5:R:50:PRO:HD3	1.93	0.49
4:Q:191:TRP:CE3	4:Q:289:LEU:HD11	2.48	0.49
4:Q:266:TRP:HD1	27:Q:407:LMG:HC3	1.76	0.49
5:R:27:ILE:HB	5:R:28:PRO:HD3	1.94	0.49
5:R:61:ARG:HH22	16:i:153:GLY:HA3	1.78	0.49
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.94	0.49
2:B:206:GLY:O	2:B:210:ILE:HG13	2.13	0.49
21:B:608:CLA:HBA2	26:B:624:SQD:H101	1.93	0.49
3:C:120:ILE:HD11	30:C:514:BCR:HC8	1.94	0.49
5:E:18:ARG:HB3	5:E:18:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:230:VAL:HG12	13:O:231:ASP:N	2.25	0.49
20:Z:55:GLY:HA2	30:Z:101:BCR:H312	1.95	0.49
1:G:238:LYS:HD2	14:g:32:LYS:HB3	1.94	0.49
1:G:240:GLY:HA3	14:g:29:ILE:HG22	1.95	0.49
4:Q:54:PHE:HB3	5:R:47:PHE:CD2	2.48	0.49
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.48	0.49
1:G:156:ALA:HA	1:G:160:ILE:HB	1.94	0.49
21:P:512:CLA:H143	21:P:513:CLA:H162	1.94	0.49
16:i:125:ASP:HA	16:i:131:ARG:HH21	1.78	0.49
17:m:39:LEU:CB	17:m:46:LEU:HD21	2.42	0.49
1:A:141:PRO:O	1:A:143:ILE:N	2.44	0.49
1:A:211:PHE:HA	1:A:214:MET:HB2	1.95	0.49
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.40	0.49
3:C:406:SER:O	3:C:418:ASN:ND2	2.43	0.49
21:C:503:CLA:H152	21:C:509:CLA:H2	1.95	0.49
12:M:20:VAL:HG11	12:e:20:VAL:HG22	1.94	0.49
1:G:78:ILE:O	1:G:176:ILE:HB	2.11	0.49
1:A:132:GLU:O	1:A:136:ARG:HG2	2.13	0.49
2:B:96:VAL:HG22	21:B:606:CLA:HBA1	1.94	0.49
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.48	0.49
21:N:606:CLA:H42	7:W:45:ILE:HD11	1.95	0.49
3:C:141:GLU:H	3:C:141:GLU:CD	2.20	0.49
3:C:259:TRP:H	3:C:259:TRP:CD1	2.30	0.49
4:D:252:PHE:O	4:D:256:ILE:HG22	2.13	0.49
11:L:7:ARG:C	11:L:8:GLN:HE21	2.21	0.49
1:G:141:PRO:O	1:G:143:ILE:N	2.44	0.49
2:N:124:ARG:HG3	2:N:124:ARG:HH11	1.77	0.49
30:B:618:BCR:HC32	27:Q:407:LMG:H392	1.95	0.48
26:B:624:SQD:H301	26:B:624:SQD:H171	1.95	0.48
21:C:503:CLA:HBB1	27:C:520:LMG:C20	2.43	0.48
4:D:55:VAL:HG21	4:D:110:LEU:HD12	1.95	0.48
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.94	0.48
13:O:190:LEU:HB2	13:O:214:LYS:HB2	1.95	0.48
26:G:410:SQD:H241	25:G:412:LHG:HC81	1.95	0.48
2:N:280:PHE:O	2:N:284:ILE:HG13	2.12	0.48
3:P:286:ALA:HB2	21:P:502:CLA:HMD1	1.94	0.48
1:A:40:THR:HG21	1:A:121:LEU:HD23	1.94	0.48
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.95	0.48
1:A:238:LYS:HD2	14:T:32:LYS:HB3	1.96	0.48
2:N:251:VAL:HA	24:W:102:DGD:HB51	1.95	0.48
31:N:625:LMT:H102	7:W:35:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:55:VAL:HG21	4:Q:110:LEU:HD12	1.94	0.48
9:b:18:GLY:HA3	30:c:101:BCR:H371	1.95	0.48
11:d:7:ARG:C	11:d:8:GLN:HE21	2.21	0.48
12:e:20:VAL:O	12:e:24:ILE:HG13	2.13	0.48
3:C:209:ILE:HG23	30:C:515:BCR:H382	1.94	0.48
27:M:101:LMG:H181	21:N:618:CLA:H61	1.96	0.48
1:G:126:TYR:O	1:G:130:GLN:HG3	2.14	0.48
1:G:183:MET:HA	21:G:402:CLA:HMD2	1.94	0.48
16:i:135:GLU:O	16:i:139:VAL:HG23	2.13	0.48
2:B:486:LEU:HD13	2:B:486:LEU:O	2.13	0.48
21:B:607:CLA:H3A	21:B:607:CLA:HBA2	1.36	0.48
3:C:72:LEU:HD11	3:C:108:THR:HB	1.95	0.48
26:N:601:SQD:H112	21:N:618:CLA:H2	1.96	0.48
21:N:606:CLA:H162	21:N:606:CLA:H122	1.55	0.48
3:P:391:ARG:NH1	3:P:391:ARG:HB2	2.28	0.48
4:Q:348:ARG:NH2	4:Q:352:LEU:O	2.41	0.48
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.48
21:A:401:CLA:H102	21:A:401:CLA:H62	1.61	0.48
2:B:191:ASN:HB2	7:H:58:VAL:CG2	2.44	0.48
21:B:606:CLA:H203	26:G:401:SQD:H332	1.94	0.48
21:C:509:CLA:CMB	21:C:511:CLA:HBB1	2.44	0.48
21:C:512:CLA:H143	21:C:513:CLA:H162	1.96	0.48
15:U:38:GLU:HG2	15:U:39:LEU:N	2.28	0.48
2:N:191:ASN:HB2	7:W:58:VAL:CG2	2.42	0.48
2:N:230:ARG:O	2:N:233:ASN:HB3	2.12	0.48
3:P:342:MET:HE3	3:P:352:GLY:HA2	1.96	0.48
30:P:514:BCR:H341	30:c:101:BCR:H322	1.94	0.48
13:f:178:ARG:HH11	13:f:178:ARG:CG	2.27	0.48
23:A:406:PL9:H33	4:D:38:PHE:HD1	1.78	0.48
18:X:12:ILE:HG12	18:X:16:LEU:HD12	1.95	0.48
2:N:7:ARG:NH2	27:N:622:LMG:O3	2.47	0.48
16:i:119:PRO:HG2	34:i:201:HEM:HMC2	1.96	0.48
18:j:17:LYS:O	18:j:21:ILE:HG13	2.14	0.48
2:B:483:ASP:CB	2:B:484:PRO:HD2	2.44	0.48
10:K:31:LEU:HB3	30:K:101:BCR:C15	2.43	0.48
2:N:243:ALA:HA	2:N:246:PHE:CE2	2.48	0.48
4:Q:18:LEU:O	4:Q:22:LEU:HG	2.13	0.48
5:R:20:TRP:HD1	9:b:8:ILE:HD13	1.77	0.48
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.95	0.48
2:B:30:VAL:HG13	21:B:613:CLA:HMC2	1.95	0.48
2:B:124:ARG:HG3	2:B:124:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.95	0.48
4:D:246:MET:HE3	4:D:262:SER:HA	1.96	0.48
7:H:3:ARG:NH2	11:L:1:MET:HE1	2.29	0.48
20:Z:28:ALA:O	20:Z:30:PRO:HD3	2.14	0.48
1:G:159:LEU:C	1:G:162:PRO:HD2	2.39	0.48
1:G:317:TRP:CD1	4:Q:177:ALA:HB2	2.49	0.48
3:P:141:GLU:CD	3:P:141:GLU:H	2.22	0.48
21:P:511:CLA:H43	17:m:46:LEU:HD22	1.94	0.48
13:f:59:ASP:C	13:f:61:SER:H	2.21	0.48
21:B:606:CLA:H18	21:B:616:CLA:H121	1.96	0.48
3:C:240:ILE:HG13	21:C:501:CLA:HBB1	1.95	0.48
4:D:39:PRO:O	4:D:43:LEU:HD22	2.13	0.48
11:L:6:ASN:O	11:L:8:GLN:NE2	2.47	0.48
17:y:41:VAL:C	17:y:43:ARG:H	2.22	0.48
1:G:131:TRP:CH2	21:P:505:CLA:HAA2	2.48	0.48
21:N:607:CLA:HBA2	21:N:608:CLA:HED3	1.95	0.48
3:P:472:LEU:HD12	3:P:473:ASP:H	1.79	0.48
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.79	0.48
8:I:6:ILE:O	8:I:10:ILE:HG12	2.13	0.48
13:O:36:ILE:HG23	13:O:41:LEU:HB3	1.96	0.48
1:G:132:GLU:O	1:G:136:ARG:HG2	2.14	0.48
2:N:184:GLU:H	2:N:200:ALA:HB2	1.79	0.48
21:N:620:CLA:HBA2	21:N:620:CLA:CGD	2.44	0.48
4:Q:152:VAL:HG21	4:Q:279:LEU:HD12	1.96	0.48
2:B:198:VAL:O	2:B:202:HIS:ND1	2.43	0.47
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.48	0.47
3:C:149:TYR:HA	3:C:156:LYS:HD3	1.96	0.47
16:V:98:LEU:O	16:V:102:MET:HG3	2.14	0.47
3:P:223:TRP:CD2	3:P:224:ILE:HG13	2.49	0.47
4:Q:199:MET:HB3	23:Q:405:PL9:H28	1.96	0.47
4:Q:246:MET:HE3	4:Q:262:SER:HA	1.95	0.47
13:f:218:LEU:HD22	15:h:119:THR:HG21	1.94	0.47
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.48	0.47
1:A:143:ILE:HD11	4:D:217:THR:HA	1.96	0.47
21:B:614:CLA:H51	30:B:617:BCR:H372	1.96	0.47
5:E:23:HIS:HA	5:E:26:THR:OG1	2.14	0.47
10:K:24:VAL:O	10:K:27:VAL:HG12	2.14	0.47
1:G:65:GLU:OE2	1:G:334:ARG:NH2	2.48	0.47
11:d:6:ASN:O	11:d:8:GLN:NE2	2.47	0.47
4:D:157:PHE:CE1	4:D:171:PRO:HG2	2.49	0.47
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:33:TRP:O	20:Z:33:TRP:HD1	1.97	0.47
4:Q:302:GLU:OE1	13:f:186:LYS:NZ	2.39	0.47
13:f:59:ASP:HB3	13:f:62:GLN:HB3	1.96	0.47
2:B:26:HIS:CE1	21:B:612:CLA:HMA2	2.50	0.47
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.96	0.47
4:D:134:ARG:HE	4:D:134:ARG:HA	1.79	0.47
27:M:101:LMG:H292	21:N:618:CLA:HMD2	1.97	0.47
2:N:329:PRO:HB3	21:N:611:CLA:HED1	1.95	0.47
3:P:223:TRP:CG	3:P:224:ILE:H	2.33	0.47
3:P:386:PRO:HB3	16:i:116:GLU:HG2	1.96	0.47
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.50	0.47
3:C:275:SER:HB3	21:C:509:CLA:HED3	1.96	0.47
7:H:19:GLY:O	7:H:21:VAL:HG13	2.14	0.47
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.50	0.47
22:G:405:PHO:H41	22:G:405:PHO:H62	1.49	0.47
3:P:275:SER:HB3	21:P:509:CLA:HED3	1.95	0.47
21:P:504:CLA:H121	24:P:518:DGD:HBE2	1.97	0.47
26:S:102:SQD:H131	18:j:36:VAL:HG11	1.96	0.47
2:B:271:THR:HG22	2:B:273:TYR:N	2.29	0.47
21:B:610:CLA:H12	21:B:610:CLA:H112	1.95	0.47
31:B:629:LMT:H122	14:g:7:VAL:HG12	1.96	0.47
3:C:130:VAL:O	3:C:134:ILE:HG12	2.14	0.47
3:C:472:LEU:HD12	3:C:473:ASP:H	1.80	0.47
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.15	0.47
7:H:3:ARG:HH21	11:L:1:MET:HE1	1.80	0.47
8:I:24:LEU:O	8:I:26:GLY:N	2.42	0.47
1:G:180:PHE:O	1:G:184:ILE:HG13	2.15	0.47
26:Q:408:SQD:H241	26:Q:408:SQD:H111	1.96	0.47
1:A:126:TYR:O	1:A:130:GLN:HG3	2.14	0.47
1:A:176:ILE:HD12	21:A:402:CLA:HED3	1.97	0.47
1:A:183:MET:HA	21:A:401:CLA:HMD2	1.97	0.47
2:B:12:LEU:HD22	2:B:18:ARG:HB2	1.97	0.47
2:B:317:ASN:HA	2:B:330:MET:HE1	1.97	0.47
31:B:626:LMT:H102	7:H:35:MET:SD	2.55	0.47
3:C:75:PHE:CD1	3:C:86:LEU:HD21	2.47	0.47
3:C:276:LEU:HD11	3:C:444:HIS:HD2	1.79	0.47
4:D:18:LEU:O	4:D:22:LEU:HG	2.15	0.47
2:N:133:LEU:HB3	2:N:138:MET:CE	2.44	0.47
2:N:198:VAL:O	2:N:202:HIS:ND1	2.41	0.47
4:Q:161:PRO:HB3	4:Q:170:ALA:HB2	1.95	0.47
4:Q:210:LEU:HA	4:Q:213:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:28:VAL:HB	6:S:29:PRO:HD3	1.97	0.47
9:b:9:PRO:HB2	9:b:12:ILE:HG13	1.96	0.47
9:b:15:THR:O	9:b:19:MET:HG3	2.15	0.47
15:h:99:GLU:HA	15:h:102:LYS:HE3	1.96	0.47
18:j:12:ILE:HG12	18:j:16:LEU:HD12	1.97	0.47
21:A:402:CLA:HBA1	21:A:402:CLA:CHA	2.44	0.47
4:D:264:LYS:O	4:D:268:HIS:ND1	2.38	0.47
6:F:21:VAL:O	6:F:25:THR:HG23	2.15	0.47
8:I:15:PHE:CE1	30:I:101:BCR:H312	2.49	0.47
11:L:5:PRO:HA	11:L:7:ARG:HH22	1.79	0.47
21:N:607:CLA:H141	21:N:607:CLA:H161	1.61	0.47
4:Q:129:GLN:HE22	4:Q:143:ALA:HA	1.80	0.47
10:c:31:LEU:HB3	30:c:101:BCR:C15	2.45	0.47
20:l:29:SER:C	20:l:31:GLN:H	2.23	0.47
21:C:509:CLA:H62	21:C:509:CLA:H92	1.70	0.47
30:C:514:BCR:H343	30:C:514:BCR:H321	1.96	0.47
3:P:305:THR:HG22	3:P:308:GLU:HB2	1.97	0.47
4:Q:87:HIS:CD2	4:Q:162:LEU:HD23	2.46	0.47
1:A:119:PHE:HZ	21:A:401:CLA:H8	1.78	0.47
3:C:342:MET:HE3	3:C:352:GLY:HA2	1.97	0.47
30:T:101:BCR:H372	21:N:618:CLA:H51	1.96	0.47
26:G:401:SQD:H321	30:a:101:BCR:H321	1.97	0.47
22:G:405:PHO:H61	22:G:405:PHO:H92	1.62	0.47
21:G:404:CLA:H202	27:Q:406:LMG:H401	1.96	0.47
26:G:410:SQD:H223	24:P:519:DGD:HAE1	1.96	0.47
3:P:75:PHE:CD1	3:P:86:LEU:HD21	2.48	0.47
3:P:135:ARG:HB2	20:l:27:TYR:HB3	1.96	0.47
5:R:23:HIS:HA	5:R:26:THR:OG1	2.14	0.47
7:W:19:GLY:O	7:W:21:VAL:HG13	2.14	0.47
13:f:147:THR:OG1	13:f:148:VAL:N	2.48	0.47
1:A:244:GLU:OE1	4:D:264:LYS:NZ	2.48	0.46
2:B:286:ARG:HG2	2:B:286:ARG:HH11	1.80	0.46
2:B:474:LEU:O	4:D:134:ARG:NH1	2.48	0.46
3:C:29:GLU:HB3	10:K:46:ARG:NH1	2.30	0.46
3:C:265:ILE:HG12	21:C:505:CLA:HED1	1.97	0.46
21:C:501:CLA:C2D	21:C:503:CLA:H2	2.45	0.46
5:E:8:ARG:HB2	6:F:13:TYR:CB	2.46	0.46
13:O:59:ASP:C	13:O:61:SER:H	2.23	0.46
14:T:22:PHE:HB3	30:T:103:BCR:H291	1.97	0.46
20:Z:29:SER:C	20:Z:31:GLN:H	2.22	0.46
2:N:271:THR:HG22	2:N:273:TYR:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:286:ARG:HG2	2:N:286:ARG:HH11	1.80	0.46
21:P:505:CLA:HBA1	21:P:505:CLA:CBD	2.41	0.46
4:Q:244:TYR:OH	4:Q:264:LYS:HE3	2.14	0.46
13:f:230:VAL:HG12	13:f:231:ASP:N	2.25	0.46
21:C:504:CLA:H121	24:C:517:DGD:HBE2	1.97	0.46
7:H:31:MET:HE3	7:H:35:MET:HE1	1.97	0.46
1:G:182:PHE:O	1:G:186:PHE:HB2	2.16	0.46
2:N:483:ASP:CB	2:N:484:PRO:HD2	2.44	0.46
3:P:461:ARG:HG3	3:P:461:ARG:HH11	1.80	0.46
7:W:55:LEU:O	7:W:58:VAL:HG12	2.15	0.46
13:f:33:TYR:O	13:f:37:VAL:HG23	2.15	0.46
1:A:38:ILE:O	1:A:42:LEU:HG	2.16	0.46
2:B:190:PHE:HE2	7:H:41:PHE:HE1	1.61	0.46
2:B:251:VAL:HA	24:B:621:DGD:HB51	1.97	0.46
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.81	0.46
1:G:27:ARG:NH1	4:Q:254:SER:O	2.48	0.46
1:G:29:TYR:CG	1:G:133:LEU:HD13	2.50	0.46
21:G:404:CLA:H93	21:Q:402:CLA:H152	1.97	0.46
3:P:197:ARG:NH2	3:P:231:GLU:OE2	2.48	0.46
4:Q:88:SER:HB2	5:R:69:ARG:NH2	2.30	0.46
6:S:11:VAL:HG12	6:S:12:SER:H	1.81	0.46
16:i:98:LEU:O	16:i:102:MET:HG3	2.15	0.46
2:B:10:THR:C	2:B:12:LEU:H	2.23	0.46
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.96	0.46
5:E:82:GLN:H	5:E:82:GLN:HG3	1.52	0.46
11:L:7:ARG:HD2	11:L:7:ARG:O	2.16	0.46
3:P:259:TRP:CD1	3:P:259:TRP:H	2.32	0.46
3:P:380:ILE:HA	3:P:384:ILE:HD11	1.97	0.46
4:Q:67:TYR:CE1	4:Q:76:VAL:HG11	2.50	0.46
1:A:92:HIS:CD2	3:C:219:GLY:HA3	2.50	0.46
1:A:257:ARG:HH22	2:B:489:GLU:HA	1.81	0.46
3:C:362:ARG:O	24:C:516:DGD:O4E	2.31	0.46
30:J:102:BCR:H15C	30:J:102:BCR:H351	1.68	0.46
13:O:77:LEU:HD23	13:O:93:PRO:HA	1.97	0.46
21:G:402:CLA:HBA1	21:G:402:CLA:H3A	1.55	0.46
22:Q:403:PHO:H151	21:Q:402:CLA:H172	1.98	0.46
10:c:18:PHE:N	10:c:18:PHE:HD2	2.14	0.46
3:C:28:GLN:HB2	21:C:511:CLA:HED3	1.97	0.46
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.16	0.46
21:G:403:CLA:CHA	21:G:403:CLA:HBA1	2.46	0.46
2:N:18:ARG:HD3	2:N:118:TRP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:405:ASN:HB2	24:P:519:DGD:HG31	1.98	0.46
5:R:18:ARG:HB3	5:R:18:ARG:NH1	2.29	0.46
30:b:102:BCR:H15C	30:b:102:BCR:H351	1.68	0.46
13:f:35:ASP:C	13:f:36:ILE:HD12	2.41	0.46
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.50	0.46
21:B:603:CLA:H141	21:B:603:CLA:H161	1.62	0.46
21:B:612:CLA:CMB	21:B:614:CLA:HBB1	2.46	0.46
30:B:618:BCR:H11C	30:B:618:BCR:H341	1.84	0.46
3:C:85:GLY:N	24:C:517:DGD:HE4	2.31	0.46
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.49	0.46
3:C:461:ARG:HH11	3:C:461:ARG:HG3	1.79	0.46
5:E:78:THR:O	5:E:81:GLU:HB2	2.15	0.46
13:O:55:ALA:HA	13:O:230:VAL:HG11	1.98	0.46
2:N:256:MET:O	2:N:448:ARG:NH1	2.42	0.46
3:P:165:LEU:HD21	21:P:506:CLA:HHC	1.98	0.46
3:P:245:ILE:O	3:P:249:ILE:HG12	2.15	0.46
2:B:150:CYS:HA	21:B:603:CLA:HBC2	1.98	0.46
9:J:9:PRO:HB2	9:J:12:ILE:HG13	1.98	0.46
9:J:14:ALA:HB3	30:K:101:BCR:H393	1.97	0.46
10:K:18:PHE:O	10:K:22:VAL:HG23	2.16	0.46
1:G:93:PHE:CD2	24:G:408:DGD:HD2	2.51	0.46
1:G:262:TYR:O	27:R:102:LMG:H112	2.16	0.46
3:P:178:LYS:HA	3:P:182:PHE:HB2	1.97	0.46
4:Q:39:PRO:O	4:Q:43:LEU:HD22	2.16	0.46
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.51	0.46
31:B:629:LMT:H3'	31:B:629:LMT:H1B	1.62	0.46
27:D:407:LMG:HC2	27:D:407:LMG:HC71	1.77	0.46
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.51	0.46
1:G:38:ILE:O	1:G:42:LEU:HG	2.15	0.46
4:Q:264:LYS:O	4:Q:268:HIS:ND1	2.32	0.46
1:A:180:PHE:O	1:A:184:ILE:HG13	2.16	0.46
23:A:406:PL9:H33	4:D:38:PHE:CD1	2.50	0.46
21:B:614:CLA:HMD2	27:e:102:LMG:H292	1.98	0.46
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.98	0.46
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.81	0.46
21:G:404:CLA:HAB	21:Q:402:CLA:H72	1.98	0.46
3:P:455:PHE:C	3:P:457:LYS:H	2.24	0.46
30:P:514:BCR:H343	30:P:514:BCR:H321	1.96	0.46
17:m:41:VAL:C	17:m:43:ARG:H	2.23	0.46
21:B:609:CLA:H62	21:B:609:CLA:H92	1.71	0.45
18:X:17:LYS:O	18:X:21:ILE:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:51:VAL:HG13	2:N:308:LYS:HB2	1.98	0.45
3:P:276:LEU:HD11	3:P:444:HIS:HD2	1.81	0.45
30:P:514:BCR:H312	20:l:9:LEU:HD11	1.98	0.45
11:d:7:ARG:HD2	11:d:7:ARG:O	2.15	0.45
12:e:29:THR:O	12:e:32:GLN:HG3	2.16	0.45
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.45
30:C:514:BCR:H312	20:Z:9:LEU:HD11	1.97	0.45
27:D:406:LMG:O4	9:J:31:GLY:O	2.34	0.45
1:G:329:GLU:O	1:G:332:HIS:ND1	2.40	0.45
4:Q:103:ARG:O	4:Q:107:LEU:HG	2.17	0.45
4:Q:239:GLN:HB3	4:Q:240:ALA:H	1.32	0.45
10:c:18:PHE:N	10:c:18:PHE:CD2	2.84	0.45
16:i:38:LEU:H	16:i:44:THR:HA	1.81	0.45
21:A:403:CLA:H202	27:D:406:LMG:H401	1.98	0.45
2:B:192:PRO:HD2	7:H:60:VAL:HG12	1.98	0.45
21:B:602:CLA:H61	7:H:46:LEU:HB2	1.97	0.45
24:B:621:DGD:HD2	4:D:87:HIS:ND1	2.32	0.45
3:C:155:ASN:HA	3:C:158:THR:HG22	1.98	0.45
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.98	0.45
13:O:33:TYR:O	13:O:37:VAL:HG23	2.17	0.45
14:T:7:VAL:HG12	31:N:603:LMT:H122	1.97	0.45
26:N:601:SQD:H112	21:N:618:CLA:H51	1.98	0.45
3:P:120:ILE:CD1	30:P:514:BCR:HC8	2.46	0.45
20:l:33:TRP:O	20:l:33:TRP:HD1	1.98	0.45
1:A:153:SER:HB3	21:A:401:CLA:HED1	1.99	0.45
1:A:249:VAL:HG11	2:B:486:LEU:HD23	1.99	0.45
3:C:305:THR:HG22	3:C:308:GLU:H	1.79	0.45
27:D:406:LMG:H171	30:D:405:BCR:H383	1.97	0.45
7:H:55:LEU:O	7:H:58:VAL:HG12	2.17	0.45
9:J:14:ALA:CB	30:K:101:BCR:H393	2.46	0.45
12:M:20:VAL:O	12:M:24:ILE:HG13	2.16	0.45
17:y:19:ILE:HG23	17:y:20:ALA:H	1.81	0.45
17:y:33:PRO:O	17:y:36:ILE:HG13	2.17	0.45
18:X:12:ILE:HA	18:X:16:LEU:HD12	1.97	0.45
26:G:410:SQD:H202	24:P:519:DGD:HAH2	1.98	0.45
2:N:23:HIS:NE2	21:N:616:CLA:C4B	2.80	0.45
21:N:611:CLA:HBA2	21:N:611:CLA:H3A	1.34	0.45
21:A:403:CLA:H93	21:D:401:CLA:H152	1.97	0.45
2:B:6:TYR:HA	21:B:611:CLA:H11	1.99	0.45
30:B:617:BCR:H333	12:M:13:LEU:HD12	1.99	0.45
27:B:623:LMG:HC3	31:M:102:LMT:H2'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:11:VAL:HG12	6:F:12:SER:H	1.81	0.45
7:H:12:ARG:HD3	7:H:12:ARG:C	2.42	0.45
12:M:27:VAL:HG12	12:e:28:GLN:CB	2.46	0.45
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.98	0.45
13:O:178:ARG:HH11	13:O:178:ARG:CG	2.26	0.45
16:V:74:THR:O	16:V:75:ASN:HB2	2.17	0.45
25:G:412:LHG:H271	25:G:412:LHG:H101	1.99	0.45
3:P:80:PRO:HB3	3:P:82:TYR:CE1	2.52	0.45
4:Q:350:ASN:O	4:Q:352:LEU:N	2.45	0.45
5:R:78:THR:O	5:R:81:GLU:HB2	2.16	0.45
9:b:11:TRP:CZ3	17:m:36:ILE:HD11	2.52	0.45
10:c:18:PHE:O	10:c:22:VAL:HG23	2.17	0.45
21:A:405:CLA:H162	21:A:405:CLA:H141	1.60	0.45
21:B:606:CLA:H3A	21:B:606:CLA:HBA2	1.31	0.45
21:B:608:CLA:H92	26:B:624:SQD:H172	1.99	0.45
3:C:135:ARG:HB2	20:Z:27:TYR:HB3	1.99	0.45
34:E:101:HEM:HBC2	6:F:31:ILE:HD13	1.99	0.45
8:I:29:ALA:HA	8:I:35:LYS:HB2	1.99	0.45
1:G:272:HIS:CD2	4:Q:218:VAL:HG21	2.51	0.45
21:N:616:CLA:CMB	21:N:618:CLA:HBB1	2.47	0.45
3:P:225:VAL:HG13	3:P:289:PHE:HA	1.98	0.45
3:P:415:ASN:O	3:P:416:SER:HB3	2.17	0.45
30:P:514:BCR:H343	30:P:514:BCR:H311	1.98	0.45
5:R:8:ARG:HB2	6:S:13:TYR:CB	2.47	0.45
13:f:36:ILE:HG23	13:f:41:LEU:HB3	1.97	0.45
13:f:77:LEU:HD23	13:f:93:PRO:HA	1.99	0.45
34:i:201:HEM:HHD	34:i:201:HEM:HBC2	1.99	0.45
17:m:19:ILE:HG23	17:m:20:ALA:H	1.82	0.45
1:A:41:LEU:O	1:A:45:THR:HG22	2.16	0.45
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.99	0.45
1:A:182:PHE:O	1:A:186:PHE:HB2	2.16	0.45
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.97	0.45
2:B:349:LYS:HG2	2:B:395:GLN:O	2.17	0.45
21:B:603:CLA:CBB	21:B:605:CLA:H152	2.47	0.45
11:L:1:MET:HE2	11:L:1:MET:HA	1.99	0.45
12:M:20:VAL:HG21	12:e:20:VAL:HG21	1.99	0.45
24:N:602:DGD:HB21	31:N:604:LMT:H72	1.99	0.45
3:P:38:GLY:HA3	21:P:511:CLA:HMD2	1.99	0.45
4:Q:172:SER:HB2	4:Q:177:ALA:HB1	1.98	0.45
21:B:602:CLA:H42	7:H:45:ILE:HD11	1.99	0.45
21:B:612:CLA:H162	21:B:612:CLA:H122	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:67:TYR:CE1	4:D:76:VAL:HG11	2.51	0.45
9:J:18:GLY:HA3	30:K:101:BCR:H371	1.99	0.45
13:O:35:ASP:C	13:O:36:ILE:HD12	2.41	0.45
13:O:126:GLY:O	13:O:128:ASP:N	2.49	0.45
15:U:97:LEU:O	15:U:102:LYS:HE2	2.17	0.45
1:G:220:THR:O	1:G:223:LEU:HG	2.16	0.45
26:Q:408:SQD:H301	26:Q:408:SQD:H171	1.99	0.45
9:b:14:ALA:CB	30:c:101:BCR:H393	2.47	0.45
15:h:38:GLU:HG2	15:h:39:LEU:H	1.82	0.45
1:A:49:VAL:O	1:A:53:ILE:HG13	2.17	0.45
2:B:122:LEU:O	7:H:15:ASN:ND2	2.49	0.45
26:B:624:SQD:H81	26:B:624:SQD:H45	1.79	0.45
3:C:53:HIS:HB3	21:C:512:CLA:OBD	2.16	0.45
1:G:69:GLY:O	1:G:81:ALA:N	2.40	0.45
2:N:103:LEU:HD21	21:N:609:CLA:HMC3	1.99	0.45
27:Q:406:LMG:O3	9:b:37:GLY:HA3	2.17	0.45
13:f:178:ARG:HD2	13:f:182:PHE:CD1	2.52	0.45
17:m:31:ALA:O	17:m:35:ILE:HG23	2.17	0.45
21:A:401:CLA:H202	21:A:402:CLA:H93	1.98	0.44
10:K:16:ALA:O	10:K:19:ASP:HB2	2.17	0.44
1:G:49:VAL:O	1:G:53:ILE:HG13	2.16	0.44
26:G:410:SQD:H132	25:G:412:LHG:H132	1.98	0.44
21:N:612:CLA:H12	4:Q:127:LEU:HD21	1.98	0.44
3:P:305:THR:HG22	3:P:308:GLU:H	1.82	0.44
3:P:425:TRP:CE2	21:P:504:CLA:HBA1	2.52	0.44
21:A:402:CLA:H62	21:A:402:CLA:H41	1.82	0.44
2:B:184:GLU:H	2:B:200:ALA:HB2	1.81	0.44
3:C:391:ARG:HB2	3:C:391:ARG:HH11	1.83	0.44
13:O:31:LEU:HB2	13:O:36:ILE:HD11	1.99	0.44
2:N:12:LEU:HD22	2:N:18:ARG:HB2	1.97	0.44
27:Q:406:LMG:H391	23:b:101:PL9:H112	1.99	0.44
5:R:20:TRP:CD1	9:b:8:ILE:HD13	2.53	0.44
16:i:147:VAL:O	16:i:150:LYS:HB2	2.17	0.44
2:B:68:ARG:NH1	2:B:262:THR:HG23	2.32	0.44
2:B:483:ASP:CG	2:B:484:PRO:HD2	2.41	0.44
3:C:245:ILE:O	3:C:249:ILE:HG12	2.17	0.44
3:C:425:TRP:HE1	24:C:517:DGD:HE62	1.82	0.44
30:I:101:BCR:H351	30:I:101:BCR:H15C	1.84	0.44
30:T:102:BCR:H19C	30:N:621:BCR:H363	1.99	0.44
17:y:19:ILE:HG23	17:y:20:ALA:N	2.32	0.44
1:G:41:LEU:O	1:G:45:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:PHE:CE2	23:G:407:PL9:H111	2.52	0.44
1:G:322:ASN:OD1	3:P:412:THR:HA	2.17	0.44
2:N:34:ALA:HB2	21:N:609:CLA:HMD2	2.00	0.44
3:P:50:LEU:HD11	21:P:513:CLA:HBB1	1.98	0.44
6:S:11:VAL:HG12	6:S:12:SER:N	2.32	0.44
8:a:24:LEU:O	8:a:26:GLY:N	2.43	0.44
17:m:19:ILE:HG23	17:m:20:ALA:N	2.32	0.44
17:m:42:ARG:HG2	17:m:42:ARG:HH11	1.83	0.44
1:A:220:THR:O	1:A:223:LEU:HG	2.17	0.44
13:O:118:SER:HA	13:O:159:VAL:HG12	2.00	0.44
15:U:64:ALA:O	15:U:67:GLN:HG2	2.18	0.44
2:N:134:ASP:OD2	2:N:137:LYS:HE3	2.16	0.44
21:N:616:CLA:H122	21:N:616:CLA:H162	1.66	0.44
3:P:363:GLY:O	3:P:367:GLU:HG2	2.17	0.44
5:R:79:PHE:HA	5:R:82:GLN:HE21	1.83	0.44
30:b:102:BCR:H20C	30:b:102:BCR:H361	1.88	0.44
18:j:12:ILE:HA	18:j:16:LEU:HD12	1.99	0.44
1:A:262:TYR:O	27:E:102:LMG:H112	2.18	0.44
1:A:283:VAL:O	1:A:286:THR:HG22	2.16	0.44
21:A:401:CLA:H122	22:A:404:PHO:H3A	2.00	0.44
22:A:404:PHO:H92	22:A:404:PHO:H61	1.63	0.44
2:B:91:TRP:HE1	31:B:625:LMT:H12	1.81	0.44
21:B:605:CLA:HMA2	21:B:606:CLA:HMA2	1.99	0.44
21:B:616:CLA:H61	26:G:401:SQD:H301	1.99	0.44
3:C:284:PHE:HB3	24:C:516:DGD:HA51	2.00	0.44
21:C:509:CLA:HMB1	21:C:511:CLA:HBB1	1.99	0.44
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.99	0.44
11:L:5:PRO:HA	11:L:7:ARG:NH2	2.32	0.44
17:y:34:MET:HE1	17:y:38:LEU:HD21	1.99	0.44
2:N:192:PRO:HD2	7:W:60:VAL:HG12	2.00	0.44
3:P:160:ILE:HA	3:P:163:PHE:CD2	2.52	0.44
30:P:514:BCR:HC7	30:P:514:BCR:H331	1.31	0.44
4:Q:294:ARG:H	4:Q:294:ARG:HG2	1.66	0.44
21:Q:402:CLA:H92	21:Q:402:CLA:H62	1.63	0.44
16:i:74:THR:O	16:i:75:ASN:HB2	2.17	0.44
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.51	0.44
3:C:143:TYR:O	3:C:144:SER:HB2	2.18	0.44
21:C:501:CLA:C3D	21:C:503:CLA:H2	2.48	0.44
22:D:402:PHO:H143	22:D:402:PHO:H111	1.87	0.44
6:F:11:VAL:HG12	6:F:12:SER:N	2.33	0.44
9:J:15:THR:O	9:J:19:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:147:VAL:O	16:V:150:LYS:HB2	2.18	0.44
17:y:20:ALA:C	17:y:22:LEU:H	2.26	0.44
1:G:265:PHE:CD1	1:G:271:LEU:HA	2.53	0.44
2:N:483:ASP:CG	2:N:484:PRO:HD2	2.42	0.44
3:P:29:GLU:HB3	10:c:46:ARG:NH1	2.33	0.44
21:P:509:CLA:CMB	21:P:511:CLA:HBB1	2.48	0.44
30:P:515:BCR:H24C	30:P:515:BCR:H371	1.81	0.44
4:Q:49:LEU:HD13	30:S:101:BCR:C15	2.48	0.44
4:Q:346:LEU:O	4:Q:348:ARG:HG3	2.18	0.44
24:Q:409:DGD:HD2	24:Q:409:DGD:HG32	1.66	0.44
17:m:33:PRO:O	17:m:36:ILE:HG13	2.18	0.44
24:B:628:DGD:HB21	31:B:630:LMT:H72	1.99	0.44
3:C:126:GLY:O	3:C:130:VAL:HG23	2.18	0.44
4:D:49:LEU:HD13	30:D:405:BCR:C15	2.47	0.44
10:K:18:PHE:HD2	10:K:18:PHE:N	2.15	0.44
16:V:135:GLU:O	16:V:139:VAL:HG23	2.18	0.44
2:N:10:THR:C	2:N:12:LEU:H	2.25	0.44
21:N:609:CLA:H141	21:N:609:CLA:H161	1.77	0.44
3:P:53:HIS:HB3	21:P:512:CLA:OBD	2.17	0.44
13:f:69:LEU:HD12	13:f:70:CYS:N	2.29	0.44
1:A:20:TRP:NE1	26:A:414:SQD:O3	2.51	0.44
21:A:401:CLA:HBA1	21:A:401:CLA:H3A	1.56	0.44
2:B:134:ASP:OD2	2:B:137:LYS:HE3	2.18	0.44
3:C:455:PHE:C	3:C:457:LYS:H	2.26	0.44
14:T:29:ILE:H	14:T:29:ILE:CD1	2.28	0.44
3:P:85:GLY:N	24:P:518:DGD:HE4	2.33	0.44
3:P:204:LEU:HD21	3:P:238:ILE:HG21	1.99	0.44
3:P:391:ARG:HD2	3:P:395:TYR:CE2	2.53	0.44
24:P:518:DGD:HB62	30:b:102:BCR:H352	2.00	0.44
4:Q:222:LEU:HD23	4:Q:244:TYR:HB3	2.00	0.44
4:Q:343:GLU:HG2	16:i:161:VAL:HG11	1.99	0.44
8:a:6:ILE:O	8:a:10:ILE:HG12	2.17	0.44
10:c:24:VAL:HG21	17:m:25:ILE:HG12	2.00	0.44
20:l:32:ASP:CB	20:l:35:ARG:HG2	2.47	0.44
2:B:464:PHE:CZ	27:B:622:LMG:H141	2.52	0.44
24:C:517:DGD:HB62	30:J:102:BCR:H352	1.99	0.44
6:F:19:ARG:O	6:F:23:VAL:HG23	2.18	0.44
26:F:101:SQD:H131	18:X:36:VAL:HG11	2.00	0.44
9:J:11:TRP:CZ3	17:y:36:ILE:HD11	2.53	0.44
13:O:69:LEU:HD12	13:O:70:CYS:N	2.28	0.44
13:O:83:LYS:HE2	2:N:338:GLN:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:G:407:PL9:H33	4:Q:38:PHE:HD1	1.83	0.44
2:N:91:TRP:HE1	31:N:624:LMT:H12	1.82	0.44
21:N:606:CLA:H61	7:W:46:LEU:HB2	2.00	0.44
21:P:502:CLA:HBD	21:P:503:CLA:H43	2.00	0.44
4:Q:93:TRP:HH2	21:Q:404:CLA:HBA2	1.83	0.44
2:B:16:PRO:HB3	2:B:133:LEU:HD21	2.00	0.43
3:C:223:TRP:CG	3:C:224:ILE:H	2.36	0.43
3:C:415:ASN:O	3:C:416:SER:HB3	2.17	0.43
21:C:507:CLA:H92	21:C:507:CLA:H62	1.75	0.43
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.83	0.43
10:K:19:ASP:N	10:K:20:PRO:HD2	2.33	0.43
21:N:608:CLA:H101	21:N:619:CLA:H42	2.01	0.43
15:h:75:LEU:HD21	15:h:101:GLN:HB3	2.00	0.43
1:A:221:SER:HB2	4:D:139:ARG:O	2.18	0.43
2:B:246:PHE:CD1	2:B:246:PHE:C	2.96	0.43
21:B:616:CLA:HBA2	21:B:616:CLA:CGD	2.48	0.43
21:C:501:CLA:H141	21:C:501:CLA:H162	1.87	0.43
13:O:94:THR:HB	13:O:135:GLN:O	2.18	0.43
1:G:92:HIS:CD2	3:P:219:GLY:HA3	2.53	0.43
1:G:129:ARG:NH2	4:Q:256:ILE:HA	2.34	0.43
2:N:235:GLU:OE1	2:N:472:ARG:NH1	2.50	0.43
21:P:504:CLA:H142	21:P:504:CLA:H112	1.82	0.43
1:A:214:MET:HE1	4:D:142:ASN:HD21	1.83	0.43
3:C:38:GLY:HA3	21:C:511:CLA:HMD2	2.00	0.43
3:C:386:PRO:HB3	16:V:116:GLU:HG2	2.00	0.43
2:N:366:PHE:CD1	2:N:367:PRO:HD2	2.53	0.43
21:N:619:CLA:H62	21:N:619:CLA:H92	1.63	0.43
3:P:186:TYR:HE2	3:P:188:THR:HG22	1.83	0.43
21:P:503:CLA:H161	21:P:503:CLA:H193	1.68	0.43
30:S:101:BCR:H15C	30:S:101:BCR:H351	1.89	0.43
11:d:1:MET:HA	11:d:1:MET:HE2	2.00	0.43
15:h:100:ARG:O	15:h:103:GLN:HB3	2.18	0.43
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.01	0.43
30:C:514:BCR:H343	30:C:514:BCR:H311	2.00	0.43
4:D:84:SER:HB2	4:D:85:MET:HE2	2.00	0.43
4:D:122:LEU:HD11	22:D:402:PHO:H92	2.00	0.43
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.99	0.43
5:E:42:LEU:O	5:E:46:VAL:HG23	2.19	0.43
12:M:19:SER:O	12:M:23:ILE:HG13	2.18	0.43
21:G:406:CLA:H141	21:G:406:CLA:H162	1.63	0.43
2:N:19:LEU:CD1	2:N:23:HIS:HE1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:25:MET:HE1	2:N:108:PHE:CE1	2.53	0.43
2:N:317:ASN:HA	2:N:330:MET:HE1	2.01	0.43
3:P:240:ILE:HG13	21:P:501:CLA:HBB1	2.00	0.43
3:P:466:VAL:HA	3:P:469:MET:SD	2.59	0.43
4:Q:153:PHE:HB2	21:Q:402:CLA:H41	2.00	0.43
34:R:101:HEM:HBC2	6:S:31:ILE:HD13	2.01	0.43
15:h:94:ILE:O	15:h:97:LEU:HG	2.18	0.43
21:B:614:CLA:H2	26:B:627:SQD:C10	2.47	0.43
3:C:405:ASN:HB2	24:C:518:DGD:HG31	2.00	0.43
5:E:30:LEU:HG	34:E:101:HEM:HBB1	2.00	0.43
17:y:39:LEU:HD23	17:y:39:LEU:HA	1.78	0.43
17:y:39:LEU:CB	17:y:46:LEU:HD21	2.46	0.43
30:Z:101:BCR:H15C	30:Z:101:BCR:H351	1.78	0.43
1:G:83:VAL:HA	1:G:84:PRO:HD3	1.91	0.43
1:G:330:VAL:HG11	4:Q:328:TRP:CZ2	2.53	0.43
2:N:464:PHE:CZ	27:N:622:LMG:H141	2.53	0.43
21:N:615:CLA:H141	21:N:615:CLA:H162	1.78	0.43
3:P:449:ARG:HE	21:P:505:CLA:CED	2.31	0.43
5:R:68:ASP:OD2	5:R:71:GLU:HB2	2.19	0.43
7:W:62:TRP:HD1	24:W:102:DGD:HE5	1.83	0.43
8:a:15:PHE:CE1	30:a:101:BCR:H312	2.53	0.43
9:b:14:ALA:HB3	30:c:101:BCR:H393	1.98	0.43
2:B:256:MET:O	2:B:448:ARG:NH1	2.44	0.43
4:D:250:ASN:ND2	4:D:262:SER:HB3	2.34	0.43
27:I:102:LMG:HC2	31:N:604:LMT:H11	1.99	0.43
9:J:11:TRP:CG	10:K:42:ALA:HA	2.54	0.43
10:K:18:PHE:N	10:K:18:PHE:CD2	2.85	0.43
4:Q:134:ARG:HE	4:Q:134:ARG:HA	1.83	0.43
7:W:12:ARG:HD3	7:W:12:ARG:C	2.44	0.43
27:a:102:LMG:H181	31:a:103:LMT:H42	2.01	0.43
16:i:119:PRO:HA	16:i:127:PHE:CD2	2.54	0.43
1:A:258:LEU:HD12	4:D:128:ARG:HD3	2.00	0.43
2:B:270:PRO:HG3	2:B:312:TYR:CD2	2.51	0.43
3:C:204:LEU:HD21	3:C:238:ILE:HG21	2.00	0.43
3:C:261:ARG:HA	3:C:266:TRP:CZ2	2.54	0.43
3:C:342:MET:HE1	3:C:356:MET:HE2	2.01	0.43
4:D:93:TRP:HH2	21:D:403:CLA:HBA2	1.83	0.43
4:D:103:ARG:NH1	5:E:77:GLU:OE2	2.50	0.43
1:G:81:ALA:HB2	1:G:175:GLY:HA3	2.00	0.43
2:N:306:PRO:HG2	2:N:309:LEU:HB2	2.00	0.43
21:N:614:CLA:H141	21:N:614:CLA:H162	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:P:514:BCR:H15C	30:P:514:BCR:H351	1.78	0.43
7:W:6:TRP:CE2	7:W:10:ILE:HD11	2.53	0.43
13:f:192:SER:OG	13:f:193:GLY:N	2.52	0.43
1:A:215:HIS:HA	23:A:406:PL9:O1	2.18	0.43
2:B:293:ALA:C	2:B:295:GLY:H	2.27	0.43
21:B:608:CLA:CHA	21:B:608:CLA:HBA1	2.48	0.43
3:C:269:GLU:O	3:C:272:LEU:HB3	2.19	0.43
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.00	0.43
13:O:123:GLU:HG2	13:O:124:GLU:N	2.34	0.43
17:y:42:ARG:HG2	17:y:42:ARG:HH11	1.83	0.43
1:G:61:ASP:HB2	1:G:63:ILE:HG12	2.00	0.43
1:G:215:HIS:HA	23:G:407:PL9:O1	2.19	0.43
2:N:30:VAL:HG13	21:N:617:CLA:HMC2	1.99	0.43
2:N:103:LEU:HD22	21:N:610:CLA:H41	2.00	0.43
21:N:614:CLA:H112	21:N:614:CLA:H12	2.01	0.43
21:N:620:CLA:HBA2	21:N:620:CLA:HBD	2.00	0.43
4:Q:84:SER:HB2	4:Q:85:MET:HE2	2.00	0.43
4:Q:275:PRO:O	4:Q:279:LEU:HD23	2.18	0.43
7:W:31:MET:HE3	7:W:35:MET:HE1	1.99	0.43
13:f:31:LEU:HB2	13:f:36:ILE:HD11	1.99	0.43
13:f:83:LYS:HG2	13:f:84:ASN:N	2.31	0.43
15:h:64:ALA:O	15:h:67:GLN:HG2	2.19	0.43
2:B:174:LEU:HD23	2:B:308:LYS:HG2	2.01	0.43
21:B:607:CLA:H193	11:L:27:LEU:HD11	2.00	0.43
3:C:291:TRP:O	3:C:305:THR:OG1	2.37	0.43
3:C:391:ARG:HD2	3:C:395:TYR:CE2	2.54	0.43
3:C:449:ARG:HE	21:C:505:CLA:CED	2.31	0.43
16:V:58:LEU:HD13	16:V:137:ASP:HB3	2.01	0.43
1:G:153:SER:HB2	21:G:402:CLA:H43	2.01	0.43
2:N:349:LYS:HG2	2:N:395:GLN:O	2.18	0.43
3:P:89:ILE:N	3:P:90:PRO:HD2	2.34	0.43
4:Q:176:ALA:HA	4:Q:179:PHE:CD2	2.54	0.43
13:f:154:SER:O	13:f:168:PHE:HA	2.18	0.43
18:j:12:ILE:O	18:j:12:ILE:HG23	2.18	0.43
1:A:51:ALA:HA	1:A:55:ALA:HB2	2.01	0.43
1:A:136:ARG:HH22	8:I:27:ASP:CG	2.27	0.43
1:A:228:THR:HG22	1:A:229:GLU:H	1.84	0.43
1:A:268:SER:O	1:A:272:HIS:ND1	2.48	0.43
2:B:25:MET:HE1	2:B:108:PHE:CE1	2.54	0.43
3:C:36:TRP:O	21:C:508:CLA:H11	2.19	0.43
21:C:508:CLA:H172	24:C:517:DGD:HBW2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:263:ASN:O	4:D:266:TRP:N	2.50	0.43
2:N:246:PHE:CD1	2:N:246:PHE:C	2.96	0.43
3:P:155:ASN:HA	3:P:158:THR:HG22	2.00	0.43
3:P:310:SER:OG	3:P:355:THR:HG23	2.19	0.43
21:P:501:CLA:H2	21:P:501:CLA:CHB	2.49	0.43
2:B:137:LYS:HD2	7:H:14:LEU:O	2.19	0.42
30:B:618:BCR:H381	14:g:4:ILE:HD13	2.01	0.42
3:C:161:LEU:HG	3:C:165:LEU:HD12	2.01	0.42
21:C:505:CLA:H193	21:C:505:CLA:H162	1.79	0.42
5:E:28:PRO:O	5:E:32:ILE:HG13	2.19	0.42
13:O:97:VAL:HG21	13:O:135:GLN:HE21	1.84	0.42
14:T:1:MET:HE2	12:e:6:LEU:HD21	2.01	0.42
20:Z:29:SER:HB2	20:Z:31:GLN:HG3	1.99	0.42
1:G:317:TRP:O	1:G:321:ILE:HG13	2.18	0.42
21:N:612:CLA:CHA	21:N:612:CLA:HBA1	2.47	0.42
4:Q:146:PHE:O	4:Q:150:ILE:HG12	2.19	0.42
1:A:93:PHE:CD2	24:A:407:DGD:HD2	2.54	0.42
21:B:608:CLA:H143	21:B:608:CLA:H161	1.84	0.42
31:B:629:LMT:H31	1:G:72:LEU:HD21	2.01	0.42
3:C:435:PHE:O	3:C:438:LEU:N	2.51	0.42
4:D:41:ALA:HB1	22:D:402:PHO:H42	2.01	0.42
4:D:107:LEU:HD21	5:E:76:VAL:HG21	2.00	0.42
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.00	0.42
15:U:38:GLU:HG2	15:U:39:LEU:H	1.84	0.42
16:V:119:PRO:HG2	34:V:201:HEM:HMC2	2.02	0.42
1:G:12:ASN:O	1:G:16:ARG:HG3	2.18	0.42
4:Q:43:LEU:HD23	4:Q:117:HIS:HE1	1.83	0.42
10:c:43:VAL:CG2	10:c:46:ARG:HE	2.32	0.42
13:f:126:GLY:O	13:f:128:ASP:N	2.52	0.42
1:A:142:TRP:HB2	4:D:220:ASN:OD1	2.19	0.42
22:A:404:PHO:H62	22:A:404:PHO:H41	1.46	0.42
2:B:103:LEU:HD22	21:B:606:CLA:H41	2.00	0.42
3:C:50:LEU:HD11	21:C:513:CLA:HBB1	2.01	0.42
3:C:363:GLY:O	3:C:367:GLU:HG2	2.19	0.42
3:C:380:ILE:HA	3:C:384:ILE:HD11	2.00	0.42
4:D:54:PHE:HB3	5:E:47:PHE:CD2	2.53	0.42
30:T:103:BCR:H393	2:N:112:CYS:HB3	2.01	0.42
16:V:83:GLU:H	16:V:83:GLU:CD	2.27	0.42
3:P:250:TRP:CD1	3:P:250:TRP:C	2.97	0.42
27:Q:406:LMG:H171	30:S:101:BCR:H383	2.01	0.42
13:f:86:ARG:C	13:f:86:ARG:HH11	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TRP:O	1:A:321:ILE:HG13	2.19	0.42
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.55	0.42
21:B:615:CLA:H62	21:B:615:CLA:H92	1.67	0.42
5:E:26:THR:HB	34:E:101:HEM:CBB	2.50	0.42
5:E:61:ARG:NH2	16:V:153:GLY:HA3	2.34	0.42
27:E:102:LMG:HC71	27:E:102:LMG:O9	2.18	0.42
15:U:94:ILE:O	15:U:97:LEU:HG	2.20	0.42
2:N:137:LYS:HD2	7:W:14:LEU:O	2.19	0.42
2:N:341:LYS:HD2	2:N:429:ILE:HG22	2.02	0.42
3:P:101:PRO:O	3:P:104:GLU:HB2	2.19	0.42
4:Q:253:TRP:HA	4:Q:256:ILE:HG23	2.01	0.42
2:B:224:ARG:HG2	7:H:24:GLY:O	2.19	0.42
2:B:341:LYS:HD2	2:B:429:ILE:HG22	2.02	0.42
2:B:462:PHE:HA	21:B:611:CLA:HMC2	2.01	0.42
30:B:619:BCR:H15C	30:B:619:BCR:H351	1.84	0.42
3:C:334:PRO:HA	13:O:179:THR:OG1	2.19	0.42
30:C:514:BCR:H391	10:K:36:ALA:HB2	2.00	0.42
6:F:45:ARG:NH2	9:J:40:LEU:O	2.52	0.42
17:y:23:THR:O	17:y:27:MET:HG3	2.20	0.42
1:G:243:GLU:CD	1:G:243:GLU:H	2.23	0.42
2:N:36:SER:HB2	31:N:603:LMT:H91	2.01	0.42
2:N:54:PRO:HD2	2:N:57:ARG:HG3	2.02	0.42
2:N:239:SER:O	2:N:466:HIS:ND1	2.47	0.42
21:N:607:CLA:CBB	21:N:609:CLA:H152	2.49	0.42
30:N:621:BCR:H351	30:N:621:BCR:H15C	1.82	0.42
3:P:240:ILE:HD13	3:P:240:ILE:HA	1.88	0.42
21:P:503:CLA:HBB1	27:P:521:LMG:C20	2.45	0.42
5:R:17:VAL:O	5:R:21:VAL:HG23	2.20	0.42
6:S:41:GLN:OE1	9:b:31:GLY:HA3	2.19	0.42
15:h:68:TYR:HB2	15:h:71:LEU:HD12	2.01	0.42
17:m:34:MET:HE1	17:m:38:LEU:HD21	2.02	0.42
1:A:232:SER:HB3	1:A:235:TYR:CD1	2.54	0.42
1:A:306:VAL:HG13	1:A:314:ILE:O	2.19	0.42
2:B:10:THR:O	2:B:13:ILE:HG13	2.20	0.42
30:C:514:BCR:H351	30:C:514:BCR:H15C	1.79	0.42
4:D:93:TRP:CH2	21:D:403:CLA:HBA2	2.54	0.42
10:K:24:VAL:HG21	17:y:25:ILE:HG12	2.02	0.42
20:Z:32:ASP:C	20:Z:34:ASP:N	2.76	0.42
1:G:161:TYR:HB3	1:G:162:PRO:HD3	2.00	0.42
5:R:30:LEU:HG	34:R:101:HEM:HBB1	2.01	0.42
16:i:160:LYS:HA	16:i:163:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LEU:HB3	2:B:138:MET:HE2	2.01	0.42
2:B:137:LYS:O	2:B:141:ILE:HG13	2.19	0.42
21:B:616:CLA:H52	26:G:401:SQD:H261	2.02	0.42
21:C:501:CLA:CHB	21:C:501:CLA:H2	2.49	0.42
5:E:26:THR:HB	34:E:101:HEM:CAB	2.50	0.42
30:T:102:BCR:H341	30:N:621:BCR:H381	2.01	0.42
1:G:76:ASN:OD1	1:G:79:THR:HG23	2.20	0.42
2:N:68:ARG:NH1	2:N:262:THR:HG23	2.35	0.42
3:P:62:PHE:HE2	10:c:29:PRO:HD3	1.85	0.42
3:P:269:GLU:O	3:P:272:LEU:HB3	2.20	0.42
20:l:29:SER:HB2	20:l:31:GLN:HG3	2.02	0.42
2:B:154:GLY:O	2:B:159:THR:HG23	2.20	0.42
2:B:262:THR:HG22	2:B:263:THR:HG23	2.02	0.42
3:C:277:GLY:C	21:C:505:CLA:HBC2	2.43	0.42
13:O:147:THR:OG1	13:O:148:VAL:N	2.52	0.42
13:O:154:SER:N	13:O:169:LYS:O	2.50	0.42
18:X:12:ILE:HG23	18:X:12:ILE:O	2.19	0.42
1:G:177:SER:HA	1:G:180:PHE:CD2	2.54	0.42
1:G:228:THR:HG22	1:G:229:GLU:H	1.84	0.42
1:G:296:ASN:HB2	3:P:400:PRO:O	2.20	0.42
1:G:306:VAL:HG13	1:G:314:ILE:O	2.19	0.42
30:N:621:BCR:H11C	30:N:621:BCR:H341	1.91	0.42
3:P:269:GLU:OE1	21:P:508:CLA:HED1	2.19	0.42
13:f:94:THR:HB	13:f:135:GLN:O	2.19	0.42
1:A:153:SER:HB2	21:A:401:CLA:H43	2.00	0.42
5:E:22:ILE:O	5:E:26:THR:HG23	2.20	0.42
13:O:59:ASP:HB3	13:O:62:GLN:HB3	2.02	0.42
20:Z:32:ASP:HB3	20:Z:35:ARG:NH1	2.35	0.42
2:N:348:ASN:OD1	2:N:352:GLU:HB2	2.20	0.42
2:N:474:LEU:O	4:Q:134:ARG:NH1	2.53	0.42
3:P:35:TRP:CG	3:P:36:TRP:N	2.88	0.42
3:P:374:GLY:O	3:P:375:LEU:C	2.63	0.42
3:P:391:ARG:HB2	3:P:391:ARG:HH11	1.84	0.42
21:P:507:CLA:H62	21:P:507:CLA:H92	1.73	0.42
30:P:515:BCR:H15C	30:P:515:BCR:H351	1.79	0.42
4:Q:146:PHE:C	4:Q:149:PRO:HD2	2.44	0.42
9:b:11:TRP:CG	10:c:42:ALA:HA	2.54	0.42
13:f:81:GLU:C	13:f:83:LYS:H	2.28	0.42
17:m:24:MET:O	17:m:28:ILE:HG23	2.20	0.42
2:B:331:ASN:HB3	2:B:437:LEU:HD12	2.01	0.42
21:B:610:CLA:H141	21:B:610:CLA:H162	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.83	0.42
3:C:120:ILE:CD1	30:C:514:BCR:HC8	2.50	0.42
3:C:303:GLY:O	3:C:423:ARG:NE	2.44	0.42
3:C:374:GLY:O	3:C:375:LEU:C	2.63	0.42
12:M:5:GLN:NE2	12:e:5:GLN:HG2	2.35	0.42
1:G:249:VAL:HG11	2:N:486:LEU:HD23	2.02	0.42
2:N:270:PRO:HG3	2:N:312:TYR:CD2	2.51	0.42
2:N:483:ASP:OD2	2:N:484:PRO:HD2	2.20	0.42
3:P:143:TYR:O	3:P:144:SER:HB2	2.19	0.42
4:Q:157:PHE:CE1	4:Q:171:PRO:HG2	2.55	0.42
27:Q:406:LMG:O4	9:b:31:GLY:O	2.37	0.42
5:R:22:ILE:O	5:R:26:THR:HG23	2.20	0.42
10:c:19:ASP:N	10:c:20:PRO:HD2	2.34	0.42
11:d:5:PRO:HA	11:d:7:ARG:HH22	1.85	0.42
16:i:103:LYS:O	16:i:122:ARG:HG2	2.20	0.42
2:B:278:SER:HB3	2:B:281:GLN:HB3	2.02	0.41
21:B:605:CLA:HMC1	21:B:615:CLA:H2	2.01	0.41
3:C:160:ILE:HA	3:C:163:PHE:CD2	2.55	0.41
3:C:162:GLY:O	3:C:166:ILE:HG13	2.20	0.41
3:C:250:TRP:CD1	3:C:250:TRP:C	2.98	0.41
3:C:418:ASN:HB2	24:C:518:DGD:HE2	2.00	0.41
3:C:466:VAL:HA	3:C:469:MET:SD	2.60	0.41
4:D:275:PRO:O	4:D:279:LEU:HD23	2.20	0.41
4:D:334:GLN:N	4:D:335:PRO:HD3	2.35	0.41
27:M:101:LMG:H292	21:N:618:CLA:CMD	2.50	0.41
13:O:192:SER:OG	13:O:193:GLY:N	2.52	0.41
17:y:31:ALA:O	17:y:35:ILE:HG23	2.19	0.41
26:N:601:SQD:C10	21:N:618:CLA:H2	2.46	0.41
3:P:28:GLN:HB2	21:P:511:CLA:HED3	2.02	0.41
3:P:142:GLU:C	3:P:144:SER:H	2.28	0.41
3:P:161:LEU:HG	3:P:165:LEU:HD12	2.02	0.41
3:P:229:ASN:HD22	3:P:231:GLU:HB2	1.85	0.41
3:P:453:ALA:O	8:a:34:ARG:HB2	2.20	0.41
4:Q:26:ARG:CD	6:S:18:VAL:HG11	2.39	0.41
4:Q:250:ASN:ND2	4:Q:262:SER:HB3	2.35	0.41
16:i:115:ALA:CB	16:i:122:ARG:HD2	2.50	0.41
1:A:20:TRP:O	1:A:23:SER:HB3	2.20	0.41
1:A:72:LEU:HD21	31:N:603:LMT:H31	2.02	0.41
2:B:124:ARG:NE	2:B:131:PRO:HD3	2.34	0.41
2:B:133:LEU:HB3	2:B:138:MET:HE1	2.02	0.41
2:B:483:ASP:OD2	2:B:484:PRO:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:ILE:N	3:C:90:PRO:HD2	2.35	0.41
30:C:515:BCR:H15C	30:C:515:BCR:H351	1.84	0.41
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.41
16:V:143:GLY:O	16:V:147:VAL:HG23	2.19	0.41
21:G:402:CLA:H191	27:Q:407:LMG:H352	2.02	0.41
2:N:10:THR:O	2:N:13:ILE:HG13	2.19	0.41
21:P:511:CLA:H43	17:m:46:LEU:HA	2.01	0.41
5:R:26:THR:HB	34:R:101:HEM:CAB	2.50	0.41
12:e:18:PRO:O	12:e:21:PHE:HB3	2.20	0.41
13:f:59:ASP:OD2	13:f:61:SER:OG	2.35	0.41
20:l:32:ASP:C	20:l:34:ASP:N	2.76	0.41
30:B:617:BCR:H15C	30:B:617:BCR:H351	1.84	0.41
30:B:617:BCR:H24C	30:B:617:BCR:H371	1.87	0.41
3:C:310:SER:OG	3:C:355:THR:HG23	2.19	0.41
3:C:375:LEU:HB3	3:C:380:ILE:HD11	2.03	0.41
30:C:514:BCR:H331	30:C:514:BCR:HC7	1.34	0.41
4:D:101:PHE:O	4:D:104:TRP:HB3	2.21	0.41
13:O:215:ARG:NH1	13:O:252:GLY:O	2.53	0.41
15:U:73:PRO:HG2	16:V:107:THR:HB	2.02	0.41
1:G:143:ILE:HD11	4:Q:217:THR:HA	2.01	0.41
2:N:224:ARG:HG2	7:W:24:GLY:O	2.20	0.41
3:P:342:MET:HE1	3:P:356:MET:HE2	2.03	0.41
7:W:12:ARG:N	7:W:13:PRO:HD2	2.35	0.41
30:c:101:BCR:H15C	30:c:101:BCR:H351	1.87	0.41
16:i:39:ASN:HD21	16:i:43:LYS:HB3	1.85	0.41
2:B:25:MET:HG2	30:B:617:BCR:H23C	2.01	0.41
3:C:35:TRP:CG	3:C:36:TRP:N	2.88	0.41
21:C:509:CLA:H161	21:C:509:CLA:H203	1.81	0.41
4:D:201:VAL:O	4:D:205:LEU:HB2	2.21	0.41
4:D:253:TRP:HA	4:D:256:ILE:HG23	2.02	0.41
30:J:102:BCR:H20C	30:J:102:BCR:H361	1.87	0.41
13:O:86:ARG:HD2	13:O:86:ARG:C	2.45	0.41
16:V:68:VAL:O	16:V:71:ILE:HG12	2.20	0.41
2:N:23:HIS:CD2	21:N:616:CLA:C1B	3.03	0.41
2:N:462:PHE:HA	21:N:615:CLA:HMC2	2.01	0.41
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.01	0.41
3:C:186:TYR:CE2	3:C:188:THR:HG22	2.55	0.41
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.73	0.41
21:C:504:CLA:H142	21:C:504:CLA:H112	1.80	0.41
4:D:320:LEU:HD23	4:D:323:GLU:OE1	2.21	0.41
9:J:14:ALA:O	9:J:18:GLY:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:J:102:BCR:C8	30:J:102:BCR:H331	2.51	0.41
13:O:86:ARG:C	13:O:86:ARG:HH11	2.28	0.41
30:T:101:BCR:H23C	2:N:25:MET:HG2	2.01	0.41
15:U:68:TYR:HB2	15:U:71:LEU:HD12	2.02	0.41
1:G:37:MET:HE1	1:G:129:ARG:CZ	2.50	0.41
1:G:93:PHE:HD2	24:G:408:DGD:HD2	1.86	0.41
22:G:405:PHO:H13	22:G:405:PHO:H102	1.81	0.41
2:N:188:ASP:OD1	7:W:58:VAL:HA	2.20	0.41
21:N:609:CLA:HMA2	21:N:610:CLA:HMA2	2.01	0.41
3:P:279:LEU:HD12	3:P:437:PHE:HE1	1.86	0.41
1:A:234:ASN:HD22	1:A:234:ASN:HA	1.63	0.41
2:B:112:CYS:HB3	30:B:620:BCR:H393	2.02	0.41
2:B:130:GLU:HB2	2:B:131:PRO:HD2	2.02	0.41
21:B:610:CLA:H62	21:B:610:CLA:H41	1.88	0.41
3:C:404:LEU:HD12	3:C:404:LEU:HA	1.92	0.41
4:D:103:ARG:O	4:D:107:LEU:HG	2.19	0.41
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.82	0.41
27:I:102:LMG:H221	31:I:103:LMT:H81	2.02	0.41
9:J:15:THR:HG23	30:K:101:BCR:H392	2.03	0.41
2:N:201:HIS:HD2	2:N:202:HIS:ND1	2.18	0.41
2:N:262:THR:HG22	2:N:263:THR:HG23	2.01	0.41
2:N:475:PHE:CD1	4:Q:140:PRO:HD3	2.56	0.41
3:P:135:ARG:HB2	20:l:27:TYR:CG	2.55	0.41
3:P:334:PRO:HA	13:f:179:THR:OG1	2.21	0.41
30:W:101:BCR:H15C	30:W:101:BCR:H351	1.95	0.41
1:A:12:ASN:O	1:A:16:ARG:HG3	2.21	0.41
1:A:296:ASN:HB2	3:C:400:PRO:O	2.20	0.41
21:A:403:CLA:H143	21:A:403:CLA:H161	1.95	0.41
2:B:153:PHE:O	2:B:157:HIS:HB3	2.21	0.41
5:E:20:TRP:HD1	9:J:8:ILE:HD13	1.85	0.41
30:I:101:BCR:H24C	30:I:101:BCR:H371	1.91	0.41
14:T:18:PHE:HB2	30:T:102:BCR:H10C	2.02	0.41
20:Z:35:ARG:O	20:Z:38:GLN:HB3	2.20	0.41
1:G:51:ALA:HA	1:G:55:ALA:HB2	2.03	0.41
1:G:191:ASN:HB2	3:P:411:ALA:HB1	2.03	0.41
23:G:407:PL9:H33	4:Q:38:PHE:CD1	2.55	0.41
2:N:18:ARG:HD2	2:N:115:TRP:CE3	2.56	0.41
3:P:277:GLY:C	21:P:505:CLA:HBC2	2.46	0.41
3:P:418:ASN:HB2	24:P:519:DGD:HE2	2.02	0.41
4:Q:43:LEU:HD12	4:Q:43:LEU:HA	1.94	0.41
18:j:11:THR:HG23	18:j:12:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:H	1:A:243:GLU:CD	2.25	0.41
1:A:271:LEU:HD21	23:A:406:PL9:HC71	2.02	0.41
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.56	0.41
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.55	0.41
8:I:8:VAL:O	8:I:12:VAL:HG23	2.21	0.41
1:G:238:LYS:HD3	1:G:238:LYS:HA	1.83	0.41
1:G:283:VAL:O	1:G:286:THR:HG22	2.20	0.41
21:G:403:CLA:H62	21:G:403:CLA:H41	1.84	0.41
3:P:62:PHE:CE2	10:c:29:PRO:HD3	2.55	0.41
3:P:332:GLN:HG3	13:f:129:PHE:CE2	2.56	0.41
3:P:348:GLU:OE2	13:f:37:VAL:HA	2.20	0.41
21:P:512:CLA:H72	21:P:512:CLA:H112	1.77	0.41
26:Q:408:SQD:H81	26:Q:408:SQD:H45	1.85	0.41
5:R:82:GLN:H	5:R:82:GLN:HG3	1.52	0.41
30:a:101:BCR:H24C	30:a:101:BCR:H371	1.90	0.41
13:f:81:GLU:HA	13:f:82:PRO:HD3	1.84	0.41
13:f:230:VAL:HG13	13:f:237:ILE:HG22	2.02	0.41
1:A:172:MET:SD	1:A:179:THR:HG23	2.60	0.41
1:A:330:VAL:HG11	4:D:328:TRP:CZ2	2.55	0.41
2:B:49:ASP:HA	2:B:50:PRO:HD2	1.98	0.41
2:B:112:CYS:HA	30:B:617:BCR:H282	2.03	0.41
2:B:275:TRP:CH2	2:B:358:ARG:HD3	2.56	0.41
3:C:256:PRO:HA	21:C:506:CLA:HED3	2.02	0.41
3:C:425:TRP:CZ2	21:C:504:CLA:HBA1	2.56	0.41
4:D:92:LEU:HA	4:D:104:TRP:CD1	2.56	0.41
4:D:146:PHE:C	4:D:149:PRO:HD2	2.46	0.41
4:D:308:ASP:HA	4:D:309:PRO:HD3	1.87	0.41
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.56	0.41
15:U:80:VAL:HG22	15:U:127:ARG:NH2	2.35	0.41
20:Z:32:ASP:CB	20:Z:35:ARG:HG2	2.50	0.41
1:G:142:TRP:HB2	4:Q:220:ASN:OD1	2.20	0.41
1:G:221:SER:HB2	4:Q:139:ARG:O	2.20	0.41
2:N:133:LEU:HB3	2:N:138:MET:HE2	2.03	0.41
2:N:234:ILE:C	2:N:236:THR:H	2.29	0.41
2:N:383:PHE:CZ	13:f:193:GLY:HA2	2.56	0.41
27:N:623:LMG:HC3	31:e:101:LMT:H2'	2.03	0.41
3:P:296:VAL:HG23	3:P:297:TYR:CD2	2.56	0.41
30:P:514:BCR:H11C	30:P:514:BCR:H341	1.92	0.41
27:R:102:LMG:O9	27:R:102:LMG:HC71	2.21	0.41
8:a:13:THR:O	8:a:17:LEU:HG	2.21	0.41
15:h:73:PRO:HG2	16:i:107:THR:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:23:UNK:O	19:k:24:UNK:C	2.69	0.41
3:C:29:GLU:HB2	3:C:30:SER:H	1.73	0.41
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.55	0.41
7:H:55:LEU:HB2	7:H:58:VAL:CG1	2.51	0.41
14:T:9:ILE:O	14:T:13:ILE:HG13	2.21	0.41
1:G:93:PHE:HZ	21:G:406:CLA:HAA1	1.85	0.41
2:N:155:ALA:O	2:N:159:THR:OG1	2.26	0.41
2:N:293:ALA:C	2:N:295:GLY:H	2.28	0.41
21:N:606:CLA:H12	7:W:49:TYR:HD2	1.85	0.41
21:N:618:CLA:OBD	11:d:10:VAL:HG21	2.21	0.41
3:P:107:ASP:OD2	3:P:110:PRO:HD3	2.20	0.41
3:P:116:VAL:CG2	30:P:515:BCR:H323	2.51	0.41
3:P:362:ARG:H	24:P:517:DGD:HE4	1.86	0.41
17:m:20:ALA:C	17:m:22:LEU:H	2.29	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.90	0.40
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.37	0.40
21:A:401:CLA:H191	27:D:407:LMG:H352	2.03	0.40
2:B:3:LEU:HA	2:B:4:PRO:HD3	1.97	0.40
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.02	0.40
5:E:17:VAL:O	5:E:21:VAL:HG23	2.21	0.40
13:O:240:THR:HG22	13:O:264:VAL:HG12	2.02	0.40
16:V:63:CYS:SG	34:V:201:HEM:CAB	3.10	0.40
1:G:300:PHE:CZ	3:P:404:LEU:HD23	2.56	0.40
3:P:421:SER:HA	3:P:422:PRO:HD3	1.90	0.40
4:Q:47:GLY:HA2	30:S:101:BCR:H332	2.03	0.40
10:c:15:TYR:HE2	20:l:62:VAL:HG21	1.86	0.40
20:l:32:ASP:HB3	20:l:35:ARG:NH1	2.37	0.40
1:A:76:ASN:OD1	1:A:79:THR:HG23	2.20	0.40
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.40
1:A:265:PHE:CD1	1:A:271:LEU:HA	2.57	0.40
2:B:12:LEU:HB2	21:B:612:CLA:HMC2	2.02	0.40
7:H:18:TYR:CG	7:H:19:GLY:N	2.89	0.40
15:U:89:GLU:H	15:U:89:GLU:CD	2.30	0.40
1:G:268:SER:O	1:G:272:HIS:ND1	2.53	0.40
1:G:308:ASP:O	6:S:45:ARG:NE	2.54	0.40
21:G:402:CLA:HBD	21:G:403:CLA:HAC2	2.03	0.40
21:G:402:CLA:HMC3	4:Q:182:LEU:HD13	2.02	0.40
21:G:402:CLA:HBB1	21:Q:402:CLA:NC	2.36	0.40
2:N:153:PHE:O	2:N:157:HIS:HB3	2.22	0.40
2:N:154:GLY:O	2:N:159:THR:HG23	2.21	0.40
21:P:511:CLA:H122	10:c:32:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:42:LEU:O	5:R:46:VAL:HG23	2.20	0.40
9:b:15:THR:HG23	30:c:101:BCR:H392	2.04	0.40
16:i:116:GLU:O	16:i:116:GLU:HG3	2.21	0.40
16:i:143:GLY:O	16:i:147:VAL:HG23	2.21	0.40
21:B:602:CLA:H122	21:B:602:CLA:H162	1.58	0.40
21:B:613:CLA:H41	21:B:613:CLA:H62	1.88	0.40
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.36	0.40
4:D:346:LEU:O	4:D:348:ARG:HG3	2.20	0.40
12:M:16:LEU:HD21	21:N:618:CLA:H202	2.02	0.40
1:G:219:VAL:HG11	4:Q:268:HIS:CD2	2.57	0.40
1:G:237:TYR:OH	4:Q:246:MET:HG2	2.20	0.40
3:P:319:ILE:HG21	3:P:389:GLU:HG3	2.04	0.40
4:Q:194:ASN:HA	4:Q:195:PRO:HD2	1.91	0.40
4:Q:334:GLN:N	4:Q:335:PRO:HD3	2.35	0.40
13:f:86:ARG:C	13:f:86:ARG:HD2	2.46	0.40
14:g:29:ILE:H	14:g:29:ILE:CD1	2.28	0.40
1:A:37:MET:HE1	1:A:129:ARG:CZ	2.52	0.40
1:A:140:ARG:NH2	25:A:408:LHG:O5	2.45	0.40
21:A:401:CLA:HBB1	21:D:401:CLA:NC	2.36	0.40
3:C:321:ASP:HA	3:C:324:LEU:HD23	2.03	0.40
4:D:146:PHE:O	4:D:150:ILE:HG12	2.22	0.40
5:E:7:GLU:HB3	6:F:19:ARG:CZ	2.52	0.40
5:E:68:ASP:OD2	5:E:71:GLU:HB2	2.21	0.40
10:K:20:PRO:O	10:K:23:ASP:HB2	2.21	0.40
13:O:31:LEU:HB2	13:O:36:ILE:CD1	2.51	0.40
30:T:102:BCR:H341	30:T:102:BCR:H11C	1.85	0.40
30:T:102:BCR:H331	30:T:102:BCR:C8	2.52	0.40
18:X:11:THR:HG23	18:X:12:ILE:HG22	2.03	0.40
21:P:509:CLA:H203	21:P:509:CLA:H161	1.87	0.40
4:Q:93:TRP:CH2	21:Q:404:CLA:HBA2	2.56	0.40
10:c:43:VAL:HG22	10:c:46:ARG:HE	1.87	0.40
17:m:25:ILE:O	17:m:29:GLY:N	2.55	0.40
1:A:269:ARG:NH1	4:D:231:THR:HB	2.37	0.40
26:A:409:SQD:H202	24:C:518:DGD:HAH2	2.03	0.40
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.57	0.40
3:C:307:PRO:HG3	3:C:358:PHE:CD1	2.57	0.40
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.52	0.40
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.57	0.40
4:D:350:ASN:O	4:D:352:LEU:N	2.45	0.40
30:T:102:BCR:H24C	30:T:102:BCR:H371	1.92	0.40
20:Z:30:PRO:C	20:Z:32:ASP:N	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:TRP:NE1	26:G:401:SQD:O3	2.55	0.40
1:G:136:ARG:HH22	8:a:27:ASP:CG	2.30	0.40
1:G:211:PHE:HA	1:G:214:MET:HB2	2.04	0.40
26:G:410:SQD:H5	4:Q:232:PHE:HB3	2.04	0.40
3:P:44:ASN:C	3:P:45:LEU:HD12	2.47	0.40
3:P:257:PHE:HB3	3:P:258:GLY:H	1.59	0.40
3:P:261:ARG:HA	3:P:266:TRP:CZ2	2.57	0.40
3:P:261:ARG:HA	3:P:266:TRP:HZ2	1.87	0.40
22:Q:403:PHO:H111	22:Q:403:PHO:H143	1.89	0.40
5:R:49:THR:HA	5:R:50:PRO:HD3	1.85	0.40
9:b:14:ALA:O	9:b:18:GLY:N	2.49	0.40
13:f:123:GLU:HG2	13:f:124:GLU:N	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:60:PHE:O	13:f:115:SER:OG[3_755]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	333/344 (97%)	297 (89%)	31 (9%)	5 (2%)	8	40
1	G	333/344 (97%)	297 (89%)	31 (9%)	5 (2%)	8	40
2	B	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	4	26
2	N	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	4	26
3	C	445/461 (96%)	375 (84%)	55 (12%)	15 (3%)	3	21
3	P	445/461 (96%)	376 (84%)	53 (12%)	16 (4%)	2	20
4	D	338/352 (96%)	292 (86%)	40 (12%)	6 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	338/352 (96%)	291 (86%)	41 (12%)	6 (2%)	6	34
5	E	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	2	19
5	R	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	2	19
6	F	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
6	S	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
7	H	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	9
7	W	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	9
8	I	33/38 (87%)	24 (73%)	7 (21%)	2 (6%)	1	13
8	a	33/38 (87%)	25 (76%)	6 (18%)	2 (6%)	1	13
9	J	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	1	12
9	b	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	1	12
10	K	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	14
10	c	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	14
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	d	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
12	e	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/246 (98%)	203 (84%)	27 (11%)	11 (5%)	2	16
13	f	241/246 (98%)	203 (84%)	29 (12%)	9 (4%)	2	19
14	T	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	3	21
14	g	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	3	21
15	U	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	2	17
15	h	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	2	17
16	V	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	18	56
16	i	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	18	56
17	m	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	10
17	y	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	10
18	X	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	5
18	j	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	5
20	Z	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	1	16
20	l	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5138/5426 (95%)	4357 (85%)	626 (12%)	155 (3%)	3	22

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	142	TRP
2	B	176	GLY
2	B	230	ARG
2	B	484	PRO
2	B	488	PRO
3	C	144	SER
3	C	257	PHE
3	C	416	SER
4	D	239	GLN
4	D	240	ALA
4	D	262	SER
7	H	18	TYR
8	I	25	SER
9	J	35	GLY
13	O	52	ALA
14	T	30	THR
15	U	72	TYR
15	U	83	ALA
16	V	75	ASN
17	y	43	ARG
18	X	45	LYS
20	Z	32	ASP
1	G	12	ASN
1	G	142	TRP
2	N	176	GLY
2	N	230	ARG
2	N	484	PRO
2	N	488	PRO
3	P	144	SER
3	P	257	PHE
3	P	416	SER
3	P	452	ALA
4	Q	239	GLN
4	Q	240	ALA
4	Q	262	SER
7	W	18	TYR

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Mol	Chain	Res	Type
8	a	25	SER
9	b	35	GLY
13	f	52	ALA
14	g	30	THR
15	h	72	TYR
15	h	83	ALA
16	i	75	ASN
17	m	43	ARG
18	j	45	LYS
20	l	32	ASP
1	A	141	PRO
2	B	349	LYS
3	C	46	SER
3	C	136	GLY
3	C	194	GLY
3	C	452	ALA
4	D	234	ALA
4	D	264	LYS
5	E	82	GLN
7	H	26	GLY
9	J	38	SER
13	O	231	ASP
15	U	73	PRO
1	G	141	PRO
2	N	349	LYS
3	P	46	SER
3	P	136	GLY
3	P	194	GLY
4	Q	234	ALA
4	Q	264	LYS
5	R	82	GLN
7	W	26	GLY
9	b	38	SER
13	f	231	ASP
15	h	73	PRO
17	m	25	ILE
2	B	436	THR
3	C	32	GLY
3	C	141	GLU
3	C	209	ILE
3	C	375	LEU
3	C	456	GLU

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Mol	Chain	Res	Type
4	D	263	ASN
5	E	9	PRO
7	H	16	SER
10	K	13	GLU
10	K	45	PHE
13	O	158	ASN
13	O	165	SER
17	y	25	ILE
18	X	43	ILE
2	N	436	THR
3	P	32	GLY
3	P	141	GLU
3	P	209	ILE
3	P	375	LEU
3	P	456	GLU
4	Q	263	ASN
5	R	9	PRO
7	W	16	SER
10	c	13	GLU
10	c	45	PHE
13	f	158	ASN
13	f	165	SER
18	j	43	ILE
20	l	28	ALA
2	B	127	ARG
2	B	183	PRO
2	B	414	PRO
13	O	60	SER
13	O	82	PRO
20	Z	24	PRO
20	Z	28	ALA
2	N	127	ARG
2	N	183	PRO
2	N	414	PRO
13	f	60	SER
13	f	82	PRO
20	l	24	PRO
1	A	334	ARG
2	B	13	ILE
2	B	173	GLY
3	C	154	LYS
3	C	462	GLU

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Mol	Chain	Res	Type
5	E	10	PHE
7	H	6	TRP
13	O	51	THR
13	O	88	GLU
1	G	334	ARG
2	N	13	ILE
2	N	173	GLY
3	P	154	LYS
3	P	411	ALA
3	P	462	GLU
5	R	10	PHE
7	W	6	TRP
13	f	51	THR
13	f	88	GLU
15	U	42	VAL
18	X	12	ILE
18	X	44	ASP
18	j	12	ILE
18	j	44	ASP
15	h	42	VAL
8	I	32	PRO
8	a	32	PRO
1	A	176	ILE
2	B	16	PRO
3	C	201	ASN
7	H	60	VAL
13	O	127	ILE
13	O	159	VAL
1	G	176	ILE
2	N	16	PRO
3	P	201	ASN
13	f	159	VAL
13	O	271	PRO
7	W	60	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	271/280 (97%)	258 (95%)	13 (5%)	23	44
1	G	271/280 (97%)	258 (95%)	13 (5%)	23	44
2	B	390/407 (96%)	373 (96%)	17 (4%)	25	47
2	N	390/407 (96%)	373 (96%)	17 (4%)	25	47
3	C	347/362 (96%)	334 (96%)	13 (4%)	30	51
3	P	347/362 (96%)	334 (96%)	13 (4%)	30	51
4	D	275/283 (97%)	257 (94%)	18 (6%)	15	37
4	Q	275/283 (97%)	257 (94%)	18 (6%)	15	37
5	E	72/72 (100%)	66 (92%)	6 (8%)	10	30
5	R	72/72 (100%)	66 (92%)	6 (8%)	10	30
6	F	29/38 (76%)	29 (100%)	0	100	100
6	S	29/38 (76%)	29 (100%)	0	100	100
7	H	53/54 (98%)	50 (94%)	3 (6%)	18	40
7	W	53/54 (98%)	49 (92%)	4 (8%)	12	33
8	I	32/35 (91%)	30 (94%)	2 (6%)	16	37
8	a	32/35 (91%)	30 (94%)	2 (6%)	16	37
9	J	24/27 (89%)	23 (96%)	1 (4%)	26	48
9	b	24/27 (89%)	23 (96%)	1 (4%)	26	48
10	K	30/30 (100%)	28 (93%)	2 (7%)	15	36
10	c	30/30 (100%)	28 (93%)	2 (7%)	15	36
11	L	35/35 (100%)	32 (91%)	3 (9%)	10	29
11	d	35/35 (100%)	32 (91%)	3 (9%)	10	29
12	M	31/33 (94%)	30 (97%)	1 (3%)	34	56
12	e	31/33 (94%)	30 (97%)	1 (3%)	34	56
13	O	202/208 (97%)	196 (97%)	6 (3%)	36	57
13	f	202/208 (97%)	196 (97%)	6 (3%)	36	57
14	T	29/29 (100%)	28 (97%)	1 (3%)	32	54
14	g	29/29 (100%)	28 (97%)	1 (3%)	32	54
15	U	84/89 (94%)	81 (96%)	3 (4%)	31	52
15	h	84/89 (94%)	81 (96%)	3 (4%)	31	52
16	V	116/117 (99%)	113 (97%)	3 (3%)	40	62
16	i	116/117 (99%)	113 (97%)	3 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	m	20/37 (54%)	16 (80%)	4 (20%)	1	7
17	y	20/37 (54%)	16 (80%)	4 (20%)	1	7
18	X	30/33 (91%)	25 (83%)	5 (17%)	2	10
18	j	30/33 (91%)	25 (83%)	5 (17%)	2	10
20	Z	52/52 (100%)	47 (90%)	5 (10%)	8	25
20	l	52/52 (100%)	47 (90%)	5 (10%)	8	25
All	All	4244/4442 (96%)	4031 (95%)	213 (5%)	22	43

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	32	TRP
1	A	157	VAL
1	A	202	VAL
1	A	210	LEU
1	A	214	MET
1	A	218	LEU
1	A	243	GLU
1	A	271	LEU
1	A	275	LEU
1	A	286	THR
1	A	292	THR
1	A	306	VAL
2	B	11	VAL
2	B	18	ARG
2	B	84	THR
2	B	116	VAL
2	B	223	GLN
2	B	262	THR
2	B	271	THR
2	B	308	LYS
2	B	309	LEU
2	B	362	PHE
2	B	414	PRO
2	B	422	ARG
2	B	433	ASP
2	B	467	ILE
2	B	486	LEU
2	B	488	PRO

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Mol	Chain	Res	Type
2	B	490	GLN
3	C	29	GLU
3	C	86	LEU
3	C	165	LEU
3	C	174	LEU
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	391	ARG
3	C	401	LEU
3	C	417	VAL
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	53	THR
4	D	60	THR
4	D	84	SER
4	D	91	LEU
4	D	130	PHE
4	D	180	ARG
4	D	201	VAL
4	D	221	THR
4	D	236	ASN
4	D	241	GLU
4	D	256	ILE
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	323	GLU
4	D	346	LEU
5	E	5	THR
5	E	9	PRO
5	E	18	ARG
5	E	77	GLU
5	E	82	GLN
5	E	84	LYS
7	H	21	VAL
7	H	27	THR
7	H	60	VAL
8	I	32	PRO

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Mol	Chain	Res	Type
8	I	33	LYS
9	J	7	ARG
10	K	18	PHE
10	K	19	ASP
11	L	8	GLN
11	L	11	GLU
11	L	15	THR
12	M	20	VAL
13	O	31	LEU
13	O	86	ARG
13	O	97	VAL
13	O	98	THR
13	O	178	ARG
13	O	219	THR
14	T	29	ILE
15	U	88	VAL
15	U	114	VAL
15	U	132	LEU
16	V	35	THR
16	V	63	CYS
16	V	116	GLU
17	y	25	ILE
17	y	28	ILE
17	y	36	ILE
17	y	46	LEU
18	X	11	THR
18	X	12	ILE
18	X	32	LEU
18	X	42	GLN
18	X	45	LYS
20	Z	14	ILE
20	Z	25	VAL
20	Z	33	TRP
20	Z	58	ASN
20	Z	62	VAL
1	G	30	VAL
1	G	32	TRP
1	G	157	VAL
1	G	202	VAL
1	G	210	LEU
1	G	214	MET
1	G	218	LEU

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Mol	Chain	Res	Type
1	G	243	GLU
1	G	271	LEU
1	G	275	LEU
1	G	286	THR
1	G	292	THR
1	G	306	VAL
2	N	11	VAL
2	N	18	ARG
2	N	84	THR
2	N	116	VAL
2	N	223	GLN
2	N	262	THR
2	N	271	THR
2	N	308	LYS
2	N	309	LEU
2	N	362	PHE
2	N	414	PRO
2	N	422	ARG
2	N	433	ASP
2	N	467	ILE
2	N	486	LEU
2	N	488	PRO
2	N	490	GLN
3	P	29	GLU
3	P	86	LEU
3	P	165	LEU
3	P	174	LEU
3	P	244	CYS
3	P	254	THR
3	P	289	PHE
3	P	305	THR
3	P	355	THR
3	P	391	ARG
3	P	401	LEU
3	P	417	VAL
3	P	472	LEU
4	Q	20	ASP
4	Q	43	LEU
4	Q	53	THR
4	Q	60	THR
4	Q	84	SER
4	Q	91	LEU

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Mol	Chain	Res	Type
4	Q	130	PHE
4	Q	180	ARG
4	Q	201	VAL
4	Q	221	THR
4	Q	236	ASN
4	Q	241	GLU
4	Q	256	ILE
4	Q	259	ILE
4	Q	279	LEU
4	Q	291	LEU
4	Q	323	GLU
4	Q	346	LEU
5	R	5	THR
5	R	9	PRO
5	R	18	ARG
5	R	77	GLU
5	R	82	GLN
5	R	84	LYS
7	W	21	VAL
7	W	27	THR
7	W	45	ILE
7	W	60	VAL
8	a	32	PRO
8	a	33	LYS
9	b	7	ARG
10	c	18	PHE
10	c	19	ASP
11	d	8	GLN
11	d	11	GLU
11	d	15	THR
12	e	20	VAL
13	f	31	LEU
13	f	86	ARG
13	f	97	VAL
13	f	98	THR
13	f	178	ARG
13	f	219	THR
14	g	29	ILE
15	h	88	VAL
15	h	114	VAL
15	h	132	LEU
16	i	35	THR

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Mol	Chain	Res	Type
16	i	63	CYS
16	i	116	GLU
17	m	25	ILE
17	m	28	ILE
17	m	36	ILE
17	m	46	LEU
18	j	11	THR
18	j	12	ILE
18	j	32	LEU
18	j	42	GLN
18	j	45	LYS
20	l	14	ILE
20	l	25	VAL
20	l	33	TRP
20	l	58	ASN
20	l	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	234	ASN
1	A	247	ASN
2	B	23	HIS
2	B	26	HIS
2	B	201	HIS
2	B	223	GLN
2	B	282	GLN
2	B	374	ASN
3	C	44	ASN
3	C	118	HIS
4	D	117	HIS
4	D	224	GLN
4	D	250	ASN
11	L	8	GLN
12	M	33	GLN
13	O	135	GLN
15	U	108	ASN
15	U	111	HIS
16	V	104	ASN
20	Z	58	ASN
1	G	165	GLN

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Mol	Chain	Res	Type
1	G	247	ASN
2	N	26	HIS
2	N	201	HIS
2	N	223	GLN
2	N	331	ASN
3	P	56	HIS
3	P	118	HIS
4	Q	117	HIS
4	Q	129	GLN
4	Q	224	GLN
4	Q	250	ASN
4	Q	301	GLN
7	W	50	ASN
11	d	8	GLN
12	e	5	GLN
13	f	130	GLN
13	f	135	GLN
15	h	111	HIS
16	i	104	ASN
20	l	58	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 182 ligands modelled in this entry, 6 are monoatomic - leaving 176 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	Q	410	-	32,32,36	0.48	0	43,43,47	0.66	1 (2%)
27	LMG	e	102	-	42,42,55	1.04	2 (4%)	50,50,63	1.32	6 (12%)
31	LMT	N	625	-	36,36,36	0.42	0	47,47,47	0.67	1 (2%)
27	LMG	B	622	-	49,49,55	0.94	2 (4%)	57,57,63	1.28	7 (12%)
24	DGD	B	628	-	53,53,67	1.03	3 (5%)	67,67,81	1.51	11 (16%)
24	DGD	P	518	-	63,63,67	0.93	3 (4%)	77,77,81	1.50	14 (18%)
21	CLA	G	404	-	69,73,73	1.54	15 (21%)	82,113,113	1.94	14 (17%)
25	LHG	G	409	-	38,38,48	1.07	2 (5%)	41,44,54	0.96	3 (7%)
21	CLA	N	619	-	69,73,73	1.52	13 (18%)	82,113,113	1.97	14 (17%)
27	LMG	D	406	-	46,46,55	0.99	2 (4%)	54,54,63	1.34	7 (12%)
27	LMG	A	410	-	51,51,55	0.96	2 (3%)	59,59,63	1.27	4 (6%)
24	DGD	A	407	-	57,57,67	0.99	4 (7%)	71,71,81	1.47	8 (11%)
26	SQD	A	409	-	49,51,54	1.14	3 (6%)	59,62,65	1.38	9 (15%)
23	PL9	J	101	-	35,35,55	1.20	5 (14%)	44,45,69	1.57	8 (18%)
21	CLA	B	606	-	69,73,73	1.55	14 (20%)	82,113,113	1.90	13 (15%)
21	CLA	N	607	-	69,73,73	1.57	16 (23%)	82,113,113	1.90	13 (15%)
21	CLA	N	616	-	69,73,73	1.54	13 (18%)	82,113,113	1.98	11 (13%)
22	PHO	Q	403	-	58,69,69	2.81	12 (20%)	55,99,99	2.59	15 (27%)
26	SQD	A	414	-	52,54,54	1.09	3 (5%)	62,65,65	1.04	3 (4%)
21	CLA	G	402	-	69,73,73	1.55	16 (23%)	82,113,113	1.91	11 (13%)
30	BCR	B	617	-	41,41,41	0.73	0	56,56,56	1.61	11 (19%)
21	CLA	B	611	-	69,73,73	1.55	14 (20%)	82,113,113	1.98	12 (14%)
21	CLA	P	501	-	69,73,73	1.54	14 (20%)	82,113,113	1.95	10 (12%)
27	LMG	P	521	-	45,45,55	1.03	2 (4%)	53,53,63	1.23	5 (9%)
21	CLA	G	406	-	69,73,73	1.53	16 (23%)	82,113,113	1.93	13 (15%)
27	LMG	R	102	-	44,44,55	1.01	2 (4%)	52,52,63	1.12	4 (7%)
26	SQD	Q	408	-	41,43,54	1.28	4 (9%)	51,54,65	1.44	7 (13%)
30	BCR	P	516	-	41,41,41	0.77	0	56,56,56	1.70	13 (23%)
21	CLA	N	614	-	69,73,73	1.56	15 (21%)	82,113,113	1.89	13 (15%)
30	BCR	C	515	-	41,41,41	0.78	0	56,56,56	1.70	11 (19%)
21	CLA	G	403	-	69,73,73	1.55	16 (23%)	82,113,113	1.95	16 (19%)
27	LMG	C	519	-	48,48,55	0.97	2 (4%)	56,56,63	1.30	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	BCT	Q	411	29	3,3,3	0.71	0	2,3,3	0.09	0
21	CLA	Q	402	-	69,73,73	1.57	13 (18%)	82,113,113	1.89	14 (17%)
30	BCR	Z	101	-	41,41,41	0.68	0	56,56,56	1.63	14 (25%)
24	DGD	P	517	-	54,54,67	1.00	3 (5%)	68,68,81	1.54	10 (14%)
30	BCR	B	618	-	41,41,41	0.72	0	56,56,56	1.91	14 (25%)
27	LMG	N	623	-	49,49,55	0.95	2 (4%)	57,57,63	1.25	8 (14%)
30	BCR	T	102	-	41,41,41	0.71	0	56,56,56	1.88	16 (28%)
24	DGD	P	519	-	67,67,67	0.90	4 (5%)	81,81,81	1.28	7 (8%)
30	BCR	a	101	-	41,41,41	0.70	0	56,56,56	1.60	14 (25%)
21	CLA	B	602	-	69,73,73	1.55	14 (20%)	82,113,113	1.90	13 (15%)
24	DGD	B	621	-	59,59,67	0.95	3 (5%)	73,73,81	1.39	9 (12%)
21	CLA	B	610	-	69,73,73	1.56	14 (20%)	82,113,113	1.93	13 (15%)
27	LMG	G	411	-	51,51,55	0.96	2 (3%)	59,59,63	1.24	4 (6%)
21	CLA	N	620	-	69,73,73	1.55	13 (18%)	82,113,113	1.94	14 (17%)
21	CLA	C	505	-	69,73,73	1.53	14 (20%)	82,113,113	1.98	10 (12%)
26	SQD	N	601	-	45,47,54	1.21	4 (8%)	55,58,65	1.47	10 (18%)
31	LMT	B	629	-	36,36,36	0.45	0	47,47,47	0.78	1 (2%)
22	PHO	A	404	-	58,69,69	2.77	12 (20%)	55,99,99	2.66	17 (30%)
30	BCR	P	514	-	41,41,41	0.70	0	56,56,56	2.41	17 (30%)
21	CLA	P	513	-	69,73,73	1.55	15 (21%)	82,113,113	1.90	12 (14%)
21	CLA	C	510	-	69,73,73	1.55	15 (21%)	82,113,113	1.91	11 (13%)
21	CLA	N	613	-	69,73,73	1.55	15 (21%)	82,113,113	1.93	10 (12%)
32	BCT	D	410	29	3,3,3	0.71	0	2,3,3	0.06	0
24	DGD	C	518	-	67,67,67	0.93	4 (5%)	81,81,81	1.33	7 (8%)
30	BCR	H	101	-	41,41,41	0.78	0	56,56,56	1.48	10 (17%)
30	BCR	T	103	-	41,41,41	0.70	0	56,56,56	1.64	11 (19%)
22	PHO	G	405	-	58,69,69	2.76	12 (20%)	55,99,99	2.73	17 (30%)
21	CLA	Q	404	-	69,73,73	1.57	15 (21%)	82,113,113	1.95	12 (14%)
21	CLA	A	405	-	69,73,73	1.56	16 (23%)	82,113,113	1.93	13 (15%)
21	CLA	C	507	-	69,73,73	1.56	15 (21%)	82,113,113	1.91	11 (13%)
21	CLA	N	605	-	69,73,73	1.54	15 (21%)	82,113,113	1.94	13 (15%)
31	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.70	1 (2%)
24	DGD	W	102	-	59,59,67	0.96	3 (5%)	73,73,81	1.41	8 (10%)
23	PL9	D	404	-	55,55,55	1.27	8 (14%)	68,69,69	1.64	18 (26%)
21	CLA	N	615	-	69,73,73	1.56	15 (21%)	82,113,113	1.94	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	b	102	-	41,41,41	0.80	0	56,56,56	3.18	20 (35%)
21	CLA	N	617	-	69,73,73	1.57	15 (21%)	82,113,113	1.91	9 (10%)
31	LMT	B	630	-	36,36,36	0.39	0	47,47,47	0.63	0
21	CLA	P	509	-	69,73,73	1.55	15 (21%)	82,113,113	1.89	13 (15%)
21	CLA	P	512	-	69,73,73	1.56	14 (20%)	82,113,113	1.93	13 (15%)
21	CLA	B	612	-	69,73,73	1.57	15 (21%)	82,113,113	1.91	12 (14%)
21	CLA	C	512	-	69,73,73	1.54	13 (18%)	82,113,113	1.94	13 (15%)
21	CLA	N	606	-	69,73,73	1.55	15 (21%)	82,113,113	1.94	12 (14%)
21	CLA	N	608	-	69,73,73	1.56	14 (20%)	82,113,113	1.93	12 (14%)
26	SQD	G	410	-	49,51,54	1.14	3 (6%)	59,62,65	1.41	9 (15%)
21	CLA	N	611	-	69,73,73	1.57	16 (23%)	82,113,113	1.92	12 (14%)
21	CLA	B	613	-	69,73,73	1.54	15 (21%)	82,113,113	1.91	11 (13%)
30	BCR	W	101	-	41,41,41	0.78	0	56,56,56	1.48	8 (14%)
30	BCR	C	514	-	41,41,41	0.73	0	56,56,56	2.38	17 (30%)
30	BCR	K	101	-	41,41,41	0.81	0	56,56,56	1.64	12 (21%)
21	CLA	P	506	-	69,73,73	1.57	15 (21%)	82,113,113	1.91	13 (15%)
21	CLA	P	505	-	69,73,73	1.56	15 (21%)	82,113,113	1.97	10 (12%)
21	CLA	D	401	-	69,73,73	1.57	14 (20%)	82,113,113	1.90	13 (15%)
26	SQD	B	627	-	45,47,54	1.21	4 (8%)	55,58,65	1.40	8 (14%)
30	BCR	J	102	-	41,41,41	0.81	0	56,56,56	3.15	20 (35%)
31	LMT	D	409	-	32,32,36	0.47	0	43,43,47	0.66	1 (2%)
21	CLA	P	510	-	69,73,73	1.55	15 (21%)	82,113,113	1.92	12 (14%)
21	CLA	B	615	-	69,73,73	1.54	14 (20%)	82,113,113	1.95	13 (15%)
24	DGD	Q	409	-	64,64,67	0.91	2 (3%)	78,78,81	1.33	9 (11%)
31	LMT	N	624	-	36,36,36	0.42	0	47,47,47	0.67	0
27	LMG	Q	406	-	46,46,55	0.99	2 (4%)	54,54,63	1.31	4 (7%)
21	CLA	C	504	-	69,73,73	1.56	15 (21%)	82,113,113	1.90	13 (15%)
26	SQD	B	624	-	41,43,54	1.27	4 (9%)	51,54,65	1.43	7 (13%)
30	BCR	c	101	-	41,41,41	0.80	0	56,56,56	1.59	12 (21%)
31	LMT	N	603	-	36,36,36	0.45	0	47,47,47	0.80	1 (2%)
27	LMG	I	102	-	43,43,55	1.01	2 (4%)	51,51,63	1.32	5 (9%)
27	LMG	N	622	-	49,49,55	0.94	2 (4%)	57,57,63	1.36	7 (12%)
26	SQD	S	102	-	43,45,54	1.25	4 (9%)	53,56,65	1.17	5 (9%)
31	LMT	B	626	-	36,36,36	0.45	0	47,47,47	0.67	1 (2%)
21	CLA	D	403	-	69,73,73	1.56	15 (21%)	82,113,113	1.95	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	403	-	69,73,73	1.56	17 (24%)	82,113,113	1.90	12 (14%)
21	CLA	A	402	-	69,73,73	1.55	16 (23%)	82,113,113	1.97	14 (17%)
31	LMT	I	103	-	36,36,36	0.48	1 (2%)	47,47,47	0.71	1 (2%)
27	LMG	E	102	-	44,44,55	1.02	2 (4%)	52,52,63	1.11	5 (9%)
31	LMT	B	625	-	36,36,36	0.41	0	47,47,47	0.70	0
21	CLA	C	511	3	69,73,73	1.55	15 (21%)	82,113,113	1.96	13 (15%)
24	DGD	C	516	-	54,54,67	0.99	3 (5%)	68,68,81	1.51	11 (16%)
34	HEM	R	101	5,6	50,50,50	1.84	8 (16%)	67,82,82	1.56	10 (14%)
26	SQD	G	401	-	52,54,54	1.10	3 (5%)	62,65,65	1.02	4 (6%)
21	CLA	B	605	-	69,73,73	1.55	16 (23%)	82,113,113	1.95	15 (18%)
21	CLA	P	507	-	69,73,73	1.56	15 (21%)	82,113,113	1.90	10 (12%)
30	BCR	N	621	-	41,41,41	0.76	0	56,56,56	1.54	12 (21%)
21	CLA	B	608	-	69,73,73	1.57	15 (21%)	82,113,113	1.90	10 (12%)
27	LMG	D	412	-	42,42,55	1.04	3 (7%)	50,50,63	1.27	5 (10%)
30	BCR	D	405	-	41,41,41	0.73	0	56,56,56	1.74	10 (17%)
30	BCR	B	619	-	41,41,41	0.76	0	56,56,56	1.52	10 (17%)
21	CLA	B	601	-	69,73,73	1.55	14 (20%)	82,113,113	1.97	12 (14%)
21	CLA	C	501	-	69,73,73	1.54	14 (20%)	82,113,113	1.93	11 (13%)
21	CLA	C	509	-	69,73,73	1.57	15 (21%)	82,113,113	1.88	13 (15%)
21	CLA	P	508	-	69,73,73	1.55	16 (23%)	82,113,113	1.96	11 (13%)
21	CLA	N	612	-	69,73,73	1.57	16 (23%)	82,113,113	1.88	11 (13%)
23	PL9	Q	405	-	55,55,55	1.27	8 (14%)	68,69,69	1.66	18 (26%)
25	LHG	G	412	-	36,36,48	1.09	2 (5%)	39,42,54	1.07	2 (5%)
27	LMG	C	520	-	45,45,55	1.04	2 (4%)	53,53,63	1.27	5 (9%)
27	LMG	D	407	-	48,48,55	0.96	2 (4%)	56,56,63	1.28	5 (8%)
21	CLA	C	508	-	69,73,73	1.55	14 (20%)	82,113,113	1.94	12 (14%)
25	LHG	A	408	-	38,38,48	1.07	2 (5%)	41,44,54	0.96	2 (4%)
21	CLA	B	614	-	69,73,73	1.55	13 (18%)	82,113,113	1.87	12 (14%)
25	LHG	A	411	-	36,36,48	1.08	2 (5%)	39,42,54	1.09	2 (5%)
24	DGD	G	408	-	57,57,67	0.98	4 (7%)	71,71,81	1.46	8 (11%)
21	CLA	A	401	-	69,73,73	1.57	16 (23%)	82,113,113	1.88	12 (14%)
27	LMG	B	623	-	49,49,55	0.95	2 (4%)	57,57,63	1.26	8 (14%)
31	LMT	e	101	-	36,36,36	0.41	0	47,47,47	0.66	1 (2%)
23	PL9	b	101	-	35,35,55	1.20	5 (14%)	44,45,69	1.59	9 (20%)
27	LMG	a	102	-	43,43,55	1.01	2 (4%)	51,51,63	1.33	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	a	103	-	36,36,36	0.46	0	47,47,47	0.70	1 (2%)
27	LMG	M	101	-	42,42,55	1.03	2 (4%)	50,50,63	1.29	6 (12%)
24	DGD	C	517	-	63,63,67	0.93	3 (4%)	77,77,81	1.49	14 (18%)
22	PHO	D	402	-	58,69,69	2.81	12 (20%)	55,99,99	2.62	16 (29%)
21	CLA	B	607	-	69,73,73	1.57	15 (21%)	82,113,113	1.93	12 (14%)
21	CLA	B	604	-	69,73,73	1.55	13 (18%)	82,113,113	1.93	12 (14%)
30	BCR	S	101	-	41,41,41	0.74	0	56,56,56	1.76	11 (19%)
21	CLA	B	603	-	69,73,73	1.57	16 (23%)	82,113,113	1.93	13 (15%)
34	HEM	V	201	16	50,50,50	1.83	10 (20%)	67,82,82	1.38	5 (7%)
21	CLA	B	616	-	69,73,73	1.55	15 (21%)	82,113,113	1.94	13 (15%)
21	CLA	P	504	-	69,73,73	1.56	14 (20%)	82,113,113	1.88	12 (14%)
30	BCR	P	515	-	41,41,41	0.69	0	56,56,56	1.58	14 (25%)
34	HEM	E	101	5,6	50,50,50	1.86	8 (16%)	67,82,82	1.55	11 (16%)
21	CLA	B	609	-	69,73,73	1.54	15 (21%)	82,113,113	1.91	10 (12%)
21	CLA	C	513	-	69,73,73	1.55	15 (21%)	82,113,113	1.91	11 (13%)
21	CLA	C	503	-	69,73,73	1.54	15 (21%)	82,113,113	1.93	14 (17%)
21	CLA	C	506	-	69,73,73	1.58	17 (24%)	82,113,113	1.92	13 (15%)
34	HEM	i	201	16	50,50,50	1.85	9 (18%)	67,82,82	1.43	6 (8%)
23	PL9	A	406	-	45,45,55	1.25	7 (15%)	56,57,69	1.70	15 (26%)
27	LMG	Q	401	-	42,42,55	1.04	2 (4%)	50,50,63	1.24	5 (10%)
30	BCR	I	101	-	41,41,41	0.70	0	56,56,56	1.58	13 (23%)
21	CLA	C	502	-	69,73,73	1.55	14 (20%)	82,113,113	1.91	10 (12%)
31	LMT	N	604	-	36,36,36	0.42	0	47,47,47	0.63	1 (2%)
27	LMG	P	520	-	48,48,55	0.96	2 (4%)	56,56,63	1.30	6 (10%)
24	DGD	D	408	-	64,64,67	0.91	2 (3%)	78,78,81	1.33	9 (11%)
21	CLA	P	503	-	69,73,73	1.54	14 (20%)	82,113,113	1.90	14 (17%)
21	CLA	N	610	-	69,73,73	1.54	14 (20%)	82,113,113	1.92	12 (14%)
23	PL9	G	407	-	45,45,55	1.25	7 (15%)	56,57,69	1.71	15 (26%)
27	LMG	Q	407	-	48,48,55	0.96	2 (4%)	56,56,63	1.30	5 (8%)
21	CLA	N	618	-	69,73,73	1.56	14 (20%)	82,113,113	1.85	12 (14%)
21	CLA	P	511	3	69,73,73	1.54	13 (18%)	82,113,113	1.93	12 (14%)
21	CLA	N	609	-	69,73,73	1.55	16 (23%)	82,113,113	1.99	16 (19%)
21	CLA	P	502	-	69,73,73	1.56	14 (20%)	82,113,113	1.93	12 (14%)
24	DGD	N	602	-	53,53,67	1.02	3 (5%)	67,67,81	1.51	10 (14%)
30	BCR	B	620	-	41,41,41	0.73	0	56,56,56	1.62	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	T	101	-	41,41,41	0.73	0	56,56,56	1.59	11 (19%)
26	SQD	F	101	-	43,45,54	1.23	3 (6%)	53,56,65	1.17	6 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	Q	410	-	-	0/17/57/61	0/2/2/2
27	LMG	e	102	-	2/2/8/8	12/37/57/70	0/1/1/1
31	LMT	N	625	-	-	2/21/61/61	0/2/2/2
27	LMG	B	622	-	2/2/8/8	24/44/64/70	0/1/1/1
24	DGD	B	628	-	3/3/13/13	22/41/81/95	0/2/2/2
24	DGD	P	518	-	3/3/13/13	19/51/91/95	0/2/2/2
21	CLA	G	404	-	1/1/15/20	12/39/115/115	-
25	LHG	G	409	-	-	13/43/43/53	-
21	CLA	N	619	-	1/1/15/20	10/39/115/115	-
27	LMG	D	406	-	2/2/8/8	13/41/61/70	0/1/1/1
27	LMG	A	410	-	2/2/8/8	22/46/66/70	0/1/1/1
24	DGD	A	407	-	3/3/13/13	13/45/85/95	0/2/2/2
26	SQD	A	409	-	-	16/46/66/69	0/1/1/1
23	PL9	J	101	-	-	12/29/49/73	0/1/1/1
21	CLA	B	606	-	1/1/15/20	15/39/115/115	-
21	CLA	N	607	-	1/1/15/20	13/39/115/115	-
21	CLA	N	616	-	1/1/15/20	12/39/115/115	-
22	PHO	Q	403	-	-	11/37/103/103	0/5/6/6
26	SQD	A	414	-	-	19/49/69/69	0/1/1/1
21	CLA	G	402	-	1/1/15/20	9/39/115/115	-
30	BCR	B	617	-	-	2/29/63/63	0/2/2/2
21	CLA	B	611	-	1/1/15/20	15/39/115/115	-
21	CLA	P	501	-	1/1/15/20	14/39/115/115	-
27	LMG	P	521	-	2/2/8/8	19/40/60/70	0/1/1/1
21	CLA	G	406	-	1/1/15/20	12/39/115/115	-
27	LMG	R	102	-	2/2/8/8	16/39/59/70	0/1/1/1
26	SQD	Q	408	-	-	10/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	P	516	-	-	8/29/63/63	0/2/2/2
21	CLA	N	614	-	1/1/15/20	19/39/115/115	-
30	BCR	C	515	-	-	8/29/63/63	0/2/2/2
21	CLA	G	403	-	1/1/15/20	14/39/115/115	-
27	LMG	C	519	-	2/2/8/8	20/43/63/70	0/1/1/1
21	CLA	Q	402	-	1/1/15/20	15/39/115/115	-
30	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
24	DGD	P	517	-	3/3/13/13	17/42/82/95	0/2/2/2
30	BCR	B	618	-	-	4/29/63/63	0/2/2/2
27	LMG	N	623	-	2/2/8/8	17/44/64/70	0/1/1/1
30	BCR	T	102	-	-	4/29/63/63	0/2/2/2
24	DGD	P	519	-	3/3/13/13	19/55/95/95	0/2/2/2
30	BCR	a	101	-	-	4/29/63/63	0/2/2/2
21	CLA	B	602	-	1/1/15/20	19/39/115/115	-
24	DGD	B	621	-	3/3/13/13	17/47/87/95	0/2/2/2
21	CLA	B	610	-	1/1/15/20	19/39/115/115	-
27	LMG	G	411	-	2/2/8/8	22/46/66/70	0/1/1/1
21	CLA	N	620	-	1/1/15/20	21/39/115/115	-
21	CLA	C	505	-	1/1/15/20	19/39/115/115	-
26	SQD	N	601	-	-	13/42/62/69	0/1/1/1
31	LMT	B	629	-	-	3/21/61/61	0/2/2/2
22	PHO	A	404	-	-	10/37/103/103	0/5/6/6
30	BCR	P	514	-	-	4/29/63/63	0/2/2/2
21	CLA	P	513	-	1/1/15/20	19/39/115/115	-
21	CLA	C	510	-	1/1/15/20	15/39/115/115	-
21	CLA	N	613	-	1/1/15/20	9/39/115/115	-
24	DGD	C	518	-	3/3/13/13	21/55/95/95	0/2/2/2
30	BCR	H	101	-	-	2/29/63/63	0/2/2/2
30	BCR	T	103	-	-	2/29/63/63	0/2/2/2
22	PHO	G	405	-	-	9/37/103/103	0/5/6/6
21	CLA	Q	404	-	1/1/15/20	7/39/115/115	-
21	CLA	A	405	-	1/1/15/20	13/39/115/115	-
21	CLA	C	507	-	1/1/15/20	13/39/115/115	-
21	CLA	N	605	-	1/1/15/20	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
24	DGD	W	102	-	3/3/13/13	17/47/87/95	0/2/2/2
23	PL9	D	404	-	-	17/53/73/73	0/1/1/1
21	CLA	N	615	-	1/1/15/20	15/39/115/115	-
30	BCR	b	102	-	-	2/29/63/63	0/2/2/2
21	CLA	N	617	-	1/1/15/20	20/39/115/115	-
31	LMT	B	630	-	-	5/21/61/61	0/2/2/2
21	CLA	P	509	-	1/1/15/20	12/39/115/115	-
21	CLA	P	512	-	1/1/15/20	20/39/115/115	-
21	CLA	B	612	-	1/1/15/20	12/39/115/115	-
21	CLA	C	512	-	1/1/15/20	21/39/115/115	-
21	CLA	N	606	-	1/1/15/20	20/39/115/115	-
21	CLA	N	608	-	1/1/15/20	10/39/115/115	-
26	SQD	G	410	-	-	15/46/66/69	0/1/1/1
21	CLA	N	611	-	1/1/15/20	9/39/115/115	-
21	CLA	B	613	-	1/1/15/20	17/39/115/115	-
30	BCR	W	101	-	-	2/29/63/63	0/2/2/2
30	BCR	C	514	-	-	4/29/63/63	0/2/2/2
30	BCR	K	101	-	-	6/29/63/63	0/2/2/2
21	CLA	P	506	-	1/1/15/20	18/39/115/115	-
21	CLA	P	505	-	1/1/15/20	20/39/115/115	-
21	CLA	D	401	-	1/1/15/20	15/39/115/115	-
26	SQD	B	627	-	-	14/42/62/69	0/1/1/1
30	BCR	J	102	-	-	2/29/63/63	0/2/2/2
31	LMT	D	409	-	-	0/17/57/61	0/2/2/2
21	CLA	P	510	-	1/1/15/20	13/39/115/115	-
21	CLA	B	615	-	1/1/15/20	10/39/115/115	-
24	DGD	Q	409	-	3/3/13/13	34/52/92/95	0/2/2/2
31	LMT	N	624	-	-	3/21/61/61	0/2/2/2
27	LMG	Q	406	-	2/2/8/8	13/41/61/70	0/1/1/1
21	CLA	C	504	-	1/1/15/20	12/39/115/115	-
26	SQD	B	624	-	-	10/38/58/69	0/1/1/1
30	BCR	c	101	-	-	6/29/63/63	0/2/2/2
31	LMT	N	603	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	I	102	-	2/2/8/8	19/38/58/70	0/1/1/1
27	LMG	N	622	-	2/2/8/8	23/44/64/70	0/1/1/1
26	SQD	S	102	-	-	13/40/60/69	0/1/1/1
31	LMT	B	626	-	-	2/21/61/61	0/2/2/2
21	CLA	D	403	-	1/1/15/20	8/39/115/115	-
21	CLA	A	403	-	1/1/15/20	13/39/115/115	-
21	CLA	A	402	-	1/1/15/20	15/39/115/115	-
31	LMT	I	103	-	-	4/21/61/61	0/2/2/2
27	LMG	E	102	-	2/2/8/8	15/39/59/70	0/1/1/1
31	LMT	B	625	-	-	3/21/61/61	0/2/2/2
21	CLA	C	511	3	1/1/15/20	16/39/115/115	-
24	DGD	C	516	-	3/3/13/13	19/42/82/95	0/2/2/2
34	HEM	R	101	5,6	-	3/14/54/54	-
26	SQD	G	401	-	-	17/49/69/69	0/1/1/1
21	CLA	B	605	-	1/1/15/20	22/39/115/115	-
21	CLA	P	507	-	1/1/15/20	13/39/115/115	-
30	BCR	N	621	-	-	0/29/63/63	0/2/2/2
21	CLA	B	608	-	1/1/15/20	18/39/115/115	-
27	LMG	D	412	-	2/2/8/8	15/37/57/70	0/1/1/1
30	BCR	D	405	-	-	6/29/63/63	0/2/2/2
30	BCR	B	619	-	-	0/29/63/63	0/2/2/2
21	CLA	B	601	-	1/1/15/20	20/39/115/115	-
21	CLA	C	501	-	1/1/15/20	14/39/115/115	-
21	CLA	C	509	-	1/1/15/20	13/39/115/115	-
21	CLA	P	508	-	1/1/15/20	13/39/115/115	-
21	CLA	N	612	-	1/1/15/20	18/39/115/115	-
27	LMG	C	520	-	2/2/8/8	17/40/60/70	0/1/1/1
23	PL9	Q	405	-	-	17/53/73/73	0/1/1/1
25	LHG	G	412	-	-	13/41/41/53	-
27	LMG	D	407	-	2/2/8/8	20/43/63/70	0/1/1/1
21	CLA	C	508	-	1/1/15/20	13/39/115/115	-
25	LHG	A	408	-	-	12/43/43/53	-
21	CLA	B	614	-	1/1/15/20	18/39/115/115	-
27	LMG	B	623	-	2/2/8/8	15/44/64/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DGD	G	408	-	3/3/13/13	13/45/85/95	0/2/2/2
21	CLA	A	401	-	1/1/15/20	9/39/115/115	-
25	LHG	A	411	-	-	12/41/41/53	-
31	LMT	e	101	-	-	0/21/61/61	0/2/2/2
23	PL9	b	101	-	-	11/29/49/73	0/1/1/1
27	LMG	a	102	-	2/2/8/8	20/38/58/70	0/1/1/1
31	LMT	a	103	-	-	4/21/61/61	0/2/2/2
27	LMG	M	101	-	2/2/8/8	14/37/57/70	0/1/1/1
24	DGD	C	517	-	3/3/13/13	18/51/91/95	0/2/2/2
22	PHO	D	402	-	-	13/37/103/103	0/5/6/6
21	CLA	B	607	-	1/1/15/20	10/39/115/115	-
21	CLA	B	604	-	1/1/15/20	10/39/115/115	-
30	BCR	S	101	-	-	6/29/63/63	0/2/2/2
21	CLA	B	603	-	1/1/15/20	15/39/115/115	-
34	HEM	V	201	16	-	3/14/54/54	-
21	CLA	B	616	-	1/1/15/20	21/39/115/115	-
21	CLA	P	504	-	1/1/15/20	12/39/115/115	-
30	BCR	P	515	-	-	4/29/63/63	0/2/2/2
34	HEM	E	101	5,6	-	4/14/54/54	-
21	CLA	B	609	-	1/1/15/20	9/39/115/115	-
21	CLA	C	513	-	1/1/15/20	20/39/115/115	-
21	CLA	C	503	-	1/1/15/20	16/39/115/115	-
21	CLA	C	506	-	1/1/15/20	18/39/115/115	-
34	HEM	i	201	16	-	3/14/54/54	-
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
27	LMG	Q	401	-	2/2/8/8	16/37/57/70	0/1/1/1
30	BCR	I	101	-	-	4/29/63/63	0/2/2/2
21	CLA	C	502	-	1/1/15/20	11/39/115/115	-
31	LMT	N	604	-	-	5/21/61/61	0/2/2/2
27	LMG	P	520	-	2/2/8/8	20/43/63/70	0/1/1/1
24	DGD	D	408	-	3/3/13/13	33/52/92/95	0/2/2/2
21	CLA	P	503	-	1/1/15/20	16/39/115/115	-
21	CLA	N	610	-	1/1/15/20	15/39/115/115	-
23	PL9	G	407	-	-	18/41/61/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	Q	407	-	2/2/8/8	18/43/63/70	0/1/1/1
21	CLA	N	618	-	1/1/15/20	19/39/115/115	-
21	CLA	P	511	3	1/1/15/20	15/39/115/115	-
21	CLA	N	609	-	1/1/15/20	23/39/115/115	-
21	CLA	P	502	-	1/1/15/20	11/39/115/115	-
24	DGD	N	602	-	3/3/13/13	22/41/81/95	0/2/2/2
30	BCR	B	620	-	-	2/29/63/63	0/2/2/2
30	BCR	T	101	-	-	2/29/63/63	0/2/2/2
26	SQD	F	101	-	-	14/40/60/69	0/1/1/1

