



Full wwPDB X-ray Structure Validation Report

Sep 14, 2020 – 03:22 AM BST

PDB ID : 4Y28
Title : The structure of plant photosystem I super-complex at 2.8 angstrom resolution.
Authors : Mazor, Y.; Brovikov, A.; Nelson, N.
Deposited on : 2015-02-09
Resolution : 2.80 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 following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

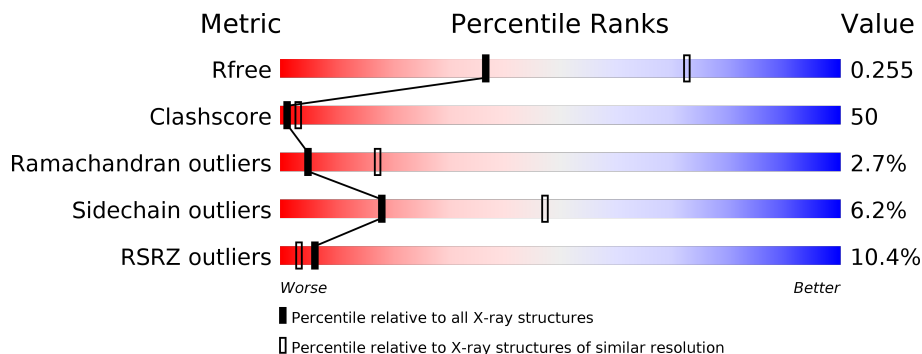
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	758	
2	B	733	
3	I	30	
4	J	42	
5	F	154	
6	G	97	

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Mol	Chain	Length	Quality of chain
7	L	167	
8	C	81	
9	D	147	
10	E	66	
11	H	90	
12	K	129	
13	2	269	
14	4	252	
15	1	202	
16	3	275	

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
17	CL0	A	1011	X	-	-	-
18	CLA	1	1001	X	-	X	-
18	CLA	1	1002	X	-	X	-
18	CLA	1	1003	X	-	X	-
18	CLA	1	1004	X	-	X	-
18	CLA	1	1005	X	-	-	-
18	CLA	1	1006	X	-	-	-
18	CLA	1	1007	X	-	-	-
18	CLA	1	1008	X	-	X	-
18	CLA	1	1011	X	-	-	-
18	CLA	1	1012	X	-	-	-
18	CLA	1	1013	X	-	-	-
18	CLA	1	1014	X	-	-	-
18	CLA	2	2001	X	-	X	-
18	CLA	2	2002	X	-	X	-
18	CLA	2	2003	X	-	X	-
18	CLA	2	2004	X	-	X	-
18	CLA	2	2005	X	-	X	-
18	CLA	2	2006	X	-	X	-
18	CLA	2	2007	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	2008	X	-	-	-
18	CLA	2	2009	X	-	-	-
18	CLA	2	2012	X	-	X	-
18	CLA	2	2016	X	-	X	-
18	CLA	2	2019	X	-	-	-
18	CLA	3	3001	X	-	X	-
18	CLA	3	3002	X	-	-	-
18	CLA	3	3003	X	-	X	-
18	CLA	3	3004	X	-	-	-
18	CLA	3	3005	X	-	-	-
18	CLA	3	3006	X	-	X	-
18	CLA	3	3007	X	-	-	-
18	CLA	3	3008	X	-	-	-
18	CLA	3	3010	X	-	X	-
18	CLA	3	3012	X	-	X	-
18	CLA	3	3013	X	-	X	-
18	CLA	3	3017	X	-	-	-
18	CLA	3	3018	X	-	-	-
18	CLA	3	3019	X	-	-	X
18	CLA	4	4001	X	-	X	-
18	CLA	4	4002	X	-	-	-
18	CLA	4	4003	X	-	-	-
18	CLA	4	4004	X	-	-	-
18	CLA	4	4005	X	-	-	-
18	CLA	4	4006	X	-	X	-
18	CLA	4	4007	X	-	-	-
18	CLA	4	4008	X	-	-	-
18	CLA	4	4009	X	-	-	-
18	CLA	4	4012	X	-	X	-
18	CLA	4	4016	X	-	X	-
18	CLA	4	4017	X	-	-	-
18	CLA	A	1013	X	-	-	-
18	CLA	A	1022	X	-	-	-
18	CLA	A	1101	X	-	-	-
18	CLA	A	1102	X	-	-	-
18	CLA	A	1103	X	-	-	-
18	CLA	A	1104	X	-	-	-
18	CLA	A	1105	X	-	-	-
18	CLA	A	1106	X	-	-	-
18	CLA	A	1107	X	-	-	-
18	CLA	A	1108	X	-	-	-
18	CLA	A	1109	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	1110	X	-	-	-
18	CLA	A	1111	X	-	-	-
18	CLA	A	1112	X	-	-	-
18	CLA	A	1113	X	-	-	-
18	CLA	A	1114	X	-	-	-
18	CLA	A	1115	X	-	-	-
18	CLA	A	1116	X	-	-	-
18	CLA	A	1117	X	-	-	-
18	CLA	A	1118	X	-	-	-
18	CLA	A	1119	X	-	-	-
18	CLA	A	1120	X	-	-	-
18	CLA	A	1121	X	-	-	-
18	CLA	A	1122	X	-	-	-
18	CLA	A	1123	X	-	-	-
18	CLA	A	1124	X	-	-	-
18	CLA	A	1125	X	-	-	-
18	CLA	A	1126	X	-	-	-
18	CLA	A	1127	X	-	-	-
18	CLA	A	1128	X	-	-	-
18	CLA	A	1129	X	-	-	-
18	CLA	A	1130	X	-	-	-
18	CLA	A	1131	X	-	-	-
18	CLA	A	1132	X	-	-	-
18	CLA	A	1133	X	-	-	-
18	CLA	A	1134	X	-	-	-
18	CLA	A	1135	X	-	-	-
18	CLA	A	1136	X	-	-	-
18	CLA	A	1137	X	-	-	-
18	CLA	A	1138	X	-	-	-
18	CLA	A	1139	X	-	-	-
18	CLA	A	1140	X	-	-	-
18	CLA	A	1151	X	-	-	-
18	CLA	A	1237	X	-	-	-
18	CLA	B	1012	X	-	-	-
18	CLA	B	1021	X	-	-	-
18	CLA	B	1023	X	-	-	-
18	CLA	B	1201	X	-	-	-
18	CLA	B	1202	X	-	-	-
18	CLA	B	1203	X	-	-	-
18	CLA	B	1204	X	-	-	-
18	CLA	B	1205	X	-	-	-
18	CLA	B	1206	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	1207	X	-	-	-
18	CLA	B	1208	X	-	-	-
18	CLA	B	1209	X	-	-	-
18	CLA	B	1210	X	-	-	-
18	CLA	B	1211	X	-	-	-
18	CLA	B	1212	X	-	-	-
18	CLA	B	1213	X	-	-	-
18	CLA	B	1214	X	-	-	-
18	CLA	B	1215	X	-	-	-
18	CLA	B	1216	X	-	-	-
18	CLA	B	1217	X	-	-	-
18	CLA	B	1218	X	-	-	-
18	CLA	B	1219	X	-	-	-
18	CLA	B	1220	X	-	-	-
18	CLA	B	1221	X	-	-	-
18	CLA	B	1222	X	-	-	-
18	CLA	B	1223	X	-	-	-
18	CLA	B	1224	X	-	-	-
18	CLA	B	1225	X	-	-	-
18	CLA	B	1226	X	-	-	-
18	CLA	B	1227	X	-	-	-
18	CLA	B	1228	X	-	-	-
18	CLA	B	1229	X	-	-	-
18	CLA	B	1230	X	-	-	-
18	CLA	B	1231	X	-	-	-
18	CLA	B	1232	X	-	-	-
18	CLA	B	1234	X	-	-	-
18	CLA	B	1235	X	-	-	-
18	CLA	B	1236	X	-	-	-
18	CLA	B	1238	X	-	-	-
18	CLA	B	1239	X	-	-	-
18	CLA	B	1240	X	-	-	-
18	CLA	F	1301	X	-	-	-
18	CLA	F	1302	X	-	-	-
18	CLA	G	1001	X	-	X	-
18	CLA	G	1002	X	-	X	-
18	CLA	G	1003	X	-	X	-
18	CLA	H	1000	X	-	-	-
18	CLA	J	1302	X	-	-	-
18	CLA	K	1001	X	-	-	-
18	CLA	L	1501	X	-	-	-
18	CLA	L	1502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	L	1503	X	-	-	-
22	BCR	3	3503	-	-	X	-
22	BCR	B	6005	-	-	-	X
22	BCR	G	2011	-	-	X	-
22	BCR	L	6019	-	-	X	-
27	LUT	1	1501	X	-	X	-
27	LUT	1	1502	X	-	-	-
27	LUT	2	2501	X	-	X	-
27	LUT	2	2502	X	-	X	-
27	LUT	3	3501	X	-	X	X
27	LUT	3	3502	X	-	X	-
27	LUT	4	4501	X	-	X	-
27	LUT	4	4502	X	-	X	-
27	LUT	4	4503	X	-	X	-
27	LUT	I	6018	X	-	-	-
28	CHL	1	1009	X	-	X	-
28	CHL	1	1010	X	-	-	-
28	CHL	2	2010	X	-	-	-
28	CHL	2	2011	X	-	-	-
28	CHL	2	2013	X	-	-	-
28	CHL	3	3011	X	-	X	-
28	CHL	4	4010	X	-	-	-
28	CHL	4	4011	X	-	-	-
28	CHL	4	4013	X	-	-	-

2 Entry composition i

There are 29 unique types of molecules in this entry. The entry contains 35653 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 I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	742	5852	3833	997	1004	18	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ILE	LEU	engineered mutation	UNP P05310
A	22	LEU	VAL	engineered mutation	UNP P05310
A	117	ARG	GLY	engineered mutation	UNP P05310
A	220	GLY	ARG	engineered mutation	UNP P05310

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	732	5856	3851	995	996	14	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	LEU	ILE	engineered mutation	UNP P05311
B	115	ILE	ASN	engineered mutation	UNP P05311
B	273	MET	VAL	engineered mutation	UNP P05311
B	471	SER	THR	engineered mutation	UNP P05311
B	476	VAL	ILE	engineered mutation	UNP P05311
B	477	LEU	PRO	engineered mutation	UNP P05311
B	635	TYR	ILE	engineered mutation	UNP P05311

- Molecule 3 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	29	224	155	35	33	1	0	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	J	41	321	217	50	54		0	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	150	1187	770	207	208	2	0	0	0

- Molecule 6 is a protein called photosystem I reaction center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	G	91	689	444	117	128		0	0	0

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	L	160	1197	791	190	215	1	0	0	0

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	C	80	612	379	107	115	11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	D	141	1116	720	192	201	3	0	0	0

- Molecule 10 is a protein called Photosystem I reaction center subunit IV A, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	E	66	530	337	93	100	0	0	0

- Molecule 11 is a protein called Photosystem I reaction center subunit VI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	H	84	642	425	97	120	0	0	0

- Molecule 12 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	57	379	241	64	71	3	0	0	0

- Molecule 13 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	2	207	1613	1057	263	289	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	133	LEU	ASN	engineered mutation	UNP Q41038

- Molecule 14 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	4	198	1544	1007	252	282	3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	128	ASP	ALA	engineered mutation	UNP Q9SQL2

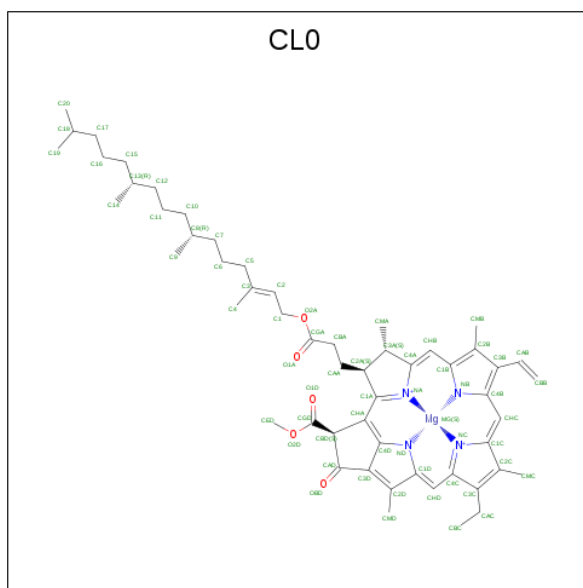
- Molecule 15 is a protein called Light-harvesting complex I chlorophyll A/B-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	1	194	1513	986	254	268	5	0	0	0

- Molecule 16 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

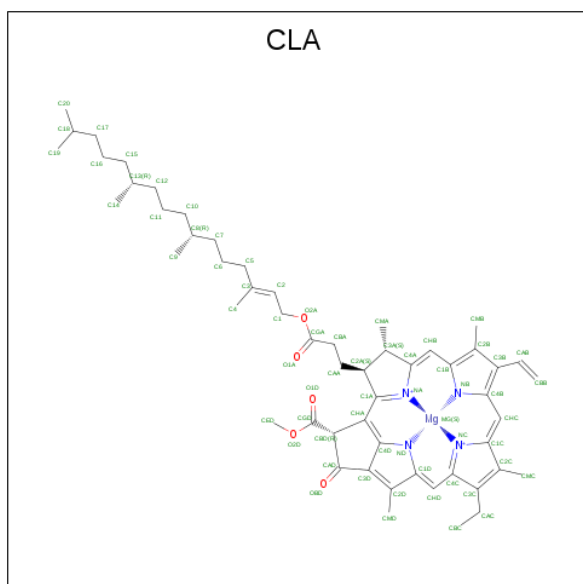
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	3	215	1619	1053	263	298	5	0	0	0

- Molecule 17 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
18	A	1	60	50	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0
18	A	1	55	45	1	4	5	0	0
18	A	1	55	45	1	4	5	0	0
18	A	1	51	41	1	4	5	0	0
18	A	1	56	46	1	4	5	0	0
18	A	1	55	45	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0
18	A	1	46	36	1	4	5	0	0
18	A	1	60	50	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0
18	A	1	46	36	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0
18	A	1	50	40	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0
18	A	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
18	B	1	65	55	1	4	5	0	0
18	B	1	50	40	1	4	5	0	0
18	B	1	65	55	1	4	5	0	0
18	B	1	65	55	1	4	5	0	0
18	B	1	55	45	1	4	5	0	0
18	B	1	46	36	1	4	5	0	0
18	B	1	65	55	1	4	5	0	0
18	B	1	65	55	1	4	5	0	0
18	B	1	55	45	1	4	5	0	0
18	B	1	60	50	1	4	5	0	0
18	B	1	59	49	1	4	5	0	0
18	B	1	60	50	1	4	5	0	0
18	B	1	65	55	1	4	5	0	0
18	B	1	65	55	1	4	5	0	0
18	B	1	65	55	1	4	5	0	0
18	B	1	65	55	1	4	5	0	0
18	B	1	60	50	1	4	5	0	0
18	B	1	65	55	1	4	5	0	0
18	B	1	58	48	1	4	5	0	0
18	B	1	55	45	1	4	5	0	0
18	B	1	60	50	1	4	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
18	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	H	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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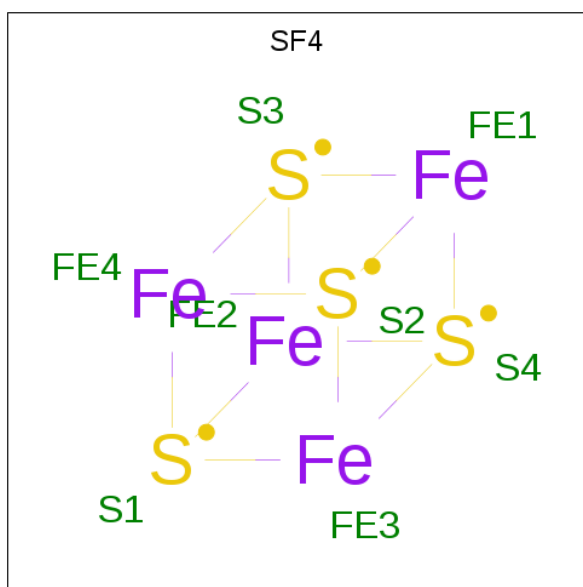
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	2	1	Total	C	Mg	N	0	0	
			27	22	1	4			
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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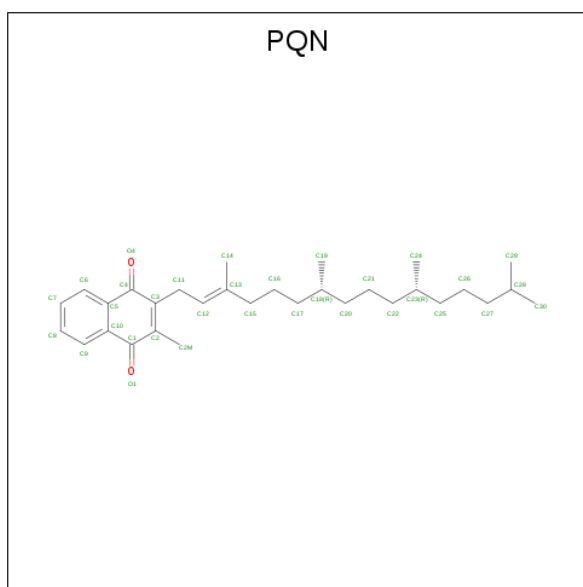
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N		0	0
			27	22	1	4			

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total Fe S 8 4 4	0	0
19	C	1	Total Fe S 8 4 4	0	0
19	C	1	Total Fe S 8 4 4	0	0

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



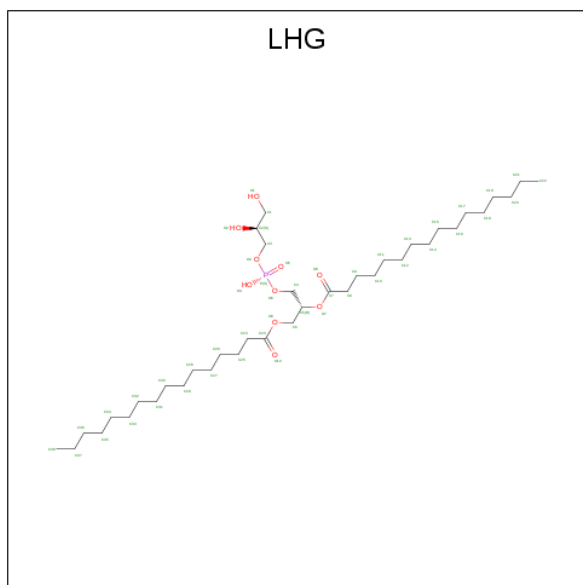
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 33 31 2	0	0

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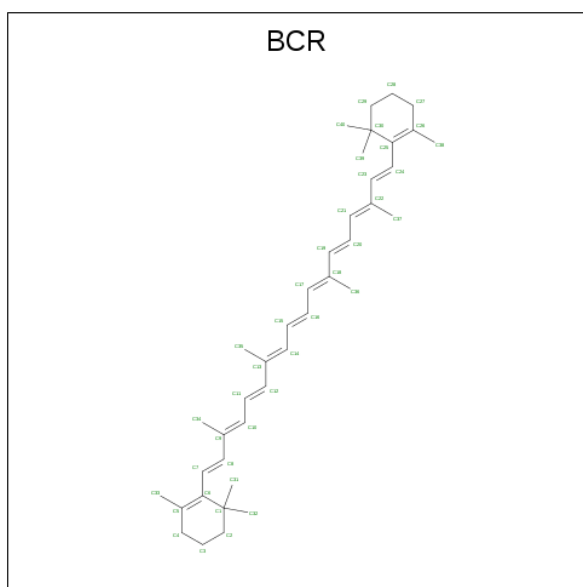
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	B	1	33	31	2	0	0

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
21	A	1	40	29	10	1	0	0
21	A	1	49	38	10	1	0	0
21	B	1	21	10	10	1	0	0
21	2	1	24	13	10	1	0	0
21	1	1	49	38	10	1	0	0

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



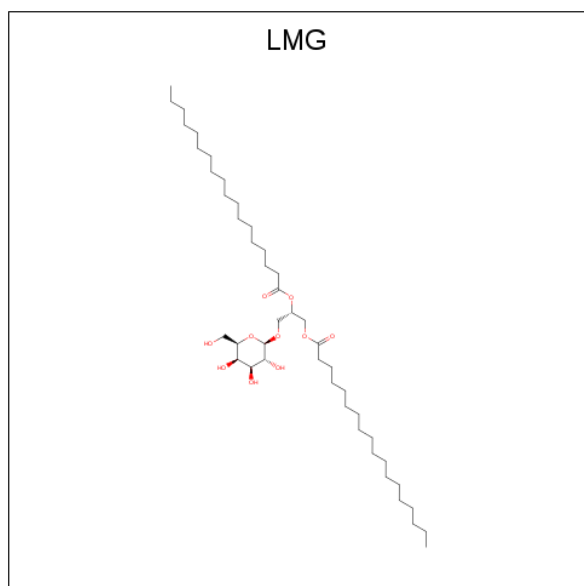
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	3	1	Total C 40 40	0	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 38 28 10	0	0
23	J	1	Total C O 55 45 10	0	0
23	F	1	Total C O 23 13 10	0	0
23	F	1	Total C O 37 27 10	0	0

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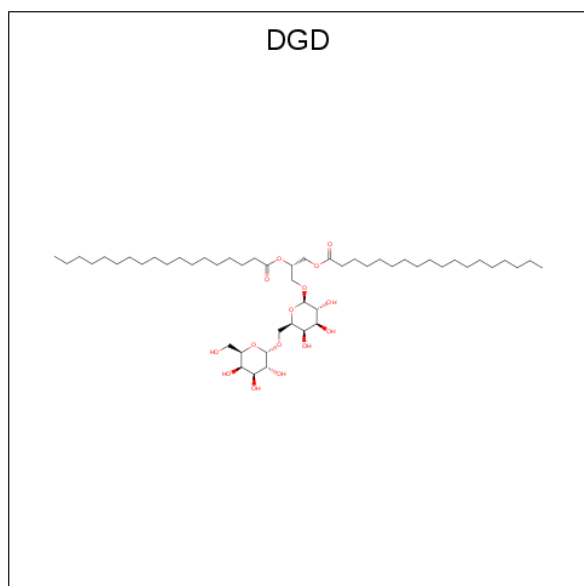
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	G	1	Total	C	O	0	0
			41	31	10		
23	2	1	Total	C	O	0	0
			35	25	10		
23	4	1	Total	C	O	0	0
			35	25	10		

- Molecule 24 is CALCIUM ION (three-letter code: CA) (formula: Ca).

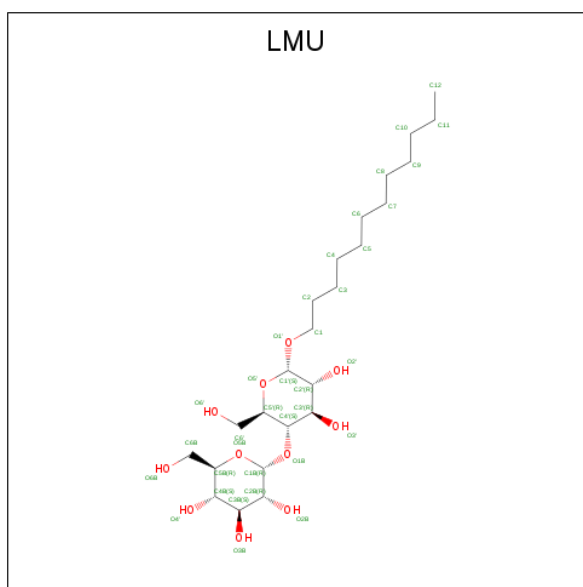
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	B	1	Total	Ca	0	0
			1	1		

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



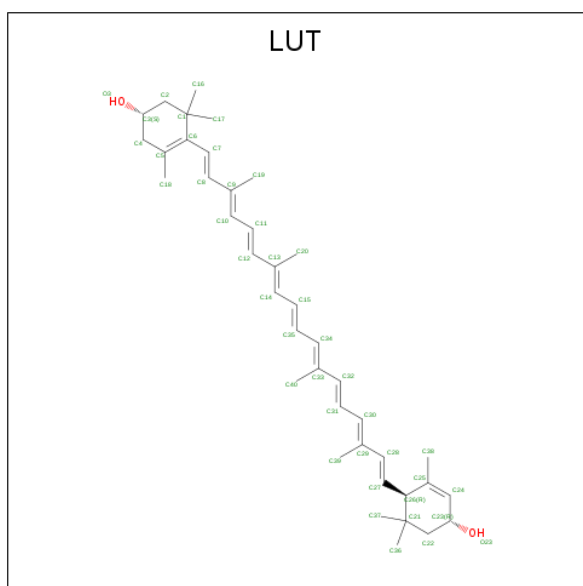
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			61	46	15		

- Molecule 26 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	B	1	Total	C O	0	0
			35	24 11		
26	B	1	Total	C O	0	0
			35	24 11		

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



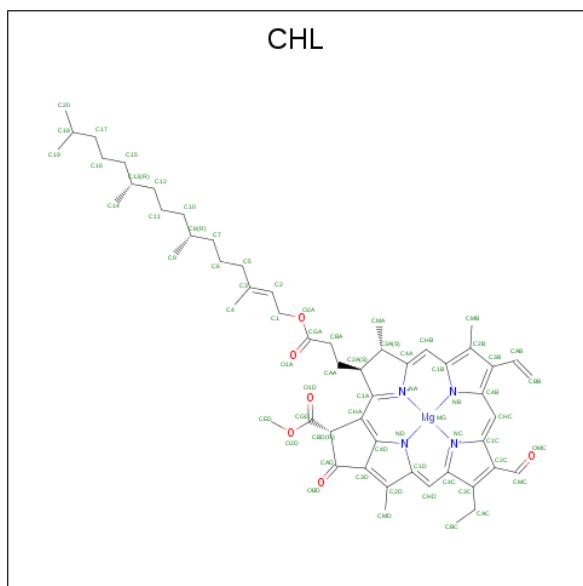
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	I	1	Total	C O	0	0
			42	40 2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	2	1	Total	C	O	0	0
			42	40	2		
27	2	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	1	1	Total	C	O	0	0
			42	40	2		
27	1	1	Total	C	O	0	0
			42	40	2		
27	3	1	Total	C	O	0	0
			42	40	2		
27	3	1	Total	C	O	0	0
			42	40	2		

- Molecule 28 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



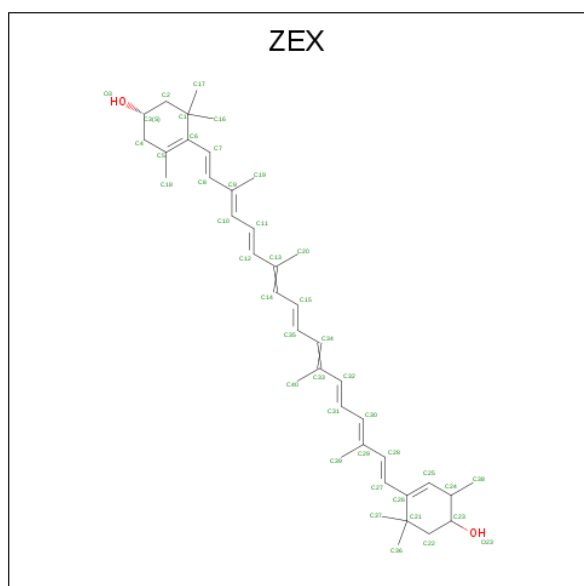
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
28	2	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	3	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		

- Molecule 29 is (1R,2S)-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl]-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: C₄₀H₅₆O₂).

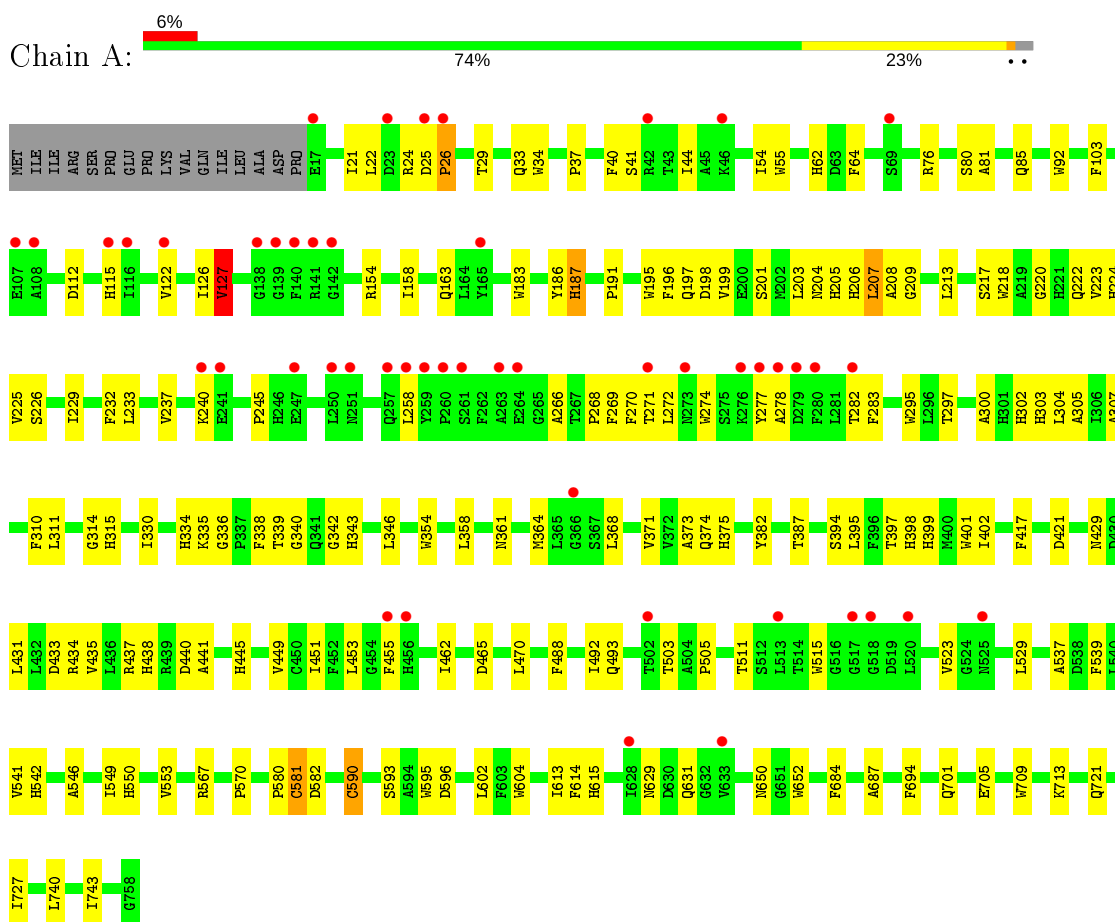


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	4	1	Total	C	O	0	0
			42	40	2		

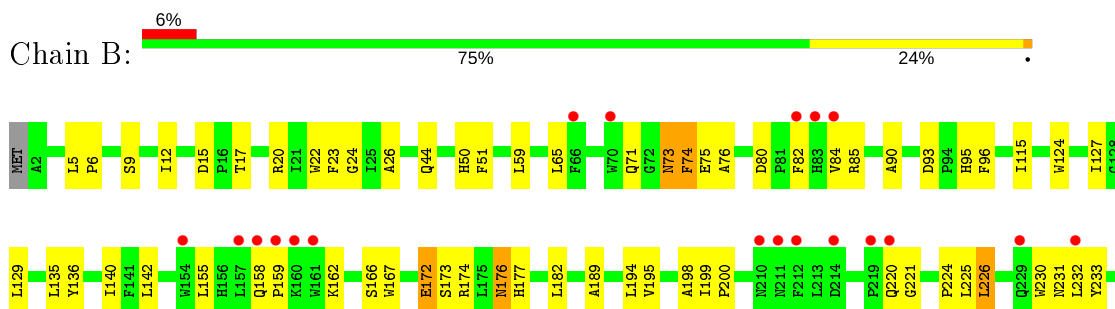
3 Residue-property plots

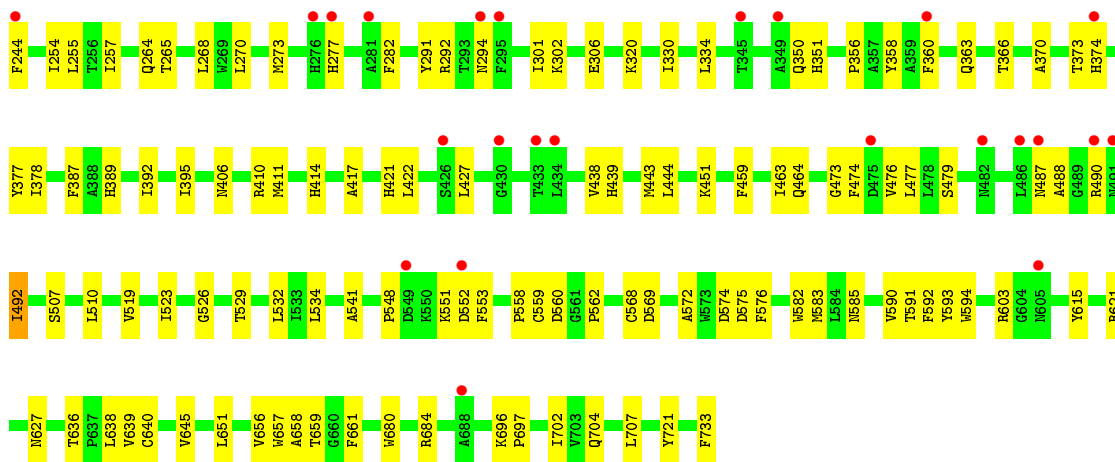
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 I P700 chlorophyll a apoprotein A1

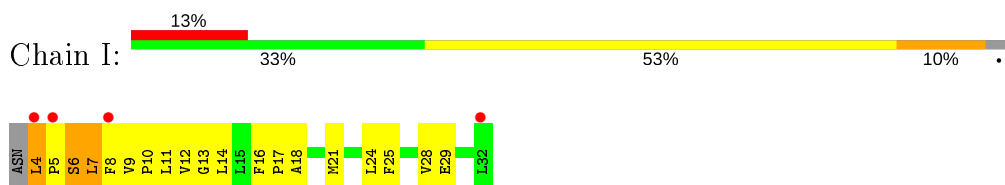


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

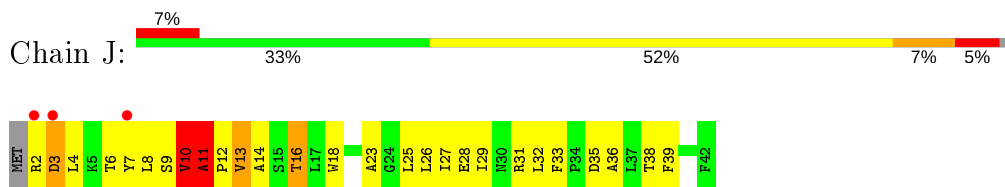




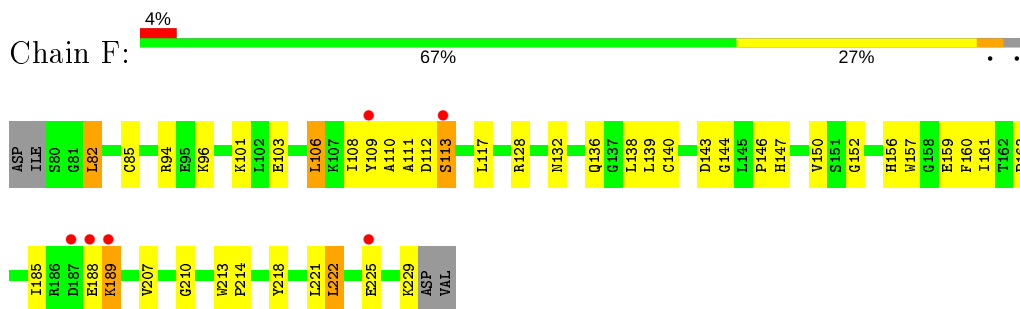
• Molecule 3: Photosystem I reaction center subunit VIII



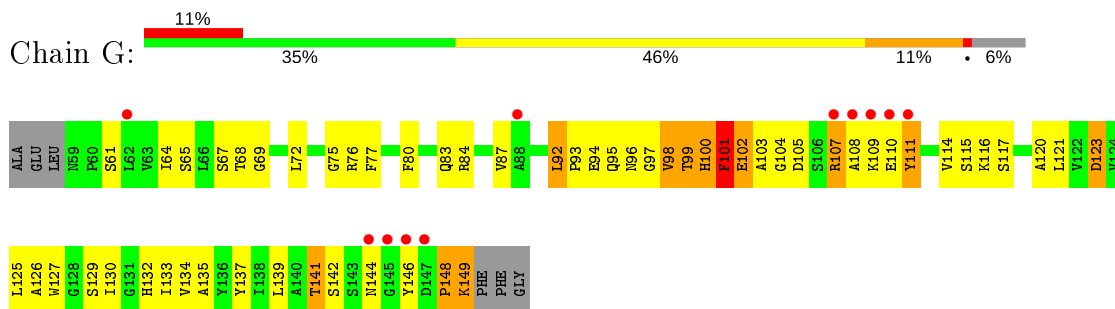
• Molecule 4: Photosystem I reaction center subunit IX



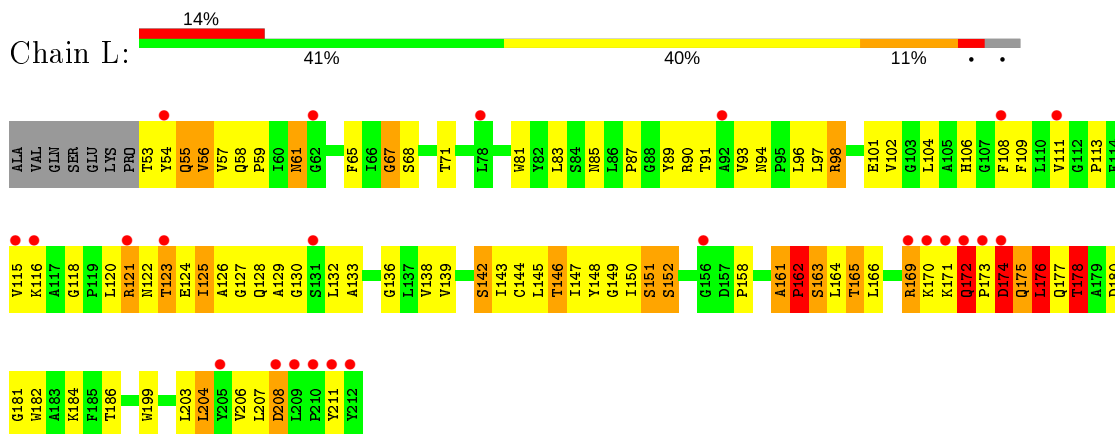
• Molecule 5: Photosystem I reaction center subunit III



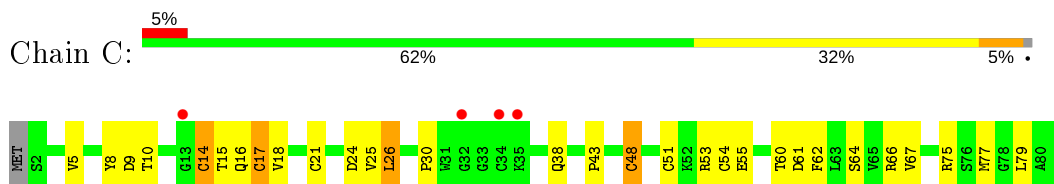
• Molecule 6: photosystem I reaction center



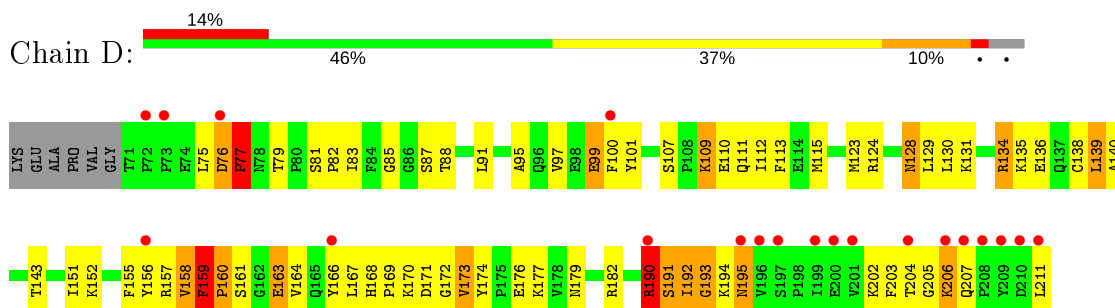
- Molecule 7: Putative uncharacterized protein



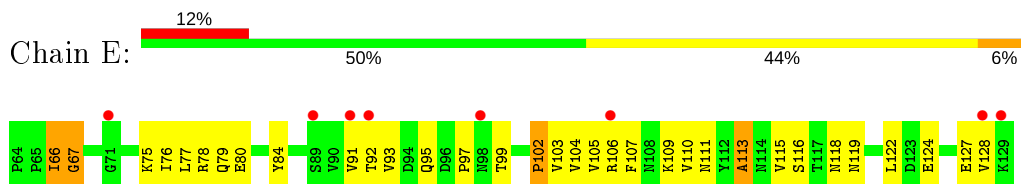
- Molecule 8: Photosystem I iron-sulfur center



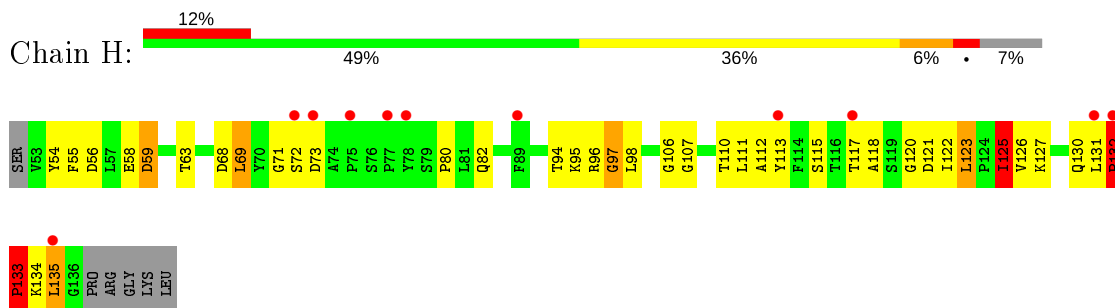
- Molecule 9: Photosystem I reaction center subunit II, chloroplastic



- Molecule 10: Photosystem I reaction center subunit IV A, chloroplastic

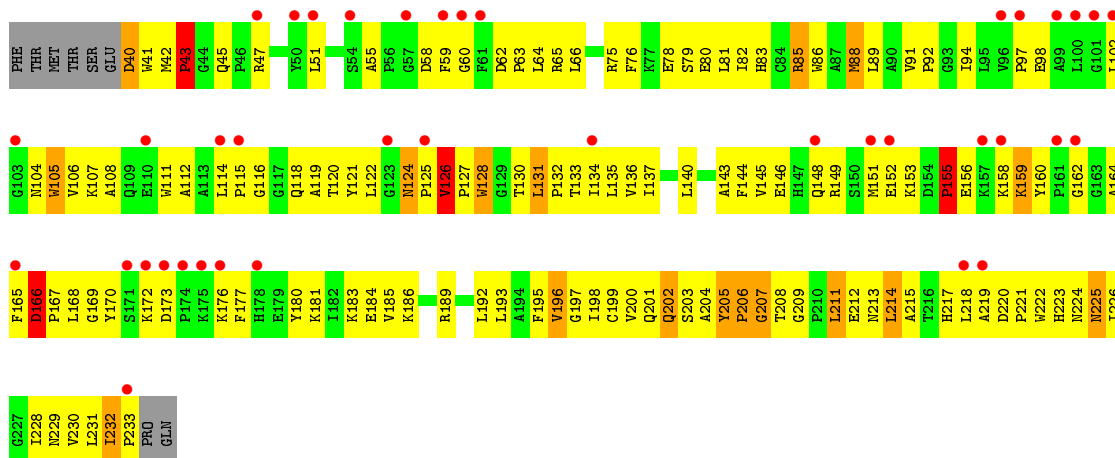


- Molecule 11: Photosystem I reaction center subunit VI





• Molecule 15: Light-harvesting complex I chlorophyll A/B-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	189.00Å 201.90Å 213.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.80 39.89 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.65-2.80) 88.8 (39.89-2.79)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.81Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.259 , 0.268 0.243 , 0.255	Depositor DCC
R_{free} test set	3977 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtrriage
Anisotropy	0.306	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	35653	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: LHG, LUT, DGD, SF4, CHL, CLA, PQN, LMU, ZEX, CL0, CA, BCR, 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	0.23	0/6049	0.40	0/8253
2	B	0.24	0/6067	0.40	0/8287
3	I	0.92	0/230	1.02	2/313 (0.6%)
4	J	0.76	0/330	0.90	2/452 (0.4%)
5	F	0.62	0/1214	0.64	0/1638
6	G	0.78	0/705	1.01	3/956 (0.3%)
7	L	0.76	0/1233	0.94	7/1690 (0.4%)
8	C	0.82	0/625	0.81	1/846 (0.1%)
9	D	1.00	0/1146	1.06	7/1550 (0.5%)
10	E	0.89	0/542	0.90	3/737 (0.4%)
11	H	0.62	0/662	0.85	4/902 (0.4%)
12	K	0.48	0/381	0.87	1/517 (0.2%)
13	2	0.94	2/1672 (0.1%)	1.09	11/2292 (0.5%)
14	4	0.93	2/1592 (0.1%)	0.99	10/2174 (0.5%)
15	1	0.86	0/1563	1.04	6/2132 (0.3%)
16	3	0.86	2/1666 (0.1%)	1.08	11/2265 (0.5%)
All	All	0.63	6/25677 (0.0%)	0.76	68/35004 (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
6	G	0	1
7	L	0	1
13	2	0	1
14	4	0	1
16	3	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	153	GLU	C-O	-10.68	1.03	1.23
13	2	164	GLU	C-O	-10.38	1.03	1.23
16	3	205	GLY	C-N	7.70	1.48	1.34
16	3	205	GLY	C-O	-7.23	1.12	1.23
13	2	164	GLU	C-N	6.29	1.44	1.33
14	4	154	ILE	C-N	5.62	1.47	1.34

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	101	PHE	C-N-CA	11.02	149.25	121.70
6	G	100	HIS	N-CA-C	-10.25	83.33	111.00
13	2	165	GLY	N-CA-C	-9.45	89.48	113.10
11	H	120	GLY	N-CA-C	-8.68	91.41	113.10
16	3	206	PRO	CA-N-CD	-8.59	99.47	111.50
13	2	164	GLU	CA-C-N	-8.50	99.19	116.20
13	2	190	GLY	N-CA-C	-8.41	92.06	113.10
15	1	155	PRO	CA-N-CD	-8.14	100.10	111.50
16	3	205	GLY	CA-C-N	-8.10	94.42	117.10
14	4	153	GLU	CA-C-N	-8.02	99.56	117.20
7	L	174	ASP	N-CA-C	7.89	132.29	111.00
16	3	205	GLY	CA-C-O	7.72	134.49	120.60
14	4	153	GLU	O-C-N	-7.71	110.37	122.70
13	2	180	ASP	N-CA-C	-7.57	90.56	111.00
13	2	165	GLY	CA-C-N	-7.52	100.66	117.20
13	2	165	GLY	C-N-CA	-7.50	102.95	121.70
15	1	43	PRO	CA-N-CD	-7.31	101.27	111.50
15	1	207	GLY	N-CA-C	-7.10	95.35	113.10
10	E	113	ALA	N-CA-C	-6.98	92.17	111.00
13	2	165	GLY	O-C-N	6.97	133.86	122.70
9	D	173	VAL	CB-CA-C	-6.87	98.35	111.40
14	4	154	ILE	N-CA-C	-6.82	92.60	111.00
16	3	249	GLY	N-CA-C	-6.78	96.14	113.10
13	2	164	GLU	O-C-N	-6.70	111.81	123.20
16	3	205	GLY	O-C-N	-6.50	108.74	121.10
15	1	43	PRO	N-CA-C	6.32	128.52	112.10
16	3	134	LEU	N-CA-C	-6.24	94.14	111.00
13	2	148	ASP	N-CA-C	6.19	127.72	111.00
7	L	55	GLN	N-CA-C	5.95	127.07	111.00
11	H	132	PRO	C-N-CD	5.95	140.89	128.40
16	3	208	PHE	C-N-CA	-5.79	107.23	121.70
13	2	147	THR	N-CA-C	5.77	126.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	190	ARG	N-CA-C	-5.72	95.56	111.00
7	L	176	LEU	N-CA-C	-5.71	95.60	111.00
14	4	154	ILE	C-N-CA	-5.70	107.45	121.70
11	H	133	PRO	CA-N-CD	-5.67	103.56	111.50
7	L	175	GLN	N-CA-C	5.61	126.14	111.00
10	E	66	ILE	N-CA-C	5.57	126.04	111.00
9	D	193	GLY	N-CA-C	-5.55	99.23	113.10
9	D	77	PRO	CA-N-CD	-5.55	103.73	111.50
14	4	198	LEU	N-CA-C	-5.55	96.02	111.00
11	H	132	PRO	CA-N-CD	-5.54	103.74	111.50
8	C	17	CYS	CA-CB-SG	-5.45	104.19	114.00
15	1	166	ASP	C-N-CD	5.39	139.72	128.40
15	1	232	ILE	C-N-CD	5.39	139.72	128.40
9	D	159	PHE	C-N-CD	5.36	139.66	128.40
7	L	178	THR	N-CA-C	-5.29	96.72	111.00
14	4	177	LEU	C-N-CD	5.28	139.50	128.40
16	3	64	SER	N-CA-C	5.27	125.24	111.00
14	4	180	GLY	N-CA-C	5.27	126.28	113.10
4	J	39	PHE	C-N-CD	5.27	139.46	128.40
16	3	262	ASP	C-N-CD	5.25	139.42	128.40
7	L	172	GLN	C-N-CD	5.25	139.41	128.40
7	L	161	ALA	C-N-CD	5.24	139.41	128.40
16	3	85	ASP	C-N-CD	5.23	139.39	128.40
9	D	158	VAL	N-CA-C	5.20	125.03	111.00
9	D	134	ARG	N-CA-C	5.16	124.93	111.00
13	2	61	GLU	C-N-CD	5.14	139.19	128.40
12	K	86	ALA	C-N-CD	5.14	139.19	128.40
16	3	118	ALA	C-N-CD	5.13	139.18	128.40
14	4	190	ASN	C-N-CD	5.11	139.13	128.40
14	4	228	GLY	C-N-CD	5.10	139.10	128.40
3	I	16	PHE	C-N-CD	5.09	139.09	128.40
6	G	98	VAL	N-CA-C	5.07	124.69	111.00
3	I	7	LEU	CA-CB-CG	-5.06	103.65	115.30
14	4	239	ASP	C-N-CD	5.06	139.02	128.40
10	E	67	GLY	C-N-CD	5.03	138.95	128.40
4	J	11	ALA	C-N-CD	5.00	138.91	128.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	2	164	GLU	Mainchain

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Mol	Chain	Res	Type	Group
16	3	205	GLY	Mainchain
14	4	153	GLU	Mainchain
6	G	101	PHE	Peptide
7	L	98	ARG	Sidechain

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5852	0	5710	169	0
2	B	5856	0	5666	146	0
3	I	224	0	247	34	0
4	J	321	0	328	48	0
5	F	1187	0	1226	39	3
6	G	689	0	675	112	0
7	L	1197	0	1187	165	3
8	C	612	0	594	36	0
9	D	1116	0	1126	103	0
10	E	530	0	530	44	0
11	H	642	0	637	48	0
12	K	379	0	386	92	0
13	2	1613	0	1554	371	0
14	4	1544	0	1489	230	0
15	1	1513	0	1495	379	0
16	3	1619	0	1554	472	0
17	A	65	0	72	6	0
18	1	615	0	511	235	0
18	2	628	0	538	255	0
18	3	698	0	559	265	0
18	4	677	0	635	195	0
18	A	2583	0	2555	197	0
18	B	2519	0	2617	217	0
18	F	95	0	72	20	0
18	G	161	0	141	92	0
18	H	46	0	33	4	0
18	J	50	0	39	7	0
18	K	46	0	33	12	0
18	L	160	0	137	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	8	0	0	1	0
19	C	16	0	0	0	0
20	A	33	0	46	3	0
20	B	33	0	46	5	0
21	1	49	0	74	15	0
21	2	24	0	18	6	0
21	A	89	0	127	12	0
21	B	21	0	12	1	0
22	3	40	0	48	21	0
22	A	240	0	292	21	0
22	B	200	0	245	24	0
22	F	80	0	98	19	0
22	G	40	0	49	29	0
22	I	40	0	49	3	0
22	J	80	0	98	15	0
22	K	40	0	49	17	0
22	L	80	0	98	28	0
23	2	35	0	40	9	0
23	4	35	0	40	6	0
23	B	38	0	46	3	0
23	F	60	0	60	13	0
23	G	41	0	52	20	0
23	J	55	0	86	9	0
24	B	1	0	0	0	0
25	B	61	0	83	4	0
26	B	70	0	92	4	0
27	1	84	0	110	48	0
27	2	84	0	110	55	0
27	3	84	0	110	62	0
27	4	126	0	165	84	0
27	I	42	0	55	14	0
28	1	103	0	78	35	0
28	2	141	0	95	39	0
28	3	56	0	47	22	0
28	4	145	0	99	44	0
29	4	42	0	56	12	0
All	All	35653	0	35119	3560	3

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 50.