All (1288) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	402	PHO	C1D-C2D	10.28	1.50	1.39
22	G	405	PHO	C1D-C2D	10.16	1.50	1.39
22	Q	403	PHO	C1D-C2D	10.11	1.50	1.39
22	A	404	PHO	C1D-C2D	10.04	1.50	1.39
22	A	404	PHO	C1B-C2B	9.39	1.49	1.39
22	D	402	PHO	C1B-C2B	9.34	1.49	1.39
22	G	405	PHO	C1B-C2B	9.28	1.49	1.39
22	Q	403	PHO	C1B-C2B	9.27	1.49	1.39
34	i	201	HEM	C3D-C2D	7.92	1.53	1.36
34	V	201	HEM	C3D-C2D	7.91	1.53	1.36
34	E	101	HEM	C3D-C2D	7.82	1.53	1.36
34	R	101	HEM	C3D-C2D	7.75	1.53	1.36
22	Q	403	PHO	C3B-C4B	7.07	1.48	1.41
22	D	402	PHO	C3B-C4B	7.07	1.48	1.41
22	G	405	PHO	C3B-C4B	6.63	1.48	1.41
22	A	404	PHO	C3B-C4B	6.52	1.48	1.41
22	Q	403	PHO	C4D-CHA	6.30	1.49	1.39
22	A	404	PHO	C4D-CHA	6.21	1.48	1.39
22	G	405	PHO	C4D-CHA	6.15	1.48	1.39
22	D	402	PHO	C4D-CHA	6.02	1.48	1.39
22	Q	403	PHO	C3B-C2B	5.41	1.47	1.40
22	D	402	PHO	C3B-C2B	5.30	1.47	1.40
22	G	405	PHO	C3B-C2B	5.28	1.47	1.40
22	A	404	PHO	C3B-C2B	5.28	1.47	1.40
22	D	402	PHO	O2D-CGD	5.12	1.45	1.33
22	Q	403	PHO	O2D-CGD	5.10	1.45	1.33
22	A	404	PHO	C3D-C4D	-5.01	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	405	PHO	O2D-CGD	4.93	1.45	1.33
22	D	402	PHO	C3D-C4D	-4.90	1.34	1.41
22	D	402	PHO	OBD-CAD	4.86	1.28	1.22
22	Q	403	PHO	OBD-CAD	4.84	1.28	1.22
22	A	404	PHO	O2D-CGD	4.83	1.45	1.33
22	G	405	PHO	OBD-CAD	4.83	1.28	1.22
22	G	405	PHO	C3D-C4D	-4.83	1.34	1.41
22	Q	403	PHO	C3D-C4D	-4.82	1.34	1.41
22	A	404	PHO	OBD-CAD	4.73	1.28	1.22
34	E	101	HEM	FE-ND	4.66	2.09	1.94
34	R	101	HEM	FE-ND	4.54	2.08	1.94
27	C	519	LMG	O8-C28	4.49	1.46	1.33
27	P	521	LMG	O8-C28	4.48	1.46	1.33
27	C	520	LMG	O8-C28	4.48	1.46	1.33
24	Q	409	DGD	O2G-C1B	4.43	1.46	1.34
24	N	602	DGD	O1G-C1A	4.42	1.46	1.33
27	C	520	LMG	O7-C10	4.41	1.46	1.34
27	G	411	LMG	O7-C10	4.41	1.46	1.34
27	P	520	LMG	O8-C28	4.41	1.46	1.33
24	D	408	DGD	O2G-C1B	4.40	1.46	1.34
24	A	407	DGD	O2G-C1B	4.40	1.46	1.34
24	D	408	DGD	O1G-C1A	4.39	1.46	1.33
27	E	102	LMG	O7-C10	4.39	1.46	1.34
24	Q	409	DGD	O1G-C1A	4.39	1.46	1.33
24	C	517	DGD	O1G-C1A	4.37	1.46	1.33
26	G	401	SQD	O8-S	4.37	1.63	1.47
27	A	410	LMG	O7-C10	4.36	1.46	1.34
24	B	628	DGD	O1G-C1A	4.36	1.46	1.33
26	G	410	SQD	O8-S	4.36	1.63	1.47
26	Q	408	SQD	O8-S	4.36	1.63	1.47
24	P	518	DGD	O1G-C1A	4.36	1.46	1.33
26	F	101	SQD	O8-S	4.36	1.63	1.47
26	B	624	SQD	O8-S	4.36	1.63	1.47
26	A	409	SQD	O48-C23	4.35	1.46	1.33
24	W	102	DGD	O1G-C1A	4.35	1.46	1.33
26	Q	408	SQD	O48-C23	4.35	1.46	1.33
27	P	521	LMG	O7-C10	4.34	1.46	1.34
25	G	409	LHG	O8-C23	4.34	1.46	1.33
26	S	102	SQD	O8-S	4.33	1.63	1.47
26	N	601	SQD	O48-C23	4.33	1.46	1.33
26	B	627	SQD	O48-C23	4.33	1.46	1.33
26	B	624	SQD	O48-C23	4.33	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	414	SQD	O8-S	4.32	1.63	1.47
24	G	408	DGD	O2G-C1B	4.32	1.46	1.34
27	R	102	LMG	O7-C10	4.32	1.46	1.34
26	G	410	SQD	O48-C23	4.32	1.45	1.33
25	A	408	LHG	O8-C23	4.32	1.45	1.33
26	A	409	SQD	O8-S	4.32	1.63	1.47
27	M	101	LMG	O7-C10	4.31	1.46	1.34
27	a	102	LMG	O8-C28	4.30	1.45	1.33
26	B	627	SQD	O8-S	4.30	1.63	1.47
24	C	518	DGD	O1G-C1A	4.29	1.45	1.33
27	E	102	LMG	O8-C28	4.29	1.45	1.33
27	I	102	LMG	O8-C28	4.28	1.45	1.33
27	N	623	LMG	O8-C28	4.28	1.45	1.33
27	Q	406	LMG	O8-C28	4.28	1.45	1.33
26	N	601	SQD	O8-S	4.28	1.63	1.47
24	B	621	DGD	O1G-C1A	4.28	1.45	1.33
22	A	404	PHO	O2A-CGA	4.28	1.45	1.33
26	A	414	SQD	O48-C23	4.27	1.45	1.33
27	B	623	LMG	O8-C28	4.27	1.45	1.33
27	A	410	LMG	O8-C28	4.27	1.45	1.33
24	C	518	DGD	O2G-C1B	4.27	1.46	1.34
26	G	401	SQD	O48-C23	4.26	1.45	1.33
25	G	412	LHG	O8-C23	4.25	1.45	1.33
34	i	201	HEM	FE-NA	4.25	2.09	1.95
27	G	411	LMG	O8-C28	4.25	1.45	1.33
27	D	406	LMG	O8-C28	4.25	1.45	1.33
27	e	102	LMG	O7-C10	4.24	1.46	1.34
27	Q	407	LMG	O8-C28	4.24	1.45	1.33
24	B	628	DGD	O2G-C1B	4.24	1.46	1.34
24	P	519	DGD	O2G-C1B	4.24	1.46	1.34
24	N	602	DGD	O2G-C1B	4.24	1.46	1.34
24	P	519	DGD	O1G-C1A	4.23	1.45	1.33
24	P	517	DGD	O2G-C1B	4.23	1.46	1.34
25	A	408	LHG	O7-C7	4.23	1.46	1.34
27	e	102	LMG	O8-C28	4.23	1.45	1.33
26	S	102	SQD	O48-C23	4.22	1.45	1.33
24	C	516	DGD	O1G-C1A	4.22	1.45	1.33
22	A	404	PHO	C3A-C2A	-4.22	1.51	1.54
26	S	102	SQD	O47-C7	4.22	1.46	1.34
25	A	411	LHG	O8-C23	4.22	1.45	1.33
24	P	517	DGD	O1G-C1A	4.21	1.45	1.33
27	D	407	LMG	O8-C28	4.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Q	401	LMG	O7-C10	4.21	1.46	1.34
27	Q	401	LMG	O8-C28	4.20	1.45	1.33
27	D	412	LMG	O7-C10	4.19	1.46	1.34
26	F	101	SQD	O48-C23	4.19	1.45	1.33
22	Q	403	PHO	C3D-C2D	4.18	1.46	1.39
27	D	412	LMG	O8-C28	4.18	1.45	1.33
24	C	517	DGD	O2G-C1B	4.18	1.46	1.34
27	B	623	LMG	O7-C10	4.18	1.46	1.34
25	G	409	LHG	O7-C7	4.18	1.46	1.34
22	D	402	PHO	O2A-CGA	4.17	1.45	1.33
22	G	405	PHO	O2A-CGA	4.17	1.45	1.33
27	Q	406	LMG	O7-C10	4.17	1.46	1.34
24	G	408	DGD	O1G-C1A	4.17	1.45	1.33
27	N	623	LMG	O7-C10	4.16	1.46	1.34
25	G	412	LHG	O7-C7	4.16	1.46	1.34
24	A	407	DGD	O1G-C1A	4.16	1.45	1.33
27	R	102	LMG	O8-C28	4.16	1.45	1.33
27	M	101	LMG	O8-C28	4.16	1.45	1.33
26	A	414	SQD	O47-C7	4.15	1.46	1.34
22	G	405	PHO	C3A-C2A	-4.14	1.51	1.54
24	C	516	DGD	O2G-C1B	4.14	1.46	1.34
21	B	612	CLA	MG-ND	-4.14	1.97	2.05
27	D	406	LMG	O7-C10	4.14	1.46	1.34
26	Q	408	SQD	O47-C7	4.14	1.46	1.34
26	F	101	SQD	O47-C7	4.13	1.45	1.34
25	A	411	LHG	O7-C7	4.12	1.45	1.34
26	G	401	SQD	O47-C7	4.12	1.45	1.34
27	I	102	LMG	O7-C10	4.12	1.45	1.34
26	B	624	SQD	O47-C7	4.12	1.45	1.34
27	B	622	LMG	O8-C28	4.11	1.45	1.33
22	Q	403	PHO	O2A-CGA	4.11	1.45	1.33
34	V	201	HEM	FE-NA	4.10	2.08	1.95
21	P	505	CLA	MG-ND	-4.10	1.97	2.05
27	B	622	LMG	O7-C10	4.09	1.45	1.34
24	P	518	DGD	O2G-C1B	4.09	1.45	1.34
27	a	102	LMG	O7-C10	4.09	1.45	1.34
21	C	506	CLA	MG-ND	-4.09	1.97	2.05
24	B	621	DGD	O2G-C1B	4.09	1.45	1.34
27	N	622	LMG	O8-C28	4.09	1.45	1.33
27	N	622	LMG	O7-C10	4.07	1.45	1.34
27	Q	407	LMG	O7-C10	4.07	1.45	1.34
26	N	601	SQD	O47-C7	4.07	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	403	PHO	C3A-C2A	-4.06	1.51	1.54
24	W	102	DGD	O2G-C1B	4.06	1.45	1.34
26	B	627	SQD	O47-C7	4.05	1.45	1.34
21	A	401	CLA	MG-ND	-4.05	1.97	2.05
21	P	506	CLA	MG-ND	-4.04	1.97	2.05
27	D	407	LMG	O7-C10	4.04	1.45	1.34
26	G	410	SQD	O47-C7	4.04	1.45	1.34
21	C	509	CLA	MG-ND	-4.03	1.97	2.05
21	P	507	CLA	MG-ND	-4.03	1.97	2.05
22	D	402	PHO	C3A-C2A	-4.03	1.51	1.54
26	A	409	SQD	O47-C7	4.02	1.45	1.34
21	N	620	CLA	MG-ND	-4.02	1.97	2.05
22	D	402	PHO	C3D-C2D	4.02	1.46	1.39
21	N	618	CLA	MG-ND	-4.02	1.97	2.05
21	C	507	CLA	MG-ND	-4.00	1.97	2.05
21	D	401	CLA	MG-ND	-3.99	1.97	2.05
21	A	403	CLA	MG-ND	-3.99	1.97	2.05
21	Q	404	CLA	MG-ND	-3.98	1.97	2.05
21	Q	402	CLA	MG-ND	-3.98	1.97	2.05
21	B	616	CLA	MG-ND	-3.97	1.97	2.05
21	N	605	CLA	MG-ND	-3.97	1.97	2.05
21	N	607	CLA	MG-ND	-3.97	1.97	2.05
21	P	512	CLA	MG-ND	-3.96	1.97	2.05
21	P	510	CLA	MG-ND	-3.95	1.97	2.05
21	N	608	CLA	MG-ND	-3.95	1.97	2.05
21	A	405	CLA	MG-ND	-3.95	1.98	2.05
21	B	602	CLA	MG-ND	-3.95	1.98	2.05
21	N	613	CLA	MG-ND	-3.94	1.98	2.05
21	D	403	CLA	MG-ND	-3.94	1.98	2.05
21	B	614	CLA	MG-ND	-3.93	1.98	2.05
21	N	615	CLA	MG-ND	-3.93	1.98	2.05
21	N	612	CLA	MG-ND	-3.93	1.98	2.05
27	C	519	LMG	O7-C10	3.93	1.45	1.34
21	C	510	CLA	MG-ND	-3.93	1.98	2.05
34	V	201	HEM	FE-ND	3.93	2.07	1.94
27	P	520	LMG	O7-C10	3.92	1.45	1.34
21	P	508	CLA	MG-ND	-3.92	1.98	2.05
21	B	606	CLA	MG-ND	-3.91	1.98	2.05
21	C	511	CLA	MG-ND	-3.91	1.98	2.05
21	B	608	CLA	MG-ND	-3.90	1.98	2.05
22	G	405	PHO	C3D-C2D	3.90	1.46	1.39
21	C	503	CLA	MG-ND	-3.89	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	504	CLA	MG-ND	-3.89	1.98	2.05
21	C	502	CLA	MG-ND	-3.89	1.98	2.05
21	G	404	CLA	MG-ND	-3.89	1.98	2.05
21	N	611	CLA	MG-ND	-3.89	1.98	2.05
21	N	614	CLA	MG-ND	-3.88	1.98	2.05
21	P	503	CLA	MG-ND	-3.88	1.98	2.05
21	B	601	CLA	MG-ND	-3.88	1.98	2.05
21	G	402	CLA	MG-ND	-3.87	1.98	2.05
21	B	603	CLA	MG-ND	-3.87	1.98	2.05
21	B	607	CLA	MG-ND	-3.86	1.98	2.05
21	B	609	CLA	MG-ND	-3.86	1.98	2.05
21	P	504	CLA	MG-ND	-3.86	1.98	2.05
21	G	403	CLA	MG-ND	-3.86	1.98	2.05
21	B	611	CLA	MG-ND	-3.86	1.98	2.05
21	N	617	CLA	MG-ND	-3.86	1.98	2.05
21	B	604	CLA	MG-ND	-3.86	1.98	2.05
21	P	509	CLA	MG-ND	-3.85	1.98	2.05
21	P	511	CLA	MG-ND	-3.85	1.98	2.05
21	B	613	CLA	MG-ND	-3.85	1.98	2.05
21	B	615	CLA	MG-ND	-3.85	1.98	2.05
21	C	508	CLA	MG-ND	-3.84	1.98	2.05
21	C	501	CLA	MG-ND	-3.84	1.98	2.05
22	A	404	PHO	C3D-C2D	3.83	1.46	1.39
21	B	610	CLA	MG-ND	-3.82	1.98	2.05
21	G	406	CLA	MG-ND	-3.82	1.98	2.05
21	P	502	CLA	MG-ND	-3.82	1.98	2.05
21	B	605	CLA	MG-ND	-3.81	1.98	2.05
21	P	513	CLA	MG-ND	-3.80	1.98	2.05
21	C	513	CLA	MG-ND	-3.80	1.98	2.05
21	C	512	CLA	MG-ND	-3.80	1.98	2.05
21	C	505	CLA	MG-ND	-3.80	1.98	2.05
21	N	606	CLA	MG-ND	-3.80	1.98	2.05
21	N	609	CLA	MG-ND	-3.77	1.98	2.05
21	N	610	CLA	MG-ND	-3.77	1.98	2.05
21	P	501	CLA	MG-ND	-3.77	1.98	2.05
21	A	402	CLA	MG-ND	-3.76	1.98	2.05
21	N	619	CLA	MG-ND	-3.75	1.98	2.05
21	N	616	CLA	MG-ND	-3.72	1.98	2.05
21	N	616	CLA	C1C-C2C	3.67	1.52	1.44
34	E	101	HEM	FE-NB	3.65	2.06	1.94
21	C	505	CLA	C1C-C2C	3.65	1.51	1.44
21	B	609	CLA	C1C-C2C	3.65	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	505	CLA	C1D-C2D	-3.64	1.38	1.45
34	R	101	HEM	FE-NB	3.63	2.06	1.94
34	E	101	HEM	FE-NA	3.63	2.07	1.95
21	Q	402	CLA	C1C-C2C	3.61	1.51	1.44
21	G	402	CLA	C1C-C2C	3.59	1.51	1.44
21	P	505	CLA	C1C-C2C	3.58	1.51	1.44
21	N	617	CLA	C1C-C2C	3.57	1.51	1.44
21	Q	404	CLA	C1C-C2C	3.55	1.51	1.44
21	B	610	CLA	C1C-C2C	3.55	1.51	1.44
21	P	511	CLA	C1C-C2C	3.55	1.51	1.44
21	D	401	CLA	C1C-C2C	3.54	1.51	1.44
21	C	513	CLA	C1C-C2C	3.53	1.51	1.44
21	B	612	CLA	C1D-C2D	-3.53	1.38	1.45
21	B	603	CLA	C1C-C2C	3.53	1.51	1.44
21	N	606	CLA	C1C-C2C	3.53	1.51	1.44
21	P	506	CLA	C1C-C2C	3.52	1.51	1.44
21	P	513	CLA	C1C-C2C	3.52	1.51	1.44
21	N	607	CLA	C1C-C2C	3.52	1.51	1.44
21	B	602	CLA	C1C-C2C	3.51	1.51	1.44
21	N	613	CLA	C1C-C2C	3.51	1.51	1.44
21	N	610	CLA	C1C-C2C	3.50	1.51	1.44
21	B	612	CLA	C1C-C2C	3.50	1.51	1.44
21	C	512	CLA	C1C-C2C	3.50	1.51	1.44
21	N	614	CLA	C1C-C2C	3.49	1.51	1.44
21	P	508	CLA	C1C-C2C	3.49	1.51	1.44
21	B	608	CLA	C1C-C2C	3.48	1.51	1.44
21	N	618	CLA	C1C-C2C	3.48	1.51	1.44
21	C	508	CLA	C1C-C2C	3.48	1.51	1.44
21	B	606	CLA	C1C-C2C	3.47	1.51	1.44
21	B	603	CLA	C2-C3	3.47	1.41	1.33
21	B	607	CLA	C2-C3	3.47	1.41	1.33
21	N	607	CLA	C2-C3	3.47	1.41	1.33
21	P	503	CLA	C1C-C2C	3.47	1.51	1.44
21	D	403	CLA	C1C-C2C	3.46	1.51	1.44
21	C	510	CLA	C1C-C2C	3.46	1.51	1.44
21	P	512	CLA	C1C-C2C	3.46	1.51	1.44
21	P	510	CLA	C1C-C2C	3.46	1.51	1.44
21	A	402	CLA	C4C-C3C	3.45	1.50	1.45
21	B	614	CLA	C1C-C2C	3.45	1.51	1.44
21	N	612	CLA	C1C-C2C	3.45	1.51	1.44
34	i	201	HEM	FE-NC	3.45	2.06	1.95
21	P	504	CLA	C2-C3	3.45	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	509	CLA	C1C-C2C	3.44	1.51	1.44
21	G	403	CLA	C4C-C3C	3.44	1.50	1.45
21	B	615	CLA	C1C-C2C	3.44	1.51	1.44
21	N	616	CLA	C1D-C2D	-3.43	1.38	1.45
21	C	503	CLA	C1C-C2C	3.43	1.51	1.44
21	B	613	CLA	C1C-C2C	3.43	1.51	1.44
21	B	608	CLA	C2-C3	3.43	1.41	1.33
21	N	609	CLA	C1C-C2C	3.43	1.51	1.44
23	A	406	PL9	C33-C34	3.43	1.41	1.33
21	N	611	CLA	C2-C3	3.42	1.40	1.33
21	C	511	CLA	C1C-C2C	3.42	1.51	1.44
21	P	501	CLA	C1C-C2C	3.42	1.51	1.44
21	P	509	CLA	C1C-C2C	3.42	1.51	1.44
21	B	604	CLA	C1C-C2C	3.41	1.51	1.44
21	B	611	CLA	C1C-C2C	3.41	1.51	1.44
21	C	505	CLA	C1D-C2D	-3.41	1.38	1.45
21	A	401	CLA	C1C-C2C	3.41	1.51	1.44
21	A	405	CLA	C1C-C2C	3.41	1.51	1.44
21	N	611	CLA	C1C-C2C	3.40	1.51	1.44
21	N	612	CLA	C2-C3	3.40	1.40	1.33
21	B	601	CLA	C4C-C3C	3.40	1.50	1.45
21	C	507	CLA	C1C-C2C	3.39	1.51	1.44
21	N	619	CLA	C1C-C2C	3.39	1.51	1.44
23	G	407	PL9	C33-C34	3.39	1.40	1.33
21	C	501	CLA	C1C-C2C	3.38	1.51	1.44
21	B	605	CLA	C1C-C2C	3.38	1.51	1.44
21	N	605	CLA	C4C-C3C	3.38	1.50	1.45
21	B	614	CLA	C4C-C3C	3.37	1.50	1.45
21	P	502	CLA	C1C-C2C	3.37	1.51	1.44
21	P	507	CLA	C1C-C2C	3.37	1.51	1.44
21	A	403	CLA	C1C-C2C	3.37	1.51	1.44
23	Q	405	PL9	C38-C39	3.36	1.40	1.33
21	N	616	CLA	C2-C3	3.36	1.40	1.33
21	C	506	CLA	C1C-C2C	3.36	1.51	1.44
21	B	604	CLA	C2-C3	3.36	1.40	1.33
21	D	401	CLA	C2-C3	3.36	1.40	1.33
21	B	607	CLA	C1C-C2C	3.36	1.51	1.44
34	R	101	HEM	FE-NA	3.35	2.06	1.95
21	N	615	CLA	C1C-C2C	3.35	1.51	1.44
21	P	510	CLA	C1D-C2D	-3.35	1.38	1.45
34	i	201	HEM	FE-ND	3.35	2.05	1.94
21	C	504	CLA	C2-C3	3.35	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	406	CLA	C1C-C2C	3.34	1.51	1.44
21	A	403	CLA	C4C-C3C	3.34	1.50	1.45
21	N	610	CLA	C4C-C3C	3.34	1.50	1.45
21	C	504	CLA	C1C-C2C	3.33	1.51	1.44
21	C	502	CLA	C1C-C2C	3.33	1.51	1.44
21	P	502	CLA	C2-C3	3.33	1.40	1.33
21	N	620	CLA	C2-C3	3.33	1.40	1.33
21	C	513	CLA	C2-C3	3.32	1.40	1.33
21	G	404	CLA	C4C-C3C	3.32	1.50	1.45
21	G	404	CLA	C1C-C2C	3.32	1.51	1.44
21	N	608	CLA	C1C-C2C	3.32	1.51	1.44
21	D	401	CLA	C1D-C2D	-3.32	1.38	1.45
21	P	508	CLA	C1D-C2D	-3.31	1.38	1.45
21	P	501	CLA	C2-C3	3.31	1.40	1.33
21	N	618	CLA	C1D-C2D	-3.31	1.38	1.45
21	N	611	CLA	C4C-C3C	3.31	1.50	1.45
21	P	509	CLA	C2-C3	3.31	1.40	1.33
21	N	608	CLA	C2-C3	3.31	1.40	1.33
23	D	404	PL9	C38-C39	3.31	1.40	1.33
21	B	614	CLA	C2-C3	3.30	1.40	1.33
21	N	618	CLA	C4C-C3C	3.30	1.50	1.45
21	B	604	CLA	C4C-C3C	3.30	1.50	1.45
21	C	505	CLA	C4C-C3C	3.30	1.50	1.45
21	N	618	CLA	C2-C3	3.30	1.40	1.33
21	P	504	CLA	C1C-C2C	3.29	1.51	1.44
21	B	615	CLA	C4C-C3C	3.29	1.50	1.45
21	C	509	CLA	C4C-C3C	3.29	1.50	1.45
21	Q	402	CLA	C2-C3	3.29	1.40	1.33
21	Q	402	CLA	C1D-C2D	-3.29	1.38	1.45
21	C	512	CLA	C2-C3	3.28	1.40	1.33
21	D	403	CLA	C2-C3	3.28	1.40	1.33
21	P	512	CLA	C2-C3	3.28	1.40	1.33
21	Q	404	CLA	C2-C3	3.28	1.40	1.33
21	N	613	CLA	C1D-C2D	-3.28	1.38	1.45
21	B	614	CLA	C1D-C2D	-3.28	1.38	1.45
21	B	605	CLA	C2-C3	3.28	1.40	1.33
21	C	501	CLA	C2-C3	3.28	1.40	1.33
21	C	507	CLA	MG-NB	-3.28	1.99	2.05
21	C	501	CLA	C4C-C3C	3.28	1.50	1.45
34	i	201	HEM	FE-NB	3.28	2.05	1.94
21	N	614	CLA	C4C-C3C	3.28	1.50	1.45
21	N	614	CLA	C2-C3	3.28	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	610	CLA	C4C-C3C	3.28	1.50	1.45
21	C	509	CLA	C2-C3	3.28	1.40	1.33
21	N	610	CLA	C2-C3	3.28	1.40	1.33
21	B	616	CLA	C2-C3	3.28	1.40	1.33
21	C	502	CLA	C1D-C2D	-3.28	1.38	1.45
21	P	507	CLA	MG-NB	-3.27	1.99	2.05
21	B	610	CLA	C2-C3	3.27	1.40	1.33
21	N	605	CLA	C2-C3	3.27	1.40	1.33
21	B	601	CLA	C2-C3	3.27	1.40	1.33
21	N	609	CLA	C2-C3	3.27	1.40	1.33
21	P	511	CLA	C2-C3	3.27	1.40	1.33
21	C	506	CLA	C2-C3	3.27	1.40	1.33
21	N	608	CLA	C4C-C3C	3.27	1.50	1.45
21	P	501	CLA	C4C-C3C	3.27	1.50	1.45
23	D	404	PL9	C33-C34	3.27	1.40	1.33
23	Q	405	PL9	C33-C34	3.26	1.40	1.33
21	P	505	CLA	C4C-C3C	3.26	1.50	1.45
21	P	502	CLA	MG-NB	-3.26	1.99	2.05
21	N	612	CLA	MG-NB	-3.26	1.99	2.05
21	B	606	CLA	C4C-C3C	3.26	1.50	1.45
21	P	513	CLA	C4C-C3C	3.26	1.50	1.45
21	C	503	CLA	C2-C3	3.25	1.40	1.33
21	N	607	CLA	C1D-C2D	-3.25	1.38	1.45
21	N	606	CLA	C2-C3	3.25	1.40	1.33
21	P	503	CLA	C2-C3	3.25	1.40	1.33
21	C	510	CLA	C1D-C2D	-3.25	1.38	1.45
21	B	609	CLA	C2-C3	3.25	1.40	1.33
21	C	502	CLA	C2-C3	3.25	1.40	1.33
21	P	509	CLA	C4C-C3C	3.25	1.50	1.45
21	B	612	CLA	C2-C3	3.24	1.40	1.33
21	A	403	CLA	C2-C3	3.24	1.40	1.33
21	A	405	CLA	C2-C3	3.24	1.40	1.33
21	P	506	CLA	C2-C3	3.24	1.40	1.33
21	B	605	CLA	C1D-C2D	-3.24	1.38	1.45
21	C	508	CLA	C1D-C2D	-3.24	1.38	1.45
21	P	512	CLA	C1D-C2D	-3.24	1.38	1.45
21	N	608	CLA	C1D-C2D	-3.24	1.38	1.45
21	G	402	CLA	C4C-C3C	3.24	1.50	1.45
21	P	513	CLA	C2-C3	3.23	1.40	1.33
21	B	603	CLA	C1D-C2D	-3.23	1.38	1.45
21	C	508	CLA	C2-C3	3.23	1.40	1.33
21	N	620	CLA	C1C-C2C	3.23	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Q	404	CLA	C1D-C2D	-3.23	1.38	1.45
21	B	613	CLA	C1D-C2D	-3.23	1.38	1.45
21	A	402	CLA	C2-C3	3.23	1.40	1.33
21	C	507	CLA	C1D-C2D	-3.23	1.38	1.45
21	P	504	CLA	C4C-C3C	3.23	1.50	1.45
21	B	615	CLA	C1D-C2D	-3.22	1.39	1.45
21	C	504	CLA	C4C-C3C	3.22	1.50	1.45
21	C	503	CLA	C1D-C2D	-3.22	1.39	1.45
21	C	511	CLA	C1D-C2D	-3.22	1.39	1.45
21	N	609	CLA	C1D-C2D	-3.22	1.39	1.45
21	C	504	CLA	C1D-C2D	-3.22	1.39	1.45
21	A	401	CLA	C2-C3	3.22	1.40	1.33
21	P	512	CLA	C4C-C3C	3.22	1.50	1.45
21	P	506	CLA	C1D-C2D	-3.22	1.39	1.45
21	A	401	CLA	MG-NB	-3.21	1.99	2.05
21	N	620	CLA	C1D-C2D	-3.21	1.39	1.45
21	C	510	CLA	C2-C3	3.21	1.40	1.33
21	P	502	CLA	C1D-C2D	-3.21	1.39	1.45
21	P	507	CLA	C1D-C2D	-3.21	1.39	1.45
21	G	403	CLA	C2-C3	3.21	1.40	1.33
21	N	606	CLA	C1D-C2D	-3.20	1.39	1.45
21	B	616	CLA	C1C-C2C	3.20	1.51	1.44
21	B	602	CLA	C2-C3	3.20	1.40	1.33
21	N	617	CLA	C1D-C2D	-3.19	1.39	1.45
21	B	608	CLA	C1D-C2D	-3.19	1.39	1.45
21	B	615	CLA	C2-C3	3.19	1.40	1.33
21	N	614	CLA	MG-NB	-3.19	1.99	2.05
21	B	612	CLA	MG-NB	-3.19	1.99	2.05
21	B	604	CLA	C1D-C2D	-3.19	1.39	1.45
21	B	616	CLA	C1D-C2D	-3.19	1.39	1.45
21	P	511	CLA	C4C-C3C	3.19	1.50	1.45
21	C	511	CLA	C2-C3	3.19	1.40	1.33
21	B	602	CLA	C4C-C3C	3.18	1.50	1.45
21	N	613	CLA	C2-C3	3.18	1.40	1.33
21	A	405	CLA	MG-NB	-3.18	1.99	2.05
21	P	508	CLA	C2-C3	3.18	1.40	1.33
21	N	617	CLA	C2-C3	3.18	1.40	1.33
21	B	607	CLA	C4C-C3C	3.18	1.50	1.45
21	C	506	CLA	C1D-C2D	-3.18	1.39	1.45
21	P	509	CLA	C1D-C2D	-3.18	1.39	1.45
21	C	509	CLA	C1D-C2D	-3.17	1.39	1.45
21	A	405	CLA	C1D-C2D	-3.17	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	402	CLA	C2-C3	3.17	1.40	1.33
21	P	507	CLA	C2-C3	3.17	1.40	1.33
21	D	401	CLA	C4C-C3C	3.17	1.50	1.45
21	P	501	CLA	C1D-C2D	-3.17	1.39	1.45
21	A	401	CLA	C1D-C2D	-3.17	1.39	1.45
21	N	620	CLA	C4C-C3C	3.17	1.50	1.45
21	G	404	CLA	C2-C3	3.17	1.40	1.33
21	N	619	CLA	C2-C3	3.16	1.40	1.33
21	B	611	CLA	C4C-C3C	3.16	1.50	1.45
21	Q	402	CLA	C4C-C3C	3.16	1.50	1.45
21	B	609	CLA	C1D-C2D	-3.16	1.39	1.45
21	C	511	CLA	C4C-C3C	3.16	1.50	1.45
21	Q	404	CLA	C4C-C3C	3.16	1.50	1.45
21	C	502	CLA	MG-NB	-3.16	1.99	2.05
21	N	608	CLA	MG-NB	-3.16	1.99	2.05
21	N	615	CLA	C1D-C2D	-3.16	1.39	1.45
21	B	606	CLA	C2-C3	3.16	1.40	1.33
21	P	507	CLA	C4C-C3C	3.15	1.50	1.45
21	P	511	CLA	C1D-C2D	-3.15	1.39	1.45
21	C	512	CLA	C1D-C2D	-3.15	1.39	1.45
21	N	612	CLA	C1D-C2D	-3.15	1.39	1.45
21	B	604	CLA	MG-NB	-3.15	1.99	2.05
21	P	510	CLA	C2-C3	3.15	1.40	1.33
21	C	513	CLA	C4C-C3C	3.15	1.50	1.45
21	A	403	CLA	MG-NB	-3.15	1.99	2.05
21	D	403	CLA	C1D-C2D	-3.15	1.39	1.45
21	P	503	CLA	C4C-C3C	3.15	1.50	1.45
21	A	402	CLA	C1C-C2C	3.15	1.50	1.44
21	G	406	CLA	C1D-C2D	-3.15	1.39	1.45
21	N	619	CLA	C4C-C3C	3.15	1.50	1.45
21	N	617	CLA	C4C-C3C	3.14	1.50	1.45
21	B	607	CLA	MG-NB	-3.14	1.99	2.05
21	C	506	CLA	MG-NB	-3.14	1.99	2.05
21	D	401	CLA	MG-NB	-3.14	1.99	2.05
21	N	612	CLA	C4C-C3C	3.14	1.50	1.45
21	C	505	CLA	C2-C3	3.14	1.40	1.33
21	D	403	CLA	C4C-C3C	3.14	1.50	1.45
21	C	503	CLA	C4C-C3C	3.13	1.50	1.45
21	N	615	CLA	C4C-C3C	3.13	1.50	1.45
21	B	601	CLA	MG-NB	-3.13	1.99	2.05
21	C	512	CLA	C4C-C3C	3.13	1.50	1.45
21	N	606	CLA	C4C-C3C	3.13	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	610	CLA	MG-NB	-3.13	1.99	2.05
21	B	606	CLA	C1D-C2D	-3.13	1.39	1.45
21	G	406	CLA	C2-C3	3.13	1.40	1.33
21	P	510	CLA	C4C-C3C	3.13	1.50	1.45
21	N	605	CLA	C1D-C2D	-3.13	1.39	1.45
21	C	507	CLA	C2-C3	3.13	1.40	1.33
21	C	509	CLA	MG-NB	-3.13	1.99	2.05
21	A	401	CLA	C4C-C3C	3.12	1.50	1.45
21	P	505	CLA	C2-C3	3.12	1.40	1.33
21	B	607	CLA	C1D-C2D	-3.12	1.39	1.45
21	B	601	CLA	C1D-C2D	-3.12	1.39	1.45
21	B	609	CLA	C4C-C3C	3.12	1.50	1.45
21	N	610	CLA	C1D-C2D	-3.12	1.39	1.45
23	Q	405	PL9	C43-C44	3.12	1.40	1.33
21	N	605	CLA	MG-NB	-3.12	1.99	2.05
21	P	503	CLA	C1D-C2D	-3.12	1.39	1.45
21	G	402	CLA	C1D-C2D	-3.11	1.39	1.45
21	B	613	CLA	C2-C3	3.11	1.40	1.33
21	A	405	CLA	C4C-C3C	3.11	1.50	1.45
21	P	504	CLA	C1D-C2D	-3.11	1.39	1.45
21	Q	404	CLA	MG-NB	-3.11	1.99	2.05
21	P	506	CLA	C4C-C3C	3.11	1.50	1.45
21	B	611	CLA	C1D-C2D	-3.11	1.39	1.45
21	N	614	CLA	C1D-C2D	-3.11	1.39	1.45
21	N	615	CLA	C2-C3	3.11	1.40	1.33
21	N	611	CLA	C1D-C2D	-3.11	1.39	1.45
21	B	616	CLA	MG-NB	-3.10	1.99	2.05
21	B	613	CLA	C4C-C3C	3.10	1.50	1.45
21	C	501	CLA	C1D-C2D	-3.10	1.39	1.45
21	N	617	CLA	MG-NB	-3.10	1.99	2.05
21	N	609	CLA	MG-NB	-3.10	1.99	2.05
21	B	602	CLA	C1D-C2D	-3.10	1.39	1.45
21	B	610	CLA	C1D-C2D	-3.10	1.39	1.45
21	P	506	CLA	MG-NB	-3.10	1.99	2.05
21	P	502	CLA	C4C-C3C	3.10	1.50	1.45
21	P	504	CLA	MG-NB	-3.10	1.99	2.05
21	B	601	CLA	C1C-C2C	3.09	1.50	1.44
21	B	608	CLA	C4C-C3C	3.09	1.50	1.45
21	D	403	CLA	MG-NB	-3.09	1.99	2.05
21	B	616	CLA	C4C-C3C	3.09	1.50	1.45
21	N	616	CLA	C4C-C3C	3.09	1.50	1.45
21	B	611	CLA	MG-NB	-3.09	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	510	CLA	C4C-C3C	3.09	1.50	1.45
21	P	512	CLA	MG-NB	-3.09	1.99	2.05
21	G	403	CLA	MG-NB	-3.08	1.99	2.05
21	P	508	CLA	C4C-C3C	3.08	1.50	1.45
21	G	404	CLA	C1D-C2D	-3.08	1.39	1.45
23	D	404	PL9	C43-C44	3.08	1.40	1.33
21	N	613	CLA	MG-NB	-3.08	1.99	2.05
21	B	611	CLA	C2-C3	3.08	1.40	1.33
21	Q	402	CLA	MG-NB	-3.08	1.99	2.05
21	P	505	CLA	MG-NB	-3.08	1.99	2.05
21	C	508	CLA	C4C-C3C	3.07	1.50	1.45
21	N	615	CLA	MG-NB	-3.07	1.99	2.05
21	C	513	CLA	C1D-C2D	-3.07	1.39	1.45
21	P	509	CLA	MG-NB	-3.07	1.99	2.05
21	C	507	CLA	C4C-C3C	3.07	1.50	1.45
21	C	506	CLA	C4C-C3C	3.07	1.50	1.45
21	B	608	CLA	MG-NB	-3.07	1.99	2.05
21	N	618	CLA	MG-NB	-3.07	1.99	2.05
21	A	403	CLA	C1D-C2D	-3.07	1.39	1.45
21	G	406	CLA	C4C-C3C	3.07	1.50	1.45
21	B	606	CLA	MG-NB	-3.06	1.99	2.05
21	C	504	CLA	MG-NB	-3.06	1.99	2.05
21	P	513	CLA	C1D-C2D	-3.06	1.39	1.45
21	N	607	CLA	C4C-C3C	3.06	1.50	1.45
21	B	602	CLA	MG-NB	-3.06	1.99	2.05
21	B	613	CLA	MG-NB	-3.06	1.99	2.05
21	N	619	CLA	C1D-C2D	-3.06	1.39	1.45
21	B	605	CLA	C4C-C3C	3.05	1.50	1.45
21	C	510	CLA	MG-NB	-3.05	1.99	2.05
21	P	510	CLA	MG-NB	-3.05	1.99	2.05
21	N	605	CLA	C1C-C2C	3.05	1.50	1.44
21	C	511	CLA	MG-NB	-3.04	1.99	2.05
21	P	513	CLA	MG-NB	-3.04	1.99	2.05
21	B	603	CLA	C4C-C3C	3.04	1.50	1.45
21	G	406	CLA	MG-NB	-3.04	1.99	2.05
21	P	503	CLA	MG-NB	-3.03	1.99	2.05
21	N	619	CLA	MG-NB	-3.03	1.99	2.05
21	G	404	CLA	MG-NB	-3.03	1.99	2.05
21	N	611	CLA	MG-NB	-3.02	1.99	2.05
21	C	501	CLA	MG-NB	-3.02	1.99	2.05
21	C	513	CLA	MG-NB	-3.01	1.99	2.05
34	E	101	HEM	CAC-C3C	3.01	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	607	CLA	MG-NB	-3.01	1.99	2.05
21	B	609	CLA	MG-NB	-3.01	1.99	2.05
21	C	502	CLA	C4C-C3C	3.01	1.50	1.45
21	C	505	CLA	MG-NB	-3.01	1.99	2.05
21	C	508	CLA	MG-NB	-3.01	1.99	2.05
21	G	403	CLA	C1C-C2C	3.00	1.50	1.44
21	N	610	CLA	MG-NB	-3.00	1.99	2.05
21	B	605	CLA	MG-NB	-2.99	1.99	2.05
21	B	615	CLA	MG-NB	-2.99	1.99	2.05
21	B	603	CLA	MG-NB	-2.99	1.99	2.05
21	A	402	CLA	MG-NB	-2.98	1.99	2.05
21	N	620	CLA	MG-NB	-2.98	1.99	2.05
21	B	614	CLA	MG-NB	-2.98	1.99	2.05
21	N	609	CLA	C4C-C3C	2.97	1.50	1.45
34	R	101	HEM	CAC-C3C	2.97	1.55	1.47
21	C	512	CLA	MG-NB	-2.97	1.99	2.05
21	C	503	CLA	MG-NB	-2.97	1.99	2.05
21	P	511	CLA	MG-NB	-2.96	1.99	2.05
34	V	201	HEM	CAC-C3C	2.96	1.55	1.47
21	B	612	CLA	C4C-C3C	2.96	1.50	1.45
21	P	508	CLA	MG-NB	-2.95	1.99	2.05
23	J	101	PL9	C23-C24	2.95	1.39	1.33
21	N	613	CLA	C4C-C3C	2.95	1.50	1.45
21	N	606	CLA	MG-NB	-2.94	2.00	2.05
21	P	501	CLA	MG-NB	-2.92	2.00	2.05
34	i	201	HEM	CAC-C3C	2.92	1.55	1.47
23	G	407	PL9	C38-C39	2.91	1.41	1.32
34	V	201	HEM	FE-NC	2.89	2.04	1.95
21	G	402	CLA	MG-NB	-2.88	2.00	2.05
23	b	101	PL9	C23-C24	2.86	1.39	1.33
23	A	406	PL9	C38-C39	2.86	1.41	1.32
23	D	404	PL9	C23-C24	2.85	1.39	1.33
21	N	616	CLA	MG-NB	-2.84	2.00	2.05
23	Q	405	PL9	C23-C24	2.83	1.39	1.33
23	b	101	PL9	C8-C9	2.83	1.39	1.33
23	b	101	PL9	C13-C14	2.83	1.39	1.33
21	G	403	CLA	C1D-C2D	-2.82	1.39	1.45
21	A	402	CLA	C1D-C2D	-2.81	1.39	1.45
23	J	101	PL9	C13-C14	2.80	1.39	1.33
34	R	101	HEM	CAB-C3B	2.80	1.54	1.47
23	J	101	PL9	C8-C9	2.79	1.39	1.33
34	E	101	HEM	CAB-C3B	2.78	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Q	402	CLA	O2D-CED	-2.77	1.39	1.45
21	D	401	CLA	O2D-CED	-2.77	1.39	1.45
23	J	101	PL9	C18-C19	2.76	1.39	1.33
23	b	101	PL9	C18-C19	2.75	1.39	1.33
23	A	406	PL9	C23-C24	2.75	1.39	1.33
23	Q	405	PL9	C8-C9	2.74	1.39	1.33
23	Q	405	PL9	C13-C14	2.74	1.39	1.33
23	D	404	PL9	C13-C14	2.74	1.39	1.33
23	G	407	PL9	C23-C24	2.73	1.39	1.33
23	D	404	PL9	C18-C19	2.73	1.39	1.33
23	D	404	PL9	C8-C9	2.71	1.39	1.33
23	A	406	PL9	C13-C14	2.67	1.39	1.33
21	P	504	CLA	O2D-CED	-2.66	1.39	1.45
23	G	407	PL9	C13-C14	2.65	1.39	1.33
21	C	509	CLA	O2D-CED	-2.64	1.39	1.45
21	C	504	CLA	O2D-CED	-2.64	1.39	1.45
34	i	201	HEM	CAB-C3B	2.64	1.54	1.47
23	Q	405	PL9	C18-C19	2.63	1.39	1.33
23	G	407	PL9	C8-C9	2.63	1.39	1.33
21	C	510	CLA	O2D-CED	-2.63	1.39	1.45
21	C	508	CLA	O2D-CED	-2.62	1.39	1.45
21	C	507	CLA	O2D-CED	-2.62	1.39	1.45
21	N	613	CLA	O2D-CED	-2.62	1.39	1.45
23	A	406	PL9	C18-C19	2.62	1.39	1.33
21	N	611	CLA	O2D-CED	-2.61	1.39	1.45
21	B	602	CLA	O2D-CED	-2.61	1.39	1.45
21	B	608	CLA	O2D-CED	-2.61	1.39	1.45
21	B	607	CLA	O2D-CED	-2.61	1.39	1.45
21	P	509	CLA	O2D-CED	-2.61	1.39	1.45
21	B	613	CLA	O2D-CED	-2.61	1.39	1.45
21	G	403	CLA	O2D-CED	-2.61	1.39	1.45
21	P	513	CLA	O2D-CED	-2.61	1.39	1.45
21	A	402	CLA	O2D-CED	-2.61	1.39	1.45
23	G	407	PL9	C18-C19	2.60	1.39	1.33
21	P	501	CLA	O2D-CED	-2.60	1.39	1.45
34	V	201	HEM	FE-NB	2.60	2.02	1.94
23	A	406	PL9	C8-C9	2.60	1.39	1.33
21	A	403	CLA	O2D-CED	-2.60	1.39	1.45
21	N	617	CLA	O2D-CED	-2.60	1.39	1.45
21	P	506	CLA	O2D-CED	-2.60	1.39	1.45
21	B	601	CLA	O2D-CED	-2.60	1.39	1.45
21	N	618	CLA	O2D-CED	-2.59	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	616	CLA	O2D-CED	-2.59	1.39	1.45
21	B	609	CLA	O2D-CED	-2.59	1.39	1.45
21	B	615	CLA	O2D-CED	-2.59	1.39	1.45
21	B	612	CLA	O2D-CED	-2.59	1.39	1.45
21	B	604	CLA	O2D-CED	-2.59	1.39	1.45
21	B	614	CLA	O2D-CED	-2.59	1.39	1.45
21	N	608	CLA	O2D-CED	-2.59	1.39	1.45
21	P	511	CLA	O2D-CED	-2.58	1.39	1.45
21	P	507	CLA	O2D-CED	-2.58	1.39	1.45
21	C	506	CLA	O2D-CED	-2.58	1.39	1.45
21	C	512	CLA	O2D-CED	-2.58	1.39	1.45
21	C	502	CLA	O2D-CED	-2.58	1.39	1.45
21	Q	404	CLA	O2D-CED	-2.58	1.39	1.45
21	C	503	CLA	O2D-CED	-2.57	1.39	1.45
21	P	508	CLA	O2D-CED	-2.57	1.39	1.45
21	G	402	CLA	O2D-CED	-2.57	1.39	1.45
21	P	510	CLA	O2D-CED	-2.57	1.39	1.45
21	D	403	CLA	O2D-CED	-2.57	1.39	1.45
21	N	619	CLA	O2D-CED	-2.57	1.39	1.45
21	N	612	CLA	O2D-CED	-2.57	1.39	1.45
34	V	201	HEM	CAB-C3B	2.56	1.54	1.47
21	C	501	CLA	O2D-CED	-2.56	1.39	1.45
21	N	605	CLA	O2D-CED	-2.56	1.39	1.45
21	N	614	CLA	O2D-CED	-2.56	1.39	1.45
21	C	511	CLA	O2D-CED	-2.55	1.39	1.45
21	B	616	CLA	O2D-CED	-2.55	1.39	1.45
24	P	517	DGD	O5D-C1E	2.55	1.44	1.40
21	N	615	CLA	O2D-CED	-2.55	1.39	1.45
21	P	503	CLA	O2D-CED	-2.55	1.39	1.45
21	G	406	CLA	O2D-CED	-2.55	1.39	1.45
21	G	402	CLA	O2A-C1	-2.55	1.39	1.46
21	N	607	CLA	O2D-CED	-2.55	1.39	1.45
24	A	407	DGD	O5D-C1E	2.55	1.44	1.40
21	B	605	CLA	O2D-CED	-2.54	1.39	1.45
21	P	512	CLA	O2D-CED	-2.54	1.39	1.45
21	P	505	CLA	O2D-CED	-2.54	1.39	1.45
24	G	408	DGD	O5D-C1E	2.54	1.44	1.40
21	B	611	CLA	O2D-CED	-2.54	1.39	1.45
21	A	401	CLA	C1A-CHA	-2.54	1.32	1.43
21	G	404	CLA	O2D-CED	-2.53	1.39	1.45
24	C	518	DGD	O5D-C1E	2.53	1.44	1.40
21	B	606	CLA	O2D-CED	-2.53	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	405	CLA	O2D-CED	-2.53	1.39	1.45
21	B	603	CLA	O2D-CED	-2.53	1.39	1.45
21	N	606	CLA	O2D-CED	-2.52	1.39	1.45
21	C	505	CLA	O2D-CED	-2.52	1.39	1.45
21	C	513	CLA	O2D-CED	-2.52	1.39	1.45
21	B	610	CLA	O2D-CED	-2.51	1.39	1.45
21	A	401	CLA	O2A-C1	-2.51	1.39	1.46
21	N	620	CLA	O2D-CED	-2.51	1.39	1.45
21	A	401	CLA	O2D-CED	-2.50	1.39	1.45
23	D	404	PL9	C28-C29	2.50	1.38	1.33
21	N	609	CLA	O2D-CED	-2.50	1.39	1.45
21	P	502	CLA	O2D-CED	-2.50	1.39	1.45
23	Q	405	PL9	C28-C29	2.49	1.38	1.33
21	G	402	CLA	C1A-CHA	-2.48	1.32	1.43
21	N	610	CLA	O2D-CED	-2.47	1.39	1.45
21	P	505	CLA	O2A-C1	-2.47	1.39	1.46
21	N	611	CLA	O2A-CGA	2.46	1.40	1.33
21	N	615	CLA	O2A-C1	-2.45	1.39	1.46
21	C	510	CLA	O2A-C1	-2.45	1.39	1.46
21	B	611	CLA	O2A-C1	-2.45	1.39	1.46
21	B	606	CLA	C1A-CHA	-2.44	1.33	1.43
21	G	406	CLA	O2A-C1	-2.44	1.39	1.46
21	C	505	CLA	O2A-C1	-2.44	1.39	1.46
21	N	607	CLA	O2A-CGA	2.43	1.40	1.33
21	B	616	CLA	O2A-C1	-2.43	1.39	1.46
24	C	516	DGD	O5D-C1E	2.43	1.44	1.40
24	P	519	DGD	O5D-C1E	2.43	1.44	1.40
21	D	401	CLA	C1A-CHA	-2.43	1.33	1.43
21	N	617	CLA	O2A-C1	-2.43	1.39	1.46
21	B	615	CLA	O2A-C1	-2.43	1.39	1.46
21	B	613	CLA	O2A-C1	-2.42	1.39	1.46
21	B	603	CLA	C5-C3	2.42	1.56	1.51
21	N	619	CLA	O2A-C1	-2.42	1.39	1.46
21	B	612	CLA	C1A-CHA	-2.41	1.33	1.43
21	N	611	CLA	C5-C3	2.41	1.56	1.51
21	P	504	CLA	C1A-CHA	-2.41	1.33	1.43
21	C	508	CLA	O2A-C1	-2.41	1.39	1.46
21	N	613	CLA	O2A-C1	-2.41	1.39	1.46
21	B	606	CLA	O2A-C1	-2.41	1.39	1.46
21	B	607	CLA	O2A-CGA	2.41	1.40	1.33
21	P	508	CLA	O2A-C1	-2.40	1.39	1.46
21	Q	402	CLA	C1A-CHA	-2.40	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	614	CLA	O2A-C1	-2.40	1.39	1.46
21	P	510	CLA	O2A-C1	-2.39	1.39	1.46
21	N	616	CLA	C1A-CHA	-2.39	1.33	1.43
21	B	607	CLA	C5-C3	2.39	1.56	1.51
21	C	511	CLA	O2A-C1	-2.39	1.39	1.46
21	P	504	CLA	C5-C3	2.39	1.56	1.51
21	P	504	CLA	O2A-CGA	2.39	1.40	1.33
21	B	614	CLA	C5-C3	2.39	1.56	1.51
21	N	618	CLA	C5-C3	2.38	1.56	1.51
21	C	504	CLA	C1A-CHA	-2.38	1.33	1.43
21	N	607	CLA	C5-C3	2.38	1.56	1.51
21	C	509	CLA	C1A-CHA	-2.37	1.33	1.43
21	B	608	CLA	C1A-CHA	-2.37	1.33	1.43
21	N	612	CLA	C1A-CHA	-2.37	1.33	1.43
21	A	405	CLA	O2A-C1	-2.37	1.39	1.46
21	G	404	CLA	O2A-C1	-2.37	1.39	1.46
21	P	513	CLA	C1A-CHA	-2.37	1.33	1.43
21	C	504	CLA	O2A-CGA	2.37	1.40	1.33
21	B	614	CLA	C1A-CHA	-2.37	1.33	1.43
21	C	510	CLA	C1A-CHA	-2.37	1.33	1.43
21	B	612	CLA	O2A-C1	-2.37	1.39	1.46
21	C	507	CLA	O2A-C1	-2.37	1.39	1.46
21	P	513	CLA	O2A-C1	-2.37	1.39	1.46
21	P	509	CLA	O2A-C1	-2.36	1.39	1.46
21	B	609	CLA	O2A-C1	-2.36	1.39	1.46
21	P	507	CLA	O2A-C1	-2.36	1.39	1.46
21	N	620	CLA	C5-C3	2.36	1.56	1.51
21	N	606	CLA	O2A-C1	-2.36	1.39	1.46
21	N	618	CLA	C1A-CHA	-2.36	1.33	1.43
21	N	620	CLA	O2A-C1	-2.36	1.39	1.46
21	G	403	CLA	C1A-CHA	-2.36	1.33	1.43
21	N	612	CLA	C5-C3	2.36	1.56	1.51
24	P	518	DGD	O5D-C1E	2.35	1.44	1.40
21	B	605	CLA	C1A-CHA	-2.35	1.33	1.43
21	B	602	CLA	O2A-C1	-2.35	1.39	1.46
21	C	509	CLA	O2A-C1	-2.35	1.39	1.46
21	D	401	CLA	C5-C3	2.35	1.56	1.51
21	B	601	CLA	O2A-C1	-2.35	1.39	1.46
21	A	403	CLA	O2A-C1	-2.35	1.39	1.46
21	P	506	CLA	O2A-C1	-2.35	1.39	1.46
21	N	616	CLA	C5-C3	2.35	1.56	1.51
21	A	403	CLA	C1A-CHA	-2.35	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	503	CLA	C1A-CHA	-2.35	1.33	1.43
21	A	402	CLA	O2A-C1	-2.35	1.39	1.46
21	P	510	CLA	C1A-CHA	-2.35	1.33	1.43
21	N	605	CLA	O2A-C1	-2.34	1.39	1.46
21	B	610	CLA	O2A-C1	-2.34	1.39	1.46
21	P	505	CLA	C1A-CHA	-2.34	1.33	1.43
21	B	603	CLA	O2A-CGA	2.34	1.40	1.33
21	B	605	CLA	O2A-C1	-2.34	1.39	1.46
21	N	610	CLA	O2A-C1	-2.34	1.39	1.46
24	W	102	DGD	O5D-C1E	2.34	1.44	1.40
21	G	403	CLA	O2A-C1	-2.34	1.39	1.46
21	P	501	CLA	C5-C3	2.34	1.56	1.51
21	C	513	CLA	C1A-CHA	-2.33	1.33	1.43
24	N	602	DGD	O5D-C1E	2.33	1.44	1.40
21	C	506	CLA	O2A-C1	-2.33	1.39	1.46
21	N	614	CLA	C1A-CHA	-2.33	1.33	1.43
21	P	506	CLA	C1A-CHA	-2.33	1.33	1.43
21	C	502	CLA	C1A-CHA	-2.33	1.33	1.43
21	P	502	CLA	C5-C3	2.33	1.56	1.51
21	N	611	CLA	C1A-CHA	-2.33	1.33	1.43
21	C	503	CLA	C1A-CHA	-2.33	1.33	1.43
21	B	608	CLA	O2A-CGA	2.33	1.40	1.33
21	N	608	CLA	C1A-CHA	-2.32	1.33	1.43
21	N	612	CLA	O2A-CGA	2.32	1.40	1.33
21	C	502	CLA	C5-C3	2.32	1.56	1.51
21	C	506	CLA	C1A-CHA	-2.32	1.33	1.43
21	Q	404	CLA	C1A-CHA	-2.32	1.33	1.43
21	N	608	CLA	O2A-C1	-2.32	1.39	1.46
21	B	604	CLA	O2A-C1	-2.32	1.39	1.46
24	B	628	DGD	O5D-C1E	2.32	1.44	1.40
24	C	517	DGD	O5D-C1E	2.32	1.44	1.40
21	B	607	CLA	C1A-CHA	-2.32	1.33	1.43
21	D	403	CLA	O2A-C1	-2.32	1.39	1.46
21	D	403	CLA	C1A-CHA	-2.31	1.33	1.43
21	Q	402	CLA	C5-C3	2.31	1.56	1.51
21	B	614	CLA	O2A-CGA	2.31	1.40	1.33
22	Q	403	PHO	CBD-CGD	-2.31	1.49	1.52
21	N	615	CLA	C1A-CHA	-2.31	1.33	1.43
21	B	608	CLA	C5-C3	2.31	1.56	1.51
21	P	511	CLA	O2A-C1	-2.31	1.39	1.46
21	Q	404	CLA	O2A-CGA	2.31	1.40	1.33
21	B	604	CLA	C1A-CHA	-2.31	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	609	CLA	O2A-C1	-2.31	1.39	1.46
21	N	609	CLA	C1A-CHA	-2.31	1.33	1.43
21	C	501	CLA	O2A-C1	-2.31	1.39	1.46
24	C	518	DGD	O3G-C1D	2.31	1.44	1.40
21	C	503	CLA	O2A-C1	-2.31	1.39	1.46
21	C	501	CLA	C5-C3	2.30	1.56	1.51
21	N	618	CLA	O2A-CGA	2.30	1.40	1.33
21	D	401	CLA	CAB-C3B	2.30	1.53	1.47
21	N	610	CLA	C5-C3	2.30	1.56	1.51
21	P	503	CLA	O2A-C1	-2.30	1.39	1.46
23	A	406	PL9	C28-C29	2.30	1.38	1.33
21	B	602	CLA	C1A-CHA	-2.30	1.33	1.43
21	B	616	CLA	C5-C3	2.30	1.56	1.51
21	P	512	CLA	C1A-CHA	-2.29	1.33	1.43
21	A	402	CLA	C1A-CHA	-2.29	1.33	1.43
21	C	508	CLA	C5-C3	2.29	1.56	1.51
21	C	513	CLA	O2A-C1	-2.29	1.40	1.46
21	B	613	CLA	C1A-CHA	-2.29	1.33	1.43
21	C	502	CLA	O2A-C1	-2.29	1.40	1.46
21	C	508	CLA	C1A-CHA	-2.29	1.33	1.43
21	N	605	CLA	C1A-CHA	-2.29	1.33	1.43
21	P	509	CLA	C1A-CHA	-2.29	1.33	1.43
21	P	512	CLA	C5-C3	2.29	1.56	1.51
21	C	507	CLA	C1A-CHA	-2.29	1.33	1.43
21	N	610	CLA	C1A-CHA	-2.29	1.33	1.43
21	N	613	CLA	C1A-CHA	-2.29	1.33	1.43
21	P	508	CLA	C1A-CHA	-2.29	1.33	1.43
21	N	605	CLA	C5-C3	2.28	1.56	1.51
21	B	610	CLA	C1A-CHA	-2.28	1.33	1.43
23	G	407	PL9	C28-C29	2.28	1.38	1.33
22	D	402	PHO	CBD-CGD	-2.28	1.49	1.52
21	C	512	CLA	O2A-CGA	2.28	1.40	1.33
21	D	401	CLA	O2A-CGA	2.28	1.40	1.33
21	B	609	CLA	C1A-CHA	-2.28	1.33	1.43
21	Q	402	CLA	CAB-C3B	2.28	1.53	1.47
21	P	502	CLA	C1A-CHA	-2.28	1.33	1.43
21	A	402	CLA	C5-C3	2.28	1.56	1.51
21	P	509	CLA	C5-C3	2.27	1.56	1.51
21	Q	404	CLA	C5-C3	2.27	1.56	1.51
21	N	616	CLA	O2A-CGA	2.27	1.40	1.33
21	B	615	CLA	C1A-CHA	-2.27	1.33	1.43
21	B	601	CLA	C5-C3	2.27	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	612	CLA	C5-C3	2.27	1.56	1.51
21	D	403	CLA	C5-C3	2.27	1.56	1.51
21	P	502	CLA	O2A-C1	-2.27	1.40	1.46
21	P	512	CLA	O2A-CGA	2.27	1.40	1.33
21	N	608	CLA	C5-C3	2.27	1.56	1.51
21	G	406	CLA	C1A-CHA	-2.27	1.33	1.43
21	A	403	CLA	C5-C3	2.27	1.56	1.51
21	A	401	CLA	C5-C3	2.27	1.56	1.51
21	P	501	CLA	O2A-CGA	2.26	1.40	1.33
21	C	504	CLA	C5-C3	2.26	1.56	1.51
21	A	405	CLA	C1A-CHA	-2.26	1.33	1.43
21	C	501	CLA	O2A-CGA	2.26	1.39	1.33
21	C	504	CLA	O2A-C1	-2.26	1.40	1.46
21	P	513	CLA	C5-C3	2.26	1.55	1.51
21	B	601	CLA	C1A-CHA	-2.26	1.33	1.43
21	G	404	CLA	C1A-CHA	-2.26	1.33	1.43
21	Q	402	CLA	O2A-C1	-2.26	1.40	1.46
21	C	505	CLA	C1A-CHA	-2.26	1.33	1.43
21	Q	404	CLA	O2A-C1	-2.25	1.40	1.46
21	N	617	CLA	C1A-CHA	-2.25	1.33	1.43
21	B	604	CLA	C5-C3	2.25	1.55	1.51
21	C	503	CLA	O2A-CGA	2.25	1.39	1.33
21	C	511	CLA	C1A-CHA	-2.25	1.33	1.43
21	N	614	CLA	C5-C3	2.25	1.55	1.51
21	A	405	CLA	C5-C3	2.25	1.55	1.51
21	B	605	CLA	O2A-CGA	2.25	1.39	1.33
21	G	402	CLA	C5-C3	2.25	1.55	1.51
21	P	503	CLA	C5-C3	2.25	1.55	1.51
21	N	616	CLA	O2A-C1	-2.24	1.40	1.46
21	N	618	CLA	O2A-C1	-2.24	1.40	1.46
21	P	501	CLA	O2A-C1	-2.24	1.40	1.46
21	P	502	CLA	O2A-CGA	2.24	1.39	1.33
21	C	501	CLA	C1A-CHA	-2.24	1.33	1.43
21	C	513	CLA	C5-C3	2.24	1.55	1.51
21	N	613	CLA	C5-C3	2.24	1.55	1.51
34	R	101	HEM	FE-NC	2.24	2.02	1.95
21	N	609	CLA	O2A-CGA	2.23	1.39	1.33
21	G	403	CLA	C5-C3	2.23	1.55	1.51
21	G	403	CLA	MG-NC	-2.23	2.01	2.06
21	C	502	CLA	O2A-CGA	2.23	1.39	1.33
21	N	606	CLA	C1A-CHA	-2.23	1.33	1.43
21	N	615	CLA	C5-C3	2.23	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	604	CLA	O2A-CGA	2.23	1.39	1.33
21	P	502	CLA	O2D-CGD	2.23	1.38	1.33
21	B	615	CLA	C5-C3	2.23	1.55	1.51
21	P	503	CLA	O2A-CGA	2.23	1.39	1.33
21	B	611	CLA	C5-C3	2.23	1.55	1.51
21	B	616	CLA	C1A-CHA	-2.23	1.33	1.43
21	C	512	CLA	C1A-CHA	-2.23	1.33	1.43
21	B	610	CLA	C5-C3	2.23	1.55	1.51
21	C	513	CLA	O2A-CGA	2.23	1.39	1.33
21	D	401	CLA	O2A-C1	-2.22	1.40	1.46
24	B	621	DGD	O5D-C1E	2.22	1.43	1.40
21	N	606	CLA	C5-C3	2.22	1.55	1.51
21	A	403	CLA	O2A-CGA	2.22	1.39	1.33
21	C	509	CLA	C5-C3	2.22	1.55	1.51
21	P	507	CLA	C1A-CHA	-2.22	1.34	1.43
21	G	406	CLA	C5-C3	2.22	1.55	1.51
21	P	507	CLA	C5-C3	2.22	1.55	1.51
21	D	403	CLA	O2A-CGA	2.22	1.39	1.33
21	A	402	CLA	MG-NC	-2.22	2.01	2.06
21	P	504	CLA	O2A-C1	-2.22	1.40	1.46
21	C	512	CLA	C5-C3	2.22	1.55	1.51
21	B	603	CLA	C1A-CHA	-2.22	1.34	1.43
21	G	403	CLA	C3D-C4D	-2.21	1.39	1.44
21	G	404	CLA	C3D-C4D	-2.21	1.39	1.44
21	P	513	CLA	O2A-CGA	2.21	1.39	1.33
21	N	620	CLA	O2A-CGA	2.21	1.39	1.33
21	B	614	CLA	O2A-C1	-2.21	1.40	1.46
21	B	605	CLA	MG-NC	-2.21	2.01	2.06
22	A	404	PHO	CBD-CGD	-2.21	1.49	1.52
21	B	609	CLA	C5-C3	2.21	1.55	1.51
21	N	608	CLA	O2A-CGA	2.21	1.39	1.33
21	B	602	CLA	O2A-CGA	2.21	1.39	1.33
21	N	606	CLA	O2A-CGA	2.21	1.39	1.33
21	P	501	CLA	C1A-CHA	-2.21	1.34	1.43
21	P	511	CLA	C1A-CHA	-2.21	1.34	1.43
21	N	618	CLA	CAB-C3B	2.21	1.53	1.47
21	C	503	CLA	C5-C3	2.21	1.55	1.51
21	N	619	CLA	C1A-CHA	-2.21	1.34	1.43
21	C	503	CLA	CAB-C3B	2.21	1.53	1.47
21	A	401	CLA	C3D-C4D	-2.20	1.39	1.44
21	N	615	CLA	MG-NC	-2.20	2.01	2.06
21	N	607	CLA	C1A-CHA	-2.20	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	512	CLA	O2A-C1	-2.20	1.40	1.46
26	Q	408	SQD	O6-C1	2.20	1.43	1.40
21	B	611	CLA	C1A-CHA	-2.20	1.34	1.43
21	B	608	CLA	O2A-C1	-2.20	1.40	1.46
21	C	509	CLA	O2A-CGA	2.20	1.39	1.33
21	G	404	CLA	C5-C3	2.20	1.55	1.51
21	A	401	CLA	O2D-CGD	2.20	1.38	1.33
21	B	609	CLA	O2A-CGA	2.20	1.39	1.33
21	N	609	CLA	O2D-CGD	2.19	1.38	1.33
21	P	503	CLA	CAB-C3B	2.19	1.53	1.47
21	N	609	CLA	C5-C3	2.19	1.55	1.51
21	B	609	CLA	O2D-CGD	2.19	1.38	1.33
21	G	402	CLA	C3D-C4D	-2.19	1.39	1.44
21	N	617	CLA	C5-C3	2.19	1.55	1.51
21	G	404	CLA	O2A-CGA	2.19	1.39	1.33
21	Q	402	CLA	O2A-CGA	2.19	1.39	1.33
23	J	101	PL9	C28-C29	2.19	1.39	1.32
21	C	505	CLA	C5-C3	2.19	1.55	1.51
21	B	610	CLA	O2A-CGA	2.19	1.39	1.33
21	P	506	CLA	C5-C3	2.19	1.55	1.51
21	P	505	CLA	C3D-C4D	-2.19	1.39	1.44
21	C	507	CLA	C5-C3	2.18	1.55	1.51
21	B	607	CLA	O2A-C1	-2.18	1.40	1.46
21	C	512	CLA	O2A-C1	-2.18	1.40	1.46
21	N	609	CLA	MG-NC	-2.18	2.01	2.06
21	N	612	CLA	O2A-C1	-2.18	1.40	1.46
21	A	402	CLA	CHB-C1B	-2.18	1.34	1.39
21	C	506	CLA	MG-NC	-2.18	2.01	2.06
26	S	102	SQD	O6-C1	2.18	1.43	1.40
21	G	403	CLA	CAB-C3B	2.18	1.53	1.47
21	A	402	CLA	O2A-CGA	2.18	1.39	1.33
34	R	101	HEM	CMC-C2C	2.18	1.55	1.50
21	A	402	CLA	CAB-C3B	2.18	1.53	1.47
21	B	613	CLA	C5-C3	2.18	1.55	1.51
21	A	401	CLA	MG-NC	-2.18	2.01	2.06
21	B	602	CLA	C5-C3	2.17	1.55	1.51
21	P	508	CLA	C5-C3	2.17	1.55	1.51
21	N	606	CLA	O2D-CGD	2.17	1.38	1.33
21	N	620	CLA	C1A-CHA	-2.17	1.34	1.43
21	P	506	CLA	O2A-CGA	2.17	1.39	1.33
21	P	511	CLA	C5-C3	2.17	1.55	1.51
21	B	605	CLA	C5-C3	2.17	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	510	CLA	C5-C3	2.17	1.55	1.51
21	N	610	CLA	O2A-CGA	2.17	1.39	1.33
21	G	403	CLA	O2A-CGA	2.17	1.39	1.33
23	b	101	PL9	C28-C29	2.17	1.39	1.32
21	B	603	CLA	O2A-C1	-2.17	1.40	1.46
21	C	508	CLA	O2A-CGA	2.17	1.39	1.33
21	B	605	CLA	O2D-CGD	2.16	1.38	1.33
21	B	608	CLA	MG-NC	-2.16	2.01	2.06
21	P	509	CLA	O2A-CGA	2.16	1.39	1.33
21	B	606	CLA	C5-C3	2.16	1.55	1.51
21	P	508	CLA	MG-NC	-2.16	2.01	2.06
21	N	614	CLA	O2A-CGA	2.16	1.39	1.33
21	P	506	CLA	O2D-CGD	2.16	1.38	1.33
21	N	613	CLA	O2A-CGA	2.16	1.39	1.33
21	N	611	CLA	C3D-C4D	-2.16	1.39	1.44
21	A	405	CLA	MG-NC	-2.15	2.01	2.06
21	B	615	CLA	CAB-C3B	2.15	1.53	1.47
21	N	610	CLA	CAB-C3B	2.15	1.53	1.47
21	N	617	CLA	O2D-CGD	2.15	1.38	1.33
21	B	612	CLA	O2A-CGA	2.15	1.39	1.33
21	B	616	CLA	O2A-CGA	2.15	1.39	1.33
21	G	406	CLA	MG-NC	-2.15	2.01	2.06
21	N	612	CLA	MG-NC	-2.15	2.01	2.06
21	C	511	CLA	C5-C3	2.15	1.55	1.51
21	N	611	CLA	O2A-C1	-2.15	1.40	1.46
21	Q	404	CLA	C3D-C4D	-2.15	1.39	1.44
21	P	511	CLA	O2A-CGA	2.15	1.39	1.33
21	N	619	CLA	C5-C3	2.15	1.55	1.51
21	B	602	CLA	CAB-C3B	2.15	1.53	1.47
21	A	403	CLA	C3D-C4D	-2.15	1.39	1.44
21	C	506	CLA	C5-C3	2.14	1.55	1.51
21	B	614	CLA	CAB-C3B	2.14	1.53	1.47
21	B	601	CLA	O2A-CGA	2.14	1.39	1.33
21	A	402	CLA	C3D-C4D	-2.14	1.39	1.44
21	N	613	CLA	O2D-CGD	2.14	1.38	1.33
21	P	508	CLA	O2A-CGA	2.14	1.39	1.33
24	P	519	DGD	O3G-C1D	2.14	1.43	1.40
21	P	510	CLA	O2A-CGA	2.14	1.39	1.33
21	P	508	CLA	CAB-C3B	2.14	1.53	1.47
21	C	503	CLA	C3D-C4D	-2.14	1.39	1.44
21	P	510	CLA	C3D-C4D	-2.14	1.39	1.44
21	N	606	CLA	CAB-C3B	2.14	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	506	CLA	O2D-CGD	2.14	1.38	1.33
21	C	513	CLA	MG-NC	-2.14	2.01	2.06
21	C	506	CLA	O2A-CGA	2.13	1.39	1.33
26	B	624	SQD	O6-C1	2.13	1.43	1.40
21	B	601	CLA	CAB-C3B	2.13	1.53	1.47
21	A	405	CLA	O2A-CGA	2.13	1.39	1.33
21	P	507	CLA	O2A-CGA	2.13	1.39	1.33
21	P	503	CLA	C3D-C4D	-2.13	1.39	1.44
21	C	508	CLA	CAB-C3B	2.13	1.53	1.47
21	P	502	CLA	MG-NC	-2.13	2.01	2.06
21	P	510	CLA	CAB-C3B	2.13	1.53	1.47
21	N	615	CLA	CAB-C3B	2.13	1.53	1.47
21	N	608	CLA	C3D-C4D	-2.13	1.39	1.44
21	C	504	CLA	MG-NC	-2.13	2.01	2.06
21	C	510	CLA	C5-C3	2.12	1.55	1.51
21	D	401	CLA	C3D-C4D	-2.12	1.39	1.44
21	N	607	CLA	CHB-C1B	-2.12	1.34	1.39
21	N	619	CLA	CAB-C3B	2.12	1.53	1.47
21	C	505	CLA	O2A-CGA	2.12	1.39	1.33
21	N	617	CLA	O2A-CGA	2.12	1.39	1.33
21	C	510	CLA	O2A-CGA	2.12	1.39	1.33
21	C	510	CLA	C3D-C4D	-2.12	1.39	1.44
21	P	504	CLA	CAB-C3B	2.12	1.53	1.47
21	P	504	CLA	MG-NC	-2.12	2.01	2.06
21	B	608	CLA	C3D-C4D	-2.12	1.39	1.44
21	C	507	CLA	MG-NC	-2.12	2.01	2.06
21	G	406	CLA	CAB-C3B	2.11	1.53	1.47
21	B	605	CLA	C3D-C4D	-2.11	1.39	1.44
21	C	509	CLA	C3D-C4D	-2.11	1.39	1.44
21	A	405	CLA	O2D-CGD	2.11	1.38	1.33
21	N	606	CLA	CHB-C1B	-2.11	1.34	1.39
21	A	405	CLA	CAB-C3B	2.11	1.53	1.47
21	D	403	CLA	C3D-C4D	-2.11	1.39	1.44
21	N	620	CLA	O2D-CGD	2.11	1.38	1.33
21	B	614	CLA	C3D-C4D	-2.11	1.39	1.44
21	B	611	CLA	O2D-CGD	2.11	1.38	1.33
21	B	603	CLA	O2D-CGD	2.11	1.38	1.33
21	C	507	CLA	O2A-CGA	2.11	1.39	1.33
21	B	610	CLA	O2D-CGD	2.11	1.38	1.33
21	N	612	CLA	O2D-CGD	2.11	1.38	1.33
21	P	505	CLA	O2D-CGD	2.11	1.38	1.33
21	C	502	CLA	MG-NC	-2.11	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	612	CLA	CAB-C3B	2.10	1.53	1.47
21	P	505	CLA	O2A-CGA	2.10	1.39	1.33
21	P	511	CLA	CAB-C3B	2.10	1.53	1.47
21	N	607	CLA	O2A-C1	-2.10	1.40	1.46
21	B	613	CLA	O2A-CGA	2.10	1.39	1.33
21	P	505	CLA	CAB-C3B	2.10	1.53	1.47
21	N	615	CLA	O2A-CGA	2.10	1.39	1.33
21	B	615	CLA	O2A-CGA	2.10	1.39	1.33
21	P	505	CLA	C5-C3	2.10	1.55	1.51
21	P	513	CLA	O2D-CGD	2.10	1.38	1.33
21	C	513	CLA	O2D-CGD	2.10	1.38	1.33
21	C	510	CLA	CAB-C3B	2.10	1.53	1.47
21	B	612	CLA	C3D-C4D	-2.10	1.39	1.44
21	B	611	CLA	MG-NC	-2.10	2.01	2.06
21	P	512	CLA	CAB-C3B	2.10	1.53	1.47
21	N	605	CLA	O2A-CGA	2.10	1.39	1.33
21	C	508	CLA	MG-NC	-2.10	2.01	2.06
21	P	509	CLA	C3D-C4D	-2.09	1.39	1.44
21	B	616	CLA	MG-NC	-2.09	2.01	2.06
21	B	615	CLA	C3D-C4D	-2.09	1.39	1.44
21	C	511	CLA	O2A-CGA	2.09	1.39	1.33
21	C	505	CLA	O2D-CGD	2.09	1.38	1.33
21	C	506	CLA	CAB-C3B	2.09	1.53	1.47
21	P	513	CLA	CAB-C3B	2.09	1.53	1.47
21	G	402	CLA	O2D-CGD	2.09	1.38	1.33
26	B	627	SQD	O6-C1	2.09	1.43	1.40
21	C	505	CLA	C3D-C4D	-2.09	1.39	1.44
21	N	608	CLA	CAB-C3B	2.09	1.53	1.47
21	G	403	CLA	CHB-C1B	-2.09	1.34	1.39
21	C	512	CLA	O2D-CGD	2.09	1.38	1.33
21	B	606	CLA	O2A-CGA	2.09	1.39	1.33
21	N	612	CLA	CAB-C3B	2.09	1.53	1.47
21	N	619	CLA	O2A-CGA	2.09	1.39	1.33
21	P	506	CLA	C3D-C4D	-2.09	1.39	1.44
21	P	503	CLA	O2D-CGD	2.09	1.38	1.33
21	B	613	CLA	CAB-C3B	2.09	1.53	1.47
21	P	509	CLA	CAB-C3B	2.09	1.53	1.47
21	N	605	CLA	C3D-C4D	-2.09	1.39	1.44
21	N	615	CLA	O2D-CGD	2.09	1.38	1.33
21	C	511	CLA	MG-NC	-2.08	2.01	2.06
21	G	404	CLA	O2D-CGD	2.08	1.38	1.33
21	G	402	CLA	MG-NC	-2.08	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	506	CLA	C3D-C4D	-2.08	1.39	1.44
21	B	606	CLA	C3D-C4D	-2.08	1.39	1.44
21	P	505	CLA	CHD-C1D	-2.08	1.34	1.38
21	C	511	CLA	CAB-C3B	2.08	1.52	1.47
21	P	504	CLA	C3D-C4D	-2.08	1.39	1.44
21	A	405	CLA	CHB-C1B	-2.08	1.34	1.39
31	I	103	LMT	O1'-C1'	2.08	1.43	1.40
21	P	506	CLA	CAB-C3B	2.08	1.52	1.47
21	N	616	CLA	C3D-C4D	-2.08	1.39	1.44
21	G	404	CLA	MG-NC	-2.08	2.01	2.06
21	D	403	CLA	CAB-C3B	2.08	1.52	1.47
21	B	607	CLA	MG-NC	-2.08	2.01	2.06
21	N	607	CLA	CAB-C3B	2.08	1.52	1.47
21	N	614	CLA	MG-NC	-2.08	2.01	2.06
26	N	601	SQD	O6-C1	2.07	1.43	1.40
21	B	607	CLA	C3D-C4D	-2.07	1.39	1.44
21	C	501	CLA	O2D-CGD	2.07	1.38	1.33
21	B	606	CLA	CAB-C3B	2.07	1.52	1.47
21	N	605	CLA	CAB-C3B	2.07	1.52	1.47
21	B	611	CLA	CAB-C3B	2.07	1.52	1.47
21	P	513	CLA	MG-NC	-2.07	2.01	2.06
21	N	605	CLA	O2D-CGD	2.07	1.38	1.33
34	E	101	HEM	CMC-C2C	2.07	1.55	1.50
21	N	613	CLA	C3D-C4D	-2.07	1.39	1.44
21	A	401	CLA	O2A-CGA	2.07	1.39	1.33
21	N	614	CLA	O2D-CGD	2.07	1.38	1.33
21	B	611	CLA	O2A-CGA	2.07	1.39	1.33
21	P	509	CLA	O2D-CGD	2.07	1.38	1.33
21	C	506	CLA	C1B-NB	-2.07	1.35	1.37
21	P	502	CLA	CAB-C3B	2.07	1.52	1.47
21	C	511	CLA	O2D-CGD	2.07	1.38	1.33
21	N	612	CLA	C3D-C4D	-2.07	1.39	1.44
21	C	507	CLA	CHB-C1B	-2.07	1.34	1.39
21	C	512	CLA	CAB-C3B	2.07	1.52	1.47
21	P	512	CLA	O2D-CGD	2.07	1.38	1.33
21	N	607	CLA	MG-NC	-2.07	2.01	2.06
21	B	601	CLA	O2D-CGD	2.07	1.38	1.33
24	G	408	DGD	O3G-C1D	2.07	1.43	1.40
21	P	507	CLA	O2D-CGD	2.06	1.38	1.33
21	P	510	CLA	O2D-CGD	2.06	1.38	1.33
21	G	406	CLA	O2D-CGD	2.06	1.38	1.33
21	N	617	CLA	CAB-C3B	2.06	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	613	CLA	CBD-CAD	-2.06	1.47	1.56
21	P	508	CLA	C3D-C4D	-2.06	1.39	1.44
21	N	619	CLA	MG-NC	-2.06	2.01	2.06
34	V	201	HEM	CMB-C2B	2.06	1.55	1.50
21	Q	404	CLA	CAB-C3B	2.06	1.52	1.47
21	C	502	CLA	CAB-C3B	2.06	1.52	1.47
21	C	504	CLA	CAB-C3B	2.06	1.52	1.47
21	B	616	CLA	O2D-CGD	2.06	1.38	1.33
21	Q	402	CLA	C3D-C4D	-2.06	1.39	1.44
21	N	615	CLA	C3D-C4D	-2.06	1.39	1.44
21	D	403	CLA	MG-NC	-2.06	2.01	2.06
21	C	513	CLA	CAB-C3B	2.06	1.52	1.47
21	N	610	CLA	O2D-CGD	2.06	1.38	1.33
21	N	610	CLA	CHB-C1B	-2.06	1.34	1.39
21	N	613	CLA	CAB-C3B	2.06	1.52	1.47
21	B	604	CLA	CAB-C3B	2.06	1.52	1.47
21	P	501	CLA	O2D-CGD	2.05	1.38	1.33
21	N	614	CLA	C3D-C4D	-2.05	1.39	1.44
21	N	608	CLA	MG-NC	-2.05	2.01	2.06
21	C	513	CLA	C3D-C4D	-2.05	1.39	1.44
21	C	503	CLA	O2D-CGD	2.05	1.38	1.33
21	B	605	CLA	CAB-C3B	2.05	1.52	1.47
21	B	601	CLA	MG-NC	-2.05	2.01	2.06
21	N	607	CLA	O2D-CGD	2.05	1.38	1.33
21	A	403	CLA	MG-NC	-2.05	2.01	2.06
21	C	504	CLA	C3D-C4D	-2.05	1.39	1.44
21	B	607	CLA	CAB-C3B	2.05	1.52	1.47
21	B	603	CLA	CHB-C1B	-2.05	1.34	1.39
21	C	502	CLA	O2D-CGD	2.05	1.38	1.33
21	B	607	CLA	CHB-C1B	-2.05	1.34	1.39
21	C	507	CLA	C3D-C4D	-2.05	1.39	1.44
21	G	406	CLA	O2A-CGA	2.05	1.39	1.33
21	B	613	CLA	O2D-CGD	2.05	1.38	1.33
21	N	609	CLA	C3D-C4D	-2.05	1.39	1.44
21	C	503	CLA	MG-NC	-2.05	2.01	2.06
21	C	501	CLA	C3D-C4D	-2.05	1.39	1.44
24	A	407	DGD	O3G-C1D	2.05	1.43	1.40
21	A	401	CLA	CAB-C3B	2.05	1.52	1.47
21	C	508	CLA	C3D-C4D	-2.05	1.39	1.44
21	B	612	CLA	O2D-CGD	2.04	1.38	1.33
21	A	403	CLA	CAB-C3B	2.04	1.52	1.47
21	B	608	CLA	O2D-CGD	2.04	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	613	CLA	MG-NC	-2.04	2.01	2.06
21	N	606	CLA	MG-NC	-2.04	2.01	2.06
21	P	511	CLA	O2D-CGD	2.04	1.38	1.33
21	N	605	CLA	MG-NC	-2.04	2.01	2.06
21	G	402	CLA	CHB-C1B	-2.04	1.34	1.39
21	N	609	CLA	CHB-C1B	-2.04	1.34	1.39
21	P	512	CLA	C3D-C4D	-2.04	1.39	1.44
21	N	609	CLA	CAB-C3B	2.04	1.52	1.47
21	N	618	CLA	C3D-C4D	-2.04	1.39	1.44
21	C	509	CLA	O2D-CGD	2.04	1.38	1.33
21	A	401	CLA	CHB-C1B	-2.04	1.34	1.39
21	P	508	CLA	CHB-C1B	-2.04	1.34	1.39
21	B	608	CLA	CAB-C3B	2.04	1.52	1.47
21	B	609	CLA	C3D-C4D	-2.04	1.39	1.44
22	G	405	PHO	CBD-CGD	-2.04	1.49	1.52
21	B	603	CLA	MG-NC	-2.03	2.01	2.06
21	N	620	CLA	CAB-C3B	2.03	1.52	1.47
21	N	616	CLA	O2D-CGD	2.03	1.38	1.33
21	P	510	CLA	MG-NC	-2.03	2.01	2.06
21	B	606	CLA	O2D-CGD	2.03	1.38	1.33
21	C	506	CLA	CBD-CAD	-2.03	1.47	1.56
21	C	509	CLA	CAB-C3B	2.03	1.52	1.47
21	G	402	CLA	O2A-CGA	2.03	1.39	1.33
21	P	501	CLA	C3D-C4D	-2.03	1.39	1.44
21	D	401	CLA	CBD-CAD	-2.03	1.47	1.56
21	G	403	CLA	CBD-CAD	-2.03	1.47	1.56
21	P	513	CLA	C3D-C4D	-2.03	1.39	1.44
21	A	402	CLA	CBD-CAD	-2.03	1.47	1.56
21	B	603	CLA	C3D-C4D	-2.03	1.39	1.44
21	B	609	CLA	CAB-C3B	2.03	1.52	1.47
21	A	403	CLA	CHB-C1B	-2.03	1.34	1.39
21	G	402	CLA	CAB-C3B	2.03	1.52	1.47
21	N	611	CLA	MG-NC	-2.03	2.01	2.06
21	B	602	CLA	CHB-C1B	-2.03	1.34	1.39
34	E	101	HEM	FE-NC	2.03	2.01	1.95
21	N	618	CLA	O2D-CGD	2.03	1.38	1.33
21	G	404	CLA	CAB-C3B	2.03	1.52	1.47
21	C	510	CLA	MG-NC	-2.03	2.01	2.06
21	B	613	CLA	C3D-C4D	-2.02	1.39	1.44
21	B	612	CLA	MG-NC	-2.02	2.01	2.06
21	P	509	CLA	MG-NC	-2.02	2.01	2.06
21	B	605	CLA	CBD-CAD	-2.02	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	i	201	HEM	CMC-C2C	2.02	1.54	1.50
21	C	511	CLA	C3D-C4D	-2.02	1.39	1.44
21	C	510	CLA	O2D-CGD	2.02	1.38	1.33
21	A	403	CLA	O2D-CGD	2.02	1.38	1.33
21	P	508	CLA	O2D-CGD	2.02	1.38	1.33
21	N	617	CLA	MG-NC	-2.02	2.01	2.06
21	P	507	CLA	CHB-C1B	-2.02	1.34	1.39
21	Q	404	CLA	MG-NC	-2.02	2.01	2.06
34	V	201	HEM	CMA-C3A	2.02	1.54	1.50
21	C	507	CLA	O2D-CGD	2.02	1.38	1.33
21	P	506	CLA	MG-NC	-2.02	2.01	2.06
21	G	406	CLA	CHB-C1B	-2.02	1.34	1.39
34	V	201	HEM	CMC-C2C	2.02	1.54	1.50
21	A	405	CLA	C3D-C4D	-2.02	1.39	1.44
21	C	501	CLA	CAB-C3B	2.02	1.52	1.47
21	C	505	CLA	CAB-C3B	2.02	1.52	1.47
21	B	604	CLA	C3D-C4D	-2.02	1.39	1.44
27	D	412	LMG	O1-C1	2.02	1.43	1.40
21	P	507	CLA	C3D-C4D	-2.02	1.39	1.44
21	P	507	CLA	MG-NC	-2.02	2.01	2.06
21	N	611	CLA	CBD-CAD	-2.02	1.47	1.56
21	B	616	CLA	C3D-C4D	-2.01	1.39	1.44
21	G	406	CLA	C3D-C4D	-2.01	1.39	1.44
21	N	611	CLA	CHB-C1B	-2.01	1.34	1.39
21	B	610	CLA	C3D-C4D	-2.01	1.39	1.44
21	B	603	CLA	CAB-C3B	2.01	1.52	1.47
21	N	611	CLA	CAB-C3B	2.01	1.52	1.47
21	A	403	CLA	CBD-CAD	-2.01	1.47	1.56
21	B	616	CLA	CAB-C3B	2.01	1.52	1.47
21	P	501	CLA	CAB-C3B	2.01	1.52	1.47
21	B	609	CLA	CBD-CAD	-2.01	1.47	1.56
21	C	509	CLA	MG-NC	-2.01	2.01	2.06
21	C	504	CLA	O2D-CGD	2.01	1.38	1.33
21	D	403	CLA	CBD-CAD	-2.01	1.47	1.56
21	N	617	CLA	CHB-C1B	-2.01	1.34	1.39
34	i	201	HEM	CMA-C3A	2.01	1.54	1.50
21	N	614	CLA	CAB-C3B	2.01	1.52	1.47
21	B	615	CLA	CBD-CAD	-2.01	1.47	1.56
21	B	610	CLA	CAB-C3B	2.01	1.52	1.47
21	B	602	CLA	O2D-CGD	2.01	1.38	1.33
21	N	612	CLA	C1B-NB	-2.01	1.35	1.37
21	Q	404	CLA	CBD-CAD	-2.01	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	607	CLA	C3D-C4D	-2.00	1.39	1.44

All (1695) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	102	BCR	C32-C1-C6	-13.90	88.45	110.24
30	J	102	BCR	C32-C1-C6	-13.83	88.56	110.24
21	C	505	CLA	C4A-NA-C1A	13.12	112.67	106.68
21	P	505	CLA	C4A-NA-C1A	12.97	112.60	106.68
21	B	611	CLA	C4A-NA-C1A	12.70	112.47	106.68
21	N	609	CLA	C4A-NA-C1A	12.69	112.47	106.68
21	P	501	CLA	C4A-NA-C1A	12.67	112.46	106.68
21	N	616	CLA	C4A-NA-C1A	12.49	112.38	106.68
21	C	511	CLA	C4A-NA-C1A	12.49	112.38	106.68
21	C	501	CLA	C4A-NA-C1A	12.45	112.36	106.68
21	B	608	CLA	C4A-NA-C1A	12.41	112.34	106.68
21	N	619	CLA	C4A-NA-C1A	12.38	112.33	106.68
21	B	605	CLA	C4A-NA-C1A	12.34	112.31	106.68
21	N	613	CLA	C4A-NA-C1A	12.33	112.30	106.68
21	B	610	CLA	C4A-NA-C1A	12.30	112.29	106.68
21	B	604	CLA	C4A-NA-C1A	12.29	112.28	106.68
21	N	608	CLA	C4A-NA-C1A	12.27	112.28	106.68
21	C	503	CLA	C4A-NA-C1A	12.26	112.27	106.68
21	C	504	CLA	C4A-NA-C1A	12.26	112.27	106.68
21	B	601	CLA	C4A-NA-C1A	12.24	112.26	106.68
21	C	513	CLA	C4A-NA-C1A	12.23	112.26	106.68
21	P	502	CLA	C4A-NA-C1A	12.23	112.26	106.68
21	C	508	CLA	C4A-NA-C1A	12.20	112.25	106.68
21	B	616	CLA	C4A-NA-C1A	12.20	112.24	106.68
21	B	615	CLA	C4A-NA-C1A	12.19	112.24	106.68
21	N	606	CLA	C4A-NA-C1A	12.19	112.24	106.68
21	B	603	CLA	C4A-NA-C1A	12.18	112.24	106.68
21	P	508	CLA	C4A-NA-C1A	12.18	112.23	106.68
21	N	617	CLA	C4A-NA-C1A	12.18	112.23	106.68
21	P	511	CLA	C4A-NA-C1A	12.17	112.23	106.68
21	D	401	CLA	C4A-NA-C1A	12.17	112.23	106.68
21	C	502	CLA	C4A-NA-C1A	12.16	112.23	106.68
21	B	609	CLA	C4A-NA-C1A	12.15	112.22	106.68
21	N	620	CLA	C4A-NA-C1A	12.15	112.22	106.68
21	P	504	CLA	C4A-NA-C1A	12.13	112.21	106.68
21	A	405	CLA	C4A-NA-C1A	12.12	112.21	106.68
21	G	406	CLA	C4A-NA-C1A	12.12	112.21	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	613	CLA	C4A-NA-C1A	12.10	112.20	106.68
21	C	507	CLA	C4A-NA-C1A	12.08	112.19	106.68
21	N	615	CLA	C4A-NA-C1A	12.06	112.18	106.68
21	B	607	CLA	C4A-NA-C1A	12.05	112.18	106.68
21	N	612	CLA	C4A-NA-C1A	12.04	112.17	106.68
21	P	513	CLA	C4A-NA-C1A	12.04	112.17	106.68
21	P	507	CLA	C4A-NA-C1A	12.00	112.15	106.68
21	A	402	CLA	C4A-NA-C1A	11.98	112.14	106.68
21	B	614	CLA	C4A-NA-C1A	11.97	112.14	106.68
21	Q	402	CLA	C4A-NA-C1A	11.94	112.13	106.68
21	D	403	CLA	C4A-NA-C1A	11.92	112.12	106.68
21	N	605	CLA	C4A-NA-C1A	11.92	112.12	106.68
21	Q	404	CLA	C4A-NA-C1A	11.91	112.11	106.68
21	B	602	CLA	C4A-NA-C1A	11.90	112.11	106.68
21	N	614	CLA	C4A-NA-C1A	11.89	112.10	106.68
21	P	509	CLA	C4A-NA-C1A	11.86	112.09	106.68
21	P	510	CLA	C4A-NA-C1A	11.86	112.09	106.68
21	N	611	CLA	C4A-NA-C1A	11.85	112.08	106.68
21	N	610	CLA	C4A-NA-C1A	11.85	112.08	106.68
21	C	512	CLA	C4A-NA-C1A	11.83	112.08	106.68
21	P	503	CLA	C4A-NA-C1A	11.80	112.06	106.68
21	P	506	CLA	C4A-NA-C1A	11.77	112.05	106.68
21	G	404	CLA	C4A-NA-C1A	11.77	112.05	106.68
21	G	402	CLA	C4A-NA-C1A	11.76	112.05	106.68
21	C	510	CLA	C4A-NA-C1A	11.75	112.04	106.68
21	N	607	CLA	C4A-NA-C1A	11.75	112.04	106.68
21	P	512	CLA	C4A-NA-C1A	11.72	112.03	106.68
21	C	506	CLA	C4A-NA-C1A	11.71	112.02	106.68
21	B	612	CLA	C4A-NA-C1A	11.69	112.01	106.68
21	G	403	CLA	C4A-NA-C1A	11.69	112.01	106.68
21	C	509	CLA	C4A-NA-C1A	11.64	111.99	106.68
21	N	618	CLA	C4A-NA-C1A	11.59	111.97	106.68
21	B	606	CLA	C4A-NA-C1A	11.56	111.95	106.68
21	A	403	CLA	C4A-NA-C1A	11.53	111.94	106.68
21	A	401	CLA	C4A-NA-C1A	11.26	111.82	106.68
30	C	514	BCR	C7-C8-C9	9.60	140.43	126.23
30	P	514	BCR	C7-C8-C9	9.41	140.16	126.23
30	b	102	BCR	C32-C1-C31	-9.17	82.38	108.63
30	J	102	BCR	C32-C1-C31	-9.16	82.42	108.63
22	G	405	PHO	O2D-CGD-CBD	8.04	119.78	110.95
22	Q	403	PHO	C3B-C4B-NB	7.78	112.53	107.46
22	G	405	PHO	C3B-C4B-NB	7.77	112.53	107.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	402	PHO	C3B-C4B-NB	7.68	112.47	107.46
22	A	404	PHO	C3B-C4B-NB	7.67	112.47	107.46
22	A	404	PHO	O2D-CGD-CBD	7.44	119.12	110.95
30	T	102	BCR	C7-C8-C9	-6.99	115.89	126.23
30	B	618	BCR	C7-C8-C9	-6.93	115.99	126.23
30	b	102	BCR	C31-C1-C6	6.89	121.04	110.24
30	J	102	BCR	C31-C1-C6	6.87	121.02	110.24
22	G	405	PHO	C2D-C1D-ND	6.73	114.29	109.43
22	A	404	PHO	C2D-C1D-ND	6.67	114.25	109.43
22	Q	403	PHO	C2B-C1B-NB	6.62	114.21	109.43
22	Q	403	PHO	C2D-C1D-ND	6.54	114.16	109.43
22	D	402	PHO	C2D-C1D-ND	6.52	114.14	109.43
22	D	402	PHO	C2B-C1B-NB	6.49	114.12	109.43
22	G	405	PHO	C2B-C1B-NB	6.47	114.11	109.43
22	D	402	PHO	C3D-C4D-ND	6.42	115.94	107.71
22	A	404	PHO	C2B-C1B-NB	6.30	113.99	109.43
22	G	405	PHO	C3D-C4D-ND	6.30	115.79	107.71
22	D	402	PHO	O2D-CGD-CBD	6.28	117.85	110.95
22	Q	403	PHO	C3D-C4D-ND	6.21	115.67	107.71
22	A	404	PHO	C3D-C4D-ND	6.20	115.66	107.71
30	S	101	BCR	C7-C8-C9	-6.07	117.26	126.23
22	Q	403	PHO	O2D-CGD-CBD	6.06	117.61	110.95
22	G	405	PHO	C4D-ND-C1D	-5.93	101.77	108.87
30	D	405	BCR	C7-C8-C9	-5.92	117.48	126.23
22	A	404	PHO	C4D-ND-C1D	-5.92	101.78	108.87
22	D	402	PHO	C4D-ND-C1D	-5.91	101.80	108.87
34	i	201	HEM	C4D-ND-C1D	5.83	112.11	105.21
22	Q	403	PHO	C4D-ND-C1D	-5.76	101.97	108.87
21	A	402	CLA	O2D-CGD-CBD	5.61	121.03	111.23
34	V	201	HEM	C4D-ND-C1D	5.55	111.78	105.21
21	G	403	CLA	O2D-CGD-CBD	5.53	120.90	111.23
30	J	102	BCR	C32-C1-C2	-5.46	87.99	108.95
30	C	514	BCR	C8-C7-C6	5.45	141.57	127.00
30	b	102	BCR	C32-C1-C2	-5.45	88.04	108.95
30	P	514	BCR	C8-C7-C6	5.42	141.49	127.00
21	N	619	CLA	O2D-CGD-CBD	5.36	120.61	111.23
21	D	403	CLA	O2D-CGD-CBD	5.35	120.58	111.23
21	B	615	CLA	O2D-CGD-CBD	5.32	120.54	111.23
21	Q	404	CLA	O2D-CGD-CBD	5.28	120.47	111.23
21	P	512	CLA	O2D-CGD-CBD	5.24	120.39	111.23
24	G	408	DGD	O6E-C5E-C4E	5.20	119.08	109.70
21	C	511	CLA	O2D-CGD-CBD	5.16	120.25	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	508	CLA	O2D-CGD-CBD	5.12	120.17	111.23
21	G	404	CLA	O2D-CGD-CBD	5.11	120.16	111.23
21	N	614	CLA	O2D-CGD-CBD	5.11	120.16	111.23
21	P	511	CLA	O2D-CGD-CBD	5.10	120.15	111.23
21	C	512	CLA	O2D-CGD-CBD	5.10	120.14	111.23
24	A	407	DGD	O6E-C5E-C4E	5.09	118.88	109.70
21	B	610	CLA	O2D-CGD-CBD	4.97	119.92	111.23
21	A	403	CLA	O2D-CGD-CBD	4.94	119.87	111.23
24	D	408	DGD	O6E-C5E-C4E	4.94	118.60	109.70
21	P	510	CLA	O2D-CGD-CBD	4.92	119.83	111.23
21	B	612	CLA	O2D-CGD-CBD	4.89	119.78	111.23
21	N	620	CLA	O2D-CGD-CBD	4.88	119.76	111.23
21	N	616	CLA	O2D-CGD-CBD	4.84	119.70	111.23
24	Q	409	DGD	O6E-C5E-C4E	4.84	118.43	109.70
26	N	601	SQD	O9-S-C6	4.84	113.99	106.76
34	R	101	HEM	C4D-ND-C1D	4.83	110.92	105.21
34	E	101	HEM	C4D-ND-C1D	4.81	110.90	105.21
21	P	502	CLA	O2D-CGD-CBD	4.81	119.63	111.23
30	P	514	BCR	C33-C5-C6	-4.80	119.25	124.48
27	e	102	LMG	O7-C10-C11	4.79	121.84	111.48
24	C	518	DGD	O6E-C5E-C4E	4.78	118.32	109.70
26	B	627	SQD	O9-S-C6	4.77	113.88	106.76
30	b	102	BCR	C15-C14-C13	-4.74	120.63	127.28
27	M	101	LMG	O7-C10-C11	4.74	121.73	111.48
21	N	606	CLA	O2D-CGD-CBD	4.73	119.51	111.23
30	b	102	BCR	C24-C23-C22	-4.71	119.26	126.23
21	B	607	CLA	O2D-CGD-CBD	4.71	119.47	111.23
21	A	405	CLA	O2D-CGD-CBD	4.70	119.45	111.23
21	C	501	CLA	O2D-CGD-CBD	4.69	119.43	111.23
21	C	502	CLA	O2D-CGD-CBD	4.69	119.42	111.23
21	C	510	CLA	O2D-CGD-CBD	4.68	119.40	111.23
21	G	406	CLA	O2D-CGD-CBD	4.67	119.39	111.23
21	P	503	CLA	O2D-CGD-CBD	4.66	119.38	111.23
30	J	102	BCR	C15-C14-C13	-4.66	120.74	127.28
30	b	102	BCR	C20-C21-C22	-4.65	120.75	127.28
21	P	513	CLA	O2D-CGD-CBD	4.64	119.35	111.23
24	P	519	DGD	O6E-C5E-C4E	4.63	118.05	109.70
21	G	402	CLA	O2D-CGD-CBD	4.62	119.31	111.23
24	A	407	DGD	O2G-C1B-C2B	4.62	121.47	111.48
23	b	101	PL9	C7-C3-C4	4.61	120.71	116.91
21	C	507	CLA	O2D-CGD-CBD	4.61	119.28	111.23
26	Q	408	SQD	O6-C1-C2	4.61	115.27	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	513	CLA	O2D-CGD-CBD	4.60	119.27	111.23
24	P	517	DGD	O6E-C5E-C4E	4.58	117.96	109.70
21	P	507	CLA	O2D-CGD-CBD	4.56	119.20	111.23
21	C	503	CLA	O2D-CGD-CBD	4.55	119.19	111.23
30	J	102	BCR	C24-C23-C22	-4.55	119.51	126.23
27	G	411	LMG	O7-C10-C11	4.54	121.30	111.48
27	A	410	LMG	O7-C10-C11	4.54	121.30	111.48
24	C	516	DGD	O6D-C5D-C6D	4.54	115.69	106.69
24	C	518	DGD	O6D-C5D-C6D	4.53	115.68	106.69
27	D	406	LMG	O7-C10-C11	4.53	121.27	111.48
26	B	624	SQD	O6-C1-C2	4.52	115.13	108.27
30	J	102	BCR	C2-C1-C6	4.51	116.99	110.44
21	P	501	CLA	O2D-CGD-CBD	4.50	119.09	111.23
21	B	616	CLA	O2D-CGD-CBD	4.49	119.08	111.23
21	B	602	CLA	O2D-CGD-CBD	4.48	119.06	111.23
21	C	508	CLA	O2D-CGD-CBD	4.48	119.06	111.23
23	Q	405	PL9	C7-C3-C4	4.48	120.60	116.91
34	R	101	HEM	CBD-CAD-C3D	-4.48	100.15	112.53
21	N	605	CLA	O2D-CGD-CBD	4.48	119.06	111.23
30	C	514	BCR	C33-C5-C6	-4.47	119.60	124.48
21	P	509	CLA	O2D-CGD-CBD	4.46	119.03	111.23
30	J	102	BCR	C20-C21-C22	-4.46	121.03	127.28
27	Q	401	LMG	O7-C10-C11	4.45	121.11	111.48
27	D	412	LMG	O7-C10-C11	4.44	121.09	111.48
24	C	516	DGD	O6E-C5E-C4E	4.44	117.70	109.70
21	C	509	CLA	O2D-CGD-CBD	4.44	118.99	111.23
27	C	520	LMG	O7-C10-C11	4.44	121.09	111.48
21	C	504	CLA	O2D-CGD-CBD	4.43	118.98	111.23
21	P	504	CLA	O2D-CGD-CBD	4.43	118.97	111.23
21	N	611	CLA	O2D-CGD-CBD	4.42	118.96	111.23
21	B	608	CLA	O2D-CGD-CBD	4.41	118.95	111.23
24	W	102	DGD	O6E-C5E-C4E	4.40	117.63	109.70
30	b	102	BCR	C2-C1-C6	4.39	116.82	110.44
24	P	519	DGD	O6D-C5D-C6D	4.39	115.40	106.69
27	Q	406	LMG	O7-C10-C11	4.39	120.98	111.48
21	A	401	CLA	O2D-CGD-CBD	4.39	118.90	111.23
24	G	408	DGD	O2G-C1B-C2B	4.38	120.96	111.48
24	N	602	DGD	O2G-C1B-C2B	4.38	120.95	111.48
24	C	517	DGD	C1E-O6E-C5E	4.37	122.25	113.72
21	N	612	CLA	O2D-CGD-CBD	4.36	118.86	111.23
24	P	517	DGD	O6D-C5D-C6D	4.35	115.33	106.69
24	B	628	DGD	O2G-C1B-C2B	4.35	120.90	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	518	DGD	C1E-O6E-C5E	4.33	122.18	113.72
23	J	101	PL9	C7-C3-C4	4.33	120.48	116.91
24	B	621	DGD	O6E-C5E-C4E	4.32	117.48	109.70
24	B	621	DGD	O6D-C5D-C6D	4.32	115.25	106.69
27	P	521	LMG	O7-C10-C11	4.30	120.79	111.48
24	W	102	DGD	O6D-C5D-C6D	4.29	115.19	106.69
24	P	518	DGD	O6E-C5E-C4E	4.28	117.41	109.70
27	Q	407	LMG	O7-C10-C11	4.25	120.67	111.48
21	N	618	CLA	O2D-CGD-CBD	4.22	118.61	111.23
30	T	103	BCR	C24-C23-C22	-4.22	119.99	126.23
21	B	606	CLA	O2D-CGD-CBD	4.21	118.58	111.23
24	C	517	DGD	O6E-C5E-C4E	4.20	117.27	109.70
21	B	601	CLA	O2D-CGD-CBD	4.19	118.56	111.23
30	P	516	BCR	C7-C8-C9	-4.19	120.04	126.23
21	C	506	CLA	O2D-CGD-CBD	4.18	118.54	111.23
24	A	407	DGD	O6D-C5D-C6D	4.18	114.98	106.69
24	G	408	DGD	O6D-C5D-C6D	4.17	114.96	106.69
30	T	102	BCR	C28-C27-C26	-4.16	106.64	114.06
21	B	614	CLA	O2D-CGD-CBD	4.14	118.46	111.23
23	G	407	PL9	C7-C3-C4	4.13	120.31	116.91
30	B	618	BCR	C28-C27-C26	-4.13	106.69	114.06
24	N	602	DGD	C1E-O6E-C5E	4.12	121.78	113.72
30	K	101	BCR	C38-C26-C25	-4.12	119.99	124.48
24	B	628	DGD	C1E-O6E-C5E	4.11	121.75	113.72
27	D	407	LMG	O7-C10-C11	4.10	120.36	111.48
21	P	505	CLA	O2D-CGD-CBD	4.10	118.40	111.23
21	N	617	CLA	O2D-CGD-CBD	4.10	118.39	111.23
21	N	609	CLA	O2D-CGD-CBD	4.10	118.39	111.23
21	C	505	CLA	O2D-CGD-CBD	4.08	118.37	111.23
30	P	516	BCR	C28-C27-C26	-4.06	106.82	114.06
30	Z	101	BCR	C15-C14-C13	-4.05	121.60	127.28
30	W	101	BCR	C33-C5-C6	-4.05	120.07	124.48
21	B	603	CLA	O2D-CGD-CBD	4.04	118.29	111.23
30	C	515	BCR	C28-C27-C26	-4.03	106.86	114.06
21	N	615	CLA	O2D-CGD-CBD	4.03	118.27	111.23
21	N	607	CLA	O2D-CGD-CBD	4.02	118.27	111.23
21	B	605	CLA	O2D-CGD-CBD	4.01	118.24	111.23
26	G	410	SQD	O6-C1-C2	4.01	114.36	108.27
34	E	101	HEM	C3B-C4B-NB	-3.99	106.60	109.47
24	C	517	DGD	O2G-C1B-C2B	3.97	120.07	111.48
27	Q	407	LMG	O6-C5-C6	3.97	116.28	106.44
27	D	407	LMG	O6-C5-C6	3.97	116.27	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	101	BCR	C38-C26-C25	-3.96	120.16	124.48
30	P	514	BCR	C1-C6-C7	3.96	126.39	115.65
22	D	402	PHO	C4D-CHA-CBD	3.94	110.35	108.45
34	R	101	HEM	C3B-C4B-NB	-3.94	106.64	109.47
30	B	620	BCR	C24-C23-C22	-3.94	120.41	126.23
30	H	101	BCR	C33-C5-C6	-3.93	120.19	124.48
30	P	514	BCR	C7-C6-C5	-3.92	112.52	121.56
23	A	406	PL9	C7-C3-C4	3.89	120.12	116.91
30	C	514	BCR	C7-C6-C5	-3.87	112.64	121.56
24	P	517	DGD	O2G-C1B-C2B	3.87	119.85	111.48
21	B	609	CLA	O2D-CGD-CBD	3.86	117.99	111.23
24	P	518	DGD	O2G-C1B-C2B	3.86	119.84	111.48
30	C	514	BCR	C1-C6-C7	3.86	126.11	115.65
30	P	516	BCR	C38-C26-C25	-3.85	120.28	124.48
25	A	411	LHG	O7-C7-C8	3.84	119.79	111.48
34	V	201	HEM	CBD-CAD-C3D	-3.82	101.96	112.53
21	P	506	CLA	O2D-CGD-CBD	3.82	117.91	111.23
30	C	515	BCR	C38-C26-C25	-3.82	120.31	124.48
25	G	412	LHG	O7-C7-C8	3.81	119.73	111.48
30	B	617	BCR	C7-C8-C9	-3.81	120.60	126.23
30	C	515	BCR	C7-C8-C9	-3.81	120.60	126.23
24	W	102	DGD	O2G-C1B-C2B	3.80	119.71	111.48
34	i	201	HEM	CBD-CAD-C3D	-3.80	102.03	112.53
30	P	515	BCR	C15-C14-C13	-3.79	121.96	127.28
24	C	518	DGD	C1E-O6E-C5E	3.79	121.13	113.72
30	T	101	BCR	C33-C5-C6	-3.79	120.35	124.48
21	B	613	CLA	O2D-CGD-CBD	3.76	117.80	111.23
24	C	516	DGD	O2G-C1B-C2B	3.76	119.61	111.48
21	N	610	CLA	O2D-CGD-CBD	3.76	117.80	111.23
26	Q	408	SQD	O47-C7-C8	3.75	119.59	111.48
27	N	622	LMG	O7-C10-C11	3.75	119.59	111.48
26	N	601	SQD	O6-C1-C2	3.75	113.96	108.27
30	b	102	BCR	C7-C8-C9	-3.75	120.69	126.23
34	E	101	HEM	CBD-CAD-C3D	-3.74	102.19	112.53
23	D	404	PL9	C7-C3-C4	3.74	119.99	116.91
21	N	608	CLA	O2D-CGD-CBD	3.74	117.76	111.23
30	P	514	BCR	C15-C14-C13	-3.73	122.05	127.28
21	N	613	CLA	O2D-CGD-CBD	3.73	117.75	111.23
24	B	621	DGD	O2G-C1B-C2B	3.72	119.53	111.48
26	G	410	SQD	O47-C7-C8	3.71	119.50	111.48
23	G	407	PL9	C35-C34-C36	3.71	121.66	115.23
26	B	624	SQD	O47-C7-C8	3.70	119.49	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	409	SQD	O47-C7-C8	3.70	119.48	111.48
21	Q	402	CLA	O2D-CGD-CBD	3.69	117.69	111.23
22	Q	403	PHO	C4D-CHA-CBD	3.69	110.23	108.45
24	N	602	DGD	O6D-C5D-C6D	3.69	114.02	106.69
23	A	406	PL9	C25-C24-C26	3.69	121.63	115.23
24	B	628	DGD	O6D-C5D-C6D	3.68	113.99	106.69
30	B	620	BCR	C3-C4-C5	-3.68	107.50	114.06
30	B	617	BCR	C33-C5-C6	-3.66	120.49	124.48
30	B	618	BCR	C3-C4-C5	-3.65	107.54	114.06
30	S	101	BCR	C28-C27-C26	-3.65	107.54	114.06
23	A	406	PL9	C35-C34-C36	3.64	121.55	115.23
30	T	101	BCR	C7-C8-C9	-3.64	120.85	126.23
21	D	401	CLA	O2D-CGD-CBD	3.64	117.58	111.23
21	A	401	CLA	C3B-C4B-NB	-3.63	107.29	110.53
30	c	101	BCR	C3-C4-C5	-3.62	107.60	114.06
23	G	407	PL9	C25-C24-C26	3.62	121.51	115.23
27	B	623	LMG	O7-C10-C11	3.61	119.29	111.48
30	D	405	BCR	C28-C27-C26	-3.60	107.64	114.06
21	B	611	CLA	O2D-CGD-CBD	3.60	117.52	111.23
24	A	407	DGD	C1E-O6E-C5E	3.60	120.75	113.72
21	G	402	CLA	C3B-C4B-NB	-3.60	107.32	110.53
21	N	616	CLA	C3B-C4B-NB	-3.60	107.32	110.53
26	G	401	SQD	O47-C7-C8	3.59	119.24	111.48
21	B	604	CLA	O2D-CGD-CBD	3.58	117.49	111.23
30	C	514	BCR	C15-C14-C13	-3.58	122.26	127.28
30	T	103	BCR	C3-C4-C5	-3.56	107.71	114.06
26	S	102	SQD	O47-C7-C8	3.56	119.17	111.48
26	A	414	SQD	O47-C7-C8	3.55	119.17	111.48
27	B	622	LMG	O7-C10-C11	3.55	119.17	111.48
24	P	517	DGD	C1E-O6E-C5E	3.54	120.63	113.72
24	P	519	DGD	O2G-C1B-C2B	3.54	119.13	111.48
30	T	102	BCR	C3-C4-C5	-3.53	107.75	114.06
24	C	518	DGD	O2G-C1B-C2B	3.52	119.09	111.48
24	Q	409	DGD	O2G-C1B-C2B	3.51	119.08	111.48
24	N	602	DGD	O6E-C5E-C4E	3.51	116.03	109.70
30	K	101	BCR	C3-C4-C5	-3.51	107.80	114.06
26	N	601	SQD	O47-C7-C8	3.51	119.07	111.48
27	N	623	LMG	O7-C10-C11	3.51	119.07	111.48
24	G	408	DGD	C1E-O6E-C5E	3.50	120.55	113.72
26	A	409	SQD	O6-C1-C2	3.49	113.57	108.27
30	P	514	BCR	C34-C9-C8	3.49	123.41	118.09
30	B	618	BCR	C38-C26-C25	-3.49	120.68	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	520	LMG	O8-C28-C29	3.48	122.46	111.83
30	J	102	BCR	C29-C30-C25	3.48	115.50	110.44
30	b	102	BCR	C29-C30-C25	3.48	115.50	110.44
25	A	408	LHG	O7-C7-C8	3.47	119.00	111.48
21	B	612	CLA	C3B-C4B-NB	-3.47	107.43	110.53
30	J	102	BCR	C7-C8-C9	-3.46	121.11	126.23
27	N	622	LMG	O6-C5-C6	3.45	114.98	106.44
27	a	102	LMG	O6-C1-O1	-3.44	101.91	110.04
21	C	512	CLA	O2A-CGA-CBA	3.43	122.30	111.83
30	T	102	BCR	C38-C26-C25	-3.42	120.75	124.48
21	N	610	CLA	O1D-CGD-CBD	-3.42	117.77	124.52
27	a	102	LMG	O1-C1-C2	3.42	113.47	108.27
24	C	517	DGD	C3G-O3G-C1D	-3.42	106.47	113.80
30	a	101	BCR	C38-C26-C25	-3.41	120.76	124.48
21	P	505	CLA	C3B-C4B-NB	-3.41	107.48	110.53
26	F	101	SQD	O47-C7-C8	3.41	118.86	111.48
24	P	518	DGD	C3G-O3G-C1D	-3.40	106.50	113.80
30	P	514	BCR	C16-C17-C18	-3.40	122.51	127.28
26	B	627	SQD	O47-C7-C8	3.40	118.83	111.48
21	N	611	CLA	O1D-CGD-CBD	-3.40	117.82	124.52
21	N	607	CLA	C3B-C4B-NB	-3.39	107.50	110.53
21	P	512	CLA	O2A-CGA-CBA	3.39	122.18	111.83
24	D	408	DGD	O2G-C1B-C2B	3.39	118.82	111.48
24	D	408	DGD	C3E-C4E-C5E	3.39	116.37	110.23
30	a	101	BCR	C33-C5-C6	-3.38	120.80	124.48
27	I	102	LMG	O6-C1-O1	-3.38	102.07	110.04
25	G	409	LHG	O7-C7-C8	3.37	118.78	111.48
21	B	602	CLA	C3B-C4B-NB	-3.37	107.52	110.53
21	B	612	CLA	C1-C2-C3	-3.37	120.68	126.20
27	N	622	LMG	C7-O1-C1	-3.37	106.58	113.80
21	N	612	CLA	C3B-C4B-NB	-3.37	107.53	110.53
21	B	613	CLA	C1-C2-C3	-3.36	120.69	126.20
30	Z	101	BCR	C33-C5-C6	-3.36	120.82	124.48
24	B	628	DGD	O6E-C5E-C4E	3.36	115.75	109.70
24	W	102	DGD	C3E-C4E-C5E	3.35	116.31	110.23
23	b	101	PL9	C25-C24-C26	3.35	121.05	115.23
21	N	610	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
24	D	408	DGD	O6D-C5D-C6D	3.35	113.33	106.69
30	B	620	BCR	C2-C1-C6	3.34	115.29	110.44
30	C	514	BCR	C34-C9-C8	3.34	123.19	118.09
26	G	410	SQD	O9-S-C6	3.34	111.74	106.76
24	P	519	DGD	C1E-O6E-C5E	3.33	120.22	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	514	BCR	C3-C4-C5	-3.33	108.12	114.06
21	N	610	CLA	C3B-C4B-NB	-3.33	107.56	110.53
27	I	102	LMG	O1-C1-C2	3.32	113.32	108.27
24	Q	409	DGD	C3E-C4E-C5E	3.32	116.26	110.23
21	B	607	CLA	O1D-CGD-CBD	-3.32	117.96	124.52
21	N	616	CLA	C2A-C3A-C4A	3.32	107.23	101.87
30	P	514	BCR	C3-C4-C5	-3.32	108.14	114.06
27	P	520	LMG	O7-C10-C11	3.31	118.65	111.48
30	T	103	BCR	C38-C26-C25	-3.31	120.87	124.48
21	P	507	CLA	C3B-C4B-NB	-3.31	107.57	110.53
30	B	620	BCR	C38-C26-C25	-3.31	120.87	124.48
30	Z	101	BCR	C24-C23-C22	-3.31	121.34	126.23
23	J	101	PL9	C25-C24-C26	3.30	120.96	115.23
21	B	603	CLA	C3B-C4B-NB	-3.30	107.58	110.53
21	C	507	CLA	C3B-C4B-NB	-3.30	107.59	110.53
21	N	617	CLA	C3B-C4B-NB	-3.29	107.59	110.53
26	B	627	SQD	O6-C1-C2	3.29	113.27	108.27
21	N	615	CLA	C1-C2-C3	-3.29	120.80	126.20
27	C	519	LMG	O7-C10-C11	3.29	118.60	111.48
30	C	515	BCR	C33-C5-C6	-3.29	120.89	124.48
21	B	611	CLA	C1-C2-C3	-3.29	120.81	126.20
21	B	606	CLA	C3B-C4B-NB	-3.29	107.59	110.53
27	D	406	LMG	O6-C5-C6	3.29	114.59	106.44
21	N	606	CLA	C3B-C4B-NB	-3.28	107.60	110.53
34	E	101	HEM	CHD-C4C-NC	3.28	128.03	124.45
27	I	102	LMG	O7-C10-C11	3.28	118.58	111.48
30	P	515	BCR	C24-C23-C22	-3.28	121.39	126.23
24	B	621	DGD	C3E-C4E-C5E	3.27	116.16	110.23
21	P	506	CLA	C3B-C4B-NB	-3.27	107.61	110.53
30	N	621	BCR	C24-C23-C22	-3.26	121.41	126.23
21	P	512	CLA	C3B-C4B-NB	-3.26	107.62	110.53
21	B	607	CLA	C3B-C4B-NB	-3.26	107.62	110.53
21	A	403	CLA	C3B-C4B-NB	-3.26	107.62	110.53
30	I	101	BCR	C33-C5-C6	-3.26	120.93	124.48
21	C	509	CLA	C3B-C4B-NB	-3.25	107.62	110.53
27	a	102	LMG	O7-C10-C11	3.25	118.52	111.48
30	K	101	BCR	C2-C1-C6	3.25	115.16	110.44
26	N	601	SQD	C1-C2-C3	-3.25	103.18	110.01
21	Q	404	CLA	C3B-C4B-NB	-3.25	107.63	110.53
27	B	622	LMG	O6-C5-C6	3.24	114.48	106.44
30	S	101	BCR	C33-C5-C6	-3.24	120.94	124.48
21	N	611	CLA	C3B-C4B-NB	-3.24	107.64	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	R	101	HEM	CHD-C4C-NC	3.24	127.98	124.45
27	P	521	LMG	O8-C28-C29	3.24	121.71	111.83
23	D	404	PL9	C25-C24-C26	3.24	120.85	115.23
21	C	510	CLA	C3B-C4B-NB	-3.24	107.64	110.53
30	I	101	BCR	C38-C26-C25	-3.24	120.95	124.48
21	C	502	CLA	C3B-C4B-NB	-3.23	107.65	110.53
22	G	405	PHO	O1D-CGD-CBD	-3.22	119.84	124.72
21	C	508	CLA	C3B-C4B-NB	-3.21	107.66	110.53
23	Q	405	PL9	C25-C24-C26	3.21	120.80	115.23
21	D	403	CLA	C3B-C4B-NB	-3.21	107.67	110.53
21	N	613	CLA	C1-C2-C3	-3.21	120.94	126.20
30	T	103	BCR	C2-C1-C6	3.21	115.09	110.44
21	C	505	CLA	C3B-C4B-NB	-3.20	107.67	110.53
23	Q	405	PL9	C7-C3-C2	-3.20	119.61	123.39
21	D	401	CLA	C2A-C3A-C4A	3.20	107.04	101.87
23	J	101	PL9	C7-C3-C2	-3.19	119.63	123.39
21	P	513	CLA	C3B-C4B-NB	-3.19	107.68	110.53
30	P	515	BCR	C33-C5-C6	-3.19	121.01	124.48
21	B	612	CLA	C2A-C3A-C4A	3.19	107.02	101.87
21	N	617	CLA	C1-C2-C3	-3.19	120.98	126.20
21	N	618	CLA	C3B-C4B-NB	-3.18	107.69	110.53
21	N	616	CLA	C1-C2-C3	-3.18	120.98	126.20
21	B	605	CLA	C2A-C3A-C4A	3.18	107.01	101.87
21	B	604	CLA	O1D-CGD-CBD	-3.18	118.24	124.52
21	B	609	CLA	C3B-C4B-NB	-3.18	107.69	110.53
21	P	510	CLA	C3B-C4B-NB	-3.18	107.69	110.53
21	G	406	CLA	C3B-C4B-NB	-3.18	107.69	110.53
23	G	407	PL9	C22-C23-C24	-3.18	120.36	127.62
21	P	502	CLA	C3B-C4B-NB	-3.17	107.70	110.53
23	b	101	PL9	C7-C3-C2	-3.17	119.65	123.39
23	D	404	PL9	C22-C23-C24	-3.17	120.36	127.62
21	C	512	CLA	C3B-C4B-NB	-3.17	107.70	110.53
21	B	613	CLA	C3B-C4B-NB	-3.17	107.70	110.53
24	Q	409	DGD	O6D-C5D-C6D	3.17	112.97	106.69
30	I	101	BCR	C3-C4-C5	-3.17	108.41	114.06
21	B	611	CLA	O1D-CGD-CBD	-3.16	118.28	124.52
21	P	508	CLA	C1-C2-C3	-3.16	121.02	126.20
27	R	102	LMG	O6-C5-C6	3.16	114.27	106.44
21	C	513	CLA	C3B-C4B-NB	-3.16	107.71	110.53
23	D	404	PL9	C35-C34-C36	3.16	120.71	115.23
21	P	511	CLA	C3B-C4B-NB	-3.16	107.71	110.53
21	N	609	CLA	C3B-C4B-NB	-3.15	107.71	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	405	PL9	C22-C23-C24	-3.15	120.41	127.62
21	P	508	CLA	C3B-C4B-NB	-3.15	107.72	110.53
21	B	610	CLA	C3B-C4B-NB	-3.15	107.72	110.53
24	N	602	DGD	C3E-C4E-C5E	3.14	115.93	110.23
23	A	406	PL9	C22-C23-C24	-3.14	120.43	127.62
21	C	506	CLA	C3B-C4B-NB	-3.14	107.72	110.53
21	B	614	CLA	C3B-C4B-NB	-3.14	107.73	110.53
21	N	607	CLA	C2A-C1A-CHA	3.14	129.31	123.87
24	Q	409	DGD	C1E-O6E-C5E	3.13	119.83	113.72
27	Q	406	LMG	O6-C5-C6	3.13	114.20	106.44
21	A	405	CLA	C3B-C4B-NB	-3.13	107.74	110.53
21	B	603	CLA	C2A-C1A-CHA	3.13	129.30	123.87
24	C	516	DGD	C3E-C4E-C5E	3.12	115.90	110.23
21	N	613	CLA	C3B-C4B-NB	-3.12	107.74	110.53
30	P	516	BCR	C33-C5-C6	-3.12	121.08	124.48
21	P	510	CLA	C1-C2-C3	-3.12	121.08	126.20
26	B	624	SQD	C45-O47-C7	-3.12	110.34	117.80
22	A	404	PHO	O2A-CGA-CBA	3.11	121.33	111.83
21	P	509	CLA	C3B-C4B-NB	-3.11	107.75	110.53
21	N	608	CLA	O1D-CGD-CBD	-3.11	118.39	124.52
21	P	504	CLA	C3B-C4B-NB	-3.11	107.76	110.53
21	G	402	CLA	C2A-C3A-C4A	3.10	106.88	101.87
21	P	503	CLA	C3B-C4B-NB	-3.10	107.76	110.53
30	B	618	BCR	C29-C30-C25	3.10	114.95	110.44
30	b	102	BCR	C31-C1-C2	3.10	120.85	108.95
21	Q	402	CLA	C2A-C3A-C4A	3.10	106.87	101.87
21	B	607	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
27	C	519	LMG	O6-C5-C6	3.09	114.10	106.44
21	N	620	CLA	C2A-C3A-C4A	3.09	106.86	101.87
21	B	616	CLA	C2A-C1A-CHA	3.09	129.23	123.87
27	A	410	LMG	O6-C5-C6	3.09	114.09	106.44
30	N	621	BCR	C15-C14-C13	-3.09	122.95	127.28
21	A	401	CLA	C2A-C3A-C4A	3.09	106.85	101.87
30	b	102	BCR	C11-C10-C9	-3.09	122.95	127.28
21	N	609	CLA	C2A-C3A-C4A	3.08	106.85	101.87
26	Q	408	SQD	C45-O47-C7	-3.08	110.42	117.80
26	G	410	SQD	C44-O6-C1	-3.08	107.19	113.80
21	B	615	CLA	C3B-C4B-NB	-3.08	107.78	110.53
21	G	404	CLA	C3B-C4B-NB	-3.08	107.78	110.53
24	C	516	DGD	C1E-O6E-C5E	3.08	119.73	113.72
24	P	518	DGD	O1G-C1A-C2A	3.08	121.22	111.83
30	C	514	BCR	C16-C17-C18	-3.08	122.96	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	606	CLA	C2A-C3A-C4A	3.07	106.83	101.87
30	c	101	BCR	C10-C11-C12	-3.07	114.31	123.20
30	J	102	BCR	C31-C1-C2	3.07	120.74	108.95
27	E	102	LMG	O6-C5-C6	3.07	114.04	106.44
21	Q	402	CLA	C3B-C4B-NB	-3.07	107.79	110.53
21	B	613	CLA	C2A-C3A-C4A	3.07	106.82	101.87
30	T	101	BCR	C15-C14-C13	-3.07	122.98	127.28
23	Q	405	PL9	C35-C34-C36	3.07	120.55	115.23
21	C	504	CLA	C3B-C4B-NB	-3.07	107.79	110.53
21	C	510	CLA	C2A-C3A-C4A	3.07	106.82	101.87
30	B	617	BCR	C15-C14-C13	-3.06	122.98	127.28
21	B	608	CLA	C3B-C4B-NB	-3.06	107.80	110.53
21	B	606	CLA	O1D-CGD-CBD	-3.06	118.48	124.52
21	N	618	CLA	O1D-CGD-CBD	-3.06	118.48	124.52
21	N	614	CLA	C3B-C4B-NB	-3.06	107.80	110.53
22	G	405	PHO	O2A-CGA-CBA	3.06	121.16	111.83
30	N	621	BCR	C29-C30-C25	3.06	114.88	110.44
21	P	507	CLA	C2A-C1A-CHA	3.05	129.17	123.87
27	C	519	LMG	O6-C1-O1	-3.05	102.84	110.04
21	P	510	CLA	C2A-C3A-C4A	3.05	106.79	101.87
21	N	608	CLA	C2A-C3A-C4A	3.05	106.79	101.87
30	B	618	BCR	C11-C10-C9	-3.05	123.01	127.28
21	P	513	CLA	C2A-C3A-C4A	3.05	106.79	101.87
21	B	604	CLA	C3B-C4B-NB	-3.04	107.81	110.53
21	C	510	CLA	C1-C2-C3	-3.04	121.21	126.20
27	C	519	LMG	O8-C28-C29	3.04	121.11	111.83
21	A	402	CLA	C3B-C4B-NB	-3.04	107.82	110.53
30	D	405	BCR	C33-C5-C6	-3.04	121.17	124.48
24	P	517	DGD	C3E-C4E-C5E	3.04	115.74	110.23
21	N	608	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
21	C	504	CLA	C2A-C3A-C4A	3.04	106.78	101.87
30	B	619	BCR	C33-C5-C6	-3.04	121.17	124.48
26	A	409	SQD	O8-S-C6	3.04	111.83	105.97
30	I	101	BCR	C15-C14-C13	-3.04	123.02	127.28
21	N	620	CLA	C2A-C1A-CHA	3.04	129.14	123.87
21	C	508	CLA	C1-C2-C3	-3.04	121.22	126.20
21	P	504	CLA	C2A-C3A-C4A	3.04	106.77	101.87
21	B	609	CLA	C1-C2-C3	-3.03	121.22	126.20
30	H	101	BCR	C10-C11-C12	-3.03	114.41	123.20
34	E	101	HEM	C3B-C2B-C1B	3.03	108.69	106.41
21	N	619	CLA	C3B-C4B-NB	-3.03	107.83	110.53
21	N	615	CLA	O1D-CGD-CBD	-3.03	118.54	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	404	PHO	O1D-CGD-CBD	-3.03	120.13	124.72
24	C	518	DGD	O1G-C1A-C2A	3.03	121.06	111.83
21	B	609	CLA	C2A-C3A-C4A	3.03	106.76	101.87
21	B	604	CLA	C2A-C3A-C4A	3.02	106.75	101.87
21	B	616	CLA	C3B-C4B-NB	-3.02	107.83	110.53
21	C	513	CLA	C2A-C3A-C4A	3.02	106.75	101.87
26	A	409	SQD	O9-S-C6	3.02	111.27	106.76
30	K	101	BCR	C10-C11-C12	-3.02	114.45	123.20
24	C	517	DGD	O1G-C1A-C2A	3.02	121.04	111.83
21	G	403	CLA	C3B-C4B-NB	-3.02	107.84	110.53
24	P	519	DGD	C3E-C4E-C5E	3.02	115.70	110.23
27	P	520	LMG	O6-C5-C6	3.01	113.90	106.44
21	B	608	CLA	C2A-C3A-C4A	3.01	106.73	101.87
21	B	605	CLA	C3B-C4B-NB	-3.01	107.84	110.53
30	T	102	BCR	C29-C30-C25	3.00	114.80	110.44
21	N	615	CLA	C2A-C3A-C4A	3.00	106.72	101.87
21	P	505	CLA	C2A-C3A-C4A	3.00	106.71	101.87
21	P	512	CLA	C2A-C3A-C4A	3.00	106.71	101.87
26	S	102	SQD	O8-S-C6	2.99	111.75	105.97
21	B	615	CLA	C2A-C3A-C4A	2.99	106.70	101.87
21	C	509	CLA	C2A-C3A-C4A	2.99	106.70	101.87
34	R	101	HEM	C3B-C2B-C1B	2.99	108.66	106.41
30	B	617	BCR	C38-C26-C25	-2.99	121.22	124.48
24	B	628	DGD	C3E-C4E-C5E	2.99	115.65	110.23
21	D	403	CLA	C2A-C3A-C4A	2.99	106.70	101.87
21	D	403	CLA	C1-C2-C3	-2.99	121.30	126.20
21	N	619	CLA	C1-C2-C3	-2.99	121.30	126.20
21	N	613	CLA	C2A-C3A-C4A	2.98	106.69	101.87
21	B	616	CLA	C2A-C3A-C4A	2.98	106.69	101.87
21	B	601	CLA	O2A-CGA-CBA	2.98	120.92	111.83
21	N	608	CLA	C3B-C4B-NB	-2.98	107.87	110.53
23	D	404	PL9	C37-C38-C39	-2.98	120.81	127.62
34	V	201	HEM	CHC-C4B-NB	2.97	127.62	124.42
30	W	101	BCR	C29-C30-C25	2.97	114.76	110.44
21	N	605	CLA	O2A-CGA-CBA	2.97	120.89	111.83
30	B	619	BCR	C29-C30-C25	2.97	114.75	110.44
21	P	509	CLA	C2A-C3A-C4A	2.97	106.67	101.87
30	a	101	BCR	C24-C23-C22	-2.97	121.84	126.23
30	P	515	BCR	C3-C4-C5	-2.97	108.76	114.06
21	C	512	CLA	C2A-C3A-C4A	2.97	106.67	101.87
21	N	610	CLA	C2A-C3A-C4A	2.97	106.66	101.87
30	T	103	BCR	C7-C8-C9	-2.97	121.84	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	520	LMG	O8-C28-C29	2.97	120.88	111.83
24	W	102	DGD	C1E-O6E-C5E	2.97	119.51	113.72
27	P	520	LMG	O6-C1-O1	-2.96	103.04	110.04
21	Q	404	CLA	C2A-C3A-C4A	2.96	106.66	101.87
21	C	503	CLA	C2A-C3A-C4A	2.96	106.65	101.87
30	W	101	BCR	C10-C11-C12	-2.96	114.62	123.20
21	P	501	CLA	C3B-C4B-NB	-2.96	107.89	110.53
21	C	507	CLA	C2A-C1A-CHA	2.96	129.01	123.87
30	b	102	BCR	C28-C27-C26	-2.96	108.78	114.06
21	D	401	CLA	C3B-C4B-NB	-2.96	107.89	110.53
30	B	619	BCR	C24-C23-C22	-2.96	121.86	126.23
24	G	408	DGD	C1D-O6D-C5D	2.96	119.50	113.72
24	P	519	DGD	O1G-C1A-C2A	2.96	120.85	111.83
21	B	601	CLA	C1-C2-C3	-2.96	121.35	126.20
30	S	101	BCR	C3-C4-C5	-2.96	108.78	114.06
21	B	611	CLA	C3B-C4B-NB	-2.96	107.89	110.53
21	C	507	CLA	C2A-C3A-C4A	2.96	106.64	101.87
21	N	620	CLA	C3B-C4B-NB	-2.95	107.89	110.53
30	N	621	BCR	C33-C5-C6	-2.95	121.26	124.48
27	N	623	LMG	C8-O7-C10	-2.95	110.73	117.80
21	N	612	CLA	C2A-C3A-C4A	2.95	106.64	101.87
21	Q	404	CLA	C1-C2-C3	-2.95	121.36	126.20
31	N	603	LMT	O1B-C4'-C3'	2.95	114.73	107.23
27	D	407	LMG	C8-O7-C10	-2.95	110.73	117.80
21	N	605	CLA	C2A-C3A-C4A	2.95	106.64	101.87
21	P	503	CLA	C2A-C3A-C4A	2.95	106.63	101.87
21	C	512	CLA	C2A-C1A-CHA	2.95	128.98	123.87
21	A	402	CLA	C2A-C1A-CHA	2.94	128.98	123.87
21	G	403	CLA	C2A-C1A-CHA	2.94	128.97	123.87
30	S	101	BCR	C29-C30-C25	2.94	114.71	110.44
30	B	619	BCR	C7-C8-C9	-2.94	121.89	126.23
21	B	616	CLA	O1D-CGD-CBD	-2.94	118.73	124.52
24	N	602	DGD	O1G-C1A-C2A	2.94	120.78	111.83
21	G	402	CLA	C1-C2-C3	-2.93	121.39	126.20
22	Q	403	PHO	C4-C3-C5	2.93	120.32	115.23
21	Q	404	CLA	O1D-CGD-CBD	-2.93	118.74	124.52
21	P	501	CLA	C2A-C1A-CHA	2.93	128.95	123.87
30	a	101	BCR	C15-C14-C13	-2.93	123.17	127.28
21	A	403	CLA	C2A-C3A-C4A	2.93	106.60	101.87
21	B	601	CLA	C2A-C3A-C4A	2.93	106.60	101.87
27	B	623	LMG	C8-O7-C10	-2.93	110.79	117.80
21	B	604	CLA	O2D-CGD-O1D	-2.92	118.16	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	403	CLA	C2A-C1A-CHA	2.92	128.94	123.87
24	C	518	DGD	C3E-C4E-C5E	2.92	115.53	110.23
21	B	611	CLA	C2A-C3A-C4A	2.92	106.59	101.87
21	C	501	CLA	C3B-C4B-NB	-2.92	107.92	110.53
21	C	501	CLA	C2A-C3A-C4A	2.92	106.58	101.87
21	N	619	CLA	C2A-C3A-C4A	2.92	106.58	101.87
21	N	619	CLA	C2A-C1A-CHA	2.92	128.93	123.87
21	A	401	CLA	C1-C2-C3	-2.92	121.42	126.20
23	G	407	PL9	C12-C13-C14	-2.92	120.95	127.62
21	C	508	CLA	O1D-CGD-CBD	-2.92	118.77	124.52
23	Q	405	PL9	C37-C38-C39	-2.92	120.95	127.62
24	C	517	DGD	O6D-C5D-C6D	2.92	112.47	106.69
21	P	501	CLA	C2A-C3A-C4A	2.91	106.58	101.87
34	E	101	HEM	C1B-NB-C4B	2.91	108.66	105.21
21	C	502	CLA	C2A-C3A-C4A	2.91	106.57	101.87
21	P	512	CLA	C2A-C1A-CHA	2.91	128.92	123.87
21	N	605	CLA	C1-C2-C3	-2.91	121.44	126.20
27	I	102	LMG	O6-C5-C6	2.91	113.64	106.44
21	P	508	CLA	C2A-C3A-C4A	2.90	106.56	101.87
21	B	601	CLA	O1D-CGD-CBD	-2.90	118.79	124.52
34	i	201	HEM	CHC-C4B-NB	2.90	127.55	124.42
23	G	407	PL9	C7-C3-C2	-2.90	119.97	123.39
21	C	503	CLA	C3B-C4B-NB	-2.90	107.94	110.53
26	F	101	SQD	O8-S-C6	2.90	111.57	105.97
21	Q	404	CLA	C2A-C1A-CHA	2.90	128.90	123.87
26	B	627	SQD	C1-C2-C3	-2.90	103.91	110.01
21	B	603	CLA	O1D-CGD-CBD	-2.90	118.81	124.52
21	N	616	CLA	O2A-CGA-CBA	2.90	120.67	111.83
30	C	515	BCR	C29-C30-C25	2.90	114.64	110.44
27	M	101	LMG	C7-O1-C1	-2.89	107.59	113.80
21	G	403	CLA	C1-C2-C3	-2.89	121.46	126.20
21	N	617	CLA	C2A-C3A-C4A	2.89	106.54	101.87
21	P	506	CLA	C2A-C3A-C4A	2.89	106.54	101.87
23	A	406	PL9	C12-C13-C14	-2.89	121.01	127.62
21	C	505	CLA	C2A-C3A-C4A	2.89	106.54	101.87
21	P	507	CLA	C2A-C3A-C4A	2.89	106.53	101.87
21	B	614	CLA	C2A-C3A-C4A	2.88	106.53	101.87
27	P	520	LMG	O1-C1-C2	2.88	112.65	108.27
21	P	502	CLA	C2A-C3A-C4A	2.88	106.53	101.87
21	P	511	CLA	C2A-C1A-CHA	2.88	128.87	123.87
30	J	102	BCR	C28-C27-C26	-2.88	108.92	114.06
30	C	514	BCR	C24-C23-C22	-2.88	121.97	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	511	CLA	C3B-C4B-NB	-2.88	107.96	110.53
21	C	508	CLA	C2A-C3A-C4A	2.88	106.52	101.87
27	A	410	LMG	O8-C28-C29	2.88	120.61	111.83
27	Q	407	LMG	C8-O7-C10	-2.88	110.91	117.80
21	N	611	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
21	G	404	CLA	C1-C2-C3	-2.88	121.48	126.20
30	B	619	BCR	C15-C14-C13	-2.87	123.25	127.28
21	Q	402	CLA	O2A-CGA-CBA	2.87	120.58	111.83
22	D	402	PHO	C4-C3-C5	2.87	120.21	115.23
30	N	621	BCR	C3-C4-C5	-2.87	108.94	114.06
21	B	615	CLA	C2A-C1A-CHA	2.87	128.84	123.87
21	C	512	CLA	O1D-CGD-CBD	-2.87	118.86	124.52
21	C	506	CLA	C2A-C3A-C4A	2.87	106.50	101.87
21	B	615	CLA	C1-C2-C3	-2.86	121.50	126.20
21	N	614	CLA	C2A-C3A-C4A	2.86	106.50	101.87
21	N	613	CLA	C2A-C1A-CHA	2.86	128.84	123.87
21	C	511	CLA	C2A-C1A-CHA	2.86	128.84	123.87
27	B	622	LMG	C7-O1-C1	-2.86	107.66	113.80
26	A	409	SQD	C44-O6-C1	-2.86	107.66	113.80
30	Z	101	BCR	C3-C4-C5	-2.86	108.95	114.06
34	R	101	HEM	C1B-NB-C4B	2.86	108.59	105.21
27	G	411	LMG	O6-C5-C6	2.86	113.52	106.44
30	D	405	BCR	C29-C30-C25	2.86	114.59	110.44
21	G	404	CLA	C2A-C3A-C4A	2.86	106.48	101.87
21	N	606	CLA	C2A-C1A-CHA	2.85	128.82	123.87
31	B	629	LMT	O1B-C4'-C3'	2.85	114.48	107.23
24	P	518	DGD	O6D-C5D-C6D	2.85	112.35	106.69
21	G	404	CLA	C2A-C1A-CHA	2.85	128.82	123.87
21	B	601	CLA	C2A-C1A-CHA	2.85	128.81	123.87
26	A	414	SQD	O9-S-C6	2.85	111.01	106.76
21	N	618	CLA	C2A-C3A-C4A	2.85	106.47	101.87
21	N	611	CLA	C2A-C1A-CHA	2.85	128.81	123.87
22	G	405	PHO	C4-C3-C5	2.85	120.17	115.23
27	a	102	LMG	O6-C5-C6	2.85	113.50	106.44
27	A	410	LMG	C8-O7-C10	-2.85	110.99	117.80
24	C	516	DGD	O1G-C1A-C2A	2.84	120.50	111.83
30	P	514	BCR	C28-C27-C26	-2.84	108.99	114.06
30	a	101	BCR	C3-C4-C5	-2.84	109.00	114.06
30	P	514	BCR	C24-C23-C22	-2.84	122.04	126.23
21	B	609	CLA	C2A-C1A-CHA	2.84	128.79	123.87
30	B	620	BCR	C15-C14-C13	-2.84	123.30	127.28
24	W	102	DGD	O1G-C1A-C2A	2.84	120.48	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	501	CLA	C2A-C1A-CHA	2.83	128.79	123.87
27	e	102	LMG	C7-O1-C1	-2.83	107.73	113.80
27	Q	406	LMG	O8-C28-C29	2.83	120.46	111.83
30	T	102	BCR	C2-C1-C6	2.83	114.55	110.44
30	B	620	BCR	C7-C8-C9	-2.83	122.06	126.23
21	C	506	CLA	C2A-C1A-CHA	2.83	128.77	123.87
30	T	103	BCR	C16-C17-C18	-2.82	123.32	127.28
21	A	401	CLA	O1D-CGD-CBD	-2.82	118.95	124.52
21	D	401	CLA	O2A-CGA-CBA	2.82	120.44	111.83
24	P	517	DGD	O1G-C1A-C2A	2.82	120.44	111.83
24	P	517	DGD	O5D-C1E-C2E	2.82	112.56	108.27
30	D	405	BCR	C3-C4-C5	-2.82	109.03	114.06
21	A	402	CLA	C1-C2-C3	-2.82	121.58	126.20
30	D	405	BCR	C24-C23-C22	-2.82	122.07	126.23
21	G	403	CLA	C2A-C3A-C4A	2.82	106.42	101.87
21	N	611	CLA	C2A-C3A-C4A	2.81	106.42	101.87
21	N	615	CLA	C3B-C4B-NB	-2.81	108.02	110.53
21	N	608	CLA	C1-C2-C3	-2.81	121.59	126.20
24	A	407	DGD	C1D-O6D-C5D	2.81	119.21	113.72
21	B	601	CLA	C3B-C4B-NB	-2.81	108.02	110.53
21	N	610	CLA	C2A-C1A-CHA	2.81	128.74	123.87
21	N	607	CLA	O1D-CGD-CBD	-2.81	118.98	124.52
30	P	516	BCR	C29-C30-C25	2.81	114.52	110.44
30	J	102	BCR	C11-C10-C9	-2.81	123.34	127.28
30	B	618	BCR	C21-C20-C19	-2.81	115.06	123.20
30	H	101	BCR	C29-C30-C25	2.81	114.52	110.44
30	c	101	BCR	C2-C1-C6	2.81	114.52	110.44
21	B	603	CLA	C2A-C3A-C4A	2.80	106.40	101.87
21	C	511	CLA	C2A-C3A-C4A	2.80	106.40	101.87
30	T	101	BCR	C38-C26-C25	-2.80	121.43	124.48
21	A	405	CLA	C2A-C1A-CHA	2.80	128.73	123.87
24	B	621	DGD	O1G-C1A-C2A	2.80	120.37	111.83
21	N	605	CLA	C3B-C4B-NB	-2.80	108.03	110.53
30	B	618	BCR	C2-C1-C6	2.80	114.50	110.44
21	A	405	CLA	O1D-CGD-CBD	-2.80	119.00	124.52
30	C	515	BCR	C15-C14-C13	-2.79	123.36	127.28
30	P	516	BCR	C15-C14-C13	-2.79	123.36	127.28
27	N	622	LMG	C9-C8-C7	-2.79	105.28	111.78
24	B	628	DGD	O1G-C1A-C2A	2.79	120.34	111.83
27	B	623	LMG	C7-O1-C1	-2.79	107.81	113.80
21	N	617	CLA	C2A-C1A-CHA	2.79	128.71	123.87
21	N	607	CLA	C2A-C3A-C4A	2.79	106.37	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	506	CLA	C2A-C1A-CHA	2.79	128.70	123.87
30	T	103	BCR	C15-C14-C13	-2.79	123.37	127.28
27	B	623	LMG	O1-C1-C2	2.78	112.50	108.27
26	A	409	SQD	C1-C2-C3	-2.78	104.16	110.01
21	G	406	CLA	C4-C3-C5	2.78	120.05	115.23
21	B	614	CLA	O1D-CGD-CBD	-2.78	119.04	124.52
30	T	102	BCR	C21-C20-C19	-2.78	115.15	123.20
27	N	623	LMG	C7-O1-C1	-2.78	107.85	113.80
30	B	617	BCR	C16-C17-C18	-2.77	123.39	127.28
21	A	402	CLA	C2A-C3A-C4A	2.77	106.35	101.87
21	B	607	CLA	C2A-C3A-C4A	2.77	106.35	101.87
26	A	414	SQD	O48-C23-C24	2.77	120.28	111.83
23	D	404	PL9	C7-C3-C2	-2.77	120.12	123.39
21	B	602	CLA	C2A-C1A-CHA	2.77	128.67	123.87
21	N	605	CLA	C2A-C1A-CHA	2.77	128.67	123.87
21	P	511	CLA	C2A-C3A-C4A	2.77	106.34	101.87
21	D	403	CLA	O1D-CGD-CBD	-2.77	119.06	124.52
30	P	516	BCR	C3-C4-C5	-2.77	109.12	114.06
21	B	610	CLA	C2A-C3A-C4A	2.77	106.34	101.87
30	T	101	BCR	C28-C27-C26	-2.77	109.12	114.06
23	A	406	PL9	C7-C3-C2	-2.77	120.13	123.39
21	B	607	CLA	C2A-C1A-CHA	2.77	128.67	123.87
21	N	618	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
30	T	102	BCR	C11-C10-C9	-2.76	123.40	127.28
24	G	408	DGD	O1G-C1A-C2A	2.76	120.26	111.83
21	B	613	CLA	C2A-C1A-CHA	2.76	128.66	123.87
26	G	401	SQD	O9-S-C6	2.76	110.88	106.76
27	G	411	LMG	C8-O7-C10	-2.76	111.19	117.80
21	N	612	CLA	O2A-CGA-CBA	2.76	120.25	111.83
27	N	623	LMG	O1-C1-C2	2.76	112.46	108.27
24	D	408	DGD	C1E-O6E-C5E	2.75	119.10	113.72
30	C	514	BCR	C28-C27-C26	-2.75	109.15	114.06
21	P	505	CLA	C2A-C1A-CHA	2.75	128.64	123.87
27	D	412	LMG	O6-C5-C6	2.75	113.26	106.44
21	G	403	CLA	CMD-C2D-C1D	2.75	129.57	124.73
27	D	406	LMG	O8-C28-C29	2.75	120.22	111.83
27	N	622	LMG	C8-O7-C10	-2.75	111.21	117.80
21	B	606	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
21	G	406	CLA	C1-C2-C3	-2.75	121.70	126.20
21	G	406	CLA	C2A-C1A-CHA	2.75	128.63	123.87
27	B	623	LMG	O6-C1-O1	-2.74	103.56	110.04
21	B	602	CLA	C2A-C3A-C4A	2.74	106.30	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	402	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
21	N	608	CLA	O2A-CGA-CBA	2.74	120.19	111.83
24	A	407	DGD	O1G-C1A-C2A	2.74	120.19	111.83
21	B	604	CLA	C1-C2-C3	-2.74	121.72	126.20
30	N	621	BCR	C7-C8-C9	-2.73	122.19	126.23
21	C	509	CLA	C2A-C1A-CHA	2.73	128.61	123.87
24	B	621	DGD	C1E-O6E-C5E	2.73	119.06	113.72
30	B	619	BCR	C3-C4-C5	-2.73	109.18	114.06
21	G	406	CLA	C2A-C3A-C4A	2.73	106.28	101.87
23	Q	405	PL9	C12-C13-C14	-2.73	121.37	127.62
21	P	509	CLA	C2A-C1A-CHA	2.73	128.61	123.87
30	B	618	BCR	C35-C13-C12	2.73	122.26	118.09
21	P	506	CLA	O2A-CGA-CBA	2.73	120.16	111.83
21	G	403	CLA	O1D-CGD-CBD	-2.73	119.14	124.52
21	B	608	CLA	C2A-C1A-CHA	2.73	128.60	123.87
30	K	101	BCR	C15-C14-C13	-2.73	123.45	127.28
21	C	506	CLA	C1-C2-C3	-2.73	121.73	126.20
21	N	606	CLA	C2A-C3A-C4A	2.73	106.27	101.87
21	C	505	CLA	C2A-C1A-CHA	2.72	128.59	123.87
21	P	511	CLA	O2A-CGA-CBA	2.72	120.14	111.83
21	C	509	CLA	C1-C2-C3	-2.72	121.74	126.20
21	B	602	CLA	C1-C2-C3	-2.72	121.74	126.20
24	P	517	DGD	C3G-O3G-C1D	-2.72	107.96	113.80
21	B	604	CLA	O2A-CGA-CBA	2.72	120.12	111.83
26	G	410	SQD	C1-C2-C3	-2.72	104.30	110.01
34	E	101	HEM	CHB-C1B-NB	2.71	127.72	124.37
22	D	402	PHO	O2A-CGA-CBA	2.71	120.08	111.83
21	A	402	CLA	CMD-C2D-C1D	2.70	129.49	124.73
30	S	101	BCR	C38-C26-C25	-2.69	121.55	124.48
21	A	403	CLA	C2A-C1A-CHA	2.69	128.54	123.87
21	B	612	CLA	O2A-CGA-CBA	2.68	120.01	111.83
21	D	401	CLA	C2A-C1A-CHA	2.68	128.51	123.87
23	A	406	PL9	C20-C19-C21	2.68	119.88	115.23
21	A	405	CLA	C2A-C3A-C4A	2.68	106.19	101.87
26	G	401	SQD	O48-C23-C24	2.67	119.99	111.83
27	G	411	LMG	O8-C28-C29	2.67	119.99	111.83
21	C	508	CLA	C2A-C1A-CHA	2.67	128.50	123.87
34	i	201	HEM	CHA-C4D-ND	2.67	127.67	124.37
21	P	503	CLA	C1-C2-C3	-2.67	121.82	126.20
30	D	405	BCR	C38-C26-C25	-2.67	121.57	124.48
24	B	628	DGD	O5D-C6D-C5D	2.67	115.43	109.42
27	C	519	LMG	O1-C1-C2	2.67	112.32	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	514	BCR	C38-C26-C25	-2.67	121.58	124.48
21	B	606	CLA	C4-C3-C5	2.66	119.85	115.23
22	D	402	PHO	CMA-C3A-C4A	-2.66	108.88	114.61
21	B	612	CLA	C2A-C1A-CHA	2.66	128.48	123.87
31	Q	410	LMT	C1B-O1B-C4'	-2.66	111.68	117.98
21	Q	402	CLA	C2A-C1A-CHA	2.66	128.47	123.87
21	B	610	CLA	O1D-CGD-CBD	-2.66	119.28	124.52
21	B	614	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
27	B	622	LMG	C9-C8-C7	-2.65	105.60	111.78
21	N	616	CLA	C2B-C1B-NB	-2.65	107.58	110.33
30	B	619	BCR	C2-C1-C6	2.65	114.28	110.44
21	N	610	CLA	C4-C3-C5	2.65	119.82	115.23
21	P	506	CLA	C1-C2-C3	-2.65	121.86	126.20
21	C	506	CLA	O2A-CGA-CBA	2.65	119.90	111.83
21	B	610	CLA	C2A-C1A-CHA	2.64	128.46	123.87
21	N	612	CLA	C2A-C1A-CHA	2.64	128.46	123.87
21	P	508	CLA	C2A-C1A-CHA	2.64	128.45	123.87
34	R	101	HEM	CHB-C1B-NB	2.64	127.63	124.37
21	C	503	CLA	O1D-CGD-CBD	-2.64	119.32	124.52
26	Q	408	SQD	O9-S-C6	2.64	110.69	106.76
26	G	410	SQD	O8-S-C6	2.64	111.06	105.97
23	D	404	PL9	C12-C13-C14	-2.64	121.59	127.62
21	C	501	CLA	C1-C2-C3	-2.63	121.88	126.20
21	B	608	CLA	O2A-CGA-CBA	2.63	119.86	111.83
21	P	503	CLA	O1D-CGD-CBD	-2.63	119.33	124.52
21	N	619	CLA	O2A-CGA-CBA	2.63	119.85	111.83
21	B	611	CLA	C2A-C1A-CHA	2.63	128.43	123.87
21	B	605	CLA	C1-C2-C3	-2.63	121.89	126.20
24	N	602	DGD	O5D-C1E-C2E	2.62	112.26	108.27
30	T	101	BCR	C16-C17-C18	-2.62	123.60	127.28
21	N	605	CLA	O1D-CGD-CBD	-2.62	119.34	124.52
24	B	628	DGD	O5D-C1E-C2E	2.62	112.25	108.27
21	B	604	CLA	C2B-C1B-NB	-2.62	107.61	110.33
27	Q	401	LMG	O6-C5-C6	2.62	112.93	106.44
21	G	402	CLA	C4-C3-C5	2.62	119.77	115.23
21	B	606	CLA	C2A-C1A-CHA	2.62	128.41	123.87
27	P	520	LMG	C8-O7-C10	-2.62	111.54	117.80
30	Z	101	BCR	C20-C21-C22	-2.62	123.61	127.28
24	P	518	DGD	C3E-C4E-C5E	2.61	114.97	110.23
21	P	509	CLA	C1-C2-C3	-2.61	121.92	126.20
34	E	101	HEM	CBA-CAA-C2A	-2.61	105.31	112.53
22	Q	403	PHO	O2A-CGA-CBA	2.61	119.80	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	510	CLA	O2A-CGA-CBA	2.61	119.79	111.83
21	N	607	CLA	O2A-CGA-CBA	2.61	119.78	111.83
22	A	404	PHO	CAA-C2A-C3A	-2.61	105.95	113.00
21	P	502	CLA	C2A-C1A-CHA	2.61	128.39	123.87
30	c	101	BCR	C15-C14-C13	-2.60	123.62	127.28
22	G	405	PHO	C1-C2-C3	-2.60	121.93	126.20
21	C	513	CLA	O2A-CGA-CBA	2.60	119.77	111.83
21	B	604	CLA	C2A-C1A-CHA	2.60	128.38	123.87
21	P	510	CLA	C4-C3-C5	2.60	119.74	115.23
27	C	519	LMG	C8-O7-C10	-2.60	111.58	117.80
22	D	402	PHO	O1D-CGD-CBD	-2.60	120.79	124.72
30	I	101	BCR	C24-C23-C22	-2.60	122.40	126.23
26	Q	408	SQD	C1-C2-C3	-2.59	104.55	110.01
21	N	611	CLA	O2A-CGA-CBA	2.59	119.75	111.83
21	N	620	CLA	O1D-CGD-CBD	-2.59	119.40	124.52
30	J	102	BCR	C35-C13-C14	-2.59	118.61	122.82
21	B	601	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
21	Q	404	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
21	D	403	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
23	J	101	PL9	C12-C13-C14	-2.59	121.69	127.62
30	C	515	BCR	C3-C4-C5	-2.59	109.44	114.06
21	P	501	CLA	C1-C2-C3	-2.59	121.96	126.20
21	G	404	CLA	C4-C3-C5	2.59	119.72	115.23
23	J	101	PL9	C20-C19-C21	2.59	119.72	115.23
21	N	609	CLA	C2A-C1A-CHA	2.58	128.35	123.87
21	B	614	CLA	C2A-C1A-CHA	2.58	128.35	123.87
22	A	404	PHO	C4D-CHA-CBD	2.58	109.69	108.45
21	N	609	CLA	C1-C2-C3	-2.58	121.97	126.20
22	Q	403	PHO	CMA-C3A-C4A	-2.58	109.05	114.61
21	G	406	CLA	O1D-CGD-CBD	-2.58	119.43	124.52
21	C	510	CLA	C4-C3-C5	2.58	119.71	115.23
27	Q	407	LMG	O8-C28-C29	2.58	119.70	111.83
30	N	621	BCR	C28-C27-C26	-2.58	109.46	114.06
30	P	515	BCR	C28-C27-C26	-2.58	109.46	114.06
21	B	606	CLA	O2A-CGA-CBA	2.58	119.70	111.83
27	B	622	LMG	C8-O7-C10	-2.58	111.63	117.80
21	C	510	CLA	C2B-C1B-NB	-2.58	107.66	110.33
21	C	501	CLA	O2A-CGA-CBA	2.57	119.69	111.83
21	P	513	CLA	O2A-CGA-CBA	2.57	119.69	111.83
24	C	517	DGD	C3E-C4E-C5E	2.57	114.90	110.23
21	N	614	CLA	C2A-C1A-CHA	2.57	128.32	123.87
26	N	601	SQD	C3-C4-C5	2.57	114.89	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	T	101	BCR	C3-C4-C5	-2.57	109.48	114.06
21	N	606	CLA	C1-C2-C3	-2.57	121.99	126.20
21	P	510	CLA	C2A-C1A-CHA	2.56	128.32	123.87
21	N	615	CLA	C2A-C1A-CHA	2.56	128.31	123.87
21	C	503	CLA	C2A-C1A-CHA	2.56	128.31	123.87
21	N	608	CLA	C2A-C1A-CHA	2.56	128.31	123.87
21	P	505	CLA	C1-C2-C3	-2.56	122.00	126.20
23	D	404	PL9	C7-C8-C9	-2.56	122.42	126.83
21	C	504	CLA	C2A-C1A-CHA	2.56	128.31	123.87
25	A	411	LHG	O8-C23-C24	2.55	119.62	111.83
24	D	408	DGD	O1G-C1A-C2A	2.55	119.61	111.83
21	P	501	CLA	O2A-CGA-CBA	2.55	119.61	111.83
21	N	616	CLA	C2A-C1A-CHA	2.55	128.29	123.87
30	N	621	BCR	C38-C26-C25	-2.55	121.70	124.48
21	P	503	CLA	C2A-C1A-CHA	2.55	128.29	123.87
23	D	404	PL9	C42-C43-C44	-2.55	121.79	127.62
21	B	615	CLA	O2A-CGA-CBA	2.55	119.60	111.83
23	b	101	PL9	C12-C13-C14	-2.55	121.79	127.62
21	Q	404	CLA	O2A-CGA-CBA	2.55	119.60	111.83
21	B	611	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
21	B	603	CLA	O2A-CGA-CBA	2.54	119.59	111.83
27	D	407	LMG	O8-C28-C29	2.54	119.58	111.83
26	B	624	SQD	O9-S-C6	2.54	110.55	106.76
22	G	405	PHO	CAA-C2A-C3A	-2.54	106.14	113.00
21	A	403	CLA	C1-C2-C3	-2.54	122.04	126.20
21	C	505	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
21	A	405	CLA	C4-C3-C5	2.54	119.64	115.23
21	C	502	CLA	C2A-C1A-CHA	2.54	128.27	123.87
30	B	619	BCR	C38-C26-C25	-2.54	121.71	124.48
21	B	603	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
30	B	617	BCR	C28-C27-C26	-2.54	109.53	114.06
23	G	407	PL9	C20-C19-C21	2.54	119.63	115.23
24	C	516	DGD	O5D-C1E-C2E	2.54	112.12	108.27
30	c	101	BCR	C29-C30-C25	2.54	114.12	110.44
22	G	405	PHO	CMA-C3A-C4A	-2.54	109.15	114.61
31	D	409	LMT	C1B-O1B-C4'	-2.54	111.97	117.98
21	N	618	CLA	C2A-C1A-CHA	2.53	128.26	123.87
23	D	404	PL9	C32-C33-C34	-2.53	121.83	127.62
23	A	406	PL9	C30-C29-C31	2.53	119.62	115.23
21	B	609	CLA	O2A-CGA-CBA	2.53	119.54	111.83
30	B	620	BCR	C28-C27-C26	-2.53	109.55	114.06
25	G	412	LHG	O8-C23-C24	2.53	119.54	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	620	BCR	C16-C17-C18	-2.53	123.74	127.28
21	B	609	CLA	CED-O2D-CGD	2.52	121.64	115.92
22	A	404	PHO	CMA-C3A-C4A	-2.52	109.17	114.61
21	B	612	CLA	C2B-C1B-NB	-2.52	107.71	110.33
21	P	513	CLA	C1-C2-C3	-2.52	122.06	126.20
24	N	602	DGD	O5D-C6D-C5D	2.52	115.10	109.42
24	A	407	DGD	C3E-C4E-C5E	2.52	114.80	110.23
27	C	520	LMG	O1-C1-C2	2.52	112.10	108.27
21	C	511	CLA	C4-C3-C5	2.52	119.60	115.23
27	D	406	LMG	C8-O7-C10	-2.52	111.77	117.80
27	N	623	LMG	O6-C5-C6	2.52	112.68	106.44
21	N	617	CLA	O2A-CGA-CBA	2.52	119.51	111.83
21	N	620	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
30	Z	101	BCR	C28-C27-C26	-2.52	109.57	114.06
22	A	404	PHO	C4-C3-C5	2.51	119.59	115.23
23	b	101	PL9	C22-C23-C24	-2.51	121.87	127.62
21	A	403	CLA	C4-C3-C5	2.51	119.59	115.23
21	D	403	CLA	O2A-CGA-CBA	2.51	119.49	111.83
21	N	615	CLA	C2B-C1B-NB	-2.51	107.72	110.33
26	N	601	SQD	C1-O5-C5	-2.51	108.82	113.72
23	Q	405	PL9	C42-C43-C44	-2.51	121.88	127.62
24	G	408	DGD	C3E-C4E-C5E	2.50	114.77	110.23
30	T	102	BCR	C35-C13-C12	2.50	121.91	118.09
24	B	628	DGD	C3D-C4D-C5D	2.50	114.77	110.23
21	B	613	CLA	C2B-C1B-NB	-2.50	107.73	110.33
21	A	401	CLA	C4-C3-C5	2.50	119.57	115.23
21	B	616	CLA	O2A-CGA-CBA	2.50	119.46	111.83
21	G	404	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
30	B	617	BCR	C3-C4-C5	-2.50	109.60	114.06
24	Q	409	DGD	O1G-C1A-C2A	2.50	119.46	111.83
30	K	101	BCR	C29-C30-C25	2.50	114.07	110.44
21	N	620	CLA	O2A-CGA-CBA	2.50	119.44	111.83
30	N	621	BCR	C2-C1-C6	2.49	114.06	110.44
22	Q	403	PHO	O1D-CGD-CBD	-2.49	120.94	124.72
27	D	412	LMG	C8-O7-C10	-2.49	111.83	117.80
21	C	510	CLA	C2A-C1A-CHA	2.49	128.19	123.87
21	N	607	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
21	C	503	CLA	C1-C2-C3	-2.49	122.12	126.20
21	P	511	CLA	C4-C3-C5	2.49	119.55	115.23
30	I	101	BCR	C16-C17-C18	-2.49	123.79	127.28
24	N	602	DGD	C3D-C4D-C5D	2.48	114.73	110.23
21	B	602	CLA	O1D-CGD-CBD	-2.48	119.62	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	405	PL9	C7-C8-C9	-2.48	122.55	126.83
23	Q	405	PL9	C32-C33-C34	-2.48	121.94	127.62
26	B	624	SQD	C1-C2-C3	-2.48	104.79	110.01
23	J	101	PL9	C22-C23-C24	-2.48	121.94	127.62
21	B	605	CLA	C2A-C1A-CHA	2.48	128.17	123.87
21	N	605	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
24	C	516	DGD	C3G-O3G-C1D	-2.48	108.48	113.80
30	a	101	BCR	C20-C21-C22	-2.48	123.80	127.28
21	N	618	CLA	O2A-CGA-CBA	2.48	119.38	111.83
31	M	102	LMT	C1B-O1B-C4'	-2.47	112.11	117.98
30	b	102	BCR	C35-C13-C14	-2.47	118.81	122.82
21	B	611	CLA	C2B-C1B-NB	-2.47	107.76	110.33
27	I	102	LMG	O8-C28-C29	2.47	119.37	111.83
21	B	614	CLA	O2A-CGA-CBA	2.47	119.36	111.83
22	G	405	PHO	C4D-CHA-CBD	2.47	109.64	108.45
21	N	610	CLA	O2A-CGA-CBA	2.47	119.36	111.83
21	A	405	CLA	O2A-CGA-CBA	2.47	119.36	111.83
21	Q	402	CLA	C4-C3-C5	2.46	119.51	115.23
30	Z	101	BCR	C10-C11-C12	-2.46	116.06	123.20
21	N	612	CLA	C1-C2-C3	-2.46	122.16	126.20
21	C	511	CLA	O2A-CGA-CBA	2.46	119.34	111.83
21	A	403	CLA	O1D-CGD-CBD	-2.46	119.66	124.52
23	A	406	PL9	C15-C14-C16	2.46	119.50	115.23
21	G	406	CLA	O2A-CGA-CBA	2.46	119.33	111.83
21	C	506	CLA	CHB-C1B-NB	2.46	127.74	124.05
21	G	402	CLA	O2A-CGA-CBA	2.46	119.33	111.83
21	C	509	CLA	O2A-CGA-CBA	2.46	119.33	111.83
30	b	102	BCR	C33-C5-C6	-2.46	121.80	124.48
21	A	401	CLA	CHB-C1B-NB	2.46	127.73	124.05
30	C	515	BCR	C2-C1-C6	2.45	114.00	110.44
21	D	403	CLA	C4D-CHA-C1A	2.45	124.17	121.24
26	B	627	SQD	C1-O5-C5	-2.45	108.93	113.72
21	D	401	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
21	P	512	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
21	N	609	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
21	B	613	CLA	O2A-CGA-CBA	2.45	119.30	111.83
21	C	513	CLA	C2A-C1A-CHA	2.45	128.11	123.87
30	T	101	BCR	C24-C23-C22	-2.45	122.62	126.23
30	B	617	BCR	C11-C10-C9	-2.44	123.85	127.28
21	C	505	CLA	C2B-C1B-NB	-2.44	107.80	110.33
27	e	102	LMG	C8-O7-C10	-2.44	111.96	117.80
21	P	504	CLA	C2A-C1A-CHA	2.44	128.10	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	618	BCR	C4-C5-C6	-2.44	119.41	122.70
21	A	405	CLA	C1-C2-C3	-2.44	122.20	126.20
27	e	102	LMG	O8-C28-C29	2.44	119.27	111.83
21	C	505	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
23	b	101	PL9	C20-C19-C21	2.44	119.46	115.23
30	H	101	BCR	C3-C4-C5	-2.43	109.72	114.06
21	N	619	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
21	N	609	CLA	C4-C3-C5	2.43	119.45	115.23
30	P	514	BCR	C35-C13-C12	2.43	121.80	118.09
30	P	514	BCR	C38-C26-C25	-2.43	121.83	124.48
30	B	619	BCR	C28-C27-C26	-2.43	109.73	114.06
30	T	102	BCR	C4-C5-C6	-2.43	119.43	122.70
27	P	521	LMG	O6-C5-C6	2.42	112.45	106.44
21	B	601	CLA	C2B-C1B-NB	-2.42	107.81	110.33
27	N	623	LMG	O6-C1-O1	-2.42	104.32	110.04
21	P	510	CLA	C2B-C1B-NB	-2.42	107.81	110.33
30	D	405	BCR	C21-C20-C19	-2.42	116.19	123.20
21	N	605	CLA	C2B-C1B-NB	-2.42	107.82	110.33
23	b	101	PL9	C15-C14-C16	2.42	119.43	115.23
24	D	408	DGD	O5D-C1E-C2E	-2.42	104.60	108.27
21	N	608	CLA	C2B-C1B-NB	-2.42	107.82	110.33
30	C	515	BCR	C21-C20-C19	-2.42	116.19	123.20
21	N	619	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
21	C	508	CLA	O2A-CGA-CBA	2.42	119.20	111.83
21	C	501	CLA	C2B-C1B-NB	-2.41	107.82	110.33
21	P	508	CLA	O2A-CGA-CBA	2.41	119.19	111.83
27	E	102	LMG	O8-C28-C29	2.41	119.19	111.83
30	B	618	BCR	C30-C25-C24	2.41	122.19	115.65
26	A	409	SQD	O48-C23-C24	2.41	119.18	111.83
27	C	520	LMG	O6-C5-C6	2.41	112.41	106.44
27	B	623	LMG	O8-C28-C29	2.41	119.18	111.83
26	B	624	SQD	O48-C23-C24	2.41	119.17	111.83
21	C	513	CLA	C1-C2-C3	-2.40	122.26	126.20
21	P	502	CLA	C2B-C1B-NB	-2.40	107.83	110.33
21	B	616	CLA	C1-C2-C3	-2.40	122.26	126.20
21	B	606	CLA	C1-C2-C3	-2.40	122.26	126.20
27	M	101	LMG	C8-O7-C10	-2.40	112.05	117.80
23	D	404	PL9	C40-C39-C41	2.40	119.39	115.23
21	P	505	CLA	O2A-CGA-CBA	2.40	119.15	111.83
21	B	615	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
21	C	511	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
21	N	618	CLA	C4-C3-C5	2.39	119.38	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	407	PL9	C17-C18-C19	-2.39	122.14	127.62
21	B	608	CLA	C1-C2-C3	-2.39	122.28	126.20
21	B	606	CLA	CHB-C1B-NB	2.39	127.64	124.05
21	C	502	CLA	C1-C2-C3	-2.39	122.28	126.20
21	C	511	CLA	C1-C2-C3	-2.39	122.28	126.20
27	Q	406	LMG	C8-O7-C10	-2.39	112.08	117.80
30	C	514	BCR	C29-C30-C25	2.39	113.91	110.44
21	P	509	CLA	O2A-CGA-CBA	2.39	119.12	111.83
30	P	515	BCR	C10-C11-C12	-2.39	116.28	123.20
21	G	402	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
30	W	101	BCR	C16-C17-C18	-2.39	123.93	127.28
30	S	101	BCR	C21-C20-C19	-2.39	116.28	123.20
21	C	505	CLA	O2A-CGA-CBA	2.39	119.11	111.83
30	S	101	BCR	C37-C22-C23	2.38	121.73	118.09
21	N	613	CLA	O2A-CGA-CBA	2.38	119.11	111.83
21	B	602	CLA	CHB-C1B-NB	2.38	127.62	124.05
21	C	510	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
22	Q	403	PHO	CBC-CAC-C3C	-2.38	109.46	112.87
21	B	616	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
21	N	614	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
21	C	502	CLA	C2B-C1B-NB	-2.38	107.86	110.33
21	P	503	CLA	C2B-C1B-NB	-2.38	107.86	110.33
27	N	623	LMG	O8-C28-C29	2.38	119.09	111.83
30	B	618	BCR	C15-C16-C17	-2.38	118.66	123.52
21	C	503	CLA	O2A-CGA-CBA	2.38	119.08	111.83
21	C	513	CLA	O1D-CGD-CBD	-2.37	119.83	124.52
30	C	515	BCR	C30-C25-C24	2.37	122.09	115.65
21	P	505	CLA	C2B-C1B-NB	-2.37	107.86	110.33
26	Q	408	SQD	O48-C23-C24	2.37	119.07	111.83
21	G	402	CLA	C2A-C1A-CHA	2.37	127.98	123.87
27	e	102	LMG	O6-C5-C6	2.37	112.32	106.44
30	P	515	BCR	C20-C21-C22	-2.37	123.95	127.28
27	R	102	LMG	O8-C28-C29	2.37	119.07	111.83
30	J	102	BCR	C33-C5-C6	-2.37	121.90	124.48
21	B	605	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
21	C	508	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
23	A	406	PL9	C17-C18-C19	-2.37	122.20	127.62
21	P	511	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
23	A	406	PL9	C27-C28-C29	-2.37	122.20	127.62
21	C	502	CLA	O2A-CGA-CBA	2.37	119.06	111.83
21	P	506	CLA	CHB-C1B-NB	2.37	127.60	124.05
21	A	401	CLA	O2A-CGA-CBA	2.37	119.06	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	613	CLA	CED-O2D-CGD	2.37	121.29	115.92
21	Q	404	CLA	C4D-CHA-C1A	2.37	124.07	121.24
30	P	516	BCR	C2-C1-C6	2.37	113.88	110.44
23	D	404	PL9	C36-C34-C33	-2.37	115.86	121.17
21	C	509	CLA	CHB-C1B-NB	2.36	127.60	124.05
23	Q	405	PL9	C17-C18-C19	-2.36	122.21	127.62
21	D	401	CLA	C4-C3-C5	2.36	119.33	115.23
21	G	403	CLA	CHB-C1B-NB	2.36	127.59	124.05
21	C	509	CLA	C4D-CHA-C1A	2.36	124.06	121.24
34	R	101	HEM	CBA-CAA-C2A	-2.36	106.00	112.53
21	C	505	CLA	C1-C2-C3	-2.36	122.33	126.20
34	V	201	HEM	CHA-C4D-ND	2.36	127.28	124.37
21	N	606	CLA	CHB-C1B-NB	2.36	127.59	124.05
30	T	101	BCR	C11-C10-C9	-2.36	123.97	127.28
21	N	610	CLA	CHB-C1B-NB	2.36	127.58	124.05
27	a	102	LMG	O8-C28-C29	2.35	119.02	111.83
23	D	404	PL9	C45-C44-C43	-2.35	117.58	123.63
30	S	101	BCR	C11-C10-C9	-2.35	123.98	127.28
21	N	606	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
23	G	407	PL9	C30-C29-C31	2.35	119.31	115.23
26	B	627	SQD	O5-C1-O6	2.35	115.59	110.04
23	Q	405	PL9	C36-C34-C33	-2.35	115.90	121.17
21	P	503	CLA	O2A-CGA-CBA	2.35	118.99	111.83
23	G	407	PL9	C15-C14-C16	2.35	119.30	115.23
21	P	513	CLA	C2A-C1A-CHA	2.35	127.94	123.87
21	P	502	CLA	O2A-CGA-CBA	2.34	118.98	111.83
23	Q	405	PL9	C20-C19-C21	2.34	119.30	115.23
23	J	101	PL9	C15-C14-C16	2.34	119.29	115.23
27	B	623	LMG	O6-C5-C6	2.34	112.24	106.44
21	C	510	CLA	O2A-CGA-CBA	2.34	118.98	111.83
24	P	518	DGD	C3G-C2G-C1G	-2.34	106.33	111.78
21	P	513	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
21	B	615	CLA	C4D-CHA-C1A	2.34	124.03	121.24
30	B	619	BCR	C16-C17-C18	-2.34	124.00	127.28
22	A	404	PHO	CBC-CAC-C3C	-2.34	109.53	112.87
31	e	101	LMT	C1B-O1B-C4'	-2.33	112.44	117.98
30	I	101	BCR	C28-C27-C26	-2.33	109.89	114.06
21	B	607	CLA	O2A-CGA-CBA	2.33	118.95	111.83
30	T	103	BCR	C28-C27-C26	-2.33	109.89	114.06
21	C	503	CLA	C4-C3-C5	2.33	119.28	115.23
21	C	509	CLA	C2B-C1B-NB	-2.33	107.91	110.33
23	G	407	PL9	C27-C28-C29	-2.33	122.29	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	518	DGD	C6E-C5E-C4E	-2.33	107.30	113.02
21	B	609	CLA	C2B-C1B-NB	-2.33	107.91	110.33
21	G	402	CLA	CHB-C1B-NB	2.33	127.54	124.05
30	T	102	BCR	C30-C25-C24	2.33	121.96	115.65
30	T	102	BCR	C36-C18-C19	2.32	121.64	118.09
21	N	607	CLA	CHB-C1B-NB	2.32	127.54	124.05
21	N	615	CLA	O2D-CGD-O1D	-2.32	119.32	123.85
27	Q	401	LMG	O8-C28-C29	2.32	118.92	111.83
21	Q	402	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
22	D	402	PHO	CBC-CAC-C3C	-2.32	109.55	112.87
21	P	511	CLA	C1-C2-C3	-2.32	122.39	126.20
21	C	506	CLA	C2B-C1B-NB	-2.32	107.92	110.33
21	P	501	CLA	C2B-C1B-NB	-2.32	107.92	110.33
30	D	405	BCR	C37-C22-C23	2.32	121.63	118.09
30	c	101	BCR	C1-C6-C5	-2.32	119.47	122.64
30	K	101	BCR	C1-C6-C5	-2.31	119.47	122.64
22	Q	403	PHO	CAA-C2A-C3A	-2.31	106.75	113.00
30	P	514	BCR	C21-C20-C19	-2.31	116.50	123.20
21	N	612	CLA	CHB-C1B-NB	2.31	127.52	124.05
30	D	405	BCR	C11-C10-C9	-2.31	124.04	127.28
30	a	101	BCR	C7-C8-C9	-2.31	122.82	126.23
30	P	514	BCR	C29-C30-C25	2.31	113.79	110.44
21	D	403	CLA	CHB-C1B-NB	2.31	127.51	124.05
30	B	617	BCR	C24-C23-C22	-2.31	122.82	126.23
21	A	405	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
21	N	617	CLA	C2B-C1B-NB	-2.31	107.94	110.33
21	C	512	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
24	C	518	DGD	O6E-C1E-O5D	2.30	115.49	110.04
21	A	401	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
21	B	612	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
21	B	603	CLA	C4-C3-C5	2.30	119.22	115.23
27	Q	401	LMG	C8-O7-C10	-2.30	112.29	117.80
21	P	503	CLA	C4-C3-C5	2.30	119.22	115.23
21	C	506	CLA	C4D-CHA-C1A	2.30	123.99	121.24
21	A	402	CLA	O2A-CGA-CBA	2.30	118.85	111.83
21	N	613	CLA	C2B-C1B-NB	-2.30	107.94	110.33
21	P	504	CLA	C2B-C1B-NB	-2.30	107.94	110.33
27	P	521	LMG	O1-C1-C2	2.30	111.76	108.27
26	G	410	SQD	O48-C23-C24	2.30	118.84	111.83
26	N	601	SQD	C44-O6-C1	-2.30	108.87	113.80
30	H	101	BCR	C28-C27-C26	-2.29	109.96	114.06
21	N	612	CLA	C2B-C1B-NB	-2.29	107.95	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	520	LMG	O8-C28-O10	-2.29	117.89	123.63
30	I	101	BCR	C2-C1-C6	2.29	113.77	110.44
21	A	402	CLA	CHB-C1B-NB	2.29	127.49	124.05
21	B	603	CLA	CHB-C1B-NB	2.29	127.49	124.05
30	H	101	BCR	C21-C20-C19	-2.29	116.55	123.20
21	N	607	CLA	C1-O2A-CGA	2.29	122.20	116.65
21	B	610	CLA	O2A-CGA-CBA	2.29	118.82	111.83
23	Q	405	PL9	C45-C44-C43	-2.29	117.75	123.63
21	P	505	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
23	J	101	PL9	C7-C8-C9	-2.28	122.90	126.83
21	B	605	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
27	D	412	LMG	O8-C28-C29	2.28	118.79	111.83
21	A	405	CLA	CHB-C1B-NB	2.28	127.47	124.05
21	B	605	CLA	C4-C3-C5	2.28	119.19	115.23
21	B	616	CLA	C2B-C1B-NB	-2.28	107.96	110.33
21	Q	402	CLA	CHB-C1B-NB	2.28	127.47	124.05
21	N	609	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
21	N	619	CLA	C4-C3-C5	2.28	119.18	115.23
26	N	601	SQD	O5-C1-O6	2.28	115.43	110.04
26	B	627	SQD	C3-C4-C5	2.28	114.36	110.23
30	a	101	BCR	C28-C27-C26	-2.28	110.00	114.06
24	C	517	DGD	C3G-C2G-C1G	-2.28	106.48	111.78
21	P	509	CLA	C4D-CHA-C1A	2.28	123.96	121.24
21	C	506	CLA	C4-C3-C5	2.28	119.18	115.23
21	P	508	CLA	CHB-C1B-NB	2.28	127.46	124.05
21	P	506	CLA	CED-O2D-CGD	2.27	121.07	115.92
21	C	503	CLA	C2B-C1B-NB	-2.27	107.97	110.33
26	A	409	SQD	O5-C5-C4	2.27	113.79	109.70
21	P	509	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
21	C	503	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
21	C	507	CLA	C4-C3-C5	2.27	119.17	115.23
31	I	103	LMT	O1B-C4'-C3'	2.27	113.00	107.23
21	G	403	CLA	O2A-CGA-CBA	2.27	118.75	111.83
21	N	614	CLA	O2A-CGA-CBA	2.27	118.75	111.83
21	B	610	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
21	N	619	CLA	C2B-C1B-NB	-2.27	107.97	110.33
21	C	508	CLA	CHB-C1B-NB	2.27	127.45	124.05
21	B	614	CLA	C4-C3-C5	2.27	119.16	115.23
23	Q	405	PL9	C27-C28-C29	-2.27	122.44	127.62
24	Q	409	DGD	C6E-C5E-C4E	-2.27	107.45	113.02
27	a	102	LMG	C7-O1-C1	-2.26	108.94	113.80
22	G	405	PHO	CBC-CAC-C3C	-2.26	109.63	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	509	CLA	CHB-C1B-NB	2.26	127.44	124.05
23	D	404	PL9	C15-C14-C16	2.26	119.15	115.23
30	b	102	BCR	C37-C22-C21	-2.26	119.15	122.82
21	P	502	CLA	CHB-C1B-NB	2.26	127.44	124.05
21	C	512	CLA	C4-C3-C5	2.26	119.15	115.23
21	A	402	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
30	Z	101	BCR	C11-C10-C9	-2.26	124.11	127.28
21	P	507	CLA	C4D-CHA-C1A	2.26	123.94	121.24
30	K	101	BCR	C15-C16-C17	-2.26	118.90	123.52
21	A	401	CLA	C2A-C1A-CHA	2.26	127.78	123.87
21	B	607	CLA	CHB-C1B-NB	2.26	127.43	124.05
21	B	611	CLA	CHB-C1B-NB	2.26	127.43	124.05
21	N	615	CLA	CHB-C1B-NB	2.25	127.43	124.05
21	B	610	CLA	C1-C2-C3	-2.25	122.50	126.20
21	P	511	CLA	C2B-C1B-NB	-2.25	107.99	110.33
21	N	612	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
21	P	506	CLA	C2B-C1B-NB	-2.25	107.99	110.33
21	G	402	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
30	K	101	BCR	C36-C18-C19	2.25	121.53	118.09
23	A	406	PL9	C7-C8-C9	-2.25	122.95	126.83
26	G	410	SQD	C45-O47-C7	-2.25	112.42	117.80
34	i	201	HEM	CHD-C1D-ND	2.25	126.84	124.42
21	B	601	CLA	CHB-C1B-NB	2.25	127.42	124.05
21	B	612	CLA	CHB-C1B-NB	2.25	127.42	124.05
23	b	101	PL9	C7-C8-C9	-2.25	122.96	126.83
30	J	102	BCR	C37-C22-C21	-2.24	119.18	122.82
30	H	101	BCR	C16-C17-C18	-2.24	124.13	127.28
21	P	504	CLA	C1-O2A-CGA	2.24	122.08	116.65
21	N	614	CLA	C2B-C1B-NB	-2.24	108.00	110.33
21	B	610	CLA	CHB-C1B-NB	2.24	127.41	124.05
21	A	402	CLA	CHD-C1D-ND	-2.24	121.65	124.80
27	M	101	LMG	O6-C5-C6	2.24	111.99	106.44
30	J	102	BCR	C12-C13-C14	2.24	122.53	119.01
22	D	402	PHO	CAA-C2A-C3A	-2.24	106.95	113.00
21	C	507	CLA	C4D-CHA-C1A	2.23	123.91	121.24
21	B	601	CLA	C4D-CHA-C1A	2.23	123.91	121.24
21	B	615	CLA	C2B-C1B-NB	-2.23	108.01	110.33
21	N	614	CLA	C1-C2-C3	-2.23	122.54	126.20
30	P	515	BCR	C15-C16-C17	-2.23	118.95	123.52
21	P	503	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
21	Q	402	CLA	C2B-C1B-NB	-2.23	108.01	110.33
21	G	406	CLA	O2D-CGD-O1D	-2.23	119.50	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	P	515	BCR	C8-C7-C6	-2.23	121.04	127.00
21	N	611	CLA	C4D-CHA-C1A	2.23	123.91	121.24
21	C	507	CLA	CHB-C1B-NB	2.23	127.40	124.05
21	C	511	CLA	C2B-C1B-NB	-2.23	108.01	110.33
21	N	613	CLA	C4D-CHA-C1A	2.23	123.90	121.24
21	N	614	CLA	CHB-C1B-NB	2.23	127.39	124.05
22	A	404	PHO	C1A-C2A-C3A	-2.23	100.72	102.84
21	N	616	CLA	CBB-CAB-C3B	-2.22	116.41	127.53
30	C	514	BCR	C21-C20-C19	-2.22	116.76	123.20
21	C	502	CLA	CHB-C1B-NB	2.22	127.38	124.05
30	P	515	BCR	C38-C26-C25	-2.22	122.06	124.48
30	B	617	BCR	C20-C21-C22	-2.22	124.16	127.28
21	D	401	CLA	C2B-C1B-NB	-2.22	108.02	110.33
23	D	404	PL9	C27-C28-C29	-2.22	122.54	127.62
30	H	101	BCR	C35-C13-C12	2.22	121.48	118.09
25	G	409	LHG	O8-C23-C24	2.22	118.60	111.83
21	N	620	CLA	C1-C2-C3	-2.22	122.56	126.20
21	P	507	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
30	T	101	BCR	C29-C30-C25	2.22	113.66	110.44
21	P	512	CLA	CHB-C1B-NB	2.21	127.37	124.05
30	Z	101	BCR	C38-C26-C25	-2.21	122.07	124.48
21	B	608	CLA	CHB-C1B-NB	2.21	127.37	124.05
21	P	502	CLA	C1-C2-C3	-2.21	122.57	126.20
21	P	512	CLA	C2B-C1B-NB	-2.21	108.03	110.33
21	D	401	CLA	C4D-CHA-C1A	2.21	123.88	121.24
24	B	621	DGD	C1E-C2E-C3E	-2.21	105.36	110.01
21	Q	402	CLA	C4D-CHA-C1A	2.21	123.88	121.24
21	N	614	CLA	C4-C3-C5	2.21	119.06	115.23
30	N	621	BCR	C20-C21-C22	-2.21	124.18	127.28
27	N	622	LMG	O6-C1-O1	-2.21	104.82	110.04
21	P	507	CLA	CHB-C1B-NB	2.21	127.36	124.05
21	N	620	CLA	C2B-C1B-NB	-2.21	108.04	110.33
30	N	621	BCR	C16-C17-C18	-2.21	124.18	127.28
21	B	610	CLA	C2B-C1B-NB	-2.21	108.04	110.33
30	I	101	BCR	C21-C20-C19	-2.21	116.81	123.20
24	P	517	DGD	O5D-C6D-C5D	2.21	114.39	109.42
23	Q	405	PL9	C40-C39-C41	2.21	119.06	115.23
21	C	504	CLA	C4-C3-C5	2.20	119.05	115.23
21	G	404	CLA	C4D-CHA-C1A	2.20	123.87	121.24
27	D	412	LMG	O7-C10-O9	-2.20	118.56	123.70
24	P	518	DGD	O6E-C1E-O5D	2.20	115.25	110.04
21	G	406	CLA	CHB-C1B-NB	2.20	127.35	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	P	516	BCR	C30-C25-C24	2.20	121.62	115.65
21	B	606	CLA	C4D-CHA-C1A	2.20	123.87	121.24
21	Q	404	CLA	CHB-C1B-NB	2.20	127.35	124.05
21	C	511	CLA	C4D-CHA-C1A	2.20	123.87	121.24
22	D	402	PHO	CMC-C2C-C1C	2.20	128.69	124.73
21	N	605	CLA	C4D-CHA-C1A	2.20	123.87	121.24
21	P	509	CLA	C2B-C1B-NB	-2.20	108.05	110.33
21	P	506	CLA	C4D-CHA-C1A	2.20	123.87	121.24
30	C	514	BCR	C35-C13-C12	2.20	121.45	118.09
21	P	513	CLA	CHB-C1B-NB	2.20	127.35	124.05
21	N	606	CLA	CED-O2D-CGD	2.20	120.90	115.92
21	C	504	CLA	C2B-C1B-NB	-2.20	108.05	110.33
21	C	512	CLA	C2B-C1B-NB	-2.20	108.05	110.33
21	P	508	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
21	B	615	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
26	B	627	SQD	O48-C23-C24	2.20	118.53	111.83
30	S	101	BCR	C24-C23-C22	-2.20	122.98	126.23
30	P	516	BCR	C16-C17-C18	-2.20	124.20	127.28
21	B	613	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
30	b	102	BCR	C12-C13-C14	2.20	122.46	119.01
21	N	611	CLA	CHB-C1B-NB	2.20	127.34	124.05
21	P	502	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
30	T	103	BCR	C20-C21-C22	-2.19	124.20	127.28
26	S	102	SQD	O6-C1-C2	2.19	111.61	108.27
21	N	615	CLA	O2A-CGA-CBA	2.19	118.53	111.83
21	N	610	CLA	C1-C2-C3	-2.19	122.60	126.20
26	S	102	SQD	C3-C4-C5	2.19	114.21	110.23
30	a	101	BCR	C16-C17-C18	-2.19	124.20	127.28
21	N	616	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
30	W	101	BCR	C21-C20-C19	-2.19	116.85	123.20
27	M	101	LMG	O7-C10-O9	-2.19	118.58	123.70
30	B	618	BCR	C36-C18-C19	2.19	121.44	118.09
25	A	408	LHG	O8-C23-C24	2.19	118.52	111.83
26	F	101	SQD	C3-C4-C5	2.19	114.20	110.23
21	C	512	CLA	CHB-C1B-NB	2.19	127.33	124.05
21	C	510	CLA	CHB-C1B-NB	2.19	127.33	124.05
23	G	407	PL9	C7-C8-C9	-2.19	123.06	126.83
21	P	510	CLA	O1D-CGD-CBD	-2.19	120.21	124.52
26	F	101	SQD	O6-C1-C2	2.19	111.59	108.27
27	M	101	LMG	O8-C28-C29	2.19	118.50	111.83
21	N	606	CLA	C4D-CHA-C1A	2.18	123.85	121.24
22	D	402	PHO	C1A-C2A-C3A	-2.18	100.76	102.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Q	401	LMG	O7-C10-O9	-2.18	118.60	123.70
21	C	509	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
24	C	517	DGD	C6D-C5D-C4D	2.18	116.65	112.07
21	P	510	CLA	CHB-C1B-NB	2.18	127.32	124.05
21	G	404	CLA	CMD-C2D-C1D	2.18	128.57	124.73
30	I	101	BCR	C7-C8-C9	-2.18	123.01	126.23
21	N	618	CLA	CHB-C1B-NB	2.18	127.32	124.05
27	e	102	LMG	O7-C10-O9	-2.18	118.61	123.70
30	b	102	BCR	C39-C30-C25	-2.18	106.83	110.24
21	P	511	CLA	CHB-C1B-NB	2.18	127.32	124.05
30	W	101	BCR	C28-C27-C26	-2.18	110.17	114.06
21	D	401	CLA	CHB-C1B-NB	2.18	127.32	124.05
30	Z	101	BCR	C16-C17-C18	-2.18	124.22	127.28
21	D	403	CLA	C2B-C1B-NB	-2.18	108.07	110.33
21	A	403	CLA	CHB-C1B-NB	2.18	127.32	124.05
26	G	401	SQD	O8-S-C6	2.18	110.18	105.97
24	Q	409	DGD	O5D-C1E-C2E	-2.18	104.97	108.27
21	P	512	CLA	C4-C3-C5	2.18	119.01	115.23
21	N	605	CLA	CHB-C1B-NB	2.18	127.31	124.05
22	G	405	PHO	C1A-C2A-C3A	-2.18	100.77	102.84
21	B	602	CLA	C4-C3-C5	2.18	119.00	115.23
21	C	511	CLA	CHB-C1B-NB	2.17	127.31	124.05
21	G	403	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
21	B	606	CLA	C2B-C1B-NB	-2.17	108.07	110.33
24	C	517	DGD	C6E-C5E-C4E	-2.17	107.69	113.02
21	B	607	CLA	C4D-CHA-C1A	2.17	123.83	121.24
21	C	513	CLA	CHD-C1D-ND	-2.17	121.75	124.80
21	B	616	CLA	C4D-CHA-C1A	2.17	123.83	121.24
30	B	617	BCR	C29-C30-C25	2.17	113.59	110.44
21	N	611	CLA	CMD-C2D-C1D	2.17	128.55	124.73
21	N	616	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
21	P	513	CLA	C2B-C1B-NB	-2.17	108.08	110.33
24	Q	409	DGD	O3G-C1D-C2D	2.17	111.57	108.27
31	a	103	LMT	O1B-C4'-C3'	2.17	112.74	107.23
31	N	625	LMT	O1B-C1B-C2B	2.17	113.42	108.09
24	C	517	DGD	C1D-O6D-C5D	2.17	117.95	113.72
21	P	508	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
21	B	611	CLA	O2A-CGA-CBA	2.17	118.44	111.83
21	B	605	CLA	C2B-C1B-NB	-2.16	108.08	110.33
34	E	101	HEM	CAB-C3B-C2B	-2.16	121.40	128.43
27	B	622	LMG	O6-C1-O1	-2.16	104.93	110.04
21	C	509	CLA	C4-C3-C5	2.16	118.98	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	T	103	BCR	C33-C5-C6	-2.16	122.13	124.48
24	C	517	DGD	O6E-C1E-O5D	2.16	115.14	110.04
21	P	513	CLA	CHD-C1D-ND	-2.16	121.77	124.80
27	R	102	LMG	C9-C8-C7	-2.16	106.75	111.78
21	N	619	CLA	C4D-CHA-C1A	2.16	123.82	121.24
21	B	615	CLA	C4-C3-C5	2.16	118.97	115.23
21	N	614	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
30	a	101	BCR	C21-C20-C19	-2.16	116.95	123.20
30	W	101	BCR	C3-C4-C5	-2.16	110.21	114.06
22	G	405	PHO	C9-C8-C10	-2.16	103.59	111.27
21	B	609	CLA	C4D-CHA-C1A	2.15	123.81	121.24
21	C	513	CLA	CHB-C1B-NB	2.15	127.28	124.05
23	G	407	PL9	C53-C6-C1	2.15	119.69	115.28
23	Q	405	PL9	C15-C14-C16	2.15	118.97	115.23
30	K	101	BCR	C24-C23-C22	-2.15	123.05	126.23
21	P	511	CLA	C4D-CHA-C1A	2.15	123.81	121.24
21	N	617	CLA	CHB-C1B-NB	2.15	127.28	124.05
21	N	615	CLA	CBA-CAA-C2A	-2.15	107.39	113.79
30	H	101	BCR	C2-C1-C6	2.15	113.56	110.44
30	P	516	BCR	C21-C20-C19	-2.15	116.97	123.20
30	W	101	BCR	C35-C13-C12	2.15	121.37	118.09
30	Z	101	BCR	C15-C16-C17	-2.15	119.12	123.52
27	E	102	LMG	O7-C10-C11	2.15	116.13	111.48
30	Z	101	BCR	C29-C30-C25	2.15	113.56	110.44
21	C	506	CLA	CBA-CAA-C2A	-2.15	107.40	113.79
21	P	509	CLA	C4-C3-C5	2.15	118.95	115.23
21	P	507	CLA	C2B-C1B-NB	-2.15	108.10	110.33
21	N	609	CLA	O2A-CGA-CBA	2.14	118.38	111.83
24	W	102	DGD	O6D-C5D-C4D	2.14	113.56	109.70
21	P	502	CLA	CED-O2D-CGD	2.14	120.78	115.92
21	B	614	CLA	C4D-CHA-C1A	2.14	123.80	121.24
21	C	504	CLA	C4D-CHA-C1A	2.14	123.80	121.24
30	Z	101	BCR	C8-C7-C6	-2.14	121.28	127.00
21	G	404	CLA	CHB-C1B-NB	2.14	127.26	124.05
21	B	608	CLA	C2B-C1B-NB	-2.14	108.11	110.33
27	Q	407	LMG	O7-C10-O9	-2.14	118.70	123.70
24	P	518	DGD	O5D-C6D-C5D	2.14	114.25	109.42
22	Q	403	PHO	CMB-C2B-C3B	2.14	128.96	124.68
26	A	409	SQD	C45-O47-C7	-2.14	112.68	117.80
21	B	604	CLA	CHB-C1B-NB	2.14	127.26	124.05
21	N	619	CLA	CHB-C1B-NB	2.14	127.26	124.05
24	C	517	DGD	O5D-C6D-C5D	2.14	114.24	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	403	CLA	CHD-C1D-ND	-2.14	121.79	124.80
26	N	601	SQD	O48-C23-C24	2.14	118.35	111.83
30	N	621	BCR	C11-C10-C9	-2.13	124.28	127.28
21	B	602	CLA	O2A-CGA-CBA	2.13	118.34	111.83
21	A	403	CLA	C2B-C1B-NB	-2.13	108.12	110.33
21	Q	404	CLA	C2B-C1B-NB	-2.13	108.12	110.33
30	b	102	BCR	C23-C22-C21	2.13	122.36	119.01
30	c	101	BCR	C36-C18-C19	2.13	121.34	118.09
21	N	609	CLA	CED-O2D-CGD	2.13	120.74	115.92
30	I	101	BCR	C10-C11-C12	-2.13	117.03	123.20
21	B	605	CLA	CED-O2D-CGD	2.13	120.74	115.92
21	A	403	CLA	CMD-C2D-C1D	2.13	128.47	124.73
23	D	404	PL9	C20-C19-C21	2.13	118.92	115.23
21	C	506	CLA	CED-O2D-CGD	2.13	120.74	115.92
30	H	101	BCR	C24-C23-C22	-2.13	123.09	126.23
23	D	404	PL9	C17-C18-C19	-2.12	122.76	127.62
30	a	101	BCR	C2-C1-C6	2.12	113.52	110.44
21	G	403	CLA	C4D-CHA-C1A	2.12	123.77	121.24
21	B	616	CLA	CHB-C1B-NB	2.12	127.23	124.05
21	B	614	CLA	CHB-C1B-NB	2.12	127.23	124.05
34	R	101	HEM	CAB-C3B-C2B	-2.12	121.54	128.43
21	N	607	CLA	CAA-C2A-C3A	-2.12	107.27	113.00
21	P	503	CLA	CHB-C1B-NB	2.12	127.23	124.05
30	J	102	BCR	C39-C30-C25	-2.12	106.92	110.24
21	A	402	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
24	D	408	DGD	O3G-C1D-C2D	2.12	111.49	108.27
34	R	101	HEM	C1D-C2D-C3D	-2.12	104.75	106.98
21	N	609	CLA	C2B-C1B-NB	-2.12	108.13	110.33
21	N	609	CLA	C4D-CHA-C1A	2.12	123.77	121.24
30	a	101	BCR	C10-C11-C12	-2.12	117.07	123.20
26	N	601	SQD	C45-O47-C7	-2.12	112.73	117.80
21	N	618	CLA	C2B-C1B-NB	-2.11	108.13	110.33
24	P	518	DGD	C6D-C5D-C4D	2.11	116.50	112.07
27	R	102	LMG	C1-O6-C5	2.11	117.85	113.72
23	G	407	PL9	C41-C39-C40	2.11	119.45	114.59
21	B	610	CLA	C4-C3-C5	2.11	118.90	115.23
31	B	626	LMT	O1B-C1B-C2B	2.11	113.29	108.09
30	T	102	BCR	C38-C26-C27	2.11	118.10	113.60
30	P	514	BCR	C35-C13-C14	-2.11	119.39	122.82
21	P	512	CLA	C4D-CHA-C1A	2.11	123.76	121.24
30	B	620	BCR	C20-C21-C22	-2.11	124.31	127.28
21	B	605	CLA	O2A-CGA-CBA	2.11	118.28	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	519	DGD	O6E-C1E-O5D	2.11	115.03	110.04
30	J	102	BCR	C1-C6-C5	-2.11	119.75	122.64
21	P	501	CLA	C4-C3-C5	2.11	118.89	115.23
21	P	504	CLA	O2A-CGA-CBA	2.11	118.27	111.83
24	D	408	DGD	C6E-C5E-C4E	-2.11	107.84	113.02
30	P	515	BCR	C36-C18-C19	2.11	121.31	118.09
24	P	517	DGD	O3D-C3D-C4D	-2.11	105.40	110.38
21	C	512	CLA	C4D-CHA-C1A	2.11	123.76	121.24
27	D	407	LMG	O7-C10-O9	-2.11	118.78	123.70
21	C	501	CLA	C4-C3-C5	2.11	118.88	115.23
21	N	614	CLA	C4D-CHA-C1A	2.11	123.76	121.24
21	A	403	CLA	C4D-CHA-C1A	2.11	123.75	121.24
21	B	613	CLA	CHB-C1B-NB	2.11	127.21	124.05
24	B	628	DGD	C2G-O2G-C1B	-2.11	112.76	117.80
30	c	101	BCR	C28-C27-C26	-2.10	110.30	114.06
27	D	406	LMG	O7-C10-O9	-2.10	118.78	123.70
21	C	504	CLA	C1-O2A-CGA	2.10	121.74	116.65
21	P	504	CLA	CHB-C1B-NB	2.10	127.20	124.05
23	Q	405	PL9	C51-C49-C50	2.10	119.42	114.59
21	N	620	CLA	CED-O2D-CGD	2.10	120.68	115.92
22	A	404	PHO	CMC-C2C-C1C	2.10	128.51	124.73
21	D	401	CLA	C1-C2-C3	-2.10	122.76	126.20
21	G	404	CLA	O2A-CGA-CBA	2.10	118.23	111.83
21	Q	402	CLA	C1-C2-C3	-2.10	122.76	126.20
21	N	606	CLA	CAA-CBA-CGA	-2.10	107.25	113.21
26	S	102	SQD	O48-C23-C24	2.10	118.23	111.83
21	P	503	CLA	C4D-CHA-C1A	2.10	123.75	121.24
21	N	609	CLA	CHB-C1B-NB	2.10	127.19	124.05
27	E	102	LMG	C1-O6-C5	2.10	117.81	113.72
30	I	101	BCR	C20-C21-C22	-2.10	124.34	127.28
21	N	608	CLA	CHB-C1B-NB	2.10	127.19	124.05
21	B	602	CLA	O2D-CGD-O1D	-2.09	119.77	123.85
24	B	628	DGD	O6D-C1D-O3G	-2.09	105.09	110.04
30	P	515	BCR	C11-C10-C9	-2.09	124.34	127.28
30	P	515	BCR	C29-C30-C25	2.09	113.48	110.44
21	P	508	CLA	C4-C3-C5	2.09	118.86	115.23
26	F	101	SQD	O48-C23-C24	2.09	118.21	111.83
21	P	507	CLA	C4-C3-C5	2.09	118.86	115.23
21	C	504	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
23	A	406	PL9	C11-C9-C8	-2.09	116.48	121.17
27	D	406	LMG	O2-C2-C1	-2.09	105.10	110.08
30	a	101	BCR	C36-C18-C19	2.09	121.28	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	502	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
30	T	103	BCR	C10-C11-C12	-2.09	117.16	123.20
21	P	509	CLA	O2D-CGD-O1D	-2.08	119.79	123.85
21	P	513	CLA	CED-O2D-CGD	2.08	120.64	115.92
21	P	502	CLA	C4D-CHA-C1A	2.08	123.73	121.24
21	N	620	CLA	C4D-CHA-C1A	2.08	123.73	121.24
27	P	521	LMG	O8-C28-O10	-2.08	118.42	123.63
22	G	405	PHO	CMB-C2B-C3B	2.08	128.84	124.68
21	B	611	CLA	CBA-CAA-C2A	-2.08	107.60	113.79
21	B	603	CLA	C1-O2A-CGA	2.08	121.69	116.65
21	B	615	CLA	CHB-C1B-NB	2.08	127.17	124.05
21	C	507	CLA	C2B-C1B-NB	-2.08	108.17	110.33
22	A	404	PHO	C1-C2-C3	-2.08	122.79	126.20
30	P	516	BCR	C23-C24-C25	-2.08	121.45	127.00
22	D	402	PHO	CMB-C2B-C3B	2.08	128.83	124.68
23	A	406	PL9	C41-C39-C40	2.08	119.36	114.59
21	B	608	CLA	C4D-CHA-C1A	2.07	123.72	121.24
21	N	608	CLA	C4-C3-C5	2.07	118.83	115.23
24	C	516	DGD	O5D-C6D-C5D	2.07	114.09	109.42
21	N	611	CLA	C2B-C1B-NB	-2.07	108.18	110.33
30	c	101	BCR	C15-C16-C17	-2.07	119.28	123.52
21	C	504	CLA	O2A-CGA-CBA	2.07	118.15	111.83
21	B	610	CLA	C4D-CHA-C1A	2.07	123.71	121.24
21	B	602	CLA	C4D-CHA-C1A	2.07	123.71	121.24
21	N	605	CLA	CMC-C2C-C1C	-2.07	121.80	125.03
24	C	516	DGD	O3D-C3D-C4D	-2.07	105.50	110.38
30	I	101	BCR	C35-C13-C12	2.07	121.24	118.09
24	W	102	DGD	C1D-O6D-C5D	2.07	117.75	113.72
21	Q	402	CLA	CED-O2D-CGD	2.06	120.60	115.92
23	D	404	PL9	C51-C49-C50	2.06	119.34	114.59
22	Q	403	PHO	CMC-C2C-C1C	2.06	128.44	124.73
34	E	101	HEM	CAC-C3C-C4C	-2.06	119.90	124.82
21	N	609	CLA	CHD-C1D-ND	-2.06	121.90	124.80
21	C	504	CLA	CHB-C1B-NB	2.06	127.14	124.05
21	A	401	CLA	C2B-C1B-NB	-2.06	108.19	110.33
23	G	407	PL9	C10-C9-C11	2.06	118.80	115.23
21	B	602	CLA	C2B-C1B-NB	-2.06	108.19	110.33
27	N	623	LMG	O2-C2-C3	-2.06	105.52	110.38
21	P	504	CLA	C4D-CHA-C1A	2.06	123.70	121.24
21	C	507	CLA	O2A-CGA-CBA	2.06	118.11	111.83
34	i	201	HEM	CAA-CBA-CGA	-2.06	108.21	113.67
34	V	201	HEM	CHD-C1D-ND	2.06	126.64	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	618	BCR	C38-C26-C27	2.06	117.98	113.60
27	B	623	LMG	O2-C2-C3	-2.06	105.53	110.38
25	G	409	LHG	C5-O7-C7	-2.05	112.88	117.80
21	G	406	CLA	C4D-CHA-C1A	2.05	123.69	121.24
21	A	402	CLA	C4D-CHA-C1A	2.05	123.69	121.24
21	C	501	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
21	C	512	CLA	C1-C2-C3	-2.05	122.84	126.20
27	N	622	LMG	O3-C3-C4	-2.05	105.55	110.38
26	G	410	SQD	O5-C5-C4	2.05	113.39	109.70
23	A	406	PL9	C53-C6-C1	2.05	119.47	115.28
23	b	101	PL9	C10-C9-C11	2.05	118.78	115.23
30	C	514	BCR	C35-C13-C14	-2.05	119.50	122.82
21	P	512	CLA	C1-C2-C3	-2.05	122.84	126.20
21	C	503	CLA	CMD-C2D-C1D	2.04	128.33	124.73
21	A	405	CLA	C2B-C1B-NB	-2.04	108.21	110.33
30	T	101	BCR	C20-C21-C22	-2.04	124.41	127.28
21	G	403	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
24	P	518	DGD	O3G-C1D-C2D	2.04	111.38	108.27
34	E	101	HEM	CHA-C4D-ND	2.04	126.89	124.37
21	P	506	CLA	C4-C3-C5	2.04	118.77	115.23
21	C	508	CLA	CBA-CAA-C2A	-2.04	107.72	113.79
30	B	620	BCR	C4-C5-C6	-2.04	119.94	122.70
30	K	101	BCR	C28-C27-C26	-2.04	110.42	114.06
21	B	616	CLA	CED-O2D-CGD	2.04	120.54	115.92
21	C	507	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
24	C	516	DGD	O3G-C1D-C2D	2.04	111.37	108.27
21	B	605	CLA	CHB-C1B-NB	2.04	127.11	124.05
21	D	401	CLA	CED-O2D-CGD	2.04	120.54	115.92
21	C	501	CLA	C4D-CHA-C1A	2.04	123.67	121.24
21	N	612	CLA	CED-O2D-CGD	2.04	120.54	115.92
21	C	511	CLA	O2D-CGD-O1D	-2.04	119.89	123.85
21	N	607	CLA	C4-C3-C5	2.04	118.76	115.23
30	c	101	BCR	C24-C23-C22	-2.04	123.22	126.23
21	B	607	CLA	C1-C2-C3	-2.03	122.86	126.20
21	P	512	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
21	G	406	CLA	C2B-C1B-NB	-2.03	108.22	110.33
27	B	622	LMG	O8-C28-C29	2.03	118.03	111.83
30	a	101	BCR	C35-C13-C12	2.03	121.19	118.09
24	G	408	DGD	C2G-O2G-C1B	-2.03	112.93	117.80
31	N	604	LMT	O1B-C4'-C3'	2.03	112.40	107.23
30	S	101	BCR	C15-C14-C13	-2.03	124.43	127.28
21	B	605	CLA	C11-C10-C8	-2.03	109.21	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	518	DGD	C1D-O6D-C5D	2.03	117.69	113.72
21	C	508	CLA	C2B-C1B-NB	-2.03	108.22	110.33
21	G	403	CLA	C2B-C1B-NB	-2.03	108.22	110.33
21	N	609	CLA	C11-C10-C8	-2.03	109.22	115.97
30	P	516	BCR	C11-C10-C9	-2.03	124.43	127.28
21	C	509	CLA	C7-C6-C5	-2.03	107.85	113.26
27	E	102	LMG	C9-C8-C7	-2.03	107.05	111.78
21	P	504	CLA	C4-C3-C5	2.03	118.75	115.23
21	C	513	CLA	C2B-C1B-NB	-2.03	108.22	110.33
21	N	607	CLA	C2B-C1B-NB	-2.03	108.22	110.33
21	C	503	CLA	C4D-CHA-C1A	2.03	123.67	121.24
30	T	102	BCR	C15-C16-C17	-2.03	119.37	123.52
21	G	403	CLA	C4-C3-C5	2.03	118.75	115.23
21	N	615	CLA	C4D-CHA-C1A	2.03	123.66	121.24
21	B	603	CLA	C2B-C1B-NB	-2.03	108.22	110.33
24	C	517	DGD	O3G-C1D-C2D	2.03	111.35	108.27
21	B	604	CLA	C4-C3-C5	2.03	118.75	115.23
21	B	607	CLA	C2B-C1B-NB	-2.03	108.22	110.33
30	b	102	BCR	C1-C6-C5	-2.02	119.87	122.64
26	Q	408	SQD	O9-S-O7	-2.02	107.24	113.82
30	Z	101	BCR	C36-C18-C19	2.02	121.18	118.09
21	C	503	CLA	CHB-C1B-NB	2.02	127.08	124.05
21	B	605	CLA	C4D-CHA-C1A	2.02	123.66	121.24
21	B	612	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
21	B	612	CLA	C4-C3-C5	2.02	118.73	115.23
30	P	514	BCR	C2-C1-C6	2.02	113.37	110.44
30	J	102	BCR	C23-C22-C21	2.02	122.19	119.01
30	C	514	BCR	C20-C21-C22	-2.02	124.45	127.28
21	N	620	CLA	CHB-C1B-NB	2.02	127.08	124.05
21	C	504	CLA	C1-C2-C3	-2.02	122.89	126.20
30	T	102	BCR	C24-C23-C22	-2.02	123.25	126.23
21	G	404	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
21	N	606	CLA	C4-C3-C5	2.02	118.73	115.23
21	N	610	CLA	C2B-C1B-NB	-2.02	108.23	110.33
26	F	101	SQD	O8-S-O7	-2.02	106.36	111.40
30	K	101	BCR	C35-C13-C12	2.02	121.17	118.09
21	P	506	CLA	CBA-CAA-C2A	-2.01	107.80	113.79
24	A	407	DGD	C2G-O2G-C1B	-2.01	112.98	117.80
26	B	624	SQD	O9-S-O7	-2.01	107.28	113.82
22	A	404	PHO	C9-C8-C10	-2.01	104.10	111.27
21	Q	402	CLA	CAA-C2A-C1A	2.01	118.56	111.97
21	P	510	CLA	O2D-CGD-O1D	-2.01	119.94	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	505	CLA	CHB-C1B-NB	2.01	127.06	124.05
30	C	515	BCR	C23-C24-C25	-2.01	121.63	127.00
27	D	406	LMG	O3-C3-C4	-2.01	105.64	110.38
30	T	102	BCR	C24-C25-C26	-2.01	116.93	121.56
21	P	501	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
21	G	404	CLA	C2B-C1B-NB	-2.01	108.24	110.33
24	B	621	DGD	O6E-C5E-C6E	2.01	111.41	106.44
21	N	618	CLA	C4D-CHA-C1A	2.01	123.64	121.24
21	N	619	CLA	CHD-C1D-ND	-2.01	121.98	124.80
24	N	602	DGD	C2G-O2G-C1B	-2.01	113.00	117.80
21	P	503	CLA	CMD-C2D-C1D	2.01	128.26	124.73
21	B	603	CLA	C3A-C2A-C1A	2.00	104.34	101.34
21	B	614	CLA	C1-O2A-CGA	2.00	121.50	116.65
21	A	405	CLA	C11-C10-C8	-2.00	109.31	115.97
24	B	621	DGD	O3G-C1D-C2D	2.00	111.31	108.27
21	N	620	CLA	CAA-C2A-C3A	-2.00	107.59	113.00
30	c	101	BCR	C20-C21-C22	-2.00	124.47	127.28
30	P	515	BCR	C16-C17-C18	-2.00	124.47	127.28
21	P	504	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
21	B	613	CLA	O2D-CGD-O1D	-2.00	119.95	123.85

All (156) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	401	CLA	ND
21	A	402	CLA	ND
21	A	403	CLA	ND
21	A	405	CLA	ND
21	B	601	CLA	ND
21	B	602	CLA	ND
21	B	603	CLA	ND
21	B	604	CLA	ND
21	B	605	CLA	ND
21	B	606	CLA	ND
21	B	607	CLA	ND
21	B	608	CLA	ND
21	B	609	CLA	ND
21	B	610	CLA	ND
21	B	611	CLA	ND
21	B	612	CLA	ND
21	B	613	CLA	ND
21	B	614	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B	615	CLA	ND
21	B	616	CLA	ND
21	C	501	CLA	ND
21	C	502	CLA	ND
21	C	503	CLA	ND
21	C	504	CLA	ND
21	C	505	CLA	ND
21	C	506	CLA	ND
21	C	507	CLA	ND
21	C	508	CLA	ND
21	C	509	CLA	ND
21	C	510	CLA	ND
21	C	511	CLA	ND
21	C	512	CLA	ND
21	C	513	CLA	ND
21	D	401	CLA	ND
21	D	403	CLA	ND
21	G	402	CLA	ND
21	G	403	CLA	ND
21	G	404	CLA	ND
21	G	406	CLA	ND
21	N	605	CLA	ND
21	N	606	CLA	ND
21	N	607	CLA	ND
21	N	608	CLA	ND
21	N	609	CLA	ND
21	N	610	CLA	ND
21	N	611	CLA	ND
21	N	612	CLA	ND
21	N	613	CLA	ND
21	N	614	CLA	ND
21	N	615	CLA	ND
21	N	616	CLA	ND
21	N	617	CLA	ND
21	N	618	CLA	ND
21	N	619	CLA	ND
21	N	620	CLA	ND
21	P	501	CLA	ND
21	P	502	CLA	ND
21	P	503	CLA	ND
21	P	504	CLA	ND
21	P	505	CLA	ND

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Mol	Chain	Res	Type	Atom
21	P	506	CLA	ND
21	P	507	CLA	ND
21	P	508	CLA	ND
21	P	509	CLA	ND
21	P	510	CLA	ND
21	P	511	CLA	ND
21	P	512	CLA	ND
21	P	513	CLA	ND
21	Q	402	CLA	ND
21	Q	404	CLA	ND
24	A	407	DGD	C5E
24	A	407	DGD	C5D
24	A	407	DGD	C2D
24	B	621	DGD	C5E
24	B	621	DGD	C5D
24	B	621	DGD	C2D
24	B	628	DGD	C5E
24	B	628	DGD	C5D
24	B	628	DGD	C2D
24	C	516	DGD	C5E
24	C	516	DGD	C5D
24	C	516	DGD	C2D
24	C	517	DGD	C5E
24	C	517	DGD	C5D
24	C	517	DGD	C2D
24	C	518	DGD	C5E
24	C	518	DGD	C5D
24	C	518	DGD	C2D
24	D	408	DGD	C5E
24	D	408	DGD	C5D
24	D	408	DGD	C2D
24	G	408	DGD	C5E
24	G	408	DGD	C5D
24	G	408	DGD	C2D
24	N	602	DGD	C5E
24	N	602	DGD	C5D
24	N	602	DGD	C2D
24	P	517	DGD	C5E
24	P	517	DGD	C5D
24	P	517	DGD	C2D
24	P	518	DGD	C5E
24	P	518	DGD	C5D

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Mol	Chain	Res	Type	Atom
24	P	518	DGD	C2D
24	P	519	DGD	C5E
24	P	519	DGD	C5D
24	P	519	DGD	C2D
24	Q	409	DGD	C5E
24	Q	409	DGD	C5D
24	Q	409	DGD	C2D
24	W	102	DGD	C5E
24	W	102	DGD	C5D
24	W	102	DGD	C2D
27	A	410	LMG	C2
27	A	410	LMG	C5
27	B	622	LMG	C2
27	B	622	LMG	C5
27	B	623	LMG	C2
27	B	623	LMG	C5
27	C	519	LMG	C2
27	C	519	LMG	C5
27	C	520	LMG	C2
27	C	520	LMG	C5
27	D	406	LMG	C2
27	D	406	LMG	C5
27	D	407	LMG	C2
27	D	407	LMG	C5
27	D	412	LMG	C2
27	D	412	LMG	C5
27	E	102	LMG	C2
27	E	102	LMG	C5
27	I	102	LMG	C2
27	I	102	LMG	C5
27	M	101	LMG	C2
27	M	101	LMG	C5
27	G	411	LMG	C2
27	G	411	LMG	C5
27	N	623	LMG	C2
27	N	623	LMG	C5
27	N	622	LMG	C2
27	N	622	LMG	C5
27	P	520	LMG	C2
27	P	520	LMG	C5
27	P	521	LMG	C2
27	P	521	LMG	C5

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Mol	Chain	Res	Type	Atom
27	Q	401	LMG	C2
27	Q	401	LMG	C5
27	Q	407	LMG	C2
27	Q	407	LMG	C5
27	Q	406	LMG	C2
27	Q	406	LMG	C5
27	R	102	LMG	C2
27	R	102	LMG	C5
27	a	102	LMG	C2
27	a	102	LMG	C5
27	e	102	LMG	C2
27	e	102	LMG	C5