All (3560) 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)
16:3:138:GLN:HB2	16:3:145:ALA:HB2	1.25	1.18
18:3:3012:CLA:HBB1	18:3:3012:CLA:HMB1	1.18	1.17
16:3:268:VAL:HG21	18:3:3003:CLA:H43	1.17	1.16
18:3:3004:CLA:HBB1	18:3:3004:CLA:HMB1	1.25	1.15
16:3:111:LEU:HD22	18:3:3006:CLA:CBB	1.74	1.15
16:3:127:LEU:HB2	18:3:3018:CLA:HBC1	1.29	1.15
7:L:85:ASN:HB3	18:L:1501:CLA:HAC1	1.26	1.14
18:4:4009:CLA:HHC	18:4:4009:CLA:HBB1	1.28	1.14
27:4:4502:LUT:H28	27:4:4502:LUT:H381	1.27	1.13
18:2:2012:CLA:HMB1	18:2:2012:CLA:HBB1	1.27	1.13
13:2:122:ILE:HG23	13:2:133:LEU:HB2	1.31	1.12
18:2:2002:CLA:HMC1	18:2:2002:CLA:HBC2	1.30	1.12
13:2:139:THR:H	28:2:2010:CHL:CED	1.61	1.12
18:2:2001:CLA:H42	18:2:2002:CLA:HBA1	1.30	1.12
12:K:69:ILE:HA	18:K:1001:CLA:O1A	1.50	1.12
22:K:2011:BCR:HC8	22:K:2011:BCR:H321	1.31	1.12
18:4:4007:CLA:HBB1	18:4:4007:CLA:HHC	1.30	1.12
14:4:118:ILE:HD13	14:4:120:ILE:HD11	1.33	1.11
13:2:126:LEU:HB3	13:2:133:LEU:HD13	1.32	1.11
7:L:113:PRO:HG3	18:L:1503:CLA:HBB1	1.21	1.11
18:2:2004:CLA:H52	27:2:2502:LUT:H383	1.32	1.10
13:2:131:ILE:HD12	13:2:133:LEU:HD21	1.15	1.10
18:4:4001:CLA:H12	27:4:4501:LUT:H373	1.24	1.10
16:3:206:PRO:HD2	16:3:207:PHE:HB2	1.17	1.10
18:3:3010:CLA:HMB1	18:3:3013:CLA:HAB	1.16	1.10
7:L:58:GLN:HG3	7:L:59:PRO:HD2	1.35	1.09
18:1:1003:CLA:HBB1	18:1:1003:CLA:H92	1.11	1.09
4:J:2:ARG:HE	4:J:4:LEU:HD12	1.17	1.08
7:L:145:LEU:HD11	22:L:6019:BCR:H392	1.34	1.08
18:2:2016:CLA:HBB1	18:2:2016:CLA:HHC	1.33	1.08
27:4:4503:LUT:H181	27:4:4503:LUT:H8	1.31	1.08
18:G:1001:CLA:H62	22:G:2011:BCR:H343	1.28	1.08
18:G:1001:CLA:HHC	18:G:1001:CLA:HBB1	1.31	1.07
15:1:114:LEU:HD23	15:1:115:PRO:HD2	1.25	1.07
18:4:4002:CLA:H12	18:4:4002:CLA:HMA2	1.13	1.07
18:2:2009:CLA:HHC	18:2:2009:CLA:HBB1	1.27	1.07
13:2:223:LYS:NZ	21:2:2801:LHG:O5	1.88	1.07
16:3:94:GLU:OE2	16:3:96:ARG:N	1.86	1.07
13:2:87:PHE:CZ	27:2:2502:LUT:H372	1.89	1.06
11:H:96:ARG:HG2	11:H:97:GLY:H	1.19	1.06
13:2:70:GLY:O	16:3:178:LYS:NZ	1.88	1.06
13:2:166:ARG:NH1	18:4:4009:CLA:OBD	1.88	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:149:ARG:NH2	18:1:1012:CLA:O1D	1.87	1.06
6:G:92:LEU:HD12	6:G:92:LEU:H	1.19	1.06
28:1:1010:CHL:HMC	28:1:1010:CHL:HBC3	1.38	1.05
18:2:2006:CLA:HBD	18:2:2006:CLA:H43	1.35	1.05
16:3:111:LEU:CD2	18:3:3006:CLA:HBB2	1.84	1.05
16:3:111:LEU:CD2	18:3:3006:CLA:CBB	2.34	1.05
12:K:137:VAL:HA	12:K:140:LEU:HD22	1.35	1.05
12:K:78:LEU:HD22	12:K:82:ARG:HG2	1.06	1.05
18:F:1302:CLA:HHD	18:F:1302:CLA:HBC2	1.35	1.04
14:4:170:PRO:HB2	18:4:4016:CLA:HMA3	1.06	1.04
7:L:94:ASN:HB2	7:L:97:LEU:HD12	1.34	1.04
18:2:2008:CLA:HHD	18:2:2008:CLA:HBC3	1.38	1.03
15:1:97:PRO:HB2	15:1:102:LEU:HB2	1.35	1.03
18:2:2001:CLA:C4	18:2:2002:CLA:HBA1	1.89	1.03
13:2:188:LEU:HD23	13:2:198:GLY:HA3	1.39	1.03
18:3:3003:CLA:H42	18:3:3003:CLA:C1D	1.88	1.03
18:4:4007:CLA:HBC2	18:4:4007:CLA:HHD	1.37	1.03
7:L:176:LEU:HD12	7:L:177:GLN:H	1.23	1.03
13:2:186:ASN:ND2	18:2:2016:CLA:O1D	1.90	1.03
16:3:164:LEU:HB3	22:3:3503:BCR:H351	1.41	1.02
12:K:72:ALA:HB3	18:K:1001:CLA:O2A	1.60	1.02
14:4:150:HIS:HA	18:4:4012:CLA:HAB	1.40	1.02
18:3:3002:CLA:HHC	18:3:3002:CLA:HBB1	1.42	1.02
13:2:186:ASN:HB3	18:2:2016:CLA:HMA3	1.40	1.02
18:3:3008:CLA:HHC	18:3:3008:CLA:HBB1	1.42	1.01
15:1:114:LEU:CD2	15:1:115:PRO:HD2	1.90	1.01
15:1:85:ARG:HB3	18:1:1001:CLA:HBC3	1.04	1.01
27:3:3501:LUT:H8	27:3:3501:LUT:H161	1.35	1.01
14:4:169:ASP:HB3	18:4:4016:CLA:C3D	1.90	1.01
13:2:114:MET:HE3	18:2:2001:CLA:HMC3	1.04	1.01
13:2:188:LEU:HD23	13:2:198:GLY:CA	1.89	1.01
21:1:1801:LHG:C38	21:1:1801:LHG:H223	1.90	1.00
14:4:63:PRO:HD2	14:4:66:LEU:HD12	1.40	1.00
10:E:66:ILE:HG22	10:E:95:GLN:HE22	1.25	1.00
13:2:200:TRP:NE1	18:2:2016:CLA:HAA2	1.76	1.00
13:2:244:THR:HG22	13:2:245:GLY:H	1.25	1.00
8:C:8:TYR:HB3	9:D:191:SER:CB	1.90	1.00
7:L:94:ASN:CB	7:L:97:LEU:HD12	1.91	1.00
13:2:122:ILE:CG2	13:2:133:LEU:HB2	1.90	1.00
15:1:209:GLY:HA3	15:1:212:GLU:HB3	1.44	1.00
16:3:65:LEU:HD13	16:3:67:TYR:CE1	1.96	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:1003:CLA:H51	23:G:2021:LMG:H311	1.42	1.00
18:3:3008:CLA:HBC2	18:3:3008:CLA:HHD	1.41	0.99
18:2:2001:CLA:H11	27:2:2501:LUT:H173	1.44	0.99
28:4:4010:CHL:HHD	28:4:4010:CHL:HBC2	1.42	0.99
12:K:78:LEU:HD22	12:K:82:ARG:CG	1.91	0.99
15:1:183:LYS:HD3	18:1:1002:CLA:HAA2	1.40	0.99
15:1:183:LYS:HG3	18:1:1007:CLA:HED2	1.41	0.99
16:3:205:GLY:HA3	16:3:208:PHE:CA	1.89	0.99
16:3:241:TYR:CE1	27:3:3501:LUT:H162	1.97	0.99
18:2:2016:CLA:HBA2	18:2:2016:CLA:HBD	1.43	0.99
18:3:3005:CLA:H93	18:3:3012:CLA:H43	1.44	0.99
15:1:85:ARG:CB	18:1:1001:CLA:HBC3	1.93	0.99
15:1:183:LYS:HD3	18:1:1002:CLA:CAA	1.92	0.99
6:G:108:ALA:HB1	6:G:111:TYR:CD1	1.98	0.98
13:2:262:ILE:HD11	18:2:2003:CLA:H11	1.45	0.98
16:3:268:VAL:HG23	18:3:3003:CLA:H12	1.41	0.98
18:3:3018:CLA:HBB1	18:3:3018:CLA:HMB1	1.45	0.98
15:1:88:MET:HB2	18:1:1001:CLA:HMC3	1.45	0.98
10:E:122:LEU:H	10:E:122:LEU:HD12	1.25	0.98
13:2:139:THR:H	28:2:2010:CHL:HED1	1.29	0.97
13:2:219:THR:HG22	18:2:2007:CLA:HED3	1.43	0.97
12:K:124:ALA:HB1	22:K:2011:BCR:HC7	1.46	0.97
15:1:97:PRO:CB	15:1:102:LEU:HB2	1.93	0.97
15:1:221:PRO:HG2	15:1:222:TRP:CE3	1.98	0.97
22:G:2011:BCR:H403	22:G:2011:BCR:H23C	1.43	0.97
16:3:138:GLN:CB	16:3:145:ALA:HB2	1.94	0.97
13:2:114:MET:HE3	18:2:2001:CLA:CMC	1.93	0.97
18:4:4003:CLA:HHC	18:4:4003:CLA:HBB1	1.46	0.97
13:2:220:LYS:HD3	18:2:2002:CLA:HED2	1.44	0.97
7:L:145:LEU:HD21	22:L:6019:BCR:H403	1.44	0.97
7:L:87:PRO:CD	18:L:1502:CLA:HED2	1.94	0.97
18:1:1008:CLA:HBB1	18:1:1008:CLA:HHC	1.47	0.96
16:3:205:GLY:HA3	16:3:208:PHE:CB	1.95	0.96
29:4:4505:ZEX:H362	29:4:4505:ZEX:H382	1.46	0.96
15:1:98:GLU:CB	15:1:211:LEU:HD21	1.94	0.96
14:4:153:GLU:OE2	14:4:156:ARG:NH1	1.98	0.96
7:L:138:VAL:O	7:L:142:SER:OG	1.84	0.96
13:2:126:LEU:HB3	13:2:133:LEU:CD1	1.96	0.95
18:2:2006:CLA:CBD	18:2:2006:CLA:H43	1.96	0.95
16:3:111:LEU:HD22	18:3:3006:CLA:HBB2	0.97	0.95
2:B:50:HIS:HB3	18:B:1210:CLA:HED3	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2001:CLA:HMB1	18:2:2001:CLA:HBB1	1.47	0.95
3:I:4:LEU:HD11	3:I:6:SER:HB2	1.48	0.95
18:4:4008:CLA:HAA1	18:4:4008:CLA:C1	1.96	0.95
9:D:192:ILE:HG22	9:D:193:GLY:H	1.29	0.95
13:2:230:LEU:HD21	18:2:2004:CLA:HMC1	1.44	0.95
16:3:205:GLY:HA3	16:3:208:PHE:HB2	1.47	0.95
13:2:116:GLY:HA2	27:2:2502:LUT:H181	1.48	0.95
18:4:4002:CLA:C1	18:4:4002:CLA:HMA2	1.96	0.94
13:2:126:LEU:HD12	13:2:127:THR:N	1.82	0.94
13:2:87:PHE:CE2	27:2:2502:LUT:H363	2.03	0.94
15:1:222:TRP:CH2	18:1:1008:CLA:HMB3	2.03	0.94
18:4:4001:CLA:C1	27:4:4501:LUT:H373	1.97	0.94
13:2:188:LEU:HD22	13:2:189:THR:N	1.82	0.94
18:4:4007:CLA:CED	18:4:4007:CLA:H2A	1.98	0.93
13:2:106:GLU:O	13:2:110:SER:OG	1.85	0.93
18:3:3010:CLA:CMB	18:3:3013:CLA:HAB	1.97	0.93
12:K:137:VAL:HA	12:K:140:LEU:CD2	1.97	0.93
13:2:220:LYS:N	18:2:2007:CLA:HED1	1.83	0.93
15:1:232:ILE:HG23	15:1:233:PRO:HD2	1.46	0.93
13:2:193:VAL:HG23	13:2:194:GLY:H	1.30	0.93
15:1:202:GLN:NE2	15:1:208:THR:HB	1.84	0.93
13:2:115:LEU:HB3	18:2:2006:CLA:HBB2	1.51	0.93
28:4:4011:CHL:HBC2	28:4:4011:CHL:HHD	1.48	0.93
16:3:136:TRP:O	27:3:3502:LUT:O3	1.85	0.92
14:4:103:MET:HE1	14:4:207:ASN:HB3	1.51	0.92
16:3:209:ASN:OD1	27:3:3501:LUT:O23	1.85	0.92
6:G:77:PHE:HE1	18:G:1002:CLA:HAB	1.33	0.92
14:4:118:ILE:HD13	14:4:120:ILE:CD1	2.00	0.92
16:3:241:TYR:HE1	27:3:3501:LUT:H162	1.28	0.92
4:J:28:GLU:OE1	18:J:1302:CLA:C4D	2.17	0.92
15:1:121:TYR:CD2	15:1:122:LEU:HG	2.04	0.92
13:2:186:ASN:CB	18:2:2016:CLA:HMA3	2.00	0.92
18:1:1011:CLA:C3	27:1:1501:LUT:H23	2.00	0.91
18:2:2003:CLA:HHB	18:2:2008:CLA:HBC3	1.53	0.91
12:K:71:VAL:HG11	12:K:129:GLY:O	1.70	0.91
16:3:206:PRO:HD2	16:3:207:PHE:CB	2.00	0.91
27:4:4501:LUT:H28	27:4:4501:LUT:H371	1.53	0.91
18:3:3010:CLA:HBB1	18:3:3010:CLA:HHC	1.51	0.91
18:2:2007:CLA:H92	18:2:2007:CLA:H51	1.53	0.91
14:4:103:MET:HE3	14:4:207:ASN:C	1.90	0.91
9:D:76:ASP:HB3	9:D:77:PRO:HB3	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:131:ILE:CD1	13:2:133:LEU:HD21	2.00	0.91
18:1:1004:CLA:CBB	27:1:1502:LUT:H12	2.01	0.91
18:1:1003:CLA:CBB	18:1:1003:CLA:H92	2.00	0.90
15:1:126:VAL:HG23	15:1:127:PRO:HA	1.53	0.90
14:4:170:PRO:CB	18:4:4016:CLA:HMA3	1.99	0.90
16:3:184:LYS:HG2	16:3:185:GLN:HG2	1.54	0.90
18:1:1008:CLA:HED2	18:1:1008:CLA:C3D	2.00	0.90
18:2:2005:CLA:HBC1	18:2:2012:CLA:HBC1	1.52	0.90
18:1:1003:CLA:CGA	18:1:1008:CLA:HED1	2.00	0.90
15:1:127:PRO:HG2	15:1:128:TRP:CD1	2.07	0.90
13:2:163:ALA:O	13:2:166:ARG:HB3	1.72	0.90
13:2:211:PRO:O	13:2:212:GLN:HG3	1.70	0.90
14:4:125:LYS:NZ	14:4:231:ASP:OD1	2.03	0.90
22:J:6012:BCR:H23C	22:J:6012:BCR:H383	1.51	0.90
16:3:102:GLU:OE2	16:3:232:ARG:NH2	2.04	0.90
18:B:1229:CLA:HAB	18:B:1230:CLA:HMB2	1.54	0.90
18:1:1001:CLA:HHC	27:1:1501:LUT:H32	1.54	0.90
18:2:2004:CLA:H8	27:2:2502:LUT:C38	2.00	0.90
18:2:2004:CLA:H8	27:2:2502:LUT:H381	1.53	0.90
27:4:4503:LUT:H363	28:1:1009:CHL:H8	1.53	0.89
13:2:115:LEU:CB	18:2:2006:CLA:HBB2	2.02	0.89
16:3:225:LEU:HB3	16:3:226:LYS:NZ	1.87	0.89
15:1:146:GLU:HG2	15:1:149:ARG:HH11	1.35	0.89
18:4:4017:CLA:HED1	21:1:1801:LHG:H151	1.54	0.89
16:3:105:ASN:ND2	18:3:3012:CLA:HMD1	1.88	0.89
16:3:248:THR:HG22	16:3:250:VAL:HG23	1.54	0.89
28:4:4013:CHL:HHD	28:4:4013:CHL:HBC2	1.54	0.89
14:4:158:GLN:HE22	14:4:161:LYS:HE3	1.36	0.89
13:2:70:GLY:HA3	16:3:174:GLN:HE21	1.36	0.89
6:G:103:ALA:O	6:G:105:ASP:N	2.04	0.89
11:H:96:ARG:O	11:H:98:LEU:N	2.05	0.89
15:1:230:VAL:C	15:1:231:LEU:HD23	1.93	0.89
16:3:268:VAL:CG2	18:3:3003:CLA:H43	2.03	0.89
14:4:170:PRO:HB2	18:4:4016:CLA:CMA	1.99	0.89
13:2:120:ILE:HG21	27:2:2501:LUT:C37	2.03	0.89
18:3:3004:CLA:C2	27:3:3502:LUT:H363	2.02	0.89
5:F:221:LEU:C	5:F:222:LEU:HD23	1.94	0.88
18:G:1001:CLA:C6	22:G:2011:BCR:H343	2.03	0.88
18:2:2004:CLA:H52	27:2:2502:LUT:C38	2.03	0.88
14:4:220:ILE:HD12	18:4:4003:CLA:HAC2	1.52	0.88
16:3:203:PRO:HD3	28:3:3011:CHL:HMD2	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:13:GLY:O	3:I:14:LEU:HD23	1.73	0.88
12:K:141:LYS:O	12:K:142:THR:OG1	1.91	0.88
12:K:124:ALA:HB1	22:K:2011:BCR:H331	1.54	0.88
15:1:183:LYS:CG	18:1:1007:CLA:HED2	2.03	0.88
13:2:220:LYS:CD	18:2:2002:CLA:HED2	2.02	0.88
14:4:94:ALA:CA	18:4:4012:CLA:HED2	2.03	0.88
12:K:128:VAL:O	12:K:132:ILE:HG13	1.74	0.88
18:1:1008:CLA:HED2	18:1:1008:CLA:C4D	2.03	0.88
15:1:232:ILE:HG23	15:1:233:PRO:CD	2.02	0.88
13:2:139:THR:N	28:2:2010:CHL:CED	2.37	0.88
16:3:110:MET:CE	16:3:230:ASN:HB3	2.02	0.88
15:1:183:LYS:HD3	18:1:1002:CLA:CBA	2.04	0.88
27:3:3502:LUT:H8	27:3:3502:LUT:H161	1.55	0.88
18:2:2003:CLA:C2B	27:2:2501:LUT:H383	2.03	0.88
18:4:4017:CLA:HMC2	29:4:4505:ZEX:H393	1.54	0.88
18:3:3003:CLA:H42	18:3:3003:CLA:C2D	2.04	0.88
16:3:127:LEU:HB2	18:3:3018:CLA:CBC	2.02	0.88
7:L:121:ARG:CG	7:L:127:GLY:HA2	2.04	0.88
18:1:1005:CLA:HMD2	18:1:1012:CLA:C1D	2.04	0.87
15:1:130:THR:HG22	15:1:132:PRO:CD	2.03	0.87
13:2:219:THR:HG22	18:2:2007:CLA:CED	2.03	0.87
16:3:65:LEU:CB	16:3:68:LEU:HD21	2.03	0.87
10:E:66:ILE:HG22	10:E:95:GLN:NE2	1.88	0.87
15:1:186:LYS:NZ	21:1:1801:LHG:O5	2.06	0.87
18:2:2001:CLA:C1	27:2:2501:LUT:H173	2.04	0.87
18:3:3003:CLA:H11	18:3:3003:CLA:C4D	2.03	0.87
18:2:2005:CLA:H41	18:2:2005:CLA:H72	1.56	0.87
28:2:2013:CHL:HHC	28:2:2013:CHL:HBB1	1.57	0.87
9:D:134:ARG:NH2	9:D:136:GLU:OE2	2.05	0.87
4:J:2:ARG:HE	4:J:4:LEU:CD1	1.88	0.87
13:2:124:GLU:O	13:2:127:THR:HG22	1.75	0.87
18:L:1502:CLA:C4C	22:L:6019:BCR:H282	2.04	0.87
15:1:111:TRP:CZ3	18:1:1006:CLA:HED1	2.10	0.87
15:1:183:LYS:HG3	18:1:1007:CLA:CED	2.04	0.87
13:2:70:GLY:HA3	16:3:174:GLN:NE2	1.90	0.86
14:4:115:PHE:O	14:4:118:ILE:HG22	1.73	0.86
18:2:2005:CLA:H41	18:2:2005:CLA:C7	2.03	0.86
14:4:94:ALA:HA	18:4:4012:CLA:HED2	1.57	0.86
5:F:138:LEU:HD23	5:F:159:GLU:OE2	1.74	0.86
15:1:226:ILE:HG21	18:1:1003:CLA:H42	1.56	0.86
15:1:152:GLU:O	15:1:153:LYS:HD3	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1001:CLA:H61	27:1:1501:LUT:C30	2.06	0.86
13:2:120:ILE:O	13:2:123:PRO:HD2	1.74	0.86
28:4:4011:CHL:HBD	28:4:4011:CHL:HAA1	1.57	0.86
28:3:3011:CHL:HBA2	28:3:3011:CHL:HBD	1.58	0.86
13:2:114:MET:CE	18:2:2001:CLA:HMC3	2.00	0.86
16:3:140:GLY:HA2	18:3:3013:CLA:HBC2	1.57	0.86
12:K:65:SER:O	12:K:69:ILE:HG22	1.74	0.86
18:A:1104:CLA:HED1	18:A:1128:CLA:H2	1.58	0.86
1:A:220:GLY:HA3	18:A:1113:CLA:HBB1	1.55	0.86
15:1:132:PRO:O	15:1:136:VAL:HG23	1.75	0.86
15:1:88:MET:HE3	18:1:1001:CLA:HHC	1.57	0.86
15:1:230:VAL:HG13	18:1:1014:CLA:C1B	2.05	0.85
16:3:220:LEU:HD23	16:3:221:LYS:N	1.91	0.85
27:2:2501:LUT:H28	27:2:2501:LUT:H371	1.55	0.85
16:3:236:LEU:HD23	18:3:3004:CLA:HMC1	1.57	0.85
16:3:131:GLU:OE2	18:3:3018:CLA:HMA3	1.76	0.85
2:B:733:PHE:HB3	11:H:134:LYS:HE2	1.58	0.85
18:1:1005:CLA:HBB1	18:1:1005:CLA:HMB1	1.58	0.85
15:1:152:GLU:C	15:1:153:LYS:HD3	1.96	0.85
7:L:146:THR:O	7:L:150:ILE:HG13	1.76	0.85
18:3:3017:CLA:H3A	18:3:3017:CLA:CGA	2.03	0.85
9:D:76:ASP:HB3	9:D:77:PRO:CB	2.07	0.85
28:2:2010:CHL:CBB	28:2:2013:CHL:HBB2	2.05	0.85
6:G:65:SER:OG	18:G:1001:CLA:HBA1	1.75	0.85
13:2:148:ASP:O	13:2:149:THR:HB	1.74	0.85
18:3:3003:CLA:CMB	27:3:3501:LUT:H173	2.05	0.85
18:G:1003:CLA:C9	18:G:1003:CLA:H13	2.06	0.85
13:2:109:HIS:CD2	18:2:2012:CLA:HMD1	2.11	0.85
16:3:226:LYS:H	16:3:226:LYS:HZ2	1.20	0.85
13:2:143:GLN:HB2	13:2:145:TYR:CE1	2.11	0.85
16:3:110:MET:HE2	16:3:230:ASN:HB3	1.59	0.85
7:L:85:ASN:HB3	18:L:1501:CLA:CAC	2.06	0.85
15:1:111:TRP:CH2	18:1:1006:CLA:HED1	2.12	0.85
16:3:248:THR:HG21	16:3:255:ASN:ND2	1.92	0.85
18:G:1003:CLA:H13	18:G:1003:CLA:H8	1.56	0.85
16:3:135:ALA:N	16:3:138:GLN:HG2	1.91	0.84
16:3:256:LEU:O	16:3:260:VAL:HG23	1.77	0.84
14:4:233:LEU:O	14:4:237:ILE:HG13	1.77	0.84
13:2:127:THR:HG21	13:2:247:ILE:CD1	2.07	0.84
12:K:86:ALA:HB1	12:K:87:PRO:HD3	1.55	0.84
14:4:217:GLY:O	14:4:221:GLN:HB2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:6:SER:O	3:I:7:LEU:HD22	1.77	0.84
12:K:137:VAL:CA	12:K:140:LEU:HD22	2.07	0.84
16:3:267:ASN:O	16:3:270:THR:OG1	1.93	0.84
15:1:85:ARG:HB3	18:1:1001:CLA:CBC	1.99	0.84
12:K:71:VAL:CG1	12:K:129:GLY:O	2.25	0.84
27:1:1501:LUT:H181	27:1:1501:LUT:C8	2.05	0.84
13:2:116:GLY:HA2	27:2:2502:LUT:C18	2.07	0.84
18:4:4001:CLA:H52	27:4:4501:LUT:H371	1.58	0.84
6:G:149:LYS:HB2	6:G:149:LYS:NZ	1.91	0.84
15:1:148:GLN:O	15:1:151:MET:HG2	1.78	0.84
16:3:146:GLY:O	16:3:147:THR:OG1	1.94	0.84
7:L:121:ARG:HG3	7:L:127:GLY:HA2	1.58	0.84
15:1:126:VAL:CG2	15:1:127:PRO:HA	2.07	0.84
18:4:4006:CLA:C1B	27:4:4503:LUT:H172	2.07	0.84
7:L:120:LEU:HB3	7:L:126:ALA:CB	2.08	0.84
13:2:200:TRP:HE1	18:2:2016:CLA:HAA2	1.41	0.83
8:C:8:TYR:HD2	9:D:191:SER:HA	1.40	0.83
18:G:1003:CLA:H13	18:G:1003:CLA:C8	2.08	0.83
16:3:164:LEU:HB3	22:3:3503:BCR:C35	2.09	0.83
28:4:4013:CHL:CHB	27:4:4503:LUT:H192	2.08	0.83
9:D:192:ILE:HG23	10:E:80:GLU:OE2	1.77	0.83
18:4:4002:CLA:HBB1	18:4:4002:CLA:HHC	1.60	0.83
12:K:64:SER:O	12:K:68:VAL:HG23	1.79	0.83
16:3:208:PHE:HB3	18:3:3001:CLA:HMD1	1.61	0.83
16:3:269:LEU:HD11	18:3:3008:CLA:HED1	1.58	0.83
22:A:6003:BCR:H23C	18:A:1103:CLA:H61	1.61	0.83
15:1:230:VAL:O	15:1:231:LEU:HD23	1.78	0.83
18:2:2002:CLA:C1	18:2:2002:CLA:HED1	2.09	0.83
18:2:2004:CLA:HMB1	18:2:2004:CLA:HBB1	1.58	0.83
18:2:2016:CLA:HHD	18:2:2016:CLA:HBC2	1.59	0.83
18:3:3013:CLA:HMA2	22:3:3503:BCR:C35	2.08	0.83
18:4:4005:CLA:OBD	18:4:4012:CLA:HBA2	1.78	0.83
6:G:116:LYS:HG3	18:G:1002:CLA:ND	1.93	0.83
15:1:88:MET:HB2	18:1:1001:CLA:CMC	2.09	0.82
13:2:186:ASN:HD21	18:2:2016:CLA:CGD	1.91	0.82
13:2:220:LYS:CE	18:2:2002:CLA:HED2	2.09	0.82
16:3:190:LEU:HB2	16:3:207:PHE:CZ	2.14	0.82
13:2:233:MET:HA	13:2:233:MET:CE	2.08	0.82
7:L:85:ASN:CB	18:L:1501:CLA:HAC1	2.07	0.82
15:1:120:THR:HG22	15:1:124:ASN:C	1.98	0.82
15:1:164:ALA:O	15:1:167:PRO:HD3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2016:CLA:CBA	18:2:2016:CLA:HBD	2.09	0.82
18:2:2009:CLA:HED3	16:3:171:ARG:CG	2.10	0.82
18:4:4005:CLA:HMD2	18:4:4012:CLA:CHD	2.09	0.82
18:4:4007:CLA:HBB1	18:4:4007:CLA:CHC	2.09	0.82
13:2:151:THR:O	13:2:154:ILE:HG22	1.78	0.82
13:2:239:HIS:O	13:2:243:GLY:N	2.11	0.82
16:3:226:LYS:CE	18:3:3007:CLA:HED2	2.09	0.82
13:2:87:PHE:CE2	27:2:2502:LUT:H372	2.15	0.82
28:4:4010:CHL:CBB	28:4:4013:CHL:HBB2	2.10	0.82
3:I:14:LEU:C	3:I:17:PRO:HD2	2.00	0.82
7:L:87:PRO:HD2	18:L:1502:CLA:HED2	1.61	0.82
18:3:3001:CLA:CGA	27:3:3501:LUT:H382	2.09	0.82
18:3:3006:CLA:HED2	18:3:3006:CLA:C1A	2.09	0.82
18:3:3001:CLA:HBA1	27:3:3501:LUT:H382	1.62	0.82
13:2:131:ILE:HG22	13:2:132:LEU:H	1.45	0.82
6:G:65:SER:CB	18:G:1001:CLA:HBA1	2.09	0.82
6:G:139:LEU:O	6:G:142:SER:OG	1.98	0.82
27:3:3502:LUT:H361	27:3:3502:LUT:H28	1.61	0.82
4:J:36:ALA:HB1	23:J:5001:LMG:H111	1.60	0.82
27:4:4503:LUT:H363	28:1:1009:CHL:C9	2.10	0.81
18:3:3004:CLA:O1A	18:3:3004:CLA:H3A	1.80	0.81
18:2:2002:CLA:HMB1	18:2:2002:CLA:HBB1	1.62	0.81
13:2:87:PHE:HE2	27:2:2502:LUT:H363	1.43	0.81
18:G:1001:CLA:H41	22:G:2011:BCR:H342	1.60	0.81
14:4:152:VAL:O	14:4:155:ARG:HB3	1.79	0.81
18:L:1501:CLA:HBA1	18:L:1501:CLA:CHA	2.08	0.81
7:L:199:TRP:O	7:L:203:LEU:HD13	1.80	0.81
15:1:106:VAL:CG2	15:1:208:THR:HG21	2.11	0.81
15:1:226:ILE:HA	18:1:1003:CLA:OBD	1.80	0.81
13:2:139:THR:HG23	13:2:142:GLU:OE2	1.80	0.81
18:2:2007:CLA:HBC2	18:2:2007:CLA:HMC1	1.63	0.81
18:3:3002:CLA:HBC2	18:3:3002:CLA:HMC1	1.62	0.81
16:3:248:THR:HG21	16:3:255:ASN:HD22	1.42	0.81
13:2:139:THR:H	28:2:2010:CHL:HED3	1.44	0.81
14:4:103:MET:CE	14:4:207:ASN:HB3	2.09	0.81
13:2:188:LEU:HD13	13:2:188:LEU:O	1.80	0.81
16:3:206:PRO:HA	16:3:209:ASN:C	2.01	0.81
7:L:87:PRO:O	7:L:98:ARG:HD2	1.80	0.81
6:G:61:SER:HB2	18:G:1001:CLA:OBD	1.81	0.81
2:B:166:SER:HB3	6:G:102:GLU:HB2	1.63	0.81
15:1:111:TRP:CD1	15:1:119:ALA:HB2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:85:ARG:HH21	18:1:1001:CLA:C4D	1.93	0.81
13:2:131:ILE:HB	13:2:133:LEU:CD1	2.10	0.81
18:G:1001:CLA:CAB	22:G:2011:BCR:H363	2.11	0.81
18:K:1001:CLA:HBB1	18:K:1001:CLA:HHC	1.62	0.81
18:2:2009:CLA:CHC	18:2:2009:CLA:HBB1	2.09	0.81
16:3:258:ASP:CB	16:3:266:ASN:HD21	1.93	0.81
4:J:6:THR:HG21	23:F:5001:LMG:HC72	1.62	0.81
15:1:202:GLN:NE2	15:1:202:GLN:O	2.12	0.80
9:D:204:THR:HG22	9:D:206:LYS:HG2	1.62	0.80
7:L:176:LEU:O	7:L:178:THR:HG22	1.80	0.80
15:1:106:VAL:HG21	15:1:208:THR:HG21	1.60	0.80
13:2:66:LEU:H	16:3:186:TYR:HE2	1.25	0.80
13:2:123:PRO:HA	13:2:126:LEU:HD21	1.62	0.80
13:2:68:PHE:HB3	13:2:71:SER:OG	1.81	0.80
18:3:3018:CLA:HBC2	18:3:3018:CLA:HMC1	1.63	0.80
3:I:6:SER:C	3:I:7:LEU:HD22	2.02	0.80
12:K:63:GLY:O	12:K:66:THR:HG22	1.82	0.80
16:3:142:ILE:HD11	18:3:3010:CLA:HBC3	1.60	0.80
18:2:2008:CLA:HBC3	18:2:2008:CLA:CHD	2.11	0.80
16:3:269:LEU:HD11	18:3:3008:CLA:CED	2.11	0.80
6:G:137:TYR:O	6:G:141:THR:HG23	1.81	0.80
13:2:219:THR:C	18:2:2007:CLA:HED1	2.01	0.80
27:3:3502:LUT:H371	27:3:3502:LUT:C28	2.11	0.80
18:3:3006:CLA:HBB1	18:3:3006:CLA:HHC	1.63	0.80
18:4:4008:CLA:HHD	18:4:4008:CLA:HBC2	1.63	0.80
15:1:130:THR:HG22	15:1:132:PRO:HD2	1.63	0.80
18:3:3003:CLA:C3B	27:3:3501:LUT:H172	2.12	0.80
18:1:1004:CLA:HMD2	28:1:1009:CHL:CBB	2.10	0.80
13:2:137:TRP:HH2	13:2:236:TRP:HA	1.46	0.80
14:4:152:VAL:C	14:4:155:ARG:HB3	2.03	0.80
9:D:76:ASP:HB3	9:D:77:PRO:CA	2.12	0.80
4:J:10:VAL:HG11	23:F:5001:LMG:O2	1.82	0.80
18:1:1004:CLA:O1A	18:1:1004:CLA:H3A	1.80	0.80
15:1:126:VAL:CB	15:1:127:PRO:HA	2.12	0.80
16:3:107:ARG:HB2	28:3:3011:CHL:HED1	1.63	0.80
23:J:5001:LMG:O3	5:F:128:ARG:NH2	2.15	0.80
13:2:68:PHE:HD2	13:2:71:SER:HB3	1.47	0.79
16:3:206:PRO:CD	16:3:207:PHE:HB2	2.07	0.79
13:2:230:LEU:CD2	18:2:2004:CLA:HMC1	2.12	0.79
15:1:111:TRP:CZ2	18:1:1013:CLA:HBC1	2.17	0.79
13:2:127:THR:HG21	13:2:247:ILE:HD13	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:106:GLY:O	16:3:110:MET:HB2	1.83	0.79
5:F:132:ASN:O	5:F:136:GLN:HG2	1.81	0.79
6:G:144:ASN:ND2	18:G:1003:CLA:HED2	1.96	0.79
6:G:76:ARG:HE	6:G:116:LYS:HE2	1.46	0.79
13:2:126:LEU:HA	13:2:130:GLY:O	1.81	0.79
13:2:120:ILE:HG21	27:2:2501:LUT:H373	1.63	0.79
18:3:3005:CLA:HMD2	18:3:3012:CLA:C1D	2.13	0.79
6:G:76:ARG:HG3	6:G:77:PHE:CE1	2.17	0.79
18:K:1001:CLA:HHH	18:K:1001:CLA:HBC2	1.62	0.79
18:4:4012:CLA:H122	18:4:4012:CLA:H91	1.65	0.79
18:2:2004:CLA:HMD2	18:2:2009:CLA:CBB	2.12	0.79
16:3:138:GLN:HB2	16:3:145:ALA:CB	2.09	0.79
18:3:3008:CLA:HBC2	18:3:3008:CLA:CHD	2.10	0.79
15:1:225:ASN:O	15:1:228:ILE:HG22	1.83	0.79
14:4:170:PRO:HB3	18:4:4016:CLA:C4A	2.13	0.79
12:K:133:GLY:O	12:K:137:VAL:HG23	1.82	0.79
28:1:1010:CHL:CBB	18:1:1013:CLA:HBB2	2.11	0.79
9:D:82:PRO:HG3	9:D:128:ASN:ND2	1.98	0.79
6:G:144:ASN:HD22	18:G:1003:CLA:HED2	1.46	0.79
15:1:133:THR:O	15:1:137:ILE:HG13	1.82	0.79
16:3:78:PHE:N	18:3:3004:CLA:OBD	2.16	0.79
27:3:3501:LUT:H171	27:3:3501:LUT:C8	2.12	0.79
7:L:120:LEU:HB3	7:L:126:ALA:HB3	1.63	0.79
15:1:85:ARG:HB2	18:1:1011:CLA:HED2	1.65	0.78
12:K:70:MET:HE2	12:K:71:VAL:CA	2.12	0.78
13:2:87:PHE:HZ	27:2:2502:LUT:H372	1.42	0.78
18:1:1003:CLA:HBA1	18:1:1008:CLA:CED	2.13	0.78
1:A:401:TRP:CD1	18:A:1126:CLA:HAB	2.19	0.78
15:1:88:MET:CB	18:1:1001:CLA:HMC3	2.13	0.78
13:2:187:LYS:O	13:2:188:LEU:HB3	1.83	0.78
6:G:114:VAL:HG11	18:G:1002:CLA:HAA2	1.66	0.78
18:1:1003:CLA:HBA1	18:1:1008:CLA:HED1	1.65	0.78
18:3:3013:CLA:HMA2	22:3:3503:BCR:H353	1.66	0.78
14:4:169:ASP:HB3	18:4:4016:CLA:C2D	2.12	0.78
18:4:4016:CLA:HBD	18:4:4016:CLA:HBA1	1.65	0.78
18:B:1238:CLA:HAB	20:B:5002:PQN:H162	1.66	0.78
12:K:70:MET:HE2	12:K:71:VAL:N	1.98	0.78
18:2:2001:CLA:HED2	18:2:2001:CLA:OBD	1.82	0.78
8:C:75:ARG:NH2	9:D:99:GLU:OE2	2.14	0.78
15:1:97:PRO:HB2	15:1:102:LEU:CB	2.12	0.78
16:3:138:GLN:O	16:3:145:ALA:HB3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:202:GLN:HE22	15:1:208:THR:HB	1.48	0.78
13:2:123:PRO:HA	13:2:126:LEU:CD2	2.14	0.78
18:3:3001:CLA:H43	18:3:3002:CLA:HBA1	1.65	0.78
14:4:208:GLY:O	14:4:212:MET:HG3	1.83	0.78
9:D:100:PHE:CE1	9:D:158:VAL:HB	2.19	0.78
15:1:146:GLU:HG2	15:1:149:ARG:NH1	1.98	0.78
13:2:262:ILE:HD11	18:2:2003:CLA:C1	2.14	0.78
7:L:132:LEU:O	7:L:132:LEU:HD12	1.82	0.78
15:1:83:HIS:CE1	18:1:1012:CLA:HMD1	2.19	0.78
15:1:114:LEU:HD23	15:1:115:PRO:CD	2.11	0.78
18:2:2003:CLA:H42	18:2:2003:CLA:C1D	2.14	0.78
16:3:182:MET:CE	16:3:182:MET:HA	2.14	0.78
2:B:73:ASN:HD22	2:B:74:PHE:H	1.28	0.78
12:K:71:VAL:HG21	12:K:133:GLY:HA2	1.66	0.78
13:2:139:THR:CA	28:2:2010:CHL:HED3	2.14	0.77
13:2:139:THR:N	28:2:2010:CHL:HED3	2.00	0.77
18:F:1302:CLA:CHD	18:F:1302:CLA:HBC2	2.14	0.77
11:H:96:ARG:HG2	11:H:97:GLY:N	1.97	0.77
16:3:139:THR:HG23	16:3:140:GLY:H	1.49	0.77
13:2:182:ILE:CD1	18:4:4007:CLA:HAB	2.14	0.77
12:K:70:MET:HE2	12:K:71:VAL:CG2	2.15	0.77
18:1:1005:CLA:H12	18:1:1005:CLA:HED1	1.64	0.77
14:4:143:VAL:O	14:4:147:ILE:HG12	1.85	0.77
18:B:1220:CLA:H42	18:B:1221:CLA:H13	1.65	0.77
6:G:121:LEU:HD23	6:G:121:LEU:O	1.83	0.77
7:L:139:VAL:O	7:L:143:ILE:HG13	1.85	0.77
27:2:2502:LUT:H28	27:2:2502:LUT:H361	1.67	0.77
16:3:222:GLU:C	16:3:226:LYS:HZ3	1.87	0.77
14:4:150:HIS:CA	18:4:4012:CLA:HAB	2.14	0.77
6:G:77:PHE:CE1	18:G:1002:CLA:HAB	2.19	0.77
18:1:1003:CLA:CBA	18:1:1008:CLA:HED1	2.14	0.77
16:3:158:PHE:HB2	18:3:3010:CLA:HMC2	1.67	0.77
16:3:101:GLY:HA2	18:3:3012:CLA:HED2	1.64	0.77
18:2:2012:CLA:CBB	18:2:2012:CLA:HMB1	2.14	0.77
16:3:205:GLY:CA	16:3:208:PHE:HB2	2.14	0.77
12:K:71:VAL:HG12	12:K:129:GLY:HA2	1.67	0.77
16:3:152:ALA:HB3	16:3:157:LEU:HD21	1.65	0.77
18:4:4012:CLA:C12	18:4:4012:CLA:H91	2.15	0.77
6:G:149:LYS:HB2	6:G:149:LYS:HZ2	1.48	0.77
27:4:4503:LUT:H363	28:1:1009:CHL:C8	2.14	0.77
13:2:131:ILE:HD12	13:2:133:LEU:CD2	2.08	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:110:MET:SD	16:3:231:GLY:HA2	2.25	0.77
6:G:64:ILE:O	6:G:68:THR:HG22	1.85	0.77
12:K:124:ALA:CB	22:K:2011:BCR:H331	2.15	0.77
7:L:87:PRO:HB3	7:L:101:GLU:OE1	1.85	0.77
16:3:162:MET:CE	16:3:162:MET:HA	2.14	0.77
6:G:115:SER:HB2	18:G:1002:CLA:OBD	1.84	0.77
15:1:232:ILE:HG22	15:1:233:PRO:O	1.85	0.76
13:2:233:MET:HA	13:2:233:MET:HE2	1.66	0.76
16:3:110:MET:HE1	16:3:230:ASN:O	1.85	0.76
16:3:120:GLU:CD	16:3:253:TYR:HB3	2.04	0.76
3:I:4:LEU:HD12	3:I:6:SER:H	1.50	0.76
18:3:3002:CLA:CHC	18:3:3002:CLA:HBB1	2.13	0.76
4:J:2:ARG:HD3	4:J:4:LEU:HB2	1.65	0.76
15:1:222:TRP:NE1	18:1:1008:CLA:HMA1	1.99	0.76
13:2:131:ILE:HB	13:2:133:LEU:HG	1.67	0.76
16:3:68:LEU:N	16:3:68:LEU:HD13	2.00	0.76
18:G:1001:CLA:CHC	18:G:1001:CLA:HBB1	2.09	0.76
3:I:14:LEU:O	3:I:17:PRO:HD2	1.86	0.76
12:K:72:ALA:CB	18:K:1001:CLA:O2A	2.32	0.76
15:1:209:GLY:CA	15:1:212:GLU:HB3	2.14	0.76
13:2:262:ILE:HD11	18:2:2003:CLA:H43	1.65	0.76
18:3:3003:CLA:H92	18:3:3003:CLA:C1C	2.14	0.76
16:3:155:TYR:CZ	18:3:3010:CLA:HAC1	2.20	0.76
7:L:178:THR:HG23	7:L:181:GLY:H	1.49	0.76
13:2:125:PHE:HB3	13:2:131:ILE:CD1	2.16	0.76
16:3:139:THR:HG23	16:3:140:GLY:N	2.01	0.76
13:2:191:THR:HG22	13:2:192:ASP:H	1.51	0.76
18:2:2012:CLA:HBB1	18:2:2012:CLA:CMB	2.08	0.76
16:3:65:LEU:HD13	16:3:67:TYR:HE1	1.49	0.76
1:A:539:PHE:HA	18:A:1136:CLA:HED1	1.65	0.76
15:1:85:ARG:CB	18:1:1011:CLA:HED2	2.15	0.76
18:2:2003:CLA:H42	18:2:2003:CLA:CHD	2.15	0.76
13:2:115:LEU:HB3	18:2:2006:CLA:CBB	2.15	0.76
13:2:246:PRO:HA	13:2:249:ASN:OD1	1.84	0.76
18:A:1123:CLA:HMA3	18:A:1119:CLA:HMB2	1.67	0.76
1:A:269:PHE:HA	1:A:274:TRP:HE1	1.50	0.76
7:L:176:LEU:HD12	7:L:177:GLN:N	2.00	0.76
13:2:178:ASN:O	13:2:187:LYS:HD2	1.85	0.76
16:3:172:ARG:NH2	18:3:3012:CLA:O1D	2.12	0.76
15:1:192:LEU:O	15:1:196:VAL:HG23	1.86	0.76
16:3:205:GLY:HA3	16:3:208:PHE:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:3011:CHL:CBA	28:3:3011:CHL:HBD	2.16	0.76
18:3:3006:CLA:HMB3	27:3:3502:LUT:H182	1.68	0.76
14:4:221:GLN:O	14:4:225:THR:HB	1.86	0.76
18:4:4007:CLA:CBB	18:4:4007:CLA:HHC	2.15	0.76
6:G:94:GLU:HB2	6:G:98:VAL:H	1.51	0.76
15:1:121:TYR:HD2	15:1:122:LEU:HG	1.50	0.75
15:1:126:VAL:HG23	15:1:127:PRO:CA	2.15	0.75
16:3:119:PRO:CB	16:3:133:ALA:HB2	2.17	0.75
16:3:161:GLU:OE1	18:3:3010:CLA:HAB	1.86	0.75
11:H:130:GLN:HB3	11:H:132:PRO:HB3	1.68	0.75
27:1:1502:LUT:H371	27:1:1502:LUT:H28	1.68	0.75
27:2:2501:LUT:H371	27:2:2501:LUT:C28	2.17	0.75
16:3:226:LYS:HE3	18:3:3007:CLA:HED2	1.67	0.75
16:3:137:PHE:O	16:3:141:VAL:HG12	1.86	0.75
18:4:4005:CLA:HMD2	18:4:4012:CLA:C4C	2.16	0.75
6:G:149:LYS:O	6:G:149:LYS:HE3	1.86	0.75
7:L:176:LEU:CD1	7:L:177:GLN:H	1.97	0.75
16:3:131:GLU:O	16:3:131:GLU:HG3	1.87	0.75
16:3:185:GLN:HB2	16:3:186:TYR:CD1	2.20	0.75
11:H:133:PRO:HD2	11:H:135:LEU:H	1.52	0.75
13:2:199:LEU:O	13:2:199:LEU:HD23	1.87	0.75
18:2:2003:CLA:HHB	18:2:2008:CLA:CBC	2.15	0.75
23:2:2802:LMG:HO5	23:2:2802:LMG:HO4	1.33	0.75
18:3:3010:CLA:CBB	18:3:3010:CLA:HHC	2.16	0.75
16:3:79:ASP:OD1	16:3:82:GLY:N	2.19	0.75
14:4:156:ARG:NH2	18:4:4012:CLA:O1D	2.19	0.75
2:B:704:GLN:HG3	25:B:7101:DGD:HA22	1.67	0.75
7:L:130:GLY:O	7:L:133:ALA:N	2.19	0.75
15:1:58:ASP:HA	18:1:1004:CLA:HED2	1.69	0.75
13:2:139:THR:HA	28:2:2010:CHL:HED3	1.68	0.75
13:2:130:GLY:O	13:2:133:LEU:HD11	1.87	0.75
16:3:120:GLU:OE1	16:3:252:PRO:HG2	1.87	0.75
18:3:3010:CLA:H93	18:3:3010:CLA:C2C	2.17	0.75
16:3:65:LEU:HB3	16:3:68:LEU:HD21	1.67	0.75
27:4:4503:LUT:C28	27:4:4503:LUT:H371	2.16	0.75
1:A:440:ASP:HB2	9:D:88:THR:HG21	1.68	0.75
16:3:225:LEU:HB3	16:3:226:LYS:CE	2.16	0.75
13:2:129:LEU:HD22	13:2:131:ILE:CG1	2.17	0.74
14:4:158:GLN:NE2	14:4:161:LYS:HE3	2.02	0.74
1:A:503:THR:HG21	18:A:1133:CLA:HMD1	1.68	0.74
6:G:84:ARG:NH2	6:G:123:ASP:OD2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:3003:CLA:H92	18:3:3003:CLA:CHC	2.18	0.74
18:3:3006:CLA:HMD2	18:3:3018:CLA:CAB	2.17	0.74
14:4:82:ALA:HB1	14:4:88:LEU:HD13	1.68	0.74
7:L:113:PRO:CG	18:L:1503:CLA:HBB1	2.12	0.74
15:1:160:TYR:HB3	18:1:1001:CLA:HED3	1.69	0.74
16:3:267:ASN:CG	16:3:270:THR:HG23	2.07	0.74
14:4:168:GLN:O	18:4:4016:CLA:HED3	1.87	0.74
22:F:6016:BCR:C8	22:F:6016:BCR:H331	2.16	0.74
12:K:130:HIS:O	12:K:134:VAL:HG23	1.86	0.74
15:1:226:ILE:N	18:1:1003:CLA:O1A	2.20	0.74
16:3:101:GLY:HA2	18:3:3012:CLA:CED	2.18	0.74
18:3:3001:CLA:HBA1	27:3:3501:LUT:C38	2.17	0.74
6:G:76:ARG:HD2	6:G:76:ARG:O	1.86	0.74
18:L:1501:CLA:HBA2	18:H:1000:CLA:HBB	1.69	0.74
18:1:1003:CLA:C9	18:1:1003:CLA:HBB1	2.04	0.74
15:1:131:LEU:HD23	15:1:131:LEU:N	2.03	0.74
15:1:165:PHE:O	15:1:167:PRO:HD2	1.88	0.74
18:2:2002:CLA:HBC2	18:2:2002:CLA:CMC	2.12	0.74
16:3:266:ASN:O	16:3:270:THR:HG21	1.87	0.74
27:3:3502:LUT:H161	27:3:3502:LUT:C8	2.12	0.74
14:4:235:GLN:HB3	14:4:243:ASN:HD22	1.51	0.74
27:4:4501:LUT:C28	27:4:4501:LUT:H371	2.11	0.74
1:A:24:ARG:HH11	1:A:76:ARG:HH12	1.34	0.74
28:1:1010:CHL:CMC	28:1:1010:CHL:HBC3	2.17	0.74
16:3:225:LEU:HB3	16:3:226:LYS:HZ1	1.51	0.74
18:2:2005:CLA:H71	23:2:2802:LMG:H132	1.70	0.74
14:4:213:LEU:HD12	23:4:4801:LMG:H302	1.68	0.74
2:B:488:ALA:O	6:G:146:TYR:OH	2.06	0.74
9:D:115:MET:HE1	9:D:130:LEU:HD11	1.68	0.74
18:3:3002:CLA:CBB	18:3:3002:CLA:HHC	2.17	0.74
13:2:105:ALA:HB2	18:2:2012:CLA:HED2	1.68	0.74
13:2:174:PRO:HD2	13:2:175:GLY:H	1.52	0.74
13:2:254:LEU:N	13:2:254:LEU:HD23	2.01	0.74
16:3:259:HIS:NE2	18:3:3008:CLA:NC	2.36	0.74
18:B:1236:CLA:HED1	18:B:1234:CLA:HMB2	1.69	0.74
9:D:191:SER:C	9:D:192:ILE:HD12	2.07	0.74
21:1:1801:LHG:HC61	21:1:1801:LHG:HC81	1.70	0.74
18:3:3013:CLA:CBB	27:3:3502:LUT:H181	2.17	0.74
14:4:215:PHE:CD2	27:4:4502:LUT:H14	2.22	0.74
28:4:4013:CHL:HHD	28:4:4013:CHL:CBC	2.18	0.74
1:A:217:SER:HA	18:A:1113:CLA:HBB2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:116:LYS:HE3	18:G:1002:CLA:NC	2.02	0.74
18:G:1003:CLA:C5	23:G:2021:LMG:H311	2.17	0.74
13:2:250:LEU:CD2	13:2:254:LEU:HD21	2.18	0.73
8:C:10:THR:HG23	8:C:64:SER:OG	1.88	0.73
18:G:1003:CLA:H93	23:G:2021:LMG:H162	1.70	0.73
15:1:88:MET:HE3	18:1:1001:CLA:CHC	2.17	0.73
14:4:151:TYR:HB2	28:1:1009:CHL:H11	1.69	0.73
21:1:1801:LHG:H383	21:1:1801:LHG:H223	1.70	0.73
18:2:2001:CLA:C4	18:2:2002:CLA:H3A	2.17	0.73
16:3:65:LEU:HD13	16:3:67:TYR:CZ	2.23	0.73
12:K:75:THR:HG21	12:K:129:GLY:CA	2.18	0.73
18:L:1501:CLA:CBD	18:L:1501:CLA:HBA1	2.18	0.73
28:1:1010:CHL:OMC	18:1:1013:CLA:HAB	1.89	0.73
18:2:2003:CLA:HMA1	18:2:2008:CLA:HBC2	1.70	0.73
8:C:61:ASP:HB2	10:E:118:ASN:ND2	2.03	0.73
12:K:71:VAL:HG12	12:K:129:GLY:CA	2.18	0.73
12:K:76:LEU:O	12:K:79:PHE:HB2	1.89	0.73
13:2:162:TRP:O	13:2:166:ARG:HB2	1.87	0.73
28:2:2010:CHL:HBB1	28:2:2013:CHL:HBB2	1.68	0.73
10:E:66:ILE:HG23	10:E:67:GLY:N	2.03	0.73
12:K:72:ALA:O	12:K:76:LEU:HG	1.89	0.73
18:4:4017:CLA:HED2	28:1:1009:CHL:HMB2	1.69	0.73
13:2:122:ILE:HG23	13:2:133:LEU:CB	2.16	0.73
18:2:2016:CLA:HBA2	18:2:2016:CLA:CBD	2.17	0.73
18:4:4003:CLA:C4B	18:4:4003:CLA:H93	2.18	0.73
16:3:103:VAL:O	16:3:107:ARG:HG3	1.89	0.73
18:L:1501:CLA:HBA1	18:L:1501:CLA:HBD	1.71	0.73
18:4:4002:CLA:HHC	18:4:4002:CLA:CBB	2.19	0.73
4:J:6:THR:CG2	23:F:5001:LMG:HC1	2.19	0.73
11:H:59:ASP:OD1	11:H:59:ASP:N	2.22	0.73
4:J:2:ARG:O	4:J:4:LEU:N	2.20	0.73
18:1:1003:CLA:C2B	27:1:1501:LUT:H173	2.18	0.73
18:B:1219:CLA:HBB2	22:B:6009:BCR:H343	1.70	0.73
7:L:121:ARG:HG2	7:L:127:GLY:H	1.53	0.73
18:3:3008:CLA:HHC	18:3:3008:CLA:CBB	2.15	0.73
7:L:91:THR:HG22	7:L:175:GLN:NE2	2.03	0.73
18:2:2002:CLA:HED1	18:2:2002:CLA:O2A	1.89	0.73
14:4:169:ASP:HB3	18:4:4016:CLA:C4D	2.19	0.73
23:J:5001:LMG:HC8	23:J:5001:LMG:O10	1.87	0.73
18:1:1005:CLA:HMD2	18:1:1012:CLA:ND	2.03	0.72
13:2:219:THR:CG2	18:2:2007:CLA:HED3	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:3001:CLA:CBA	27:3:3501:LUT:H382	2.19	0.72
18:B:1216:CLA:HMB2	18:B:1221:CLA:HMA3	1.71	0.72
5:F:222:LEU:HD23	5:F:222:LEU:N	2.03	0.72
28:2:2011:CHL:HAA1	28:2:2011:CHL:HBD	1.69	0.72
13:2:120:ILE:HD13	27:2:2501:LUT:H373	1.71	0.72
16:3:187:PHE:O	16:3:188:LEU:HB2	1.88	0.72
27:1:1501:LUT:H8	27:1:1501:LUT:H181	1.69	0.72
13:2:131:ILE:HB	13:2:133:LEU:CG	2.20	0.72
18:4:4016:CLA:HED2	18:4:4016:CLA:OBD	1.89	0.72
7:L:116:LYS:HD3	18:L:1503:CLA:HMB2	1.71	0.72
7:L:87:PRO:HD3	18:L:1502:CLA:HED2	1.69	0.72
13:2:118:ALA:CB	18:2:2006:CLA:HMC3	2.19	0.72
14:4:236:HIS:NE2	18:4:4008:CLA:NC	2.38	0.72
18:G:1001:CLA:HAB	22:G:2011:BCR:H363	1.71	0.72
11:H:132:PRO:CD	11:H:133:PRO:HD3	2.19	0.72
7:L:166:LEU:O	7:L:166:LEU:HD23	1.90	0.72
2:B:684:ARG:HH21	7:L:67:GLY:HA3	1.55	0.72
13:2:177:VAL:O	13:2:179:THR:N	2.22	0.72
16:3:166:GLY:HA2	18:3:3012:CLA:CBB	2.19	0.72
14:4:225:THR:CG2	14:4:227:LYS:H	2.00	0.72
18:K:1001:CLA:CBB	18:K:1001:CLA:HHC	2.19	0.72
16:3:184:LYS:CG	16:3:185:GLN:HE21	2.02	0.72
18:3:3004:CLA:CBB	18:3:3004:CLA:HMB1	2.14	0.72
7:L:128:GLN:CB	7:L:204:LEU:HG	2.19	0.72
16:3:244:GLN:O	16:3:248:THR:HB	1.90	0.72
9:D:195:ASN:HD22	9:D:195:ASN:H	1.37	0.72
11:H:112:ALA:O	11:H:115:SER:HB3	1.88	0.72
13:2:191:THR:HG22	13:2:192:ASP:N	2.03	0.72
18:2:2006:CLA:CAD	18:2:2006:CLA:H43	2.18	0.72
16:3:122:LEU:O	16:3:126:GLY:N	2.23	0.72
18:2:2009:CLA:HED3	16:3:171:ARG:HG3	1.70	0.72
16:3:268:VAL:CG2	18:3:3003:CLA:H12	2.19	0.72
7:L:121:ARG:HA	7:L:124:GLU:O	1.89	0.72
15:1:82:ILE:HD12	15:1:149:ARG:NH2	2.05	0.72
18:2:2001:CLA:H42	18:2:2002:CLA:CBA	2.15	0.72
18:2:2016:CLA:CHC	18:2:2016:CLA:HBB1	2.12	0.72
16:3:169:GLU:CD	16:3:172:ARG:HH11	1.92	0.72
27:1:1502:LUT:H371	27:1:1502:LUT:C28	2.18	0.72
22:L:6020:BCR:H19C	18:L:1501:CLA:HMB2	1.72	0.72
18:1:1001:CLA:O1A	18:1:1001:CLA:H3A	1.88	0.71
15:1:211:LEU:HD12	15:1:212:GLU:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:202:TYR:HB3	18:3:3001:CLA:O1D	1.90	0.71
16:3:206:PRO:HA	16:3:209:ASN:O	1.90	0.71
14:4:151:TYR:O	14:4:155:ARG:HB2	1.89	0.71
15:1:200:VAL:HG11	18:1:1003:CLA:HAC2	1.71	0.71
16:3:263:PRO:CG	18:3:3008:CLA:HMB3	2.20	0.71
18:A:1102:CLA:HBA2	18:A:1109:CLA:H51	1.72	0.71
14:4:140:THR:HB	15:1:225:ASN:OD1	1.90	0.71
21:2:2801:LHG:O4	21:2:2801:LHG:O2	2.07	0.71
13:2:163:ALA:C	13:2:166:ARG:HB3	2.10	0.71
16:3:223:LEU:CA	16:3:226:LYS:HG2	2.20	0.71
1:A:37:PRO:HA	18:A:1101:CLA:HBC1	1.72	0.71
9:D:112:ILE:HD12	9:D:112:ILE:N	2.04	0.71
10:E:122:LEU:HD12	10:E:122:LEU:N	2.02	0.71
18:F:1301:CLA:HHC	18:F:1301:CLA:HBB1	1.72	0.71
6:G:149:LYS:C	6:G:149:LYS:HE3	2.11	0.71
13:2:148:ASP:O	13:2:149:THR:CB	2.38	0.71
13:2:193:VAL:HG23	13:2:194:GLY:N	2.04	0.71
18:3:3003:CLA:CAB	27:3:3501:LUT:H172	2.20	0.71
14:4:168:GLN:OE1	14:4:171:ILE:HA	1.89	0.71
18:B:1204:CLA:H2	3:I:8:PHE:HD2	1.53	0.71
18:G:1001:CLA:C3D	18:G:1001:CLA:HED2	2.21	0.71
22:J:6013:BCR:H392	22:J:6013:BCR:H23C	1.71	0.71
13:2:177:VAL:HG23	13:2:178:ASN:N	2.05	0.71
16:3:169:GLU:OE2	16:3:172:ARG:NH1	2.22	0.71
18:1:1011:CLA:C5	27:1:1501:LUT:H23	2.18	0.71
16:3:141:VAL:HG22	16:3:143:PRO:HD2	1.72	0.71
14:4:118:ILE:CD1	14:4:120:ILE:HD11	2.06	0.71
15:1:186:LYS:HD3	18:1:1007:CLA:O1D	1.90	0.71
15:1:88:MET:HE3	18:1:1001:CLA:CAB	2.20	0.71
18:B:1220:CLA:HAB	18:B:1227:CLA:HMD2	1.73	0.71
18:B:1235:CLA:HBB1	18:B:1235:CLA:H72	1.71	0.71
7:L:102:VAL:HG13	7:L:106:HIS:CE1	2.26	0.71
23:G:2021:LMG:HC61	15:1:115:PRO:HA	1.71	0.71
15:1:125:PRO:O	15:1:126:VAL:HG22	1.89	0.71
16:3:223:LEU:HA	16:3:226:LYS:HG2	1.73	0.71
14:4:60:LEU:HG	14:4:61:ALA:N	2.06	0.71
18:L:1502:CLA:HAC2	22:L:6019:BCR:H292	1.72	0.71
16:3:142:ILE:O	16:3:146:GLY:HA2	1.90	0.70
16:3:265:ASN:O	16:3:270:THR:HB	1.91	0.70
18:3:3006:CLA:H43	18:3:3018:CLA:O2A	1.90	0.70
16:3:67:TYR:HE2	16:3:84:SER:CB	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:152:VAL:HG13	28:4:4011:CHL:NB	2.06	0.70
4:J:28:GLU:OE1	18:J:1302:CLA:CHA	2.39	0.70
18:2:2005:CLA:C7	23:2:2802:LMG:H132	2.21	0.70
18:A:1114:CLA:HHC	18:A:1114:CLA:HBB1	1.73	0.70
22:K:2011:BCR:C32	22:K:2011:BCR:HC8	2.16	0.70
22:L:6019:BCR:H393	22:L:6019:BCR:C27	2.21	0.70
15:1:202:GLN:HE21	15:1:202:GLN:C	1.94	0.70
18:2:2016:CLA:CBB	18:2:2016:CLA:HHC	2.14	0.70
16:3:226:LYS:N	16:3:226:LYS:HZ2	1.89	0.70
18:3:3001:CLA:C4	18:3:3002:CLA:HBA1	2.20	0.70
18:4:4016:CLA:HMC1	18:4:4016:CLA:HBC2	1.73	0.70
9:D:192:ILE:HG22	9:D:193:GLY:N	2.03	0.70
18:L:1501:CLA:HAA1	18:H:1000:CLA:HMB2	1.73	0.70
13:2:200:TRP:CD1	18:2:2016:CLA:HAA2	2.25	0.70
28:2:2010:CHL:HHC	28:2:2010:CHL:HBB1	1.71	0.70
16:3:226:LYS:NZ	16:3:226:LYS:H	1.88	0.70
18:4:4003:CLA:HBB1	18:4:4003:CLA:CHC	2.19	0.70
18:1:1001:CLA:ND	27:1:1501:LUT:H383	2.06	0.70
18:1:1008:CLA:CBB	18:1:1008:CLA:HHC	2.22	0.70
6:G:75:GLY:O	6:G:80:PHE:HB2	1.90	0.70
15:1:41:TRP:CD1	15:1:59:PHE:HA	2.26	0.70
18:3:3006:CLA:CHA	18:3:3006:CLA:HED2	2.21	0.70
18:4:4002:CLA:OBD	18:4:4007:CLA:HBD	1.92	0.70
15:1:121:TYR:O	15:1:122:LEU:HD23	1.91	0.70
13:2:77:LEU:CD1	13:2:86:GLY:HA2	2.22	0.70
18:3:3012:CLA:H12	18:3:3017:CLA:CBB	2.22	0.70
28:4:4013:CHL:HHB	27:4:4503:LUT:H192	1.72	0.70
18:2:2003:CLA:C3B	27:2:2501:LUT:H383	2.21	0.70
16:3:120:GLU:CD	16:3:253:TYR:H	1.95	0.70
28:4:4013:CHL:HHB	27:4:4503:LUT:C19	2.22	0.70
2:B:582:TRP:CH2	18:B:1012:CLA:HAB	2.27	0.70
27:I:6018:LUT:C8	27:I:6018:LUT:H181	2.21	0.70
18:1:1008:CLA:HBB1	18:1:1008:CLA:CHC	2.19	0.70
9:D:169:PRO:O	9:D:170:LYS:HB3	1.90	0.70
10:E:111:ASN:ND2	10:E:113:ALA:O	2.24	0.70
4:J:38:THR:C	23:J:5001:LMG:H122	2.11	0.70
28:2:2013:CHL:HBC2	28:2:2013:CHL:OMC	1.92	0.70
16:3:107:ARG:CB	28:3:3011:CHL:HED1	2.21	0.70
14:4:150:HIS:O	14:4:154:ILE:HG22	1.91	0.70
11:H:72:SER:OG	11:H:73:ASP:N	2.25	0.70
18:1:1004:CLA:HMD2	28:1:1009:CHL:HBB1	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:104:ASN:CG	15:1:208:THR:HG23	2.11	0.69
15:1:126:VAL:HB	15:1:127:PRO:HA	1.73	0.69
13:2:141:GLY:HA2	28:2:2013:CHL:HBC1	1.72	0.69
7:L:91:THR:HA	7:L:175:GLN:NE2	2.05	0.69
15:1:167:PRO:HD2	27:1:1501:LUT:O23	1.91	0.69
18:2:2003:CLA:CHB	18:2:2008:CLA:HMD3	2.22	0.69
1:A:593:SER:OG	1:A:596:ASP:OD2	2.10	0.69
2:B:294:ASN:HB3	6:G:107:ARG:HA	1.74	0.69
18:A:1131:CLA:HMA1	27:I:6018:LUT:H22	1.74	0.69
7:L:83:LEU:O	7:L:89:TYR:HD2	1.75	0.69
27:2:2501:LUT:H28	27:2:2501:LUT:C37	2.22	0.69
16:3:135:ALA:H	16:3:138:GLN:HG2	1.55	0.69
16:3:166:GLY:O	16:3:170:HIS:ND1	2.23	0.69
27:3:3502:LUT:H371	27:3:3502:LUT:H28	1.73	0.69
15:1:89:LEU:O	15:1:92:PRO:HD2	1.92	0.69
18:3:3008:CLA:CHC	18:3:3008:CLA:HBB1	2.16	0.69
18:2:2002:CLA:HED1	18:2:2002:CLA:CGA	2.22	0.69
18:2:2016:CLA:HBD	18:2:2016:CLA:CGA	2.22	0.69
16:3:259:HIS:CG	18:3:3003:CLA:HAA2	2.28	0.69
16:3:155:TYR:CE1	18:3:3010:CLA:HAC1	2.27	0.69
14:4:94:ALA:N	18:4:4012:CLA:HED2	2.07	0.69
10:E:111:ASN:HD22	10:E:113:ALA:H	1.40	0.69
11:H:68:ASP:OD1	11:H:71:GLY:HA3	1.92	0.69
16:3:117:ILE:HD11	16:3:252:PRO:HB2	1.73	0.69
14:4:120:ILE:N	14:4:120:ILE:HD12	2.07	0.69
5:F:106:LEU:HD13	5:F:106:LEU:O	1.91	0.69
15:1:202:GLN:CD	15:1:208:THR:HB	2.12	0.69
18:3:3003:CLA:C9	18:3:3003:CLA:H122	2.23	0.69
14:4:136:ALA:HB1	14:4:140:THR:HG21	1.75	0.69
14:4:197:THR:OG1	14:4:200:ALA:HB2	1.93	0.69
17:A:1011:CL0:H2	17:A:1011:CL0:H15	1.75	0.69
28:4:4011:CHL:HAA1	28:4:4011:CHL:CB	2.21	0.69
13:2:123:PRO:HA	13:2:126:LEU:CG	2.22	0.69
18:3:3004:CLA:H3A	18:3:3004:CLA:CGA	2.22	0.69
18:G:1001:CLA:HHC	18:G:1001:CLA:CBB	2.15	0.69
15:1:232:ILE:HD11	18:1:1014:CLA:HMD2	1.74	0.69
15:1:75:ARG:NH1	18:1:1005:CLA:O1A	2.26	0.69
18:2:2005:CLA:HBC1	18:2:2012:CLA:CBC	2.23	0.69
18:2:2008:CLA:HAA2	16:3:160:LEU:HB2	1.74	0.69
16:3:110:MET:HA	16:3:234:ALA:CB	2.23	0.69
18:A:1013:CLA:H203	18:A:1140:CLA:H51	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:209:GLY:O	15:1:213:ASN:N	2.19	0.69
27:2:2502:LUT:C28	27:2:2502:LUT:H361	2.22	0.69
13:2:77:LEU:HD12	13:2:86:GLY:HA2	1.75	0.69
16:3:259:HIS:HA	16:3:266:ASN:CB	2.23	0.69
14:4:212:MET:HE3	18:4:4004:CLA:HMC3	1.74	0.69
18:4:4007:CLA:O2D	18:4:4007:CLA:H2A	1.93	0.69
18:1:1004:CLA:H2	27:1:1502:LUT:H182	1.74	0.68
15:1:193:LEU:O	15:1:193:LEU:HD23	1.93	0.68
16:3:258:ASP:HB2	16:3:266:ASN:HD21	1.58	0.68
6:G:76:ARG:HE	6:G:116:LYS:CE	2.04	0.68
15:1:144:PHE:O	15:1:148:GLN:HG2	1.93	0.68
16:3:155:TYR:CE1	18:3:3010:CLA:CAC	2.76	0.68
18:3:3006:CLA:CBB	18:3:3006:CLA:HHC	2.22	0.68
18:4:4002:CLA:HBB1	18:4:4002:CLA:CHC	2.23	0.68
18:4:4007:CLA:HBC2	18:4:4007:CLA:CHD	2.13	0.68
18:4:4017:CLA:CED	28:1:1009:CHL:HMB2	2.23	0.68
22:A:6017:BCR:H362	18:B:1023:CLA:H112	1.75	0.68
12:K:124:ALA:O	12:K:128:VAL:HG23	1.94	0.68
13:2:131:ILE:CG2	13:2:133:LEU:HG	2.23	0.68
13:2:186:ASN:OD1	18:2:2016:CLA:H2A	1.93	0.68
13:2:117:ALA:HB1	27:2:2501:LUT:H32	1.75	0.68
27:3:3501:LUT:C8	27:3:3501:LUT:H161	2.17	0.68
18:4:4006:CLA:C3B	27:4:4502:LUT:H183	2.23	0.68
6:G:76:ARG:HG2	6:G:116:LYS:HZ1	1.58	0.68
12:K:71:VAL:HG21	12:K:133:GLY:CA	2.23	0.68
7:L:98:ARG:HH22	7:L:175:GLN:HE22	1.41	0.68
18:1:1002:CLA:HED2	18:1:1002:CLA:O1A	1.94	0.68
13:2:125:PHE:HB3	13:2:131:ILE:HD11	1.75	0.68
18:3:3004:CLA:HBB1	18:3:3004:CLA:CMB	2.08	0.68
18:3:3012:CLA:HBB1	18:3:3012:CLA:CMB	2.03	0.68
22:L:6019:BCR:H23C	22:L:6019:BCR:C38	2.23	0.68
15:1:177:PHE:CE2	15:1:181:LYS:HE2	2.28	0.68
13:2:68:PHE:CD2	13:2:71:SER:HB3	2.29	0.68
13:2:69:PRO:HD2	18:2:2009:CLA:O1D	1.93	0.68
16:3:246:LEU:HD23	16:3:246:LEU:C	2.14	0.68
18:3:3010:CLA:CHC	18:3:3010:CLA:HBB1	2.20	0.68
14:4:132:GLU:HB2	14:4:133:GLU:OE2	1.94	0.68
27:4:4502:LUT:C28	27:4:4502:LUT:H381	2.06	0.68
18:A:1022:CLA:H122	22:A:6017:BCR:H352	1.75	0.68
12:K:66:THR:O	12:K:69:ILE:HG23	1.94	0.68
7:L:91:THR:HA	7:L:98:ARG:NH2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1002:CLA:HMC1	18:1:1002:CLA:HBC2	1.75	0.68
15:1:58:ASP:HA	18:1:1004:CLA:CED	2.23	0.68
13:2:186:ASN:CG	18:2:2016:CLA:HMA3	2.14	0.68
18:2:2008:CLA:HBB1	18:2:2008:CLA:HHC	1.75	0.68
11:H:132:PRO:HD2	11:H:133:PRO:CD	2.23	0.68
13:2:211:PRO:O	13:2:212:GLN:CG	2.42	0.68
18:3:3005:CLA:HMD2	18:3:3012:CLA:CHD	2.23	0.68
16:3:155:TYR:HA	18:3:3010:CLA:HMC1	1.74	0.68
29:4:4505:ZEX:H362	29:4:4505:ZEX:C38	2.22	0.68
14:4:213:LEU:CD1	23:4:4801:LMG:H302	2.24	0.68
4:J:2:ARG:NE	4:J:4:LEU:HD12	2.01	0.68
7:L:162:PRO:HG2	11:H:68:ASP:HB2	1.75	0.68
28:2:2013:CHL:O2A	28:2:2013:CHL:HMA2	1.94	0.68
18:3:3007:CLA:HBC2	18:3:3007:CLA:HMC1	1.76	0.68
10:E:111:ASN:ND2	10:E:113:ALA:H	1.91	0.68
5:F:139:LEU:HD23	5:F:139:LEU:N	2.07	0.68
3:I:4:LEU:HD12	3:I:4:LEU:C	2.14	0.68
7:L:109:PHE:HE1	18:L:1503:CLA:C2C	2.06	0.68
15:1:106:VAL:HG21	15:1:202:GLN:OE1	1.94	0.68
14:4:203:LYS:HA	18:4:4007:CLA:O1D	1.92	0.68
18:G:1001:CLA:H41	22:G:2011:BCR:C34	2.22	0.68
13:2:130:GLY:C	13:2:131:ILE:HG13	2.14	0.68
13:2:177:VAL:HG23	13:2:178:ASN:H	1.59	0.68
16:3:237:ALA:HB1	27:3:3501:LUT:H161	1.76	0.68
18:3:3013:CLA:CMA	22:3:3503:BCR:H353	2.23	0.68
1:A:387:THR:HG21	1:A:523:VAL:HB	1.75	0.68
22:L:6019:BCR:H271	22:L:6019:BCR:H393	1.76	0.68
15:1:80:GLU:HG3	18:1:1004:CLA:C1B	2.24	0.67
15:1:130:THR:HG22	15:1:132:PRO:HD3	1.76	0.67
18:2:2009:CLA:HED3	16:3:171:ARG:HG2	1.76	0.67
9:D:195:ASN:ND2	9:D:195:ASN:H	1.92	0.67
11:H:106:GLY:O	11:H:110:THR:HG22	1.94	0.67
18:K:1001:CLA:HBB1	18:K:1001:CLA:CHC	2.24	0.67
12:K:78:LEU:HB3	12:K:82:ARG:HB2	1.75	0.67
7:L:161:ALA:HB3	7:L:174:ASP:OD1	1.94	0.67
15:1:221:PRO:HG2	15:1:222:TRP:CZ3	2.30	0.67
13:2:129:LEU:HD23	13:2:129:LEU:C	2.15	0.67
13:2:175:GLY:O	13:2:176:CYS:HB3	1.92	0.67
14:4:209:ARG:HD3	18:4:4004:CLA:CHD	2.24	0.67
9:D:160:PRO:HD2	9:D:161:SER:H	1.60	0.67
18:G:1003:CLA:H91	18:G:1003:CLA:H13	1.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:131:ILE:HG22	13:2:132:LEU:N	2.09	0.67
2:B:15:ASP:HB3	2:B:20:ARG:HB3	1.76	0.67
18:K:1001:CLA:H2A	18:K:1001:CLA:O2D	1.93	0.67
16:3:183:GLY:HA2	16:3:194:PHE:CB	2.23	0.67
15:1:85:ARG:HH11	15:1:85:ARG:CG	2.08	0.67
18:2:2001:CLA:H11	27:2:2501:LUT:C17	2.24	0.67
14:4:198:LEU:O	14:4:199:GLU:HB2	1.94	0.67
14:4:197:THR:O	14:4:200:ALA:HB3	1.95	0.67
15:1:131:LEU:HD23	15:1:131:LEU:H	1.58	0.67
18:2:2005:CLA:HMD2	18:2:2012:CLA:C1D	2.24	0.67
16:3:119:PRO:HB2	16:3:133:ALA:CB	2.25	0.67
16:3:218:LYS:HD3	16:3:218:LYS:C	2.15	0.67
16:3:249:GLY:O	16:3:250:VAL:HG23	1.94	0.67
6:G:120:ALA:HB3	6:G:123:ASP:OD1	1.95	0.67
22:G:2011:BCR:C23	22:G:2011:BCR:H403	2.19	0.67
7:L:166:LEU:HD23	7:L:166:LEU:C	2.15	0.67
15:1:152:GLU:CG	15:1:156:GLU:HA	2.25	0.67
13:2:188:LEU:C	13:2:188:LEU:HD22	2.15	0.67
13:2:64:ARG:NH2	13:2:77:LEU:O	2.28	0.67
16:3:138:GLN:CG	16:3:145:ALA:HB2	2.24	0.67
14:4:170:PRO:HA	18:4:4016:CLA:O1D	1.95	0.67
18:4:4003:CLA:HBC2	18:4:4003:CLA:HHD	1.77	0.67
18:4:4001:CLA:H52	27:4:4501:LUT:H28	1.75	0.67
9:D:129:LEU:HD23	9:D:129:LEU:C	2.14	0.67
12:K:86:ALA:CB	12:K:87:PRO:HD3	2.25	0.67
7:L:90:ARG:O	7:L:98:ARG:NH2	2.27	0.67
15:1:195:PHE:O	15:1:198:ILE:HB	1.95	0.67
16:3:251:GLY:O	16:3:255:ASN:N	2.24	0.67
14:4:220:ILE:HD12	18:4:4003:CLA:CAC	2.23	0.67
14:4:229:PRO:HA	14:4:232:ASN:HD22	1.59	0.67
18:1:1001:CLA:CHC	27:1:1501:LUT:H32	2.25	0.67
15:1:130:THR:HG22	15:1:131:LEU:N	2.10	0.67
13:2:203:PRO:HD2	27:2:2501:LUT:O3	1.95	0.67
18:3:3004:CLA:H2	27:3:3502:LUT:H363	1.77	0.67
18:4:4003:CLA:H11	18:4:4008:CLA:OBD	1.94	0.67
1:A:208:ALA:HB2	1:A:314:GLY:HA3	1.76	0.67
12:K:66:THR:HA	12:K:69:ILE:CG2	2.23	0.67
12:K:76:LEU:N	12:K:76:LEU:HD23	2.10	0.67
13:2:262:ILE:HA	18:2:2003:CLA:OBD	1.94	0.66
18:2:2009:CLA:CED	16:3:171:ARG:HG3	2.25	0.66
16:3:220:LEU:HD23	16:3:220:LEU:C	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:267:ASN:O	16:3:271:SER:N	2.28	0.66
6:G:116:LYS:HE3	18:G:1002:CLA:C1C	2.23	0.66
12:K:136:VAL:O	12:K:140:LEU:HD22	1.94	0.66
14:4:112:PRO:O	14:4:116:THR:OG1	2.13	0.66
18:B:1210:CLA:HBB1	18:B:1210:CLA:HHC	1.76	0.66
9:D:192:ILE:CG2	9:D:193:GLY:H	2.07	0.66
18:B:1204:CLA:H2	3:I:8:PHE:CD2	2.31	0.66
18:1:1011:CLA:HMB1	18:1:1011:CLA:HBB1	1.77	0.66
15:1:85:ARG:HB2	18:1:1011:CLA:CED	2.25	0.66
18:3:3001:CLA:HBB2	27:3:3501:LUT:H34	1.77	0.66
18:1:1003:CLA:C3B	27:1:1501:LUT:H173	2.26	0.66
13:2:70:GLY:CA	16:3:174:GLN:HE21	2.05	0.66
1:A:34:TRP:CE3	4:J:8:LEU:HD22	2.30	0.66
7:L:102:VAL:HG22	18:L:1502:CLA:O1D	1.94	0.66
13:2:222:ILE:N	13:2:222:ILE:HD12	2.09	0.66
14:4:105:GLY:O	14:4:109:MET:HE2	1.95	0.66
18:4:4003:CLA:HHC	18:4:4003:CLA:CBB	2.23	0.66
9:D:157:ARG:HB2	9:D:167:LEU:HD11	1.76	0.66
6:G:132:HIS:CE1	22:G:2011:BCR:H19C	2.29	0.66
7:L:96:LEU:C	7:L:96:LEU:HD23	2.15	0.66
18:1:1005:CLA:HMD2	18:1:1012:CLA:CHD	2.26	0.66
1:A:462:ILE:HG22	18:A:1132:CLA:HBC2	1.78	0.66
4:J:6:THR:HG22	23:F:5001:LMG:HC1	1.76	0.66
7:L:204:LEU:HD13	7:L:204:LEU:O	1.95	0.66
15:1:226:ILE:HG13	18:1:1003:CLA:HMD2	1.76	0.66
21:1:1801:LHG:O1	21:1:1801:LHG:O3	2.10	0.66
13:2:188:LEU:HD23	13:2:198:GLY:N	2.09	0.66
16:3:223:LEU:N	16:3:226:LYS:HZ3	1.93	0.66
16:3:258:ASP:HB3	16:3:266:ASN:HD21	1.61	0.66
16:3:268:VAL:HG23	18:3:3003:CLA:C1	2.21	0.66
14:4:105:GLY:HA2	18:4:4006:CLA:CBB	2.25	0.66
11:H:131:LEU:HB2	11:H:132:PRO:HA	1.78	0.66
7:L:129:ALA:O	7:L:132:LEU:HB3	1.96	0.66
15:1:94:ILE:HG13	27:1:1502:LUT:H382	1.78	0.66
13:2:119:GLY:O	13:2:123:PRO:HD3	1.96	0.66
13:2:160:ILE:CD1	28:2:2013:CHL:HMB3	2.25	0.66
16:3:155:TYR:CD1	18:3:3010:CLA:HAC2	2.31	0.66
16:3:268:VAL:HG21	18:3:3003:CLA:C4	2.11	0.66
14:4:235:GLN:HB3	14:4:243:ASN:ND2	2.10	0.66
5:F:94:ARG:NH1	5:F:143:ASP:O	2.26	0.66
18:1:1004:CLA:CGA	18:1:1004:CLA:H3A	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:1009:CHL:O2D	28:1:1009:CHL:H2A	1.96	0.66
15:1:120:THR:HG22	15:1:124:ASN:O	1.94	0.66
15:1:204:ALA:C	15:1:206:PRO:HD3	2.16	0.66
15:1:43:PRO:HB2	28:1:1009:CHL:O1D	1.96	0.66
13:2:244:THR:HG22	13:2:245:GLY:N	2.03	0.66
16:3:223:LEU:HA	16:3:226:LYS:CG	2.26	0.66
14:4:212:MET:HB3	27:4:4502:LUT:C34	2.26	0.66
18:4:4001:CLA:HBC2	28:4:4011:CHL:O1A	1.96	0.66
2:B:12:ILE:HD11	2:B:23:PHE:HB3	1.77	0.66
8:C:8:TYR:CD2	9:D:191:SER:HA	2.27	0.66
18:1:1006:CLA:HMA2	18:1:1013:CLA:HBC2	1.76	0.66
15:1:98:GLU:HA	15:1:102:LEU:HB3	1.77	0.66
16:3:267:ASN:OD1	16:3:270:THR:HG23	1.94	0.66
18:3:3008:CLA:HBA1	18:3:3008:CLA:HBD	1.77	0.66
18:4:4005:CLA:HMD2	18:4:4012:CLA:C1D	2.25	0.66
18:4:4001:CLA:H52	27:4:4501:LUT:C37	2.26	0.66
8:C:14:CYS:C	8:C:15:THR:HG23	2.16	0.66
8:C:25:VAL:HG21	8:C:48:CYS:HB2	1.77	0.66
6:G:76:ARG:NE	6:G:116:LYS:HE2	2.11	0.66
5:F:138:LEU:CD2	5:F:159:GLU:OE2	2.44	0.65
18:G:1003:CLA:H91	18:G:1003:CLA:C13	2.26	0.65
7:L:91:THR:HG22	7:L:175:GLN:HE21	1.61	0.65
18:1:1014:CLA:O2D	18:1:1014:CLA:HBA2	1.94	0.65
16:3:178:LYS:HB2	16:3:181:SER:OG	1.96	0.65
16:3:184:LYS:HG2	16:3:185:GLN:HE21	1.59	0.65
16:3:94:GLU:OE2	16:3:95:PRO:HD2	1.96	0.65
1:A:453:LEU:HD21	18:A:1136:CLA:HAB	1.78	0.65
13:2:174:PRO:CD	13:2:175:GLY:H	2.08	0.65
13:2:256:ASP:OD1	13:2:259:HIS:HD2	1.79	0.65
16:3:267:ASN:OD1	16:3:269:LEU:HG	1.95	0.65
16:3:78:PHE:HB3	18:3:3004:CLA:OBD	1.96	0.65
2:B:603:ARG:HH22	2:B:627:ASN:HD21	1.43	0.65
10:E:111:ASN:HD21	10:E:113:ALA:HB3	1.60	0.65
13:2:111:ARG:NH1	28:2:2011:CHL:OBD	2.27	0.65
18:2:2016:CLA:HBC2	18:2:2016:CLA:CHD	2.25	0.65
1:A:567:ARG:NH2	9:D:88:THR:O	2.29	0.65
2:B:487:ASN:HB3	6:G:149:LYS:HB3	1.77	0.65
23:2:2802:LMG:O5	23:2:2802:LMG:O4	2.10	0.65
22:B:6006:BCR:H362	18:B:1211:CLA:H2	1.79	0.65
3:I:5:PRO:O	3:I:7:LEU:N	2.29	0.65
18:2:2002:CLA:O1D	18:2:2007:CLA:H42	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:3002:CLA:HMD2	18:3:3007:CLA:C4D	2.27	0.65
18:3:3001:CLA:HBA2	27:3:3501:LUT:H24	1.78	0.65
2:B:176:ASN:HD21	2:B:291:TYR:H	1.43	0.65
18:1:1003:CLA:HBD	18:1:1003:CLA:O1A	1.97	0.65
15:1:146:GLU:OE2	15:1:149:ARG:NH1	2.29	0.65
15:1:85:ARG:HD2	18:1:1001:CLA:C3C	2.26	0.65
13:2:191:THR:O	13:2:192:ASP:HB2	1.96	0.65
18:3:3013:CLA:HMA2	22:3:3503:BCR:H352	1.77	0.65
22:A:6011:BCR:H24C	18:B:1230:CLA:HMC2	1.79	0.65
22:B:6004:BCR:H24C	18:B:1218:CLA:HMD2	1.78	0.65
12:K:72:ALA:HB3	18:K:1001:CLA:CGA	2.26	0.65
13:2:239:HIS:ND1	13:2:244:THR:O	2.29	0.65
16:3:65:LEU:O	16:3:68:LEU:HD22	1.97	0.65
14:4:140:THR:O	14:4:144:ILE:HG13	1.96	0.65
1:A:441:ALA:O	1:A:445:HIS:ND1	2.30	0.65
12:K:70:MET:CE	12:K:71:VAL:HA	2.26	0.65
18:2:2004:CLA:H13	27:2:2502:LUT:H393	1.78	0.65
18:3:3005:CLA:H93	18:3:3012:CLA:C4	2.25	0.65
14:4:104:LEU:C	18:4:4006:CLA:HBB2	2.17	0.65
12:K:75:THR:HG21	12:K:129:GLY:N	2.12	0.65
22:L:6019:BCR:H311	22:L:6019:BCR:HC8	1.79	0.65
13:2:262:ILE:CD1	18:2:2003:CLA:H43	2.27	0.65
16:3:234:ALA:O	16:3:238:ILE:HG22	1.97	0.65
18:4:4002:CLA:HMC2	27:4:4501:LUT:C11	2.26	0.65
27:4:4503:LUT:H28	27:4:4503:LUT:H361	1.79	0.65
3:I:6:SER:O	3:I:9:VAL:HG23	1.97	0.65
16:3:74:GLY:HA2	16:3:225:LEU:CD2	2.27	0.64
16:3:231:GLY:O	16:3:235:MET:HG3	1.97	0.64
18:3:3005:CLA:H12	18:3:3005:CLA:HED1	1.79	0.64
16:3:63:GLN:OE1	16:3:78:PHE:HD2	1.80	0.64
14:4:223:ASN:O	14:4:225:THR:N	2.30	0.64
18:4:4009:CLA:H2A	18:4:4009:CLA:O2D	1.98	0.64
18:F:1302:CLA:HBB1	18:F:1302:CLA:HHC	1.79	0.64
15:1:98:GLU:CA	15:1:102:LEU:HB3	2.26	0.64
16:3:121:TYR:O	16:3:124:LYS:HB2	1.96	0.64
28:4:4010:CHL:HBB1	28:4:4013:CHL:HBB2	1.79	0.64
1:A:629:ASN:ND2	1:A:631:GLN:OE1	2.30	0.64
15:1:202:GLN:CA	15:1:202:GLN:HE21	2.10	0.64
18:2:2002:CLA:H2A	18:2:2002:CLA:O1A	1.96	0.64
28:2:2010:CHL:O2D	28:2:2010:CHL:H2A	1.96	0.64
16:3:184:LYS:C	16:3:185:GLN:HG2	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:114:VAL:HG11	18:G:1002:CLA:CAA	2.26	0.64
16:3:117:ILE:HD13	16:3:252:PRO:HG2	1.78	0.64
16:3:216:ASP:OD1	16:3:216:ASP:N	2.27	0.64
16:3:75:ASP:OD1	16:3:77:GLY:N	2.30	0.64
18:4:4006:CLA:NB	27:4:4503:LUT:H172	2.13	0.64
18:B:1229:CLA:H61	22:F:6016:BCR:H393	1.79	0.64
18:2:2007:CLA:O1D	18:2:2007:CLA:H2A	1.98	0.64
13:2:218:ARG:O	13:2:222:ILE:HD13	1.98	0.64
16:3:225:LEU:N	16:3:226:LYS:HZ2	1.94	0.64
16:3:105:ASN:ND2	18:3:3012:CLA:OBD	2.30	0.64
18:4:4008:CLA:HBB1	18:4:4008:CLA:HHC	1.78	0.64
28:4:4010:CHL:HBB1	28:4:4013:CHL:CBB	2.27	0.64
2:B:656:VAL:HG22	18:B:1239:CLA:HMB3	1.79	0.64
7:L:169:ARG:HD2	7:L:171:LYS:CB	2.28	0.64
15:1:98:GLU:N	15:1:102:LEU:HB3	2.12	0.64
16:3:144:PRO:HG2	16:3:145:ALA:H	1.61	0.64
18:3:3006:CLA:HMB2	18:3:3013:CLA:C4B	2.27	0.64
5:F:207:VAL:HB	18:F:1301:CLA:HED2	1.79	0.64
22:L:6019:BCR:H23C	22:L:6019:BCR:H382	1.79	0.64
18:1:1002:CLA:O2D	18:1:1002:CLA:H2A	1.98	0.64
21:2:2801:LHG:HC42	22:3:3503:BCR:H281	1.80	0.64
14:4:225:THR:HG22	14:4:227:LYS:H	1.61	0.64
14:4:72:GLY:HA2	23:4:4801:LMG:O5	1.97	0.64
11:H:132:PRO:HD2	11:H:133:PRO:HD3	1.79	0.64
29:4:4505:ZEX:H41	18:1:1014:CLA:O1A	1.98	0.64
16:3:158:PHE:CB	18:3:3010:CLA:HMC2	2.28	0.64
18:4:4005:CLA:HMC2	27:4:4502:LUT:C12	2.28	0.64
1:A:24:ARG:HD3	1:A:76:ARG:HH22	1.63	0.64
6:G:95:GLN:O	6:G:95:GLN:HG3	1.98	0.64
13:2:135:PRO:HG2	18:2:2006:CLA:CED	2.27	0.64
16:3:259:HIS:HA	16:3:266:ASN:HB2	1.80	0.64
18:3:3003:CLA:H91	18:3:3003:CLA:H122	1.80	0.64
18:3:3003:CLA:HMB3	27:3:3501:LUT:H173	1.80	0.64
18:A:1131:CLA:HAB	18:A:1132:CLA:HHB	1.79	0.64
18:A:1151:CLA:HAB	18:A:1122:CLA:HHB	1.80	0.64
13:2:131:ILE:HB	13:2:133:LEU:HD11	1.78	0.63
4:J:10:VAL:HA	4:J:14:ALA:HB2	1.79	0.63
7:L:211:TYR:HE2	18:L:1503:CLA:C2	2.12	0.63
15:1:79:SER:HB2	18:1:1012:CLA:HED2	1.80	0.63
18:3:3001:CLA:HBB1	27:3:3501:LUT:H32	1.79	0.63
16:3:111:LEU:CD2	18:3:3006:CLA:HBB1	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:4501:LUT:H28	27:4:4501:LUT:C37	2.28	0.63
1:A:34:TRP:HE3	4:J:8:LEU:HD22	1.63	0.63
18:4:4009:CLA:HBB1	18:4:4009:CLA:CHC	2.11	0.63
7:L:211:TYR:HE2	18:L:1503:CLA:C3	2.12	0.63
28:1:1010:CHL:HHC	28:1:1010:CHL:HBB1	1.78	0.63
15:1:130:THR:CG2	15:1:132:PRO:HD2	2.26	0.63
15:1:97:PRO:HB2	15:1:102:LEU:HD22	1.79	0.63
27:1:1502:LUT:H28	27:1:1502:LUT:C37	2.28	0.63
13:2:202:ASP:OD2	13:2:205:GLY:HA2	1.99	0.63
16:3:136:TRP:CG	16:3:137:PHE:N	2.66	0.63
7:L:96:LEU:HD12	11:H:94:THR:HG21	1.81	0.63
15:1:146:GLU:CG	15:1:149:ARG:HH11	2.10	0.63
15:1:169:GLY:O	15:1:172:LYS:HG3	1.99	0.63
13:2:204:LEU:HB3	13:2:206:TRP:NE1	2.14	0.63
18:B:1204:CLA:H51	27:I:6018:LUT:O23	1.99	0.63
13:2:131:ILE:CB	13:2:133:LEU:HG	2.28	0.63
12:K:71:VAL:CG1	12:K:132:ILE:HB	2.29	0.63
18:L:1502:CLA:HBA1	18:L:1502:CLA:CHA	2.27	0.63
15:1:193:LEU:C	15:1:193:LEU:HD23	2.18	0.63
18:3:3003:CLA:H92	18:3:3003:CLA:C2C	2.29	0.63
16:3:65:LEU:HD23	16:3:66:SER:H	1.63	0.63
18:A:1139:CLA:H43	18:A:1138:CLA:H171	1.80	0.63
8:C:54:CYS:SG	8:C:55:GLU:N	2.72	0.63
6:G:94:GLU:HB2	6:G:98:VAL:N	2.13	0.63
18:1:1007:CLA:HBC2	18:1:1007:CLA:HMC1	1.81	0.63
15:1:211:LEU:CD1	15:1:212:GLU:H	2.12	0.63
2:B:351:HIS:HB3	18:B:1214:CLA:HED2	1.80	0.63
4:J:16:THR:HG21	22:J:6013:BCR:C40	2.29	0.63
7:L:133:ALA:O	7:L:136:GLY:N	2.30	0.63
7:L:163:SER:O	7:L:172:GLN:HG2	1.99	0.63
7:L:145:LEU:CD2	22:L:6019:BCR:H403	2.26	0.63
15:1:151:MET:HG3	15:1:151:MET:O	1.97	0.62
15:1:158:LYS:C	15:1:159:LYS:HD3	2.19	0.62
16:3:257:LEU:O	16:3:261:ALA:N	2.30	0.62
18:3:3006:CLA:CHC	18:3:3006:CLA:HBB1	2.27	0.62
14:4:105:GLY:N	18:4:4006:CLA:HBB2	2.14	0.62
14:4:170:PRO:HB3	18:4:4016:CLA:NA	2.12	0.62
1:A:604:TRP:CH2	18:A:1022:CLA:HAB	2.34	0.62
1:A:546:ALA:HB1	18:A:1136:CLA:HMB3	1.79	0.62
18:2:2003:CLA:C1B	27:2:2501:LUT:H383	2.28	0.62
18:2:2006:CLA:C4	18:2:2006:CLA:H71	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:2:2802:LMG:O2	23:2:2802:LMG:H292	1.98	0.62
16:3:193:GLY:HA3	16:3:207:PHE:CD2	2.33	0.62
9:D:139:LEU:HD23	9:D:139:LEU:O	1.99	0.62
12:K:85:LEU:CB	12:K:118:THR:HG21	2.29	0.62
15:1:143:ALA:HA	18:1:1012:CLA:HAB	1.79	0.62
15:1:111:TRP:NE1	15:1:119:ALA:HB2	2.14	0.62
15:1:127:PRO:HG2	15:1:128:TRP:NE1	2.14	0.62
16:3:190:LEU:HB2	16:3:207:PHE:HZ	1.63	0.62
6:G:76:ARG:HG3	6:G:77:PHE:CD1	2.34	0.62
18:L:1501:CLA:CBA	18:L:1501:CLA:HBD	2.29	0.62
15:1:146:GLU:O	15:1:149:ARG:HB2	1.98	0.62
13:2:197:GLY:CA	18:2:2001:CLA:HED1	2.29	0.62
28:4:4013:CHL:HBB1	28:4:4013:CHL:HHC	1.80	0.62
6:G:116:LYS:HB2	18:G:1002:CLA:C4D	2.29	0.62
15:1:183:LYS:CD	18:1:1002:CLA:HAA2	2.23	0.62
15:1:155:PRO:O	15:1:158:LYS:N	2.33	0.62
15:1:162:GLY:N	18:1:1001:CLA:HED2	2.14	0.62
13:2:104:GLN:NE2	13:2:193:VAL:HB	2.15	0.62
18:2:2005:CLA:H41	18:2:2005:CLA:H92	1.79	0.62
13:2:88:ASP:OD1	27:2:2502:LUT:O23	2.16	0.62
16:3:225:LEU:O	16:3:225:LEU:HD13	1.99	0.62
16:3:262:ASP:HB3	16:3:265:ASN:ND2	2.15	0.62
18:3:3003:CLA:H11	18:3:3003:CLA:C3D	2.27	0.62
18:A:1110:CLA:HBC3	18:A:1111:CLA:HAB	1.81	0.62
2:B:5:LEU:HD22	3:I:28:VAL:HG22	1.82	0.62
16:3:134:LEU:CB	16:3:138:GLN:HG3	2.30	0.62
18:3:3017:CLA:HBB1	18:3:3017:CLA:HHC	1.82	0.62
18:3:3003:CLA:HAB	27:3:3501:LUT:H172	1.82	0.62
6:G:133:ILE:HA	22:G:2011:BCR:H401	1.81	0.62
18:1:1005:CLA:HMB1	18:1:1005:CLA:CBB	2.28	0.62
13:2:87:PHE:HB3	18:2:2004:CLA:CAD	2.29	0.62
18:4:4016:CLA:CB	18:4:4016:CLA:HBA1	2.29	0.62
9:D:173:VAL:HG12	9:D:174:TYR:N	2.14	0.62
14:4:177:LEU:HD13	18:4:4016:CLA:HMD3	1.81	0.62
14:4:239:ASP:OD2	14:4:242:HIS:HD2	1.82	0.62
18:A:1110:CLA:CB	18:A:1111:CLA:HAB	2.29	0.62
13:2:220:LYS:HG2	18:2:2007:CLA:O2D	1.99	0.62
18:3:3001:CLA:O1A	18:3:3001:CLA:H3A	1.99	0.62
28:3:3011:CHL:CGD	28:3:3011:CHL:HAA1	2.29	0.62
22:B:6006:BCR:H311	18:B:1212:CLA:HMB2	1.82	0.62
13:2:104:GLN:HE22	13:2:193:VAL:CG2	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:220:LYS:HA	18:2:2007:CLA:CED	2.30	0.62
13:2:220:LYS:CA	18:2:2007:CLA:HED1	2.30	0.62
16:3:169:GLU:OE2	16:3:169:GLU:HA	1.99	0.62
18:A:1138:CLA:H111	18:A:1138:CLA:HAB	1.82	0.62
2:B:85:ARG:HD2	2:B:115:ILE:HD13	1.82	0.62
10:E:66:ILE:HG23	10:E:93:VAL:HG11	1.81	0.62
5:F:163:PRO:O	5:F:166:LEU:HB3	1.99	0.62
7:L:109:PHE:CE1	18:L:1503:CLA:C2C	2.83	0.62
13:2:109:HIS:NE2	18:2:2012:CLA:HMD1	2.15	0.61
13:2:123:PRO:HA	13:2:126:LEU:HG	1.82	0.61
16:3:164:LEU:HD13	22:3:3503:BCR:C35	2.30	0.61
16:3:164:LEU:CB	22:3:3503:BCR:H351	2.26	0.61
18:4:4003:CLA:CHC	18:4:4003:CLA:H93	2.30	0.61
13:2:165:GLY:O	18:4:4009:CLA:HED2	1.99	0.61
18:A:1130:CLA:HMB1	18:A:1130:CLA:HBB1	1.81	0.61
9:D:111:GLN:O	9:D:123:MET:N	2.31	0.61
9:D:158:VAL:O	9:D:159:PHE:HB2	1.99	0.61
9:D:75:LEU:O	9:D:76:ASP:HB2	1.98	0.61
11:H:123:LEU:HD12	11:H:123:LEU:H	1.64	0.61
15:1:158:LYS:HD3	15:1:159:LYS:NZ	2.15	0.61
18:2:2001:CLA:H41	18:2:2002:CLA:H3A	1.81	0.61
13:2:89:PRO:HD2	27:2:2502:LUT:H221	1.82	0.61
7:L:90:ARG:C	7:L:98:ARG:HH21	2.04	0.61
18:2:2005:CLA:C4	18:2:2005:CLA:H72	2.29	0.61
1:A:354:TRP:HB3	18:A:1103:CLA:HAC1	1.81	0.61
18:B:1222:CLA:H41	18:B:1234:CLA:H43	1.82	0.61
1:A:361:ASN:ND2	18:A:1103:CLA:OBD	2.29	0.61
1:A:590:CYS:HB3	19:A:3001:SF4:S2	2.41	0.61
22:B:6005:BCR:H311	18:B:1202:CLA:H42	1.83	0.61
10:E:95:GLN:HA	10:E:95:GLN:OE1	2.00	0.61
18:B:1206:CLA:H18	27:I:6018:LUT:H403	1.82	0.61
15:1:85:ARG:HD2	18:1:1001:CLA:C4C	2.30	0.61
18:B:1205:CLA:H2	18:B:1205:CLA:H102	1.83	0.61
10:E:76:ILE:C	10:E:77:LEU:HD12	2.20	0.61
11:H:122:ILE:HG22	11:H:122:ILE:O	1.99	0.61
15:1:230:VAL:HG12	15:1:231:LEU:HD23	1.82	0.61
13:2:105:ALA:CB	18:2:2012:CLA:HED2	2.31	0.61
18:2:2009:CLA:HED1	16:3:167:PHE:O	2.01	0.61
18:B:1229:CLA:HAB	18:B:1230:CLA:CMB	2.27	0.61
6:G:98:VAL:O	6:G:99:THR:HG22	2.00	0.61
3:I:13:GLY:C	3:I:14:LEU:HD23	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2012:CLA:H12	23:2:2802:LMG:C36	2.30	0.61
18:3:3003:CLA:C2B	27:3:3501:LUT:H173	2.29	0.61
1:A:222:GLN:HA	1:A:226:SER:HB2	1.83	0.61
9:D:134:ARG:O	9:D:135:LYS:HB3	2.01	0.61
13:2:127:THR:HG21	13:2:247:ILE:HD11	1.83	0.61
18:2:2002:CLA:HMC1	18:2:2002:CLA:CBC	2.19	0.61
18:2:2006:CLA:HMA2	28:2:2013:CHL:HAC2	1.83	0.61
16:3:182:MET:HE1	16:3:182:MET:HA	1.81	0.61
16:3:184:LYS:HG2	16:3:185:GLN:CG	2.29	0.61
2:B:173:SER:O	2:B:177:HIS:ND1	2.20	0.61
15:1:111:TRP:CE2	15:1:119:ALA:CB	2.84	0.61
1:A:358:LEU:HD11	18:A:1128:CLA:HBB1	1.82	0.61
9:D:140:ALA:O	9:D:143:THR:HG22	2.00	0.61
6:G:121:LEU:HD23	6:G:121:LEU:C	2.22	0.61
4:J:7:TYR:CZ	23:F:5001:LMG:HC4	2.36	0.61
12:K:81:GLY:O	12:K:82:ARG:HD3	1.99	0.61
15:1:211:LEU:N	15:1:211:LEU:HD12	2.16	0.60
13:2:115:LEU:HB2	18:2:2006:CLA:HBB2	1.82	0.60
16:3:110:MET:HE1	16:3:230:ASN:C	2.22	0.60
18:3:3004:CLA:H93	18:3:3005:CLA:HMB3	1.83	0.60
16:3:155:TYR:CZ	18:3:3010:CLA:CAC	2.83	0.60
16:3:67:TYR:HE2	16:3:84:SER:HB2	1.66	0.60
18:L:1502:CLA:CHD	22:L:6019:BCR:H282	2.31	0.60
18:2:2004:CLA:CMB	18:2:2004:CLA:HBB1	2.31	0.60
16:3:120:GLU:OE2	16:3:253:TYR:N	2.33	0.60
18:3:3005:CLA:O2D	18:3:3005:CLA:HBA2	2.00	0.60
16:3:175:ASP:HB2	28:3:3011:CHL:HAC2	1.82	0.60
2:B:451:LYS:NZ	18:B:1230:CLA:O1D	2.35	0.60
18:G:1001:CLA:HED2	18:G:1001:CLA:CAD	2.31	0.60
18:3:3010:CLA:HMB1	18:3:3013:CLA:CAB	2.10	0.60
14:4:167:ASN:CG	14:4:168:GLN:H	2.03	0.60
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.83	0.60
22:F:6016:BCR:H382	22:F:6016:BCR:C23	2.32	0.60
12:K:83:PHE:HB2	22:K:2011:BCR:C4	2.31	0.60
15:1:217:HIS:CE1	15:1:221:PRO:CB	2.85	0.60
13:2:105:ALA:CA	18:2:2012:CLA:HED2	2.31	0.60
14:4:103:MET:CG	18:4:4001:CLA:HMC3	2.31	0.60
18:A:1104:CLA:HAB	18:A:1127:CLA:HMC2	1.83	0.60
1:A:205:HIS:CD2	18:A:1111:CLA:HMC2	2.36	0.60
18:B:1218:CLA:H41	18:B:1218:CLA:H92	1.84	0.60
18:F:1302:CLA:HHD	18:F:1302:CLA:CBC	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:150:VAL:HG12	5:F:160:PHE:HB2	1.84	0.60
6:G:116:LYS:HG3	18:G:1002:CLA:C1D	2.30	0.60
12:K:136:VAL:C	12:K:140:LEU:HD22	2.21	0.60
7:L:172:GLN:HG3	7:L:172:GLN:O	2.00	0.60
27:4:4503:LUT:C36	28:1:1009:CHL:H93	2.32	0.60
2:B:273:MET:O	2:B:277:HIS:ND1	2.34	0.60
18:1:1002:CLA:HMD2	18:1:1007:CLA:ND	2.16	0.60
15:1:41:TRP:HD1	15:1:59:PHE:C	2.04	0.60
13:2:199:LEU:C	13:2:199:LEU:HD23	2.22	0.60
16:3:137:PHE:CE1	16:3:138:GLN:HB3	2.37	0.60
1:A:274:TRP:O	12:K:141:LYS:HD2	2.01	0.60
2:B:422:LEU:HG	18:B:1236:CLA:HAB	1.82	0.60
28:1:1009:CHL:HBB1	28:1:1009:CHL:HHC	1.83	0.60
13:2:154:ILE:HG21	18:4:4008:CLA:HED1	1.83	0.60
28:2:2011:CHL:HAA1	28:2:2011:CHL:CB D	2.30	0.60
16:3:74:GLY:CA	16:3:225:LEU:HD22	2.31	0.60
27:3:3501:LUT:H171	27:3:3501:LUT:H8	1.82	0.60
27:4:4503:LUT:H8	27:4:4503:LUT:C18	2.19	0.60
18:B:1205:CLA:HAB	18:B:1206:CLA:HAA2	1.83	0.60
22:J:6013:BCR:C23	22:J:6013:BCR:H403	2.31	0.60
12:K:70:MET:CE	12:K:71:VAL:HG22	2.31	0.60
15:1:166:ASP:CG	15:1:169:GLY:HA2	2.21	0.60
15:1:55:ALA:HB3	15:1:58:ASP:HB2	1.84	0.60
13:2:139:THR:HG22	13:2:139:THR:O	2.01	0.60
18:3:3017:CLA:H2A	18:3:3017:CLA:O2D	2.02	0.60
18:3:3001:CLA:O2A	27:3:3501:LUT:H382	2.01	0.60
14:4:154:ILE:HG13	28:1:1009:CHL:HED1	1.82	0.60
15:1:120:THR:HG22	15:1:125:PRO:HA	1.84	0.60
28:4:4011:CHL:CBC	28:4:4011:CHL:HHD	2.28	0.60
22:A:6008:BCR:C23	18:A:1124:CLA:HAB	2.31	0.60
20:A:5001:PQN:H141	18:A:1139:CLA:HBB2	1.83	0.60
22:B:6004:BCR:H14C	18:B:1217:CLA:HBB1	1.83	0.60
2:B:560:ASP:CG	8:C:66:ARG:HH12	2.05	0.60
3:I:24:LEU:HD22	22:L:6019:BCR:H333	1.82	0.60
16:3:107:ARG:NH1	16:3:227:GLU:OE1	2.35	0.60
2:B:73:ASN:O	2:B:75:GLU:N	2.35	0.60
2:B:172:GLU:HG3	6:G:93:PRO:HG2	1.84	0.60
15:1:80:GLU:HG3	18:1:1004:CLA:NB	2.17	0.59
15:1:41:TRP:CD1	15:1:59:PHE:CA	2.85	0.59
13:2:181:PRO:HD2	18:2:2016:CLA:CBB	2.32	0.59
18:3:3003:CLA:HMB2	18:3:3008:CLA:HBC1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:3502:LUT:H361	27:3:3502:LUT:C28	2.32	0.59
28:4:4010:CHL:HHD	28:4:4010:CHL:CBC	2.23	0.59
18:B:1206:CLA:HBB1	18:B:1206:CLA:HMB1	1.83	0.59
15:1:226:ILE:HG13	18:1:1003:CLA:CMD	2.32	0.59
22:3:3503:BCR:C23	22:3:3503:BCR:H403	2.32	0.59
16:3:74:GLY:O	16:3:232:ARG:NH1	2.35	0.59
18:A:1106:CLA:HAB	18:A:1126:CLA:H13	1.83	0.59
2:B:51:PHE:CE1	18:B:1208:CLA:HBB1	2.36	0.59
9:D:100:PHE:CE1	9:D:158:VAL:CB	2.85	0.59
15:1:58:ASP:CA	18:1:1004:CLA:HED2	2.32	0.59
13:2:85:PHE:HZ	13:2:223:LYS:HE3	1.66	0.59
16:3:162:MET:HA	16:3:162:MET:HE1	1.83	0.59
14:4:158:GLN:NE2	14:4:158:GLN:HA	2.17	0.59
2:B:174:ARG:HE	18:B:1221:CLA:HMD1	1.67	0.59
9:D:176:GLU:H	9:D:176:GLU:CD	2.06	0.59
15:1:111:TRP:HZ3	18:1:1006:CLA:HED1	1.66	0.59
28:2:2013:CHL:HBD	28:2:2013:CHL:HAA2	1.85	0.59
14:4:170:PRO:HD2	14:4:172:PHE:O	2.02	0.59
18:4:4004:CLA:H3A	18:4:4004:CLA:O1A	2.01	0.59
14:4:84:ASP:OD1	14:4:86:GLU:N	2.35	0.59
1:A:546:ALA:O	1:A:550:HIS:ND1	2.34	0.59
22:B:6004:BCR:H311	18:B:1212:CLA:H8	1.84	0.59
18:4:4001:CLA:C5	27:4:4501:LUT:H28	2.31	0.59
11:H:72:SER:O	11:H:73:ASP:HB3	2.01	0.59
18:2:2004:CLA:HMB1	18:2:2004:CLA:CBB	2.32	0.59
18:2:2016:CLA:O2A	18:2:2016:CLA:H2A	2.01	0.59
16:3:135:ALA:H	16:3:138:GLN:CG	2.15	0.59
16:3:268:VAL:HA	16:3:271:SER:HB3	1.84	0.59
18:3:3005:CLA:HMD2	18:3:3012:CLA:ND	2.16	0.59
16:3:67:TYR:CE2	16:3:84:SER:CB	2.86	0.59
6:G:114:VAL:HG12	6:G:116:LYS:H	1.68	0.59
16:3:137:PHE:CD1	16:3:138:GLN:N	2.71	0.59
16:3:155:TYR:CE1	18:3:3010:CLA:HAC2	2.38	0.59
2:B:377:TYR:CD2	18:B:1224:CLA:HAB	2.37	0.59
7:L:176:LEU:C	7:L:178:THR:HG22	2.23	0.59
15:1:183:LYS:HD3	18:1:1002:CLA:HBA2	1.83	0.59
15:1:80:GLU:OE2	15:1:189:ARG:NE	2.35	0.59
16:3:104:ILE:HD12	16:3:172:ARG:CZ	2.33	0.59
9:D:100:PHE:CE1	9:D:158:VAL:CG1	2.85	0.59
4:J:25:LEU:O	4:J:29:ILE:HG12	2.02	0.59
18:1:1003:CLA:C2	18:1:1008:CLA:HMD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:160:TYR:CZ	15:1:181:LYS:HD3	2.38	0.59
15:1:85:ARG:O	18:1:1001:CLA:HBC2	2.03	0.59
16:3:100:TYR:OH	16:3:172:ARG:HD2	2.03	0.59
16:3:263:PRO:HG2	18:3:3008:CLA:HMB3	1.84	0.59
18:3:3006:CLA:HMA1	18:3:3013:CLA:C3C	2.32	0.59
18:B:1222:CLA:HAA2	18:B:1223:CLA:OBD	2.03	0.59
2:B:334:LEU:HD11	18:B:1226:CLA:HBB1	1.85	0.59
18:B:1240:CLA:HED3	18:B:1220:CLA:HMA1	1.85	0.59
18:K:1001:CLA:HBC2	18:K:1001:CLA:CHD	2.30	0.59
12:K:70:MET:HE2	12:K:71:VAL:HA	1.82	0.59
15:1:111:TRP:CZ2	18:1:1013:CLA:CBC	2.85	0.59
16:3:243:ILE:CG2	18:3:3003:CLA:HMD3	2.33	0.59
16:3:246:LEU:HD23	16:3:246:LEU:O	2.03	0.59
16:3:127:LEU:O	18:3:3018:CLA:HBC3	2.02	0.59
9:D:91:LEU:N	9:D:91:LEU:HD23	2.18	0.59
10:E:111:ASN:OD1	10:E:115:VAL:HG22	2.02	0.59
6:G:129:SER:O	6:G:133:ILE:HG13	2.03	0.59
7:L:124:GLU:O	7:L:126:ALA:N	2.36	0.59
18:1:1001:CLA:HBA1	27:1:1501:LUT:H382	1.85	0.58
15:1:221:PRO:CG	15:1:222:TRP:CZ3	2.86	0.58
13:2:110:SER:HB3	13:2:225:GLY:HA3	1.85	0.58
16:3:134:LEU:HB3	16:3:138:GLN:HG3	1.85	0.58
14:4:225:THR:HG23	14:4:227:LYS:H	1.68	0.58
18:B:1211:CLA:CMC	18:B:1212:CLA:HAB	2.33	0.58
7:L:211:TYR:CE2	18:L:1503:CLA:C2	2.85	0.58
18:1:1001:CLA:H61	27:1:1501:LUT:H30	1.82	0.58
18:2:2007:CLA:H51	18:2:2007:CLA:C9	2.31	0.58
16:3:141:VAL:HG22	16:3:143:PRO:CD	2.32	0.58
16:3:267:ASN:ND2	16:3:270:THR:HG23	2.18	0.58
2:B:582:TRP:HH2	18:B:1012:CLA:HAB	1.68	0.58
5:F:82:LEU:HB3	5:F:140:CYS:O	2.02	0.58
15:1:186:LYS:CE	21:1:1801:LHG:HC41	2.33	0.58
16:3:248:THR:HG22	16:3:249:GLY:O	2.03	0.58
23:4:4801:LMG:O5	23:4:4801:LMG:O4	2.14	0.58
6:G:76:ARG:CG	6:G:77:PHE:CE1	2.86	0.58
12:K:83:PHE:HB2	22:K:2011:BCR:HC42	1.84	0.58
12:K:86:ALA:HB1	12:K:87:PRO:CD	2.28	0.58
13:2:125:PHE:O	13:2:130:GLY:N	2.30	0.58
14:4:95:GLU:HG3	18:4:4004:CLA:C4B	2.33	0.58
1:A:41:SER:HB3	1:A:44:ILE:HG22	1.84	0.58
18:B:1207:CLA:HMC3	27:I:6018:LUT:C14	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:1001:CLA:H51	22:G:2011:BCR:H341	1.85	0.58
6:G:123:ASP:N	6:G:123:ASP:OD1	2.31	0.58
12:K:71:VAL:HG11	12:K:132:ILE:HB	1.85	0.58
13:2:126:LEU:HD23	13:2:133:LEU:O	2.04	0.58
18:A:1129:CLA:HMA2	7:L:71:THR:HG21	1.84	0.58
8:C:26:LEU:H	8:C:26:LEU:HD22	1.68	0.58
6:G:111:TYR:N	6:G:111:TYR:CD1	2.71	0.58
14:4:120:ILE:HD12	14:4:120:ILE:H	1.68	0.58
27:4:4501:LUT:C8	27:4:4501:LUT:H171	2.34	0.58
1:A:218:TRP:HD1	1:A:303:HIS:CD2	2.21	0.58
18:B:1209:CLA:HBB1	18:B:1209:CLA:HMB1	1.85	0.58
3:I:5:PRO:C	3:I:7:LEU:H	2.07	0.58
18:B:1203:CLA:HHB	18:B:1226:CLA:HAB	1.86	0.58
2:B:492:ILE:HD11	6:G:146:TYR:CE1	2.38	0.58
15:1:41:TRP:CE3	28:1:1009:CHL:HBC3	2.38	0.58
13:2:145:TYR:CB	18:2:2006:CLA:H92	2.34	0.58
16:3:142:ILE:HD11	18:3:3010:CLA:CBC	2.33	0.58
16:3:203:PRO:HD3	28:3:3011:CHL:CMD	2.29	0.58
28:3:3011:CHL:HHC	28:3:3011:CHL:HBB1	1.84	0.58
14:4:223:ASN:O	14:4:224:VAL:HB	2.03	0.58
18:G:1003:CLA:C4B	23:G:2021:LMG:H151	2.33	0.58
15:1:134:ILE:HD11	18:1:1013:CLA:C2D	2.34	0.58
13:2:135:PRO:HG2	18:2:2006:CLA:HED1	1.86	0.58
22:3:3503:BCR:H323	22:3:3503:BCR:HC8	1.85	0.58
16:3:76:TYR:HB2	18:3:3004:CLA:HMD1	1.85	0.58
18:A:1022:CLA:CAD	18:B:1021:CLA:HMB3	2.33	0.58
15:1:165:PHE:O	27:1:1501:LUT:H24	2.04	0.58
15:1:177:PHE:CD2	15:1:181:LYS:HE2	2.38	0.58
18:3:3001:CLA:CBA	27:3:3501:LUT:H24	2.34	0.58
16:3:62:LYS:O	16:3:63:GLN:HB2	2.04	0.58
14:4:153:GLU:CG	14:4:156:ARG:HH11	2.17	0.58
2:B:659:THR:HA	18:B:1023:CLA:HAB	1.85	0.58
5:F:109:TYR:O	5:F:110:ALA:HB3	2.04	0.58
5:F:160:PHE:O	5:F:163:PRO:HD2	2.04	0.58
6:G:92:LEU:HD12	6:G:92:LEU:N	2.02	0.58
12:K:72:ALA:CB	18:K:1001:CLA:CGA	2.81	0.58
7:L:121:ARG:C	7:L:124:GLU:H	2.07	0.58
7:L:143:ILE:O	7:L:146:THR:HG22	2.04	0.58
15:1:85:ARG:HE	18:1:1001:CLA:C4C	2.17	0.57
16:3:197:SER:OG	16:3:198:GLY:N	2.37	0.57
16:3:210:PRO:HB2	16:3:211:LEU:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:4:4011:CHL:HHC	28:4:4011:CHL:HBB1	1.85	0.57
18:2:2008:CLA:CBB	18:2:2008:CLA:HHC	2.34	0.57
16:3:119:PRO:HB2	16:3:133:ALA:HB2	1.86	0.57
16:3:94:GLU:OE1	16:3:96:ARG:HB2	2.04	0.57
14:4:178:PRO:O	14:4:179:ALA:HB2	2.04	0.57
2:B:707:LEU:HD23	25:B:7101:DGD:HA21	1.85	0.57
9:D:88:THR:O	9:D:88:THR:HG22	2.04	0.57
7:L:91:THR:HA	7:L:175:GLN:HE22	1.69	0.57
13:2:110:SER:O	13:2:114:MET:HG3	2.04	0.57
13:2:224:ASN:OD1	18:2:2007:CLA:HMD1	2.04	0.57
16:3:62:LYS:HB2	16:3:63:GLN:OE1	2.04	0.57
12:K:90:ASN:O	16:3:64:SER:HB3	2.04	0.57
14:4:103:MET:HB2	18:4:4001:CLA:CMC	2.34	0.57
14:4:57:LEU:HD11	18:4:4009:CLA:CED	2.35	0.57
18:B:1204:CLA:H3A	18:B:1205:CLA:HMB3	1.86	0.57
10:E:104:VAL:HG12	10:E:119:ASN:OD1	2.03	0.57
18:G:1003:CLA:C14	18:G:1003:CLA:H91	2.35	0.57
4:J:36:ALA:CB	23:J:5001:LMG:H111	2.30	0.57
15:1:58:ASP:CB	18:1:1004:CLA:HED2	2.35	0.57
16:3:267:ASN:HA	18:3:3003:CLA:O1A	2.05	0.57
18:B:1216:CLA:HAA2	18:B:1221:CLA:HBB1	1.86	0.57
9:D:155:PHE:CZ	9:D:168:HIS:HB3	2.39	0.57
11:H:132:PRO:N	11:H:133:PRO:HD3	2.18	0.57
22:J:6012:BCR:C23	22:J:6012:BCR:H383	2.28	0.57
12:K:136:VAL:HG12	12:K:140:LEU:HD21	1.86	0.57
7:L:121:ARG:HG2	7:L:127:GLY:N	2.20	0.57
18:L:1502:CLA:HHD	22:L:6019:BCR:H292	1.87	0.57
16:3:263:PRO:HG3	18:3:3008:CLA:HMB3	1.85	0.57
16:3:110:MET:CE	27:3:3501:LUT:H201	2.35	0.57
9:D:76:ASP:CB	9:D:77:PRO:HB3	2.30	0.57
18:G:1003:CLA:H62	23:G:2021:LMG:H132	1.84	0.57
15:1:124:ASN:OD1	15:1:124:ASN:N	2.38	0.57
13:2:87:PHE:HE2	27:2:2502:LUT:C36	2.14	0.57
16:3:100:TYR:HD1	16:3:100:TYR:O	1.87	0.57
16:3:136:TRP:CD2	16:3:137:PHE:N	2.72	0.57
18:3:3010:CLA:C3C	18:3:3010:CLA:H93	2.35	0.57
14:4:101:TRP:CE2	28:4:4011:CHL:HED3	2.39	0.57
14:4:184:TYR:O	18:4:4001:CLA:HED2	2.04	0.57
18:4:4006:CLA:C1B	27:4:4503:LUT:C17	2.83	0.57
1:A:24:ARG:NH1	1:A:76:ARG:HH12	2.03	0.57
3:I:4:LEU:CD1	3:I:6:SER:H	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:127:PRO:CG	15:1:128:TRP:CD1	2.85	0.57
18:2:2005:CLA:O1D	18:2:2012:CLA:H61	2.05	0.57
16:3:101:GLY:CA	18:3:3012:CLA:HED2	2.35	0.57
18:4:4003:CLA:H91	18:4:4003:CLA:H121	1.85	0.57
18:4:4008:CLA:CHD	18:4:4008:CLA:HBC2	2.34	0.57
28:4:4013:CHL:HBB1	27:4:4502:LUT:H161	1.86	0.57
18:A:1127:CLA:H91	18:A:1117:CLA:H92	1.86	0.57
1:A:338:PHE:HB2	21:A:5003:LHG:HC42	1.86	0.57
18:B:1211:CLA:HHC	18:B:1211:CLA:HBB1	1.85	0.57
18:1:1011:CLA:H43	27:1:1501:LUT:O23	2.04	0.57
15:1:111:TRP:CD1	15:1:112:ALA:N	2.72	0.57
16:3:253:TYR:O	16:3:256:LEU:HB3	2.04	0.57
16:3:270:THR:HG1	16:3:271:SER:N	2.01	0.57
16:3:65:LEU:HB3	16:3:68:LEU:CD2	2.34	0.57
9:D:167:LEU:O	9:D:170:LYS:HB2	2.04	0.57
15:1:205:TYR:HE2	18:1:1003:CLA:O1D	1.88	0.57
15:1:223:HIS:CD2	15:1:223:HIS:N	2.73	0.57
13:2:197:GLY:HA2	18:2:2001:CLA:HED1	1.86	0.57
13:2:114:MET:HE1	18:2:2001:CLA:CHC	2.34	0.57
18:2:2005:CLA:HED2	18:2:2012:CLA:O1A	2.05	0.57
18:B:1240:CLA:HED3	18:B:1220:CLA:HBB	1.86	0.57
18:G:1003:CLA:H51	23:G:2021:LMG:C31	2.25	0.57
6:G:102:GLU:O	6:G:103:ALA:HB3	2.05	0.57
7:L:115:VAL:HG13	7:L:127:GLY:O	2.05	0.57
15:1:133:THR:HG22	15:1:137:ILE:HD11	1.87	0.56
15:1:167:PRO:HD2	27:1:1501:LUT:H1	1.70	0.56
18:2:2001:CLA:CGA	18:2:2001:CLA:H3A	2.35	0.56
16:3:136:TRP:CE2	16:3:137:PHE:HB3	2.38	0.56
14:4:147:ILE:HD11	21:1:1801:LHG:C36	2.35	0.56
14:4:240:PRO:HG2	18:4:4008:CLA:C2B	2.34	0.56
18:L:1501:CLA:HED2	11:H:82:GLN:NE2	2.20	0.56
7:L:171:LYS:O	7:L:172:GLN:HB3	2.04	0.56
18:1:1002:CLA:HMD2	18:1:1007:CLA:C4D	2.35	0.56
13:2:143:GLN:CB	13:2:145:TYR:CE1	2.85	0.56
13:2:164:GLU:HA	13:2:167:ARG:H	1.70	0.56
13:2:211:PRO:O	13:2:212:GLN:CB	2.52	0.56
16:3:185:GLN:HB2	16:3:186:TYR:CE1	2.39	0.56
28:4:4013:CHL:CBB	27:4:4502:LUT:H161	2.34	0.56
1:A:493:GLN:HG3	1:A:515:TRP:HD1	1.68	0.56
15:1:41:TRP:HD1	15:1:59:PHE:O	1.87	0.56
13:2:186:ASN:CG	18:2:2016:CLA:H2A	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:110:MET:SD	16:3:231:GLY:CA	2.92	0.56
16:3:259:HIS:ND1	18:3:3003:CLA:HAA2	2.20	0.56
16:3:105:ASN:CG	18:3:3012:CLA:HMD1	2.25	0.56
18:4:4005:CLA:HAB	27:4:4502:LUT:H35	1.86	0.56
14:4:88:LEU:O	14:4:92:VAL:HG23	2.05	0.56
18:G:1003:CLA:C3	23:G:2021:LMG:H331	2.35	0.56
27:I:6018:LUT:H162	22:I:6020:BCR:H353	1.87	0.56
15:1:83:HIS:HD2	27:1:1502:LUT:H35	1.69	0.56
18:2:2009:CLA:HHC	18:2:2009:CLA:CBB	2.18	0.56
16:3:173:PHE:HD2	18:3:3012:CLA:HMA2	1.70	0.56
1:A:310:PHE:HZ	18:A:1117:CLA:H121	1.70	0.56
22:B:6004:BCR:H371	18:B:1218:CLA:HMD2	1.87	0.56
9:D:97:VAL:HG12	9:D:97:VAL:O	2.05	0.56
18:G:1003:CLA:H52	23:G:2021:LMG:C33	2.35	0.56
18:G:1003:CLA:C4	23:G:2021:LMG:H332	2.36	0.56
13:2:125:PHE:HB3	13:2:131:ILE:HD12	1.88	0.56
13:2:160:ILE:HD11	28:2:2013:CHL:HMB3	1.86	0.56
16:3:65:LEU:HB2	16:3:68:LEU:HD21	1.83	0.56
1:A:40:PHE:HB3	18:A:1102:CLA:HED2	1.87	0.56
15:1:111:TRP:CE2	15:1:119:ALA:HB1	2.40	0.56
15:1:170:TYR:HE2	27:1:1501:LUT:H372	1.70	0.56
13:2:129:LEU:HD22	13:2:131:ILE:HG13	1.87	0.56
1:A:183:TRP:HB2	18:A:1109:CLA:HMC3	1.86	0.56
1:A:394:SER:HB3	18:A:1126:CLA:HMA1	1.88	0.56
18:G:1001:CLA:C4	22:G:2011:BCR:H342	2.35	0.56
11:H:133:PRO:HD2	11:H:135:LEU:N	2.21	0.56
15:1:180:TYR:HB3	18:1:1001:CLA:HMA1	1.86	0.56
18:3:3003:CLA:H42	18:3:3003:CLA:CHD	2.35	0.56
16:3:226:LYS:HE2	18:3:3007:CLA:HED2	1.84	0.56
18:4:4017:CLA:H3A	29:4:4505:ZEX:H202	1.88	0.56
2:B:476:VAL:HG12	2:B:477:LEU:H	1.71	0.56
10:E:102:PRO:HG2	10:E:103:VAL:HG23	1.88	0.56
28:1:1010:CHL:HBB2	18:1:1013:CLA:HBB2	1.88	0.56
15:1:160:TYR:CE2	15:1:181:LYS:HD3	2.40	0.56
15:1:203:SER:O	15:1:204:ALA:HB3	2.05	0.56
13:2:141:GLY:HA2	28:2:2013:CHL:CBC	2.35	0.56
14:4:215:PHE:CE1	27:4:4502:LUT:H10	2.40	0.56
18:4:4005:CLA:CMD	18:4:4012:CLA:C1D	2.83	0.56
27:4:4503:LUT:H28	27:4:4503:LUT:H371	1.86	0.56
14:4:52:LYS:O	14:4:53:LYS:HB3	2.06	0.56
18:2:2003:CLA:C1B	18:2:2008:CLA:HMD3	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:167:PHE:O	16:3:171:ARG:HG3	2.05	0.56
14:4:97:VAL:HG21	14:4:156:ARG:NH2	2.21	0.56
1:A:373:ALA:HB2	1:A:399:HIS:HB2	1.88	0.56
18:B:1238:CLA:H13	27:I:6018:LUT:C19	2.36	0.56
9:D:202:LYS:O	9:D:203:PHE:HB2	2.04	0.56
18:G:1002:CLA:HBC3	18:G:1002:CLA:HMC1	1.86	0.56
15:1:222:TRP:CH2	18:1:1008:CLA:CMB	2.85	0.56
18:2:2005:CLA:OBD	18:2:2012:CLA:HBA2	2.05	0.56
16:3:225:LEU:HB3	16:3:226:LYS:HE3	1.88	0.56
22:B:6004:BCR:H292	18:B:1218:CLA:C4D	2.36	0.56
11:H:107:GLY:HA2	11:H:110:THR:CG2	2.36	0.56
12:K:86:ALA:CB	12:K:87:PRO:CD	2.84	0.56
18:2:2001:CLA:C3A	18:2:2001:CLA:CGA	2.83	0.56
16:3:190:LEU:O	16:3:194:PHE:N	2.38	0.56
10:E:78:ARG:O	10:E:79:GLN:HB2	2.05	0.56
13:2:126:LEU:HB2	13:2:134:THR:HA	1.87	0.55
18:2:2004:CLA:HHC	27:2:2502:LUT:H32	1.88	0.55
16:3:235:MET:O	16:3:238:ILE:HG23	2.06	0.55
18:3:3003:CLA:C3B	27:3:3501:LUT:C17	2.84	0.55
16:3:263:PRO:HG3	18:3:3008:CLA:CMB	2.36	0.55
14:4:169:ASP:HA	18:4:4016:CLA:O1D	2.06	0.55
18:B:1204:CLA:O2A	3:I:12:VAL:HG21	2.05	0.55
18:G:1001:CLA:HED3	18:G:1001:CLA:CHA	2.35	0.55
7:L:145:LEU:HD11	22:L:6019:BCR:C39	2.20	0.55
13:2:174:PRO:CD	13:2:175:GLY:N	2.70	0.55
28:4:4011:CHL:CHD	28:4:4011:CHL:HBC2	2.29	0.55
21:A:5003:LHG:H302	18:A:1122:CLA:H152	1.89	0.55
1:A:21:ILE:HD13	18:A:1108:CLA:HAA2	1.87	0.55
18:B:1021:CLA:HBB1	18:B:1021:CLA:HMB1	1.88	0.55
22:F:6014:BCR:C40	22:F:6014:BCR:H23C	2.36	0.55
11:H:95:LYS:O	11:H:96:ARG:HB3	2.06	0.55
7:L:90:ARG:O	7:L:98:ARG:HD3	2.06	0.55
18:1:1001:CLA:CGA	18:1:1001:CLA:H3A	2.35	0.55
15:1:118:GLN:O	15:1:119:ALA:HB3	2.06	0.55
18:4:4007:CLA:H2A	18:4:4007:CLA:HED2	1.87	0.55
18:A:1105:CLA:HBB1	18:A:1105:CLA:HHC	1.89	0.55
18:A:1134:CLA:H92	18:A:1134:CLA:H2	1.87	0.55
2:B:26:ALA:HB2	25:B:7101:DGD:HA32	1.89	0.55
2:B:292:ARG:HH21	6:G:107:ARG:NH1	2.04	0.55
22:K:2011:BCR:H321	22:K:2011:BCR:C8	2.15	0.55
15:1:112:ALA:HB3	28:1:1010:CHL:HMD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:142:GLU:O	13:2:142:GLU:HG3	2.06	0.55
16:3:134:LEU:CB	16:3:138:GLN:CG	2.84	0.55
16:3:236:LEU:CD2	18:3:3004:CLA:HMC1	2.33	0.55
1:A:92:TRP:HE1	18:A:1106:CLA:HBA1	1.72	0.55
18:A:1022:CLA:H161	22:A:6017:BCR:H321	1.89	0.55
22:A:6017:BCR:H292	20:B:5002:PQN:H142	1.89	0.55
4:J:38:THR:O	23:J:5001:LMG:H122	2.05	0.55
13:2:197:GLY:HA2	18:2:2001:CLA:CED	2.36	0.55
18:2:2016:CLA:CAD	18:2:2016:CLA:HED2	2.36	0.55
18:3:3010:CLA:H93	18:3:3010:CLA:C1C	2.37	0.55
18:3:3006:CLA:C1D	18:3:3018:CLA:CBB	2.84	0.55
16:3:65:LEU:CD2	16:3:66:SER:H	2.19	0.55
16:3:74:GLY:HA2	16:3:225:LEU:HD22	1.87	0.55
18:4:4001:CLA:H51	27:4:4501:LUT:H30	1.89	0.55
1:A:223:VAL:HG23	1:A:224:HIS:CD2	2.42	0.55
18:G:1003:CLA:H91	18:G:1003:CLA:H142	1.88	0.55
7:L:169:ARG:CZ	7:L:171:LYS:CB	2.85	0.55
18:1:1001:CLA:HMC1	18:1:1001:CLA:HBC2	1.89	0.55
13:2:139:THR:HA	28:2:2010:CHL:CED	2.35	0.55
16:3:140:GLY:HA2	18:3:3013:CLA:CBC	2.32	0.55
14:4:98:ASN:ND2	18:4:4012:CLA:HMD1	2.22	0.55
9:D:109:LYS:HG2	9:D:110:GLU:N	2.22	0.55
9:D:100:PHE:CE1	9:D:158:VAL:HG11	2.41	0.55
11:H:134:LYS:O	11:H:135:LEU:HG	2.06	0.55
27:4:4503:LUT:H361	28:1:1009:CHL:H62	1.89	0.55
15:1:126:VAL:CB	15:1:127:PRO:CA	2.83	0.55
18:2:2004:CLA:HHD	18:2:2004:CLA:HBC2	1.88	0.55
16:3:267:ASN:HB2	18:3:3003:CLA:O1A	2.07	0.55
16:3:110:MET:CE	27:3:3501:LUT:C20	2.85	0.55
18:B:1204:CLA:H11	27:I:6018:LUT:O23	2.07	0.55
22:J:6012:BCR:H23C	22:J:6012:BCR:C38	2.30	0.55
18:4:4004:CLA:CBB	27:4:4502:LUT:H32	2.36	0.55
18:4:4017:CLA:OBD	28:1:1009:CHL:HMA1	2.06	0.55
18:A:1102:CLA:HMA2	18:A:1109:CLA:HMD2	1.87	0.55
12:K:132:ILE:O	12:K:136:VAL:HG23	2.07	0.55
18:1:1001:CLA:CBB	27:1:1501:LUT:C32	2.85	0.55
18:2:2003:CLA:C3B	27:2:2501:LUT:C38	2.85	0.55
18:3:3005:CLA:CMD	18:3:3012:CLA:C1D	2.84	0.55
18:3:3006:CLA:CHA	18:3:3006:CLA:CED	2.85	0.55
18:3:3003:CLA:C2B	27:3:3501:LUT:C17	2.84	0.55
16:3:65:LEU:CD1	16:3:67:TYR:HE1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:104:LEU:C	18:4:4006:CLA:CBB	2.74	0.55
27:4:4501:LUT:C8	27:4:4501:LUT:C17	2.85	0.55
22:G:2011:BCR:C23	22:G:2011:BCR:C40	2.85	0.55
11:H:110:THR:HG23	11:H:111:LEU:N	2.20	0.55
18:2:2001:CLA:O1A	18:2:2001:CLA:H3A	2.06	0.55
16:3:134:LEU:HB3	16:3:138:GLN:CG	2.36	0.55
9:D:100:PHE:CD1	9:D:158:VAL:HB	2.41	0.55
22:F:6014:BCR:C40	22:F:6014:BCR:C23	2.85	0.55
7:L:94:ASN:HB3	7:L:97:LEU:HD12	1.83	0.55
15:1:134:ILE:CD1	18:1:1013:CLA:C2D	2.85	0.54
15:1:230:VAL:HG12	15:1:231:LEU:CD2	2.36	0.54
18:2:2002:CLA:CGA	18:2:2002:CLA:CED	2.84	0.54
16:3:232:ARG:HD2	18:3:3004:CLA:C4C	2.37	0.54
18:3:3003:CLA:CHC	18:3:3003:CLA:C9	2.85	0.54
14:4:186:GLY:O	14:4:189:PHE:HB2	2.07	0.54
27:4:4502:LUT:C8	27:4:4502:LUT:C17	2.86	0.54
1:A:434:ARG:O	1:A:438:HIS:ND1	2.33	0.54
1:A:54:ILE:HD12	18:A:1139:CLA:HMB3	1.89	0.54
18:G:1001:CLA:CED	18:G:1001:CLA:CHA	2.85	0.54
7:L:121:ARG:O	7:L:124:GLU:N	2.38	0.54
18:1:1001:CLA:C3A	18:1:1001:CLA:CGA	2.85	0.54
13:2:118:ALA:CB	18:2:2006:CLA:CMC	2.85	0.54
13:2:256:ASP:CG	13:2:259:HIS:HD2	2.10	0.54
16:3:129:PRO:O	16:3:132:THR:HG22	2.07	0.54
16:3:141:VAL:HG13	16:3:144:PRO:HD2	1.88	0.54
16:3:146:GLY:C	16:3:147:THR:HG1	2.02	0.54
16:3:104:ILE:HD12	16:3:172:ARG:NH2	2.21	0.54
16:3:196:GLY:O	16:3:197:SER:HB3	2.06	0.54
28:3:3011:CHL:CAA	28:3:3011:CHL:CBD	2.85	0.54
18:3:3017:CLA:H3A	18:3:3017:CLA:O2A	2.06	0.54
14:4:118:ILE:HG23	14:4:120:ILE:H	1.72	0.54
18:4:4006:CLA:C4B	27:4:4503:LUT:C17	2.86	0.54
17:A:1011:CL0:H13	18:B:1012:CLA:OBD	2.07	0.54
8:C:14:CYS:SG	8:C:16:GLN:HG2	2.48	0.54
10:E:78:ARG:NH1	10:E:124:GLU:OE1	2.40	0.54
12:K:75:THR:HG21	12:K:129:GLY:HA2	1.88	0.54
15:1:85:ARG:NE	18:1:1001:CLA:C4C	2.71	0.54
13:2:125:PHE:CB	13:2:131:ILE:HD12	2.37	0.54
16:3:183:GLY:HA3	16:3:194:PHE:C	2.28	0.54
18:4:4007:CLA:CAA	18:4:4007:CLA:HED2	2.37	0.54
1:A:274:TRP:CH2	18:A:1115:CLA:HBB1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:ILE:HG13	2:B:255:LEU:HG	1.88	0.54
15:1:205:TYR:OH	18:1:1003:CLA:OBD	2.18	0.54
18:2:2016:CLA: CBD	18:2:2016:CLA:CGA	2.85	0.54
13:2:92:LEU:CD1	27:2:2502:LUT:C24	2.85	0.54
16:3:101:GLY:CA	18:3:3012:CLA: CED	2.85	0.54
18:3:3003:CLA:C12	18:3:3003:CLA:C9	2.85	0.54
18:4:4003:CLA:C1C	18:4:4003:CLA:H61	2.38	0.54
1:A:195:TRP:CZ2	18:A:1108:CLA:HMA1	2.42	0.54
18:B:1207:CLA:H92	7:L:132:LEU:HG	1.90	0.54
18:G:1001:CLA:C5	22:G:2011:BCR:C34	2.85	0.54
6:G:95:GLN:O	6:G:96:ASN:HB2	2.07	0.54
22:L:6020:BCR:C19	18:L:1501:CLA:HMB2	2.37	0.54
7:L:116:LYS:HD3	18:L:1503:CLA:CMB	2.35	0.54
15:1:183:LYS:HG2	18:1:1007:CLA:HED2	1.89	0.54
23:F:5002:LMG:H292	18:1:1014:CLA:C1D	2.38	0.54
15:1:80:GLU:OE2	15:1:189:ARG:NH2	2.39	0.54
18:2:2003:CLA:CHD	18:2:2003:CLA:C4	2.85	0.54
28:2:2011:CHL:CBB	18:2:2016:CLA:CAB	2.86	0.54
14:4:198:LEU:N	14:4:198:LEU:HD12	2.21	0.54
18:A:1106:CLA:H62	18:A:1126:CLA:H92	1.89	0.54
1:A:213:LEU:HD22	22:A:6002:BCR:H361	1.89	0.54
18:B:1224:CLA:CGA	18:B:1224:CLA:H3A	2.37	0.54
18:1:1006:CLA:HMA2	18:1:1013:CLA:CBC	2.38	0.54
18:1:1003:CLA:H12	18:1:1008:CLA:CMD	2.37	0.54
14:4:155:ARG:NH1	28:1:1009:CHL:OBD	2.41	0.54
15:1:134:ILE:HD11	18:1:1013:CLA:C3D	2.38	0.54
15:1:88:MET:CE	18:1:1001:CLA:CAB	2.85	0.54
13:2:197:GLY:CA	18:2:2001:CLA: CED	2.85	0.54
16:3:117:ILE:CD1	16:3:252:PRO:HB2	2.38	0.54
14:4:152:VAL:CG1	28:4:4011:CHL:C1B	2.85	0.54
18:4:4012:CLA:HMC1	18:4:4012:CLA:HBC3	1.90	0.54
18:G:1001:CLA:HMB2	22:G:2011:BCR:C15	2.37	0.54
15:1:88:MET:CE	18:1:1001:CLA:CHC	2.86	0.54
13:2:178:ASN:HD22	13:2:179:THR:N	2.05	0.54
16:3:120:GLU:OE2	16:3:254:GLN:N	2.31	0.54
16:3:179:PRO:HG2	16:3:180:GLY:H	1.71	0.54
18:3:3010:CLA:C9	18:3:3010:CLA:C1C	2.85	0.54
16:3:67:TYR:HE2	16:3:84:SER:HB3	1.72	0.54
14:4:126:TRP:C	14:4:128:ASP:H	2.11	0.54
2:B:124:TRP:HB3	2:B:129:LEU:HD12	1.90	0.54
2:B:225:LEU:O	2:B:230:TRP:NE1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:120:THR:HG22	15:1:125:PRO:N	2.23	0.54
18:2:2005:CLA:CBC	18:2:2012:CLA:CBC	2.85	0.54
18:3:3013:CLA:CBB	27:3:3502:LUT:C18	2.86	0.54
18:2:2007:CLA:CBB	22:3:3503:BCR:C26	2.85	0.54
22:3:3503:BCR:C8	22:3:3503:BCR:C32	2.86	0.54
14:4:152:VAL:HG11	28:4:4011:CHL:CHB	2.38	0.54
18:4:4016:CLA:C4D	18:4:4016:CLA:C1	2.86	0.54
1:A:268:PRO:HD2	1:A:277:TYR:CZ	2.43	0.54
18:G:1002:CLA:HBA2	18:G:1002:CLA:HBD	1.89	0.54
18:G:1003:CLA:C5	23:G:2021:LMG:C33	2.85	0.54
3:I:4:LEU:HD11	3:I:6:SER:CB	2.29	0.54
15:1:202:GLN:CA	15:1:202:GLN:NE2	2.71	0.54
15:1:40:ASP:N	15:1:47:ARG:HD2	2.23	0.54
13:2:125:PHE:CB	13:2:131:ILE:CD1	2.86	0.54
18:2:2003:CLA:HMB3	18:2:2008:CLA:HBC1	1.89	0.54
13:2:233:MET:HG2	18:2:2004:CLA:H193	1.89	0.54
28:2:2013:CHL:O2A	28:2:2013:CHL:H2A	2.07	0.54
13:2:225:GLY:O	13:2:229:MET:HG3	2.08	0.54
14:4:170:PRO:CB	18:4:4016:CLA:C4A	2.85	0.54
18:4:4007:CLA:CBC	18:4:4007:CLA:CHD	2.86	0.54
14:4:169:ASP:CB	18:4:4016:CLA:C2D	2.85	0.54
18:G:1001:CLA:H51	22:G:2011:BCR:C34	2.38	0.54
22:J:6012:BCR:C38	22:J:6012:BCR:C23	2.85	0.54
12:K:79:PHE:O	12:K:80:ALA:HB2	2.07	0.54
18:1:1003:CLA:C2	18:1:1008:CLA:CMD	2.85	0.54
28:2:2011:CHL:HBB2	18:2:2016:CLA:CBB	2.38	0.54
16:3:134:LEU:HB3	16:3:138:GLN:OE1	2.07	0.54
16:3:132:THR:O	16:3:134:LEU:HD23	2.07	0.54
1:A:266:ALA:HB3	16:3:272:LEU:HD13	1.90	0.54
2:B:306:GLU:HA	2:B:320:LYS:HG2	1.90	0.54
18:B:1240:CLA:HED1	22:B:6009:BCR:H353	1.89	0.54
22:F:6014:BCR:H23C	22:F:6014:BCR:H402	1.88	0.54
18:4:4002:CLA:H12	18:4:4002:CLA:CMA	2.09	0.53
18:4:4006:CLA:C3B	27:4:4502:LUT:C18	2.85	0.53
18:4:4008:CLA:CBB	18:4:4008:CLA:HHC	2.37	0.53
2:B:6:PRO:HG3	2:B:24:GLY:HA2	1.88	0.53
2:B:523:ILE:HD13	18:B:1234:CLA:HAB	1.90	0.53
6:G:114:VAL:HG11	18:G:1002:CLA:CBA	2.38	0.53
28:1:1009:CHL:CED	28:1:1009:CHL:H2A	2.39	0.53
13:2:104:GLN:NE2	13:2:193:VAL:CG2	2.72	0.53
14:4:225:THR:HG21	14:4:232:ASN:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:4001:CLA:HHD	18:4:4001:CLA:HBC2	1.89	0.53
14:4:101:TRP:CZ2	28:4:4011:CHL:HED3	2.43	0.53
18:B:1240:CLA:H142	18:B:1227:CLA:HMC2	1.90	0.53
18:G:1002:CLA:HMB1	18:G:1002:CLA:HBB1	1.90	0.53
18:G:1003:CLA:C3	23:G:2021:LMG:C33	2.85	0.53
7:L:169:ARG:HD2	7:L:171:LYS:H	1.72	0.53
15:1:58:ASP:CB	18:1:1004:CLA:CED	2.86	0.53
18:2:2008:CLA:CBC	18:2:2008:CLA:CHD	2.85	0.53
13:2:67:TRP:NE1	13:2:86:GLY:O	2.41	0.53
18:3:3006:CLA:CMA	18:3:3013:CLA:C3C	2.85	0.53
18:3:3006:CLA:CMD	18:3:3018:CLA:CAB	2.87	0.53
16:3:161:GLU:CD	18:3:3010:CLA:HAB	2.29	0.53
27:4:4503:LUT:H181	27:4:4503:LUT:C8	2.10	0.53
1:A:126:ILE:HB	22:J:6013:BCR:H322	1.90	0.53
7:L:94:ASN:HB2	7:L:97:LEU:CD1	2.23	0.53
13:2:188:LEU:CD2	13:2:198:GLY:HA3	2.24	0.53
28:3:3011:CHL:CBA	28:3:3011:CHL:CBD	2.85	0.53
21:A:7001:LHG:H252	18:A:1128:CLA:H42	1.89	0.53
18:B:1216:CLA:HMC2	18:B:1221:CLA:H18	1.91	0.53
7:L:91:THR:HA	7:L:98:ARG:HH21	1.71	0.53
18:2:2001:CLA:H43	18:2:2002:CLA:HBA1	1.85	0.53
18:3:3008:CLA:HBA1	18:3:3008:CLA:CBD	2.38	0.53
14:4:120:ILE:CD1	14:4:120:ILE:H	2.22	0.53
14:4:199:GLU:HA	14:4:202:GLU:HG3	1.90	0.53
18:4:4004:CLA:CGA	18:4:4004:CLA:H3A	2.38	0.53
22:A:6002:BCR:H331	18:A:1112:CLA:HBB	1.90	0.53
1:A:269:PHE:HD2	1:A:270:PHE:HD1	1.55	0.53
9:D:82:PRO:HG3	9:D:128:ASN:HD21	1.72	0.53
15:1:152:GLU:HG3	15:1:156:GLU:HA	1.91	0.53
15:1:58:ASP:CG	18:1:1004:CLA:HED2	2.29	0.53
13:2:220:LYS:CE	18:2:2002:CLA:CED	2.85	0.53
13:2:242:THR:HG22	13:2:242:THR:O	2.08	0.53
13:2:246:PRO:O	13:2:249:ASN:HB2	2.09	0.53
16:3:110:MET:SD	16:3:231:GLY:N	2.82	0.53
16:3:67:TYR:CE2	16:3:84:SER:HB2	2.43	0.53
14:4:135:PHE:O	14:4:136:ALA:HB3	2.09	0.53
18:4:4005:CLA:CMD	18:4:4012:CLA:ND	2.72	0.53
18:4:4016:CLA:CHA	18:4:4016:CLA:HBA1	2.39	0.53
23:4:4801:LMG:HC72	23:4:4801:LMG:O2	2.07	0.53
9:D:76:ASP:HB3	9:D:77:PRO:HA	1.88	0.53
7:L:206:VAL:O	7:L:207:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:90:ARG:HA	11:H:72:SER:OG	2.09	0.53
15:1:221:PRO:CG	15:1:222:TRP:CE3	2.85	0.53
13:2:122:ILE:HG23	13:2:133:LEU:HD22	1.90	0.53
13:2:177:VAL:CG2	13:2:178:ASN:N	2.72	0.53
13:2:197:GLY:N	18:2:2001:CLA:CED	2.72	0.53
18:2:2005:CLA:H41	18:2:2005:CLA:C9	2.39	0.53
16:3:119:PRO:HB2	16:3:133:ALA:HB1	1.89	0.53
16:3:185:GLN:C	16:3:186:TYR:HD1	2.12	0.53
16:3:193:GLY:HA3	16:3:207:PHE:CE2	2.44	0.53
16:3:227:GLU:HB2	18:3:3001:CLA:C1B	2.39	0.53
16:3:259:HIS:N	16:3:266:ASN:ND2	2.57	0.53
1:A:209:GLY:HA2	18:A:1118:CLA:HBC1	1.91	0.53
1:A:493:GLN:HG3	1:A:515:TRP:CD1	2.43	0.53
2:B:167:TRP:CZ2	18:B:1208:CLA:HMA1	2.44	0.53
27:I:6018:LUT:H181	27:I:6018:LUT:H8	1.90	0.53
18:1:1001:CLA:C4D	27:1:1501:LUT:H383	2.39	0.53
15:1:120:THR:HG22	15:1:125:PRO:CA	2.38	0.53
18:1:1004:CLA:HBB2	27:1:1502:LUT:H12	1.86	0.53
15:1:104:ASN:ND2	15:1:208:THR:HG23	2.24	0.53
18:2:2002:CLA:HMB1	18:2:2002:CLA:CBB	2.34	0.53
18:2:2003:CLA:CGA	18:2:2003:CLA:C1A	2.87	0.53
13:2:181:PRO:HD2	18:2:2016:CLA:HBB1	1.91	0.53
18:3:3012:CLA:HMC1	18:3:3012:CLA:HBC2	1.91	0.53
14:4:245:ILE:HG12	14:4:249:LEU:HD12	1.89	0.53
2:B:177:HIS:CG	18:B:1210:CLA:HMC2	2.44	0.53
16:3:226:LYS:N	16:3:226:LYS:CE	2.72	0.53
18:A:1121:CLA:C2D	22:K:2011:BCR:H323	2.38	0.53
2:B:389:HIS:HA	2:B:392:ILE:HD12	1.91	0.53
8:C:26:LEU:N	8:C:26:LEU:HD22	2.23	0.53
10:E:66:ILE:HB	10:E:95:GLN:OE1	2.08	0.53
18:F:1301:CLA:HHC	18:F:1301:CLA:CBB	2.37	0.53
18:B:1238:CLA:H18	27:I:6018:LUT:H203	1.90	0.53
18:L:1502:CLA:C3C	22:L:6019:BCR:H282	2.39	0.53
22:L:6019:BCR:C38	22:L:6019:BCR:C23	2.85	0.53
13:2:250:LEU:HD23	13:2:254:LEU:HD21	1.89	0.53
13:2:87:PHE:CE2	27:2:2502:LUT:C36	2.86	0.53
9:D:173:VAL:HG12	9:D:174:TYR:H	1.72	0.53
3:I:29:GLU:HB2	7:L:151:SER:OG	2.08	0.53
4:J:9:SER:O	4:J:10:VAL:HG22	2.09	0.53
15:1:145:VAL:O	15:1:148:GLN:HB2	2.08	0.52
18:3:3006:CLA:HMA2	18:3:3013:CLA:HAC2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:212:MET:HB2	18:4:4004:CLA:HMC3	1.90	0.52
18:A:1134:CLA:H3A	18:A:1116:CLA:H93	1.91	0.52
7:L:204:LEU:HD13	7:L:204:LEU:C	2.28	0.52
15:1:42:MET:SD	15:1:45:GLN:HG3	2.50	0.52
13:2:139:THR:CA	28:2:2010:CHL:CED	2.84	0.52
18:2:2002:CLA:HMD2	18:2:2007:CLA:ND	2.24	0.52
28:3:3011:CHL:O1D	28:3:3011:CHL:H2A	2.09	0.52
18:4:4004:CLA:HMC2	27:4:4502:LUT:C32	2.39	0.52
1:A:268:PRO:HA	1:A:271:THR:HG22	1.91	0.52
18:B:1221:CLA:HMA1	18:B:1221:CLA:H92	1.90	0.52
2:B:422:LEU:HG	18:B:1236:CLA:CAB	2.39	0.52
6:G:108:ALA:HB1	6:G:111:TYR:CE1	2.41	0.52
18:2:2012:CLA:C1	23:2:2802:LMG:C36	2.87	0.52
18:3:3004:CLA:CGA	18:3:3004:CLA:C3A	2.87	0.52
18:4:4001:CLA:CHD	18:4:4001:CLA:HBC2	2.40	0.52
18:4:4003:CLA:O1A	18:4:4003:CLA:HBD	2.08	0.52
1:A:401:TRP:NE1	18:A:1126:CLA:HAB	2.24	0.52
2:B:373:THR:HG23	2:B:591:THR:HG21	1.91	0.52
2:B:636:THR:HG22	2:B:638:LEU:H	1.75	0.52
8:C:21:CYS:SG	8:C:24:ASP:N	2.83	0.52
18:G:1001:CLA:CAB	22:G:2011:BCR:C36	2.86	0.52
18:A:1101:CLA:ND	4:J:12:PRO:HG3	2.24	0.52
18:2:2006:CLA:C4	18:2:2006:CLA:CAD	2.85	0.52
18:2:2008:CLA:HBB1	18:2:2008:CLA:CHC	2.38	0.52
13:2:85:PHE:CD2	18:2:2009:CLA:HBC2	2.44	0.52
28:2:2010:CHL:HBB2	18:2:2012:CLA:HBC1	1.91	0.52
13:2:186:ASN:ND2	18:2:2016:CLA:C1A	2.73	0.52
27:2:2501:LUT:C37	27:2:2501:LUT:C28	2.85	0.52
18:3:3008:CLA:HBA1	18:3:3008:CLA:CHA	2.38	0.52
16:3:171:ARG:HD3	28:3:3011:CHL:OMC	2.09	0.52
23:B:5005:LMG:H111	18:B:1227:CLA:HAA2	1.91	0.52
8:C:51:CYS:SG	8:C:53:ARG:HD3	2.49	0.52
10:E:66:ILE:CG2	10:E:67:GLY:N	2.72	0.52
18:A:1138:CLA:H121	18:F:1301:CLA:HAC1	1.90	0.52
7:L:90:ARG:HB3	7:L:93:VAL:HG23	1.91	0.52
15:1:41:TRP:CE3	28:1:1009:CHL:CBC	2.91	0.52
15:1:94:ILE:HG23	15:1:105:TRP:HB3	1.91	0.52
13:2:204:LEU:HB3	13:2:206:TRP:CD1	2.45	0.52
16:3:121:TYR:HA	16:3:253:TYR:CD2	2.44	0.52
18:3:3005:CLA:CMD	18:3:3012:CLA:ND	2.72	0.52
14:4:94:ALA:HB2	18:4:4012:CLA:CED	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:TRP:CD1	18:A:1128:CLA:HMD1	2.45	0.52
18:1:1006:CLA:HBC2	18:1:1006:CLA:HMC1	1.89	0.52
15:1:134:ILE:CD1	18:1:1013:CLA:C3D	2.88	0.52
15:1:211:LEU:H	15:1:211:LEU:HD12	1.75	0.52
15:1:226:ILE:O	15:1:229:ASN:N	2.43	0.52
13:2:89:PRO:HD2	27:2:2502:LUT:C22	2.40	0.52
16:3:104:ILE:CD1	16:3:172:ARG:NH2	2.72	0.52
16:3:184:LYS:HG2	16:3:185:GLN:NE2	2.25	0.52
16:3:262:ASP:CB	16:3:265:ASN:ND2	2.73	0.52
16:3:263:PRO:HD2	16:3:264:VAL:H	1.75	0.52
16:3:267:ASN:ND2	16:3:270:THR:CG2	2.73	0.52
18:3:3006:CLA:CMB	18:3:3013:CLA:C4B	2.87	0.52
18:3:3017:CLA:HAA2	18:3:3017:CLA:CED	2.38	0.52
16:3:164:LEU:HD13	22:3:3503:BCR:H352	1.91	0.52
14:4:94:ALA:N	18:4:4012:CLA:CED	2.73	0.52
18:B:1232:CLA:O1A	18:G:1003:CLA:HHB	2.09	0.52
2:B:182:LEU:HD13	18:B:1210:CLA:HHB	1.92	0.52
9:D:204:THR:O	9:D:206:LYS:N	2.42	0.52
10:E:79:GLN:HG3	10:E:84:TYR:CZ	2.45	0.52
22:L:6020:BCR:H342	18:H:1000:CLA:HAB	1.92	0.52
4:J:38:THR:OG1	5:F:136:GLN:NE2	2.42	0.52
15:1:130:THR:CG2	15:1:131:LEU:N	2.73	0.52
14:4:147:ILE:HD11	21:1:1801:LHG:H361	1.92	0.52
13:2:134:THR:N	13:2:135:PRO:HD2	2.25	0.52
16:3:139:THR:CG2	16:3:140:GLY:N	2.73	0.52
16:3:94:GLU:OE2	16:3:95:PRO:CD	2.57	0.52
2:B:680:TRP:NE1	9:D:88:THR:HG23	2.25	0.52
9:D:135:LYS:O	9:D:138:CYS:N	2.43	0.52
9:D:155:PHE:CZ	9:D:168:HIS:CB	2.93	0.52
12:K:120:ALA:HA	12:K:123:LEU:HD12	1.92	0.52
18:1:1011:CLA:HMB1	18:1:1011:CLA:CBB	2.38	0.52
15:1:85:ARG:CB	18:1:1011:CLA:CED	2.85	0.52
18:1:1005:CLA:CMD	18:1:1012:CLA:ND	2.72	0.52
15:1:82:ILE:CD1	15:1:149:ARG:NH2	2.73	0.52
18:1:1001:CLA:CBB	27:1:1501:LUT:H32	2.40	0.52
15:1:166:ASP:OD2	15:1:169:GLY:HA2	2.10	0.52
18:2:2005:CLA:OBD	18:2:2012:CLA:H2	2.09	0.52
18:2:2003:CLA:H2	18:2:2008:CLA:OBD	2.09	0.52
18:2:2007:CLA:C4C	21:2:2801:LHG:HC62	2.40	0.52
16:3:210:PRO:HB2	16:3:211:LEU:HD13	1.90	0.52
18:3:3010:CLA:HBD	18:3:3010:CLA:HAA1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:100:ARG:HA	14:4:103:MET:HG3	1.91	0.52
14:4:171:ILE:HD13	18:4:4016:CLA:HMA2	1.91	0.52
1:A:342:GLY:O	1:A:343:HIS:HB2	2.09	0.52
26:B:8002:LMU:O2B	26:B:8002:LMU:O3'	2.19	0.52
10:E:122:LEU:H	10:E:122:LEU:CD1	2.05	0.52
6:G:116:LYS:NZ	18:G:1002:CLA:C4B	2.73	0.52
18:G:1003:CLA:H52	23:G:2021:LMG:C32	2.39	0.52
6:G:77:PHE:N	6:G:77:PHE:CD1	2.78	0.52
7:L:176:LEU:CG	7:L:177:GLN:N	2.73	0.52
18:1:1003:CLA:H11	18:1:1008:CLA:OBD	2.09	0.52
15:1:108:ALA:HA	15:1:111:TRP:CZ3	2.45	0.52
13:2:122:ILE:HG21	13:2:133:LEU:HB2	1.89	0.52
13:2:177:VAL:CG2	13:2:178:ASN:H	2.22	0.52
13:2:220:LYS:HD3	18:2:2002:CLA:CED	2.29	0.52
13:2:234:GLY:O	13:2:238:GLN:HB2	2.10	0.52
16:3:115:GLY:O	16:3:119:PRO:CD	2.57	0.52
16:3:223:LEU:HB3	18:3:3001:CLA:HMA1	1.92	0.52
18:3:3013:CLA:H2A	18:3:3013:CLA:O2D	2.09	0.52
18:3:3006:CLA:H12	22:3:3503:BCR:H313	1.91	0.52
14:4:103:MET:CE	14:4:207:ASN:CB	2.85	0.52
1:A:397:THR:HG22	18:A:1126:CLA:HAB	1.91	0.52
18:B:1220:CLA:H13	22:B:6009:BCR:H312	1.92	0.52
8:C:17:CYS:SG	8:C:18:VAL:N	2.83	0.52
3:I:9:VAL:O	3:I:13:GLY:N	2.34	0.52
15:1:116:GLY:O	15:1:118:GLN:HG2	2.10	0.52
13:2:188:LEU:HD22	13:2:189:THR:CA	2.39	0.52
13:2:216:GLU:O	13:2:220:LYS:HG3	2.09	0.52
18:3:3002:CLA:CMC	18:3:3002:CLA:HBC2	2.37	0.52
18:3:3003:CLA:CGA	18:3:3003:CLA:CHA	2.88	0.52
18:3:3006:CLA:CED	18:3:3006:CLA:C1A	2.85	0.52
16:3:164:LEU:CB	22:3:3503:BCR:C35	2.85	0.52
1:A:272:LEU:HD13	18:K:1001:CLA:HBC1	1.92	0.52
8:C:10:THR:HG23	8:C:64:SER:CB	2.40	0.52
4:J:36:ALA:CB	23:J:5001:LMG:HC72	2.40	0.52
15:1:111:TRP:CE2	15:1:119:ALA:HB2	2.43	0.51
15:1:104:ASN:ND2	15:1:208:THR:CG2	2.73	0.51
15:1:211:LEU:CD1	15:1:212:GLU:N	2.73	0.51
16:3:174:GLN:HA	16:3:174:GLN:OE1	2.10	0.51
18:3:3003:CLA:C4	18:3:3003:CLA:C2D	2.85	0.51
18:3:3005:CLA:H12	18:3:3005:CLA:CED	2.39	0.51
27:3:3501:LUT:C16	27:3:3501:LUT:H8	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:103:MET:HG3	18:4:4001:CLA:HMC3	1.92	0.51
28:4:4013:CHL:CHD	28:4:4013:CHL:HBC2	2.32	0.51
1:A:33:GLN:HB2	18:A:1109:CLA:HBA1	1.91	0.51
9:D:204:THR:HG22	9:D:206:LYS:CG	2.38	0.51
7:L:98:ARG:HH22	7:L:175:GLN:NE2	2.08	0.51
18:1:1011:CLA:HBC2	18:1:1011:CLA:HMC1	1.91	0.51
15:1:127:PRO:CG	15:1:128:TRP:NE1	2.73	0.51
15:1:196:VAL:O	15:1:199:CYS:N	2.43	0.51
14:4:199:GLU:HG2	14:4:202:GLU:OE1	2.10	0.51
14:4:219:ILE:HG23	14:4:220:ILE:N	2.25	0.51
18:A:1139:CLA:H61	4:J:18:TRP:CG	2.45	0.51
18:A:1022:CLA:OBD	18:B:1021:CLA:HMB3	2.10	0.51
9:D:163:GLU:OE2	9:D:164:VAL:N	2.42	0.51
18:G:1003:CLA:C5	23:G:2021:LMG:C31	2.85	0.51
11:H:107:GLY:C	11:H:110:THR:HG22	2.30	0.51
7:L:121:ARG:CG	7:L:127:GLY:CA	2.84	0.51
7:L:169:ARG:NH1	7:L:171:LYS:CB	2.73	0.51
15:1:127:PRO:C	15:1:128:TRP:CD1	2.83	0.51
15:1:232:ILE:CG2	15:1:233:PRO:N	2.73	0.51
13:2:131:ILE:CG2	13:2:132:LEU:H	2.20	0.51
13:2:178:ASN:O	13:2:179:THR:HG23	2.11	0.51
13:2:232:VAL:HG11	27:2:2502:LUT:H12	1.92	0.51
16:3:211:LEU:N	16:3:211:LEU:CD1	2.72	0.51
14:4:148:LEU:HB3	27:4:4503:LUT:H15	1.91	0.51
14:4:171:ILE:CD1	14:4:171:ILE:N	2.73	0.51
2:B:615:TYR:OH	2:B:621:ARG:NH2	2.39	0.51
9:D:192:ILE:HG23	10:E:80:GLU:CD	2.31	0.51
9:D:211:LEU:CD1	9:D:211:LEU:N	2.72	0.51
18:F:1302:CLA:HHC	18:F:1302:CLA:CBB	2.40	0.51
14:4:147:ILE:HD13	21:1:1801:LHG:H351	1.92	0.51
13:2:220:LYS:NZ	18:2:2002:CLA:CED	2.73	0.51
18:2:2002:CLA:OBD	18:2:2007:CLA:HBD	2.10	0.51
13:2:222:ILE:N	13:2:222:ILE:CD1	2.73	0.51
27:2:2502:LUT:C8	27:2:2502:LUT:H181	2.40	0.51
16:3:153:ASP:OD1	16:3:154:ASN:N	2.44	0.51
14:4:120:ILE:N	14:4:120:ILE:CD1	2.72	0.51
27:4:4503:LUT:H363	28:1:1009:CHL:H93	1.86	0.51
6:G:92:LEU:CD1	6:G:92:LEU:H	1.98	0.51
7:L:91:THR:CB	7:L:175:GLN:NE2	2.73	0.51
13:2:129:LEU:CD2	13:2:131:ILE:CG1	2.86	0.51
13:2:262:ILE:CD1	18:2:2003:CLA:H11	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2016:CLA:HBA2	18:2:2016:CLA:CHA	2.40	0.51
13:2:241:TYR:CE1	13:2:265:ALA:HB3	2.46	0.51
14:4:171:ILE:HD12	14:4:171:ILE:N	2.25	0.51
14:4:101:TRP:CE2	28:4:4011:CHL:CED	2.94	0.51
18:4:4005:CLA:HBC1	18:4:4012:CLA:HBC1	1.92	0.51
2:B:255:LEU:HD11	18:B:1212:CLA:HBC1	1.91	0.51
6:G:64:ILE:HD12	18:G:1001:CLA:C3D	2.40	0.51
18:2:2004:CLA:H12	18:2:2004:CLA:CHB	2.40	0.51
13:2:85:PHE:HD2	18:2:2009:CLA:HBC2	1.75	0.51
27:3:3501:LUT:H371	27:3:3501:LUT:H28	1.92	0.51
16:3:65:LEU:HD13	16:3:67:TYR:OH	2.09	0.51
14:4:113:GLU:OE1	14:4:229:PRO:HG2	2.11	0.51
18:A:1110:CLA:HBD	18:A:1110:CLA:HBA1	1.93	0.51
1:A:208:ALA:HB1	18:A:1118:CLA:HBC3	1.93	0.51
1:A:346:LEU:HG	1:A:429:ASN:ND2	2.25	0.51
2:B:177:HIS:HB3	18:B:1210:CLA:HBB1	1.93	0.51
9:D:135:LYS:O	9:D:138:CYS:HB2	2.10	0.51
9:D:191:SER:O	9:D:192:ILE:HB	2.11	0.51
18:F:1301:CLA:HBB1	18:F:1301:CLA:CHC	2.39	0.51
4:J:6:THR:CG2	23:F:5001:LMG:HC72	2.39	0.51
15:1:81:LEU:CD1	15:1:159:LYS:HG3	2.41	0.51
15:1:88:MET:CE	18:1:1001:CLA:HAB	2.41	0.51
13:2:108:VAL:HG12	13:2:112:TRP:HD1	1.76	0.51
14:4:206:ALA:HB2	23:4:4801:LMG:HC62	1.92	0.51
17:A:1011:CL0:H13	18:B:1012:CLA:CAD	2.41	0.51
6:G:116:LYS:HE3	18:G:1002:CLA:CHC	2.40	0.51
18:1:1008:CLA:CHA	18:1:1008:CLA:CED	2.89	0.51
15:1:202:GLN:HA	15:1:202:GLN:HE21	1.75	0.51
15:1:222:TRP:NE1	18:1:1008:CLA:CMA	2.73	0.51
13:2:122:ILE:N	13:2:122:ILE:CD1	2.73	0.51
18:2:2005:CLA:C4	18:2:2005:CLA:H92	2.40	0.51
16:3:183:GLY:HA3	16:3:194:PHE:O	2.11	0.51
18:3:3005:CLA:HBC3	18:3:3005:CLA:HMC1	1.93	0.51
18:3:3012:CLA:C1	18:3:3017:CLA:CBB	2.89	0.51
27:3:3502:LUT:C16	27:3:3502:LUT:C8	2.86	0.51
14:4:113:GLU:CD	14:4:230:PHE:HB3	2.30	0.51
1:A:629:ASN:HD21	1:A:631:GLN:HB2	1.75	0.51
1:A:743:ILE:HG21	18:A:1126:CLA:HMC2	1.93	0.51
10:E:91:VAL:HB	10:E:104:VAL:HG23	1.92	0.51
18:B:1230:CLA:H91	18:F:1301:CLA:HMA1	1.93	0.51
18:G:1001:CLA:HMB2	22:G:2011:BCR:C16	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:187:LYS:CG	13:2:188:LEU:H	2.23	0.51
18:2:2002:CLA:C1	18:2:2002:CLA:CED	2.85	0.51
16:3:134:LEU:HB2	16:3:138:GLN:HG3	1.92	0.51
16:3:197:SER:HB2	16:3:203:PRO:C	2.32	0.51
16:3:248:THR:CG2	16:3:255:ASN:HD22	2.17	0.51
16:3:266:ASN:O	16:3:267:ASN:ND2	2.44	0.51
27:3:3502:LUT:C36	27:3:3502:LUT:H28	2.37	0.51
9:D:168:HIS:HA	9:D:169:PRO:C	2.30	0.51
6:G:114:VAL:CG1	18:G:1002:CLA:HBA1	2.41	0.51
6:G:76:ARG:NE	6:G:116:LYS:NZ	2.59	0.51
11:H:132:PRO:CD	11:H:133:PRO:CD	2.84	0.51
7:L:207:LEU:O	7:L:208:ASP:HB3	2.11	0.51
15:1:152:GLU:HA	15:1:152:GLU:OE1	2.11	0.51
13:2:120:ILE:C	13:2:123:PRO:HD2	2.31	0.51
13:2:130:GLY:O	13:2:131:ILE:HG13	2.10	0.51
18:2:2001:CLA:C4A	18:2:2001:CLA:CGA	2.89	0.51
18:2:2002:CLA:H2A	18:2:2002:CLA:O2D	2.11	0.51
16:3:115:GLY:O	16:3:119:PRO:HD3	2.11	0.51
16:3:171:ARG:HD3	28:3:3011:CHL:HBB1	1.93	0.51
16:3:184:LYS:CG	16:3:185:GLN:NE2	2.73	0.51
16:3:230:ASN:OD1	18:3:3007:CLA:HMD1	2.10	0.51
1:A:64:PHE:CD2	18:A:1103:CLA:HMC2	2.46	0.51
18:B:1216:CLA:CGA	18:B:1221:CLA:HBB1	2.41	0.51
11:H:123:LEU:O	11:H:123:LEU:HD13	2.10	0.51
15:1:230:VAL:CG1	18:1:1014:CLA:C1B	2.86	0.50
14:4:228:GLY:O	14:4:232:ASN:ND2	2.45	0.50
14:4:55:GLU:OE1	14:4:58:PRO:HA	2.11	0.50
18:A:1105:CLA:H12	22:J:6013:BCR:H14C	1.93	0.50
4:J:28:GLU:CD	18:J:1302:CLA:ND	2.64	0.50
12:K:127:THR:O	12:K:131:ILE:HG12	2.11	0.50
13:2:85:PHE:CZ	13:2:223:LYS:HE3	2.47	0.50
14:4:152:VAL:HG13	28:4:4011:CHL:C1B	2.41	0.50
14:4:177:LEU:HD13	18:4:4016:CLA:CMD	2.41	0.50
18:4:4001:CLA:CGA	18:4:4001:CLA:H3A	2.41	0.50
28:4:4013:CHL:HBA1	27:4:4503:LUT:C10	2.40	0.50
1:A:330:ILE:O	1:A:334:HIS:ND1	2.40	0.50
18:G:1003:CLA:C13	18:G:1003:CLA:H8	2.33	0.50
22:L:6019:BCR:C8	22:L:6019:BCR:H321	2.41	0.50
7:L:96:LEU:O	7:L:96:LEU:HD23	2.11	0.50
18:1:1011:CLA:CHA	18:1:1011:CLA:HBA1	2.39	0.50
15:1:83:HIS:CE1	18:1:1012:CLA:CMD	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:182:MET:CA	16:3:182:MET:CE	2.88	0.50
16:3:232:ARG:NH2	18:3:3004:CLA:ND	2.60	0.50
28:4:4013:CHL:CBC	28:4:4013:CHL:CHD	2.85	0.50
1:A:25:ASP:HB3	1:A:26:PRO:HD2	1.94	0.50
18:B:1238:CLA:H191	3:I:18:ALA:HB2	1.93	0.50
12:K:137:VAL:N	12:K:140:LEU:HD22	2.26	0.50
18:1:1005:CLA:C3B	27:1:1502:LUT:C14	2.90	0.50
15:1:158:LYS:HD3	15:1:159:LYS:HZ1	1.73	0.50
18:2:2002:CLA:HMD2	18:2:2007:CLA:C1D	2.42	0.50
18:2:2009:CLA:HBD	18:2:2009:CLA:HAA1	1.92	0.50
13:2:92:LEU:HD12	27:2:2502:LUT:C24	2.41	0.50
16:3:224:LYS:O	16:3:228:VAL:HG23	2.10	0.50
16:3:182:MET:HB3	28:3:3011:CHL:HMC	1.94	0.50
14:4:60:LEU:HG	14:4:61:ALA:O	2.10	0.50
1:A:604:TRP:HH2	18:A:1022:CLA:HAB	1.74	0.50
1:A:305:ALA:HA	18:A:1115:CLA:HMC3	1.93	0.50
2:B:71:GLN:OE1	2:B:90:ALA:N	2.37	0.50
9:D:171:ASP:O	9:D:173:VAL:N	2.44	0.50
15:1:218:LEU:O	15:1:221:PRO:HD3	2.12	0.50
18:2:2002:CLA:HBB1	18:2:2002:CLA:CMB	2.34	0.50
16:3:135:ALA:H	16:3:138:GLN:CD	2.14	0.50
16:3:152:ALA:HB3	16:3:157:LEU:CD2	2.38	0.50
16:3:208:PHE:HB3	18:3:3001:CLA:CMD	2.37	0.50
16:3:205:GLY:CA	16:3:208:PHE:N	2.73	0.50
18:3:3003:CLA:C1A	18:3:3003:CLA:CGA	2.89	0.50
18:A:1013:CLA:H3A	18:A:1013:CLA:CGA	2.41	0.50
2:B:194:LEU:HA	2:B:198:ALA:HB3	1.92	0.50
7:L:65:PHE:O	9:D:91:LEU:HG	2.11	0.50
15:1:192:LEU:HD13	18:1:1004:CLA:HMC3	1.93	0.50
15:1:225:ASN:C	15:1:225:ASN:HD22	2.15	0.50
13:2:180:ASP:HB3	13:2:183:PHE:O	2.11	0.50
13:2:220:LYS:HE2	18:2:2002:CLA:HED2	1.91	0.50
14:4:103:MET:HE3	14:4:208:GLY:N	2.26	0.50
14:4:236:HIS:CE1	14:4:240:PRO:HB3	2.46	0.50
28:4:4010:CHL:HBB1	28:4:4010:CHL:HHC	1.94	0.50
2:B:438:VAL:HG13	18:B:1012:CLA:H61	1.94	0.50
2:B:377:TYR:HD2	18:B:1224:CLA:HAB	1.75	0.50
2:B:572:ALA:HA	2:B:575:ASP:OD2	2.11	0.50
23:F:5002:LMG:H292	18:1:1014:CLA:C4D	2.42	0.50
6:G:94:GLU:CB	6:G:98:VAL:H	2.21	0.50
18:A:1101:CLA:C4D	4:J:12:PRO:HG3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:118:THR:OG1	12:K:121:ASP:HB3	2.12	0.50
18:1:1003:CLA:HBA1	18:1:1008:CLA:HED2	1.93	0.50
15:1:76:PHE:HB3	18:1:1004:CLA:HMA1	1.92	0.50
18:1:1003:CLA:H2	18:1:1008:CLA:HMD3	1.93	0.50
15:1:89:LEU:C	15:1:92:PRO:HD2	2.32	0.50
16:3:221:LYS:C	16:3:223:LEU:H	2.14	0.50
18:4:4006:CLA:C2B	27:4:4502:LUT:H183	2.41	0.50
22:A:6008:BCR:H402	18:A:1119:CLA:H122	1.93	0.50
2:B:459:PHE:HD1	18:F:1302:CLA:HMC2	1.76	0.50
2:B:65:LEU:HD21	22:B:6006:BCR:H291	1.93	0.50
11:H:58:GLU:HA	11:H:58:GLU:OE1	2.10	0.50
15:1:114:LEU:HD22	15:1:115:PRO:HD2	1.88	0.50
15:1:202:GLN:HA	15:1:202:GLN:NE2	2.27	0.50
13:2:126:LEU:CB	13:2:133:LEU:HD13	2.24	0.50
13:2:138:TYR:O	13:2:139:THR:HB	2.11	0.50
13:2:161:GLY:HA2	18:2:2012:CLA:CBB	2.42	0.50
16:3:269:LEU:HD11	18:3:3008:CLA:HED3	1.92	0.50
18:3:3003:CLA:O1A	18:3:3003:CLA:HBD	2.10	0.50
14:4:74:ASN:ND2	14:4:74:ASN:N	2.60	0.50
1:A:511:THR:HG23	18:A:1116:CLA:O1A	2.11	0.50
18:B:1221:CLA:HBA2	18:B:1202:CLA:H8	1.92	0.50
23:B:5005:LMG:H172	18:B:1228:CLA:HBD	1.93	0.50
3:I:29:GLU:OE2	3:I:29:GLU:HA	2.11	0.50
12:K:78:LEU:O	12:K:80:ALA:N	2.42	0.50
15:1:102:LEU:O	15:1:104:ASN:N	2.41	0.50
18:2:2009:CLA:CED	16:3:171:ARG:CG	2.86	0.50
16:3:185:GLN:C	16:3:186:TYR:CD1	2.85	0.50
16:3:225:LEU:HD12	16:3:226:LYS:HE3	1.94	0.50
18:3:3003:CLA:C4D	18:3:3003:CLA:C1	2.85	0.50
16:3:127:LEU:CB	18:3:3018:CLA:CBC	2.85	0.50
28:4:4013:CHL:HBD	28:4:4013:CHL:HAA2	1.93	0.50
21:A:7001:LHG:H331	18:A:1104:CLA:H92	1.93	0.50
18:A:1123:CLA:HBB1	18:A:1119:CLA:H2	1.94	0.50
18:A:1122:CLA:H71	18:A:1122:CLA:H41	1.93	0.50
2:B:270:LEU:HD23	2:B:273:MET:HE3	1.93	0.50
9:D:160:PRO:CD	9:D:161:SER:H	2.25	0.50
7:L:91:THR:CA	7:L:175:GLN:NE2	2.73	0.50
13:2:118:ALA:HB3	18:2:2006:CLA:HMC3	1.92	0.49
13:2:79:GLY:HA2	13:2:84:ASP:OD2	2.11	0.49
18:4:4004:CLA:H111	27:4:4502:LUT:H393	1.94	0.49
18:A:1106:CLA:H2A	18:A:1106:CLA:HED2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:LEU:HD22	18:A:1140:CLA:HMA1	1.94	0.49
2:B:721:TYR:HB2	18:B:1021:CLA:HED3	1.94	0.49
2:B:529:THR:HG21	2:B:582:TRP:CE2	2.47	0.49
6:G:76:ARG:NE	6:G:116:LYS:CE	2.73	0.49
12:K:61:PHE:O	12:K:64:SER:HB3	2.12	0.49
7:L:91:THR:CG2	7:L:175:GLN:NE2	2.73	0.49
18:3:3006:CLA:HMA2	18:3:3013:CLA:CAC	2.41	0.49
2:B:592:PHE:HE2	18:B:1021:CLA:H62	1.76	0.49
22:B:6006:BCR:H392	18:B:1211:CLA:H3A	1.94	0.49
9:D:112:ILE:CD1	9:D:112:ILE:N	2.72	0.49
9:D:163:GLU:OE1	9:D:164:VAL:O	2.30	0.49
9:D:195:ASN:ND2	9:D:195:ASN:N	2.60	0.49
7:L:85:ASN:HB2	18:L:1501:CLA:HMC1	1.94	0.49
18:2:2002:CLA:O2D	18:2:2002:CLA:HAA2	2.13	0.49
13:2:77:LEU:HD13	13:2:86:GLY:HA2	1.93	0.49
2:B:657:TRP:CE3	18:B:1021:CLA:HMA1	2.48	0.49
8:C:61:ASP:HB2	10:E:118:ASN:CG	2.32	0.49
22:F:6016:BCR:H382	22:F:6016:BCR:H23C	1.94	0.49
7:L:111:VAL:O	7:L:115:VAL:HG23	2.12	0.49
18:1:1008:CLA:HED2	18:1:1008:CLA:CAD	2.43	0.49
15:1:202:GLN:OE1	15:1:208:THR:HB	2.11	0.49
18:2:2004:CLA:CGA	18:2:2004:CLA:H3A	2.42	0.49
18:2:2016:CLA:CBA	18:2:2016:CLA:CBF	2.85	0.49
18:4:4003:CLA:HBC2	18:4:4003:CLA:CHD	2.41	0.49
14:4:57:LEU:HD11	18:4:4009:CLA:HED1	1.95	0.49
18:A:1110:CLA:H42	18:A:1110:CLA:C4C	2.42	0.49
18:B:1216:CLA:CMB	18:B:1221:CLA:HMA3	2.40	0.49
18:B:1238:CLA:H13	27:I:6018:LUT:H193	1.94	0.49
23:G:2021:LMG:O9	23:G:2021:LMG:HC92	2.13	0.49
11:H:123:LEU:HD12	11:H:123:LEU:N	2.26	0.49
22:K:2011:BCR:C32	22:K:2011:BCR:C8	2.85	0.49
12:K:70:MET:HE2	12:K:71:VAL:HG23	1.91	0.49
7:L:90:ARG:HB2	7:L:98:ARG:HD3	1.95	0.49
15:1:183:LYS:NZ	18:1:1002:CLA:O1D	2.44	0.49
15:1:111:TRP:CG	15:1:119:ALA:HB2	2.47	0.49
13:2:238:GLN:NE2	18:2:2003:CLA:NA	2.60	0.49
13:2:211:PRO:C	13:2:212:GLN:HG3	2.32	0.49
2:B:439:HIS:O	2:B:443:MET:HG2	2.12	0.49
11:H:131:LEU:HB3	11:H:135:LEU:HD22	1.94	0.49
12:K:124:ALA:CB	22:K:2011:BCR:H343	2.42	0.49
12:K:70:MET:HE1	12:K:71:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:6020:BCR:H342	18:H:1000:CLA:CAB	2.42	0.49
7:L:81:TRP:O	7:L:85:ASN:ND2	2.43	0.49
15:1:88:MET:CE	18:1:1001:CLA:HHC	2.38	0.49
15:1:140:LEU:HD23	15:1:140:LEU:O	2.12	0.49
15:1:226:ILE:HG12	15:1:230:VAL:HG23	1.94	0.49
13:2:147:THR:HG21	14:4:241:TRP:HE3	1.78	0.49
13:2:66:LEU:N	16:3:186:TYR:HE2	2.03	0.49
14:4:241:TRP:CD2	18:4:4008:CLA:HMA1	2.47	0.49
1:A:336:GLY:N	21:A:5003:LHG:HC32	2.27	0.49
18:G:1002:CLA:HMB1	18:G:1002:CLA:CBB	2.42	0.49
4:J:2:ARG:O	4:J:3:ASP:HB2	2.11	0.49
4:J:36:ALA:HB1	23:J:5001:LMG:HC72	1.94	0.49
15:1:158:LYS:O	15:1:159:LYS:HE2	2.13	0.49
15:1:217:HIS:ND1	15:1:221:PRO:HA	2.28	0.49
13:2:145:TYR:HB2	18:2:2006:CLA:H92	1.95	0.49
13:2:188:LEU:HD13	13:2:188:LEU:C	2.32	0.49
18:2:2005:CLA:H72	23:2:2802:LMG:H132	1.93	0.49
18:2:2007:CLA:C5	18:2:2007:CLA:C9	2.90	0.49
13:2:198:GLY:O	13:2:202:ASP:N	2.42	0.49
16:3:225:LEU:N	16:3:226:LYS:NZ	2.60	0.49
16:3:243:ILE:HG22	18:3:3003:CLA:HMD3	1.95	0.49
16:3:151:TRP:NE1	18:3:3013:CLA:OBD	2.37	0.49
9:D:173:VAL:HG21	9:D:179:ASN:OD1	2.13	0.49
6:G:130:ILE:O	6:G:134:VAL:HG23	2.12	0.49
18:3:3018:CLA:HBC2	18:3:3018:CLA:CMC	2.39	0.49
16:3:187:PHE:CZ	18:3:3019:CLA:C4B	2.95	0.49
18:3:3005:CLA:HMB2	27:3:3502:LUT:C32	2.43	0.49
14:4:147:ILE:CD1	21:1:1801:LHG:C36	2.91	0.49
28:4:4010:CHL:HBC2	28:4:4010:CHL:CHD	2.26	0.49
18:B:1213:CLA:HBB1	18:B:1213:CLA:HMB1	1.95	0.49
18:B:1222:CLA:CAD	18:B:1234:CLA:HBB1	2.43	0.49
9:D:131:LYS:NZ	11:H:63:THR:O	2.46	0.49
28:2:2013:CHL:O1D	28:2:2013:CHL:H2A	2.12	0.49
13:2:232:VAL:HG11	27:2:2502:LUT:H10	1.94	0.49
16:3:67:TYR:CE1	16:3:85:ASP:HA	2.48	0.49
14:4:151:TYR:C	14:4:151:TYR:CD1	2.85	0.49
28:4:4011:CHL:H11	27:4:4501:LUT:H383	1.93	0.49
18:4:4004:CLA:HBB1	27:4:4502:LUT:H30	1.95	0.49
14:4:94:ALA:CA	18:4:4012:CLA:CED	2.85	0.49
18:A:1123:CLA:HBA1	18:A:1127:CLA:H191	1.94	0.49
1:A:80:SER:OG	1:A:186:TYR:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD11	18:A:1117:CLA:H71	1.95	0.49
1:A:684:PHE:CG	22:A:6011:BCR:H363	2.48	0.49
18:B:1205:CLA:O1A	18:B:1224:CLA:HBD	2.13	0.49
1:A:713:LYS:NZ	5:F:229:LYS:O	2.40	0.49
7:L:125:ILE:HG22	7:L:125:ILE:O	2.12	0.49
18:1:1008:CLA:C4D	18:1:1008:CLA:CED	2.85	0.49
13:2:118:ALA:O	13:2:121:PHE:N	2.46	0.49
16:3:169:GLU:HG3	18:3:3012:CLA:C4B	2.43	0.49
16:3:68:LEU:N	16:3:68:LEU:CD1	2.73	0.49
14:4:133:GLU:C	14:4:134:TYR:CD1	2.86	0.49
18:B:1208:CLA:H12	18:B:1209:CLA:C4D	2.43	0.49
7:L:67:GLY:O	9:D:88:THR:HA	2.12	0.49
7:L:90:ARG:NH2	18:L:1501:CLA:HAC2	2.28	0.49
15:1:106:VAL:HG23	15:1:208:THR:HG21	1.89	0.48
15:1:222:TRP:CD1	18:1:1008:CLA:CMA	2.96	0.48
28:3:3011:CHL:HBD	28:3:3011:CHL:CAA	2.43	0.48
14:4:103:MET:HE1	27:4:4501:LUT:H15	1.95	0.48
1:A:438:HIS:HA	9:D:88:THR:OG1	2.13	0.48
18:B:1203:CLA:H8	25:B:7101:DGD:HBH2	1.95	0.48
2:B:224:PRO:HB3	2:B:232:LEU:HD22	1.93	0.48
22:B:6004:BCR:H351	22:B:6004:BCR:H15C	1.59	0.48
10:E:76:ILE:HG22	10:E:78:ARG:H	1.78	0.48
11:H:107:GLY:HA2	11:H:110:THR:HG21	1.94	0.48
7:L:118:GLY:O	7:L:122:ASN:ND2	2.46	0.48
15:1:214:LEU:HA	18:1:1003:CLA:HMA2	1.94	0.48
29:4:4505:ZEX:H173	15:1:200:VAL:HG13	1.95	0.48
28:2:2013:CHL:CB	28:2:2013:CHL:HAA2	2.43	0.48
23:2:2802:LMG:HC92	23:2:2802:LMG:O9	2.14	0.48
16:3:119:PRO:C	16:3:133:ALA:CB	2.82	0.48
18:3:3012:CLA:H12	18:3:3017:CLA:HBB2	1.94	0.48
18:A:1110:CLA:O1A	16:3:81:LEU:HD22	2.13	0.48
18:B:1218:CLA:H41	18:B:1218:CLA:H61	1.67	0.48
18:L:1502:CLA:HAC2	22:L:6019:BCR:C29	2.42	0.48
7:L:90:ARG:HB3	7:L:93:VAL:CG2	2.43	0.48
13:2:220:LYS:HA	18:2:2007:CLA:HED2	1.94	0.48
18:3:3013:CLA:CMA	22:3:3503:BCR:C35	2.85	0.48
18:G:1001:CLA:C6	22:G:2011:BCR:C34	2.85	0.48
6:G:132:HIS:ND1	22:G:2011:BCR:H19C	2.27	0.48
16:3:270:THR:HG1	16:3:271:SER:H	1.60	0.48
18:3:3003:CLA:CAB	27:3:3501:LUT:C17	2.90	0.48
16:3:70:GLY:HA2	16:3:75:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:4503:LUT:C28	27:4:4503:LUT:C37	2.86	0.48
18:A:1013:CLA:O2A	2:B:427:LEU:HA	2.12	0.48
2:B:350:GLN:HG3	18:B:1222:CLA:HED2	1.95	0.48
2:B:414:HIS:O	2:B:414:HIS:ND1	2.46	0.48
9:D:129:LEU:HD23	9:D:129:LEU:O	2.12	0.48
9:D:166:TYR:CE2	9:D:170:LYS:HA	2.49	0.48
4:J:16:THR:HG21	22:J:6013:BCR:H401	1.95	0.48
15:1:88:MET:HB3	27:1:1501:LUT:C34	2.43	0.48
18:2:2005:CLA:H41	18:2:2005:CLA:C8	2.44	0.48
18:2:2004:CLA:C5	27:2:2502:LUT:C38	2.85	0.48
16:3:136:TRP:CZ2	16:3:137:PHE:HB3	2.49	0.48
18:3:3003:CLA:C12	18:3:3003:CLA:H93	2.44	0.48
18:3:3006:CLA:C2D	18:3:3018:CLA:CBB	2.91	0.48
16:3:94:GLU:CD	16:3:96:ARG:N	2.65	0.48
28:4:4011:CHL:CHD	28:4:4011:CHL:CBC	2.89	0.48
18:A:1106:CLA:H203	18:A:1101:CLA:HMA1	1.95	0.48
1:A:218:TRP:HA	18:A:1112:CLA:HBB1	1.94	0.48
1:A:581:CYS:SG	2:B:562:PRO:HG3	2.53	0.48
18:F:1302:CLA:CHD	18:F:1302:CLA:CBC	2.86	0.48
4:J:23:ALA:O	4:J:27:ILE:HG13	2.13	0.48
18:B:1230:CLA:O1D	4:J:35:ASP:HA	2.13	0.48
12:K:137:VAL:HA	12:K:140:LEU:HD23	1.89	0.48
7:L:102:VAL:HG13	7:L:106:HIS:ND1	2.29	0.48
15:1:222:TRP:CE2	18:1:1008:CLA:HMA1	2.48	0.48
13:2:102:ASN:OD1	18:2:2004:CLA:H11	2.12	0.48
16:3:253:TYR:C	16:3:253:TYR:CD1	2.85	0.48
16:3:250:VAL:HG12	16:3:254:GLN:HG2	1.94	0.48
1:A:81:ALA:HB1	18:A:1103:CLA:HBB1	1.96	0.48
7:L:149:GLY:HA3	7:L:182:TRP:CD1	2.47	0.48
13:2:191:THR:CG2	13:2:192:ASP:H	2.24	0.48
13:2:233:MET:CA	13:2:233:MET:CE	2.85	0.48
16:3:158:PHE:HB2	18:3:3010:CLA:CMC	2.42	0.48
16:3:197:SER:HB2	16:3:203:PRO:O	2.14	0.48
18:4:4001:CLA:HMB2	18:4:4002:CLA:HBA2	1.95	0.48
18:A:1022:CLA:H143	18:B:1207:CLA:HBC3	1.95	0.48
18:A:1125:CLA:H11	18:A:1125:CLA:H51	1.69	0.48
18:B:1240:CLA:C1D	18:B:1219:CLA:HMB3	2.44	0.48
2:B:44:GLN:NE2	2:B:162:LYS:HD2	2.29	0.48
2:B:387:PHE:HB3	2:B:534:LEU:HB3	1.96	0.48
3:I:17:PRO:O	3:I:21:MET:HG3	2.13	0.48
18:1:1005:CLA:HBB1	18:1:1005:CLA:CMB	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:181:LYS:O	15:1:185:VAL:HG23	2.13	0.48
15:1:218:LEU:CD2	18:1:1008:CLA:HBB1	2.44	0.48
15:1:91:VAL:HB	15:1:92:PRO:HD3	1.96	0.48
13:2:238:GLN:NE2	18:2:2003:CLA:C4D	2.77	0.48
13:2:120:ILE:CG2	27:2:2501:LUT:H373	2.38	0.48
16:3:139:THR:O	16:3:147:THR:HG22	2.14	0.48
14:4:108:GLY:O	14:4:112:PRO:HD2	2.14	0.48
2:B:59:LEU:HG	18:B:1204:CLA:HBB2	1.96	0.48
10:E:107:PHE:N	10:E:107:PHE:CD1	2.82	0.48
6:G:109:LYS:HG3	6:G:110:GLU:HG3	1.96	0.48
6:G:144:ASN:ND2	18:G:1003:CLA:CED	2.73	0.48
18:G:1001:CLA:C5	22:G:2011:BCR:H343	2.44	0.48
12:K:71:VAL:HG12	12:K:129:GLY:O	2.09	0.48
15:1:94:ILE:HG12	27:1:1502:LUT:H24	1.95	0.48
13:2:117:ALA:O	13:2:120:ILE:HB	2.14	0.48
18:2:2002:CLA:HMC2	27:2:2501:LUT:H31	1.95	0.48
16:3:268:VAL:CG2	18:3:3003:CLA:C1	2.87	0.48
14:4:193:ASN:OD1	14:4:193:ASN:N	2.46	0.48
18:4:4006:CLA:CBB	27:4:4502:LUT:H181	2.44	0.48
8:C:8:TYR:C	8:C:10:THR:H	2.17	0.48
9:D:211:LEU:HD12	9:D:211:LEU:N	2.28	0.48
10:E:104:VAL:HG12	10:E:119:ASN:CG	2.34	0.48
18:G:1001:CLA:CED	18:G:1001:CLA:CAD	2.92	0.48
6:G:111:TYR:HD1	6:G:111:TYR:H	1.52	0.48
15:1:41:TRP:HD1	15:1:59:PHE:CA	2.25	0.48
15:1:97:PRO:C	15:1:102:LEU:HB2	2.34	0.48
13:2:176:CYS:HA	13:2:178:ASN:HD21	1.79	0.48
18:2:2002:CLA:CBC	18:2:2002:CLA:CMC	2.86	0.48
18:2:2005:CLA:HAB	27:2:2502:LUT:C40	2.43	0.48
16:3:223:LEU:C	16:3:226:LYS:HG2	2.34	0.48