All (2177) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	401	CLA	C1A-C2A-CAA-CBA
21	A	401	CLA	C3A-C2A-CAA-CBA
21	A	401	CLA	CBD-CGD-O2D-CED
21	A	402	CLA	C1A-C2A-CAA-CBA
21	A	402	CLA	C1-C2-C3-C4
21	A	402	CLA	C1-C2-C3-C5
21	A	403	CLA	C2B-C3B-CAB-CBB
21	A	403	CLA	C4B-C3B-CAB-CBB
21	A	403	CLA	C1-C2-C3-C5
21	B	601	CLA	C4B-C3B-CAB-CBB
21	B	601	CLA	CBD-CGD-O2D-CED
21	B	602	CLA	C1A-C2A-CAA-CBA
21	B	602	CLA	C4B-C3B-CAB-CBB
21	B	602	CLA	C1-C2-C3-C4
21	B	602	CLA	C1-C2-C3-C5
21	B	602	CLA	C6-C7-C8-C9
21	B	603	CLA	C4B-C3B-CAB-CBB
21	B	604	CLA	C2B-C3B-CAB-CBB
21	B	604	CLA	C4B-C3B-CAB-CBB
21	B	604	CLA	CBD-CGD-O2D-CED
21	B	605	CLA	C2B-C3B-CAB-CBB
21	B	605	CLA	C4B-C3B-CAB-CBB
21	B	605	CLA	C1-C2-C3-C5
21	B	606	CLA	C3A-C2A-CAA-CBA
21	B	606	CLA	C2B-C3B-CAB-CBB
21	B	606	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	B	606	CLA	C1-C2-C3-C4
21	B	606	CLA	C1-C2-C3-C5
21	B	607	CLA	C1A-C2A-CAA-CBA
21	B	607	CLA	C3A-C2A-CAA-CBA
21	B	607	CLA	C2B-C3B-CAB-CBB
21	B	607	CLA	C4B-C3B-CAB-CBB
21	B	608	CLA	C1A-C2A-CAA-CBA
21	B	609	CLA	C2B-C3B-CAB-CBB
21	B	609	CLA	C4B-C3B-CAB-CBB
21	B	610	CLA	C2B-C3B-CAB-CBB
21	B	610	CLA	C4B-C3B-CAB-CBB
21	B	610	CLA	C1-C2-C3-C4
21	B	610	CLA	C1-C2-C3-C5
21	B	611	CLA	C2B-C3B-CAB-CBB
21	B	611	CLA	C4B-C3B-CAB-CBB
21	B	612	CLA	C2B-C3B-CAB-CBB
21	B	612	CLA	C4B-C3B-CAB-CBB
21	B	613	CLA	CBD-CGD-O2D-CED
21	B	614	CLA	CAD-CBD-CGD-O2D
21	B	615	CLA	C4B-C3B-CAB-CBB
21	B	615	CLA	C1-C2-C3-C4
21	B	615	CLA	C1-C2-C3-C5
21	B	616	CLA	C1A-C2A-CAA-CBA
21	B	616	CLA	C2B-C3B-CAB-CBB
21	B	616	CLA	C4B-C3B-CAB-CBB
21	B	616	CLA	CBD-CGD-O2D-CED
21	B	616	CLA	O1D-CGD-O2D-CED
21	B	616	CLA	C1-C2-C3-C4
21	B	616	CLA	C1-C2-C3-C5
21	C	501	CLA	C2B-C3B-CAB-CBB
21	C	501	CLA	C4B-C3B-CAB-CBB
21	C	502	CLA	C2B-C3B-CAB-CBB
21	C	502	CLA	C4B-C3B-CAB-CBB
21	C	502	CLA	C1-C2-C3-C4
21	C	502	CLA	C1-C2-C3-C5
21	C	503	CLA	C2B-C3B-CAB-CBB
21	C	503	CLA	C4B-C3B-CAB-CBB
21	C	504	CLA	C2B-C3B-CAB-CBB
21	C	504	CLA	C4B-C3B-CAB-CBB
21	C	504	CLA	CBD-CGD-O2D-CED
21	C	505	CLA	C1A-C2A-CAA-CBA
21	C	505	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	C	505	CLA	C2B-C3B-CAB-CBB
21	C	505	CLA	C4B-C3B-CAB-CBB
21	C	505	CLA	CBD-CGD-O2D-CED
21	C	505	CLA	C1-C2-C3-C4
21	C	505	CLA	C1-C2-C3-C5
21	C	506	CLA	C2B-C3B-CAB-CBB
21	C	506	CLA	C4B-C3B-CAB-CBB
21	C	508	CLA	CBD-CGD-O2D-CED
21	C	509	CLA	CHA-CBD-CGD-O1D
21	C	509	CLA	C1-C2-C3-C4
21	C	509	CLA	C1-C2-C3-C5
21	C	510	CLA	C2B-C3B-CAB-CBB
21	C	510	CLA	C4B-C3B-CAB-CBB
21	C	510	CLA	C1-C2-C3-C5
21	C	511	CLA	C1-C2-C3-C5
21	C	512	CLA	C2B-C3B-CAB-CBB
21	C	512	CLA	C4B-C3B-CAB-CBB
21	C	513	CLA	C1A-C2A-CAA-CBA
21	C	513	CLA	C4B-C3B-CAB-CBB
21	D	401	CLA	C1-C2-C3-C4
21	D	401	CLA	C1-C2-C3-C5
21	D	403	CLA	C2B-C3B-CAB-CBB
21	D	403	CLA	C4B-C3B-CAB-CBB
21	G	402	CLA	C1A-C2A-CAA-CBA
21	G	402	CLA	C3A-C2A-CAA-CBA
21	G	402	CLA	CBD-CGD-O2D-CED
21	G	403	CLA	C1A-C2A-CAA-CBA
21	G	403	CLA	C1-C2-C3-C4
21	G	403	CLA	C1-C2-C3-C5
21	G	403	CLA	C2-C3-C5-C6
21	G	404	CLA	C2B-C3B-CAB-CBB
21	G	404	CLA	C4B-C3B-CAB-CBB
21	G	404	CLA	C1-C2-C3-C5
21	N	605	CLA	C4B-C3B-CAB-CBB
21	N	605	CLA	CBD-CGD-O2D-CED
21	N	606	CLA	C4B-C3B-CAB-CBB
21	N	606	CLA	C1-C2-C3-C4
21	N	606	CLA	C1-C2-C3-C5
21	N	606	CLA	C6-C7-C8-C9
21	N	607	CLA	C4B-C3B-CAB-CBB
21	N	608	CLA	C2B-C3B-CAB-CBB
21	N	608	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	N	608	CLA	CBD-CGD-O2D-CED
21	N	609	CLA	C1A-C2A-CAA-CBA
21	N	609	CLA	C2B-C3B-CAB-CBB
21	N	609	CLA	C4B-C3B-CAB-CBB
21	N	609	CLA	C1-C2-C3-C5
21	N	610	CLA	C3A-C2A-CAA-CBA
21	N	610	CLA	C2B-C3B-CAB-CBB
21	N	610	CLA	C4B-C3B-CAB-CBB
21	N	610	CLA	C1-C2-C3-C4
21	N	610	CLA	C1-C2-C3-C5
21	N	611	CLA	C1A-C2A-CAA-CBA
21	N	611	CLA	C3A-C2A-CAA-CBA
21	N	611	CLA	C2B-C3B-CAB-CBB
21	N	611	CLA	C4B-C3B-CAB-CBB
21	N	612	CLA	C1A-C2A-CAA-CBA
21	N	613	CLA	C2B-C3B-CAB-CBB
21	N	613	CLA	C4B-C3B-CAB-CBB
21	N	614	CLA	C2B-C3B-CAB-CBB
21	N	614	CLA	C4B-C3B-CAB-CBB
21	N	614	CLA	C1-C2-C3-C4
21	N	614	CLA	C1-C2-C3-C5
21	N	615	CLA	C2B-C3B-CAB-CBB
21	N	615	CLA	C4B-C3B-CAB-CBB
21	N	616	CLA	C2B-C3B-CAB-CBB
21	N	616	CLA	C4B-C3B-CAB-CBB
21	N	617	CLA	CBD-CGD-O2D-CED
21	N	618	CLA	CAD-CBD-CGD-O2D
21	N	619	CLA	C4B-C3B-CAB-CBB
21	N	619	CLA	C1-C2-C3-C4
21	N	619	CLA	C1-C2-C3-C5
21	N	620	CLA	C1A-C2A-CAA-CBA
21	N	620	CLA	C2B-C3B-CAB-CBB
21	N	620	CLA	C4B-C3B-CAB-CBB
21	N	620	CLA	CBD-CGD-O2D-CED
21	N	620	CLA	C1-C2-C3-C4
21	N	620	CLA	C1-C2-C3-C5
21	P	501	CLA	C2B-C3B-CAB-CBB
21	P	501	CLA	C4B-C3B-CAB-CBB
21	P	502	CLA	C2B-C3B-CAB-CBB
21	P	502	CLA	C4B-C3B-CAB-CBB
21	P	502	CLA	C1-C2-C3-C4
21	P	502	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
21	P	503	CLA	C2B-C3B-CAB-CBB
21	P	503	CLA	C4B-C3B-CAB-CBB
21	P	504	CLA	C4B-C3B-CAB-CBB
21	P	505	CLA	C1A-C2A-CAA-CBA
21	P	505	CLA	C3A-C2A-CAA-CBA
21	P	505	CLA	C2B-C3B-CAB-CBB
21	P	505	CLA	C4B-C3B-CAB-CBB
21	P	505	CLA	CBD-CGD-O2D-CED
21	P	505	CLA	O1D-CGD-O2D-CED
21	P	506	CLA	C2B-C3B-CAB-CBB
21	P	506	CLA	C4B-C3B-CAB-CBB
21	P	508	CLA	CBD-CGD-O2D-CED
21	P	509	CLA	CHA-CBD-CGD-O1D
21	P	509	CLA	C1-C2-C3-C4
21	P	509	CLA	C1-C2-C3-C5
21	P	510	CLA	C2B-C3B-CAB-CBB
21	P	510	CLA	C4B-C3B-CAB-CBB
21	P	510	CLA	C1-C2-C3-C5
21	P	511	CLA	C1-C2-C3-C5
21	P	512	CLA	C2B-C3B-CAB-CBB
21	P	512	CLA	C4B-C3B-CAB-CBB
21	P	513	CLA	C1A-C2A-CAA-CBA
21	Q	402	CLA	C1-C2-C3-C4
21	Q	402	CLA	C1-C2-C3-C5
21	Q	404	CLA	C2B-C3B-CAB-CBB
21	Q	404	CLA	C4B-C3B-CAB-CBB
23	A	406	PL9	C7-C8-C9-C11
23	A	406	PL9	C12-C13-C14-C15
23	A	406	PL9	C12-C13-C14-C16
23	A	406	PL9	C17-C18-C19-C20
23	A	406	PL9	C17-C18-C19-C21
23	A	406	PL9	C27-C28-C29-C30
23	A	406	PL9	C27-C28-C29-C31
23	A	406	PL9	C37-C38-C39-C41
23	D	404	PL9	C12-C13-C14-C15
23	D	404	PL9	C12-C13-C14-C16
23	D	404	PL9	C34-C36-C37-C38
23	D	404	PL9	C42-C43-C44-C46
23	J	101	PL9	C7-C8-C9-C10
23	J	101	PL9	C7-C8-C9-C11
23	J	101	PL9	C12-C13-C14-C15
23	J	101	PL9	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
23	J	101	PL9	C17-C18-C19-C21
23	J	101	PL9	C22-C23-C24-C25
23	J	101	PL9	C22-C23-C24-C26
23	G	407	PL9	C7-C8-C9-C11
23	G	407	PL9	C12-C13-C14-C15
23	G	407	PL9	C12-C13-C14-C16
23	G	407	PL9	C17-C18-C19-C21
23	G	407	PL9	C27-C28-C29-C30
23	G	407	PL9	C27-C28-C29-C31
23	G	407	PL9	C37-C38-C39-C41
23	Q	405	PL9	C12-C13-C14-C15
23	Q	405	PL9	C12-C13-C14-C16
23	Q	405	PL9	C27-C28-C29-C31
23	Q	405	PL9	C42-C43-C44-C46
23	b	101	PL9	C7-C8-C9-C10
23	b	101	PL9	C7-C8-C9-C11
23	b	101	PL9	C12-C13-C14-C15
23	b	101	PL9	C12-C13-C14-C16
23	b	101	PL9	C17-C18-C19-C21
23	b	101	PL9	C22-C23-C24-C25
23	b	101	PL9	C22-C23-C24-C26
24	A	407	DGD	O6D-C1D-O3G-C3G
24	A	407	DGD	C4D-C5D-C6D-O5D
24	B	621	DGD	C2E-C1E-O5D-C6D
24	B	621	DGD	O6E-C1E-O5D-C6D
24	B	628	DGD	O1B-C1B-O2G-C2G
24	B	628	DGD	O2G-C2G-C3G-O3G
24	B	628	DGD	C2E-C1E-O5D-C6D
24	C	517	DGD	C2B-C1B-O2G-C2G
24	C	517	DGD	C4D-C5D-C6D-O5D
24	C	518	DGD	O6D-C1D-O3G-C3G
24	D	408	DGD	O6D-C1D-O3G-C3G
24	G	408	DGD	O6D-C1D-O3G-C3G
24	G	408	DGD	C4D-C5D-C6D-O5D
24	N	602	DGD	O1B-C1B-O2G-C2G
24	N	602	DGD	O2G-C2G-C3G-O3G
24	N	602	DGD	C2E-C1E-O5D-C6D
24	P	518	DGD	C2B-C1B-O2G-C2G
24	P	518	DGD	C4D-C5D-C6D-O5D
24	P	519	DGD	O6D-C1D-O3G-C3G
24	Q	409	DGD	O6D-C1D-O3G-C3G
24	W	102	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
24	W	102	DGD	O6E-C1E-O5D-C6D
25	A	408	LHG	C1-C2-C3-O3
25	G	409	LHG	C1-C2-C3-O3
26	A	409	SQD	C5-C6-S-O7
26	A	409	SQD	C5-C6-S-O8
26	A	409	SQD	C5-C6-S-O9
26	A	414	SQD	C5-C6-S-O9
26	B	624	SQD	C2-C1-O6-C44
26	B	624	SQD	O5-C1-O6-C44
26	B	624	SQD	O49-C7-O47-C45
26	B	624	SQD	C8-C7-O47-C45
26	B	627	SQD	O5-C5-C6-S
26	G	401	SQD	C5-C6-S-O9
26	G	410	SQD	C5-C6-S-O7
26	G	410	SQD	C5-C6-S-O8
26	G	410	SQD	C5-C6-S-O9
26	N	601	SQD	O5-C5-C6-S
26	Q	408	SQD	C2-C1-O6-C44
26	Q	408	SQD	O5-C1-O6-C44
26	Q	408	SQD	O49-C7-O47-C45
27	B	622	LMG	C11-C10-O7-C8
27	B	623	LMG	C11-C10-O7-C8
27	C	520	LMG	C11-C10-O7-C8
27	D	406	LMG	C11-C10-O7-C8
27	D	407	LMG	O6-C1-O1-C7
27	E	102	LMG	C2-C1-O1-C7
27	E	102	LMG	O6-C1-O1-C7
27	M	101	LMG	O6-C1-O1-C7
27	M	101	LMG	O9-C10-O7-C8
27	N	623	LMG	C11-C10-O7-C8
27	N	622	LMG	C11-C10-O7-C8
27	N	622	LMG	O10-C28-O8-C9
27	P	521	LMG	C11-C10-O7-C8
27	Q	407	LMG	O6-C1-O1-C7
27	Q	406	LMG	C11-C10-O7-C8
27	R	102	LMG	C2-C1-O1-C7
27	R	102	LMG	O6-C1-O1-C7
27	e	102	LMG	O6-C1-O1-C7
27	e	102	LMG	O9-C10-O7-C8
30	C	514	BCR	C7-C8-C9-C10
30	C	514	BCR	C7-C8-C9-C34
30	C	515	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
30	D	405	BCR	C7-C8-C9-C10
30	D	405	BCR	C7-C8-C9-C34
30	K	101	BCR	C21-C22-C23-C24
30	K	101	BCR	C37-C22-C23-C24
30	T	103	BCR	C21-C22-C23-C24
30	P	514	BCR	C7-C8-C9-C10
30	P	514	BCR	C7-C8-C9-C34
30	P	514	BCR	C11-C12-C13-C14
30	P	516	BCR	C7-C8-C9-C10
30	S	101	BCR	C7-C8-C9-C10
30	S	101	BCR	C7-C8-C9-C34
30	c	101	BCR	C21-C22-C23-C24
30	c	101	BCR	C37-C22-C23-C24
34	E	101	HEM	C3D-CAD-CBD-CGD
31	B	629	LMT	C3'-C4'-O1B-C1B
21	A	401	CLA	O1D-CGD-O2D-CED
21	B	610	CLA	O1D-CGD-O2D-CED
21	C	505	CLA	O1D-CGD-O2D-CED
21	C	508	CLA	O1D-CGD-O2D-CED
21	N	614	CLA	O1D-CGD-O2D-CED
21	N	620	CLA	O1D-CGD-O2D-CED
21	P	511	CLA	O1D-CGD-O2D-CED
31	N	603	LMT	C3'-C4'-O1B-C1B
21	B	605	CLA	O1D-CGD-O2D-CED
21	C	511	CLA	O1D-CGD-O2D-CED
21	G	402	CLA	O1D-CGD-O2D-CED
21	N	609	CLA	O1D-CGD-O2D-CED
21	B	603	CLA	CBD-CGD-O2D-CED
21	B	605	CLA	CBD-CGD-O2D-CED
21	B	606	CLA	CBD-CGD-O2D-CED
21	B	607	CLA	CBD-CGD-O2D-CED
21	B	610	CLA	CBD-CGD-O2D-CED
21	C	501	CLA	CBD-CGD-O2D-CED
21	C	503	CLA	CBD-CGD-O2D-CED
21	C	507	CLA	CBD-CGD-O2D-CED
21	C	511	CLA	CBD-CGD-O2D-CED
21	C	512	CLA	CBD-CGD-O2D-CED
21	N	607	CLA	CBD-CGD-O2D-CED
21	N	609	CLA	CBD-CGD-O2D-CED
21	N	610	CLA	CBD-CGD-O2D-CED
21	N	611	CLA	CBD-CGD-O2D-CED
21	N	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	P	501	CLA	CBD-CGD-O2D-CED
21	P	503	CLA	CBD-CGD-O2D-CED
21	P	504	CLA	CBD-CGD-O2D-CED
21	P	507	CLA	CBD-CGD-O2D-CED
21	P	511	CLA	CBD-CGD-O2D-CED
21	P	512	CLA	CBD-CGD-O2D-CED
26	A	414	SQD	O10-C23-O48-C46
26	G	401	SQD	O10-C23-O48-C46
27	A	410	LMG	O10-C28-O8-C9
27	B	622	LMG	O10-C28-O8-C9
21	B	604	CLA	O1D-CGD-O2D-CED
21	C	503	CLA	O1D-CGD-O2D-CED
21	N	608	CLA	O1D-CGD-O2D-CED
21	P	503	CLA	O1D-CGD-O2D-CED
23	A	406	PL9	C37-C38-C39-C40
23	J	101	PL9	C27-C28-C29-C31
23	G	407	PL9	C37-C38-C39-C40
23	b	101	PL9	C27-C28-C29-C31
27	C	520	LMG	C8-C9-O8-C28
27	P	521	LMG	C8-C9-O8-C28
26	A	414	SQD	C24-C23-O48-C46
26	G	401	SQD	C24-C23-O48-C46
27	A	410	LMG	C29-C28-O8-C9
26	F	101	SQD	O10-C23-O48-C46
26	S	102	SQD	O10-C23-O48-C46
27	C	520	LMG	O10-C28-O8-C9
27	D	407	LMG	O10-C28-O8-C9
27	G	411	LMG	O10-C28-O8-C9
27	P	521	LMG	O10-C28-O8-C9
21	P	507	CLA	O1D-CGD-O2D-CED
21	C	504	CLA	O1D-CGD-O2D-CED
21	C	512	CLA	O1D-CGD-O2D-CED
21	P	504	CLA	O1D-CGD-O2D-CED
27	P	521	LMG	C4-C5-C6-O5
21	C	506	CLA	CBD-CGD-O2D-CED
24	C	517	DGD	O1B-C1B-O2G-C2G
24	P	518	DGD	O1B-C1B-O2G-C2G
24	Q	409	DGD	O1B-C1B-O2G-C2G
27	B	622	LMG	O9-C10-O7-C8
27	B	623	LMG	O9-C10-O7-C8
27	C	520	LMG	O9-C10-O7-C8
27	D	406	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
27	N	623	LMG	O9-C10-O7-C8
27	N	622	LMG	O9-C10-O7-C8
27	P	521	LMG	O9-C10-O7-C8
27	Q	406	LMG	O9-C10-O7-C8
27	C	520	LMG	C4-C5-C6-O5
21	B	608	CLA	C3-C5-C6-C7
27	B	622	LMG	C29-C28-O8-C9
27	C	519	LMG	C29-C28-O8-C9
27	C	520	LMG	C29-C28-O8-C9
27	G	411	LMG	C29-C28-O8-C9
27	N	622	LMG	C29-C28-O8-C9
27	P	520	LMG	C29-C28-O8-C9
27	P	521	LMG	C29-C28-O8-C9
21	B	614	CLA	CBD-CGD-O2D-CED
21	C	509	CLA	CBD-CGD-O2D-CED
21	C	510	CLA	CBD-CGD-O2D-CED
21	N	618	CLA	CBD-CGD-O2D-CED
21	P	509	CLA	CBD-CGD-O2D-CED
21	P	513	CLA	CBD-CGD-O2D-CED
24	B	628	DGD	C2B-C1B-O2G-C2G
24	N	602	DGD	C2B-C1B-O2G-C2G
24	Q	409	DGD	C2B-C1B-O2G-C2G
26	Q	408	SQD	C8-C7-O47-C45
27	M	101	LMG	C11-C10-O7-C8
27	e	102	LMG	C11-C10-O7-C8
21	P	508	CLA	O1D-CGD-O2D-CED
21	B	603	CLA	C4-C3-C5-C6
21	N	607	CLA	C4-C3-C5-C6
22	A	404	PHO	C4-C3-C5-C6
21	A	402	CLA	C2-C3-C5-C6
21	B	608	CLA	C2-C3-C5-C6
21	B	610	CLA	C2-C3-C5-C6
21	N	612	CLA	C2-C3-C5-C6
21	N	614	CLA	C2-C3-C5-C6
21	N	612	CLA	C3-C5-C6-C7
21	C	507	CLA	O1D-CGD-O2D-CED
24	Q	409	DGD	C2A-C1A-O1G-C1G
26	F	101	SQD	C24-C23-O48-C46
26	S	102	SQD	C24-C23-O48-C46
27	D	407	LMG	C29-C28-O8-C9
27	E	102	LMG	C29-C28-O8-C9
27	C	520	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
23	A	406	PL9	C22-C23-C24-C25
23	D	404	PL9	C27-C28-C29-C30
23	G	407	PL9	C17-C18-C19-C20
23	G	407	PL9	C22-C23-C24-C25
23	Q	405	PL9	C27-C28-C29-C30
23	A	406	PL9	C22-C23-C24-C26
23	D	404	PL9	C27-C28-C29-C31
23	G	407	PL9	C22-C23-C24-C26
27	P	520	LMG	O10-C28-O8-C9
27	Q	407	LMG	O10-C28-O8-C9
31	B	630	LMT	C3'-C4'-O1B-C1B
31	N	604	LMT	C3'-C4'-O1B-C1B
21	C	501	CLA	O1D-CGD-O2D-CED
21	C	512	CLA	C3-C5-C6-C7
21	P	512	CLA	C3-C5-C6-C7
21	P	506	CLA	CBD-CGD-O2D-CED
31	I	103	LMT	C3'-C4'-O1B-C1B
31	a	103	LMT	C3'-C4'-O1B-C1B
25	A	408	LHG	O2-C2-C3-O3
25	G	409	LHG	O2-C2-C3-O3
21	N	605	CLA	O1D-CGD-O2D-CED
21	P	512	CLA	O1D-CGD-O2D-CED
24	D	408	DGD	C2A-C1A-O1G-C1G
27	I	102	LMG	C29-C28-O8-C9
27	R	102	LMG	C29-C28-O8-C9
27	C	519	LMG	O10-C28-O8-C9
27	A	410	LMG	C4-C5-C6-O5
27	C	519	LMG	O6-C5-C6-O5
27	P	521	LMG	O6-C5-C6-O5
27	C	519	LMG	C4-C5-C6-O5
21	B	608	CLA	CBD-CGD-O2D-CED
21	C	513	CLA	CBD-CGD-O2D-CED
24	C	516	DGD	C2B-C1B-O2G-C2G
24	D	408	DGD	C2B-C1B-O2G-C2G
24	P	517	DGD	C2B-C1B-O2G-C2G
24	Q	409	DGD	O1A-C1A-O1G-C1G
27	N	622	LMG	O6-C5-C6-O5
27	P	520	LMG	C4-C5-C6-O5
21	P	510	CLA	CBD-CGD-O2D-CED
27	A	410	LMG	O6-C5-C6-O5
27	B	622	LMG	O6-C5-C6-O5
21	C	513	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	Q	407	LMG	C29-C28-O8-C9
21	B	603	CLA	C2-C3-C5-C6
22	A	404	PHO	C2-C3-C5-C6
27	E	102	LMG	O10-C28-O8-C9
24	D	408	DGD	O1B-C1B-O2G-C2G
24	D	408	DGD	O6E-C5E-C6E-O5E
23	D	404	PL9	C24-C26-C27-C28
23	D	404	PL9	C29-C31-C32-C33
23	Q	405	PL9	C29-C31-C32-C33
23	Q	405	PL9	C34-C36-C37-C38
27	G	411	LMG	C4-C5-C6-O5
27	D	407	LMG	O6-C5-C6-O5
27	G	411	LMG	O6-C5-C6-O5
34	R	101	HEM	C3D-CAD-CBD-CGD
21	B	610	CLA	C2A-CAA-CBA-CGA
23	J	101	PL9	C27-C28-C29-C30
24	D	408	DGD	O1A-C1A-O1G-C1G
24	B	628	DGD	O6D-C1D-O3G-C3G
24	C	516	DGD	O6D-C1D-O3G-C3G
24	C	517	DGD	O6D-C1D-O3G-C3G
24	N	602	DGD	O6D-C1D-O3G-C3G
24	P	517	DGD	O6D-C1D-O3G-C3G
24	P	518	DGD	O6D-C1D-O3G-C3G
26	A	409	SQD	O5-C1-O6-C44
26	G	410	SQD	O5-C1-O6-C44
27	B	623	LMG	O6-C1-O1-C7
27	C	519	LMG	O6-C1-O1-C7
27	C	520	LMG	O6-C1-O1-C7
27	N	623	LMG	O6-C1-O1-C7
27	P	520	LMG	O6-C1-O1-C7
27	P	521	LMG	O6-C1-O1-C7
24	Q	409	DGD	O6E-C5E-C6E-O5E
27	P	520	LMG	O6-C5-C6-O5
21	B	611	CLA	CBD-CGD-O2D-CED
21	N	612	CLA	CBD-CGD-O2D-CED
21	N	615	CLA	CBD-CGD-O2D-CED
22	D	402	PHO	CBD-CGD-O2D-CED
22	Q	403	PHO	CBD-CGD-O2D-CED
27	Q	407	LMG	O6-C5-C6-O5
21	N	617	CLA	O1D-CGD-O2D-CED
23	Q	405	PL9	C47-C48-C49-C51
23	b	101	PL9	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
21	N	618	CLA	C3-C5-C6-C7
24	D	408	DGD	C4E-C5E-C6E-O5E
27	I	102	LMG	O10-C28-O8-C9
27	R	102	LMG	O10-C28-O8-C9
24	C	516	DGD	O1B-C1B-O2G-C2G
24	P	517	DGD	O1B-C1B-O2G-C2G
22	A	404	PHO	CBA-CGA-O2A-C1
22	G	405	PHO	CBA-CGA-O2A-C1
27	a	102	LMG	C29-C28-O8-C9
21	B	601	CLA	O1D-CGD-O2D-CED
21	P	501	CLA	O1D-CGD-O2D-CED
21	P	513	CLA	O1D-CGD-O2D-CED
22	G	405	PHO	C4-C3-C5-C6
21	B	613	CLA	C2-C3-C5-C6
21	N	607	CLA	C2-C3-C5-C6
22	G	405	PHO	C2-C3-C5-C6
21	A	402	CLA	C6-C7-C8-C9
21	B	608	CLA	C6-C7-C8-C9
21	B	610	CLA	C14-C13-C15-C16
21	C	511	CLA	C6-C7-C8-C9
21	G	403	CLA	C6-C7-C8-C9
21	N	612	CLA	C6-C7-C8-C9
21	N	614	CLA	C14-C13-C15-C16
21	P	511	CLA	C6-C7-C8-C9
27	Q	406	LMG	O6-C5-C6-O5
27	D	407	LMG	C4-C5-C6-O5
27	Q	407	LMG	C4-C5-C6-O5
24	A	407	DGD	C2D-C1D-O3G-C3G
24	B	628	DGD	C2D-C1D-O3G-C3G
24	C	516	DGD	C2D-C1D-O3G-C3G
24	C	517	DGD	C2D-C1D-O3G-C3G
24	D	408	DGD	C2D-C1D-O3G-C3G
24	G	408	DGD	C2D-C1D-O3G-C3G
24	N	602	DGD	C2D-C1D-O3G-C3G
24	P	517	DGD	C2D-C1D-O3G-C3G
24	P	518	DGD	C2D-C1D-O3G-C3G
24	Q	409	DGD	C2D-C1D-O3G-C3G
26	A	409	SQD	C2-C1-O6-C44
26	G	410	SQD	C2-C1-O6-C44
27	B	623	LMG	C2-C1-O1-C7
27	C	519	LMG	C2-C1-O1-C7
27	C	520	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
27	N	623	LMG	C2-C1-O1-C7
27	P	520	LMG	C2-C1-O1-C7
27	P	521	LMG	C2-C1-O1-C7
27	C	519	LMG	C10-C11-C12-C13
24	C	517	DGD	O6D-C5D-C6D-O5D
24	P	518	DGD	O6D-C5D-C6D-O5D
25	A	411	LHG	O2-C2-C3-O3
25	G	412	LHG	O2-C2-C3-O3
21	B	613	CLA	O1D-CGD-O2D-CED
22	A	404	PHO	O1A-CGA-O2A-C1
24	Q	409	DGD	C4E-C5E-C6E-O5E
30	B	620	BCR	C37-C22-C23-C24
30	C	514	BCR	C11-C12-C13-C35
30	C	515	BCR	C7-C8-C9-C34
30	K	101	BCR	C7-C8-C9-C34
30	T	103	BCR	C37-C22-C23-C24
30	P	514	BCR	C11-C12-C13-C35
30	P	515	BCR	C7-C8-C9-C34
30	P	516	BCR	C7-C8-C9-C34
30	b	102	BCR	C7-C8-C9-C34
30	c	101	BCR	C7-C8-C9-C34
30	K	101	BCR	C7-C8-C9-C10
30	c	101	BCR	C7-C8-C9-C10
21	B	601	CLA	C2A-CAA-CBA-CGA
21	N	605	CLA	C2A-CAA-CBA-CGA
27	B	623	LMG	C10-C11-C12-C13
27	a	102	LMG	O10-C28-O8-C9
21	B	614	CLA	C3-C5-C6-C7
27	D	406	LMG	O6-C5-C6-O5
26	F	101	SQD	C8-C7-O47-C45
26	S	102	SQD	C8-C7-O47-C45
27	Q	401	LMG	C11-C10-O7-C8
26	G	410	SQD	O47-C45-C46-O48
21	B	608	CLA	C15-C16-C17-C18
27	P	520	LMG	C10-C11-C12-C13
21	D	401	CLA	O1D-CGD-O2D-CED
27	I	102	LMG	C4-C5-C6-O5
23	b	101	PL9	C17-C18-C19-C20
21	C	505	CLA	C10-C11-C12-C13
21	C	512	CLA	C13-C15-C16-C17
21	N	606	CLA	C5-C6-C7-C8
21	N	620	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	P	501	CLA	C15-C16-C17-C18
23	Q	405	PL9	C47-C48-C49-C50
21	C	506	CLA	O1D-CGD-O2D-CED
21	C	501	CLA	C15-C16-C17-C18
21	A	403	CLA	CBD-CGD-O2D-CED
24	Q	409	DGD	C1B-C2B-C3B-C4B
24	W	102	DGD	C1B-C2B-C3B-C4B
27	N	623	LMG	C10-C11-C12-C13
21	G	404	CLA	CBD-CGD-O2D-CED
27	M	101	LMG	O6-C5-C6-O5
26	S	102	SQD	C24-C25-C26-C27
21	C	510	CLA	C15-C16-C17-C18
21	N	616	CLA	C13-C15-C16-C17
26	F	101	SQD	C24-C25-C26-C27
24	C	516	DGD	C1A-C2A-C3A-C4A
24	C	516	DGD	C1B-C2B-C3B-C4B
27	B	622	LMG	C10-C11-C12-C13
27	C	520	LMG	C28-C29-C30-C31
27	D	407	LMG	C10-C11-C12-C13
27	P	521	LMG	C28-C29-C30-C31
22	G	405	PHO	O1A-CGA-O2A-C1
27	D	412	LMG	C11-C10-O7-C8
21	B	613	CLA	C5-C6-C7-C8
21	D	401	CLA	C13-C15-C16-C17
21	N	606	CLA	C13-C15-C16-C17
21	N	615	CLA	C15-C16-C17-C18
21	P	506	CLA	C5-C6-C7-C8
21	P	508	CLA	C15-C16-C17-C18
21	P	510	CLA	C15-C16-C17-C18
21	P	512	CLA	C13-C15-C16-C17
21	Q	402	CLA	C13-C15-C16-C17
22	D	402	PHO	C15-C16-C17-C18
24	A	407	DGD	O6D-C5D-C6D-O5D
24	G	408	DGD	O6D-C5D-C6D-O5D
21	A	401	CLA	C2A-CAA-CBA-CGA
21	C	508	CLA	C2A-CAA-CBA-CGA
21	C	511	CLA	C2A-CAA-CBA-CGA
21	G	402	CLA	C2A-CAA-CBA-CGA
21	N	611	CLA	C2A-CAA-CBA-CGA
21	N	614	CLA	C2A-CAA-CBA-CGA
21	P	508	CLA	C2A-CAA-CBA-CGA
21	B	601	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	B	602	CLA	C5-C6-C7-C8
21	B	612	CLA	C13-C15-C16-C17
21	B	616	CLA	C5-C6-C7-C8
21	B	616	CLA	C10-C11-C12-C13
21	B	616	CLA	C13-C15-C16-C17
21	C	503	CLA	C10-C11-C12-C13
21	C	504	CLA	C13-C15-C16-C17
21	C	506	CLA	C5-C6-C7-C8
21	G	403	CLA	C15-C16-C17-C18
21	N	608	CLA	C13-C15-C16-C17
21	N	612	CLA	C15-C16-C17-C18
21	P	505	CLA	C10-C11-C12-C13
21	Q	402	CLA	C15-C16-C17-C18
22	Q	403	PHO	C15-C16-C17-C18
24	P	518	DGD	O6E-C5E-C6E-O5E
24	B	621	DGD	C1B-C2B-C3B-C4B
24	D	408	DGD	C1B-C2B-C3B-C4B
24	P	517	DGD	C1B-C2B-C3B-C4B
27	D	406	LMG	C10-C11-C12-C13
27	N	622	LMG	C10-C11-C12-C13
27	Q	407	LMG	C10-C11-C12-C13
24	B	628	DGD	O6E-C1E-O5D-C6D
21	A	402	CLA	C15-C16-C17-C18
21	B	601	CLA	C13-C15-C16-C17
21	B	602	CLA	C13-C15-C16-C17
21	B	604	CLA	C13-C15-C16-C17
21	B	611	CLA	C15-C16-C17-C18
21	B	615	CLA	C13-C15-C16-C17
21	C	504	CLA	C15-C16-C17-C18
21	C	507	CLA	C5-C6-C7-C8
21	C	508	CLA	C10-C11-C12-C13
21	C	508	CLA	C15-C16-C17-C18
21	C	513	CLA	C15-C16-C17-C18
21	D	401	CLA	C15-C16-C17-C18
21	N	605	CLA	C10-C11-C12-C13
21	N	611	CLA	C15-C16-C17-C18
21	N	619	CLA	C13-C15-C16-C17
21	N	620	CLA	C5-C6-C7-C8
21	N	620	CLA	C10-C11-C12-C13
21	P	504	CLA	C13-C15-C16-C17
21	P	504	CLA	C15-C16-C17-C18
21	P	508	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	P	513	CLA	C15-C16-C17-C18
24	N	602	DGD	C1A-C2A-C3A-C4A
27	Q	406	LMG	C10-C11-C12-C13
21	B	607	CLA	C13-C15-C16-C17
21	N	605	CLA	C13-C15-C16-C17
21	N	611	CLA	C13-C15-C16-C17
21	P	503	CLA	C10-C11-C12-C13
21	P	507	CLA	C5-C6-C7-C8
27	Q	401	LMG	O9-C10-O7-C8
23	D	404	PL9	C47-C48-C49-C50
21	P	510	CLA	O1D-CGD-O2D-CED
21	B	607	CLA	C15-C16-C17-C18
21	B	610	CLA	C8-C10-C11-C12
21	B	614	CLA	C15-C16-C17-C18
21	D	403	CLA	C15-C16-C17-C18
21	N	618	CLA	C15-C16-C17-C18
21	P	501	CLA	C10-C11-C12-C13
24	G	408	DGD	C4E-C5E-C6E-O5E
24	B	628	DGD	C1A-C2A-C3A-C4A
24	G	408	DGD	C1B-C2B-C3B-C4B
21	B	602	CLA	O1D-CGD-O2D-CED
21	A	403	CLA	C15-C16-C17-C18
21	B	604	CLA	C8-C10-C11-C12
21	B	605	CLA	C5-C6-C7-C8
21	B	613	CLA	C13-C15-C16-C17
21	C	501	CLA	C10-C11-C12-C13
21	C	509	CLA	C15-C16-C17-C18
21	C	513	CLA	C13-C15-C16-C17
21	N	609	CLA	C5-C6-C7-C8
21	N	614	CLA	C8-C10-C11-C12
21	N	617	CLA	C5-C6-C7-C8
21	P	509	CLA	C15-C16-C17-C18
21	Q	404	CLA	C15-C16-C17-C18
25	A	408	LHG	C24-C23-O8-C6
25	G	409	LHG	C24-C23-O8-C6
24	A	407	DGD	C4E-C5E-C6E-O5E
27	a	102	LMG	C11-C10-O7-C8
27	B	622	LMG	C4-C5-C6-O5
24	B	621	DGD	O6D-C5D-C6D-O5D
21	C	506	CLA	C15-C16-C17-C18
21	G	404	CLA	C10-C11-C12-C13
26	F	101	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
26	S	102	SQD	O49-C7-O47-C45
27	D	412	LMG	O9-C10-O7-C8
27	a	102	LMG	O9-C10-O7-C8
25	A	411	LHG	C1-C2-C3-O3
25	G	412	LHG	C1-C2-C3-O3
21	B	607	CLA	C2A-CAA-CBA-CGA
21	C	512	CLA	C2A-CAA-CBA-CGA
25	G	412	LHG	C24-C23-O8-C6
21	A	405	CLA	C13-C15-C16-C17
21	C	506	CLA	C13-C15-C16-C17
21	N	608	CLA	C8-C10-C11-C12
21	N	612	CLA	C5-C6-C7-C8
21	N	613	CLA	C13-C15-C16-C17
21	N	618	CLA	C5-C6-C7-C8
21	P	501	CLA	C8-C10-C11-C12
21	P	504	CLA	C10-C11-C12-C13
21	P	513	CLA	C13-C15-C16-C17
24	W	102	DGD	O6D-C5D-C6D-O5D
21	B	608	CLA	O1D-CGD-O2D-CED
21	A	403	CLA	C10-C11-C12-C13
21	C	501	CLA	C8-C10-C11-C12
21	C	504	CLA	C10-C11-C12-C13
21	N	616	CLA	C5-C6-C7-C8
21	P	503	CLA	C5-C6-C7-C8
21	P	506	CLA	C13-C15-C16-C17
21	P	511	CLA	C5-C6-C7-C8
21	G	404	CLA	O1D-CGD-O2D-CED
21	B	608	CLA	C5-C6-C7-C8
21	B	612	CLA	C5-C6-C7-C8
21	B	616	CLA	C15-C16-C17-C18
21	G	406	CLA	C10-C11-C12-C13
21	G	406	CLA	C13-C15-C16-C17
21	N	617	CLA	C13-C15-C16-C17
24	C	516	DGD	O6D-C5D-C6D-O5D
23	G	407	PL9	C35-C34-C36-C37
21	B	609	CLA	C13-C15-C16-C17
21	B	614	CLA	C5-C6-C7-C8
21	G	406	CLA	C5-C6-C7-C8
21	P	506	CLA	C15-C16-C17-C18
27	I	102	LMG	C11-C10-O7-C8
23	D	404	PL9	C22-C23-C24-C25
23	G	407	PL9	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	Q	405	PL9	C22-C23-C24-C25
27	I	102	LMG	O9-C10-O7-C8
27	I	102	LMG	C2-C1-O1-C7
27	a	102	LMG	C2-C1-O1-C7
27	e	102	LMG	C2-C1-O1-C7
23	Q	405	PL9	C24-C26-C27-C28
24	P	517	DGD	O6D-C5D-C6D-O5D
25	A	411	LHG	C24-C23-O8-C6
27	I	102	LMG	O6-C5-C6-O5
27	e	102	LMG	O6-C5-C6-O5
21	C	503	CLA	C5-C6-C7-C8
30	B	618	BCR	C7-C8-C9-C34
30	C	515	BCR	C37-C22-C23-C24
30	D	405	BCR	C37-C22-C23-C24
30	T	102	BCR	C7-C8-C9-C34
30	Z	101	BCR	C7-C8-C9-C34
30	P	516	BCR	C37-C22-C23-C24
30	B	618	BCR	C7-C8-C9-C10
30	C	514	BCR	C11-C12-C13-C14
30	D	405	BCR	C21-C22-C23-C24
30	T	102	BCR	C7-C8-C9-C10
21	C	504	CLA	C2A-CAA-CBA-CGA
21	D	403	CLA	C2A-CAA-CBA-CGA
21	P	504	CLA	C2A-CAA-CBA-CGA
21	P	511	CLA	C2A-CAA-CBA-CGA
21	P	512	CLA	C2A-CAA-CBA-CGA
21	P	513	CLA	C2A-CAA-CBA-CGA
21	Q	404	CLA	C2A-CAA-CBA-CGA
21	B	604	CLA	C15-C16-C17-C18
25	A	411	LHG	O1-C1-C2-C3
25	G	412	LHG	O1-C1-C2-C3
21	P	509	CLA	O2A-C1-C2-C3
21	N	606	CLA	O1D-CGD-O2D-CED
24	N	602	DGD	O6E-C1E-O5D-C6D
27	I	102	LMG	O6-C1-O1-C7
27	a	102	LMG	O6-C1-O1-C7
25	G	409	LHG	C8-C7-O7-C5
24	P	517	DGD	C1A-C2A-C3A-C4A
21	G	404	CLA	C15-C16-C17-C18
21	B	604	CLA	C2-C3-C5-C6
21	Q	402	CLA	O1D-CGD-O2D-CED
21	A	405	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	C	511	CLA	C5-C6-C7-C8
24	C	517	DGD	O6E-C5E-C6E-O5E
24	P	517	DGD	C4E-C5E-C6E-O5E
21	A	405	CLA	C5-C6-C7-C8
21	C	506	CLA	C10-C11-C12-C13
24	B	621	DGD	C6B-C7B-C8B-C9B
24	D	408	DGD	CAB-CBB-CCB-CDB
27	Q	407	LMG	C15-C16-C17-C18
27	N	622	LMG	C4-C5-C6-O5
31	N	624	LMT	C1-C2-C3-C4
24	A	407	DGD	C8B-C9B-CAB-CBB
25	A	411	LHG	C11-C10-C9-C8
27	D	407	LMG	C15-C16-C17-C18
27	Q	401	LMG	C18-C19-C20-C21
27	a	102	LMG	C12-C13-C14-C15
24	C	516	DGD	C3A-C4A-C5A-C6A
24	D	408	DGD	CDB-CEB-CFB-CGB
24	G	408	DGD	C8B-C9B-CAB-CBB
24	Q	409	DGD	CAB-CBB-CCB-CDB
25	A	411	LHG	C25-C26-C27-C28
27	D	412	LMG	C18-C19-C20-C21
27	I	102	LMG	C12-C13-C14-C15
27	G	411	LMG	C34-C35-C36-C37
27	Q	401	LMG	C32-C33-C34-C35
23	D	404	PL9	C47-C48-C49-C51
27	B	623	LMG	C29-C28-O8-C9
31	B	625	LMT	C1-C2-C3-C4
24	C	516	DGD	C3B-C4B-C5B-C6B
24	C	518	DGD	C9B-CAB-CBB-CCB
25	A	408	LHG	C30-C31-C32-C33
25	G	412	LHG	C25-C26-C27-C28
27	A	410	LMG	C34-C35-C36-C37
27	C	520	LMG	C29-C30-C31-C32
31	I	103	LMT	C6-C7-C8-C9
24	C	517	DGD	CAB-CBB-CCB-CDB
24	P	517	DGD	C3B-C4B-C5B-C6B
25	G	409	LHG	C30-C31-C32-C33
25	G	412	LHG	C24-C25-C26-C27
27	C	520	LMG	C12-C13-C14-C15
27	I	102	LMG	C14-C15-C16-C17
21	C	509	CLA	O1D-CGD-O2D-CED
21	B	608	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	B	613	CLA	C4B-C3B-CAB-CBB
21	C	507	CLA	C4B-C3B-CAB-CBB
21	C	509	CLA	C4B-C3B-CAB-CBB
21	C	511	CLA	C4B-C3B-CAB-CBB
21	N	612	CLA	C4B-C3B-CAB-CBB
21	N	617	CLA	C4B-C3B-CAB-CBB
21	P	507	CLA	C4B-C3B-CAB-CBB
21	P	509	CLA	C4B-C3B-CAB-CBB
21	P	511	CLA	C4B-C3B-CAB-CBB
21	P	513	CLA	C4B-C3B-CAB-CBB
24	D	408	DGD	C1A-C2A-C3A-C4A
24	B	628	DGD	C9B-CAB-CBB-CCB
24	C	518	DGD	C3B-C4B-C5B-C6B
26	S	102	SQD	C27-C28-C29-C30
27	N	622	LMG	C31-C32-C33-C34
21	C	513	CLA	C2A-CAA-CBA-CGA
27	D	412	LMG	C11-C12-C13-C14
21	P	503	CLA	C8-C10-C11-C12
24	P	519	DGD	C2B-C1B-O2G-C2G
27	C	519	LMG	C11-C10-O7-C8
27	D	407	LMG	C11-C10-O7-C8
27	Q	407	LMG	C11-C10-O7-C8
24	P	519	DGD	C9B-CAB-CBB-CCB
24	Q	409	DGD	CDB-CEB-CFB-CGB
24	W	102	DGD	C6B-C7B-C8B-C9B
27	D	407	LMG	C19-C20-C21-C22
27	P	521	LMG	C12-C13-C14-C15
31	N	603	LMT	C2-C3-C4-C5
21	C	503	CLA	C11-C12-C13-C15
21	N	606	CLA	C12-C13-C15-C16
21	P	503	CLA	C11-C12-C13-C15
22	Q	403	PHO	C11-C10-C8-C7
24	D	408	DGD	C3B-C4B-C5B-C6B
24	D	408	DGD	CEB-CFB-CGB-CHB
24	N	602	DGD	C9B-CAB-CBB-CCB
24	Q	409	DGD	C3B-C4B-C5B-C6B
25	A	411	LHG	C24-C25-C26-C27
31	a	103	LMT	C6-C7-C8-C9
24	A	407	DGD	C1B-C2B-C3B-C4B
24	Q	409	DGD	C1A-C2A-C3A-C4A
27	N	623	LMG	C29-C28-O8-C9
21	N	607	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	P	506	CLA	C10-C11-C12-C13
27	D	412	LMG	C32-C33-C34-C35
27	M	101	LMG	C29-C30-C31-C32
27	Q	407	LMG	C19-C20-C21-C22
27	e	102	LMG	C29-C30-C31-C32
25	G	409	LHG	O10-C23-O8-C6
21	A	402	CLA	C3A-C2A-CAA-CBA
21	B	602	CLA	C3A-C2A-CAA-CBA
21	B	608	CLA	C3A-C2A-CAA-CBA
21	C	507	CLA	C3A-C2A-CAA-CBA
21	C	512	CLA	C3A-C2A-CAA-CBA
21	G	403	CLA	C3A-C2A-CAA-CBA
21	N	612	CLA	C3A-C2A-CAA-CBA
21	P	507	CLA	C3A-C2A-CAA-CBA
21	P	512	CLA	C3A-C2A-CAA-CBA
24	P	517	DGD	C4A-C5A-C6A-C7A
25	A	408	LHG	C25-C26-C27-C28
25	G	409	LHG	C25-C26-C27-C28
27	E	102	LMG	C15-C16-C17-C18
21	N	607	CLA	O1D-CGD-O2D-CED
25	A	408	LHG	O10-C23-O8-C6
24	C	516	DGD	C4A-C5A-C6A-C7A
24	D	408	DGD	C7B-C8B-C9B-CAB
24	Q	409	DGD	C7B-C8B-C9B-CAB
24	W	102	DGD	C7A-C8A-C9A-CAA
27	D	412	LMG	C30-C31-C32-C33
27	a	102	LMG	C14-C15-C16-C17
25	G	409	LHG	O9-C7-O7-C5
24	P	517	DGD	C3A-C4A-C5A-C6A
24	Q	409	DGD	C5A-C6A-C7A-C8A
27	A	410	LMG	O1-C7-C8-C9
27	M	101	LMG	C7-C8-C9-O8
24	D	408	DGD	C6B-C7B-C8B-C9B
24	P	518	DGD	C2B-C3B-C4B-C5B
24	W	102	DGD	C5B-C6B-C7B-C8B
27	D	407	LMG	C36-C37-C38-C39
27	Q	401	LMG	C30-C31-C32-C33
27	Q	407	LMG	C36-C37-C38-C39
27	C	520	LMG	C10-C11-C12-C13
24	D	408	DGD	C3A-C4A-C5A-C6A
24	P	517	DGD	C4B-C5B-C6B-C7B
24	Q	409	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
27	P	521	LMG	C29-C30-C31-C32
27	R	102	LMG	C15-C16-C17-C18
27	B	623	LMG	C13-C14-C15-C16
27	N	623	LMG	C31-C32-C33-C34
27	Q	401	LMG	C11-C12-C13-C14
24	D	408	DGD	C5A-C6A-C7A-C8A
22	Q	403	PHO	O1D-CGD-O2D-CED
24	Q	409	DGD	C3A-C4A-C5A-C6A
24	Q	409	DGD	CEB-CFB-CGB-CHB
26	N	601	SQD	C11-C10-C9-C8
23	J	101	PL9	C17-C18-C19-C20
25	G	412	LHG	O10-C23-O8-C6
21	B	601	CLA	C2B-C3B-CAB-CBB
21	B	602	CLA	C2B-C3B-CAB-CBB
21	B	603	CLA	C2B-C3B-CAB-CBB
21	B	615	CLA	C2B-C3B-CAB-CBB
21	C	509	CLA	C2B-C3B-CAB-CBB
21	C	513	CLA	C2B-C3B-CAB-CBB
21	N	605	CLA	C2B-C3B-CAB-CBB
21	N	606	CLA	C2B-C3B-CAB-CBB
21	N	607	CLA	C2B-C3B-CAB-CBB
21	N	619	CLA	C2B-C3B-CAB-CBB
21	P	504	CLA	C2B-C3B-CAB-CBB
21	P	509	CLA	C2B-C3B-CAB-CBB
21	P	513	CLA	C2B-C3B-CAB-CBB
30	B	618	BCR	C23-C24-C25-C26
30	B	618	BCR	C23-C24-C25-C30
30	H	101	BCR	C1-C6-C7-C8
30	H	101	BCR	C5-C6-C7-C8
30	K	101	BCR	C23-C24-C25-C26
30	K	101	BCR	C23-C24-C25-C30
30	T	102	BCR	C23-C24-C25-C26
30	T	102	BCR	C23-C24-C25-C30
30	W	101	BCR	C1-C6-C7-C8
30	W	101	BCR	C5-C6-C7-C8
30	c	101	BCR	C23-C24-C25-C26
30	c	101	BCR	C23-C24-C25-C30
25	A	408	LHG	C8-C7-O7-C5
24	C	517	DGD	C2A-C3A-C4A-C5A
24	P	518	DGD	C2A-C3A-C4A-C5A
24	Q	409	DGD	CCB-CDB-CEB-CFB
27	B	622	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
24	B	621	DGD	C5B-C6B-C7B-C8B
24	D	408	DGD	CCB-CDB-CEB-CFB
25	G	412	LHG	C11-C10-C9-C8
27	N	623	LMG	C15-C16-C17-C18
25	A	411	LHG	O10-C23-O8-C6
23	G	407	PL9	C4-C3-C7-C8
24	P	519	DGD	C3B-C4B-C5B-C6B
27	B	623	LMG	C31-C32-C33-C34
27	C	519	LMG	O9-C10-O7-C8
27	D	407	LMG	O9-C10-O7-C8
27	Q	407	LMG	O9-C10-O7-C8
24	P	518	DGD	CAB-CBB-CCB-CDB
26	F	101	SQD	C27-C28-C29-C30
27	B	622	LMG	C15-C16-C17-C18
21	N	608	CLA	C15-C16-C17-C18
21	P	505	CLA	C15-C16-C17-C18
21	N	617	CLA	C2-C3-C5-C6
23	D	404	PL9	C18-C19-C21-C22
24	Q	409	DGD	C2A-C3A-C4A-C5A
27	D	412	LMG	C31-C32-C33-C34
24	B	621	DGD	C7A-C8A-C9A-CAA
24	C	517	DGD	C2B-C3B-C4B-C5B
27	A	410	LMG	C14-C15-C16-C17
27	D	407	LMG	C13-C14-C15-C16
27	Q	401	LMG	C31-C32-C33-C34
31	B	629	LMT	C2-C3-C4-C5
27	M	101	LMG	C2-C1-O1-C7
21	N	620	CLA	C15-C16-C17-C18
27	N	622	LMG	C15-C16-C17-C18
24	C	516	DGD	C4B-C5B-C6B-C7B
24	N	602	DGD	C8B-C9B-CAB-CBB
27	I	102	LMG	C13-C14-C15-C16
27	I	102	LMG	C16-C17-C18-C19
27	N	622	LMG	C36-C37-C38-C39
31	B	629	LMT	C7-C8-C9-C10
31	N	603	LMT	C7-C8-C9-C10
24	N	602	DGD	O6E-C5E-C6E-O5E
24	C	518	DGD	C2B-C1B-O2G-C2G
26	B	627	SQD	C8-C7-O47-C45
26	N	601	SQD	C8-C7-O47-C45
27	P	520	LMG	C11-C10-O7-C8
27	P	521	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	P	519	DGD	O1B-C1B-O2G-C2G
25	A	408	LHG	O9-C7-O7-C5
26	B	627	SQD	O49-C7-O47-C45
26	N	601	SQD	O49-C7-O47-C45
27	P	520	LMG	O9-C10-O7-C8
24	D	408	DGD	C2A-C3A-C4A-C5A
27	B	622	LMG	C17-C18-C19-C20
27	G	411	LMG	C30-C31-C32-C33
23	A	406	PL9	C7-C8-C9-C10
30	b	102	BCR	C7-C8-C9-C10
27	A	410	LMG	C29-C30-C31-C32
27	D	407	LMG	C32-C33-C34-C35
27	G	411	LMG	C14-C15-C16-C17
21	N	613	CLA	C4-C3-C5-C6
27	D	412	LMG	C28-C29-C30-C31
27	E	102	LMG	C28-C29-C30-C31
24	C	517	DGD	C4B-C5B-C6B-C7B
27	N	623	LMG	C13-C14-C15-C16
27	a	102	LMG	C13-C14-C15-C16
27	a	102	LMG	C16-C17-C18-C19
21	P	509	CLA	O1D-CGD-O2D-CED
27	N	622	LMG	C17-C18-C19-C20
27	B	623	LMG	O10-C28-O8-C9
27	N	623	LMG	O10-C28-O8-C9
24	W	102	DGD	C4B-C5B-C6B-C7B
24	C	518	DGD	O1B-C1B-O2G-C2G
27	D	412	LMG	O6-C5-C6-O5
24	B	628	DGD	C8B-C9B-CAB-CBB
27	A	410	LMG	C30-C31-C32-C33
27	B	622	LMG	C36-C37-C38-C39
26	B	627	SQD	C11-C10-C9-C8
27	Q	407	LMG	C32-C33-C34-C35
27	B	622	LMG	C28-C29-C30-C31
27	G	411	LMG	C29-C30-C31-C32
24	C	517	DGD	O2G-C2G-C3G-O3G
24	P	518	DGD	O2G-C2G-C3G-O3G
26	A	409	SQD	O47-C45-C46-O48
26	B	624	SQD	O6-C44-C45-O47
26	Q	408	SQD	O6-C44-C45-O47
27	A	410	LMG	O1-C7-C8-O7
27	G	411	LMG	O1-C7-C8-O7
27	a	102	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
24	B	621	DGD	C4B-C5B-C6B-C7B
26	A	409	SQD	C15-C16-C17-C18
21	B	615	CLA	C5-C6-C7-C8
26	G	410	SQD	C17-C18-C19-C20
21	N	605	CLA	C2C-C3C-CAC-CBC
21	C	503	CLA	C8-C10-C11-C12
22	Q	403	PHO	C10-C11-C12-C13
27	N	622	LMG	C18-C19-C20-C21
27	Q	401	LMG	C28-C29-C30-C31
23	Q	405	PL9	C42-C43-C44-C45
27	E	102	LMG	O6-C5-C6-O5
26	B	627	SQD	C11-C12-C13-C14
24	C	516	DGD	C4D-C5D-C6D-O5D
24	P	517	DGD	C4D-C5D-C6D-O5D
21	A	403	CLA	O1D-CGD-O2D-CED
22	D	402	PHO	O1D-CGD-O2D-CED
24	P	519	DGD	C8B-C9B-CAB-CBB
27	B	623	LMG	C15-C16-C17-C18
21	A	402	CLA	C5-C6-C7-C8
21	C	502	CLA	C13-C15-C16-C17
21	G	403	CLA	C5-C6-C7-C8
21	N	614	CLA	C10-C11-C12-C13
27	E	102	LMG	C17-C18-C19-C20
21	B	612	CLA	CBD-CGD-O2D-CED
27	B	622	LMG	C18-C19-C20-C21
21	N	609	CLA	C15-C16-C17-C18
21	B	606	CLA	C1A-C2A-CAA-CBA
21	C	507	CLA	C1A-C2A-CAA-CBA
21	C	512	CLA	C1A-C2A-CAA-CBA
21	D	401	CLA	C1A-C2A-CAA-CBA
21	N	610	CLA	C1A-C2A-CAA-CBA
21	P	507	CLA	C1A-C2A-CAA-CBA
21	P	512	CLA	C1A-C2A-CAA-CBA
27	Q	401	LMG	O6-C5-C6-O5
21	B	610	CLA	C10-C11-C12-C13
21	N	619	CLA	C5-C6-C7-C8
21	P	505	CLA	C8-C10-C11-C12
24	C	516	DGD	C2A-C3A-C4A-C5A
24	Q	409	DGD	C4B-C5B-C6B-C7B
27	B	622	LMG	C20-C21-C22-C23
24	C	518	DGD	CAB-CBB-CCB-CDB
21	B	602	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	B	606	CLA	C12-C13-C15-C16
21	B	609	CLA	C12-C13-C15-C16
21	B	613	CLA	C11-C10-C8-C7
21	B	615	CLA	C12-C13-C15-C16
21	C	502	CLA	C12-C13-C15-C16
21	C	503	CLA	C11-C10-C8-C7
21	C	505	CLA	C12-C13-C15-C16
21	C	511	CLA	C11-C10-C8-C7
21	C	513	CLA	C11-C10-C8-C7
21	D	401	CLA	C12-C13-C15-C16
21	G	404	CLA	C6-C7-C8-C10
21	N	610	CLA	C12-C13-C15-C16
21	N	617	CLA	C11-C10-C8-C7
21	N	619	CLA	C12-C13-C15-C16
21	P	502	CLA	C12-C13-C15-C16
21	P	503	CLA	C11-C10-C8-C7
21	P	511	CLA	C11-C10-C8-C7
21	P	513	CLA	C11-C10-C8-C7
21	Q	402	CLA	C12-C13-C15-C16
24	D	408	DGD	C4B-C5B-C6B-C7B
21	B	603	CLA	C5-C6-C7-C8
21	B	605	CLA	C15-C16-C17-C18
26	S	102	SQD	C15-C16-C17-C18
21	N	613	CLA	C5-C6-C7-C8
21	Q	402	CLA	C5-C6-C7-C8
21	B	609	CLA	C4-C3-C5-C6
27	Q	407	LMG	C14-C15-C16-C17
21	C	505	CLA	C8-C10-C11-C12
21	N	610	CLA	C2A-CAA-CBA-CGA
21	B	602	CLA	C11-C10-C8-C9
21	B	608	CLA	C11-C12-C13-C14
21	B	609	CLA	C14-C13-C15-C16
21	B	615	CLA	C11-C10-C8-C9
21	C	503	CLA	C11-C12-C13-C14
21	C	508	CLA	C11-C10-C8-C9
21	G	404	CLA	C6-C7-C8-C9
21	N	613	CLA	C14-C13-C15-C16
21	N	619	CLA	C14-C13-C15-C16
21	P	503	CLA	C11-C12-C13-C14
21	P	505	CLA	C14-C13-C15-C16
21	P	513	CLA	C11-C10-C8-C9
27	E	102	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
27	G	411	LMG	C31-C32-C33-C34
27	N	622	LMG	C20-C21-C22-C23
24	B	621	DGD	C3B-C4B-C5B-C6B
27	R	102	LMG	O6-C5-C6-O5
24	W	102	DGD	C3B-C4B-C5B-C6B
27	D	407	LMG	C2-C1-O1-C7
27	Q	407	LMG	C2-C1-O1-C7
21	N	614	CLA	C13-C15-C16-C17
21	P	502	CLA	C13-C15-C16-C17
21	C	510	CLA	O1D-CGD-O2D-CED
23	G	407	PL9	C24-C26-C27-C28
24	B	621	DGD	O1G-C1G-C2G-C3G
24	C	517	DGD	C1G-C2G-C3G-O3G
24	P	518	DGD	C1G-C2G-C3G-O3G
26	G	410	SQD	C44-C45-C46-O48
27	C	519	LMG	C7-C8-C9-O8
27	P	520	LMG	C7-C8-C9-O8
27	e	102	LMG	C7-C8-C9-O8
21	B	610	CLA	C13-C15-C16-C17
22	D	402	PHO	C10-C11-C12-C13
24	P	517	DGD	C2A-C3A-C4A-C5A
27	N	622	LMG	C28-C29-C30-C31
24	A	407	DGD	C5B-C6B-C7B-C8B
26	G	410	SQD	C15-C16-C17-C18
26	N	601	SQD	C11-C12-C13-C14
21	N	610	CLA	C10-C11-C12-C13
23	Q	405	PL9	C35-C34-C36-C37
27	B	622	LMG	C19-C20-C21-C22
27	R	102	LMG	C18-C19-C20-C21
27	N	622	LMG	C19-C20-C21-C22
30	B	620	BCR	C21-C22-C23-C24
21	N	607	CLA	C13-C15-C16-C17
24	G	408	DGD	C5B-C6B-C7B-C8B
27	D	407	LMG	C14-C15-C16-C17
31	N	625	LMT	C2B-C1B-O1B-C4'
21	C	505	CLA	C15-C16-C17-C18
26	F	101	SQD	C11-C12-C13-C14
21	A	402	CLA	O2A-C1-C2-C3
21	C	509	CLA	O2A-C1-C2-C3
24	D	408	DGD	C1G-C2G-O2G-C1B
24	Q	409	DGD	C1G-C2G-O2G-C1B
24	P	518	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
26	A	409	SQD	C27-C28-C29-C30
26	G	410	SQD	C7-C8-C9-C10
26	G	410	SQD	C27-C28-C29-C30
26	B	627	SQD	C24-C23-O48-C46
26	N	601	SQD	C24-C23-O48-C46
27	R	102	LMG	C17-C18-C19-C20
23	A	406	PL9	C35-C34-C36-C37
23	D	404	PL9	C35-C34-C36-C37
24	B	621	DGD	CAB-CBB-CCB-CDB
26	N	601	SQD	C9-C10-C11-C12
26	S	102	SQD	C11-C12-C13-C14
24	A	407	DGD	C3B-C4B-C5B-C6B
24	P	518	DGD	C4A-C5A-C6A-C7A
24	P	519	DGD	O1G-C1G-C2G-O2G
26	A	414	SQD	O6-C44-C45-O47
26	G	401	SQD	O6-C44-C45-O47
27	M	101	LMG	C29-C28-O8-C9
27	D	406	LMG	C38-C39-C40-C41
21	B	601	CLA	C2C-C3C-CAC-CBC
24	D	408	DGD	C7A-C8A-C9A-CAA
26	A	409	SQD	C17-C18-C19-C20
27	N	623	LMG	C12-C13-C14-C15
27	Q	406	LMG	C31-C32-C33-C34
24	W	102	DGD	CAB-CBB-CCB-CDB
21	P	501	CLA	C13-C15-C16-C17
24	C	517	DGD	C3A-C4A-C5A-C6A
24	G	408	DGD	C7B-C8B-C9B-CAB
24	P	518	DGD	C4B-C5B-C6B-C7B
23	A	406	PL9	C32-C33-C34-C35
23	G	407	PL9	C32-C33-C34-C35
24	C	517	DGD	CCB-CDB-CEB-CFB
21	B	614	CLA	C2C-C3C-CAC-CBC
21	B	605	CLA	C10-C11-C12-C13
21	B	609	CLA	C5-C6-C7-C8
21	B	612	CLA	C4-C3-C5-C6
24	P	519	DGD	CFA-CGA-CHA-CIA
24	B	628	DGD	C4A-C5A-C6A-C7A
31	I	103	LMT	C5'-C4'-O1B-C1B
24	C	518	DGD	C8B-C9B-CAB-CBB
27	D	412	LMG	C15-C16-C17-C18
27	Q	407	LMG	C13-C14-C15-C16
31	B	626	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
24	C	518	DGD	CDB-CEB-CFB-CGB
27	N	622	LMG	C30-C31-C32-C33
21	A	403	CLA	C6-C7-C8-C9
21	B	606	CLA	C14-C13-C15-C16
21	B	615	CLA	C14-C13-C15-C16
21	C	502	CLA	C14-C13-C15-C16
21	C	505	CLA	C14-C13-C15-C16
21	C	511	CLA	C11-C10-C8-C9
21	D	401	CLA	C14-C13-C15-C16
21	N	606	CLA	C11-C10-C8-C9
21	N	610	CLA	C14-C13-C15-C16
21	N	619	CLA	C11-C10-C8-C9
21	P	502	CLA	C14-C13-C15-C16
21	P	508	CLA	C11-C10-C8-C9
21	P	511	CLA	C11-C10-C8-C9
21	Q	402	CLA	C14-C13-C15-C16
22	Q	403	PHO	C6-C7-C8-C9
22	Q	403	PHO	C11-C10-C8-C9
26	N	601	SQD	C12-C13-C14-C15
21	D	401	CLA	C5-C6-C7-C8
21	B	614	CLA	C4B-C3B-CAB-CBB
21	C	508	CLA	C4B-C3B-CAB-CBB
21	G	406	CLA	C4B-C3B-CAB-CBB
21	N	618	CLA	C4B-C3B-CAB-CBB
21	P	508	CLA	C4B-C3B-CAB-CBB
27	A	410	LMG	C31-C32-C33-C34
31	N	604	LMT	C5'-C4'-O1B-C1B
31	a	103	LMT	C5'-C4'-O1B-C1B
21	B	606	CLA	C10-C11-C12-C13
21	N	609	CLA	C10-C11-C12-C13
21	N	620	CLA	C8-C10-C11-C12
27	E	102	LMG	C19-C20-C21-C22
21	B	616	CLA	C2A-CAA-CBA-CGA
21	B	603	CLA	C13-C15-C16-C17
26	B	627	SQD	C9-C10-C11-C12
27	B	622	LMG	C30-C31-C32-C33
27	Q	406	LMG	C36-C37-C38-C39
26	A	409	SQD	C7-C8-C9-C10
27	N	623	LMG	C4-C5-C6-O5
24	W	102	DGD	C4D-C5D-C6D-O5D
27	Q	406	LMG	C38-C39-C40-C41
21	A	402	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	A	403	CLA	C6-C7-C8-C10
21	B	602	CLA	C6-C7-C8-C10
21	B	602	CLA	C11-C10-C8-C7
21	B	608	CLA	C11-C12-C13-C15
21	B	610	CLA	C12-C13-C15-C16
21	B	613	CLA	C11-C12-C13-C15
21	B	615	CLA	C11-C10-C8-C7
21	C	504	CLA	C6-C7-C8-C10
21	C	506	CLA	C11-C12-C13-C15
21	C	506	CLA	C12-C13-C15-C16
21	C	508	CLA	C11-C10-C8-C7
21	C	510	CLA	C6-C7-C8-C10
21	G	403	CLA	C6-C7-C8-C10
21	G	406	CLA	C11-C10-C8-C7
21	N	605	CLA	C6-C7-C8-C10
21	N	606	CLA	C6-C7-C8-C10
21	N	606	CLA	C11-C10-C8-C7
21	N	613	CLA	C12-C13-C15-C16
21	N	614	CLA	C12-C13-C15-C16
21	N	615	CLA	C6-C7-C8-C10
21	P	504	CLA	C6-C7-C8-C10
21	P	505	CLA	C12-C13-C15-C16
21	P	506	CLA	C12-C13-C15-C16
21	P	508	CLA	C11-C10-C8-C7
21	P	508	CLA	C12-C13-C15-C16
21	C	501	CLA	C13-C15-C16-C17
21	C	509	CLA	C10-C11-C12-C13
26	S	102	SQD	C29-C30-C31-C32
27	I	102	LMG	C18-C19-C20-C21
21	B	616	CLA	C8-C10-C11-C12
27	R	102	LMG	C19-C20-C21-C22
24	B	621	DGD	C4D-C5D-C6D-O5D
21	C	513	CLA	C3A-C2A-CAA-CBA
21	N	609	CLA	C3A-C2A-CAA-CBA
21	N	615	CLA	C4-C3-C5-C6
21	N	616	CLA	C4-C3-C5-C6
21	P	504	CLA	C3A-C2A-CAA-CBA
21	P	513	CLA	C3A-C2A-CAA-CBA
22	A	404	PHO	C5-C6-C7-C8
24	G	408	DGD	C7A-C8A-C9A-CAA
24	P	518	DGD	C3A-C4A-C5A-C6A
26	N	601	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
26	F	101	SQD	C15-C16-C17-C18
27	A	410	LMG	C19-C20-C21-C22
24	B	628	DGD	O6E-C5E-C6E-O5E
24	B	628	DGD	C5B-C6B-C7B-C8B
23	A	406	PL9	C24-C26-C27-C28
24	N	602	DGD	C1G-C2G-C3G-O3G
24	Q	409	DGD	C1G-C2G-C3G-O3G
24	W	102	DGD	O1G-C1G-C2G-C3G
26	A	409	SQD	C44-C45-C46-O48
26	B	624	SQD	O6-C44-C45-C46
26	Q	408	SQD	O6-C44-C45-C46
27	B	623	LMG	C7-C8-C9-O8
27	G	411	LMG	O1-C7-C8-C9
27	N	623	LMG	C7-C8-C9-O8
24	C	518	DGD	CFA-CGA-CHA-CIA
24	C	518	DGD	CEA-CFA-CGA-CHA
21	A	403	CLA	C1-C2-C3-C4
21	B	604	CLA	C1-C2-C3-C4
21	B	605	CLA	C1-C2-C3-C4
21	B	608	CLA	C1-C2-C3-C4
21	B	611	CLA	C1-C2-C3-C4
21	B	612	CLA	C1-C2-C3-C4
21	C	506	CLA	C1-C2-C3-C4
21	C	511	CLA	C1-C2-C3-C4
21	G	404	CLA	C1-C2-C3-C4
21	N	609	CLA	C1-C2-C3-C4
21	N	612	CLA	C1-C2-C3-C4
21	N	615	CLA	C1-C2-C3-C4
21	N	616	CLA	C1-C2-C3-C4
21	P	505	CLA	C1-C2-C3-C4
21	P	506	CLA	C1-C2-C3-C4
27	B	623	LMG	C12-C13-C14-C15
21	B	611	CLA	C4-C3-C5-C6
27	N	622	LMG	C32-C33-C34-C35
21	N	613	CLA	C2-C3-C5-C6
24	Q	409	DGD	C8B-C9B-CAB-CBB
21	B	603	CLA	O1D-CGD-O2D-CED
27	G	411	LMG	C19-C20-C21-C22
27	D	406	LMG	C36-C37-C38-C39
24	P	519	DGD	CAB-CBB-CCB-CDB
24	C	516	DGD	C4E-C5E-C6E-O5E
30	B	617	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	C	515	BCR	C23-C24-C25-C30
30	D	405	BCR	C1-C6-C7-C8
30	T	101	BCR	C1-C6-C7-C8
30	Z	101	BCR	C1-C6-C7-C8
30	P	515	BCR	C1-C6-C7-C8
30	P	516	BCR	C23-C24-C25-C30
30	S	101	BCR	C1-C6-C7-C8
21	N	609	CLA	C13-C15-C16-C17
22	G	405	PHO	C5-C6-C7-C8
31	B	630	LMT	C1-C2-C3-C4
27	D	406	LMG	C31-C32-C33-C34
31	B	630	LMT	C5'-C4'-O1B-C1B
26	B	627	SQD	O10-C23-O48-C46
27	Q	401	LMG	C12-C13-C14-C15
24	D	408	DGD	C8B-C9B-CAB-CBB
24	P	519	DGD	CEA-CFA-CGA-CHA
21	B	606	CLA	C2A-CAA-CBA-CGA
24	C	518	DGD	O1G-C1G-C2G-O2G
27	B	622	LMG	O1-C7-C8-O7
27	C	519	LMG	O7-C8-C9-O8
23	A	406	PL9	C4-C3-C7-C8
24	D	408	DGD	CBA-CCA-CDA-CEA
26	G	401	SQD	C17-C18-C19-C20
26	G	410	SQD	C24-C25-C26-C27
24	A	407	DGD	C7A-C8A-C9A-CAA
24	B	621	DGD	C2A-C3A-C4A-C5A
24	N	602	DGD	C4A-C5A-C6A-C7A
27	A	410	LMG	C20-C21-C22-C23
24	Q	409	DGD	CBA-CCA-CDA-CEA
21	B	608	CLA	C1-C2-C3-C5
21	B	614	CLA	C1-C2-C3-C5
21	C	506	CLA	C1-C2-C3-C5
21	N	612	CLA	C1-C2-C3-C5
21	N	618	CLA	C1-C2-C3-C5
21	P	505	CLA	C1-C2-C3-C5
21	P	506	CLA	C1-C2-C3-C5
21	P	512	CLA	C1-C2-C3-C5
24	G	408	DGD	C3B-C4B-C5B-C6B
24	N	602	DGD	C2A-C3A-C4A-C5A
27	D	412	LMG	C12-C13-C14-C15
21	N	606	CLA	CBD-CGD-O2D-CED
21	A	402	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	B	605	CLA	C11-C10-C8-C9
21	B	613	CLA	C11-C12-C13-C14
21	C	503	CLA	C11-C10-C8-C9
21	C	506	CLA	C14-C13-C15-C16
21	C	512	CLA	C14-C13-C15-C16
21	C	513	CLA	C11-C10-C8-C9
21	N	609	CLA	C11-C10-C8-C9
21	N	617	CLA	C11-C12-C13-C14
21	N	620	CLA	C11-C10-C8-C9
21	P	506	CLA	C14-C13-C15-C16
26	B	627	SQD	C10-C11-C12-C13
27	C	519	LMG	C34-C35-C36-C37
31	N	625	LMT	O5B-C1B-O1B-C4'
27	a	102	LMG	C18-C19-C20-C21
24	P	519	DGD	CDB-CEB-CFB-CGB
26	N	601	SQD	C10-C11-C12-C13
24	W	102	DGD	C2A-C3A-C4A-C5A
31	B	626	LMT	O5B-C1B-O1B-C4'
26	F	101	SQD	C29-C30-C31-C32
21	N	611	CLA	O1D-CGD-O2D-CED
27	P	520	LMG	C34-C35-C36-C37
24	A	407	DGD	C7B-C8B-C9B-CAB
21	C	513	CLA	C5-C6-C7-C8
21	P	509	CLA	C10-C11-C12-C13
24	A	407	DGD	C4B-C5B-C6B-C7B
21	P	512	CLA	CAA-CBA-CGA-O2A
21	N	615	CLA	C8-C10-C11-C12
21	P	508	CLA	C5-C6-C7-C8
21	P	510	CLA	C13-C15-C16-C17
22	D	402	PHO	C13-C15-C16-C17
27	A	410	LMG	C15-C16-C17-C18
21	P	503	CLA	C15-C16-C17-C18
26	B	627	SQD	C12-C13-C14-C15
21	B	605	CLA	C11-C10-C8-C7
21	B	608	CLA	C6-C7-C8-C10
21	B	616	CLA	C11-C10-C8-C7
21	C	511	CLA	C6-C7-C8-C10
21	C	512	CLA	C11-C12-C13-C15
21	C	512	CLA	C12-C13-C15-C16
21	G	403	CLA	C12-C13-C15-C16
21	N	609	CLA	C11-C10-C8-C7
21	N	612	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	N	612	CLA	C11-C12-C13-C15
21	N	617	CLA	C11-C12-C13-C15
21	N	619	CLA	C11-C10-C8-C7
21	N	620	CLA	C11-C10-C8-C7
21	P	506	CLA	C11-C12-C13-C15
21	P	511	CLA	C6-C7-C8-C10
21	P	512	CLA	C11-C12-C13-C15
21	P	512	CLA	C12-C13-C15-C16
22	D	402	PHO	C12-C13-C15-C16
22	Q	403	PHO	C6-C7-C8-C10
31	N	604	LMT	C1-C2-C3-C4
24	G	408	DGD	C4B-C5B-C6B-C7B
30	P	515	BCR	C7-C8-C9-C10
27	G	411	LMG	C20-C21-C22-C23
24	B	628	DGD	C5D-C6D-O5D-C1E
24	N	602	DGD	C5D-C6D-O5D-C1E
26	A	414	SQD	C5-C6-S-O8
26	B	624	SQD	C45-C44-O6-C1
26	G	401	SQD	C5-C6-S-O8
26	Q	408	SQD	C45-C44-O6-C1
27	D	407	LMG	C8-C7-O1-C1
27	Q	407	LMG	C8-C7-O1-C1
24	B	628	DGD	C4B-C5B-C6B-C7B
27	M	101	LMG	O10-C28-O8-C9
21	B	605	CLA	C13-C15-C16-C17
21	C	510	CLA	C13-C15-C16-C17
24	P	519	DGD	C3G-C2G-O2G-C1B
27	E	102	LMG	C7-C8-O7-C10
27	R	102	LMG	C7-C8-O7-C10
27	Q	401	LMG	C15-C16-C17-C18
27	B	623	LMG	C4-C5-C6-O5
24	N	602	DGD	C5B-C6B-C7B-C8B
26	F	101	SQD	C12-C13-C14-C15
22	A	404	PHO	C3-C5-C6-C7
26	S	102	SQD	C10-C11-C12-C13
21	C	512	CLA	CAA-CBA-CGA-O2A
24	Q	409	DGD	O6E-C1E-O5D-C6D
24	B	628	DGD	C1G-C2G-C3G-O3G
24	D	408	DGD	C1G-C2G-C3G-O3G
27	B	622	LMG	O1-C7-C8-C9
34	E	101	HEM	C4B-C3B-CAB-CBB
34	R	101	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	C	511	CLA	C10-C11-C12-C13
21	N	608	CLA	C2-C3-C5-C6
23	G	407	PL9	C33-C34-C36-C37
24	D	408	DGD	CBB-CCB-CDB-CEB
24	B	621	DGD	O1G-C1G-C2G-O2G
24	D	408	DGD	O2G-C2G-C3G-O3G
24	Q	409	DGD	O2G-C2G-C3G-O3G
24	W	102	DGD	O1G-C1G-C2G-O2G
27	B	623	LMG	O7-C8-C9-O8
27	M	101	LMG	O7-C8-C9-O8
27	N	623	LMG	O7-C8-C9-O8
27	P	521	LMG	O7-C8-C9-O8
21	B	616	CLA	C11-C10-C8-C9
21	C	512	CLA	C11-C12-C13-C14
21	G	403	CLA	C14-C13-C15-C16
21	N	605	CLA	C6-C7-C8-C9
21	N	617	CLA	C11-C10-C8-C9
21	P	512	CLA	C11-C12-C13-C14
21	P	512	CLA	C14-C13-C15-C16
21	P	512	CLA	C16-C17-C18-C19
26	A	409	SQD	C24-C25-C26-C27
27	e	102	LMG	C30-C31-C32-C33
21	B	606	CLA	C15-C16-C17-C18
21	C	510	CLA	C5-C6-C7-C8
24	B	628	DGD	C2A-C3A-C4A-C5A
27	N	622	LMG	C13-C14-C15-C16
25	G	412	LHG	C7-C8-C9-C10
26	S	102	SQD	C12-C13-C14-C15
27	B	622	LMG	C16-C17-C18-C19
27	N	622	LMG	C16-C17-C18-C19
27	G	411	LMG	C15-C16-C17-C18
27	E	102	LMG	O7-C10-C11-C12
27	a	102	LMG	C19-C20-C21-C22
21	N	618	CLA	C16-C17-C18-C20
21	N	614	CLA	C5-C6-C7-C8
24	C	517	DGD	C4A-C5A-C6A-C7A
23	D	404	PL9	C22-C23-C24-C26
26	A	414	SQD	C10-C11-C12-C13
24	P	519	DGD	C1A-C2A-C3A-C4A
25	A	411	LHG	C7-C8-C9-C10
21	A	403	CLA	C5-C6-C7-C8
21	B	614	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	N	605	CLA	C4C-C3C-CAC-CBC
21	P	512	CLA	C16-C17-C18-C20
27	a	102	LMG	C10-C11-C12-C13
24	N	602	DGD	C4B-C5B-C6B-C7B
27	D	412	LMG	C13-C14-C15-C16
22	A	404	PHO	CBD-CGD-O2D-CED
21	C	501	CLA	C1A-C2A-CAA-CBA
21	N	606	CLA	C1A-C2A-CAA-CBA
21	B	606	CLA	O1D-CGD-O2D-CED
24	C	518	DGD	CBA-CCA-CDA-CEA
27	R	102	LMG	O7-C10-C11-C12
23	A	406	PL9	C33-C34-C36-C37
30	Z	101	BCR	C7-C8-C9-C10
24	Q	409	DGD	C7A-C8A-C9A-CAA
27	C	520	LMG	C13-C14-C15-C16
21	N	615	CLA	C16-C17-C18-C19
21	N	620	CLA	C2A-CAA-CBA-CGA
27	C	519	LMG	C16-C17-C18-C19
21	A	402	CLA	C6-C7-C8-C10
21	A	405	CLA	C11-C10-C8-C7
21	B	603	CLA	C11-C12-C13-C15
21	B	611	CLA	C6-C7-C8-C10
21	B	611	CLA	C11-C10-C8-C7
21	C	501	CLA	C11-C12-C13-C15
21	C	502	CLA	C11-C10-C8-C7
21	C	508	CLA	C12-C13-C15-C16
21	C	513	CLA	C6-C7-C8-C10
21	D	403	CLA	C11-C10-C8-C7
21	N	609	CLA	C11-C12-C13-C15
21	N	615	CLA	C11-C10-C8-C7
21	N	620	CLA	C12-C13-C15-C16
21	P	501	CLA	C11-C12-C13-C15
21	P	502	CLA	C11-C10-C8-C7
21	P	510	CLA	C6-C7-C8-C10
21	P	513	CLA	C6-C7-C8-C10
21	Q	404	CLA	C11-C10-C8-C7
22	D	402	PHO	C6-C7-C8-C10
22	D	402	PHO	C11-C10-C8-C7
21	C	512	CLA	C16-C17-C18-C19
21	C	512	CLA	C16-C17-C18-C20
21	N	615	CLA	C16-C17-C18-C20
21	N	618	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
21	B	614	CLA	C4C-C3C-CAC-CBC
27	B	622	LMG	C32-C33-C34-C35
25	A	408	LHG	C9-C10-C11-C12
26	A	414	SQD	C12-C13-C14-C15
27	P	520	LMG	C16-C17-C18-C19
27	P	521	LMG	C13-C14-C15-C16
27	M	101	LMG	C4-C5-C6-O5
27	B	622	LMG	C13-C14-C15-C16
21	B	616	CLA	C3A-C2A-CAA-CBA
21	C	504	CLA	C3A-C2A-CAA-CBA
26	G	401	SQD	C26-C27-C28-C29
26	G	410	SQD	C29-C30-C31-C32
21	B	609	CLA	C2-C3-C5-C6
27	Q	406	LMG	C4-C5-C6-O5
21	B	613	CLA	C11-C10-C8-C9
21	C	501	CLA	C11-C12-C13-C14
21	C	504	CLA	C6-C7-C8-C9
21	C	510	CLA	C6-C7-C8-C9
21	G	406	CLA	C11-C10-C8-C9
21	N	612	CLA	C11-C12-C13-C14
21	N	615	CLA	C6-C7-C8-C9
21	P	503	CLA	C11-C10-C8-C9
21	P	504	CLA	C6-C7-C8-C9
21	P	506	CLA	C11-C12-C13-C14
22	D	402	PHO	C11-C10-C8-C9
21	B	608	CLA	C13-C15-C16-C17
26	B	624	SQD	O5-C5-C6-S
26	Q	408	SQD	O5-C5-C6-S
27	Q	401	LMG	C13-C14-C15-C16
21	N	620	CLA	C3-C5-C6-C7
26	G	410	SQD	C10-C11-C12-C13
27	I	102	LMG	C19-C20-C21-C22
27	M	101	LMG	C13-C14-C15-C16
21	C	508	CLA	C5-C6-C7-C8
21	C	511	CLA	O1A-CGA-O2A-C1
26	B	627	SQD	O47-C45-C46-O48
26	F	101	SQD	O47-C45-C46-O48
26	N	601	SQD	O47-C45-C46-O48
26	S	102	SQD	O47-C45-C46-O48
27	N	622	LMG	O1-C7-C8-O7
27	P	520	LMG	O7-C8-C9-O8
27	D	406	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
26	B	627	SQD	C44-C45-C46-O48
26	N	601	SQD	C44-C45-C46-O48
27	N	622	LMG	O1-C7-C8-C9
21	B	610	CLA	C5-C6-C7-C8
22	G	405	PHO	C3-C5-C6-C7
21	B	605	CLA	CAD-CBD-CGD-O2D
21	C	506	CLA	CAD-CBD-CGD-O2D
21	N	609	CLA	CAD-CBD-CGD-O2D
21	B	607	CLA	O1D-CGD-O2D-CED
21	P	506	CLA	O1D-CGD-O2D-CED
26	A	409	SQD	C29-C30-C31-C32
21	G	404	CLA	C5-C6-C7-C8
21	B	611	CLA	C16-C17-C18-C20
24	B	621	DGD	C5A-C6A-C7A-C8A
21	B	613	CLA	C8-C10-C11-C12
25	G	409	LHG	C9-C10-C11-C12
27	a	102	LMG	O6-C5-C6-O5
21	B	614	CLA	CAD-CBD-CGD-O1D
21	C	506	CLA	CAD-CBD-CGD-O1D
21	C	508	CLA	CHA-CBD-CGD-O1D
21	C	509	CLA	CHA-CBD-CGD-O2D
21	C	512	CLA	CHA-CBD-CGD-O1D
21	N	617	CLA	CHA-CBD-CGD-O1D
21	N	618	CLA	CAD-CBD-CGD-O1D
21	P	506	CLA	CAD-CBD-CGD-O1D
21	P	509	CLA	CHA-CBD-CGD-O2D
25	A	408	LHG	C3-O3-P-O5
25	A	411	LHG	C3-O3-P-O5
25	G	409	LHG	C3-O3-P-O5
21	B	601	CLA	C4C-C3C-CAC-CBC
21	B	611	CLA	C16-C17-C18-C19
26	A	409	SQD	C10-C11-C12-C13
27	D	407	LMG	C11-C12-C13-C14
21	C	505	CLA	C4-C3-C5-C6
23	D	404	PL9	C15-C14-C16-C17
21	B	608	CLA	C2B-C3B-CAB-CBB
21	B	613	CLA	C2B-C3B-CAB-CBB
21	C	507	CLA	C2B-C3B-CAB-CBB
21	C	511	CLA	C2B-C3B-CAB-CBB
21	N	612	CLA	C2B-C3B-CAB-CBB
21	N	617	CLA	C2B-C3B-CAB-CBB
21	P	507	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	P	511	CLA	C2B-C3B-CAB-CBB
30	C	515	BCR	C1-C6-C7-C8
21	N	616	CLA	C2-C3-C5-C6
25	A	408	LHG	C2-C3-O3-P
25	G	409	LHG	C2-C3-O3-P
30	J	102	BCR	C7-C8-C9-C34
30	S	101	BCR	C37-C22-C23-C24
21	N	610	CLA	C15-C16-C17-C18
21	P	511	CLA	C10-C11-C12-C13
27	D	406	LMG	C34-C35-C36-C37
24	P	519	DGD	C4B-C5B-C6B-C7B
24	N	602	DGD	C5A-C6A-C7A-C8A
26	G	401	SQD	C12-C13-C14-C15
27	I	102	LMG	C29-C30-C31-C32
26	G	401	SQD	C10-C11-C12-C13
24	P	518	DGD	C1A-C2A-C3A-C4A
21	N	617	CLA	C8-C10-C11-C12
24	C	518	DGD	C3G-C2G-O2G-C1B
25	A	408	LHG	C4-C5-O7-C7
25	G	409	LHG	C4-C5-O7-C7
27	C	520	LMG	C7-C8-O7-C10
21	N	616	CLA	C8-C10-C11-C12
21	B	612	CLA	C8-C10-C11-C12
21	C	509	CLA	C5-C6-C7-C8
24	W	102	DGD	C7B-C8B-C9B-CAB
24	C	518	DGD	C1A-C2A-C3A-C4A
21	D	401	CLA	O1A-CGA-O2A-C1
21	A	405	CLA	C11-C10-C8-C9
21	B	603	CLA	C11-C12-C13-C14
21	B	611	CLA	C6-C7-C8-C9
21	C	506	CLA	C11-C12-C13-C14
21	C	513	CLA	C6-C7-C8-C9
21	D	403	CLA	C11-C10-C8-C9
21	N	620	CLA	C11-C12-C13-C14
21	P	501	CLA	C11-C12-C13-C14
21	P	508	CLA	C14-C13-C15-C16
21	P	513	CLA	C6-C7-C8-C9
22	D	402	PHO	C6-C7-C8-C9
22	D	402	PHO	C14-C13-C15-C16
22	Q	403	PHO	C14-C13-C15-C16
21	B	601	CLA	C6-C7-C8-C10
21	B	616	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	G	406	CLA	C11-C12-C13-C15
22	Q	403	PHO	C12-C13-C15-C16
21	N	618	CLA	C2C-C3C-CAC-CBC
27	I	102	LMG	C10-C11-C12-C13
27	G	411	LMG	C35-C36-C37-C38
22	G	405	PHO	CBD-CGD-O2D-CED
21	B	601	CLA	C16-C17-C18-C19
25	A	411	LHG	C11-C12-C13-C14
27	A	410	LMG	C38-C39-C40-C41
27	R	102	LMG	O7-C8-C9-O8
27	e	102	LMG	O7-C8-C9-O8
21	N	610	CLA	C13-C15-C16-C17
31	B	625	LMT	C4-C5-C6-C7
21	B	601	CLA	C16-C17-C18-C20
24	B	621	DGD	C7B-C8B-C9B-CAB
27	A	410	LMG	C11-C10-O7-C8
26	A	414	SQD	C7-C8-C9-C10
21	N	618	CLA	C13-C15-C16-C17
26	A	414	SQD	O6-C44-C45-C46
27	P	521	LMG	C7-C8-C9-O8
27	R	102	LMG	C28-C29-C30-C31
21	C	503	CLA	C15-C16-C17-C18
24	B	628	DGD	CAB-CBB-CCB-CDB
24	W	102	DGD	C5A-C6A-C7A-C8A
26	F	101	SQD	C10-C11-C12-C13
23	Q	405	PL9	C22-C23-C24-C26
30	S	101	BCR	C21-C22-C23-C24
21	C	501	CLA	C2A-CAA-CBA-CGA
21	N	609	CLA	C2A-CAA-CBA-CGA
21	N	618	CLA	C2A-CAA-CBA-CGA
21	P	501	CLA	C2A-CAA-CBA-CGA
24	C	517	DGD	CBB-CCB-CDB-CEB
27	D	412	LMG	C10-C11-C12-C13
24	A	407	DGD	C2A-C3A-C4A-C5A
21	B	601	CLA	C6-C7-C8-C9
21	C	508	CLA	C14-C13-C15-C16
21	N	615	CLA	C11-C10-C8-C9
21	P	510	CLA	C6-C7-C8-C9
21	Q	404	CLA	C11-C10-C8-C9
21	B	616	CLA	CBA-CGA-O2A-C1
21	B	611	CLA	C8-C10-C11-C12
21	A	405	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	Q	409	DGD	CBB-CCB-CDB-CEB
27	P	520	LMG	C30-C31-C32-C33
21	P	509	CLA	C5-C6-C7-C8
21	P	505	CLA	C4-C3-C5-C6
23	Q	405	PL9	C15-C14-C16-C17
21	B	616	CLA	C3-C5-C6-C7
26	A	414	SQD	C26-C27-C28-C29
21	B	614	CLA	C16-C17-C18-C19
24	N	602	DGD	C3A-C4A-C5A-C6A
21	A	405	CLA	C11-C12-C13-C15
21	B	602	CLA	C11-C12-C13-C15
21	C	502	CLA	C11-C12-C13-C15
21	C	505	CLA	C6-C7-C8-C10
21	N	606	CLA	C11-C12-C13-C15
21	P	505	CLA	C6-C7-C8-C10
21	P	513	CLA	C12-C13-C15-C16
24	P	518	DGD	CBB-CCB-CDB-CEB
27	G	411	LMG	C16-C17-C18-C19
27	C	519	LMG	C30-C31-C32-C33
27	I	102	LMG	C17-C18-C19-C20
26	A	414	SQD	C17-C18-C19-C20
27	a	102	LMG	C17-C18-C19-C20
21	B	614	CLA	C16-C17-C18-C20
27	Q	401	LMG	C10-C11-C12-C13
22	Q	403	PHO	C13-C15-C16-C17
21	B	614	CLA	O1A-CGA-O2A-C1
21	A	402	CLA	C3-C5-C6-C7
24	C	516	DGD	O2G-C2G-C3G-O3G
27	E	102	LMG	O7-C8-C9-O8
21	B	605	CLA	C3A-C2A-CAA-CBA
21	N	620	CLA	C3A-C2A-CAA-CBA
27	M	101	LMG	C30-C31-C32-C33
23	Q	405	PL9	C13-C14-C16-C17
21	B	610	CLA	C16-C17-C18-C19
24	D	408	DGD	O6E-C1E-O5D-C6D
21	B	613	CLA	C2-C1-O2A-CGA
21	N	617	CLA	C2-C1-O2A-CGA
21	N	618	CLA	C2-C1-O2A-CGA
21	P	505	CLA	C2-C1-O2A-CGA
21	P	510	CLA	C2-C1-O2A-CGA
21	G	403	CLA	C3-C5-C6-C7
27	C	519	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
25	G	412	LHG	C11-C12-C13-C14
21	B	612	CLA	C2-C3-C5-C6
24	P	519	DGD	O1G-C1G-C2G-C3G
24	N	602	DGD	CAB-CBB-CCB-CDB
24	D	408	DGD	C2B-C3B-C4B-C5B
26	A	409	SQD	C11-C10-C9-C8
31	N	624	LMT	C4-C5-C6-C7
21	N	608	CLA	O1A-CGA-O2A-C1
21	A	401	CLA	C11-C12-C13-C14
21	B	602	CLA	C11-C12-C13-C14
21	B	611	CLA	C11-C10-C8-C9
21	C	502	CLA	C11-C10-C8-C9
21	C	502	CLA	C11-C12-C13-C14
21	C	505	CLA	C6-C7-C8-C9
21	C	511	CLA	C14-C13-C15-C16
21	G	402	CLA	C11-C12-C13-C14
21	N	606	CLA	C11-C12-C13-C14
21	N	607	CLA	C11-C12-C13-C14
21	P	502	CLA	C11-C12-C13-C14
21	P	505	CLA	C6-C7-C8-C9
26	N	601	SQD	C15-C16-C17-C18
24	G	408	DGD	C2A-C3A-C4A-C5A
21	G	403	CLA	O2A-C1-C2-C3
27	A	410	LMG	O9-C10-O7-C8
21	B	613	CLA	C1-C2-C3-C4
21	C	510	CLA	C1-C2-C3-C4
21	C	513	CLA	C1-C2-C3-C4
21	N	608	CLA	C1-C2-C3-C4
21	N	617	CLA	C1-C2-C3-C4
21	P	510	CLA	C1-C2-C3-C4
21	P	511	CLA	C1-C2-C3-C4
21	P	513	CLA	C1-C2-C3-C4
23	D	404	PL9	C13-C14-C16-C17
24	P	519	DGD	CCB-CDB-CEB-CFB
27	a	102	LMG	C31-C32-C33-C34
25	G	412	LHG	O1-C1-C2-O2
24	C	516	DGD	C5A-C6A-C7A-C8A
21	A	403	CLA	C1A-C2A-CAA-CBA
21	B	605	CLA	C1A-C2A-CAA-CBA
21	C	504	CLA	C1A-C2A-CAA-CBA
21	P	501	CLA	C1A-C2A-CAA-CBA
21	P	504	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	Q	402	CLA	C1A-C2A-CAA-CBA
21	N	618	CLA	C4C-C3C-CAC-CBC
24	D	408	DGD	CAA-CBA-CCA-CDA
21	N	614	CLA	C16-C17-C18-C19
21	N	617	CLA	C16-C17-C18-C20
24	Q	409	DGD	C2B-C3B-C4B-C5B
27	G	411	LMG	C38-C39-C40-C41
24	C	518	DGD	C4B-C5B-C6B-C7B
24	P	519	DGD	CBA-CCA-CDA-CEA
21	A	405	CLA	C2B-C3B-CAB-CBB
21	B	614	CLA	C2B-C3B-CAB-CBB
21	C	508	CLA	C2B-C3B-CAB-CBB
21	P	508	CLA	C2B-C3B-CAB-CBB
30	B	617	BCR	C5-C6-C7-C8
30	C	515	BCR	C23-C24-C25-C26
30	D	405	BCR	C5-C6-C7-C8
30	I	101	BCR	C1-C6-C7-C8
30	I	101	BCR	C23-C24-C25-C30
30	T	101	BCR	C5-C6-C7-C8
30	Z	101	BCR	C5-C6-C7-C8
30	P	515	BCR	C5-C6-C7-C8
30	P	516	BCR	C1-C6-C7-C8
30	P	516	BCR	C23-C24-C25-C26
30	S	101	BCR	C5-C6-C7-C8
30	a	101	BCR	C1-C6-C7-C8
30	a	101	BCR	C23-C24-C25-C30
21	C	509	CLA	O1A-CGA-O2A-C1
31	B	630	LMT	C4-C5-C6-C7
26	G	401	SQD	C23-C24-C25-C26
27	P	520	LMG	C32-C33-C34-C35
21	P	512	CLA	C4-C3-C5-C6
27	D	412	LMG	C17-C18-C19-C20
23	Q	405	PL9	C18-C19-C21-C22
21	B	605	CLA	C11-C12-C13-C15
21	C	513	CLA	C12-C13-C15-C16
21	D	401	CLA	C11-C10-C8-C7
21	N	607	CLA	C11-C12-C13-C15
21	N	609	CLA	C6-C7-C8-C10
21	N	612	CLA	C11-C10-C8-C7
21	N	616	CLA	C12-C13-C15-C16
21	Q	402	CLA	C11-C10-C8-C7
31	B	630	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	N	604	LMT	C4-C5-C6-C7
27	D	412	LMG	C29-C30-C31-C32
27	G	411	LMG	C11-C12-C13-C14
27	a	102	LMG	C29-C30-C31-C32
27	C	519	LMG	C20-C21-C22-C23
27	B	623	LMG	C34-C35-C36-C37
24	C	517	DGD	C1A-C2A-C3A-C4A
21	B	604	CLA	O1A-CGA-O2A-C1
21	N	612	CLA	C13-C15-C16-C17
21	B	611	CLA	C2-C3-C5-C6
21	N	615	CLA	C2-C3-C5-C6
21	B	611	CLA	C1-C2-C3-C5
21	C	513	CLA	C1-C2-C3-C5
21	N	615	CLA	C1-C2-C3-C5
21	P	513	CLA	C1-C2-C3-C5
27	D	406	LMG	C4-C5-C6-O5
21	B	605	CLA	O1A-CGA-O2A-C1
21	P	507	CLA	C3-C5-C6-C7
21	A	405	CLA	C2A-CAA-CBA-CGA
21	B	605	CLA	C2A-CAA-CBA-CGA
21	C	513	CLA	C14-C13-C15-C16
21	P	513	CLA	C14-C13-C15-C16
27	e	102	LMG	C13-C14-C15-C16
26	A	414	SQD	C25-C26-C27-C28
27	A	410	LMG	C35-C36-C37-C38
26	A	409	SQD	C31-C32-C33-C34
21	P	506	CLA	C4-C3-C5-C6
27	C	519	LMG	C12-C13-C14-C15
21	B	614	CLA	C13-C15-C16-C17
27	A	410	LMG	C16-C17-C18-C19
21	C	512	CLA	CAA-CBA-CGA-O1A
21	G	406	CLA	C2A-CAA-CBA-CGA
26	B	627	SQD	C17-C18-C19-C20
24	D	408	DGD	C5B-C6B-C7B-C8B
21	P	513	CLA	C5-C6-C7-C8
21	C	512	CLA	C4-C3-C5-C6
21	C	512	CLA	C10-C11-C12-C13
27	e	102	LMG	C29-C28-O8-C9
27	N	623	LMG	C34-C35-C36-C37
27	P	521	LMG	C36-C37-C38-C39
21	A	401	CLA	C16-C17-C18-C20
21	B	610	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
21	G	402	CLA	C16-C17-C18-C20
21	N	617	CLA	C16-C17-C18-C19
22	D	402	PHO	CHA-CBD-CGD-O1D
24	P	517	DGD	C5A-C6A-C7A-C8A
31	N	604	LMT	O1'-C1-C2-C3
27	P	520	LMG	C12-C13-C14-C15
27	D	407	LMG	O1-C7-C8-O7
21	B	606	CLA	C13-C15-C16-C17
34	V	201	HEM	CAD-CBD-CGD-O2D
27	B	622	LMG	O6-C1-O1-C7
21	C	511	CLA	C12-C13-C15-C16
21	N	605	CLA	C12-C13-C15-C16
21	P	502	CLA	C11-C12-C13-C15
21	P	505	CLA	C11-C10-C8-C7
27	P	520	LMG	C17-C18-C19-C20
21	N	617	CLA	C10-C11-C12-C13
21	C	505	CLA	C2C-C3C-CAC-CBC
21	B	603	CLA	C6-C7-C8-C9
21	C	503	CLA	C6-C7-C8-C9
21	C	506	CLA	C11-C10-C8-C9
21	N	605	CLA	C11-C12-C13-C14
21	N	607	CLA	C6-C7-C8-C9
21	P	505	CLA	C11-C10-C8-C9
21	P	511	CLA	C14-C13-C15-C16
21	Q	402	CLA	C6-C7-C8-C9
24	B	621	DGD	C5D-C6D-O5D-C1E
27	I	102	LMG	C8-C7-O1-C1
27	Q	401	LMG	C8-C7-O1-C1
27	a	102	LMG	C8-C7-O1-C1
27	Q	401	LMG	C17-C18-C19-C20
21	C	510	CLA	C2-C1-O2A-CGA
21	N	616	CLA	C2-C1-O2A-CGA
21	A	405	CLA	C16-C17-C18-C20
21	N	606	CLA	C3A-C2A-CAA-CBA
27	C	520	LMG	C9-C8-O7-C10
34	i	201	HEM	CAD-CBD-CGD-O2D
21	A	401	CLA	C13-C15-C16-C17
21	N	614	CLA	C16-C17-C18-C20
21	A	401	CLA	C3-C5-C6-C7
26	G	410	SQD	C31-C32-C33-C34
21	N	605	CLA	C15-C16-C17-C18
34	V	201	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	F	101	SQD	C44-C45-C46-O48
26	G	401	SQD	O6-C44-C45-C46
26	S	102	SQD	C44-C45-C46-O48
27	C	520	LMG	C7-C8-C9-O8
27	D	407	LMG	O1-C7-C8-C9
27	Q	407	LMG	O1-C7-C8-C9
21	N	609	CLA	O1A-CGA-O2A-C1
21	Q	402	CLA	O1A-CGA-O2A-C1
27	e	102	LMG	O10-C28-O8-C9
21	B	612	CLA	C3-C5-C6-C7
27	Q	406	LMG	C14-C15-C16-C17
21	B	601	CLA	C4-C3-C5-C6
21	N	614	CLA	C4-C3-C5-C6
21	C	507	CLA	CAA-CBA-CGA-O2A
25	G	409	LHG	C35-C36-C37-C38
24	B	628	DGD	C3A-C4A-C5A-C6A
21	N	609	CLA	C16-C17-C18-C20
27	D	406	LMG	C14-C15-C16-C17
21	B	606	CLA	C5-C6-C7-C8
26	G	401	SQD	C32-C33-C34-C35
21	P	507	CLA	CAA-CBA-CGA-O2A
24	B	628	DGD	O2G-C1B-C2B-C3B
26	Q	408	SQD	O47-C7-C8-C9
27	P	520	LMG	O8-C28-C29-C30
21	P	512	CLA	CAA-CBA-CGA-O1A
27	Q	407	LMG	O1-C7-C8-O7
34	i	201	HEM	CAD-CBD-CGD-O1D
21	A	405	CLA	C11-C12-C13-C14
21	B	601	CLA	C11-C12-C13-C14
21	B	605	CLA	C11-C12-C13-C14
21	D	401	CLA	C11-C10-C8-C9
21	G	406	CLA	C11-C12-C13-C14
21	N	606	CLA	C14-C13-C15-C16
21	N	609	CLA	C11-C12-C13-C14
21	N	620	CLA	C14-C13-C15-C16
21	P	503	CLA	C6-C7-C8-C9
21	P	506	CLA	C11-C10-C8-C9
21	Q	402	CLA	C11-C10-C8-C9
21	B	605	CLA	C16-C17-C18-C20
31	B	625	LMT	O1'-C1-C2-C3
21	B	602	CLA	CAA-CBA-CGA-O2A
21	N	617	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	A	414	SQD	O47-C7-C8-C9
27	A	410	LMG	O7-C10-C11-C12
26	A	414	SQD	C33-C34-C35-C36
30	J	102	BCR	C7-C8-C9-C10
21	P	510	CLA	C4-C3-C5-C6
26	G	401	SQD	O47-C7-C8-C9
27	G	411	LMG	O7-C10-C11-C12
31	a	103	LMT	C7-C8-C9-C10
21	P	503	CLA	C2A-CAA-CBA-CGA
21	B	601	CLA	C12-C13-C15-C16
21	B	603	CLA	C6-C7-C8-C10
21	B	603	CLA	C11-C10-C8-C7
21	B	605	CLA	C6-C7-C8-C10
21	B	608	CLA	C11-C10-C8-C7
21	B	610	CLA	C11-C12-C13-C15
21	C	503	CLA	C6-C7-C8-C10
21	C	506	CLA	C11-C10-C8-C7
21	C	507	CLA	C12-C13-C15-C16
21	C	513	CLA	C11-C12-C13-C15
21	N	605	CLA	C11-C12-C13-C15
21	N	607	CLA	C6-C7-C8-C10
21	P	506	CLA	C11-C10-C8-C7
21	P	507	CLA	C11-C10-C8-C7
21	P	507	CLA	C11-C12-C13-C15
21	P	511	CLA	C12-C13-C15-C16
21	G	406	CLA	C2B-C3B-CAB-CBB
21	N	618	CLA	C2B-C3B-CAB-CBB
30	C	515	BCR	C5-C6-C7-C8
30	I	101	BCR	C5-C6-C7-C8
30	I	101	BCR	C23-C24-C25-C26
30	P	516	BCR	C5-C6-C7-C8
30	a	101	BCR	C5-C6-C7-C8
30	a	101	BCR	C23-C24-C25-C26
21	C	501	CLA	CAA-CBA-CGA-O2A
26	B	624	SQD	O47-C7-C8-C9
27	Q	406	LMG	C32-C33-C34-C35
21	A	403	CLA	C2-C1-O2A-CGA
21	B	614	CLA	C2-C1-O2A-CGA
21	C	512	CLA	C2-C1-O2A-CGA
22	A	404	PHO	C2-C1-O2A-CGA
21	C	507	CLA	C3-C5-C6-C7
27	D	406	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
27	D	407	LMG	C29-C30-C31-C32
21	P	501	CLA	CBA-CGA-O2A-C1
24	Q	409	DGD	C5B-C6B-C7B-C8B
26	A	414	SQD	C23-C24-C25-C26
21	P	501	CLA	CAA-CBA-CGA-O2A
24	N	602	DGD	O2G-C1B-C2B-C3B
24	C	518	DGD	C4E-C5E-C6E-O5E
21	P	512	CLA	C10-C11-C12-C13
24	B	628	DGD	C5A-C6A-C7A-C8A
21	N	606	CLA	C3-C5-C6-C7
21	G	406	CLA	C16-C17-C18-C20
21	N	605	CLA	C16-C17-C18-C19
21	B	601	CLA	C15-C16-C17-C18
27	C	519	LMG	C17-C18-C19-C20
21	G	402	CLA	C13-C15-C16-C17
21	B	610	CLA	CAA-CBA-CGA-O2A
24	P	519	DGD	O2G-C1B-C2B-C3B
21	N	605	CLA	C4-C3-C5-C6
31	I	103	LMT	C7-C8-C9-C10
21	B	613	CLA	CAA-CBA-CGA-O2A
31	N	624	LMT	O1'-C1-C2-C3
21	B	613	CLA	C10-C11-C12-C13
21	C	503	CLA	C2A-CAA-CBA-CGA
27	Q	406	LMG	C17-C18-C19-C20
21	B	602	CLA	C14-C13-C15-C16
21	B	605	CLA	C6-C7-C8-C9
21	B	616	CLA	C14-C13-C15-C16
21	D	401	CLA	C6-C7-C8-C9
21	N	605	CLA	C11-C10-C8-C9
21	P	502	CLA	C11-C10-C8-C9
21	P	507	CLA	C11-C10-C8-C9
21	N	614	CLA	CAA-CBA-CGA-O2A
27	N	623	LMG	C36-C37-C38-C39
27	R	102	LMG	C7-C8-C9-O8
21	N	607	CLA	C15-C16-C17-C18
21	B	601	CLA	C1A-C2A-CAA-CBA
21	D	403	CLA	C1A-C2A-CAA-CBA
22	A	404	PHO	O1D-CGD-O2D-CED
21	N	616	CLA	C3-C5-C6-C7
21	P	505	CLA	C2C-C3C-CAC-CBC
27	N	622	LMG	O6-C1-O1-C7
24	C	516	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
27	C	519	LMG	O8-C28-C29-C30
23	J	101	PL9	C21-C22-C23-C24
23	b	101	PL9	C21-C22-C23-C24
30	C	515	BCR	C21-C22-C23-C24
30	P	516	BCR	C21-C22-C23-C24
21	P	510	CLA	C5-C6-C7-C8
27	A	410	LMG	C11-C12-C13-C14
24	C	518	DGD	O2G-C1B-C2B-C3B
24	P	517	DGD	O2G-C1B-C2B-C3B
26	A	414	SQD	C32-C33-C34-C35
27	B	622	LMG	C2-C1-O1-C7
26	G	401	SQD	C33-C34-C35-C36
23	D	404	PL9	C42-C43-C44-C45
24	C	518	DGD	O1G-C1A-C2A-C3A
26	A	414	SQD	C5-C6-S-O7
26	G	401	SQD	C5-C6-S-O7
21	B	612	CLA	C2-C1-O2A-CGA
21	G	404	CLA	C2-C1-O2A-CGA
21	N	610	CLA	C2-C1-O2A-CGA
22	G	405	PHO	C2-C1-O2A-CGA
21	D	401	CLA	CAA-CBA-CGA-O2A
21	A	405	CLA	C6-C7-C8-C10
21	B	601	CLA	C11-C12-C13-C15
21	B	612	CLA	C12-C13-C15-C16
21	C	505	CLA	C11-C10-C8-C7
21	C	507	CLA	C11-C12-C13-C15
21	C	510	CLA	C11-C12-C13-C15
21	G	406	CLA	C6-C7-C8-C10
21	N	605	CLA	C11-C10-C8-C7
21	N	614	CLA	C11-C12-C13-C15
21	P	503	CLA	C6-C7-C8-C10
21	P	513	CLA	C11-C12-C13-C15
26	G	401	SQD	C25-C26-C27-C28
22	D	402	PHO	O2A-C1-C2-C3
27	P	521	LMG	C7-C8-O7-C10
27	P	521	LMG	C9-C8-O7-C10
27	I	102	LMG	C31-C32-C33-C34
21	N	606	CLA	CAA-CBA-CGA-O2A
24	P	518	DGD	C6B-C7B-C8B-C9B
21	B	603	CLA	C15-C16-C17-C18
27	R	102	LMG	C30-C31-C32-C33
21	Q	402	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	Q	409	DGD	CAA-CBA-CCA-CDA
21	C	507	CLA	O1A-CGA-O2A-C1
21	N	616	CLA	CBD-CGD-O2D-CED
27	Q	406	LMG	C34-C35-C36-C37
21	B	610	CLA	C4-C3-C5-C6
23	J	101	PL9	C15-C14-C16-C17
27	E	102	LMG	O9-C10-C11-C12
27	Q	401	LMG	C29-C30-C31-C32
21	G	403	CLA	CAA-CBA-CGA-O1A
24	N	602	DGD	O1B-C1B-C2B-C3B
27	C	519	LMG	O10-C28-C29-C30
27	R	102	LMG	O9-C10-C11-C12
21	C	501	CLA	CBA-CGA-O2A-C1
21	D	401	CLA	CAA-CBA-CGA-O1A
21	N	617	CLA	CAA-CBA-CGA-O1A
21	N	618	CLA	CAA-CBA-CGA-O1A
27	A	410	LMG	O9-C10-C11-C12
27	G	411	LMG	C11-C10-O7-C8
21	B	603	CLA	C11-C10-C8-C9
21	C	507	CLA	C14-C13-C15-C16
21	C	510	CLA	C11-C12-C13-C14
21	C	513	CLA	C11-C12-C13-C14
21	N	605	CLA	C14-C13-C15-C16
21	N	609	CLA	C6-C7-C8-C9
21	N	612	CLA	C11-C10-C8-C9
21	P	507	CLA	C11-C12-C13-C14
21	Q	402	CLA	CAA-CBA-CGA-O1A
21	D	403	CLA	C8-C10-C11-C12
34	R	101	HEM	CAA-CBA-CGA-O2A
21	G	402	CLA	C3-C5-C6-C7
22	A	404	PHO	C13-C15-C16-C17
21	B	614	CLA	CAA-CBA-CGA-O1A
26	F	101	SQD	O5-C5-C6-S
34	i	201	HEM	CAA-CBA-CGA-O2A
21	B	613	CLA	CAA-CBA-CGA-O1A
26	A	414	SQD	O49-C7-C8-C9
25	A	411	LHG	O1-C1-C2-O2
21	C	510	CLA	C16-C17-C18-C20
26	B	624	SQD	O49-C7-C8-C9
26	G	401	SQD	O49-C7-C8-C9
26	Q	408	SQD	O49-C7-C8-C9
27	P	520	LMG	O10-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	P	520	LMG	C20-C21-C22-C23
24	D	408	DGD	C2G-C3G-O3G-C1D
24	Q	409	DGD	C2G-C3G-O3G-C1D
24	Q	409	DGD	C5D-C6D-O5D-C1E
24	W	102	DGD	C5D-C6D-O5D-C1E
27	B	622	LMG	C8-C7-O1-C1
27	D	406	LMG	C8-C7-O1-C1
27	N	622	LMG	C8-C7-O1-C1
27	G	411	LMG	O9-C10-O7-C8
24	B	628	DGD	O1B-C1B-C2B-C3B
24	P	517	DGD	O1B-C1B-C2B-C3B
21	N	610	CLA	C5-C6-C7-C8
27	Q	406	LMG	C13-C14-C15-C16
27	a	102	LMG	C20-C21-C22-C23
24	C	516	DGD	C1G-C2G-C3G-O3G
27	E	102	LMG	C7-C8-C9-O8
34	E	101	HEM	CAA-CBA-CGA-O2A
24	C	516	DGD	O1B-C1B-C2B-C3B
27	G	411	LMG	O9-C10-C11-C12
27	N	623	LMG	C11-C12-C13-C14
27	M	101	LMG	O8-C28-C29-C30
21	A	402	CLA	CAA-CBA-CGA-O1A
21	C	503	CLA	CAD-CBD-CGD-O2D
21	P	503	CLA	CAD-CBD-CGD-O2D
21	P	508	CLA	CAD-CBD-CGD-O2D
22	G	405	PHO	O1D-CGD-O2D-CED
21	N	618	CLA	CAA-CBA-CGA-O2A
21	B	609	CLA	C15-C16-C17-C18
21	N	613	CLA	C15-C16-C17-C18
26	A	414	SQD	C18-C19-C20-C21
21	B	616	CLA	C2-C1-O2A-CGA
21	C	505	CLA	C2-C1-O2A-CGA
21	N	620	CLA	C2-C1-O2A-CGA
24	P	519	DGD	O1B-C1B-C2B-C3B
21	B	607	CLA	C1-C2-C3-C4
21	N	618	CLA	C1-C2-C3-C4
21	A	405	CLA	C16-C17-C18-C19
21	N	609	CLA	C16-C17-C18-C19
24	C	518	DGD	O1A-C1A-C2A-C3A
21	Q	404	CLA	C8-C10-C11-C12
23	G	407	PL9	C15-C14-C16-C17
25	G	412	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
21	A	402	CLA	CBA-CGA-O2A-C1
21	B	601	CLA	CAA-CBA-CGA-O2A
25	G	412	LHG	O7-C7-C8-C9
34	E	101	HEM	CAA-CBA-CGA-O1A
34	V	201	HEM	CAA-CBA-CGA-O2A
21	B	602	CLA	C3-C5-C6-C7
24	C	518	DGD	C1B-C2B-C3B-C4B
26	B	627	SQD	C15-C16-C17-C18
24	C	518	DGD	O1B-C1B-C2B-C3B

There are no ring outliers.

165 monomers are involved in 586 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	e	102	LMG	3	0
31	N	625	LMT	1	0
27	B	622	LMG	1	0
24	B	628	DGD	3	0
24	P	518	DGD	5	0
21	G	404	CLA	4	0
25	G	409	LHG	1	0
21	N	619	CLA	3	0
27	D	406	LMG	4	0
27	A	410	LMG	2	0
24	A	407	DGD	1	0
26	A	409	SQD	5	0
23	J	101	PL9	1	0
21	B	606	CLA	8	0
21	N	607	CLA	7	0
21	N	616	CLA	8	0
22	Q	403	PHO	5	0
26	A	414	SQD	8	0
21	G	402	CLA	12	0
30	B	617	BCR	8	0
21	B	611	CLA	3	0
21	P	501	CLA	2	0
27	P	521	LMG	4	0
21	G	406	CLA	4	0
27	R	102	LMG	2	0
26	Q	408	SQD	3	0
30	P	516	BCR	3	0
21	N	614	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	C	515	BCR	4	0
21	G	403	CLA	8	0
21	Q	402	CLA	10	0
30	Z	101	BCR	3	0
24	P	517	DGD	2	0
30	B	618	BCR	5	0
27	N	623	LMG	1	0
30	T	102	BCR	9	0
24	P	519	DGD	7	0
30	a	101	BCR	4	0
21	B	602	CLA	4	0
24	B	621	DGD	2	0
21	B	610	CLA	4	0
27	G	411	LMG	2	0
21	N	620	CLA	4	0
21	C	505	CLA	7	0
26	N	601	SQD	7	0
31	B	629	LMT	3	0
22	A	404	PHO	6	0
30	P	514	BCR	12	0
21	P	513	CLA	3	0
21	C	510	CLA	2	0
21	N	613	CLA	2	0
24	C	518	DGD	7	0
30	H	101	BCR	2	0
30	T	103	BCR	3	0
22	G	405	PHO	7	0
21	Q	404	CLA	4	0
21	A	405	CLA	3	0
21	C	507	CLA	3	0
31	M	102	LMT	1	0
24	W	102	DGD	3	0
23	D	404	PL9	6	0
21	N	615	CLA	3	0
30	b	102	BCR	3	0
21	N	617	CLA	2	0
31	B	630	LMT	3	0
21	P	509	CLA	5	0
21	P	512	CLA	4	0
21	B	612	CLA	6	0
21	C	512	CLA	3	0
21	N	606	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	N	608	CLA	6	0
26	G	410	SQD	7	0
21	N	611	CLA	5	0
21	B	613	CLA	3	0
30	W	101	BCR	3	0
30	C	514	BCR	12	0
30	K	101	BCR	11	0
21	P	506	CLA	1	0
21	P	505	CLA	6	0
21	D	401	CLA	7	0
26	B	627	SQD	5	0
30	J	102	BCR	4	0
21	P	510	CLA	2	0
21	B	615	CLA	3	0
24	Q	409	DGD	1	0
31	N	624	LMT	1	0
27	Q	406	LMG	5	0
21	C	504	CLA	6	0
26	B	624	SQD	5	0
30	c	101	BCR	12	0
31	N	603	LMT	3	0
27	I	102	LMG	4	0
27	N	622	LMG	2	0
26	S	102	SQD	2	0
31	B	626	LMT	1	0
21	D	403	CLA	4	0
21	A	403	CLA	5	0
21	A	402	CLA	8	0
31	I	103	LMT	2	0
27	E	102	LMG	2	0
31	B	625	LMT	1	0
21	C	511	CLA	8	0
24	C	516	DGD	3	0
34	R	101	HEM	6	0
26	G	401	SQD	9	0
21	B	605	CLA	5	0
21	P	507	CLA	3	0
30	N	621	BCR	4	0
21	B	608	CLA	9	0
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30	D	405	BCR	3	0
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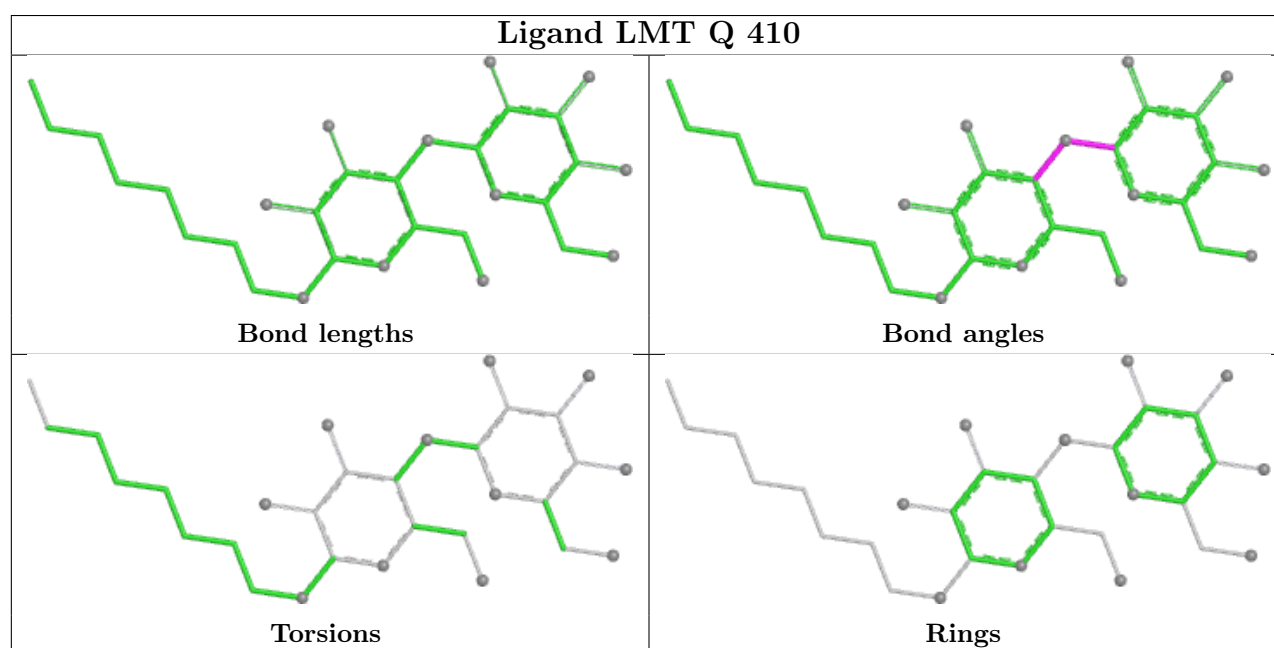
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21	N	612	CLA	6	0
23	Q	405	PL9	5	0
25	G	412	LHG	3	0
27	C	520	LMG	4	0
27	D	407	LMG	9	0
21	C	508	CLA	5	0
25	A	408	LHG	2	0
21	B	614	CLA	7	0
25	A	411	LHG	2	0
24	G	408	DGD	2	0
21	A	401	CLA	12	0
27	B	623	LMG	1	0
31	e	101	LMT	1	0
23	b	101	PL9	2	0
27	a	102	LMG	2	0
31	a	103	LMT	1	0
27	M	101	LMG	4	0
24	C	517	DGD	7	0
22	D	402	PHO	5	0
21	B	607	CLA	6	0
21	B	604	CLA	5	0
30	S	101	BCR	5	0
21	B	603	CLA	7	0
34	V	201	HEM	5	0
21	B	616	CLA	6	0
21	P	504	CLA	5	0
30	P	515	BCR	5	0
34	E	101	HEM	7	0
21	B	609	CLA	3	0
21	C	513	CLA	3	0
21	C	503	CLA	6	0
21	C	506	CLA	2	0
34	i	201	HEM	4	0
23	A	406	PL9	5	0
27	Q	401	LMG	2	0
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21	C	502	CLA	1	0
31	N	604	LMT	4	0
21	P	503	CLA	6	0

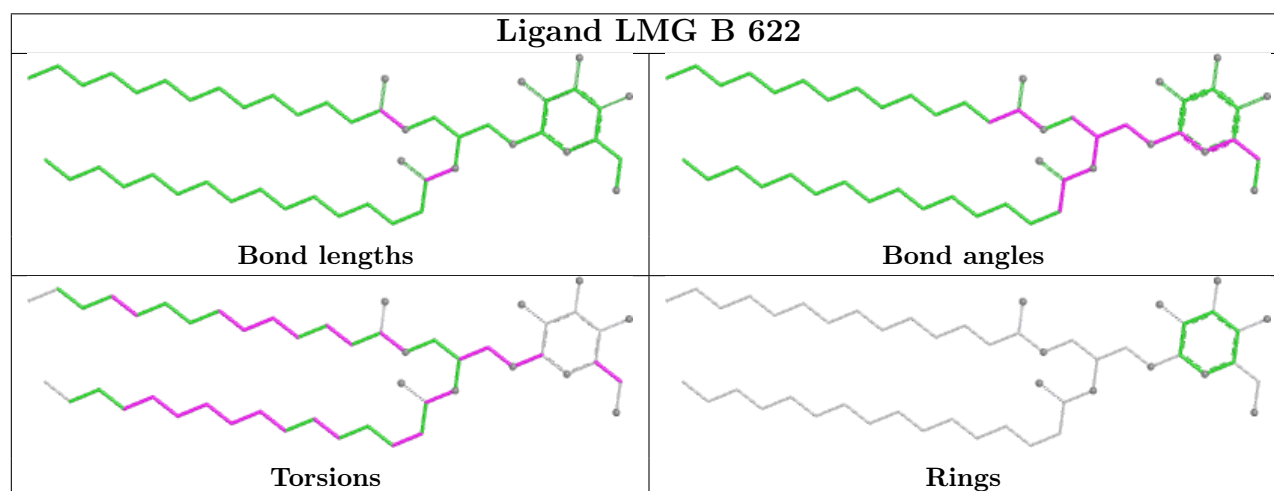
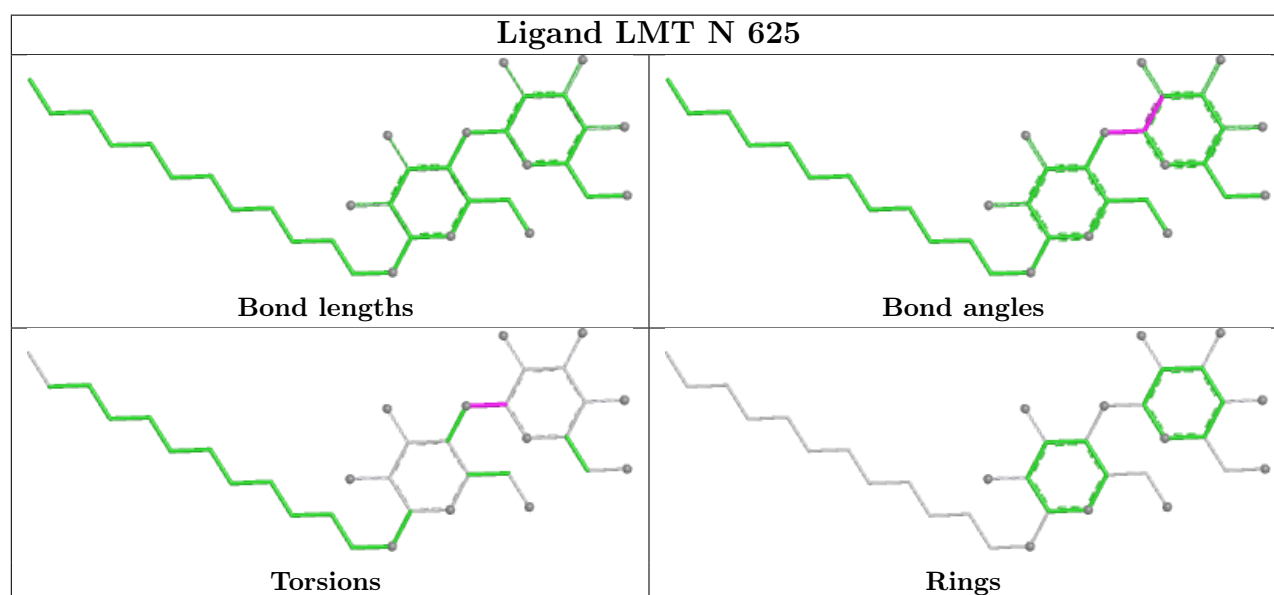
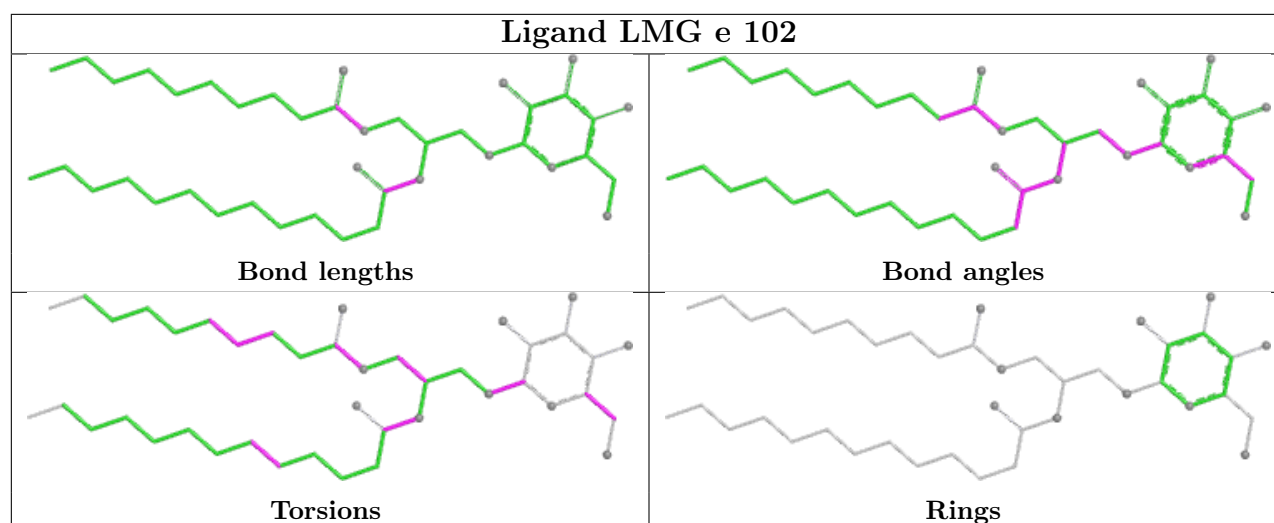
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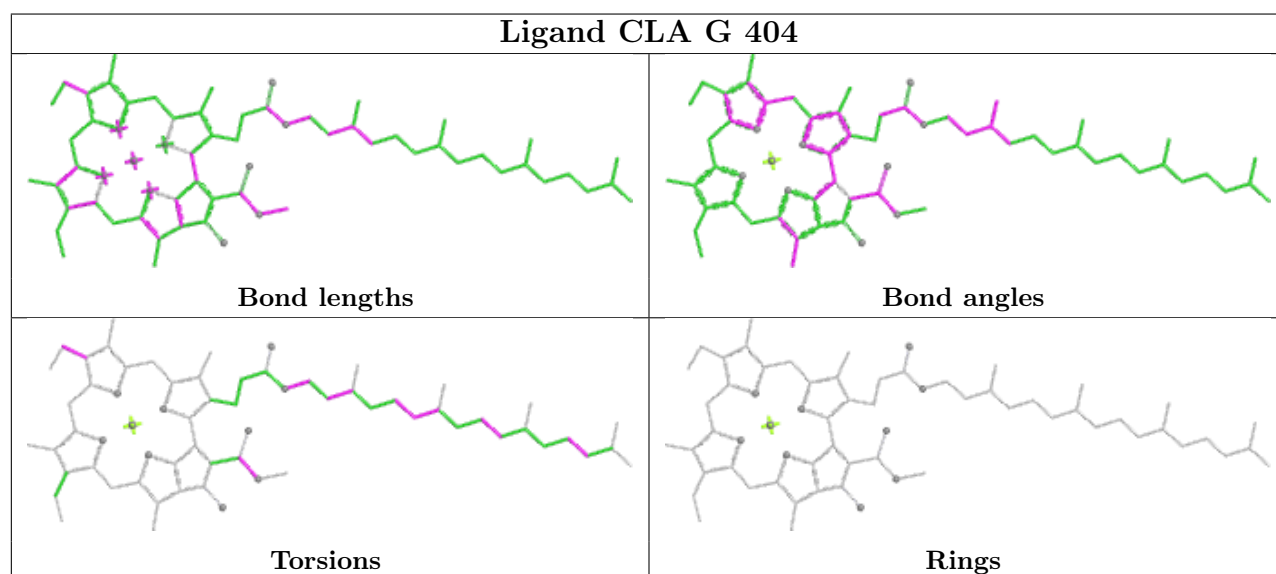
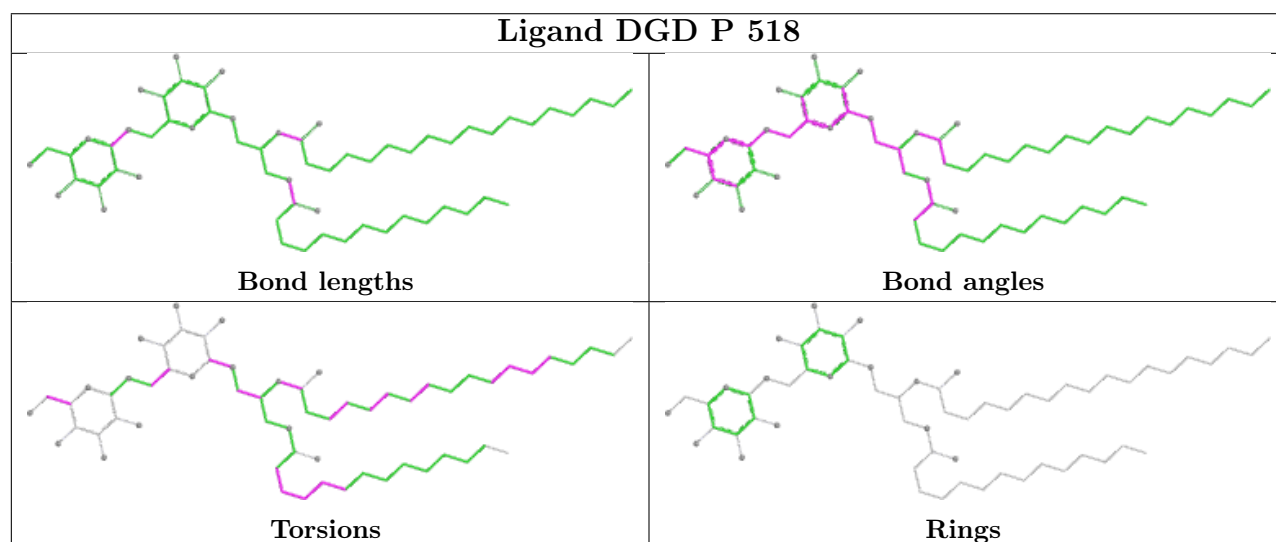
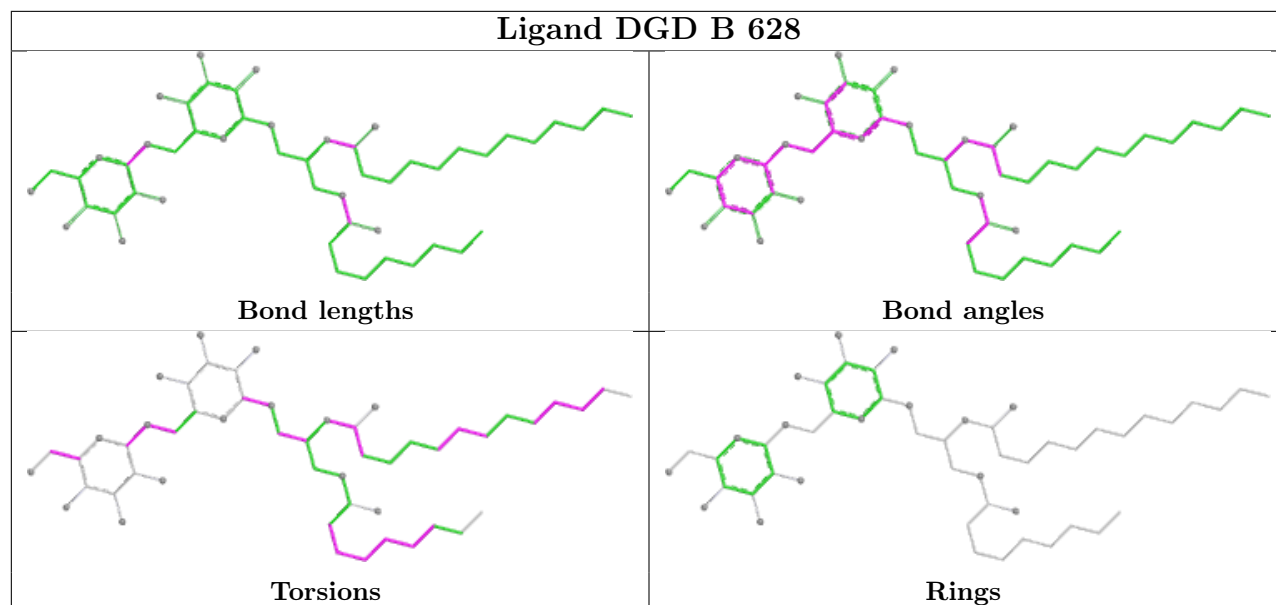
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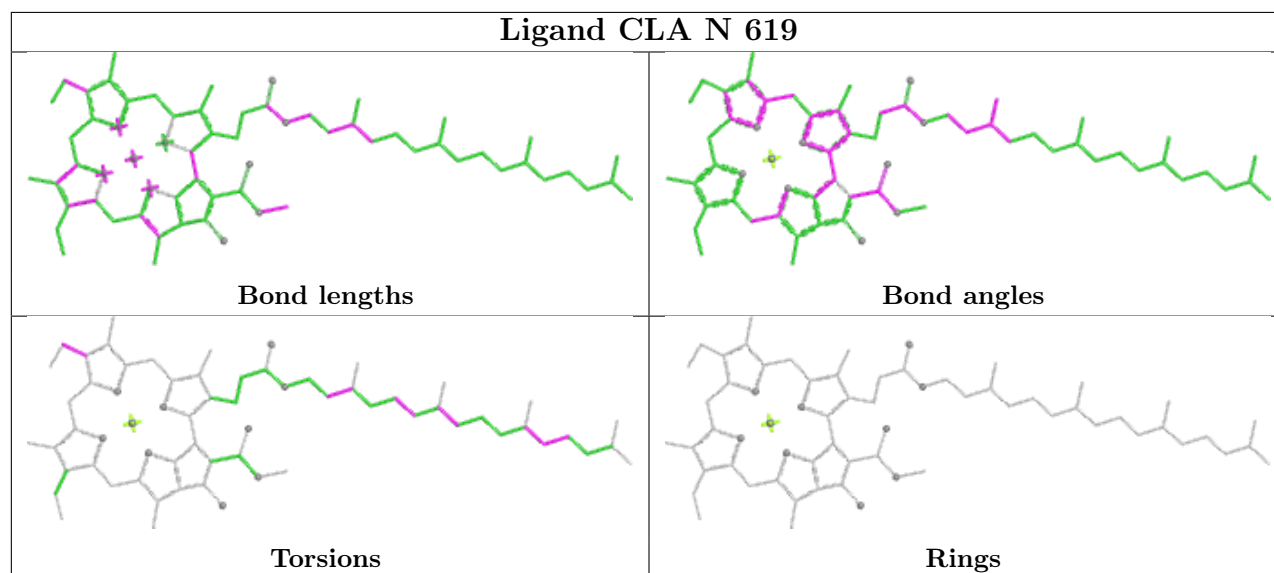
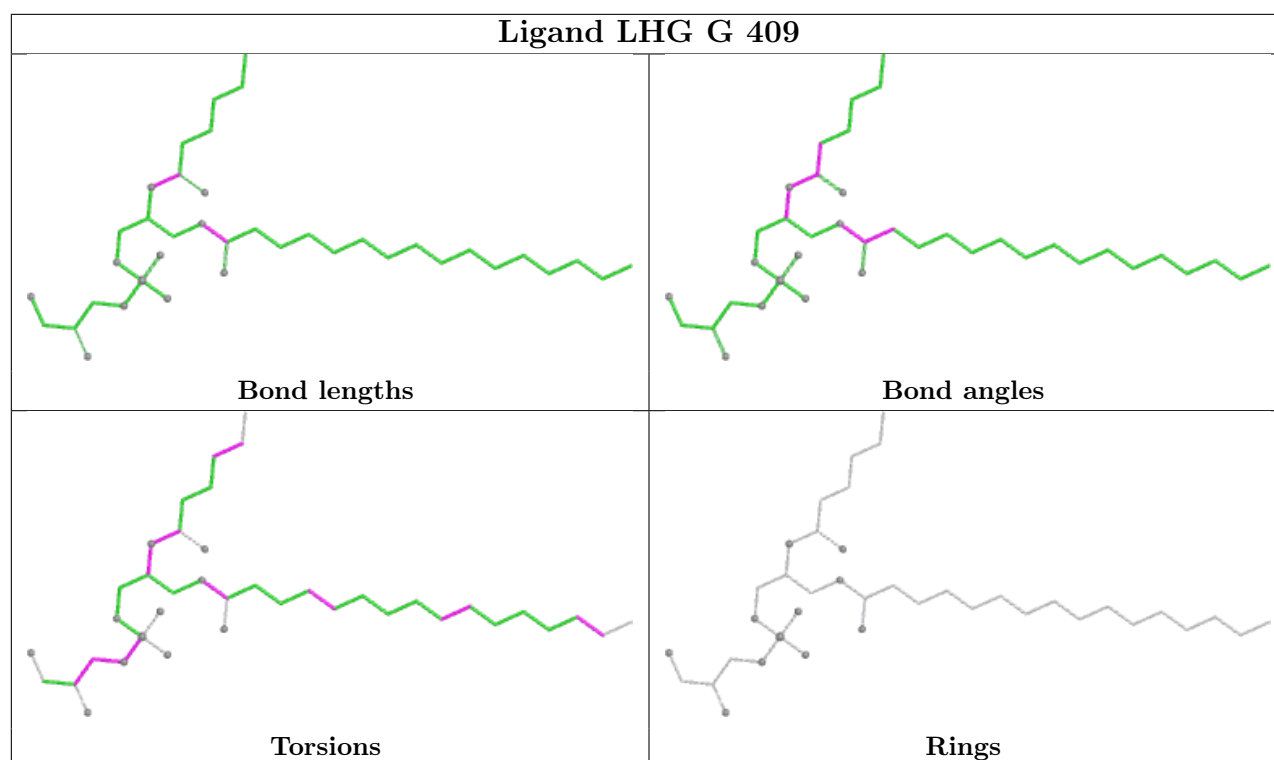
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	N	610	CLA	5	0
23	G	407	PL9	5	0
27	Q	407	LMG	8	0
21	N	618	CLA	11	0
21	P	511	CLA	9	0
21	N	609	CLA	7	0
21	P	502	CLA	2	0
24	N	602	DGD	4	0
30	B	620	BCR	2	0
30	T	101	BCR	5	0
26	F	101	SQD	2	0

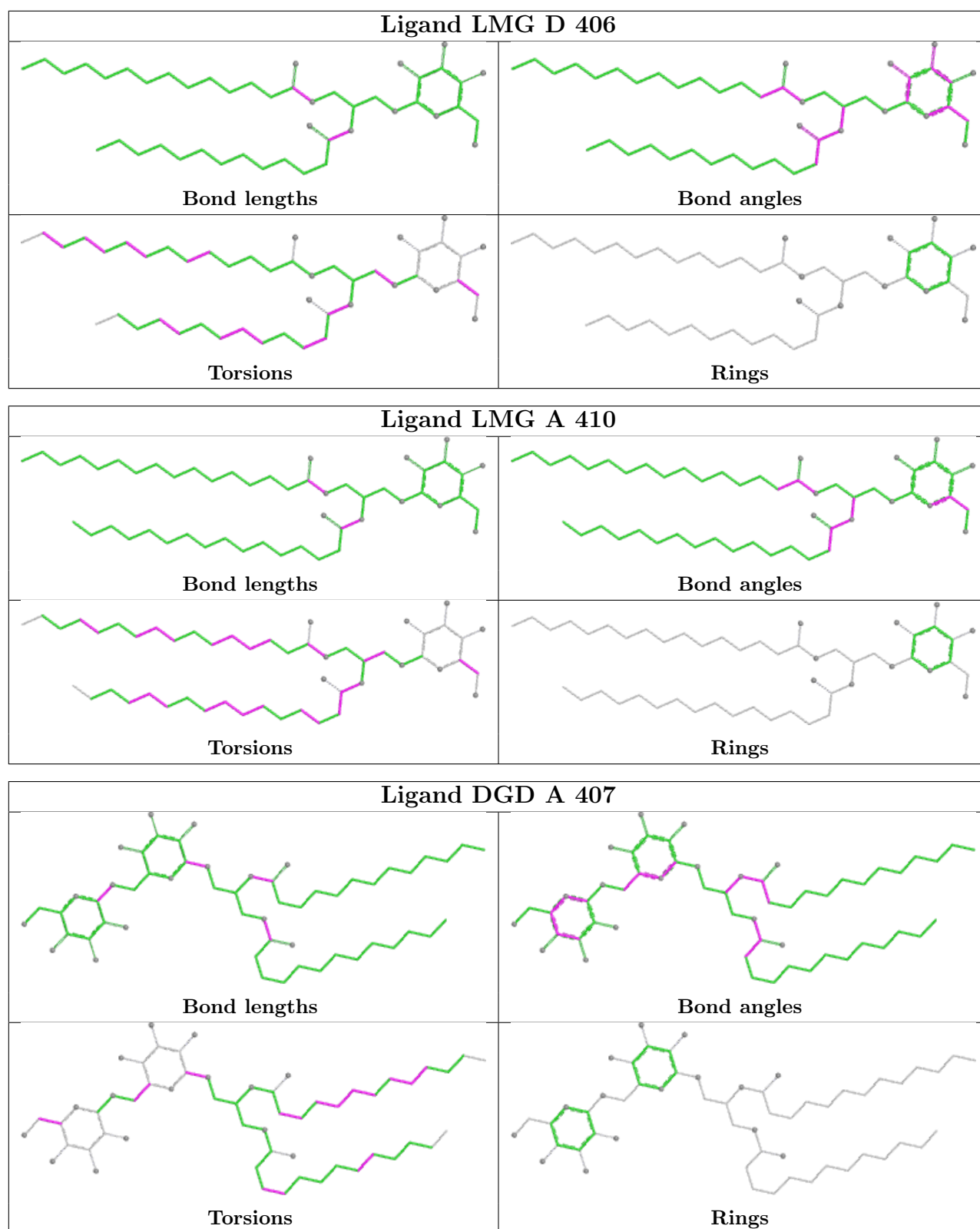
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

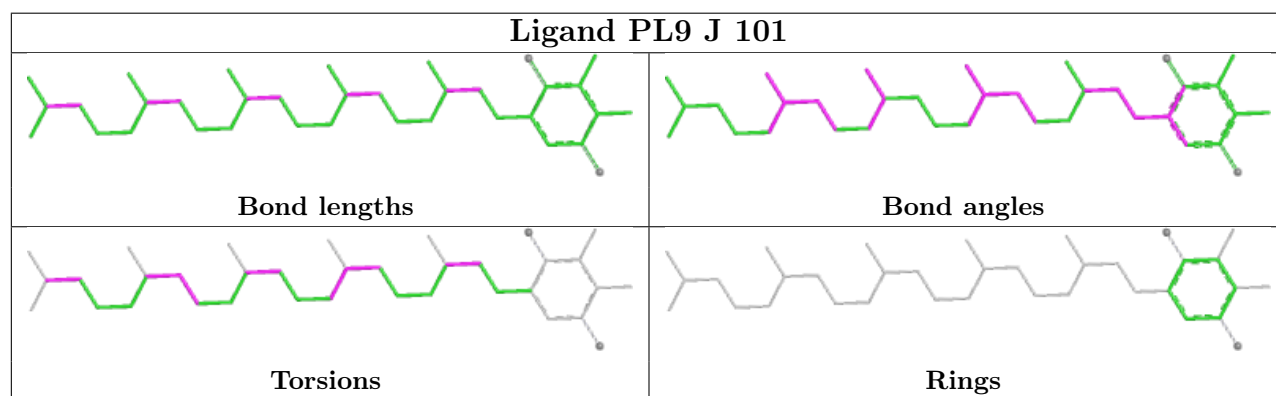
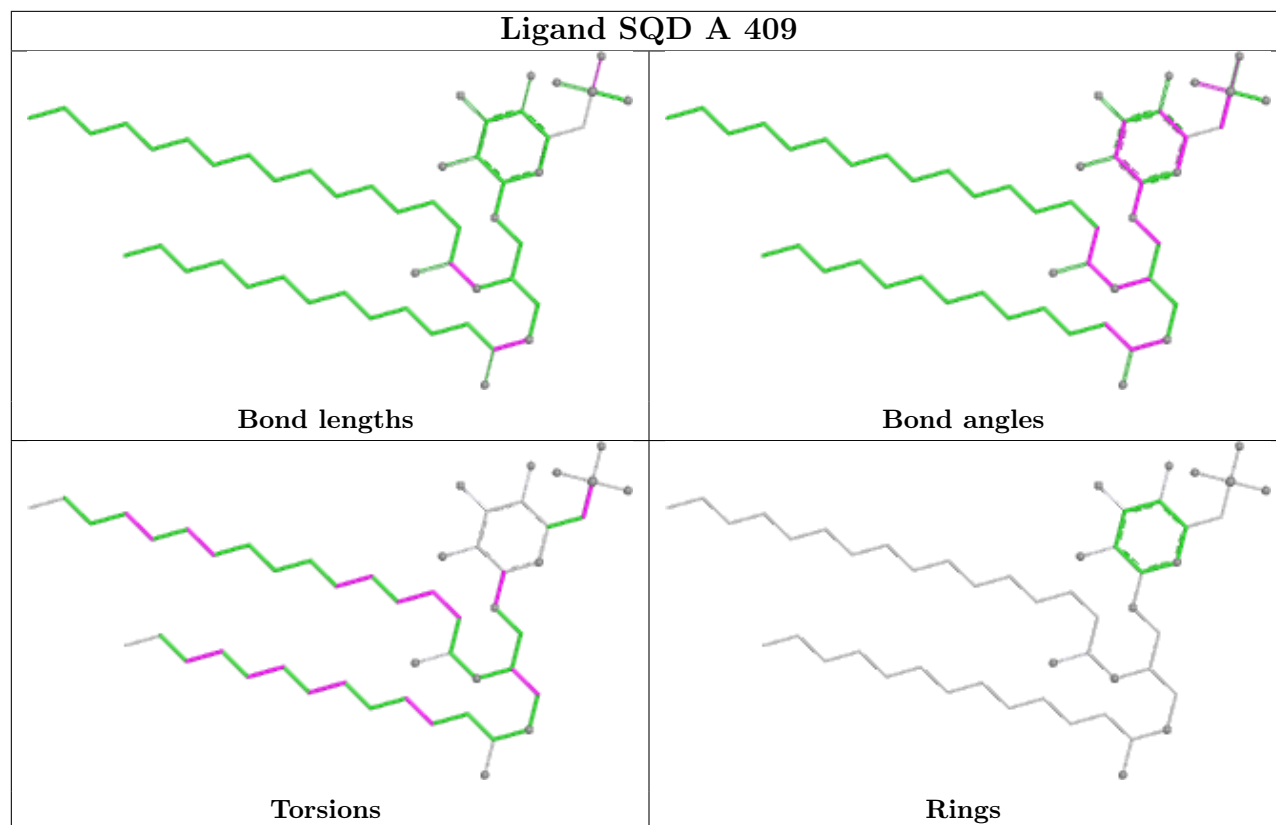




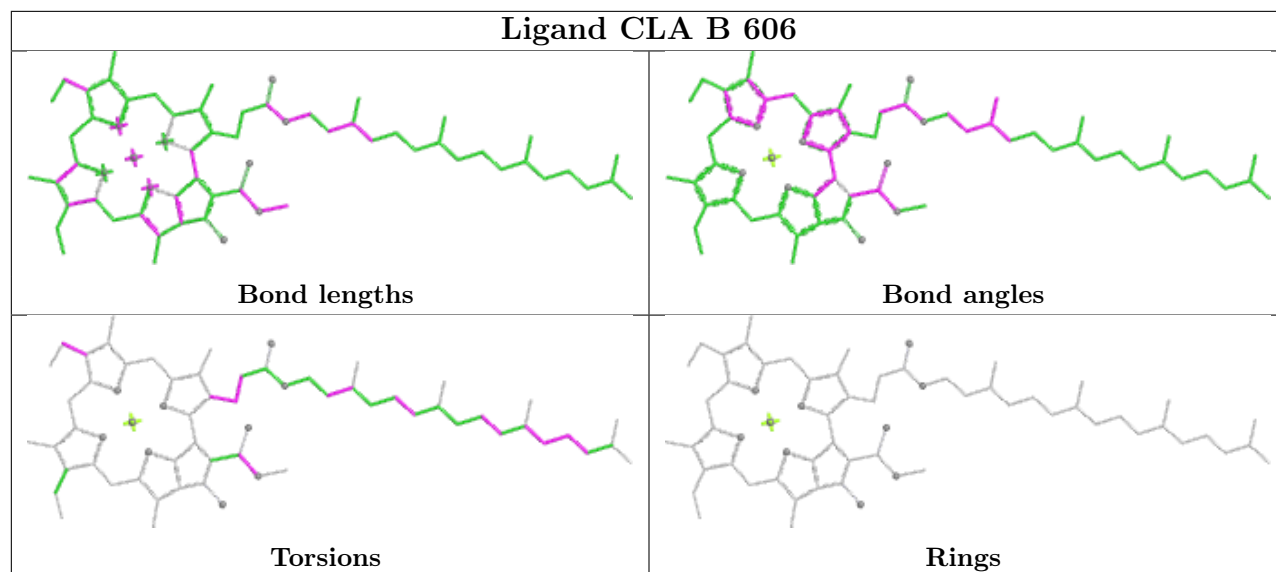




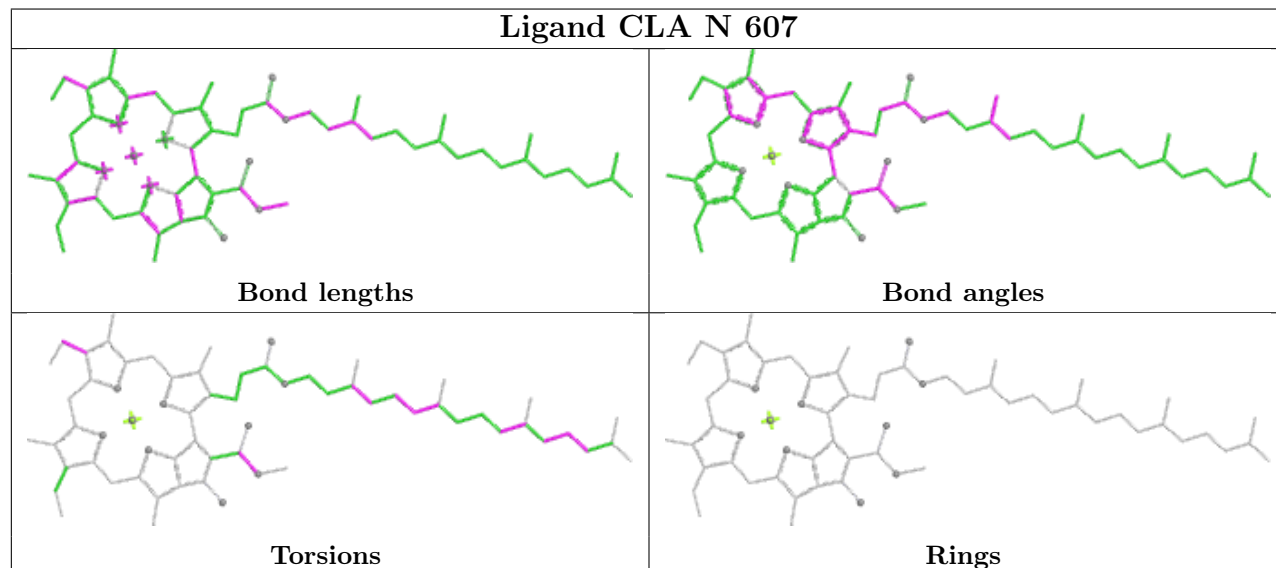




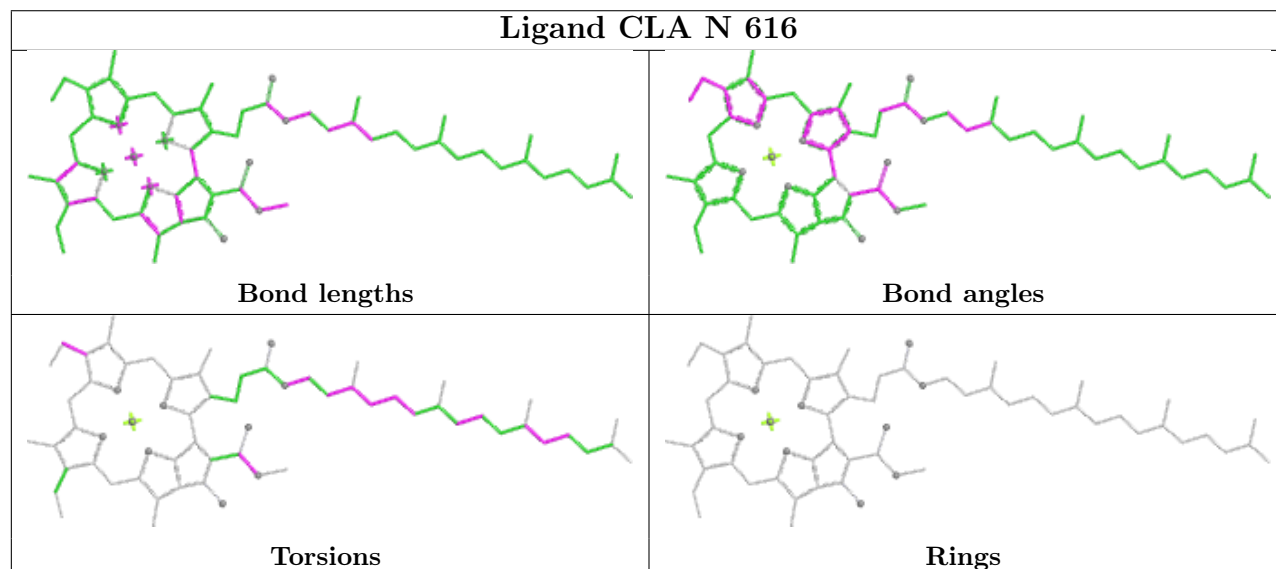
Ligand CLA B 606

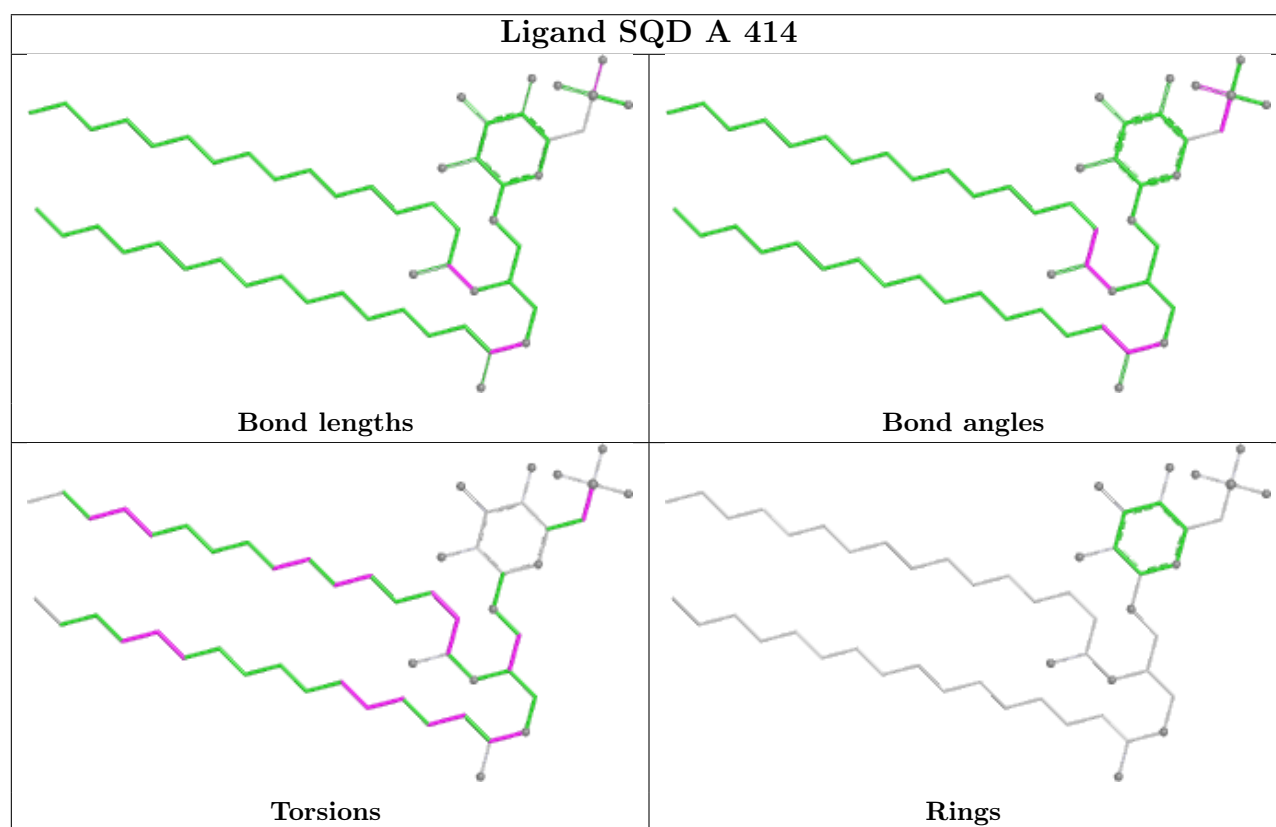
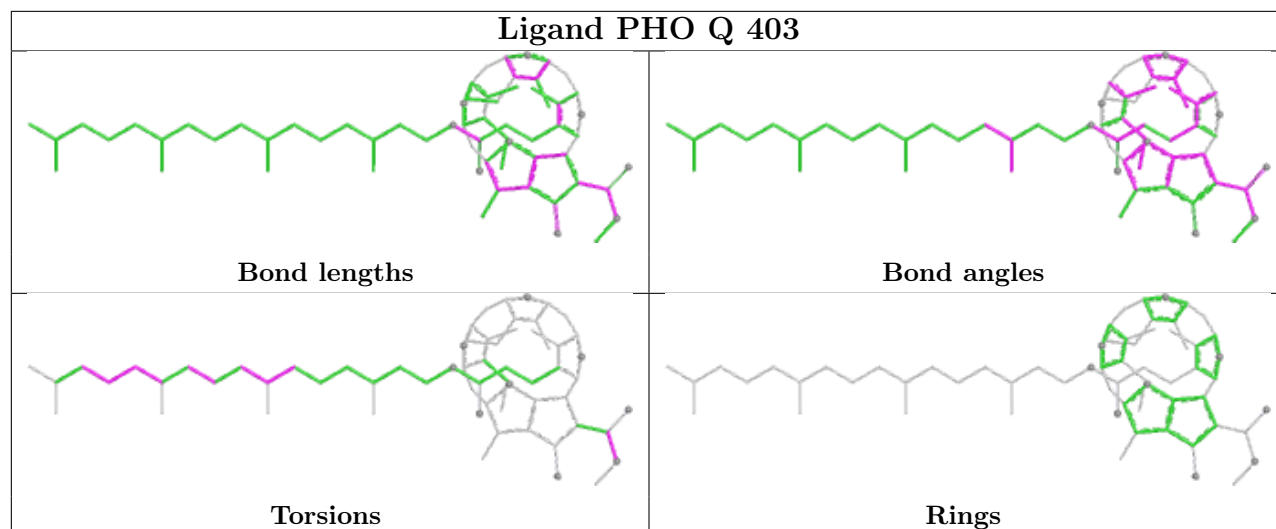


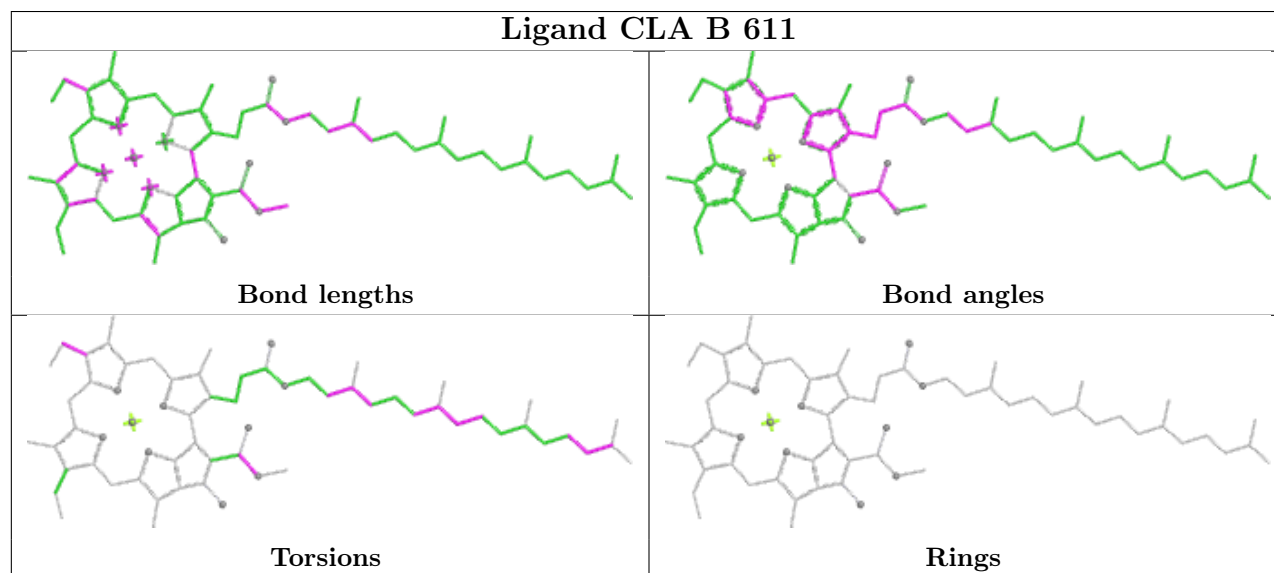
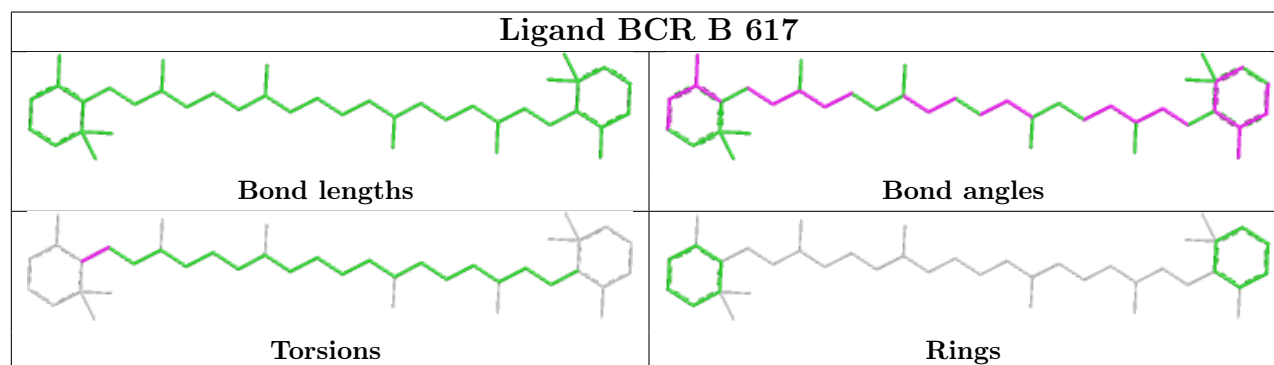
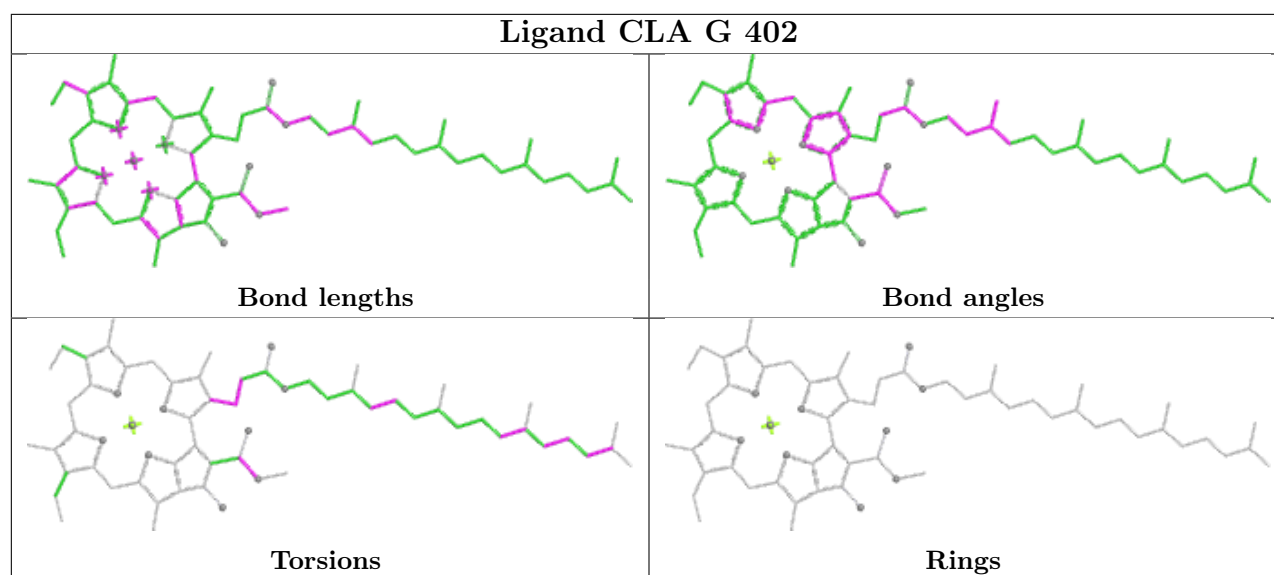
Ligand CLA N 607

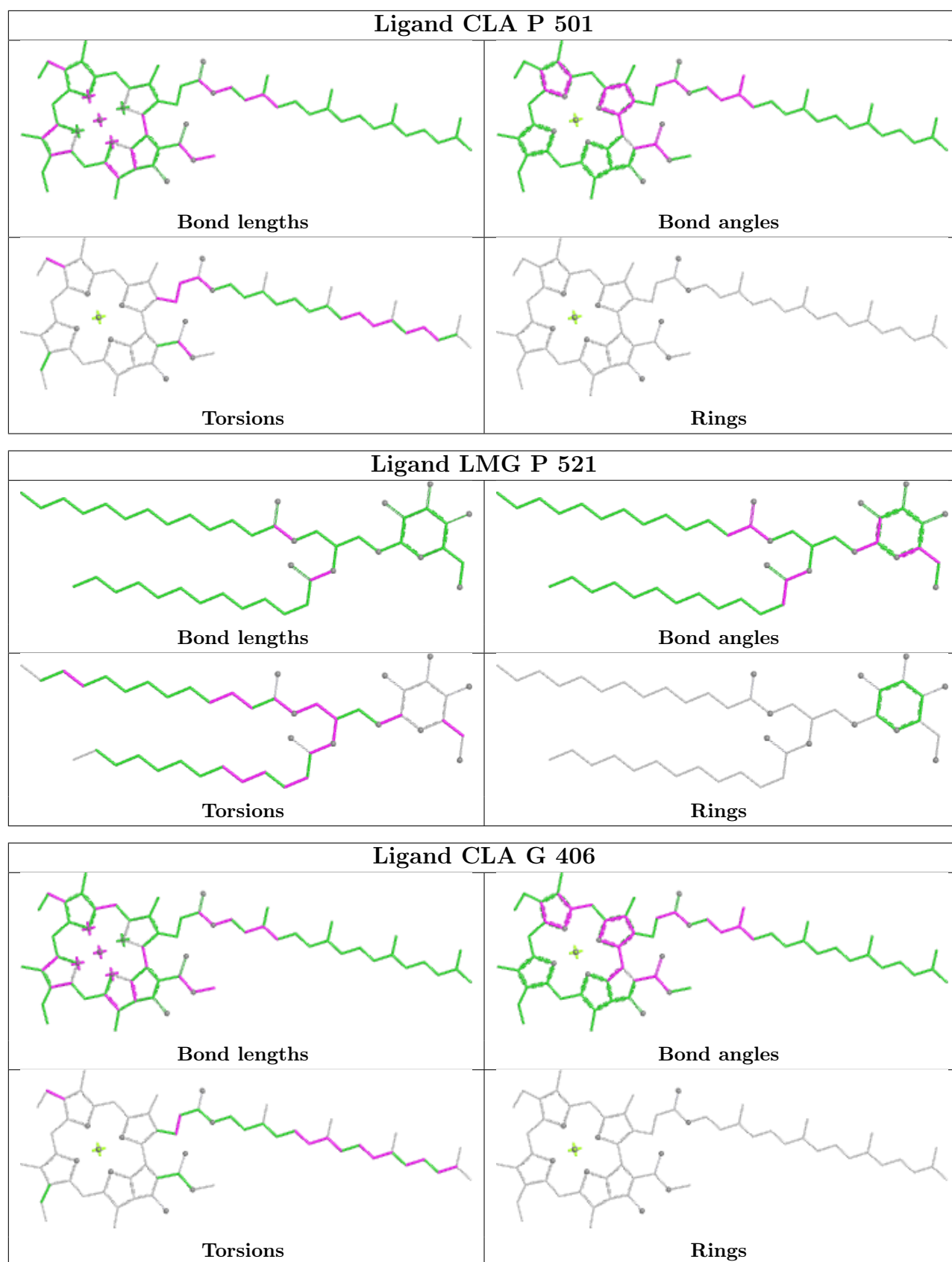


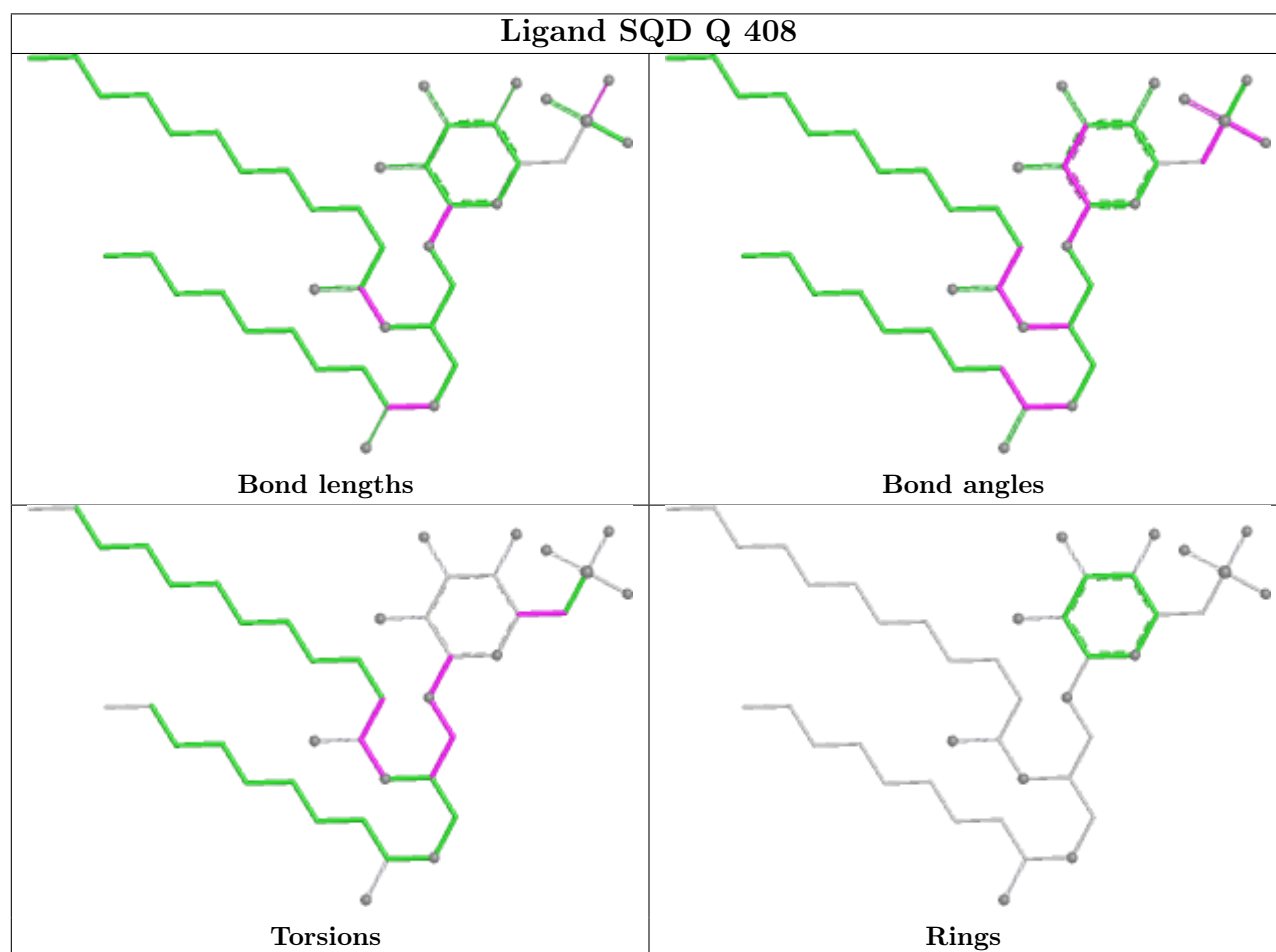
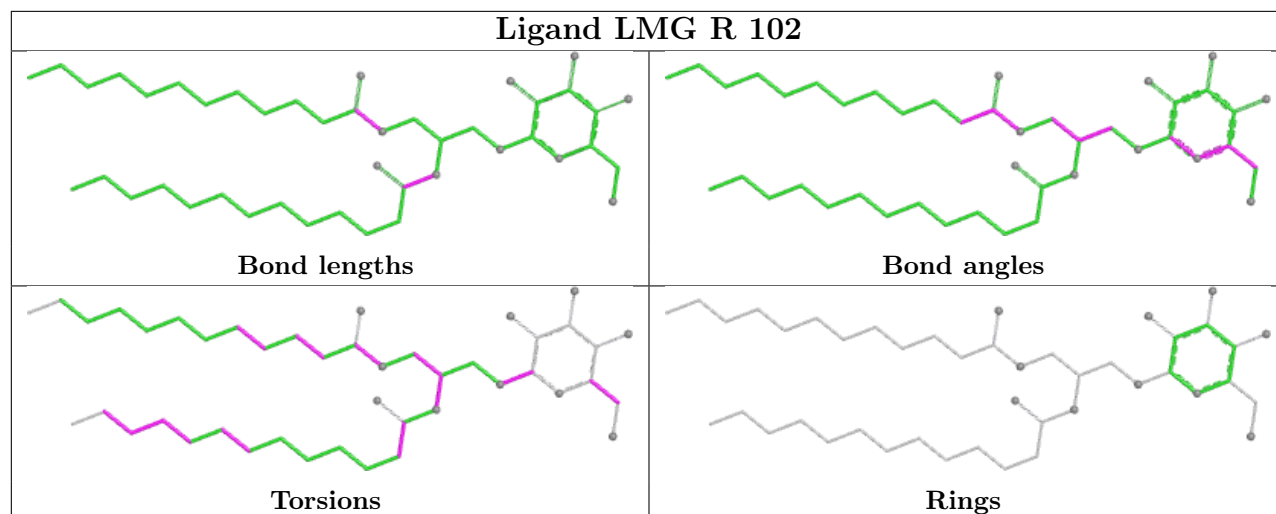
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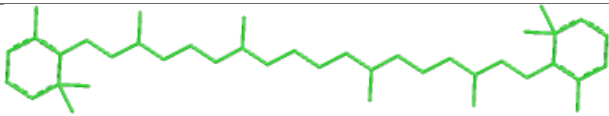
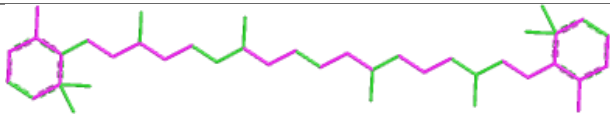
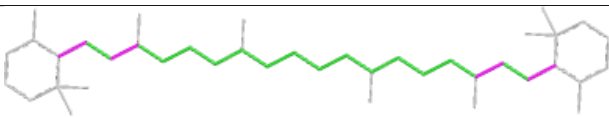
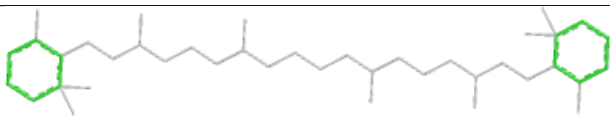


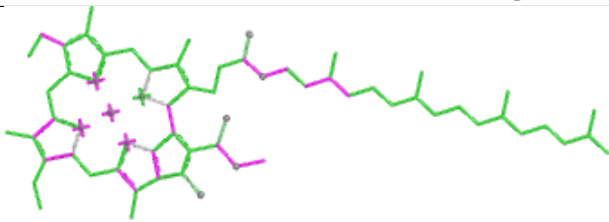
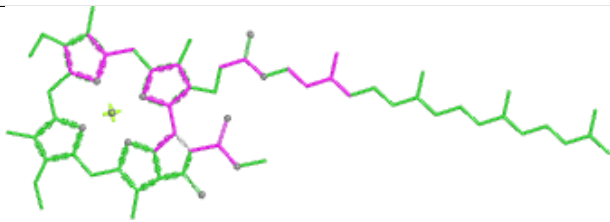
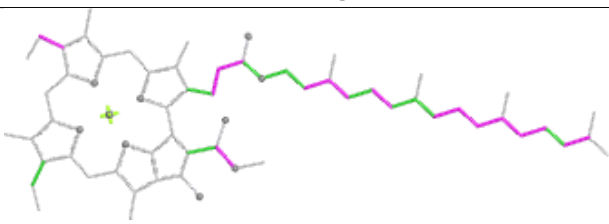
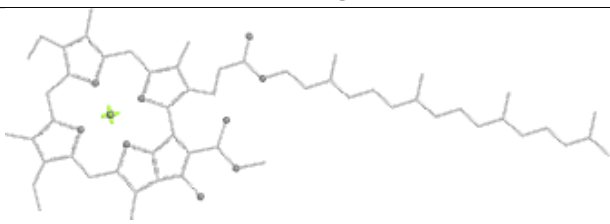


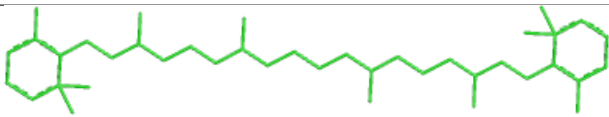
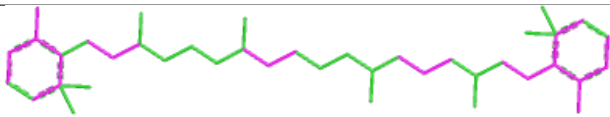
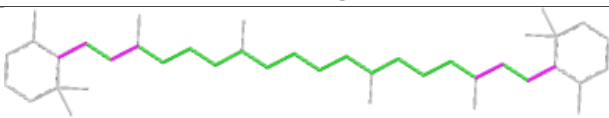
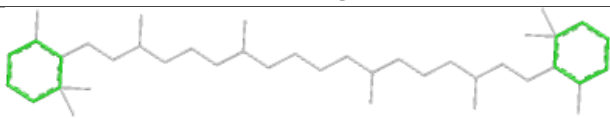




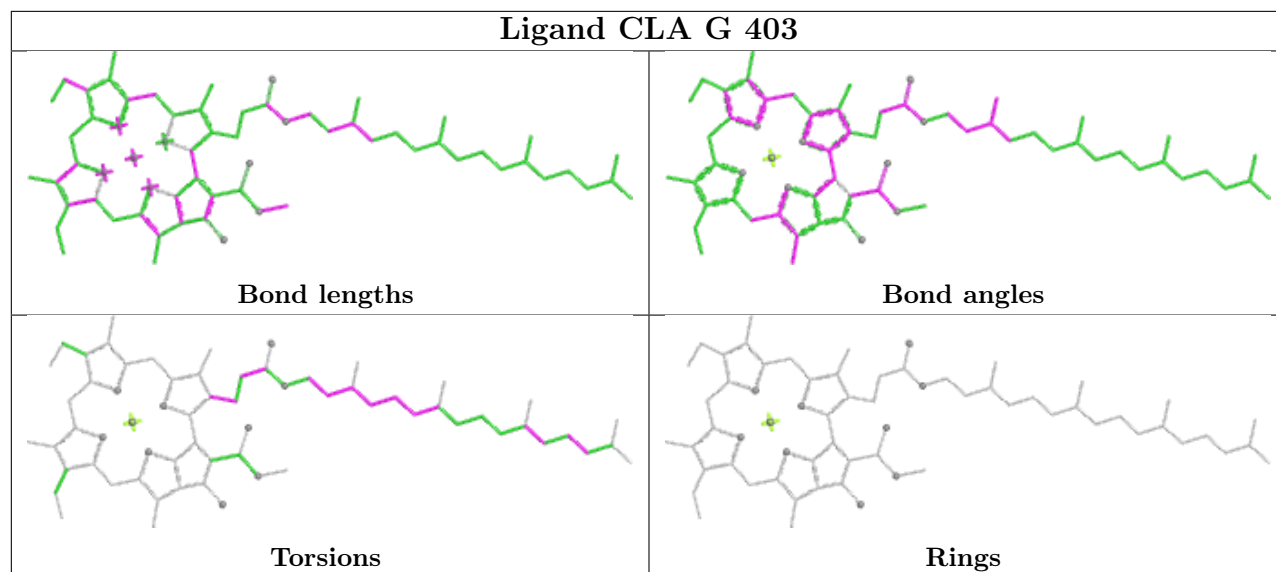


Ligand BCR P 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

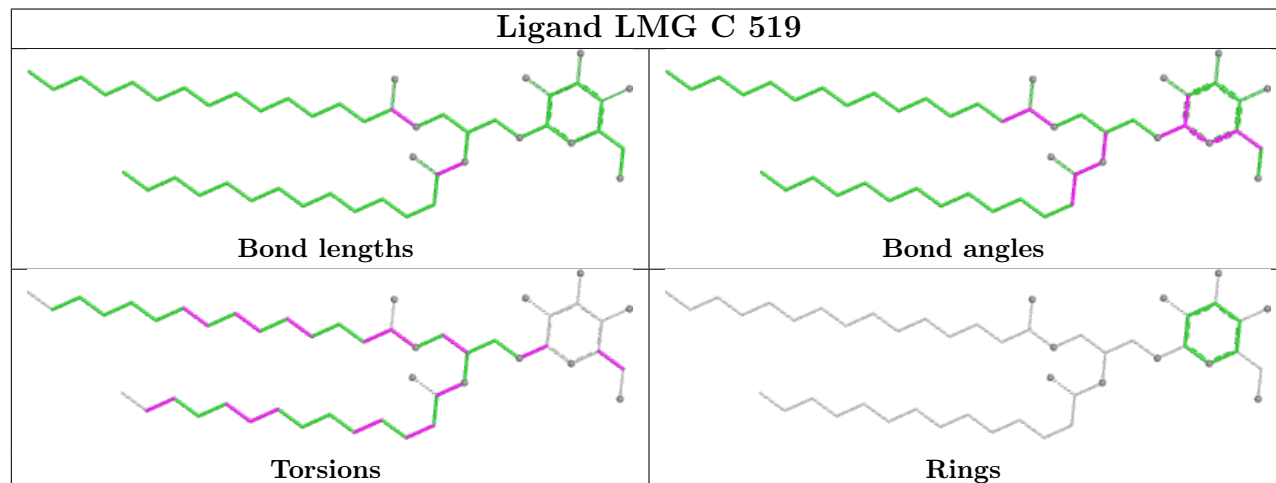
Ligand CLA N 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

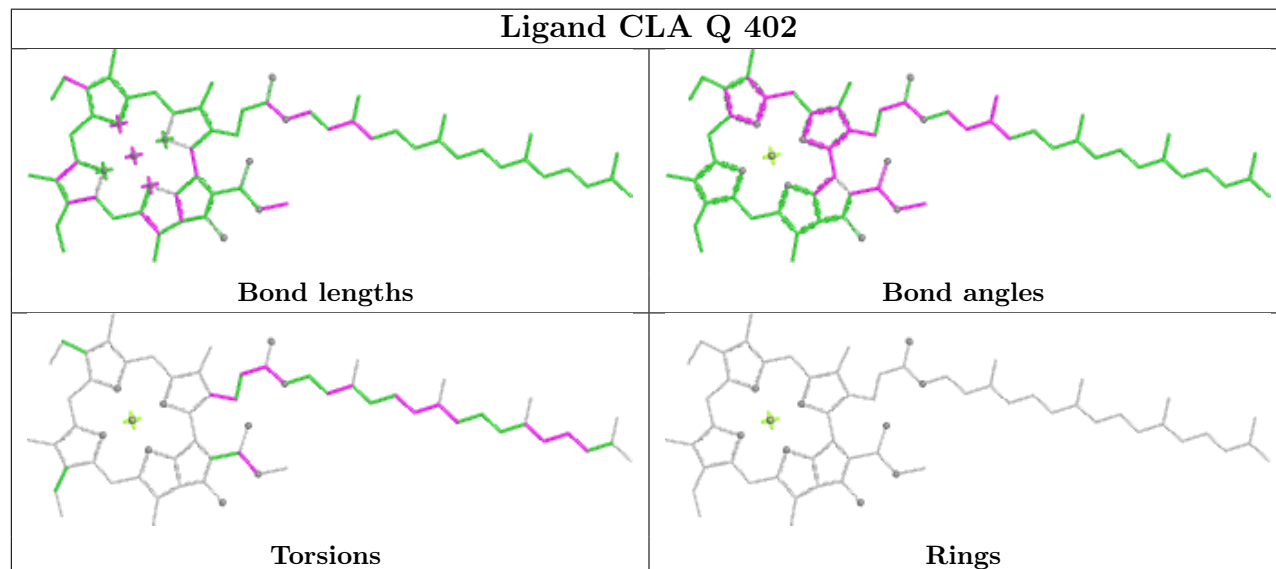
Ligand CLA G 403



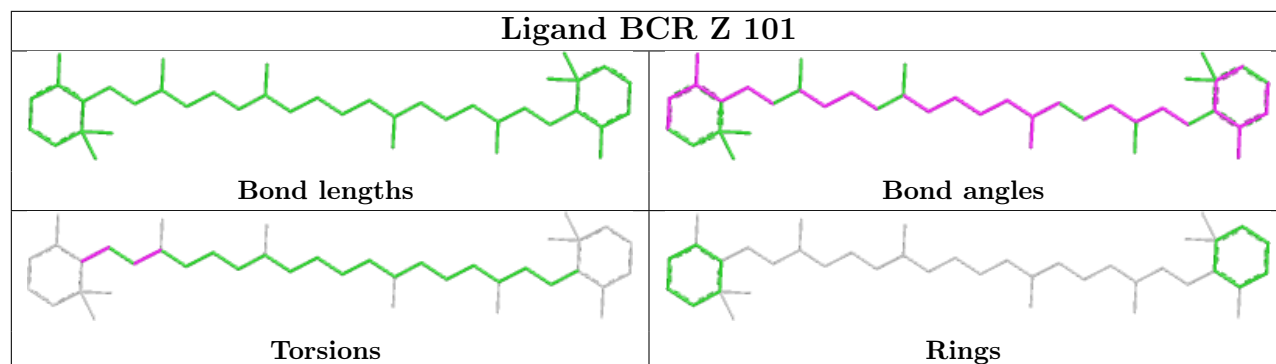
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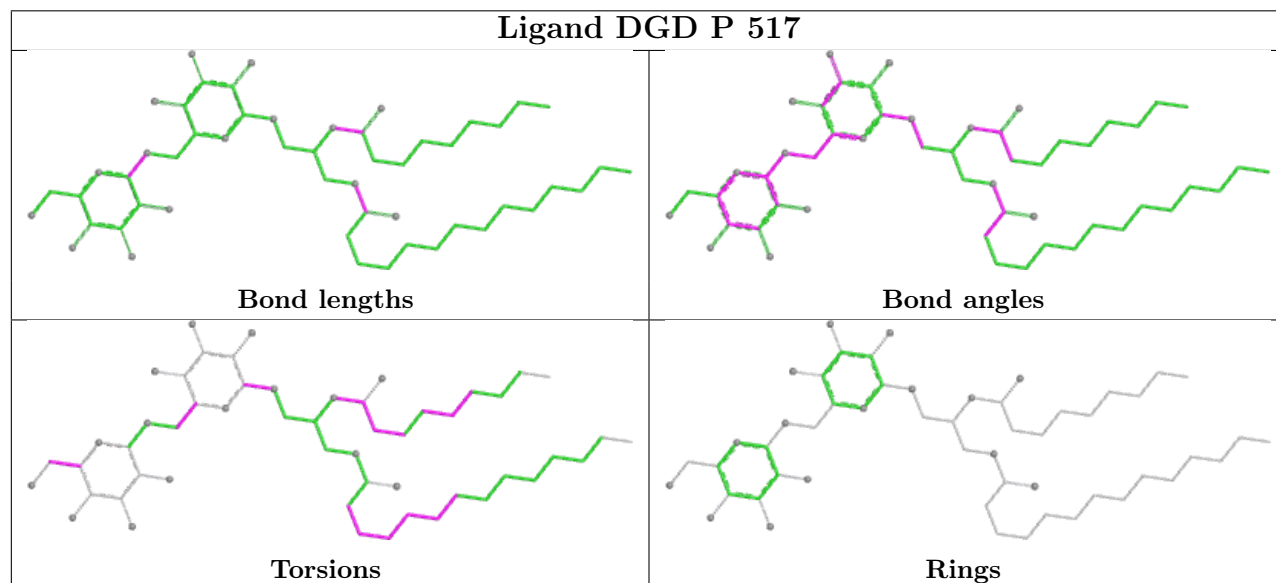
Ligand CLA Q 402



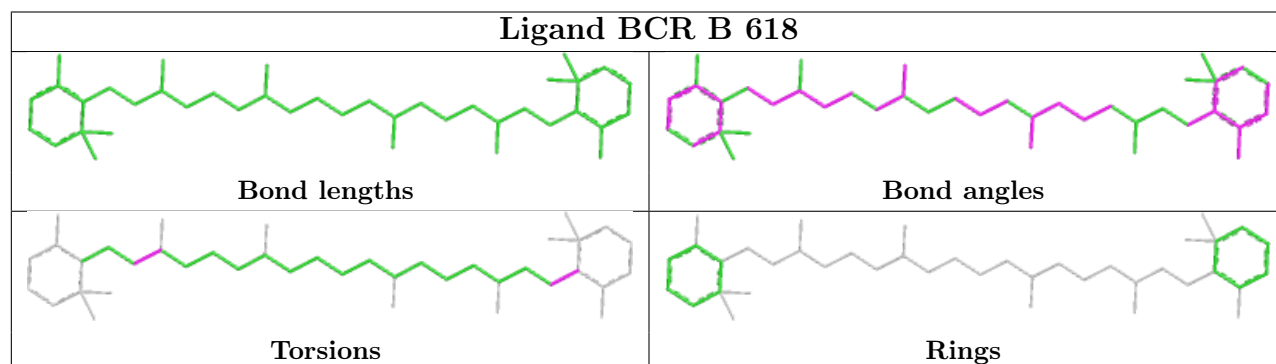
Ligand BCR Z 101

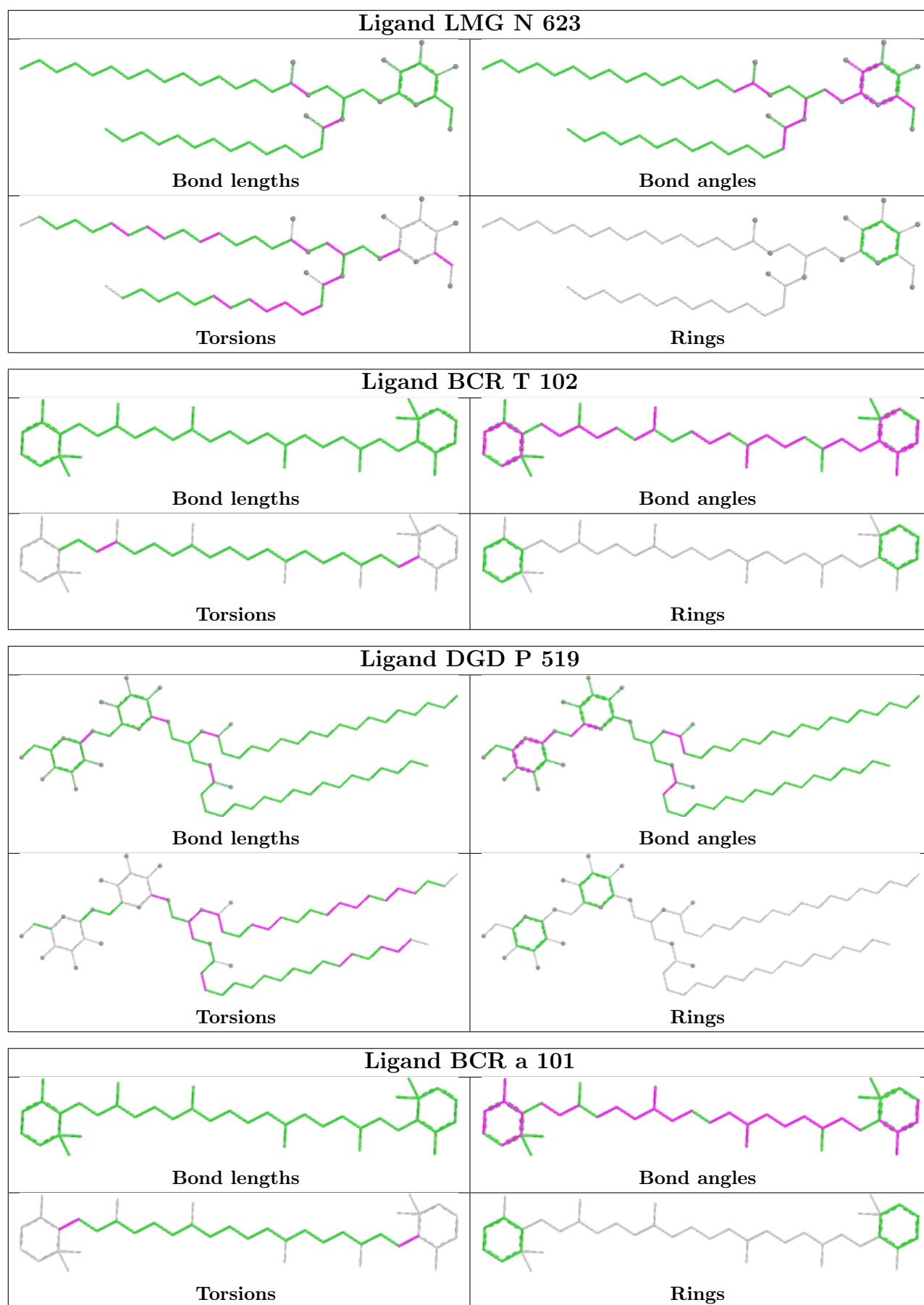


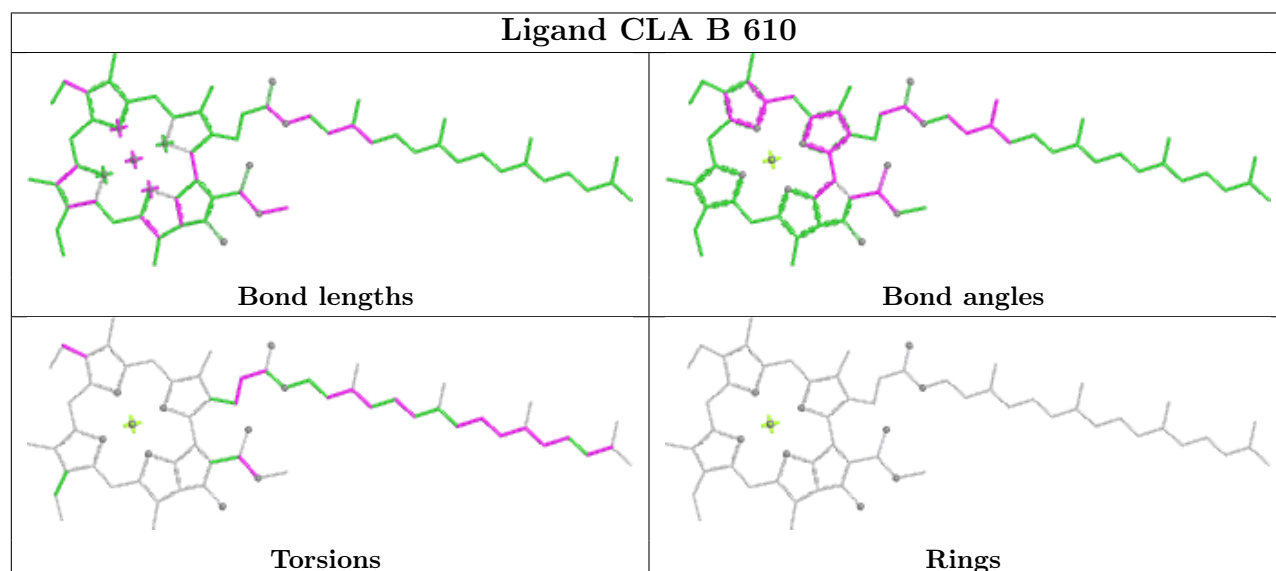
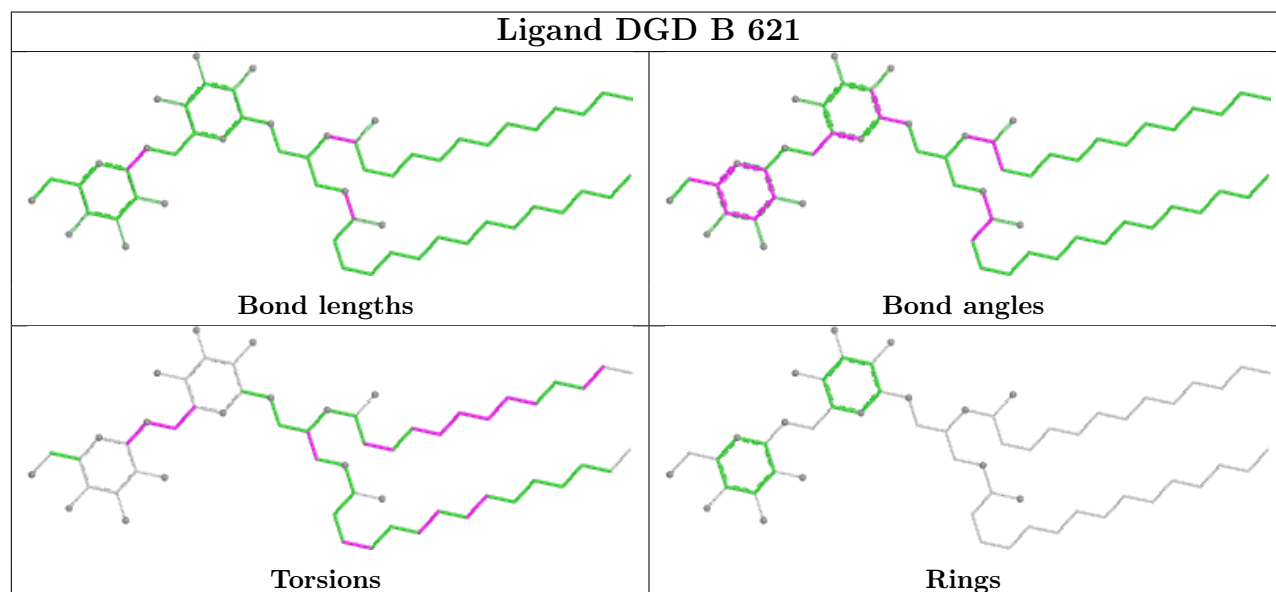
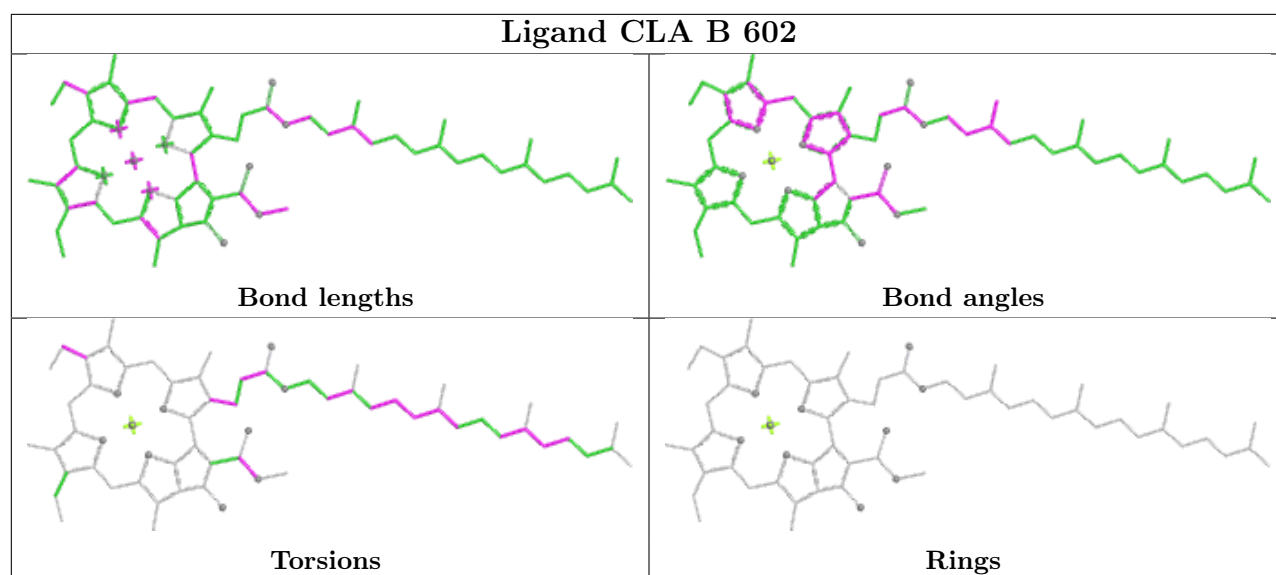
Ligand DGD P 517

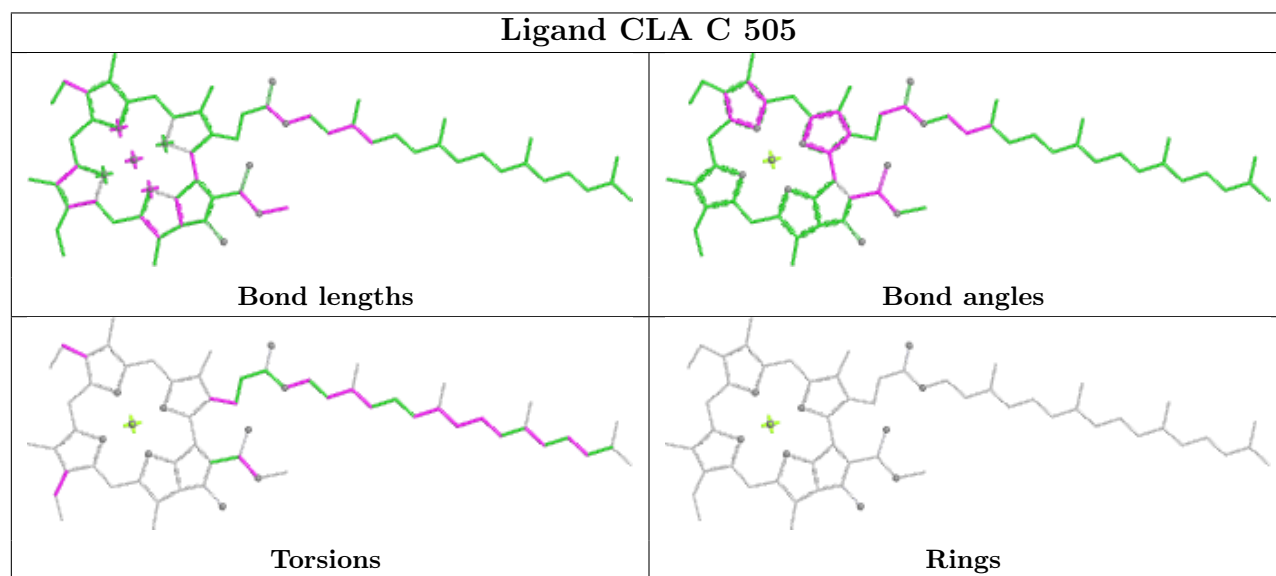
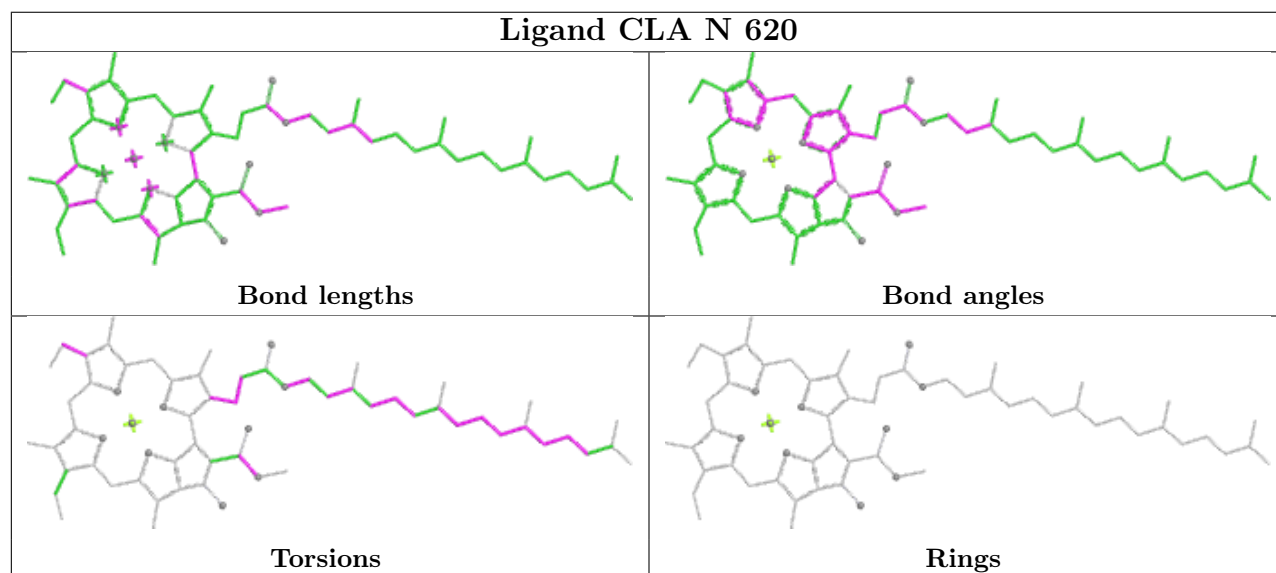
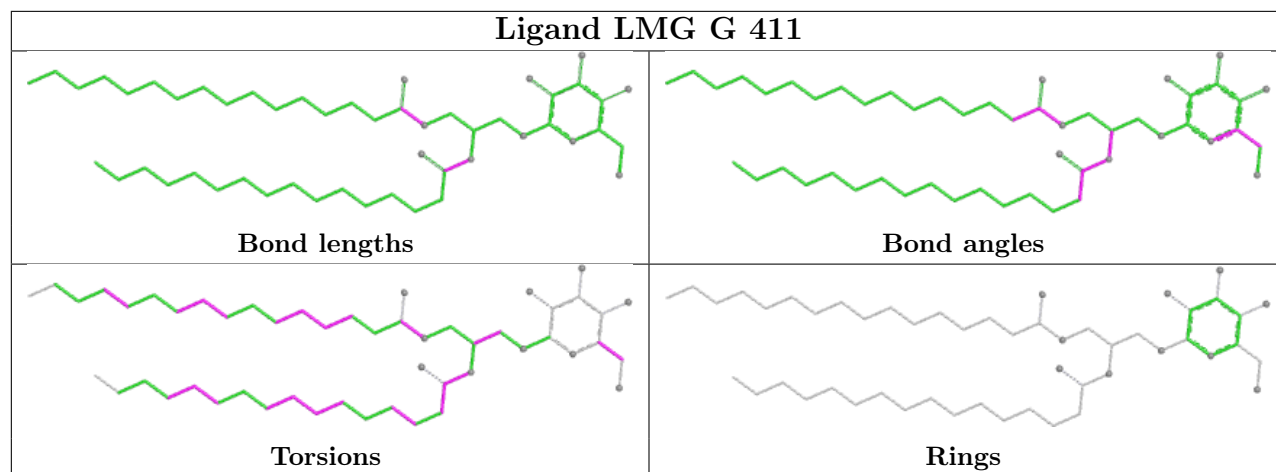


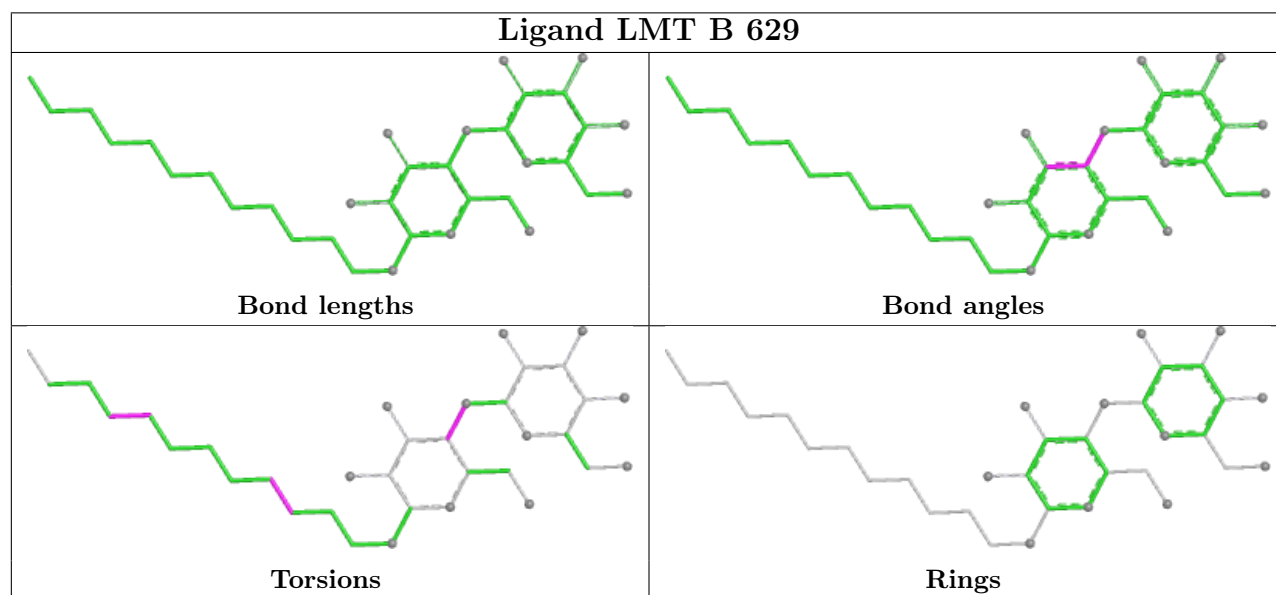
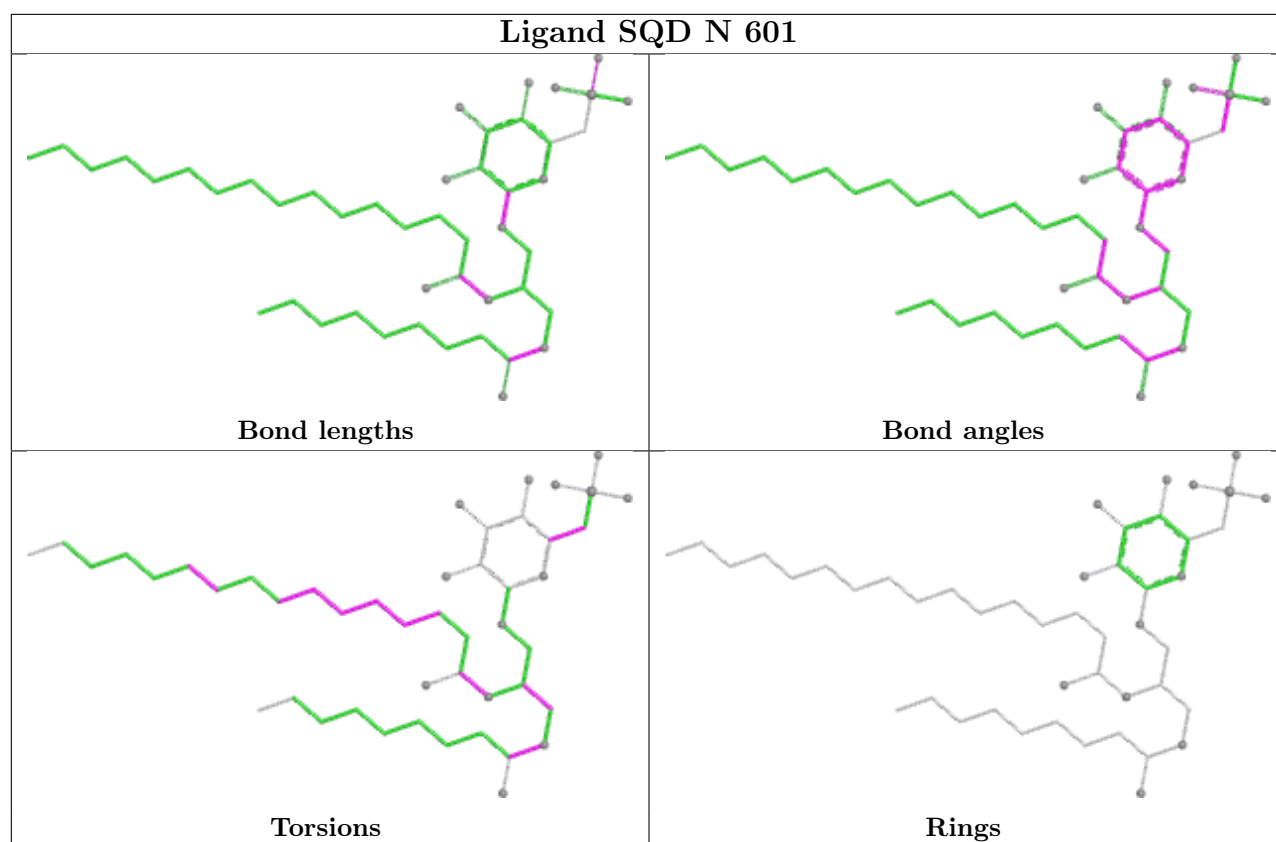
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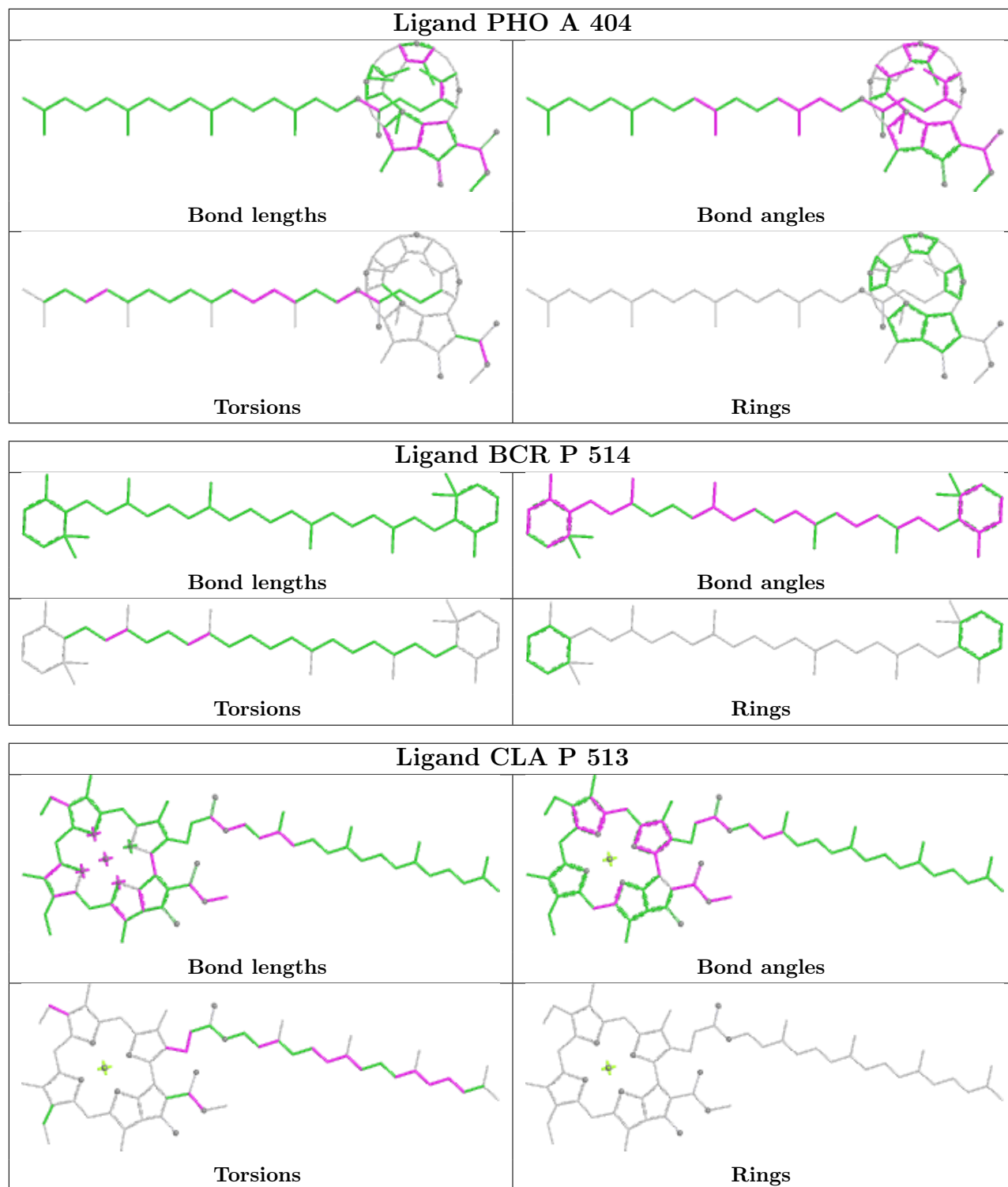


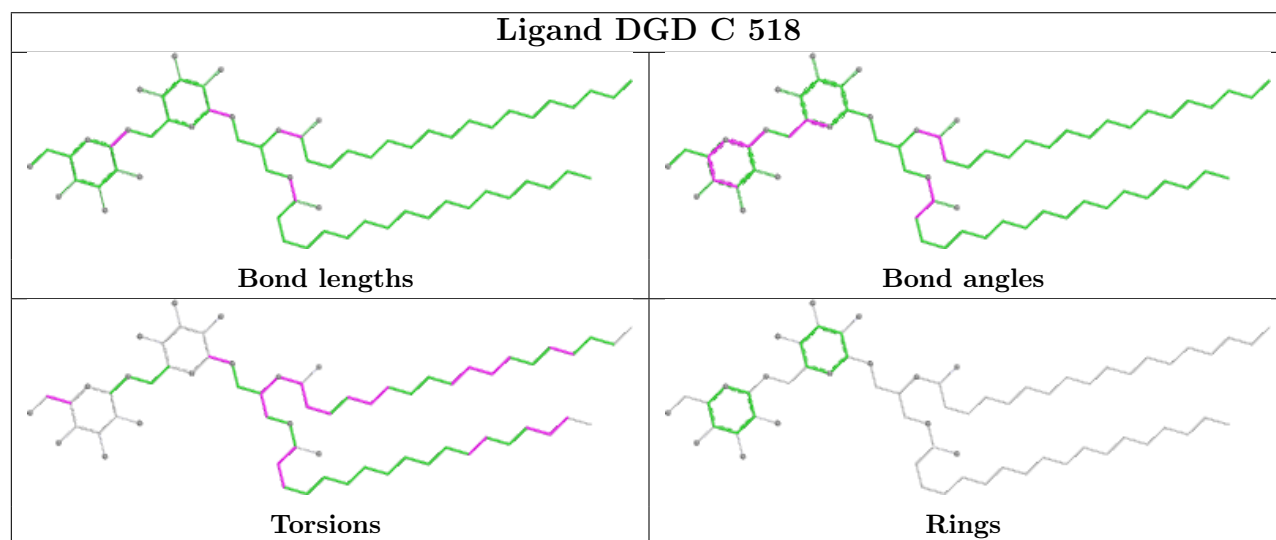
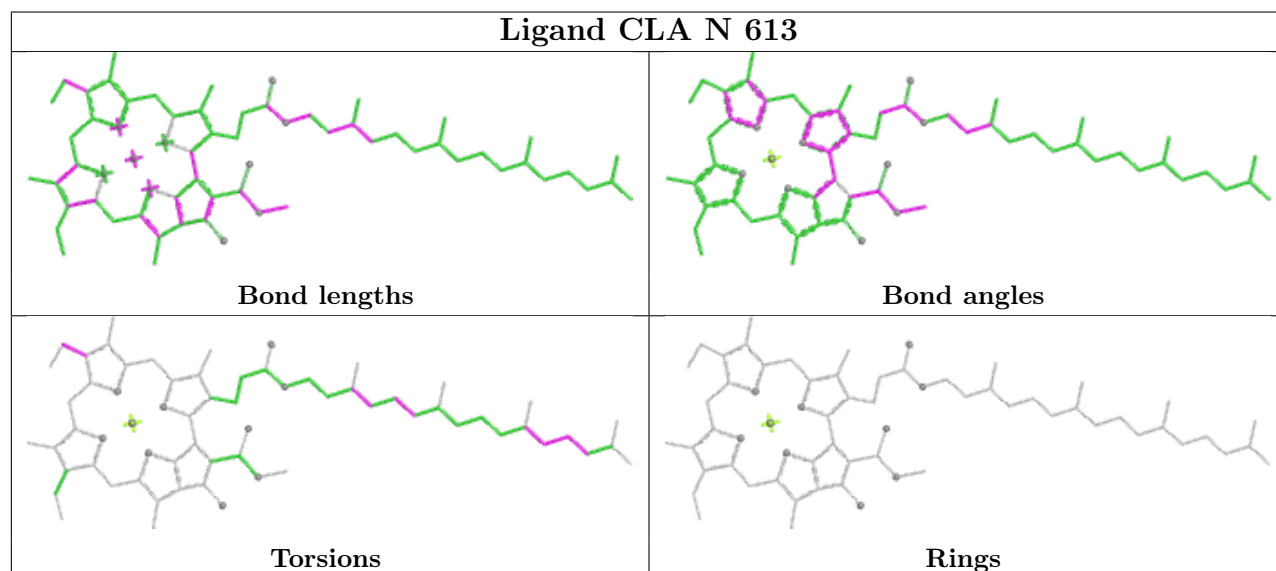
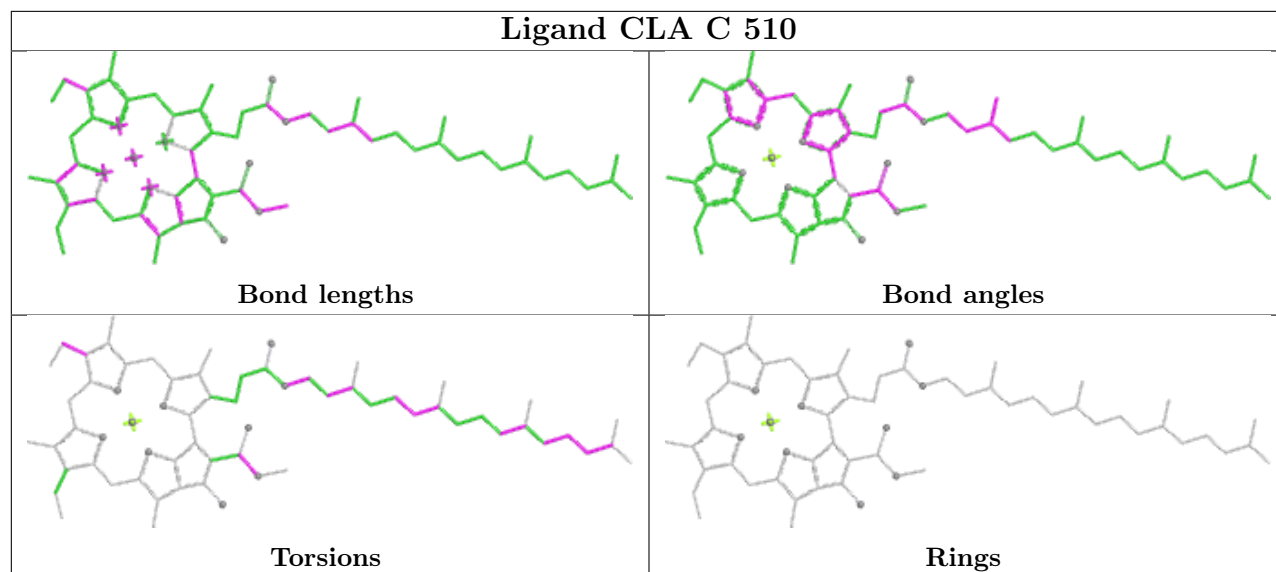


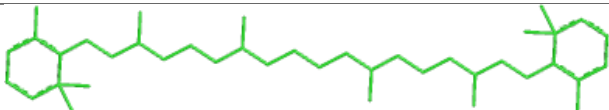
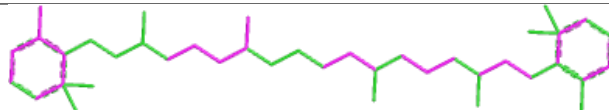
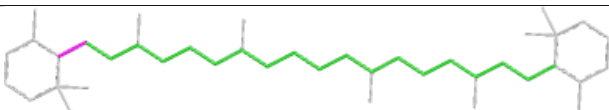
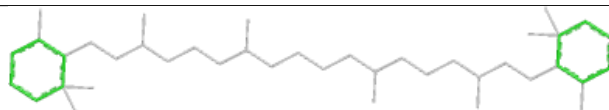


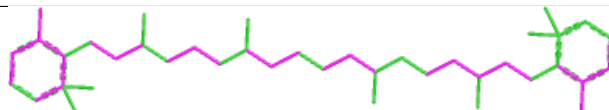
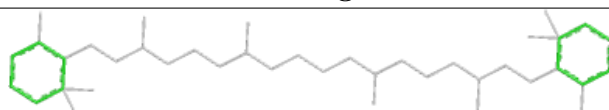


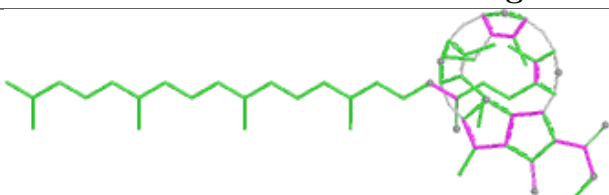
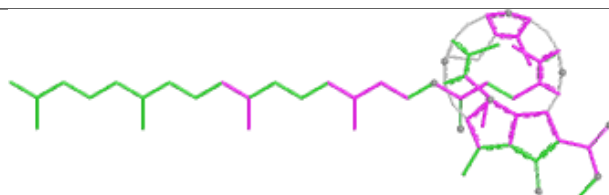
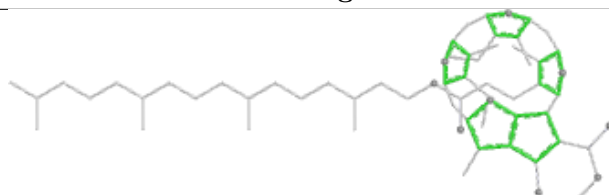




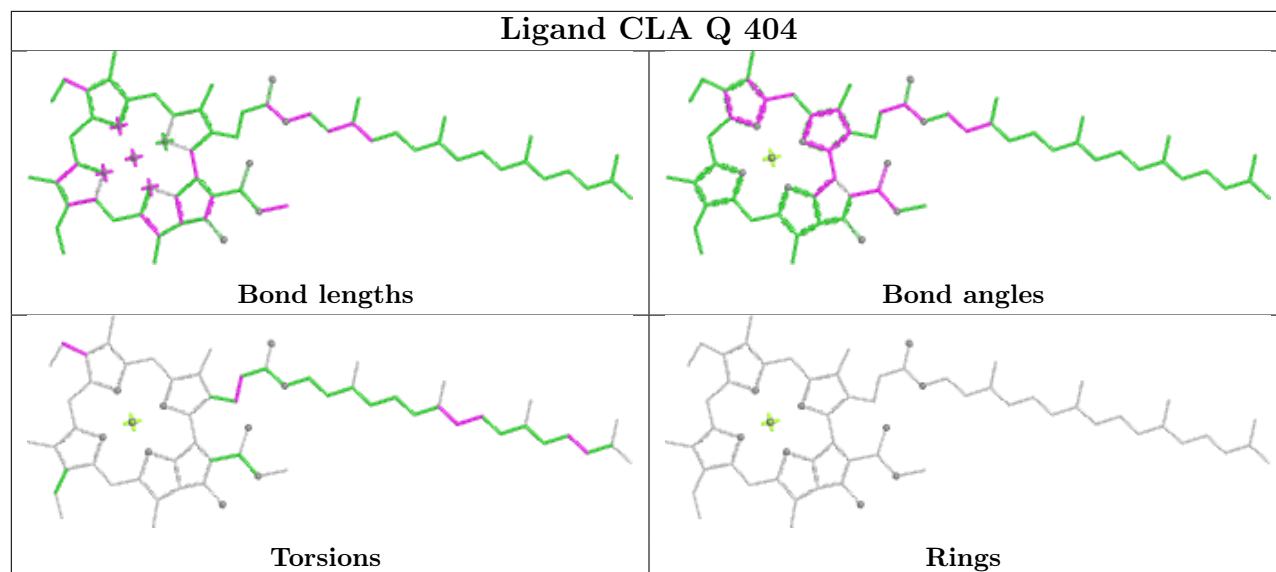


Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

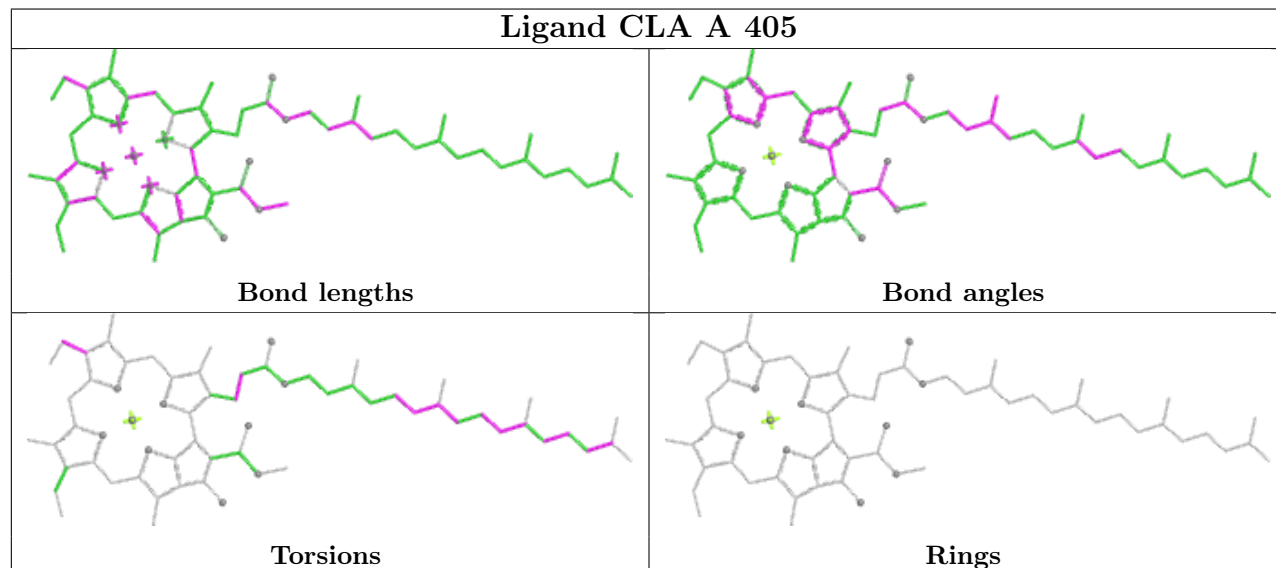
Ligand BCR T 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO G 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

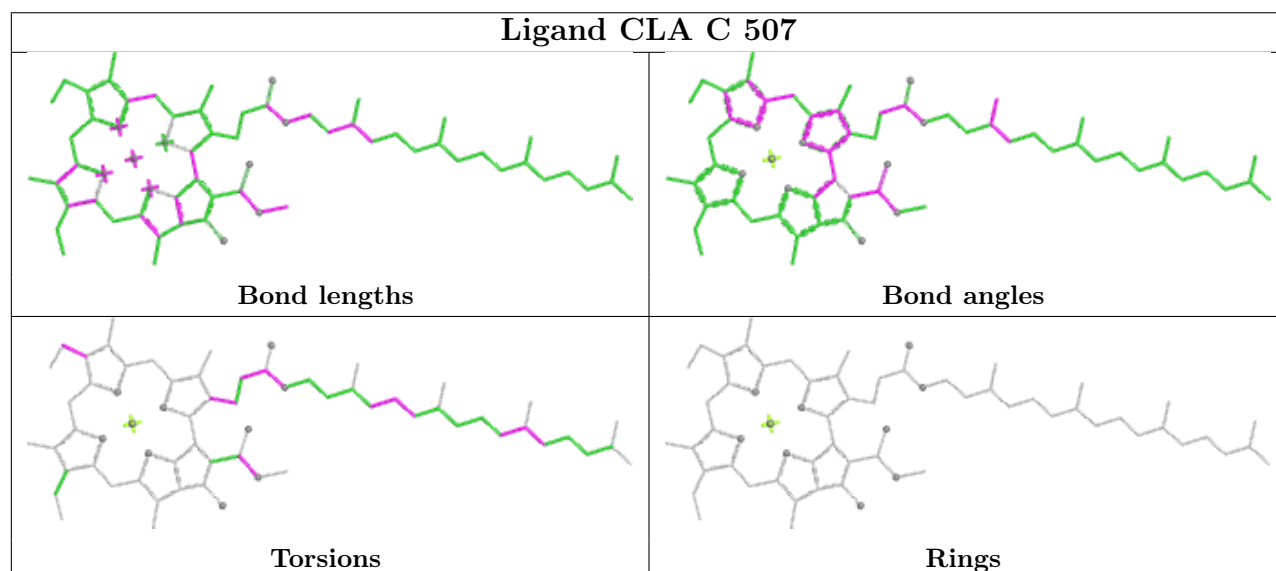
Ligand CLA Q 404

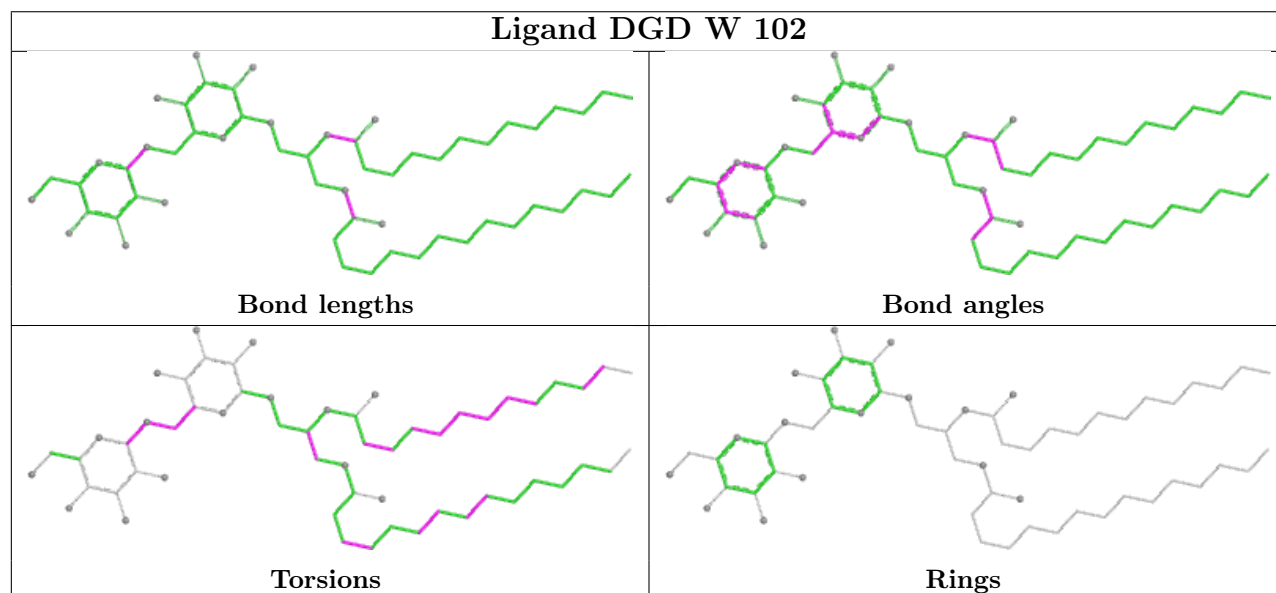
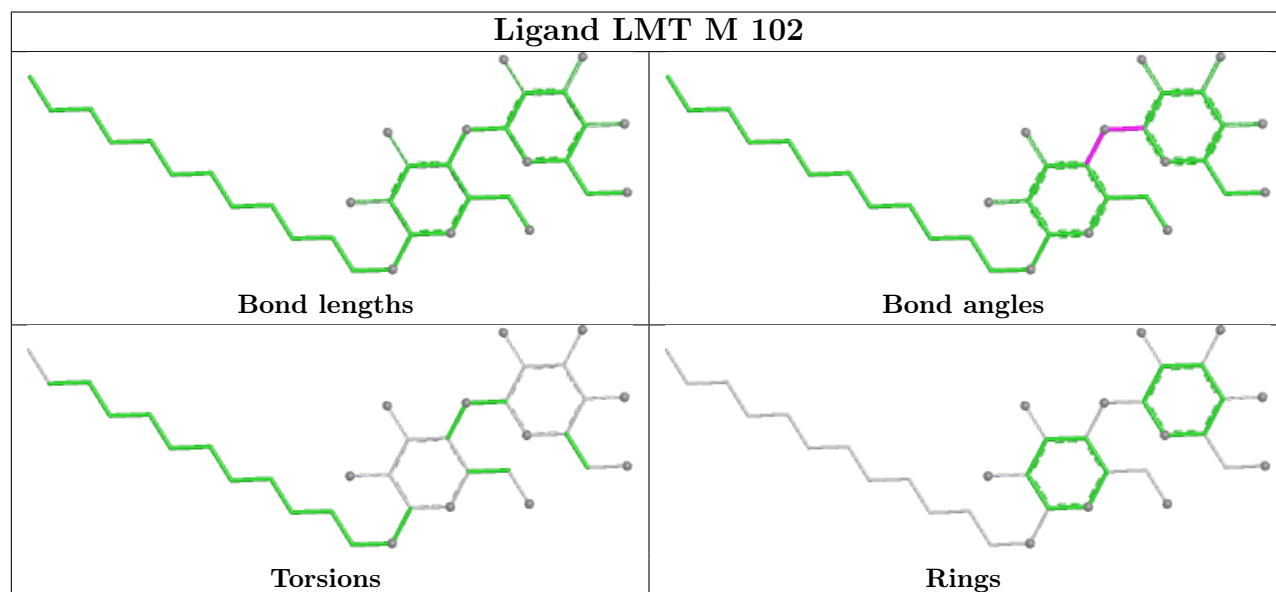
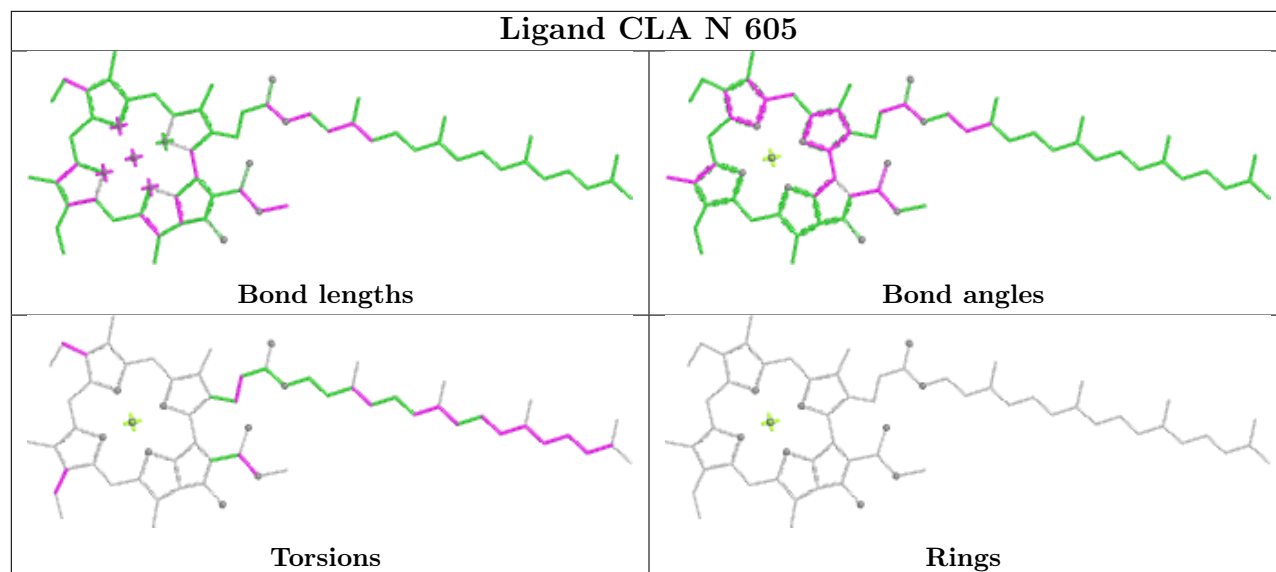


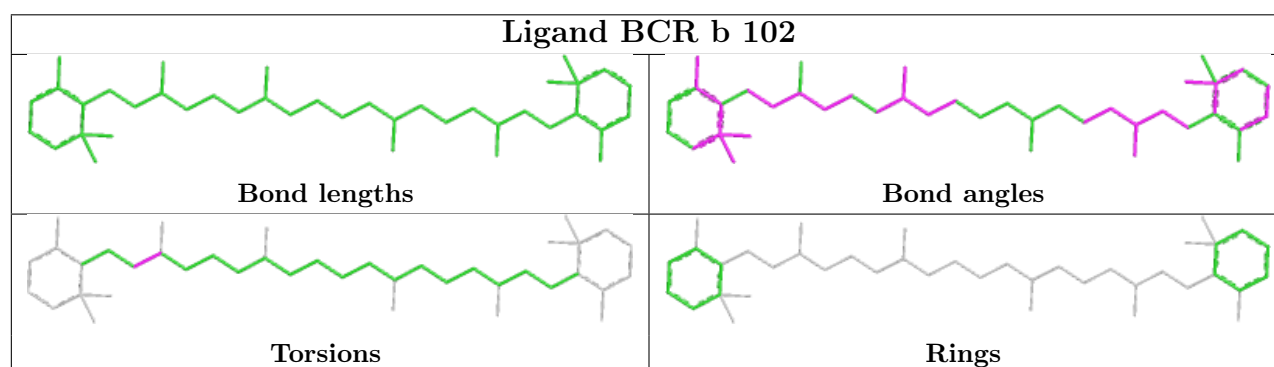
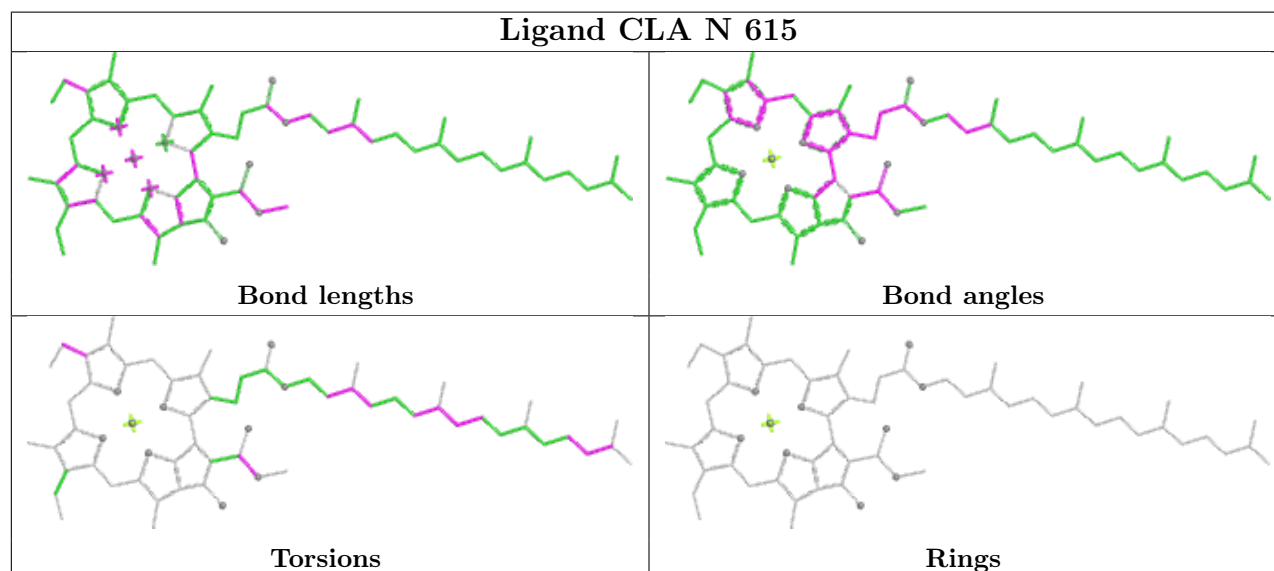
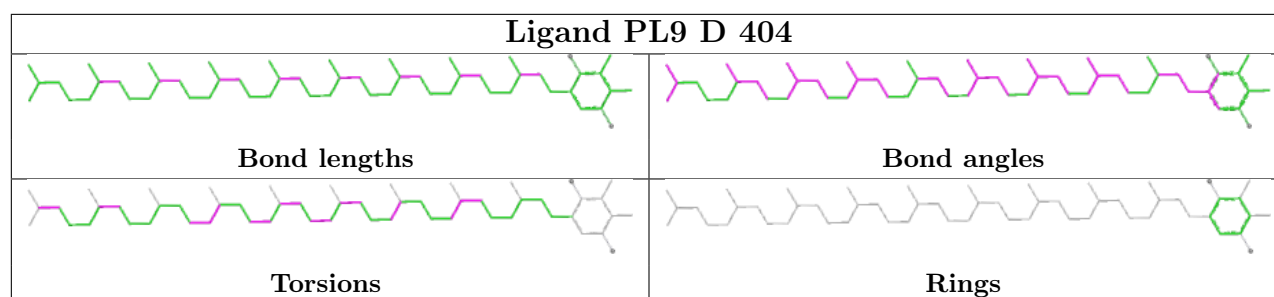
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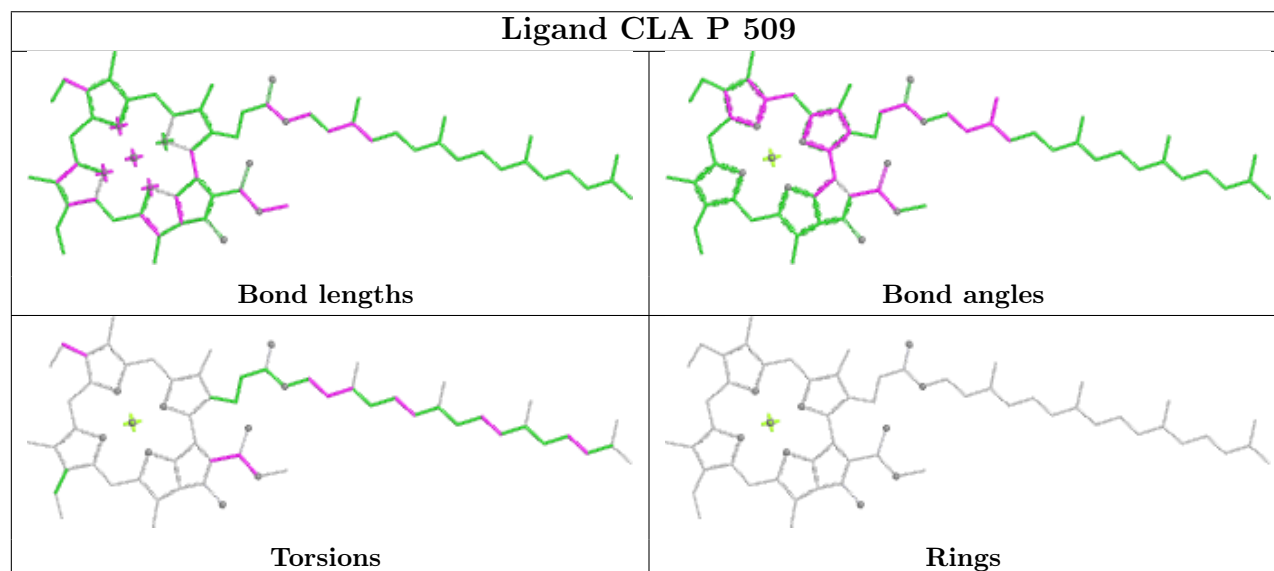
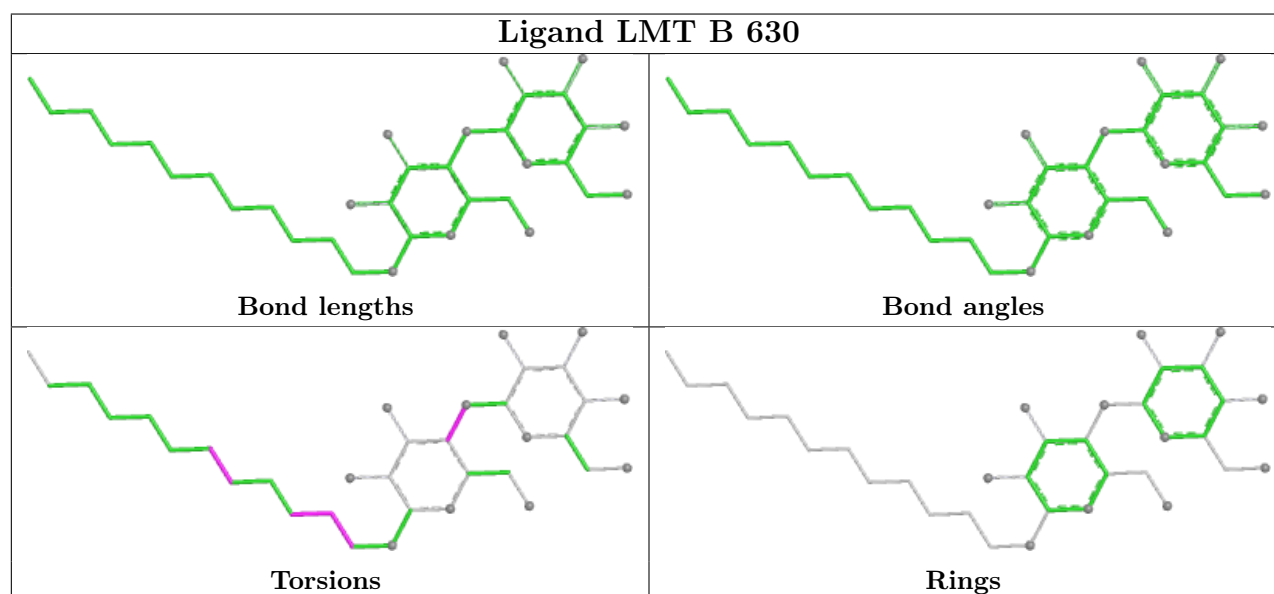
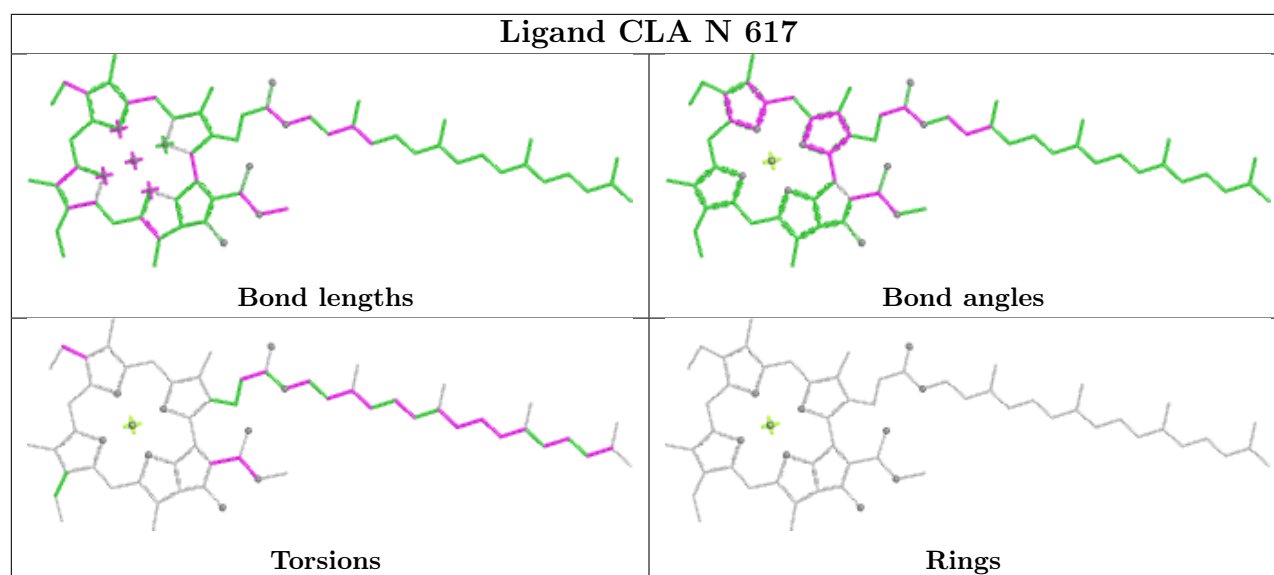


Ligand CLA C 507

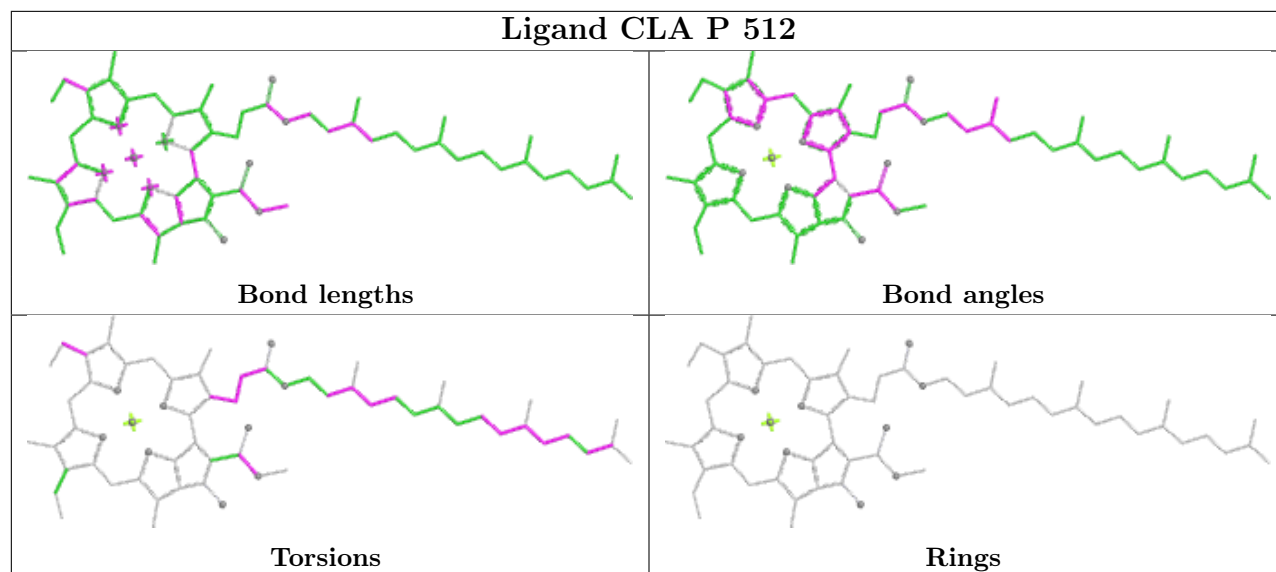




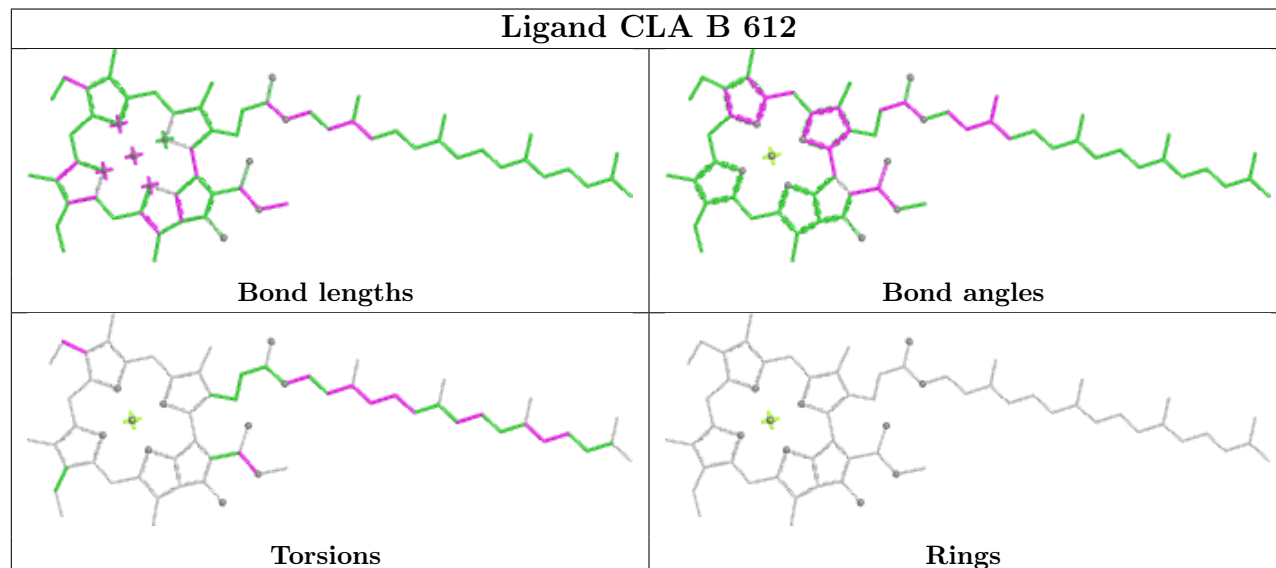




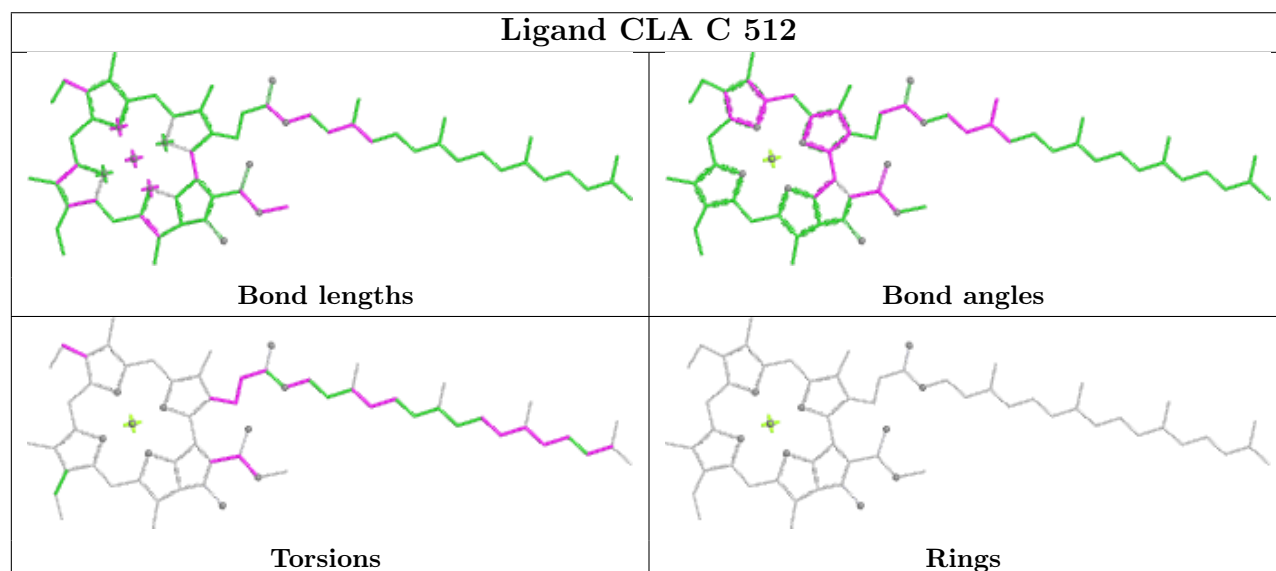
Ligand CLA P 512

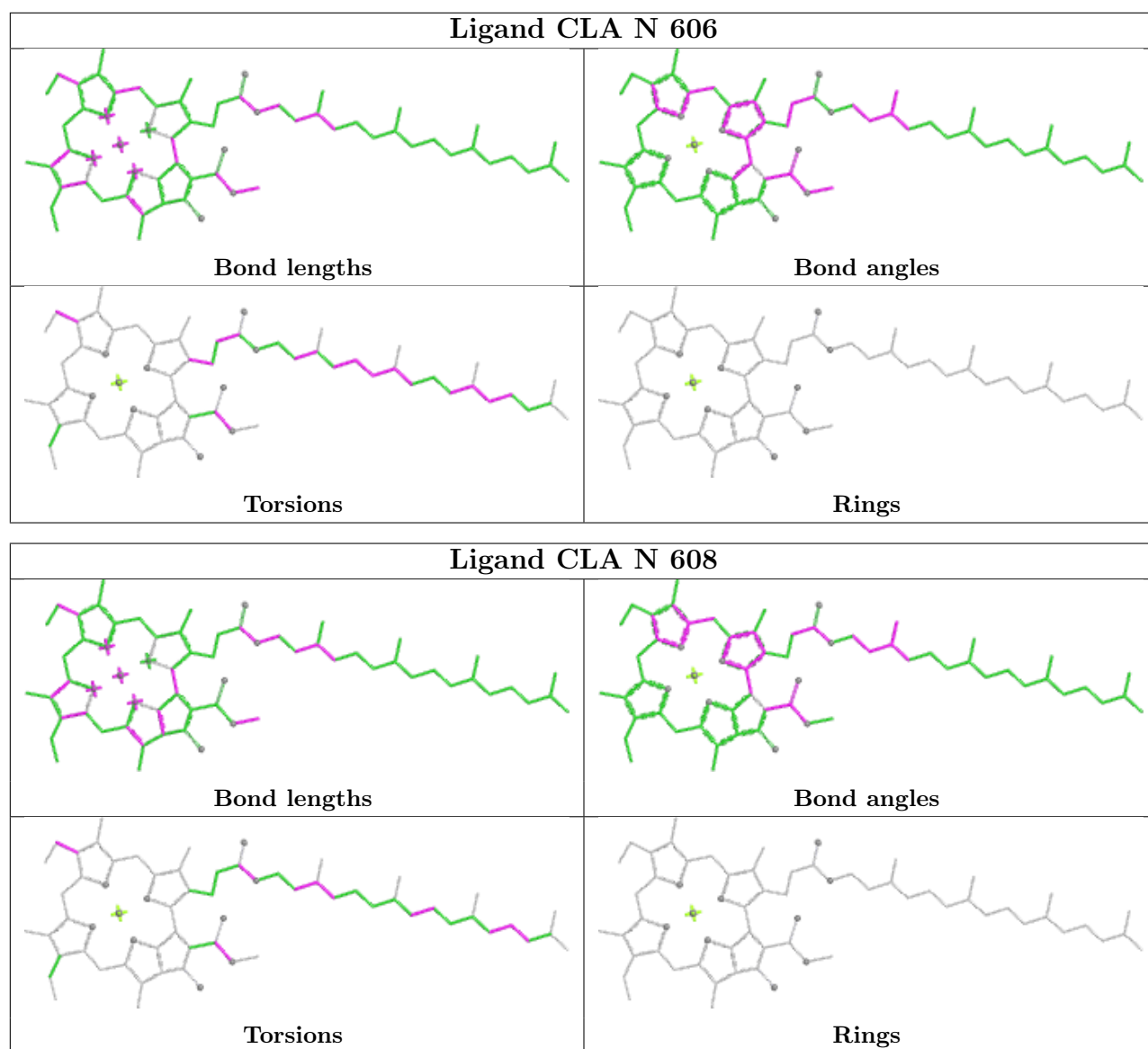


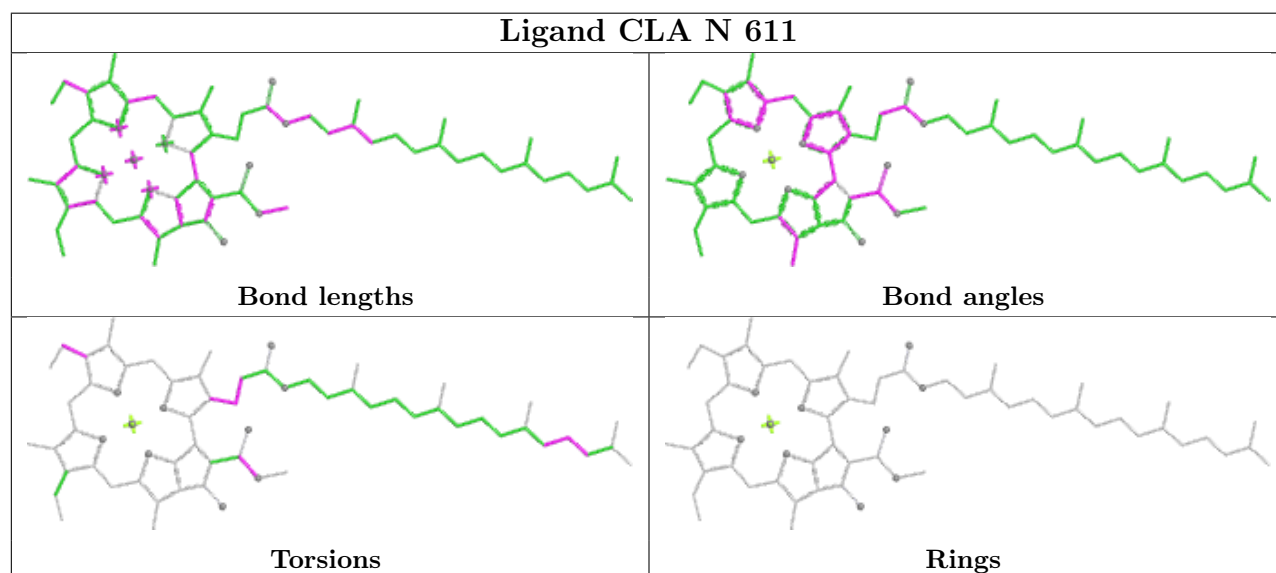
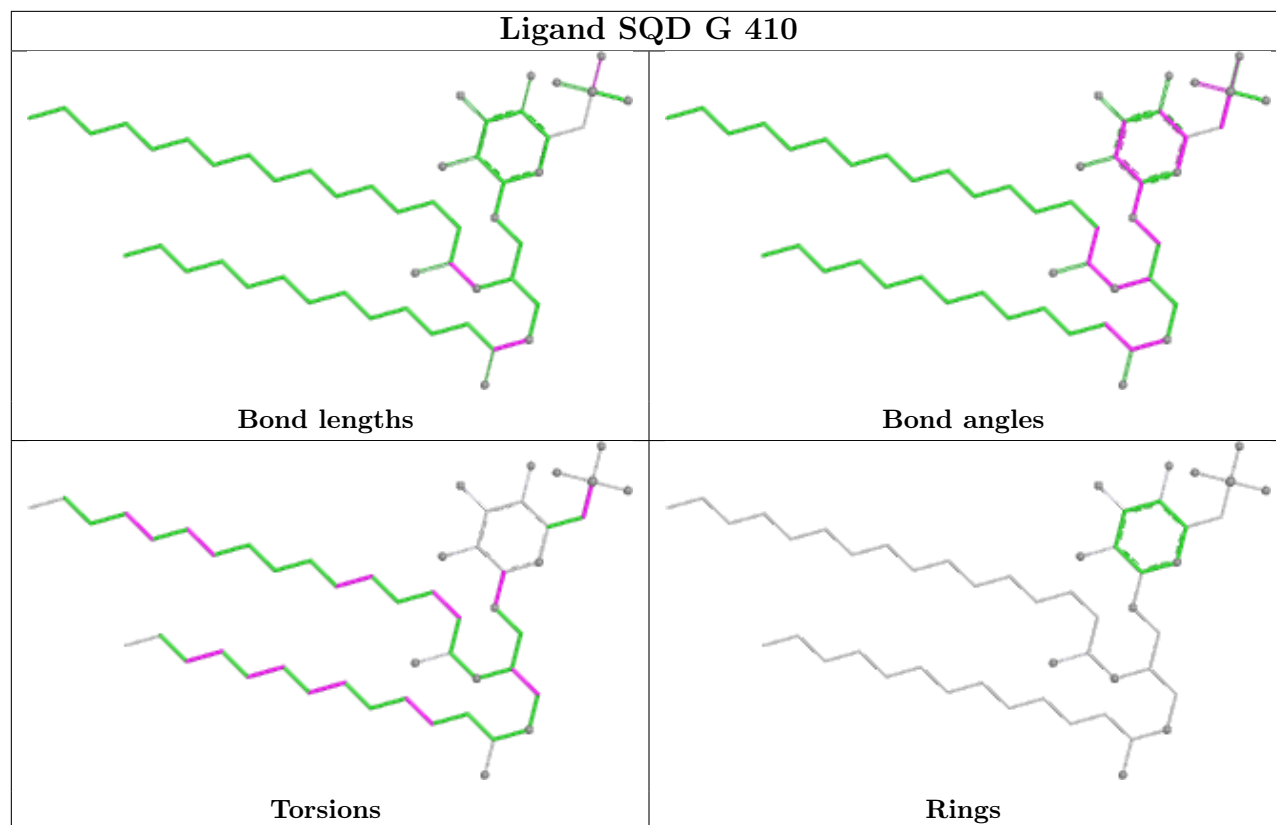
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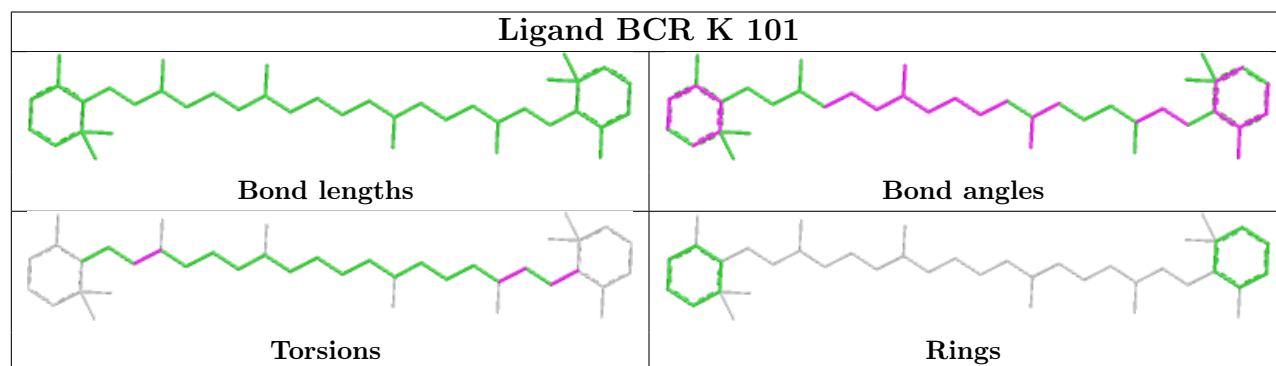
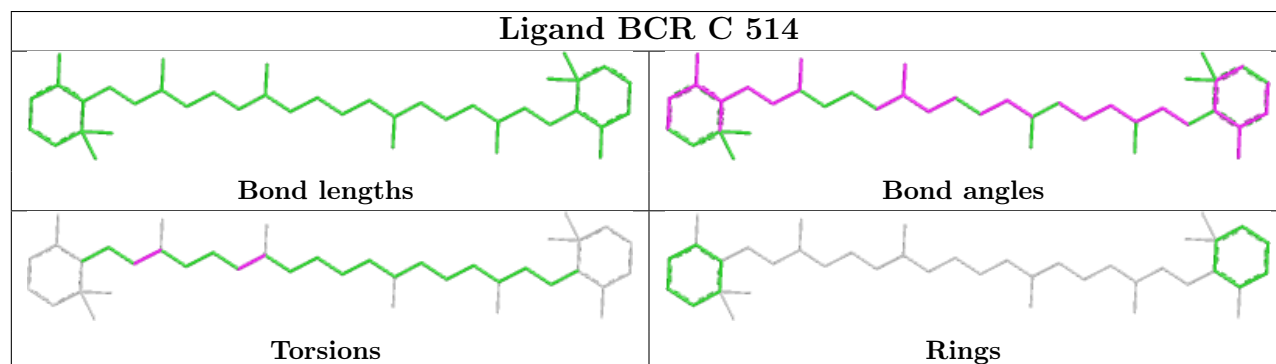
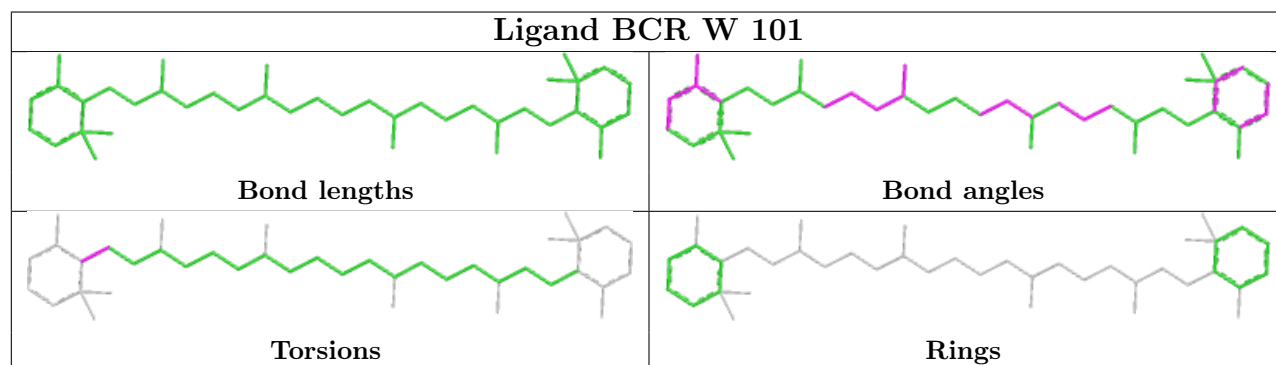
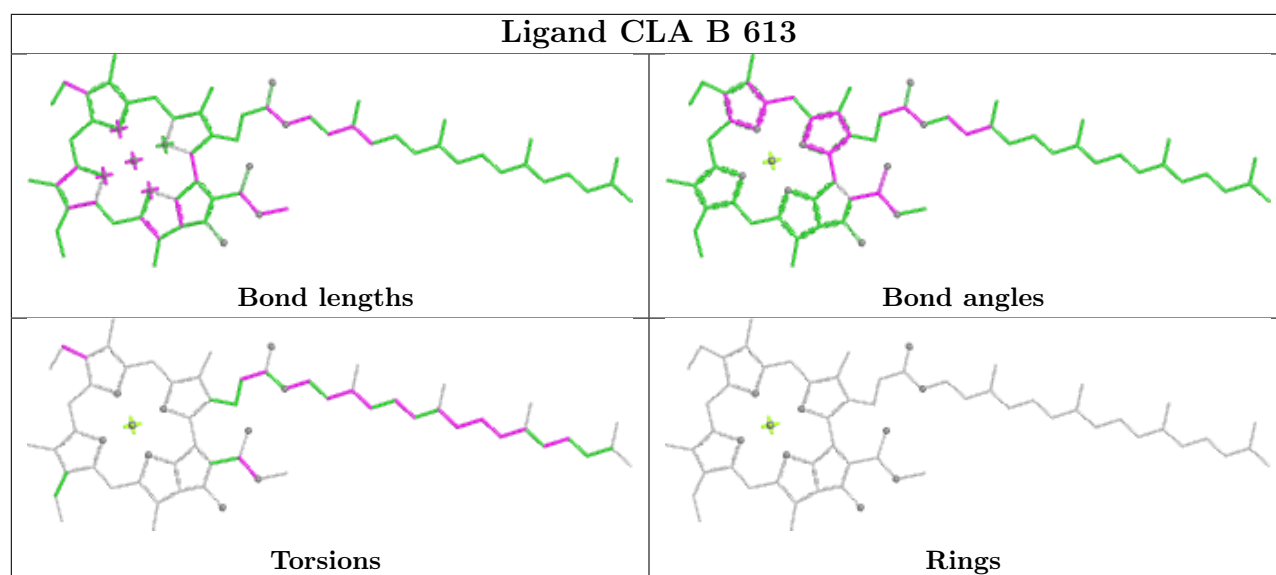


Ligand CLA C 512

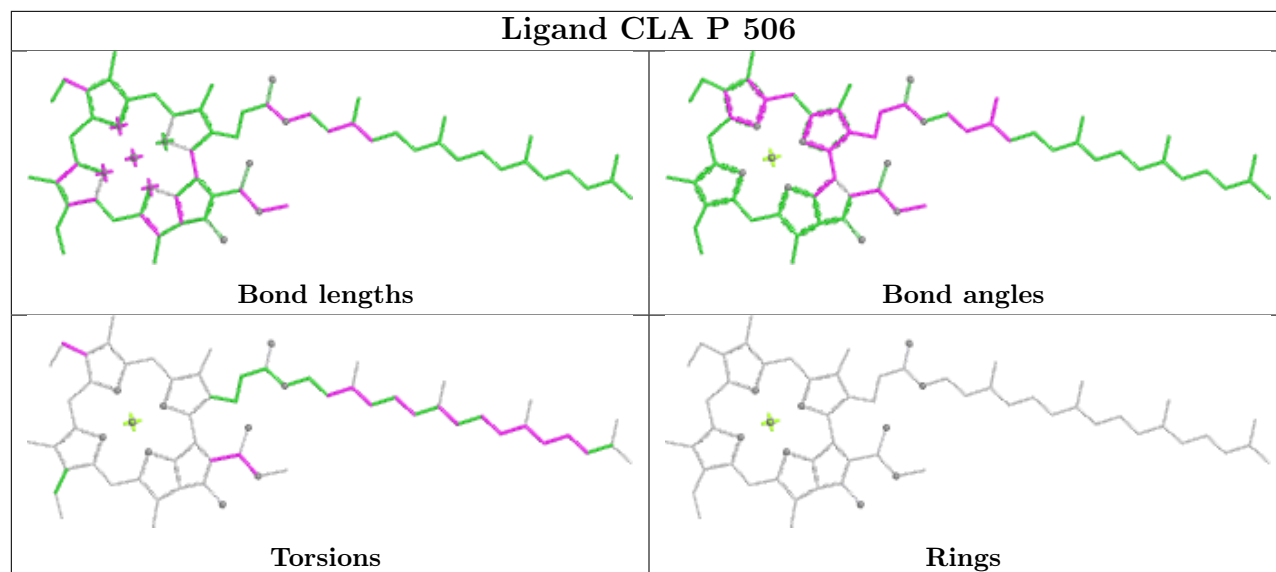




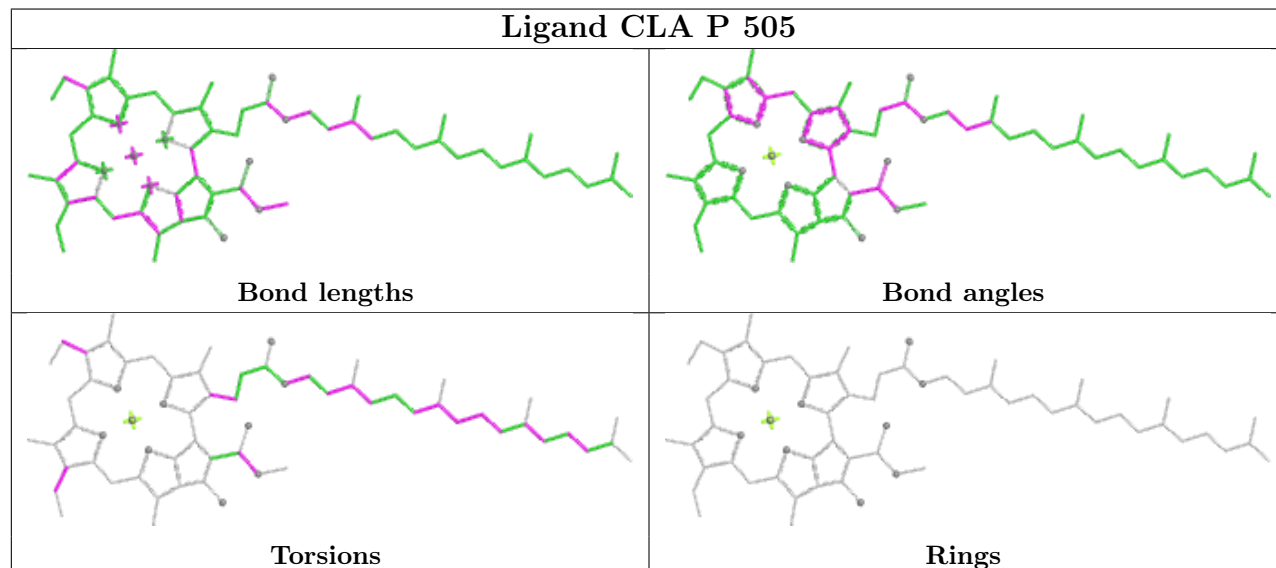




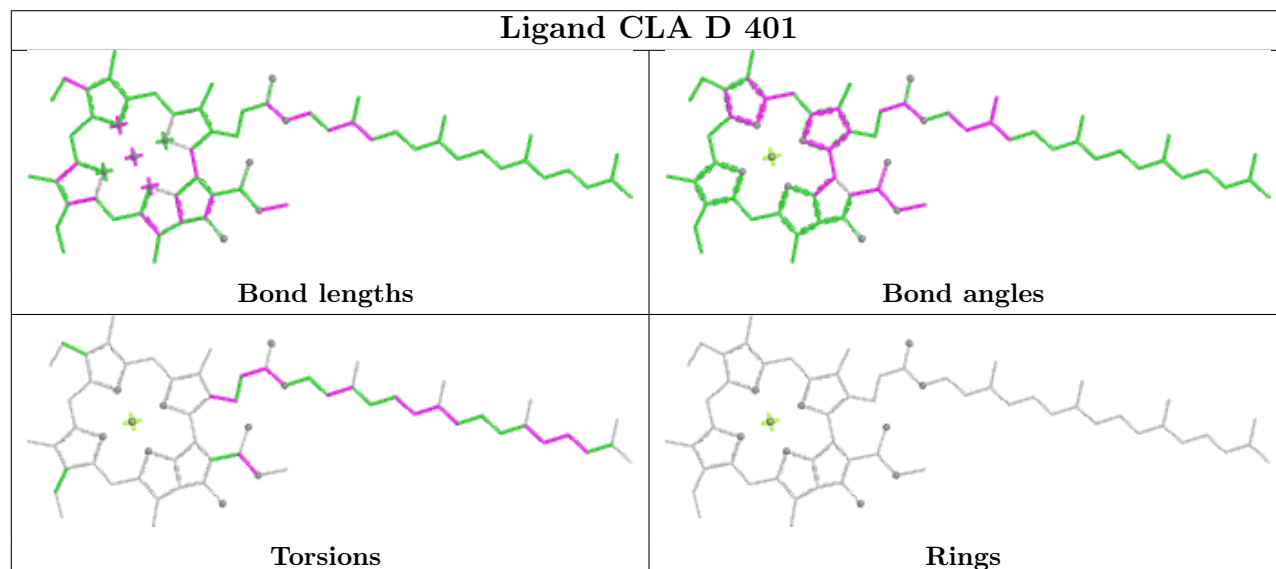
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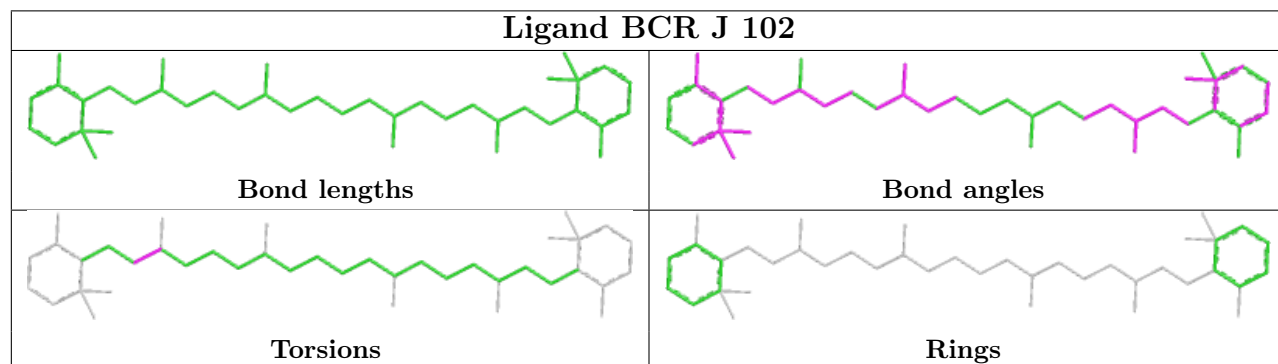
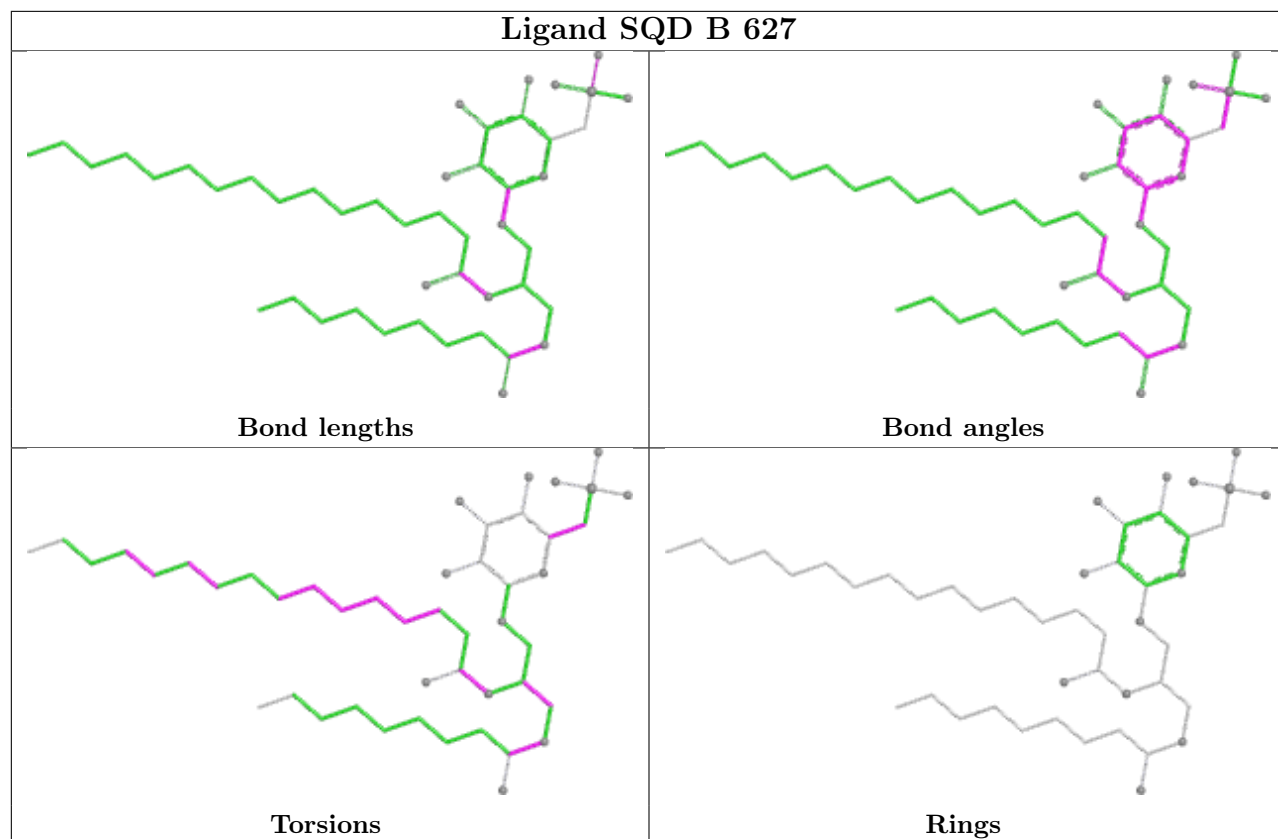


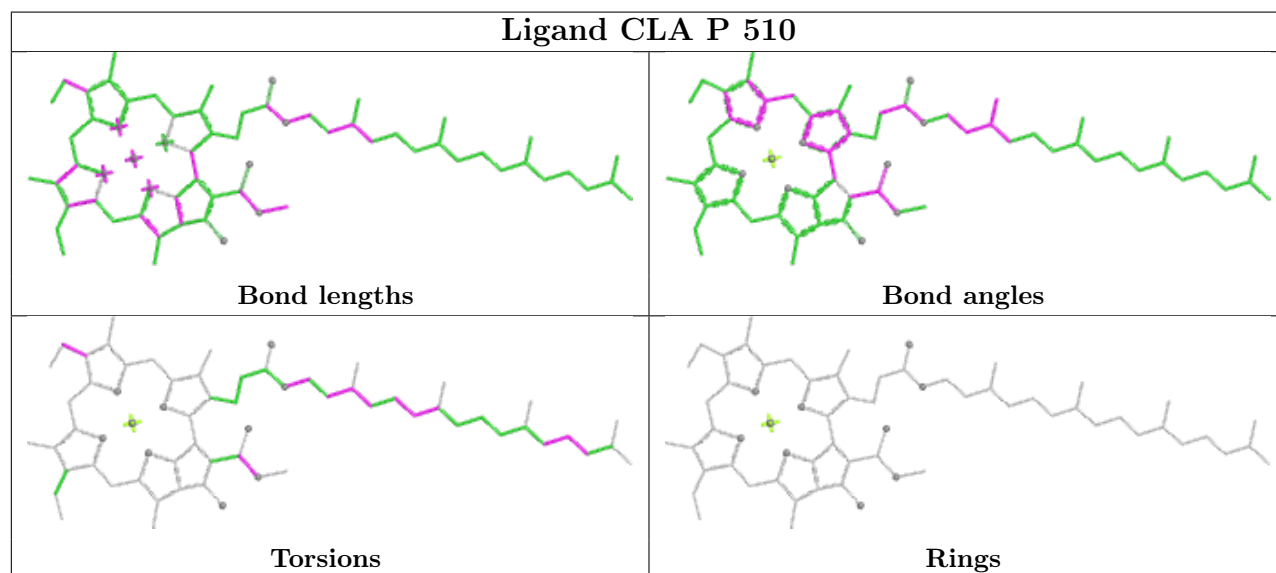
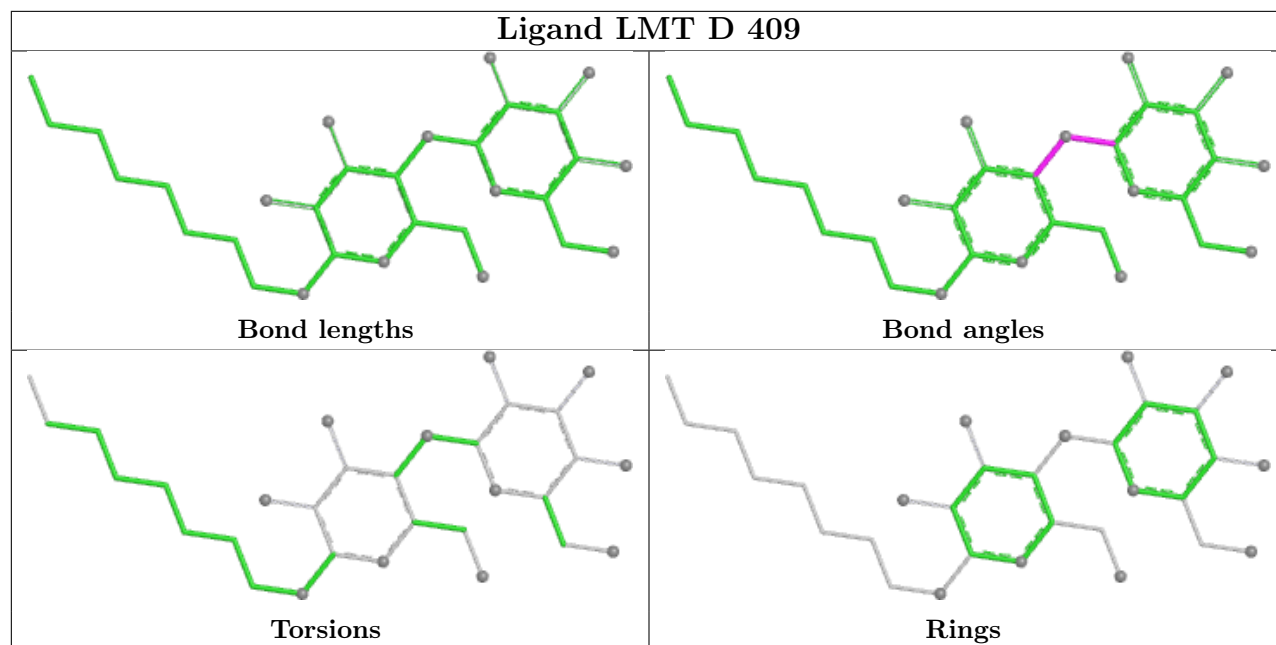
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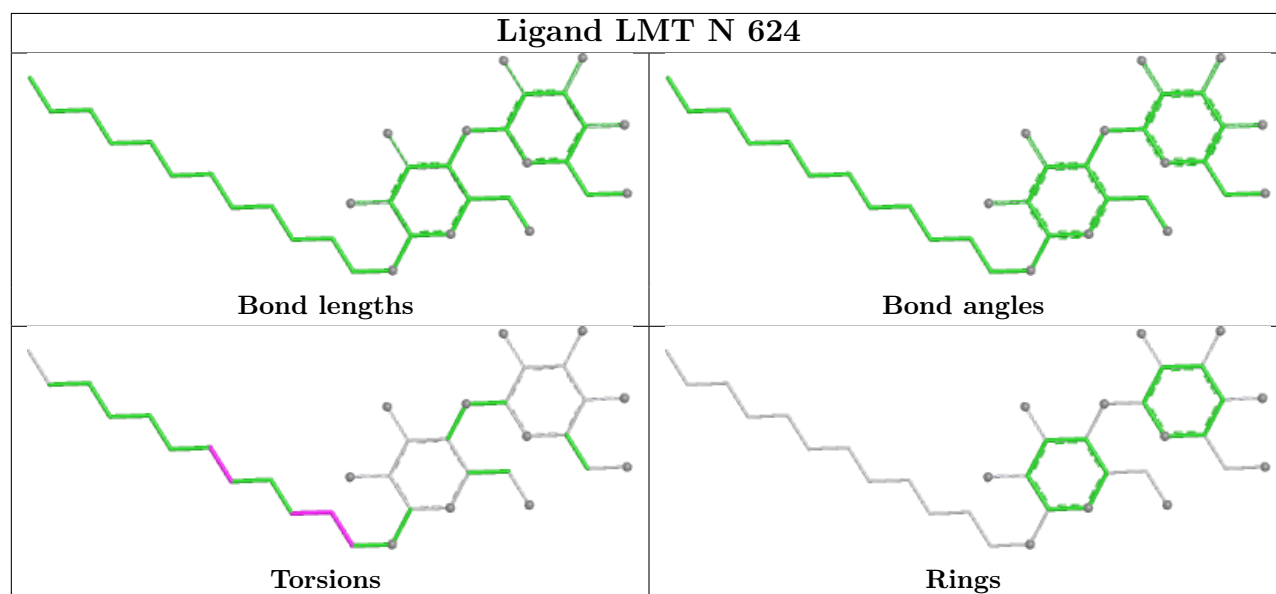
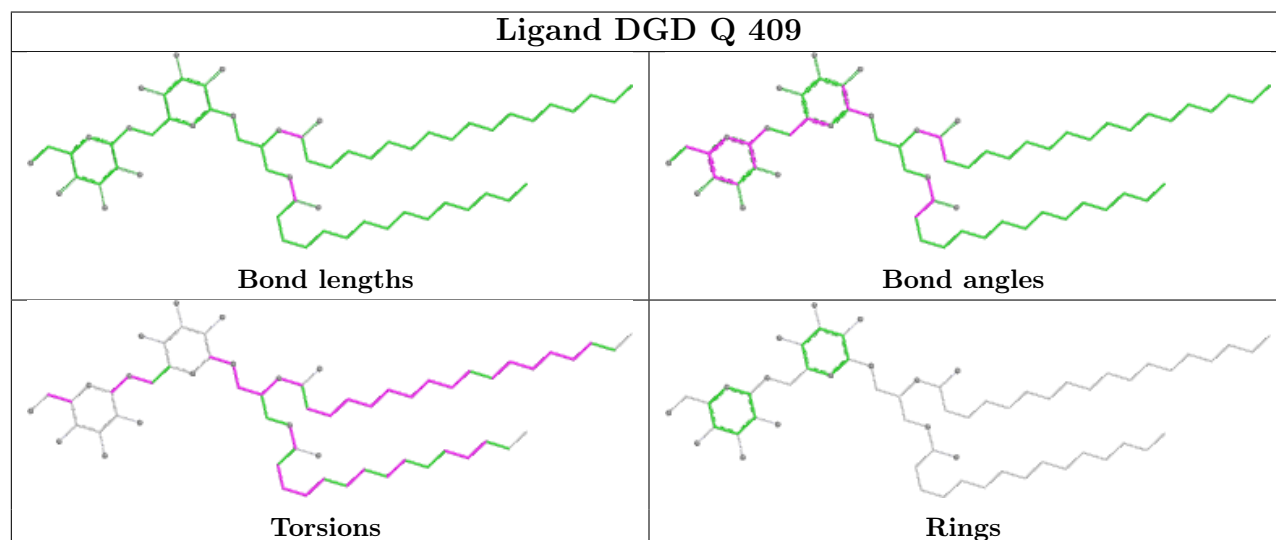
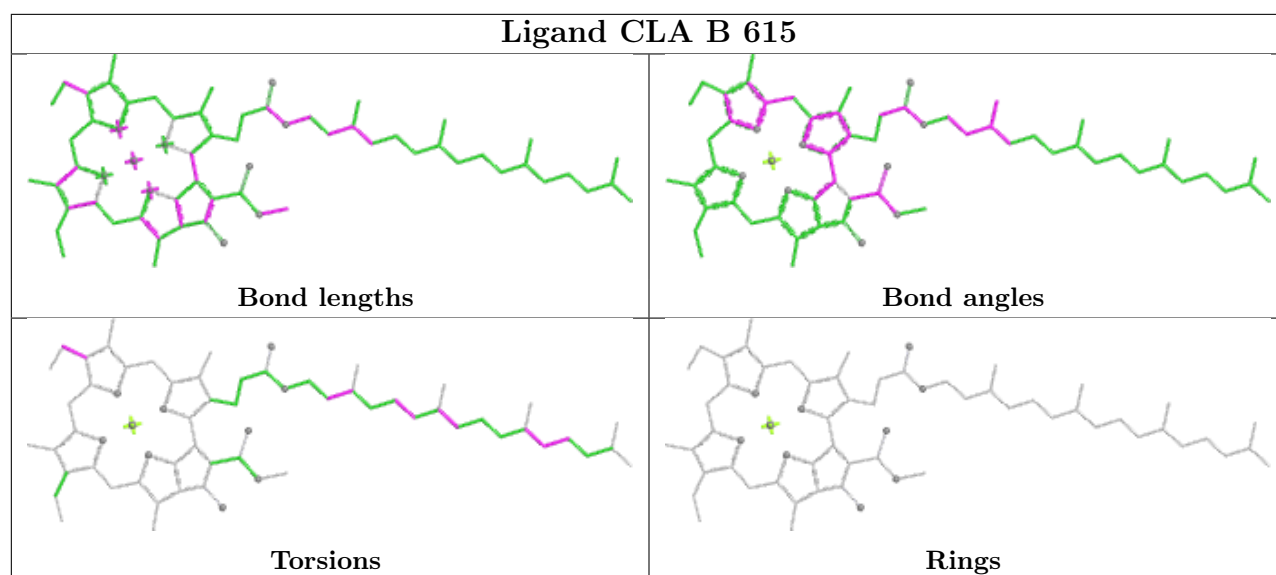