16:3:236:LEU:HD21	18:3:3004:CLA:HBC3	1.96	0.48
16:3:65:LEU:CB	16:3:68:LEU:CD2	2.85	0.48
14:4:144:ILE:HD13	18:1:1008:CLA:HAA2	1.94	0.48
14:4:239:ASP:CG	14:4:242:HIS:HD2	2.17	0.48
14:4:95:GLU:HG3	18:4:4004:CLA:NB	2.29	0.48
13:2:145:TYR:HB3	18:2:2006:CLA:C9	2.44	0.47
18:2:2016:CLA:HED2	18:2:2016:CLA:OBD	2.14	0.47
16:3:174:GLN:HB2	16:3:182:MET:HG2	1.96	0.47
16:3:217:GLU:C	16:3:219:SER:H	2.17	0.47
22:3:3503:BCR:HC8	22:3:3503:BCR:C32	2.44	0.47
1:A:709:TRP:CD1	5:F:229:LYS:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:66:ILE:HG23	10:E:67:GLY:H	1.79	0.47
18:G:1001:CLA:C2B	22:G:2011:BCR:C17	2.91	0.47
6:G:134:VAL:O	6:G:137:TYR:HB3	2.14	0.47
6:G:76:ARG:CD	6:G:116:LYS:HZ3	2.27	0.47
7:L:176:LEU:CG	7:L:177:GLN:H	2.26	0.47
15:1:111:TRP:HH2	18:1:1006:CLA:HED1	1.70	0.47
18:2:2004:CLA:CHD	18:2:2004:CLA:HBC2	2.44	0.47
18:2:2005:CLA:HBA1	18:2:2005:CLA:H3A	1.70	0.47
16:3:271:SER:HB2	18:3:3003:CLA:CED	2.44	0.47
18:3:3010:CLA:H2A	18:3:3010:CLA:CED	2.44	0.47
1:A:338:PHE:O	1:A:434:ARG:NH1	2.47	0.47
22:B:6010:BCR:H321	22:B:6010:BCR:HC8	1.95	0.47
7:L:108:PHE:HZ	18:L:1503:CLA:OBD	1.97	0.47
7:L:165:THR:OG1	7:L:169:ARG:HB3	2.14	0.47
15:1:226:ILE:HG22	18:1:1003:CLA:O2A	2.14	0.47
18:1:1006:CLA:H43	18:1:1013:CLA:HBD	1.96	0.47
15:1:158:LYS:O	15:1:159:LYS:HG2	2.15	0.47
13:2:246:PRO:HG2	13:2:247:ILE:H	1.80	0.47
16:3:106:GLY:O	16:3:110:MET:N	2.42	0.47
16:3:249:GLY:C	16:3:250:VAL:CG2	2.83	0.47
16:3:249:GLY:C	16:3:250:VAL:HG23	2.35	0.47
18:A:1125:CLA:HED1	18:A:1133:CLA:HAB	1.97	0.47
1:A:205:HIS:O	1:A:209:GLY:N	2.46	0.47
1:A:232:PHE:O	1:A:237:VAL:HG12	2.14	0.47
8:C:77:MET:HB3	8:C:79:LEU:HG	1.97	0.47
18:F:1302:CLA:CHC	18:F:1302:CLA:HBB1	2.44	0.47
22:F:6016:BCR:C8	22:F:6016:BCR:C33	2.85	0.47
6:G:68:THR:HG23	18:G:1001:CLA:O2A	2.14	0.47
11:H:113:TYR:C	11:H:115:SER:H	2.16	0.47
7:L:121:ARG:HG2	7:L:127:GLY:HA2	1.93	0.47
18:1:1004:CLA:C3A	18:1:1004:CLA:CGA	2.92	0.47
18:3:3002:CLA:HBD	18:3:3002:CLA:HAA2	1.94	0.47
14:4:190:ASN:OD1	27:4:4501:LUT:O23	2.23	0.47
18:A:1122:CLA:H202	18:A:1122:CLA:H101	1.96	0.47
20:A:5001:PQN:H201	18:A:1138:CLA:HBC1	1.95	0.47
1:A:22:LEU:HA	16:3:88:GLY:HA3	1.96	0.47
9:D:101:TYR:CE2	9:D:135:LYS:HB2	2.50	0.47
18:G:1001:CLA:O1A	22:G:2011:BCR:H352	2.15	0.47
15:1:180:TYR:HB3	18:1:1001:CLA:CMA	2.45	0.47
15:1:166:ASP:OD1	15:1:169:GLY:N	2.48	0.47
13:2:177:VAL:C	13:2:179:THR:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:168:TRP:CE3	18:2:2012:CLA:HMA1	2.48	0.47
13:2:68:PHE:HD2	13:2:71:SER:CB	2.23	0.47
18:3:3006:CLA:HAA1	18:3:3006:CLA:HBD	1.97	0.47
16:3:155:TYR:CE1	18:3:3010:CLA:H102	2.49	0.47
14:4:158:GLN:CA	14:4:158:GLN:NE2	2.77	0.47
18:4:4017:CLA:HAC2	29:4:4505:ZEX:H373	1.96	0.47
1:A:595:TRP:NE1	18:A:1128:CLA:HMD1	2.29	0.47
18:B:1220:CLA:CAB	18:B:1227:CLA:HMD2	2.44	0.47
22:J:6013:BCR:H351	22:J:6013:BCR:H15C	1.67	0.47
15:1:43:PRO:HG2	28:1:1009:CHL:C3D	2.45	0.47
21:1:1801:LHG:H381	21:1:1801:LHG:H223	1.89	0.47
16:3:139:THR:CG2	16:3:140:GLY:H	2.23	0.47
16:3:110:MET:SD	16:3:230:ASN:C	2.93	0.47
14:4:240:PRO:HG2	18:4:4008:CLA:C3B	2.44	0.47
14:4:156:ARG:HB3	28:4:4011:CHL:CHD	2.45	0.47
18:B:1213:CLA:NC	18:B:1213:CLA:H52	2.29	0.47
18:F:1302:CLA:O1D	23:F:5002:LMG:HC91	2.14	0.47
7:L:116:LYS:HB3	18:L:1503:CLA:HMB3	1.97	0.47
18:1:1008:CLA:CHA	18:1:1008:CLA:HED2	2.45	0.47
15:1:62:ASP:OD2	15:1:65:ARG:HA	2.15	0.47
13:2:87:PHE:CE2	27:2:2502:LUT:C37	2.94	0.47
16:3:217:GLU:C	16:3:219:SER:N	2.68	0.47
16:3:136:TRP:HB2	27:3:3502:LUT:H22	1.97	0.47
14:4:118:ILE:CD1	14:4:120:ILE:CD1	2.76	0.47
14:4:172:PHE:HD1	14:4:173:LYS:H	1.63	0.47
18:4:4001:CLA:C4D	27:4:4501:LUT:H382	2.45	0.47
28:4:4013:CHL:HBA1	28:4:4013:CHL:H3A	1.70	0.47
18:B:1218:CLA:H192	18:1:1012:CLA:HMC2	1.96	0.47
9:D:83:ILE:HG12	9:D:124:ARG:HH11	1.80	0.47
6:G:65:SER:HB3	18:G:1001:CLA:HBA1	1.91	0.47
18:B:1213:CLA:C3D	18:G:1003:CLA:HED1	2.44	0.47
16:3:62:LYS:NZ	16:3:76:TYR:CD2	2.83	0.47
18:A:1120:CLA:H112	18:A:1120:CLA:H91	1.73	0.47
18:B:1234:CLA:H101	18:B:1234:CLA:H41	1.95	0.47
2:B:417:ALA:O	2:B:421:HIS:ND1	2.46	0.47
18:B:1218:CLA:H151	18:G:1003:CLA:C15	2.45	0.47
22:G:2011:BCR:H15C	22:G:2011:BCR:H351	1.69	0.47
22:I:6020:BCR:H351	22:I:6020:BCR:H15C	1.68	0.47
12:K:71:VAL:HG13	12:K:132:ILE:HB	1.97	0.47
18:1:1001:CLA:C4D	27:1:1501:LUT:C38	2.93	0.47
13:2:129:LEU:HD22	13:2:131:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2001:CLA:H41	18:2:2002:CLA:CMA	2.45	0.47
16:3:214:GLY:O	16:3:220:LEU:CB	2.62	0.47
18:B:1220:CLA:H62	18:B:1220:CLA:H101	1.64	0.47
2:B:73:ASN:HB2	2:B:76:ALA:HB3	1.96	0.47
9:D:171:ASP:OD1	9:D:179:ASN:ND2	2.48	0.47
18:F:1302:CLA:HMB2	22:F:6016:BCR:HC7	1.97	0.47
22:L:6019:BCR:H371	22:L:6019:BCR:H24C	1.68	0.47
15:1:222:TRP:CZ2	18:1:1008:CLA:HMB3	2.48	0.47
18:1:1011:CLA:HBA2	18:1:1011:CLA:HBD	1.95	0.47
15:1:85:ARG:HH11	15:1:85:ARG:HG2	1.79	0.47
15:1:85:ARG:NE	18:1:1001:CLA:CHD	2.78	0.47
13:2:256:ASP:O	13:2:260:ALA:HB3	2.14	0.47
18:4:4005:CLA:HMD2	18:4:4012:CLA:NC	2.30	0.47
21:A:7001:LHG:H191	18:A:1128:CLA:H111	1.97	0.47
1:A:371:VAL:HG12	18:A:1124:CLA:HED3	1.96	0.47
1:A:582:ASP:OD1	8:C:53:ARG:HD2	2.15	0.47
18:B:1239:CLA:HBA2	18:B:1239:CLA:H3A	1.47	0.47
2:B:576:PHE:CE1	18:B:1226:CLA:HAC2	2.49	0.47
8:C:14:CYS:O	8:C:15:THR:OG1	2.15	0.47
4:J:7:TYR:CE2	23:F:5001:LMG:HC4	2.50	0.47
15:1:85:ARG:CD	18:1:1001:CLA:C4C	2.93	0.47
13:2:114:MET:CE	18:2:2001:CLA:HHC	2.44	0.47
16:3:111:LEU:HD21	18:3:3006:CLA:HBB1	1.97	0.47
28:3:3011:CHL:CBA	28:3:3011:CHL:CHA	2.93	0.47
16:3:80:PRO:CG	27:3:3502:LUT:H24	2.45	0.47
18:3:3006:CLA:NC	22:3:3503:BCR:HC31	2.29	0.47
16:3:70:GLY:N	16:3:75:ASP:OD2	2.48	0.47
27:4:4502:LUT:H171	27:4:4502:LUT:C8	2.45	0.47
18:A:1105:CLA:H3A	18:A:1105:CLA:HBA2	1.59	0.47
1:A:282:THR:OG1	1:A:283:PHE:N	2.48	0.47
1:A:602:LEU:HD21	18:A:1128:CLA:HBC1	1.95	0.47
2:B:82:PHE:CZ	2:B:363:GLN:HG2	2.49	0.47
9:D:151:ILE:HG22	9:D:152:LYS:N	2.29	0.47
11:H:132:PRO:N	11:H:133:PRO:CD	2.78	0.47
18:1:1001:CLA:ND	27:1:1501:LUT:C38	2.75	0.46
15:1:149:ARG:HA	18:1:1011:CLA:HBC3	1.96	0.46
15:1:111:TRP:HZ2	18:1:1013:CLA:CBC	2.26	0.46
15:1:232:ILE:CG2	15:1:233:PRO:CD	2.84	0.46
13:2:207:GLY:HA2	18:2:2001:CLA:HAA2	1.97	0.46
13:2:69:PRO:HA	16:3:186:TYR:CZ	2.50	0.46
16:3:92:PHE:HB3	18:3:3005:CLA:H11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1110:CLA:H52	16:3:81:LEU:HD13	1.98	0.46
14:4:176:SER:OG	14:4:177:LEU:N	2.49	0.46
18:4:4006:CLA:C4B	27:4:4502:LUT:H183	2.45	0.46
18:A:1107:CLA:H151	18:A:1109:CLA:H142	1.95	0.46
1:A:203:LEU:O	1:A:207:LEU:HB2	2.15	0.46
1:A:335:LYS:O	18:A:1151:CLA:HBC3	2.15	0.46
2:B:576:PHE:HE1	18:B:1226:CLA:HAC2	1.79	0.46
18:B:1240:CLA:H161	18:B:1240:CLA:H143	1.76	0.46
2:B:282:PHE:HE2	22:G:2011:BCR:H281	1.79	0.46
11:H:107:GLY:O	11:H:110:THR:CG2	2.63	0.46
7:L:61:ASN:OD1	7:L:166:LEU:HD21	2.14	0.46
16:3:141:VAL:HG13	16:3:141:VAL:O	2.15	0.46
16:3:267:ASN:N	16:3:270:THR:OG1	2.48	0.46
18:3:3010:CLA:H2A	18:3:3010:CLA:O2D	2.15	0.46
28:3:3011:CHL:HBA1	28:3:3011:CHL:CHA	2.44	0.46
18:3:3018:CLA:CMB	18:3:3018:CLA:HBB1	2.29	0.46
14:4:103:MET:HE3	14:4:207:ASN:O	2.14	0.46
14:4:68:GLY:HA2	14:4:73:ASP:OD2	2.16	0.46
18:B:1208:CLA:H2A	18:B:1208:CLA:HED2	1.97	0.46
22:B:6004:BCR:H282	18:B:1218:CLA:HBA2	1.96	0.46
7:L:120:LEU:HD23	7:L:120:LEU:HA	1.72	0.46
18:2:2005:CLA:HMD2	18:2:2012:CLA:CHD	2.45	0.46
13:2:137:TRP:CH2	13:2:236:TRP:HA	2.38	0.46
14:4:166:VAL:HB	14:4:177:LEU:HB2	1.97	0.46
2:B:294:ASN:HA	6:G:107:ARG:HG2	1.98	0.46
2:B:459:PHE:O	2:B:463:ILE:HG12	2.15	0.46
18:1:1002:CLA:HAA2	18:1:1002:CLA:HBD	1.98	0.46
18:2:2002:CLA:HAA2	18:2:2002:CLA:HBD	1.97	0.46
13:2:152:LEU:HD11	28:2:2013:CHL:HMD3	1.97	0.46
16:3:80:PRO:HG2	27:3:3502:LUT:H24	1.96	0.46
14:4:125:LYS:O	14:4:128:ASP:HB2	2.16	0.46
18:4:4001:CLA:H61	18:4:4001:CLA:H41	1.60	0.46
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.50	0.46
18:B:1021:CLA:H3A	18:B:1021:CLA:HBA2	1.68	0.46
18:B:1215:CLA:CGA	18:B:1215:CLA:H3A	2.42	0.46
5:F:213:TRP:CD1	5:F:214:PRO:HD3	2.51	0.46
18:A:1121:CLA:H52	12:K:82:ARG:HG3	1.97	0.46
15:1:143:ALA:CA	18:1:1012:CLA:HAB	2.46	0.46
15:1:97:PRO:C	15:1:102:LEU:CB	2.84	0.46
13:2:129:LEU:HD22	13:2:131:ILE:CD1	2.46	0.46
13:2:173:ASN:HB3	13:2:174:PRO:CD	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:2502:LUT:H15	27:2:2502:LUT:H201	1.81	0.46
18:3:3004:CLA:H61	27:3:3502:LUT:C36	2.45	0.46
14:4:135:PHE:CD1	14:4:135:PHE:C	2.89	0.46
18:B:1240:CLA:H62	18:B:1240:CLA:H41	1.74	0.46
9:D:151:ILE:CG2	9:D:152:LYS:N	2.79	0.46
6:G:100:HIS:O	6:G:101:PHE:CD2	2.69	0.46
18:1:1005:CLA:CMD	18:1:1012:CLA:C1D	2.85	0.46
15:1:183:LYS:HZ2	18:1:1002:CLA:CGD	2.26	0.46
13:2:203:PRO:HD2	27:2:2501:LUT:C3	2.44	0.46
18:4:4017:CLA:H3A	18:4:4017:CLA:HBA2	1.66	0.46
18:4:4005:CLA:HMB1	27:4:4502:LUT:H403	1.97	0.46
2:B:224:PRO:HG2	2:B:233:TYR:CZ	2.51	0.46
9:D:166:TYR:OH	9:D:169:PRO:HD2	2.16	0.46
9:D:177:LYS:O	9:D:182:ARG:NH1	2.47	0.46
6:G:149:LYS:O	6:G:149:LYS:HG3	2.14	0.46
18:1:1002:CLA:HMD2	18:1:1007:CLA:C1D	2.45	0.46
28:1:1009:CHL:HBA1	28:1:1009:CHL:H3A	1.67	0.46
15:1:97:PRO:HB2	15:1:102:LEU:CG	2.45	0.46
13:2:111:ARG:HA	13:2:114:MET:HE2	1.97	0.46
18:2:2004:CLA:HHD	18:2:2009:CLA:HBB2	1.98	0.46
27:2:2502:LUT:C36	27:2:2502:LUT:H28	2.42	0.46
16:3:94:GLU:CD	16:3:96:ARG:H	2.01	0.46
14:4:132:GLU:O	14:4:134:TYR:CD1	2.69	0.46
18:A:1151:CLA:HBC2	18:A:1151:CLA:HMC1	1.97	0.46
18:B:1214:CLA:HBA2	18:B:1214:CLA:H3A	1.58	0.46
22:B:6005:BCR:H15C	22:B:6005:BCR:H351	1.74	0.46
9:D:81:SER:HB3	9:D:129:LEU:O	2.16	0.46
7:L:145:LEU:HB3	7:L:186:THR:CG2	2.45	0.46
7:L:85:ASN:HA	7:L:90:ARG:NH2	2.30	0.46
15:1:104:ASN:OD1	15:1:208:THR:HG23	2.15	0.46
15:1:173:ASP:HB3	15:1:176:LYS:HB3	1.97	0.46
13:2:126:LEU:CB	13:2:134:THR:HA	2.45	0.46
18:2:2001:CLA:H41	18:2:2001:CLA:H62	1.63	0.46
13:2:127:THR:CG2	13:2:247:ILE:HD13	2.39	0.46
13:2:91:GLY:O	13:2:94:SER:HB2	2.16	0.46
18:4:4006:CLA:C3B	27:4:4503:LUT:C17	2.93	0.46
5:F:146:PRO:O	5:F:147:HIS:HD2	1.99	0.46
18:G:1003:CLA:H52	23:G:2021:LMG:H332	1.98	0.46
1:A:272:LEU:HD11	12:K:134:VAL:HG13	1.97	0.46
15:1:97:PRO:HB2	15:1:102:LEU:CD2	2.43	0.46
13:2:126:LEU:HD12	13:2:126:LEU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:154:ILE:CG2	18:4:4008:CLA:HED1	2.46	0.46
13:2:59:VAL:O	13:2:59:VAL:HG12	2.16	0.46
16:3:225:LEU:CB	16:3:226:LYS:NZ	2.71	0.46
18:4:4006:CLA:C2B	27:4:4503:LUT:C17	2.93	0.46
18:A:1151:CLA:C2C	18:A:1120:CLA:HMB3	2.46	0.46
18:1:1002:CLA:CMC	18:1:1002:CLA:HBC2	2.45	0.46
15:1:200:VAL:CG1	18:1:1003:CLA:HAC2	2.44	0.46
15:1:183:LYS:HD3	18:1:1002:CLA:CGA	2.45	0.46
13:2:188:LEU:CD2	13:2:197:GLY:C	2.84	0.46
16:3:225:LEU:C	16:3:225:LEU:HD13	2.36	0.46
18:3:3005:CLA:HMD2	18:3:3012:CLA:C4C	2.45	0.46
16:3:67:TYR:CZ	16:3:84:SER:C	2.89	0.46
14:4:204:GLU:HG3	18:4:4001:CLA:NB	2.31	0.46
17:A:1011:CL0:H7	18:B:1021:CLA:HBB1	1.97	0.46
18:A:1013:CLA:HMA1	18:A:1013:CLA:H51	1.97	0.46
18:A:1104:CLA:H192	18:A:1104:CLA:H162	1.72	0.46
18:A:1122:CLA:H111	18:A:1122:CLA:H72	1.70	0.46
18:A:1132:CLA:H141	18:A:1132:CLA:H161	1.61	0.46
1:A:197:GLN:O	1:A:199:VAL:N	2.49	0.46
2:B:231:ASN:HA	18:B:1213:CLA:HAA2	1.98	0.46
10:E:76:ILE:O	10:E:77:LEU:HD12	2.16	0.46
18:G:1001:CLA:C4D	18:G:1001:CLA:CED	2.94	0.46
7:L:203:LEU:HD12	7:L:203:LEU:N	2.30	0.46
7:L:96:LEU:C	7:L:96:LEU:CD2	2.85	0.46
27:4:4503:LUT:C36	28:1:1009:CHL:H8	2.36	0.45
15:1:108:ALA:O	15:1:111:TRP:CZ3	2.69	0.45
21:1:1801:LHG:C6	21:1:1801:LHG:HC81	2.39	0.45
15:1:183:LYS:HE3	18:1:1002:CLA:O1A	2.16	0.45
13:2:60:ALA:HB2	13:2:78:ASP:OD1	2.16	0.45
16:3:135:ALA:HB1	16:3:137:PHE:CE2	2.52	0.45
16:3:72:LEU:HA	16:3:72:LEU:HD23	1.73	0.45
14:4:152:VAL:HG11	28:4:4011:CHL:C1B	2.45	0.45
14:4:204:GLU:HG3	18:4:4001:CLA:C4B	2.46	0.45
18:A:1140:CLA:HBA2	18:A:1140:CLA:H3A	1.69	0.45
2:B:142:LEU:HD21	22:B:6006:BCR:H24C	1.97	0.45
12:K:71:VAL:CG1	12:K:129:GLY:HA2	2.42	0.45
18:1:1006:CLA:O1A	18:1:1013:CLA:HMD2	2.15	0.45
15:1:232:ILE:CD1	18:1:1014:CLA:HMD2	2.45	0.45
23:G:2021:LMG:O5	15:1:131:LEU:HD11	2.15	0.45
15:1:148:GLN:HA	15:1:148:GLN:NE2	2.31	0.45
15:1:230:VAL:CG1	18:1:1014:CLA:C4B	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:131:ILE:HG21	13:2:133:LEU:HG	1.98	0.45
18:2:2016:CLA:CED	18:2:2016:CLA:CAD	2.94	0.45
16:3:226:LYS:H	16:3:226:LYS:CE	2.29	0.45
18:3:3013:CLA:HBA1	18:3:3013:CLA:H3A	1.54	0.45
14:4:54:GLY:O	14:4:74:ASN:HA	2.16	0.45
18:A:1119:CLA:H111	18:A:1119:CLA:H143	1.67	0.45
18:A:1132:CLA:H193	18:A:1132:CLA:H162	1.70	0.45
18:B:1229:CLA:H121	22:F:6016:BCR:H271	1.98	0.45
2:B:560:ASP:OD1	8:C:66:ARG:NH1	2.47	0.45
2:B:9:SER:O	2:B:12:ILE:HG22	2.16	0.45
4:J:28:GLU:OE1	18:J:1302:CLA:ND	2.49	0.45
15:1:104:ASN:CG	15:1:208:THR:CG2	2.84	0.45
15:1:127:PRO:O	15:1:128:TRP:CD1	2.70	0.45
15:1:212:GLU:O	15:1:215:ALA:HB3	2.16	0.45
15:1:225:ASN:N	15:1:225:ASN:ND2	2.60	0.45
15:1:63:PRO:HD2	27:1:1502:LUT:C3	2.47	0.45
13:2:186:ASN:CG	18:2:2016:CLA:CMA	2.84	0.45
16:3:205:GLY:HA2	16:3:206:PRO:HD3	1.66	0.45
16:3:190:LEU:HA	16:3:207:PHE:CE2	2.51	0.45
16:3:262:ASP:CB	16:3:265:ASN:HD22	2.29	0.45
16:3:110:MET:HE2	27:3:3501:LUT:H201	1.98	0.45
14:4:154:ILE:O	28:1:1009:CHL:HED1	2.15	0.45
1:A:397:THR:HG23	1:A:613:ILE:HG21	1.97	0.45
18:B:1240:CLA:CED	18:B:1220:CLA:HBB	2.46	0.45
18:1:1002:CLA:CMD	18:1:1007:CLA:C4D	2.95	0.45
18:1:1011:CLA:CBA	18:1:1011:CLA:HBD	2.46	0.45
15:1:146:GLU:CG	15:1:149:ARG:NH1	2.73	0.45
15:1:158:LYS:C	15:1:159:LYS:CD	2.85	0.45
15:1:218:LEU:HD21	18:1:1008:CLA:HMC3	1.98	0.45
16:3:121:TYR:C	16:3:121:TYR:CD1	2.89	0.45
18:3:3008:CLA:CHD	18:3:3008:CLA:CBC	2.85	0.45
18:A:1110:CLA:H52	16:3:81:LEU:CD1	2.47	0.45
1:A:205:HIS:CE1	18:A:1118:CLA:HMD2	2.51	0.45
1:A:503:THR:O	1:A:505:PRO:HD3	2.16	0.45
1:A:570:PRO:HD2	9:D:136:GLU:OE1	2.15	0.45
22:A:6017:BCR:H392	22:A:6017:BCR:H23C	1.99	0.45
2:B:265:THR:HG22	2:B:360:PHE:CE1	2.52	0.45
2:B:551:LYS:C	2:B:553:PHE:H	2.20	0.45
9:D:211:LEU:CD1	9:D:211:LEU:H	2.28	0.45
13:2:164:GLU:O	13:2:168:TRP:HB2	2.16	0.45
16:3:149:ASN:O	16:3:150:TYR:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:157:LEU:O	16:3:161:GLU:N	2.37	0.45
14:4:74:ASN:N	14:4:74:ASN:HD22	2.14	0.45
18:A:1108:CLA:HED2	16:3:93:ILE:HB	1.98	0.45
1:A:225:VAL:HG22	1:A:245:PRO:HB3	1.97	0.45
2:B:282:PHE:CE2	22:G:2011:BCR:H281	2.51	0.45
18:B:1240:CLA:HBA1	21:B:5004:LHG:HC42	1.98	0.45
10:E:111:ASN:ND2	10:E:113:ALA:N	2.60	0.45
5:F:111:ALA:O	5:F:113:SER:N	2.50	0.45
22:F:6014:BCR:H331	22:F:6014:BCR:C8	2.46	0.45
7:L:166:LEU:CD2	7:L:166:LEU:C	2.85	0.45
18:1:1001:CLA:CGA	18:1:1001:CLA:C4A	2.95	0.45
15:1:127:PRO:C	15:1:128:TRP:CG	2.87	0.45
13:2:140:ALA:O	13:2:143:GLN:HG3	2.17	0.45
13:2:231:ALA:HA	18:2:2003:CLA:HBB1	1.99	0.45
13:2:76:TRP:CD1	13:2:93:GLY:O	2.69	0.45
16:3:225:LEU:CD1	16:3:225:LEU:C	2.84	0.45
16:3:263:PRO:CD	16:3:264:VAL:H	2.30	0.45
18:4:4007:CLA:H92	18:4:4007:CLA:H52	1.99	0.45
22:A:6007:BCR:H351	22:A:6007:BCR:H15C	1.65	0.45
1:A:62:HIS:HB2	18:A:1128:CLA:CGA	2.46	0.45
23:B:5005:LMG:H212	22:F:6016:BCR:H362	1.98	0.45
22:B:6004:BCR:H383	6:G:126:ALA:HB1	1.98	0.45
6:G:76:ARG:HE	6:G:116:LYS:NZ	2.14	0.45
3:I:24:LEU:O	3:I:28:VAL:HG23	2.16	0.45
4:J:32:LEU:HB3	4:J:33:PHE:CD1	2.52	0.45
13:2:129:LEU:CD2	13:2:131:ILE:HG13	2.47	0.45
18:2:2002:CLA:HMC2	27:2:2501:LUT:C31	2.46	0.45
16:3:137:PHE:CD1	16:3:137:PHE:C	2.90	0.45
16:3:253:TYR:CD1	16:3:253:TYR:O	2.70	0.45
16:3:202:TYR:CD1	18:3:3001:CLA:O1D	2.70	0.45
18:3:3003:CLA:H62	18:3:3003:CLA:H2	1.79	0.45
18:3:3018:CLA:HBA1	18:3:3018:CLA:C4A	2.45	0.45
14:4:215:PHE:CE1	27:4:4502:LUT:H12	2.51	0.45
29:4:4505:ZEX:H191	29:4:4505:ZEX:H11	1.79	0.45
18:A:1130:CLA:C2	18:L:1502:CLA:H93	2.47	0.45
18:A:1237:CLA:HMC3	18:B:1238:CLA:ND	2.32	0.45
1:A:222:GLN:NE2	1:A:300:ALA:HA	2.32	0.45
18:B:1207:CLA:H91	18:B:1207:CLA:H112	1.61	0.45
2:B:473:GLY:O	2:B:474:PHE:HB2	2.17	0.45
2:B:548:PRO:HD2	8:C:62:PHE:CZ	2.52	0.45
18:G:1001:CLA:C4	22:G:2011:BCR:C34	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:32:LEU:HD21	18:J:1302:CLA:C2	2.46	0.45
7:L:121:ARG:HG3	7:L:127:GLY:CA	2.39	0.45
7:L:148:TYR:CE1	7:L:152:SER:OG	2.70	0.45
15:1:130:THR:HG22	15:1:131:LEU:H	1.80	0.45
15:1:51:LEU:HD12	15:1:60:GLY:HA2	1.99	0.45
13:2:122:ILE:N	13:2:122:ILE:HD12	2.31	0.45
16:3:130:GLN:C	16:3:132:THR:H	2.18	0.45
16:3:183:GLY:CA	16:3:194:PHE:C	2.85	0.45
16:3:186:TYR:CD1	16:3:186:TYR:N	2.85	0.45
16:3:62:LYS:HZ3	16:3:76:TYR:HD2	1.63	0.45
14:4:132:GLU:O	14:4:134:TYR:CE1	2.70	0.45
14:4:99:GLY:O	14:4:103:MET:HG2	2.17	0.45
1:A:304:LEU:HA	1:A:304:LEU:HD23	1.83	0.45
2:B:374:HIS:O	2:B:378:ILE:HG12	2.17	0.45
18:F:1302:CLA:H3A	18:F:1302:CLA:HBA1	1.74	0.45
5:F:167:PHE:HB2	22:F:6014:BCR:C40	2.47	0.45
6:G:114:VAL:CG1	18:G:1002:CLA:CBA	2.95	0.45
3:I:9:VAL:HB	3:I:10:PRO:CD	2.47	0.45
4:J:31:ARG:HH22	18:J:1302:CLA:H3A	1.81	0.45
4:J:2:ARG:CD	4:J:4:LEU:HB2	2.42	0.45
4:J:9:SER:HA	4:J:13:VAL:HG21	1.99	0.45
22:K:2011:BCR:H24C	22:K:2011:BCR:H371	1.73	0.45
7:L:145:LEU:CD1	22:L:6019:BCR:H392	2.25	0.45
15:1:220:ASP:OD2	15:1:223:HIS:CD2	2.70	0.45
13:2:220:LYS:CA	18:2:2007:CLA:CED	2.90	0.45
16:3:229:LYS:HD2	16:3:229:LYS:HA	1.67	0.45
28:3:3011:CHL:HBC2	28:3:3011:CHL:HHD	1.99	0.45
18:3:3001:CLA:CBB	27:3:3501:LUT:H34	2.44	0.45
16:3:94:GLU:OE2	16:3:95:PRO:N	2.50	0.45
14:4:167:ASN:OD1	14:4:168:GLN:N	2.49	0.45
18:4:4008:CLA:H3A	18:4:4008:CLA:HBA2	1.59	0.45
14:4:60:LEU:CG	14:4:61:ALA:N	2.79	0.45
18:B:1205:CLA:CGA	18:B:1205:CLA:C1A	2.94	0.45
18:B:1207:CLA:H111	18:B:1207:CLA:H142	1.68	0.45
18:B:1223:CLA:H143	22:B:6009:BCR:C19	2.46	0.45
2:B:172:GLU:HB3	2:B:291:TYR:HB3	1.98	0.45
2:B:301:ILE:HG21	18:B:1221:CLA:HAC1	1.97	0.45
2:B:226:LEU:HD13	26:B:8002:LMU:H5B	1.99	0.45
8:C:5:VAL:HG22	8:C:67:VAL:HG22	1.98	0.45
22:F:6016:BCR:C38	22:F:6016:BCR:C23	2.91	0.45
12:K:136:VAL:O	12:K:140:LEU:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:70:MET:CE	12:K:71:VAL:CA	2.85	0.45
7:L:98:ARG:NH2	7:L:175:GLN:OE1	2.50	0.45
7:L:204:LEU:CD1	7:L:204:LEU:C	2.85	0.45
7:L:55:GLN:O	7:L:56:VAL:HB	2.16	0.45
15:1:126:VAL:HG23	15:1:127:PRO:N	2.31	0.45
15:1:217:HIS:O	15:1:221:PRO:HA	2.17	0.45
13:2:177:VAL:C	13:2:179:THR:N	2.70	0.45
13:2:185:ASN:OD1	13:2:186:ASN:N	2.50	0.45
13:2:120:ILE:CG2	27:2:2501:LUT:C37	2.86	0.45
14:4:199:GLU:O	14:4:202:GLU:HB2	2.16	0.45
1:A:229:ILE:HD11	1:A:245:PRO:HG3	1.99	0.45
1:A:346:LEU:HG	1:A:429:ASN:HD21	1.81	0.45
2:B:585:ASN:HB2	18:B:1012:CLA:HBC2	1.98	0.45
2:B:358:TYR:CE2	18:B:1225:CLA:HED2	2.52	0.45
18:B:1235:CLA:H203	18:B:1235:CLA:H161	1.87	0.45
22:B:6009:BCR:H351	22:B:6009:BCR:H15C	1.71	0.45
10:E:66:ILE:CG2	10:E:93:VAL:HG11	2.45	0.45
5:F:157:TRP:CH2	18:F:1302:CLA:O1A	2.70	0.45
23:F:5002:LMG:H172	23:F:5002:LMG:H141	1.68	0.45
7:L:164:LEU:HD23	7:L:164:LEU:N	2.31	0.45
15:1:105:TRP:HD1	15:1:105:TRP:H	1.62	0.44
13:2:194:GLY:O	13:2:195:TYR:CD1	2.70	0.44
16:3:100:TYR:CE1	16:3:104:ILE:HG13	2.52	0.44
16:3:242:PHE:O	16:3:246:LEU:HB2	2.17	0.44
14:4:169:ASP:HB3	18:4:4016:CLA:C1D	2.47	0.44
14:4:239:ASP:OD1	14:4:242:HIS:CD2	2.70	0.44
18:4:4001:CLA:CGA	18:4:4001:CLA:C3A	2.95	0.44
14:4:98:ASN:ND2	18:4:4012:CLA:OBD	2.50	0.44
18:A:1131:CLA:C3B	18:A:1132:CLA:HMB2	2.47	0.44
1:A:453:LEU:HD21	18:A:1136:CLA:CAB	2.46	0.44
2:B:645:VAL:HG21	18:B:1205:CLA:HAC1	1.99	0.44
18:B:1202:CLA:HBA2	18:B:1210:CLA:CED	2.47	0.44
2:B:22:TRP:CZ2	18:B:1238:CLA:HMB1	2.53	0.44
2:B:603:ARG:HH22	2:B:627:ASN:ND2	2.14	0.44
2:B:6:PRO:HG3	2:B:24:GLY:CA	2.47	0.44
2:B:93:ASP:O	2:B:96:PHE:HB2	2.17	0.44
18:G:1003:CLA:HBA2	18:G:1003:CLA:H3A	1.57	0.44
11:H:107:GLY:CA	11:H:110:THR:HG22	2.47	0.44
18:A:1237:CLA:H143	22:I:6020:BCR:H363	1.99	0.44
18:2:2004:CLA:H61	18:2:2004:CLA:H41	1.67	0.44
28:2:2010:CHL:HBB1	28:2:2013:CHL:CBB	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:3003:CLA:HAB	27:3:3501:LUT:C17	2.47	0.44
18:3:3012:CLA:CBB	18:3:3012:CLA:HMB1	2.12	0.44
27:3:3502:LUT:C28	27:3:3502:LUT:C37	2.85	0.44
14:4:135:PHE:O	14:4:135:PHE:CG	2.71	0.44
28:4:4013:CHL:HHB	27:4:4503:LUT:H191	1.98	0.44
27:4:4502:LUT:H401	27:4:4502:LUT:H35	1.77	0.44
18:A:1237:CLA:H62	18:A:1237:CLA:H92	1.86	0.44
1:A:382:TYR:CE2	18:A:1127:CLA:HED2	2.52	0.44
1:A:614:PHE:HB3	1:A:652:TRP:HZ3	1.82	0.44
18:B:1214:CLA:H92	18:B:1214:CLA:H61	1.74	0.44
9:D:113:PHE:N	9:D:113:PHE:CD1	2.85	0.44
1:A:721:GLN:NE2	10:E:109:LYS:HB2	2.32	0.44
4:J:2:ARG:O	4:J:2:ARG:HG2	2.16	0.44
12:K:78:LEU:HD23	12:K:78:LEU:HA	1.75	0.44
18:1:1001:CLA:C1D	27:1:1501:LUT:H383	2.47	0.44
13:2:129:LEU:HD23	13:2:129:LEU:O	2.17	0.44
13:2:238:GLN:NE2	18:2:2003:CLA:C1A	2.81	0.44
13:2:219:THR:CG2	18:2:2007:CLA:CED	2.86	0.44
13:2:250:LEU:C	13:2:250:LEU:CD2	2.85	0.44
13:2:256:ASP:OD2	13:2:259:HIS:CD2	2.70	0.44
13:2:79:GLY:N	13:2:84:ASP:OD2	2.50	0.44
13:2:95:ASP:OD1	13:2:98:SER:HB2	2.17	0.44
16:3:120:GLU:OE2	16:3:253:TYR:HB3	2.16	0.44
16:3:267:ASN:C	18:3:3003:CLA:HED2	2.37	0.44
18:3:3006:CLA:HMB1	18:3:3013:CLA:HBB1	1.99	0.44
18:3:3006:CLA:C4	18:3:3018:CLA:C1	2.94	0.44
14:4:219:ILE:CG2	14:4:220:ILE:N	2.81	0.44
14:4:76:PHE:HB3	18:4:4004:CLA:CAD	2.48	0.44
18:B:1207:CLA:H92	18:B:1207:CLA:H61	1.65	0.44
18:B:1215:CLA:H111	18:B:1215:CLA:H143	1.72	0.44
6:G:114:VAL:HG11	18:G:1002:CLA:HBA1	1.99	0.44
18:G:1002:CLA:O2D	18:G:1002:CLA:HBA2	2.18	0.44
6:G:132:HIS:CG	22:G:2011:BCR:H19C	2.53	0.44
12:K:128:VAL:CG2	22:K:2011:BCR:H311	2.47	0.44
7:L:204:LEU:O	7:L:207:LEU:HD23	2.17	0.44
15:1:120:THR:CG2	15:1:125:PRO:HA	2.48	0.44
15:1:42:MET:O	15:1:42:MET:HE2	2.17	0.44
13:2:162:TRP:O	13:2:162:TRP:CD1	2.70	0.44
18:2:2005:CLA:HMD2	18:2:2012:CLA:ND	2.33	0.44
18:A:1107:CLA:HMA1	4:J:27:ILE:HD13	2.00	0.44
18:A:1132:CLA:H143	18:A:1132:CLA:H111	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1235:CLA:H162	18:B:1235:CLA:H141	1.70	0.44
9:D:207:GLN:O	9:D:211:LEU:HD13	2.17	0.44
6:G:100:HIS:O	6:G:101:PHE:CG	2.70	0.44
6:G:125:LEU:HD23	6:G:125:LEU:HA	1.77	0.44
6:G:72:LEU:HD23	6:G:127:TRP:HB2	1.99	0.44
6:G:95:GLN:C	6:G:97:GLY:H	2.20	0.44
18:B:1207:CLA:HAC2	27:I:6018:LUT:H181	1.99	0.44
12:K:124:ALA:HA	12:K:127:THR:OG1	2.17	0.44
12:K:126:GLY:O	12:K:130:HIS:CD2	2.70	0.44
15:1:85:ARG:HH21	18:1:1001:CLA:C1D	2.29	0.44
13:2:133:LEU:CD1	13:2:133:LEU:C	2.85	0.44
13:2:146:PHE:CD1	13:2:147:THR:N	2.85	0.44
13:2:188:LEU:O	13:2:189:THR:HG23	2.18	0.44
13:2:220:LYS:HD3	18:2:2002:CLA:HAA2	1.99	0.44
13:2:239:HIS:CE1	13:2:244:THR:O	2.70	0.44
16:3:135:ALA:CB	16:3:137:PHE:CE2	3.00	0.44
16:3:236:LEU:HD11	18:3:3003:CLA:C15	2.48	0.44
18:3:3005:CLA:OBD	18:3:3012:CLA:HBA2	2.18	0.44
14:4:153:GLU:HG3	14:4:156:ARG:HH11	1.82	0.44
22:A:6007:BCR:C11	18:A:1119:CLA:H112	2.47	0.44
21:A:5003:LHG:H371	18:A:1137:CLA:C4D	2.48	0.44
22:A:6003:BCR:H351	22:A:6003:BCR:H15C	1.72	0.44
18:B:1221:CLA:H2	18:B:1210:CLA:H92	1.99	0.44
11:H:55:PHE:CD2	11:H:55:PHE:O	2.70	0.44
7:L:102:VAL:CG1	7:L:106:HIS:ND1	2.81	0.44
23:F:5002:LMG:H292	18:1:1014:CLA:ND	2.32	0.44
15:1:116:GLY:O	15:1:118:GLN:HA	2.18	0.44
15:1:180:TYR:CD2	18:1:1001:CLA:O1A	2.71	0.44
15:1:98:GLU:N	15:1:102:LEU:CB	2.81	0.44
27:2:2502:LUT:H391	27:2:2502:LUT:H31	1.88	0.44
18:A:1110:CLA:H8	18:A:1110:CLA:HBB1	1.99	0.44
18:B:1236:CLA:H52	18:B:1227:CLA:H191	1.99	0.44
9:D:192:ILE:CG2	9:D:193:GLY:N	2.73	0.44
5:F:167:PHE:HB2	22:F:6014:BCR:H401	1.99	0.44
7:L:174:ASP:CG	7:L:175:GLN:HG2	2.38	0.44
15:1:79:SER:CB	18:1:1012:CLA:HED2	2.47	0.44
13:2:105:ALA:O	13:2:109:HIS:HD2	2.00	0.44
13:2:199:LEU:C	13:2:199:LEU:CD2	2.85	0.44
16:3:117:ILE:HG23	16:3:253:TYR:HB2	1.99	0.44
16:3:174:GLN:HB2	16:3:182:MET:CG	2.48	0.44
18:3:3012:CLA:HBC2	18:3:3013:CLA:HMB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:168:GLN:NE2	14:4:171:ILE:O	2.34	0.44
18:A:1112:CLA:H112	18:A:1112:CLA:H142	1.78	0.44
1:A:269:PHE:HA	1:A:274:TRP:NE1	2.27	0.44
18:B:1207:CLA:H51	18:B:1207:CLA:H11	1.77	0.44
18:B:1225:CLA:H161	18:B:1225:CLA:H202	1.76	0.44
2:B:166:SER:OG	6:G:95:GLN:NE2	2.51	0.44
20:B:5002:PQN:H292	20:B:5002:PQN:H261	1.71	0.44
6:G:116:LYS:HZ1	18:G:1002:CLA:C4B	2.30	0.44
7:L:91:THR:CG2	7:L:175:GLN:HE21	2.30	0.44
16:3:171:ARG:HB3	28:3:3011:CHL:CMC	2.48	0.44
16:3:205:GLY:O	16:3:209:ASN:HB3	2.17	0.44
16:3:241:TYR:CE1	27:3:3501:LUT:C16	2.85	0.44
16:3:268:VAL:HG22	18:3:3003:CLA:C3D	2.48	0.44
18:3:3006:CLA:C2D	18:3:3018:CLA:CAB	2.95	0.44
14:4:113:GLU:CD	14:4:230:PHE:CB	2.86	0.44
1:A:375:HIS:ND1	18:A:1116:CLA:OBD	2.50	0.44
1:A:492:ILE:HD11	18:A:1135:CLA:H11	1.99	0.44
27:I:6018:LUT:H381	27:I:6018:LUT:C28	2.45	0.44
12:K:70:MET:CE	12:K:71:VAL:CG2	2.85	0.44
7:L:132:LEU:C	7:L:132:LEU:HD12	2.35	0.44
18:1:1004:CLA:H52	27:1:1502:LUT:H8	2.00	0.44
15:1:106:VAL:HG21	15:1:208:THR:CG2	2.40	0.44
15:1:193:LEU:C	15:1:193:LEU:CD2	2.85	0.44
18:2:2006:CLA:CMA	28:2:2013:CHL:HAC2	2.46	0.44
18:2:2016:CLA:CGD	18:2:2016:CLA:CGA	2.96	0.44
13:2:223:LYS:HZ3	21:2:2801:LHG:P	2.23	0.44
16:3:78:PHE:CD1	16:3:78:PHE:O	2.70	0.44
1:A:374:GLN:HG3	18:A:1124:CLA:HED2	2.00	0.44
22:A:6007:BCR:H24C	22:A:6007:BCR:H371	1.59	0.44
1:A:85:GLN:HG2	18:A:1103:CLA:HMA1	2.00	0.44
2:B:370:ALA:HB1	18:B:1224:CLA:HMA1	2.00	0.44
18:B:1229:CLA:H2	18:B:1229:CLA:H62	1.67	0.44
9:D:95:ALA:HA	9:D:99:GLU:O	2.16	0.44
15:1:205:TYR:C	15:1:207:GLY:N	2.71	0.43
16:3:202:TYR:HB3	18:3:3001:CLA:CGD	2.47	0.43
14:4:221:GLN:HE21	14:4:221:GLN:HB2	1.60	0.43
18:A:1013:CLA:H71	18:A:1140:CLA:HMC3	2.00	0.43
8:C:14:CYS:O	8:C:15:THR:HG23	2.17	0.43
6:G:126:ALA:O	6:G:130:ILE:HG13	2.17	0.43
27:I:6018:LUT:H31	27:I:6018:LUT:H391	1.89	0.43
7:L:122:ASN:N	7:L:122:ASN:HD22	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1801:LHG:H382	21:1:1801:LHG:H223	1.88	0.43
13:2:209:ALA:HB3	13:2:214:LEU:CD2	2.48	0.43
16:3:183:GLY:HA2	16:3:191:GLU:O	2.18	0.43
16:3:225:LEU:CA	16:3:226:LYS:HZ2	2.31	0.43
16:3:62:LYS:NZ	16:3:76:TYR:HD2	2.16	0.43
14:4:118:ILE:CG2	14:4:120:ILE:H	2.30	0.43
27:4:4503:LUT:H191	27:4:4503:LUT:H11	1.80	0.43
1:A:240:LYS:HB2	1:A:240:LYS:HE3	1.83	0.43
1:A:295:TRP:HB3	1:A:297:THR:HG22	2.00	0.43
1:A:615:HIS:CD2	18:A:1135:CLA:HMC2	2.53	0.43
18:B:1226:CLA:H141	18:B:1226:CLA:H161	1.70	0.43
18:1:1004:CLA:H2	27:1:1502:LUT:C18	2.47	0.43
15:1:222:TRP:CD1	18:1:1008:CLA:HMA1	2.54	0.43
27:1:1502:LUT:H11	27:1:1502:LUT:H191	1.83	0.43
27:4:4503:LUT:H391	27:4:4503:LUT:H31	1.79	0.43
18:B:1204:CLA:H12	18:B:1204:CLA:C4D	2.48	0.43
18:B:1208:CLA:HBA2	18:B:1208:CLA:H3A	1.35	0.43
5:F:143:ASP:OD1	5:F:144:GLY:N	2.51	0.43
6:G:65:SER:HA	6:G:68:THR:CG2	2.48	0.43
3:I:4:LEU:HD12	3:I:5:PRO:N	2.34	0.43
15:1:148:GLN:HE21	15:1:148:GLN:HA	1.83	0.43
13:2:253:HIS:CG	18:2:2003:CLA:HAA2	2.54	0.43
18:2:2003:CLA:HMA1	18:2:2008:CLA:CBC	2.42	0.43
18:2:2005:CLA:H61	18:2:2005:CLA:H93	1.79	0.43
13:2:217:LEU:HD12	13:2:217:LEU:HA	1.77	0.43
16:3:100:TYR:CE1	16:3:104:ILE:CG1	3.01	0.43
16:3:184:LYS:CE	16:3:185:GLN:HE21	2.32	0.43
14:4:135:PHE:O	14:4:135:PHE:CD1	2.70	0.43
14:4:103:MET:CB	18:4:4001:CLA:HMC3	2.47	0.43
17:A:1011:CL0:H10	17:A:1011:CL0:H72	1.55	0.43
18:A:1127:CLA:H62	18:A:1127:CLA:H102	1.81	0.43
18:A:1128:CLA:H122	18:A:1128:CLA:H162	1.70	0.43
1:A:158:ILE:HD11	18:A:1112:CLA:HMA2	1.99	0.43
1:A:55:TRP:HE3	21:A:7001:LHG:H111	1.84	0.43
18:B:1218:CLA:H52	18:B:1218:CLA:H8	1.80	0.43
18:B:1232:CLA:H11	18:B:1232:CLA:H52	1.62	0.43
2:B:195:VAL:HA	2:B:199:ILE:HD12	2.00	0.43
2:B:244:PHE:N	2:B:264:GLN:OE1	2.32	0.43
10:E:79:GLN:HG3	10:E:84:TYR:OH	2.17	0.43
6:G:67:SER:HB2	6:G:135:ALA:HB2	2.00	0.43
15:1:230:VAL:HG13	18:1:1014:CLA:NB	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:41:TRP:CD1	15:1:59:PHE:O	2.70	0.43
16:3:257:LEU:HA	16:3:260:VAL:HB	1.99	0.43
18:3:3006:CLA:CHC	22:3:3503:BCR:HC41	2.48	0.43
14:4:144:ILE:CD1	18:1:1008:CLA:HAA2	2.48	0.43
14:4:243:ASN:C	14:4:244:THR:HG23	2.39	0.43
18:4:4008:CLA:CHC	18:4:4008:CLA:HBB1	2.43	0.43
18:A:1109:CLA:H102	18:A:1101:CLA:HBB2	1.99	0.43
18:B:1220:CLA:H141	22:B:6009:BCR:HC32	1.99	0.43
22:G:2011:BCR:H321	22:G:2011:BCR:C8	2.48	0.43
15:1:85:ARG:NH2	18:1:1001:CLA:C4D	2.72	0.43
15:1:58:ASP:CA	18:1:1004:CLA:CED	2.92	0.43
27:1:1501:LUT:H15	27:1:1501:LUT:H201	1.76	0.43
15:1:168:LEU:HA	15:1:168:LEU:HD13	1.79	0.43
14:4:136:ALA:HA	15:1:223:HIS:NE2	2.33	0.43
13:2:129:LEU:CD2	13:2:131:ILE:HG12	2.49	0.43
14:4:105:GLY:CA	18:4:4006:CLA:CBB	2.95	0.43
14:4:154:ILE:HD12	14:4:157:TRP:HE3	1.83	0.43
18:4:4006:CLA:C2B	27:4:4503:LUT:H171	2.48	0.43
18:A:1237:CLA:HAA2	18:A:1130:CLA:HMB1	2.00	0.43
1:A:417:PHE:CD1	1:A:421:ASP:HB2	2.54	0.43
18:B:1224:CLA:O1D	18:B:1225:CLA:HMA1	2.19	0.43
2:B:406:ASN:O	2:B:410:ARG:HG2	2.18	0.43
5:F:117:LEU:HD23	5:F:117:LEU:HA	1.77	0.43
6:G:148:PRO:O	6:G:148:PRO:HD2	2.18	0.43
12:K:70:MET:CE	12:K:71:VAL:N	2.77	0.43
3:I:25:PHE:CE1	7:L:147:ILE:HG22	2.54	0.43
7:L:85:ASN:CB	18:L:1501:CLA:HMC1	2.48	0.43
7:L:57:VAL:HG23	7:L:57:VAL:O	2.18	0.43
13:2:160:ILE:O	13:2:163:ALA:HB3	2.18	0.43
13:2:188:LEU:HD23	13:2:197:GLY:C	2.38	0.43
18:4:4005:CLA:HMD2	18:4:4012:CLA:ND	2.33	0.43
18:4:4005:CLA:O1A	18:4:4005:CLA:H2A	2.17	0.43
14:4:141:LEU:HD22	28:4:4013:CHL:C2D	2.49	0.43
28:4:4013:CHL:OMC	28:4:4013:CHL:HAC1	2.19	0.43
27:4:4503:LUT:H15	27:4:4503:LUT:H201	1.80	0.43
18:A:1122:CLA:H162	18:A:1122:CLA:H143	1.86	0.43
18:A:1140:CLA:H62	18:A:1140:CLA:H41	1.63	0.43
1:A:103:PHE:HB3	1:A:122:VAL:HG23	2.00	0.43
1:A:445:HIS:O	1:A:449:VAL:HG23	2.19	0.43
18:B:1211:CLA:HMC1	18:B:1212:CLA:HAB	2.00	0.43
18:B:1222:CLA:H61	18:B:1222:CLA:H41	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1222:CLA:H92	18:B:1222:CLA:H62	1.75	0.43
18:B:1231:CLA:H112	18:B:1231:CLA:H142	1.83	0.43
5:F:221:LEU:HB2	5:F:222:LEU:HD23	1.99	0.43
22:F:6016:BCR:H24C	22:F:6016:BCR:H371	1.79	0.43
6:G:116:LYS:HA	18:G:1002:CLA:C2D	2.49	0.43
6:G:68:THR:HG23	6:G:69:GLY:N	2.34	0.43
7:L:181:GLY:O	7:L:184:LYS:HB2	2.18	0.43
15:1:85:ARG:HB3	18:1:1011:CLA:HED2	1.98	0.43
15:1:230:VAL:CG1	18:1:1014:CLA:NB	2.82	0.43
15:1:108:ALA:O	15:1:111:TRP:CE3	2.72	0.43
15:1:217:HIS:CE1	15:1:221:PRO:HB2	2.54	0.43
15:1:224:ASN:OD1	15:1:224:ASN:N	2.51	0.43
15:1:81:LEU:O	15:1:85:ARG:HG2	2.18	0.43
13:2:181:PRO:CD	18:2:2016:CLA:CBB	2.95	0.43
18:3:3006:CLA:H43	18:3:3018:CLA:C1	2.48	0.43
27:3:3502:LUT:H31	27:3:3502:LUT:H391	1.88	0.43
14:4:171:ILE:HD13	18:4:4016:CLA:CMA	2.49	0.43
18:4:4007:CLA:HAA1	18:4:4007:CLA:HED2	2.00	0.43
22:A:6011:BCR:H15C	22:A:6011:BCR:H351	1.80	0.43
18:B:1205:CLA:H143	18:B:1205:CLA:H161	1.80	0.43
11:H:80:PRO:O	11:H:82:GLN:N	2.47	0.43
7:L:169:ARG:C	7:L:171:LYS:N	2.72	0.43
28:1:1010:CHL:CMC	28:1:1010:CHL:CBC	2.86	0.43
15:1:64:LEU:O	15:1:65:ARG:HB2	2.19	0.43
15:1:85:ARG:HG3	15:1:85:ARG:NH1	2.34	0.43
16:3:148:TYR:O	16:3:150:TYR:CD1	2.72	0.43
16:3:185:GLN:HB2	16:3:186:TYR:HD1	1.77	0.43
28:4:4010:CHL:HAB	28:4:4010:CHL:HMB1	1.89	0.43
18:A:1120:CLA:H62	18:A:1120:CLA:H41	1.52	0.43
1:A:434:ARG:HA	1:A:437:ARG:HB2	2.01	0.43
18:B:1239:CLA:H62	18:B:1023:CLA:H201	2.00	0.43
2:B:95:HIS:NE2	18:B:1206:CLA:HMB3	2.33	0.43
18:B:1227:CLA:H62	18:B:1227:CLA:H102	1.74	0.43
2:B:17:THR:HA	2:B:696:LYS:HB2	2.01	0.43
5:F:213:TRP:CG	5:F:214:PRO:HD3	2.54	0.43
6:G:116:LYS:HG2	6:G:117:SER:N	2.34	0.43
12:K:78:LEU:C	12:K:80:ALA:N	2.72	0.43
18:1:1003:CLA:H2	18:1:1008:CLA:CMD	2.48	0.43
27:4:4503:LUT:C36	28:1:1009:CHL:C9	2.85	0.43
23:F:5002:LMG:O9	18:1:1014:CLA:HED3	2.19	0.43
13:2:104:GLN:NE2	13:2:193:VAL:CB	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2006:CLA:O1A	28:2:2013:CHL:HMD2	2.19	0.43
14:4:103:MET:HE3	14:4:207:ASN:CB	2.48	0.43
14:4:103:MET:HE3	14:4:207:ASN:HB3	1.96	0.43
18:4:4005:CLA:C2D	18:4:4012:CLA:C1D	2.97	0.43
18:A:1110:CLA:C1	16:3:81:LEU:HD13	2.49	0.43
1:A:154:ARG:NH2	1:A:233:LEU:HB3	2.34	0.43
1:A:342:GLY:HA3	1:A:431:LEU:HG	2.00	0.43
18:B:1231:CLA:HAB	18:B:1223:CLA:HED1	2.01	0.43
5:F:103:GLU:O	5:F:106:LEU:HB3	2.19	0.43
12:K:119:LEU:HD12	12:K:119:LEU:HA	1.80	0.43
15:1:63:PRO:HD2	27:1:1502:LUT:O3	2.19	0.42
15:1:78:GLU:O	15:1:82:ILE:HG12	2.19	0.42
13:2:137:TRP:HH2	13:2:236:TRP:CA	2.24	0.42
13:2:254:LEU:HD23	13:2:254:LEU:H	1.83	0.42
13:2:262:ILE:HD11	18:2:2003:CLA:C4	2.41	0.42
16:3:138:GLN:CB	16:3:145:ALA:CB	2.82	0.42
27:3:3501:LUT:H8	27:3:3501:LUT:C17	2.46	0.42
27:3:3502:LUT:H201	27:3:3502:LUT:H15	1.92	0.42
18:4:4001:CLA:HHD	28:4:4011:CHL:O1A	2.18	0.42
18:A:1112:CLA:C2	18:A:1114:CLA:HMB2	2.49	0.42
18:B:1203:CLA:OBD	18:B:1201:CLA:HMC3	2.19	0.42
18:B:1224:CLA:HBA2	18:B:1224:CLA:H3A	1.75	0.42
2:B:464:GLN:NE2	18:B:1234:CLA:HMD1	2.34	0.42
20:B:5002:PQN:H243	20:B:5002:PQN:H262	1.72	0.42
2:B:22:TRP:HZ3	20:B:5002:PQN:H302	1.84	0.42
9:D:163:GLU:CD	9:D:164:VAL:N	2.72	0.42
10:E:66:ILE:CG2	10:E:95:GLN:NE2	2.72	0.42
6:G:121:LEU:CD2	6:G:121:LEU:C	2.84	0.42
6:G:141:THR:OG1	23:G:2021:LMG:HC91	2.18	0.42
3:I:7:LEU:HG	11:H:115:SER:HB2	2.00	0.42
4:J:16:THR:HG21	22:J:6013:BCR:H403	1.97	0.42
22:L:6020:BCR:H371	22:L:6020:BCR:H24C	1.79	0.42
18:1:1001:CLA:HHC	27:1:1501:LUT:C32	2.38	0.42
13:2:123:PRO:CA	13:2:126:LEU:HG	2.49	0.42
13:2:238:GLN:HE21	18:2:2003:CLA:CHA	2.31	0.42
16:3:128:ILE:HG22	16:3:132:THR:HA	2.01	0.42
18:3:3002:CLA:HMD1	18:3:3007:CLA:HBA2	1.99	0.42
14:4:136:ALA:HB1	14:4:140:THR:CG2	2.46	0.42
18:4:4017:CLA:HED1	21:1:1801:LHG:C15	2.37	0.42
14:4:57:LEU:HD12	14:4:57:LEU:HA	1.72	0.42
1:A:302:HIS:HB2	18:A:1116:CLA:C1B	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1121:CLA:H61	18:A:1121:CLA:H41	1.59	0.42
18:A:1126:CLA:H192	22:J:6012:BCR:H14C	2.01	0.42
1:A:455:PHE:HB3	18:A:1132:CLA:HBB2	2.01	0.42
1:A:205:HIS:HB3	18:A:1111:CLA:HBB1	2.01	0.42
1:A:580:PRO:HB3	1:A:727:ILE:HB	2.01	0.42
18:B:1208:CLA:H41	18:B:1208:CLA:H62	1.56	0.42
18:B:1227:CLA:H121	18:B:1227:CLA:H162	1.78	0.42
2:B:302:LYS:O	2:B:306:GLU:HG2	2.19	0.42
2:B:366:THR:HG1	2:B:733:PHE:HE1	1.67	0.42
2:B:658:ALA:O	2:B:661:PHE:HB2	2.19	0.42
8:C:30:PRO:HD3	9:D:179:ASN:O	2.18	0.42
22:F:6014:BCR:H403	22:F:6014:BCR:C23	2.48	0.42
6:G:116:LYS:CG	18:G:1002:CLA:ND	2.76	0.42
11:H:56:ASP:HB2	11:H:59:ASP:OD1	2.18	0.42
4:J:11:ALA:HB1	4:J:12:PRO:HD2	2.01	0.42
12:K:124:ALA:CB	22:K:2011:BCR:C33	2.92	0.42
7:L:130:GLY:C	7:L:132:LEU:N	2.72	0.42
7:L:176:LEU:CD1	7:L:177:GLN:HG2	2.49	0.42
15:1:183:LYS:HZ3	18:1:1002:CLA:HBD	1.82	0.42
13:2:118:ALA:HB2	18:2:2006:CLA:HMC3	2.01	0.42
16:3:240:GLY:HA2	18:3:3003:CLA:C3C	2.49	0.42
16:3:81:LEU:HA	16:3:81:LEU:HD23	1.75	0.42
14:4:153:GLU:CG	14:4:156:ARG:NH1	2.82	0.42
18:4:4004:CLA:CBB	27:4:4502:LUT:C32	2.97	0.42
18:4:4007:CLA:H91	18:4:4007:CLA:H112	1.74	0.42
29:4:4505:ZEX:C24	29:4:4505:ZEX:H362	2.49	0.42
29:4:4505:ZEX:H201	29:4:4505:ZEX:H15	1.81	0.42
18:B:1204:CLA:H42	3:I:8:PHE:HE2	1.84	0.42
2:B:590:VAL:HG22	18:B:1234:CLA:HAB	2.01	0.42
2:B:594:TRP:HB2	18:B:1234:CLA:HMC1	2.02	0.42
18:B:1239:CLA:HED1	18:B:1226:CLA:H102	2.01	0.42
18:A:1013:CLA:HED2	2:B:532:LEU:HD21	2.01	0.42
8:C:9:ASP:OD1	9:D:191:SER:N	2.52	0.42
6:G:76:ARG:CD	6:G:116:LYS:NZ	2.82	0.42
12:K:71:VAL:HG12	12:K:129:GLY:C	2.40	0.42
7:L:94:ASN:O	7:L:98:ARG:HG3	2.19	0.42
15:1:130:THR:CG2	15:1:132:PRO:CD	2.85	0.42
13:2:188:LEU:C	13:2:188:LEU:CD2	2.84	0.42
13:2:222:ILE:H	13:2:222:ILE:CD1	2.32	0.42
16:3:120:GLU:CD	16:3:253:TYR:CB	2.81	0.42
16:3:218:LYS:O	16:3:221:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:268:VAL:HG22	18:3:3003:CLA:CAD	2.49	0.42
16:3:169:GLU:HB3	18:3:3012:CLA:C1B	2.50	0.42
1:A:398:HIS:O	1:A:402:ILE:HG12	2.19	0.42
1:A:740:LEU:HD11	22:A:6011:BCR:HC8	2.02	0.42
18:B:1220:CLA:H51	18:B:1220:CLA:H11	1.86	0.42
2:B:199:ILE:HB	2:B:200:PRO:HD3	2.00	0.42
2:B:221:GLY:O	26:B:8002:LMU:H6D	2.19	0.42
9:D:192:ILE:HB	9:D:194:LYS:HG3	2.02	0.42
10:E:75:LYS:HB2	10:E:128:VAL:HG21	2.02	0.42
5:F:157:TRP:CZ2	18:F:1302:CLA:O1A	2.72	0.42
18:G:1003:CLA:C3	23:G:2021:LMG:H332	2.49	0.42
4:J:2:ARG:C	4:J:4:LEU:N	2.71	0.42
7:L:174:ASP:O	7:L:175:GLN:HB2	2.19	0.42
22:L:6019:BCR:C39	22:L:6019:BCR:C27	2.90	0.42
15:1:58:ASP:HB2	18:1:1004:CLA:CED	2.48	0.42
18:1:1003:CLA:H12	18:1:1008:CLA:C2D	2.49	0.42
15:1:131:LEU:CD2	15:1:131:LEU:N	2.72	0.42
27:1:1502:LUT:H35	27:1:1502:LUT:H401	1.80	0.42
27:4:4502:LUT:H162	27:4:4502:LUT:H3	1.84	0.42
10:E:105:VAL:HG12	10:E:106:ARG:N	2.35	0.42
7:L:53:THR:O	7:L:53:THR:HG22	2.19	0.42
13:2:228:ALA:O	13:2:231:ALA:HB3	2.20	0.42
18:2:2001:CLA:H12	27:2:2501:LUT:H173	1.98	0.42
14:4:103:MET:HB2	18:4:4001:CLA:HMC3	2.01	0.42
14:4:108:GLY:HA2	18:4:4006:CLA:C2C	2.50	0.42
14:4:222:HIS:C	14:4:222:HIS:HD1	2.23	0.42
18:A:1102:CLA:HBA1	18:A:1102:CLA:H3A	1.66	0.42
18:A:1106:CLA:H93	18:A:1106:CLA:H61	1.76	0.42
22:A:6002:BCR:C33	18:A:1112:CLA:HNB	2.48	0.42
1:A:340:GLY:HA2	7:L:55:GLN:OE1	2.20	0.42
1:A:364:MET:HE3	18:A:1119:CLA:H93	2.02	0.42
18:B:1202:CLA:H112	18:B:1202:CLA:H142	1.80	0.42
18:B:1202:CLA:H122	18:B:1202:CLA:HBD	2.02	0.42
18:B:1208:CLA:C4D	26:B:8001:LMU:H32	2.50	0.42
18:B:1216:CLA:H91	18:B:1216:CLA:H111	1.64	0.42
2:B:136:TYR:O	2:B:140:ILE:HG12	2.19	0.42
8:C:8:TYR:C	8:C:10:THR:N	2.72	0.42
5:F:85:CYS:SG	5:F:138:LEU:O	2.78	0.42
7:L:96:LEU:HB2	7:L:184:LYS:HB3	2.01	0.42
15:1:121:TYR:CE1	18:1:1006:CLA:H2	2.53	0.42
15:1:66:LEU:HD12	27:1:1502:LUT:H41	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2008:CLA:O2A	16:3:160:LEU:HD13	2.20	0.42
13:2:211:PRO:O	13:2:212:GLN:HB2	2.19	0.42
16:3:111:LEU:HD21	18:3:3006:CLA:CBB	2.39	0.42
18:A:1112:CLA:H112	18:A:1112:CLA:H91	1.82	0.42
18:A:1135:CLA:O1A	18:A:1136:CLA:HBD	2.20	0.42
1:A:205:HIS:CG	18:A:1111:CLA:HMC2	2.54	0.42
1:A:232:PHE:HD1	1:A:237:VAL:HG11	1.85	0.42
1:A:440:ASP:HB2	9:D:88:THR:CG2	2.43	0.42
21:A:7001:LHG:H202	18:A:1128:CLA:H13	2.02	0.42
2:B:395:ILE:HD11	2:B:541:ALA:HB1	2.00	0.42
8:C:8:TYR:HB3	9:D:191:SER:CA	2.47	0.42
9:D:77:PRO:CD	9:D:77:PRO:O	2.68	0.42
18:B:1207:CLA:C3B	3:I:14:LEU:HD21	2.50	0.42
15:1:119:ALA:O	15:1:120:THR:HG23	2.19	0.42
15:1:229:ASN:O	15:1:229:ASN:ND2	2.53	0.42
13:2:133:LEU:C	13:2:135:PRO:HD2	2.39	0.42
13:2:186:ASN:ND2	18:2:2016:CLA:H2A	2.35	0.42
13:2:233:MET:CA	13:2:233:MET:HE3	2.50	0.42
27:3:3501:LUT:H401	27:3:3501:LUT:H35	1.80	0.42
14:4:223:ASN:OD1	14:4:223:ASN:N	2.53	0.42
18:4:4006:CLA:NB	27:4:4503:LUT:C17	2.80	0.42
18:4:4002:CLA:C1D	18:4:4007:CLA:H71	2.50	0.42
18:A:1112:CLA:H162	18:A:1112:CLA:H141	1.70	0.42
1:A:191:PRO:HB2	1:A:196:PHE:CE2	2.54	0.42
1:A:34:TRP:HE1	18:A:1109:CLA:CHB	2.33	0.42
18:B:1207:CLA:H41	7:L:133:ALA:HB2	2.01	0.42
8:C:10:THR:CG2	8:C:64:SER:CB	2.97	0.42
5:F:173:TRP:CD1	5:F:210:GLY:HA3	2.55	0.42
15:1:200:VAL:HG21	18:1:1003:CLA:HAC1	2.02	0.42
15:1:205:TYR:CE2	18:1:1003:CLA:O1D	2.70	0.42
18:1:1011:CLA:C3	27:1:1501:LUT:C23	2.86	0.42
15:1:51:LEU:CD1	15:1:60:GLY:HA2	2.50	0.42
16:3:162:MET:HE2	16:3:162:MET:HA	1.98	0.42
16:3:102:GLU:OE2	16:3:232:ARG:HD3	2.20	0.42
16:3:102:GLU:CD	16:3:232:ARG:HH21	2.23	0.42
14:4:156:ARG:O	14:4:160:ILE:HG13	2.20	0.42
18:A:1106:CLA:H3A	18:A:1106:CLA:HBA2	1.48	0.42
18:A:1109:CLA:HHC	18:A:1109:CLA:HBB1	2.01	0.42
18:A:1110:CLA:HBC2	18:A:1111:CLA:HAB	2.00	0.42
18:B:1215:CLA:H3A	18:B:1215:CLA:HBA2	1.76	0.42
6:G:83:GLN:O	6:G:87:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:7:LEU:HA	3:I:7:LEU:HD13	1.65	0.42
12:K:79:PHE:CD2	12:K:121:ASP:OD2	2.73	0.42
18:A:1130:CLA:H11	7:L:83:LEU:HD11	2.01	0.42
15:1:83:HIS:ND1	18:1:1012:CLA:HMD1	2.34	0.42
15:1:158:LYS:C	15:1:160:TYR:H	2.22	0.42
15:1:166:ASP:O	15:1:169:GLY:N	2.52	0.42
13:2:197:GLY:N	18:2:2001:CLA:HED2	2.35	0.42
13:2:207:GLY:CA	18:2:2001:CLA:HAA2	2.49	0.42
13:2:254:LEU:N	13:2:254:LEU:CD2	2.73	0.42
13:2:64:ARG:HE	13:2:79:GLY:HA3	1.85	0.42
16:3:122:LEU:C	16:3:124:LYS:N	2.73	0.42
16:3:119:PRO:HB3	16:3:133:ALA:HB2	1.95	0.42
16:3:206:PRO:HD2	16:3:207:PHE:CA	2.49	0.42
16:3:222:GLU:O	16:3:222:GLU:HG2	2.20	0.42
16:3:231:GLY:O	16:3:235:MET:CG	2.68	0.42
16:3:110:MET:HB3	18:3:3001:CLA:HMC3	2.02	0.42
14:4:167:ASN:CG	14:4:168:GLN:N	2.72	0.42
14:4:95:GLU:HG3	18:4:4004:CLA:C1B	2.50	0.42
17:A:1011:CL0:H53	17:A:1011:CL0:H61	1.83	0.42
18:A:1106:CLA:H42	18:A:1126:CLA:HMD2	2.02	0.42
1:A:112:ASP:OD2	1:A:115:HIS:HB3	2.19	0.42
18:B:1226:CLA:H143	18:B:1226:CLA:H111	1.85	0.42
2:B:129:LEU:HD13	2:B:135:LEU:HD23	2.01	0.42
2:B:6:PRO:HD2	2:B:12:ILE:HG23	2.01	0.42
9:D:190:ARG:HG3	9:D:190:ARG:H	1.62	0.42
1:A:437:ARG:HG2	9:D:87:SER:HB2	2.02	0.42
10:E:92:THR:OG1	10:E:93:VAL:N	2.53	0.42
6:G:64:ILE:HD12	18:G:1001:CLA:C2D	2.50	0.42
4:J:28:GLU:HG3	18:J:1302:CLA:C1D	2.49	0.42
1:A:315:HIS:NE2	22:K:2011:BCR:H352	2.34	0.42
18:1:1005:CLA:H43	18:1:1005:CLA:HED1	2.02	0.41
15:1:130:THR:CG2	15:1:131:LEU:H	2.32	0.41
15:1:112:ALA:O	15:1:131:LEU:HD11	2.20	0.41
15:1:229:ASN:C	15:1:229:ASN:ND2	2.72	0.41
16:3:142:ILE:HA	16:3:147:THR:HG23	2.02	0.41
16:3:151:TRP:CE3	16:3:152:ALA:HB2	2.55	0.41
16:3:188:LEU:HA	16:3:188:LEU:HD22	1.88	0.41
16:3:205:GLY:O	16:3:209:ASN:CB	2.68	0.41
14:4:105:GLY:C	14:4:109:MET:HE2	2.40	0.41
14:4:136:ALA:HB2	15:1:222:TRP:HB3	2.01	0.41
14:4:73:ASP:HA	18:4:4004:CLA:O1D	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD11	18:A:1119:CLA:C3B	2.49	0.41
1:A:266:ALA:O	1:A:269:PHE:HB3	2.19	0.41
1:A:470:LEU:HG	18:B:1206:CLA:HMC3	2.02	0.41
1:A:650:ASN:HB2	2:B:651:LEU:HD11	2.02	0.41
2:B:115:ILE:O	18:B:1205:CLA:HMD3	2.21	0.41
22:A:6011:BCR:H402	18:B:1229:CLA:HMB3	2.02	0.41
2:B:487:ASN:HA	2:B:490:ARG:HB2	2.01	0.41
15:1:170:TYR:CE2	27:1:1501:LUT:C37	3.03	0.41
15:1:200:VAL:HG21	18:1:1003:CLA:CAC	2.50	0.41
16:3:110:MET:CE	16:3:230:ASN:C	2.89	0.41
16:3:258:ASP:C	16:3:266:ASN:ND2	2.73	0.41
16:3:93:ILE:HG23	16:3:93:ILE:O	2.21	0.41
14:4:113:GLU:OE2	14:4:230:PHE:HB3	2.20	0.41
14:4:241:TRP:CE2	18:4:4008:CLA:HMA1	2.54	0.41
18:4:4004:CLA:HHC	27:4:4502:LUT:H32	2.02	0.41
13:2:182:ILE:HD12	18:4:4007:CLA:HAB	1.97	0.41
27:4:4501:LUT:H201	27:4:4501:LUT:H15	1.88	0.41
1:A:694:PHE:HB2	18:A:1013:CLA:HBC2	2.02	0.41
1:A:163:GLN:CD	18:A:1112:CLA:HED1	2.40	0.41
1:A:29:THR:HG23	1:A:187:HIS:HD2	1.84	0.41
18:B:1201:CLA:HBA2	18:B:1201:CLA:H3A	1.38	0.41
2:B:411:MET:HE3	18:B:1227:CLA:HMD3	2.01	0.41
2:B:569:ASP:HA	2:B:574:ASP:OD2	2.20	0.41
2:B:519:VAL:HG11	2:B:593:TYR:HB2	2.03	0.41
2:B:73:ASN:HD22	2:B:74:PHE:N	2.07	0.41
8:C:14:CYS:O	8:C:15:THR:CB	2.69	0.41
8:C:60:THR:HG1	8:C:64:SER:HG	1.55	0.41
6:G:100:HIS:O	6:G:101:PHE:CB	2.67	0.41
22:J:6012:BCR:H371	22:J:6012:BCR:H24C	1.75	0.41
18:1:1004:CLA:HAA1	18:1:1004:CLA:HBD	2.01	0.41
15:1:158:LYS:C	15:1:160:TYR:N	2.73	0.41
15:1:167:PRO:C	15:1:169:GLY:N	2.72	0.41
15:1:197:GLY:O	15:1:201:GLN:HB2	2.20	0.41
13:2:115:LEU:HD21	18:2:2001:CLA:HBC3	2.02	0.41
16:3:116:ALA:HA	16:3:136:TRP:HB3	2.03	0.41
16:3:267:ASN:O	18:3:3003:CLA:HED2	2.21	0.41
18:4:4017:CLA:HMC2	29:4:4505:ZEX:C39	2.38	0.41
27:4:4502:LUT:H15	27:4:4502:LUT:H201	1.84	0.41
1:A:395:LEU:HD11	18:A:1127:CLA:HED3	2.02	0.41
1:A:687:ALA:C	18:A:1013:CLA:HAB	2.41	0.41
1:A:701:GLN:O	1:A:705:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1213:CLA:H41	18:B:1213:CLA:H61	1.95	0.41
2:B:697:PRO:HB3	18:B:1238:CLA:C2C	2.50	0.41
2:B:80:ASP:HB2	2:B:84:VAL:HG23	2.01	0.41
5:F:188:GLU:HG3	5:F:189:LYS:HG3	2.03	0.41
6:G:149:LYS:C	6:G:149:LYS:CE	2.85	0.41
6:G:65:SER:HA	18:G:1001:CLA:O2A	2.20	0.41
15:1:104:ASN:HB2	15:1:107:LYS:HB2	2.01	0.41
15:1:153:LYS:N	15:1:153:LYS:HD3	2.31	0.41
15:1:165:PHE:O	27:1:1501:LUT:O23	2.21	0.41
15:1:211:LEU:HD12	15:1:212:GLU:N	2.30	0.41
13:2:157:LEU:HD23	13:2:157:LEU:HA	1.84	0.41
18:2:2007:CLA:CMC	18:2:2007:CLA:HBC2	2.42	0.41
13:2:221:GLU:HB3	13:2:222:ILE:HD12	2.02	0.41
27:2:2501:LUT:H201	27:2:2501:LUT:H15	1.74	0.41
16:3:121:TYR:HA	16:3:253:TYR:HD2	1.84	0.41
16:3:129:PRO:O	16:3:132:THR:CB	2.69	0.41
16:3:93:ILE:HA	16:3:93:ILE:HD12	1.85	0.41
14:4:135:PHE:O	14:4:136:ALA:CB	2.68	0.41
18:4:4012:CLA:HHB	18:4:4017:CLA:HBC2	2.01	0.41
18:A:1126:CLA:H162	18:A:1126:CLA:H143	1.68	0.41
1:A:201:SER:O	1:A:205:HIS:HD2	2.03	0.41
1:A:209:GLY:HA3	18:A:1111:CLA:CBB	2.50	0.41
22:A:6002:BCR:H342	18:A:1112:CLA:CHB	2.51	0.41
18:B:1222:CLA:H3A	18:B:1222:CLA:HBA2	1.61	0.41
22:B:6004:BCR:H24C	22:B:6004:BCR:H371	1.82	0.41
2:B:5:LEU:HA	2:B:6:PRO:HA	1.80	0.41
6:G:116:LYS:HB2	18:G:1002:CLA:CHA	2.50	0.41
3:I:4:LEU:HD12	3:I:6:SER:N	2.26	0.41
15:1:58:ASP:OD1	18:1:1004:CLA:HED2	2.19	0.41
18:1:1004:CLA:HHD	28:1:1009:CHL:HBB2	2.02	0.41
15:1:79:SER:OG	18:1:1012:CLA:OBD	2.33	0.41
15:1:226:ILE:O	15:1:229:ASN:HB3	2.20	0.41
15:1:85:ARG:CG	15:1:85:ARG:NH1	2.72	0.41
13:2:125:PHE:O	13:2:129:LEU:N	2.53	0.41
13:2:135:PRO:HG2	18:2:2006:CLA:HED3	2.01	0.41
28:2:2010:CHL:HMB1	28:2:2010:CHL:HAB	1.95	0.41
13:2:242:THR:CG2	13:2:242:THR:O	2.68	0.41
16:3:161:GLU:OE2	18:3:3010:CLA:HAB	2.20	0.41
16:3:102:GLU:CD	16:3:232:ARG:NH2	2.72	0.41
16:3:258:ASP:CB	16:3:266:ASN:ND2	2.73	0.41
14:4:111:LEU:HD12	18:4:4006:CLA:HBC1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:182:ILE:HD13	18:4:4007:CLA:HAB	1.98	0.41
21:A:7001:LHG:H161	18:A:1101:CLA:HMB2	2.02	0.41
18:B:1240:CLA:HMC3	18:1:1005:CLA:H11	2.02	0.41
9:D:107:SER:OG	9:D:109:LYS:O	2.36	0.41
11:H:125:ILE:O	11:H:127:LYS:N	2.54	0.41
23:J:5001:LMG:H453	23:J:5001:LMG:H422	1.81	0.41
15:1:85:ARG:HE	18:1:1001:CLA:CHD	2.33	0.41
18:1:1005:CLA:H3A	18:1:1005:CLA:HBA1	1.76	0.41
13:2:167:ARG:O	13:2:171:ILE:HG12	2.21	0.41
13:2:186:ASN:CG	18:2:2016:CLA:C2A	2.89	0.41
13:2:188:LEU:HD21	13:2:197:GLY:O	2.20	0.41
16:3:209:ASN:OD1	27:3:3501:LUT:C24	2.69	0.41
16:3:212:GLY:O	16:3:215:LYS:CB	2.68	0.41
16:3:223:LEU:HA	16:3:226:LYS:HG3	1.99	0.41
16:3:227:GLU:N	18:3:3001:CLA:HMB3	2.35	0.41
18:3:3005:CLA:O1D	18:3:3012:CLA:H2	2.21	0.41
16:3:80:PRO:HD2	27:3:3502:LUT:H24	2.02	0.41
18:4:4005:CLA:ND	18:4:4012:CLA:H112	2.36	0.41
14:4:98:ASN:CG	18:4:4012:CLA:HMD1	2.41	0.41
18:4:4001:CLA:H71	27:4:4501:LUT:C30	2.51	0.41
14:4:70:LEU:HD23	14:4:70:LEU:HA	1.85	0.41
18:A:1237:CLA:H62	18:B:1238:CLA:H43	2.01	0.41
1:A:127:VAL:HG22	18:B:1230:CLA:OBD	2.21	0.41
18:B:1221:CLA:CBA	18:B:1202:CLA:H8	2.51	0.41
18:B:1211:CLA:CBB	18:B:1225:CLA:H162	2.51	0.41
18:B:1235:CLA:H111	18:B:1235:CLA:H91	1.88	0.41
2:B:158:GLN:HA	2:B:159:PRO:HD3	1.92	0.41
2:B:507:SER:HA	2:B:510:LEU:HD21	2.02	0.41
9:D:204:THR:C	9:D:206:LYS:N	2.72	0.41
7:L:176:LEU:CD1	7:L:177:GLN:N	2.71	0.41
18:1:1011:CLA:CMB	18:1:1011:CLA:HBB1	2.45	0.41
15:1:118:GLN:O	15:1:119:ALA:CB	2.69	0.41
13:2:195:TYR:C	18:2:2001:CLA:HED3	2.41	0.41
13:2:219:THR:HG22	18:2:2007:CLA:HED1	1.99	0.41
13:2:254:LEU:O	13:2:257:PRO:HD3	2.21	0.41
18:3:3003:CLA:O2A	18:3:3003:CLA:CHA	2.69	0.41
14:4:111:LEU:HD12	18:4:4006:CLA:CBC	2.49	0.41
18:A:1116:CLA:NB	18:A:1116:CLA:H43	2.36	0.41
18:A:1117:CLA:H3A	18:A:1117:CLA:HBA2	1.65	0.41
2:B:12:ILE:HD11	2:B:23:PHE:CB	2.47	0.41
18:F:1302:CLA:HMB2	22:F:6016:BCR:C7	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:114:VAL:HG12	6:G:115:SER:N	2.36	0.41
7:L:120:LEU:O	7:L:124:GLU:CB	2.69	0.41
7:L:121:ARG:HG2	7:L:127:GLY:CA	2.48	0.41
7:L:121:ARG:HB3	7:L:122:ASN:H	1.66	0.41
7:L:175:GLN:HB3	7:L:176:LEU:H	1.70	0.41
7:L:91:THR:CA	7:L:98:ARG:HH21	2.32	0.41
18:1:1002:CLA:HHC	18:1:1002:CLA:CBB	2.50	0.41
18:1:1004:CLA:H112	18:1:1004:CLA:H91	1.77	0.41
23:G:2021:LMG:C6	15:1:115:PRO:HA	2.44	0.41
13:2:131:ILE:CD1	13:2:133:LEU:CD2	2.85	0.41
27:2:2502:LUT:C28	27:2:2502:LUT:C36	2.94	0.41
16:3:117:ILE:O	16:3:117:ILE:HG22	2.20	0.41
16:3:222:GLU:O	16:3:226:LYS:HD2	2.21	0.41
16:3:246:LEU:CD2	16:3:246:LEU:C	2.85	0.41
16:3:250:VAL:CG1	16:3:254:GLN:HG2	2.50	0.41
18:3:3007:CLA:HBC2	18:3:3007:CLA:CMC	2.49	0.41
16:3:141:VAL:HG23	18:3:3010:CLA:CAD	2.51	0.41
28:3:3011:CHL:HMB3	22:3:3503:BCR:C16	2.51	0.41
14:4:212:MET:HB2	18:4:4004:CLA:CMC	2.49	0.41
18:A:1112:CLA:HBA1	18:A:1112:CLA:H3A	1.77	0.41
18:A:1124:CLA:CHB	18:A:1137:CLA:HAA2	2.51	0.41
1:A:334:HIS:O	21:A:5003:LHG:O1	2.38	0.41
18:B:1204:CLA:H11	18:B:1204:CLA:H51	1.80	0.41
18:A:1107:CLA:HAB	18:B:1230:CLA:HMD2	2.02	0.41
9:D:77:PRO:O	9:D:77:PRO:HD2	2.20	0.41
10:E:103:VAL:O	10:E:105:VAL:HG23	2.21	0.41
10:E:97:PRO:C	10:E:99:THR:H	2.24	0.41
5:F:101:LYS:HB3	5:F:101:LYS:HE2	1.88	0.41
5:F:152:GLY:HA2	5:F:161:ILE:HD11	2.02	0.41
5:F:156:HIS:HB3	5:F:159:GLU:OE1	2.21	0.41
6:G:116:LYS:NZ	18:G:1002:CLA:NB	2.69	0.41
18:1:1012:CLA:HBA2	18:1:1012:CLA:H3A	1.76	0.41
15:1:146:GLU:HG2	15:1:149:ARG:HD3	2.02	0.41
15:1:158:LYS:O	15:1:159:LYS:CG	2.69	0.41
15:1:204:ALA:C	15:1:206:PRO:CD	2.87	0.41
15:1:215:ALA:O	15:1:218:LEU:N	2.54	0.41
13:2:153:PHE:CD1	28:2:2010:CHL:HAC2	2.55	0.41
16:3:134:LEU:HB2	16:3:138:GLN:CG	2.49	0.41
14:4:126:TRP:O	27:4:4502:LUT:O3	2.36	0.41
14:4:209:ARG:NH1	18:4:4004:CLA:C2D	2.83	0.41
18:A:1106:CLA:H193	18:A:1106:CLA:H162	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1111:CLA:H62	18:A:1111:CLA:H101	1.89	0.41
18:A:1112:CLA:H192	18:A:1112:CLA:H162	1.83	0.41
1:A:283:PHE:CZ	18:A:1116:CLA:H42	2.56	0.41
1:A:542:HIS:HB2	18:A:1136:CLA:HED2	2.03	0.41
1:A:549:ILE:O	1:A:553:VAL:HG23	2.21	0.41
18:B:1221:CLA:H112	18:B:1221:CLA:H142	1.69	0.41
2:B:189:ALA:O	18:B:1211:CLA:HMC3	2.21	0.41
2:B:268:LEU:HG	2:B:356:PRO:O	2.21	0.41
8:C:9:ASP:OD1	9:D:191:SER:CB	2.69	0.41
5:F:85:CYS:SG	5:F:139:LEU:O	2.78	0.41
2:B:292:ARG:NH2	6:G:107:ARG:NH1	2.69	0.41
18:1:1005:CLA:H12	18:1:1005:CLA:CED	2.43	0.41
16:3:228:VAL:O	16:3:232:ARG:HG2	2.20	0.41
18:3:3010:CLA:H61	18:3:3010:CLA:H41	1.74	0.41
18:3:3012:CLA:C1	18:3:3017:CLA:HBB2	2.50	0.41
18:3:3017:CLA:HHC	18:3:3017:CLA:CBB	2.50	0.41
16:3:83:LEU:HD23	16:3:83:LEU:HA	1.82	0.41
18:A:1116:CLA:H112	18:A:1116:CLA:H91	1.66	0.41
1:A:206:HIS:ND1	18:A:1123:CLA:OBD	2.49	0.41
18:A:1137:CLA:H61	18:A:1137:CLA:H41	1.83	0.41
18:B:1209:CLA:O1D	18:B:1210:CLA:HMC1	2.20	0.41
18:B:1218:CLA:H202	18:B:1218:CLA:H161	1.75	0.41
18:B:1221:CLA:H41	18:B:1221:CLA:H61	1.77	0.41
18:B:1223:CLA:H62	18:B:1223:CLA:H92	1.86	0.41
22:K:2011:BCR:H15C	22:K:2011:BCR:H351	1.82	0.41
7:L:173:PRO:CD	7:L:173:PRO:O	2.69	0.41
7:L:182:TRP:O	7:L:186:THR:HG23	2.21	0.41
7:L:104:LEU:O	22:L:6020:BCR:H14C	2.20	0.41
15:1:170:TYR:CE2	27:1:1501:LUT:H372	2.52	0.41
15:1:85:ARG:NH2	18:1:1001:CLA:C1D	2.83	0.41
13:2:125:PHE:HB2	13:2:133:LEU:HD21	2.03	0.41
18:3:3004:CLA:H2	27:3:3502:LUT:C36	2.49	0.41
18:3:3006:CLA:CHA	18:3:3018:CLA:HMB3	2.51	0.41
16:3:161:GLU:OE2	18:3:3010:CLA:CAB	2.69	0.41
18:4:4005:CLA:HMC2	27:4:4502:LUT:H12	2.01	0.41
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.83	0.41
1:A:266:ALA:HB1	1:A:270:PHE:CD1	2.56	0.41
1:A:307:ALA:O	1:A:311:LEU:HG	2.21	0.41
18:B:1023:CLA:H143	18:B:1023:CLA:H111	1.82	0.41
18:B:1236:CLA:HED2	18:B:1235:CLA:CMA	2.51	0.41
2:B:526:GLY:HA2	2:B:582:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:25:VAL:O	8:C:43:PRO:HD2	2.22	0.41
10:E:106:ARG:HA	10:E:116:SER:O	2.21	0.41
10:E:78:ARG:O	10:E:79:GLN:CB	2.69	0.41
18:G:1001:CLA:HBC2	18:G:1001:CLA:HMC1	2.02	0.41
11:H:111:LEU:HA	11:H:111:LEU:HD12	1.91	0.41
18:1:1006:CLA:O1A	18:1:1013:CLA:C2D	2.70	0.40
15:1:94:ILE:O	15:1:102:LEU:CD2	2.69	0.40
15:1:205:TYR:O	15:1:207:GLY:N	2.54	0.40
18:2:2005:CLA:CBC	18:2:2012:CLA:HBC2	2.51	0.40
13:2:204:LEU:HD12	13:2:206:TRP:CE2	2.56	0.40
13:2:250:LEU:O	13:2:254:LEU:HG	2.21	0.40
16:3:168:ALA:HB1	28:3:3011:CHL:C1B	2.51	0.40
16:3:248:THR:CG2	16:3:250:VAL:HG23	2.39	0.40
16:3:248:THR:CG2	16:3:255:ASN:ND2	2.73	0.40
18:3:3005:CLA:H61	18:3:3005:CLA:H41	1.80	0.40
18:3:3010:CLA:CB D	18:3:3010:CLA:HAA1	2.50	0.40
16:3:161:GLU:OE2	18:3:3010:CLA:HBB2	2.22	0.40
18:3:3012:CLA:CBA	18:3:3017:CLA:HBB2	2.51	0.40
14:4:212:MET:HB3	27:4:4502:LUT:C33	2.49	0.40
14:4:152:VAL:CG1	28:4:4011:CHL:NB	2.81	0.40
27:4:4501:LUT:H8	27:4:4501:LUT:C17	2.51	0.40
21:A:7001:LHG:H101	18:A:1128:CLA:H41	2.03	0.40
18:A:1139:CLA:H41	18:A:1139:CLA:H62	1.50	0.40
20:A:5001:PQN:H141	20:A:5001:PQN:H161	1.60	0.40
1:A:529:LEU:HD12	1:A:529:LEU:HA	1.86	0.40
1:A:451:ILE:HA	18:B:1023:CLA:CGA	2.51	0.40
18:B:1213:CLA:H51	18:B:1213:CLA:H11	1.71	0.40
18:B:1231:CLA:HBA2	18:B:1232:CLA:HMB3	2.03	0.40
2:B:477:LEU:C	2:B:479:SER:H	2.25	0.40
9:D:77:PRO:O	9:D:77:PRO:CG	2.69	0.40
5:F:160:PHE:C	5:F:163:PRO:HD2	2.41	0.40
22:F:6014:BCR:H15C	22:F:6014:BCR:H351	1.87	0.40
12:K:77:MET:SD	12:K:77:MET:O	2.79	0.40
7:L:203:LEU:CD1	7:L:203:LEU:N	2.84	0.40
7:L:207:LEU:O	7:L:208:ASP:CB	2.69	0.40
7:L:59:PRO:HD3	9:D:85:GLY:O	2.21	0.40
15:1:80:GLU:CD	15:1:189:ARG:HH21	2.23	0.40
13:2:149:THR:HG21	28:2:2010:CHL:CMD	2.52	0.40
18:2:2003:CLA:O2A	18:2:2003:CLA:C1A	2.70	0.40
21:2:2801:LHG:P	21:2:2801:LHG:O2	2.79	0.40
16:3:107:ARG:CZ	16:3:227:GLU:OE1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:4004:CLA:C3A	18:4:4004:CLA:CGA	2.99	0.40
18:4:4009:CLA:HBA2	18:4:4009:CLA:H3A	1.79	0.40
14:4:52:LYS:O	14:4:53:LYS:CB	2.69	0.40
18:A:1112:CLA:H2	18:A:1114:CLA:HMB2	2.02	0.40
18:A:1121:CLA:HAA1	12:K:83:PHE:CE2	2.56	0.40
2:B:330:ILE:HG22	18:B:1202:CLA:HHD	2.02	0.40
18:B:1216:CLA:C1D	18:B:1220:CLA:H43	2.50	0.40
2:B:387:PHE:HZ	18:B:1222:CLA:HAB	1.87	0.40
8:C:60:THR:CB	8:C:64:SER:HG	2.34	0.40
9:D:174:TYR:HB3	9:D:176:GLU:OE2	2.22	0.40
12:K:128:VAL:HG21	22:K:2011:BCR:C31	2.51	0.40
12:K:75:THR:O	12:K:78:LEU:HB2	2.21	0.40
18:L:1502:CLA:CHD	22:L:6019:BCR:H292	2.50	0.40
15:1:183:LYS:CE	18:1:1002:CLA:O1A	2.70	0.40
14:4:154:ILE:O	28:1:1009:CHL:CED	2.69	0.40
18:1:1013:CLA:HBA1	18:1:1013:CLA:H3A	1.80	0.40
15:1:85:ARG:CZ	15:1:184:GLU:OE1	2.70	0.40
13:2:102:ASN:OD1	18:2:2004:CLA:C1	2.70	0.40
13:2:147:THR:O	13:2:148:ASP:CB	2.69	0.40
16:3:227:GLU:HB2	18:3:3001:CLA:C2B	2.52	0.40
16:3:266:ASN:O	16:3:267:ASN:CB	2.69	0.40
16:3:272:LEU:HA	16:3:272:LEU:HD23	1.96	0.40
16:3:102:GLU:HB2	18:3:3004:CLA:C1B	2.51	0.40
16:3:114:VAL:HG12	18:3:3006:CLA:HAC1	2.02	0.40
14:4:153:GLU:OE1	18:4:4012:CLA:C4B	2.70	0.40
14:4:222:HIS:C	14:4:222:HIS:ND1	2.72	0.40
18:4:4002:CLA:OBD	18:4:4007:CLA:CGA	2.70	0.40
18:4:4009:CLA:CBB	18:4:4009:CLA:HHC	2.20	0.40
1:A:278:ALA:HA	18:A:1115:CLA:HMA2	2.02	0.40
1:A:343:HIS:CE1	1:A:431:LEU:HD11	2.55	0.40
18:B:1207:CLA:CAB	3:I:14:LEU:HD21	2.51	0.40
18:B:1210:CLA:H193	18:B:1210:CLA:H161	1.80	0.40
18:B:1215:CLA:H61	18:B:1215:CLA:H41	1.66	0.40
5:F:221:LEU:CB	5:F:222:LEU:HD23	2.50	0.40
11:H:95:LYS:O	11:H:96:ARG:CB	2.69	0.40
7:L:122:ASN:O	7:L:123:THR:OG1	2.35	0.40
15:1:218:LEU:HA	15:1:218:LEU:HD23	1.82	0.40
15:1:230:VAL:HG13	18:1:1014:CLA:C2B	2.48	0.40
15:1:40:ASP:OD1	15:1:40:ASP:N	2.54	0.40
15:1:66:LEU:HG	15:1:66:LEU:H	1.73	0.40
15:1:86:TRP:O	15:1:89:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:223:LYS:HB3	18:2:2007:CLA:HMD3	2.03	0.40
16:3:227:GLU:OE2	18:3:3001:CLA:C4A	2.69	0.40
29:4:4505:ZEX:H27	29:4:4505:ZEX:H391	1.75	0.40
18:A:1125:CLA:HBB1	18:A:1133:CLA:HAA2	2.04	0.40
1:A:537:ALA:O	1:A:541:VAL:HG23	2.21	0.40
22:B:6004:BCR:H402	18:B:1218:CLA:C1D	2.50	0.40
18:B:1239:CLA:H172	7:L:144:CYS:SG	2.62	0.40
12:K:123:LEU:O	12:K:127:THR:HG23	2.21	0.40
7:L:128:GLN:CB	7:L:204:LEU:CG	2.97	0.40
7:L:145:LEU:HB3	7:L:186:THR:HG22	2.04	0.40
18:1:1011:CLA:C2	27:1:1501:LUT:H23	2.47	0.40
15:1:203:SER:O	15:1:204:ALA:CB	2.69	0.40
15:1:204:ALA:O	15:1:206:PRO:CD	2.70	0.40
15:1:218:LEU:HD22	18:1:1008:CLA:CBB	2.51	0.40
13:2:182:ILE:CG2	13:2:183:PHE:CE1	3.05	0.40
18:2:2002:CLA:O2D	18:2:2002:CLA:CGA	2.69	0.40
28:2:2011:CHL:HMB1	28:2:2011:CHL:HAB	1.84	0.40
13:2:246:PRO:HG2	13:2:247:ILE:N	2.36	0.40
16:3:210:PRO:HD2	27:3:3501:LUT:O23	2.21	0.40
18:3:3008:CLA:C4A	18:3:3008:CLA:O1A	2.70	0.40
27:4:4501:LUT:H31	27:4:4501:LUT:H391	1.81	0.40
27:4:4502:LUT:H11	27:4:4502:LUT:H191	1.98	0.40
18:A:1136:CLA:H61	18:A:1136:CLA:H92	1.89	0.40
1:A:488:PHE:HB3	18:A:1135:CLA:H2	2.04	0.40
18:B:1021:CLA:H161	18:B:1021:CLA:H202	1.76	0.40
18:B:1206:CLA:CMA	18:B:1207:CLA:HBB1	2.52	0.40
2:B:558:PRO:HB3	2:B:702:ILE:HB	2.03	0.40
10:E:84:TYR:CD1	10:E:84:TYR:C	2.95	0.40
11:H:117:THR:OG1	11:H:118:ALA:N	2.54	0.40
4:J:26:LEU:HD23	4:J:26:LEU:HA	1.86	0.40
22:J:6012:BCR:H15C	22:J:6012:BCR:H351	1.70	0.40
7:L:122:ASN:O	7:L:123:THR:CB	2.69	0.40
7:L:162:PRO:O	7:L:162:PRO:CG	2.70	0.40