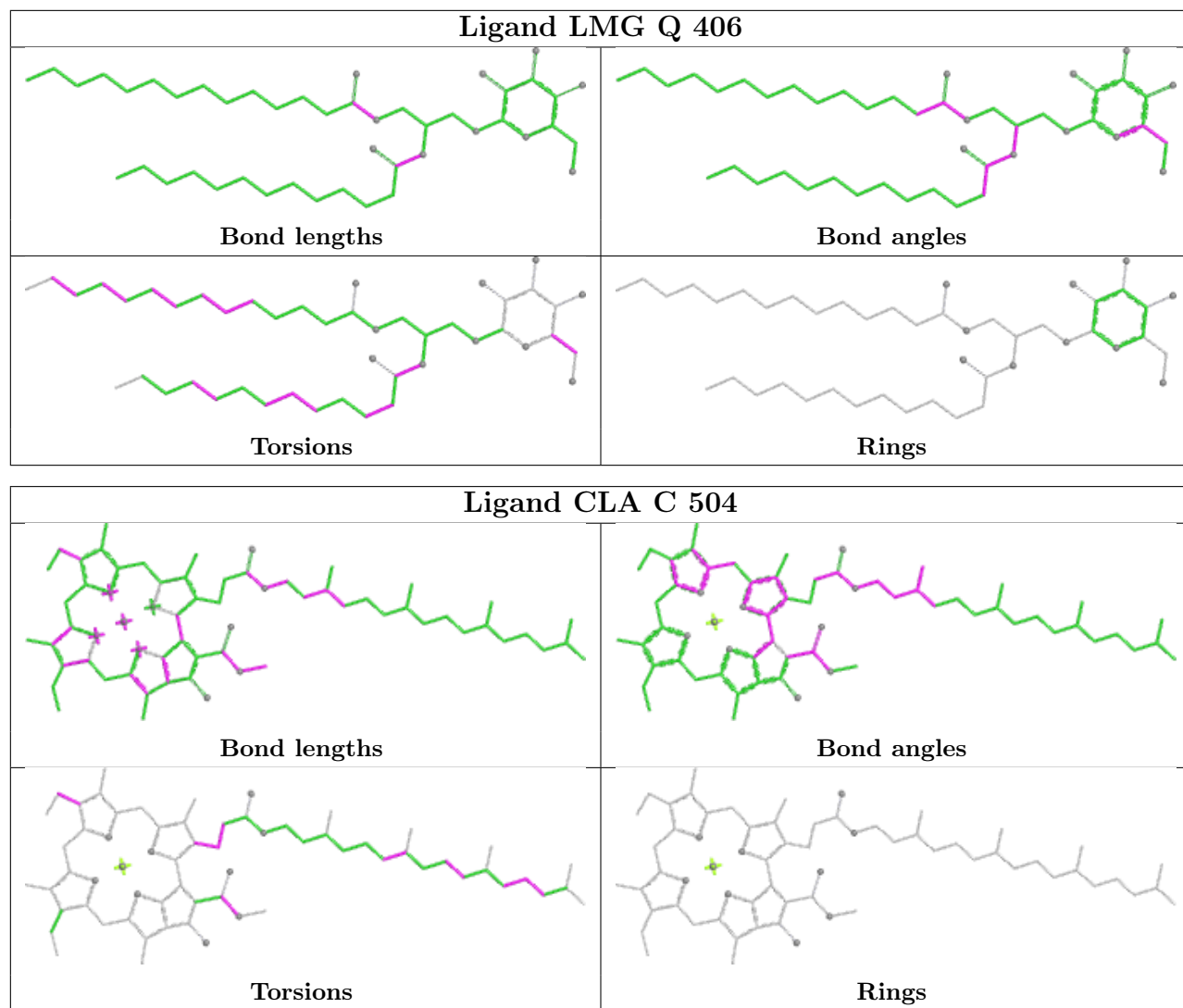
Ligand CLA D 401

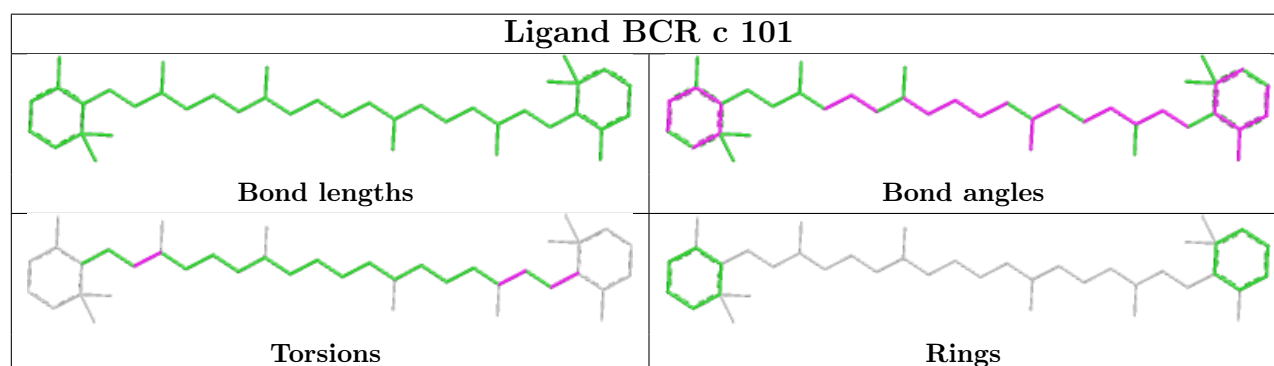
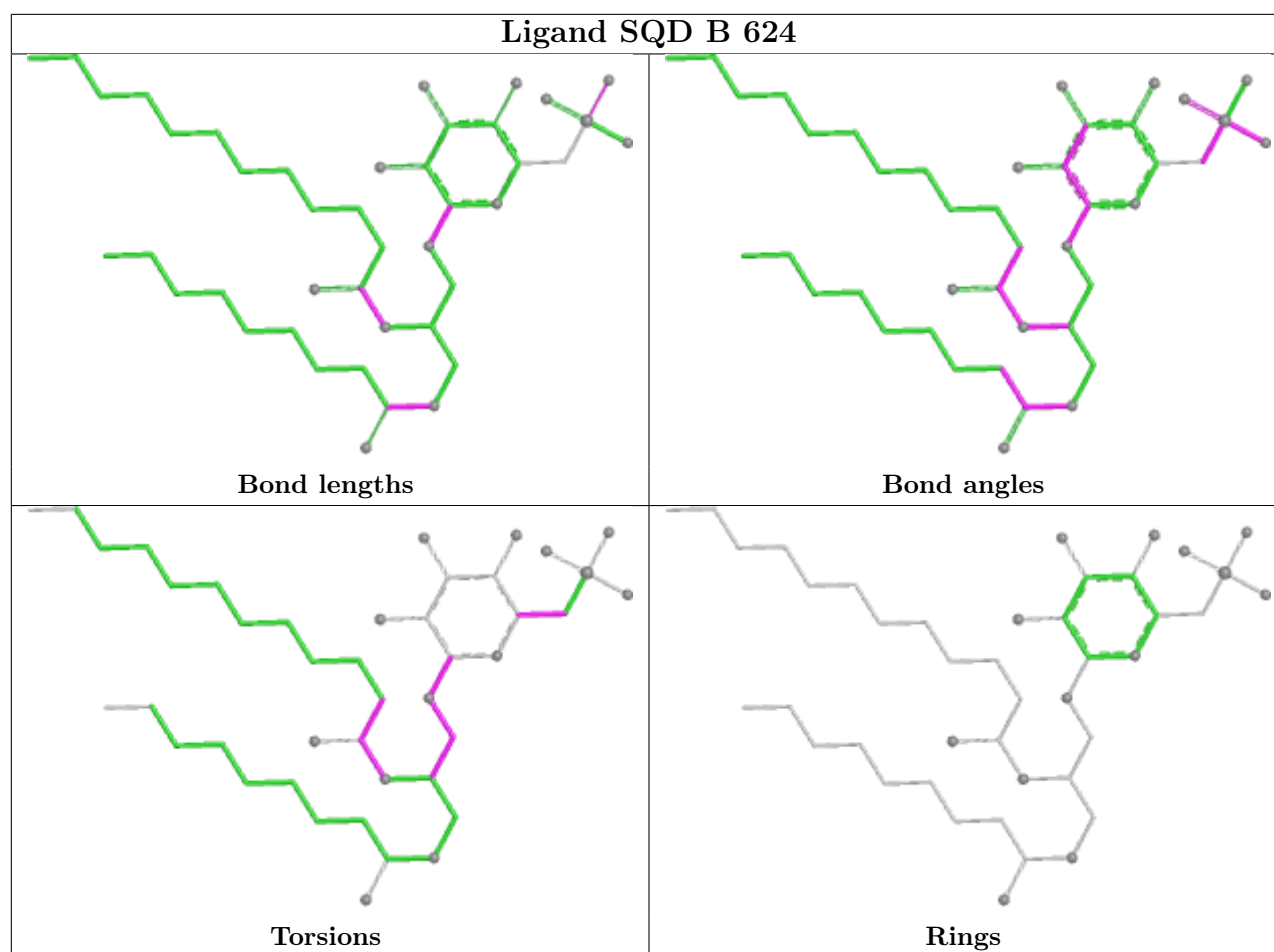


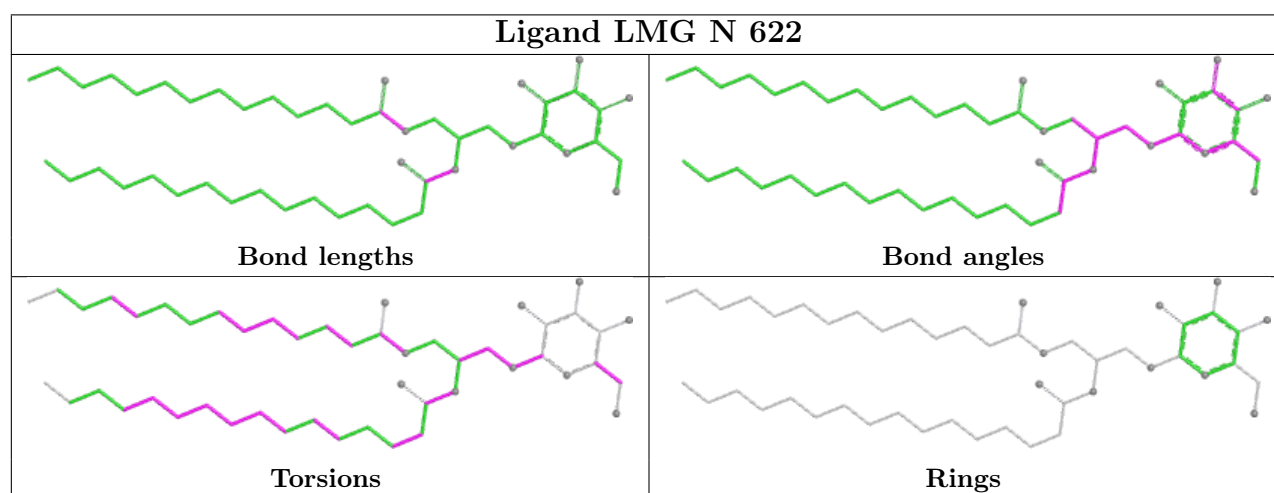
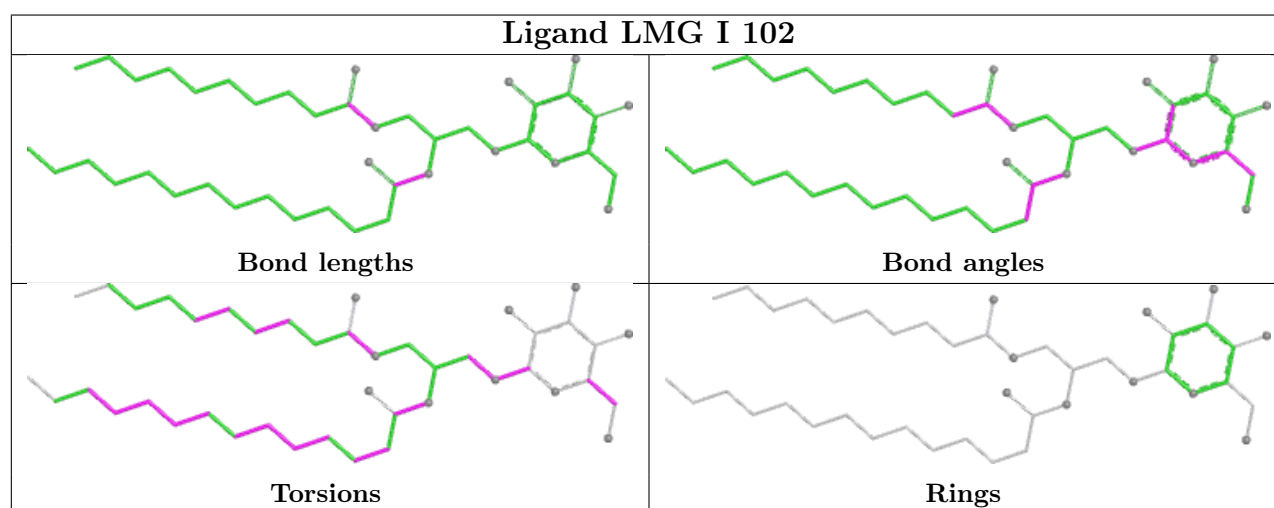
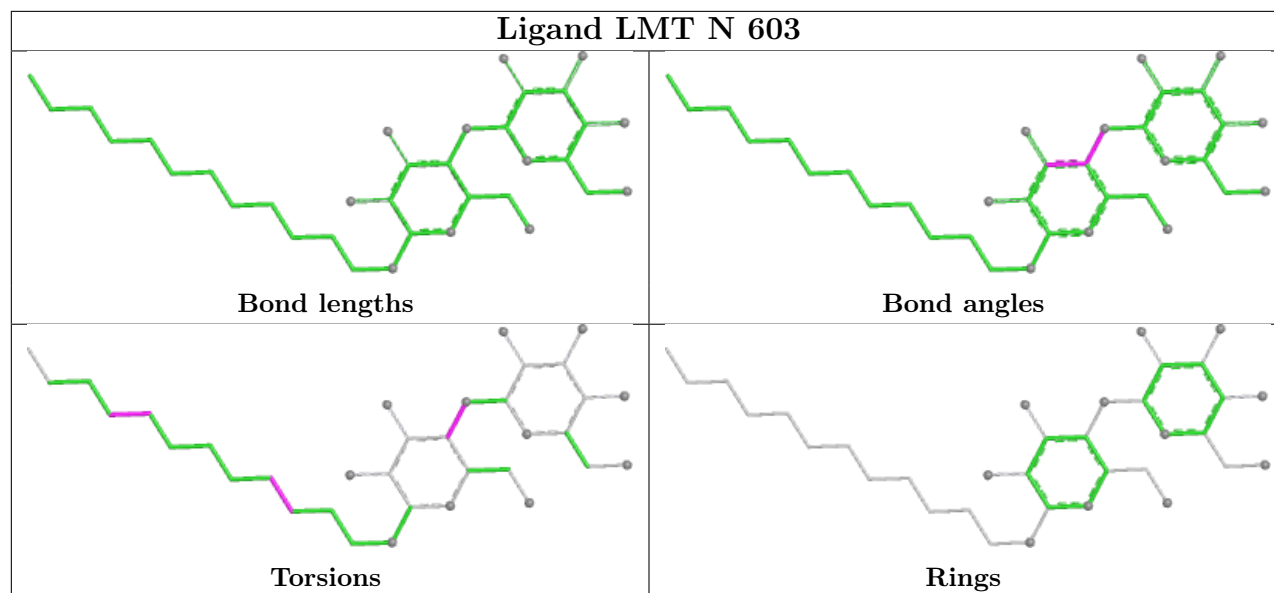


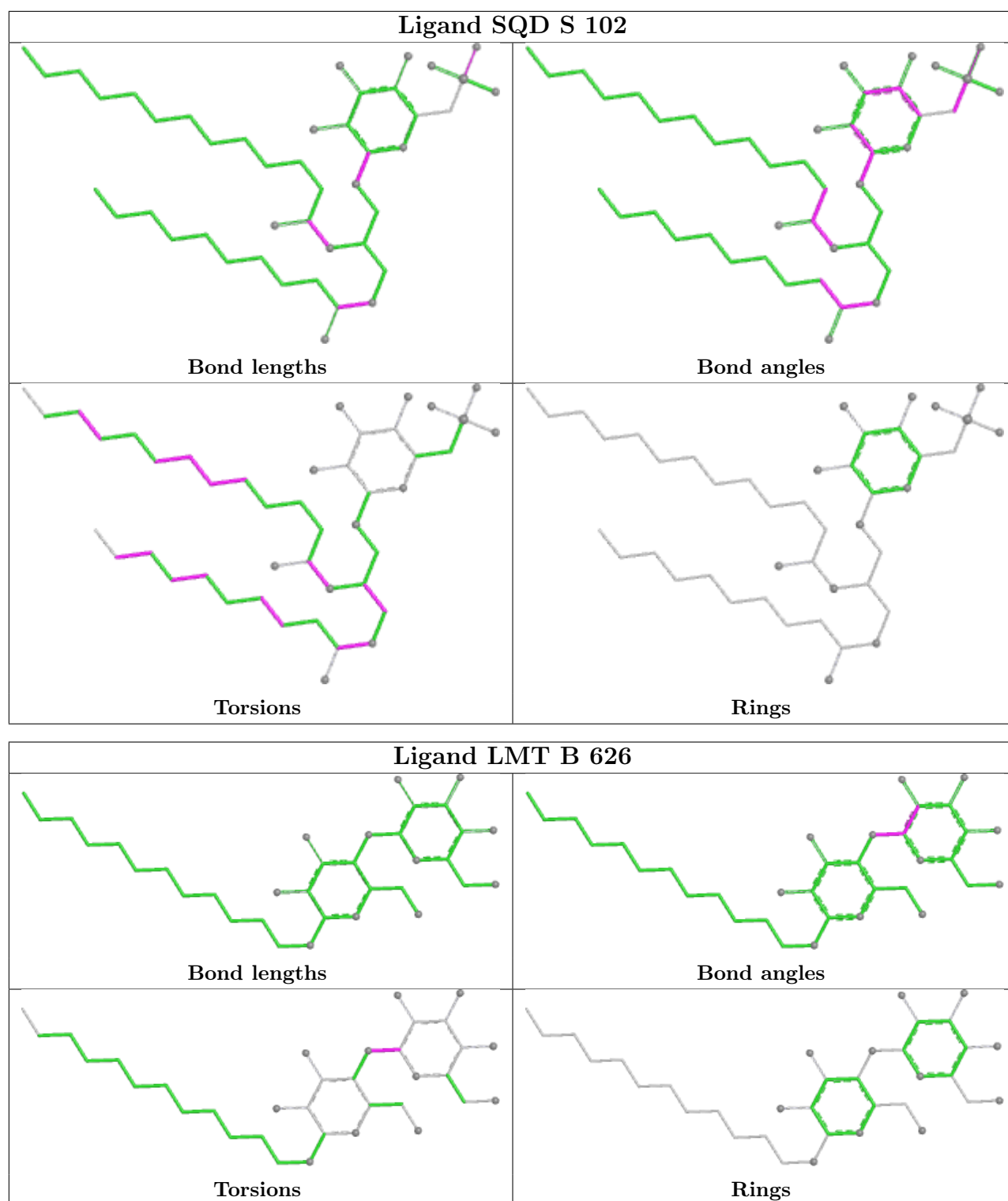


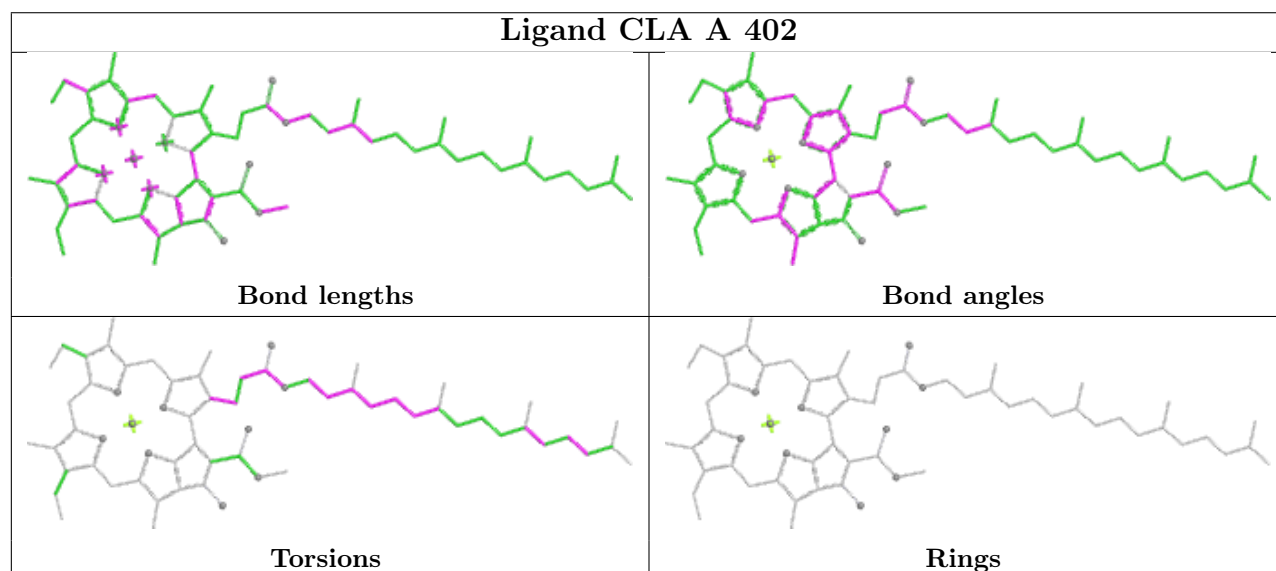
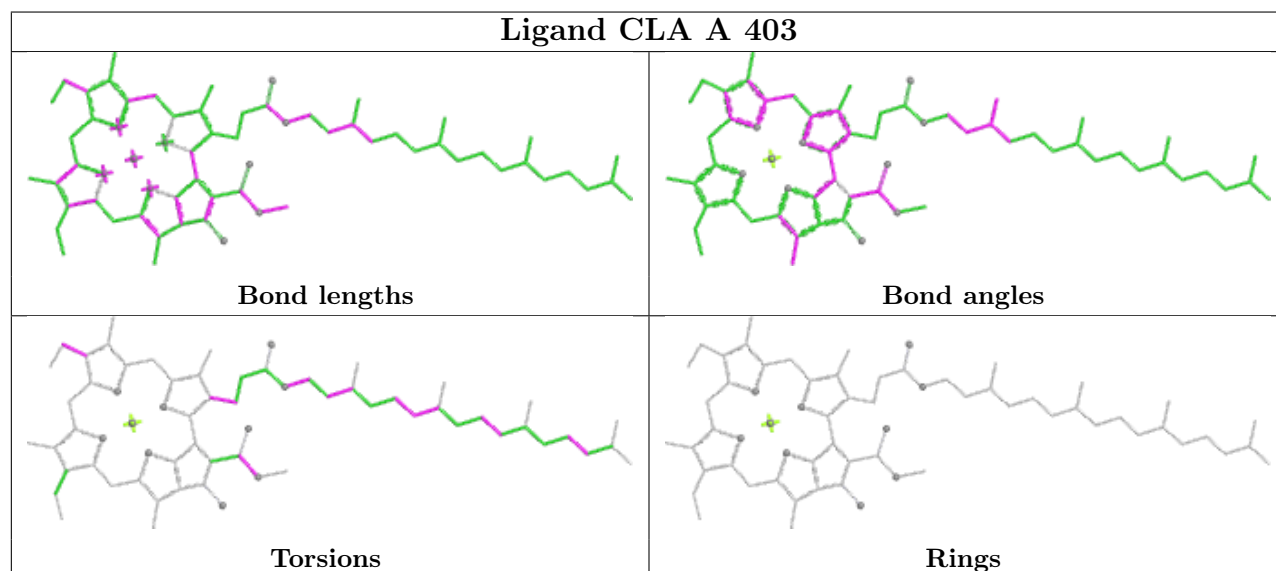
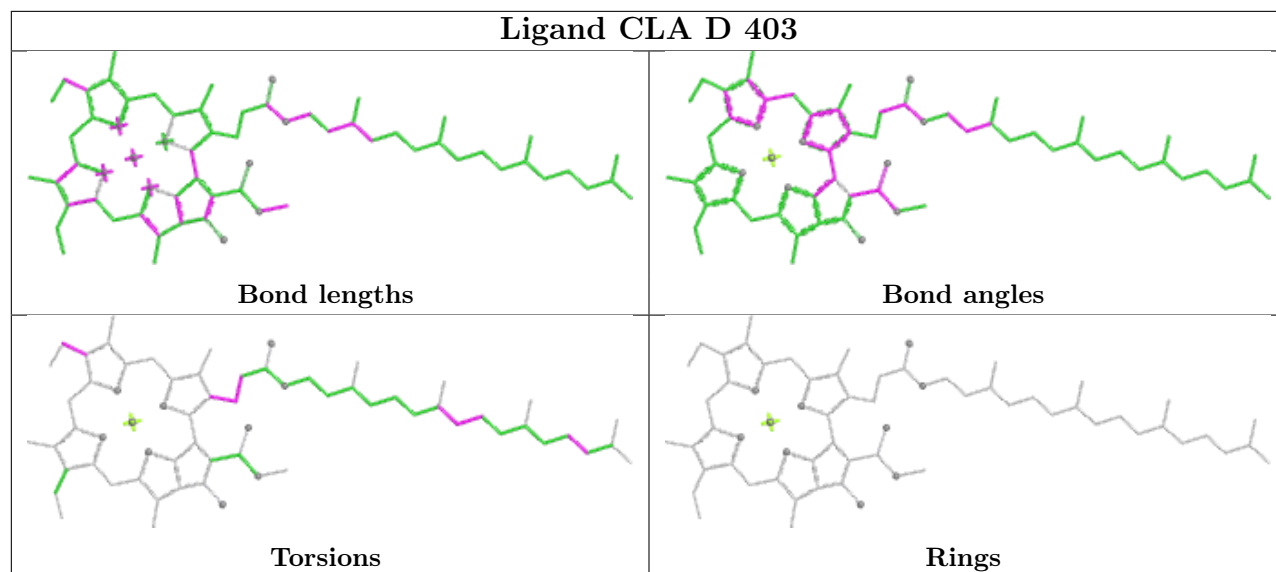


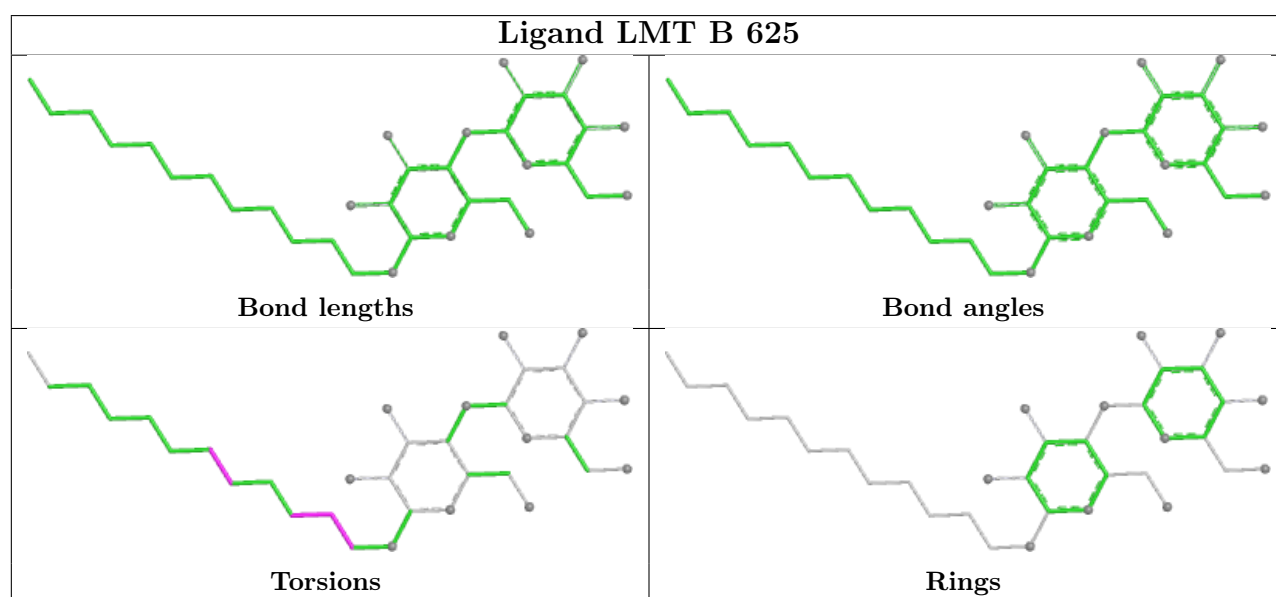
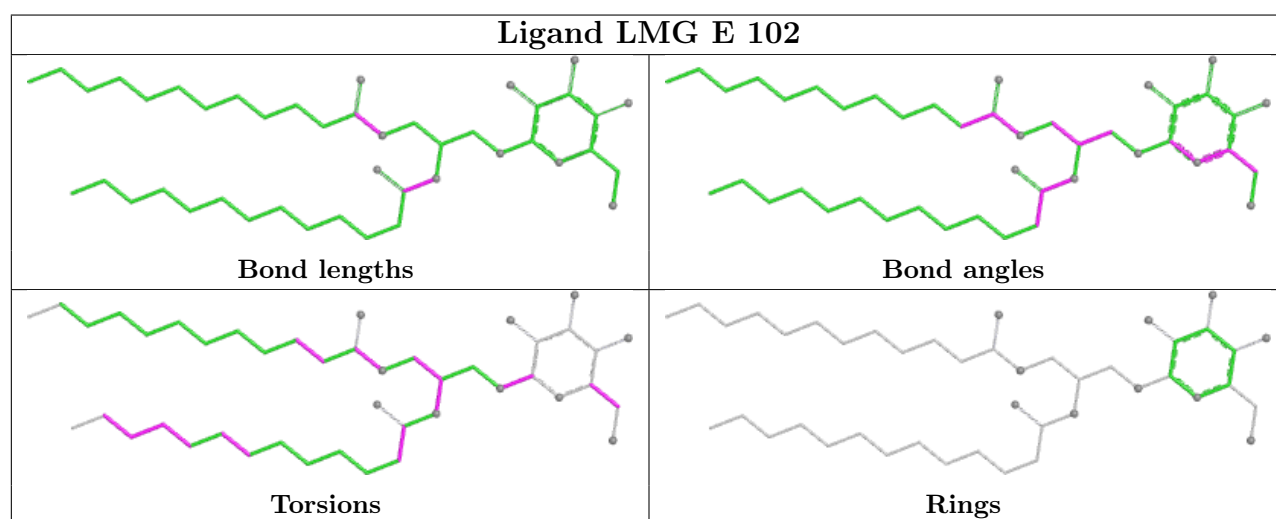
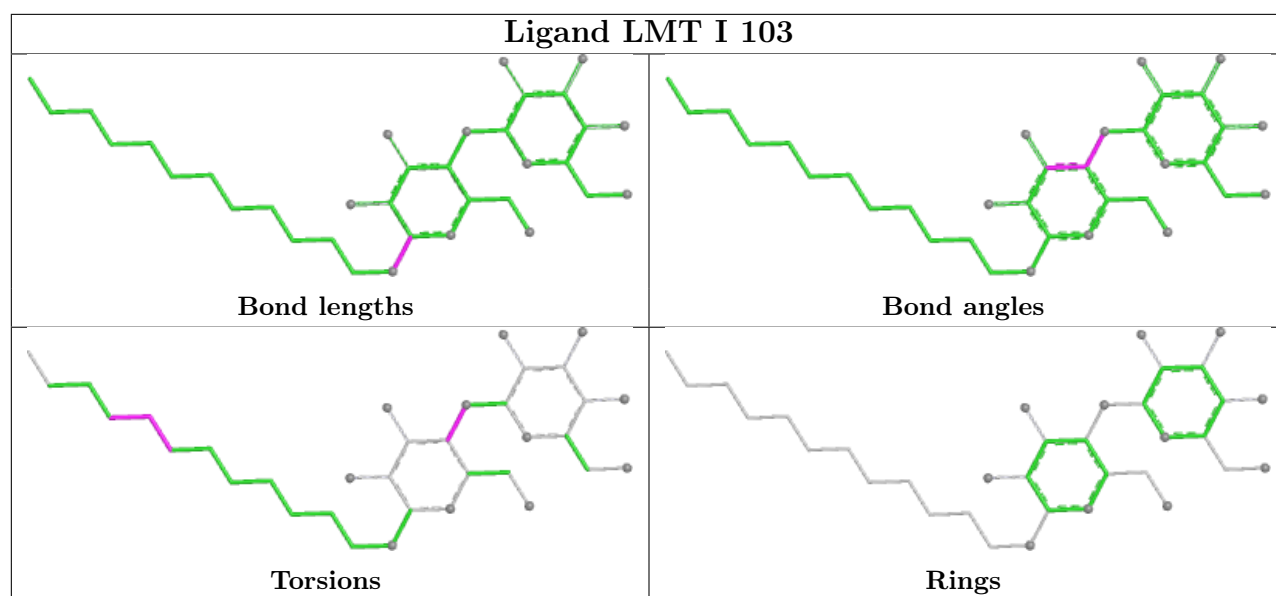


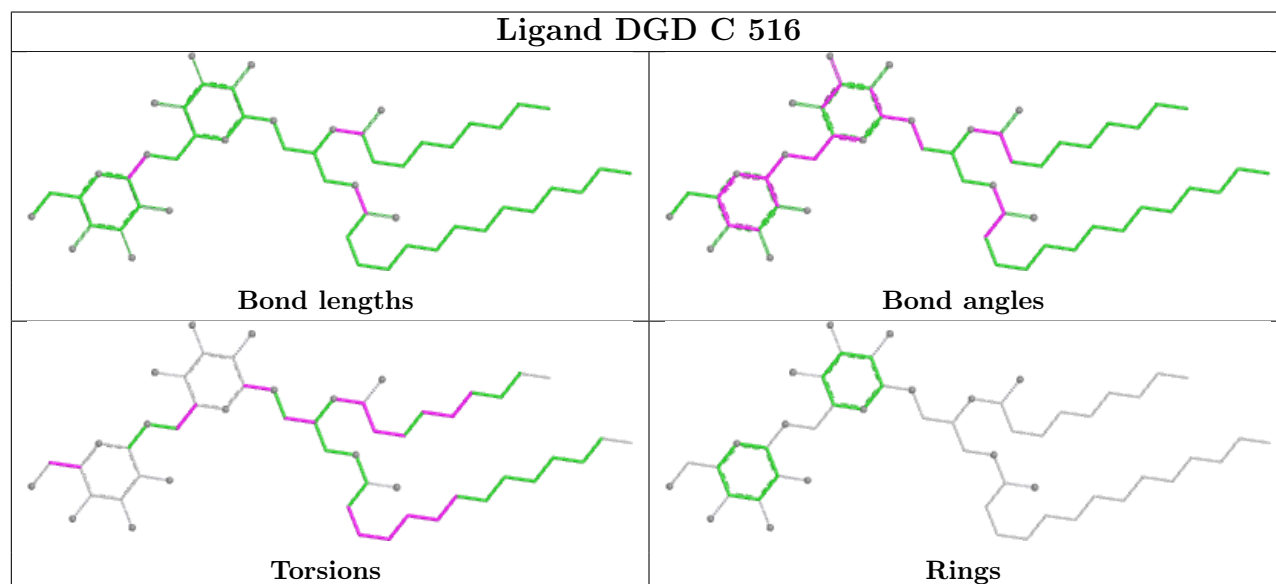
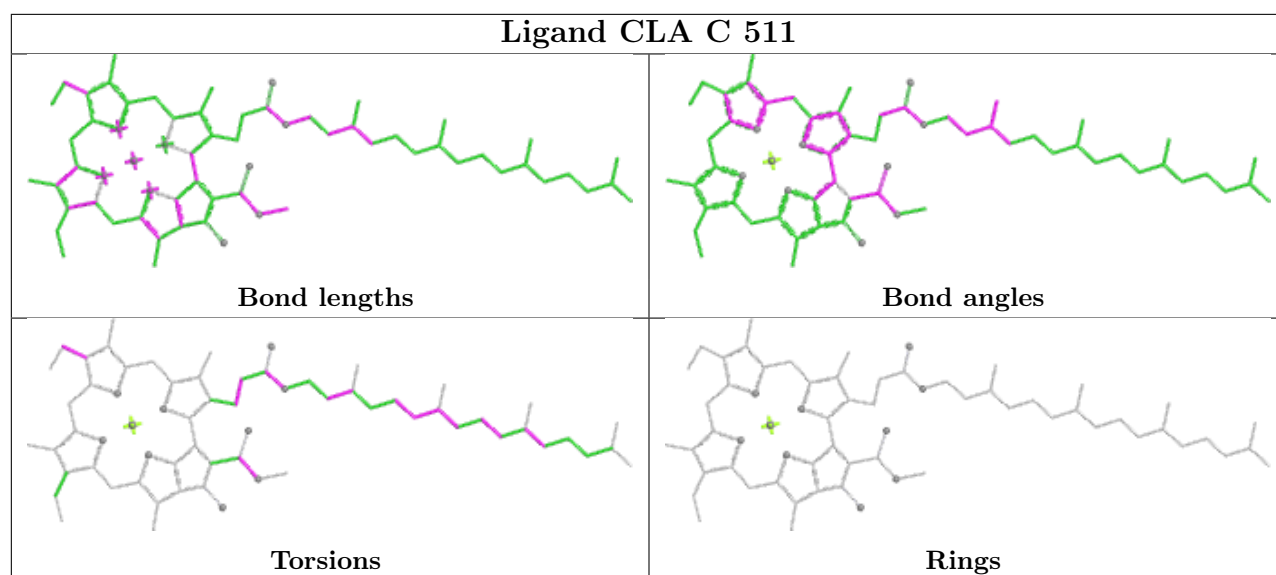


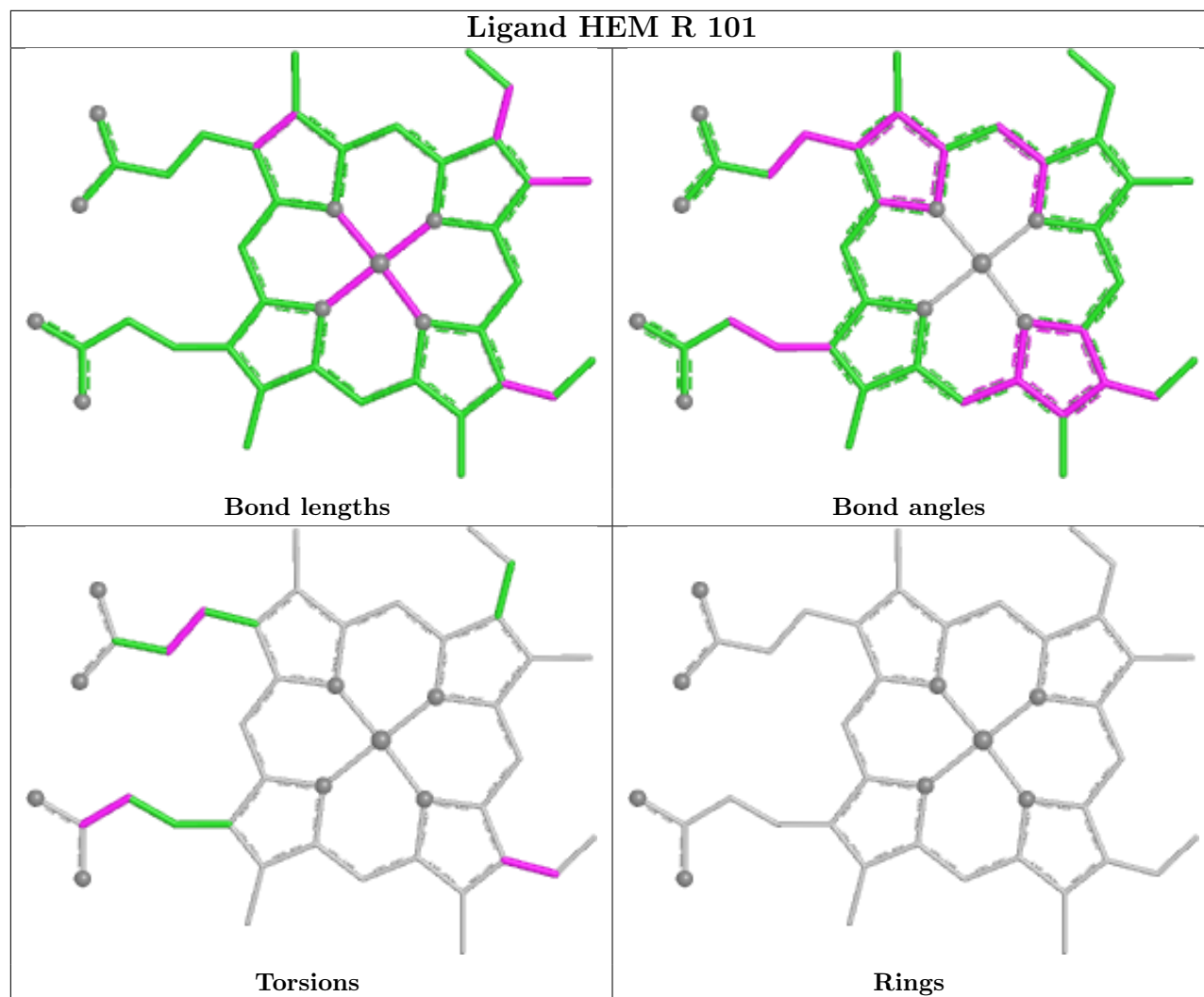


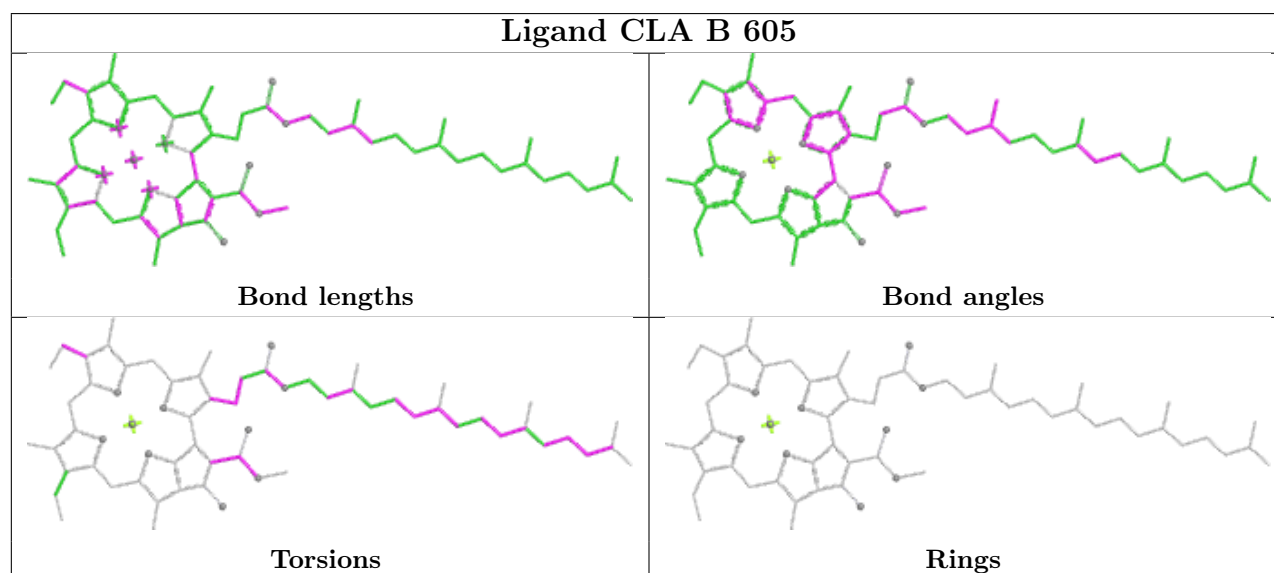
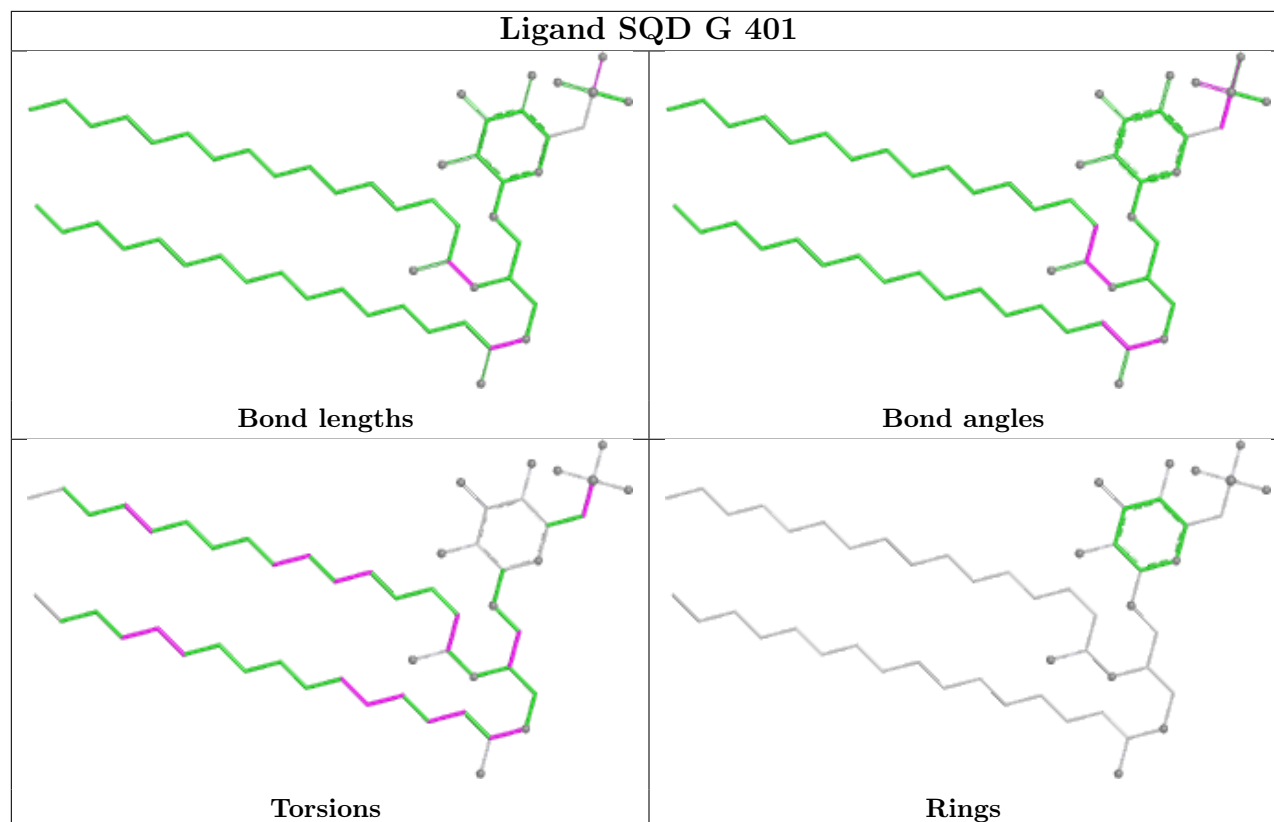


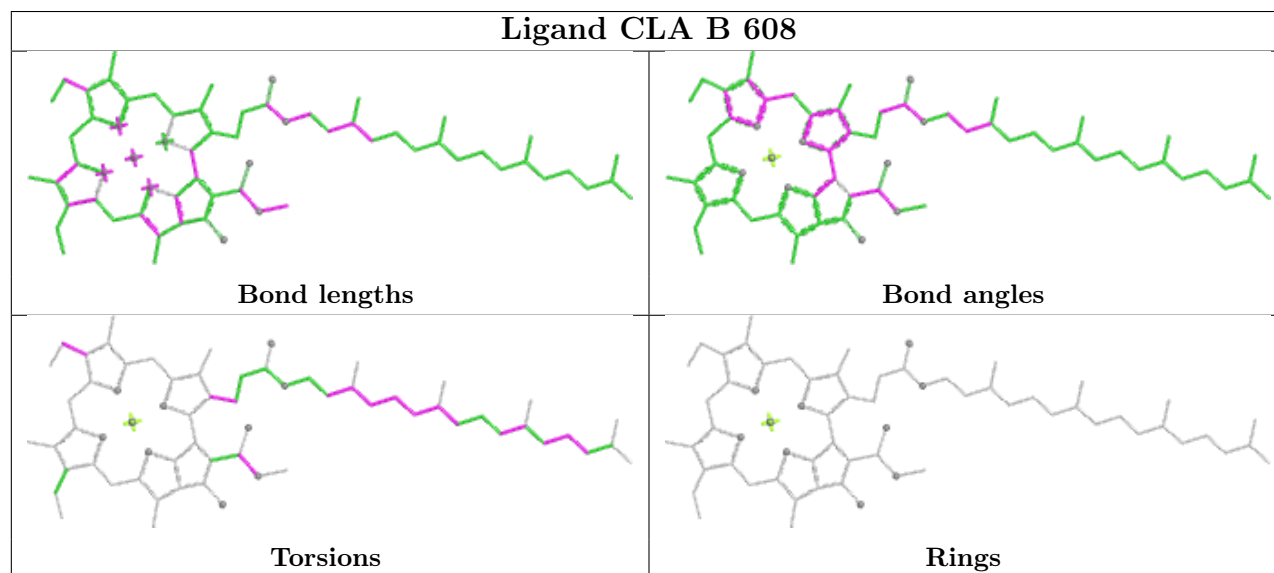
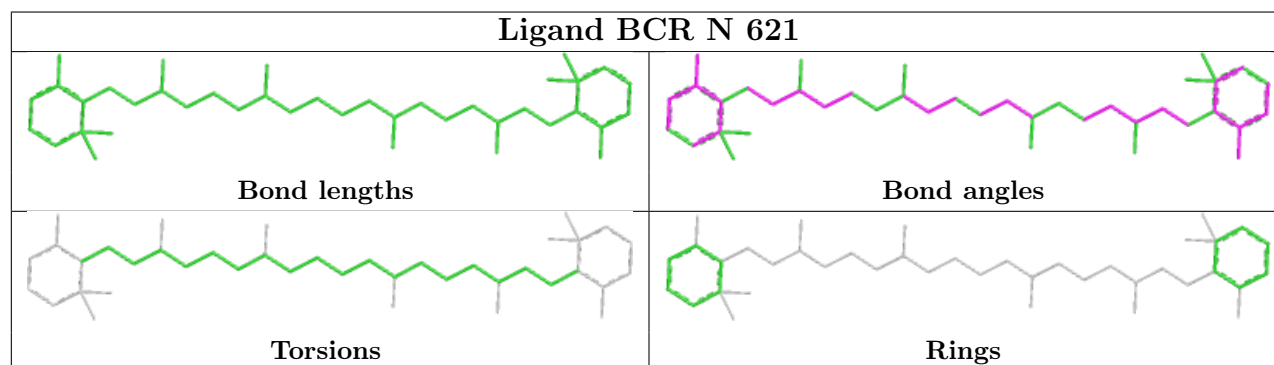
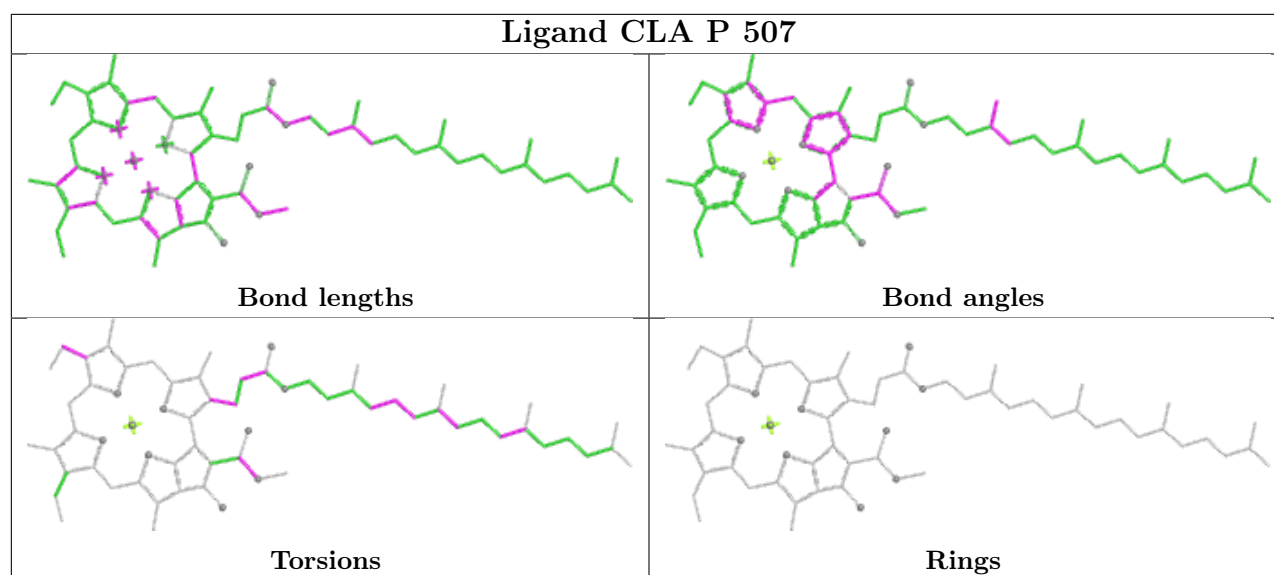


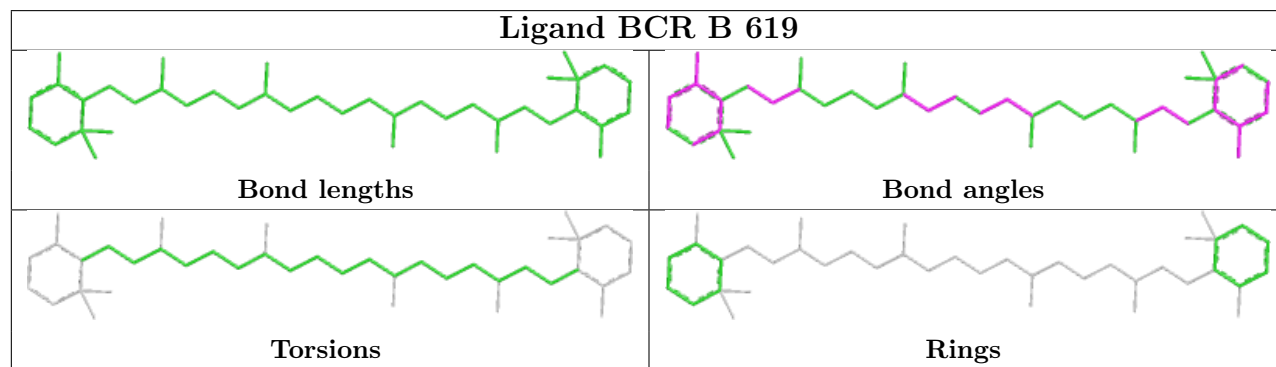
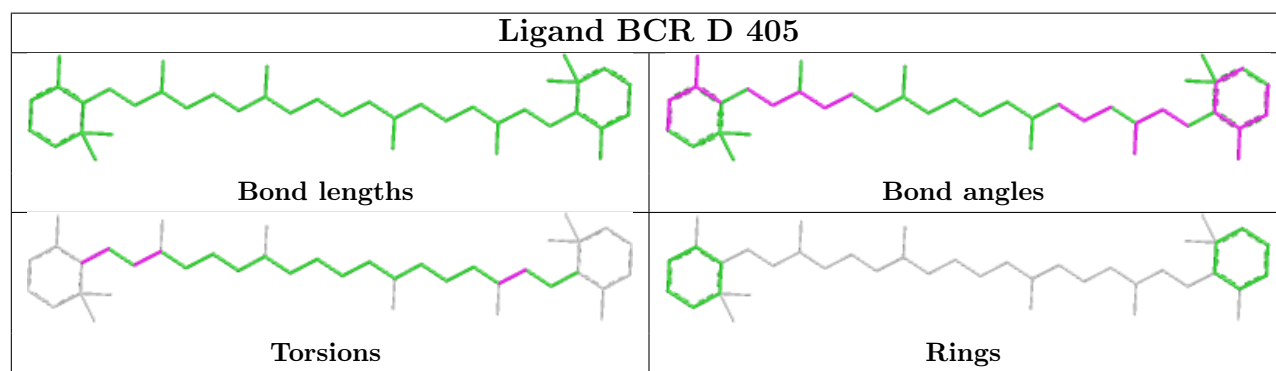
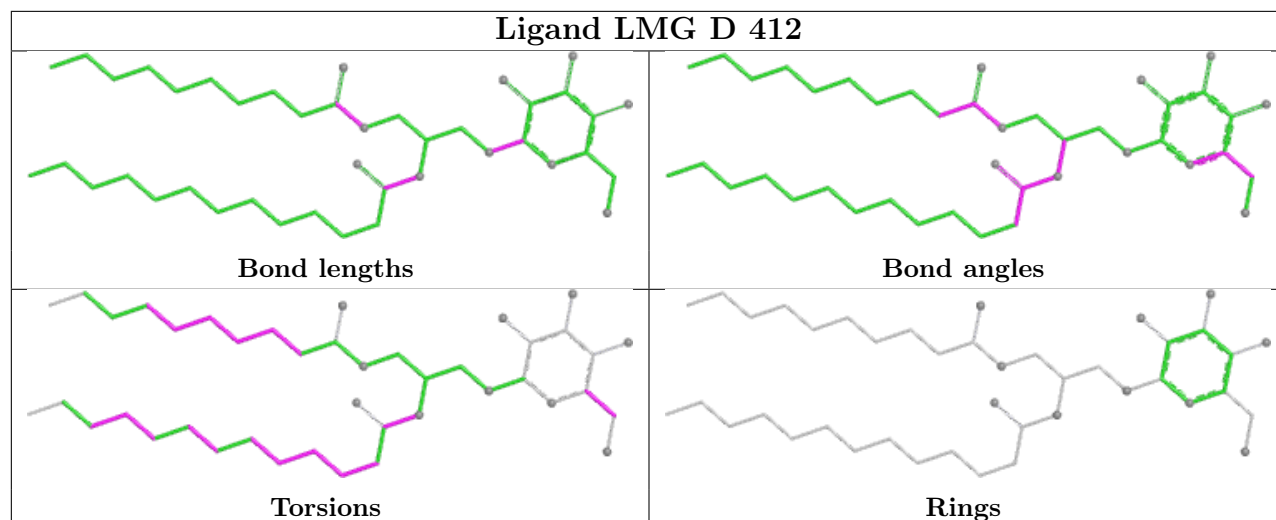




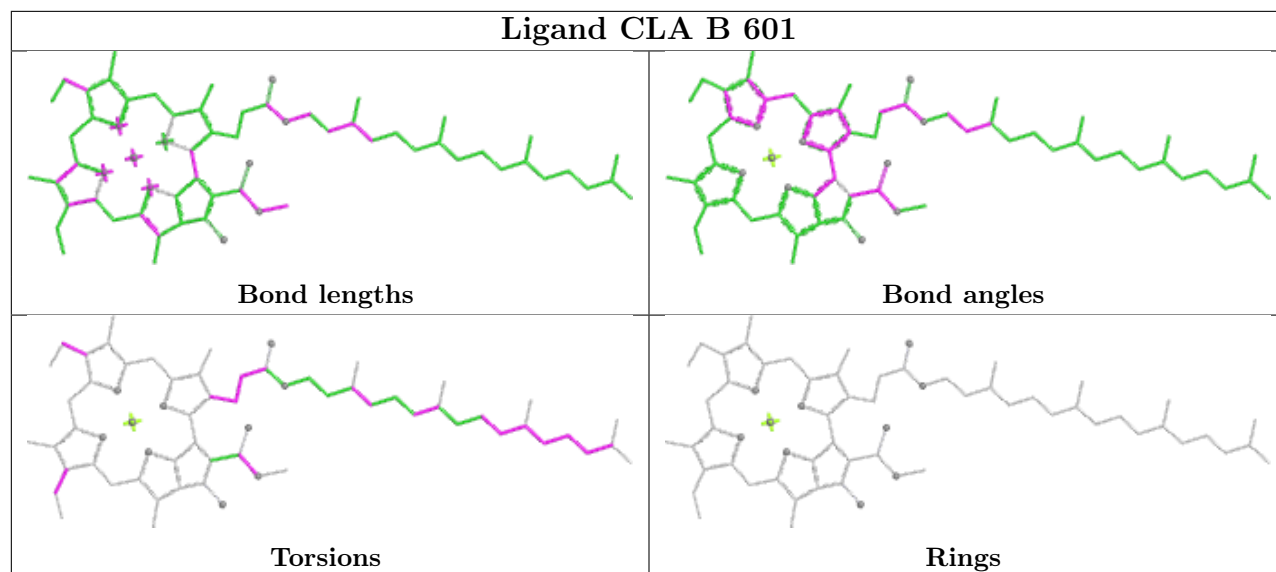




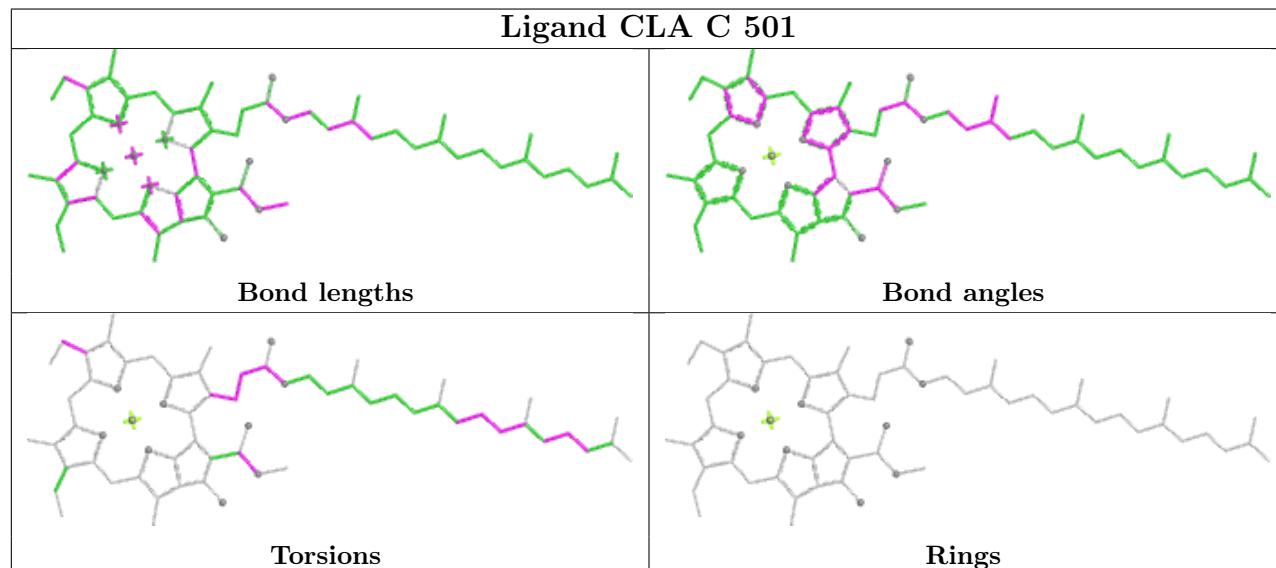




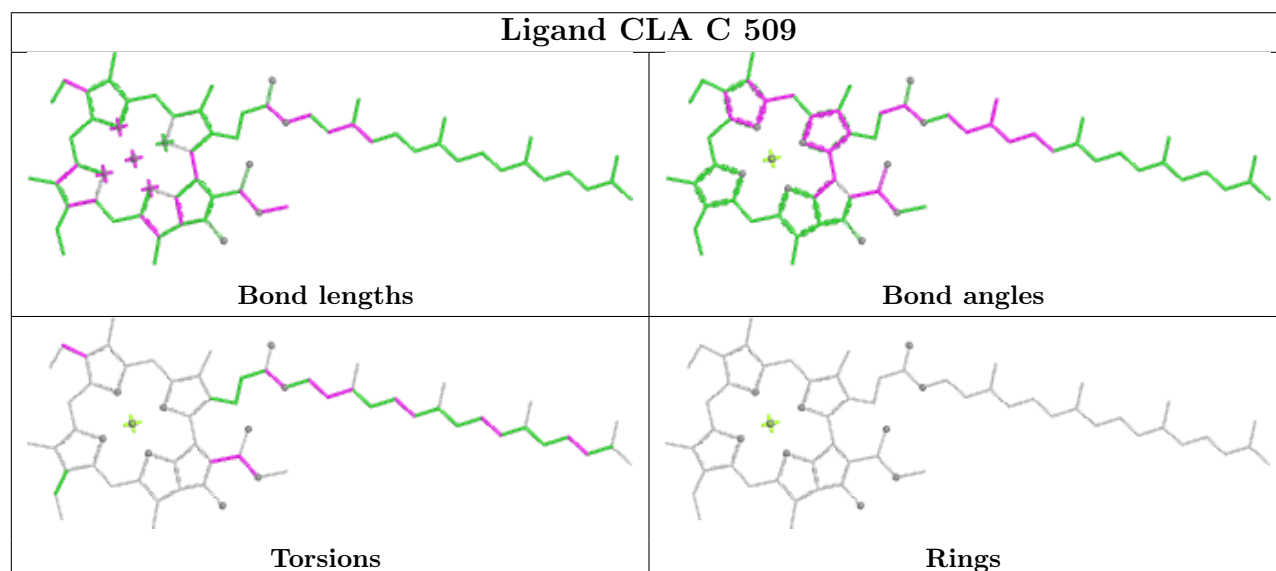
Ligand CLA B 601

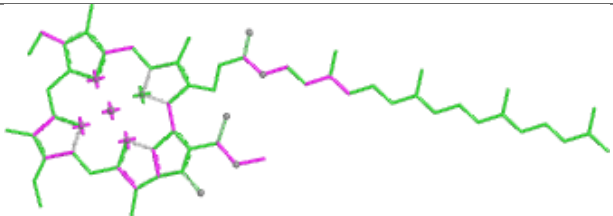
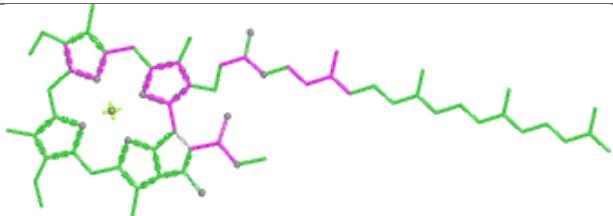
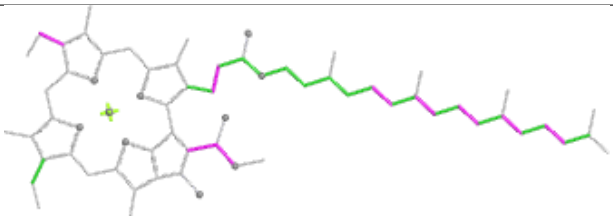
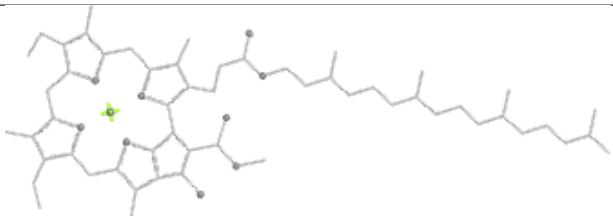


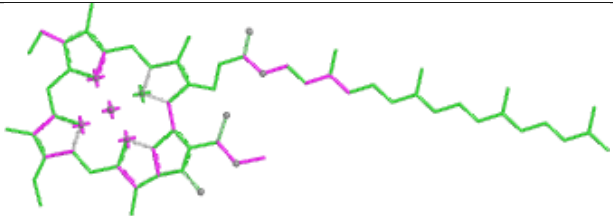
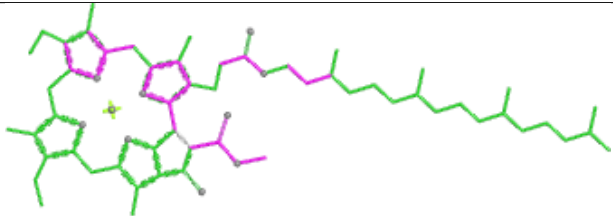
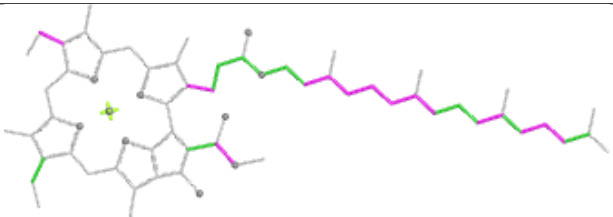
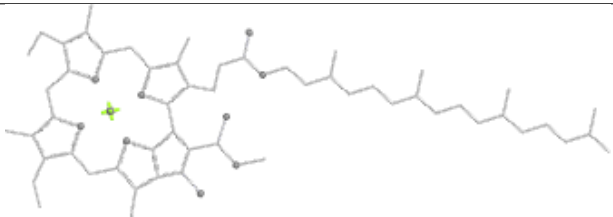
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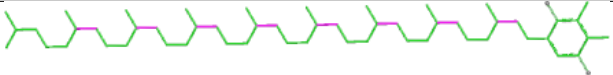
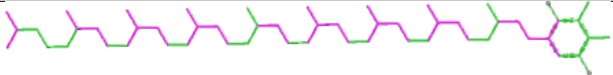
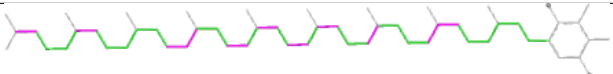
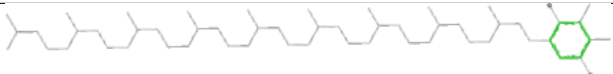


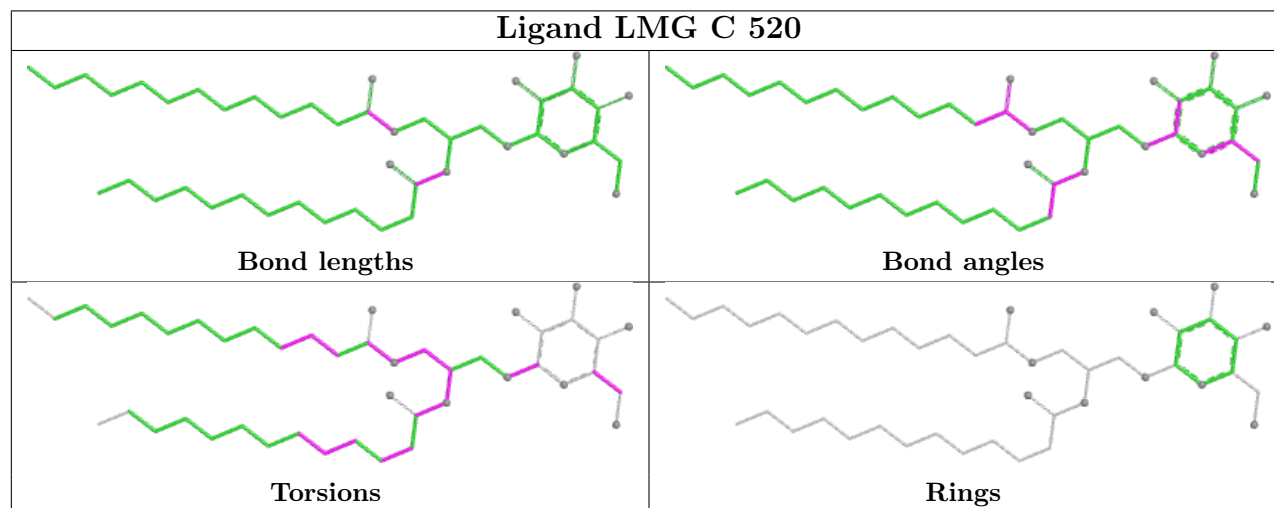
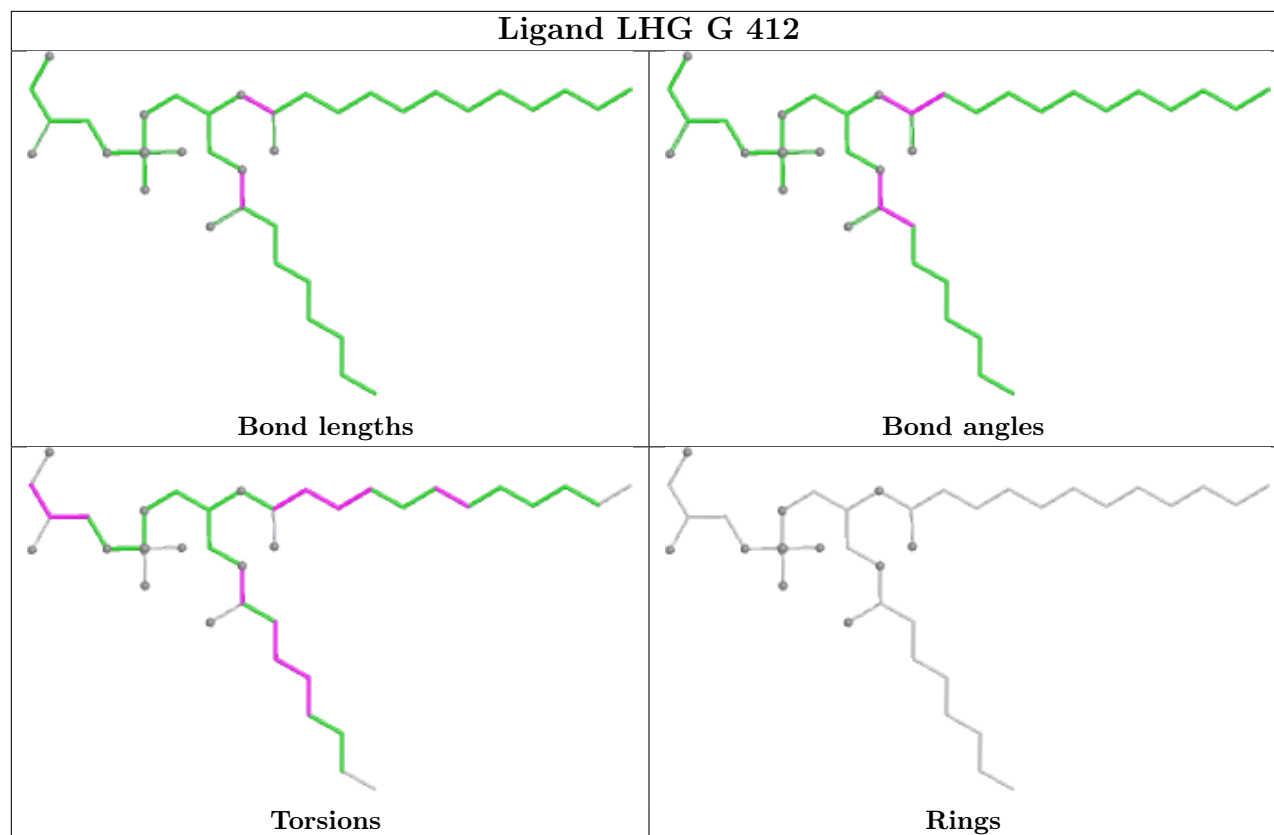
Ligand CLA C 509

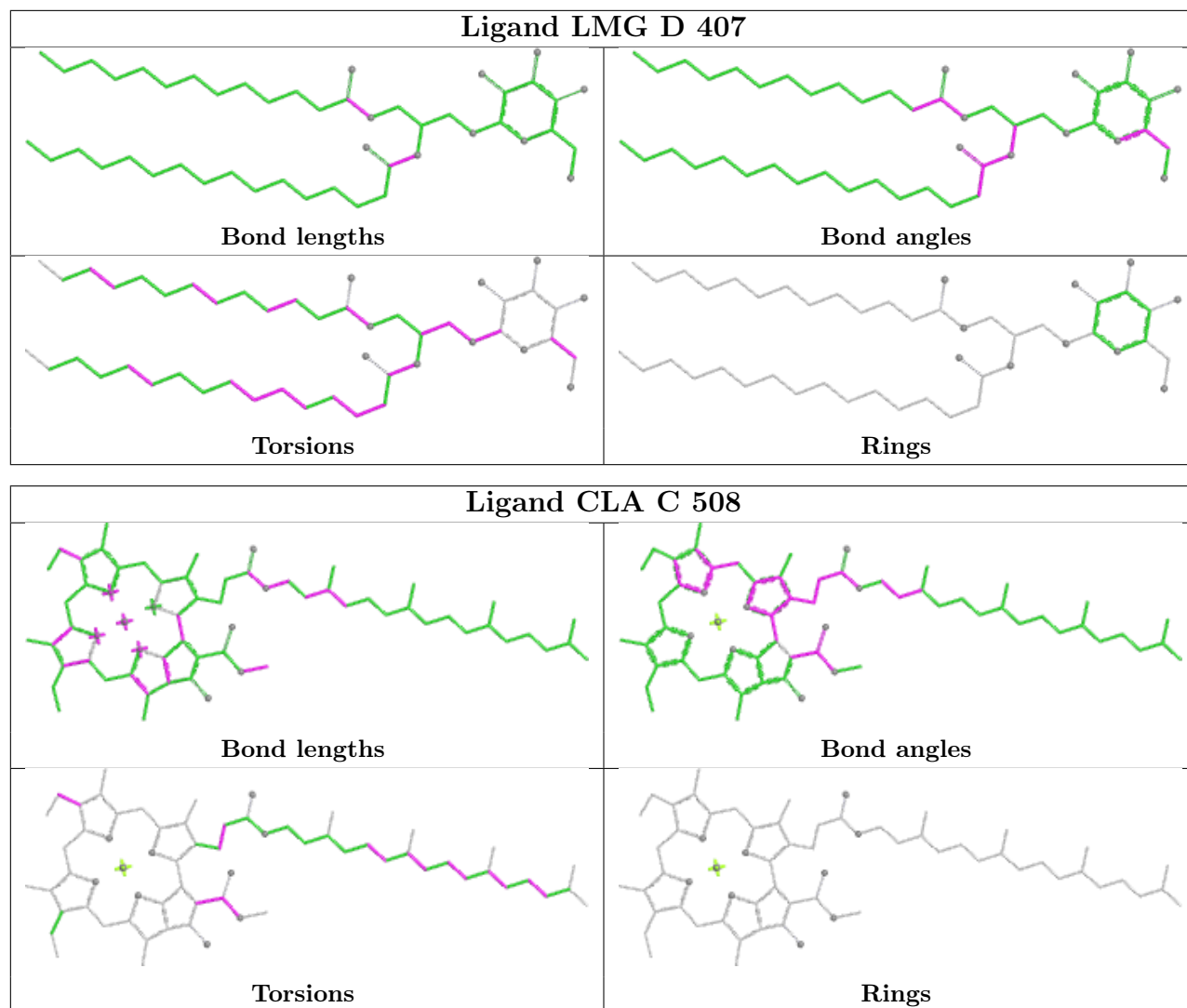


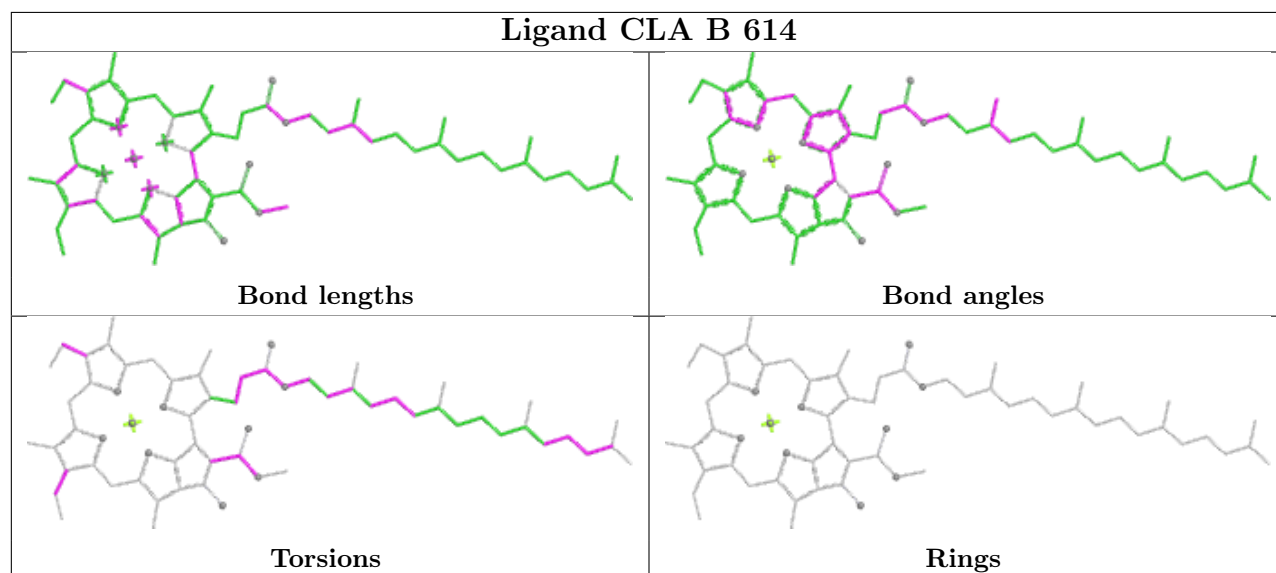
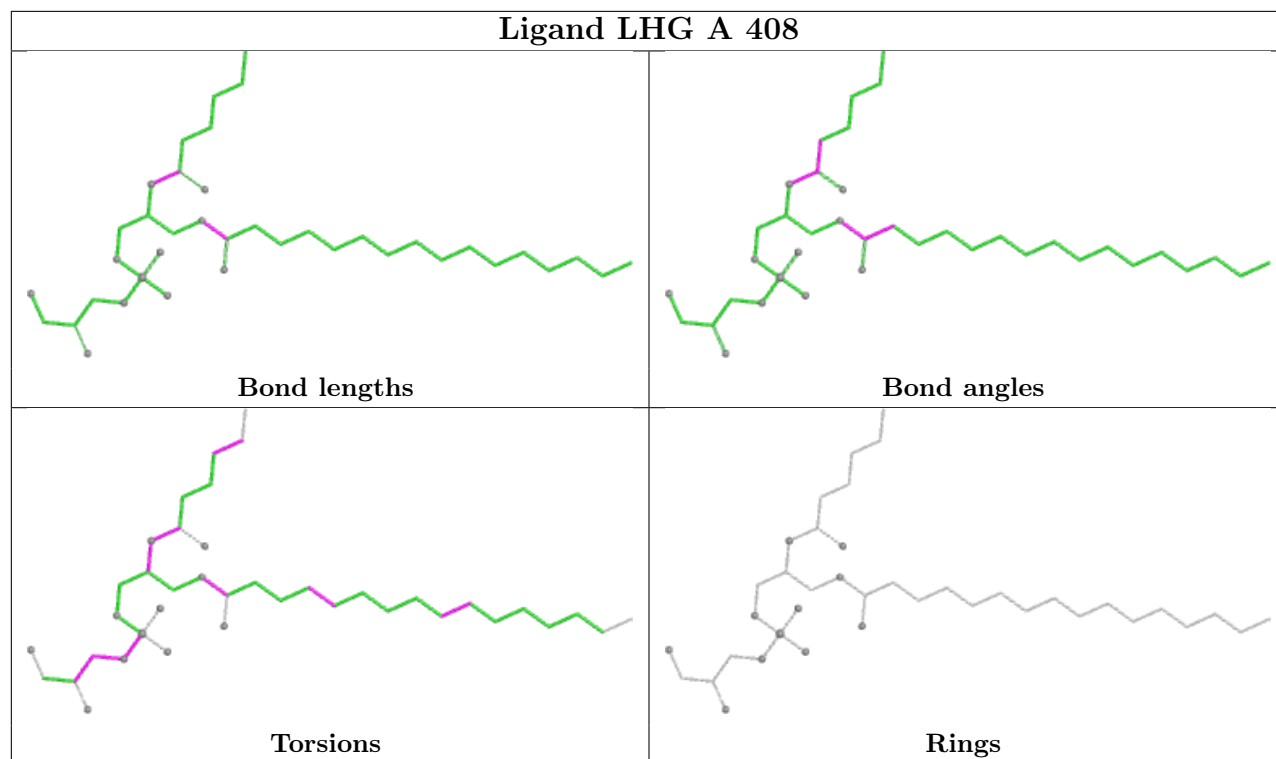
Ligand CLA P 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

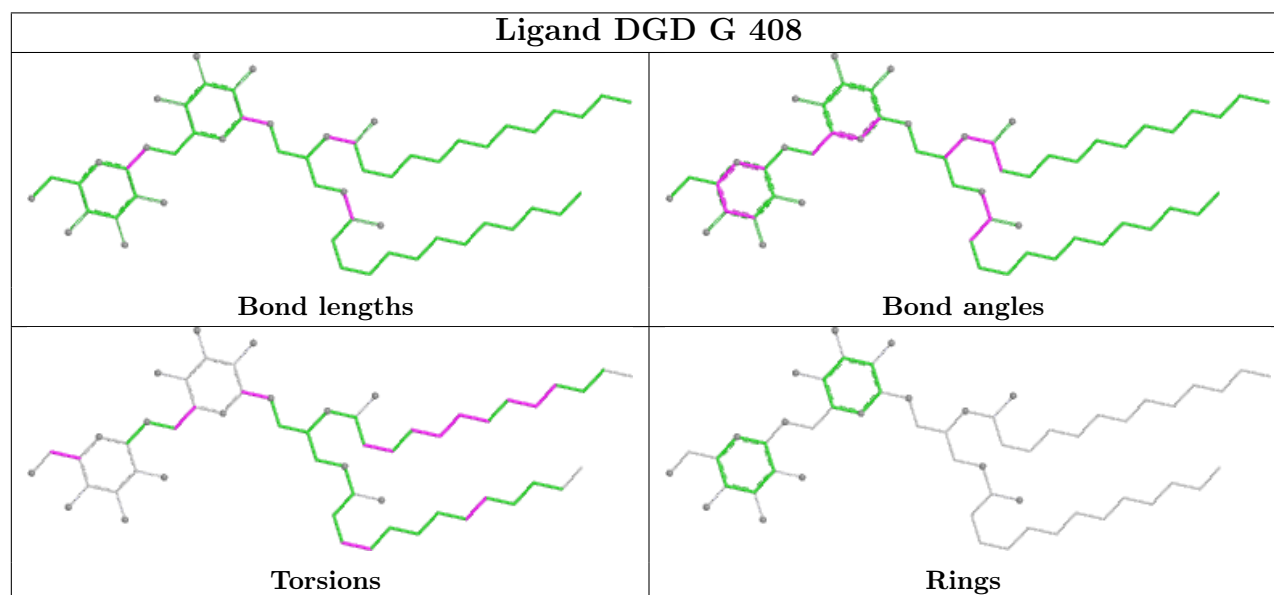
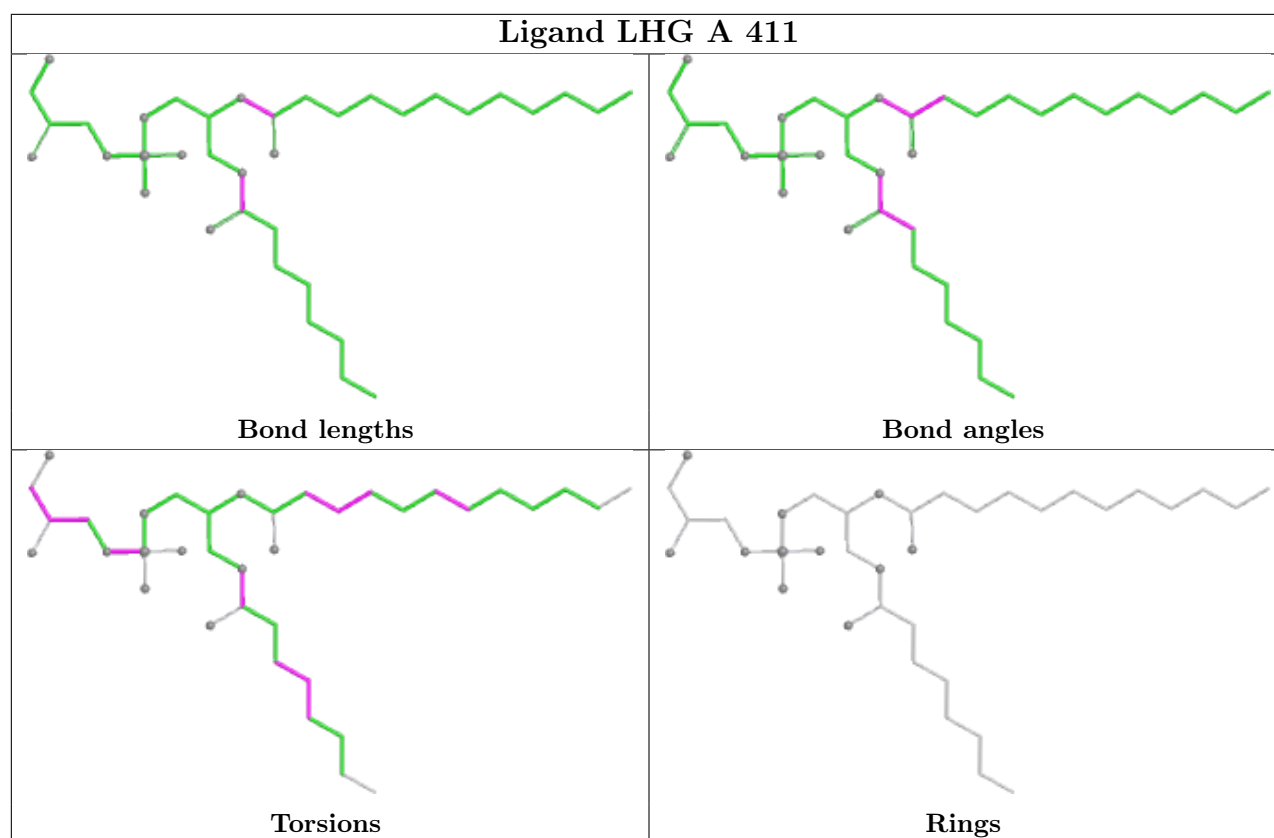
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Bond lengths	Bond angles
	
Torsions	Rings

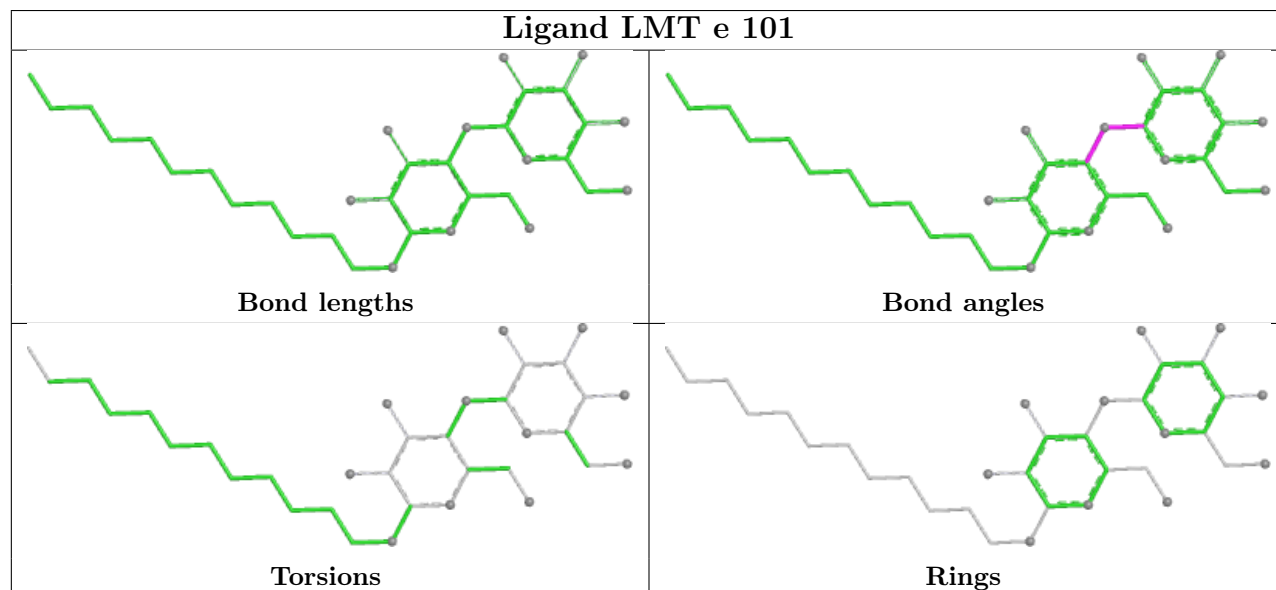
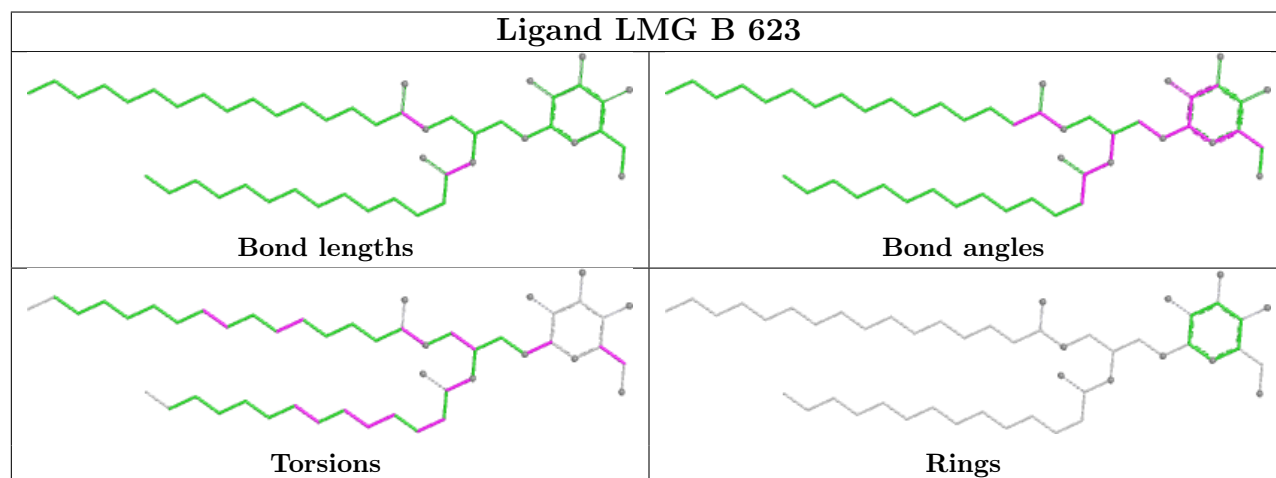
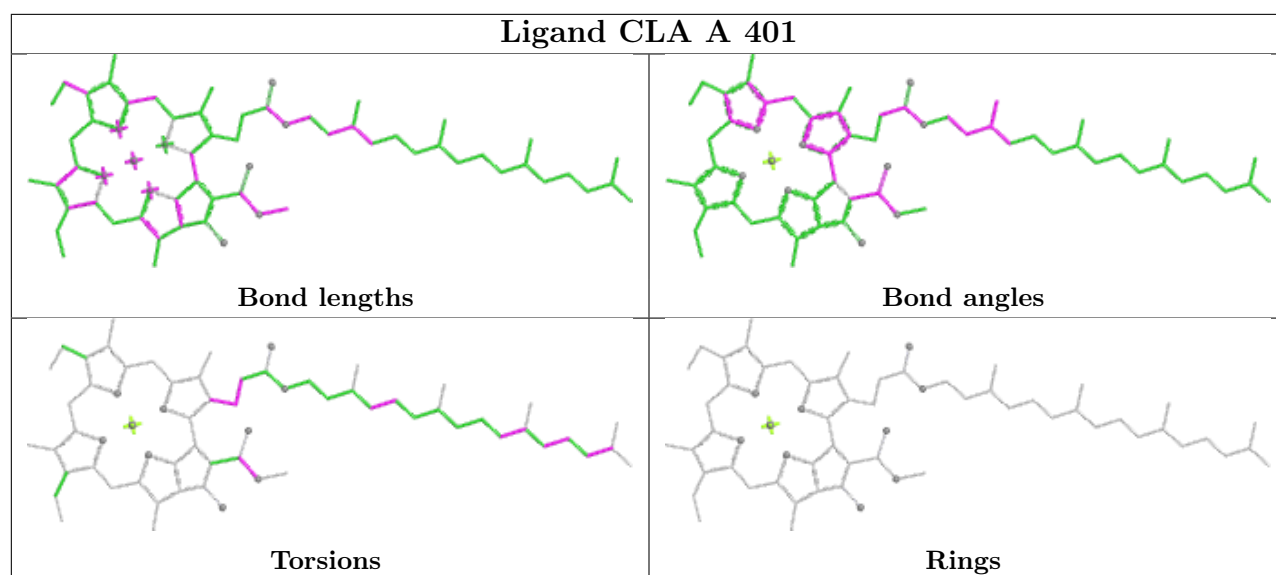
Ligand PL9 Q 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

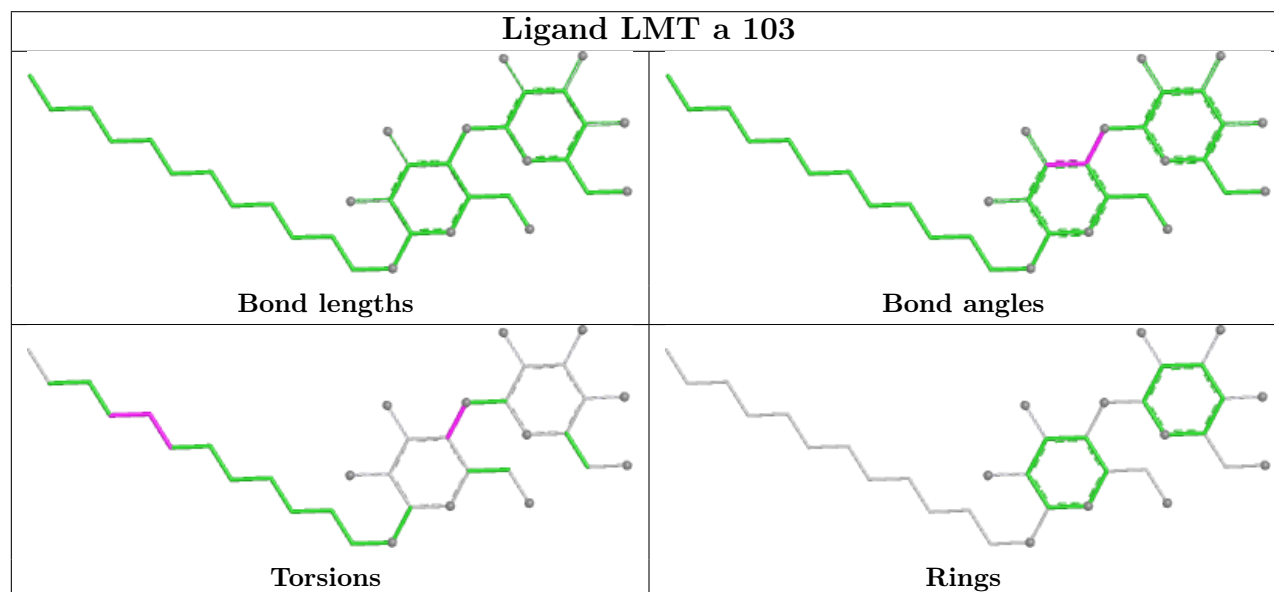
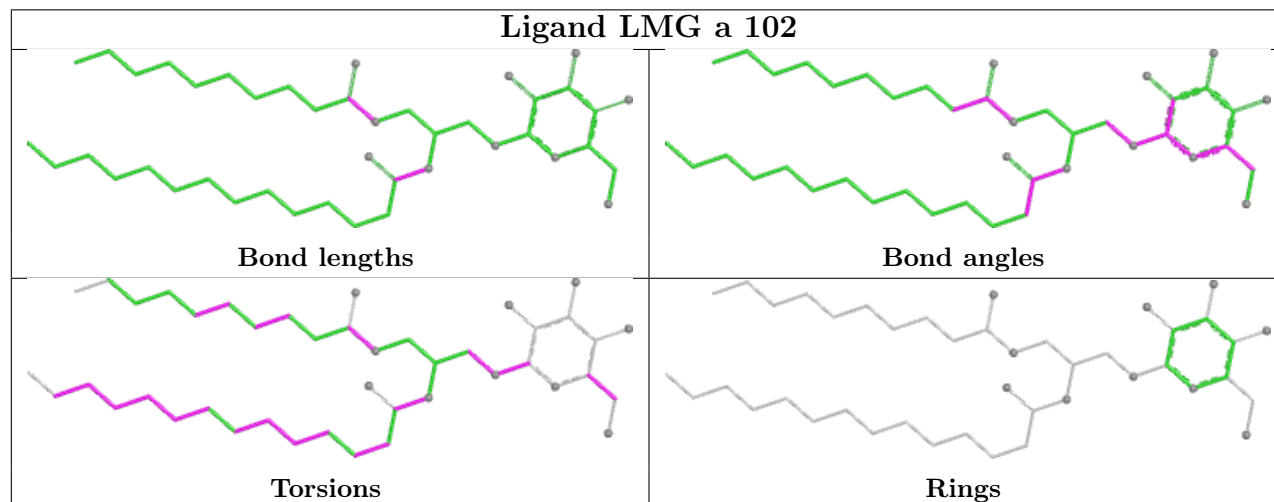
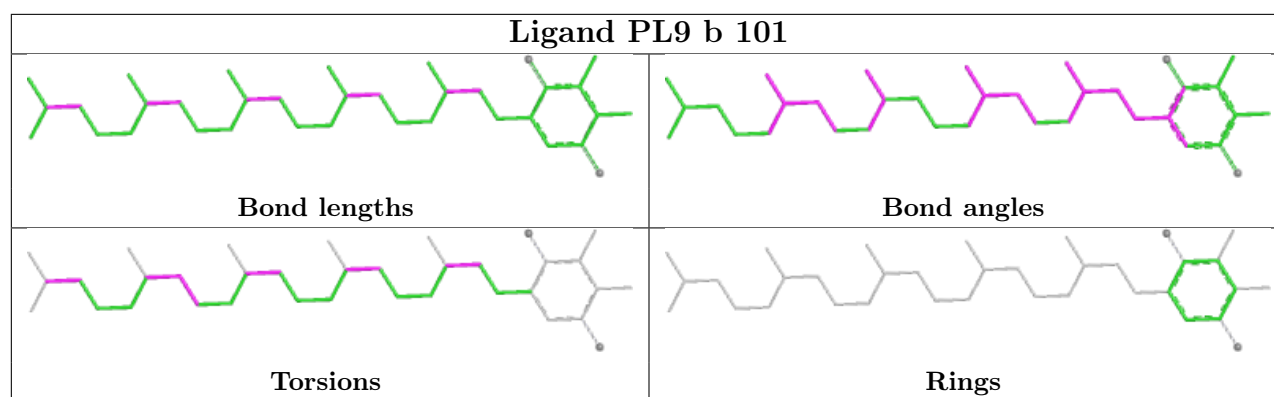


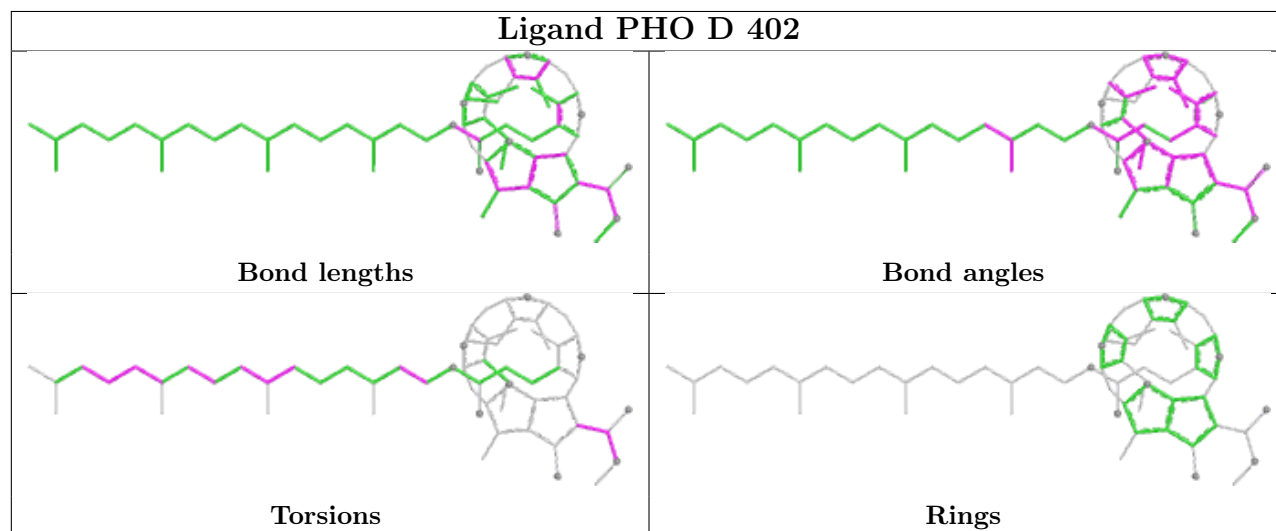
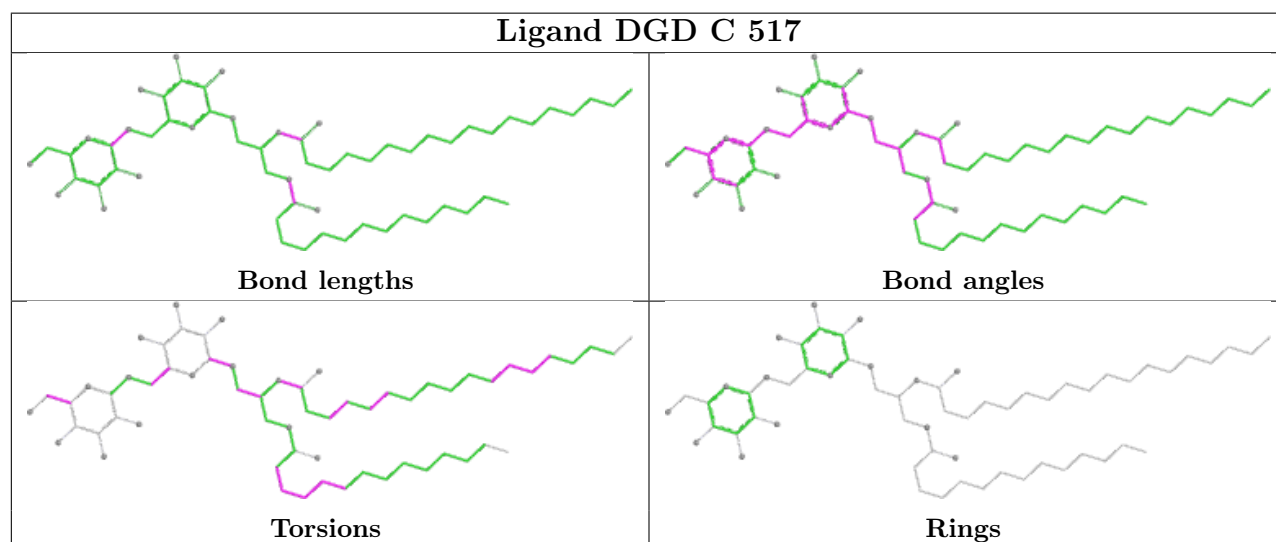
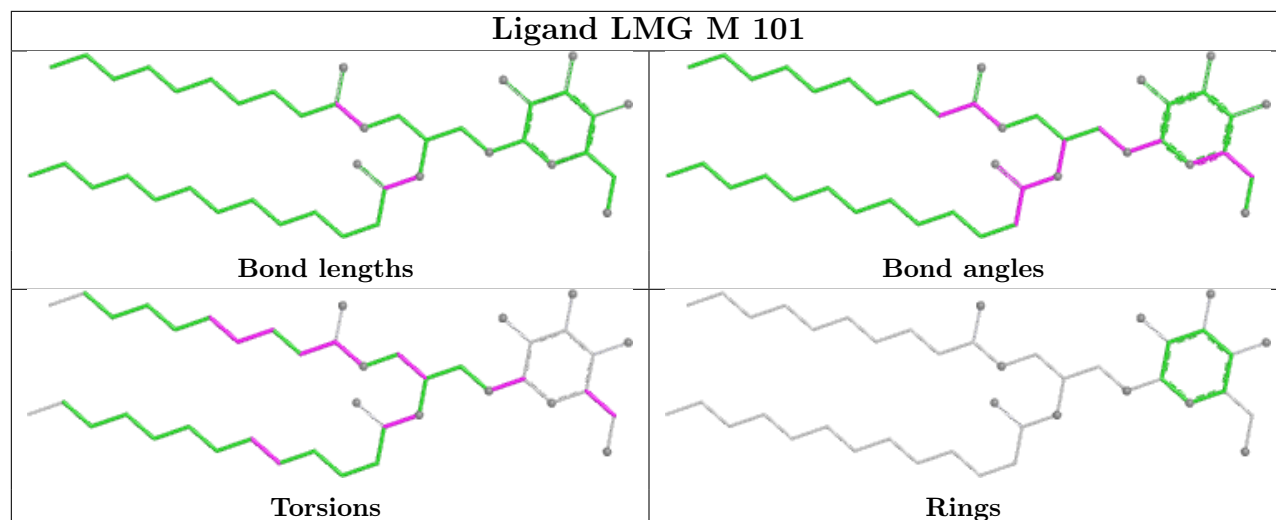


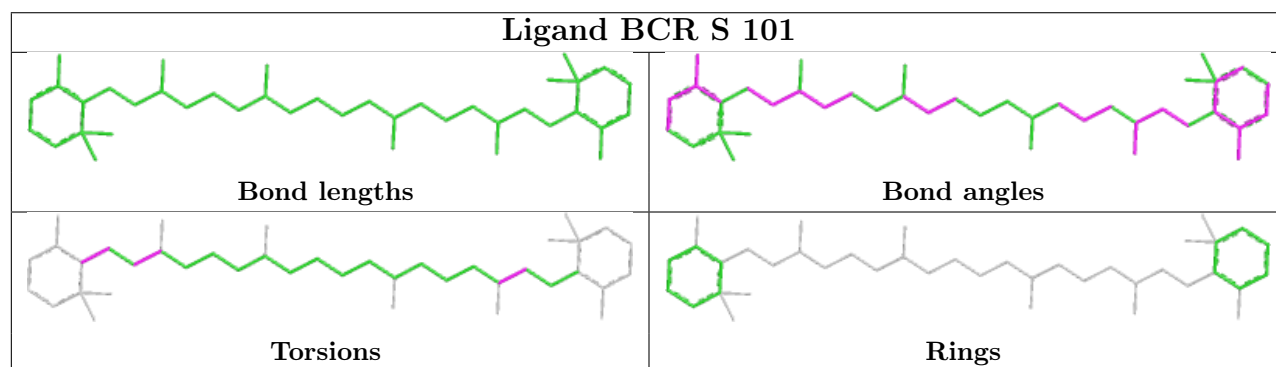
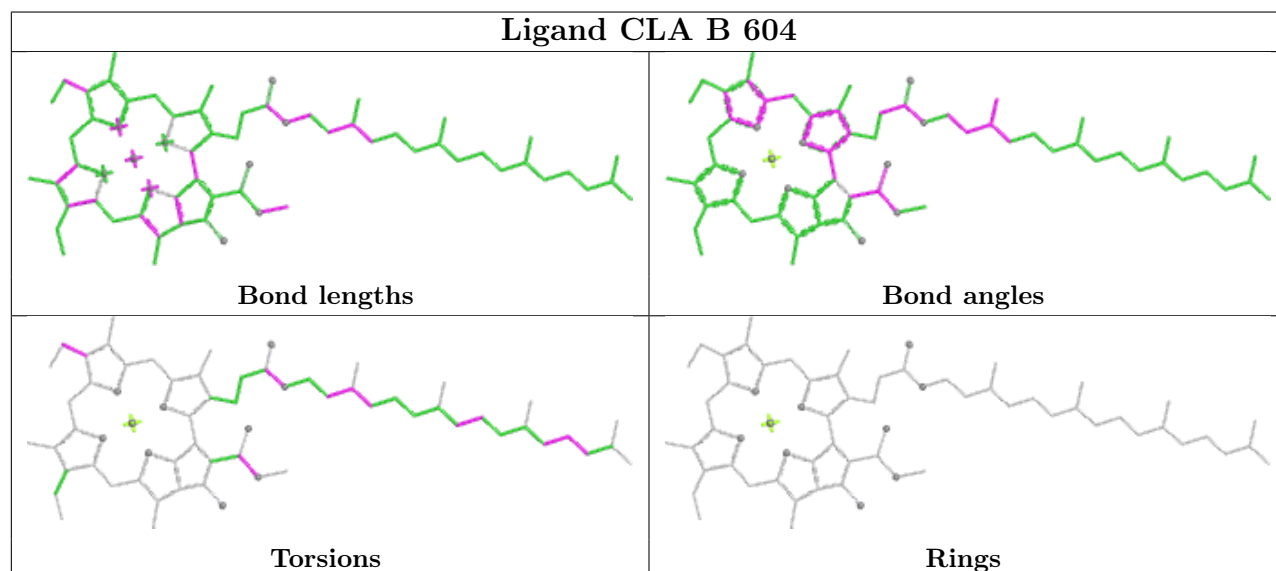
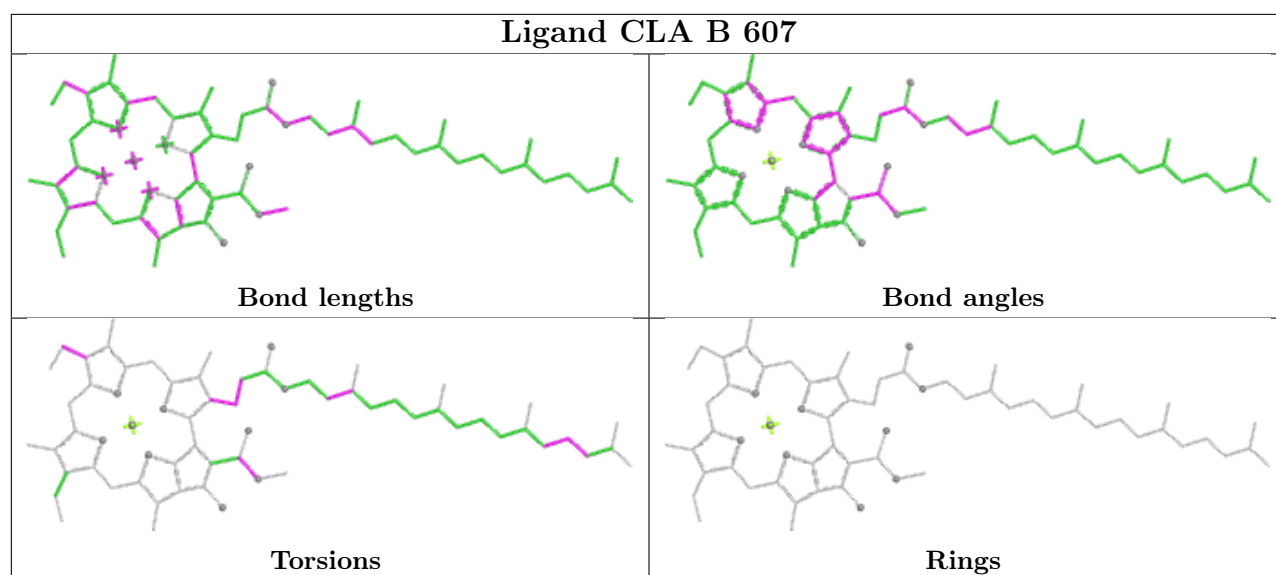




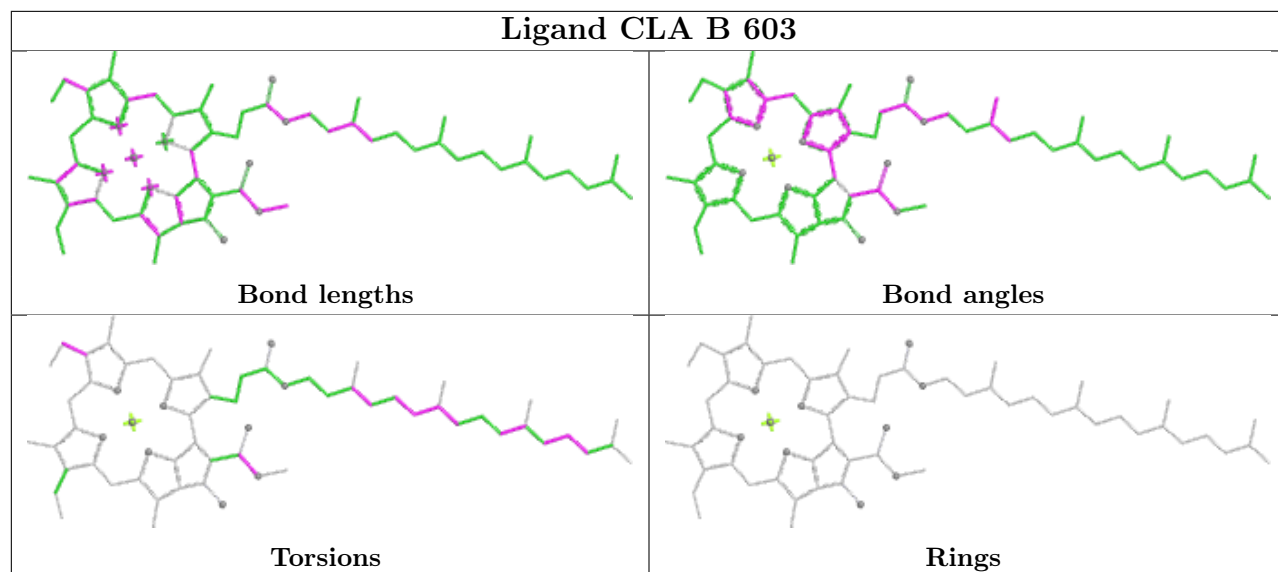




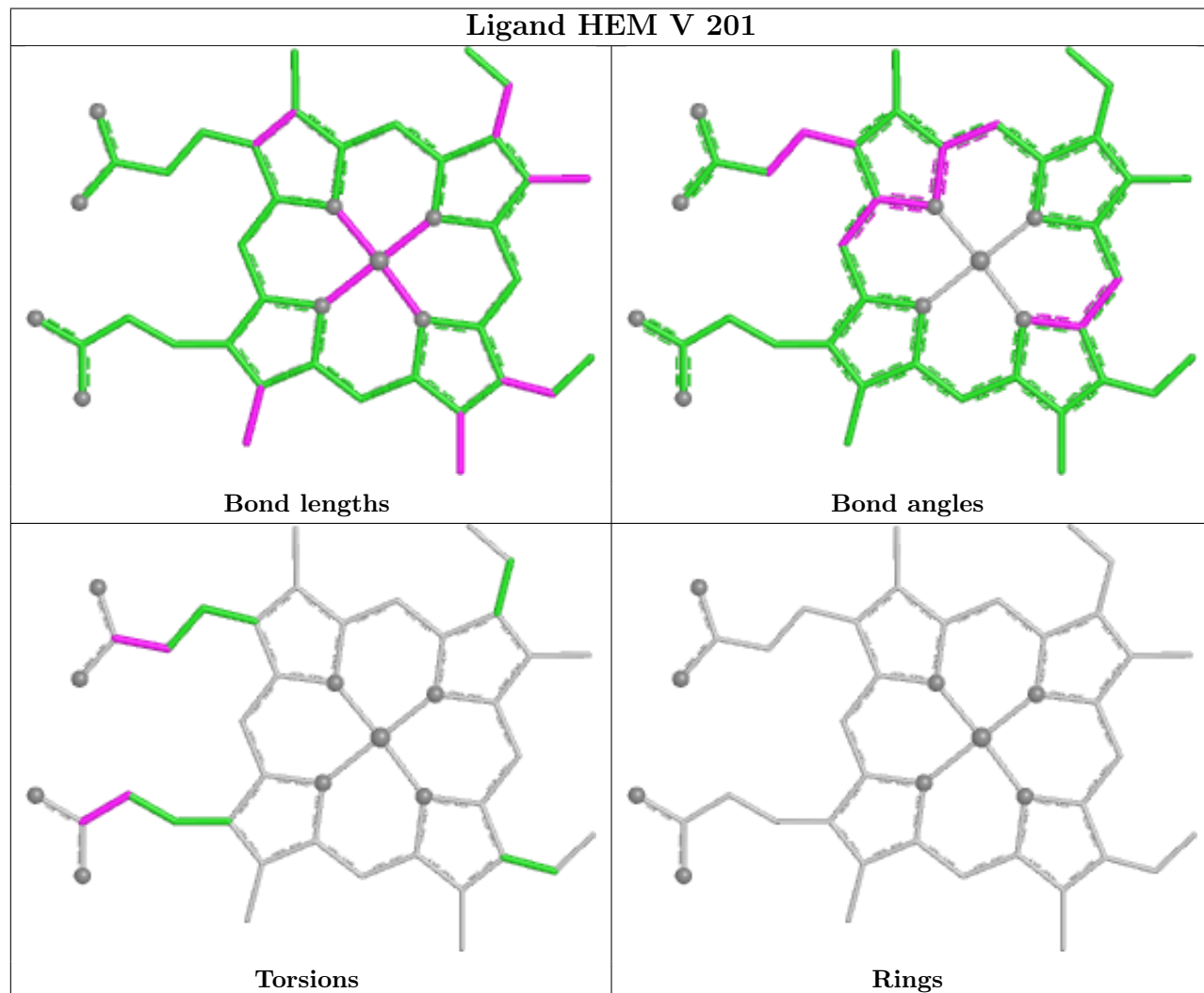


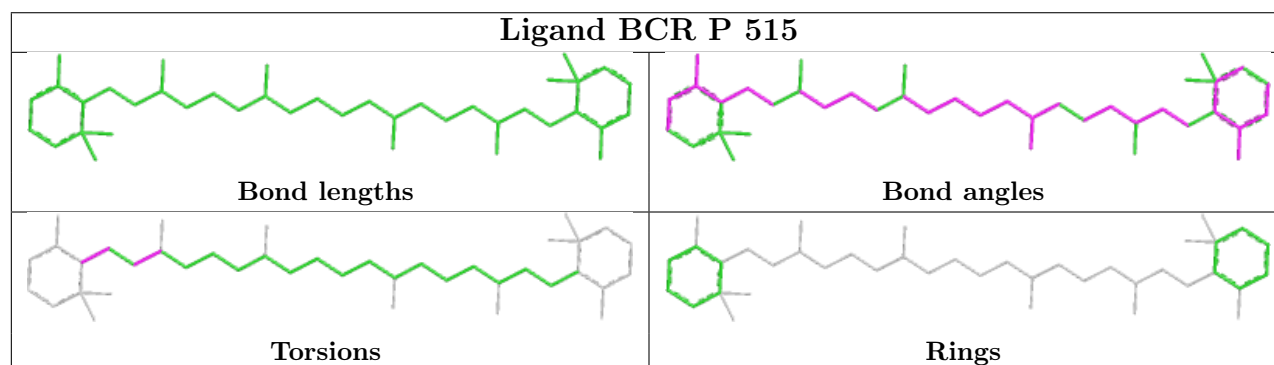
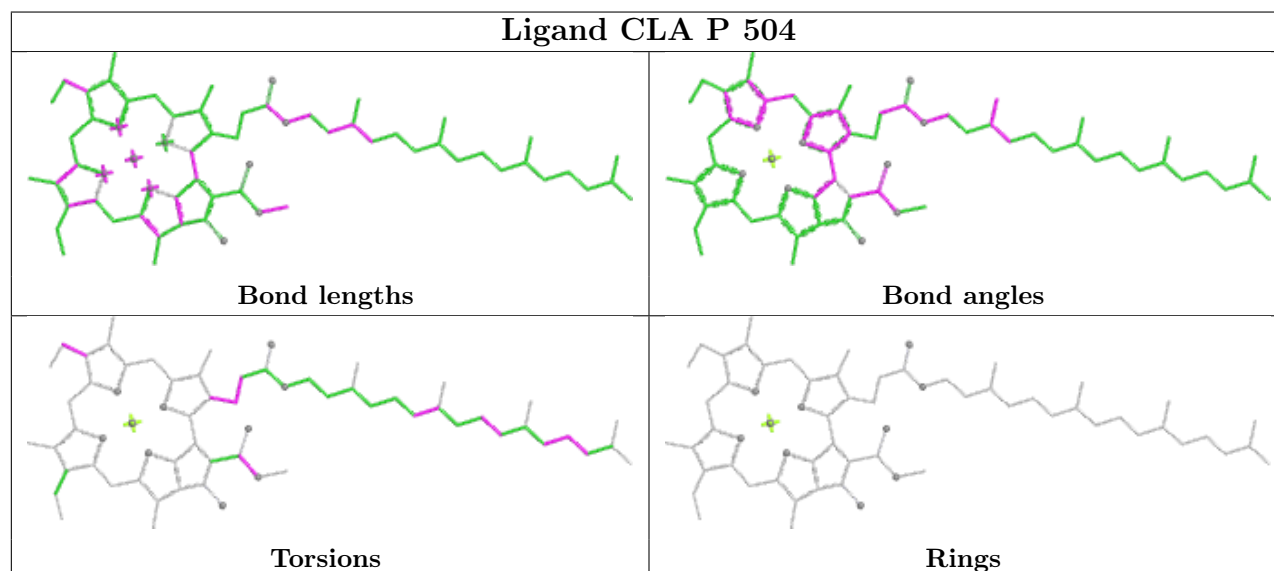
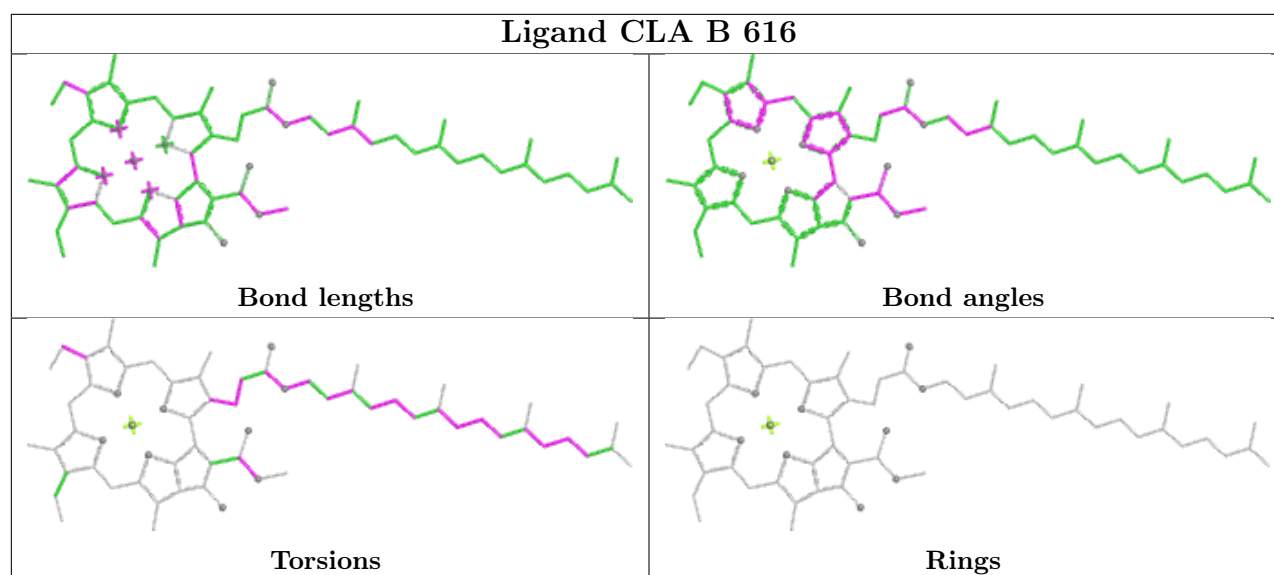