All (3) 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)
5:F:96:LYS:CD	7:L:170:LYS:NZ[3_555]	1.69	0.51
5:F:96:LYS:CE	7:L:170:LYS:NZ[3_555]	1.86	0.34
5:F:96:LYS:CG	7:L:170:LYS:NZ[3_555]	1.99	0.21

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	740/758 (98%)	691 (93%)	45 (6%)	4 (0%)	29	61
2	B	730/733 (100%)	695 (95%)	30 (4%)	5 (1%)	22	53
3	I	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	3	11
4	J	39/42 (93%)	34 (87%)	3 (8%)	2 (5%)	2	6
5	F	148/154 (96%)	138 (93%)	8 (5%)	2 (1%)	11	34
6	G	89/97 (92%)	76 (85%)	8 (9%)	5 (6%)	2	5
7	L	158/167 (95%)	133 (84%)	15 (10%)	10 (6%)	1	3
8	C	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
9	D	139/147 (95%)	116 (84%)	14 (10%)	9 (6%)	1	3
10	E	64/66 (97%)	57 (89%)	6 (9%)	1 (2%)	9	31
11	H	82/90 (91%)	65 (79%)	10 (12%)	7 (8%)	1	1
12	K	53/129 (41%)	49 (92%)	2 (4%)	2 (4%)	3	10
13	2	205/269 (76%)	184 (90%)	7 (3%)	14 (7%)	1	3
14	4	196/252 (78%)	174 (89%)	15 (8%)	7 (4%)	3	11
15	1	192/202 (95%)	168 (88%)	17 (9%)	7 (4%)	3	11
16	3	213/275 (78%)	189 (89%)	15 (7%)	9 (4%)	3	9
All	All	3153/3492 (90%)	2866 (91%)	202 (6%)	85 (3%)	5	17