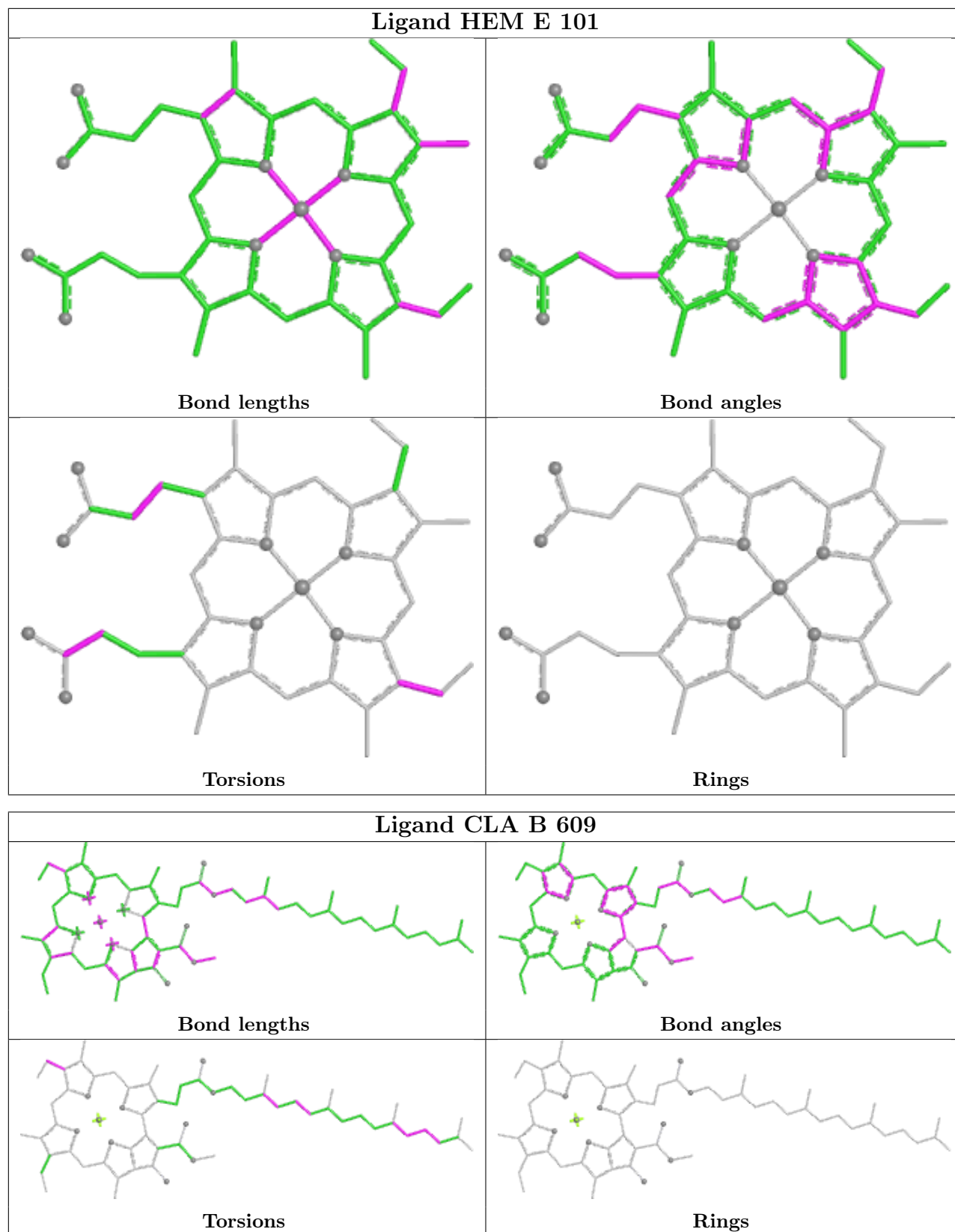
Ligand CLA B 603

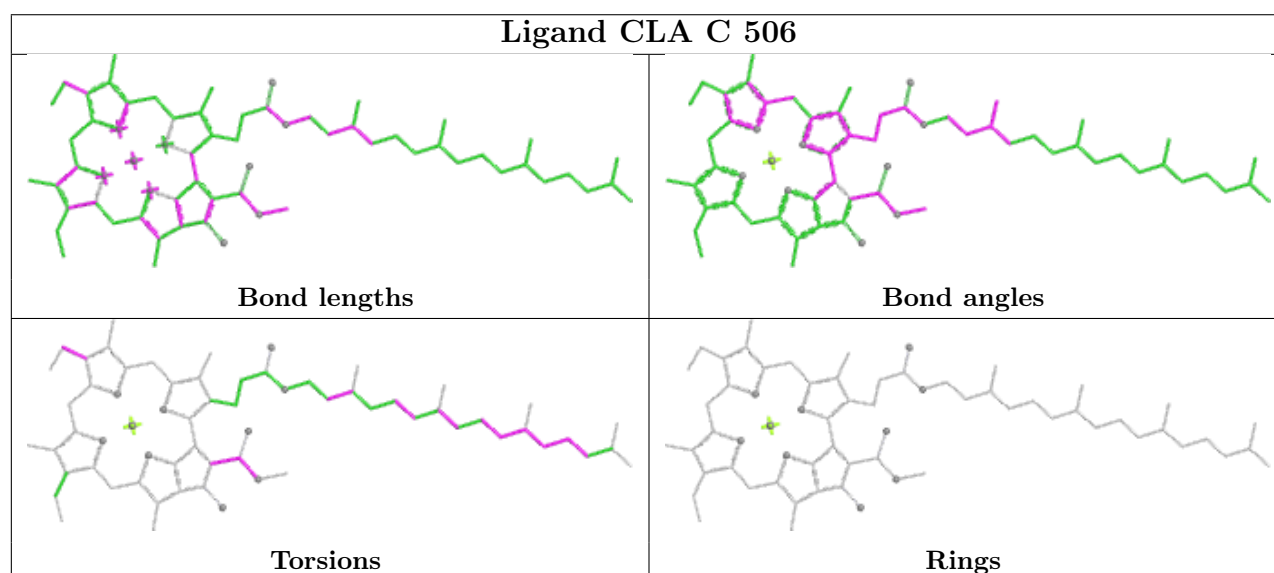
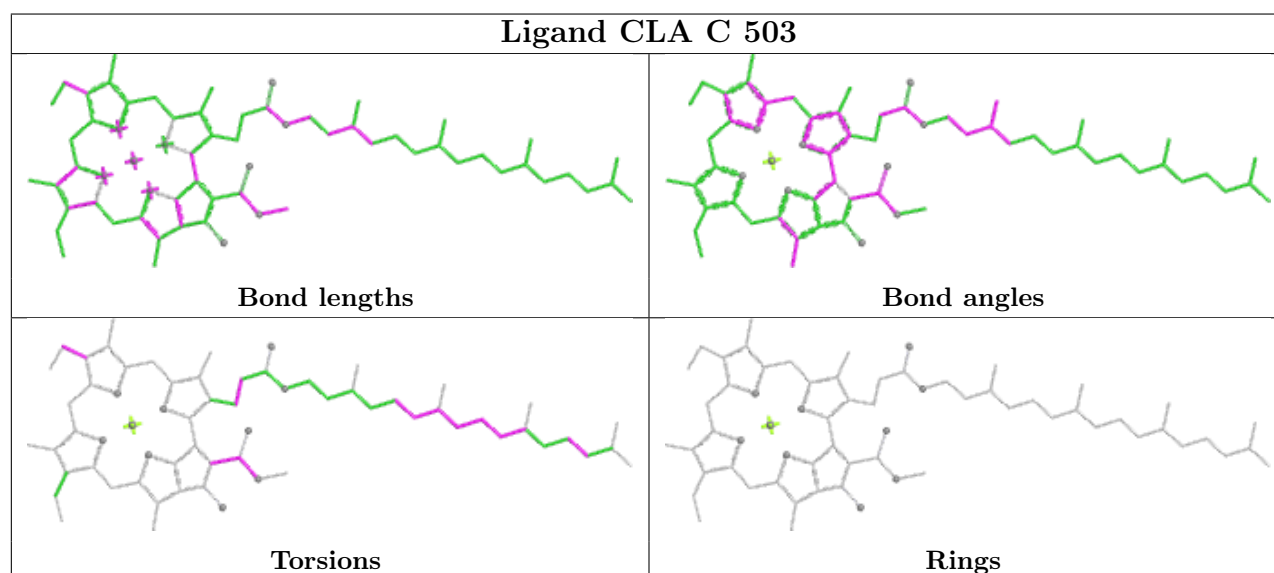
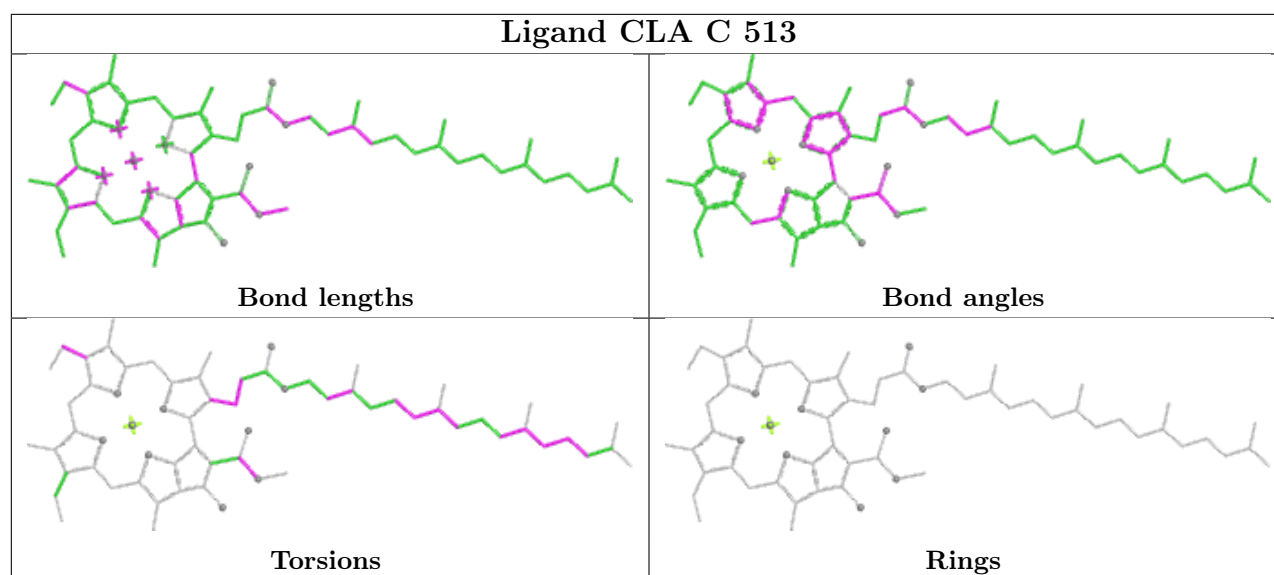


Ligand HEM V 201

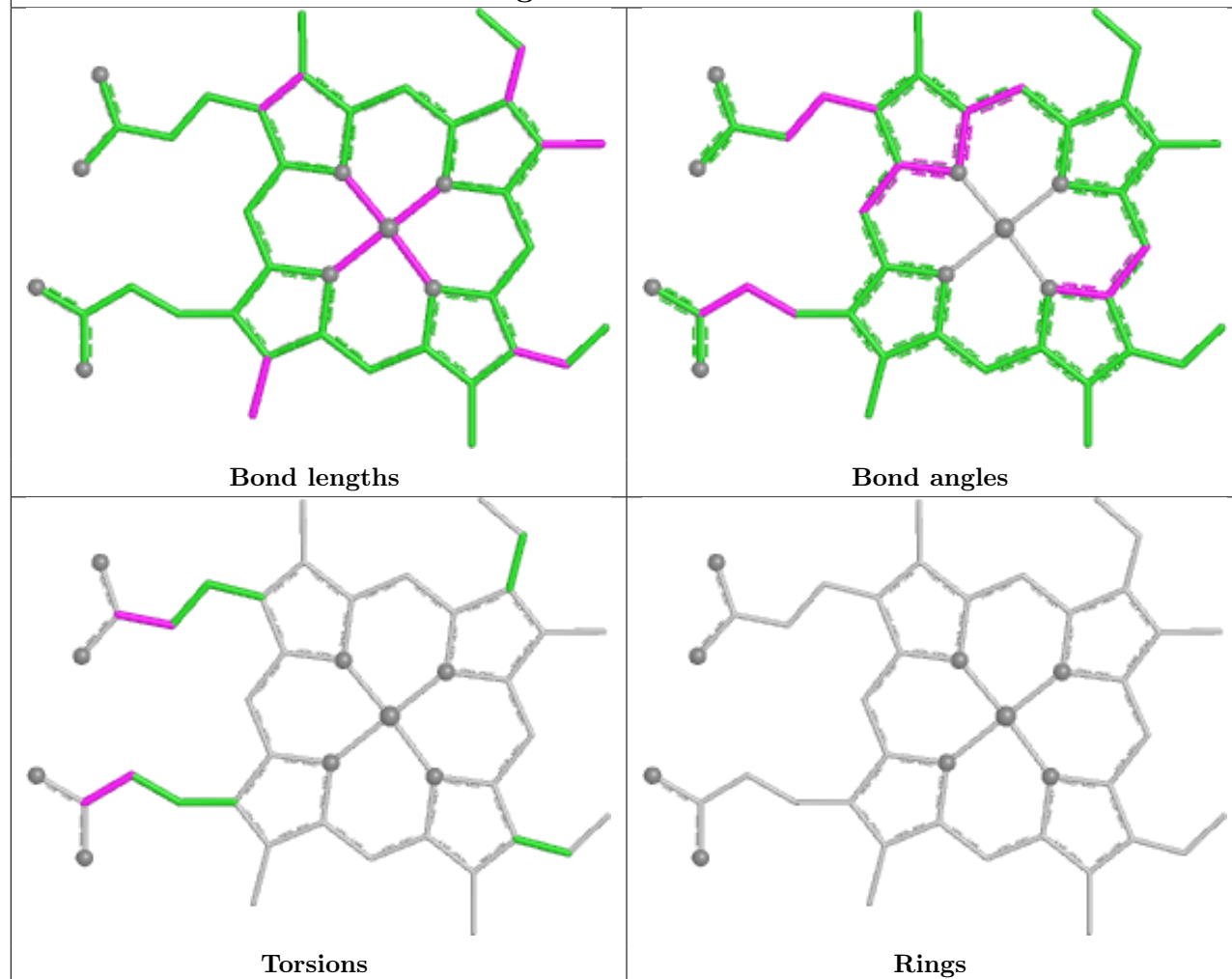




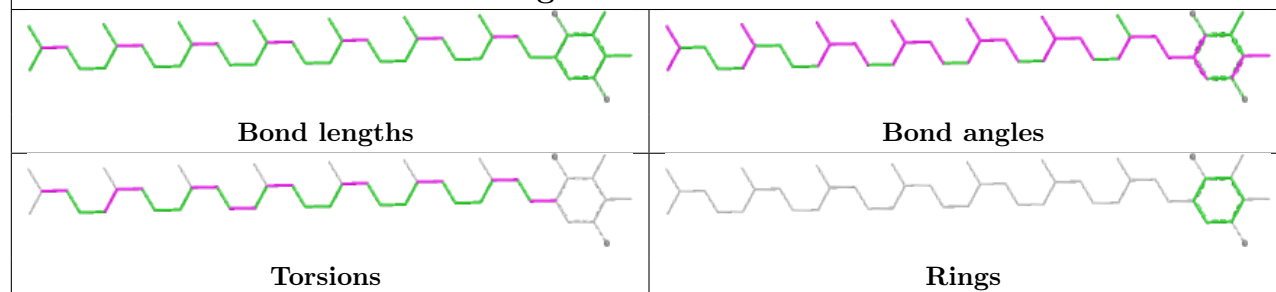


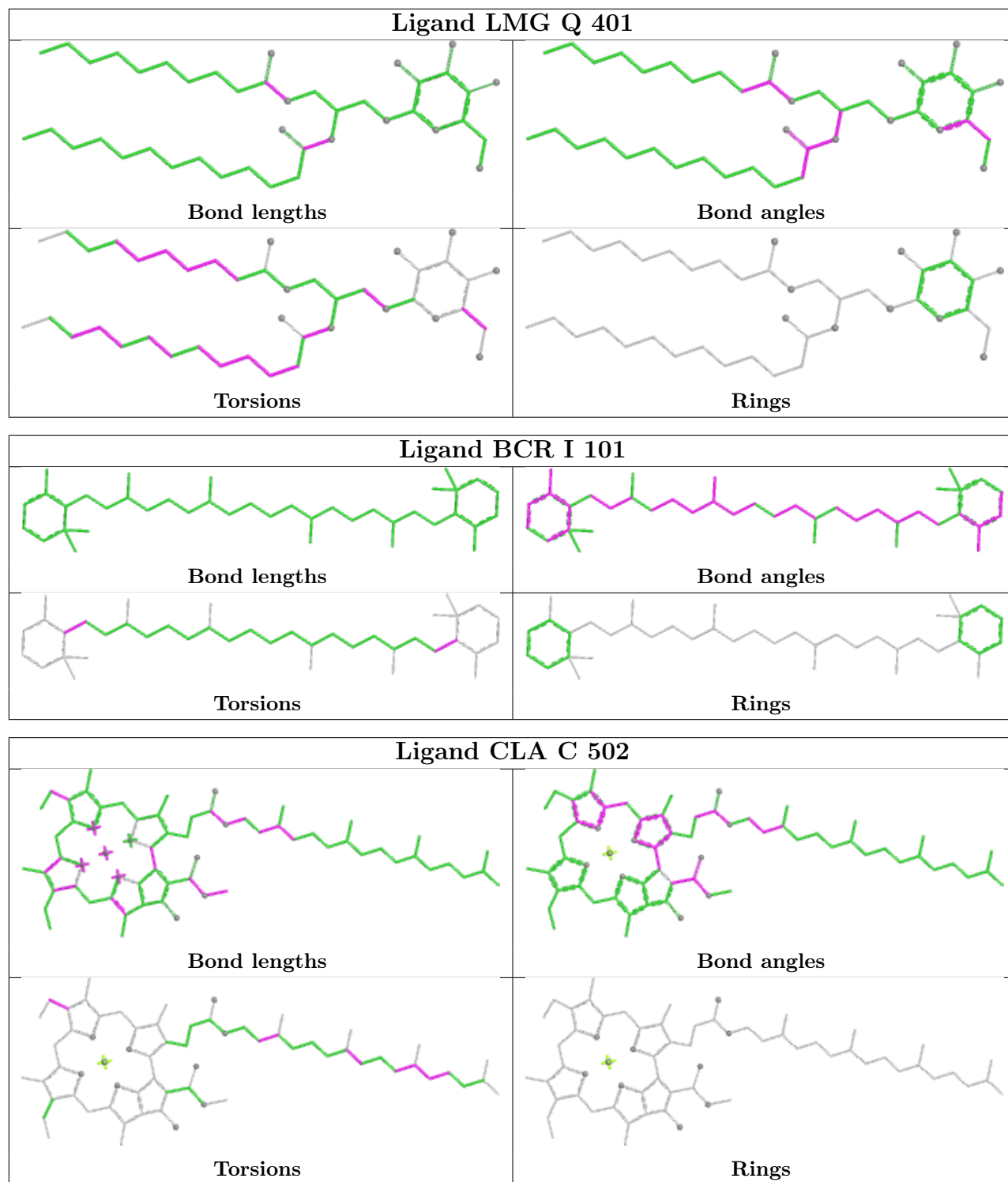


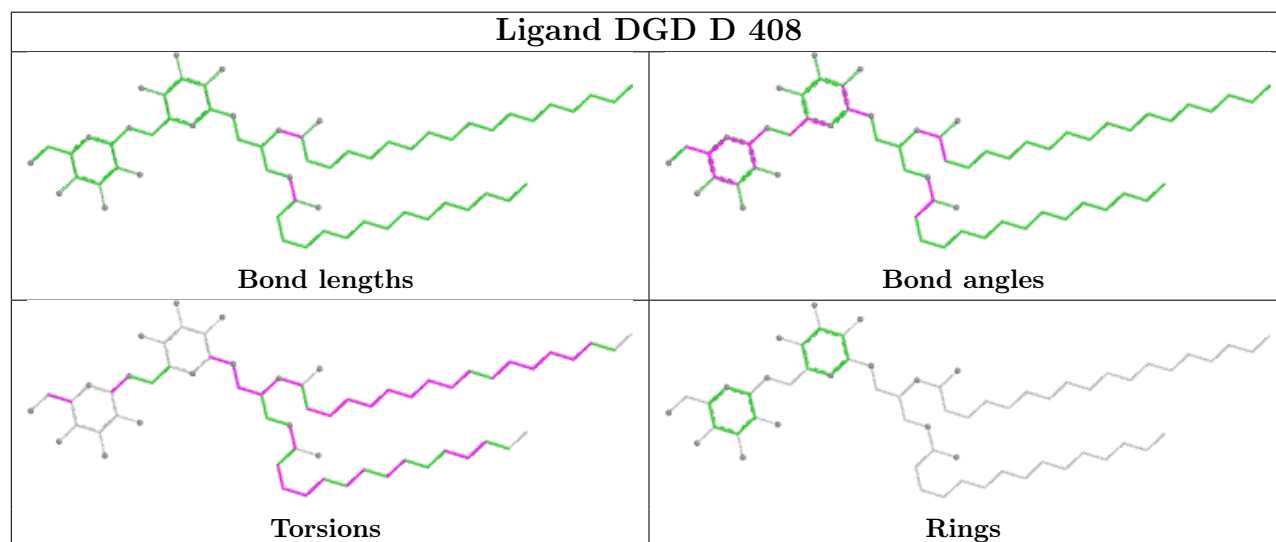
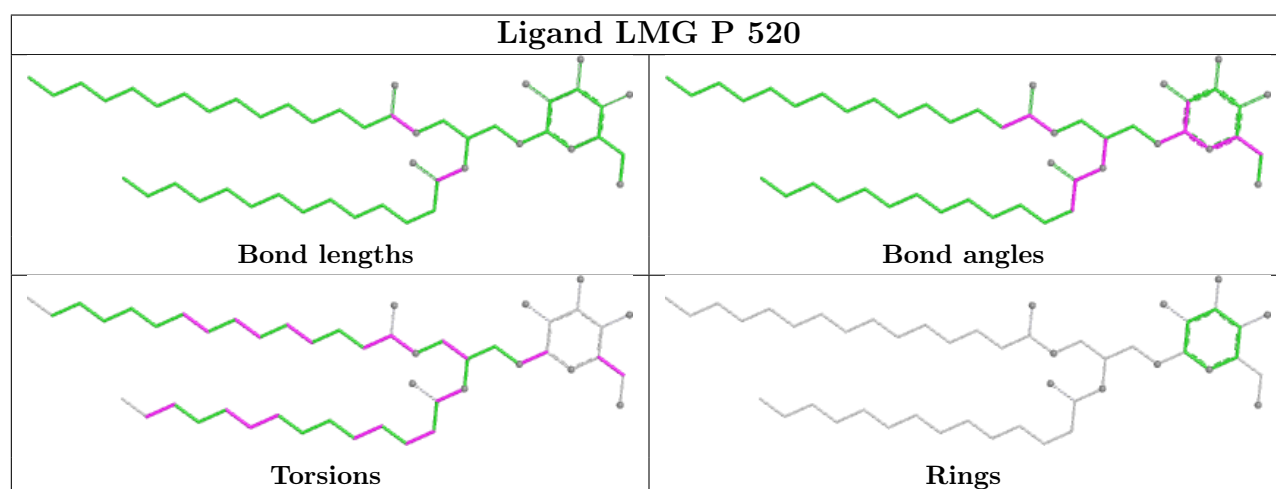
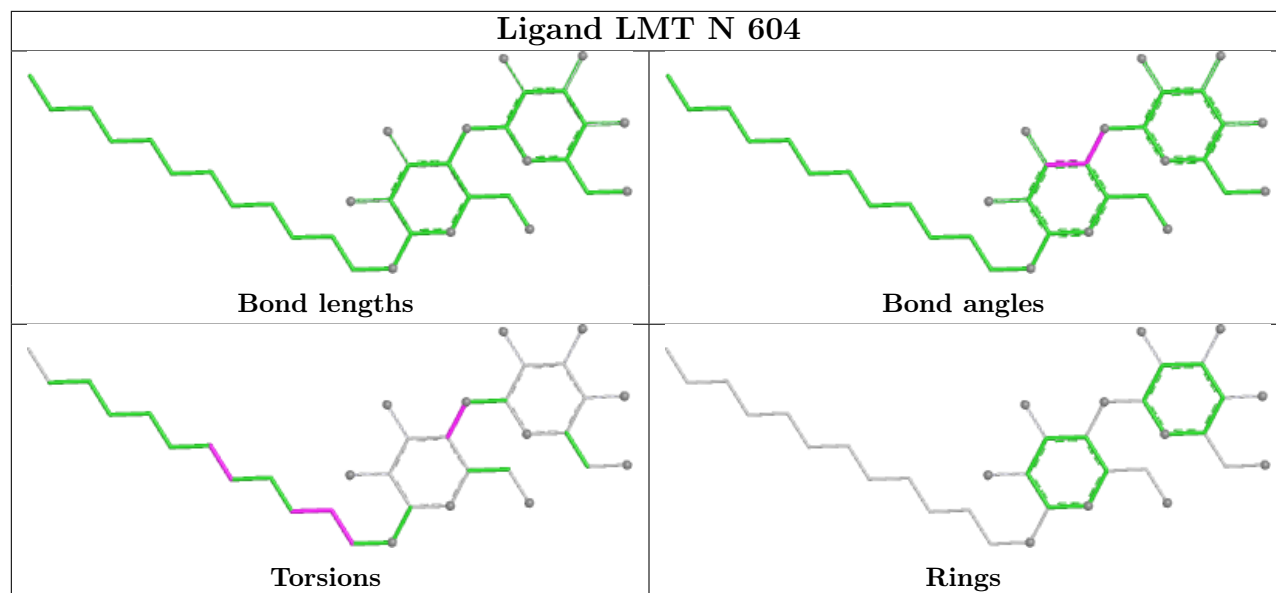
Ligand HEM i 201

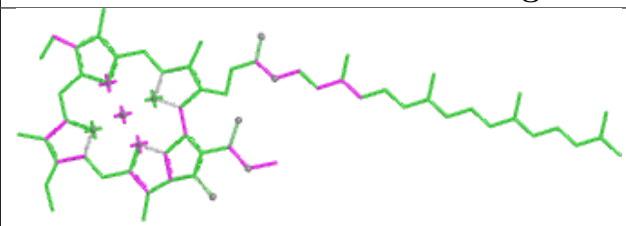
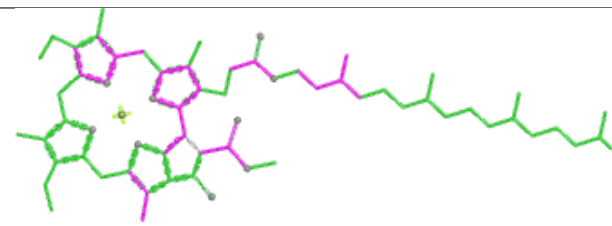
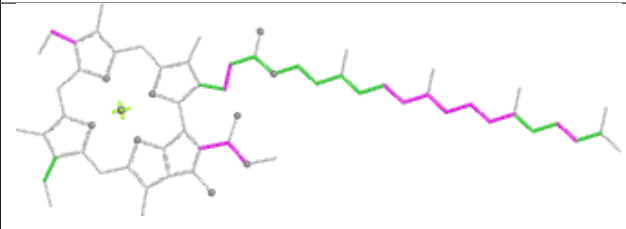
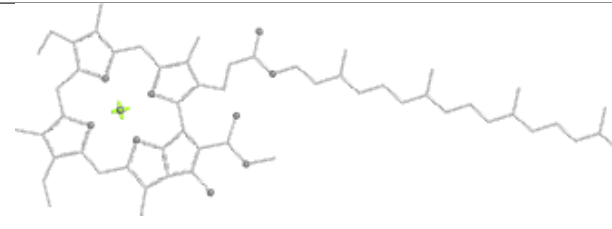


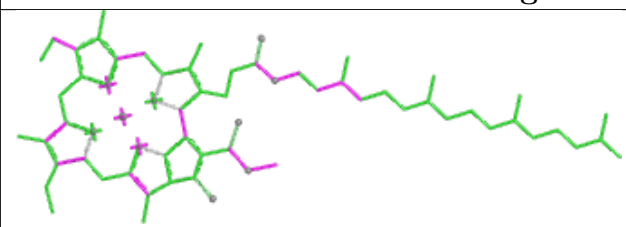
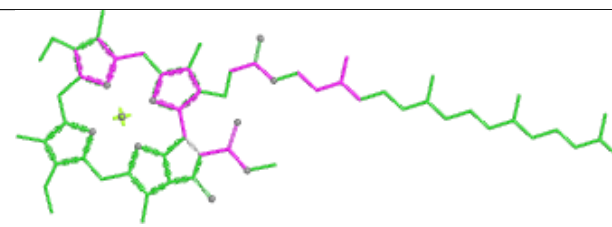
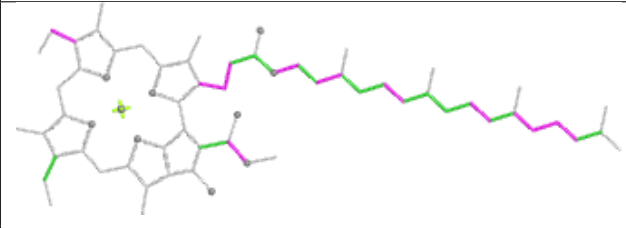
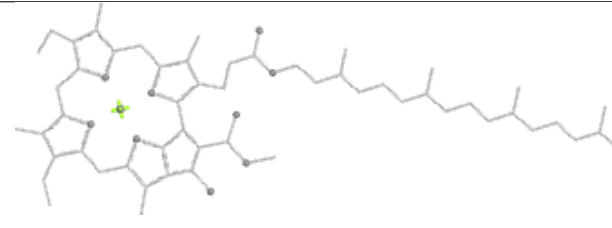
Ligand PL9 A 406

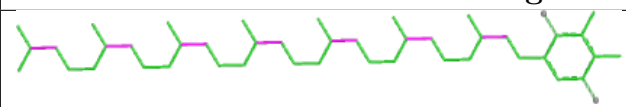
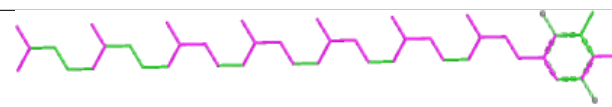
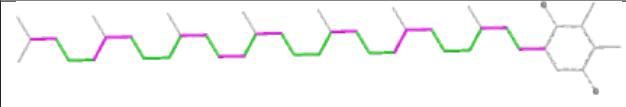
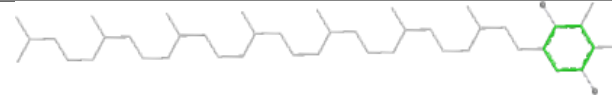


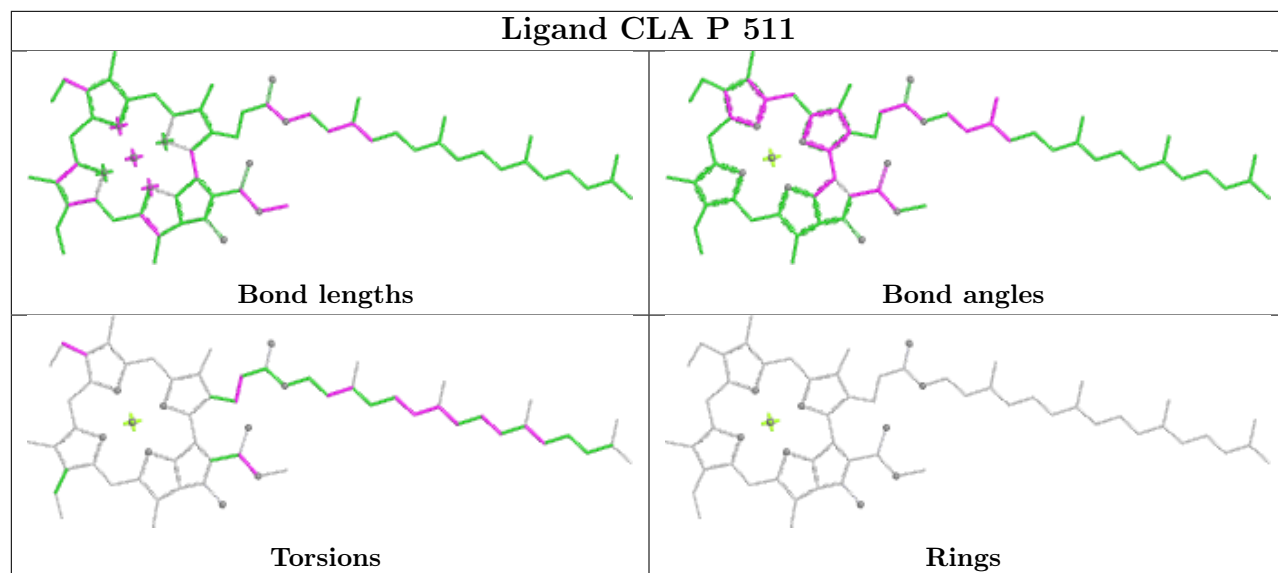
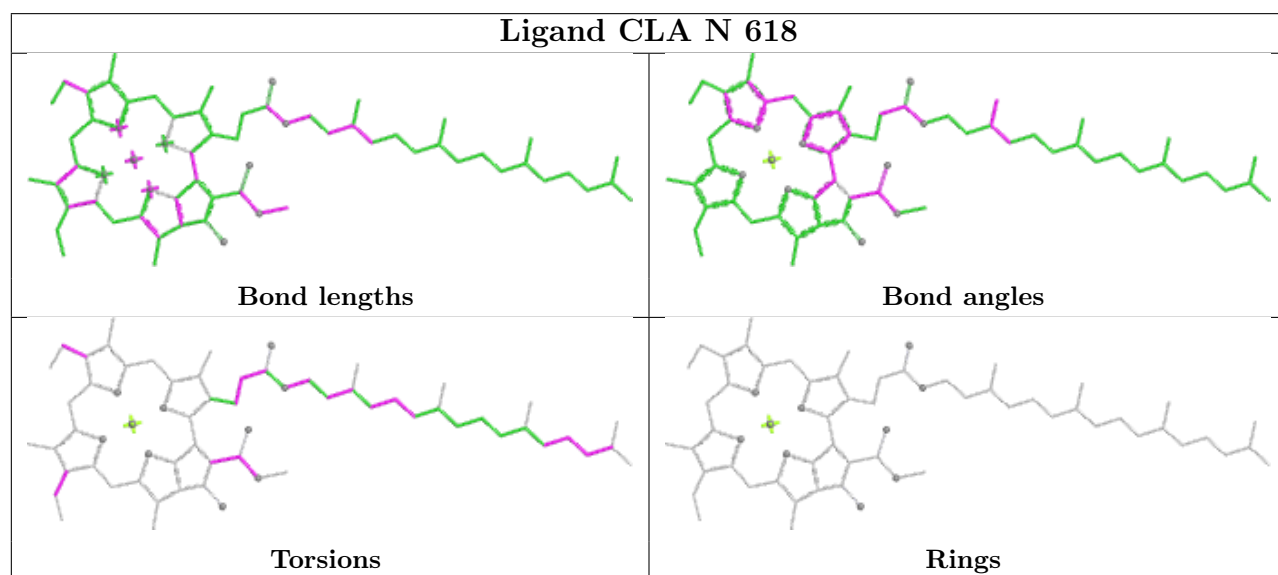
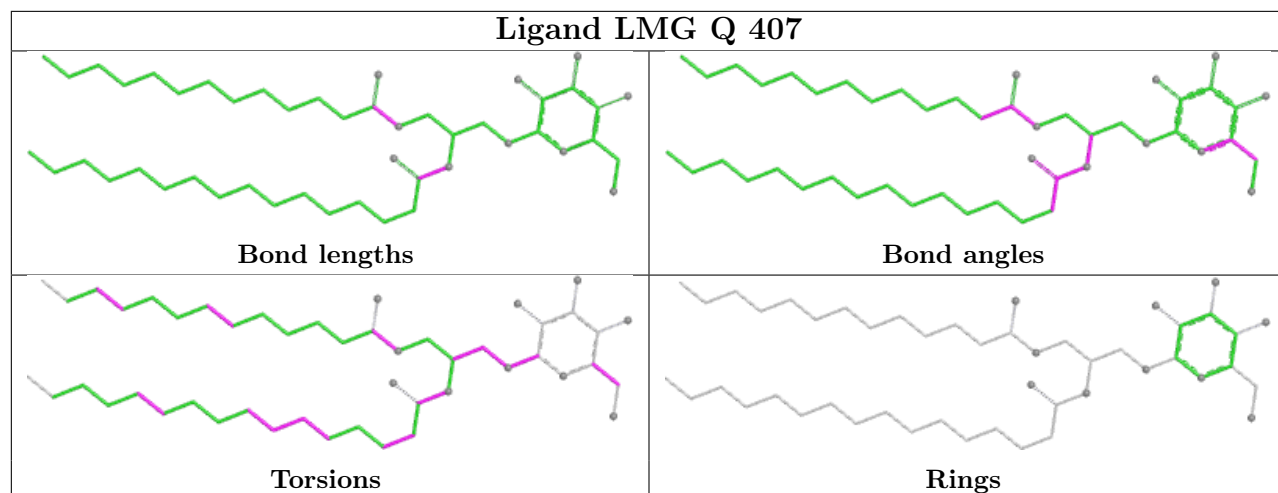


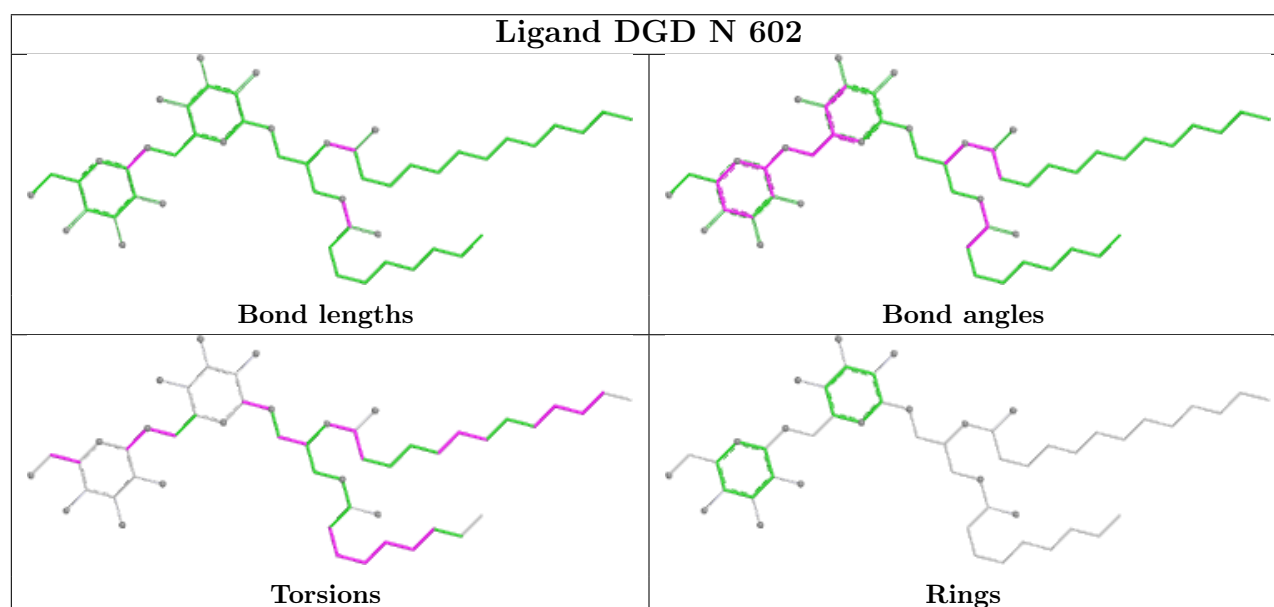
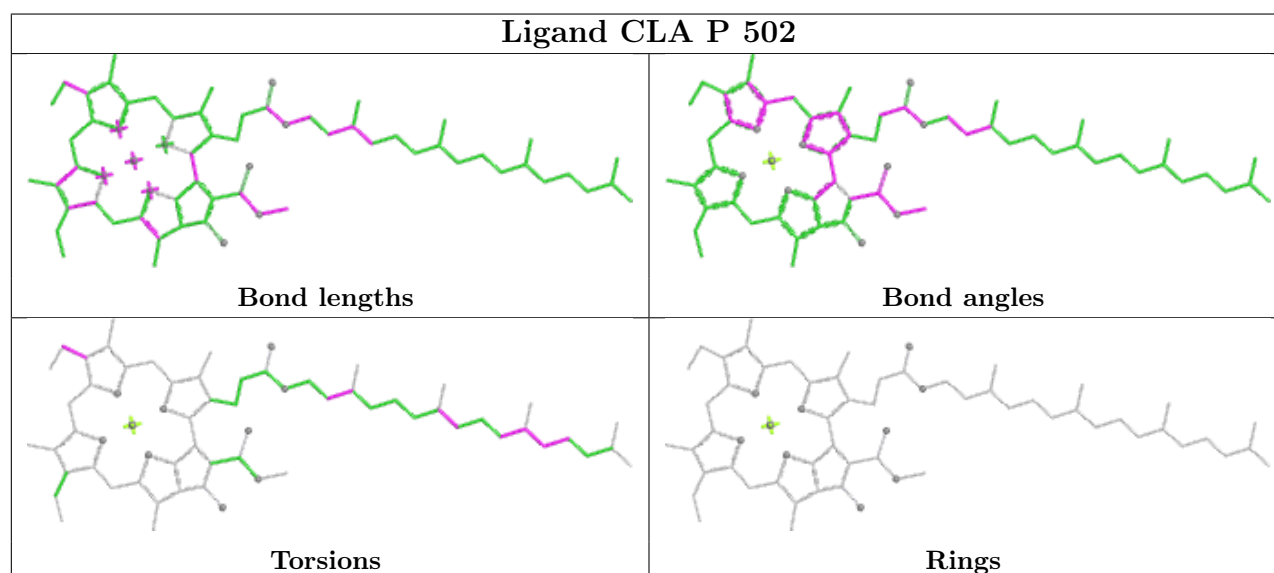
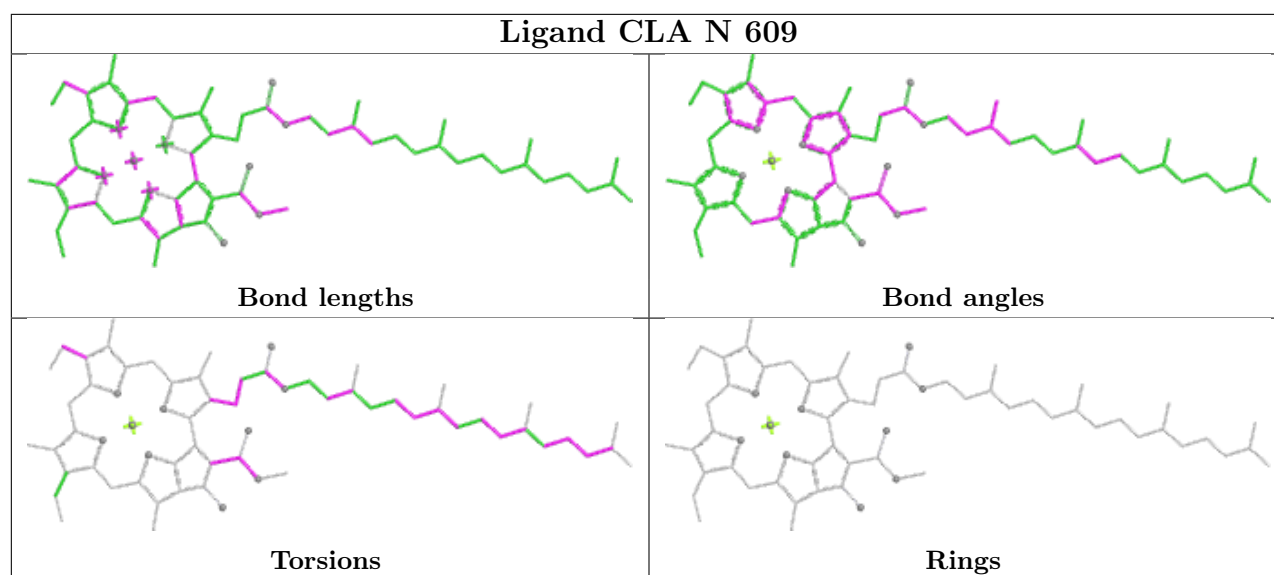


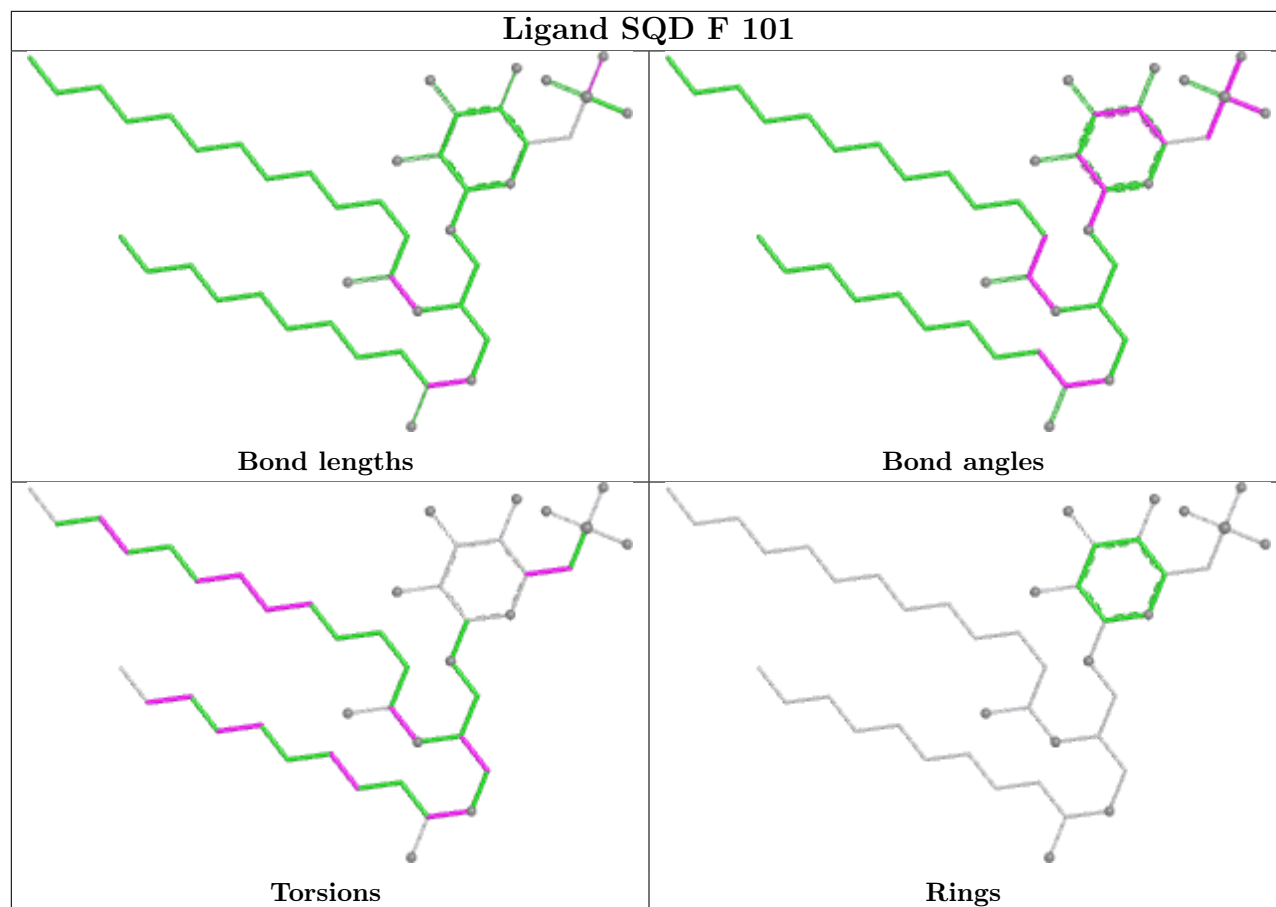
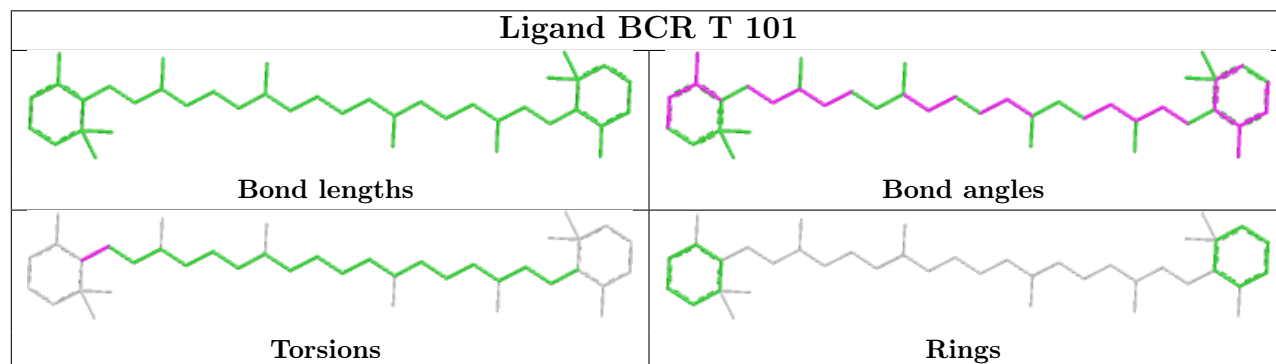
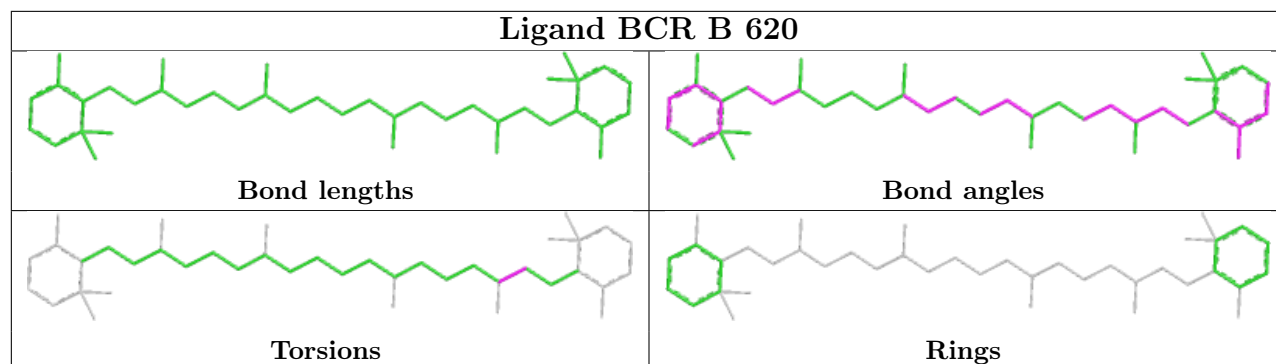
Ligand CLA P 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA N 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 G 407	
	
Bond lengths	Bond angles
	
Torsions	Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	335/344 (97%)	-0.17	3 (0%) 81 70	131, 152, 182, 204	0
1	G	335/344 (97%)	0.06	15 (4%) 38 38	128, 156, 184, 213	0
2	B	490/510 (96%)	-0.17	11 (2%) 62 53	128, 158, 178, 195	0
2	N	490/510 (96%)	-0.07	13 (2%) 56 48	129, 160, 180, 207	0
3	C	447/461 (96%)	-0.14	6 (1%) 75 64	129, 164, 183, 211	0
3	P	447/461 (96%)	-0.07	5 (1%) 78 66	139, 165, 183, 197	0
4	D	340/352 (96%)	-0.15	7 (2%) 63 54	125, 152, 176, 198	0
4	Q	340/352 (96%)	-0.07	10 (2%) 53 47	130, 155, 175, 184	0
5	E	82/83 (98%)	-0.33	0 100 100	148, 171, 188, 198	0
5	R	82/83 (98%)	0.14	5 (6%) 27 32	148, 171, 188, 195	0
6	F	35/44 (79%)	-0.31	0 100 100	140, 168, 185, 199	0
6	S	35/44 (79%)	0.14	0 100 100	148, 165, 187, 188	0
7	H	65/65 (100%)	-0.05	2 (3%) 51 46	154, 172, 189, 195	0
7	W	65/65 (100%)	0.28	5 (7%) 19 26	154, 173, 188, 196	0
8	I	35/38 (92%)	0.09	0 100 100	147, 163, 174, 178	0
8	a	35/38 (92%)	0.07	0 100 100	148, 164, 179, 190	0
9	J	34/39 (87%)	-0.13	0 100 100	155, 165, 183, 189	0
9	b	34/39 (87%)	0.99	4 (11%) 9 17	156, 176, 190, 190	0
10	K	37/37 (100%)	-0.15	0 100 100	158, 170, 181, 185	0
10	c	37/37 (100%)	0.10	1 (2%) 56 48	152, 171, 187, 195	0
11	L	37/37 (100%)	0.15	2 (5%) 31 34	137, 155, 186, 190	0
11	d	37/37 (100%)	0.08	2 (5%) 31 34	143, 158, 194, 201	0
12	M	34/36 (94%)	0.18	2 (5%) 28 32	147, 163, 179, 195	0
12	e	34/36 (94%)	0.16	2 (5%) 28 32	147, 159, 176, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/246 (98%)	-0.06	1 (0%) 88 79	132, 162, 190, 201	0
13	f	243/246 (98%)	-0.08	3 (1%) 76 65	127, 164, 191, 211	0
14	T	32/32 (100%)	-0.23	0 100 100	144, 157, 187, 198	0
14	g	32/32 (100%)	-0.13	0 100 100	145, 158, 179, 198	0
15	U	97/104 (93%)	-0.14	1 (1%) 79 68	136, 154, 173, 177	0
15	h	97/104 (93%)	-0.12	1 (1%) 79 68	140, 154, 165, 174	0
16	V	137/137 (100%)	-0.20	0 100 100	135, 156, 170, 180	0
16	i	137/137 (100%)	-0.15	0 100 100	131, 158, 176, 185	0
17	m	28/46 (60%)	0.85	2 (7%) 22 28	167, 183, 198, 205	0
17	y	28/46 (60%)	0.05	0 100 100	164, 182, 197, 200	0
18	X	37/40 (92%)	0.01	1 (2%) 56 48	158, 173, 188, 190	0
18	j	37/40 (92%)	0.06	1 (2%) 56 48	161, 175, 191, 202	0
19	Y	0/28	-	-	-	-
19	k	0/28	-	-	-	-
20	Z	62/62 (100%)	0.02	2 (3%) 50 45	159, 178, 198, 208	0
20	l	62/62 (100%)	0.08	3 (4%) 35 37	164, 178, 199, 208	0
All	All	5214/5482 (95%)	-0.07	110 (2%) 63 54	125, 161, 185, 213	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	44	ALA	6.2
7	W	30	LEU	5.7
17	m	30	ILE	5.7
2	N	211	ILE	5.3
1	G	43	ALA	5.2
1	G	42	LEU	5.2
3	P	341	LEU	4.8
2	N	393	GLU	4.5
1	G	279	PRO	4.2
20	l	17	PHE	4.1
9	b	16	VAL	4.1
2	B	421	ALA	4.0
2	B	368	VAL	4.0
1	G	277	ALA	3.9
5	R	27	ILE	3.8
4	D	270	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
5	R	28	PRO	3.7
2	B	417	VAL	3.7
2	B	397	VAL	3.6
1	G	45	THR	3.6
13	f	251	MET	3.5
5	R	31	PHE	3.5
3	C	160	ILE	3.4
4	D	208	ALA	3.4
4	Q	212	ALA	3.3
12	e	13	LEU	3.3
1	G	205	VAL	3.3
13	f	190	LEU	3.3
4	Q	210	LEU	3.3
1	G	276	ALA	3.3
2	N	415	PRO	3.2
2	B	309	LEU	3.2
3	P	367	GLU	3.2
20	Z	17	PHE	3.1
18	j	35	ALA	3.1
15	h	44	ASP	3.1
7	H	6	TRP	3.1
4	Q	343	GLU	3.1
4	Q	342	PRO	3.1
7	W	36	GLY	3.1
5	R	32	ILE	3.0
4	Q	45	LEU	3.0
2	B	5	TRP	3.0
1	A	222	SER	3.0
9	b	25	VAL	2.9
20	l	20	VAL	2.9
1	A	77	ILE	2.8
20	l	21	ILE	2.8
2	N	381	ILE	2.8
7	W	34	PHE	2.8
1	G	41	LEU	2.8
3	C	168	LEU	2.7
1	G	280	VAL	2.7
1	A	206	PHE	2.7
11	d	30	LEU	2.7
3	P	315	MET	2.7
3	C	164	HIS	2.7
2	N	407	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	351	GLY	2.6
2	N	382	PRO	2.6
4	Q	42	TYR	2.6
2	B	348	ASN	2.6
2	N	421	ALA	2.6
1	G	50	ILE	2.5
3	C	355	THR	2.5
2	N	418	LYS	2.5
5	R	38	VAL	2.5
1	G	204	GLY	2.5
1	G	46	ILE	2.5
15	U	122	VAL	2.5
3	C	275	SER	2.4
3	C	327	ASN	2.4
12	e	12	ALA	2.4
4	Q	271	MET	2.3
2	N	112	CYS	2.3
2	B	438	ASN	2.3
9	b	17	ALA	2.3
12	M	2	GLU	2.3
4	D	144	ILE	2.3
7	H	10	ILE	2.3
7	W	11	LEU	2.3
4	D	206	GLY	2.3
11	L	25	LEU	2.3
11	d	28	ALA	2.3
4	D	205	LEU	2.3
9	b	15	THR	2.2
17	m	27	MET	2.2
2	N	306	PRO	2.2
12	M	21	PHE	2.2
7	W	14	LEU	2.2
4	D	211	CYS	2.2
1	G	118	HIS	2.1
4	D	149	PRO	2.1
2	B	412	THR	2.1
2	N	391	SER	2.1
3	P	318	LEU	2.1
18	X	24	LEU	2.1
2	N	380	ASP	2.1
2	B	354	LEU	2.1
13	f	176	SER	2.1

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Mol	Chain	Res	Type	RSRZ
20	Z	53	VAL	2.1
11	L	22	LEU	2.1
13	O	67	ALA	2.1
2	N	388	SER	2.1
3	P	410	VAL	2.1
4	Q	39	PRO	2.0
4	Q	239	GLN	2.0
4	Q	171	PRO	2.0
1	G	47	CYS	2.0
10	c	10	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	CL	D	411	1/1	-0.16	0.17	121,121,121,121	0
35	CA	O	301	1/1	0.33	0.13	138,138,138,138	0
31	LMT	Q	410	31/35	0.34	0.17	165,182,193,197	0
31	LMT	I	103	35/35	0.42	0.20	153,189,201,206	0
21	CLA	N	605	65/65	0.47	0.17	170,189,202,205	0
31	LMT	D	409	31/35	0.48	0.11	162,187,202,208	0
31	LMT	N	624	35/35	0.53	0.14	166,201,210,213	0
21	CLA	B	601	65/65	0.53	0.15	167,188,199,203	0
30	BCR	H	101	40/40	0.61	0.19	165,178,188,190	0
30	BCR	b	102	40/40	0.61	0.34	158,178,202,203	0
31	LMT	N	625	35/35	0.63	0.11	165,184,206,216	0
31	LMT	N	604	35/35	0.65	0.12	145,180,209,212	0
31	LMT	B	625	35/35	0.66	0.12	163,196,218,227	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	SQD	B	627	47/54	0.68	0.15	143,179,209,227	0
31	LMT	a	103	35/35	0.68	0.13	169,180,206,216	0
27	LMG	C	520	45/55	0.69	0.16	164,178,186,187	0
30	BCR	c	101	40/40	0.69	0.18	151,171,188,190	0
21	CLA	B	604	65/65	0.69	0.15	148,158,172,182	0
33	CL	G	415	1/1	0.70	0.20	122,122,122,122	0
26	SQD	N	601	47/54	0.71	0.17	141,176,198,202	0
21	CLA	C	507	65/65	0.71	0.17	159,172,185,187	0
30	BCR	a	101	40/40	0.73	0.25	139,159,176,181	0
21	CLA	N	607	65/65	0.73	0.14	133,163,170,175	0
22	PHO	A	404	64/64	0.74	0.14	129,151,167,177	0
30	BCR	J	102	40/40	0.74	0.25	167,182,207,208	0
21	CLA	G	406	65/65	0.76	0.16	145,159,181,186	0
31	LMT	B	630	35/35	0.76	0.18	157,169,199,220	0
30	BCR	P	514	40/40	0.77	0.14	139,152,173,175	0
23	PL9	b	101	35/55	0.77	0.28	168,188,199,208	0
21	CLA	C	509	65/65	0.77	0.16	145,170,180,183	0
22	PHO	D	402	64/64	0.77	0.12	135,155,161,168	0
25	LHG	G	412	37/49	0.78	0.20	147,176,193,204	0
30	BCR	T	103	40/40	0.78	0.21	155,168,181,184	0
31	LMT	B	626	35/35	0.79	0.11	163,194,202,213	0
30	BCR	I	101	40/40	0.79	0.22	143,155,171,183	0
27	LMG	I	102	43/55	0.79	0.18	152,184,203,207	0
21	CLA	P	509	65/65	0.80	0.13	152,174,181,184	0
27	LMG	P	521	45/55	0.80	0.14	149,175,191,198	0
21	CLA	C	513	65/65	0.80	0.13	173,193,206,213	0
31	LMT	N	603	35/35	0.80	0.16	153,179,189,190	0
21	CLA	N	620	65/65	0.81	0.17	156,175,192,194	0
21	CLA	P	507	65/65	0.81	0.14	162,172,191,194	0
34	HEM	i	201	43/43	0.81	0.15	131,158,169,172	0
31	LMT	B	629	35/35	0.81	0.18	153,166,181,185	0
21	CLA	C	512	65/65	0.82	0.13	173,183,196,199	0
32	BCT	Q	411	4/4	0.82	0.13	164,166,168,173	0
21	CLA	B	609	65/65	0.82	0.14	162,177,185,186	0
30	BCR	B	618	40/40	0.83	0.19	149,162,168,169	0
21	CLA	P	501	65/65	0.83	0.13	149,170,185,188	0
30	BCR	P	516	40/40	0.83	0.18	164,173,180,187	0
30	BCR	S	101	40/40	0.83	0.21	145,159,176,178	0
26	SQD	A	414	54/54	0.83	0.26	139,173,190,200	0
27	LMG	B	623	49/55	0.83	0.19	128,147,164,167	0
30	BCR	W	101	40/40	0.84	0.12	164,176,182,186	0
24	DGD	C	518	66/66	0.84	0.14	139,157,179,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	DGD	D	408	63/66	0.84	0.18	167,181,198,212	0
27	LMG	a	102	43/55	0.84	0.16	160,179,196,200	0
21	CLA	N	610	65/65	0.84	0.15	152,178,191,194	0
30	BCR	C	514	40/40	0.84	0.13	153,160,171,173	0
24	DGD	B	628	52/66	0.84	0.15	148,173,194,200	0
21	CLA	C	505	65/65	0.85	0.17	147,172,186,188	0
21	CLA	P	513	65/65	0.85	0.13	168,182,207,216	0
27	LMG	D	412	42/55	0.85	0.17	147,178,195,199	0
21	CLA	N	609	65/65	0.85	0.12	148,165,174,178	0
27	LMG	P	520	48/55	0.86	0.29	147,168,177,184	0
30	BCR	T	101	40/40	0.86	0.16	144,167,181,184	0
24	DGD	Q	409	63/66	0.86	0.20	157,183,208,238	0
27	LMG	Q	401	42/55	0.86	0.15	131,168,174,183	0
24	DGD	C	516	53/66	0.86	0.17	141,158,168,170	0
24	DGD	B	621	58/66	0.86	0.14	142,158,168,171	0
27	LMG	D	407	48/55	0.86	0.20	145,159,169,175	0
23	PL9	J	101	35/55	0.86	0.21	177,190,200,204	0
26	SQD	G	401	54/54	0.86	0.19	158,176,209,210	0
21	CLA	B	607	65/65	0.87	0.13	135,152,161,165	0
30	BCR	B	619	40/40	0.87	0.24	140,156,169,178	0
26	SQD	F	101	45/54	0.87	0.17	157,176,196,198	0
24	DGD	A	407	56/66	0.87	0.14	147,171,188,195	0
21	CLA	B	608	65/65	0.87	0.15	147,165,180,186	0
21	CLA	B	605	65/65	0.87	0.11	156,167,176,179	0
27	LMG	C	519	48/55	0.87	0.18	132,169,183,188	0
21	CLA	B	610	65/65	0.87	0.11	146,163,174,176	0
24	DGD	C	517	62/66	0.87	0.12	145,169,193,200	0
21	CLA	B	615	65/65	0.87	0.12	162,178,191,194	0
21	CLA	N	616	65/65	0.87	0.10	156,167,181,184	0
31	LMT	e	101	35/35	0.87	0.20	164,176,191,195	0
22	PHO	Q	403	64/64	0.87	0.11	144,155,164,168	0
25	LHG	A	411	37/49	0.87	0.13	156,178,214,232	0
23	PL9	A	406	45/55	0.87	0.18	152,174,185,188	0
21	CLA	D	401	65/65	0.87	0.15	137,149,176,181	0
30	BCR	B	617	40/40	0.87	0.14	151,158,176,180	0
35	CA	f	301	1/1	0.87	0.09	210,210,210,210	0
22	PHO	G	405	64/64	0.88	0.12	131,149,159,162	0
21	CLA	N	608	65/65	0.88	0.12	146,158,176,191	0
21	CLA	N	618	65/65	0.88	0.13	153,171,180,185	0
31	LMT	M	102	35/35	0.88	0.16	134,165,196,205	0
30	BCR	T	102	40/40	0.88	0.18	143,167,176,178	0
21	CLA	P	511	65/65	0.88	0.10	156,174,184,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	SQD	G	410	51/54	0.88	0.18	161,172,184,190	0
30	BCR	P	515	40/40	0.88	0.13	165,176,185,189	0
27	LMG	Q	407	48/55	0.88	0.13	142,156,168,176	0
23	PL9	Q	405	55/55	0.88	0.13	137,146,166,170	0
27	LMG	B	622	49/55	0.88	0.18	148,163,174,176	0
24	DGD	P	519	66/66	0.88	0.14	142,157,177,186	0
21	CLA	D	403	65/65	0.88	0.13	153,160,181,189	0
21	CLA	C	501	65/65	0.88	0.13	160,174,184,185	0
30	BCR	C	515	40/40	0.88	0.13	139,164,177,180	0
30	BCR	D	405	40/40	0.88	0.14	145,161,176,179	0
21	CLA	P	502	65/65	0.88	0.11	146,161,175,182	0
21	CLA	B	614	65/65	0.89	0.13	157,172,181,184	0
21	CLA	P	505	65/65	0.89	0.15	134,164,180,183	0
26	SQD	B	624	43/54	0.89	0.13	150,181,199,206	0
21	CLA	A	405	65/65	0.89	0.12	144,155,176,187	0
24	DGD	N	602	52/66	0.89	0.13	154,176,204,206	0
27	LMG	N	623	49/55	0.89	0.17	139,152,164,171	0
24	DGD	P	518	62/66	0.89	0.19	144,168,195,200	0
21	CLA	C	506	65/65	0.89	0.15	159,175,202,211	0
21	CLA	G	402	65/65	0.89	0.12	136,148,155,166	0
26	SQD	Q	408	43/54	0.89	0.15	143,180,193,194	0
27	LMG	Q	406	46/55	0.89	0.16	135,162,171,180	0
24	DGD	W	102	58/66	0.89	0.17	145,157,168,172	0
21	CLA	G	403	65/65	0.89	0.12	123,139,149,162	0
27	LMG	G	411	51/55	0.90	0.14	152,164,177,178	0
21	CLA	P	503	65/65	0.90	0.11	144,174,187,195	0
21	CLA	P	504	65/65	0.90	0.14	155,169,181,186	0
21	CLA	A	403	65/65	0.90	0.15	142,161,183,185	0
26	SQD	S	102	45/54	0.90	0.14	160,188,201,203	0
21	CLA	N	619	65/65	0.90	0.11	158,180,190,193	0
26	SQD	A	409	51/54	0.90	0.15	156,178,191,194	0
21	CLA	C	511	65/65	0.90	0.12	155,172,181,184	0
21	CLA	P	510	65/65	0.90	0.11	145,161,170,178	0
34	HEM	V	201	43/43	0.90	0.12	139,151,166,173	0
21	CLA	N	614	65/65	0.90	0.11	150,162,173,178	0
21	CLA	P	512	65/65	0.90	0.10	172,184,194,199	0
21	CLA	B	603	65/65	0.90	0.11	147,166,178,179	0
21	CLA	G	404	65/65	0.91	0.12	141,159,179,181	0
21	CLA	N	611	65/65	0.91	0.11	145,156,164,166	0
21	CLA	B	612	65/65	0.91	0.09	152,163,174,176	0
23	PL9	D	404	55/55	0.91	0.15	129,150,158,160	0
25	LHG	A	408	39/49	0.91	0.12	146,167,179,179	0

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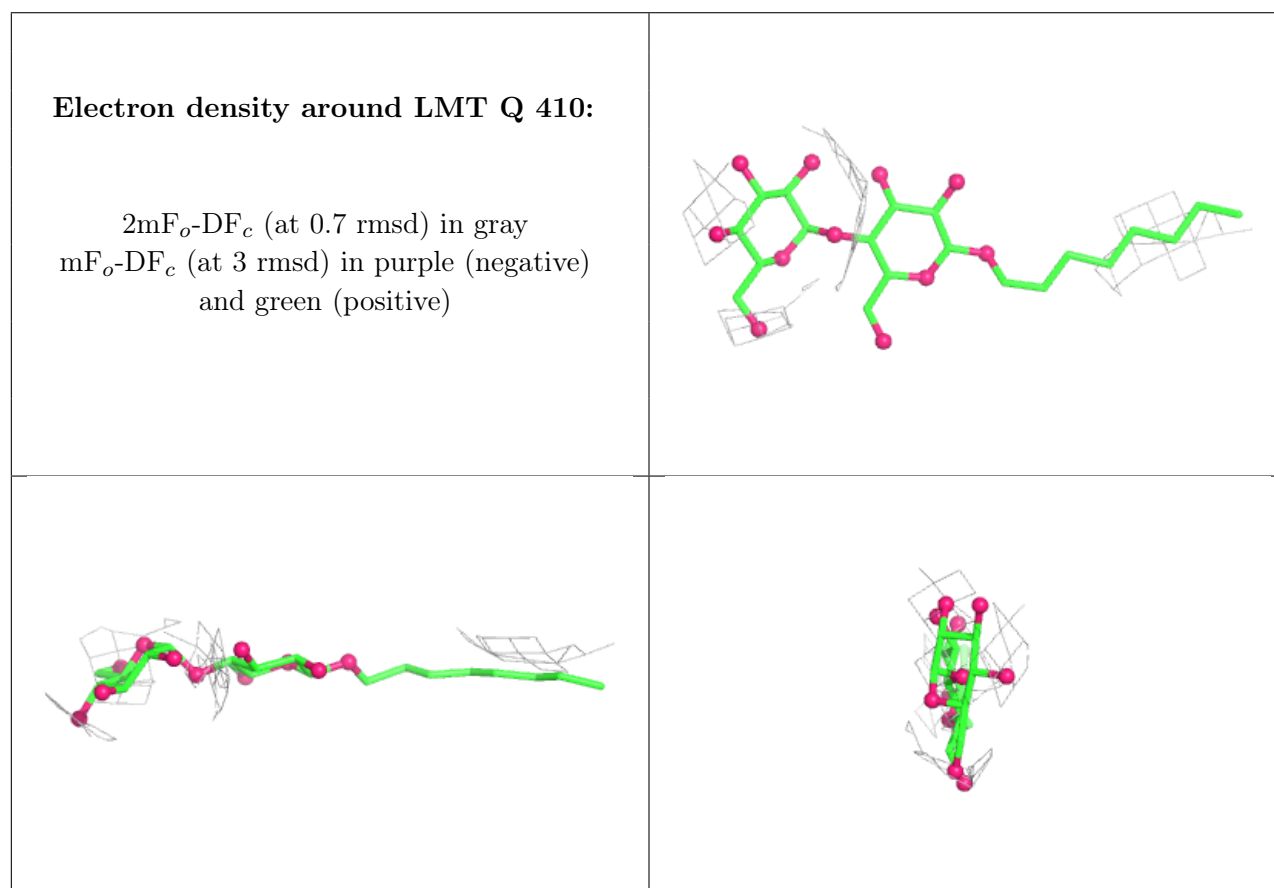
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	DGD	G	408	56/66	0.91	0.14	163,179,188,193	0
21	CLA	B	616	65/65	0.91	0.13	155,166,199,214	0
27	LMG	R	102	44/55	0.91	0.17	161,177,189,192	0
27	LMG	E	102	44/55	0.91	0.13	168,188,198,203	0
24	DGD	P	517	53/66	0.91	0.14	141,160,173,176	0
21	CLA	N	612	65/65	0.92	0.13	151,164,181,190	0
21	CLA	P	508	65/65	0.92	0.13	157,168,182,193	0
21	CLA	B	611	65/65	0.92	0.11	149,160,167,169	0
21	CLA	B	602	65/65	0.92	0.11	152,172,182,185	0
21	CLA	N	617	65/65	0.92	0.13	149,168,182,188	0
30	BCR	K	101	40/40	0.92	0.14	154,167,176,181	0
27	LMG	e	102	42/55	0.92	0.20	155,166,183,191	0
27	LMG	A	410	51/55	0.92	0.14	138,157,168,171	0
21	CLA	N	606	65/65	0.92	0.10	152,172,178,182	0
30	BCR	N	621	40/40	0.92	0.17	132,154,165,172	0
34	HEM	R	101	43/43	0.92	0.12	164,184,192,199	0
21	CLA	A	401	65/65	0.92	0.11	138,146,156,160	0
30	BCR	B	620	40/40	0.92	0.15	161,168,186,196	0
23	PL9	G	407	45/55	0.92	0.17	148,160,183,188	0
21	CLA	C	510	65/65	0.93	0.09	149,161,171,178	0
21	CLA	A	402	65/65	0.93	0.10	139,147,158,164	0
21	CLA	B	613	65/65	0.93	0.11	148,160,171,175	0
21	CLA	N	613	65/65	0.93	0.10	160,170,177,182	0
34	HEM	E	101	43/43	0.93	0.09	166,179,188,190	0
30	BCR	Z	101	40/40	0.93	0.10	163,178,192,197	0
21	CLA	Q	402	65/65	0.93	0.12	136,144,158,169	0
21	CLA	Q	404	65/65	0.93	0.13	152,162,187,194	0
21	CLA	C	503	65/65	0.93	0.10	155,171,181,183	0
21	CLA	C	504	65/65	0.93	0.11	153,172,198,204	0
21	CLA	C	502	65/65	0.94	0.09	142,157,179,185	0
28	OEC	G	413	5/9	0.94	0.14	91,102,115,124	0
21	CLA	N	615	65/65	0.94	0.09	152,158,168,173	0
21	CLA	C	508	65/65	0.94	0.09	154,170,194,203	0
27	LMG	M	101	42/55	0.94	0.15	166,174,184,188	0
27	LMG	D	406	46/55	0.94	0.13	140,153,176,181	0
21	CLA	P	506	65/65	0.94	0.14	159,176,194,202	0
27	LMG	N	622	49/55	0.94	0.16	145,154,172,174	0
32	BCT	D	410	4/4	0.94	0.07	166,167,167,169	0
21	CLA	B	606	65/65	0.95	0.10	156,173,194,204	0
25	LHG	G	409	39/49	0.95	0.11	156,168,188,191	0
29	FE2	A	413	1/1	0.97	0.07	166,166,166,166	0
28	OEC	A	412	5/9	0.99	0.05	122,122,126,129	0

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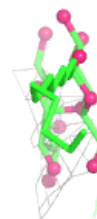
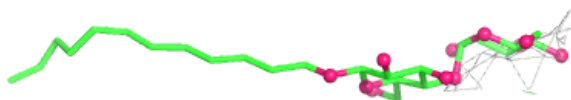
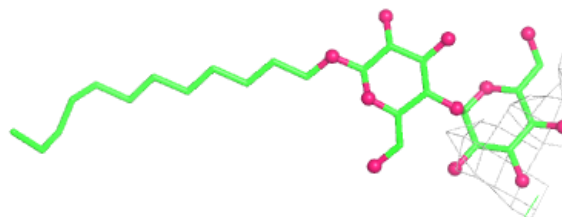
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	FE2	G	414	1/1	0.99	0.07	149,149,149,149	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



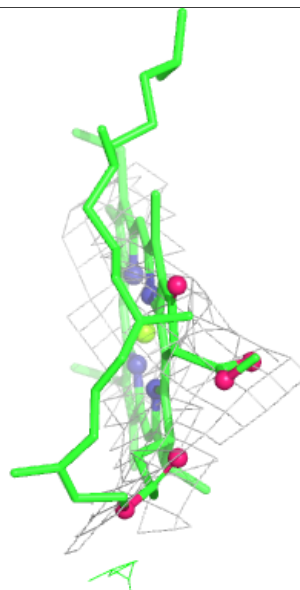
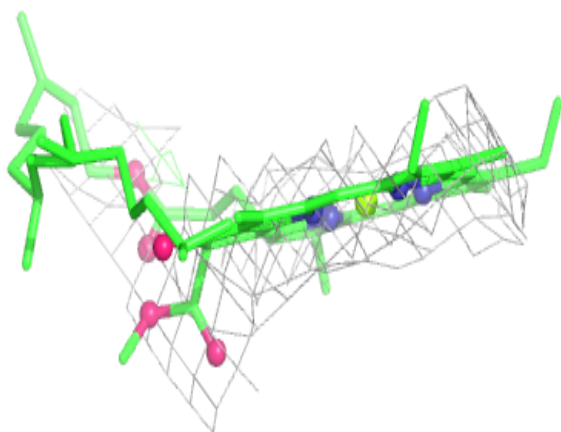
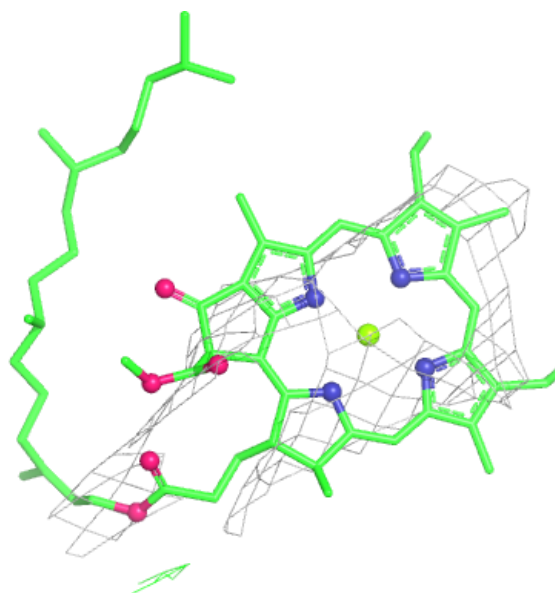
Electron density around LMT I 103:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



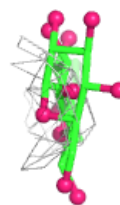
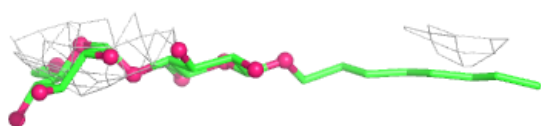
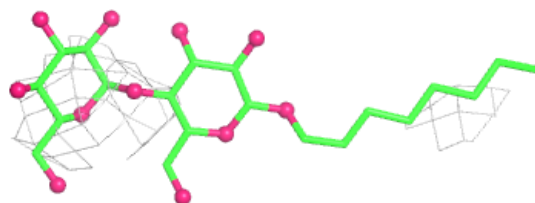
Electron density around CLA N 605:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

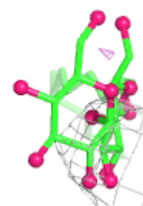
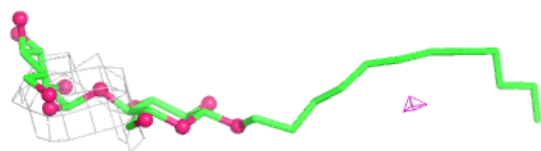
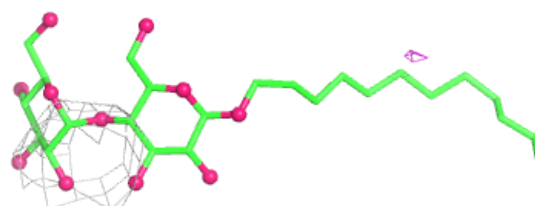


Electron density around LMT D 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

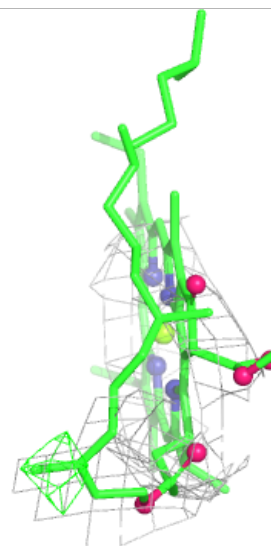
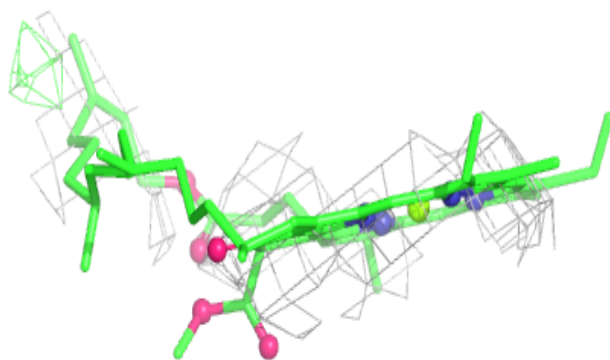
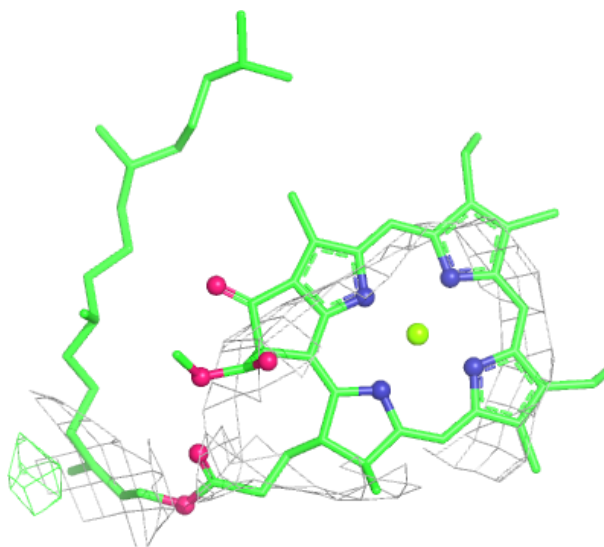
**Electron density around LMT N 624:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



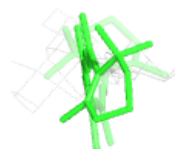
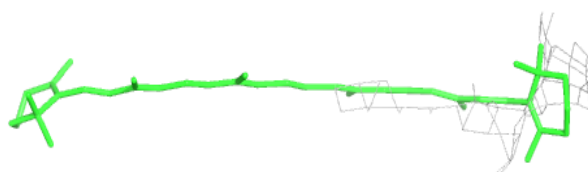
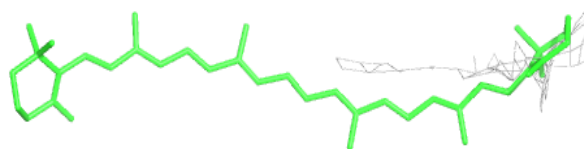
Electron density around CLA B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

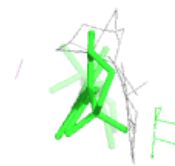
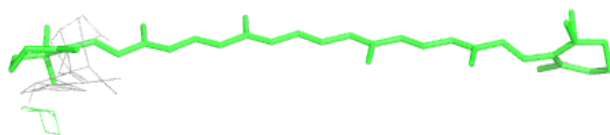
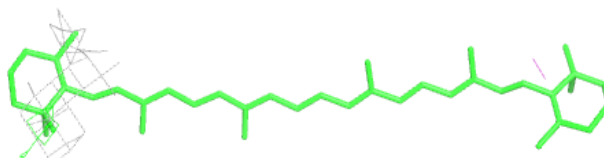


Electron density around BCR H 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

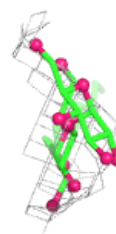
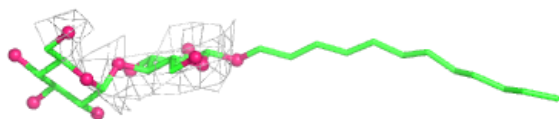
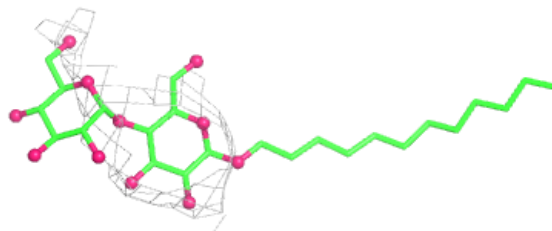
**Electron density around BCR b 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

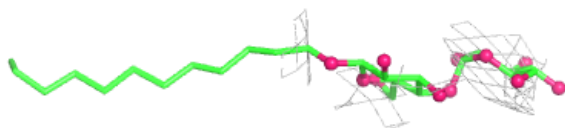
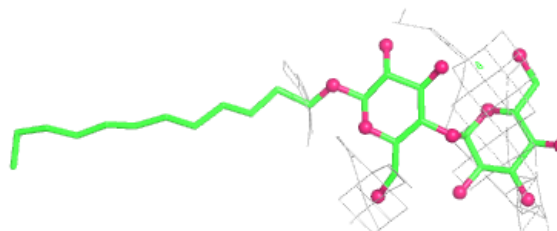


Electron density around LMT N 625:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

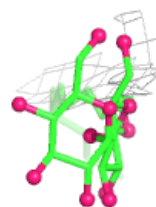
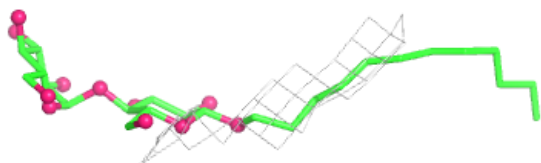
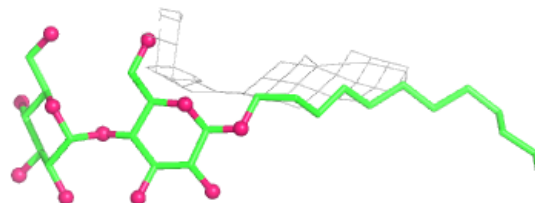
**Electron density around LMT N 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

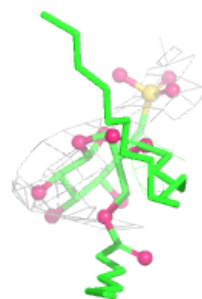
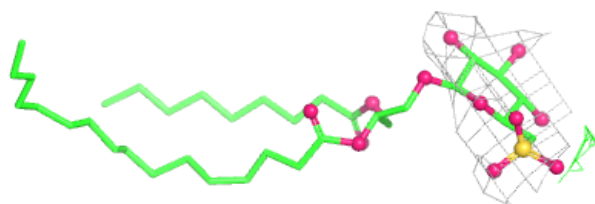
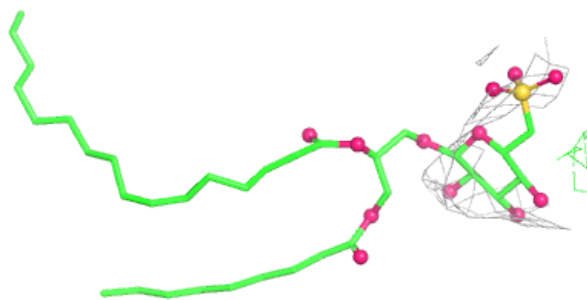


Electron density around LMT B 625:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

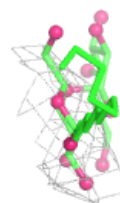
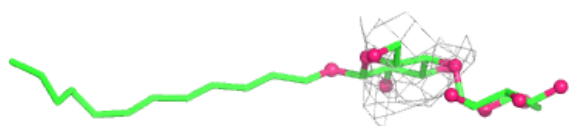
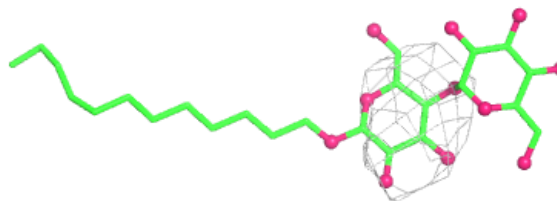
**Electron density around SQD B 627:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

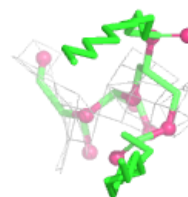
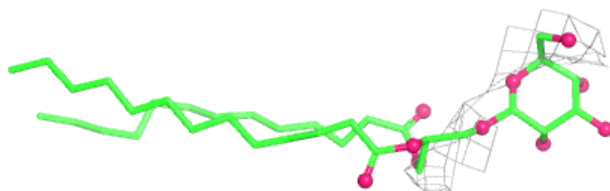
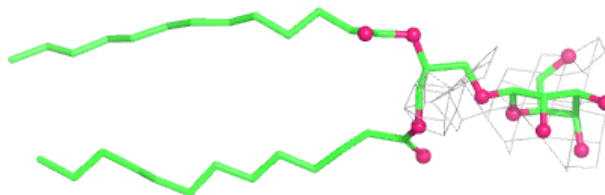


Electron density around LMT a 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

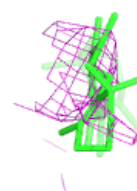
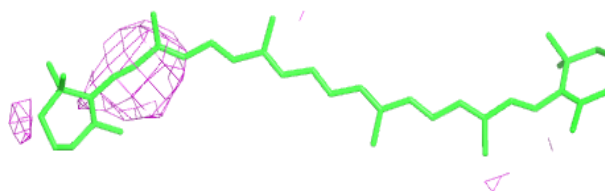
**Electron density around LMG C 520:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

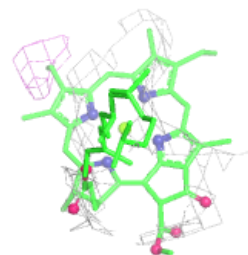
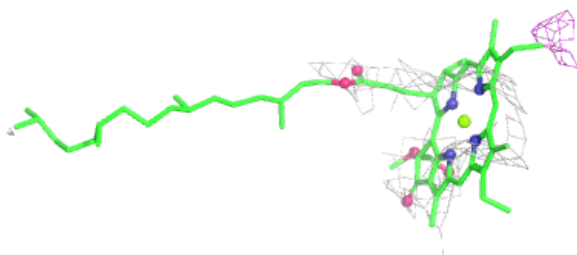
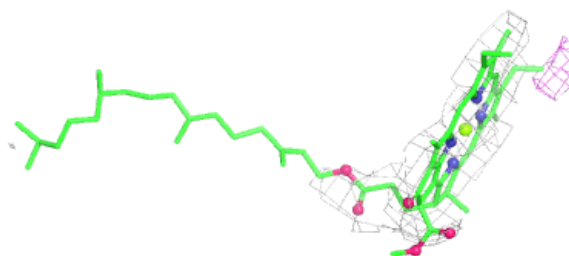


Electron density around BCR c 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

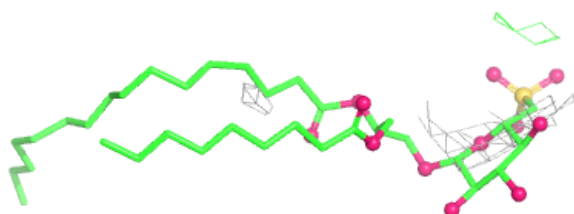
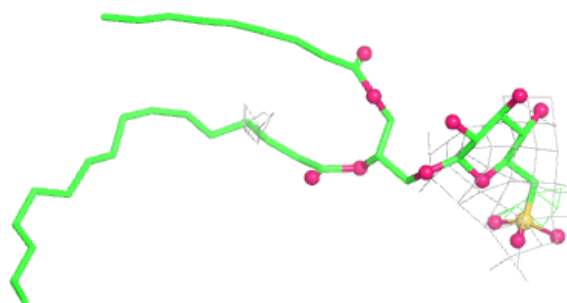
**Electron density around CLA B 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



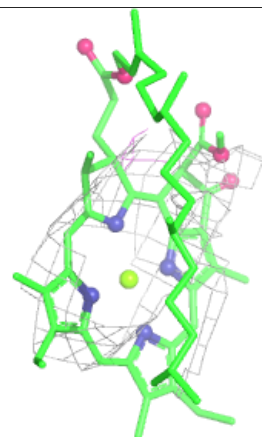
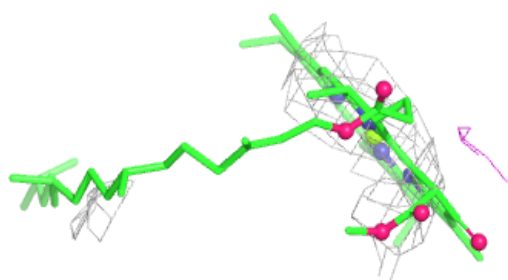
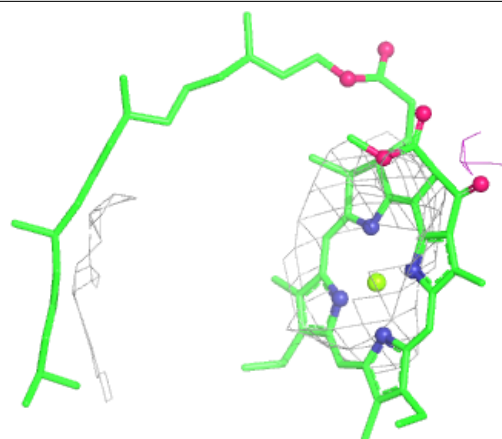
Electron density around SQD N 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

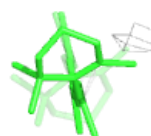


Electron density around CLA C 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

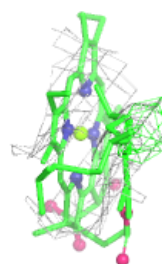
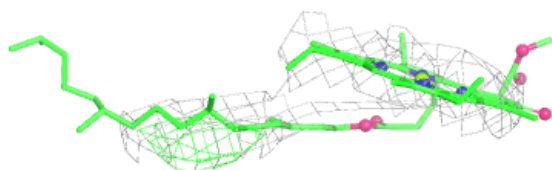
**Electron density around BCR a 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



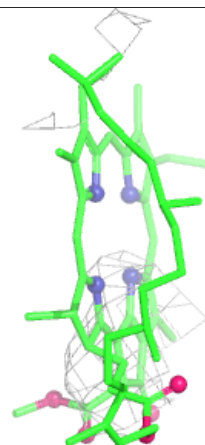
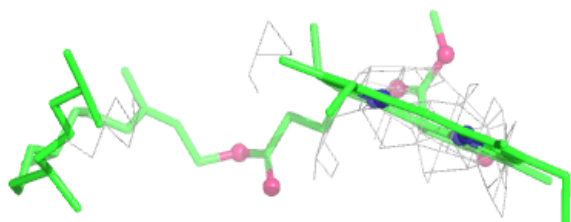
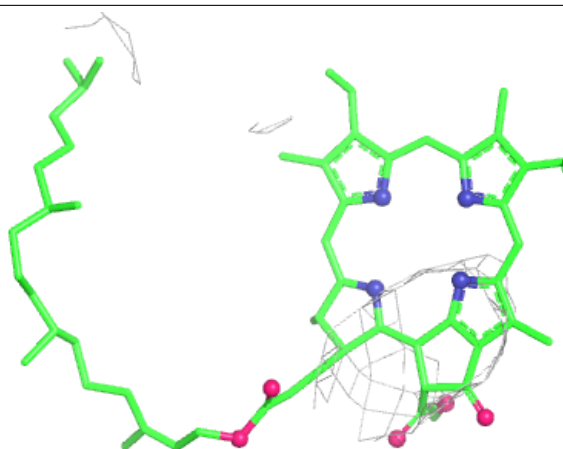
Electron density around CLA N 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

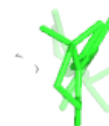
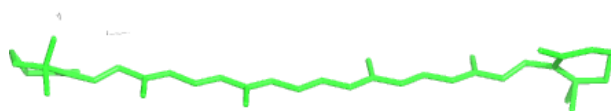
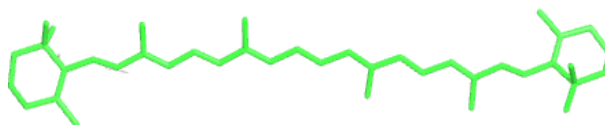


Electron density around PHO A 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

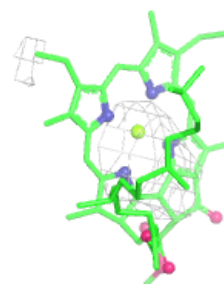
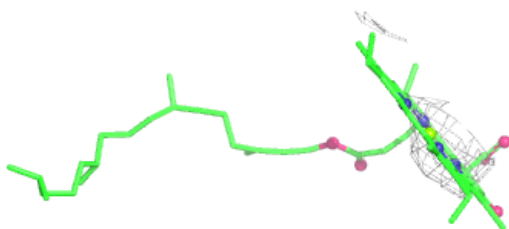
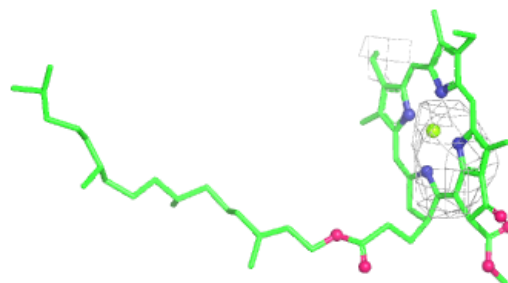
**Electron density around BCR J 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

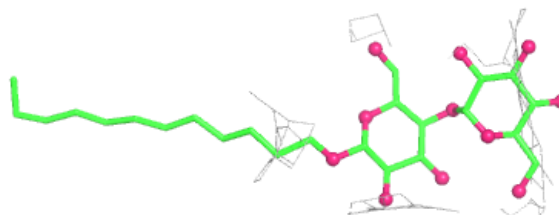


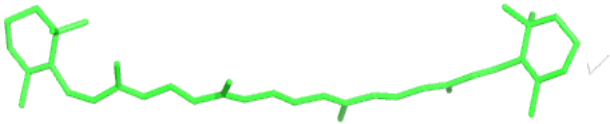
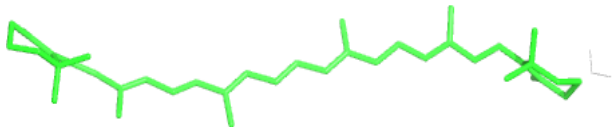
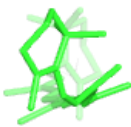
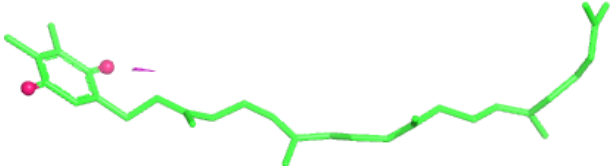
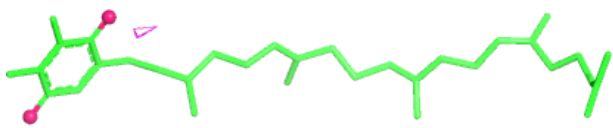
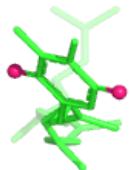
Electron density around CLA G 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LMT B 630:**

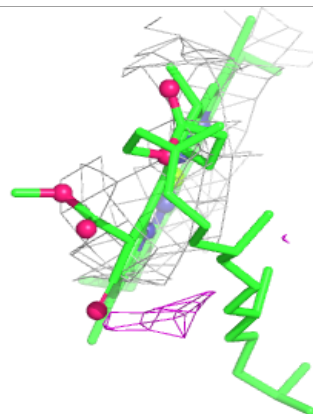
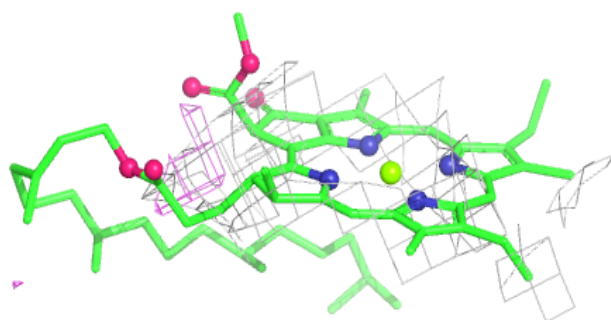
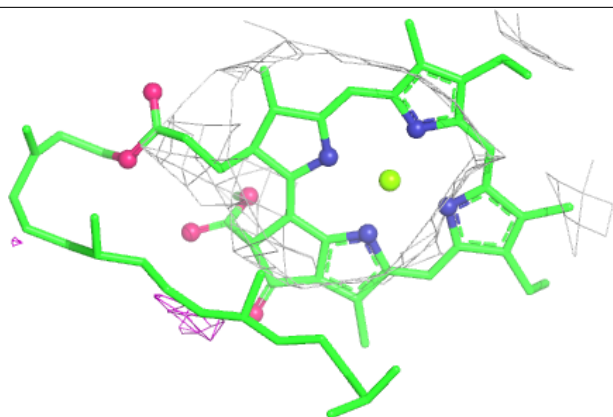
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



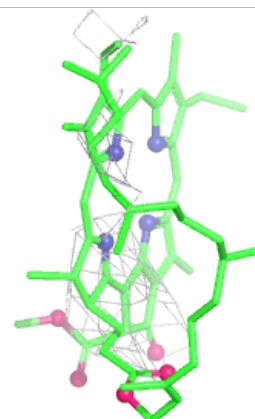
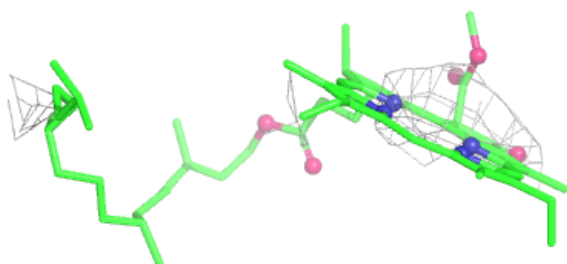
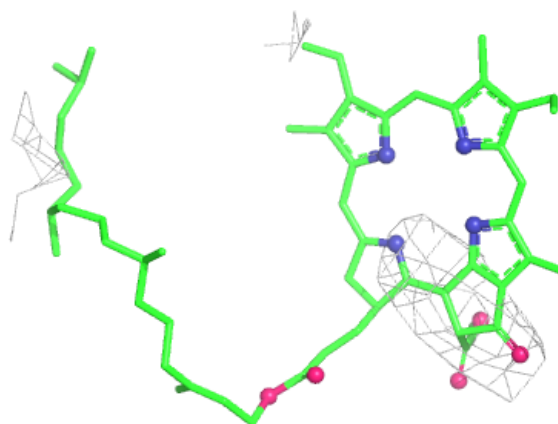
Electron density around BCR P 514: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	
Electron density around PL9 b 101: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around CLA C 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

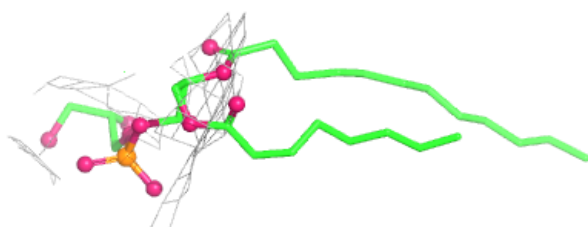
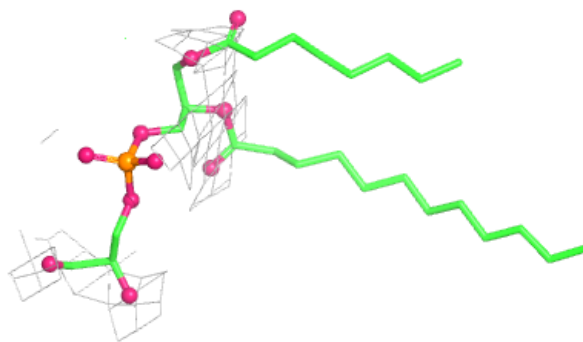
**Electron density around PHO D 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

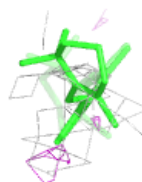
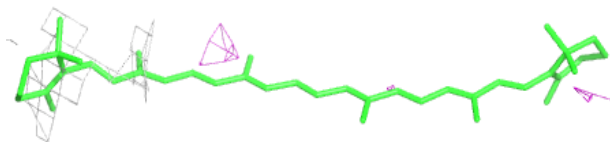
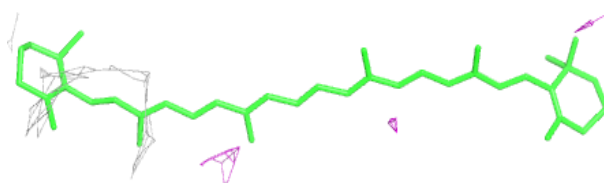


Electron density around LHG G 412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

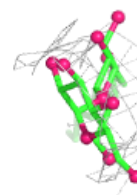
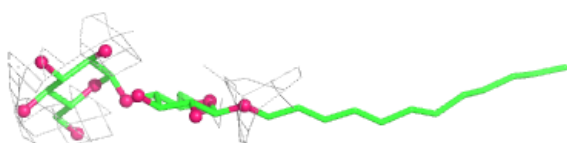
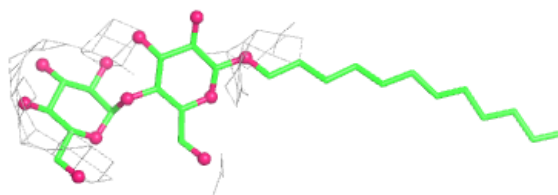
**Electron density around BCR T 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

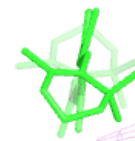
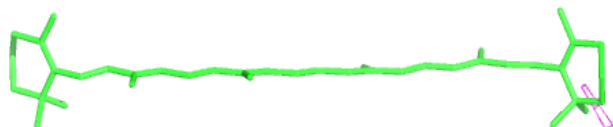
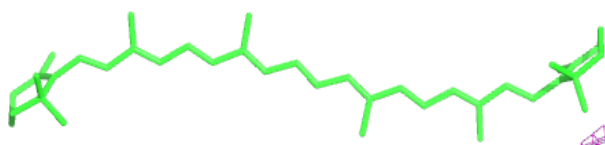


Electron density around LMT B 626:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

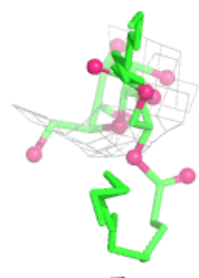
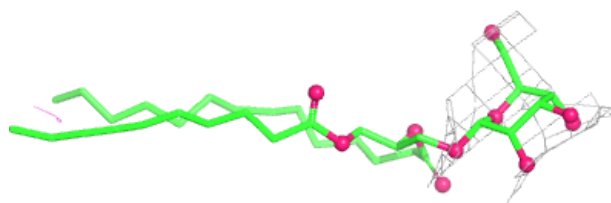
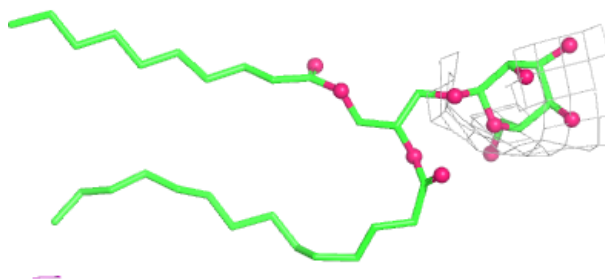
**Electron density around BCR I 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



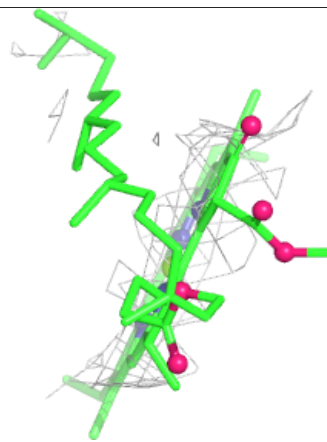
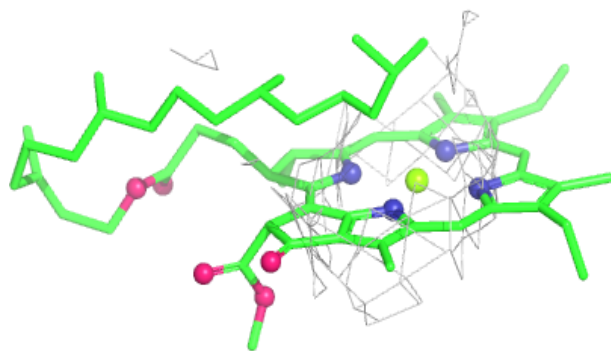
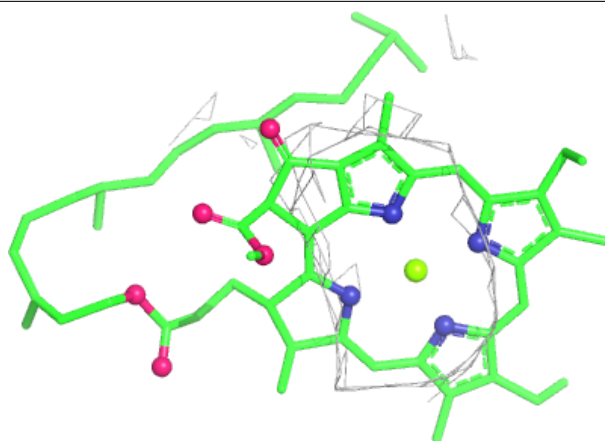
Electron density around LMG I 102:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

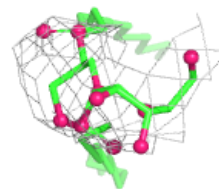
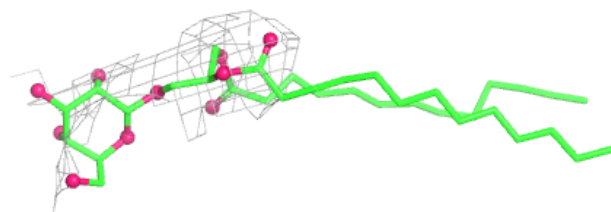
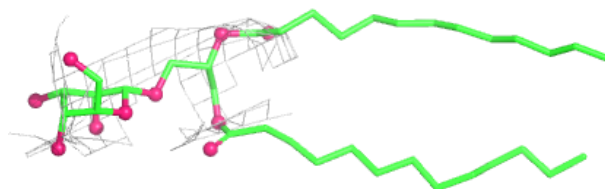


Electron density around CLA P 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

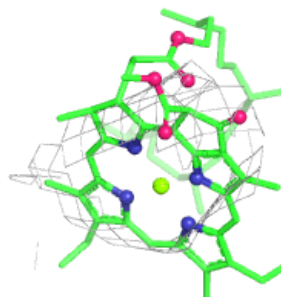
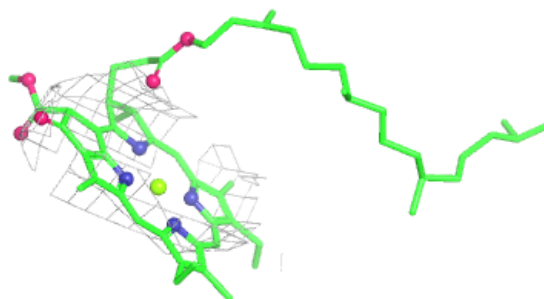
**Electron density around LMG P 521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

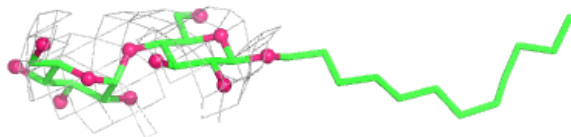
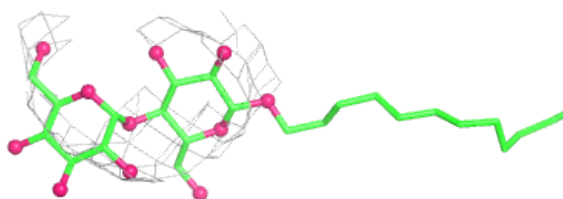


Electron density around CLA C 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

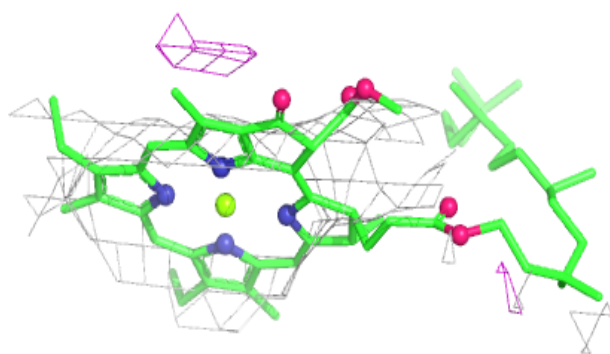
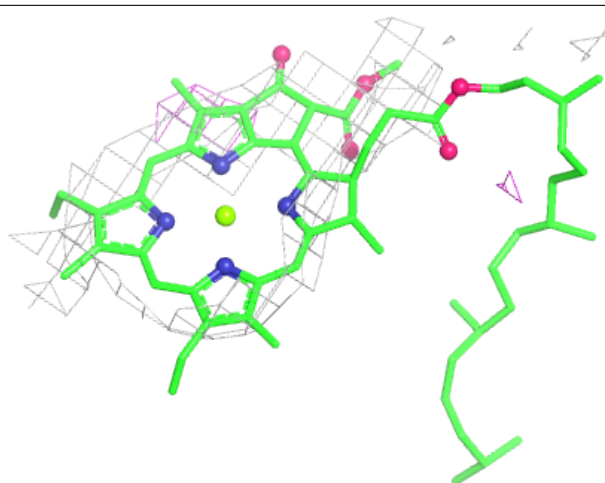
**Electron density around LMT N 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



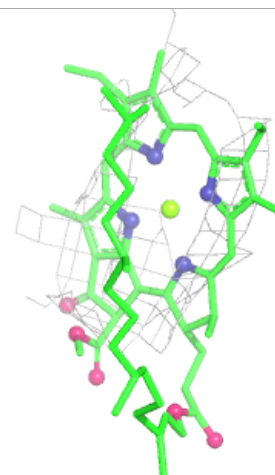
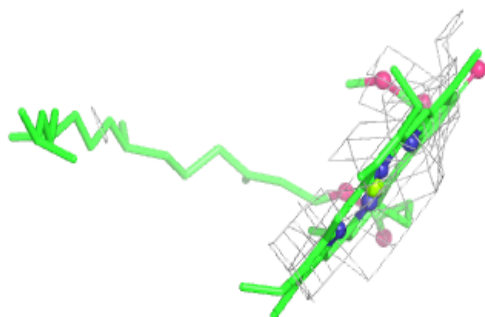
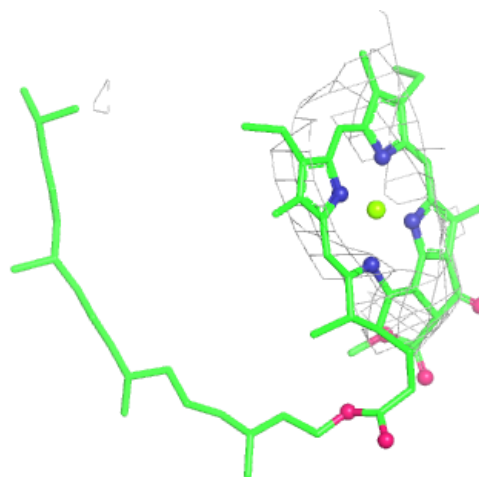
Electron density around CLA N 620:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



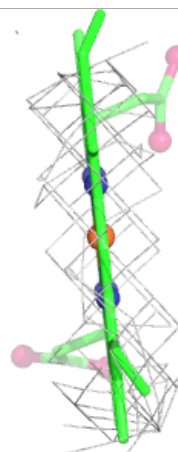
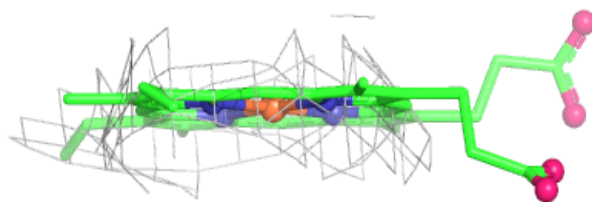
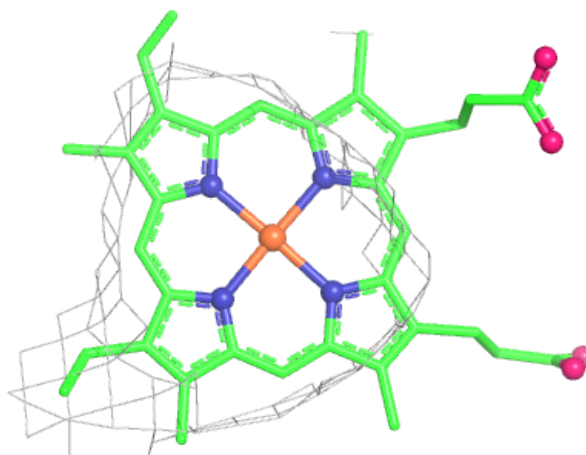
Electron density around CLA P 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



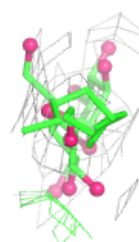
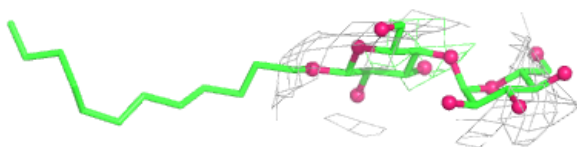
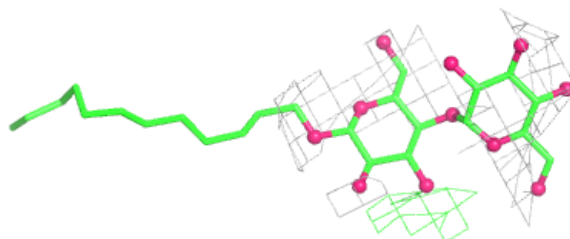
Electron density around HEM i 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



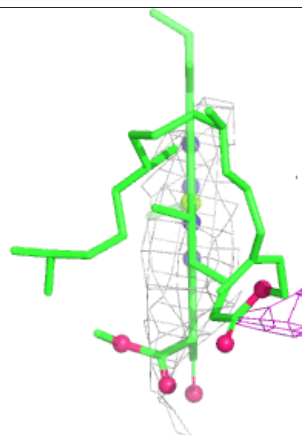
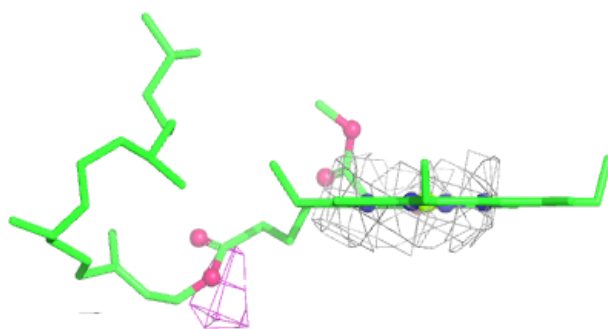
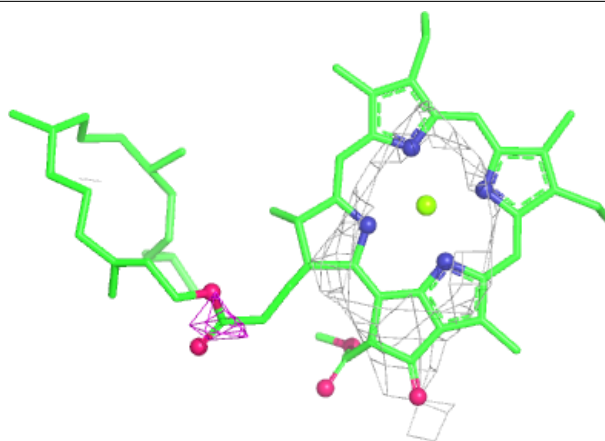
Electron density around LMT B 629:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



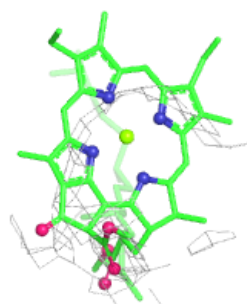
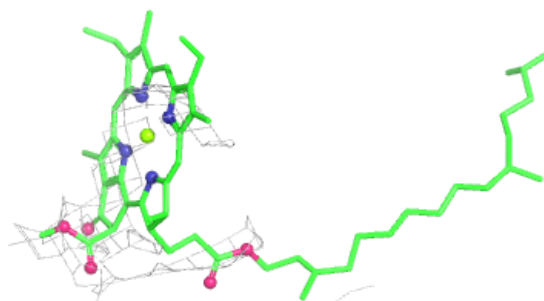
Electron density around CLA C 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

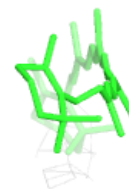
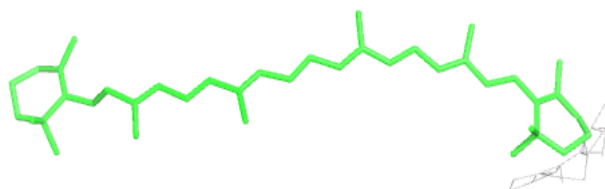


Electron density around CLA B 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

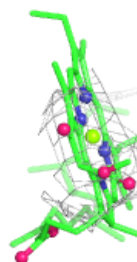
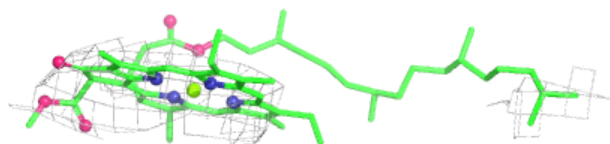
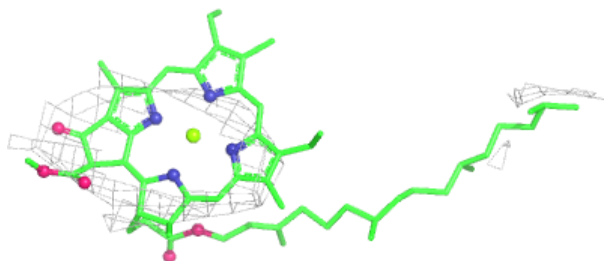
**Electron density around BCR B 618:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

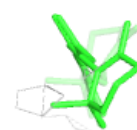
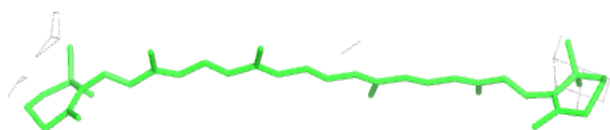
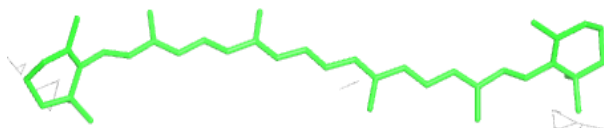


Electron density around CLA P 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

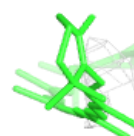
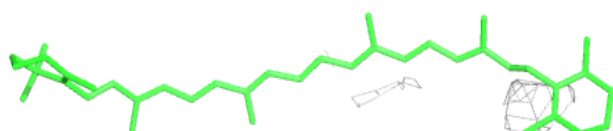
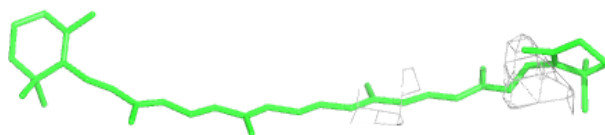
**Electron density around BCR P 516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

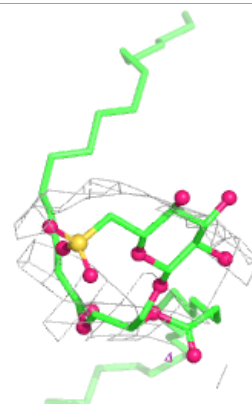
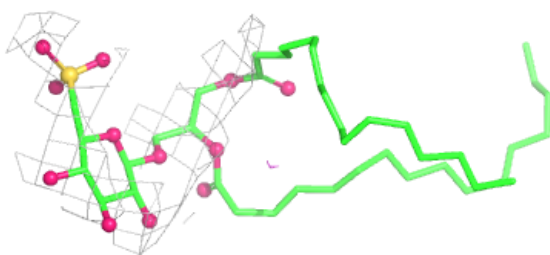
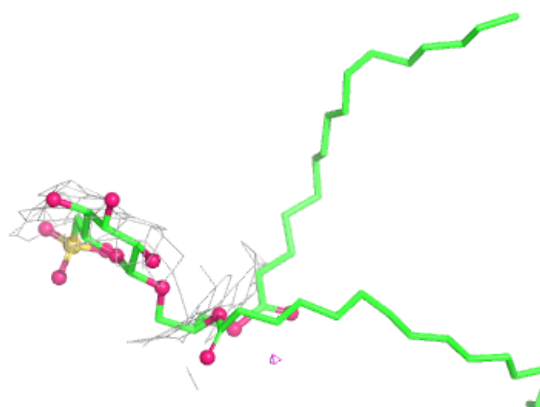


Electron density around BCR S 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

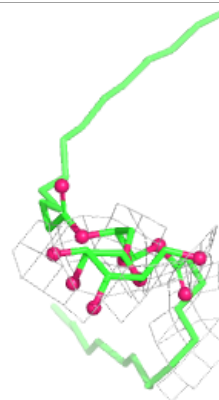
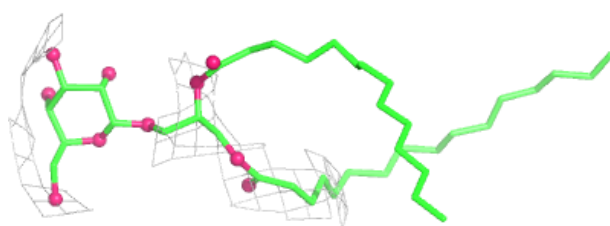
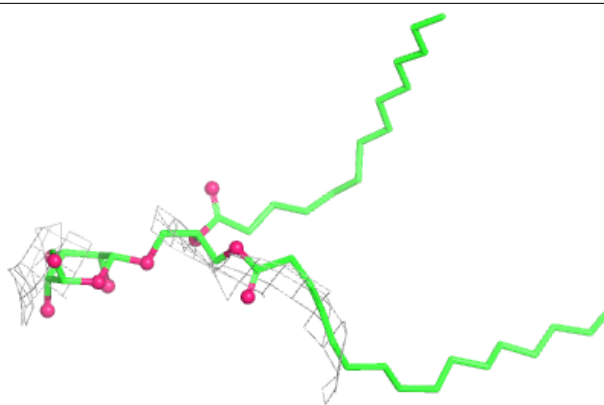
**Electron density around SQD A 414:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

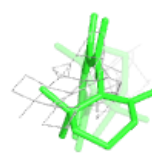
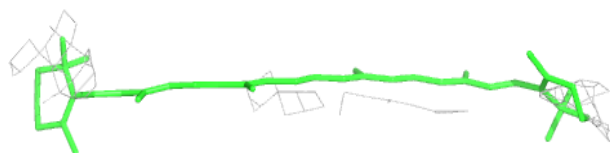
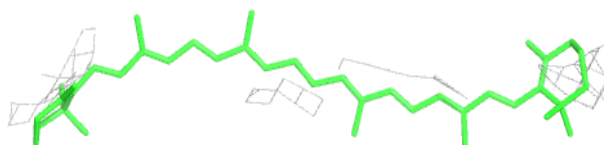


Electron density around LMG B 623:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

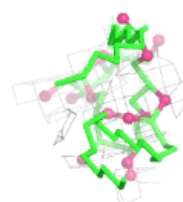
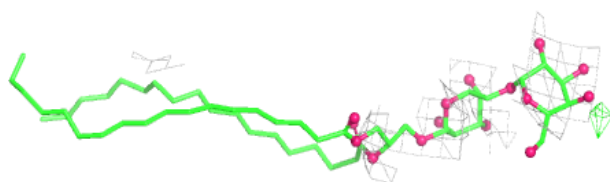
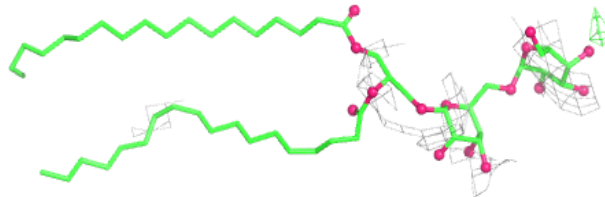
**Electron density around BCR W 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

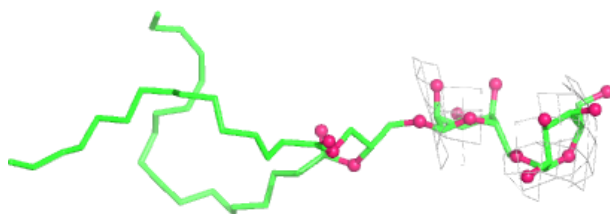
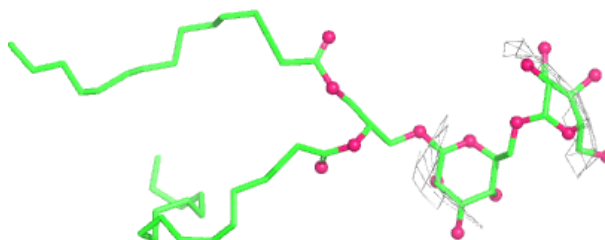


Electron density around DGD C 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

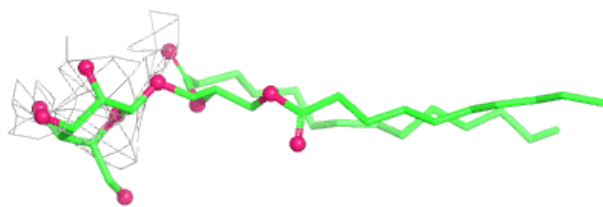
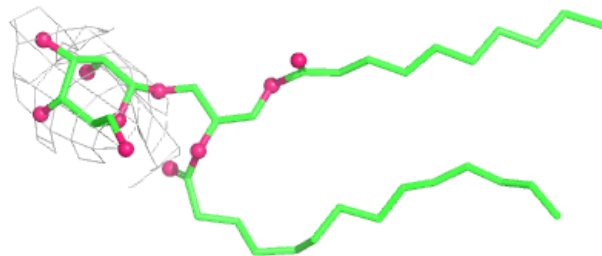
**Electron density around DGD D 408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

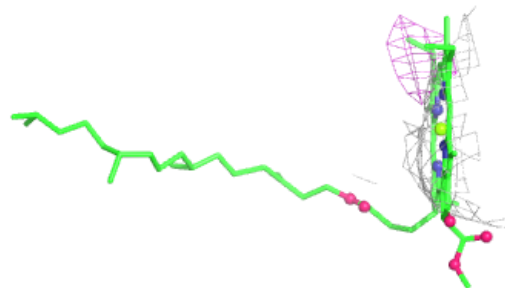


Electron density around LMG a 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

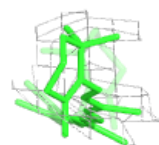
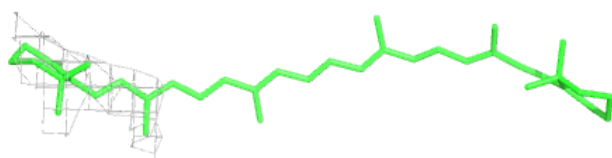
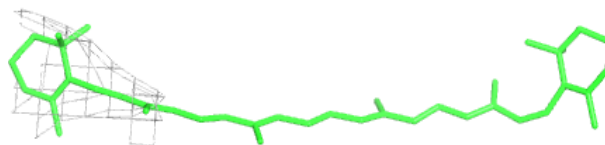
**Electron density around CLA N 610:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

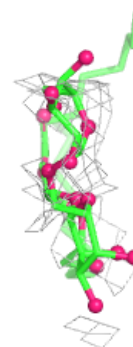
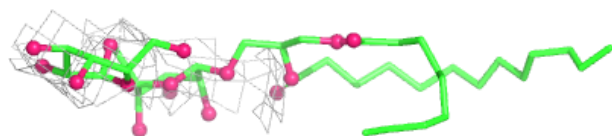
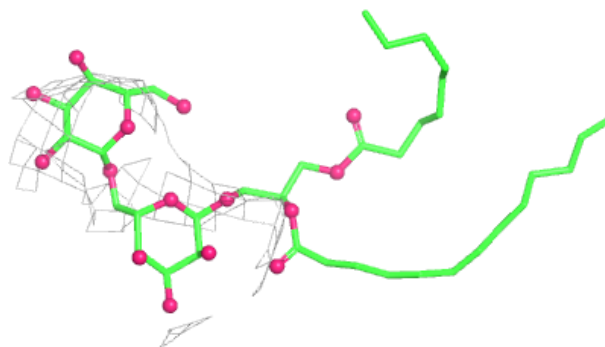