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
3	I	6	SER
4	J	11	ALA
6	G	101	PHE
6	G	102	GLU
6	G	104	GLY

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Mol	Chain	Res	Type
7	L	67	GLY
7	L	125	ILE
7	L	152	SER
9	D	77	PRO
9	D	192	ILE
11	H	69	LEU
11	H	97	GLY
11	H	125	ILE
11	H	126	VAL
11	H	133	PRO
11	H	135	LEU
12	K	80	ALA
12	K	86	ALA
13	2	71	SER
13	2	131	ILE
13	2	176	CYS
13	2	178	ASN
13	2	188	LEU
13	2	193	VAL
13	2	212	GLN
14	4	154	ILE
15	1	43	PRO
15	1	155	PRO
16	3	129	PRO
16	3	206	PRO
16	3	250	VAL
16	3	267	ASN
2	B	74	PHE
5	F	112	ASP
7	L	208	ASP
9	D	205	GLY
10	E	102	PRO
13	2	148	ASP
14	4	179	ALA
15	1	219	ALA
16	3	144	PRO
1	A	198	ASP
1	A	581	CYS
2	B	559	CYS
6	G	107	ARG
6	G	148	PRO
7	L	61	ASN

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Mol	Chain	Res	Type
9	D	76	ASP
13	2	174	PRO
13	2	209	ALA
14	4	167	ASN
14	4	199	GLU
15	1	126	VAL
15	1	166	ASP
16	3	179	PRO
16	3	263	PRO
5	F	189	LYS
9	D	160	PRO
9	D	191	SER
9	D	206	LYS
13	2	185	ASN
14	4	170	PRO
14	4	178	PRO
16	3	188	LEU
7	L	158	PRO
7	L	176	LEU
9	D	159	PHE
13	2	165	GLY
16	3	120	GLU
7	L	172	GLN
14	4	127	TYR
15	1	205	TYR
7	L	162	PRO
13	2	203	PRO
2	B	257	ILE
2	B	639	VAL
7	L	56	VAL
15	1	196	VAL
2	B	492	ILE
4	J	10	VAL
13	2	173	ASN
1	A	26	PRO
9	D	172	GLY
11	H	132	PRO

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	603/619 (97%)	595 (99%)	8 (1%)	69	91
2	B	599/600 (100%)	587 (98%)	12 (2%)	55	84
3	I	25/26 (96%)	23 (92%)	2 (8%)	12	34
4	J	33/35 (94%)	29 (88%)	4 (12%)	5	15
5	F	123/127 (97%)	115 (94%)	8 (6%)	17	44
6	G	71/76 (93%)	65 (92%)	6 (8%)	10	31
7	L	124/133 (93%)	107 (86%)	17 (14%)	3	11
8	C	69/70 (99%)	65 (94%)	4 (6%)	20	50
9	D	120/125 (96%)	110 (92%)	10 (8%)	11	32
10	E	59/59 (100%)	57 (97%)	2 (3%)	37	71
11	H	69/74 (93%)	63 (91%)	6 (9%)	10	30
12	K	38/99 (38%)	32 (84%)	6 (16%)	2	8
13	2	166/216 (77%)	148 (89%)	18 (11%)	6	19
14	4	161/202 (80%)	145 (90%)	16 (10%)	8	23
15	1	158/167 (95%)	141 (89%)	17 (11%)	6	19
16	3	159/213 (75%)	135 (85%)	24 (15%)	3	9
All	All	2577/2841 (91%)	2417 (94%)	160 (6%)	18	47

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
1	A	187	HIS
1	A	204	ASN
1	A	207	LEU
1	A	339	THR
1	A	433	ASP
1	A	465	ASP
1	A	590	CYS
2	B	73	ASN
2	B	127	ILE
2	B	155	LEU
2	B	172	GLU

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Mol	Chain	Res	Type
2	B	176	ASN
2	B	220	GLN
2	B	226	LEU
2	B	444	LEU
2	B	552	ASP
2	B	568	CYS
2	B	583	MET
2	B	640	CYS
3	I	4	LEU
3	I	11	LEU
4	J	3	ASP
4	J	10	VAL
4	J	13	VAL
4	J	16	THR
5	F	82	LEU
5	F	106	LEU
5	F	108	ILE
5	F	113	SER
5	F	185	ILE
5	F	218	TYR
5	F	222	LEU
5	F	225	GLU
6	G	92	LEU
6	G	99	THR
6	G	111	TYR
6	G	123	ASP
6	G	141	THR
6	G	149	LYS
7	L	54	TYR
7	L	68	SER
7	L	121	ARG
7	L	123	THR
7	L	142	SER
7	L	146	THR
7	L	151	SER
7	L	162	PRO
7	L	163	SER
7	L	165	THR
7	L	169	ARG
7	L	172	GLN
7	L	174	ASP
7	L	176	LEU

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Mol	Chain	Res	Type
7	L	178	THR
7	L	180	ASP
7	L	204	LEU
8	C	14	CYS
8	C	26	LEU
8	C	38	GLN
8	C	48	CYS
9	D	77	PRO
9	D	79	THR
9	D	99	GLU
9	D	109	LYS
9	D	128	ASN
9	D	139	LEU
9	D	156	TYR
9	D	163	GLU
9	D	190	ARG
9	D	195	ASN
10	E	110	VAL
10	E	127	GLU
11	H	54	TYR
11	H	59	ASP
11	H	69	LEU
11	H	121	ASP
11	H	123	LEU
11	H	125	ILE
12	K	62	ILE
12	K	69	ILE
12	K	70	MET
12	K	79	PHE
12	K	88	SER
12	K	140	LEU
13	2	102	ASN
13	2	110	SER
13	2	133	LEU
13	2	134	THR
13	2	138	TYR
13	2	145	TYR
13	2	146	PHE
13	2	148	ASP
13	2	164	GLU
13	2	173	ASN
13	2	176	CYS

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Mol	Chain	Res	Type
13	2	178	ASN
13	2	188	LEU
13	2	189	THR
13	2	233	MET
13	2	238	GLN
13	2	250	LEU
13	2	254	LEU
14	4	74	ASN
14	4	103	MET
14	4	116	THR
14	4	135	PHE
14	4	140	THR
14	4	156	ARG
14	4	162	ASN
14	4	168	GLN
14	4	169	ASP
14	4	172	PHE
14	4	174	GLN
14	4	193	ASN
14	4	221	GLN
14	4	222	HIS
14	4	225	THR
14	4	234	LEU
15	1	40	ASP
15	1	43	PRO
15	1	85	ARG
15	1	88	MET
15	1	105	TRP
15	1	124	ASN
15	1	126	VAL
15	1	128	TRP
15	1	131	LEU
15	1	135	LEU
15	1	155	PRO
15	1	159	LYS
15	1	202	GLN
15	1	206	PRO
15	1	211	LEU
15	1	214	LEU
15	1	225	ASN
16	3	68	LEU
16	3	87	GLU

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Mol	Chain	Res	Type
16	3	93	ILE
16	3	100	TYR
16	3	131	GLU
16	3	132	THR
16	3	138	GLN
16	3	148	TYR
16	3	149	ASN
16	3	188	LEU
16	3	190	LEU
16	3	206	PRO
16	3	211	LEU
16	3	220	LEU
16	3	225	LEU
16	3	226	LYS
16	3	232	ARG
16	3	235	MET
16	3	236	LEU
16	3	238	ILE
16	3	244	GLN
16	3	250	VAL
16	3	253	TYR
16	3	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	A	204	ASN
1	A	205	HIS
1	A	222	GLN
1	A	224	HIS
1	A	234	ASN
1	A	303	HIS
1	A	325	HIS
1	A	485	GLN
1	A	615	HIS
1	A	629	ASN
1	A	631	GLN
2	B	14	GLN
2	B	44	GLN
2	B	73	ASN
2	B	95	HIS

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Mol	Chain	Res	Type
2	B	176	ASN
2	B	276	HIS
2	B	294	ASN
2	B	368	GLN
2	B	627	ASN
5	F	132	ASN
5	F	136	GLN
6	G	59	ASN
6	G	95	GLN
6	G	132	HIS
6	G	144	ASN
7	L	122	ASN
8	C	71	HIS
9	D	78	ASN
9	D	96	GLN
9	D	137	GLN
9	D	195	ASN
10	E	111	ASN
11	H	82	GLN
12	K	130	HIS
13	2	104	GLN
13	2	109	HIS
13	2	178	ASN
13	2	238	GLN
13	2	259	HIS
14	4	98	ASN
14	4	158	GLN
14	4	162	ASN
14	4	174	GLN
14	4	242	HIS
15	1	83	HIS
15	1	148	GLN
15	1	187	ASN
15	1	201	GLN
15	1	225	ASN
15	1	229	ASN
16	3	105	ASN
16	3	154	ASN
16	3	174	GLN
16	3	185	GLN
16	3	255	ASN
16	3	265	ASN

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Mol	Chain	Res	Type
16	3	266	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 209 ligands modelled in this entry, 1 is monoatomic - leaving 208 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$
21	LHG	B	5004	18	20,20,48	1.34	2 (10%)	23,26,54	1.53	3 (13%)
21	LHG	1	1801	18	48,48,48	0.91	2 (4%)	51,54,54	1.20	5 (9%)
18	CLA	A	1132	-	59,73,73	2.35	16 (27%)	67,113,113	2.11	17 (25%)
18	CLA	B	1220	-	59,73,73	2.34	16 (27%)	67,113,113	2.01	16 (23%)
18	CLA	B	1201	-	44,58,73	2.71	16 (36%)	49,95,113	2.42	17 (34%)
22	BCR	I	6020	-	41,41,41	2.77	7 (17%)	56,56,56	6.64	20 (35%)
22	BCR	A	6003	-	41,41,41	2.79	6 (14%)	56,56,56	6.48	20 (35%)
18	CLA	4	4001	14	54,68,73	2.20	15 (27%)	61,107,113	2.44	19 (31%)
18	CLA	1	1005	-	49,63,73	2.29	15 (30%)	55,101,113	2.50	19 (34%)
18	CLA	3	3004	16	54,68,73	2.24	16 (29%)	61,107,113	2.37	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	1222	-	59,73,73	2.33	15 (25%)	67,113,113	2.20	18 (26%)
18	CLA	B	1240	21	59,73,73	2.33	15 (25%)	67,113,113	2.13	18 (26%)
19	SF4	C	3003	8	0,12,12	0.00	-	-		
18	CLA	B	1225	-	59,73,73	2.35	16 (27%)	67,113,113	2.15	15 (22%)
18	CLA	1	1003	15	49,63,73	2.35	17 (34%)	55,101,113	2.49	21 (38%)
18	CLA	4	4009	14	44,58,73	2.39	15 (34%)	49,95,113	2.51	14 (28%)
18	CLA	A	1013	-	59,73,73	2.33	16 (27%)	67,113,113	2.14	17 (25%)
18	CLA	J	1302	4	44,58,73	2.74	16 (36%)	49,95,113	2.60	17 (34%)
18	CLA	B	1211	-	59,73,73	2.31	15 (25%)	67,113,113	2.24	19 (28%)
18	CLA	A	1126	-	59,73,73	2.35	16 (27%)	67,113,113	2.17	16 (23%)
18	CLA	A	1111	-	54,68,73	2.44	15 (27%)	61,107,113	2.21	17 (27%)
28	CHL	4	4011	-	45,59,74	1.64	9 (20%)	46,96,114	1.47	10 (21%)
22	BCR	B	6004	-	41,41,41	2.78	6 (14%)	56,56,56	6.67	29 (51%)
18	CLA	1	1013	-	40,54,73	2.70	16 (40%)	44,90,113	2.68	12 (27%)
18	CLA	A	1114	-	40,54,73	2.91	15 (37%)	44,90,113	2.36	13 (29%)
18	CLA	2	2001	13	54,68,73	2.20	16 (29%)	61,107,113	2.57	21 (34%)
18	CLA	A	1237	-	54,68,73	2.43	15 (27%)	61,107,113	2.34	17 (27%)
18	CLA	A	1121	-	49,63,73	2.57	16 (32%)	55,101,113	2.43	17 (30%)
18	CLA	2	2004	13	59,73,73	2.26	14 (23%)	67,113,113	2.18	16 (23%)
26	LMU	B	8001	-	36,36,36	0.49	0	47,47,47	1.18	5 (10%)
18	CLA	3	3008	-	42,56,73	2.52	14 (33%)	46,92,113	3.21	19 (41%)
18	CLA	G	1003	-	54,68,73	2.28	15 (27%)	61,107,113	2.32	19 (31%)
27	LUT	2	2502	-	42,43,43	2.47	3 (7%)	51,60,60	2.10	16 (31%)
27	LUT	2	2501	-	42,43,43	2.43	1 (2%)	51,60,60	2.11	14 (27%)
18	CLA	3	3002	-	40,54,73	2.60	16 (40%)	44,90,113	2.58	18 (40%)
19	SF4	C	3002	8	0,12,12	0.00	-	-		
18	CLA	3	3013	-	40,54,73	2.74	16 (40%)	44,90,113	2.24	14 (31%)
18	CLA	2	2009	13	44,58,73	2.50	16 (36%)	49,95,113	2.53	16 (32%)
18	CLA	2	2008	-	44,58,73	2.37	15 (34%)	49,95,113	2.96	23 (46%)
18	CLA	B	1228	-	54,68,73	2.46	15 (27%)	61,107,113	2.17	15 (24%)
22	BCR	B	6006	-	41,41,41	2.79	6 (14%)	56,56,56	6.86	28 (50%)
18	CLA	A	1112	-	59,73,73	2.32	16 (27%)	67,113,113	2.14	16 (23%)
18	CLA	A	1118	-	40,54,73	2.89	14 (35%)	44,90,113	2.42	13 (29%)
18	CLA	A	1139	-	59,73,73	2.34	16 (27%)	67,113,113	2.15	16 (23%)
27	LUT	3	3502	-	42,43,43	2.39	3 (7%)	51,60,60	2.28	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1130	-	44,58,73	2.74	16 (36%)	49,95,113	2.46	14 (28%)
18	CLA	4	4003	14	59,73,73	2.17	16 (27%)	67,113,113	2.22	17 (25%)
18	CLA	A	1107	1	59,73,73	2.35	16 (27%)	67,113,113	2.18	16 (23%)
18	CLA	2	2019	-	23,35,73	3.17	12 (52%)	26,60,113	3.36	15 (57%)
22	BCR	J	6013	-	41,41,41	2.89	8 (19%)	56,56,56	6.55	30 (53%)
21	LHG	A	7001	-	48,48,48	0.96	2 (4%)	51,54,54	1.13	4 (7%)
18	CLA	B	1221	-	59,73,73	2.35	15 (25%)	67,113,113	2.25	18 (26%)
18	CLA	4	4016	-	40,54,73	2.75	14 (35%)	44,90,113	2.42	17 (38%)
27	LUT	1	1502	-	42,43,43	2.47	4 (9%)	51,60,60	2.21	18 (35%)
26	LMU	B	8002	-	36,36,36	0.45	0	47,47,47	1.06	3 (6%)
21	LHG	2	2801	-	23,23,48	1.32	2 (8%)	26,29,54	1.21	4 (15%)
18	CLA	B	1208	-	49,63,73	2.60	16 (32%)	55,101,113	2.38	15 (27%)
23	LMG	F	5002	-	37,37,55	1.07	2 (5%)	45,45,63	1.27	5 (11%)
18	CLA	A	1116	-	54,68,73	2.45	15 (27%)	61,107,113	2.35	15 (24%)
18	CLA	B	1204	-	49,63,73	2.59	15 (30%)	55,101,113	2.32	14 (25%)
18	CLA	2	2006	-	49,63,73	2.45	14 (28%)	55,101,113	2.42	15 (27%)
25	DGD	B	7101	-	62,62,67	0.91	1 (1%)	76,76,81	1.33	11 (14%)
22	BCR	F	6014	-	41,41,41	3.05	7 (17%)	56,56,56	6.69	23 (41%)
18	CLA	A	1137	-	49,63,73	2.58	16 (32%)	55,101,113	2.26	15 (27%)
18	CLA	2	2003	-	49,63,73	2.31	14 (28%)	55,101,113	2.63	17 (30%)
22	BCR	J	6012	-	41,41,41	2.91	8 (19%)	56,56,56	6.56	29 (51%)
22	BCR	L	6019	-	41,41,41	2.93	7 (17%)	56,56,56	6.55	24 (42%)
18	CLA	1	1001	15	54,68,73	2.25	15 (27%)	61,107,113	2.37	15 (24%)
29	ZEX	4	4505	-	42,43,43	1.08	3 (7%)	55,60,60	2.17	19 (34%)
18	CLA	4	4007	-	54,68,73	2.18	13 (24%)	61,107,113	2.54	15 (24%)
18	CLA	A	1123	-	59,73,73	2.36	16 (27%)	67,113,113	2.22	17 (25%)
18	CLA	A	1115	-	40,54,73	2.91	16 (40%)	44,90,113	2.25	12 (27%)
18	CLA	H	1000	11	40,54,73	2.90	15 (37%)	44,90,113	2.34	12 (27%)
18	CLA	A	1134	-	49,63,73	2.58	15 (30%)	55,101,113	2.34	15 (27%)
18	CLA	3	3010	-	54,68,73	2.24	14 (25%)	61,107,113	2.39	16 (26%)
27	LUT	4	4503	-	42,43,43	2.41	3 (7%)	51,60,60	2.42	15 (29%)
18	CLA	1	1006	-	44,58,73	2.49	17 (38%)	49,95,113	2.59	17 (34%)
18	CLA	2	2005	-	49,63,73	2.46	14 (28%)	55,101,113	2.30	17 (30%)
18	CLA	A	1022	-	59,73,73	2.35	15 (25%)	67,113,113	2.18	17 (25%)
18	CLA	B	1232	-	49,63,73	2.58	16 (32%)	55,101,113	2.29	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1129	-	44,58,73	2.70	15 (34%)	49,95,113	2.52	16 (32%)
28	CHL	1	1010	15	41,55,74	1.43	6 (14%)	41,91,114	1.40	7 (17%)
18	CLA	F	1301	-	36,53,73	2.72	13 (36%)	39,89,113	2.39	11 (28%)
18	CLA	L	1502	-	54,68,73	2.26	15 (27%)	61,107,113	2.33	17 (27%)
27	LUT	1	1501	-	42,43,43	2.50	4 (9%)	51,60,60	2.31	14 (27%)
18	CLA	2	2007	-	54,68,73	2.32	15 (27%)	61,107,113	2.26	15 (24%)
18	CLA	3	3007	-	44,58,73	2.55	16 (36%)	49,95,113	2.57	17 (34%)
18	CLA	2	2002	-	40,54,73	2.59	15 (37%)	44,90,113	2.46	16 (36%)
18	CLA	B	1223	-	59,73,73	2.29	15 (25%)	67,113,113	2.21	16 (23%)
18	CLA	A	1133	-	49,63,73	2.56	16 (32%)	55,101,113	2.42	17 (30%)
23	LMG	4	4801	-	35,35,55	1.04	2 (5%)	43,43,63	1.63	10 (23%)
28	CHL	1	1009	-	50,64,74	1.33	6 (12%)	52,102,114	1.34	10 (19%)
18	CLA	A	1151	21	44,58,73	2.77	16 (36%)	49,95,113	2.46	13 (26%)
18	CLA	A	1104	-	59,73,73	2.35	16 (27%)	67,113,113	2.12	15 (22%)
18	CLA	B	1023	-	59,73,73	2.34	15 (25%)	67,113,113	2.18	19 (28%)
18	CLA	3	3018	16	44,58,73	2.50	17 (38%)	49,95,113	2.65	18 (36%)
18	CLA	3	3019	-	23,35,73	3.36	13 (56%)	26,60,113	3.39	14 (53%)
18	CLA	2	2012	13	49,63,73	2.29	15 (30%)	55,101,113	2.38	18 (32%)
18	CLA	B	1238	-	59,73,73	2.35	16 (27%)	67,113,113	2.12	14 (20%)
18	CLA	A	1135	-	45,59,73	2.68	15 (33%)	50,96,113	2.53	15 (30%)
20	PQN	A	5001	-	34,34,34	1.62	2 (5%)	42,45,45	1.19	3 (7%)
22	BCR	B	6005	-	41,41,41	2.71	6 (14%)	56,56,56	6.79	23 (41%)
18	CLA	A	1102	-	44,58,73	2.73	15 (34%)	49,95,113	2.45	14 (28%)
18	CLA	A	1127	-	59,73,73	2.35	15 (25%)	67,113,113	2.17	16 (23%)
18	CLA	3	3017	-	40,54,73	2.68	15 (37%)	44,90,113	2.30	13 (29%)
18	CLA	4	4005	14	54,68,73	2.19	14 (25%)	61,107,113	2.50	20 (32%)
17	CL0	A	1011	-	59,73,73	2.34	16 (27%)	67,113,113	2.25	16 (23%)
22	BCR	A	6017	-	41,41,41	2.67	6 (14%)	56,56,56	7.12	27 (48%)
23	LMG	F	5001	-	23,23,55	1.24	3 (13%)	31,31,63	1.72	6 (19%)
27	LUT	4	4502	-	42,43,43	2.38	3 (7%)	51,60,60	1.95	15 (29%)
18	CLA	4	4004	14	54,68,73	2.22	14 (25%)	61,107,113	2.28	17 (27%)
18	CLA	B	1202	-	59,73,73	2.31	15 (25%)	67,113,113	2.30	16 (23%)
18	CLA	B	1227	-	59,73,73	2.33	16 (27%)	67,113,113	2.18	17 (25%)
18	CLA	B	1230	-	52,66,73	2.48	14 (26%)	58,104,113	2.44	16 (27%)
18	CLA	A	1120	-	54,68,73	2.43	15 (27%)	61,107,113	2.25	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CHL	4	4013	-	41,55,74	1.79	7 (17%)	41,91,114	1.57	10 (24%)
18	CLA	A	1108	-	40,54,73	2.93	16 (40%)	44,90,113	2.30	14 (31%)
28	CHL	4	4010	-	41,55,74	1.86	10 (24%)	41,91,114	1.91	14 (34%)
18	CLA	4	4002	-	44,58,73	2.44	14 (31%)	49,95,113	2.70	19 (38%)
18	CLA	A	1125	-	54,68,73	2.40	15 (27%)	61,107,113	2.25	16 (26%)
18	CLA	B	1206	2	59,73,73	2.35	15 (25%)	67,113,113	2.28	18 (26%)
18	CLA	A	1117	-	59,73,73	2.34	15 (25%)	67,113,113	2.13	15 (22%)
18	CLA	B	1207	-	59,73,73	2.34	16 (27%)	67,113,113	2.19	16 (23%)
23	LMG	J	5001	-	55,55,55	0.88	2 (3%)	63,63,63	1.44	7 (11%)
18	CLA	3	3012	16	44,58,73	2.45	15 (34%)	49,95,113	2.65	16 (32%)
18	CLA	A	1140	-	59,73,73	2.36	16 (27%)	67,113,113	2.11	16 (23%)
18	CLA	1	1004	15	59,73,73	2.14	15 (25%)	67,113,113	2.25	16 (23%)
18	CLA	4	4008	-	40,54,73	2.53	14 (35%)	44,90,113	2.93	18 (40%)
22	BCR	L	6020	-	41,41,41	2.83	7 (17%)	56,56,56	6.55	29 (51%)
18	CLA	2	2016	13	44,58,73	2.57	15 (34%)	49,95,113	3.36	21 (42%)
27	LUT	4	4501	-	42,43,43	2.44	3 (7%)	51,60,60	2.19	16 (31%)
28	CHL	2	2010	-	41,55,74	1.72	7 (17%)	41,91,114	1.61	9 (21%)
18	CLA	3	3005	-	49,63,73	2.32	15 (30%)	55,101,113	2.60	17 (30%)
18	CLA	B	1214	-	53,67,73	2.47	15 (28%)	59,105,113	2.34	17 (28%)
18	CLA	A	1110	-	49,63,73	2.59	16 (32%)	55,101,113	2.29	16 (29%)
18	CLA	L	1503	-	44,58,73	2.53	15 (34%)	49,95,113	2.55	17 (34%)
18	CLA	A	1131	-	59,73,73	2.35	16 (27%)	67,113,113	2.11	14 (20%)
18	CLA	B	1231	-	54,68,73	2.48	16 (29%)	61,107,113	2.16	16 (26%)
18	CLA	B	1234	-	54,68,73	2.48	16 (29%)	61,107,113	2.32	18 (29%)
27	LUT	I	6018	-	42,43,43	2.46	1 (2%)	51,60,60	2.21	18 (35%)
18	CLA	3	3006	-	44,58,73	2.50	16 (36%)	49,95,113	2.73	17 (34%)
18	CLA	3	3003	16	54,68,73	2.26	16 (29%)	61,107,113	2.44	17 (27%)
18	CLA	B	1209	-	40,54,73	2.94	15 (37%)	44,90,113	2.38	12 (27%)
23	LMG	G	2021	-	41,41,55	0.95	2 (4%)	49,49,63	1.16	5 (10%)
18	CLA	1	1014	15	40,54,73	2.66	15 (37%)	44,90,113	2.51	15 (34%)
18	CLA	B	1236	-	49,63,73	2.58	15 (30%)	55,101,113	2.35	15 (27%)
18	CLA	B	1235	-	59,73,73	2.33	15 (25%)	67,113,113	2.22	15 (22%)
18	CLA	1	1011	-	44,58,73	2.47	15 (34%)	49,95,113	2.52	17 (34%)
18	CLA	B	1219	-	54,68,73	2.46	16 (29%)	61,107,113	2.21	14 (22%)
23	LMG	B	5005	-	38,38,55	1.08	2 (5%)	46,46,63	1.04	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	1218	-	59,73,73	2.34	16 (27%)	67,113,113	2.22	16 (23%)
18	CLA	A	1109	-	59,73,73	2.34	15 (25%)	67,113,113	2.13	15 (22%)
18	CLA	B	1203	2	59,73,73	2.29	15 (25%)	67,113,113	2.15	15 (22%)
18	CLA	1	1012	15	44,58,73	2.48	16 (36%)	49,95,113	2.47	16 (32%)
18	CLA	A	1106	1	59,73,73	2.36	16 (27%)	67,113,113	2.23	16 (23%)
18	CLA	G	1002	-	40,54,73	2.71	16 (40%)	44,90,113	2.51	14 (31%)
28	CHL	3	3011	-	50,64,74	1.65	8 (16%)	52,102,114	1.39	10 (19%)
22	BCR	A	6008	-	41,41,41	2.83	6 (14%)	56,56,56	6.57	26 (46%)
18	CLA	A	1103	-	59,73,73	2.31	16 (27%)	67,113,113	2.21	17 (25%)
18	CLA	B	1224	-	59,73,73	2.32	15 (25%)	67,113,113	2.21	16 (23%)
18	CLA	4	4006	-	44,58,73	2.43	14 (31%)	49,95,113	2.51	18 (36%)
18	CLA	F	1302	5	44,58,73	2.60	14 (31%)	49,95,113	2.53	14 (28%)
28	CHL	2	2013	-	37,54,74	1.25	4 (10%)	36,90,114	1.40	8 (22%)
18	CLA	4	4017	-	59,73,73	2.13	16 (27%)	67,113,113	2.22	17 (25%)
18	CLA	A	1122	-	59,73,73	2.34	15 (25%)	67,113,113	2.10	15 (22%)
27	LUT	3	3501	-	42,43,43	2.34	1 (2%)	51,60,60	2.37	19 (37%)
22	BCR	B	6010	-	41,41,41	2.73	6 (14%)	56,56,56	6.56	23 (41%)
18	CLA	B	1239	-	59,73,73	2.34	16 (27%)	67,113,113	2.16	15 (22%)
28	CHL	2	2011	-	42,56,74	1.81	9 (21%)	42,92,114	1.47	9 (21%)
18	CLA	B	1216	-	59,73,73	2.34	16 (27%)	67,113,113	2.16	16 (23%)
23	LMG	2	2802	-	35,35,55	1.08	2 (5%)	43,43,63	1.33	7 (16%)
18	CLA	1	1007	21	40,54,73	2.59	15 (37%)	44,90,113	2.64	15 (34%)
18	CLA	A	1124	-	49,63,73	2.58	16 (32%)	55,101,113	2.36	16 (29%)
18	CLA	1	1008	-	40,54,73	2.63	15 (37%)	44,90,113	2.58	16 (36%)
18	CLA	A	1113	-	40,54,73	2.91	15 (37%)	44,90,113	2.32	14 (31%)
18	CLA	1	1002	-	40,54,73	2.63	14 (35%)	44,90,113	2.58	15 (34%)
18	CLA	B	1213	-	54,68,73	2.45	14 (25%)	61,107,113	2.22	15 (24%)
19	SF4	A	3001	1,2	0,12,12	0.00	-	-	-	-
18	CLA	A	1105	-	45,59,73	2.70	16 (35%)	50,96,113	2.44	18 (36%)
22	BCR	B	6009	-	41,41,41	2.81	6 (14%)	56,56,56	6.39	23 (41%)
22	BCR	K	2011	-	41,41,41	2.71	6 (14%)	56,56,56	6.74	27 (48%)
22	BCR	A	6002	-	41,41,41	2.74	6 (14%)	56,56,56	6.45	22 (39%)
18	CLA	L	1501	7	44,58,73	2.47	16 (36%)	49,95,113	2.57	20 (40%)
18	CLA	A	1136	-	50,64,73	2.54	16 (32%)	56,102,113	2.34	18 (32%)
18	CLA	B	1021	-	59,73,73	2.34	14 (23%)	67,113,113	2.25	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	1215	-	54,68,73	2.48	16 (29%)	61,107,113	2.24	15 (24%)
18	CLA	A	1128	-	59,73,73	2.34	15 (25%)	67,113,113	2.17	16 (23%)
20	PQN	B	5002	-	34,34,34	1.69	2 (5%)	42,45,45	1.07	3 (7%)
18	CLA	3	3001	16	44,58,73	2.49	15 (34%)	49,95,113	2.57	15 (30%)
22	BCR	3	3503	-	41,41,41	2.95	9 (21%)	56,56,56	6.43	31 (55%)
18	CLA	4	4012	14	59,73,73	2.09	15 (25%)	67,113,113	2.29	19 (28%)
21	LHG	A	5003	18	39,39,48	1.04	2 (5%)	42,45,54	1.18	4 (9%)
22	BCR	A	6011	-	41,41,41	2.89	6 (14%)	56,56,56	6.72	24 (42%)
18	CLA	A	1119	-	59,73,73	2.32	15 (25%)	67,113,113	2.11	16 (23%)
22	BCR	F	6016	-	41,41,41	3.07	9 (21%)	56,56,56	6.70	24 (42%)
18	CLA	B	1217	-	40,54,73	2.91	16 (40%)	44,90,113	2.35	12 (27%)
18	CLA	A	1101	-	59,73,73	2.33	15 (25%)	67,113,113	2.24	15 (22%)
18	CLA	A	1138	-	59,73,73	2.37	15 (25%)	67,113,113	2.05	17 (25%)
22	BCR	G	2011	-	41,41,41	3.05	7 (17%)	56,56,56	6.73	29 (51%)
18	CLA	K	1001	-	40,54,73	2.68	15 (37%)	44,90,113	2.76	14 (31%)
18	CLA	B	1212	-	49,63,73	2.56	16 (32%)	55,101,113	2.41	17 (30%)
18	CLA	B	1012	-	59,73,73	2.33	15 (25%)	67,113,113	2.22	17 (25%)
18	CLA	G	1001	-	49,63,73	2.34	15 (30%)	55,101,113	2.61	20 (36%)
18	CLA	B	1205	-	59,73,73	2.32	15 (25%)	67,113,113	2.09	17 (25%)
18	CLA	B	1210	-	59,73,73	2.31	15 (25%)	67,113,113	2.15	17 (25%)
22	BCR	A	6007	-	41,41,41	2.75	7 (17%)	56,56,56	6.52	23 (41%)
18	CLA	B	1229	-	59,73,73	2.36	16 (27%)	67,113,113	2.14	17 (25%)
18	CLA	B	1226	-	59,73,73	2.29	15 (25%)	67,113,113	2.20	15 (22%)

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
21	LHG	B	5004	18	-	15/23/23/53	-
21	LHG	1	1801	18	-	24/53/53/53	-
18	CLA	A	1132	-	3/3/20/25	13/37/135/135	-
18	CLA	B	1220	-	2/2/20/25	16/37/135/135	-
18	CLA	B	1201	-	3/3/17/25	10/19/117/135	-
22	BCR	I	6020	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	A	6003	-	-	13/29/63/63	0/2/2/2
18	CLA	4	4001	14	3/3/19/25	13/31/129/135	-
18	CLA	1	1005	-	3/3/18/25	10/25/123/135	-
18	CLA	3	3004	16	3/3/19/25	10/31/129/135	-
18	CLA	B	1222	-	3/3/20/25	16/37/135/135	-
18	CLA	B	1240	21	2/2/20/25	17/37/135/135	-
19	SF4	C	3003	8	-	-	0/6/5/5
18	CLA	B	1225	-	3/3/20/25	16/37/135/135	-
18	CLA	1	1003	15	3/3/18/25	7/25/123/135	-
18	CLA	4	4009	14	3/3/17/25	4/19/117/135	-
18	CLA	A	1013	-	3/3/20/25	12/37/135/135	-
18	CLA	J	1302	4	3/3/17/25	11/19/117/135	-
18	CLA	A	1126	-	3/3/20/25	15/37/135/135	-
18	CLA	A	1111	-	2/2/19/25	11/31/129/135	-
28	CHL	4	4011	-	3/3/17/26	3/21/119/137	-
22	BCR	B	6004	-	-	10/29/63/63	0/2/2/2
18	CLA	1	1013	-	3/3/16/25	8/15/113/135	-
18	CLA	A	1114	-	3/3/16/25	6/15/113/135	-
18	CLA	2	2001	13	3/3/19/25	18/31/129/135	-
18	CLA	A	1237	-	3/3/19/25	13/31/129/135	-
18	CLA	A	1121	-	3/3/18/25	15/25/123/135	-
18	CLA	2	2004	13	3/3/20/25	13/37/135/135	-
26	LMU	B	8001	-	-	8/21/61/61	0/2/2/2
18	CLA	3	3008	-	3/3/16/25	12/17/115/135	-
18	CLA	G	1003	-	3/3/19/25	13/31/129/135	-
22	BCR	G	2011	-	-	11/29/63/63	0/2/2/2
27	LUT	2	2501	-	1/1/12/27	3/29/67/67	0/2/2/2
18	CLA	3	3002	-	3/3/16/25	6/15/113/135	-
18	CLA	A	1137	-	3/3/18/25	12/25/123/135	-
18	CLA	3	3013	-	3/3/16/25	11/15/113/135	-
18	CLA	2	2009	13	3/3/17/25	7/19/117/135	-
19	SF4	C	3002	8	-	-	0/6/5/5
18	CLA	2	2008	-	3/3/17/25	9/19/117/135	-
18	CLA	B	1228	-	3/3/19/25	15/31/129/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	B	6006	-	-	10/29/63/63	0/2/2/2
18	CLA	A	1112	-	2/2/20/25	14/37/135/135	-
18	CLA	A	1118	-	3/3/16/25	8/15/113/135	-
18	CLA	A	1139	-	3/3/20/25	14/37/135/135	-
27	LUT	3	3502	-	1/1/12/27	8/29/67/67	0/2/2/2
18	CLA	A	1130	-	2/2/17/25	7/19/117/135	-
18	CLA	4	4003	14	3/3/20/25	17/37/135/135	-
18	CLA	A	1107	1	3/3/20/25	14/37/135/135	-
18	CLA	2	2019	-	3/3/8/25	-	-
22	BCR	B	6009	-	-	7/29/63/63	0/2/2/2
22	BCR	J	6013	-	-	13/29/63/63	0/2/2/2
21	LHG	A	7001	-	-	30/53/53/53	-
18	CLA	B	1221	-	3/3/20/25	19/37/135/135	-
18	CLA	4	4016	-	3/3/16/25	11/15/113/135	-
27	LUT	1	1502	-	1/1/12/27	3/29/67/67	0/2/2/2
26	LMU	B	8002	-	-	14/21/61/61	0/2/2/2
21	LHG	2	2801	-	-	15/28/28/53	-
22	BCR	K	2011	-	-	11/29/63/63	0/2/2/2
18	CLA	B	1208	-	3/3/18/25	15/25/123/135	-
23	LMG	F	5002	-	-	15/32/52/70	0/1/1/1
18	CLA	A	1116	-	3/3/19/25	17/31/129/135	-
18	CLA	B	1204	-	2/2/18/25	12/25/123/135	-
18	CLA	2	2006	-	3/3/18/25	10/25/123/135	-
25	DGD	B	7101	-	-	23/50/90/95	0/2/2/2
22	BCR	F	6014	-	-	12/29/63/63	0/2/2/2
18	CLA	2	2003	-	3/3/18/25	11/25/123/135	-
22	BCR	J	6012	-	-	11/29/63/63	0/2/2/2
22	BCR	L	6019	-	-	11/29/63/63	0/2/2/2
18	CLA	1	1001	15	3/3/19/25	14/31/129/135	-
29	ZEX	4	4505	-	-	2/29/67/67	0/2/2/2
18	CLA	4	4007	-	3/3/19/25	14/31/129/135	-
18	CLA	A	1123	-	2/2/20/25	16/37/135/135	-
18	CLA	A	1115	-	3/3/16/25	6/15/113/135	-
18	CLA	H	1000	11	3/3/16/25	10/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1134	-	2/2/18/25	15/25/123/135	-
18	CLA	3	3010	-	3/3/19/25	17/31/129/135	-
27	LUT	4	4503	-	1/1/12/27	10/29/67/67	0/2/2/2
18	CLA	1	1006	-	3/3/17/25	8/19/117/135	-
18	CLA	2	2005	-	3/3/18/25	14/25/123/135	-
18	CLA	A	1022	-	2/2/20/25	12/37/135/135	-
18	CLA	B	1232	-	3/3/18/25	6/25/123/135	-
18	CLA	A	1129	-	2/2/17/25	9/19/117/135	-
28	CHL	1	1010	15	3/3/16/26	5/17/115/137	-
18	CLA	F	1301	-	3/3/16/25	2/11/111/135	-
18	CLA	L	1502	-	3/3/19/25	15/31/129/135	-
27	LUT	1	1501	-	1/1/12/27	8/29/67/67	0/2/2/2
18	CLA	2	2007	-	3/3/19/25	13/31/129/135	-
18	CLA	3	3007	-	3/3/17/25	6/19/117/135	-
18	CLA	2	2002	-	3/3/16/25	8/15/113/135	-
18	CLA	B	1223	-	2/2/20/25	14/37/135/135	-
18	CLA	A	1133	-	2/2/18/25	10/25/123/135	-
23	LMG	4	4801	-	-	16/30/50/70	0/1/1/1
28	CHL	1	1009	-	4/4/18/26	8/27/125/137	-
18	CLA	A	1151	21	3/3/17/25	11/19/117/135	-
18	CLA	B	1238	-	3/3/20/25	15/37/135/135	-
18	CLA	A	1104	-	3/3/20/25	16/37/135/135	-
18	CLA	B	1023	-	3/3/20/25	10/37/135/135	-
18	CLA	3	3018	16	3/3/17/25	7/19/117/135	-
18	CLA	3	3019	-	3/3/8/25	-	-
18	CLA	2	2012	13	3/3/18/25	9/25/123/135	-
18	CLA	B	1229	-	3/3/20/25	15/37/135/135	-
18	CLA	A	1135	-	2/2/17/25	6/21/119/135	-
20	PQN	A	5001	-	-	10/23/43/43	0/2/2/2
22	BCR	B	6005	-	-	13/29/63/63	0/2/2/2
18	CLA	A	1102	-	3/3/17/25	7/19/117/135	-
18	CLA	A	1127	-	3/3/20/25	19/37/135/135	-
18	CLA	3	3017	-	3/3/16/25	9/15/113/135	-
18	CLA	4	4005	14	3/3/19/25	12/31/129/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CL0	A	1011	-	3/3/20/25	8/37/135/135	-
22	BCR	A	6017	-	-	10/29/63/63	0/2/2/2
23	LMG	F	5001	-	-	9/16/36/70	0/1/1/1
27	LUT	4	4502	-	1/1/12/27	8/29/67/67	0/2/2/2
18	CLA	4	4004	14	3/3/19/25	10/31/129/135	-
18	CLA	B	1227	-	3/3/20/25	11/37/135/135	-
18	CLA	B	1230	-	3/3/18/25	16/29/127/135	-
18	CLA	A	1120	-	3/3/19/25	16/31/129/135	-
18	CLA	A	1108	-	3/3/16/25	6/15/113/135	-
28	CHL	4	4010	-	3/3/16/26	4/17/115/137	-
18	CLA	4	4002	-	3/3/17/25	7/19/117/135	-
18	CLA	A	1125	-	3/3/19/25	19/31/129/135	-
18	CLA	B	1206	2	2/2/20/25	15/37/135/135	-
18	CLA	A	1117	-	2/2/20/25	13/37/135/135	-
18	CLA	B	1207	-	2/2/20/25	18/37/135/135	-
23	LMG	J	5001	-	-	36/50/70/70	0/1/1/1
18	CLA	B	1235	-	2/2/20/25	17/37/135/135	-
18	CLA	A	1140	-	3/3/20/25	16/37/135/135	-
18	CLA	1	1004	15	3/3/20/25	18/37/135/135	-
18	CLA	4	4008	-	3/3/16/25	12/15/113/135	-
18	CLA	B	1211	-	3/3/20/25	11/37/135/135	-
18	CLA	2	2016	13	3/3/17/25	9/19/117/135	-
27	LUT	4	4501	-	1/1/12/27	4/29/67/67	0/2/2/2
28	CHL	2	2010	-	3/3/16/26	2/17/115/137	-
18	CLA	3	3005	-	3/3/18/25	17/25/123/135	-
18	CLA	B	1214	-	3/3/18/25	10/30/128/135	-
18	CLA	A	1110	-	3/3/18/25	10/25/123/135	-
18	CLA	L	1503	-	3/3/17/25	5/19/117/135	-
18	CLA	A	1131	-	3/3/20/25	12/37/135/135	-
18	CLA	B	1231	-	3/3/19/25	11/31/129/135	-
18	CLA	B	1234	-	3/3/19/25	11/31/129/135	-
27	LUT	I	6018	-	1/1/12/27	3/29/67/67	0/2/2/2
18	CLA	3	3006	-	3/3/17/25	6/19/117/135	-
18	CLA	3	3003	16	3/3/19/25	10/31/129/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	1209	-	3/3/16/25	5/15/113/135	-
23	LMG	G	2021	-	-	24/36/56/70	0/1/1/1
18	CLA	1	1014	15	3/3/16/25	9/15/113/135	-
18	CLA	B	1236	-	2/2/18/25	10/25/123/135	-
18	CLA	3	3012	16	3/3/17/25	7/19/117/135	-
18	CLA	1	1011	-	3/3/17/25	10/19/117/135	-
18	CLA	B	1219	-	3/3/19/25	17/31/129/135	-
23	LMG	B	5005	-	-	17/33/53/70	0/1/1/1
18	CLA	B	1218	-	3/3/20/25	16/37/135/135	-
18	CLA	A	1109	-	3/3/20/25	11/37/135/135	-
18	CLA	B	1203	2	2/2/20/25	14/37/135/135	-
22	BCR	F	6016	-	-	8/29/63/63	0/2/2/2
18	CLA	1	1012	15	3/3/17/25	8/19/117/135	-
18	CLA	A	1106	1	3/3/20/25	14/37/135/135	-
18	CLA	G	1002	-	3/3/16/25	8/15/113/135	-
28	CHL	3	3011	-	4/4/18/26	6/27/125/137	-
22	BCR	A	6008	-	-	9/29/63/63	0/2/2/2
18	CLA	A	1103	-	2/2/20/25	21/37/135/135	-
18	CLA	B	1224	-	3/3/20/25	21/37/135/135	-
18	CLA	4	4006	-	3/3/17/25	6/19/117/135	-
18	CLA	F	1302	5	3/3/17/25	10/19/117/135	-
28	CHL	2	2013	-	3/3/16/26	2/13/113/137	-
18	CLA	4	4017	-	3/3/20/25	19/37/135/135	-
18	CLA	A	1122	-	3/3/20/25	24/37/135/135	-
27	LUT	3	3501	-	1/1/12/27	5/29/67/67	0/2/2/2
22	BCR	B	6010	-	-	10/29/63/63	0/2/2/2
18	CLA	B	1239	-	3/3/20/25	18/37/135/135	-
28	CHL	2	2011	-	3/3/16/26	2/18/116/137	-
18	CLA	B	1216	-	3/3/20/25	13/37/135/135	-
23	LMG	2	2802	-	-	12/30/50/70	0/1/1/1
18	CLA	1	1007	21	3/3/16/25	8/15/113/135	-
18	CLA	A	1124	-	3/3/18/25	10/25/123/135	-
18	CLA	1	1008	-	3/3/16/25	9/15/113/135	-
18	CLA	A	1113	-	2/2/16/25	11/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	1002	-	3/3/16/25	6/15/113/135	-
18	CLA	B	1213	-	2/2/19/25	13/31/129/135	-
19	SF4	A	3001	1,2	-	-	0/6/5/5
18	CLA	A	1105	-	3/3/17/25	12/21/119/135	-
27	LUT	2	2502	-	1/1/12/27	4/29/67/67	0/2/2/2
28	CHL	4	4013	-	3/3/16/26	4/17/115/137	-
22	BCR	A	6002	-	-	11/29/63/63	0/2/2/2
18	CLA	L	1501	7	3/3/17/25	7/19/117/135	-
18	CLA	A	1136	-	3/3/18/25	9/27/125/135	-
18	CLA	B	1021	-	3/3/20/25	14/37/135/135	-
18	CLA	B	1215	-	2/2/19/25	15/31/129/135	-
18	CLA	A	1128	-	3/3/20/25	13/37/135/135	-
20	PQN	B	5002	-	-	13/23/43/43	0/2/2/2
18	CLA	3	3001	16	3/3/17/25	4/19/117/135	-
22	BCR	3	3503	-	-	14/29/63/63	0/2/2/2
18	CLA	4	4012	14	3/3/20/25	17/37/135/135	-
21	LHG	A	5003	18	-	21/44/44/53	-
22	BCR	A	6011	-	-	18/29/63/63	0/2/2/2
18	CLA	A	1119	-	3/3/20/25	24/37/135/135	-
22	BCR	L	6020	-	-	9/29/63/63	0/2/2/2
18	CLA	B	1217	-	3/3/16/25	8/15/113/135	-
18	CLA	A	1101	-	2/2/20/25	15/37/135/135	-
18	CLA	A	1138	-	3/3/20/25	19/37/135/135	-
18	CLA	B	1202	-	2/2/20/25	18/37/135/135	-
18	CLA	K	1001	-	3/3/16/25	11/15/113/135	-
18	CLA	B	1212	-	3/3/18/25	7/25/123/135	-
18	CLA	B	1012	-	2/2/20/25	15/37/135/135	-
18	CLA	G	1001	-	3/3/18/25	18/25/123/135	-
18	CLA	B	1205	-	3/3/20/25	10/37/135/135	-
18	CLA	B	1210	-	3/3/20/25	15/37/135/135	-
22	BCR	A	6007	-	-	6/29/63/63	0/2/2/2
18	CLA	B	1226	-	3/3/20/25	19/37/135/135	-

All (2508) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	2502	LUT	C24-C25	14.89	1.51	1.33
27	I	6018	LUT	C24-C25	14.89	1.51	1.33
27	2	2501	LUT	C24-C25	14.81	1.51	1.33
27	1	1501	LUT	C24-C25	14.74	1.51	1.33
27	1	1502	LUT	C24-C25	14.31	1.51	1.33
27	4	4503	LUT	C24-C25	14.30	1.50	1.33
27	4	4501	LUT	C24-C25	14.29	1.50	1.33
27	3	3502	LUT	C24-C25	14.09	1.50	1.33
27	4	4502	LUT	C24-C25	14.08	1.50	1.33
27	3	3501	LUT	C24-C25	14.04	1.50	1.33
18	J	1302	CLA	MG-NA	9.71	2.29	2.06
18	A	1022	CLA	MG-NA	9.69	2.29	2.06
18	2	2004	CLA	MG-NA	9.68	2.29	2.06
18	B	1229	CLA	MG-NA	9.66	2.29	2.06
18	A	1105	CLA	MG-NA	9.65	2.29	2.06
18	A	1127	CLA	MG-NA	9.63	2.29	2.06
18	B	1232	CLA	MG-NA	9.62	2.29	2.06
18	A	1102	CLA	MG-NA	9.62	2.29	2.06
18	A	1151	CLA	MG-NA	9.61	2.29	2.06
18	B	1215	CLA	MG-NA	9.61	2.29	2.06
18	A	1114	CLA	MG-NA	9.61	2.29	2.06
18	B	1012	CLA	MG-NA	9.61	2.29	2.06
18	B	1221	CLA	MG-NA	9.60	2.29	2.06
18	B	1206	CLA	MG-NA	9.59	2.29	2.06
18	A	1140	CLA	MG-NA	9.59	2.29	2.06
18	B	1217	CLA	MG-NA	9.58	2.29	2.06
18	A	1126	CLA	MG-NA	9.58	2.29	2.06
18	B	1234	CLA	MG-NA	9.57	2.29	2.06
18	B	1236	CLA	MG-NA	9.56	2.29	2.06
18	B	1228	CLA	MG-NA	9.56	2.29	2.06
17	A	1011	CL0	MG-NA	9.56	2.29	2.06
18	B	1220	CLA	MG-NA	9.56	2.29	2.06
18	B	1238	CLA	MG-NA	9.56	2.29	2.06
18	A	1135	CLA	MG-NA	9.55	2.29	2.06
18	A	1110	CLA	MG-NA	9.55	2.29	2.06
18	A	1129	CLA	MG-NA	9.55	2.28	2.06
18	A	1122	CLA	MG-NA	9.54	2.28	2.06
18	B	1218	CLA	MG-NA	9.54	2.28	2.06
18	A	1130	CLA	MG-NA	9.54	2.28	2.06
18	A	1137	CLA	MG-NA	9.53	2.28	2.06
18	A	1117	CLA	MG-NA	9.53	2.28	2.06
18	A	1107	CLA	MG-NA	9.53	2.28	2.06
18	A	1112	CLA	MG-NA	9.52	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1104	CLA	MG-NA	9.52	2.28	2.06
18	A	1119	CLA	MG-NA	9.52	2.28	2.06
18	B	1219	CLA	MG-NA	9.51	2.28	2.06
18	A	1134	CLA	MG-NA	9.51	2.28	2.06
18	A	1109	CLA	MG-NA	9.51	2.28	2.06
18	A	1124	CLA	MG-NA	9.51	2.28	2.06
18	A	1113	CLA	MG-NA	9.51	2.28	2.06
18	B	1222	CLA	MG-NA	9.51	2.28	2.06
18	A	1139	CLA	MG-NA	9.51	2.28	2.06
18	B	1239	CLA	MG-NA	9.50	2.28	2.06
18	A	1133	CLA	MG-NA	9.50	2.28	2.06
18	B	1231	CLA	MG-NA	9.50	2.28	2.06
18	H	1000	CLA	MG-NA	9.50	2.28	2.06
18	B	1214	CLA	MG-NA	9.50	2.28	2.06
18	B	1216	CLA	MG-NA	9.49	2.28	2.06
18	B	1225	CLA	MG-NA	9.49	2.28	2.06
18	A	1128	CLA	MG-NA	9.49	2.28	2.06
18	A	1123	CLA	MG-NA	9.49	2.28	2.06
18	B	1240	CLA	MG-NA	9.48	2.28	2.06
18	A	1116	CLA	MG-NA	9.48	2.28	2.06
18	B	1201	CLA	MG-NA	9.48	2.28	2.06
18	B	1209	CLA	MG-NA	9.48	2.28	2.06
18	A	1121	CLA	MG-NA	9.48	2.28	2.06
18	A	1115	CLA	MG-NA	9.48	2.28	2.06
18	B	1208	CLA	MG-NA	9.47	2.28	2.06
18	B	1223	CLA	MG-NA	9.46	2.28	2.06
18	A	1131	CLA	MG-NA	9.45	2.28	2.06
18	B	1213	CLA	MG-NA	9.45	2.28	2.06
18	A	1125	CLA	MG-NA	9.45	2.28	2.06
18	A	1106	CLA	MG-NA	9.45	2.28	2.06
18	A	1132	CLA	MG-NA	9.45	2.28	2.06
18	A	1120	CLA	MG-NA	9.45	2.28	2.06
18	A	1136	CLA	MG-NA	9.45	2.28	2.06
18	B	1205	CLA	MG-NA	9.44	2.28	2.06
18	B	1023	CLA	MG-NA	9.44	2.28	2.06
18	B	1207	CLA	MG-NA	9.44	2.28	2.06
18	A	1108	CLA	MG-NA	9.44	2.28	2.06
18	B	1226	CLA	MG-NA	9.44	2.28	2.06
18	B	1230	CLA	MG-NA	9.43	2.28	2.06
18	A	1118	CLA	MG-NA	9.43	2.28	2.06
18	A	1111	CLA	MG-NA	9.41	2.28	2.06
18	B	1021	CLA	MG-NA	9.41	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1237	CLA	MG-NA	9.40	2.28	2.06
18	B	1224	CLA	MG-NA	9.40	2.28	2.06
18	B	1204	CLA	MG-NA	9.40	2.28	2.06
18	B	1235	CLA	MG-NA	9.39	2.28	2.06
18	B	1210	CLA	MG-NA	9.35	2.28	2.06
18	B	1227	CLA	MG-NA	9.33	2.28	2.06
18	B	1203	CLA	MG-NA	9.32	2.28	2.06
18	B	1212	CLA	MG-NA	9.31	2.28	2.06
18	A	1138	CLA	MG-NA	9.31	2.28	2.06
18	A	1101	CLA	MG-NA	9.29	2.28	2.06
18	A	1013	CLA	MG-NA	9.26	2.28	2.06
18	A	1103	CLA	MG-NA	9.22	2.28	2.06
18	B	1211	CLA	MG-NA	9.15	2.28	2.06
18	3	3019	CLA	MG-NA	9.10	2.27	2.06
18	B	1202	CLA	MG-NA	9.05	2.27	2.06
18	F	1301	CLA	MG-NA	8.82	2.27	2.06
18	2	2019	CLA	MG-NA	8.82	2.27	2.06
18	F	1302	CLA	MG-NA	8.80	2.27	2.06
18	3	3003	CLA	MG-NA	8.80	2.27	2.06
22	G	2011	BCR	C10-C9	-8.76	1.24	1.35
18	2	2005	CLA	MG-NA	8.71	2.27	2.06
18	1	1013	CLA	MG-NA	8.70	2.26	2.06
22	G	2011	BCR	C11-C10	-8.70	1.16	1.43
18	2	2007	CLA	MG-NA	8.70	2.26	2.06
18	G	1003	CLA	MG-NA	8.69	2.26	2.06
18	4	4002	CLA	MG-NA	8.67	2.26	2.06
18	2	2006	CLA	MG-NA	8.67	2.26	2.06
18	3	3013	CLA	MG-NA	8.61	2.26	2.06
18	L	1503	CLA	MG-NA	8.59	2.26	2.06
18	3	3018	CLA	MG-NA	8.57	2.26	2.06
18	1	1012	CLA	MG-NA	8.57	2.26	2.06
18	L	1502	CLA	MG-NA	8.56	2.26	2.06
18	2	2009	CLA	MG-NA	8.52	2.26	2.06
18	4	4016	CLA	MG-NA	8.52	2.26	2.06
18	1	1006	CLA	MG-NA	8.51	2.26	2.06
22	F	6014	BCR	C10-C9	-8.49	1.24	1.35
18	3	3001	CLA	MG-NA	8.49	2.26	2.06
22	A	6011	BCR	C8-C9	-8.48	1.27	1.45
22	F	6016	BCR	C11-C10	-8.47	1.17	1.43
18	3	3005	CLA	MG-NA	8.46	2.26	2.06
22	F	6016	BCR	C10-C9	-8.45	1.24	1.35
18	G	1002	CLA	MG-NA	8.44	2.26	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2016	CLA	MG-NA	8.43	2.26	2.06
18	4	4003	CLA	MG-NA	8.42	2.26	2.06
18	4	4007	CLA	MG-NA	8.40	2.26	2.06
18	G	1001	CLA	MG-NA	8.38	2.26	2.06
22	G	2011	BCR	C8-C9	-8.37	1.28	1.45
22	B	6006	BCR	C8-C9	-8.36	1.28	1.45
18	4	4017	CLA	MG-NA	8.34	2.26	2.06
18	L	1501	CLA	MG-NA	8.33	2.26	2.06
22	A	6003	BCR	C8-C9	-8.33	1.28	1.45
18	1	1011	CLA	MG-NA	8.31	2.26	2.06
22	F	6014	BCR	C11-C10	-8.31	1.17	1.43
18	K	1001	CLA	MG-NA	8.30	2.26	2.06
22	F	6014	BCR	C8-C9	-8.30	1.28	1.45
18	3	3007	CLA	MG-NA	8.30	2.26	2.06
22	A	6008	BCR	C8-C9	-8.29	1.28	1.45
18	1	1004	CLA	MG-NA	8.29	2.26	2.06
18	1	1001	CLA	MG-NA	8.29	2.26	2.06
18	3	3017	CLA	MG-NA	8.27	2.25	2.06
22	B	6004	BCR	C8-C9	-8.26	1.28	1.45
22	F	6016	BCR	C8-C9	-8.25	1.28	1.45
22	A	6011	BCR	C11-C10	-8.25	1.17	1.43
18	4	4004	CLA	MG-NA	8.24	2.25	2.06
22	L	6019	BCR	C8-C9	-8.23	1.28	1.45
22	B	6009	BCR	C8-C9	-8.22	1.28	1.45
18	4	4001	CLA	MG-NA	8.21	2.25	2.06
18	1	1008	CLA	MG-NA	8.20	2.25	2.06
22	3	3503	BCR	C10-C9	-8.19	1.24	1.35
22	B	6010	BCR	C8-C9	-8.19	1.28	1.45
22	A	6008	BCR	C11-C10	-8.19	1.18	1.43
18	4	4005	CLA	MG-NA	8.17	2.25	2.06
18	3	3006	CLA	MG-NA	8.15	2.25	2.06
22	L	6019	BCR	C11-C10	-8.11	1.18	1.43
22	L	6019	BCR	C10-C9	-8.11	1.25	1.35
22	A	6007	BCR	C8-C9	-8.10	1.28	1.45
18	1	1003	CLA	MG-NA	8.09	2.25	2.06
22	3	3503	BCR	C11-C10	-8.09	1.18	1.43
18	1	1014	CLA	MG-NA	8.09	2.25	2.06
18	1	1005	CLA	MG-NA	8.08	2.25	2.06
22	L	6020	BCR	C8-C9	-8.08	1.28	1.45
22	J	6012	BCR	C8-C9	-8.07	1.28	1.45
22	3	3503	BCR	C8-C9	-8.06	1.28	1.45
22	K	2011	BCR	C8-C9	-8.06	1.28	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	6020	BCR	C8-C9	-8.06	1.28	1.45
18	1	1002	CLA	MG-NA	8.05	2.25	2.06
22	J	6012	BCR	C11-C10	-8.04	1.18	1.43
18	4	4009	CLA	MG-NA	8.04	2.25	2.06
22	A	6002	BCR	C8-C9	-8.03	1.28	1.45
22	B	6005	BCR	C8-C9	-8.03	1.28	1.45
22	J	6013	BCR	C11-C10	-8.02	1.18	1.43
22	A	6003	BCR	C11-C10	-8.01	1.18	1.43
22	B	6009	BCR	C11-C10	-7.98	1.18	1.43
22	J	6013	BCR	C8-C9	-7.96	1.28	1.45
22	B	6006	BCR	C11-C10	-7.95	1.18	1.43
18	3	3012	CLA	MG-NA	7.95	2.25	2.06
18	3	3002	CLA	MG-NA	7.95	2.25	2.06
20	B	5002	PQN	C3-C2	7.93	1.49	1.35
22	I	6020	BCR	C11-C10	-7.93	1.18	1.43
22	A	6007	BCR	C11-C10	-7.91	1.19	1.43
22	B	6004	BCR	C11-C10	-7.90	1.19	1.43
22	A	6002	BCR	C11-C10	-7.86	1.19	1.43
18	3	3004	CLA	MG-NA	7.83	2.24	2.06
18	1	1007	CLA	MG-NA	7.82	2.24	2.06
18	4	4006	CLA	MG-NA	7.82	2.24	2.06
18	2	2012	CLA	MG-NA	7.82	2.24	2.06
22	A	6011	BCR	C10-C9	-7.81	1.25	1.35
18	4	4012	CLA	MG-NA	7.81	2.24	2.06
22	B	6005	BCR	C11-C10	-7.80	1.19	1.43
22	B	6010	BCR	C11-C10	-7.80	1.19	1.43
18	2	2001	CLA	MG-NA	7.80	2.24	2.06
22	F	6016	BCR	C16-C17	-7.80	1.19	1.43
18	2	2002	CLA	MG-NA	7.78	2.24	2.06
22	A	6017	BCR	C11-C10	-7.78	1.19	1.43
20	A	5001	PQN	C3-C2	7.78	1.49	1.35
22	A	6017	BCR	C8-C9	-7.75	1.29	1.45
22	K	2011	BCR	C11-C10	-7.75	1.19	1.43
18	3	3008	CLA	MG-NA	7.74	2.24	2.06
22	L	6020	BCR	C11-C10	-7.72	1.19	1.43
18	2	2008	CLA	MG-NA	7.71	2.24	2.06
18	3	3010	CLA	MG-NA	7.71	2.24	2.06
22	J	6013	BCR	C10-C9	-7.68	1.25	1.35
18	2	2003	CLA	MG-NA	7.67	2.24	2.06
22	B	6009	BCR	C10-C9	-7.65	1.25	1.35
22	L	6020	BCR	C10-C9	-7.62	1.25	1.35
22	G	2011	BCR	C20-C21	-7.58	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	J	6012	BCR	C20-C21	-7.56	1.20	1.43
22	3	3503	BCR	C16-C17	-7.55	1.20	1.43
22	A	6008	BCR	C10-C9	-7.54	1.25	1.35
22	A	6011	BCR	C20-C21	-7.53	1.20	1.43
22	3	3503	BCR	C20-C21	-7.50	1.20	1.43
22	F	6014	BCR	C16-C17	-7.46	1.20	1.43
18	4	4008	CLA	MG-NA	7.46	2.24	2.06
22	B	6010	BCR	C20-C21	-7.44	1.20	1.43
22	A	6011	BCR	C16-C17	-7.44	1.20	1.43
22	F	6016	BCR	C20-C21	-7.42	1.20	1.43
22	I	6020	BCR	C20-C21	-7.41	1.20	1.43
22	J	6012	BCR	C10-C9	-7.41	1.26	1.35
22	A	6003	BCR	C10-C9	-7.39	1.26	1.35
22	A	6008	BCR	C16-C17	-7.38	1.20	1.43
22	L	6020	BCR	C20-C21	-7.37	1.20	1.43
22	G	2011	BCR	C16-C17	-7.36	1.20	1.43
22	B	6006	BCR	C20-C21	-7.36	1.20	1.43
22	L	6019	BCR	C20-C21	-7.36	1.20	1.43
22	B	6004	BCR	C20-C21	-7.35	1.20	1.43
22	A	6008	BCR	C20-C21	-7.34	1.20	1.43
22	F	6014	BCR	C20-C21	-7.32	1.20	1.43
22	J	6013	BCR	C16-C17	-7.30	1.20	1.43
22	J	6013	BCR	C20-C21	-7.29	1.20	1.43
22	B	6009	BCR	C16-C17	-7.29	1.20	1.43
22	B	6009	BCR	C20-C21	-7.29	1.20	1.43
22	L	6020	BCR	C16-C17	-7.28	1.20	1.43
22	A	6003	BCR	C20-C21	-7.27	1.20	1.43
22	A	6007	BCR	C20-C21	-7.26	1.21	1.43
22	B	6004	BCR	C16-C17	-7.25	1.21	1.43
22	A	6002	BCR	C20-C21	-7.24	1.21	1.43
22	B	6006	BCR	C16-C17	-7.23	1.21	1.43
22	B	6006	BCR	C10-C9	-7.22	1.26	1.35
22	I	6020	BCR	C16-C17	-7.22	1.21	1.43
22	B	6005	BCR	C20-C21	-7.20	1.21	1.43
22	K	2011	BCR	C20-C21	-7.19	1.21	1.43
22	A	6017	BCR	C20-C21	-7.19	1.21	1.43
22	A	6007	BCR	C10-C9	-7.19	1.26	1.35
22	A	6003	BCR	C16-C17	-7.17	1.21	1.43
22	B	6004	BCR	C10-C9	-7.17	1.26	1.35
22	L	6019	BCR	C16-C17	-7.17	1.21	1.43
22	K	2011	BCR	C16-C17	-7.16	1.21	1.43
22	A	6007	BCR	C16-C17	-7.15	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	J	6012	BCR	C16-C17	-7.15	1.21	1.43
22	A	6017	BCR	C16-C17	-7.15	1.21	1.43
22	A	6002	BCR	C16-C17	-7.13	1.21	1.43
22	I	6020	BCR	C10-C9	-7.13	1.26	1.35
22	B	6005	BCR	C16-C17	-7.10	1.21	1.43
22	B	6010	BCR	C16-C17	-7.09	1.21	1.43
22	A	6002	BCR	C10-C9	-7.04	1.26	1.35
22	K	2011	BCR	C10-C9	-6.97	1.26	1.35
22	B	6005	BCR	C10-C9	-6.95	1.26	1.35
22	B	6010	BCR	C10-C9	-6.92	1.26	1.35
22	A	6017	BCR	C10-C9	-6.65	1.27	1.35
18	1	1014	CLA	O2A-C1	6.61	1.60	1.45
18	G	1002	CLA	O2A-C1	6.49	1.60	1.45
18	A	1114	CLA	O2A-C1	6.49	1.60	1.45
18	A	1118	CLA	O2A-C1	6.48	1.60	1.45
18	B	1209	CLA	O2A-C1	6.46	1.60	1.45
18	A	1113	CLA	O2A-C1	6.45	1.60	1.45
18	4	4016	CLA	O2A-C1	6.45	1.60	1.45
18	3	3013	CLA	O2A-C1	6.45	1.60	1.45
18	A	1115	CLA	O2A-C1	6.45	1.60	1.45
18	H	1000	CLA	O2A-C1	6.44	1.60	1.45
18	2	2002	CLA	O2A-C1	6.43	1.60	1.45
18	A	1108	CLA	O2A-C1	6.42	1.60	1.45
18	K	1001	CLA	O2A-C1	6.41	1.60	1.45
18	3	3017	CLA	O2A-C1	6.40	1.60	1.45
18	B	1217	CLA	O2A-C1	6.38	1.60	1.45
18	1	1013	CLA	O2A-C1	6.38	1.60	1.45
18	1	1007	CLA	O2A-C1	6.38	1.60	1.45
18	1	1008	CLA	O2A-C1	6.30	1.60	1.45
18	1	1002	CLA	O2A-C1	6.30	1.60	1.45
18	3	3002	CLA	O2A-C1	6.27	1.60	1.45
18	4	4008	CLA	O2A-C1	6.17	1.59	1.45
18	2	2016	CLA	O2D-CGD	5.81	1.47	1.33
18	3	3019	CLA	C2B-C1B	5.70	1.49	1.39
18	B	1231	CLA	CHC-C1C	5.58	1.49	1.35
18	2	2016	CLA	OBD-CAD	5.55	1.30	1.22
18	A	1104	CLA	CHC-C1C	5.53	1.49	1.35
18	B	1211	CLA	CHC-C1C	5.51	1.49	1.35
18	B	1234	CLA	CHC-C1C	5.48	1.49	1.35
18	A	1013	CLA	CHC-C1C	5.47	1.49	1.35
28	2	2010	CHL	C3B-C2B	-5.45	1.32	1.40
28	4	4013	CHL	C3B-C2B	-5.44	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1107	CLA	O2A-C1	5.43	1.61	1.46
18	B	1208	CLA	CHC-C1C	5.41	1.48	1.35
18	4	4007	CLA	O2A-C1	5.40	1.61	1.46
18	B	1235	CLA	CHC-C1C	5.40	1.48	1.35
18	A	1108	CLA	CHC-C1C	5.40	1.48	1.35
18	B	1230	CLA	CHC-C1C	5.39	1.48	1.35
18	A	1124	CLA	CHC-C1C	5.38	1.48	1.35
18	A	1107	CLA	CHC-C1C	5.37	1.48	1.35
18	B	1221	CLA	CHC-C1C	5.37	1.48	1.35
18	B	1229	CLA	CHC-C1C	5.37	1.48	1.35
18	2	2004	CLA	CHC-C1C	5.36	1.48	1.35
18	A	1138	CLA	CHC-C1C	5.36	1.48	1.35
18	B	1238	CLA	CHC-C1C	5.34	1.48	1.35
18	B	1227	CLA	CHC-C1C	5.34	1.48	1.35
18	B	1201	CLA	CHC-C1C	5.34	1.48	1.35
18	A	1110	CLA	CHC-C1C	5.34	1.48	1.35
18	A	1140	CLA	CHC-C1C	5.33	1.48	1.35
18	2	2016	CLA	O2A-C1	5.33	1.61	1.46
18	B	1216	CLA	CHC-C1C	5.33	1.48	1.35
18	A	1022	CLA	CHC-C1C	5.33	1.48	1.35
18	B	1215	CLA	CHC-C1C	5.32	1.48	1.35
18	B	1213	CLA	CHC-C1C	5.32	1.48	1.35
18	B	1012	CLA	CHC-C1C	5.32	1.48	1.35
18	A	1102	CLA	CHC-C1C	5.32	1.48	1.35
18	A	1132	CLA	CHC-C1C	5.32	1.48	1.35
18	B	1236	CLA	CHC-C1C	5.31	1.48	1.35
18	B	1240	CLA	CHC-C1C	5.31	1.48	1.35
18	A	1131	CLA	CHC-C1C	5.31	1.48	1.35
18	1	1011	CLA	CHC-C1C	5.31	1.48	1.35
18	B	1221	CLA	O2A-C1	5.31	1.61	1.46
18	A	1112	CLA	CHC-C1C	5.31	1.48	1.35
18	A	1138	CLA	O2D-CGD	5.30	1.46	1.33
18	A	1110	CLA	O2A-C1	5.30	1.61	1.46
18	B	1232	CLA	CHC-C1C	5.30	1.48	1.35
18	B	1222	CLA	CHC-C1C	5.30	1.48	1.35
18	B	1203	CLA	CHC-C1C	5.30	1.48	1.35
18	A	1136	CLA	CHC-C1C	5.30	1.48	1.35
18	B	1023	CLA	CHC-C1C	5.30	1.48	1.35
18	B	1225	CLA	CHC-C1C	5.29	1.48	1.35
18	B	1228	CLA	CHC-C1C	5.29	1.48	1.35
18	A	1129	CLA	CHC-C1C	5.29	1.48	1.35
18	A	1111	CLA	O2A-C1	5.29	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3007	CLA	O2A-C1	5.29	1.61	1.46
18	A	1125	CLA	CHC-C1C	5.29	1.48	1.35
28	4	4010	CHL	C3B-C2B	-5.29	1.33	1.40
18	B	1204	CLA	CHC-C1C	5.28	1.48	1.35
18	B	1220	CLA	CHC-C1C	5.28	1.48	1.35
18	A	1151	CLA	CHC-C1C	5.28	1.48	1.35
18	H	1000	CLA	O2D-CGD	5.28	1.46	1.33
18	B	1204	CLA	O2A-C1	5.28	1.61	1.46
18	A	1130	CLA	CHC-C1C	5.28	1.48	1.35
18	B	1218	CLA	CHC-C1C	5.28	1.48	1.35
18	B	1238	CLA	O2A-C1	5.28	1.61	1.46
18	B	1225	CLA	O2A-C1	5.28	1.61	1.46
18	A	1126	CLA	CHC-C1C	5.27	1.48	1.35
17	A	1011	CL0	CHC-C1C	5.27	1.48	1.35
18	A	1133	CLA	O2D-CGD	5.27	1.46	1.33
18	A	1140	CLA	O2A-C1	5.27	1.61	1.46
18	A	1115	CLA	CHC-C1C	5.27	1.48	1.35
18	A	1139	CLA	CHC-C1C	5.27	1.48	1.35
18	L	1502	CLA	CHC-C1C	5.27	1.48	1.35
18	A	1103	CLA	CHC-C1C	5.26	1.48	1.35
28	3	3011	CHL	C3B-C2B	-5.26	1.33	1.40
18	A	1120	CLA	CHC-C1C	5.26	1.48	1.35
20	B	5002	PQN	C10-C5	5.26	1.49	1.40
18	A	1105	CLA	CHC-C1C	5.26	1.48	1.35
18	A	1106	CLA	O2D-CGD	5.25	1.46	1.33
18	B	1236	CLA	O2A-C1	5.25	1.60	1.46
18	B	1207	CLA	CHC-C1C	5.25	1.48	1.35
18	B	1215	CLA	O2A-C1	5.25	1.60	1.46
18	A	1022	CLA	O2D-CGD	5.25	1.46	1.33
18	A	1120	CLA	O2D-CGD	5.24	1.46	1.33
18	A	1101	CLA	CHC-C1C	5.24	1.48	1.35
18	B	1212	CLA	CHC-C1C	5.24	1.48	1.35
18	3	3008	CLA	O2A-C1	5.24	1.60	1.46
18	B	1214	CLA	CHC-C1C	5.24	1.48	1.35
18	B	1205	CLA	CHC-C1C	5.23	1.48	1.35
18	A	1109	CLA	CHC-C1C	5.23	1.48	1.35
18	L	1503	CLA	CHC-C1C	5.23	1.48	1.35
18	B	1201	CLA	O2A-C1	5.23	1.60	1.46
18	A	1113	CLA	O2D-CGD	5.23	1.46	1.33
18	A	1106	CLA	CHC-C1C	5.23	1.48	1.35
18	A	1117	CLA	CHC-C1C	5.23	1.48	1.35
18	A	1113	CLA	CHC-C1C	5.22	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	1302	CLA	O2A-C1	5.22	1.60	1.46
18	3	3004	CLA	O2A-C1	5.22	1.60	1.46
18	B	1219	CLA	O2D-CGD	5.22	1.45	1.33
18	1	1001	CLA	O2A-C1	5.22	1.60	1.46
18	A	1122	CLA	CHC-C1C	5.22	1.48	1.35
18	A	1111	CLA	CHC-C1C	5.22	1.48	1.35
18	A	1121	CLA	CHC-C1C	5.22	1.48	1.35
18	B	1219	CLA	CHC-C1C	5.22	1.48	1.35
18	B	1205	CLA	O2A-C1	5.21	1.60	1.46
18	A	1132	CLA	O2A-C1	5.21	1.60	1.46
18	B	1225	CLA	O2D-CGD	5.21	1.45	1.33
18	B	1204	CLA	O2D-CGD	5.21	1.45	1.33
18	A	1151	CLA	O2D-CGD	5.21	1.45	1.33
18	A	1137	CLA	O2A-C1	5.21	1.60	1.46
18	B	1238	CLA	O2D-CGD	5.21	1.45	1.33
18	B	1239	CLA	O2A-C1	5.21	1.60	1.46
18	A	1137	CLA	CHC-C1C	5.21	1.48	1.35
18	F	1301	CLA	CHC-C1C	5.21	1.48	1.35
18	3	3001	CLA	O2A-C1	5.21	1.60	1.46
18	A	1237	CLA	CHC-C1C	5.21	1.48	1.35
18	B	1217	CLA	CHC-C1C	5.21	1.48	1.35
18	A	1130	CLA	O2A-C1	5.21	1.60	1.46
18	B	1223	CLA	CHC-C1C	5.20	1.48	1.35
18	A	1130	CLA	O2D-CGD	5.20	1.45	1.33
18	B	1208	CLA	O2A-C1	5.20	1.60	1.46
18	B	1230	CLA	O2D-CGD	5.20	1.45	1.33
18	4	4004	CLA	CHC-C1C	5.20	1.48	1.35
18	B	1211	CLA	O2A-C1	5.20	1.60	1.46
18	A	1108	CLA	O2D-CGD	5.20	1.45	1.33
18	B	1207	CLA	O2A-C1	5.20	1.60	1.46
18	A	1119	CLA	O2D-CGD	5.20	1.45	1.33
18	A	1128	CLA	O2A-C1	5.20	1.60	1.46
18	B	1206	CLA	O2A-C1	5.19	1.60	1.46
18	A	1116	CLA	CHC-C1C	5.19	1.48	1.35
18	A	1103	CLA	O2D-CGD	5.19	1.45	1.33
18	A	1102	CLA	O2A-C1	5.19	1.60	1.46
18	B	1021	CLA	O2D-CGD	5.19	1.45	1.33
18	B	1216	CLA	O2D-CGD	5.19	1.45	1.33
18	A	1105	CLA	O2D-CGD	5.19	1.45	1.33
18	A	1123	CLA	CHC-C1C	5.19	1.48	1.35
18	A	1120	CLA	O2A-C1	5.18	1.60	1.46
18	A	1121	CLA	O2D-CGD	5.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1105	CLA	O2A-C1	5.18	1.60	1.46
18	B	1239	CLA	CHC-C1C	5.18	1.48	1.35
18	A	1134	CLA	CHC-C1C	5.18	1.48	1.35
18	A	1140	CLA	O2D-CGD	5.18	1.45	1.33
18	A	1127	CLA	O2D-CGD	5.18	1.45	1.33
18	B	1212	CLA	O2A-C1	5.18	1.60	1.46
18	A	1111	CLA	O2D-CGD	5.18	1.45	1.33
18	B	1023	CLA	O2D-CGD	5.18	1.45	1.33
18	A	1129	CLA	O2A-C1	5.18	1.60	1.46
18	B	1206	CLA	O2D-CGD	5.18	1.45	1.33
18	A	1119	CLA	CHC-C1C	5.18	1.48	1.35
18	A	1114	CLA	O2D-CGD	5.17	1.45	1.33
18	2	2005	CLA	CHC-C1C	5.17	1.48	1.35
18	A	1101	CLA	O2A-C1	5.17	1.60	1.46
18	B	1209	CLA	O2D-CGD	5.17	1.45	1.33
18	J	1302	CLA	CHC-C1C	5.17	1.48	1.35
18	B	1213	CLA	O2D-CGD	5.17	1.45	1.33
18	B	1209	CLA	C3B-C2B	5.17	1.47	1.40
18	A	1115	CLA	O2D-CGD	5.17	1.45	1.33
18	B	1209	CLA	CHC-C1C	5.17	1.48	1.35
18	F	1302	CLA	CHC-C1C	5.17	1.48	1.35
18	B	1234	CLA	O2D-CGD	5.16	1.45	1.33
18	B	1021	CLA	CHC-C1C	5.16	1.48	1.35
18	G	1003	CLA	O2A-C1	5.16	1.60	1.46
18	B	1214	CLA	O2A-C1	5.16	1.60	1.46
18	B	1207	CLA	O2D-CGD	5.16	1.45	1.33
18	B	1224	CLA	CHC-C1C	5.16	1.48	1.35
18	B	1220	CLA	O2A-C1	5.16	1.60	1.46
18	B	1214	CLA	O2D-CGD	5.16	1.45	1.33
18	B	1228	CLA	O2D-CGD	5.16	1.45	1.33
18	A	1138	CLA	O2A-C1	5.15	1.60	1.46
18	A	1135	CLA	CHC-C1C	5.15	1.48	1.35
18	A	1128	CLA	O2D-CGD	5.15	1.45	1.33
18	A	1109	CLA	O2A-C1	5.15	1.60	1.46
18	A	1125	CLA	O2A-C1	5.15	1.60	1.46
18	B	1227	CLA	O2D-CGD	5.15	1.45	1.33
18	A	1118	CLA	CHC-C1C	5.15	1.48	1.35
18	A	1131	CLA	O2A-C1	5.14	1.60	1.46
18	A	1123	CLA	O2D-CGD	5.14	1.45	1.33
18	B	1228	CLA	O2A-C1	5.14	1.60	1.46
18	4	4003	CLA	CHC-C1C	5.14	1.48	1.35
18	3	3019	CLA	C3C-C2C	5.14	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1217	CLA	O2D-CGD	5.14	1.45	1.33
18	A	1130	CLA	C3B-C2B	5.14	1.47	1.40
18	A	1118	CLA	O2D-CGD	5.14	1.45	1.33
18	B	1208	CLA	O2D-CGD	5.14	1.45	1.33
18	A	1013	CLA	O2D-CGD	5.14	1.45	1.33
18	G	1003	CLA	CHC-C1C	5.14	1.48	1.35
18	B	1224	CLA	O2D-CGD	5.14	1.45	1.33
18	A	1151	CLA	C3C-C2C	5.14	1.47	1.36
18	A	1151	CLA	O2A-C1	5.13	1.60	1.46
18	B	1219	CLA	O2A-C1	5.13	1.60	1.46
18	H	1000	CLA	CHC-C1C	5.13	1.48	1.35
18	B	1236	CLA	O2D-CGD	5.13	1.45	1.33
18	2	2001	CLA	O2A-C1	5.12	1.60	1.46
18	A	1124	CLA	O2A-C1	5.12	1.60	1.46
18	2	2007	CLA	CHC-C1C	5.12	1.48	1.35
18	A	1237	CLA	O2D-CGD	5.12	1.45	1.33
18	B	1224	CLA	O2A-C1	5.12	1.60	1.46
18	A	1127	CLA	CHC-C1C	5.12	1.48	1.35
18	B	1210	CLA	CHC-C1C	5.12	1.48	1.35
18	J	1302	CLA	O2D-CGD	5.12	1.45	1.33
18	B	1202	CLA	CHC-C1C	5.12	1.48	1.35
18	B	1021	CLA	O2A-C1	5.12	1.60	1.46
18	A	1116	CLA	O2D-CGD	5.12	1.45	1.33
18	A	1134	CLA	O2A-C1	5.12	1.60	1.46
18	B	1229	CLA	O2A-C1	5.12	1.60	1.46
18	A	1135	CLA	O2A-C1	5.12	1.60	1.46
18	B	1232	CLA	O2D-CGD	5.12	1.45	1.33
18	A	1117	CLA	O2A-C1	5.12	1.60	1.46
18	A	1136	CLA	O2A-C1	5.11	1.60	1.46
18	2	2006	CLA	CHC-C1C	5.11	1.48	1.35
18	4	4016	CLA	O2D-CGD	5.11	1.45	1.33
18	B	1239	CLA	O2D-CGD	5.11	1.45	1.33
18	B	1215	CLA	O2D-CGD	5.11	1.45	1.33
18	A	1131	CLA	O2D-CGD	5.11	1.45	1.33
18	A	1109	CLA	O2D-CGD	5.11	1.45	1.33
18	A	1133	CLA	CHC-C1C	5.11	1.48	1.35
18	B	1213	CLA	O2A-C1	5.10	1.60	1.46
18	B	1231	CLA	O2D-CGD	5.10	1.45	1.33
18	B	1012	CLA	O2D-CGD	5.10	1.45	1.33
17	A	1011	CL0	O2D-CGD	5.10	1.45	1.33
18	2	2004	CLA	O2A-C1	5.10	1.60	1.46
18	A	1134	CLA	O2D-CGD	5.10	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1101	CLA	O2D-CGD	5.10	1.45	1.33
17	A	1011	CL0	O2A-C1	5.10	1.60	1.46
18	A	1123	CLA	O2A-C1	5.10	1.60	1.46
18	A	1117	CLA	O2D-CGD	5.09	1.45	1.33
18	4	4016	CLA	CHC-C1C	5.09	1.48	1.35
18	B	1223	CLA	O2A-C1	5.09	1.60	1.46
18	A	1022	CLA	O2A-C1	5.09	1.60	1.46
18	A	1121	CLA	O2A-C1	5.09	1.60	1.46
18	B	1202	CLA	O2D-CGD	5.09	1.45	1.33
18	B	1210	CLA	O2A-C1	5.09	1.60	1.46
18	A	1237	CLA	O2A-C1	5.09	1.60	1.46
18	A	1139	CLA	O2A-C1	5.09	1.60	1.46
18	B	1226	CLA	O2A-C1	5.09	1.60	1.46
18	A	1122	CLA	O2D-CGD	5.09	1.45	1.33
18	B	1203	CLA	O2A-C1	5.09	1.60	1.46
18	A	1133	CLA	O2A-C1	5.09	1.60	1.46
18	A	1122	CLA	O2A-C1	5.08	1.60	1.46
18	3	3001	CLA	CHC-C1C	5.08	1.48	1.35
18	A	1123	CLA	C3B-C2B	5.08	1.47	1.40
18	A	1106	CLA	O2A-C1	5.08	1.60	1.46
18	3	3012	CLA	O2A-C1	5.08	1.60	1.46
18	A	1128	CLA	CHC-C1C	5.08	1.48	1.35
18	B	1023	CLA	O2A-C1	5.08	1.60	1.46
18	A	1110	CLA	O2D-CGD	5.08	1.45	1.33
18	A	1104	CLA	O2A-C1	5.07	1.60	1.46
18	B	1227	CLA	O2A-C1	5.07	1.60	1.46
18	A	1135	CLA	O2D-CGD	5.07	1.45	1.33
18	3	3010	CLA	O2A-C1	5.07	1.60	1.46
18	4	4001	CLA	O2A-C1	5.07	1.60	1.46
18	B	1235	CLA	O2D-CGD	5.07	1.45	1.33
18	L	1501	CLA	O2A-C1	5.07	1.60	1.46
18	3	3017	CLA	CHC-C1C	5.07	1.48	1.35
18	A	1119	CLA	O2A-C1	5.07	1.60	1.46
18	B	1218	CLA	O2A-C1	5.07	1.60	1.46
18	B	1212	CLA	O2D-CGD	5.06	1.45	1.33
18	B	1203	CLA	O2D-CGD	5.06	1.45	1.33
18	4	4002	CLA	O2A-C1	5.06	1.60	1.46
18	4	4012	CLA	O2A-C1	5.06	1.60	1.46
18	A	1126	CLA	O2D-CGD	5.06	1.45	1.33
18	L	1503	CLA	O2A-C1	5.06	1.60	1.46
18	A	1137	CLA	O2D-CGD	5.05	1.45	1.33
18	F	1302	CLA	O2A-C1	5.05	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1112	CLA	O2A-C1	5.05	1.60	1.46
18	B	1220	CLA	O2D-CGD	5.05	1.45	1.33
18	A	1114	CLA	CHC-C1C	5.05	1.47	1.35
18	B	1232	CLA	O2A-C1	5.04	1.60	1.46
18	B	1223	CLA	O2D-CGD	5.04	1.45	1.33
18	B	1221	CLA	O2D-CGD	5.04	1.45	1.33
18	K	1001	CLA	O2D-CGD	5.04	1.45	1.33
18	3	3007	CLA	CHC-C1C	5.04	1.47	1.35
18	B	1235	CLA	O2A-C1	5.04	1.60	1.46
18	B	1202	CLA	O2A-C1	5.04	1.60	1.46
28	2	2011	CHL	C3B-C2B	-5.04	1.33	1.40
18	A	1127	CLA	O2A-C1	5.04	1.60	1.46
18	2	2005	CLA	O2A-C1	5.04	1.60	1.46
18	B	1230	CLA	O2A-C1	5.03	1.60	1.46
18	B	1211	CLA	O2D-CGD	5.03	1.45	1.33
18	2	2009	CLA	CHC-C1C	5.03	1.47	1.35
18	A	1106	CLA	C3B-C2B	5.03	1.47	1.40
18	A	1124	CLA	O2D-CGD	5.02	1.45	1.33
18	B	1213	CLA	C3B-C2B	5.02	1.47	1.40
18	2	2007	CLA	O2A-C1	5.02	1.60	1.46
18	B	1201	CLA	O2D-CGD	5.02	1.45	1.33
18	B	1240	CLA	O2D-CGD	5.02	1.45	1.33
18	G	1002	CLA	CHC-C1C	5.02	1.47	1.35
18	4	4005	CLA	O2A-C1	5.02	1.60	1.46
18	A	1125	CLA	O2D-CGD	5.02	1.45	1.33
18	B	1222	CLA	C3B-C2B	5.01	1.47	1.40
18	A	1129	CLA	O2D-CGD	5.01	1.45	1.33
18	3	3013	CLA	CHC-C1C	5.01	1.47	1.35
18	A	1139	CLA	O2D-CGD	5.01	1.45	1.33
18	2	2006	CLA	O2A-C1	5.01	1.60	1.46
18	3	3005	CLA	CHC-C1C	5.00	1.47	1.35
18	B	1229	CLA	O2D-CGD	5.00	1.45	1.33
18	A	1103	CLA	O2A-C1	5.00	1.60	1.46
18	4	4017	CLA	CHC-C1C	5.00	1.47	1.35
18	A	1107	CLA	O2D-CGD	5.00	1.45	1.33
18	B	1231	CLA	OBD-CAD	4.99	1.29	1.22
18	1	1005	CLA	CHC-C1C	4.99	1.47	1.35
18	B	1012	CLA	O2A-C1	4.99	1.60	1.46
18	2	2019	CLA	C3C-C2C	4.99	1.46	1.35
18	B	1231	CLA	O2A-C1	4.99	1.60	1.46
18	G	1001	CLA	O2A-C1	4.99	1.60	1.46
18	A	1136	CLA	O2D-CGD	4.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1102	CLA	O2D-CGD	4.98	1.45	1.33
18	2	2019	CLA	C2B-C1B	4.97	1.48	1.39
18	B	1240	CLA	O2A-C1	4.97	1.60	1.46
18	B	1218	CLA	O2D-CGD	4.97	1.45	1.33
18	1	1001	CLA	CHC-C1C	4.97	1.47	1.35
18	A	1102	CLA	C3B-C2B	4.97	1.47	1.40
18	L	1501	CLA	CHC-C1C	4.97	1.47	1.35
18	3	3012	CLA	CHC-C1C	4.97	1.47	1.35
18	B	1216	CLA	O2A-C1	4.96	1.60	1.46
18	B	1206	CLA	CHC-C1C	4.96	1.47	1.35
18	F	1301	CLA	O2D-CGD	4.95	1.45	1.33
18	L	1502	CLA	O2A-C1	4.95	1.60	1.46
18	1	1005	CLA	O2A-C1	4.94	1.60	1.46
18	A	1126	CLA	O2A-C1	4.94	1.60	1.46
18	3	3003	CLA	O2D-CGD	4.94	1.45	1.33
18	A	1013	CLA	O2A-C1	4.93	1.60	1.46
18	B	1226	CLA	CHC-C1C	4.93	1.47	1.35
18	B	1234	CLA	O2A-C1	4.93	1.60	1.46
18	A	1116	CLA	O2A-C1	4.93	1.60	1.46
18	A	1132	CLA	O2D-CGD	4.92	1.45	1.33
18	B	1234	CLA	C3B-C2B	4.92	1.47	1.40
18	3	3004	CLA	CHC-C1C	4.92	1.47	1.35
18	3	3003	CLA	O2A-C1	4.91	1.60	1.46
18	1	1006	CLA	CHC-C1C	4.90	1.47	1.35
18	B	1202	CLA	OBD-CAD	4.90	1.29	1.22
18	A	1106	CLA	OBD-CAD	4.90	1.29	1.22
18	4	4009	CLA	O2A-C1	4.90	1.59	1.46
18	3	3008	CLA	C3B-C2B	4.90	1.47	1.40
18	B	1021	CLA	OBD-CAD	4.90	1.29	1.22
18	B	1230	CLA	OBD-CAD	4.90	1.29	1.22
18	1	1008	CLA	CHC-C1C	4.89	1.47	1.35
18	B	1021	CLA	C3B-C2B	4.89	1.47	1.40
18	1	1014	CLA	CHC-C1C	4.89	1.47	1.35
18	A	1108	CLA	C3B-C2B	4.88	1.47	1.40
18	B	1222	CLA	O2A-C1	4.88	1.59	1.46
18	G	1002	CLA	O2D-CGD	4.88	1.45	1.33
18	2	2009	CLA	O2A-C1	4.88	1.59	1.46
18	B	1210	CLA	O2D-CGD	4.88	1.45	1.33
18	1	1007	CLA	CHC-C1C	4.87	1.47	1.35
18	F	1302	CLA	O2D-CGD	4.87	1.45	1.33
18	2	2006	CLA	O2D-CGD	4.87	1.45	1.33
18	1	1003	CLA	O2D-CGD	4.87	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4009	CLA	CHC-C1C	4.87	1.47	1.35
18	2	2002	CLA	CHC-C1C	4.87	1.47	1.35
18	A	1237	CLA	OBD-CAD	4.87	1.29	1.22
18	1	1006	CLA	O2A-C1	4.86	1.59	1.46
18	B	1215	CLA	OBD-CAD	4.86	1.29	1.22
18	2	2005	CLA	O2D-CGD	4.86	1.45	1.33
18	1	1004	CLA	O2A-C1	4.85	1.59	1.46
18	A	1138	CLA	C3B-C2B	4.85	1.47	1.40
18	3	3018	CLA	O2D-CGD	4.85	1.45	1.33
18	B	1221	CLA	OBD-CAD	4.85	1.29	1.22
18	A	1127	CLA	C3B-C2B	4.85	1.47	1.40
18	3	3008	CLA	O2D-CGD	4.84	1.45	1.33
18	B	1222	CLA	O2D-CGD	4.84	1.45	1.33
18	1	1004	CLA	CHC-C1C	4.84	1.47	1.35
18	B	1225	CLA	OBD-CAD	4.84	1.29	1.22
18	A	1123	CLA	OBD-CAD	4.83	1.29	1.22
18	B	1210	CLA	OBD-CAD	4.83	1.29	1.22
18	4	4003	CLA	O2D-CGD	4.83	1.45	1.33
18	3	3018	CLA	CHC-C1C	4.83	1.47	1.35
18	B	1208	CLA	OBD-CAD	4.83	1.29	1.22
18	3	3017	CLA	O2D-CGD	4.83	1.45	1.33
18	4	4001	CLA	CHC-C1C	4.83	1.47	1.35
18	2	2007	CLA	O2D-CGD	4.83	1.45	1.33
18	3	3005	CLA	O2A-C1	4.82	1.59	1.46
20	A	5001	PQN	C10-C5	4.82	1.48	1.40
18	1	1012	CLA	CHC-C1C	4.82	1.47	1.35
18	2	2003	CLA	CHC-C1C	4.82	1.47	1.35
18	B	1228	CLA	C3C-C2C	4.82	1.47	1.36
18	3	3002	CLA	CHC-C1C	4.82	1.47	1.35
18	B	1230	CLA	C3B-C2B	4.82	1.47	1.40
18	A	1134	CLA	OBD-CAD	4.82	1.29	1.22
18	B	1240	CLA	OBD-CAD	4.81	1.29	1.22
18	A	1101	CLA	OBD-CAD	4.81	1.29	1.22
18	A	1118	CLA	OBD-CAD	4.80	1.29	1.22
18	A	1104	CLA	OBD-CAD	4.80	1.29	1.22
18	A	1102	CLA	OBD-CAD	4.80	1.29	1.22
18	B	1212	CLA	OBD-CAD	4.80	1.29	1.22
18	2	2008	CLA	CHC-C1C	4.80	1.47	1.35
18	1	1003	CLA	CHC-C1C	4.80	1.47	1.35
18	A	1104	CLA	O2D-CGD	4.80	1.44	1.33
18	B	1234	CLA	C3C-C2C	4.80	1.46	1.36
18	J	1302	CLA	OBD-CAD	4.80	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1219	CLA	OBD-CAD	4.80	1.29	1.22
18	3	3019	CLA	C3B-C4B	4.79	1.48	1.39
18	3	3018	CLA	OBD-CAD	4.79	1.29	1.22
18	B	1229	CLA	OBD-CAD	4.79	1.29	1.22
18	1	1002	CLA	CHC-C1C	4.79	1.47	1.35
18	A	1127	CLA	OBD-CAD	4.79	1.29	1.22
18	A	1116	CLA	OBD-CAD	4.79	1.29	1.22
18	B	1215	CLA	C3B-C2B	4.79	1.47	1.40
18	B	1207	CLA	C3B-C2B	4.79	1.47	1.40
18	B	1202	CLA	C3B-C2B	4.78	1.47	1.40
18	B	1201	CLA	C3B-C2B	4.78	1.47	1.40
18	B	1204	CLA	OBD-CAD	4.78	1.29	1.22
18	B	1227	CLA	OBD-CAD	4.78	1.29	1.22
18	A	1138	CLA	OBD-CAD	4.78	1.29	1.22
18	A	1121	CLA	OBD-CAD	4.78	1.29	1.22
18	2	2003	CLA	O2A-C1	4.78	1.59	1.46
18	B	1206	CLA	C3B-C2B	4.78	1.47	1.40
18	B	1206	CLA	OBD-CAD	4.77	1.29	1.22
18	A	1136	CLA	OBD-CAD	4.77	1.29	1.22
18	B	1229	CLA	C3B-C2B	4.77	1.47	1.40
18	A	1124	CLA	OBD-CAD	4.77	1.29	1.22
18	A	1151	CLA	OBD-CAD	4.77	1.29	1.22
18	B	1217	CLA	OBD-CAD	4.77	1.29	1.22
18	4	4017	CLA	O2A-C1	4.77	1.59	1.46
17	A	1011	CL0	OBD-CAD	4.77	1.29	1.22
18	A	1137	CLA	C3B-C2B	4.76	1.47	1.40
18	A	1122	CLA	OBD-CAD	4.76	1.29	1.22
18	1	1013	CLA	CHC-C1C	4.76	1.47	1.35
18	A	1132	CLA	OBD-CAD	4.76	1.29	1.22
18	B	1218	CLA	OBD-CAD	4.76	1.29	1.22
18	3	3006	CLA	CHC-C1C	4.76	1.47	1.35
18	4	4003	CLA	O2A-C1	4.76	1.59	1.46
18	B	1234	CLA	OBD-CAD	4.76	1.29	1.22
18	A	1107	CLA	OBD-CAD	4.76	1.29	1.22
18	B	1209	CLA	OBD-CAD	4.76	1.29	1.22
18	B	1205	CLA	O2D-CGD	4.75	1.44	1.33
18	A	1105	CLA	OBD-CAD	4.75	1.28	1.22
18	A	1130	CLA	C3C-C2C	4.75	1.46	1.36
21	B	5004	LHG	O7-C7	4.75	1.45	1.35
18	4	4001	CLA	O2D-CGD	4.75	1.44	1.33
18	A	1151	CLA	C3B-C2B	4.75	1.47	1.40
18	A	1013	CLA	OBD-CAD	4.75	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1117	CLA	C3B-C2B	4.74	1.46	1.40
18	A	1113	CLA	OBD-CAD	4.74	1.28	1.22
18	B	1012	CLA	C3D-C2D	4.74	1.47	1.39
18	H	1000	CLA	OBD-CAD	4.74	1.28	1.22
18	A	1129	CLA	OBD-CAD	4.74	1.28	1.22
18	B	1232	CLA	OBD-CAD	4.74	1.28	1.22
18	B	1023	CLA	OBD-CAD	4.74	1.28	1.22
18	4	4002	CLA	O2D-CGD	4.74	1.44	1.33
18	B	1204	CLA	C3C-C2C	4.74	1.46	1.36
18	A	1112	CLA	OBD-CAD	4.74	1.28	1.22
18	A	1022	CLA	OBD-CAD	4.73	1.28	1.22
18	3	3010	CLA	CHC-C1C	4.73	1.47	1.35
18	A	1115	CLA	OBD-CAD	4.73	1.28	1.22
18	B	1216	CLA	OBD-CAD	4.73	1.28	1.22
18	B	1224	CLA	C3C-C2C	4.73	1.46	1.36
18	A	1128	CLA	C3C-C2C	4.73	1.46	1.36
18	B	1222	CLA	OBD-CAD	4.72	1.28	1.22
18	A	1135	CLA	C3B-C2B	4.72	1.46	1.40
18	A	1117	CLA	OBD-CAD	4.72	1.28	1.22
18	B	1226	CLA	O2D-CGD	4.72	1.44	1.33
18	B	1214	CLA	OBD-CAD	4.72	1.28	1.22
18	B	1207	CLA	OBD-CAD	4.72	1.28	1.22
18	B	1218	CLA	C3B-C2B	4.72	1.46	1.40
18	A	1135	CLA	C3C-C2C	4.72	1.46	1.36
18	B	1235	CLA	C3C-C2C	4.72	1.46	1.36
18	A	1108	CLA	C3C-C2C	4.72	1.46	1.36
18	A	1110	CLA	C3C-C2C	4.71	1.46	1.36
18	A	1111	CLA	OBD-CAD	4.71	1.28	1.22
18	A	1108	CLA	OBD-CAD	4.71	1.28	1.22
18	A	1131	CLA	C3C-C2C	4.71	1.46	1.36
18	B	1219	CLA	C3C-C2C	4.71	1.46	1.36
18	A	1138	CLA	C3C-C2C	4.71	1.46	1.36
18	K	1001	CLA	CHC-C1C	4.71	1.47	1.35
18	A	1124	CLA	C3C-C2C	4.71	1.46	1.36
18	B	1212	CLA	C3B-C2B	4.70	1.46	1.40
18	B	1228	CLA	OBD-CAD	4.70	1.28	1.22
17	A	1011	CL0	C3C-C2C	4.70	1.46	1.36
18	B	1213	CLA	OBD-CAD	4.70	1.28	1.22
18	B	1012	CLA	OBD-CAD	4.70	1.28	1.22
18	B	1232	CLA	C3C-C2C	4.70	1.46	1.36
18	A	1112	CLA	O2D-CGD	4.69	1.44	1.33
18	B	1231	CLA	C3C-C2C	4.69	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1110	CLA	OBD-CAD	4.69	1.28	1.22
18	3	3018	CLA	O2A-C1	4.69	1.59	1.46
18	B	1208	CLA	C3C-C2C	4.69	1.46	1.36
18	A	1115	CLA	C3C-C2C	4.69	1.46	1.36
18	A	1118	CLA	C3B-C2B	4.69	1.46	1.40
18	B	1212	CLA	C3C-C2C	4.69	1.46	1.36
18	B	1228	CLA	C3B-C2B	4.69	1.46	1.40
18	3	3006	CLA	O2D-CGD	4.69	1.44	1.33
18	1	1001	CLA	O2D-CGD	4.69	1.44	1.33
18	A	1107	CLA	C3C-C2C	4.68	1.46	1.36
18	B	1217	CLA	C3B-C2B	4.68	1.46	1.40
18	A	1128	CLA	C3D-C2D	4.68	1.47	1.39
18	A	1104	CLA	C3C-C2C	4.68	1.46	1.36
18	B	1239	CLA	OBD-CAD	4.68	1.28	1.22
18	A	1132	CLA	C3C-C2C	4.68	1.46	1.36
18	A	1022	CLA	C3C-C2C	4.68	1.46	1.36
18	A	1139	CLA	OBD-CAD	4.68	1.28	1.22
18	G	1001	CLA	O2D-CGD	4.68	1.44	1.33
18	A	1126	CLA	C3C-C2C	4.67	1.46	1.36
18	A	1136	CLA	C3C-C2C	4.67	1.46	1.36
18	A	1119	CLA	C3C-C2C	4.67	1.46	1.36
18	B	1225	CLA	C3C-C2C	4.67	1.46	1.36
18	2	2016	CLA	CHC-C1C	4.67	1.46	1.35
18	A	1140	CLA	OBD-CAD	4.67	1.28	1.22
18	A	1121	CLA	C3C-C2C	4.67	1.46	1.36
18	B	1238	CLA	C3B-C2B	4.66	1.46	1.40
18	A	1137	CLA	OBD-CAD	4.66	1.28	1.22
18	A	1134	CLA	C3B-C2B	4.66	1.46	1.40
18	A	1103	CLA	OBD-CAD	4.66	1.28	1.22
18	A	1136	CLA	C3B-C2B	4.66	1.46	1.40
18	B	1239	CLA	C3C-C2C	4.66	1.46	1.36
18	B	1218	CLA	C3C-C2C	4.66	1.46	1.36
18	3	3007	CLA	O2D-CGD	4.65	1.44	1.33
18	A	1114	CLA	OBD-CAD	4.65	1.28	1.22
18	A	1133	CLA	C3D-C2D	4.65	1.47	1.39
18	A	1139	CLA	C3B-C2B	4.65	1.46	1.40
18	A	1110	CLA	C3B-C2B	4.65	1.46	1.40
18	B	1238	CLA	C3C-C2C	4.65	1.46	1.36
18	B	1236	CLA	OBD-CAD	4.65	1.28	1.22
18	A	1118	CLA	C3C-C2C	4.65	1.46	1.36
18	A	1125	CLA	C3B-C2B	4.65	1.46	1.40
18	A	1120	CLA	C3C-C2C	4.65	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1106	CLA	C3C-C2C	4.65	1.46	1.36
18	A	1131	CLA	OBD-CAD	4.65	1.28	1.22
18	3	3010	CLA	O2D-CGD	4.65	1.44	1.33
18	A	1116	CLA	C3C-C2C	4.65	1.46	1.36
18	B	1211	CLA	C3C-C2C	4.65	1.46	1.36
18	A	1140	CLA	C3B-C2B	4.65	1.46	1.40
18	B	1201	CLA	OBD-CAD	4.65	1.28	1.22
18	3	3006	CLA	C3B-C2B	4.64	1.46	1.40
18	H	1000	CLA	C3C-C2C	4.64	1.46	1.36
18	A	1129	CLA	C3C-C2C	4.64	1.46	1.36
18	A	1109	CLA	C3C-C2C	4.64	1.46	1.36
18	A	1112	CLA	C3C-C2C	4.64	1.46	1.36
18	B	1238	CLA	OBD-CAD	4.64	1.28	1.22
18	A	1105	CLA	C3C-C2C	4.64	1.46	1.36
18	2	2008	CLA	O2A-C1	4.64	1.59	1.46
18	1	1003	CLA	O2A-C1	4.64	1.59	1.46
18	B	1209	CLA	C3C-C2C	4.64	1.46	1.36
18	4	4006	CLA	CHC-C1C	4.64	1.46	1.35
18	1	1006	CLA	O2D-CGD	4.64	1.44	1.33
18	J	1302	CLA	C3C-C2C	4.64	1.46	1.36
18	A	1122	CLA	C3C-C2C	4.64	1.46	1.36
18	A	1126	CLA	OBD-CAD	4.64	1.28	1.22
18	B	1208	CLA	C3B-C2B	4.64	1.46	1.40
18	B	1205	CLA	C3C-C2C	4.63	1.46	1.36
18	A	1128	CLA	OBD-CAD	4.63	1.28	1.22
18	1	1013	CLA	O2D-CGD	4.63	1.44	1.33
18	B	1217	CLA	C3C-C2C	4.63	1.46	1.36
18	B	1222	CLA	C3C-C2C	4.63	1.46	1.36
18	B	1236	CLA	C3C-C2C	4.63	1.46	1.36
18	B	1229	CLA	C3C-C2C	4.63	1.46	1.36
18	B	1224	CLA	OBD-CAD	4.63	1.28	1.22
18	A	1109	CLA	OBD-CAD	4.63	1.28	1.22
18	L	1502	CLA	O2D-CGD	4.62	1.44	1.33
18	B	1220	CLA	C3C-C2C	4.62	1.46	1.36
18	A	1120	CLA	C3B-C2B	4.62	1.46	1.40
18	A	1013	CLA	C3C-C2C	4.62	1.46	1.36
18	B	1236	CLA	C3B-C2B	4.62	1.46	1.40
18	B	1202	CLA	C3C-C2C	4.62	1.46	1.36
18	A	1116	CLA	C3B-C2B	4.62	1.46	1.40
18	2	2012	CLA	CHC-C1C	4.62	1.46	1.35
18	A	1137	CLA	C3C-C2C	4.62	1.46	1.36
18	A	1131	CLA	C3B-C2B	4.62	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	1302	CLA	C3B-C2B	4.62	1.46	1.40
18	B	1023	CLA	C3C-C2C	4.61	1.46	1.36
18	A	1135	CLA	OBD-CAD	4.61	1.28	1.22
18	A	1101	CLA	C3B-C2B	4.61	1.46	1.40
18	A	1013	CLA	C3B-C2B	4.61	1.46	1.40
18	B	1205	CLA	OBD-CAD	4.61	1.28	1.22
18	A	1102	CLA	C3C-C2C	4.61	1.46	1.36
18	A	1104	CLA	C3B-C2B	4.61	1.46	1.40
18	B	1235	CLA	C3B-C2B	4.60	1.46	1.40
18	A	1133	CLA	C3C-C2C	4.60	1.46	1.36
18	B	1227	CLA	C3C-C2C	4.60	1.46	1.36
18	A	1113	CLA	C3C-C2C	4.60	1.46	1.36
18	A	1123	CLA	C3C-C2C	4.60	1.46	1.36
18	A	1127	CLA	C3C-C2C	4.60	1.46	1.36
18	A	1115	CLA	C3B-C2B	4.60	1.46	1.40
18	A	1130	CLA	OBD-CAD	4.59	1.28	1.22
18	4	4016	CLA	C3B-C2B	4.59	1.46	1.40
18	B	1203	CLA	C3B-C2B	4.59	1.46	1.40
18	3	3006	CLA	O2A-C1	4.59	1.59	1.46
18	B	1012	CLA	C3C-C2C	4.59	1.46	1.36
18	B	1204	CLA	C3B-C2B	4.59	1.46	1.40
18	B	1215	CLA	C3C-C2C	4.59	1.46	1.36
18	B	1220	CLA	OBD-CAD	4.59	1.28	1.22
18	A	1132	CLA	C3D-C2D	4.58	1.47	1.39
18	A	1121	CLA	C3B-C2B	4.58	1.46	1.40
18	B	1240	CLA	C3C-C2C	4.58	1.46	1.36
18	A	1114	CLA	C3C-C2C	4.58	1.46	1.36
18	A	1101	CLA	C3C-C2C	4.58	1.46	1.36
18	4	4006	CLA	O2D-CGD	4.58	1.44	1.33
18	B	1203	CLA	C3C-C2C	4.58	1.46	1.36
18	A	1117	CLA	C3C-C2C	4.58	1.46	1.36
18	A	1102	CLA	C3D-C2D	4.58	1.47	1.39
18	A	1103	CLA	C3B-C2B	4.58	1.46	1.40
18	B	1219	CLA	C3B-C2B	4.57	1.46	1.40
18	3	3008	CLA	CHC-C1C	4.57	1.46	1.35
18	A	1129	CLA	C3B-C2B	4.57	1.46	1.40
18	B	1231	CLA	C3B-C2B	4.57	1.46	1.40
18	3	3001	CLA	OBD-CAD	4.57	1.28	1.22
18	A	1109	CLA	C3B-C2B	4.57	1.46	1.40
18	A	1139	CLA	C3C-C2C	4.57	1.46	1.36
18	B	1235	CLA	OBD-CAD	4.57	1.28	1.22
18	B	1221	CLA	C3C-C2C	4.56	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3012	CLA	O2D-CGD	4.56	1.44	1.33
18	A	1140	CLA	C3C-C2C	4.56	1.46	1.36
18	A	1134	CLA	C3C-C2C	4.56	1.46	1.36
18	A	1237	CLA	C3C-C2C	4.55	1.46	1.36
18	4	4005	CLA	CHC-C1C	4.55	1.46	1.35
18	1	1014	CLA	O2D-CGD	4.55	1.44	1.33
18	B	1216	CLA	C3C-C2C	4.55	1.46	1.36
18	B	1223	CLA	C3C-C2C	4.55	1.46	1.36
18	B	1240	CLA	C3B-C2B	4.55	1.46	1.40
18	A	1022	CLA	C3D-C2D	4.54	1.47	1.39
18	B	1023	CLA	C3D-C2D	4.54	1.47	1.39
18	A	1125	CLA	C3C-C2C	4.54	1.46	1.36
18	2	2003	CLA	C3B-C2B	4.54	1.46	1.40
18	B	1211	CLA	OBD-CAD	4.54	1.28	1.22
18	B	1226	CLA	OBD-CAD	4.54	1.28	1.22
18	A	1107	CLA	C3B-C2B	4.54	1.46	1.40
18	1	1011	CLA	O2A-C1	4.53	1.58	1.46
18	A	1113	CLA	C3B-C2B	4.53	1.46	1.40
18	2	2009	CLA	O2D-CGD	4.52	1.44	1.33
18	B	1214	CLA	C3B-C2B	4.52	1.46	1.40
17	A	1011	CL0	C3D-C2D	4.52	1.47	1.39
18	B	1227	CLA	C3B-C2B	4.52	1.46	1.40
18	A	1138	CLA	C3D-C2D	4.52	1.47	1.39
18	3	3004	CLA	O2D-CGD	4.52	1.44	1.33
18	2	2012	CLA	O2A-C1	4.51	1.58	1.46
18	4	4006	CLA	O2A-C1	4.51	1.58	1.46
18	B	1206	CLA	C3C-C2C	4.51	1.46	1.36
18	B	1214	CLA	C3C-C2C	4.51	1.46	1.36
18	B	1202	CLA	C3D-C2D	4.51	1.47	1.39
18	A	1237	CLA	C3B-C2B	4.51	1.46	1.40
18	B	1239	CLA	C3B-C2B	4.51	1.46	1.40
18	A	1114	CLA	C3B-C2B	4.50	1.46	1.40
18	A	1111	CLA	C3B-C2B	4.49	1.46	1.40
18	A	1122	CLA	C3B-C2B	4.49	1.46	1.40
18	B	1210	CLA	C3C-C2C	4.49	1.46	1.36
18	F	1302	CLA	OBD-CAD	4.49	1.28	1.22
18	B	1225	CLA	C3B-C2B	4.49	1.46	1.40
18	B	1206	CLA	C3D-C2D	4.49	1.47	1.39
18	A	1105	CLA	C3B-C2B	4.49	1.46	1.40
18	A	1126	CLA	C3B-C2B	4.49	1.46	1.40
18	A	1133	CLA	OBD-CAD	4.49	1.28	1.22
18	B	1215	CLA	C3D-C2D	4.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1132	CLA	C3B-C2B	4.48	1.46	1.40
18	B	1213	CLA	C3C-C2C	4.48	1.46	1.36
18	3	3005	CLA	O2D-CGD	4.48	1.44	1.33
18	A	1111	CLA	C3C-C2C	4.48	1.46	1.36
18	B	1216	CLA	C3D-C2D	4.48	1.47	1.39
18	A	1013	CLA	C3D-C2D	4.48	1.47	1.39
18	1	1004	CLA	O2D-CGD	4.48	1.44	1.33
18	G	1001	CLA	CHC-C1C	4.48	1.46	1.35
18	1	1008	CLA	O2D-CGD	4.48	1.44	1.33
18	B	1201	CLA	C3C-C2C	4.47	1.46	1.36
18	L	1503	CLA	O2D-CGD	4.47	1.44	1.33
18	1	1012	CLA	O2A-C1	4.47	1.58	1.46
18	1	1007	CLA	O2D-CGD	4.47	1.44	1.33
18	A	1124	CLA	C3B-C2B	4.47	1.46	1.40
18	4	4008	CLA	CHC-C1C	4.47	1.46	1.35
18	A	1127	CLA	C3D-C2D	4.47	1.47	1.39
18	A	1140	CLA	C3D-C2D	4.47	1.47	1.39
18	A	1133	CLA	C3B-C2B	4.46	1.46	1.40
18	B	1207	CLA	C3C-C2C	4.46	1.46	1.36
18	A	1126	CLA	C3D-C2D	4.46	1.47	1.39
18	B	1021	CLA	C3D-C2D	4.45	1.47	1.39
18	B	1021	CLA	C3C-C2C	4.45	1.46	1.36
18	B	1226	CLA	C3C-C2C	4.45	1.46	1.36
18	2	2005	CLA	OBD-CAD	4.45	1.28	1.22
18	A	1116	CLA	C3D-C2D	4.45	1.47	1.39
18	B	1224	CLA	C3D-C2D	4.45	1.47	1.39
18	B	1209	CLA	C3D-C2D	4.45	1.47	1.39
18	4	4004	CLA	O2A-C1	4.45	1.58	1.46
18	B	1228	CLA	C3D-C2D	4.45	1.47	1.39
18	B	1223	CLA	C3B-C2B	4.44	1.46	1.40
18	1	1002	CLA	OBD-CAD	4.44	1.28	1.22
18	B	1023	CLA	C3B-C2B	4.44	1.46	1.40
18	B	1220	CLA	C3D-C2D	4.44	1.47	1.39
18	B	1222	CLA	C3D-C2D	4.43	1.47	1.39
18	A	1119	CLA	C3B-C2B	4.43	1.46	1.40
18	3	3013	CLA	O2D-CGD	4.43	1.44	1.33
18	B	1221	CLA	C3B-C2B	4.43	1.46	1.40
18	A	1115	CLA	C3D-C2D	4.43	1.47	1.39
18	B	1235	CLA	C3D-C2D	4.43	1.47	1.39
18	A	1112	CLA	C3D-C2D	4.42	1.47	1.39
18	B	1204	CLA	C3D-C2D	4.42	1.47	1.39
18	B	1211	CLA	C3B-C2B	4.42	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1106	CLA	C3D-C2D	4.42	1.47	1.39
18	3	3002	CLA	O2D-CGD	4.42	1.44	1.33
18	A	1128	CLA	C3B-C2B	4.41	1.46	1.40
28	1	1009	CHL	C3B-C2B	-4.41	1.34	1.40
18	L	1501	CLA	O2D-CGD	4.41	1.44	1.33
18	B	1230	CLA	C3C-C2C	4.41	1.46	1.36
18	2	2006	CLA	OBD-CAD	4.41	1.28	1.22
18	2	2007	CLA	C3B-C2B	4.40	1.46	1.40
18	1	1012	CLA	O2D-CGD	4.40	1.43	1.33
18	F	1302	CLA	C3C-C2C	4.40	1.46	1.36
18	4	4012	CLA	CHC-C1C	4.40	1.46	1.35
18	2	2006	CLA	C3C-C2C	4.40	1.46	1.36
18	B	1232	CLA	C3D-C2D	4.40	1.47	1.39
18	A	1120	CLA	OBD-CAD	4.40	1.28	1.22
18	2	2001	CLA	CHC-C1C	4.40	1.46	1.35
18	A	1139	CLA	C3D-C2D	4.40	1.47	1.39
18	2	2004	CLA	O2D-CGD	4.40	1.43	1.33
18	A	1110	CLA	C3D-C2D	4.39	1.47	1.39
18	B	1219	CLA	C3D-C2D	4.39	1.47	1.39
18	3	3007	CLA	OBD-CAD	4.39	1.28	1.22
21	A	7001	LHG	O8-C23	4.39	1.46	1.33
18	B	1225	CLA	C3D-C2D	4.39	1.47	1.39
18	A	1151	CLA	C3D-C2D	4.39	1.47	1.39
18	H	1000	CLA	C3D-C2D	4.39	1.47	1.39
18	A	1111	CLA	C3D-C2D	4.39	1.47	1.39
18	B	1205	CLA	C3B-C2B	4.39	1.46	1.40
18	A	1131	CLA	C3D-C2D	4.39	1.47	1.39
18	A	1124	CLA	C3D-C2D	4.39	1.47	1.39
18	B	1229	CLA	C3D-C2D	4.39	1.47	1.39
18	A	1103	CLA	C3C-C2C	4.39	1.46	1.36
18	B	1236	CLA	C3D-C2D	4.38	1.47	1.39
18	A	1134	CLA	C3D-C2D	4.38	1.47	1.39
18	3	3008	CLA	C3C-C2C	4.38	1.46	1.36
18	A	1122	CLA	C3D-C2D	4.38	1.47	1.39
18	A	1117	CLA	C3D-C2D	4.38	1.47	1.39
18	4	4005	CLA	O2D-CGD	4.38	1.43	1.33
18	A	1119	CLA	OBD-CAD	4.38	1.28	1.22
18	G	1003	CLA	O2D-CGD	4.38	1.43	1.33
18	B	1210	CLA	C3D-C2D	4.37	1.47	1.39
18	2	2009	CLA	C3C-C2C	4.37	1.46	1.36
18	B	1208	CLA	C3D-C2D	4.37	1.47	1.39
18	B	1218	CLA	C3D-C2D	4.37	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1212	CLA	C3D-C2D	4.37	1.47	1.39
18	3	3013	CLA	C3C-C2C	4.37	1.46	1.36
18	B	1224	CLA	C3B-C2B	4.37	1.46	1.40
18	B	1230	CLA	C3D-C2D	4.36	1.47	1.39
18	B	1221	CLA	C3D-C2D	4.36	1.47	1.39
18	B	1210	CLA	C3B-C2B	4.36	1.46	1.40
18	B	1220	CLA	C3B-C2B	4.36	1.46	1.40
18	A	1105	CLA	C3D-C2D	4.36	1.47	1.39
18	2	2007	CLA	OBD-CAD	4.36	1.28	1.22
18	B	1232	CLA	C3B-C2B	4.35	1.46	1.40
18	A	1123	CLA	C3D-C2D	4.35	1.47	1.39
18	J	1302	CLA	C3D-C2D	4.35	1.47	1.39
18	A	1104	CLA	C3D-C2D	4.35	1.47	1.39
18	H	1000	CLA	C3B-C2B	4.35	1.46	1.40
18	4	4007	CLA	CHC-C1C	4.34	1.46	1.35
18	3	3004	CLA	OBD-CAD	4.34	1.28	1.22
18	A	1108	CLA	C3D-C2D	4.34	1.47	1.39
18	B	1211	CLA	C3D-C2D	4.33	1.47	1.39
18	2	2005	CLA	C3C-C2C	4.33	1.45	1.36
18	A	1113	CLA	C3D-C2D	4.33	1.47	1.39
18	2	2007	CLA	C3C-C2C	4.33	1.45	1.36
18	A	1109	CLA	C3D-C2D	4.32	1.47	1.39
18	B	1239	CLA	C3D-C2D	4.32	1.47	1.39
18	1	1012	CLA	OBD-CAD	4.32	1.28	1.22
18	A	1137	CLA	C3D-C2D	4.32	1.47	1.39
18	B	1213	CLA	C3D-C2D	4.31	1.47	1.39
18	A	1119	CLA	C3D-C2D	4.31	1.47	1.39
18	1	1011	CLA	O2D-CGD	4.31	1.43	1.33
18	B	1231	CLA	C3D-C2D	4.31	1.47	1.39
18	1	1008	CLA	C3B-C2B	4.31	1.46	1.40
18	B	1226	CLA	C3D-C2D	4.31	1.47	1.39
18	A	1121	CLA	C3D-C2D	4.31	1.47	1.39
18	B	1205	CLA	C3D-C2D	4.31	1.47	1.39
18	4	4003	CLA	OBD-CAD	4.31	1.28	1.22
18	B	1223	CLA	OBD-CAD	4.30	1.28	1.22
18	A	1114	CLA	C3D-C2D	4.30	1.47	1.39
18	2	2006	CLA	C3B-C2B	4.30	1.46	1.40
18	4	4002	CLA	CHC-C1C	4.30	1.46	1.35
18	K	1001	CLA	OBD-CAD	4.29	1.28	1.22
18	3	3012	CLA	OBD-CAD	4.29	1.28	1.22
18	A	1136	CLA	C3D-C2D	4.29	1.47	1.39
18	B	1214	CLA	C3D-C2D	4.29	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1101	CLA	C3D-C2D	4.28	1.47	1.39
18	B	1234	CLA	C3D-C2D	4.28	1.47	1.39
18	4	4016	CLA	OBD-CAD	4.28	1.28	1.22
23	B	5005	LMG	O8-C28	4.28	1.45	1.33
18	G	1003	CLA	C3C-C2C	4.28	1.45	1.36
18	A	1135	CLA	C3D-C2D	4.27	1.47	1.39
28	1	1010	CHL	O2D-CGD	4.27	1.43	1.33
18	B	1217	CLA	C3D-C2D	4.27	1.47	1.39
18	3	3004	CLA	C3C-C2C	4.27	1.45	1.36
18	4	4017	CLA	O2D-CGD	4.27	1.43	1.33
18	2	2005	CLA	C3B-C2B	4.27	1.46	1.40
18	B	1227	CLA	C3D-C2D	4.27	1.47	1.39
18	B	1201	CLA	C3D-C2D	4.26	1.47	1.39
18	A	1130	CLA	C3D-C2D	4.26	1.47	1.39
18	1	1003	CLA	OBD-CAD	4.26	1.28	1.22
18	A	1103	CLA	C3D-C2D	4.26	1.47	1.39
18	4	4016	CLA	C3C-C2C	4.25	1.45	1.36
18	4	4002	CLA	C3B-C2B	4.25	1.46	1.40
18	3	3003	CLA	C3C-C2C	4.25	1.45	1.36
18	F	1301	CLA	C3C-C2C	4.25	1.45	1.36
18	4	4007	CLA	OBD-CAD	4.25	1.28	1.22
28	4	4010	CHL	C3A-C2A	-4.25	1.42	1.54
18	3	3008	CLA	OBD-CAD	4.25	1.28	1.22
18	A	1118	CLA	C3D-C2D	4.25	1.47	1.39
18	3	3010	CLA	C3C-C2C	4.24	1.45	1.36
18	B	1012	CLA	C3B-C2B	4.24	1.46	1.40
21	A	5003	LHG	O8-C23	4.24	1.45	1.33
18	F	1301	CLA	OBD-CAD	4.23	1.28	1.22
18	K	1001	CLA	C3C-C2C	4.23	1.45	1.36
18	B	1240	CLA	C3D-C2D	4.23	1.47	1.39
18	B	1226	CLA	C3B-C2B	4.23	1.46	1.40
18	A	1112	CLA	C3B-C2B	4.23	1.46	1.40
18	B	1216	CLA	C3B-C2B	4.23	1.46	1.40
18	4	4004	CLA	O2D-CGD	4.23	1.43	1.33
18	1	1003	CLA	C3C-C2C	4.22	1.45	1.36
18	A	1107	CLA	C3D-C2D	4.22	1.47	1.39
18	1	1004	CLA	OBD-CAD	4.22	1.28	1.22
18	2	2003	CLA	OBD-CAD	4.22	1.28	1.22
28	3	3011	CHL	O2A-CGA	4.22	1.45	1.33
28	2	2011	CHL	C1B-NB	-4.20	1.31	1.35
18	1	1002	CLA	O2D-CGD	4.20	1.43	1.33
18	A	1129	CLA	C3D-C2D	4.20	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	2	2013	CHL	O2D-CGD	4.20	1.43	1.33
18	B	1207	CLA	C3D-C2D	4.20	1.47	1.39
18	B	1238	CLA	C3D-C2D	4.19	1.46	1.39
18	2	2003	CLA	O2D-CGD	4.19	1.43	1.33
18	2	2002	CLA	O2D-CGD	4.19	1.43	1.33
18	2	2006	CLA	C3D-C2D	4.18	1.46	1.39
18	F	1302	CLA	C3B-C2B	4.18	1.46	1.40
18	1	1004	CLA	C3C-C2C	4.18	1.45	1.36
18	G	1002	CLA	OBD-CAD	4.18	1.28	1.22
18	A	1125	CLA	OBD-CAD	4.17	1.28	1.22
28	4	4010	CHL	O2A-CGA	4.17	1.46	1.33
28	4	4010	CHL	O2D-CGD	4.16	1.43	1.33
18	B	1203	CLA	OBD-CAD	4.16	1.28	1.22
21	2	2801	LHG	O8-C23	4.16	1.45	1.33
18	3	3013	CLA	OBD-CAD	4.15	1.28	1.22
18	4	4008	CLA	O2D-CGD	4.15	1.43	1.33
18	4	4017	CLA	OBD-CAD	4.15	1.28	1.22
18	L	1502	CLA	C3B-C2B	4.15	1.46	1.40
18	F	1302	CLA	C3D-C2D	4.15	1.46	1.39
18	A	1120	CLA	C3D-C2D	4.15	1.46	1.39
18	B	1223	CLA	C3D-C2D	4.14	1.46	1.39
18	4	4003	CLA	C3B-C2B	4.14	1.46	1.40
21	A	7001	LHG	O7-C7	4.14	1.46	1.34
18	1	1001	CLA	C3D-C2D	4.14	1.46	1.39
21	A	5003	LHG	O7-C7	4.14	1.46	1.34
18	2	2007	CLA	C3D-C2D	4.13	1.46	1.39
18	2	2005	CLA	C3D-C2D	4.13	1.46	1.39
23	B	5005	LMG	O7-C10	4.12	1.45	1.34
18	L	1502	CLA	OBD-CAD	4.12	1.28	1.22
28	4	4011	CHL	C3B-C2B	-4.12	1.34	1.40
18	3	3018	CLA	C3C-C2C	4.11	1.45	1.36
18	2	2008	CLA	O2D-CGD	4.11	1.43	1.33
28	2	2010	CHL	O2A-CGA	4.11	1.46	1.33
18	4	4007	CLA	O2D-CGD	4.10	1.43	1.33
18	4	4012	CLA	O2D-CGD	4.10	1.43	1.33
18	B	1203	CLA	C3D-C2D	4.10	1.46	1.39
18	2	2019	CLA	C3B-C4B	4.10	1.47	1.39
18	G	1003	CLA	OBD-CAD	4.09	1.28	1.22
28	3	3011	CHL	O2D-CGD	4.08	1.43	1.33
18	3	3006	CLA	C3C-C2C	4.08	1.45	1.36
18	F	1301	CLA	C3B-C2B	4.08	1.46	1.40
18	3	3007	CLA	C3C-C2C	4.07	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3001	CLA	O2D-CGD	4.07	1.43	1.33
18	4	4003	CLA	C3C-C2C	4.07	1.45	1.36
18	2	2001	CLA	O2D-CGD	4.06	1.43	1.33
18	1	1005	CLA	O2D-CGD	4.06	1.43	1.33
18	4	4004	CLA	C3C-C2C	4.06	1.45	1.36
18	1	1002	CLA	C3D-C2D	4.06	1.46	1.39
18	1	1007	CLA	OBD-CAD	4.06	1.28	1.22
18	3	3012	CLA	C3C-C2C	4.05	1.45	1.36
18	2	2008	CLA	C3B-C2B	4.05	1.46	1.40
18	1	1003	CLA	C3D-C2D	4.05	1.46	1.39
18	2	2004	CLA	C1C-NC	-4.05	1.31	1.37
18	1	1013	CLA	OBD-CAD	4.05	1.28	1.22
18	L	1503	CLA	OBD-CAD	4.05	1.28	1.22
18	L	1502	CLA	C3C-C2C	4.04	1.45	1.36
18	3	3007	CLA	C3D-C2D	4.04	1.46	1.39
17	A	1011	CL0	C3B-C2B	4.04	1.46	1.40
18	A	1237	CLA	C3D-C2D	4.04	1.46	1.39
18	4	4009	CLA	O2D-CGD	4.04	1.43	1.33
18	3	3003	CLA	C3B-C2B	4.04	1.46	1.40
18	A	1125	CLA	C3D-C2D	4.03	1.46	1.39
22	G	2011	BCR	C11-C12	-4.03	1.24	1.34
18	4	4017	CLA	C3C-C2C	4.02	1.45	1.36
18	4	4001	CLA	C3C-C2C	4.01	1.45	1.36
18	F	1301	CLA	C3D-C2D	4.01	1.46	1.39
28	2	2011	CHL	O2D-CGD	4.00	1.43	1.33
18	A	1022	CLA	MG-NC	4.00	2.15	2.06
18	3	3001	CLA	C3C-C2C	4.00	1.45	1.36
21	1	1801	LHG	O7-C7	4.00	1.45	1.34
23	2	2802	LMG	O7-C10	4.00	1.45	1.34
18	1	1014	CLA	OBD-CAD	4.00	1.27	1.22
18	1	1011	CLA	C3C-C2C	4.00	1.45	1.36
18	1	1011	CLA	OBD-CAD	3.99	1.27	1.22
18	4	4004	CLA	OBD-CAD	3.99	1.27	1.22
18	L	1503	CLA	C3D-C2D	3.99	1.46	1.39
23	2	2802	LMG	O8-C28	3.99	1.45	1.33
18	3	3013	CLA	C3D-C2D	3.99	1.46	1.39
18	G	1002	CLA	C3C-C2C	3.98	1.45	1.36
18	L	1503	CLA	C3B-C2B	3.98	1.45	1.40
18	3	3002	CLA	C3C-C2C	3.98	1.45	1.36
28	1	1009	CHL	O2A-CGA	3.98	1.45	1.33
18	3	3003	CLA	CHC-C1C	3.98	1.45	1.35
18	3	3019	CLA	MG-NC	3.98	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1014	CLA	C3B-C2B	3.97	1.45	1.40
28	4	4011	CHL	O2A-CGA	3.97	1.45	1.33
18	1	1004	CLA	C3B-C2B	3.97	1.45	1.40
18	4	4006	CLA	C3B-C2B	3.97	1.45	1.40
23	F	5002	LMG	O8-C28	3.97	1.44	1.33
23	F	5001	LMG	O7-C10	3.96	1.44	1.35
28	4	4011	CHL	O2D-CGD	3.96	1.42	1.33
18	2	2009	CLA	OBD-CAD	3.96	1.27	1.22
18	1	1003	CLA	C3B-C2B	3.95	1.45	1.40
18	J	1302	CLA	MG-NC	3.95	2.15	2.06
18	4	4017	CLA	C3D-C2D	3.95	1.46	1.39
28	2	2010	CHL	O2D-CGD	3.94	1.42	1.33
21	2	2801	LHG	O7-C7	3.94	1.45	1.34
21	1	1801	LHG	O8-C23	3.93	1.44	1.33
18	A	1022	CLA	C3B-C2B	3.93	1.45	1.40
18	2	2004	CLA	C3C-C2C	3.93	1.45	1.36
18	4	4012	CLA	C1B-NB	-3.93	1.31	1.35
18	1	1011	CLA	C3B-C2B	3.92	1.45	1.40
28	2	2011	CHL	O2A-CGA	3.92	1.44	1.33
18	1	1013	CLA	C3C-C2C	3.92	1.45	1.36
28	4	4013	CHL	O2A-CGA	3.92	1.45	1.33
18	4	4005	CLA	C3D-C2D	3.92	1.46	1.39
28	4	4013	CHL	O2D-CGD	3.91	1.42	1.33
18	A	1151	CLA	MG-NC	3.91	2.15	2.06
18	A	1123	CLA	MG-NC	3.91	2.15	2.06
18	4	4006	CLA	C3D-C2D	3.91	1.46	1.39
18	2	2012	CLA	O2D-CGD	3.91	1.42	1.33
28	1	1010	CHL	O2A-CGA	3.90	1.45	1.33
18	2	2012	CLA	C3D-C2D	3.89	1.46	1.39
18	2	2012	CLA	C3C-C2C	3.88	1.45	1.36
18	B	1206	CLA	MG-NC	3.88	2.15	2.06
18	1	1012	CLA	C3D-C2D	3.88	1.46	1.39
18	1	1012	CLA	C3C-C2C	3.87	1.45	1.36
18	A	1134	CLA	MG-NC	3.87	2.15	2.06
18	1	1005	CLA	C3C-C2C	3.87	1.44	1.36
18	3	3010	CLA	C1B-NB	-3.87	1.31	1.35
18	B	1229	CLA	MG-NC	3.87	2.15	2.06
18	B	1012	CLA	MG-NC	3.86	2.15	2.06
18	4	4003	CLA	C3D-C2D	3.86	1.46	1.39
18	A	1126	CLA	MG-NC	3.86	2.15	2.06
18	3	3007	CLA	C3B-C2B	3.86	1.45	1.40
28	1	1009	CHL	O2D-CGD	3.85	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	1002	CLA	C3D-C2D	3.85	1.46	1.39
18	A	1139	CLA	MG-NC	3.85	2.15	2.06
18	1	1001	CLA	OBD-CAD	3.84	1.27	1.22
23	J	5001	LMG	O7-C10	3.84	1.45	1.34
18	A	1131	CLA	MG-NC	3.84	2.15	2.06
18	2	2012	CLA	C1C-NC	-3.84	1.32	1.37
18	B	1219	CLA	MG-NC	3.84	2.15	2.06
18	1	1008	CLA	C3C-C2C	3.83	1.44	1.36
18	A	1116	CLA	MG-NC	3.83	2.15	2.06
18	2	2001	CLA	C3D-C2D	3.83	1.46	1.39
17	A	1011	CL0	MG-NC	3.83	2.15	2.06
18	B	1216	CLA	MG-NC	3.83	2.15	2.06
18	4	4008	CLA	C4B-NB	-3.82	1.31	1.35
18	B	1214	CLA	MG-NC	3.82	2.15	2.06
18	L	1501	CLA	OBD-CAD	3.82	1.27	1.22
18	3	3017	CLA	C3C-C2C	3.82	1.44	1.36
18	3	3001	CLA	C3B-C2B	3.82	1.45	1.40
18	A	1114	CLA	MG-NC	3.82	2.15	2.06
18	3	3010	CLA	C4B-NB	-3.82	1.31	1.35
18	A	1113	CLA	MG-NC	3.82	2.15	2.06
18	1	1008	CLA	OBD-CAD	3.82	1.27	1.22
18	A	1108	CLA	MG-NC	3.82	2.15	2.06
18	G	1001	CLA	C1C-NC	-3.81	1.32	1.37
18	A	1133	CLA	MG-NC	3.81	2.15	2.06
18	G	1003	CLA	C3B-C2B	3.81	1.45	1.40
23	G	2021	LMG	O7-C10	3.81	1.45	1.34
18	3	3019	CLA	CHC-C1C	3.81	1.48	1.39
18	A	1137	CLA	MG-NC	3.80	2.15	2.06
18	A	1119	CLA	MG-NC	3.80	2.15	2.06
18	3	3004	CLA	C3D-C2D	3.80	1.46	1.39
18	L	1503	CLA	C3C-C2C	3.80	1.44	1.36
18	A	1127	CLA	MG-NC	3.80	2.15	2.06
18	B	1221	CLA	MG-NC	3.80	2.15	2.06
18	B	1225	CLA	MG-NC	3.80	2.15	2.06
18	1	1006	CLA	OBD-CAD	3.80	1.27	1.22
18	H	1000	CLA	MG-NC	3.80	2.15	2.06
18	B	1217	CLA	MG-NC	3.80	2.15	2.06
18	B	1238	CLA	MG-NC	3.80	2.15	2.06
18	4	4006	CLA	C3C-C2C	3.80	1.44	1.36
18	B	1232	CLA	MG-NC	3.79	2.15	2.06
18	A	1124	CLA	MG-NC	3.78	2.15	2.06
18	A	1107	CLA	MG-NC	3.78	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1236	CLA	MG-NC	3.78	2.15	2.06
18	3	3010	CLA	OBD-CAD	3.78	1.27	1.22
18	A	1135	CLA	MG-NC	3.78	2.15	2.06
18	B	1222	CLA	MG-NC	3.77	2.15	2.06
18	A	1104	CLA	MG-NC	3.77	2.15	2.06
18	2	2001	CLA	C3C-C2C	3.77	1.44	1.36
18	1	1006	CLA	C3B-C2B	3.77	1.45	1.40
18	B	1209	CLA	MG-NC	3.77	2.15	2.06
18	B	1215	CLA	MG-NC	3.77	2.15	2.06
18	G	1001	CLA	OBD-CAD	3.77	1.27	1.22
18	A	1112	CLA	MG-NC	3.77	2.15	2.06
18	1	1006	CLA	C3C-C2C	3.77	1.44	1.36
18	B	1208	CLA	MG-NC	3.76	2.15	2.06
23	F	5002	LMG	O7-C10	3.76	1.44	1.34
18	A	1122	CLA	MG-NC	3.76	2.15	2.06
18	B	1223	CLA	MG-NC	3.76	2.15	2.06
18	1	1002	CLA	C3B-C2B	3.75	1.45	1.40
18	B	1201	CLA	MG-NC	3.75	2.15	2.06
18	B	1212	CLA	MG-NC	3.75	2.15	2.06
18	2	2008	CLA	OBD-CAD	3.75	1.27	1.22
18	B	1234	CLA	MG-NC	3.75	2.15	2.06
18	A	1136	CLA	MG-NC	3.75	2.15	2.06
28	4	4011	CHL	C3A-C2A	-3.75	1.44	1.54
18	1	1011	CLA	C3D-C2D	3.75	1.46	1.39
18	4	4004	CLA	C4B-NB	-3.74	1.31	1.35
18	A	1140	CLA	MG-NC	3.74	2.15	2.06
18	A	1105	CLA	MG-NC	3.74	2.15	2.06
18	B	1207	CLA	MG-NC	3.74	2.15	2.06
18	4	4005	CLA	C4B-NB	-3.74	1.31	1.35
18	3	3005	CLA	C3C-C2C	3.73	1.44	1.36
18	4	4007	CLA	C1C-NC	-3.73	1.32	1.37
18	4	4007	CLA	C3C-C2C	3.72	1.44	1.36
18	2	2008	CLA	C3C-C2C	3.72	1.44	1.36
18	A	1115	CLA	MG-NC	3.72	2.15	2.06
18	4	4017	CLA	C3B-C2B	3.72	1.45	1.40
18	A	1111	CLA	MG-NC	3.72	2.15	2.06
18	B	1235	CLA	MG-NC	3.72	2.15	2.06
18	A	1109	CLA	MG-NC	3.72	2.15	2.06
22	F	6016	BCR	C11-C12	-3.72	1.25	1.34
18	B	1218	CLA	MG-NC	3.72	2.15	2.06
18	4	4012	CLA	C3D-C2D	3.71	1.46	1.39
18	L	1501	CLA	C1C-NC	-3.71	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1220	CLA	MG-NC	3.71	2.15	2.06
18	A	1130	CLA	MG-NC	3.71	2.15	2.06
18	1	1014	CLA	C3C-C2C	3.71	1.44	1.36
18	A	1117	CLA	MG-NC	3.71	2.15	2.06
18	4	4008	CLA	C1B-NB	-3.71	1.31	1.35
18	2	2009	CLA	C3B-C2B	3.70	1.45	1.40
18	3	3018	CLA	C3B-C2B	3.70	1.45	1.40
18	A	1125	CLA	MG-NC	3.70	2.15	2.06
18	3	3017	CLA	C1B-NB	-3.70	1.31	1.35
18	A	1128	CLA	MG-NC	3.70	2.15	2.06
18	A	1118	CLA	MG-NC	3.70	2.15	2.06
18	A	1106	CLA	MG-NC	3.70	2.15	2.06
18	4	4004	CLA	C1C-NC	-3.70	1.32	1.37
18	A	1132	CLA	MG-NC	3.70	2.15	2.06
18	4	4006	CLA	OBD-CAD	3.69	1.27	1.22
18	3	3002	CLA	C3B-C2B	3.69	1.45	1.40
18	G	1001	CLA	C3D-C2D	3.69	1.46	1.39
18	2	2004	CLA	C4B-NB	-3.69	1.31	1.35
18	A	1103	CLA	MG-NC	3.69	2.15	2.06
18	A	1237	CLA	MG-NC	3.69	2.15	2.06
18	A	1129	CLA	MG-NC	3.69	2.15	2.06
18	1	1014	CLA	C3D-C2D	3.69	1.46	1.39
18	1	1001	CLA	C3C-C2C	3.68	1.44	1.36
18	A	1138	CLA	MG-NC	3.68	2.15	2.06
18	2	2004	CLA	OBD-CAD	3.68	1.27	1.22
18	B	1203	CLA	MG-NC	3.68	2.15	2.06
18	4	4008	CLA	C3B-C2B	3.68	1.45	1.40
18	1	1012	CLA	C3B-C2B	3.68	1.45	1.40
18	B	1228	CLA	MG-NC	3.68	2.15	2.06
18	2	2004	CLA	C3D-C2D	3.68	1.46	1.39
18	A	1110	CLA	MG-NC	3.68	2.15	2.06
18	4	4002	CLA	C1C-NC	-3.67	1.32	1.37
18	B	1231	CLA	MG-NC	3.67	2.15	2.06
18	A	1120	CLA	MG-NC	3.67	2.15	2.06
23	G	2021	LMG	O8-C28	3.67	1.44	1.33
18	1	1004	CLA	C3D-C2D	3.67	1.46	1.39
18	B	1227	CLA	C1D-C2D	3.67	1.50	1.42
18	B	1204	CLA	MG-NC	3.66	2.15	2.06
18	B	1023	CLA	MG-NC	3.66	2.15	2.06
18	B	1205	CLA	MG-NC	3.66	2.15	2.06
18	1	1002	CLA	C3C-C2C	3.66	1.44	1.36
18	B	1226	CLA	MG-NC	3.66	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1239	CLA	MG-NC	3.65	2.15	2.06
18	B	1240	CLA	MG-NC	3.65	2.14	2.06
18	4	4005	CLA	C3C-C2C	3.65	1.44	1.36
18	2	2002	CLA	OBD-CAD	3.64	1.27	1.22
18	3	3017	CLA	C3D-C2D	3.64	1.46	1.39
18	L	1501	CLA	C3C-C2C	3.64	1.44	1.36
18	2	2012	CLA	OBD-CAD	3.63	1.27	1.22
18	2	2009	CLA	C3D-C2D	3.63	1.45	1.39
18	4	4009	CLA	C1C-NC	-3.63	1.32	1.37
18	3	3003	CLA	C3D-C2D	3.63	1.45	1.39
18	B	1227	CLA	MG-NC	3.63	2.14	2.06
18	4	4006	CLA	C1C-NC	-3.63	1.32	1.37
28	4	4013	CHL	C1B-NB	-3.63	1.32	1.35
18	4	4016	CLA	C3D-C2D	3.63	1.45	1.39
18	4	4009	CLA	C3C-C2C	3.62	1.44	1.36
18	A	1102	CLA	MG-NC	3.62	2.14	2.06
18	A	1121	CLA	MG-NC	3.62	2.14	2.06
18	G	1002	CLA	C3B-C2B	3.62	1.45	1.40
18	2	2003	CLA	C3C-C2C	3.61	1.44	1.36
18	3	3003	CLA	C4B-NB	-3.61	1.32	1.35
18	1	1008	CLA	MG-NC	3.61	2.14	2.06
18	2	2002	CLA	C3B-C2B	3.61	1.45	1.40
18	4	4005	CLA	C1C-NC	-3.61	1.32	1.37
18	4	4002	CLA	C3C-C2C	3.61	1.44	1.36
18	2	2001	CLA	C3B-C2B	3.60	1.45	1.40
18	B	1231	CLA	C1D-C2D	3.60	1.50	1.42
18	2	2001	CLA	C1C-NC	-3.60	1.32	1.37
18	B	1213	CLA	MG-NC	3.60	2.14	2.06
18	3	3012	CLA	C1C-NC	-3.59	1.32	1.37
22	F	6014	BCR	C11-C12	-3.59	1.25	1.34
18	3	3006	CLA	OBD-CAD	3.59	1.27	1.22
18	B	1021	CLA	MG-NC	3.59	2.14	2.06
18	B	1230	CLA	MG-NC	3.59	2.14	2.06
18	G	1001	CLA	C3B-C2B	3.58	1.45	1.40
18	2	2008	CLA	C1C-NC	-3.58	1.32	1.37
18	A	1101	CLA	C1D-C2D	3.58	1.50	1.42
18	1	1001	CLA	C3B-C2B	3.58	1.45	1.40
23	4	4801	LMG	O7-C10	3.58	1.44	1.34
28	3	3011	CHL	C1B-NB	-3.58	1.32	1.35
18	1	1008	CLA	C3D-C2D	3.57	1.45	1.39
18	B	1202	CLA	MG-NC	3.57	2.14	2.06
22	A	6011	BCR	C11-C12	-3.57	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3019	CLA	C4D-C3D	-3.57	1.34	1.42
18	B	1210	CLA	MG-NC	3.56	2.14	2.06
18	K	1001	CLA	C3B-C2B	3.56	1.45	1.40
18	3	3012	CLA	C3D-C2D	3.55	1.45	1.39
18	4	4012	CLA	C1C-NC	-3.55	1.32	1.37
18	1	1005	CLA	OBD-CAD	3.55	1.27	1.22
18	3	3010	CLA	C3B-C2B	3.55	1.45	1.40
18	G	1003	CLA	C3D-C2D	3.54	1.45	1.39
18	4	4001	CLA	OBD-CAD	3.54	1.27	1.22
18	2	2003	CLA	C3D-C2D	3.54	1.45	1.39
22	J	6012	BCR	C11-C12	-3.54	1.25	1.34
18	B	1224	CLA	MG-NC	3.54	2.14	2.06
18	3	3010	CLA	C3D-C2D	3.53	1.45	1.39
18	A	1101	CLA	MG-NC	3.53	2.14	2.06
18	A	1237	CLA	C1D-C2D	3.53	1.50	1.42
18	1	1007	CLA	C3C-C2C	3.53	1.44	1.36
18	1	1001	CLA	C1C-NC	-3.53	1.32	1.37
18	B	1204	CLA	C1D-C2D	3.53	1.50	1.42
18	A	1112	CLA	C1D-C2D	3.53	1.50	1.42
18	1	1013	CLA	C3B-C2B	3.53	1.45	1.40
18	4	4012	CLA	C3C-C2C	3.52	1.44	1.36
18	2	2012	CLA	C4B-NB	-3.52	1.32	1.35
18	B	1214	CLA	C1D-C2D	3.52	1.50	1.42
18	1	1013	CLA	MG-NC	3.51	2.14	2.06
18	A	1134	CLA	C1D-C2D	3.50	1.50	1.42
18	2	2016	CLA	C3C-C2C	3.50	1.44	1.36
18	A	1108	CLA	C1D-C2D	3.50	1.50	1.42
18	A	1132	CLA	C1D-C2D	3.49	1.50	1.42
18	1	1013	CLA	C1D-C2D	3.48	1.50	1.42
18	B	1210	CLA	C1D-C2D	3.48	1.50	1.42
18	A	1117	CLA	C1D-C2D	3.48	1.50	1.42
18	F	1301	CLA	MG-NC	3.48	2.14	2.06
18	L	1502	CLA	C3D-C2D	3.48	1.45	1.39
18	2	2002	CLA	C3C-C2C	3.48	1.44	1.36
18	2	2001	CLA	OBD-CAD	3.47	1.27	1.22
22	A	6008	BCR	C11-C12	-3.47	1.25	1.34
18	1	1005	CLA	C1C-NC	-3.47	1.32	1.37
18	1	1005	CLA	C3B-C2B	3.47	1.45	1.40
23	J	5001	LMG	O8-C28	3.46	1.43	1.33
18	2	2019	CLA	MG-NC	3.46	2.14	2.06
18	4	4002	CLA	C3D-C2D	3.45	1.45	1.39
18	A	1116	CLA	C1D-C2D	3.45	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1013	CLA	MG-NC	3.45	2.14	2.06
18	B	1240	CLA	C1D-C2D	3.45	1.50	1.42
18	2	2016	CLA	C3B-C2B	3.45	1.45	1.40
18	B	1216	CLA	C1D-C2D	3.45	1.50	1.42
18	B	1208	CLA	C1D-C2D	3.44	1.50	1.42
18	2	2003	CLA	MG-NC	3.44	2.14	2.06
18	4	4009	CLA	OBD-CAD	3.44	1.27	1.22
18	B	1201	CLA	C1D-C2D	3.44	1.50	1.42
22	L	6019	BCR	C11-C12	-3.44	1.25	1.34
18	A	1114	CLA	C1D-C2D	3.44	1.50	1.42
18	A	1151	CLA	C1D-C2D	3.44	1.50	1.42
18	3	3003	CLA	OBD-CAD	3.44	1.27	1.22
18	G	1002	CLA	C1D-C2D	3.44	1.50	1.42
18	4	4012	CLA	C4B-NB	-3.44	1.32	1.35
18	4	4007	CLA	C3B-C2B	3.44	1.45	1.40
18	A	1131	CLA	C1D-C2D	3.43	1.50	1.42
18	B	1215	CLA	C1D-C2D	3.43	1.50	1.42
28	2	2013	CHL	C3B-C2B	-3.43	1.35	1.40
18	3	3006	CLA	C4B-NB	-3.43	1.32	1.35
18	A	1115	CLA	C1D-C2D	3.43	1.50	1.42
18	3	3005	CLA	C3B-C2B	3.43	1.45	1.40
18	4	4012	CLA	OBD-CAD	3.43	1.27	1.22
18	A	1105	CLA	C1D-C2D	3.43	1.50	1.42
18	1	1007	CLA	C1C-NC	-3.42	1.32	1.37
28	3	3011	CHL	C3A-C2A	-3.42	1.44	1.54
18	A	1121	CLA	C1D-C2D	3.41	1.50	1.42
18	B	1236	CLA	C1D-C2D	3.41	1.50	1.42
18	A	1122	CLA	C1D-C2D	3.41	1.50	1.42
18	A	1138	CLA	C1D-C2D	3.41	1.50	1.42
18	2	2007	CLA	MG-NC	3.41	2.14	2.06
18	A	1139	CLA	C1D-C2D	3.41	1.50	1.42
18	1	1014	CLA	C1C-NC	-3.41	1.32	1.37
18	3	3017	CLA	C3B-C2B	3.40	1.45	1.40
18	B	1228	CLA	C1D-C2D	3.40	1.50	1.42
18	H	1000	CLA	C1D-C2D	3.40	1.50	1.42
18	B	1211	CLA	MG-NC	3.40	2.14	2.06
18	2	2019	CLA	C4D-C3D	-3.40	1.34	1.42
18	A	1109	CLA	C1D-C2D	3.40	1.50	1.42
18	G	1002	CLA	MG-NC	3.39	2.14	2.06
18	B	1232	CLA	C1D-C2D	3.39	1.50	1.42
18	G	1001	CLA	C3C-C2C	3.39	1.43	1.36
18	B	1235	CLA	C1D-C2D	3.38	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1004	CLA	C1C-NC	-3.38	1.32	1.37
18	A	1140	CLA	C1D-C2D	3.38	1.50	1.42
18	4	4009	CLA	C3B-C2B	3.38	1.45	1.40
18	1	1013	CLA	C3D-C2D	3.38	1.45	1.39
18	A	1120	CLA	C1D-C2D	3.38	1.50	1.42
18	4	4008	CLA	C1C-NC	-3.37	1.32	1.37
18	A	1130	CLA	C1D-C2D	3.37	1.50	1.42
18	B	1209	CLA	C1D-C2D	3.37	1.50	1.42
18	4	4002	CLA	C4B-NB	-3.37	1.32	1.35
18	A	1111	CLA	C1D-C2D	3.36	1.50	1.42
18	A	1110	CLA	C1D-C2D	3.36	1.50	1.42
18	2	2006	CLA	MG-NC	3.36	2.14	2.06
18	J	1302	CLA	C1D-C2D	3.36	1.50	1.42
18	A	1104	CLA	C1D-C2D	3.35	1.50	1.42
18	2	2012	CLA	C1B-NB	-3.35	1.32	1.35
18	A	1106	CLA	C1D-C2D	3.35	1.50	1.42
18	A	1113	CLA	C1D-C2D	3.35	1.50	1.42
18	3	3005	CLA	OBD-CAD	3.35	1.27	1.22
18	2	2019	CLA	CHC-C1C	3.35	1.47	1.39
18	L	1501	CLA	C3D-C2D	3.35	1.45	1.39
18	B	1224	CLA	C1D-C2D	3.35	1.50	1.42
18	4	4017	CLA	C1C-NC	-3.34	1.32	1.37
18	A	1107	CLA	C1D-C2D	3.34	1.50	1.42
18	A	1103	CLA	C1D-C2D	3.34	1.50	1.42
18	B	1239	CLA	C1D-C2D	3.34	1.50	1.42
18	4	4004	CLA	C3D-C2D	3.34	1.45	1.39
18	B	1218	CLA	C1D-C2D	3.34	1.50	1.42
18	A	1119	CLA	C1D-C2D	3.34	1.50	1.42
18	A	1124	CLA	C1D-C2D	3.34	1.50	1.42
18	3	3008	CLA	C3D-C2D	3.34	1.45	1.39
18	G	1003	CLA	C1D-C2D	3.33	1.50	1.42
18	B	1238	CLA	C1D-C2D	3.33	1.50	1.42
18	A	1126	CLA	C1D-C2D	3.33	1.50	1.42
18	A	1135	CLA	C1D-C2D	3.33	1.50	1.42
18	B	1211	CLA	C1D-C2D	3.33	1.50	1.42
18	A	1137	CLA	C1D-C2D	3.33	1.50	1.42
22	J	6013	BCR	C11-C12	-3.33	1.26	1.34
18	B	1217	CLA	C1D-C2D	3.33	1.50	1.42
18	4	4016	CLA	C1D-C2D	3.32	1.50	1.42
18	F	1302	CLA	MG-NC	3.32	2.14	2.06
18	B	1213	CLA	C1D-C2D	3.32	1.50	1.42
18	1	1007	CLA	C3B-C2B	3.31	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3005	CLA	MG-NC	3.31	2.14	2.06
18	3	3006	CLA	C1C-NC	-3.31	1.32	1.37
18	A	1136	CLA	C1D-C2D	3.31	1.50	1.42
28	2	2011	CHL	C1A-CHA	-3.31	1.29	1.43
18	3	3004	CLA	C1C-NC	-3.31	1.32	1.37
18	4	4001	CLA	C3B-C2B	3.30	1.45	1.40
18	3	3013	CLA	C3B-C2B	3.30	1.44	1.40
18	4	4004	CLA	C1B-NB	-3.30	1.32	1.35
18	3	3002	CLA	C1D-C2D	3.30	1.50	1.42
18	B	1226	CLA	C1D-C2D	3.30	1.50	1.42
18	K	1001	CLA	C3D-C2D	3.30	1.45	1.39
18	B	1207	CLA	C1D-C2D	3.29	1.50	1.42
18	3	3017	CLA	C1C-NC	-3.29	1.32	1.37
18	1	1012	CLA	C1C-NC	-3.29	1.32	1.37
22	A	6003	BCR	C11-C12	-3.29	1.26	1.34
18	3	3013	CLA	C1B-NB	-3.28	1.32	1.35
18	B	1219	CLA	C1D-C2D	3.28	1.50	1.42
18	B	1202	CLA	C1D-C2D	3.28	1.50	1.42
18	3	3002	CLA	C3D-C2D	3.28	1.45	1.39
18	4	4009	CLA	C3D-C2D	3.28	1.45	1.39
18	L	1501	CLA	C3B-C2B	3.28	1.44	1.40
18	4	4008	CLA	OBD-CAD	3.28	1.26	1.22
18	2	2002	CLA	MG-NC	3.27	2.14	2.06
18	L	1501	CLA	C1B-NB	-3.27	1.32	1.35
18	B	1234	CLA	C1D-C2D	3.27	1.50	1.42
18	3	3001	CLA	C1C-NC	-3.27	1.32	1.37
18	A	1123	CLA	C1D-C2D	3.27	1.50	1.42
18	3	3018	CLA	C3D-C2D	3.27	1.45	1.39
18	3	3006	CLA	C3D-C2D	3.27	1.45	1.39
18	A	1118	CLA	C1D-C2D	3.27	1.50	1.42
18	3	3012	CLA	C3B-C2B	3.27	1.44	1.40
18	B	1212	CLA	C1D-C2D	3.26	1.50	1.42
18	A	1013	CLA	C1D-C2D	3.26	1.49	1.42
18	4	4001	CLA	C3D-C2D	3.26	1.45	1.39
22	3	3503	BCR	C11-C12	-3.24	1.26	1.34
18	3	3017	CLA	OBD-CAD	3.24	1.26	1.22
18	F	1302	CLA	C1D-C2D	3.24	1.49	1.42
18	3	3010	CLA	C1C-NC	-3.23	1.33	1.37
18	2	2005	CLA	C1D-C2D	3.23	1.49	1.42
18	4	4003	CLA	MG-NC	3.23	2.13	2.06
18	B	1220	CLA	C1D-C2D	3.23	1.49	1.42
22	A	6007	BCR	C11-C12	-3.22	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	1503	CLA	MG-NC	3.22	2.13	2.06
28	4	4010	CHL	C3D-C2D	-3.22	1.33	1.39
18	2	2005	CLA	MG-NC	3.21	2.13	2.06
18	B	1205	CLA	C1D-C2D	3.21	1.49	1.42
22	B	6006	BCR	C11-C12	-3.21	1.26	1.34
18	1	1005	CLA	C3D-C2D	3.21	1.45	1.39
18	B	1229	CLA	C1D-C2D	3.21	1.49	1.42
18	4	4008	CLA	C3C-C2C	3.21	1.43	1.36
18	A	1022	CLA	C1D-C2D	3.21	1.49	1.42
18	B	1221	CLA	C1D-C2D	3.20	1.49	1.42
18	B	1203	CLA	C1D-C2D	3.20	1.49	1.42
28	3	3011	CHL	C1A-CHA	-3.20	1.29	1.43
18	3	3003	CLA	MG-NC	3.20	2.13	2.06
22	F	6014	BCR	C1-C6	-3.20	1.49	1.53
18	1	1002	CLA	C1C-NC	-3.20	1.33	1.37
18	B	1021	CLA	C1D-C2D	3.20	1.49	1.42
18	1	1005	CLA	C4B-NB	-3.20	1.32	1.35
18	1	1003	CLA	C1C-NC	-3.20	1.33	1.37
18	2	2007	CLA	C1D-C2D	3.20	1.49	1.42
18	B	1206	CLA	C1D-C2D	3.20	1.49	1.42
22	B	6009	BCR	C11-C12	-3.19	1.26	1.34
18	2	2001	CLA	C1B-NB	-3.19	1.32	1.35
18	2	2016	CLA	C1C-NC	-3.19	1.33	1.37
18	A	1133	CLA	C1D-C2D	3.19	1.49	1.42
18	3	3005	CLA	C1C-NC	-3.19	1.33	1.37
18	A	1102	CLA	C1D-C2D	3.19	1.49	1.42
18	2	2002	CLA	C3D-C2D	3.19	1.45	1.39
18	4	4009	CLA	C1B-NB	-3.19	1.32	1.35
18	3	3005	CLA	C3D-C2D	3.19	1.45	1.39
18	2	2006	CLA	C1D-C2D	3.19	1.49	1.42
18	L	1502	CLA	MG-NC	3.18	2.13	2.06
18	1	1007	CLA	C4B-NB	-3.18	1.32	1.35
18	3	3003	CLA	C1C-NC	-3.18	1.33	1.37
18	F	1301	CLA	C1D-C2D	3.18	1.49	1.42
18	3	3007	CLA	C1C-NC	-3.18	1.33	1.37
18	1	1006	CLA	MG-NC	3.17	2.13	2.06
18	B	1023	CLA	C1D-C2D	3.17	1.49	1.42
18	A	1127	CLA	C1D-C2D	3.17	1.49	1.42
18	4	4016	CLA	MG-NC	3.16	2.13	2.06
18	2	2016	CLA	MG-NC	3.16	2.13	2.06
18	2	2009	CLA	C1D-C2D	3.16	1.49	1.42
22	I	6020	BCR	C11-C12	-3.15	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4005	CLA	C3B-C2B	3.15	1.44	1.40
18	2	2009	CLA	C1C-NC	-3.15	1.33	1.37
18	1	1006	CLA	C3D-C2D	3.15	1.45	1.39
18	4	4012	CLA	C3B-C2B	3.14	1.44	1.40
18	3	3018	CLA	C1C-NC	-3.14	1.33	1.37
18	K	1001	CLA	C1C-NC	-3.14	1.33	1.37
18	G	1001	CLA	C4B-NB	-3.14	1.32	1.35
18	4	4006	CLA	C1B-NB	-3.14	1.32	1.35
18	B	1222	CLA	C1D-C2D	3.14	1.49	1.42
18	A	1129	CLA	C1D-C2D	3.14	1.49	1.42
18	3	3013	CLA	C1C-NC	-3.13	1.33	1.37
18	2	2002	CLA	C1C-NC	-3.13	1.33	1.37
18	4	4001	CLA	C1C-NC	-3.13	1.33	1.37
22	B	6004	BCR	C11-C12	-3.12	1.26	1.34
22	A	6002	BCR	C11-C12	-3.12	1.26	1.34
18	1	1007	CLA	C3D-C2D	3.12	1.45	1.39
28	4	4010	CHL	C1B-NB	-3.12	1.32	1.35
18	4	4005	CLA	OBD-CAD	3.12	1.26	1.22
18	3	3013	CLA	MG-NC	3.11	2.13	2.06
18	4	4008	CLA	C3D-C2D	3.10	1.45	1.39
18	3	3018	CLA	C1D-C2D	3.10	1.49	1.42
18	2	2003	CLA	C1B-NB	-3.10	1.32	1.35
23	4	4801	LMG	O8-C28	3.10	1.42	1.33
22	B	6010	BCR	C11-C12	-3.10	1.26	1.34
18	3	3007	CLA	C1D-C2D	3.09	1.49	1.42
18	B	1225	CLA	C1D-C2D	3.09	1.49	1.42
18	3	3001	CLA	C3D-C2D	3.09	1.45	1.39
29	4	4505	ZEX	C1-C6	-3.08	1.49	1.53
18	3	3002	CLA	OBD-CAD	3.08	1.26	1.22
18	2	2016	CLA	C1B-NB	-3.08	1.32	1.35
22	J	6013	BCR	C30-C25	-3.08	1.49	1.53
18	4	4006	CLA	C4B-NB	-3.07	1.32	1.35
18	A	1125	CLA	C1D-C2D	3.07	1.49	1.42
18	A	1128	CLA	C1D-C2D	3.07	1.49	1.42
18	G	1003	CLA	MG-NC	3.07	2.13	2.06
18	4	4001	CLA	C1B-NB	-3.07	1.32	1.35
18	3	3019	CLA	CAD-CBD	-3.07	1.50	1.54
18	2	2004	CLA	C1B-NB	-3.07	1.32	1.35
18	4	4007	CLA	C3D-C2D	3.06	1.44	1.39
18	3	3001	CLA	C1D-C2D	3.06	1.49	1.42
18	4	4004	CLA	C3B-C2B	3.06	1.44	1.40
18	3	3006	CLA	C1D-C2D	3.06	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1011	CL0	C1D-C2D	3.06	1.49	1.42
18	3	3002	CLA	MG-NC	3.05	2.13	2.06
22	K	2011	BCR	C11-C12	-3.05	1.26	1.34
18	B	1012	CLA	C1D-C2D	3.04	1.49	1.42
18	1	1006	CLA	C1D-C2D	3.04	1.49	1.42
18	B	1223	CLA	C1D-C2D	3.04	1.49	1.42
18	2	2009	CLA	MG-NC	3.03	2.13	2.06
18	2	2002	CLA	C4B-NB	-3.03	1.32	1.35
18	3	3004	CLA	C4B-NB	-3.03	1.32	1.35
18	3	3007	CLA	MG-NC	3.03	2.13	2.06
22	B	6005	BCR	C11-C12	-3.02	1.26	1.34
18	4	4003	CLA	C1D-C2D	3.02	1.49	1.42
18	1	1003	CLA	C1D-C2D	3.01	1.49	1.42
18	3	3013	CLA	C1D-C2D	3.00	1.49	1.42
18	1	1006	CLA	C1C-NC	-3.00	1.33	1.37
18	1	1011	CLA	C1C-NC	-3.00	1.33	1.37
18	3	3008	CLA	MG-NC	3.00	2.13	2.06
18	4	4005	CLA	C1B-NB	-3.00	1.32	1.35
18	1	1012	CLA	C1D-C2D	2.99	1.49	1.42
18	K	1001	CLA	C1D-C2D	2.99	1.49	1.42
22	L	6020	BCR	C11-C12	-2.99	1.26	1.34
18	1	1001	CLA	MG-NC	2.99	2.13	2.06
22	A	6017	BCR	C11-C12	-2.98	1.26	1.34
18	2	2004	CLA	C3B-C2B	2.98	1.44	1.40
18	3	3012	CLA	C4B-NB	-2.98	1.32	1.35
18	K	1001	CLA	MG-NC	2.98	2.13	2.06
18	L	1503	CLA	C1C-NC	-2.97	1.33	1.37
18	B	1231	CLA	C4B-CHC	2.96	1.49	1.41
18	3	3002	CLA	C1C-NC	-2.96	1.33	1.37
18	3	3005	CLA	C1B-NB	-2.96	1.32	1.35
18	L	1502	CLA	C1C-NC	-2.95	1.33	1.37
28	4	4013	CHL	C1C-NC	-2.95	1.33	1.37
28	2	2011	CHL	C3A-C2A	-2.95	1.46	1.54
18	3	3004	CLA	C1D-C2D	2.95	1.49	1.42
18	2	2008	CLA	C3D-C2D	2.95	1.44	1.39
28	1	1010	CHL	C3B-C2B	-2.95	1.36	1.40
18	G	1003	CLA	C1C-NC	-2.93	1.33	1.37
18	4	4016	CLA	C1C-NC	-2.93	1.33	1.37
18	2	2008	CLA	C4B-NB	-2.93	1.32	1.35
18	2	2001	CLA	C4B-NB	-2.93	1.32	1.35
18	K	1001	CLA	C4B-NB	-2.92	1.32	1.35
18	B	1230	CLA	C1D-C2D	2.92	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4017	CLA	MG-NC	2.91	2.13	2.06
28	2	2010	CHL	C1B-NB	-2.91	1.32	1.35
18	4	4001	CLA	C1D-C2D	2.90	1.49	1.42
18	1	1011	CLA	C1D-C2D	2.90	1.49	1.42
18	3	3006	CLA	MG-NC	2.90	2.13	2.06
18	3	3005	CLA	C4B-NB	-2.88	1.32	1.35
18	3	3004	CLA	C1B-NB	-2.88	1.32	1.35
18	1	1004	CLA	C1D-C2D	2.88	1.49	1.42
18	3	3008	CLA	C1D-C2D	2.88	1.49	1.42
18	3	3003	CLA	C1B-CHB	2.87	1.49	1.41
18	4	4002	CLA	MG-NC	2.87	2.13	2.06
18	4	4008	CLA	MG-NC	2.87	2.13	2.06
18	2	2002	CLA	C1D-C2D	2.86	1.49	1.42
28	2	2010	CHL	C3A-C2A	-2.85	1.46	1.54
18	1	1012	CLA	MG-NC	2.85	2.13	2.06
18	1	1013	CLA	C1B-CHB	2.85	1.48	1.41
28	4	4011	CHL	C1A-CHA	-2.85	1.31	1.43
28	2	2011	CHL	C3D-C2D	-2.85	1.34	1.39
18	4	4017	CLA	C1D-C2D	2.85	1.49	1.42
18	3	3008	CLA	C1B-CHB	2.85	1.48	1.41
18	B	1211	CLA	C4B-CHC	2.84	1.48	1.41
18	B	1234	CLA	C4B-CHC	2.84	1.48	1.41
18	2	2001	CLA	C1D-C2D	2.84	1.49	1.42
18	4	4002	CLA	C1B-CHB	2.84	1.48	1.41
18	1	1002	CLA	C4B-NB	-2.84	1.32	1.35
28	2	2010	CHL	C1A-CHA	-2.84	1.31	1.43
18	2	2005	CLA	C1C-NC	-2.83	1.33	1.37
18	2	2002	CLA	C1B-NB	-2.83	1.32	1.35
18	A	1132	CLA	C4B-CHC	2.82	1.48	1.41
18	L	1502	CLA	C1D-C2D	2.82	1.49	1.42
18	2	2003	CLA	C1B-CHB	2.82	1.48	1.41
18	A	1104	CLA	C4B-CHC	2.82	1.48	1.41
18	3	3018	CLA	MG-NC	2.82	2.13	2.06
18	1	1014	CLA	C1D-C2D	2.82	1.48	1.42
18	G	1001	CLA	C1B-NB	-2.82	1.32	1.35
18	B	1208	CLA	C4B-CHC	2.81	1.48	1.41
18	B	1232	CLA	C4B-CHC	2.81	1.48	1.41
18	A	1105	CLA	C4B-CHC	2.80	1.48	1.41
18	A	1137	CLA	C4B-CHC	2.80	1.48	1.41
18	A	1109	CLA	C4B-CHC	2.80	1.48	1.41
18	A	1013	CLA	C4B-CHC	2.80	1.48	1.41
18	F	1301	CLA	C1B-CHB	2.80	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	1010	CHL	C4B-NB	2.80	1.37	1.35
18	1	1011	CLA	MG-NC	2.79	2.12	2.06
18	A	1110	CLA	C4B-CHC	2.79	1.48	1.41
18	B	1236	CLA	C4B-CHC	2.79	1.48	1.41
18	F	1302	CLA	C1C-NC	-2.78	1.33	1.37
18	3	3008	CLA	C1B-NB	-2.78	1.32	1.35
18	A	1124	CLA	C4B-CHC	2.78	1.48	1.41
18	A	1108	CLA	C4B-CHC	2.78	1.48	1.41
18	4	4005	CLA	MG-NC	2.78	2.12	2.06
18	B	1235	CLA	C4B-CHC	2.77	1.48	1.41
28	4	4011	CHL	C1B-NB	-2.77	1.32	1.35
18	1	1013	CLA	C1C-NC	-2.77	1.33	1.37
18	3	3017	CLA	MG-NC	2.77	2.12	2.06
18	B	1238	CLA	C4B-CHC	2.77	1.48	1.41
18	1	1014	CLA	C1B-NB	-2.76	1.32	1.35
18	2	2019	CLA	CAD-CBD	-2.76	1.50	1.54
18	B	1227	CLA	C4B-CHC	2.76	1.48	1.41
18	A	1138	CLA	C4B-CHC	2.76	1.48	1.41
18	A	1140	CLA	C4B-CHC	2.76	1.48	1.41
18	B	1239	CLA	C4B-CHC	2.76	1.48	1.41
18	A	1120	CLA	C4B-CHC	2.76	1.48	1.41
18	B	1206	CLA	C1B-CHB	2.76	1.48	1.41
17	A	1011	CL0	C4B-CHC	2.76	1.48	1.41
18	B	1012	CLA	C4B-CHC	2.76	1.48	1.41
18	L	1501	CLA	C1D-C2D	2.75	1.48	1.42
18	1	1007	CLA	C1D-C2D	2.75	1.48	1.42
18	1	1003	CLA	MG-NC	2.75	2.12	2.06
18	1	1004	CLA	MG-NC	2.75	2.12	2.06
18	B	1230	CLA	C4B-CHC	2.75	1.48	1.41
18	B	1229	CLA	C4B-CHC	2.75	1.48	1.41
18	B	1218	CLA	C4B-CHC	2.75	1.48	1.41
18	2	2016	CLA	C1B-CHB	2.74	1.48	1.41
18	A	1022	CLA	C4B-CHC	2.74	1.48	1.41
18	4	4009	CLA	C4B-NB	-2.74	1.32	1.35
18	A	1107	CLA	C4B-CHC	2.74	1.48	1.41
18	F	1301	CLA	C1C-NC	-2.74	1.33	1.37
18	1	1007	CLA	MG-NC	2.73	2.12	2.06
18	A	1134	CLA	C4B-CHC	2.73	1.48	1.41
18	A	1116	CLA	C4B-CHC	2.73	1.48	1.41
18	A	1126	CLA	C4B-CHC	2.73	1.48	1.41
18	A	1131	CLA	C4B-CHC	2.73	1.48	1.41
18	B	1221	CLA	C4B-CHC	2.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3017	CLA	C4B-NB	-2.73	1.32	1.35
18	A	1139	CLA	C4B-CHC	2.72	1.48	1.41
18	A	1121	CLA	C4B-CHC	2.72	1.48	1.41
18	1	1014	CLA	MG-NC	2.72	2.12	2.06
18	B	1240	CLA	C4B-CHC	2.72	1.48	1.41
18	2	2006	CLA	C1B-CHB	2.71	1.48	1.41
18	1	1005	CLA	MG-NC	2.71	2.12	2.06
18	L	1501	CLA	C4B-NB	-2.71	1.32	1.35
18	A	1136	CLA	C4B-CHC	2.71	1.48	1.41
18	3	3010	CLA	C1D-C2D	2.71	1.48	1.42
18	A	1115	CLA	C4B-CHC	2.71	1.48	1.41
18	A	1112	CLA	C4B-CHC	2.71	1.48	1.41
18	B	1023	CLA	C4B-CHC	2.70	1.48	1.41
18	B	1201	CLA	C4B-CHC	2.70	1.48	1.41
18	B	1225	CLA	C1B-CHB	2.70	1.48	1.41
18	B	1204	CLA	C4B-CHC	2.70	1.48	1.41
18	A	1130	CLA	C4B-CHC	2.70	1.48	1.41
18	A	1129	CLA	C4B-CHC	2.70	1.48	1.41
18	3	3003	CLA	C1D-C2D	2.70	1.48	1.42
18	2	2007	CLA	C1B-CHB	2.70	1.48	1.41
18	2	2005	CLA	C1B-CHB	2.70	1.48	1.41
18	B	1236	CLA	C1B-CHB	2.70	1.48	1.41
18	B	1207	CLA	C4B-CHC	2.70	1.48	1.41
18	B	1216	CLA	C4B-CHC	2.70	1.48	1.41
18	A	1113	CLA	C4B-CHC	2.69	1.48	1.41
18	A	1137	CLA	C1B-CHB	2.69	1.48	1.41
28	4	4013	CHL	C1A-CHA	-2.69	1.31	1.43
18	2	2016	CLA	C4B-NB	-2.69	1.32	1.35
18	B	1213	CLA	C4B-CHC	2.69	1.48	1.41
18	B	1205	CLA	C4B-CHC	2.69	1.48	1.41
18	A	1140	CLA	C1B-CHB	2.69	1.48	1.41
18	L	1503	CLA	C1D-C2D	2.69	1.48	1.42
18	2	2012	CLA	C3B-C2B	2.69	1.44	1.40
18	A	1102	CLA	C4B-CHC	2.69	1.48	1.41
18	B	1222	CLA	C4B-CHC	2.69	1.48	1.41
18	B	1225	CLA	C4B-CHC	2.68	1.48	1.41
18	A	1118	CLA	C4B-CHC	2.68	1.48	1.41
18	1	1008	CLA	C1B-CHB	2.68	1.48	1.41
28	2	2013	CHL	C4B-NB	2.68	1.37	1.35
18	A	1103	CLA	C1B-CHB	2.68	1.48	1.41
18	4	4001	CLA	MG-NC	2.68	2.12	2.06
18	4	4012	CLA	C1D-C2D	2.68	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1131	CLA	C1B-CHB	2.68	1.48	1.41
18	B	1217	CLA	C4B-CHC	2.67	1.48	1.41
18	B	1228	CLA	C4B-CHC	2.67	1.48	1.41
18	L	1501	CLA	MG-NC	2.67	2.12	2.06
18	4	4001	CLA	C4B-NB	-2.66	1.32	1.35
18	2	2008	CLA	C1B-NB	-2.66	1.32	1.35
18	A	1130	CLA	C1B-CHB	2.66	1.48	1.41
18	1	1008	CLA	C1D-C2D	2.66	1.48	1.42
18	B	1219	CLA	C4B-CHC	2.66	1.48	1.41
18	B	1230	CLA	C1B-CHB	2.66	1.48	1.41
18	1	1001	CLA	C1D-C2D	2.66	1.48	1.42
18	A	1114	CLA	C4B-CHC	2.66	1.48	1.41
18	B	1223	CLA	C4B-CHC	2.66	1.48	1.41
18	A	1118	CLA	C1B-CHB	2.66	1.48	1.41
18	B	1234	CLA	C1B-CHB	2.66	1.48	1.41
18	3	3007	CLA	C1B-NB	-2.66	1.32	1.35
18	A	1151	CLA	C4B-CHC	2.66	1.48	1.41
18	B	1210	CLA	C1C-NC	-2.65	1.33	1.37
18	4	4003	CLA	C1C-NC	-2.65	1.33	1.37
18	B	1209	CLA	C4B-CHC	2.65	1.48	1.41
18	B	1203	CLA	C4B-CHC	2.65	1.48	1.41
18	J	1302	CLA	C4B-CHC	2.65	1.48	1.41
28	3	3011	CHL	C3D-C2D	-2.65	1.34	1.39
18	2	2003	CLA	C1C-NC	-2.65	1.33	1.37
18	B	1220	CLA	C4B-CHC	2.65	1.48	1.41
18	L	1502	CLA	C4B-CHC	2.65	1.48	1.41
18	4	4007	CLA	C4B-NB	-2.65	1.32	1.35
18	1	1002	CLA	C1B-CHB	2.64	1.48	1.41
18	3	3017	CLA	C1D-C2D	2.64	1.48	1.42
18	A	1114	CLA	C1B-CHB	2.64	1.48	1.41
18	A	1134	CLA	C1B-CHB	2.64	1.48	1.41
18	2	2006	CLA	C1C-NC	-2.64	1.33	1.37
18	A	1237	CLA	C1B-CHB	2.64	1.48	1.41
18	A	1107	CLA	C1B-CHB	2.64	1.48	1.41
18	A	1125	CLA	C4B-CHC	2.64	1.48	1.41
18	A	1122	CLA	C4B-CHC	2.64	1.48	1.41
18	B	1021	CLA	C4B-CHC	2.64	1.48	1.41
18	B	1215	CLA	C4B-CHC	2.64	1.48	1.41
18	G	1002	CLA	C1C-NC	-2.64	1.33	1.37
18	A	1123	CLA	C4B-CHC	2.63	1.48	1.41
18	B	1214	CLA	C4B-CHC	2.63	1.48	1.41
18	B	1212	CLA	C4B-CHC	2.63	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1210	CLA	C4B-CHC	2.63	1.48	1.41
18	A	1103	CLA	C4B-CHC	2.63	1.48	1.41
18	B	1211	CLA	C1C-NC	-2.63	1.33	1.37
18	4	4007	CLA	C1B-CHB	2.63	1.48	1.41
18	3	3004	CLA	MG-NC	2.62	2.12	2.06
18	B	1229	CLA	C1B-CHB	2.62	1.48	1.41
18	2	2012	CLA	C1D-C2D	2.62	1.48	1.42
18	B	1217	CLA	C1B-CHB	2.62	1.48	1.41
18	L	1503	CLA	C4B-CHC	2.62	1.48	1.41
18	B	1235	CLA	C1B-CHB	2.62	1.48	1.41
18	4	4009	CLA	C1D-C2D	2.62	1.48	1.42
18	B	1231	CLA	CHD-C4C	2.62	1.48	1.41
18	B	1239	CLA	C1B-CHB	2.62	1.48	1.41
18	A	1120	CLA	C1B-CHB	2.62	1.48	1.41
18	2	2016	CLA	C3D-C2D	2.62	1.44	1.39
18	A	1151	CLA	C1B-CHB	2.62	1.48	1.41
18	A	1129	CLA	C1B-CHB	2.62	1.48	1.41
18	B	1208	CLA	C1B-CHB	2.61	1.48	1.41
18	B	1218	CLA	C1B-CHB	2.61	1.48	1.41
18	1	1002	CLA	C1D-C2D	2.61	1.48	1.42
18	4	4016	CLA	C1B-CHB	2.61	1.48	1.41
18	A	1115	CLA	CHD-C4C	2.61	1.48	1.41
18	B	1226	CLA	CHD-C4C	2.61	1.48	1.41
18	B	1212	CLA	C1B-CHB	2.61	1.48	1.41
18	B	1213	CLA	C1B-CHB	2.61	1.48	1.41
18	B	1205	CLA	C1B-CHB	2.61	1.48	1.41
18	A	1117	CLA	C4B-CHC	2.61	1.48	1.41
18	A	1127	CLA	C1B-CHB	2.61	1.48	1.41
18	A	1119	CLA	C4B-CHC	2.61	1.48	1.41
18	G	1001	CLA	C1D-C2D	2.60	1.48	1.42
18	A	1127	CLA	C4B-CHC	2.60	1.48	1.41
18	3	3006	CLA	C1B-CHB	2.60	1.48	1.41
18	1	1005	CLA	C1B-NB	-2.60	1.32	1.35
18	A	1135	CLA	C1B-CHB	2.60	1.48	1.41
22	J	6012	BCR	C30-C25	-2.60	1.50	1.53
18	4	4006	CLA	MG-NC	2.60	2.12	2.06
18	1	1001	CLA	C1B-NB	-2.59	1.32	1.35
18	2	2004	CLA	C4B-CHC	2.59	1.48	1.41
18	A	1135	CLA	C4B-CHC	2.59	1.48	1.41
18	4	4005	CLA	C1B-CHB	2.59	1.48	1.41
18	B	1203	CLA	C1B-CHB	2.59	1.48	1.41
18	A	1134	CLA	CHD-C4C	2.59	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4003	CLA	C1B-CHB	2.59	1.48	1.41
18	B	1201	CLA	C1B-CHB	2.59	1.48	1.41
18	B	1202	CLA	C4B-CHC	2.59	1.48	1.41
18	G	1001	CLA	MG-NC	2.59	2.12	2.06
18	J	1302	CLA	C1B-CHB	2.59	1.48	1.41
18	A	1237	CLA	C4B-CHC	2.58	1.48	1.41
18	4	4007	CLA	C1D-C2D	2.58	1.48	1.42
18	A	1138	CLA	CHD-C4C	2.58	1.48	1.41
18	A	1122	CLA	C1B-CHB	2.58	1.48	1.41
18	A	1101	CLA	C4B-CHC	2.58	1.48	1.41
18	B	1219	CLA	C1B-CHB	2.58	1.48	1.41
18	3	3007	CLA	C4B-NB	-2.58	1.32	1.35
18	F	1302	CLA	C1B-CHB	2.58	1.48	1.41
18	A	1125	CLA	C1B-CHB	2.58	1.48	1.41
18	1	1008	CLA	C1C-NC	-2.58	1.34	1.37
18	A	1116	CLA	C1B-CHB	2.58	1.48	1.41
18	4	4009	CLA	MG-NC	2.58	2.12	2.06
18	A	1115	CLA	C1B-CHB	2.58	1.48	1.41
18	A	1106	CLA	C4B-CHC	2.58	1.48	1.41
18	1	1013	CLA	CHD-C4C	2.57	1.48	1.41
18	2	2001	CLA	C2A-C1A	-2.57	1.46	1.52
18	A	1022	CLA	CHD-C4C	2.57	1.48	1.41
18	A	1117	CLA	CHD-C4C	2.57	1.48	1.41
18	A	1105	CLA	C1B-CHB	2.57	1.48	1.41
18	A	1124	CLA	CHD-C4C	2.57	1.48	1.41
28	4	4013	CHL	C3A-C2A	-2.57	1.47	1.54
18	H	1000	CLA	C1B-CHB	2.57	1.48	1.41
18	1	1004	CLA	C1B-CHB	2.57	1.48	1.41
18	2	2007	CLA	C1C-NC	-2.57	1.34	1.37
18	B	1204	CLA	CHD-C4C	2.57	1.48	1.41
18	3	3002	CLA	C1B-CHB	2.56	1.48	1.41
18	A	1137	CLA	C1C-NC	-2.56	1.34	1.37
28	3	3011	CHL	C1C-NC	-2.56	1.34	1.37
18	A	1136	CLA	C1B-CHB	2.56	1.48	1.41
18	H	1000	CLA	CHD-C4C	2.56	1.48	1.41
28	2	2010	CHL	C1C-NC	-2.56	1.34	1.37
18	A	1133	CLA	C1B-CHB	2.56	1.48	1.41
18	A	1113	CLA	C1B-CHB	2.56	1.48	1.41
18	A	1116	CLA	CHD-C4C	2.56	1.48	1.41
18	B	1207	CLA	C1B-CHB	2.56	1.48	1.41
18	B	1216	CLA	CHD-C4C	2.56	1.48	1.41
18	4	4007	CLA	MG-NC	2.56	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1139	CLA	C1B-CHB	2.56	1.48	1.41
18	B	1238	CLA	C1B-CHB	2.55	1.48	1.41
18	A	1112	CLA	CHD-C4C	2.55	1.48	1.41
18	F	1302	CLA	C4B-CHC	2.55	1.48	1.41
18	3	3013	CLA	C4B-CHC	2.55	1.48	1.41
18	B	1204	CLA	C1B-CHB	2.55	1.48	1.41
18	L	1501	CLA	C4B-CHC	2.55	1.48	1.41
18	F	1301	CLA	C4B-CHC	2.55	1.48	1.41
18	A	1126	CLA	CHD-C4C	2.55	1.48	1.41
18	B	1202	CLA	C1B-CHB	2.55	1.48	1.41
18	B	1202	CLA	CHD-C4C	2.55	1.48	1.41
18	B	1214	CLA	CHD-C4C	2.55	1.48	1.41
18	B	1215	CLA	C1B-CHB	2.55	1.48	1.41
18	B	1240	CLA	C1B-CHB	2.55	1.48	1.41
18	B	1240	CLA	CHD-C4C	2.54	1.48	1.41
18	B	1218	CLA	CHD-C4C	2.54	1.48	1.41
18	B	1208	CLA	CHD-C4C	2.54	1.48	1.41
18	A	1117	CLA	C1B-CHB	2.54	1.48	1.41
18	A	1128	CLA	C1B-CHB	2.54	1.48	1.41
18	2	2003	CLA	C1D-C2D	2.54	1.48	1.42
18	A	1139	CLA	CHD-C4C	2.54	1.48	1.41
18	B	1228	CLA	CHD-C4C	2.54	1.48	1.41
18	A	1109	CLA	CHD-C4C	2.54	1.48	1.41
18	A	1133	CLA	C4B-CHC	2.54	1.48	1.41
18	L	1502	CLA	C1B-CHB	2.54	1.48	1.41
18	B	1209	CLA	CHD-C4C	2.54	1.48	1.41
18	B	1021	CLA	C1B-CHB	2.53	1.48	1.41
18	4	4017	CLA	C1B-NB	-2.53	1.32	1.35
18	A	1102	CLA	C1B-CHB	2.53	1.48	1.41
18	G	1001	CLA	C1B-CHB	2.53	1.48	1.41
28	4	4010	CHL	C1A-CHA	-2.53	1.32	1.43
18	B	1214	CLA	C1B-CHB	2.53	1.48	1.41
18	A	1107	CLA	CHD-C4C	2.53	1.48	1.41
18	H	1000	CLA	C4B-CHC	2.53	1.48	1.41
18	B	1220	CLA	CHD-C4C	2.53	1.48	1.41
18	A	1111	CLA	C4B-CHC	2.53	1.48	1.41
18	1	1002	CLA	MG-NC	2.53	2.12	2.06
18	3	3004	CLA	C3B-C2B	2.53	1.43	1.40
18	J	1302	CLA	CHD-C4C	2.53	1.48	1.41
18	A	1124	CLA	C1B-CHB	2.53	1.48	1.41
18	A	1013	CLA	CHD-C4C	2.53	1.48	1.41
18	2	2004	CLA	C1D-C2D	2.53	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3006	CLA	C1B-NB	-2.53	1.33	1.35
18	3	3019	CLA	C1B-CHB	2.53	1.48	1.43
18	2	2005	CLA	C4B-CHC	2.53	1.48	1.41
18	B	1012	CLA	C1B-CHB	2.53	1.48	1.41
18	B	1226	CLA	C1B-CHB	2.53	1.48	1.41
18	B	1023	CLA	CHD-C4C	2.52	1.48	1.41
18	1	1001	CLA	C4B-NB	-2.52	1.33	1.35
18	A	1106	CLA	CHD-C4C	2.52	1.48	1.41
18	A	1108	CLA	CHD-C4C	2.52	1.48	1.41
18	B	1209	CLA	C1B-CHB	2.52	1.48	1.41
18	G	1003	CLA	C4B-CHC	2.52	1.48	1.41
18	2	2006	CLA	C4B-CHC	2.52	1.48	1.41
18	A	1123	CLA	C1B-CHB	2.52	1.48	1.41
18	A	1237	CLA	CHD-C4C	2.52	1.48	1.41
18	A	1122	CLA	CHD-C4C	2.52	1.48	1.41
18	A	1104	CLA	C1B-CHB	2.52	1.48	1.41
18	A	1130	CLA	CHD-C4C	2.52	1.48	1.41
18	A	1138	CLA	C1B-CHB	2.51	1.48	1.41
18	B	1220	CLA	C1B-CHB	2.51	1.48	1.41
18	B	1223	CLA	C1C-NC	-2.51	1.34	1.37
18	B	1215	CLA	CHD-C4C	2.51	1.48	1.41
21	B	5004	LHG	O8-C23	2.51	1.45	1.33
18	2	2007	CLA	C4B-CHC	2.51	1.48	1.41
18	A	1114	CLA	CHD-C4C	2.51	1.48	1.41
18	A	1121	CLA	C1B-CHB	2.51	1.48	1.41
18	B	1224	CLA	C4C-C3C	2.51	1.49	1.45
18	A	1105	CLA	CHD-C4C	2.51	1.48	1.41
18	4	4006	CLA	C1D-C2D	2.51	1.48	1.42
18	A	1126	CLA	C4C-C3C	2.51	1.49	1.45
18	A	1132	CLA	CHD-C4C	2.50	1.48	1.41
18	B	1223	CLA	C1B-CHB	2.50	1.48	1.41
18	A	1121	CLA	CHD-C4C	2.50	1.48	1.41
18	B	1205	CLA	CHD-C4C	2.50	1.48	1.41
18	B	1224	CLA	C4B-CHC	2.50	1.47	1.41
18	A	1108	CLA	C1B-CHB	2.50	1.47	1.41
18	A	1101	CLA	CHD-C4C	2.50	1.48	1.41
18	B	1023	CLA	C4C-C3C	2.50	1.49	1.45
18	2	2002	CLA	C1B-CHB	2.50	1.47	1.41
18	A	1106	CLA	C1B-CHB	2.50	1.47	1.41
18	1	1012	CLA	C1B-NB	-2.50	1.33	1.35
18	B	1211	CLA	CHD-C4C	2.50	1.48	1.41
18	A	1113	CLA	CHD-C4C	2.50	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1210	CLA	CHD-C4C	2.50	1.48	1.41
18	B	1222	CLA	C1B-CHB	2.49	1.47	1.41
28	4	4011	CHL	C4B-NB	2.49	1.37	1.35
18	A	1135	CLA	CHD-C4C	2.49	1.48	1.41
18	B	1227	CLA	CHD-C4C	2.49	1.48	1.41
18	3	3012	CLA	C1D-C2D	2.49	1.48	1.42
18	B	1224	CLA	CHD-C4C	2.49	1.48	1.41
18	2	2019	CLA	CHD-C4C	2.49	1.48	1.41
29	4	4505	ZEX	C21-C26	-2.49	1.50	1.53
18	A	1125	CLA	C1C-NC	-2.49	1.34	1.37
18	A	1119	CLA	C1B-CHB	2.49	1.47	1.41
18	B	1217	CLA	CHD-C4C	2.49	1.48	1.41
18	B	1232	CLA	CHD-C4C	2.48	1.48	1.41
18	A	1151	CLA	CHD-C4C	2.48	1.48	1.41
18	2	2001	CLA	MG-NC	2.48	2.12	2.06
18	A	1127	CLA	CHD-C4C	2.48	1.48	1.41
18	A	1022	CLA	C1B-CHB	2.48	1.47	1.41
18	B	1221	CLA	C1B-CHB	2.48	1.47	1.41
18	B	1232	CLA	C1B-CHB	2.48	1.47	1.41
18	A	1110	CLA	CHD-C4C	2.48	1.48	1.41
18	A	1151	CLA	C4C-C3C	2.48	1.49	1.45
18	B	1231	CLA	C1B-CHB	2.48	1.47	1.41
18	A	1136	CLA	CHD-C4C	2.48	1.48	1.41
18	B	1201	CLA	CHD-C4C	2.48	1.48	1.41
18	3	3005	CLA	C4B-CHC	2.48	1.47	1.41
18	A	1119	CLA	CHD-C4C	2.48	1.48	1.41
18	1	1007	CLA	C1B-NB	-2.47	1.33	1.35
18	A	1140	CLA	CHD-C4C	2.47	1.48	1.41
18	B	1219	CLA	CHD-C4C	2.47	1.48	1.41
18	1	1006	CLA	C1B-NB	-2.47	1.33	1.35
18	B	1228	CLA	C1B-CHB	2.47	1.47	1.41
18	B	1227	CLA	C1B-CHB	2.47	1.47	1.41
18	A	1151	CLA	C1C-NC	-2.47	1.34	1.37
18	A	1110	CLA	C1B-CHB	2.47	1.47	1.41
18	A	1133	CLA	CHD-C4C	2.47	1.48	1.41
18	1	1005	CLA	C1B-CHB	2.47	1.47	1.41
18	L	1503	CLA	C1B-CHB	2.47	1.47	1.41
18	A	1111	CLA	C1C-NC	-2.47	1.34	1.37
18	G	1002	CLA	C1B-CHB	2.47	1.47	1.41
18	B	1220	CLA	C1C-NC	-2.46	1.34	1.37
18	B	1238	CLA	CHD-C4C	2.46	1.48	1.41
18	1	1006	CLA	C4B-CHC	2.46	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1239	CLA	CHD-C4C	2.46	1.48	1.41
18	B	1234	CLA	CHD-C4C	2.46	1.48	1.41
18	A	1103	CLA	CHD-C4C	2.45	1.48	1.41
18	1	1011	CLA	C4B-CHC	2.45	1.47	1.41
18	4	4017	CLA	C4B-CHC	2.45	1.47	1.41
18	B	1229	CLA	C1C-NC	-2.45	1.34	1.37
18	A	1111	CLA	CHD-C4C	2.45	1.48	1.41
18	B	1023	CLA	C1B-CHB	2.45	1.47	1.41
18	3	3017	CLA	C4B-CHC	2.45	1.47	1.41
18	B	1206	CLA	CHD-C4C	2.45	1.48	1.41
18	3	3005	CLA	C1B-CHB	2.44	1.47	1.41
18	A	1128	CLA	CHD-C4C	2.44	1.48	1.41
18	B	1207	CLA	C1C-NC	-2.44	1.34	1.37
18	A	1132	CLA	C1C-NC	-2.44	1.34	1.37
18	4	4002	CLA	C1D-C2D	2.44	1.48	1.42
18	2	2016	CLA	C1D-C2D	2.44	1.48	1.42
18	3	3007	CLA	C4B-CHC	2.44	1.47	1.41
18	A	1131	CLA	CHD-C4C	2.44	1.48	1.41
18	B	1213	CLA	CHD-C4C	2.44	1.48	1.41
22	G	2011	BCR	C1-C6	-2.44	1.50	1.53
18	B	1206	CLA	C4B-CHC	2.44	1.47	1.41
18	A	1101	CLA	C1B-CHB	2.44	1.47	1.41
18	A	1109	CLA	C1B-CHB	2.44	1.47	1.41
18	A	1123	CLA	CHD-C4C	2.44	1.48	1.41
18	A	1120	CLA	CHD-C4C	2.44	1.48	1.41
18	B	1236	CLA	CHD-C4C	2.44	1.48	1.41
18	A	1133	CLA	C1C-NC	-2.44	1.34	1.37
18	B	1205	CLA	C1C-NC	-2.44	1.34	1.37
18	2	2012	CLA	MG-NC	2.44	2.12	2.06
18	B	1204	CLA	C1C-NC	-2.43	1.34	1.37
18	A	1128	CLA	C4B-CHC	2.43	1.47	1.41
18	1	1003	CLA	CHD-C4C	2.43	1.48	1.41
18	A	1113	CLA	C4C-C3C	2.43	1.49	1.45
18	A	1114	CLA	C4C-C3C	2.43	1.49	1.45
18	3	3019	CLA	CHD-C4C	2.43	1.48	1.41
18	3	3008	CLA	C4B-NB	-2.43	1.33	1.35
18	A	1126	CLA	C1B-CHB	2.43	1.47	1.41
18	A	1101	CLA	C1C-NC	-2.43	1.34	1.37
18	B	1225	CLA	CHD-C4C	2.42	1.48	1.41
18	1	1006	CLA	CHD-C4C	2.42	1.48	1.41
18	A	1118	CLA	CHD-C4C	2.42	1.48	1.41
18	A	1129	CLA	CHD-C4C	2.42	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	5001	LMG	O7-C8	-2.42	1.40	1.46
18	3	3001	CLA	MG-NC	2.42	2.12	2.06
18	3	3001	CLA	C4B-CHC	2.42	1.47	1.41
18	B	1235	CLA	CHD-C4C	2.42	1.48	1.41
17	A	1011	CL0	C1B-CHB	2.41	1.47	1.41
18	A	1110	CLA	C1C-NC	-2.41	1.34	1.37
18	A	1237	CLA	C1C-NC	-2.41	1.34	1.37
18	1	1004	CLA	C4B-NB	-2.41	1.33	1.35
18	4	4004	CLA	C4B-CHC	2.41	1.47	1.41
18	B	1221	CLA	CHD-C4C	2.41	1.48	1.41
18	3	3010	CLA	MG-NC	2.41	2.12	2.06
18	L	1503	CLA	C1B-NB	-2.41	1.33	1.35
18	1	1005	CLA	C1D-C2D	2.41	1.48	1.42
18	2	2009	CLA	C1B-NB	-2.41	1.33	1.35
18	3	3008	CLA	C1C-NC	-2.41	1.34	1.37
18	B	1210	CLA	C1B-CHB	2.41	1.47	1.41
18	A	1132	CLA	C1B-CHB	2.40	1.47	1.41
18	A	1115	CLA	C4C-C3C	2.40	1.49	1.45
28	1	1010	CHL	C3D-C2D	-2.40	1.35	1.39
18	2	2009	CLA	C1B-CHB	2.40	1.47	1.41
25	B	7101	DGD	O2G-C2G	-2.40	1.40	1.46
18	3	3018	CLA	C4B-NB	-2.39	1.33	1.35
18	4	4008	CLA	C1B-CHB	2.39	1.47	1.41
18	B	1210	CLA	C4C-C3C	2.39	1.49	1.45
17	A	1011	CL0	CHD-C4C	2.39	1.48	1.41
18	3	3012	CLA	MG-NC	2.39	2.12	2.06
18	B	1209	CLA	C4C-C3C	2.39	1.49	1.45
18	A	1137	CLA	CHD-C4C	2.39	1.48	1.41
18	A	1114	CLA	C1C-NC	-2.39	1.34	1.37
18	3	3005	CLA	C1D-C2D	2.39	1.48	1.42
18	3	3004	CLA	C1B-CHB	2.39	1.47	1.41
18	A	1119	CLA	C1C-NC	-2.39	1.34	1.37
27	1	1502	LUT	C10-C9	-2.39	1.32	1.35
18	3	3019	CLA	C3C-C4C	2.39	1.48	1.43
18	B	1236	CLA	C1C-NC	-2.38	1.34	1.37
18	B	1213	CLA	C1C-NC	-2.38	1.34	1.37
18	2	2009	CLA	C4B-CHC	2.38	1.47	1.41
18	A	1121	CLA	C1C-NC	-2.38	1.34	1.37
18	G	1003	CLA	C1B-CHB	2.38	1.47	1.41
18	4	4003	CLA	C4B-CHC	2.38	1.47	1.41
18	2	2008	CLA	C1D-C2D	2.38	1.48	1.42
18	A	1101	CLA	C4C-C3C	2.38	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1217	CLA	C1C-NC	-2.38	1.34	1.37
18	B	1021	CLA	CHD-C4C	2.38	1.47	1.41
18	B	1023	CLA	C1C-NC	-2.38	1.34	1.37
18	B	1212	CLA	CHD-C4C	2.38	1.47	1.41
22	F	6016	BCR	C1-C6	-2.38	1.50	1.53
18	2	2008	CLA	C1B-CHB	2.38	1.47	1.41
18	H	1000	CLA	C1C-NC	-2.38	1.34	1.37
18	4	4008	CLA	C1D-C2D	2.37	1.47	1.42
18	A	1113	CLA	C1C-NC	-2.37	1.34	1.37
18	A	1105	CLA	C1C-NC	-2.37	1.34	1.37
18	B	1203	CLA	CHD-C4C	2.37	1.47	1.41
18	B	1228	CLA	C1C-NC	-2.37	1.34	1.37
18	A	1022	CLA	C4C-C3C	2.37	1.49	1.45
22	L	6019	BCR	C1-C6	-2.37	1.50	1.53
18	B	1232	CLA	C1C-NC	-2.37	1.34	1.37
18	2	2006	CLA	CHD-C4C	2.37	1.47	1.41
18	4	4012	CLA	MG-NC	2.37	2.11	2.06
18	3	3001	CLA	C4B-NB	-2.37	1.33	1.35
18	A	1128	CLA	C1C-NC	-2.37	1.34	1.37
18	3	3013	CLA	CHD-C4C	2.37	1.47	1.41
27	3	3502	LUT	C1-C6	-2.37	1.50	1.53
18	A	1109	CLA	C1C-NC	-2.36	1.34	1.37
18	4	4005	CLA	C1D-C2D	2.36	1.47	1.42
18	B	1224	CLA	C1B-CHB	2.36	1.47	1.41
18	A	1120	CLA	C1C-NC	-2.36	1.34	1.37
18	B	1207	CLA	CHD-C4C	2.36	1.47	1.41
18	B	1226	CLA	C4B-CHC	2.36	1.47	1.41
18	1	1003	CLA	C1B-CHB	2.36	1.47	1.41
18	F	1302	CLA	CHD-C4C	2.36	1.47	1.41
18	B	1209	CLA	C1C-NC	-2.36	1.34	1.37
18	A	1106	CLA	C1C-NC	-2.36	1.34	1.37
27	1	1501	LUT	C23-C24	2.36	1.53	1.50
18	4	4016	CLA	C4B-CHC	2.36	1.47	1.41
18	A	1112	CLA	C1C-NC	-2.36	1.34	1.37
18	B	1012	CLA	CHD-C4C	2.36	1.47	1.41
18	1	1012	CLA	C1B-CHB	2.36	1.47	1.41
18	A	1135	CLA	C4C-C3C	2.35	1.49	1.45
18	A	1013	CLA	C1B-CHB	2.35	1.47	1.41
18	B	1202	CLA	C1C-NC	-2.35	1.34	1.37
18	B	1214	CLA	C1C-NC	-2.35	1.34	1.37
27	1	1501	LUT	C1-C6	-2.35	1.50	1.53
18	A	1103	CLA	C1C-NC	-2.35	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	3503	BCR	C1-C6	-2.35	1.50	1.53
18	A	1138	CLA	C1C-NC	-2.35	1.34	1.37
18	1	1012	CLA	C4B-NB	-2.35	1.33	1.35
18	B	1238	CLA	C1C-NC	-2.35	1.34	1.37
18	2	2009	CLA	C4B-NB	-2.35	1.33	1.35
18	G	1002	CLA	C4B-CHC	2.35	1.47	1.41
18	2	2019	CLA	C1C-NC	-2.35	1.33	1.38
17	A	1011	CL0	C1C-NC	-2.35	1.34	1.37
18	3	3019	CLA	C2C-C1C	2.34	1.48	1.43
18	A	1112	CLA	C1B-CHB	2.34	1.47	1.41
18	4	4004	CLA	C1D-C2D	2.34	1.47	1.42
18	B	1229	CLA	CHD-C4C	2.34	1.47	1.41
18	B	1239	CLA	C1C-NC	-2.34	1.34	1.37
18	3	3019	CLA	C4B-CHC	2.34	1.48	1.43
18	B	1234	CLA	C4C-C3C	2.34	1.49	1.45
18	A	1111	CLA	C1B-CHB	2.34	1.47	1.41
18	A	1108	CLA	C1C-NC	-2.34	1.34	1.37
18	B	1204	CLA	C4C-C3C	2.34	1.49	1.45
18	B	1223	CLA	CHD-C4C	2.34	1.47	1.41
18	J	1302	CLA	C4C-C3C	2.34	1.49	1.45
28	4	4011	CHL	C3D-C2D	-2.34	1.35	1.39
18	A	1140	CLA	C1C-NC	-2.33	1.34	1.37
18	2	2005	CLA	CHD-C4C	2.33	1.47	1.41
18	B	1216	CLA	C1B-CHB	2.33	1.47	1.41
18	A	1134	CLA	C4C-C3C	2.33	1.49	1.45
18	A	1112	CLA	C4C-C3C	2.33	1.49	1.45
18	H	1000	CLA	C4C-C3C	2.33	1.49	1.45
18	B	1230	CLA	C1C-NC	-2.33	1.34	1.37
18	B	1203	CLA	C1C-NC	-2.33	1.34	1.37
18	G	1003	CLA	CHD-C4C	2.33	1.47	1.41
18	1	1006	CLA	C1B-CHB	2.33	1.47	1.41
18	A	1122	CLA	C4C-C3C	2.33	1.49	1.45
18	B	1222	CLA	C1C-NC	-2.33	1.34	1.37
18	A	1102	CLA	CHD-C4C	2.33	1.47	1.41
18	B	1212	CLA	C1C-NC	-2.33	1.34	1.37
18	A	1123	CLA	C4C-C3C	2.33	1.49	1.45
18	4	4012	CLA	C1B-CHB	2.33	1.47	1.41
28	1	1009	CHL	C1A-CHA	-2.32	1.33	1.43
22	J	6013	BCR	C1-C6	-2.32	1.50	1.53
18	3	3002	CLA	C4B-CHC	2.32	1.47	1.41
18	A	1104	CLA	CHD-C4C	2.32	1.47	1.41
18	B	1222	CLA	CHD-C4C	2.32	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3002	CLA	CHD-C4C	2.32	1.47	1.41
18	B	1240	CLA	C1C-NC	-2.32	1.34	1.37
18	2	2019	CLA	C4C-NC	-2.32	1.33	1.37
18	3	3018	CLA	C4B-CHC	2.31	1.47	1.41
18	A	1136	CLA	C4C-C3C	2.31	1.49	1.45
18	A	1118	CLA	C1C-NC	-2.31	1.34	1.37
18	1	1007	CLA	C1B-CHB	2.31	1.47	1.41
18	K	1001	CLA	C1B-CHB	2.31	1.47	1.41
18	A	1126	CLA	C1C-NC	-2.31	1.34	1.37
18	A	1133	CLA	C4C-C3C	2.31	1.49	1.45
18	A	1013	CLA	C1C-NC	-2.31	1.34	1.37
18	1	1014	CLA	C4B-NB	-2.31	1.33	1.35
18	A	1138	CLA	C4C-C3C	2.31	1.49	1.45
18	A	1104	CLA	C1C-C2C	2.30	1.49	1.44
18	A	1130	CLA	C1C-NC	-2.30	1.34	1.37
27	4	4503	LUT	C1-C6	-2.30	1.50	1.53
18	A	1116	CLA	C1C-NC	-2.30	1.34	1.37
18	A	1136	CLA	C1C-NC	-2.30	1.34	1.37
18	B	1226	CLA	C1C-NC	-2.30	1.34	1.37
18	A	1119	CLA	C4C-C3C	2.30	1.49	1.45
18	4	4009	CLA	C4B-CHC	2.29	1.47	1.41
18	1	1012	CLA	C4B-CHC	2.29	1.47	1.41
28	4	4011	CHL	C1C-NC	-2.29	1.34	1.37
18	A	1123	CLA	C1C-NC	-2.29	1.34	1.37
18	B	1211	CLA	C1B-CHB	2.29	1.47	1.41
18	A	1102	CLA	C1C-NC	-2.29	1.34	1.37
18	3	3018	CLA	C1B-NB	-2.29	1.33	1.35
18	L	1501	CLA	CHD-C4C	2.29	1.47	1.41
18	B	1012	CLA	C1C-NC	-2.29	1.34	1.37
18	B	1232	CLA	C4C-C3C	2.29	1.49	1.45
18	A	1139	CLA	C1C-NC	-2.29	1.34	1.37
18	A	1127	CLA	C1C-NC	-2.29	1.34	1.37
18	1	1004	CLA	C4B-CHC	2.29	1.47	1.41
18	A	1105	CLA	C4C-C3C	2.29	1.49	1.45
18	A	1108	CLA	C4C-C3C	2.29	1.49	1.45
18	B	1226	CLA	C4C-C3C	2.29	1.49	1.45
22	3	3503	BCR	C17-C18	-2.28	1.32	1.35
18	3	3012	CLA	C4B-CHC	2.28	1.47	1.41
17	A	1011	CL0	C1C-C2C	2.28	1.49	1.44
18	3	3012	CLA	C1B-CHB	2.28	1.47	1.41
18	A	1117	CLA	C1C-NC	-2.28	1.34	1.37
18	B	1235	CLA	C1C-NC	-2.28	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2009	CLA	CHD-C4C	2.28	1.47	1.41
28	1	1009	CHL	C4B-NB	2.28	1.37	1.35
18	3	3007	CLA	C1B-CHB	2.28	1.47	1.41
18	B	1219	CLA	C1C-NC	-2.28	1.34	1.37
18	2	2007	CLA	CHD-C4C	2.28	1.47	1.41
18	4	4002	CLA	OBD-CAD	2.28	1.25	1.22
18	B	1205	CLA	C4C-C3C	2.28	1.49	1.45
18	B	1208	CLA	C1C-NC	-2.28	1.34	1.37
18	4	4016	CLA	CHD-C4C	2.27	1.47	1.41
18	B	1202	CLA	C4C-C3C	2.27	1.49	1.45
18	B	1230	CLA	CHD-C4C	2.27	1.47	1.41
18	2	2003	CLA	C4B-CHC	2.27	1.47	1.41
18	B	1214	CLA	C4C-C3C	2.27	1.48	1.45
18	A	1125	CLA	CHD-C4C	2.27	1.47	1.41
28	4	4010	CHL	C1C-NC	-2.26	1.34	1.37
18	B	1216	CLA	C1C-NC	-2.26	1.34	1.37
18	A	1122	CLA	C1C-NC	-2.26	1.34	1.37
18	A	1124	CLA	C4C-C3C	2.26	1.48	1.45
18	A	1139	CLA	C4C-C3C	2.26	1.48	1.45
18	1	1001	CLA	C4B-CHC	2.26	1.47	1.41
18	3	3012	CLA	C1B-NB	-2.26	1.33	1.35
18	A	1135	CLA	C1C-NC	-2.26	1.34	1.37
18	A	1134	CLA	C1C-NC	-2.26	1.34	1.37
18	1	1014	CLA	C1B-CHB	2.26	1.47	1.41
18	4	4017	CLA	C1B-CHB	2.26	1.47	1.41
18	A	1127	CLA	C4C-C3C	2.25	1.48	1.45
18	A	1110	CLA	C4C-C3C	2.25	1.48	1.45
18	A	1109	CLA	C4C-C3C	2.25	1.48	1.45
18	J	1302	CLA	C1C-NC	-2.25	1.34	1.37
18	A	1104	CLA	C1C-NC	-2.25	1.34	1.37
18	4	4017	CLA	C4B-NB	-2.25	1.33	1.35
18	G	1002	CLA	CHD-C4C	2.25	1.47	1.41
18	B	1231	CLA	C4C-C3C	2.25	1.48	1.45
18	1	1011	CLA	C1B-CHB	2.24	1.47	1.41
18	3	3017	CLA	CHD-C4C	2.24	1.47	1.41
27	1	1502	LUT	C1-C6	-2.24	1.50	1.53
28	4	4010	CHL	C2C-C3C	-2.24	1.32	1.36
18	L	1501	CLA	C1B-CHB	2.24	1.47	1.41
18	B	1201	CLA	C1C-NC	-2.24	1.34	1.37
18	B	1201	CLA	C4C-C3C	2.24	1.48	1.45
18	2	2019	CLA	C4B-NB	-2.24	1.33	1.35
18	B	1218	CLA	C1C-NC	-2.24	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1206	CLA	C1C-NC	-2.24	1.34	1.37
18	B	1215	CLA	C1C-NC	-2.23	1.34	1.37
18	3	3006	CLA	CHD-C4C	2.23	1.47	1.41
18	B	1219	CLA	C4C-C3C	2.23	1.48	1.45
18	3	3004	CLA	C4B-CHC	2.23	1.47	1.41
18	A	1124	CLA	C1C-NC	-2.23	1.34	1.37
18	3	3006	CLA	C4B-CHC	2.23	1.47	1.41
18	A	1107	CLA	C4C-C3C	2.23	1.48	1.45
18	B	1220	CLA	C4C-C3C	2.22	1.48	1.45
18	4	4001	CLA	C4B-CHC	2.22	1.47	1.41
18	A	1104	CLA	C4C-C3C	2.22	1.48	1.45
18	3	3002	CLA	C4B-NB	-2.22	1.33	1.35
18	B	1227	CLA	C1C-NC	-2.22	1.34	1.37
18	B	1206	CLA	C4C-C3C	2.22	1.48	1.45
18	B	1021	CLA	C1C-NC	-2.22	1.34	1.37
18	1	1013	CLA	C4C-C3C	2.22	1.48	1.45
18	1	1011	CLA	C4B-NB	-2.22	1.33	1.35
18	A	1121	CLA	C4C-C3C	2.22	1.48	1.45
18	A	1131	CLA	C1C-NC	-2.21	1.34	1.37
18	F	1301	CLA	CHD-C4C	2.21	1.47	1.41
18	A	1116	CLA	C4C-C3C	2.21	1.48	1.45
18	A	1117	CLA	C4C-C3C	2.21	1.48	1.45
18	A	1111	CLA	C4C-C3C	2.20	1.48	1.45
18	A	1115	CLA	C1C-NC	-2.20	1.34	1.37
18	3	3001	CLA	CHD-C4C	2.20	1.47	1.41
27	1	1502	LUT	C26-C27	-2.20	1.47	1.50
22	F	6016	BCR	C30-C25	-2.20	1.50	1.53
18	B	1222	CLA	C1C-C2C	2.20	1.48	1.44
18	B	1221	CLA	C4C-C3C	2.20	1.48	1.45
22	3	3503	BCR	C30-C25	-2.20	1.50	1.53
18	A	1129	CLA	C4C-C3C	2.20	1.48	1.45
18	B	1207	CLA	C4C-C3C	2.20	1.48	1.45
18	B	1239	CLA	C4C-C3C	2.19	1.48	1.45
18	B	1232	CLA	C1C-C2C	2.19	1.48	1.44
18	3	3003	CLA	C4C-C3C	2.19	1.48	1.45
18	A	1132	CLA	C4C-C3C	2.19	1.48	1.45
18	A	1129	CLA	C1C-NC	-2.19	1.34	1.37
18	3	3018	CLA	CHD-C4C	2.19	1.47	1.41
18	B	1217	CLA	C4C-C3C	2.19	1.48	1.45
18	2	2008	CLA	C4B-CHC	2.19	1.47	1.41
18	B	1218	CLA	C4C-C3C	2.18	1.48	1.45
27	1	1501	LUT	C26-C27	-2.18	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3007	CLA	CHD-C4C	2.18	1.47	1.41
18	B	1225	CLA	C1C-NC	-2.18	1.34	1.37
18	2	2004	CLA	CHD-C4C	2.18	1.47	1.41
18	1	1008	CLA	C4B-CHC	2.18	1.47	1.41
18	K	1001	CLA	C4B-CHC	2.18	1.47	1.41
18	B	1224	CLA	C1C-NC	-2.18	1.34	1.37
18	L	1503	CLA	CHD-C4C	2.18	1.47	1.41
18	4	4006	CLA	C1B-CHB	2.18	1.47	1.41
18	2	2008	CLA	MG-NC	2.18	2.11	2.06
18	A	1237	CLA	C4C-C3C	2.18	1.48	1.45
28	2	2011	CHL	C1C-NC	-2.18	1.34	1.37
18	A	1128	CLA	C4C-C3C	2.17	1.48	1.45
18	A	1103	CLA	C4C-C3C	2.17	1.48	1.45
18	A	1013	CLA	C1C-C2C	2.17	1.48	1.44
18	1	1013	CLA	C4B-CHC	2.17	1.47	1.41
18	B	1208	CLA	C1C-C2C	2.17	1.48	1.44
18	B	1231	CLA	C1C-NC	-2.17	1.34	1.37
18	4	4003	CLA	CHD-C4C	2.17	1.47	1.41
18	1	1011	CLA	CHD-C4C	2.17	1.47	1.41
18	1	1002	CLA	C4B-CHC	2.17	1.47	1.41
18	B	1216	CLA	C4C-C3C	2.17	1.48	1.45
18	2	2002	CLA	C4B-CHC	2.16	1.47	1.41
18	B	1234	CLA	C1C-NC	-2.16	1.34	1.37
18	B	1208	CLA	C4C-C3C	2.16	1.48	1.45
28	2	2011	CHL	C4B-NB	2.16	1.37	1.35
18	B	1215	CLA	C4C-C3C	2.15	1.48	1.45
18	B	1231	CLA	C1C-C2C	2.15	1.48	1.44
18	3	3018	CLA	C1B-CHB	2.15	1.47	1.41
22	I	6020	BCR	C30-C25	-2.15	1.50	1.53
28	1	1009	CHL	C1C-NC	-2.15	1.34	1.37
18	4	4009	CLA	C1B-CHB	2.15	1.47	1.41
18	1	1003	CLA	C4B-NB	-2.15	1.33	1.35
18	B	1235	CLA	C1C-C2C	2.15	1.48	1.44
18	B	1227	CLA	C4C-C3C	2.15	1.48	1.45
18	1	1003	CLA	C4B-CHC	2.14	1.47	1.41
18	4	4001	CLA	C1B-CHB	2.14	1.47	1.41
27	4	4503	LUT	C26-C27	-2.14	1.47	1.50
27	4	4501	LUT	C1-C6	-2.14	1.50	1.53
18	B	1221	CLA	C1C-NC	-2.14	1.34	1.37
18	A	1130	CLA	C4C-C3C	2.14	1.48	1.45
18	K	1001	CLA	CHD-C4C	2.14	1.47	1.41
18	B	1201	CLA	C1C-C2C	2.14	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1011	CL0	C4C-C3C	2.14	1.48	1.45
18	B	1212	CLA	C4C-C3C	2.14	1.48	1.45
18	4	4004	CLA	MG-NC	2.14	2.11	2.06
18	B	1207	CLA	C1C-C2C	2.13	1.48	1.44
18	1	1001	CLA	C1B-CHB	2.13	1.46	1.41
18	A	1102	CLA	C1C-C2C	2.13	1.48	1.44
18	4	4012	CLA	CHD-C4C	2.13	1.47	1.41
18	2	2012	CLA	C1B-CHB	2.13	1.46	1.41
18	B	1227	CLA	C1C-C2C	2.13	1.48	1.44
18	A	1139	CLA	C1C-C2C	2.13	1.48	1.44
18	A	1106	CLA	C4C-C3C	2.13	1.48	1.45
18	B	1229	CLA	C1C-C2C	2.12	1.48	1.44
29	4	4505	ZEX	C30-C29	-2.12	1.33	1.35
28	4	4010	CHL	C4B-NB	2.12	1.37	1.35
18	A	1107	CLA	C1C-C2C	2.12	1.48	1.44
18	1	1005	CLA	C4B-CHC	2.11	1.46	1.41
18	B	1203	CLA	C1C-C2C	2.11	1.48	1.44
18	3	3001	CLA	C1B-CHB	2.11	1.46	1.41
18	2	2001	CLA	C1B-CHB	2.11	1.46	1.41
18	A	1137	CLA	C4C-C3C	2.11	1.48	1.45
18	A	1131	CLA	C1C-C2C	2.11	1.48	1.44
18	3	3013	CLA	C1B-CHB	2.11	1.46	1.41
27	3	3502	LUT	C21-C26	-2.10	1.50	1.56
18	A	1137	CLA	C1C-C2C	2.10	1.48	1.44
18	1	1008	CLA	C4B-NB	-2.10	1.33	1.35
18	4	4002	CLA	C1B-NB	-2.10	1.33	1.35
18	1	1006	CLA	C4C-C3C	2.10	1.48	1.45
18	A	1151	CLA	C1C-C2C	2.10	1.48	1.44
27	4	4501	LUT	C10-C9	-2.10	1.33	1.35
18	B	1211	CLA	C4C-C3C	2.10	1.48	1.45
18	A	1125	CLA	C1C-C2C	2.10	1.48	1.44
18	B	1236	CLA	C1C-C2C	2.10	1.48	1.44
18	A	1140	CLA	C4C-C3C	2.10	1.48	1.45
18	3	3004	CLA	CHD-C4C	2.10	1.47	1.41
18	B	1215	CLA	C1C-C2C	2.10	1.48	1.44
18	A	1107	CLA	C1C-NC	-2.10	1.34	1.37
18	3	3010	CLA	C1B-CHB	2.10	1.46	1.41
18	A	1130	CLA	C1C-C2C	2.09	1.48	1.44
18	1	1007	CLA	C4B-CHC	2.09	1.46	1.41
18	B	1216	CLA	C1C-C2C	2.09	1.48	1.44
18	B	1238	CLA	C1C-C2C	2.09	1.48	1.44
18	1	1003	CLA	C4C-C3C	2.09	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4003	CLA	C1B-NB	-2.09	1.33	1.35
18	1	1012	CLA	CHD-C4C	2.08	1.47	1.41
22	F	6016	BCR	C14-C13	-2.08	1.33	1.35
18	L	1502	CLA	C4B-NB	-2.08	1.33	1.35
18	G	1002	CLA	C4C-C3C	2.08	1.48	1.45
18	B	1219	CLA	C1C-C2C	2.08	1.48	1.44
27	2	2502	LUT	C21-C26	-2.08	1.50	1.56
18	2	2001	CLA	CHD-C4C	2.08	1.47	1.41
18	A	1131	CLA	C4C-C3C	2.08	1.48	1.45
18	B	1239	CLA	C1C-C2C	2.08	1.48	1.44
18	B	1225	CLA	C4C-C3C	2.08	1.48	1.45
18	B	1228	CLA	C4C-C3C	2.08	1.48	1.45
18	3	3013	CLA	C4B-NB	-2.08	1.33	1.35
18	B	1218	CLA	C1C-C2C	2.07	1.48	1.44
18	A	1105	CLA	C1C-C2C	2.07	1.48	1.44
18	G	1003	CLA	C4B-NB	-2.07	1.33	1.35
18	B	1229	CLA	C4C-C3C	2.07	1.48	1.45
23	F	5001	LMG	O8-C28	2.07	1.43	1.33
18	4	4003	CLA	C4B-NB	-2.07	1.33	1.35
18	B	1234	CLA	C1C-C2C	2.07	1.48	1.44
18	G	1002	CLA	C1B-NB	-2.07	1.33	1.35
18	A	1120	CLA	C1C-C2C	2.07	1.48	1.44
18	1	1006	CLA	C4B-NB	-2.06	1.33	1.35
27	2	2502	LUT	C1-C6	-2.06	1.50	1.53
18	A	1022	CLA	C1C-C2C	2.06	1.48	1.44
22	J	6012	BCR	C14-C13	-2.06	1.33	1.35
18	A	1126	CLA	C1C-C2C	2.06	1.48	1.44
18	A	1123	CLA	C1C-C2C	2.06	1.48	1.44
18	1	1014	CLA	C4B-CHC	2.06	1.46	1.41
18	A	1106	CLA	C1C-C2C	2.05	1.48	1.44
18	2	2016	CLA	C1A-CHA	2.05	1.51	1.43
28	1	1010	CHL	CHC-C1C	2.05	1.40	1.35
18	A	1108	CLA	C1C-C2C	2.05	1.48	1.44
18	3	3003	CLA	CHD-C4C	2.05	1.47	1.41
18	3	3018	CLA	C4C-C3C	2.05	1.48	1.45
18	B	1012	CLA	C1C-C2C	2.05	1.48	1.44
27	4	4502	LUT	C22-C21	-2.05	1.52	1.54
18	A	1013	CLA	C4C-C3C	2.05	1.48	1.45
18	B	1240	CLA	C4C-C3C	2.04	1.48	1.45
18	A	1132	CLA	C1C-C2C	2.04	1.48	1.44
18	A	1124	CLA	C1C-C2C	2.04	1.48	1.44
18	L	1502	CLA	CHD-C4C	2.04	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2012	CLA	CHD-C4C	2.03	1.46	1.41
18	B	1220	CLA	C1C-C2C	2.03	1.48	1.44
18	A	1140	CLA	C1C-C2C	2.03	1.48	1.44
18	B	1212	CLA	C1C-C2C	2.03	1.48	1.44
18	1	1008	CLA	CHD-C4C	2.03	1.46	1.41
18	B	1238	CLA	C4C-C3C	2.03	1.48	1.45
18	A	1121	CLA	C1C-C2C	2.03	1.48	1.44
18	A	1115	CLA	C1C-C2C	2.02	1.48	1.44
22	A	6007	BCR	C30-C25	-2.02	1.51	1.53
18	4	4017	CLA	CHD-C4C	2.02	1.46	1.41
18	1	1003	CLA	C1B-NB	-2.02	1.33	1.35
18	B	1225	CLA	C1C-C2C	2.02	1.48	1.44
18	A	1110	CLA	C1C-C2C	2.02	1.48	1.44
18	G	1001	CLA	CHD-C4C	2.02	1.46	1.41
18	3	3003	CLA	C1B-NB	-2.02	1.33	1.35
18	J	1302	CLA	C1C-C2C	2.01	1.48	1.44
18	A	1136	CLA	C1C-C2C	2.01	1.48	1.44
18	3	3002	CLA	C4C-C3C	2.01	1.48	1.45
28	2	2013	CHL	C1A-CHA	-2.01	1.34	1.43
18	B	1217	CLA	C1C-C2C	2.01	1.48	1.44
18	B	1223	CLA	C4C-C3C	2.01	1.48	1.45
27	4	4502	LUT	C1-C6	-2.01	1.51	1.53
18	A	1133	CLA	C1C-C2C	2.01	1.48	1.44
18	2	2007	CLA	C4C-C3C	2.01	1.48	1.45
18	1	1013	CLA	C1B-NB	-2.01	1.33	1.35
18	1	1004	CLA	C1B-NB	-2.00	1.33	1.35
18	A	1103	CLA	C1C-C2C	2.00	1.48	1.44
22	L	6020	BCR	C1-C6	-2.00	1.51	1.53
18	A	1112	CLA	C1C-C2C	2.00	1.48	1.44