Electron density around BCR C 514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

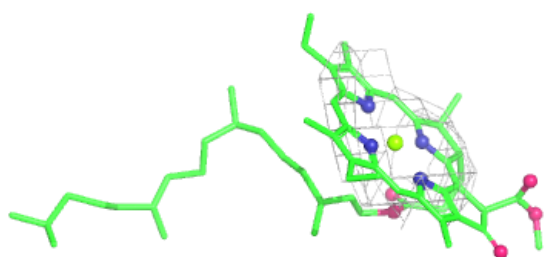
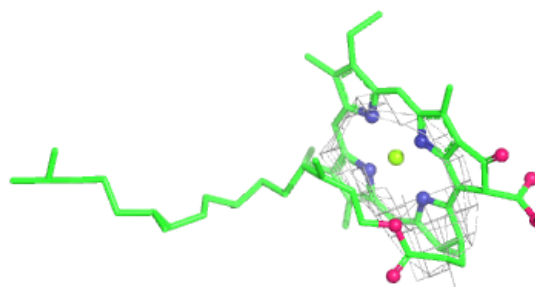
**Electron density around DGD B 628:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

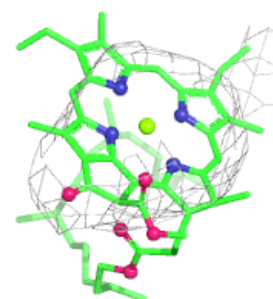
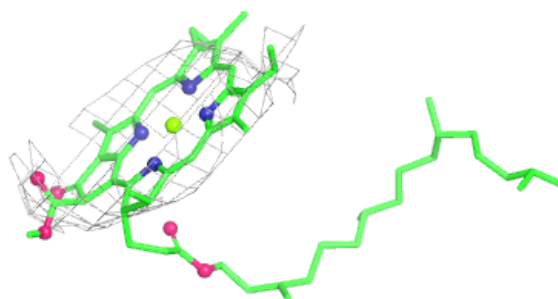


Electron density around CLA C 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

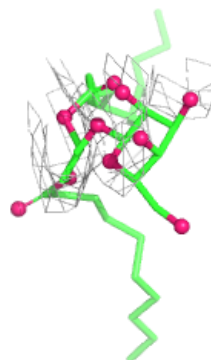
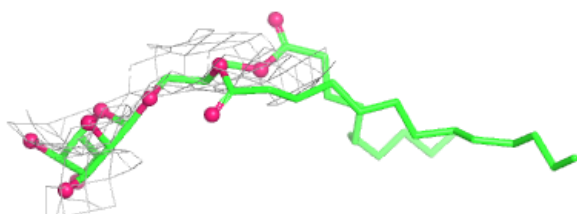
**Electron density around CLA P 513:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

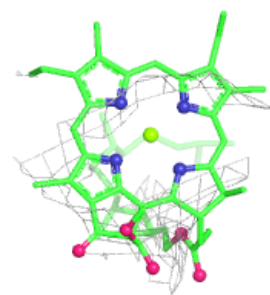
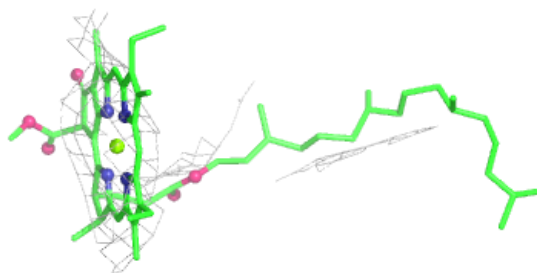
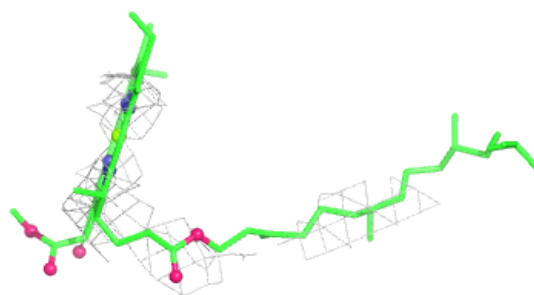


Electron density around LMG D 412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

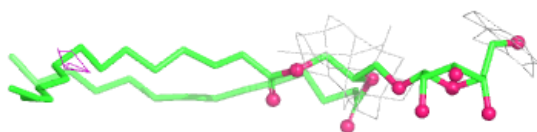
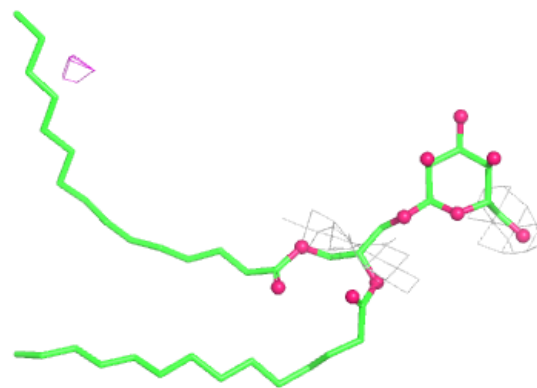
**Electron density around CLA N 609:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

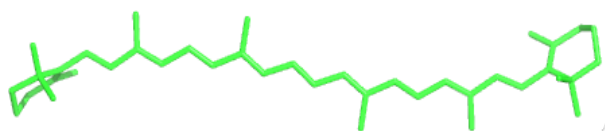


Electron density around LMG P 520:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BCR T 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

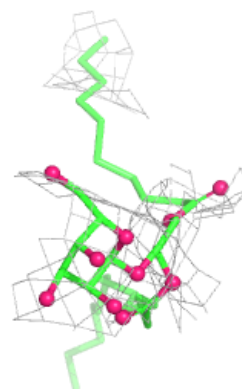
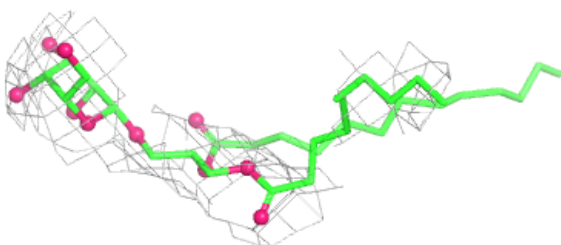
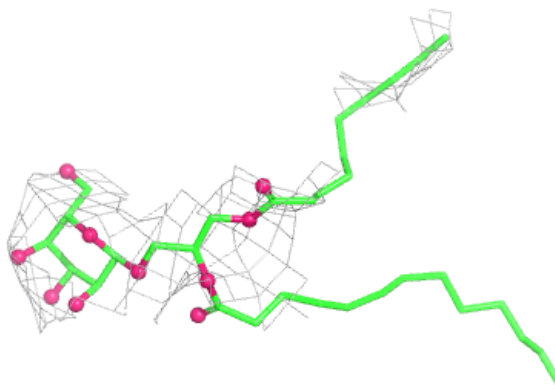


Electron density around DGD Q 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

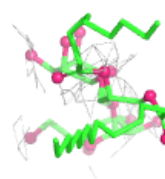
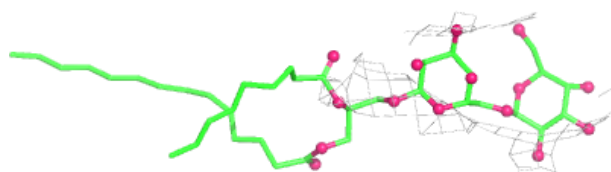
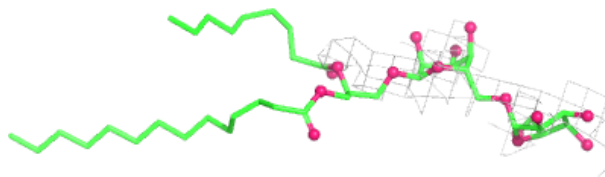
**Electron density around LMG Q 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

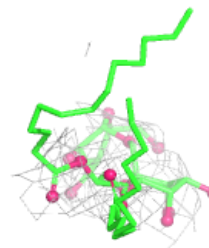
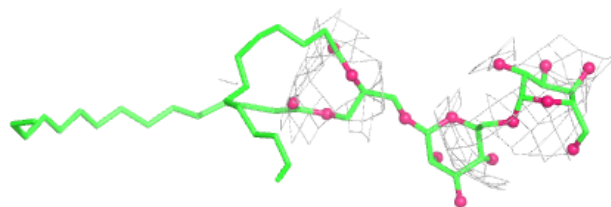
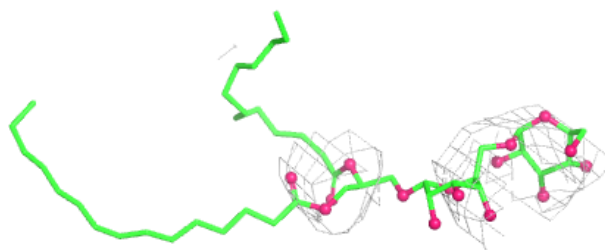


Electron density around DGD C 516:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

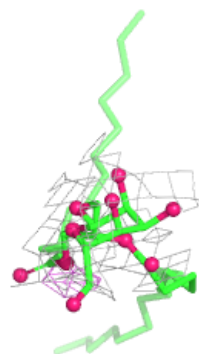
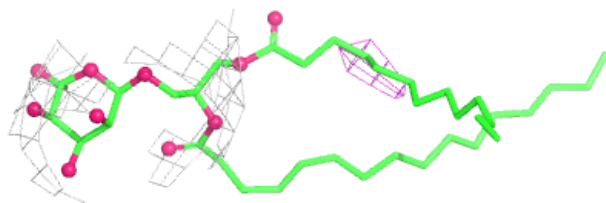
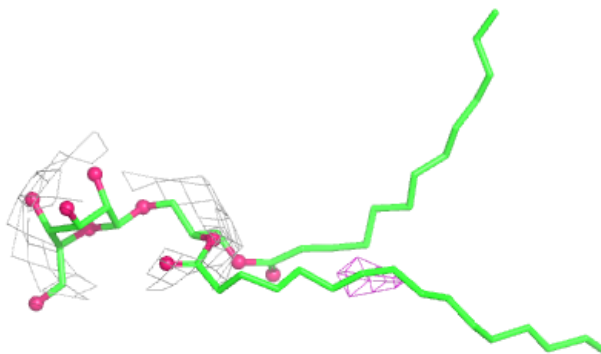
**Electron density around DGD B 621:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

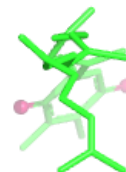
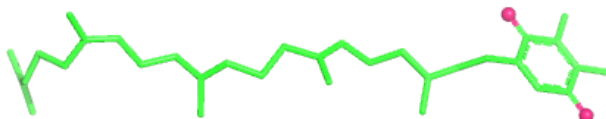
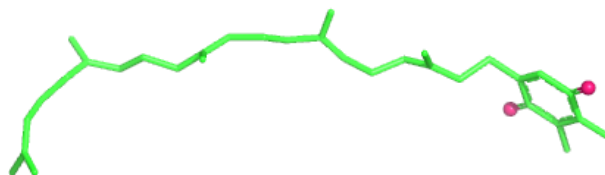


Electron density around LMG D 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

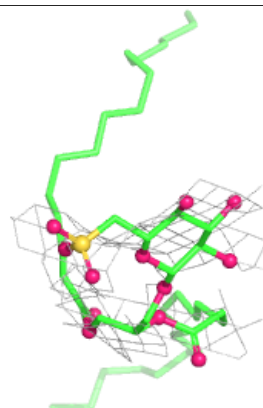
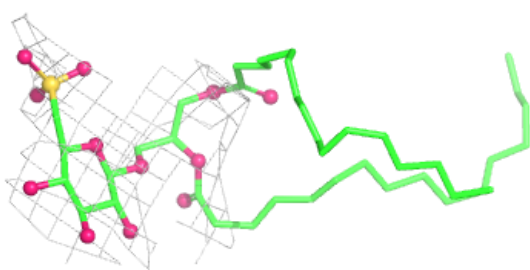
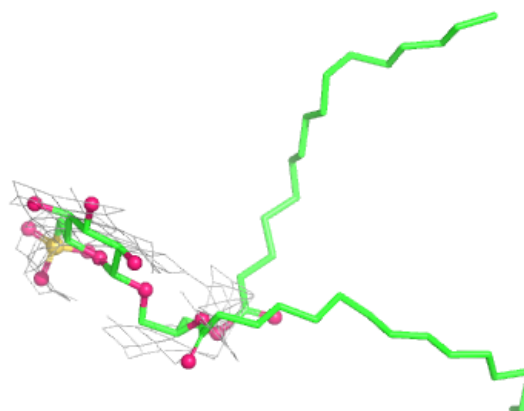
**Electron density around PL9 J 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

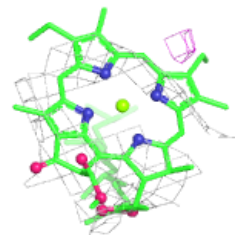
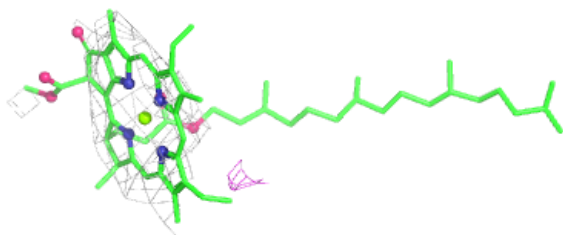
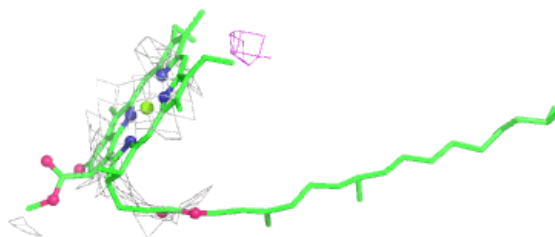


Electron density around SQD G 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

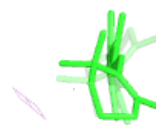
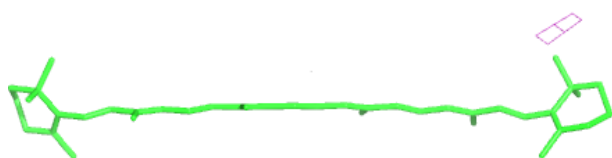
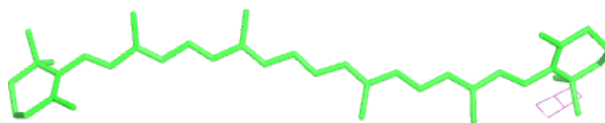
**Electron density around CLA B 607:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

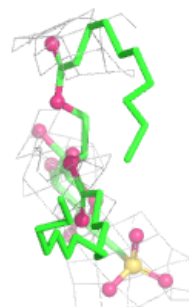
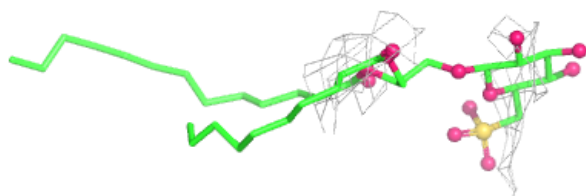
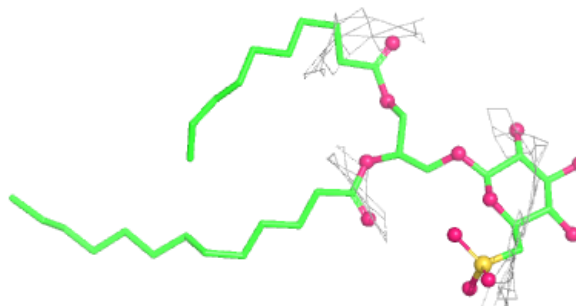


Electron density around BCR B 619:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

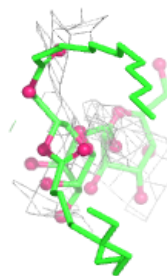
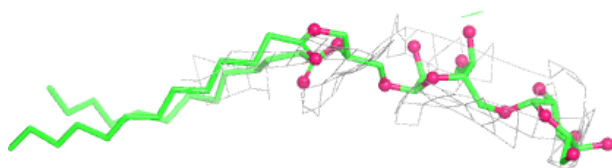
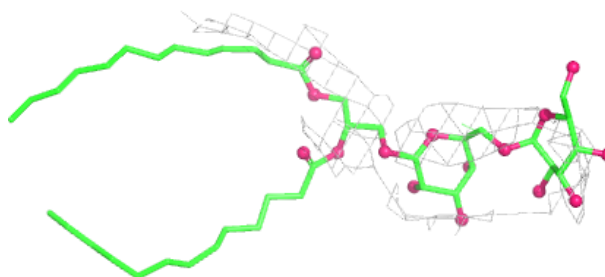
**Electron density around SQD F 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

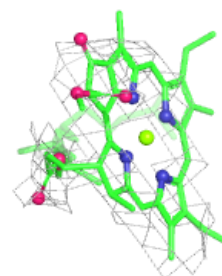
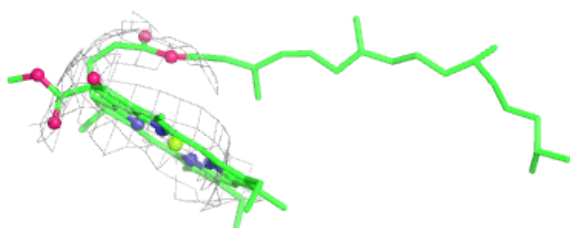
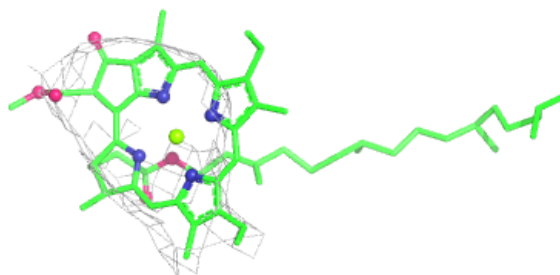


Electron density around DGD A 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

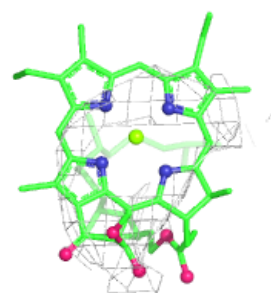
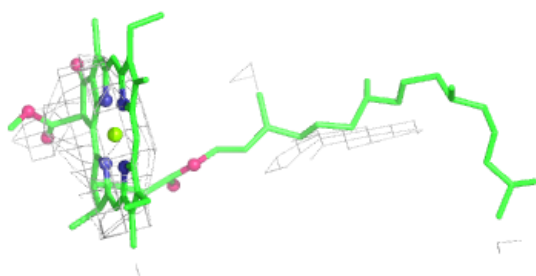
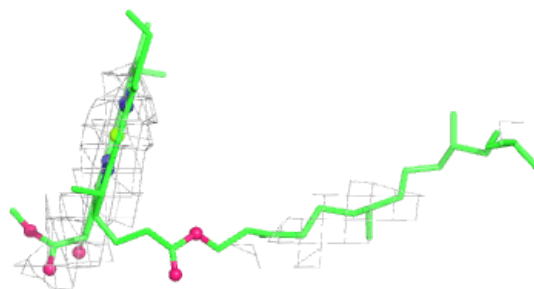
**Electron density around CLA B 608:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

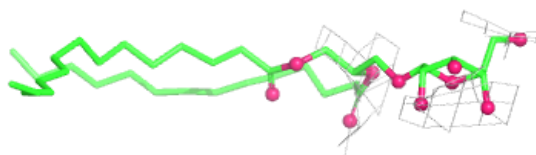
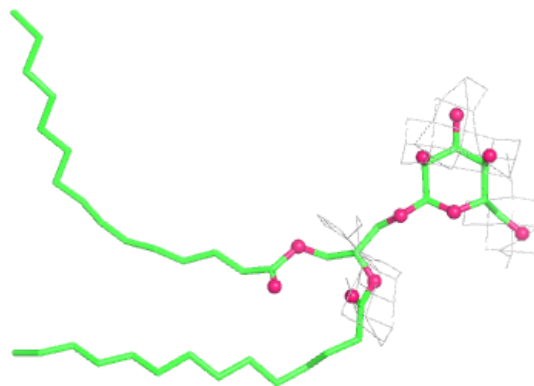


Electron density around CLA B 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

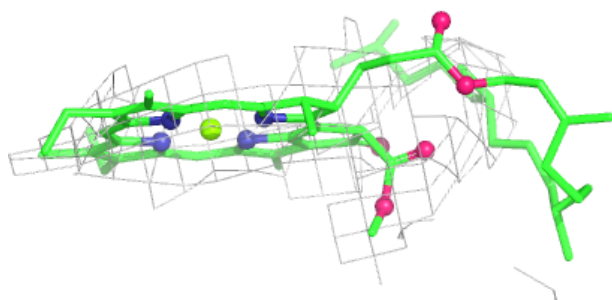
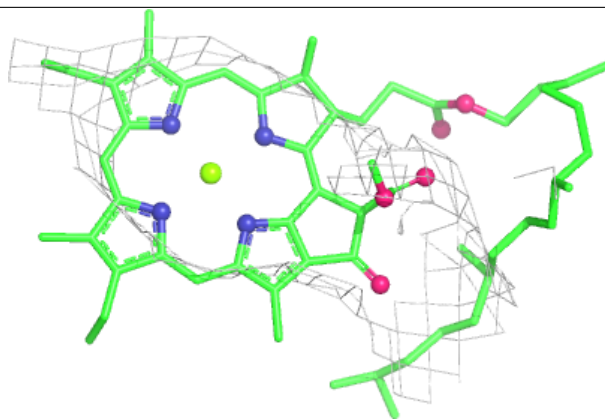
**Electron density around LMG C 519:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

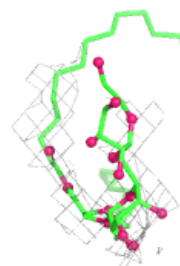
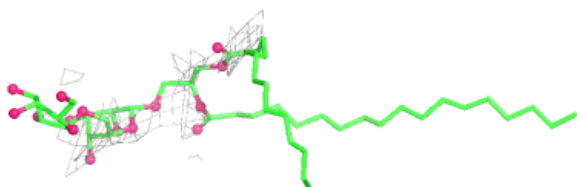


Electron density around CLA B 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

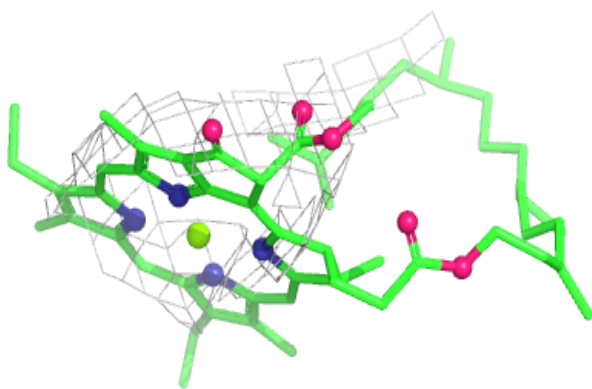
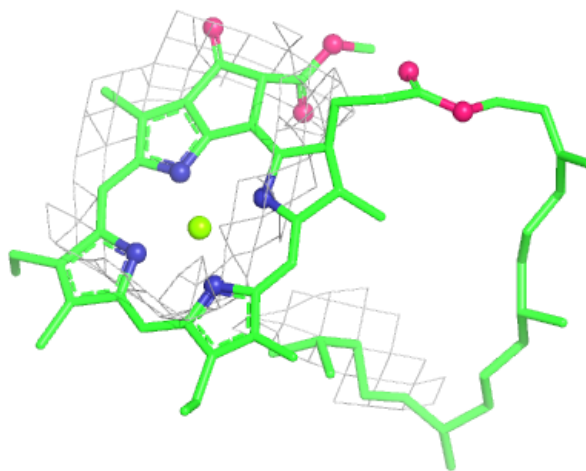
**Electron density around DGD C 517:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



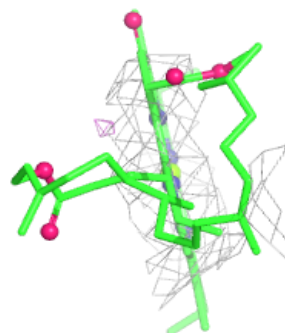
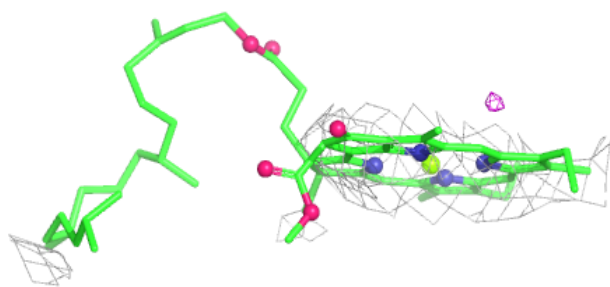
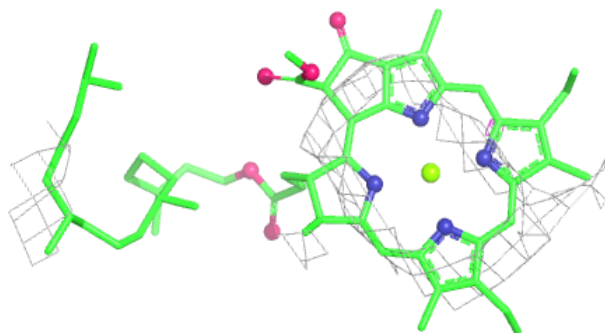
Electron density around CLA B 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

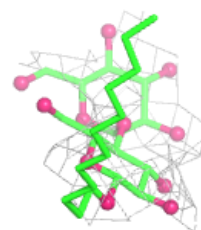
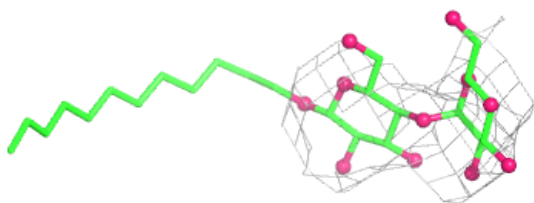
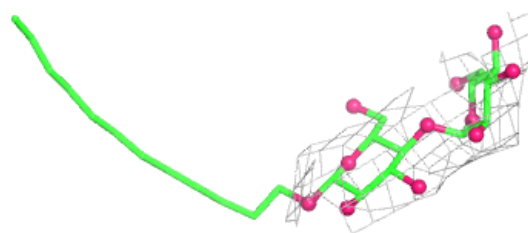


Electron density around CLA N 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

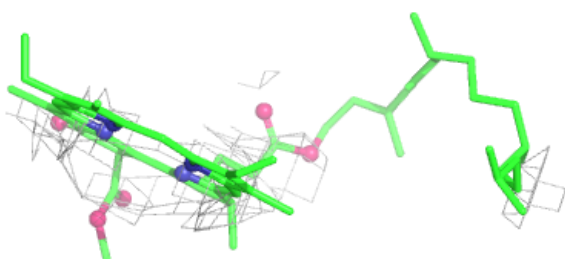
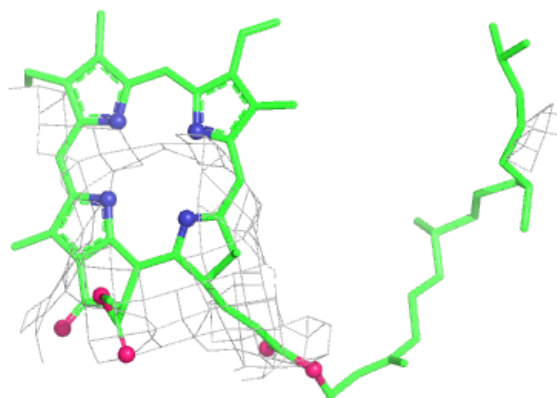
**Electron density around LMT e 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

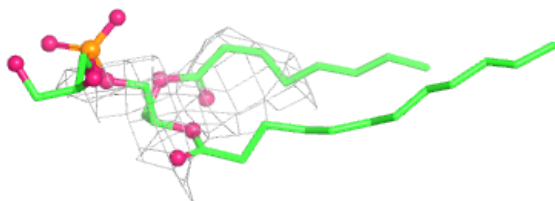


Electron density around PHO Q 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

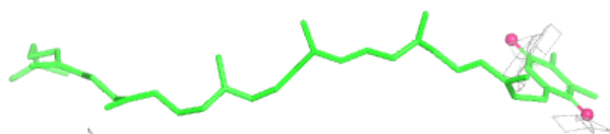
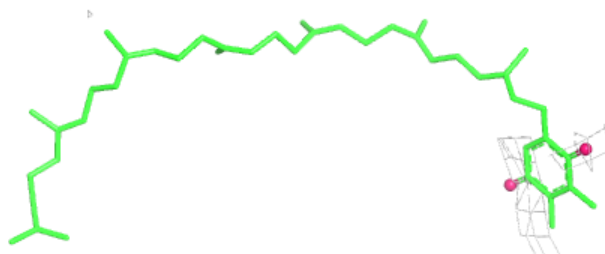
**Electron density around LHG A 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

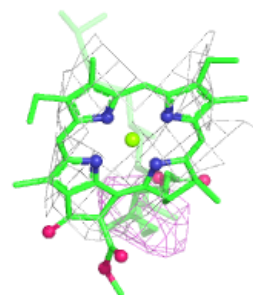
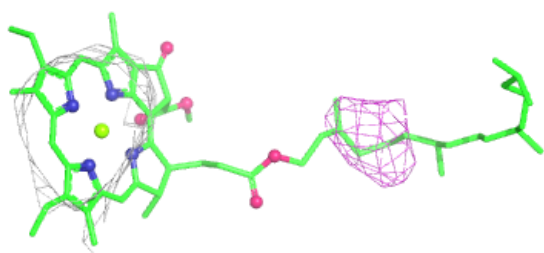
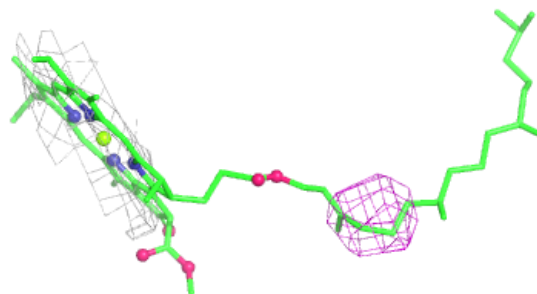


Electron density around PL9 A 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

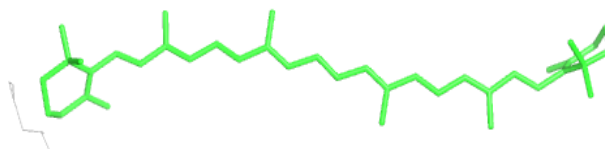
**Electron density around CLA D 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

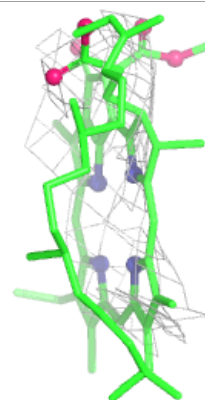
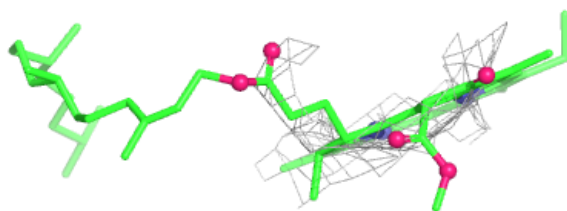
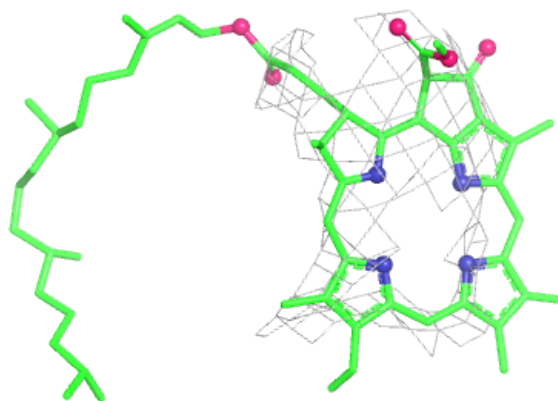


Electron density around BCR B 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

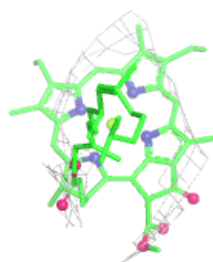
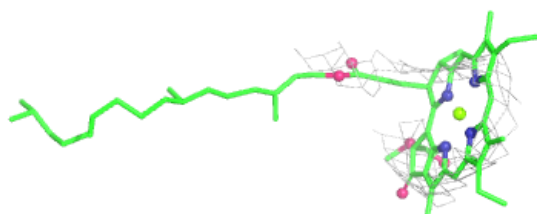
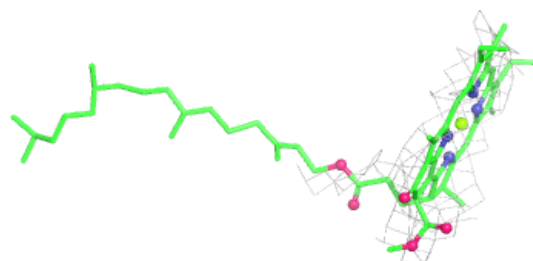
**Electron density around PHO G 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

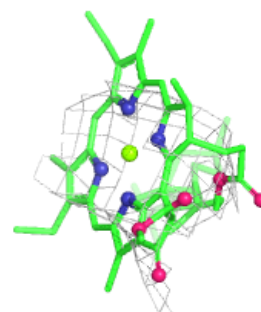
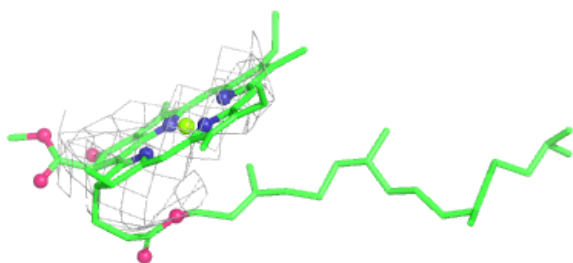
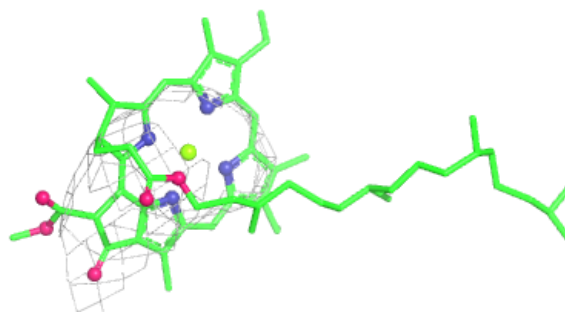


Electron density around CLA N 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

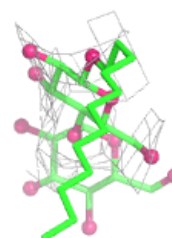
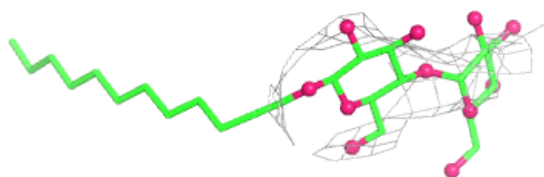
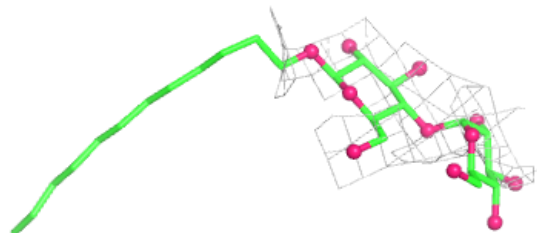
**Electron density around CLA N 618:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

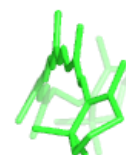
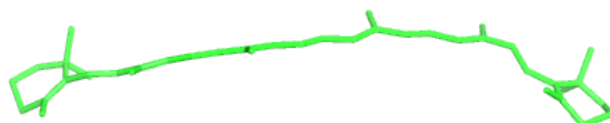
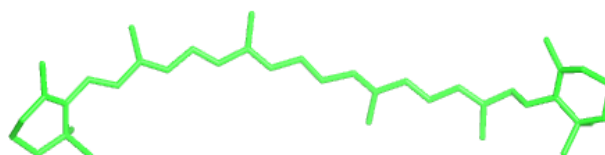


Electron density around LMT M 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

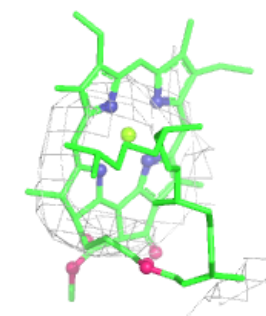
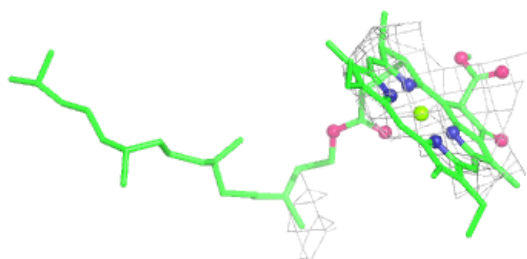
**Electron density around BCR T 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

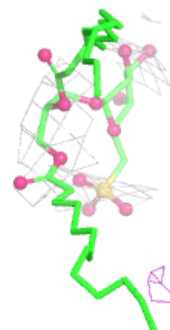
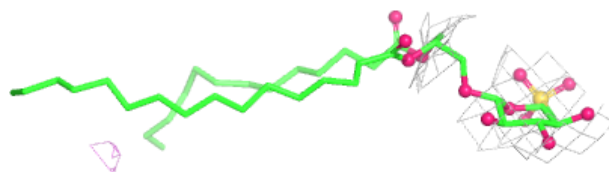
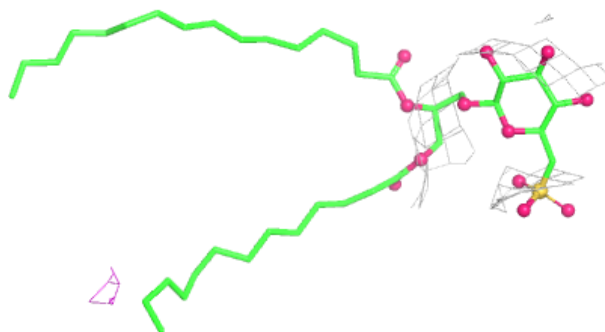


Electron density around CLA P 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

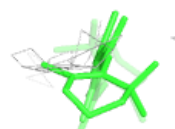
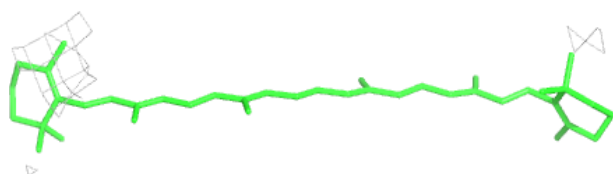
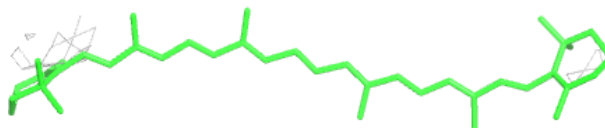
**Electron density around SQD G 410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

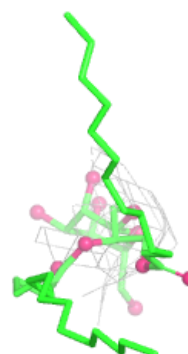
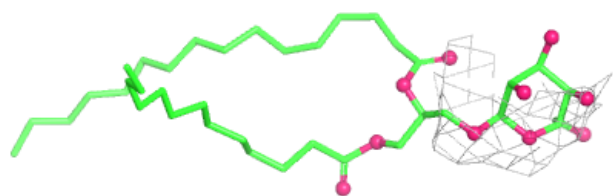
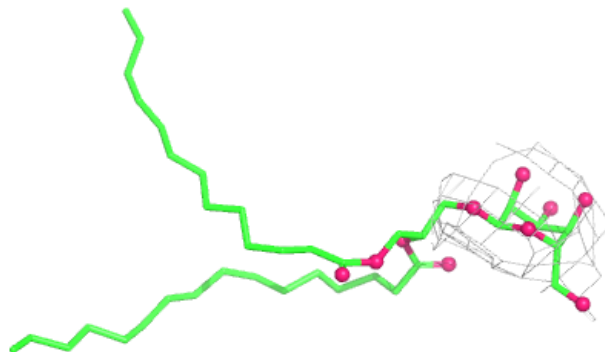


Electron density around BCR P 515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

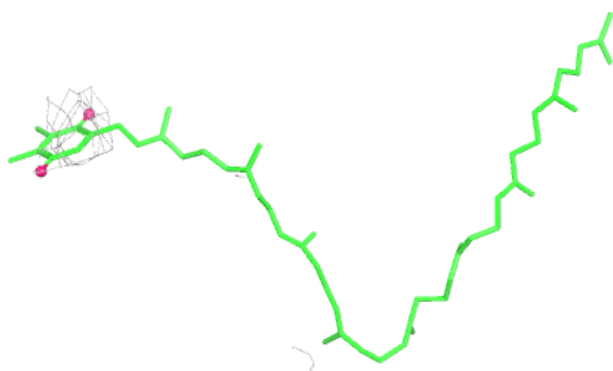
**Electron density around LMG Q 407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

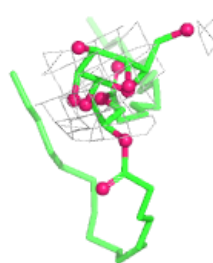
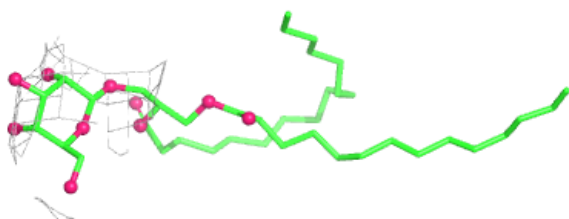
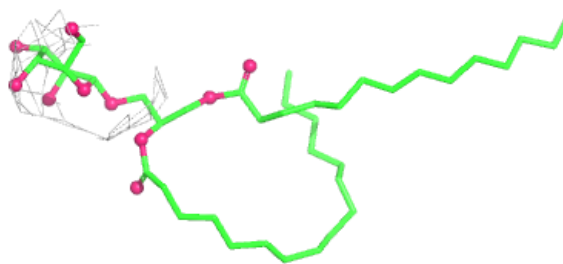


Electron density around PL9 Q 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

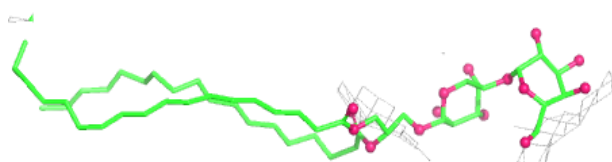
**Electron density around LMG B 622:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

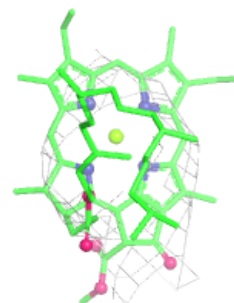
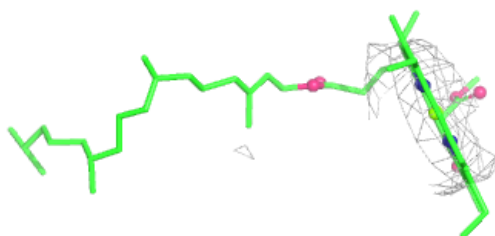
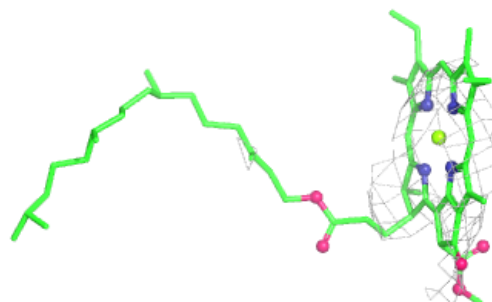


Electron density around DGD P 519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

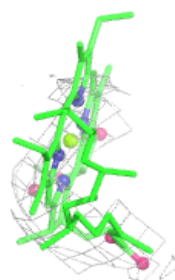
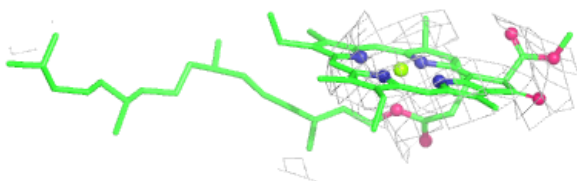
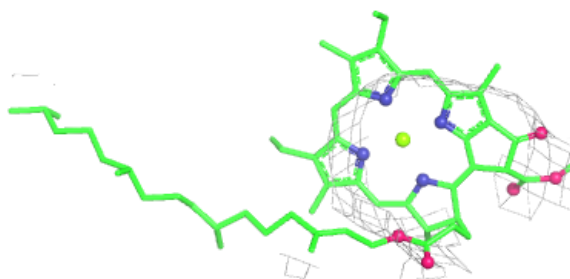
**Electron density around CLA D 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

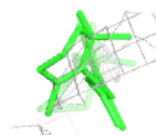
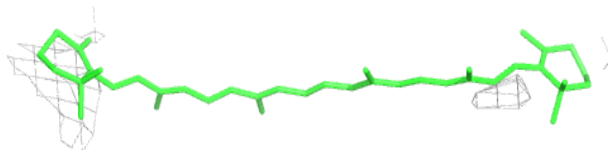
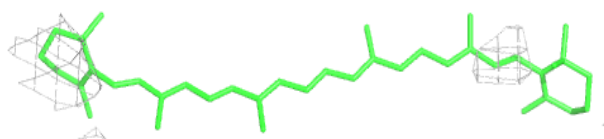


Electron density around CLA C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

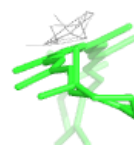
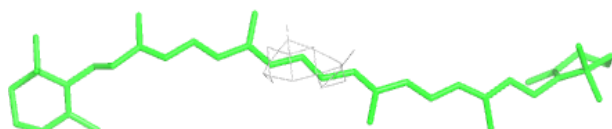
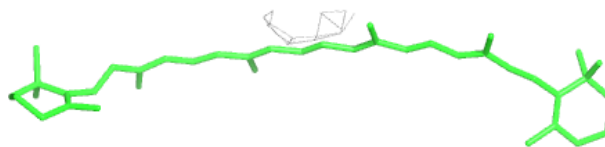
**Electron density around BCR C 515:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

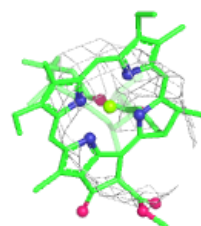
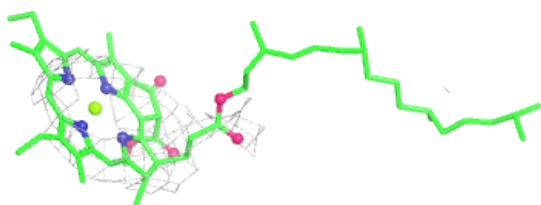


Electron density around BCR D 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

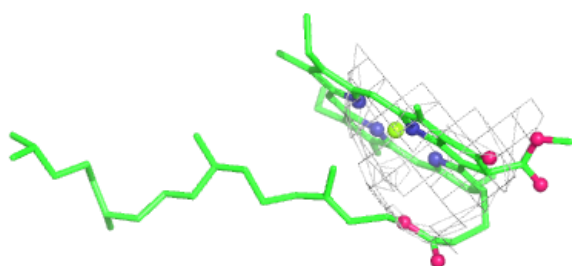
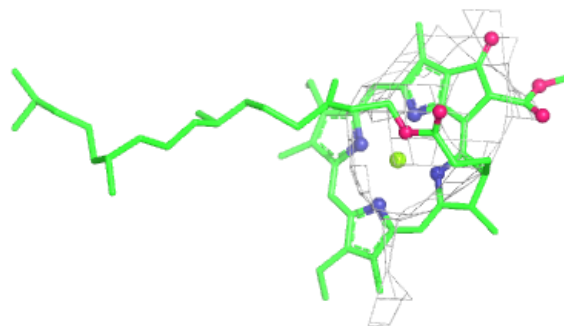
**Electron density around CLA P 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

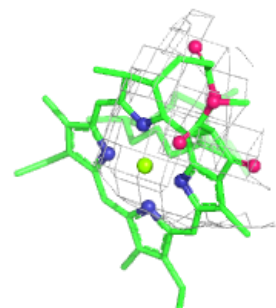
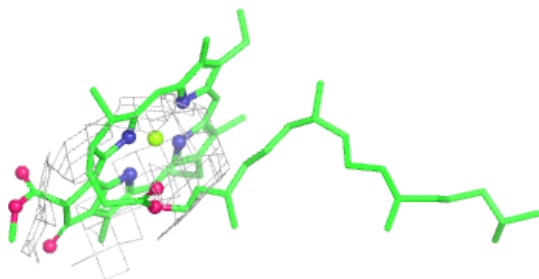
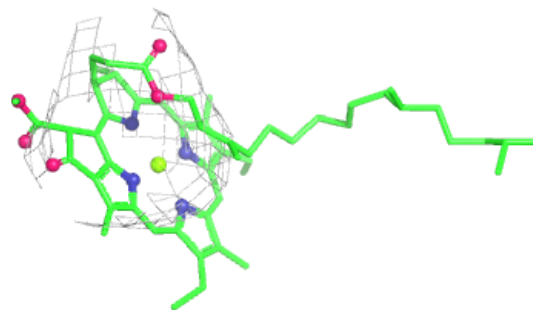


Electron density around CLA B 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

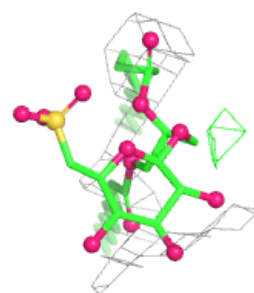
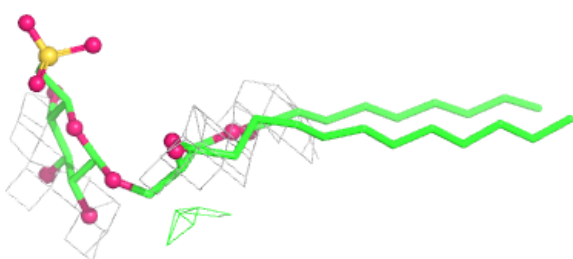
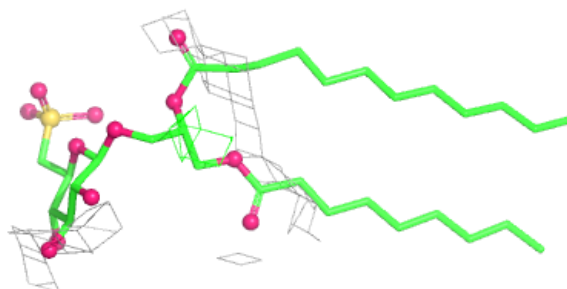
**Electron density around CLA P 505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

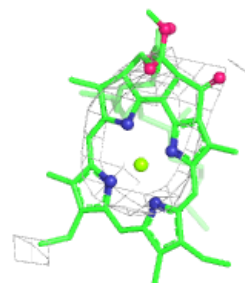
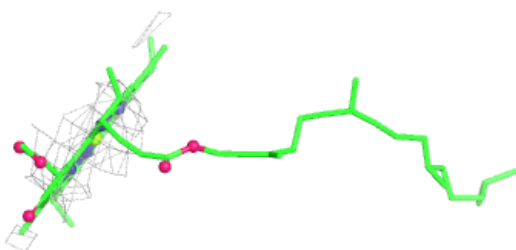
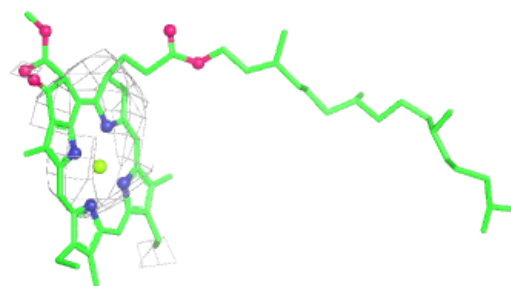


Electron density around SQD B 624:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

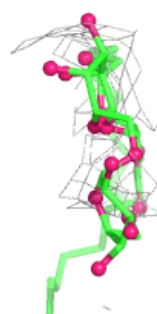
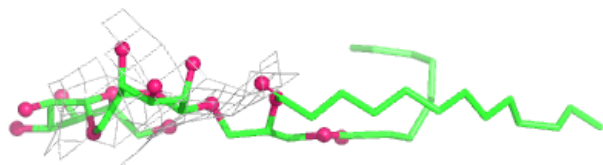
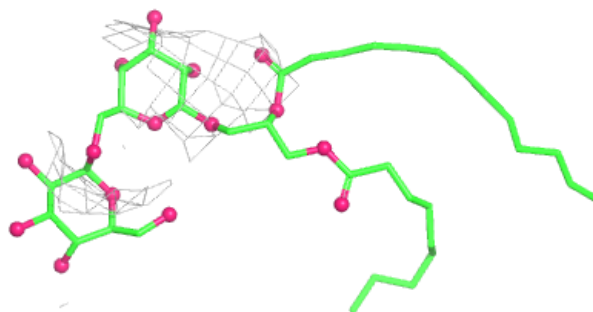
**Electron density around CLA A 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

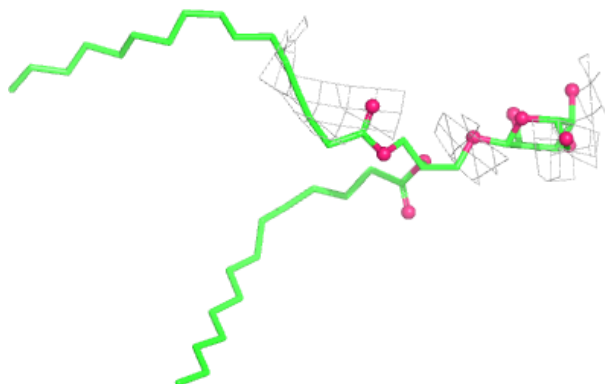


Electron density around DGD N 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

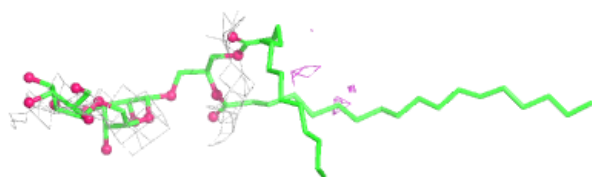
**Electron density around LMG N 623:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

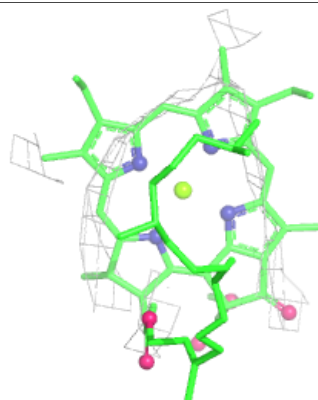
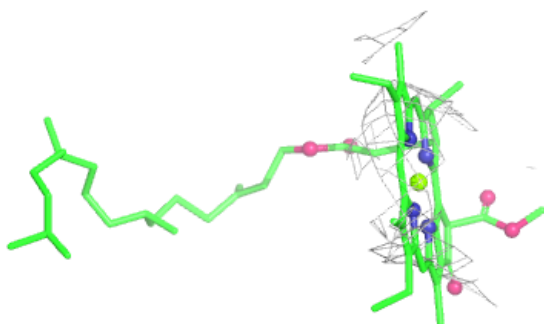
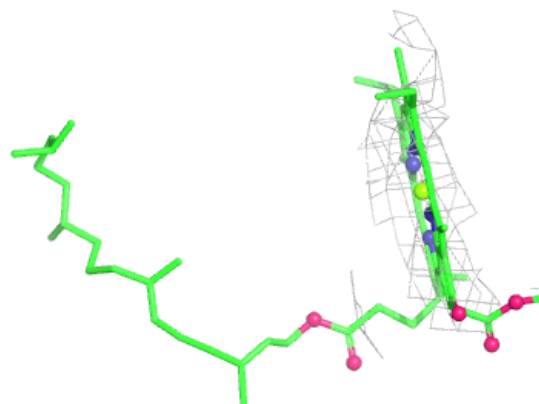


Electron density around DGD P 518:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

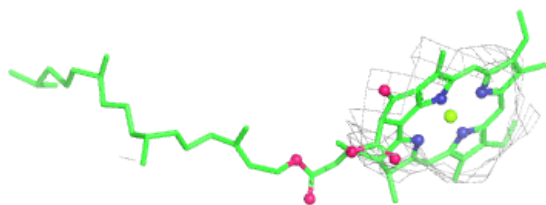
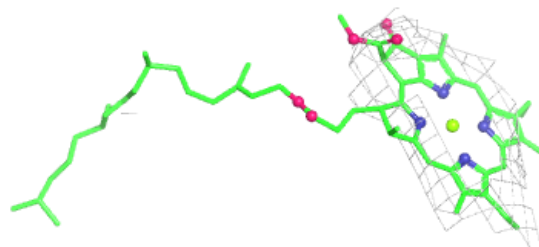
**Electron density around CLA C 506:**

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

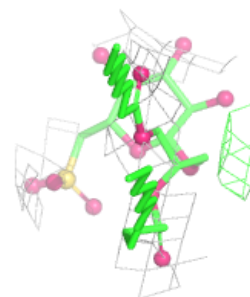
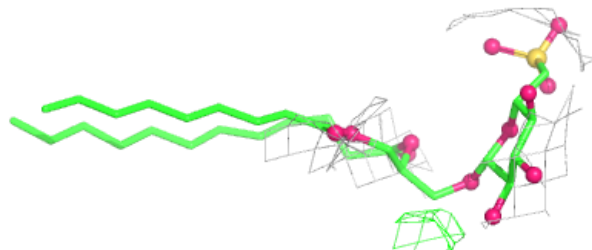
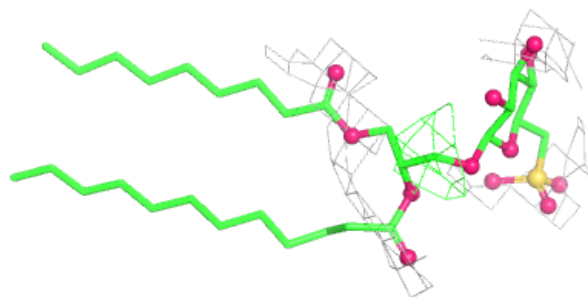


Electron density around CLA G 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

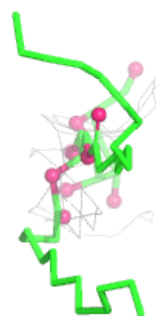
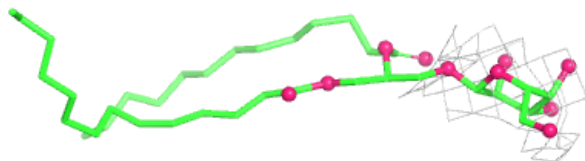
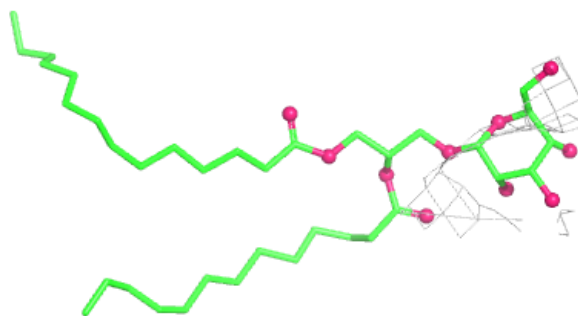
**Electron density around SQD Q 408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

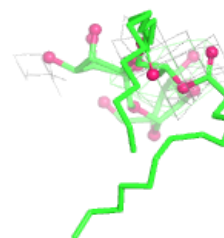
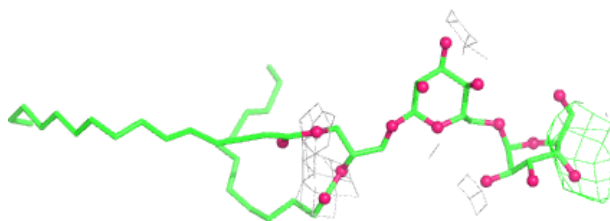


Electron density around LMG Q 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

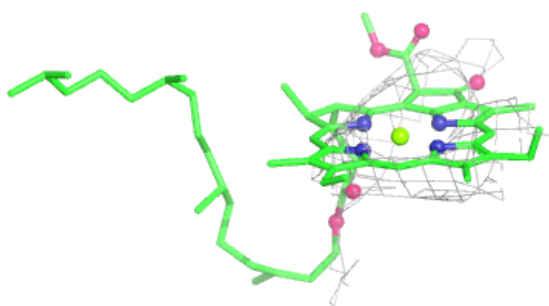
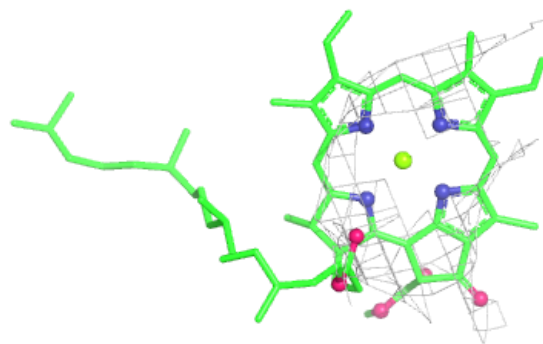
**Electron density around DGD W 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



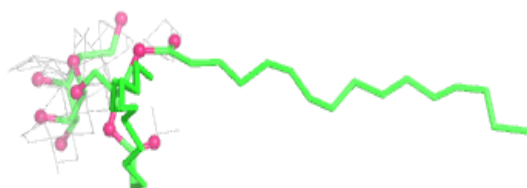
Electron density around CLA G 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



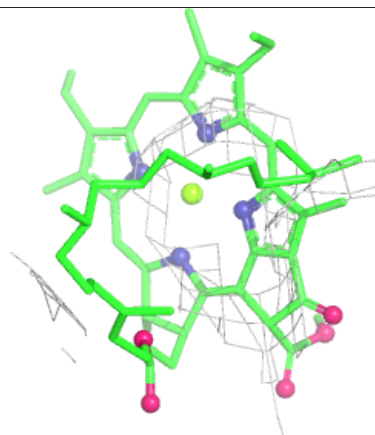
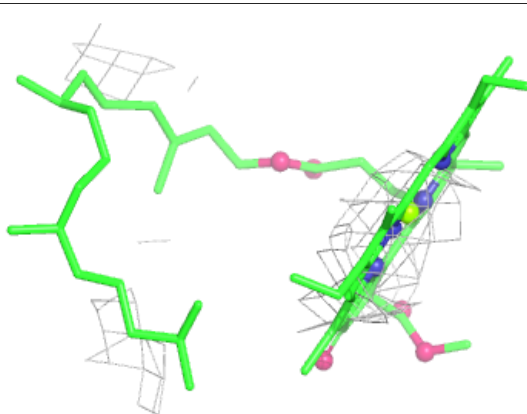
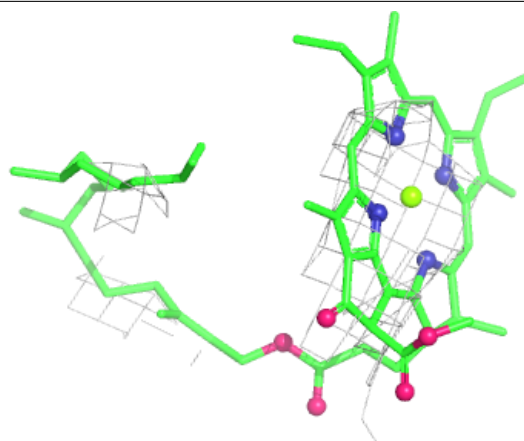
Electron density around LMG G 411:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



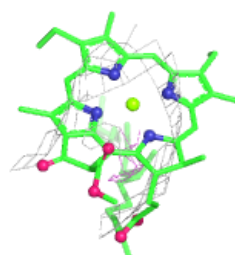
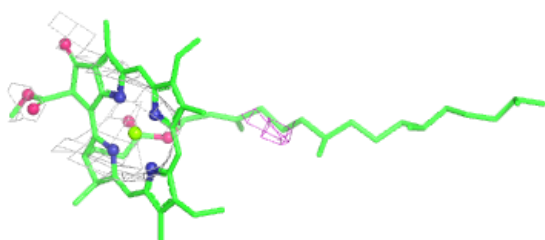
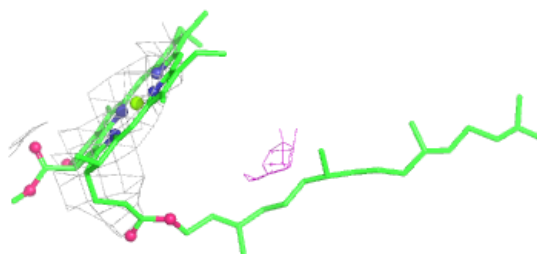
Electron density around CLA P 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

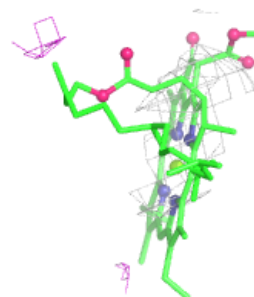
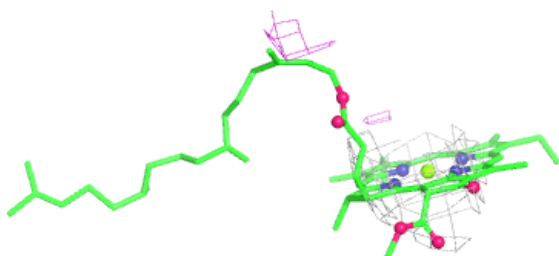
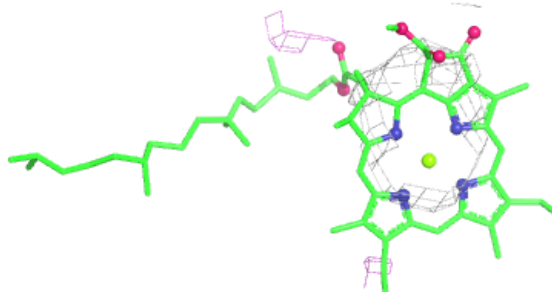


Electron density around CLA P 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

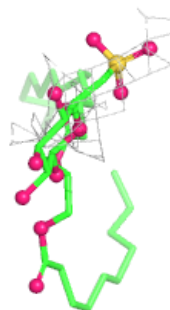
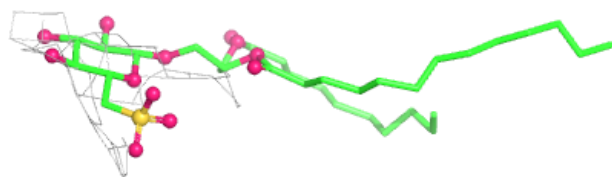
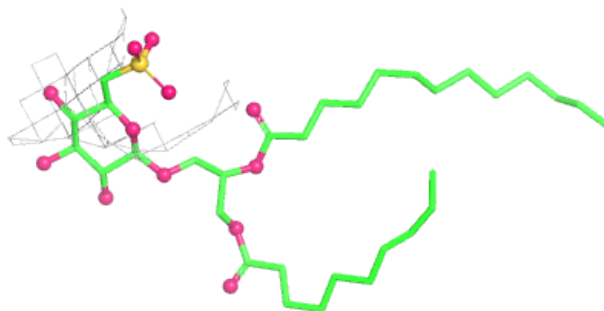
**Electron density around CLA A 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



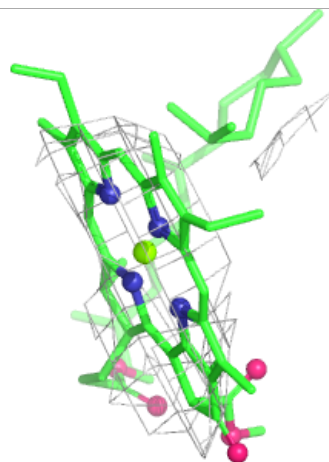
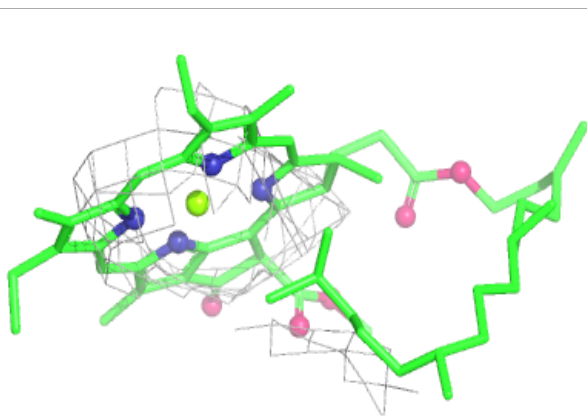
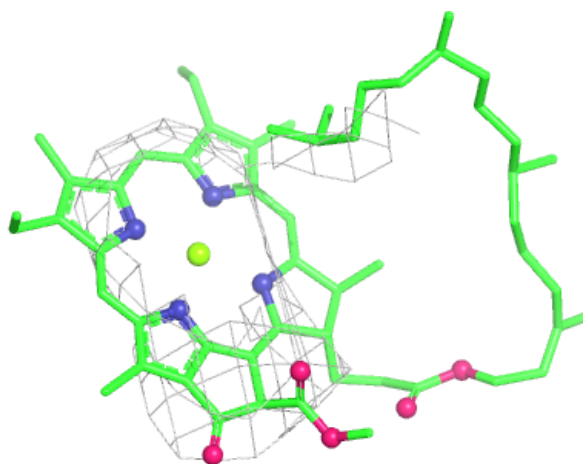
Electron density around SQD S 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



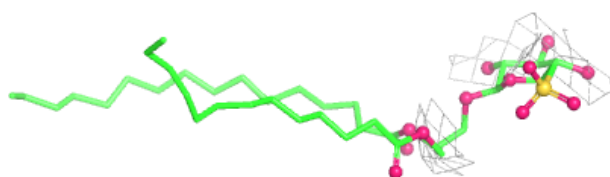
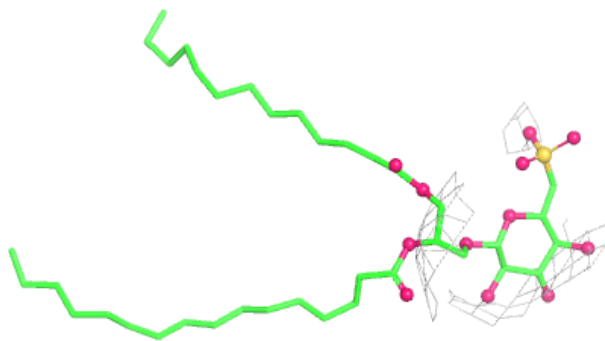
Electron density around CLA N 619:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

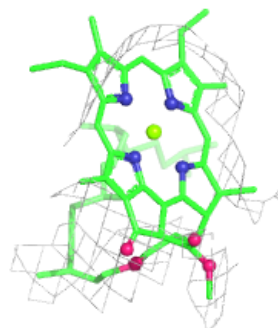
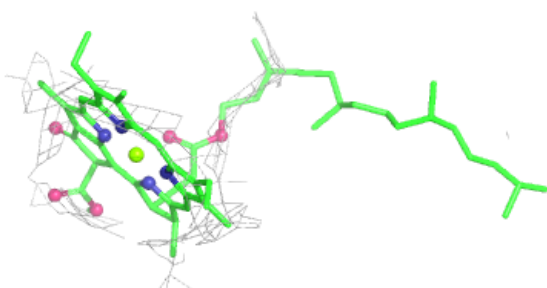
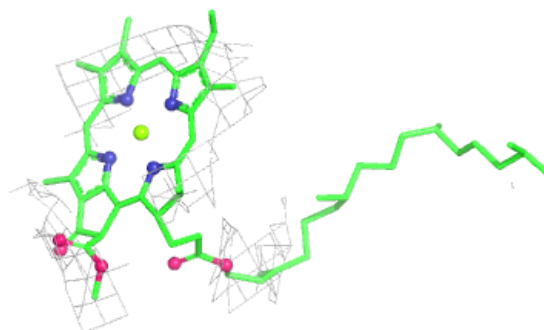


Electron density around SQD A 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

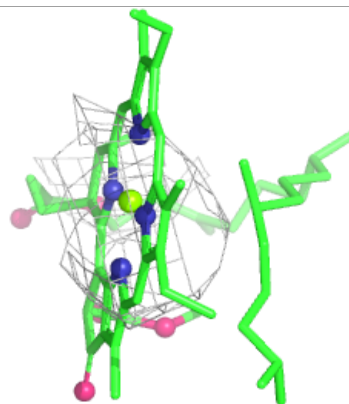
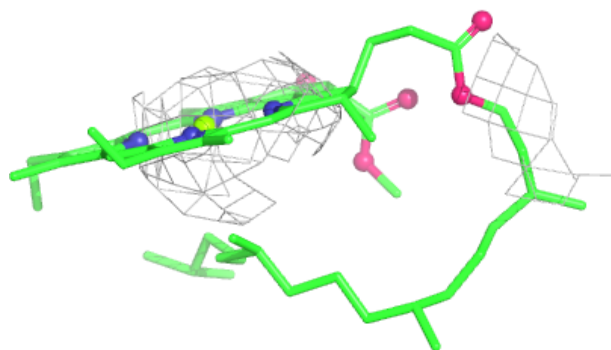
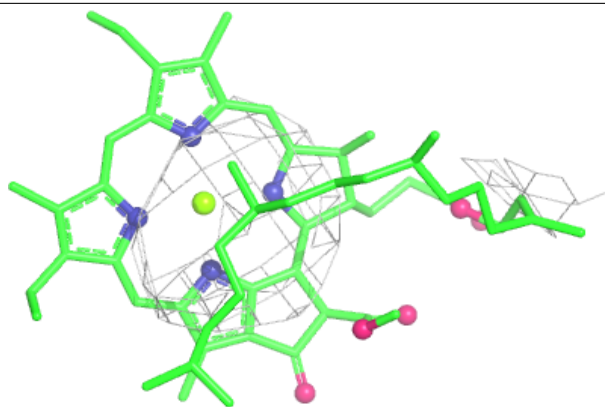
**Electron density around CLA C 511:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



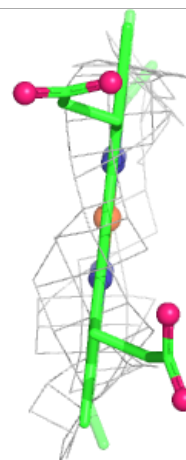
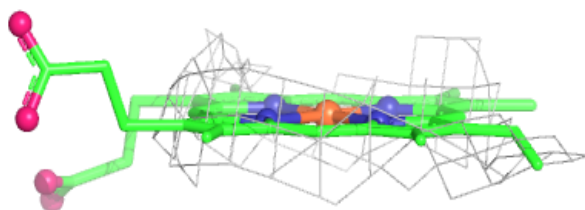
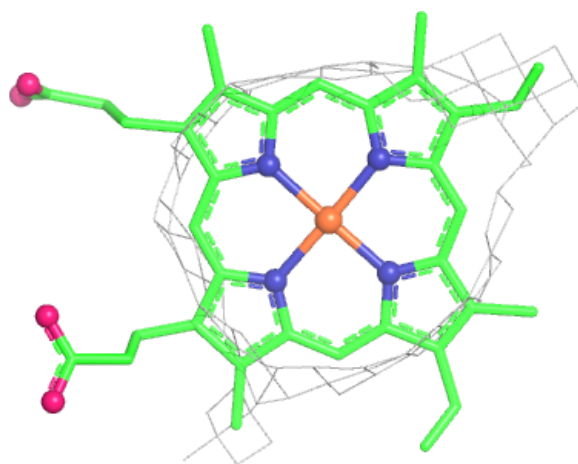
Electron density around CLA P 510:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



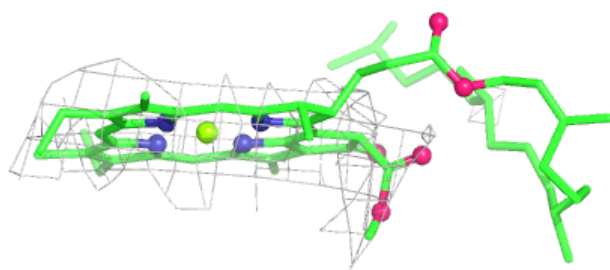
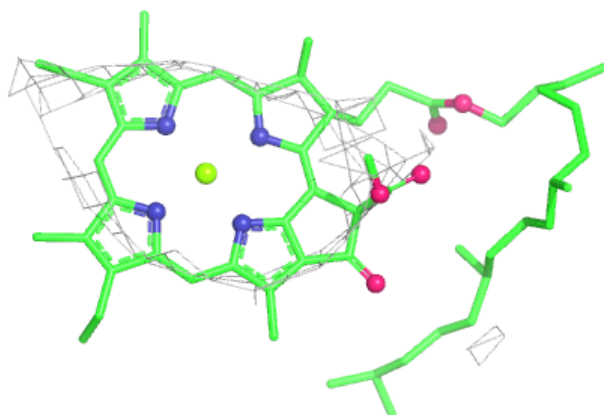
Electron density around HEM V 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

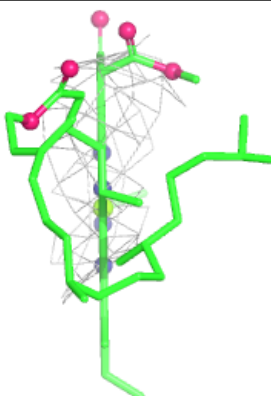
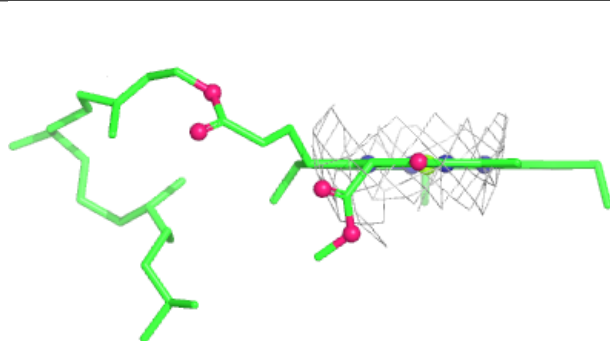
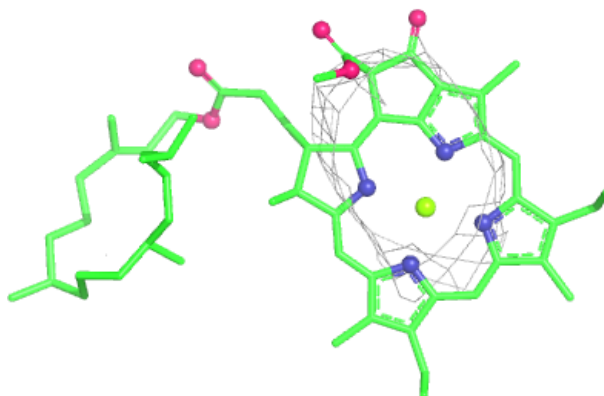


Electron density around CLA N 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

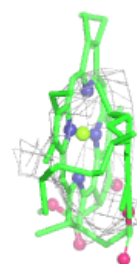
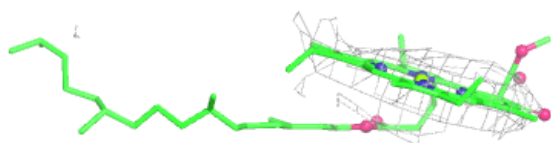
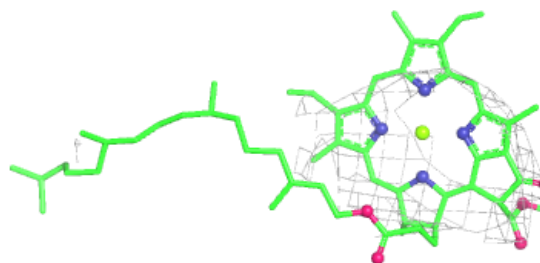
**Electron density around CLA P 512:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

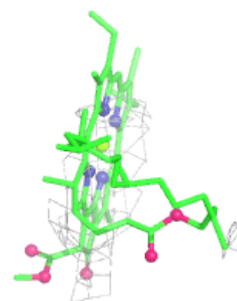
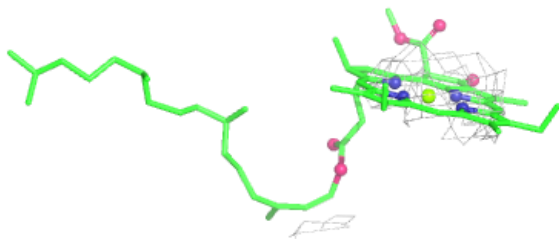
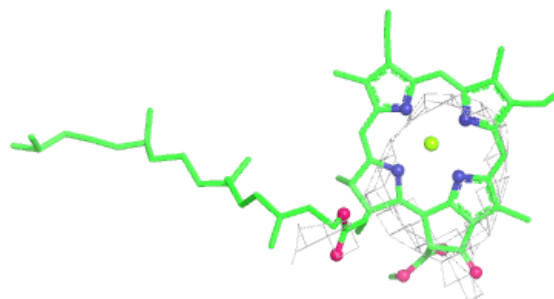


Electron density around CLA B 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

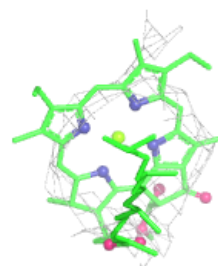
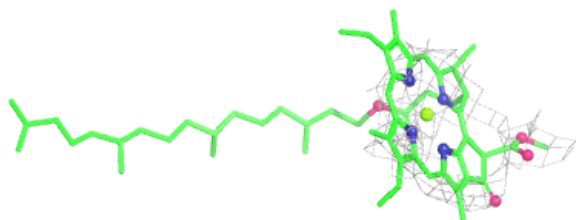
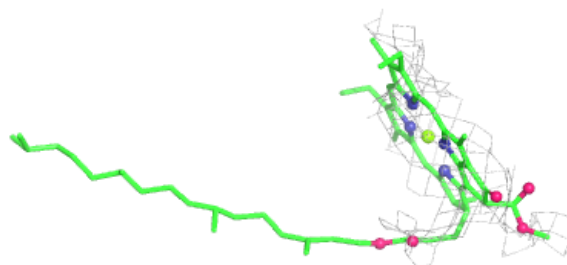
**Electron density around CLA G 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

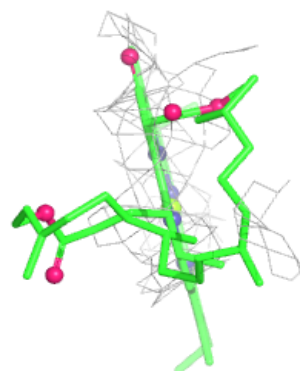
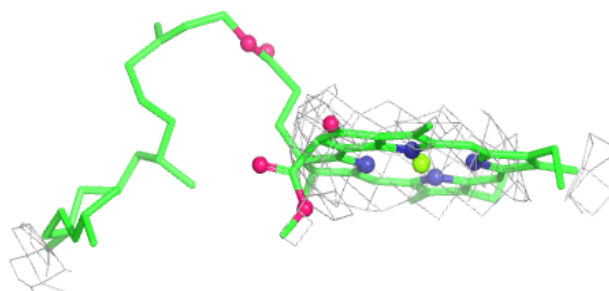
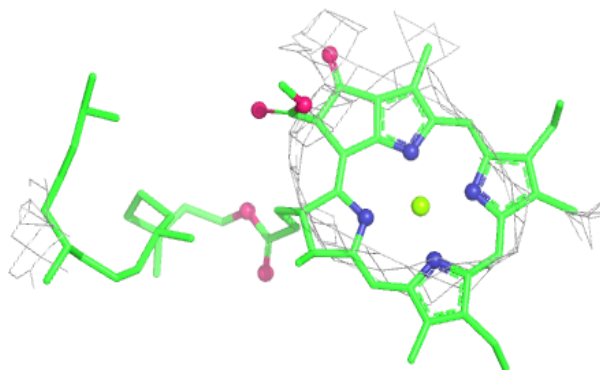


Electron density around CLA N 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

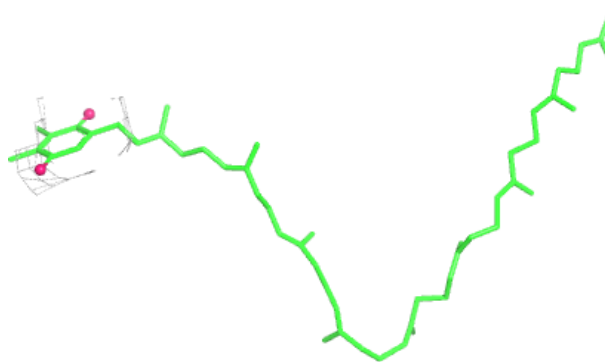
**Electron density around CLA B 612:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

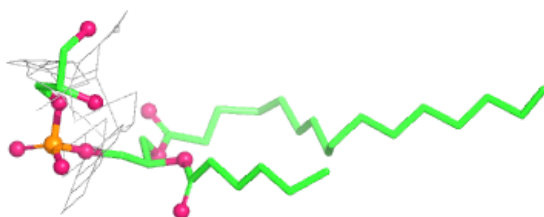


Electron density around PL9 D 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

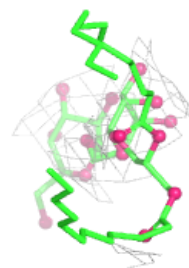
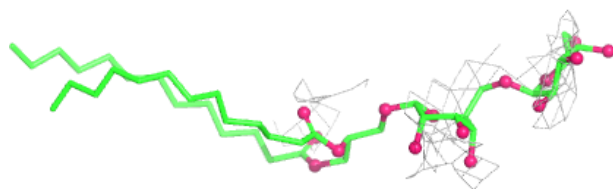
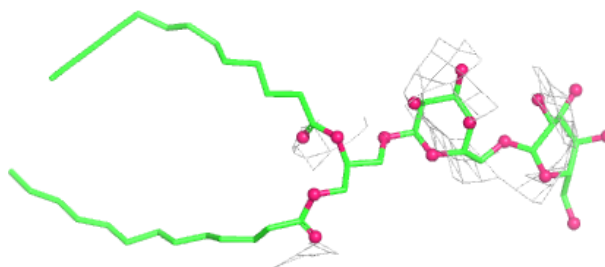
**Electron density around LHG A 408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



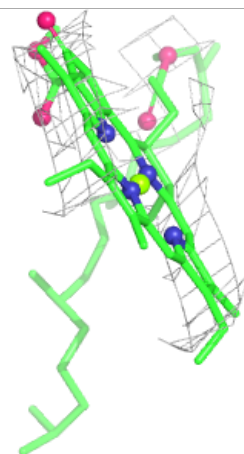
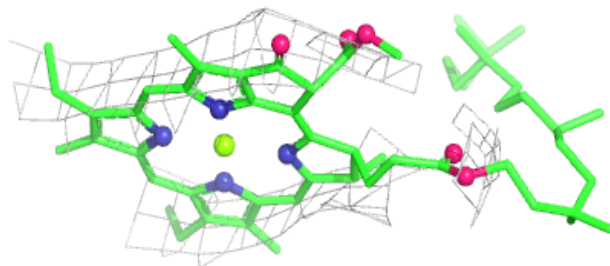
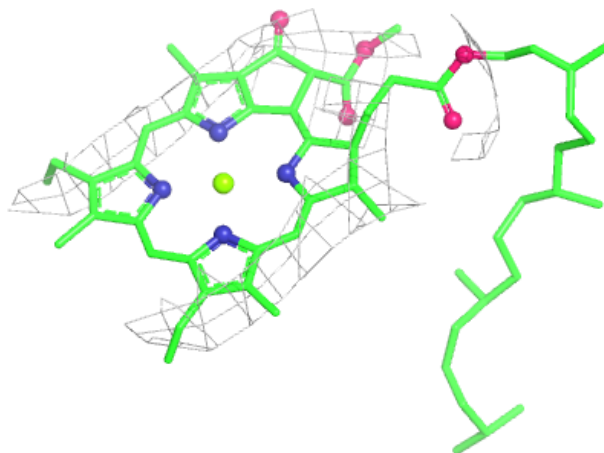
Electron density around DGD G 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



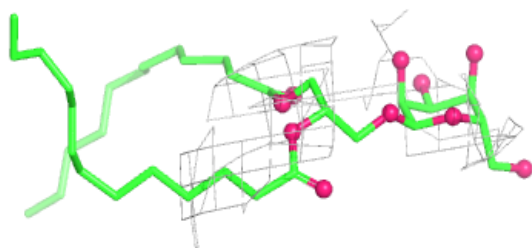
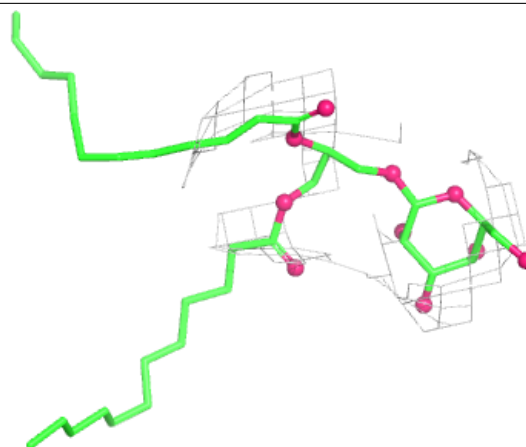
Electron density around CLA B 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



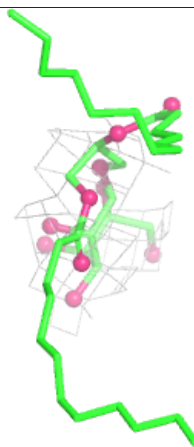
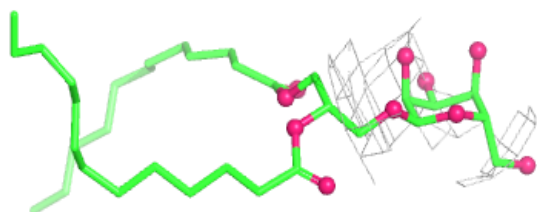
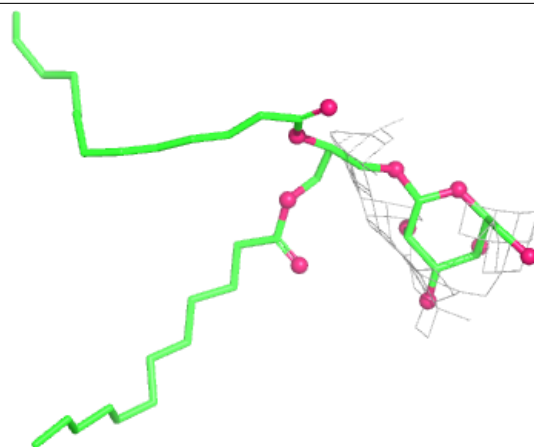
Electron density around LMG R 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

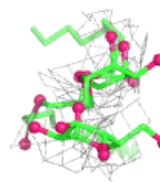
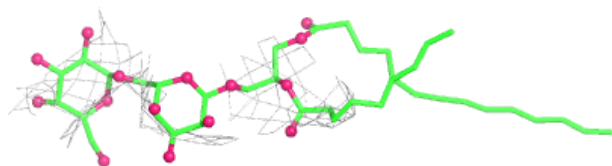
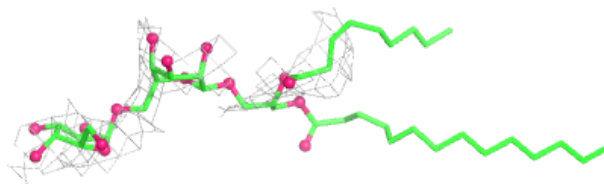


Electron density around LMG E 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

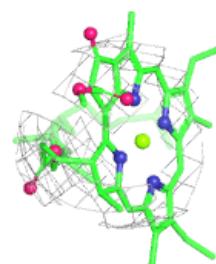
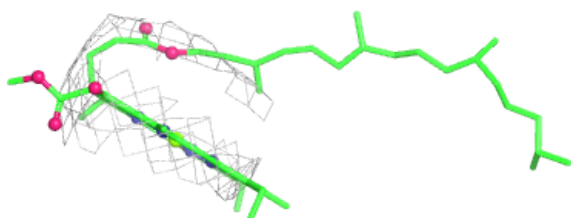
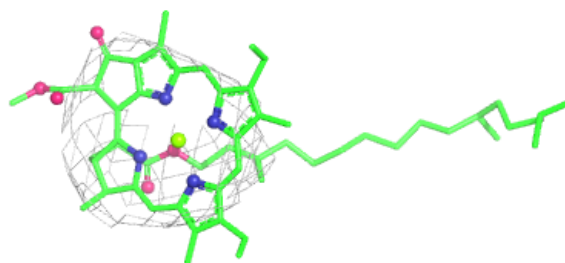
**Electron density around DGD P 517:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

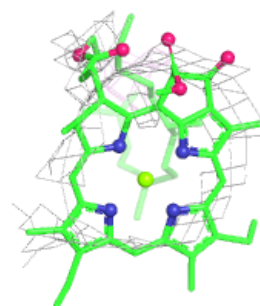
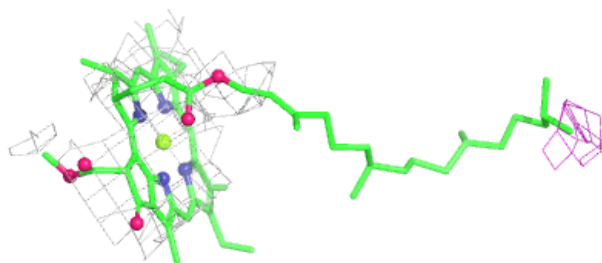


Electron density around CLA N 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

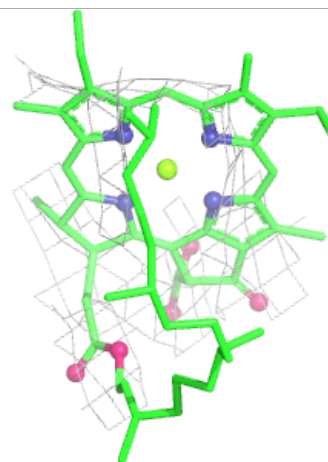
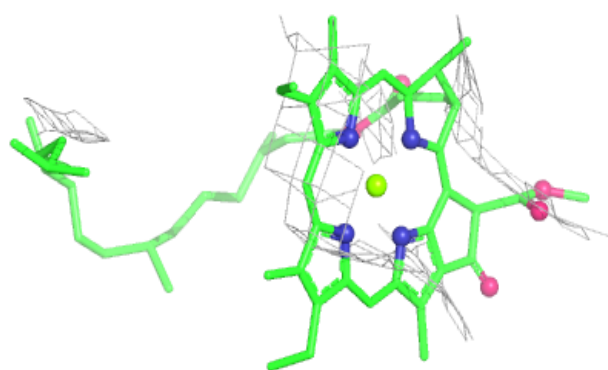
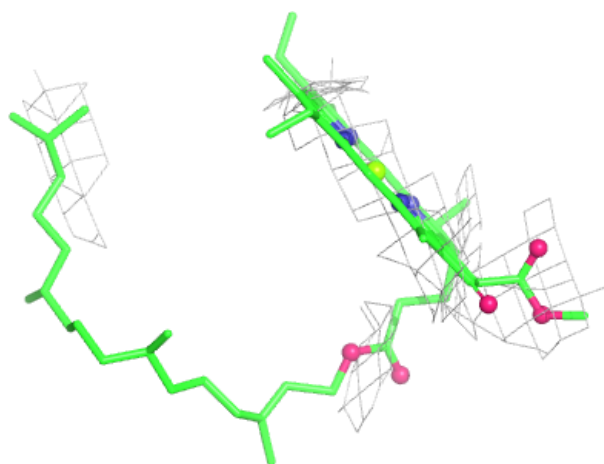
**Electron density around CLA P 508:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



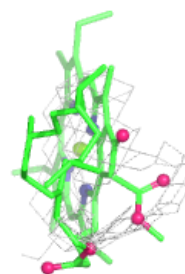
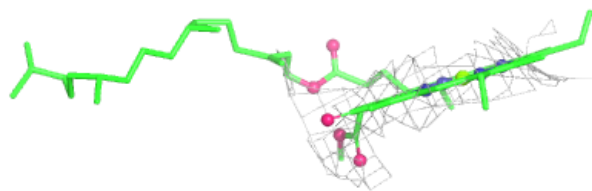
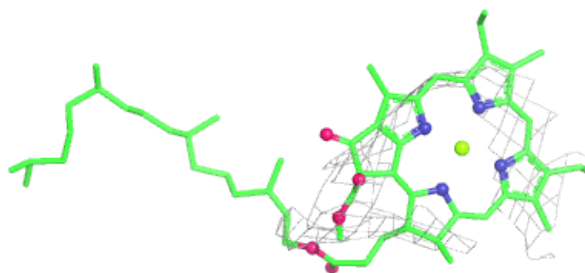
Electron density around CLA B 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



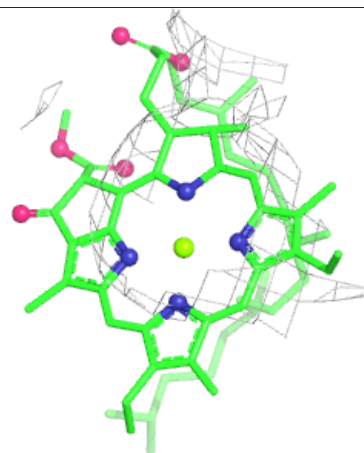
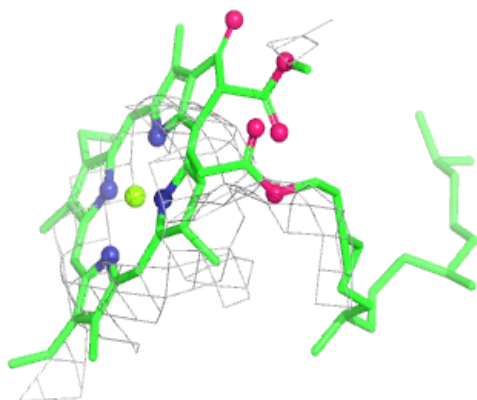
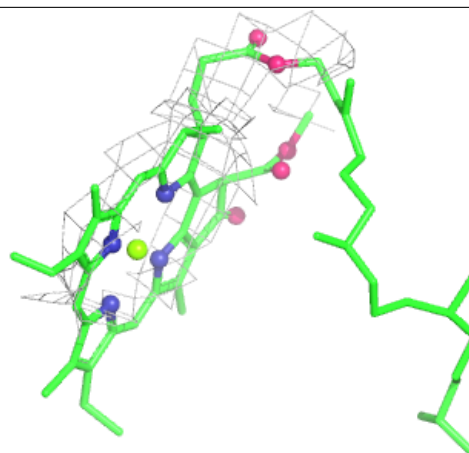
Electron density around CLA B 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

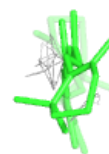
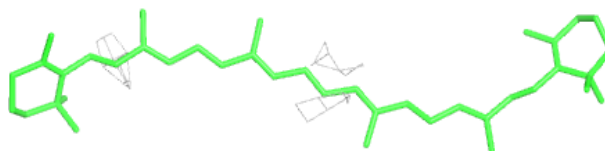


Electron density around CLA N 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

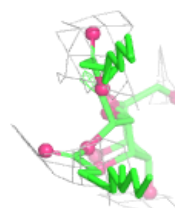
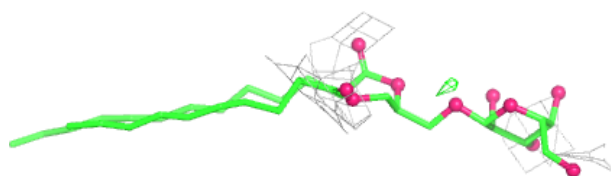
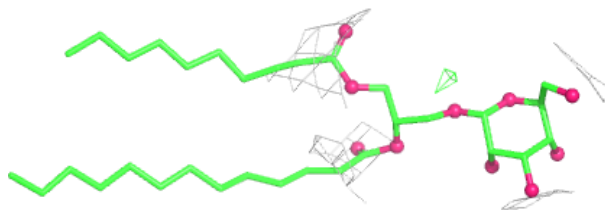
**Electron density around BCR K 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



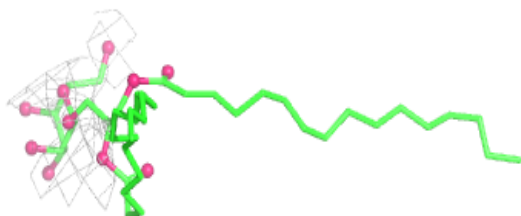
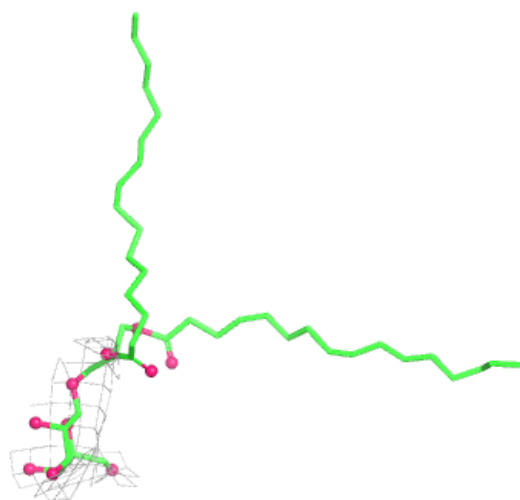
Electron density around LMG e 102:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



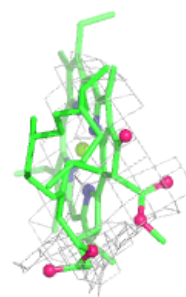
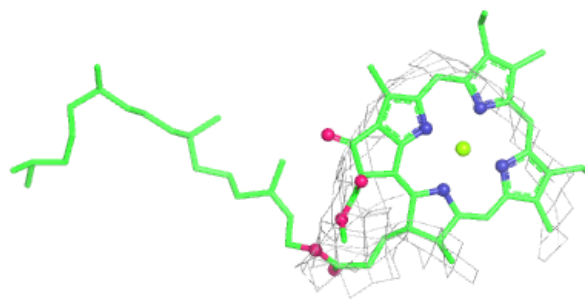
Electron density around LMG A 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

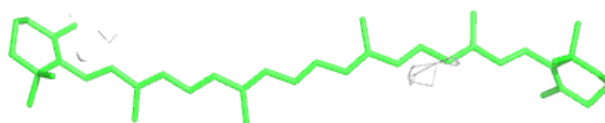


Electron density around CLA N 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

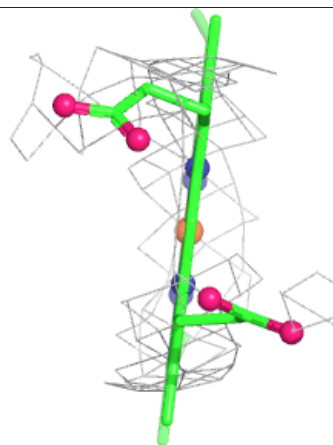
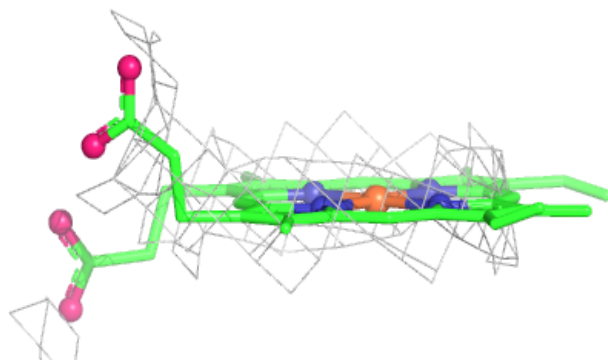
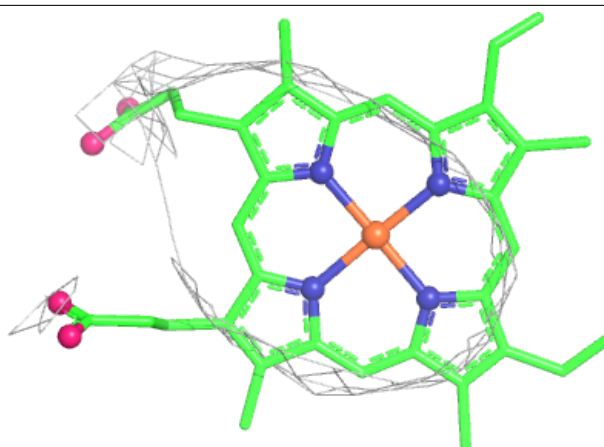
**Electron density around BCR N 621:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



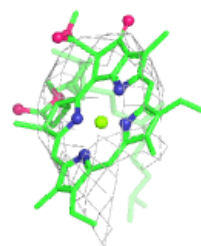
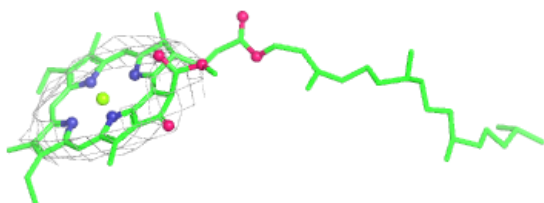
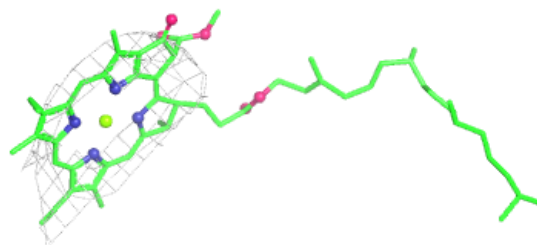
Electron density around HEM R 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

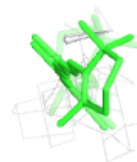
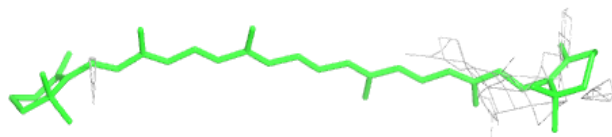
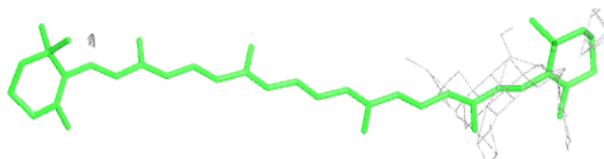


Electron density around CLA A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

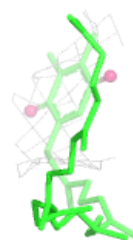
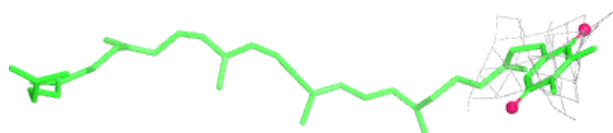
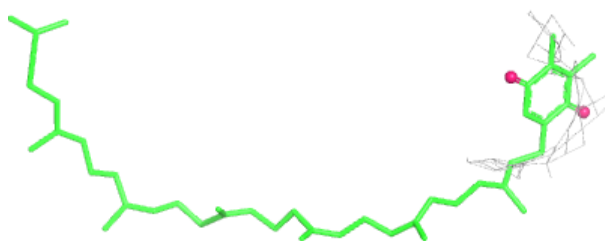
**Electron density around BCR B 620:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

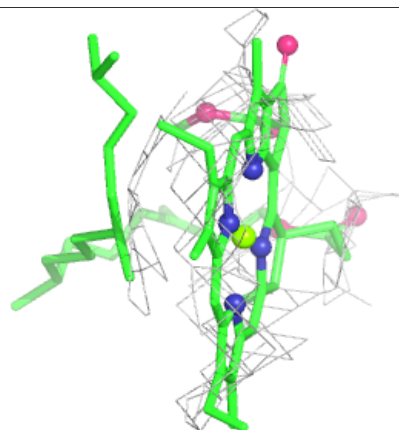
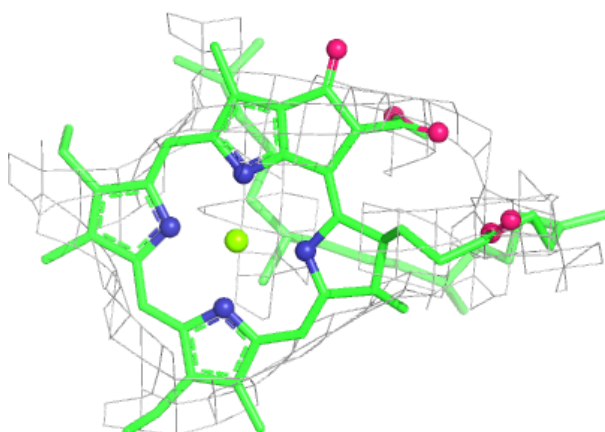


Electron density around PL9 G 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

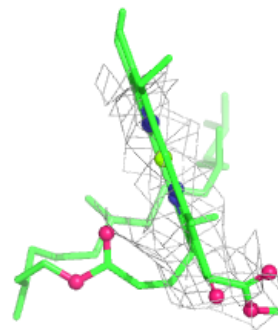
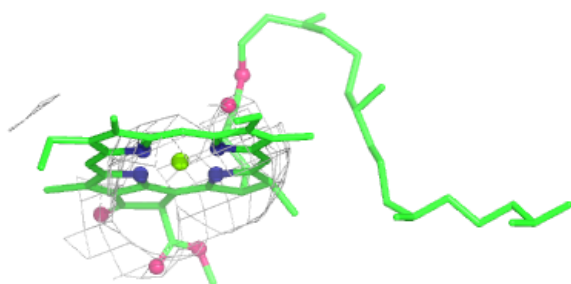
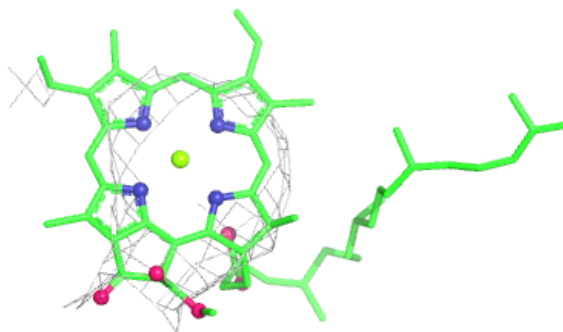
**Electron density around CLA C 510:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



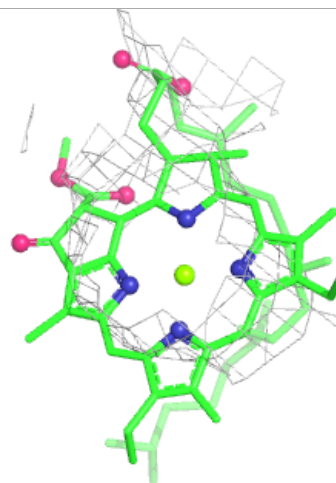
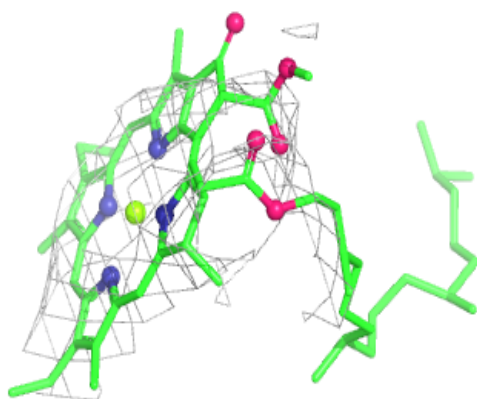
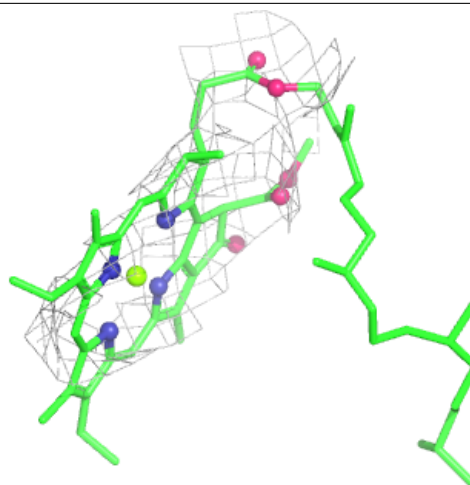
Electron density around CLA A 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



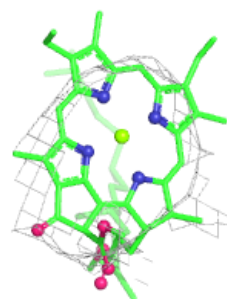
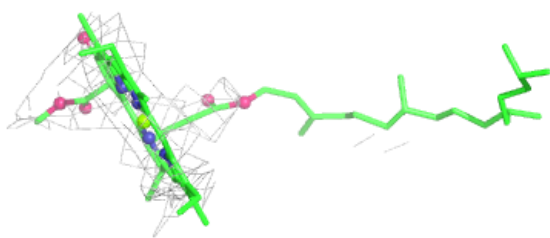
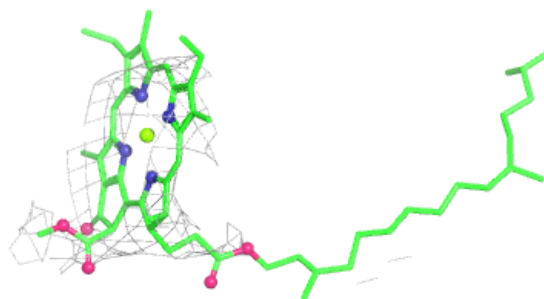
Electron density around CLA B 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



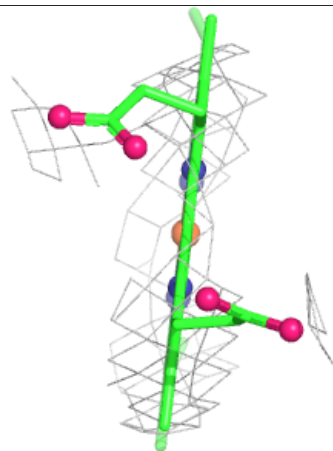
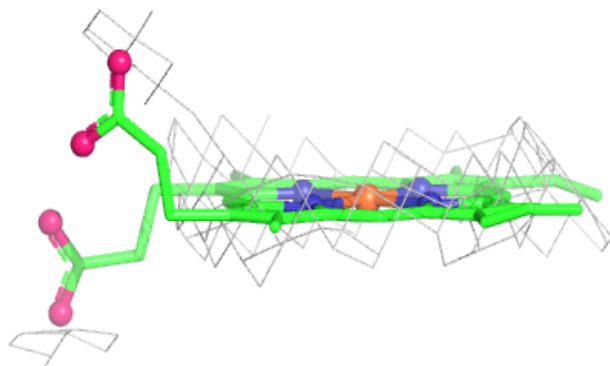
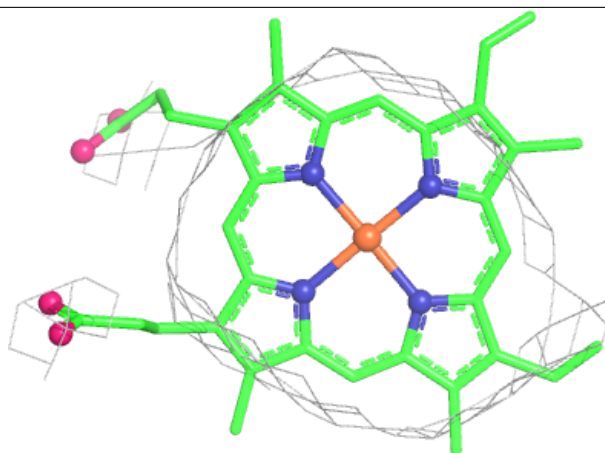
Electron density around CLA N 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

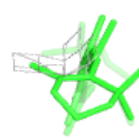
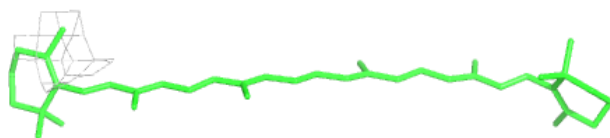
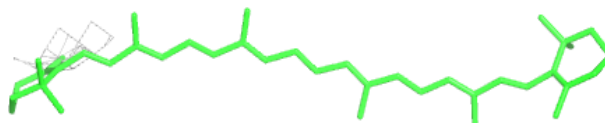


Electron density around HEM E 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

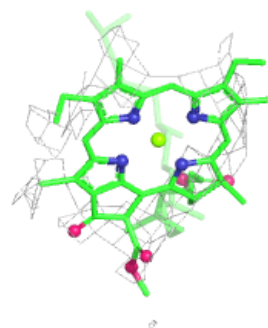
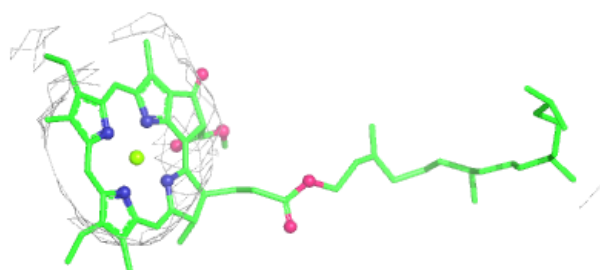
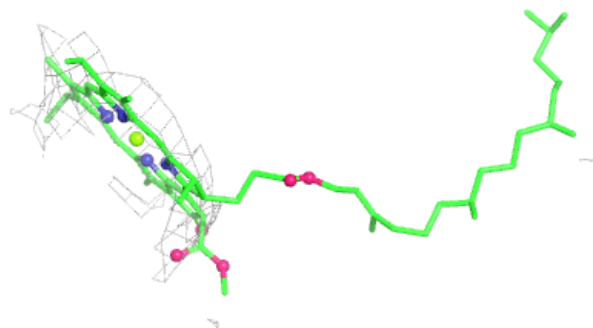
**Electron density around BCR Z 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

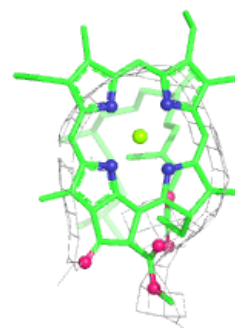
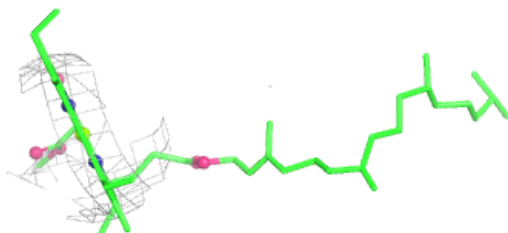
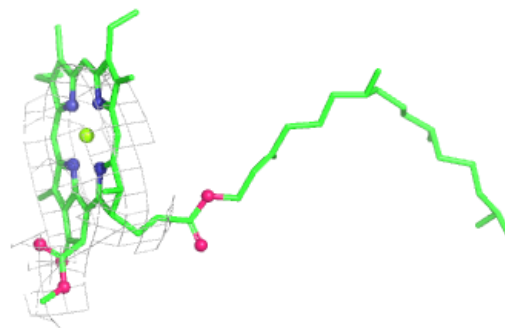


Electron density around CLA Q 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

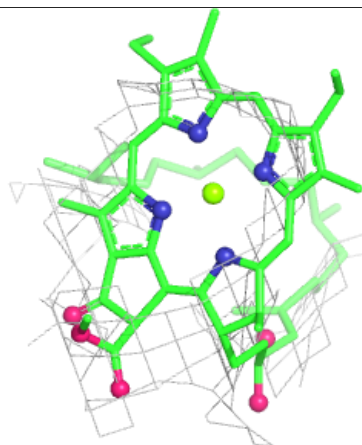
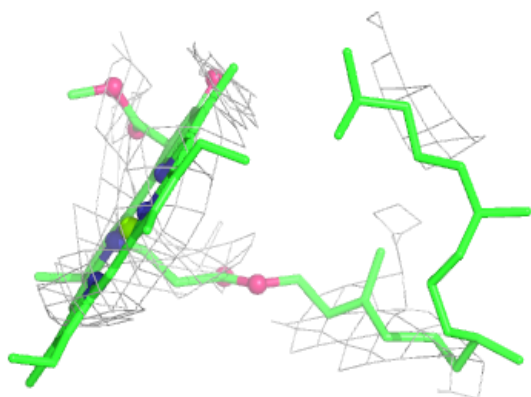
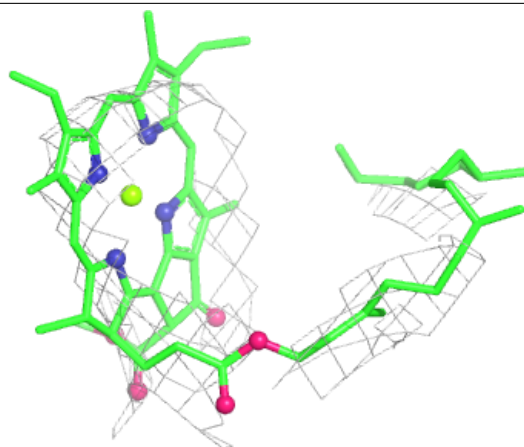
**Electron density around CLA Q 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



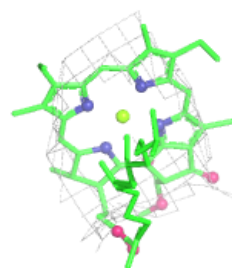
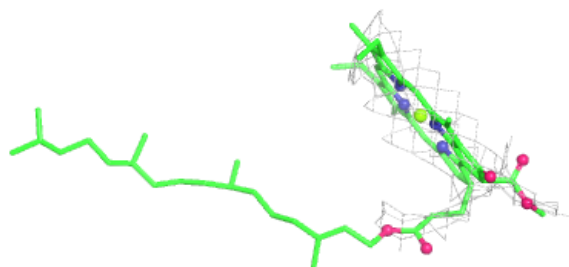
Electron density around CLA C 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

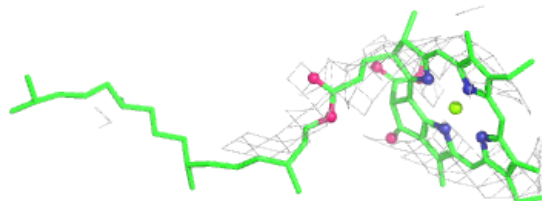
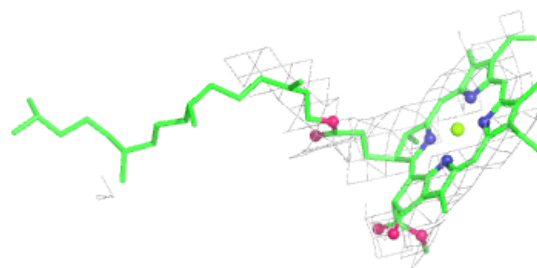


Electron density around CLA C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

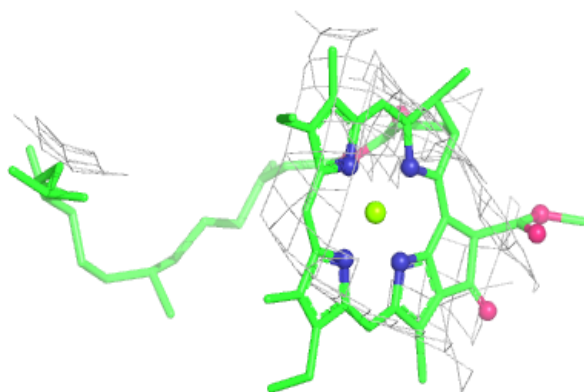
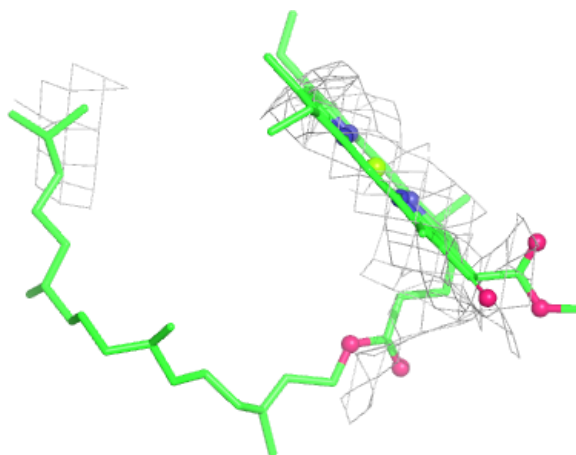
**Electron density around CLA C 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



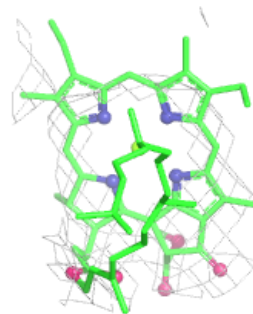
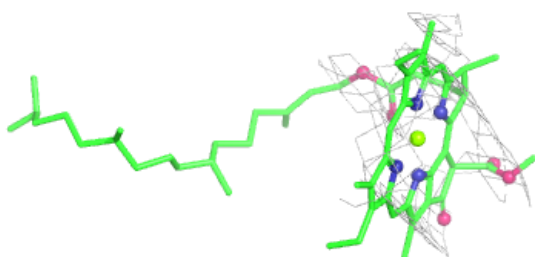
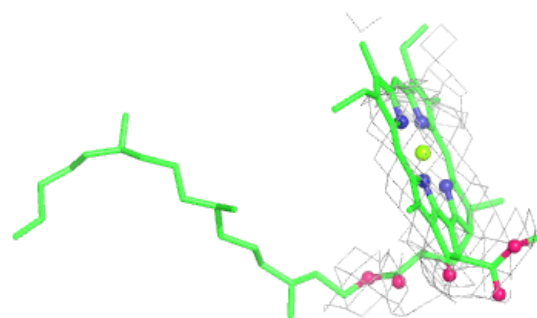
Electron density around CLA N 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

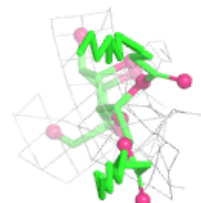
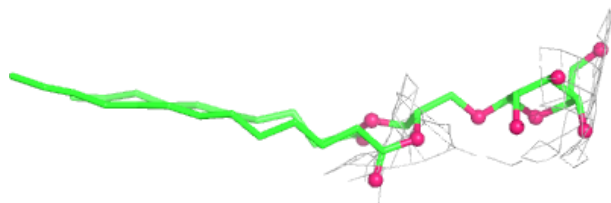
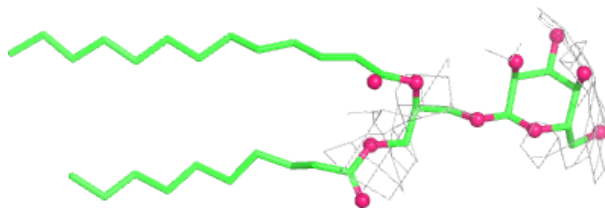


Electron density around CLA C 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

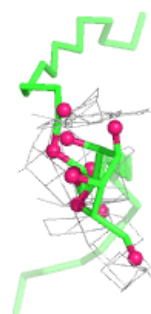
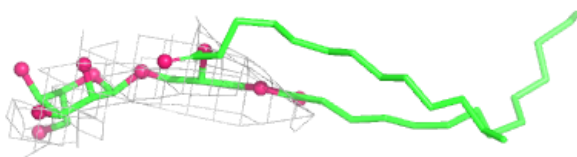
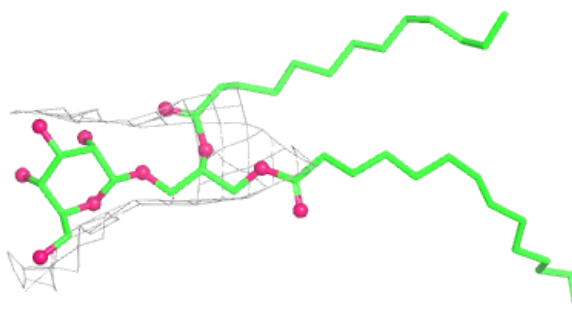
**Electron density around LMG M 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

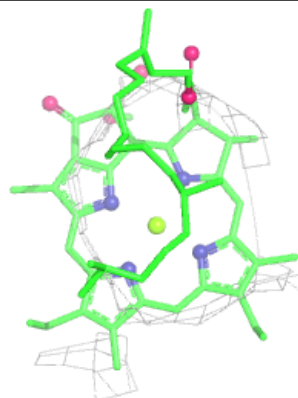
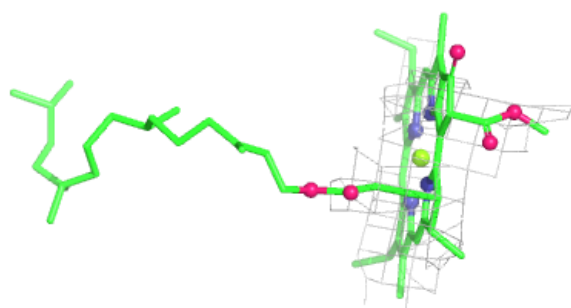


Electron density around LMG D 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

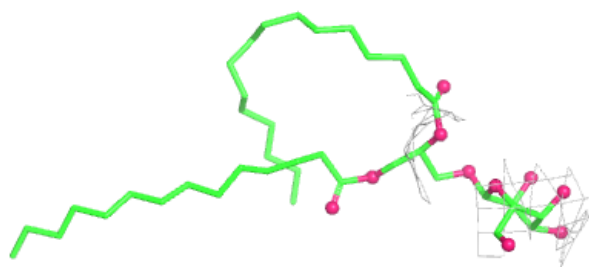
**Electron density around CLA P 506:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

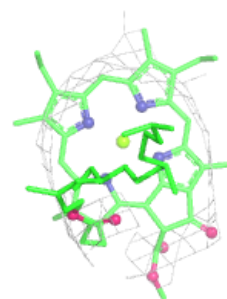
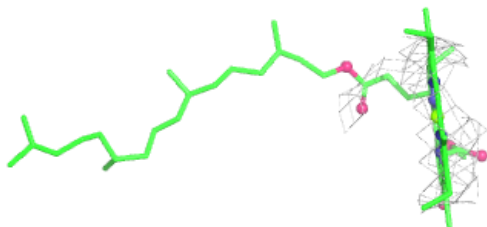
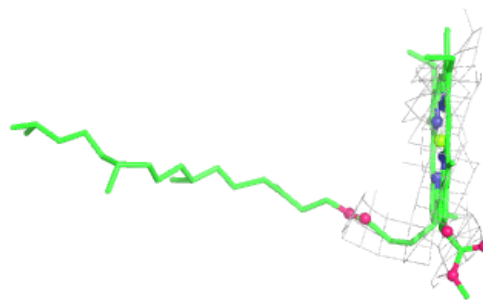


Electron density around LMG N 622:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

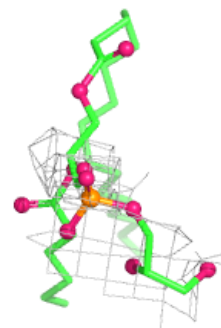
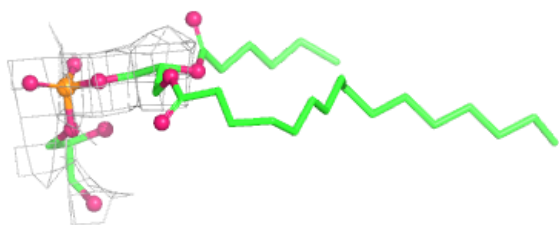
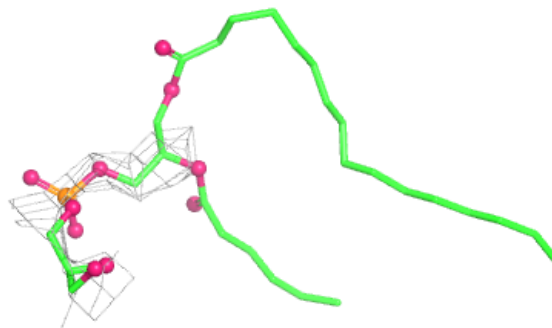
**Electron density around CLA B 606:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LHG G 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.