All (3260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6017	BCR	C16-C17-C18	29.85	169.91	127.31
22	G	2011	BCR	C16-C17-C18	27.95	167.20	127.31
22	B	6005	BCR	C16-C17-C18	27.71	166.86	127.31
22	K	2011	BCR	C16-C17-C18	27.60	166.70	127.31
22	I	6020	BCR	C16-C17-C18	27.15	166.06	127.31
22	B	6004	BCR	C16-C17-C18	26.98	165.82	127.31
22	B	6006	BCR	C20-C21-C22	24.99	162.98	127.31
22	F	6016	BCR	C16-C17-C18	23.71	161.15	127.31
22	A	6011	BCR	C16-C17-C18	23.52	160.87	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	6010	BCR	C20-C21-C22	22.95	160.06	127.31
22	F	6014	BCR	C16-C17-C18	22.33	159.18	127.31
22	F	6016	BCR	C20-C21-C22	21.97	158.67	127.31
22	A	6011	BCR	C20-C21-C22	21.62	158.17	127.31
22	J	6013	BCR	C15-C16-C17	21.47	167.46	123.47
22	K	2011	BCR	C20-C21-C22	21.32	157.73	127.31
22	A	6002	BCR	C15-C16-C17	21.13	166.77	123.47
22	L	6019	BCR	C20-C21-C22	20.91	157.16	127.31
22	A	6008	BCR	C20-C21-C22	20.84	157.06	127.31
22	F	6014	BCR	C20-C21-C22	20.77	156.95	127.31
22	F	6014	BCR	C15-C16-C17	20.74	165.97	123.47
22	A	6003	BCR	C20-C21-C22	20.68	156.82	127.31
22	A	6003	BCR	C15-C16-C17	20.59	165.65	123.47
22	B	6005	BCR	C20-C21-C22	20.41	156.43	127.31
22	L	6020	BCR	C20-C21-C22	20.35	156.36	127.31
22	B	6009	BCR	C15-C16-C17	20.35	165.16	123.47
22	B	6009	BCR	C20-C21-C22	20.33	156.32	127.31
22	J	6012	BCR	C15-C16-C17	20.26	164.97	123.47
22	B	6010	BCR	C15-C16-C17	20.21	164.87	123.47
22	3	3503	BCR	C20-C21-C22	20.15	156.07	127.31
22	B	6006	BCR	C15-C16-C17	20.10	164.64	123.47
22	A	6007	BCR	C15-C16-C17	20.09	164.63	123.47
22	A	6008	BCR	C16-C17-C18	20.09	155.97	127.31
22	A	6007	BCR	C16-C17-C18	20.08	155.96	127.31
22	B	6010	BCR	C16-C17-C18	19.94	155.77	127.31
22	L	6019	BCR	C16-C17-C18	19.91	155.72	127.31
22	B	6006	BCR	C16-C17-C18	19.84	155.62	127.31
22	J	6012	BCR	C20-C21-C22	19.83	155.61	127.31
22	L	6019	BCR	C15-C16-C17	19.78	164.00	123.47
22	B	6009	BCR	C16-C17-C18	19.70	155.43	127.31
22	L	6020	BCR	C15-C16-C17	19.70	163.82	123.47
22	B	6004	BCR	C20-C21-C22	19.61	155.30	127.31
22	A	6003	BCR	C16-C17-C18	19.61	155.29	127.31
22	J	6012	BCR	C16-C17-C18	19.60	155.28	127.31
22	A	6007	BCR	C20-C21-C22	19.53	155.18	127.31
22	G	2011	BCR	C20-C21-C22	19.51	155.16	127.31
22	L	6020	BCR	C16-C17-C18	19.37	154.95	127.31
22	A	6002	BCR	C20-C21-C22	19.36	154.94	127.31
22	J	6013	BCR	C20-C21-C22	19.17	154.66	127.31
22	3	3503	BCR	C16-C17-C18	18.99	154.41	127.31
22	3	3503	BCR	C15-C16-C17	18.71	161.80	123.47
22	F	6016	BCR	C15-C16-C17	18.54	161.46	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6008	BCR	C15-C16-C17	18.40	161.17	123.47
22	I	6020	BCR	C20-C21-C22	18.22	153.32	127.31
22	K	2011	BCR	C10-C11-C12	18.19	179.97	123.22
22	G	2011	BCR	C10-C11-C12	18.18	179.94	123.22
22	A	6011	BCR	C15-C16-C17	18.07	160.50	123.47
22	A	6017	BCR	C16-C15-C14	17.86	160.05	123.47
22	L	6020	BCR	C10-C11-C12	17.84	178.90	123.22
22	A	6002	BCR	C16-C17-C18	17.83	152.76	127.31
22	A	6017	BCR	C20-C21-C22	17.63	152.47	127.31
22	L	6019	BCR	C10-C11-C12	17.50	177.82	123.22
22	F	6016	BCR	C10-C11-C12	17.46	177.72	123.22
22	J	6013	BCR	C16-C17-C18	17.40	152.14	127.31
22	A	6007	BCR	C10-C11-C12	17.38	177.47	123.22
22	J	6013	BCR	C10-C11-C12	17.30	177.20	123.22
22	A	6003	BCR	C10-C11-C12	17.28	177.14	123.22
22	F	6014	BCR	C10-C11-C12	17.11	176.62	123.22
22	J	6012	BCR	C10-C11-C12	17.07	176.49	123.22
22	B	6005	BCR	C10-C11-C12	17.06	176.46	123.22
22	3	3503	BCR	C10-C11-C12	17.04	176.40	123.22
22	A	6002	BCR	C10-C11-C12	16.98	176.19	123.22
22	A	6008	BCR	C10-C11-C12	16.98	176.19	123.22
22	I	6020	BCR	C10-C11-C12	16.79	175.61	123.22
22	B	6009	BCR	C10-C11-C12	16.71	175.35	123.22
22	B	6010	BCR	C10-C11-C12	16.67	175.24	123.22
22	A	6017	BCR	C10-C11-C12	16.64	175.16	123.22
22	B	6006	BCR	C11-C10-C9	16.13	150.33	127.31
22	B	6004	BCR	C15-C16-C17	16.09	156.44	123.47
22	B	6006	BCR	C10-C11-C12	15.98	173.10	123.22
22	G	2011	BCR	C15-C16-C17	15.74	155.72	123.47
22	B	6004	BCR	C10-C11-C12	15.74	172.34	123.22
22	A	6011	BCR	C10-C11-C12	15.63	172.00	123.22
22	I	6020	BCR	C15-C16-C17	15.51	155.26	123.47
22	B	6005	BCR	C15-C16-C17	15.49	155.21	123.47
22	K	2011	BCR	C15-C16-C17	15.43	155.08	123.47
22	A	6011	BCR	C11-C10-C9	15.35	149.22	127.31
22	A	6008	BCR	C16-C15-C14	15.19	154.59	123.47
22	J	6012	BCR	C11-C10-C9	14.81	148.44	127.31
22	A	6017	BCR	C21-C20-C19	14.65	168.93	123.22
22	I	6020	BCR	C11-C10-C9	14.58	148.12	127.31
22	3	3503	BCR	C16-C15-C14	14.54	153.26	123.47
22	L	6020	BCR	C16-C15-C14	14.52	153.22	123.47
22	B	6004	BCR	C21-C20-C19	14.41	168.18	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	6014	BCR	C11-C10-C9	14.20	147.57	127.31
22	I	6020	BCR	C21-C20-C19	14.13	167.30	123.22
22	A	6017	BCR	C15-C16-C17	14.10	152.35	123.47
22	A	6002	BCR	C11-C10-C9	14.05	147.36	127.31
22	B	6005	BCR	C21-C20-C19	13.88	166.53	123.22
22	A	6007	BCR	C21-C20-C19	13.82	166.34	123.22
22	B	6004	BCR	C16-C15-C14	13.74	151.61	123.47
22	A	6002	BCR	C21-C20-C19	13.53	165.45	123.22
22	A	6017	BCR	C11-C10-C9	13.44	146.49	127.31
22	B	6010	BCR	C21-C20-C19	13.40	165.04	123.22
22	L	6019	BCR	C16-C15-C14	13.35	150.81	123.47
22	F	6016	BCR	C11-C10-C9	13.34	146.34	127.31
22	G	2011	BCR	C16-C15-C14	13.33	150.78	123.47
22	A	6007	BCR	C11-C10-C9	13.29	146.28	127.31
22	G	2011	BCR	C21-C20-C19	13.27	164.64	123.22
22	3	3503	BCR	C21-C20-C19	13.18	164.34	123.22
22	A	6007	BCR	C16-C15-C14	13.13	150.38	123.47
22	B	6005	BCR	C11-C10-C9	13.13	146.05	127.31
22	A	6003	BCR	C21-C20-C19	13.13	164.18	123.22
22	F	6014	BCR	C21-C20-C19	13.10	164.10	123.22
22	I	6020	BCR	C16-C15-C14	13.06	150.22	123.47
22	J	6012	BCR	C21-C20-C19	13.05	163.94	123.22
22	K	2011	BCR	C16-C15-C14	12.97	150.05	123.47
22	A	6008	BCR	C21-C20-C19	12.95	163.62	123.22
22	B	6005	BCR	C16-C15-C14	12.94	149.99	123.47
22	J	6013	BCR	C21-C20-C19	12.93	163.58	123.22
22	J	6013	BCR	C11-C10-C9	12.91	145.73	127.31
22	L	6019	BCR	C21-C20-C19	12.89	163.46	123.22
22	J	6013	BCR	C16-C15-C14	12.84	149.78	123.47
22	B	6010	BCR	C16-C15-C14	12.83	149.76	123.47
22	A	6008	BCR	C11-C10-C9	12.73	145.48	127.31
22	L	6020	BCR	C21-C20-C19	12.73	162.95	123.22
22	A	6011	BCR	C16-C15-C14	12.72	149.53	123.47
22	A	6003	BCR	C11-C10-C9	12.61	145.30	127.31
22	A	6003	BCR	C16-C15-C14	12.58	149.24	123.47
22	B	6006	BCR	C16-C15-C14	12.57	149.23	123.47
22	B	6009	BCR	C21-C20-C19	12.54	162.34	123.22
22	F	6016	BCR	C16-C15-C14	12.54	149.15	123.47
22	B	6009	BCR	C16-C15-C14	12.42	148.92	123.47
22	A	6011	BCR	C11-C12-C13	12.27	160.88	126.42
22	J	6012	BCR	C16-C15-C14	12.21	148.49	123.47
22	A	6002	BCR	C16-C15-C14	12.21	148.49	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	6016	BCR	C21-C20-C19	12.02	160.73	123.22
22	B	6006	BCR	C11-C12-C13	11.98	160.07	126.42
22	A	6011	BCR	C21-C20-C19	11.96	160.56	123.22
22	F	6014	BCR	C16-C15-C14	11.79	147.62	123.47
18	3	3008	CLA	C4A-NA-C1A	11.77	112.00	106.71
22	L	6020	BCR	C11-C10-C9	11.65	143.94	127.31
22	B	6010	BCR	C11-C10-C9	11.46	143.66	127.31
18	2	2016	CLA	C4A-NA-C1A	11.40	111.83	106.71
22	L	6019	BCR	C11-C10-C9	11.35	143.51	127.31
22	B	6005	BCR	C11-C12-C13	11.09	157.56	126.42
22	K	2011	BCR	C11-C10-C9	11.02	143.04	127.31
22	A	6002	BCR	C11-C12-C13	10.99	157.30	126.42
22	L	6019	BCR	C11-C12-C13	10.94	157.16	126.42
22	B	6006	BCR	C21-C20-C19	10.93	157.33	123.22
22	I	6020	BCR	C11-C12-C13	10.83	156.83	126.42
22	B	6009	BCR	C11-C12-C13	10.81	156.78	126.42
22	B	6009	BCR	C11-C10-C9	10.78	142.70	127.31
22	J	6013	BCR	C11-C12-C13	10.77	156.68	126.42
22	K	2011	BCR	C21-C20-C19	10.77	156.81	123.22
22	A	6003	BCR	C11-C12-C13	10.62	156.26	126.42
22	F	6014	BCR	C11-C12-C13	10.46	155.81	126.42
22	F	6016	BCR	C11-C12-C13	10.43	155.71	126.42
27	1	1501	LUT	C21-C26-C27	10.37	125.81	112.70
18	4	4008	CLA	C4A-NA-C1A	10.12	111.25	106.71
22	A	6017	BCR	C11-C12-C13	10.08	154.75	126.42
22	B	6010	BCR	C11-C12-C13	10.08	154.74	126.42
22	A	6008	BCR	C11-C12-C13	10.08	154.72	126.42
22	K	2011	BCR	C11-C12-C13	10.03	154.59	126.42
22	J	6012	BCR	C11-C12-C13	10.03	154.59	126.42
22	B	6004	BCR	C11-C10-C9	10.00	141.58	127.31
22	3	3503	BCR	C11-C12-C13	9.98	154.46	126.42
18	2	2003	CLA	C4A-NA-C1A	9.83	111.13	106.71
22	A	6007	BCR	C11-C12-C13	9.65	153.53	126.42
22	B	6004	BCR	C11-C12-C13	9.65	153.52	126.42
22	3	3503	BCR	C11-C10-C9	9.56	140.95	127.31
22	L	6020	BCR	C11-C12-C13	9.35	152.69	126.42
18	2	2008	CLA	C4A-NA-C1A	9.35	110.91	106.71
18	1	1007	CLA	C4A-NA-C1A	9.24	110.86	106.71
22	G	2011	BCR	C11-C12-C13	9.07	151.91	126.42
18	4	4007	CLA	C4A-NA-C1A	9.04	110.77	106.71
18	1	1002	CLA	C4A-NA-C1A	8.91	110.71	106.71
18	1	1008	CLA	C4A-NA-C1A	8.82	110.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1001	CLA	C4A-NA-C1A	8.79	110.66	106.71
18	2	2016	CLA	C4D-C3D-CAD	8.77	113.36	108.47
22	G	2011	BCR	C11-C10-C9	8.68	139.70	127.31
18	2	2002	CLA	C4A-NA-C1A	8.35	110.46	106.71
22	F	6016	BCR	C20-C19-C18	8.32	149.79	126.42
18	4	4005	CLA	C4A-NA-C1A	8.25	110.42	106.71
18	3	3003	CLA	C2C-C1C-NC	8.25	117.70	109.97
18	3	3003	CLA	C4A-NA-C1A	8.19	110.39	106.71
18	1	1014	CLA	C4A-NA-C1A	8.11	110.35	106.71
18	3	3012	CLA	C4A-NA-C1A	8.05	110.32	106.71
18	1	1013	CLA	C4A-NA-C1A	7.98	110.29	106.71
18	3	3008	CLA	C2C-C1C-NC	7.95	117.42	109.97
22	L	6019	BCR	C20-C19-C18	7.85	148.48	126.42
22	A	6017	BCR	C15-C14-C13	-7.85	116.11	127.31
18	1	1001	CLA	C4A-NA-C1A	7.84	110.23	106.71
27	3	3501	LUT	C21-C26-C27	7.79	122.55	112.70
18	3	3005	CLA	C4A-NA-C1A	7.76	110.19	106.71
18	4	4001	CLA	C4A-NA-C1A	7.56	110.10	106.71
18	2	2019	CLA	C3B-C2B-C1B	-7.52	99.86	106.29
22	B	6009	BCR	C20-C19-C18	7.51	147.52	126.42
18	3	3019	CLA	C3B-C2B-C1B	-7.51	99.86	106.29
22	A	6011	BCR	C20-C19-C18	7.47	147.41	126.42
18	4	4008	CLA	C2C-C1C-NC	7.46	116.96	109.97
22	F	6014	BCR	C20-C19-C18	7.42	147.27	126.42
18	2	2012	CLA	C4A-NA-C1A	7.40	110.03	106.71
18	4	4012	CLA	C4A-NA-C1A	7.38	110.02	106.71
18	3	3001	CLA	C4D-C3D-CAD	7.34	112.56	108.47
18	B	1202	CLA	C4A-NA-C1A	7.34	110.01	106.71
18	2	2007	CLA	C4A-NA-C1A	7.26	109.97	106.71
22	B	6006	BCR	C20-C19-C18	7.22	146.71	126.42
18	2	2016	CLA	O2D-CGD-CBD	7.20	124.06	111.27
18	1	1005	CLA	C4A-NA-C1A	7.19	109.94	106.71
18	4	4009	CLA	C4A-NA-C1A	7.18	109.94	106.71
22	J	6012	BCR	C20-C19-C18	7.16	146.53	126.42
18	4	4003	CLA	C4A-NA-C1A	7.16	109.92	106.71
18	2	2001	CLA	C2C-C1C-NC	7.12	116.64	109.97
18	4	4002	CLA	C2C-C1C-NC	7.12	116.64	109.97
22	J	6013	BCR	C20-C19-C18	7.09	146.34	126.42
18	G	1001	CLA	C4A-NA-C1A	7.08	109.89	106.71
18	B	1206	CLA	C2C-C1C-NC	7.05	116.57	109.97
18	1	1013	CLA	C2C-C1C-NC	7.03	116.56	109.97
18	2	2001	CLA	C4A-NA-C1A	7.02	109.86	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3018	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	A	6008	BCR	C20-C19-C18	6.98	146.01	126.42
18	4	4002	CLA	C4A-NA-C1A	6.96	109.83	106.71
18	2	2016	CLA	C2C-C1C-NC	6.92	116.46	109.97
18	B	1230	CLA	O2D-CGD-CBD	6.92	123.56	111.27
18	4	4005	CLA	C2C-C1C-NC	6.91	116.45	109.97
27	4	4503	LUT	C7-C8-C9	-6.91	115.80	126.23
18	1	1008	CLA	C2C-C1C-NC	6.90	116.43	109.97
18	2	2006	CLA	C4A-NA-C1A	6.90	109.81	106.71
18	1	1004	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	A	6003	BCR	C20-C19-C18	6.86	145.68	126.42
18	3	3019	CLA	C4A-NA-C1A	6.85	109.79	106.71
18	A	1114	CLA	C2C-C1C-NC	6.85	116.39	109.97
18	2	2019	CLA	C4A-NA-C1A	6.85	109.78	106.71
22	K	2011	BCR	C20-C19-C18	6.82	145.58	126.42
27	3	3502	LUT	C7-C8-C9	-6.82	115.93	126.23
18	B	1226	CLA	C2C-C1C-NC	6.82	116.36	109.97
18	A	1151	CLA	C2C-C1C-NC	6.79	116.33	109.97
18	H	1000	CLA	C2C-C1C-NC	6.77	116.32	109.97
18	4	4016	CLA	C4A-NA-C1A	6.77	109.75	106.71
18	4	4001	CLA	C2C-C1C-NC	6.77	116.31	109.97
22	L	6020	BCR	C20-C19-C18	6.75	145.39	126.42
18	4	4007	CLA	C2C-C1C-NC	6.75	116.30	109.97
18	L	1503	CLA	C4A-NA-C1A	6.74	109.73	106.71
18	G	1001	CLA	C2C-C1C-NC	6.73	116.28	109.97
18	1	1012	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	K	1001	CLA	C2C-C1C-NC	6.71	116.26	109.97
18	2	2004	CLA	O2D-CGD-CBD	6.70	123.17	111.27
18	K	1001	CLA	C4D-C3D-CAD	6.67	112.19	108.47
18	3	3005	CLA	C2C-C1C-NC	6.67	116.22	109.97
18	B	1224	CLA	C2C-C1C-NC	6.66	116.21	109.97
18	A	1135	CLA	C2C-C1C-NC	6.65	116.20	109.97
18	A	1123	CLA	C2C-C1C-NC	6.65	116.20	109.97
18	4	4006	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	3	3002	CLA	C2C-C1C-NC	6.64	116.19	109.97
18	3	3010	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	B	1211	CLA	O2D-CGD-CBD	6.63	123.05	111.27
18	4	4012	CLA	C2C-C1C-NC	6.61	116.17	109.97
18	1	1003	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	3	3010	CLA	C2C-C1C-NC	6.61	116.16	109.97
18	F	1301	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	B	1221	CLA	O2D-CGD-CBD	6.59	122.98	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1128	CLA	C2C-C1C-NC	6.59	116.15	109.97
18	J	1302	CLA	C2C-C1C-NC	6.59	116.15	109.97
18	A	1133	CLA	C2C-C1C-NC	6.59	116.14	109.97
18	A	1119	CLA	C2C-C1C-NC	6.58	116.14	109.97
18	A	1134	CLA	C2C-C1C-NC	6.58	116.14	109.97
18	3	3008	CLA	C1C-C2C-C3C	-6.58	100.04	106.96
18	3	3008	CLA	C4D-C3D-CAD	6.57	112.14	108.47
18	1	1003	CLA	C2C-C1C-NC	6.57	116.12	109.97
18	B	1202	CLA	C2C-C1C-NC	6.56	116.12	109.97
18	B	1209	CLA	C2C-C1C-NC	6.54	116.10	109.97
18	A	1127	CLA	C2C-C1C-NC	6.54	116.10	109.97
22	A	6002	BCR	C20-C19-C18	6.54	144.78	126.42
18	1	1013	CLA	C4D-C3D-CAD	6.53	112.11	108.47
18	4	4001	CLA	C1C-C2C-C3C	-6.52	100.10	106.96
18	3	3004	CLA	C4A-NA-C1A	6.51	109.64	106.71
18	A	1139	CLA	C2C-C1C-NC	6.51	116.07	109.97
18	G	1002	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	A	1118	CLA	C2C-C1C-NC	6.50	116.06	109.97
18	F	1302	CLA	C4A-NA-C1A	6.49	109.63	106.71
18	2	2005	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	4	4017	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	B	1217	CLA	C2C-C1C-NC	6.47	116.03	109.97
18	3	3004	CLA	C2C-C1C-NC	6.47	116.03	109.97
18	2	2003	CLA	C2C-C1C-NC	6.47	116.03	109.97
18	G	1002	CLA	C2C-C1C-NC	6.47	116.03	109.97
18	2	2008	CLA	C4D-C3D-CAD	6.46	112.07	108.47
17	A	1011	CL0	C2C-C1C-NC	6.45	116.02	109.97
18	A	1113	CLA	C2C-C1C-NC	6.44	116.01	109.97
18	3	3002	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	A	1116	CLA	C2C-C1C-NC	6.43	115.99	109.97
18	3	3018	CLA	C2C-C1C-NC	6.42	115.99	109.97
18	B	1239	CLA	C2C-C1C-NC	6.41	115.98	109.97
18	A	1117	CLA	C2C-C1C-NC	6.41	115.98	109.97
18	A	1137	CLA	C2C-C1C-NC	6.41	115.97	109.97
18	2	2009	CLA	C2C-C1C-NC	6.39	115.96	109.97
22	B	6010	BCR	C20-C19-C18	6.39	144.35	126.42
18	A	1022	CLA	C2C-C1C-NC	6.38	115.95	109.97
18	3	3006	CLA	OBD-CAD-C3D	-6.38	117.38	127.98
18	3	3007	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	B	1230	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	B	1214	CLA	C2C-C1C-NC	6.35	115.92	109.97
18	A	1101	CLA	C2C-C1C-NC	6.35	115.92	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1128	CLA	O2D-CGD-CBD	6.35	122.55	111.27
18	A	1112	CLA	C2C-C1C-NC	6.34	115.91	109.97
18	2	2007	CLA	C2C-C1C-NC	6.34	115.91	109.97
18	B	1219	CLA	C2C-C1C-NC	6.34	115.91	109.97
18	B	1235	CLA	C4A-NA-C1A	6.33	109.55	106.71
18	L	1501	CLA	O2D-CGD-CBD	6.33	122.52	111.27
18	A	1106	CLA	C2C-C1C-NC	6.33	115.90	109.97
18	A	1126	CLA	C2C-C1C-NC	6.31	115.88	109.97
22	A	6007	BCR	C20-C19-C18	6.30	144.13	126.42
18	B	1215	CLA	C2C-C1C-NC	6.30	115.88	109.97
18	B	1223	CLA	C2C-C1C-NC	6.30	115.88	109.97
18	A	1124	CLA	C2C-C1C-NC	6.30	115.87	109.97
18	B	1021	CLA	C4A-NA-C1A	6.29	109.53	106.71
18	A	1129	CLA	C2C-C1C-NC	6.29	115.86	109.97
18	A	1105	CLA	C2C-C1C-NC	6.29	115.86	109.97
18	A	1109	CLA	C2C-C1C-NC	6.28	115.86	109.97
18	B	1240	CLA	C2C-C1C-NC	6.28	115.86	109.97
18	1	1007	CLA	C2C-C1C-NC	6.27	115.85	109.97
18	A	1237	CLA	O2A-C1-C2	6.27	125.11	108.64
18	2	2009	CLA	C4A-NA-C1A	6.26	109.52	106.71
18	A	1115	CLA	C2C-C1C-NC	6.26	115.84	109.97
18	A	1122	CLA	C2C-C1C-NC	6.26	115.84	109.97
18	B	1210	CLA	C2C-C1C-NC	6.26	115.83	109.97
18	A	1237	CLA	C2C-C1C-NC	6.25	115.83	109.97
18	B	1212	CLA	C2C-C1C-NC	6.25	115.83	109.97
18	B	1225	CLA	C2C-C1C-NC	6.25	115.83	109.97
18	A	1111	CLA	C2C-C1C-NC	6.25	115.82	109.97
18	F	1301	CLA	C2C-C1C-NC	6.24	115.81	109.97
18	1	1012	CLA	C2C-C1C-NC	6.23	115.81	109.97
18	B	1216	CLA	C2C-C1C-NC	6.23	115.81	109.97
18	A	1136	CLA	C2C-C1C-NC	6.23	115.81	109.97
18	B	1204	CLA	C2C-C1C-NC	6.23	115.81	109.97
18	A	1130	CLA	C2C-C1C-NC	6.22	115.80	109.97
18	1	1011	CLA	C4A-NA-C1A	6.22	109.50	106.71
18	B	1218	CLA	C2C-C1C-NC	6.22	115.80	109.97
18	A	1121	CLA	C2C-C1C-NC	6.22	115.80	109.97
18	B	1206	CLA	C4A-NA-C1A	6.21	109.50	106.71
22	A	6008	BCR	C15-C14-C13	-6.21	118.44	127.31
18	B	1012	CLA	C2C-C1C-NC	6.21	115.79	109.97
18	1	1006	CLA	C2C-C1C-NC	6.21	115.79	109.97
18	4	4006	CLA	C2C-C1C-NC	6.21	115.79	109.97
22	3	3503	BCR	C20-C19-C18	6.21	143.85	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6007	BCR	C24-C23-C22	-6.20	116.86	126.23
18	1	1005	CLA	C2C-C1C-NC	6.18	115.76	109.97
18	A	1104	CLA	C2C-C1C-NC	6.18	115.76	109.97
18	A	1132	CLA	C2C-C1C-NC	6.18	115.76	109.97
18	B	1023	CLA	C4A-NA-C1A	6.18	109.48	106.71
18	4	4016	CLA	C2C-C1C-NC	6.17	115.75	109.97
18	A	1103	CLA	C2C-C1C-NC	6.16	115.75	109.97
18	B	1222	CLA	C2C-C1C-NC	6.16	115.74	109.97
18	B	1221	CLA	C2C-C1C-NC	6.16	115.74	109.97
18	B	1232	CLA	C2C-C1C-NC	6.14	115.73	109.97
18	A	1108	CLA	C2C-C1C-NC	6.14	115.72	109.97
18	B	1229	CLA	C2C-C1C-NC	6.14	115.72	109.97
18	A	1120	CLA	C2C-C1C-NC	6.12	115.70	109.97
18	B	1205	CLA	C2C-C1C-NC	6.11	115.70	109.97
18	4	4009	CLA	C2C-C1C-NC	6.11	115.70	109.97
18	2	2006	CLA	C2C-C1C-NC	6.11	115.69	109.97
18	3	3006	CLA	C4D-C3D-CAD	6.10	111.87	108.47
18	4	4007	CLA	O2A-CGA-O1A	-6.10	108.20	123.59
22	B	6005	BCR	C20-C19-C18	6.10	143.55	126.42
18	2	2019	CLA	C3C-C2C-C1C	-6.10	99.90	107.21
18	G	1003	CLA	C4A-NA-C1A	6.10	109.45	106.71
18	2	2008	CLA	C2C-C1C-NC	6.10	115.68	109.97
18	B	1207	CLA	C2C-C1C-NC	6.09	115.68	109.97
18	B	1203	CLA	C2C-C1C-NC	6.09	115.68	109.97
18	4	4017	CLA	C2C-C1C-NC	6.09	115.67	109.97
18	A	1107	CLA	C2C-C1C-NC	6.09	115.67	109.97
18	A	1129	CLA	C4A-NA-C1A	6.08	109.44	106.71
18	B	1220	CLA	C2C-C1C-NC	6.08	115.67	109.97
18	3	3007	CLA	C2C-C1C-NC	6.07	115.66	109.97
18	G	1003	CLA	C2C-C1C-NC	6.07	115.66	109.97
18	A	1131	CLA	C2C-C1C-NC	6.06	115.65	109.97
18	2	2001	CLA	C1C-C2C-C3C	-6.06	100.58	106.96
18	B	1238	CLA	C2C-C1C-NC	6.05	115.64	109.97
18	L	1503	CLA	C2C-C1C-NC	6.04	115.63	109.97
18	B	1208	CLA	C2C-C1C-NC	6.04	115.63	109.97
18	A	1125	CLA	C2C-C1C-NC	6.03	115.62	109.97
18	B	1204	CLA	O2A-C1-C2	6.03	124.48	108.64
18	B	1021	CLA	C2C-C1C-NC	6.03	115.62	109.97
18	B	1207	CLA	O2A-C1-C2	6.03	124.47	108.64
18	G	1002	CLA	O2D-CGD-CBD	6.03	121.98	111.27
18	2	2005	CLA	C2C-C1C-NC	6.02	115.61	109.97
18	A	1102	CLA	C2C-C1C-NC	6.02	115.61	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3006	CLA	C2C-C1C-NC	6.02	115.61	109.97
18	F	1302	CLA	C2C-C1C-NC	6.02	115.61	109.97
27	3	3501	LUT	C22-C23-C24	-6.02	104.89	111.74
18	A	1102	CLA	C4A-NA-C1A	6.01	109.41	106.71
18	4	4002	CLA	O2A-C1-C2	6.01	124.44	108.64
22	J	6012	BCR	C24-C23-C22	-6.01	117.15	126.23
18	B	1235	CLA	C2C-C1C-NC	6.01	115.60	109.97
18	A	1140	CLA	O2A-C1-C2	6.00	124.42	108.64
18	K	1001	CLA	C1C-C2C-C3C	-6.00	100.64	106.96
18	B	1236	CLA	C2C-C1C-NC	6.00	115.59	109.97
18	A	1106	CLA	O2D-CGD-CBD	6.00	121.93	111.27
18	A	1116	CLA	O2A-C1-C2	5.99	124.39	108.64
18	B	1228	CLA	C2C-C1C-NC	5.98	115.57	109.97
18	A	1123	CLA	C4A-NA-C1A	5.98	109.39	106.71
18	A	1132	CLA	O2D-CGD-CBD	5.97	121.88	111.27
18	3	3018	CLA	C4D-C3D-CAD	5.97	111.80	108.47
18	4	4004	CLA	O2D-CGD-CBD	5.97	121.87	111.27
18	2	2004	CLA	O2A-C1-C2	5.96	124.30	108.64
18	2	2002	CLA	C2C-C1C-NC	5.96	115.56	109.97
18	3	3013	CLA	C2C-C1C-NC	5.95	115.55	109.97
18	1	1014	CLA	C2C-C1C-NC	5.95	115.55	109.97
18	B	1212	CLA	C4A-NA-C1A	5.95	109.38	106.71
18	1	1004	CLA	C2C-C1C-NC	5.95	115.55	109.97
18	2	2009	CLA	C1C-C2C-C3C	-5.95	100.70	106.96
18	3	3010	CLA	C1C-C2C-C3C	-5.95	100.70	106.96
18	4	4001	CLA	C4D-C3D-CAD	5.95	111.79	108.47
18	A	1123	CLA	O2D-CGD-CBD	5.94	121.83	111.27
18	4	4004	CLA	C4A-NA-C1A	5.94	109.38	106.71
18	3	3001	CLA	C1C-C2C-C3C	-5.94	100.71	106.96
18	3	3001	CLA	C2C-C1C-NC	5.93	115.53	109.97
18	2	2016	CLA	C1C-C2C-C3C	-5.93	100.72	106.96
18	A	1110	CLA	C2C-C1C-NC	5.93	115.52	109.97
18	A	1112	CLA	O2D-CGD-CBD	5.93	121.80	111.27
18	A	1107	CLA	O2A-C1-C2	5.92	124.20	108.64
18	4	4003	CLA	C2C-C1C-NC	5.91	115.51	109.97
18	B	1227	CLA	C2C-C1C-NC	5.91	115.51	109.97
18	2	2019	CLA	CBD-CAD-C3D	5.91	108.58	104.34
18	A	1118	CLA	C4A-NA-C1A	5.90	109.36	106.71
18	B	1234	CLA	C2C-C1C-NC	5.90	115.50	109.97
18	A	1103	CLA	C4A-NA-C1A	5.89	109.36	106.71
18	3	3003	CLA	C1C-C2C-C3C	-5.89	100.77	106.96
18	4	4002	CLA	C1C-C2C-C3C	-5.89	100.77	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3004	CLA	C4D-C3D-CAD	5.88	111.75	108.47
22	J	6013	BCR	C24-C23-C22	-5.88	117.35	126.23
18	B	1221	CLA	C4A-NA-C1A	5.87	109.35	106.71
18	3	3019	CLA	CBD-CAD-C3D	5.87	108.55	104.34
18	3	3012	CLA	C2C-C1C-NC	5.87	115.47	109.97
18	A	1138	CLA	C2C-C1C-NC	5.87	115.47	109.97
18	A	1140	CLA	C2C-C1C-NC	5.86	115.47	109.97
18	3	3017	CLA	C2C-C1C-NC	5.85	115.45	109.97
18	B	1023	CLA	C2C-C1C-NC	5.85	115.45	109.97
18	B	1201	CLA	C2C-C1C-NC	5.85	115.45	109.97
18	1	1003	CLA	O2A-CGA-O1A	-5.83	108.87	123.59
18	B	1224	CLA	C4A-NA-C1A	5.83	109.33	106.71
18	4	4007	CLA	C4D-C3D-CAD	5.83	111.72	108.47
18	L	1502	CLA	C4A-NA-C1A	5.83	109.33	106.71
18	3	3017	CLA	C4A-NA-C1A	5.82	109.32	106.71
18	B	1223	CLA	O2D-CGD-CBD	5.81	121.59	111.27
22	G	2011	BCR	C20-C19-C18	5.81	142.74	126.42
18	4	4016	CLA	C4D-C3D-CAD	5.80	111.71	108.47
18	A	1122	CLA	C4A-NA-C1A	5.80	109.31	106.71
18	1	1001	CLA	C2C-C1C-NC	5.80	115.41	109.97
18	1	1004	CLA	O2A-CGA-O1A	-5.80	108.95	123.59
18	2	2012	CLA	C2C-C1C-NC	5.78	115.39	109.97
18	B	1225	CLA	C4A-NA-C1A	5.78	109.31	106.71
18	B	1218	CLA	O2D-CGD-CBD	5.77	121.53	111.27
27	2	2502	LUT	C22-C23-C24	-5.77	105.17	111.74
18	B	1208	CLA	O2A-C1-C2	5.77	123.79	108.64
18	B	1208	CLA	O2D-CGD-CBD	5.76	121.50	111.27
18	3	3006	CLA	C4A-NA-C1A	5.75	109.29	106.71
18	1	1013	CLA	C1C-C2C-C3C	-5.75	100.91	106.96
18	J	1302	CLA	O2A-C1-C2	5.74	123.72	108.64
18	B	1213	CLA	C2C-C1C-NC	5.73	115.34	109.97
18	L	1502	CLA	C4D-C3D-CAD	5.73	111.67	108.47
18	A	1120	CLA	C4A-NA-C1A	5.73	109.28	106.71
18	2	2008	CLA	C1C-C2C-C3C	-5.73	100.94	106.96
18	A	1118	CLA	O2D-CGD-CBD	5.72	121.44	111.27
18	L	1502	CLA	C2C-C1C-NC	5.71	115.32	109.97
22	A	6017	BCR	C19-C18-C17	5.71	127.70	118.94
18	3	3012	CLA	C4D-C3D-CAD	5.71	111.65	108.47
18	2	2001	CLA	O2A-CGA-O1A	-5.70	109.20	123.59
18	A	1125	CLA	C4A-NA-C1A	5.70	109.27	106.71
18	3	3004	CLA	C1C-C2C-C3C	-5.69	100.97	106.96
18	B	1227	CLA	O2D-CGD-CBD	5.69	121.38	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1236	CLA	O2A-C1-C2	5.69	123.58	108.64
18	A	1101	CLA	O2A-C1-C2	5.68	123.56	108.64
18	B	1211	CLA	C4A-NA-C1A	5.67	109.26	106.71
18	A	1103	CLA	O2A-C1-C2	5.67	123.53	108.64
18	3	3005	CLA	C1C-C2C-C3C	-5.67	101.00	106.96
18	4	4007	CLA	C1C-C2C-C3C	-5.66	101.00	106.96
18	B	1201	CLA	C4A-NA-C1A	5.66	109.25	106.71
18	1	1002	CLA	C2C-C1C-NC	5.65	115.27	109.97
18	A	1140	CLA	C4A-NA-C1A	5.65	109.25	106.71
18	A	1110	CLA	O2A-C1-C2	5.64	123.47	108.64
18	A	1116	CLA	C1-C2-C3	-5.64	116.29	126.04
18	B	1228	CLA	C4A-NA-C1A	5.64	109.24	106.71
18	B	1206	CLA	C1C-C2C-C3C	-5.64	101.03	106.96
18	B	1229	CLA	C4A-NA-C1A	5.63	109.24	106.71
18	B	1205	CLA	O2A-CGA-O1A	-5.63	109.38	123.59
18	A	1118	CLA	C1C-C2C-C3C	-5.62	101.05	106.96
18	B	1226	CLA	O2A-CGA-O1A	-5.61	109.44	123.59
18	B	1226	CLA	C1C-C2C-C3C	-5.61	101.06	106.96
18	4	4004	CLA	C1C-C2C-C3C	-5.60	101.07	106.96
18	B	1231	CLA	C2C-C1C-NC	5.59	115.21	109.97
18	A	1101	CLA	O2D-CGD-CBD	5.59	121.21	111.27
27	2	2501	LUT	C21-C26-C25	5.59	121.43	111.42
18	4	4007	CLA	O2A-C1-C2	5.59	123.33	108.64
18	G	1001	CLA	O2A-CGA-O1A	-5.59	109.48	123.59
18	1	1004	CLA	O2D-CGD-CBD	5.59	121.19	111.27
22	L	6020	BCR	C24-C23-C22	-5.58	117.80	126.23
18	B	1235	CLA	O2A-CGA-O1A	-5.57	109.53	123.59
18	4	4004	CLA	C2C-C1C-NC	5.57	115.19	109.97
18	A	1126	CLA	C4A-NA-C1A	5.57	109.21	106.71
18	2	2008	CLA	O2A-CGA-O1A	-5.56	109.55	123.59
18	3	3001	CLA	C4A-NA-C1A	5.56	109.21	106.71
18	4	4012	CLA	C1C-C2C-C3C	-5.56	101.11	106.96
18	A	1013	CLA	C2C-C1C-NC	5.55	115.17	109.97
18	1	1012	CLA	C1C-C2C-C3C	-5.54	101.13	106.96
18	B	1240	CLA	C4A-NA-C1A	5.53	109.19	106.71
27	1	1502	LUT	C7-C8-C9	-5.53	117.88	126.23
18	A	1139	CLA	C1C-C2C-C3C	-5.53	101.15	106.96
18	A	1109	CLA	C4A-NA-C1A	5.53	109.19	106.71
18	4	4005	CLA	C1C-C2C-C3C	-5.52	101.15	106.96
18	B	1229	CLA	O2A-CGA-O1A	-5.52	109.65	123.59
18	A	1013	CLA	C4A-NA-C1A	5.52	109.19	106.71
18	A	1127	CLA	C4A-NA-C1A	5.52	109.19	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4017	CLA	O2A-CGA-O1A	-5.52	109.67	123.59
18	3	3001	CLA	O2A-C1-C2	5.51	123.13	108.64
18	B	1202	CLA	O2A-C1-C2	5.51	123.13	108.64
18	B	1212	CLA	O2D-CGD-CBD	5.51	121.06	111.27
18	L	1502	CLA	O2A-CGA-O1A	-5.51	109.68	123.59
27	4	4501	LUT	C22-C23-C24	-5.51	105.47	111.74
18	2	2016	CLA	O2A-C1-C2	5.51	123.11	108.64
18	3	3007	CLA	O2A-C1-C2	5.51	123.11	108.64
18	1	1003	CLA	C1C-C2C-C3C	-5.50	101.17	106.96
18	B	1023	CLA	O2A-C1-C2	5.50	123.08	108.64
23	F	5001	LMG	O7-C10-C11	5.50	121.20	111.09
18	B	1212	CLA	O2A-C1-C2	5.49	123.06	108.64
18	A	1013	CLA	O2A-C1-C2	5.49	123.06	108.64
18	A	1113	CLA	C4A-NA-C1A	5.48	109.17	106.71
18	B	1234	CLA	O2A-C1-C2	5.48	123.04	108.64
18	3	3018	CLA	C1C-C2C-C3C	-5.48	101.20	106.96
18	A	1101	CLA	O2A-CGA-O1A	-5.48	109.77	123.59
18	4	4009	CLA	C1C-C2C-C3C	-5.47	101.20	106.96
18	A	1136	CLA	C4A-NA-C1A	5.47	109.17	106.71
27	I	6018	LUT	C21-C26-C25	5.47	121.21	111.42
18	A	1131	CLA	C4A-NA-C1A	5.46	109.16	106.71
18	A	1114	CLA	O2D-CGD-CBD	5.46	120.96	111.27
18	L	1501	CLA	O2A-C1-C2	5.45	122.96	108.64
22	B	6009	BCR	C24-C23-C22	-5.45	118.00	126.23
18	A	1121	CLA	O2A-C1-C2	5.45	122.96	108.64
18	L	1503	CLA	O2A-CGA-O1A	-5.45	109.84	123.59
18	4	4005	CLA	O2D-CGD-CBD	5.45	120.95	111.27
23	J	5001	LMG	O7-C10-C11	5.45	123.24	111.50
18	A	1135	CLA	O2D-CGD-CBD	5.44	120.94	111.27
18	B	1217	CLA	C1C-C2C-C3C	-5.44	101.24	106.96
18	A	1121	CLA	O2D-CGD-CBD	5.44	120.93	111.27
18	1	1007	CLA	C4D-C3D-CAD	5.44	111.50	108.47
18	B	1209	CLA	O2D-CGD-CBD	5.43	120.92	111.27
18	4	4017	CLA	O2D-CGD-CBD	5.43	120.92	111.27
27	2	2502	LUT	C21-C26-C25	5.43	121.14	111.42
18	B	1239	CLA	C1C-C2C-C3C	-5.42	101.26	106.96
18	1	1005	CLA	O2A-CGA-O1A	-5.42	109.92	123.59
23	4	4801	LMG	O7-C10-C11	5.42	123.17	111.50
18	1	1006	CLA	C1C-C2C-C3C	-5.41	101.26	106.96
18	B	1230	CLA	C2C-C1C-NC	5.41	115.04	109.97
18	A	1111	CLA	C4A-NA-C1A	5.41	109.14	106.71
18	B	1218	CLA	C1C-C2C-C3C	-5.41	101.27	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1234	CLA	O2D-CGD-CBD	5.41	120.89	111.27
18	2	2004	CLA	O2A-CGA-O1A	-5.41	109.94	123.59
18	4	4008	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
18	B	1222	CLA	C4A-NA-C1A	5.41	109.14	106.71
18	B	1203	CLA	C4A-NA-C1A	5.41	109.14	106.71
18	H	1000	CLA	C4A-NA-C1A	5.41	109.14	106.71
18	B	1239	CLA	O2A-C1-C2	5.40	122.84	108.64
18	H	1000	CLA	C1C-C2C-C3C	-5.40	101.28	106.96
18	1	1008	CLA	C1C-C2C-C3C	-5.40	101.28	106.96
18	B	1229	CLA	O2D-CGD-CBD	5.40	120.87	111.27
27	3	3502	LUT	C21-C26-C25	5.40	121.10	111.42
18	B	1223	CLA	C4A-NA-C1A	5.40	109.14	106.71
17	A	1011	CL0	O2A-CGA-O1A	-5.40	109.97	123.59
18	A	1105	CLA	O2A-C1-C2	5.40	122.82	108.64
18	J	1302	CLA	O2A-CGA-O1A	-5.40	109.97	123.59
17	A	1011	CL0	C1C-C2C-C3C	-5.40	101.28	106.96
18	G	1001	CLA	C1C-C2C-C3C	-5.39	101.29	106.96
18	A	1128	CLA	O2A-CGA-O1A	-5.39	109.98	123.59
18	B	1221	CLA	O2A-C1-C2	5.39	122.80	108.64
18	3	3002	CLA	C4D-C3D-CAD	5.39	111.48	108.47
18	3	3003	CLA	C4D-C3D-CAD	5.39	111.48	108.47
18	B	1234	CLA	C1-C2-C3	-5.39	116.72	126.04
18	A	1135	CLA	O2A-C1-C2	5.39	122.80	108.64
18	2	2008	CLA	O2D-CGD-CBD	5.38	120.84	111.27
18	3	3002	CLA	O2D-CGD-CBD	5.38	120.84	111.27
18	1	1011	CLA	C2C-C1C-NC	5.38	115.02	109.97
27	4	4503	LUT	C21-C26-C27	5.38	119.51	112.70
18	B	1211	CLA	C4D-C3D-CAD	5.38	111.47	108.47
18	3	3012	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
18	B	1213	CLA	O2A-C1-C2	5.37	122.76	108.64
18	A	1134	CLA	C4A-NA-C1A	5.37	109.12	106.71
18	B	1012	CLA	C4A-NA-C1A	5.37	109.12	106.71
18	3	3019	CLA	C3C-C2C-C1C	-5.37	100.78	107.21
18	3	3006	CLA	O2A-CGA-O1A	-5.37	110.04	123.59
18	G	1003	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
29	4	4505	ZEX	C7-C8-C9	-5.36	118.13	126.23
18	A	1109	CLA	O2A-C1-C2	5.36	122.73	108.64
18	2	2005	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
18	A	1106	CLA	O2A-C1-C2	5.36	122.72	108.64
18	F	1302	CLA	O2D-CGD-CBD	5.36	120.79	111.27
18	A	1151	CLA	C1C-C2C-C3C	-5.35	101.34	106.96
18	B	1224	CLA	O2A-CGA-O1A	-5.35	110.10	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1123	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
18	A	1135	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
18	A	1114	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
18	A	1130	CLA	C4A-NA-C1A	5.34	109.11	106.71
18	3	3005	CLA	O2D-CGD-CBD	5.34	120.76	111.27
18	A	1116	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
18	A	1106	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
18	3	3019	CLA	C1C-NC-C4C	-5.33	104.31	106.71
18	2	2001	CLA	C4D-C3D-CAD	5.33	111.44	108.47
18	A	1132	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
18	B	1235	CLA	O2D-CGD-CBD	5.33	120.74	111.27
18	B	1201	CLA	O2A-C1-C2	5.33	122.63	108.64
18	A	1130	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
18	B	1224	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
18	A	1103	CLA	O2D-CGD-CBD	5.32	120.72	111.27
18	A	1134	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
18	A	1111	CLA	O2D-CGD-CBD	5.32	120.72	111.27
18	3	3005	CLA	O2A-C1-C2	5.32	122.61	108.64
18	A	1133	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
18	A	1119	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
18	A	1101	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
18	G	1002	CLA	C1C-C2C-C3C	-5.31	101.38	106.96
18	B	1215	CLA	O2A-C1-C2	5.30	122.58	108.64
18	B	1234	CLA	C4A-NA-C1A	5.30	109.09	106.71
18	1	1004	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
18	B	1214	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
18	J	1302	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
18	B	1209	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
18	B	1215	CLA	C1C-C2C-C3C	-5.30	101.39	106.96
18	4	4012	CLA	O2A-C1-C2	5.29	122.54	108.64
18	A	1121	CLA	C1C-C2C-C3C	-5.29	101.39	106.96
18	B	1238	CLA	O2D-CGD-CBD	5.29	120.67	111.27
17	A	1011	CL0	C4A-NA-C1A	5.29	109.08	106.71
18	A	1109	CLA	C1C-C2C-C3C	-5.29	101.40	106.96
18	B	1021	CLA	C1C-C2C-C3C	-5.28	101.40	106.96
18	B	1203	CLA	C1C-C2C-C3C	-5.28	101.40	106.96
18	B	1217	CLA	O2D-CGD-CBD	5.28	120.65	111.27
18	B	1225	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
18	A	1116	CLA	O2A-CGA-O1A	-5.28	110.27	123.59
18	3	3002	CLA	C1C-C2C-C3C	-5.27	101.41	106.96
18	A	1124	CLA	C1C-C2C-C3C	-5.27	101.41	106.96
18	B	1218	CLA	O2A-CGA-O1A	-5.27	110.29	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	1003	CLA	C4D-C3D-CAD	5.27	111.41	108.47
22	B	6004	BCR	C24-C23-C22	-5.27	118.28	126.23
18	A	1115	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
18	4	4006	CLA	C4D-C3D-CAD	5.27	111.41	108.47
18	B	1227	CLA	O2A-C1-C2	5.27	122.48	108.64
27	1	1502	LUT	C21-C26-C25	5.27	120.85	111.42
18	A	1121	CLA	C4A-NA-C1A	5.26	109.07	106.71
22	G	2011	BCR	C19-C18-C17	5.26	127.02	118.94
18	4	4001	CLA	O2A-CGA-O1A	-5.26	110.31	123.59
18	4	4005	CLA	O2A-CGA-O1A	-5.26	110.31	123.59
18	3	3007	CLA	C4D-C3D-CAD	5.26	111.40	108.47
18	A	1137	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
18	A	1124	CLA	O2A-CGA-O1A	-5.26	110.32	123.59
18	1	1006	CLA	C4D-C3D-CAD	5.26	111.40	108.47
18	2	2004	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
18	1	1007	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
22	3	3503	BCR	C34-C9-C10	-5.25	115.56	122.92
18	J	1302	CLA	C4A-NA-C1A	5.25	109.07	106.71
18	4	4004	CLA	O2A-CGA-O1A	-5.25	110.34	123.59
18	B	1240	CLA	O2D-CGD-CBD	5.25	120.60	111.27
22	B	6004	BCR	C20-C19-C18	5.25	141.17	126.42
18	2	2007	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
18	2	2006	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
18	A	1117	CLA	C4A-NA-C1A	5.25	109.07	106.71
18	2	2001	CLA	CAA-C2A-C1A	-5.24	94.79	111.97
18	1	1011	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
18	3	3012	CLA	O2A-CGA-O1A	-5.24	110.37	123.59
18	A	1107	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
18	1	1005	CLA	O2A-C1-C2	5.24	122.40	108.64
18	B	1202	CLA	C1C-C2C-C3C	-5.23	101.45	106.96
18	A	1122	CLA	O2A-CGA-O1A	-5.23	110.38	123.59
21	B	5004	LHG	O7-C7-C8	5.23	120.72	111.09
18	A	1128	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
18	A	1139	CLA	C4A-NA-C1A	5.23	109.06	106.71
18	B	1225	CLA	O2D-CGD-CBD	5.23	120.56	111.27
18	A	1117	CLA	O2D-CGD-CBD	5.23	120.56	111.27
18	B	1219	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
18	B	1224	CLA	O2D-CGD-CBD	5.23	120.56	111.27
18	A	1125	CLA	O2D-CGD-CBD	5.23	120.55	111.27
18	3	3007	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
18	1	1001	CLA	O2A-C1-C2	5.22	122.36	108.64
18	A	1120	CLA	C1C-C2C-C3C	-5.22	101.47	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	1302	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
18	G	1001	CLA	C4D-C3D-CAD	5.22	111.38	108.47
18	B	1213	CLA	C4A-NA-C1A	5.22	109.05	106.71
18	4	4008	CLA	O2D-CGD-CBD	5.22	120.54	111.27
18	B	1205	CLA	C4A-NA-C1A	5.22	109.05	106.71
18	B	1210	CLA	O2A-C1-C2	5.22	122.34	108.64
18	B	1222	CLA	C1C-C2C-C3C	-5.21	101.47	106.96
18	B	1227	CLA	C1C-C2C-C3C	-5.21	101.47	106.96
18	B	1208	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
18	A	1136	CLA	O2A-CGA-O1A	-5.21	110.44	123.59
18	A	1237	CLA	C4A-NA-C1A	5.21	109.05	106.71
18	A	1138	CLA	C4A-NA-C1A	5.20	109.05	106.71
18	1	1002	CLA	C1C-C2C-C3C	-5.20	101.48	106.96
18	B	1219	CLA	C4A-NA-C1A	5.20	109.05	106.71
18	2	2006	CLA	O2A-CGA-O1A	-5.20	110.46	123.59
18	A	1125	CLA	O2A-C1-C2	5.20	122.31	108.64
18	B	1230	CLA	O2A-CGA-O1A	-5.20	110.47	123.59
22	3	3503	BCR	C33-C5-C6	-5.20	118.69	124.53
18	A	1121	CLA	O2A-CGA-O1A	-5.20	110.47	123.59
22	A	6017	BCR	C20-C19-C18	5.20	141.02	126.42
18	A	1117	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
18	1	1001	CLA	O2A-CGA-O1A	-5.20	110.48	123.59
18	A	1127	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
18	B	1235	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
18	4	4006	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
18	B	1211	CLA	C2C-C1C-NC	5.19	114.84	109.97
18	B	1211	CLA	O2A-C1-C2	5.19	122.28	108.64
18	2	2009	CLA	C4D-C3D-CAD	5.19	111.36	108.47
18	B	1215	CLA	O2D-CGD-CBD	5.19	120.49	111.27
18	4	4009	CLA	O2A-CGA-O1A	-5.19	110.49	123.59
18	B	1240	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
18	B	1223	CLA	O2A-C1-C2	5.19	122.27	108.64
18	A	1134	CLA	O2A-CGA-O1A	-5.19	110.50	123.59
18	B	1206	CLA	O2A-C1-C2	5.19	122.27	108.64
18	B	1238	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
18	L	1503	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
18	4	4003	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
18	A	1140	CLA	O2D-CGD-CBD	5.18	120.48	111.27
18	3	3005	CLA	C4D-C3D-CAD	5.18	111.36	108.47
18	B	1239	CLA	C4A-NA-C1A	5.18	109.03	106.71
18	A	1237	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
18	B	1204	CLA	C4A-NA-C1A	5.18	109.03	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4002	CLA	O2A-CGA-O1A	-5.18	110.52	123.59
18	B	1202	CLA	O2D-CGD-CBD	5.18	120.47	111.27
18	A	1105	CLA	C1C-C2C-C3C	-5.17	101.52	106.96
18	B	1232	CLA	O2A-CGA-O1A	-5.17	110.53	123.59
18	G	1001	CLA	O2D-CGD-CBD	5.17	120.46	111.27
18	A	1131	CLA	O2A-CGA-O1A	-5.17	110.54	123.59
18	B	1236	CLA	O2A-CGA-O1A	-5.17	110.54	123.59
18	B	1210	CLA	O2A-CGA-O1A	-5.17	110.55	123.59
18	B	1236	CLA	C4A-NA-C1A	5.17	109.03	106.71
18	B	1212	CLA	C1C-C2C-C3C	-5.17	101.53	106.96
18	A	1104	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
18	A	1108	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
18	A	1133	CLA	O2A-CGA-O1A	-5.16	110.56	123.59
18	A	1127	CLA	O2A-CGA-O1A	-5.16	110.57	123.59
18	B	1239	CLA	O2D-CGD-CBD	5.16	120.44	111.27
27	I	6018	LUT	C22-C23-C24	-5.16	105.87	111.74
18	B	1232	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
18	A	1114	CLA	C4A-NA-C1A	5.16	109.02	106.71
18	F	1301	CLA	C1C-C2C-C3C	-5.16	101.54	106.96
18	A	1136	CLA	O2D-CGD-CBD	5.16	120.43	111.27
18	B	1214	CLA	C4A-NA-C1A	5.15	109.02	106.71
18	B	1216	CLA	O2D-CGD-CBD	5.15	120.42	111.27
18	B	1214	CLA	O2A-CGA-O1A	-5.15	110.59	123.59
18	A	1130	CLA	O2D-CGD-CBD	5.15	120.42	111.27
18	A	1106	CLA	C4A-NA-C1A	5.15	109.02	106.71
18	B	1232	CLA	O2A-C1-C2	5.15	122.17	108.64
18	B	1216	CLA	O2A-C1-C2	5.15	122.16	108.64
29	4	4505	ZEX	C28-C27-C26	-5.14	118.30	127.09
18	L	1502	CLA	C1C-C2C-C3C	-5.14	101.55	106.96
18	A	1133	CLA	O2A-C1-C2	5.14	122.16	108.64
18	A	1131	CLA	C1C-C2C-C3C	-5.14	101.55	106.96
18	A	1112	CLA	C1C-C2C-C3C	-5.14	101.55	106.96
18	B	1214	CLA	C4D-C3D-CAD	5.14	111.34	108.47
18	2	2002	CLA	C1C-C2C-C3C	-5.14	101.55	106.96
18	A	1237	CLA	C4D-C3D-CAD	5.14	111.33	108.47
18	B	1231	CLA	C4D-C3D-CAD	5.14	111.33	108.47
18	1	1012	CLA	C4D-C3D-CAD	5.13	111.33	108.47
18	B	1204	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
18	A	1102	CLA	O2D-CGD-CBD	5.13	120.39	111.27
18	B	1236	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
18	A	1122	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
22	I	6020	BCR	C20-C19-C18	5.13	140.82	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1236	CLA	O2D-CGD-CBD	5.13	120.38	111.27
18	1	1013	CLA	O2D-CGD-CBD	5.13	120.38	111.27
18	B	1217	CLA	C4A-NA-C1A	5.12	109.01	106.71
18	L	1502	CLA	O2D-CGD-CBD	5.12	120.37	111.27
18	A	1107	CLA	O2D-CGD-CBD	5.12	120.36	111.27
18	A	1110	CLA	C4A-NA-C1A	5.12	109.01	106.71
18	A	1109	CLA	O2A-CGA-O1A	-5.12	110.68	123.59
18	B	1012	CLA	O2A-CGA-O1A	-5.12	110.68	123.59
18	L	1501	CLA	C2C-C1C-NC	5.12	114.76	109.97
18	A	1110	CLA	O2D-CGD-CBD	5.11	120.36	111.27
18	1	1014	CLA	O2D-CGD-CBD	5.11	120.35	111.27
18	B	1206	CLA	O2A-CGA-O1A	-5.11	110.69	123.59
18	A	1102	CLA	C1C-C2C-C3C	-5.11	101.58	106.96
18	A	1151	CLA	C4A-NA-C1A	5.11	109.00	106.71
18	A	1133	CLA	C4A-NA-C1A	5.10	109.00	106.71
18	B	1221	CLA	C1C-C2C-C3C	-5.10	101.59	106.96
18	A	1119	CLA	O2A-CGA-O1A	-5.10	110.72	123.59
22	A	6008	BCR	C24-C23-C22	-5.10	118.54	126.23
18	A	1103	CLA	C1C-C2C-C3C	-5.09	101.60	106.96
18	B	1238	CLA	O2A-CGA-O1A	-5.09	110.73	123.59
18	3	3004	CLA	O2A-CGA-O1A	-5.09	110.74	123.59
18	B	1216	CLA	C1C-C2C-C3C	-5.09	101.61	106.96
18	1	1006	CLA	O2A-CGA-O1A	-5.09	110.75	123.59
18	B	1205	CLA	C4D-C3D-CAD	5.09	111.31	108.47
18	B	1227	CLA	C4A-NA-C1A	5.08	108.99	106.71
18	4	4003	CLA	O2A-CGA-O1A	-5.08	110.76	123.59
18	B	1218	CLA	C4A-NA-C1A	5.08	108.99	106.71
18	A	1138	CLA	C1C-C2C-C3C	-5.08	101.61	106.96
18	F	1302	CLA	O2A-CGA-O1A	-5.08	110.77	123.59
18	L	1501	CLA	C4D-C3D-CAD	5.07	111.30	108.47
18	A	1136	CLA	C1C-C2C-C3C	-5.07	101.62	106.96
18	A	1117	CLA	O2A-C1-C2	5.07	121.96	108.64
18	A	1132	CLA	O2A-CGA-O1A	-5.07	110.79	123.59
22	K	2011	BCR	C24-C23-C22	-5.07	118.57	126.23
18	2	2009	CLA	O2A-CGA-O1A	-5.07	110.80	123.59
18	A	1151	CLA	O2A-CGA-O1A	-5.07	110.80	123.59
18	A	1123	CLA	O2A-CGA-O1A	-5.07	110.80	123.59
18	A	1129	CLA	O2A-C1-C2	5.06	121.94	108.64
18	A	1106	CLA	O2A-CGA-O1A	-5.06	110.81	123.59
18	B	1220	CLA	C1C-C2C-C3C	-5.06	101.63	106.96
18	B	1228	CLA	C1C-C2C-C3C	-5.06	101.63	106.96
22	F	6014	BCR	C24-C23-C22	-5.06	118.59	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1107	CLA	C4A-NA-C1A	5.06	108.98	106.71
18	B	1238	CLA	O2A-C1-C2	5.06	121.92	108.64
18	A	1134	CLA	O2D-CGD-CBD	5.05	120.25	111.27
18	3	3013	CLA	C1C-C2C-C3C	-5.05	101.65	106.96
18	B	1215	CLA	C4A-NA-C1A	5.04	108.97	106.71
18	1	1003	CLA	C4D-C3D-CAD	5.04	111.28	108.47
18	A	1128	CLA	C4A-NA-C1A	5.04	108.97	106.71
18	A	1237	CLA	O2A-CGA-O1A	-5.04	110.87	123.59
18	A	1124	CLA	O2A-C1-C2	5.04	121.88	108.64
18	1	1014	CLA	C4D-C3D-CAD	5.04	111.28	108.47
18	A	1126	CLA	C1C-C2C-C3C	-5.04	101.66	106.96
18	A	1135	CLA	C4A-NA-C1A	5.04	108.97	106.71
18	B	1209	CLA	C4A-NA-C1A	5.04	108.97	106.71
27	2	2501	LUT	C22-C23-C24	-5.04	106.01	111.74
18	4	4017	CLA	C1C-C2C-C3C	-5.04	101.66	106.96
18	A	1131	CLA	O2D-CGD-CBD	5.04	120.22	111.27
18	B	1211	CLA	O2A-CGA-O1A	-5.04	110.88	123.59
18	2	2003	CLA	C1C-C2C-C3C	-5.04	101.66	106.96
18	A	1130	CLA	O2A-CGA-O1A	-5.03	110.89	123.59
18	B	1223	CLA	O2A-CGA-O1A	-5.03	110.91	123.59
18	A	1129	CLA	C1C-C2C-C3C	-5.02	101.67	106.96
18	A	1129	CLA	O2D-CGD-CBD	5.02	120.19	111.27
18	4	4003	CLA	C4D-C3D-CAD	5.02	111.27	108.47
18	A	1137	CLA	C4A-NA-C1A	5.02	108.96	106.71
18	A	1135	CLA	O2A-CGA-O1A	-5.02	110.93	123.59
27	4	4501	LUT	C21-C26-C25	5.02	120.40	111.42
17	A	1011	CL0	O2D-CGD-CBD	5.01	120.18	111.27
18	A	1101	CLA	C4A-NA-C1A	5.01	108.96	106.71
18	3	3006	CLA	C1C-C2C-C3C	-5.01	101.69	106.96
18	A	1133	CLA	O2D-CGD-CBD	5.01	120.17	111.27
27	4	4503	LUT	C1-C6-C5	-5.01	115.56	122.61
22	B	6004	BCR	C19-C18-C17	5.01	126.62	118.94
18	A	1022	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
18	A	1013	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
18	A	1139	CLA	O2A-C1-C2	5.00	121.78	108.64
18	B	1207	CLA	C4A-NA-C1A	5.00	108.95	106.71
18	4	4016	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
18	B	1205	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
18	G	1003	CLA	O2D-CGD-CBD	5.00	120.15	111.27
18	B	1201	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
18	1	1011	CLA	C4D-C3D-CAD	5.00	111.26	108.47
18	B	1208	CLA	O2A-CGA-O1A	-5.00	110.98	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1023	CLA	O2A-CGA-O1A	-4.99	110.99	123.59
18	B	1222	CLA	O2A-CGA-O1A	-4.99	110.99	123.59
18	F	1302	CLA	O2A-C1-C2	4.99	121.76	108.64
18	B	1021	CLA	O2A-C1-C2	4.99	121.76	108.64
18	F	1301	CLA	C4D-C3D-CAD	4.99	111.25	108.47
18	3	3017	CLA	C1C-C2C-C3C	-4.99	101.72	106.96
18	2	2007	CLA	O2A-CGA-O1A	-4.98	111.01	123.59
18	L	1503	CLA	O2A-C1-C2	4.98	121.73	108.64
18	A	1111	CLA	C1C-C2C-C3C	-4.98	101.72	106.96
18	B	1219	CLA	O2A-C1-C2	4.98	121.72	108.64
18	2	2008	CLA	O2A-C1-C2	4.98	121.71	108.64
27	3	3502	LUT	C18-C5-C6	-4.98	118.94	124.53
18	B	1207	CLA	C1C-C2C-C3C	-4.97	101.73	106.96
18	A	1124	CLA	O2D-CGD-CBD	4.97	120.10	111.27
18	A	1116	CLA	C4A-NA-C1A	4.97	108.94	106.71
18	B	1213	CLA	O2A-CGA-O1A	-4.97	111.05	123.59
18	A	1134	CLA	O2A-C1-C2	4.97	121.70	108.64
18	2	2012	CLA	O2A-CGA-O1A	-4.97	111.05	123.59
18	L	1501	CLA	C1C-C2C-C3C	-4.97	101.73	106.96
18	A	1115	CLA	C4A-NA-C1A	4.96	108.94	106.71
27	4	4503	LUT	C21-C26-C25	4.96	120.31	111.42
18	B	1214	CLA	O2A-C1-C2	4.96	121.67	108.64
22	L	6019	BCR	C24-C23-C22	-4.96	118.74	126.23
18	B	1012	CLA	C1C-C2C-C3C	-4.95	101.75	106.96
18	1	1005	CLA	C4D-C3D-CAD	4.95	111.23	108.47
18	B	1234	CLA	O2A-CGA-O1A	-4.95	111.11	123.59
27	1	1502	LUT	C22-C23-C24	-4.95	106.11	111.74
18	A	1110	CLA	C1C-C2C-C3C	-4.94	101.76	106.96
18	B	1218	CLA	C4D-C3D-CAD	4.94	111.23	108.47
27	4	4503	LUT	C35-C34-C33	-4.93	120.27	127.31
18	A	1139	CLA	C4D-C3D-CAD	4.93	111.22	108.47
18	3	3005	CLA	O2A-CGA-O1A	-4.93	111.15	123.59
18	A	1107	CLA	O2A-CGA-O1A	-4.93	111.15	123.59
18	3	3008	CLA	O2A-CGA-O1A	-4.93	111.15	123.59
18	B	1231	CLA	C1C-C2C-C3C	-4.93	101.77	106.96
18	B	1227	CLA	C4D-C3D-CAD	4.93	111.22	108.47
18	2	2006	CLA	O2D-CGD-CBD	4.93	120.02	111.27
18	A	1110	CLA	O2A-CGA-O1A	-4.92	111.16	123.59
18	A	1137	CLA	O2D-CGD-CBD	4.92	120.01	111.27
18	G	1002	CLA	C4D-C3D-CAD	4.92	111.21	108.47
18	B	1207	CLA	O2D-CGD-CBD	4.92	120.01	111.27
18	B	1223	CLA	C1C-C2C-C3C	-4.92	101.78	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1129	CLA	O2A-CGA-O1A	-4.92	111.18	123.59
18	G	1003	CLA	O2A-C1-C2	4.92	121.56	108.64
18	B	1234	CLA	C4D-C3D-CAD	4.92	111.21	108.47
18	2	2005	CLA	O2A-C1-C2	4.92	121.56	108.64
18	3	3018	CLA	O2A-CGA-O1A	-4.91	111.19	123.59
18	A	1112	CLA	O2A-CGA-O1A	-4.91	111.19	123.59
18	1	1002	CLA	C4D-C3D-CAD	4.91	111.21	108.47
18	A	1102	CLA	O2A-C1-C2	4.91	121.55	108.64
17	A	1011	CL0	O2A-C1-C2	4.91	121.55	108.64
18	A	1113	CLA	C1C-C2C-C3C	-4.91	101.80	106.96
18	J	1302	CLA	O2D-CGD-CBD	4.91	119.99	111.27
22	A	6002	BCR	C24-C23-C22	-4.91	118.82	126.23
18	A	1104	CLA	O2A-C1-C2	4.91	121.53	108.64
18	B	1234	CLA	C1C-C2C-C3C	-4.90	101.80	106.96
18	A	1237	CLA	C1-C2-C3	-4.90	117.57	126.04
18	A	1111	CLA	O2A-CGA-O1A	-4.90	111.22	123.59
18	B	1204	CLA	O2D-CGD-CBD	4.90	119.97	111.27
18	A	1113	CLA	O2D-CGD-CBD	4.90	119.97	111.27
18	A	1120	CLA	O2A-CGA-O1A	-4.90	111.23	123.59
18	B	1210	CLA	C4D-C3D-CAD	4.90	111.20	108.47
18	4	4017	CLA	O2A-C1-C2	4.90	121.51	108.64
18	A	1127	CLA	O2D-CGD-CBD	4.90	119.97	111.27
18	A	1125	CLA	C1C-C2C-C3C	-4.90	101.81	106.96
18	B	1202	CLA	C1-C2-C3	-4.90	117.58	126.04
18	B	1229	CLA	C1C-C2C-C3C	-4.89	101.81	106.96
18	A	1138	CLA	O2A-CGA-O1A	-4.89	111.25	123.59
18	4	4001	CLA	O2A-C1-C2	4.89	121.49	108.64
18	A	1130	CLA	O2A-C1-C2	4.89	121.49	108.64
18	A	1151	CLA	O2D-CGD-CBD	4.89	119.95	111.27
18	B	1226	CLA	O2D-CGD-CBD	4.89	119.95	111.27
18	B	1210	CLA	O2D-CGD-CBD	4.88	119.94	111.27
18	2	2006	CLA	O2A-C1-C2	4.88	121.46	108.64
18	1	1006	CLA	C4A-NA-C1A	4.88	108.90	106.71
18	A	1120	CLA	O2A-C1-C2	4.88	121.46	108.64
18	B	1203	CLA	O2A-CGA-O1A	-4.88	111.28	123.59
22	G	2011	BCR	C37-C22-C21	-4.87	116.09	122.92
18	J	1302	CLA	C4D-C3D-CAD	4.87	111.19	108.47
18	A	1120	CLA	C4D-C3D-CAD	4.87	111.19	108.47
18	A	1116	CLA	O2D-CGD-CBD	4.87	119.93	111.27
18	A	1107	CLA	C4D-C3D-CAD	4.87	111.19	108.47
18	4	4007	CLA	O2D-CGD-CBD	4.87	119.93	111.27
22	L	6020	BCR	C19-C18-C17	4.87	126.41	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	6013	BCR	C34-C9-C10	-4.86	116.11	122.92
18	A	1151	CLA	O2A-C1-C2	4.86	121.41	108.64
18	A	1108	CLA	C4A-NA-C1A	4.86	108.89	106.71
18	4	4003	CLA	O2D-CGD-CBD	4.86	119.90	111.27
18	B	1219	CLA	O2A-CGA-O1A	-4.86	111.33	123.59
18	B	1225	CLA	O2A-CGA-O1A	-4.86	111.33	123.59
18	1	1011	CLA	O2D-CGD-CBD	4.86	119.90	111.27
27	1	1501	LUT	C22-C23-C24	-4.86	106.21	111.74
18	1	1005	CLA	C1C-C2C-C3C	-4.85	101.85	106.96
18	4	4008	CLA	C4D-C3D-CAD	4.85	111.18	108.47
18	B	1217	CLA	C4D-C3D-CAD	4.85	111.18	108.47
18	A	1140	CLA	C1C-C2C-C3C	-4.85	101.86	106.96
18	2	2003	CLA	O2A-CGA-O1A	-4.85	111.35	123.59
18	H	1000	CLA	O2D-CGD-CBD	4.85	119.89	111.27
18	B	1021	CLA	O2A-CGA-O1A	-4.84	111.36	123.59
18	B	1216	CLA	O2A-CGA-O1A	-4.84	111.37	123.59
18	A	1105	CLA	C4A-NA-C1A	4.84	108.88	106.71
18	4	4012	CLA	C4D-C3D-CAD	4.84	111.17	108.47
18	A	1102	CLA	O2A-CGA-O1A	-4.84	111.39	123.59
18	B	1203	CLA	O2A-C1-C2	4.84	121.34	108.64
18	1	1014	CLA	C1C-C2C-C3C	-4.84	101.87	106.96
18	A	1013	CLA	O2A-CGA-O1A	-4.83	111.39	123.59
18	A	1108	CLA	O2D-CGD-CBD	4.83	119.86	111.27
18	3	3010	CLA	O2A-CGA-O1A	-4.83	111.39	123.59
18	1	1007	CLA	O2D-CGD-CBD	4.83	119.85	111.27
18	B	1212	CLA	O2A-CGA-O1A	-4.83	111.40	123.59
18	B	1207	CLA	C4D-C3D-CAD	4.83	111.16	108.47
18	A	1022	CLA	O2A-C1-C2	4.83	121.32	108.64
18	A	1137	CLA	O2A-C1-C2	4.83	121.32	108.64
18	B	1228	CLA	O2A-CGA-O1A	-4.82	111.42	123.59
18	B	1228	CLA	O2A-C1-C2	4.82	121.31	108.64
18	4	4005	CLA	O2A-C1-C2	4.82	121.31	108.64
22	A	6011	BCR	C3-C4-C5	-4.82	105.47	114.08
18	B	1220	CLA	O2A-CGA-O1A	-4.81	111.44	123.59
18	1	1001	CLA	C1C-C2C-C3C	-4.81	101.90	106.96
18	A	1139	CLA	O2D-CGD-CBD	4.81	119.81	111.27
18	B	1213	CLA	C1C-C2C-C3C	-4.81	101.90	106.96
18	B	1230	CLA	C4D-C3D-CAD	4.80	111.15	108.47
18	L	1502	CLA	O2A-C1-C2	4.80	121.26	108.64
18	2	2004	CLA	C4D-C3D-CAD	4.80	111.15	108.47
18	3	3010	CLA	O2A-C1-C2	4.80	121.24	108.64
18	A	1131	CLA	O2A-C1-C2	4.79	121.23	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1232	CLA	C4A-NA-C1A	4.79	108.86	106.71
18	B	1238	CLA	C4D-C3D-CAD	4.79	111.14	108.47
18	A	1022	CLA	O2A-CGA-O1A	-4.78	111.52	123.59
18	A	1136	CLA	C4D-C3D-CAD	4.78	111.14	108.47
18	A	1104	CLA	C4D-C3D-CAD	4.78	111.13	108.47
18	B	1226	CLA	C4D-C3D-CAD	4.78	111.13	108.47
18	B	1023	CLA	O2D-CGD-CBD	4.78	119.76	111.27
18	A	1237	CLA	O2D-CGD-CBD	4.77	119.75	111.27
18	2	2001	CLA	O2A-C1-C2	4.77	121.18	108.64
18	B	1214	CLA	O2D-CGD-CBD	4.77	119.75	111.27
18	B	1202	CLA	O2A-CGA-O1A	-4.77	111.55	123.59
18	2	2003	CLA	O2D-CGD-CBD	4.76	119.73	111.27
18	B	1220	CLA	C4A-NA-C1A	4.76	108.85	106.71
18	B	1226	CLA	C4A-NA-C1A	4.76	108.84	106.71
18	3	3018	CLA	O2D-CGD-CBD	4.75	119.72	111.27
18	A	1119	CLA	C4A-NA-C1A	4.75	108.84	106.71
18	A	1101	CLA	C4D-C3D-CAD	4.75	111.12	108.47
27	2	2501	LUT	C15-C14-C13	-4.74	120.54	127.31
18	B	1021	CLA	O2D-CGD-CBD	4.74	119.70	111.27
18	1	1006	CLA	O2A-CGA-CBA	4.74	126.79	111.91
18	B	1201	CLA	O2A-CGA-O1A	-4.74	111.63	123.59
18	2	2006	CLA	C4D-C3D-CAD	4.74	111.11	108.47
18	A	1126	CLA	O2D-CGD-CBD	4.74	119.69	111.27
18	A	1022	CLA	C4A-NA-C1A	4.74	108.84	106.71
18	B	1210	CLA	C1C-C2C-C3C	-4.73	101.98	106.96
18	A	1125	CLA	O2A-CGA-O1A	-4.73	111.66	123.59
18	4	4004	CLA	O2A-C1-C2	4.73	121.06	108.64
22	G	2011	BCR	C34-C9-C10	-4.73	116.30	122.92
18	A	1104	CLA	O2A-CGA-O1A	-4.73	111.67	123.59
18	B	1204	CLA	C4D-C3D-CAD	4.73	111.11	108.47
22	A	6002	BCR	C7-C8-C9	-4.73	119.09	126.23
28	4	4013	CHL	C3C-C4C-NC	-4.72	105.27	110.57
18	B	1208	CLA	C4A-NA-C1A	4.72	108.83	106.71
18	A	1138	CLA	C4D-C3D-CAD	4.72	111.10	108.47
18	A	1123	CLA	C4D-C3D-CAD	4.72	111.10	108.47
18	A	1104	CLA	C4A-NA-C1A	4.72	108.83	106.71
18	B	1208	CLA	C4D-C3D-CAD	4.71	111.10	108.47
18	A	1105	CLA	C4D-C3D-CAD	4.71	111.10	108.47
18	B	1012	CLA	O2D-CGD-CBD	4.71	119.63	111.27
18	B	1225	CLA	C4D-C3D-CAD	4.70	111.09	108.47
27	4	4501	LUT	C21-C26-C27	4.70	118.64	112.70
18	B	1232	CLA	C4D-C3D-CAD	4.70	111.09	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4003	CLA	O2A-C1-C2	4.70	120.98	108.64
27	3	3501	LUT	C18-C5-C6	-4.70	119.25	124.53
18	B	1213	CLA	C4D-C3D-CAD	4.70	111.09	108.47
18	B	1225	CLA	O2A-C1-C2	4.70	120.97	108.64
18	A	1136	CLA	O2A-C1-C2	4.69	120.97	108.64
27	2	2501	LUT	C21-C26-C27	4.69	118.63	112.70
18	B	1235	CLA	O2A-C1-C2	4.69	120.96	108.64
18	B	1231	CLA	C4A-NA-C1A	4.69	108.81	106.71
18	A	1126	CLA	C1-C2-C3	-4.68	117.94	126.04
18	A	1120	CLA	O2D-CGD-CBD	4.68	119.59	111.27
21	1	1801	LHG	O7-C7-C8	4.68	121.59	111.50
18	A	1115	CLA	O2D-CGD-CBD	4.67	119.57	111.27
18	2	2002	CLA	C4D-C3D-CAD	4.67	111.08	108.47
27	4	4502	LUT	C21-C26-C25	4.67	119.79	111.42
18	F	1301	CLA	O2D-CGD-CBD	4.67	119.57	111.27
18	2	2003	CLA	O2A-C1-C2	4.67	120.91	108.64
18	A	1127	CLA	O2A-C1-C2	4.67	120.90	108.64
18	B	1203	CLA	O2D-CGD-CBD	4.66	119.56	111.27
18	B	1206	CLA	O2D-CGD-CBD	4.66	119.55	111.27
18	A	1111	CLA	O2A-C1-C2	4.66	120.88	108.64
18	B	1231	CLA	O2D-CGD-CBD	4.66	119.54	111.27
18	B	1230	CLA	C1C-C2C-C3C	-4.65	102.06	106.96
18	1	1011	CLA	O2A-CGA-O1A	-4.65	111.84	123.59
18	B	1230	CLA	O2A-C1-C2	4.65	120.87	108.64
18	1	1003	CLA	O2A-CGA-CBA	4.65	126.51	111.91
18	2	2012	CLA	C1C-C2C-C3C	-4.65	102.06	106.96
18	B	1239	CLA	O2A-CGA-O1A	-4.64	111.87	123.59
27	I	6018	LUT	C15-C35-C34	-4.64	113.96	123.47
18	A	1114	CLA	C4D-C3D-CAD	4.64	111.06	108.47
18	B	1219	CLA	C4D-C3D-CAD	4.64	111.06	108.47
18	A	1112	CLA	C4D-C3D-CAD	4.64	111.06	108.47
18	B	1204	CLA	O2A-CGA-O1A	-4.64	111.89	123.59
18	A	1126	CLA	O2A-CGA-O1A	-4.64	111.89	123.59
22	B	6006	BCR	C7-C8-C9	-4.63	119.24	126.23
18	2	2003	CLA	C4D-C3D-CAD	4.63	111.05	108.47
18	A	1118	CLA	C4D-C3D-CAD	4.63	111.05	108.47
18	3	3004	CLA	O2A-C1-C2	4.62	120.79	108.64
27	1	1502	LUT	C21-C26-C27	4.62	118.54	112.70
18	3	3013	CLA	C4D-C3D-CAD	4.62	111.04	108.47
18	2	2007	CLA	O2A-C1-C2	4.62	120.77	108.64
18	B	1210	CLA	C4A-NA-C1A	4.61	108.78	106.71
18	A	1119	CLA	O2D-CGD-CBD	4.61	119.45	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	1004	CLA	O2A-CGA-CBA	4.60	126.36	111.91
18	A	1137	CLA	O2A-CGA-O1A	-4.60	111.98	123.59
18	G	1003	CLA	O2A-CGA-O1A	-4.60	111.98	123.59
18	A	1139	CLA	O2A-CGA-O1A	-4.60	111.98	123.59
18	A	1124	CLA	O2A-CGA-CBA	4.60	126.34	111.91
18	B	1214	CLA	C1-C2-C3	-4.60	118.09	126.04
18	B	1239	CLA	C4D-C3D-CAD	4.60	111.03	108.47
22	B	6010	BCR	C38-C26-C25	-4.60	119.37	124.53
23	F	5002	LMG	O7-C10-C11	4.59	121.40	111.50
18	4	4006	CLA	O2A-CGA-O1A	-4.59	112.01	123.59
18	B	1215	CLA	O2A-CGA-O1A	-4.58	112.02	123.59
18	A	1119	CLA	O2A-C1-C2	4.58	120.68	108.64
22	B	6010	BCR	C33-C5-C6	-4.58	119.39	124.53
22	L	6020	BCR	C34-C9-C10	-4.58	116.51	122.92
18	A	1132	CLA	O2A-C1-C2	4.58	120.66	108.64
22	3	3503	BCR	C24-C23-C22	-4.58	119.32	126.23
18	2	2005	CLA	O2A-CGA-O1A	-4.57	112.05	123.59
18	A	1126	CLA	O2A-C1-C2	4.57	120.65	108.64
18	A	1135	CLA	C4D-C3D-CAD	4.57	111.02	108.47
18	4	4002	CLA	C4D-C3D-CAD	4.57	111.02	108.47
18	B	1206	CLA	C4D-C3D-CAD	4.57	111.02	108.47
18	A	1022	CLA	O2D-CGD-CBD	4.57	119.38	111.27
18	2	2005	CLA	C4D-C3D-CAD	4.56	111.02	108.47
18	B	1224	CLA	O2A-C1-C2	4.56	120.61	108.64
18	B	1209	CLA	C4D-C3D-CAD	4.56	111.01	108.47
18	A	1121	CLA	C4D-C3D-CAD	4.55	111.01	108.47
18	3	3007	CLA	O2A-CGA-O1A	-4.55	112.10	123.59
18	1	1005	CLA	O2D-CGD-CBD	4.55	119.36	111.27
18	B	1231	CLA	O2A-C1-C2	4.55	120.60	108.64
18	L	1501	CLA	C4A-NA-C1A	4.55	108.75	106.71
22	A	6008	BCR	C7-C8-C9	-4.55	119.36	126.23
18	A	1105	CLA	O2A-CGA-O1A	-4.55	112.12	123.59
22	B	6006	BCR	C33-C5-C6	-4.55	119.42	124.53
18	J	1302	CLA	O2A-CGA-CBA	4.54	126.17	111.91
18	A	1105	CLA	O2D-CGD-CBD	4.54	119.33	111.27
18	A	1132	CLA	C4A-NA-C1A	4.54	108.75	106.71
18	B	1227	CLA	O2A-CGA-O1A	-4.54	112.14	123.59
18	A	1138	CLA	O2D-CGD-CBD	4.53	119.33	111.27
18	L	1501	CLA	O2A-CGA-O1A	-4.53	112.16	123.59
18	4	4004	CLA	C4D-C3D-CAD	4.53	111.00	108.47
18	B	1240	CLA	O2A-CGA-O1A	-4.52	112.17	123.59
18	3	3013	CLA	C4A-NA-C1A	4.51	108.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3004	CLA	O2D-CGD-CBD	4.51	119.29	111.27
18	A	1122	CLA	O2D-CGD-CBD	4.51	119.28	111.27
22	B	6006	BCR	C39-C30-C25	4.51	117.61	110.30
18	H	1000	CLA	C4D-C3D-CAD	4.50	110.98	108.47
18	B	1224	CLA	O2A-CGA-CBA	4.50	126.03	111.91
18	B	1201	CLA	C4D-C3D-CAD	4.50	110.98	108.47
18	A	1127	CLA	C4D-C3D-CAD	4.50	110.98	108.47
18	A	1117	CLA	C4D-C3D-CAD	4.50	110.98	108.47
18	A	1151	CLA	C4D-C3D-CAD	4.50	110.98	108.47
18	A	1104	CLA	O2D-CGD-CBD	4.49	119.25	111.27
18	3	3010	CLA	C4D-C3D-CAD	4.48	110.97	108.47
18	B	1207	CLA	O2A-CGA-O1A	-4.48	112.28	123.59
18	A	1103	CLA	O2A-CGA-O1A	-4.48	112.28	123.59
18	F	1302	CLA	C4D-C3D-CAD	4.48	110.97	108.47
22	A	6003	BCR	C7-C8-C9	-4.48	119.47	126.23
18	3	3001	CLA	O2A-CGA-O1A	-4.48	112.30	123.59
18	G	1001	CLA	O2A-CGA-CBA	4.47	125.95	111.91
18	A	1112	CLA	O2A-C1-C2	4.47	120.39	108.64
18	B	1012	CLA	OBD-CAD-CBD	-4.47	119.50	125.89
18	A	1122	CLA	C4D-C3D-CAD	4.47	110.96	108.47
18	A	1123	CLA	O2A-C1-C2	4.47	120.39	108.64
27	3	3501	LUT	C11-C10-C9	-4.47	120.93	127.31
18	2	2009	CLA	O2A-C1-C2	4.47	120.37	108.64
22	A	6017	BCR	C7-C8-C9	-4.46	119.49	126.23
18	B	1212	CLA	C4D-C3D-CAD	4.46	110.96	108.47
18	A	1124	CLA	C4A-NA-C1A	4.46	108.71	106.71
18	3	3004	CLA	OBD-CAD-CBD	-4.46	119.52	125.89
18	B	1231	CLA	O2A-CGA-O1A	-4.46	112.34	123.59
18	B	1219	CLA	O2D-CGD-CBD	4.45	119.18	111.27
22	J	6013	BCR	C37-C22-C21	-4.45	116.69	122.92
18	1	1006	CLA	O2D-CGD-CBD	4.45	119.18	111.27
18	A	1108	CLA	C4D-C3D-CAD	4.45	110.95	108.47
22	A	6007	BCR	C38-C26-C25	-4.45	119.53	124.53
18	A	1013	CLA	C4D-C3D-CAD	4.44	110.95	108.47
18	1	1006	CLA	O2A-C1-C2	4.44	120.31	108.64
22	A	6003	BCR	C38-C26-C25	-4.44	119.55	124.53
22	B	6004	BCR	C33-C5-C6	-4.44	119.55	124.53
18	2	2007	CLA	O2D-CGD-CBD	4.43	119.15	111.27
27	3	3502	LUT	C21-C26-C27	4.43	118.30	112.70
18	2	2012	CLA	O2D-CGD-CBD	4.43	119.14	111.27
18	B	1228	CLA	O2D-CGD-CBD	4.42	119.13	111.27
18	A	1133	CLA	O2A-CGA-CBA	4.42	125.77	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1022	CLA	C4D-C3D-CAD	4.42	110.93	108.47
27	4	4503	LUT	C31-C30-C29	-4.41	121.01	127.31
18	1	1004	CLA	C4D-C3D-CAD	4.41	110.93	108.47
22	A	6003	BCR	C33-C5-C6	-4.41	119.58	124.53
22	A	6011	BCR	C7-C8-C9	-4.41	119.58	126.23
21	A	5003	LHG	O7-C7-C8	4.40	120.99	111.50
22	A	6007	BCR	C7-C8-C9	-4.40	119.58	126.23
18	A	1140	CLA	O2A-CGA-O1A	-4.40	112.48	123.59
18	A	1130	CLA	C4D-C3D-CAD	4.40	110.92	108.47
18	B	1211	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
22	B	6005	BCR	C19-C18-C17	4.40	125.69	118.94
18	2	2004	CLA	C2C-C1C-NC	4.40	114.09	109.97
29	4	4505	ZEX	C27-C28-C29	-4.39	119.59	126.23
18	2	2019	CLA	C2C-C1C-NC	4.39	116.96	109.51
18	A	1117	CLA	O2A-CGA-O1A	-4.39	112.50	123.59
18	A	1112	CLA	C4A-NA-C1A	4.39	108.68	106.71
22	I	6020	BCR	C19-C18-C17	4.39	125.68	118.94
18	2	2001	CLA	O2A-CGA-CBA	4.39	125.68	111.91
18	B	1240	CLA	C4D-C3D-CAD	4.39	110.92	108.47
18	1	1004	CLA	O2A-C1-C2	4.39	120.16	108.64
18	B	1235	CLA	C4D-C3D-CAD	4.38	110.92	108.47
18	B	1229	CLA	O2A-CGA-CBA	4.38	125.67	111.91
18	3	3006	CLA	C1-C2-C3	-4.38	119.66	126.75
18	A	1124	CLA	C4D-C3D-CAD	4.38	110.91	108.47
18	B	1221	CLA	C4D-C3D-CAD	4.37	110.91	108.47
18	B	1023	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
18	A	1122	CLA	O2A-C1-C2	4.37	120.12	108.64
18	B	1021	CLA	C4D-C3D-CAD	4.37	110.91	108.47
18	B	1214	CLA	O2A-CGA-CBA	4.37	125.61	111.91
18	3	3006	CLA	O2D-CGD-CBD	4.36	119.02	111.27
18	B	1213	CLA	O2D-CGD-CBD	4.36	119.02	111.27
18	4	4012	CLA	O2A-CGA-O1A	-4.36	112.59	123.59
18	B	1226	CLA	O2A-C1-C2	4.36	120.09	108.64
18	B	1205	CLA	O2A-C1-C2	4.36	120.08	108.64
18	3	3004	CLA	O2A-CGA-CBA	4.35	125.57	111.91
18	A	1129	CLA	C4D-C3D-CAD	4.35	110.90	108.47
22	J	6013	BCR	C19-C18-C17	4.35	125.61	118.94
18	1	1002	CLA	O2D-CGD-CBD	4.35	118.99	111.27
18	B	1218	CLA	O2A-CGA-CBA	4.35	125.55	111.91
18	B	1215	CLA	O2A-CGA-CBA	4.34	125.53	111.91
22	A	6002	BCR	C36-C18-C17	-4.34	116.84	122.92
18	2	2008	CLA	OBD-CAD-C3D	-4.34	120.78	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	3503	BCR	C36-C18-C17	-4.34	116.85	122.92
18	3	3007	CLA	O2D-CGD-CBD	4.34	118.98	111.27
18	B	1238	CLA	C4A-NA-C1A	4.33	108.65	106.71
18	B	1222	CLA	O2A-C1-C2	4.33	120.02	108.64
18	A	1106	CLA	C4D-C3D-CAD	4.33	110.88	108.47
17	A	1011	CL0	C4D-C3D-CAD	4.33	110.88	108.47
17	A	1011	CL0	O2A-CGA-CBA	4.32	125.47	111.91
27	4	4501	LUT	C18-C5-C6	-4.32	119.68	124.53
18	B	1218	CLA	O2A-C1-C2	4.32	119.98	108.64
18	B	1203	CLA	C4D-C3D-CAD	4.31	110.88	108.47
18	B	1222	CLA	C1-C2-C3	-4.31	118.59	126.04
18	B	1023	CLA	C4D-C3D-CAD	4.31	110.87	108.47
18	A	1131	CLA	C4D-C3D-CAD	4.31	110.87	108.47
28	2	2011	CHL	C3C-C4C-NC	-4.30	105.74	110.57
22	B	6009	BCR	C33-C5-C6	-4.30	119.70	124.53
22	L	6019	BCR	C34-C9-C10	-4.30	116.90	122.92
18	B	1228	CLA	C4D-C3D-CAD	4.30	110.87	108.47
18	B	1222	CLA	O2D-CGD-CBD	4.30	118.90	111.27
22	J	6013	BCR	C36-C18-C17	-4.29	116.91	122.92
18	A	1113	CLA	C4D-C3D-CAD	4.29	110.86	108.47
18	3	3010	CLA	O2D-CGD-CBD	4.29	118.89	111.27
18	B	1230	CLA	C4-C3-C5	4.29	122.49	115.27
28	4	4011	CHL	C3C-C4C-NC	-4.29	105.76	110.57
18	A	1122	CLA	O2A-CGA-CBA	4.29	125.36	111.91
18	A	1116	CLA	C4D-C3D-CAD	4.28	110.86	108.47
18	B	1216	CLA	C4A-NA-C1A	4.28	108.63	106.71
18	2	2007	CLA	C4D-C3D-CAD	4.28	110.86	108.47
18	2	2004	CLA	O2A-CGA-CBA	4.28	125.32	111.91
22	L	6020	BCR	C37-C22-C21	-4.27	116.94	122.92
18	B	1226	CLA	O2A-CGA-CBA	4.27	125.31	111.91
18	B	1215	CLA	C4D-C3D-CAD	4.27	110.85	108.47
18	A	1109	CLA	O2D-CGD-CBD	4.26	118.84	111.27
18	B	1224	CLA	C4D-C3D-CAD	4.26	110.85	108.47
18	A	1107	CLA	O2A-CGA-CBA	4.26	125.28	111.91
22	A	6017	BCR	C36-C18-C17	-4.26	116.96	122.92
18	4	4009	CLA	O2D-CGD-CBD	4.26	118.84	111.27
18	B	1235	CLA	O2A-CGA-CBA	4.26	125.27	111.91
18	B	1220	CLA	O2A-C1-C2	4.25	119.81	108.64
18	3	3010	CLA	O2A-CGA-CBA	4.25	125.24	111.91
18	2	2012	CLA	C4D-C3D-CAD	4.24	110.84	108.47
18	A	1128	CLA	O2A-C1-C2	4.24	119.79	108.64
18	A	1102	CLA	C4D-C3D-CAD	4.24	110.84	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1125	CLA	C4D-C3D-CAD	4.24	110.83	108.47
18	4	4002	CLA	OBD-CAD-C3D	-4.24	120.94	127.98
18	3	3008	CLA	O2A-CGA-CBA	4.24	125.21	111.91
18	4	4009	CLA	C4D-C3D-CAD	4.24	110.83	108.47
18	A	1110	CLA	C4D-C3D-CAD	4.24	110.83	108.47
18	1	1003	CLA	O2D-CGD-CBD	4.24	118.80	111.27
18	A	1134	CLA	O2A-CGA-CBA	4.24	125.20	111.91
18	B	1201	CLA	O2D-CGD-CBD	4.23	118.79	111.27
18	J	1302	CLA	C1-C2-C3	-4.23	119.92	126.75
18	4	4009	CLA	O2A-CGA-CBA	4.22	125.16	111.91
18	2	2008	CLA	C1-C2-C3	-4.22	119.92	126.75
18	A	1111	CLA	C4D-C3D-CAD	4.22	110.82	108.47
18	3	3017	CLA	O2A-CGA-O1A	-4.22	109.92	123.14
18	3	3007	CLA	C1-C2-C3	-4.21	119.94	126.75
27	4	4503	LUT	C15-C14-C13	-4.21	121.30	127.31
22	A	6007	BCR	C33-C5-C6	-4.21	119.80	124.53
18	L	1503	CLA	O2D-CGD-CBD	4.21	118.75	111.27
18	A	1127	CLA	O2A-CGA-CBA	4.21	125.12	111.91
18	G	1001	CLA	CAA-C2A-C3A	-4.21	101.25	112.78
18	B	1222	CLA	C4D-C3D-CAD	4.21	110.82	108.47
18	F	1302	CLA	O2A-CGA-CBA	4.21	125.11	111.91
18	1	1008	CLA	C4D-C3D-CAD	4.21	110.81	108.47
18	1	1006	CLA	CMC-C2C-C1C	4.20	131.44	125.04
18	B	1240	CLA	O2A-C1-C2	4.20	119.68	108.64
18	A	1115	CLA	C4D-C3D-CAD	4.20	110.81	108.47
27	3	3502	LUT	C22-C23-C24	-4.20	106.96	111.74
22	L	6019	BCR	C36-C18-C17	-4.20	117.04	122.92
18	1	1001	CLA	O2A-CGA-CBA	4.20	125.08	111.91
22	3	3503	BCR	C19-C18-C17	4.20	125.38	118.94
22	3	3503	BCR	C7-C8-C9	-4.19	119.90	126.23
18	1	1012	CLA	C1-C2-C3	-4.19	119.97	126.75
22	A	6008	BCR	C38-C26-C25	-4.19	119.83	124.53
18	A	1116	CLA	O2A-CGA-CBA	4.19	125.04	111.91
22	J	6013	BCR	C1-C6-C5	-4.17	116.73	122.61
18	B	1230	CLA	O2A-CGA-CBA	4.17	124.99	111.91
23	B	5005	LMG	O7-C10-C11	4.17	120.48	111.50
18	A	1140	CLA	C4D-C3D-CAD	4.16	110.79	108.47
18	2	2007	CLA	O2A-CGA-CBA	4.16	124.97	111.91
18	B	1232	CLA	O2D-CGD-CBD	4.16	118.66	111.27
18	B	1211	CLA	O2A-CGA-CBA	4.16	124.95	111.91
18	A	1126	CLA	C4D-C3D-CAD	4.16	110.79	108.47
18	A	1121	CLA	O2A-CGA-CBA	4.15	124.94	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6011	BCR	C28-C27-C26	-4.15	106.66	114.08
18	B	1012	CLA	C4D-C3D-CAD	4.15	110.79	108.47
18	4	4017	CLA	O2A-CGA-CBA	4.15	124.93	111.91
18	1	1008	CLA	O2A-CGA-O1A	-4.15	110.14	123.14
18	2	2016	CLA	CMC-C2C-C1C	4.15	131.35	125.04
18	1	1001	CLA	C4D-C3D-CAD	4.14	110.78	108.47
18	3	3012	CLA	O2A-C1-C2	4.14	119.52	108.64
27	2	2502	LUT	C15-C14-C13	-4.14	121.40	127.31
18	3	3019	CLA	C2C-C1C-NC	4.14	116.53	109.51
18	3	3008	CLA	OBD-CAD-C3D	-4.14	121.11	127.98
18	A	1136	CLA	O2A-CGA-CBA	4.13	124.88	111.91
18	A	1134	CLA	C4D-C3D-CAD	4.13	110.77	108.47
22	B	6004	BCR	C7-C8-C9	-4.13	119.99	126.23
22	F	6016	BCR	C34-C9-C10	-4.13	117.14	122.92
22	J	6013	BCR	C7-C8-C9	-4.12	120.01	126.23
18	B	1222	CLA	O2A-CGA-CBA	4.12	124.84	111.91
27	4	4503	LUT	C11-C10-C9	-4.12	121.43	127.31
18	B	1238	CLA	O2A-CGA-CBA	4.12	124.84	111.91
18	4	4009	CLA	O2A-C1-C2	4.12	119.46	108.64
22	3	3503	BCR	C37-C22-C21	-4.12	117.15	122.92
22	A	6002	BCR	C38-C26-C25	-4.12	119.90	124.53
18	A	1132	CLA	O2A-CGA-CBA	4.12	124.83	111.91
18	L	1503	CLA	O2A-CGA-CBA	4.12	124.83	111.91
18	2	2009	CLA	O2A-CGA-CBA	4.11	124.80	111.91
18	4	4005	CLA	O2A-CGA-CBA	4.11	124.80	111.91
18	1	1011	CLA	C1-C2-C3	-4.11	120.11	126.75
18	B	1220	CLA	O2D-CGD-CBD	4.10	118.56	111.27
22	A	6002	BCR	C19-C18-C17	4.10	125.23	118.94
18	A	1119	CLA	C4D-C3D-CAD	4.10	110.75	108.47
18	B	1229	CLA	O2A-C1-C2	4.09	119.39	108.64
18	B	1202	CLA	C4D-C3D-CAD	4.09	110.75	108.47
28	4	4010	CHL	C3C-C4C-NC	-4.09	105.99	110.57
28	3	3011	CHL	C3C-C4C-NC	-4.09	105.99	110.57
22	A	6017	BCR	C38-C26-C25	-4.09	119.94	124.53
22	B	6005	BCR	C38-C26-C25	-4.09	119.94	124.53
18	B	1221	CLA	O2A-CGA-O1A	-4.08	113.29	123.59
22	B	6010	BCR	C7-C8-C9	-4.08	120.07	126.23
18	1	1001	CLA	C1-C2-C3	-4.08	118.99	126.04
18	2	2003	CLA	O2A-CGA-CBA	4.08	124.70	111.91
18	4	4017	CLA	C4D-C3D-CAD	4.07	110.74	108.47
18	B	1210	CLA	O2A-CGA-CBA	4.07	124.69	111.91
22	J	6013	BCR	C23-C22-C21	4.07	125.19	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1229	CLA	C4D-C3D-CAD	4.07	110.74	108.47
18	B	1223	CLA	O2A-CGA-CBA	4.07	124.68	111.91
22	G	2011	BCR	C33-C5-C6	-4.07	119.96	124.53
18	A	1013	CLA	O2D-CGD-CBD	4.07	118.50	111.27
22	F	6016	BCR	C24-C23-C22	-4.07	120.09	126.23
18	B	1223	CLA	C4D-C3D-CAD	4.07	110.74	108.47
18	4	4006	CLA	C1-C2-C3	-4.06	120.17	126.75
18	K	1001	CLA	O2D-CGD-CBD	4.06	118.49	111.27
18	A	1133	CLA	C4D-C3D-CAD	4.06	110.73	108.47
18	A	1137	CLA	C4D-C3D-CAD	4.06	110.73	108.47
29	4	4505	ZEX	C18-C5-C6	-4.06	119.97	124.53
18	B	1225	CLA	O2A-CGA-CBA	4.06	124.64	111.91
28	4	4010	CHL	C2C-C3C-C4C	4.05	109.38	106.49
18	G	1003	CLA	O2A-CGA-CBA	4.05	124.62	111.91
27	I	6018	LUT	C21-C26-C27	4.05	117.82	112.70
27	1	1502	LUT	C15-C14-C13	-4.05	121.53	127.31
18	2	2006	CLA	O2A-CGA-CBA	4.05	124.61	111.91
18	A	1106	CLA	O2A-CGA-CBA	4.04	124.60	111.91
18	B	1205	CLA	O2A-CGA-CBA	4.04	124.59	111.91
20	A	5001	PQN	C14-C13-C15	4.03	122.05	115.27
18	B	1012	CLA	O2A-CGA-CBA	4.03	124.55	111.91
27	4	4502	LUT	C22-C23-C24	-4.03	107.16	111.74
22	G	2011	BCR	C36-C18-C17	-4.03	117.28	122.92
18	A	1110	CLA	O2A-CGA-CBA	4.03	124.54	111.91
22	3	3503	BCR	C33-C5-C4	4.02	121.35	113.62
18	B	1216	CLA	C4D-C3D-CAD	4.02	110.71	108.47
18	A	1119	CLA	O2A-CGA-CBA	4.02	124.53	111.91
18	A	1131	CLA	O2A-CGA-CBA	4.02	124.52	111.91
18	A	1103	CLA	C4D-C3D-CAD	4.02	110.71	108.47
18	B	1220	CLA	C4D-C3D-CAD	4.02	110.71	108.47
18	2	2016	CLA	O2A-CGA-O1A	-4.02	113.46	123.59
22	A	6017	BCR	C34-C9-C10	-4.02	117.30	122.92
18	B	1236	CLA	O2A-CGA-CBA	4.01	124.51	111.91
18	3	3001	CLA	O2A-CGA-CBA	4.01	124.50	111.91
18	A	1140	CLA	O2A-CGA-CBA	4.01	124.50	111.91
18	3	3008	CLA	O2D-CGD-CBD	4.01	118.39	111.27
18	1	1001	CLA	CAA-C2A-C3A	-4.01	101.80	112.78
18	A	1121	CLA	C1-C2-C3	-4.01	119.11	126.04
18	A	1022	CLA	OBD-CAD-C3D	-4.00	121.33	127.98
18	A	1109	CLA	C4D-C3D-CAD	4.00	110.70	108.47
18	L	1503	CLA	C1-C2-C3	-4.00	120.28	126.75
18	A	1101	CLA	O2A-CGA-CBA	4.00	124.47	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4006	CLA	O2A-C1-C2	4.00	119.14	108.64
18	B	1219	CLA	O2A-CGA-CBA	4.00	124.45	111.91
18	A	1151	CLA	O2A-CGA-CBA	3.99	124.44	111.91
18	4	4007	CLA	O2A-CGA-CBA	3.99	124.43	111.91
27	4	4502	LUT	C31-C30-C29	-3.99	121.61	127.31
18	2	2009	CLA	O2D-CGD-CBD	3.99	118.36	111.27
18	B	1206	CLA	O2A-CGA-CBA	3.99	124.43	111.91
18	A	1237	CLA	O2A-CGA-CBA	3.99	124.42	111.91
18	B	1208	CLA	O2A-CGA-CBA	3.99	124.42	111.91
18	A	1126	CLA	O2A-CGA-CBA	3.99	124.42	111.91
22	A	6007	BCR	C15-C14-C13	-3.99	121.62	127.31
18	A	1123	CLA	O2A-CGA-CBA	3.98	124.41	111.91
18	3	3005	CLA	O2A-CGA-CBA	3.98	124.40	111.91
18	A	1137	CLA	O2A-CGA-CBA	3.98	124.39	111.91
18	B	1232	CLA	O2A-CGA-CBA	3.98	124.39	111.91
18	A	1120	CLA	O2A-CGA-CBA	3.98	124.38	111.91
18	B	1021	CLA	O2A-CGA-CBA	3.97	124.38	111.91
22	G	2011	BCR	C23-C22-C21	3.97	125.04	118.94
18	A	1104	CLA	O2A-CGA-CBA	3.97	124.38	111.91
18	A	1118	CLA	O2A-CGA-O1A	-3.97	110.69	123.14
18	4	4016	CLA	O2A-CGA-O1A	-3.97	110.70	123.14
18	B	1213	CLA	C1-C2-C3	-3.97	119.18	126.04
18	2	2005	CLA	O2D-CGD-CBD	3.97	118.31	111.27
18	3	3003	CLA	O2A-C1-C2	3.96	119.05	108.64
18	2	2009	CLA	C1-C2-C3	-3.96	120.34	126.75
18	1	1001	CLA	O2D-CGD-CBD	3.96	118.31	111.27
18	F	1302	CLA	C1-C2-C3	-3.96	120.35	126.75
18	K	1001	CLA	OBD-CAD-C3D	-3.96	121.41	127.98
18	B	1220	CLA	O2A-CGA-CBA	3.96	124.32	111.91
18	3	3018	CLA	O2A-CGA-CBA	3.96	124.32	111.91
18	3	3007	CLA	O2A-CGA-CBA	3.96	124.32	111.91
18	H	1000	CLA	O2A-CGA-O1A	-3.95	110.75	123.14
18	A	1129	CLA	O2A-CGA-CBA	3.95	124.31	111.91
26	B	8001	LMU	C1B-O1B-C4'	-3.95	108.19	117.96
22	A	6003	BCR	C24-C23-C22	-3.95	120.27	126.23
18	3	3018	CLA	O2A-C1-C2	3.95	119.00	108.64
22	J	6012	BCR	C34-C9-C10	-3.95	117.40	122.92
18	A	1130	CLA	O2A-CGA-CBA	3.94	124.29	111.91
18	A	1108	CLA	O2A-CGA-O1A	-3.94	110.78	123.14
18	1	1012	CLA	O2D-CGD-CBD	3.94	118.27	111.27
18	A	1112	CLA	O2A-CGA-CBA	3.94	124.28	111.91
18	B	1012	CLA	O2A-C1-C2	3.94	118.99	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1236	CLA	C1-C2-C3	-3.94	119.23	126.04
18	1	1005	CLA	O2A-CGA-CBA	3.94	124.26	111.91
18	3	3006	CLA	O2A-C1-C2	3.94	118.98	108.64
18	3	3013	CLA	O2D-CGD-CBD	3.93	118.26	111.27
28	2	2010	CHL	C3C-C4C-NC	-3.93	106.16	110.57
18	2	2012	CLA	O2A-CGA-CBA	3.93	124.24	111.91
18	A	1109	CLA	O2A-CGA-CBA	3.93	124.23	111.91
18	B	1023	CLA	O2A-CGA-CBA	3.92	124.22	111.91
22	B	6005	BCR	C36-C18-C17	-3.92	117.43	122.92
18	2	2016	CLA	O2A-CGA-CBA	3.92	124.22	111.91
18	B	1228	CLA	O2A-CGA-CBA	3.92	124.22	111.91
18	L	1503	CLA	C4D-C3D-CAD	3.92	110.66	108.47
18	4	4012	CLA	O2D-CGD-CBD	3.92	118.23	111.27
18	4	4002	CLA	O2A-CGA-CBA	3.92	124.20	111.91
27	1	1501	LUT	C31-C30-C29	-3.91	121.73	127.31
27	2	2502	LUT	C31-C30-C29	-3.91	121.73	127.31
18	3	3019	CLA	C2B-C1B-NB	3.91	113.53	110.11
18	2	2016	CLA	C1-C2-C3	-3.90	120.43	126.75
18	B	1202	CLA	O2A-CGA-CBA	3.90	124.16	111.91
18	B	1217	CLA	O2A-CGA-O1A	-3.90	110.91	123.14
18	2	2019	CLA	C1C-NC-C4C	-3.90	104.95	106.71
18	1	1003	CLA	O2A-C1-C2	3.90	118.89	108.64
18	A	1135	CLA	O2A-CGA-CBA	3.90	124.14	111.91
21	A	7001	LHG	O7-C7-C8	3.90	119.90	111.50
18	4	4001	CLA	O2A-CGA-CBA	3.89	124.11	111.91
18	B	1216	CLA	C1-C2-C3	-3.89	119.32	126.04
27	3	3501	LUT	C35-C34-C33	-3.89	121.76	127.31
17	A	1011	CL0	C1-C2-C3	-3.88	119.33	126.04
22	A	6008	BCR	C33-C5-C6	-3.88	120.17	124.53
18	A	1111	CLA	O2A-CGA-CBA	3.88	124.08	111.91
18	B	1239	CLA	O2A-CGA-CBA	3.88	124.08	111.91
18	3	3012	CLA	O2D-CGD-CBD	3.88	118.16	111.27
18	3	3018	CLA	CAA-C2A-C3A	-3.88	102.17	112.78
22	F	6014	BCR	C2-C1-C6	3.87	116.44	110.48
22	K	2011	BCR	C36-C18-C17	-3.86	117.52	122.92
18	3	3006	CLA	OBD-CAD-CBD	-3.86	120.38	125.89
18	3	3010	CLA	CMB-C2B-C3B	3.86	131.90	124.68
27	2	2501	LUT	C18-C5-C6	-3.86	120.19	124.53
18	3	3012	CLA	O2A-CGA-CBA	3.86	124.02	111.91
22	K	2011	BCR	C19-C18-C17	3.86	124.86	118.94
18	A	1115	CLA	O2A-CGA-O1A	-3.86	111.06	123.14
18	B	1236	CLA	C4D-C3D-CAD	3.85	110.62	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3019	CLA	C3C-C4C-NC	3.85	113.53	109.97
18	2	2002	CLA	O2D-CGD-CBD	3.85	118.11	111.27
22	A	6017	BCR	C23-C22-C21	3.84	124.84	118.94
27	I	6018	LUT	C2-C3-C4	3.84	115.56	110.30
18	3	3002	CLA	OBD-CAD-C3D	-3.84	121.61	127.98
28	1	1010	CHL	C2C-C3C-C4C	3.83	109.22	106.49
18	A	1113	CLA	O2A-CGA-O1A	-3.83	111.15	123.14
18	A	1105	CLA	O2A-CGA-CBA	3.83	123.91	111.91
18	1	1002	CLA	OBD-CAD-CBD	-3.82	120.43	125.89
18	B	1203	CLA	C1-C2-C3	-3.82	119.43	126.04
18	1	1006	CLA	CAC-C3C-C4C	3.82	129.76	124.81
22	B	6004	BCR	C36-C18-C17	-3.82	117.58	122.92
20	B	5002	PQN	C14-C13-C15	3.81	121.69	115.27
18	4	4005	CLA	C4D-C3D-CAD	3.81	110.60	108.47
18	B	1208	CLA	C1-C2-C3	-3.81	119.45	126.04
18	A	1128	CLA	O2A-CGA-CBA	3.81	123.87	111.91
22	B	6009	BCR	C3-C4-C5	-3.81	107.27	114.08
18	B	1201	CLA	O2A-CGA-CBA	3.81	123.86	111.91
27	2	2501	LUT	C7-C8-C9	-3.81	120.48	126.23
22	A	6017	BCR	C35-C13-C14	-3.81	117.59	122.92
18	L	1501	CLA	C1-C2-C3	-3.80	120.60	126.75
22	G	2011	BCR	C33-C5-C4	3.80	120.92	113.62
18	A	1125	CLA	O2A-CGA-CBA	3.80	123.84	111.91
22	J	6012	BCR	C7-C8-C9	-3.80	120.49	126.23
28	1	1009	CHL	C3C-C4C-NC	-3.80	106.31	110.57
22	B	6009	BCR	C38-C26-C25	-3.80	120.27	124.53
18	2	2008	CLA	O2A-CGA-CBA	3.79	123.81	111.91
18	3	3008	CLA	O2A-C1-C2	3.79	122.31	109.49
18	3	3017	CLA	O2D-CGD-CBD	3.79	118.01	111.27
18	3	3013	CLA	O2A-CGA-O1A	-3.79	111.27	123.14
18	4	4006	CLA	O2D-CGD-CBD	3.78	117.99	111.27
18	K	1001	CLA	OBD-CAD-CBD	-3.78	120.49	125.89
18	A	1114	CLA	O2A-CGA-O1A	-3.78	111.29	123.14
18	A	1105	CLA	C4-C3-C5	3.78	120.30	115.98
18	A	1022	CLA	O2A-CGA-CBA	3.77	123.74	111.91
18	4	4008	CLA	O2A-CGA-O1A	-3.77	111.33	123.14
18	B	1234	CLA	O2A-CGA-CBA	3.77	123.73	111.91
22	G	2011	BCR	C8-C9-C10	3.77	124.72	118.94
22	3	3503	BCR	C8-C9-C10	3.76	124.72	118.94
18	B	1203	CLA	O2A-CGA-CBA	3.76	123.72	111.91
18	1	1011	CLA	O2A-C1-C2	3.76	118.53	108.64
18	B	1209	CLA	O2A-CGA-O1A	-3.76	111.34	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3006	CLA	O2A-CGA-CBA	3.76	123.71	111.91
18	A	1109	CLA	C1-C2-C3	-3.76	119.54	126.04
18	4	4016	CLA	O2D-CGD-CBD	3.76	117.95	111.27
28	4	4010	CHL	CGD-CBD-CAD	-3.75	98.58	110.73
22	J	6013	BCR	C33-C5-C4	3.75	120.82	113.62
18	2	2001	CLA	C1-C2-C3	-3.75	119.56	126.04
22	B	6005	BCR	C7-C8-C9	-3.75	120.57	126.23
22	B	6009	BCR	C7-C8-C9	-3.75	120.57	126.23
27	1	1501	LUT	C15-C14-C13	-3.75	121.96	127.31
18	B	1212	CLA	O2A-CGA-CBA	3.75	123.67	111.91
18	4	4004	CLA	O2A-CGA-CBA	3.74	123.66	111.91
22	L	6020	BCR	C36-C18-C17	-3.74	117.69	122.92
18	K	1001	CLA	O2A-CGA-O1A	-3.73	111.44	123.14
22	B	6006	BCR	C8-C9-C10	3.73	124.67	118.94
23	2	2802	LMG	O7-C10-C11	3.73	119.54	111.50
22	L	6019	BCR	C33-C5-C6	-3.73	120.34	124.53
18	4	4005	CLA	OBD-CAD-C3D	-3.73	121.80	127.98
18	A	1133	CLA	C1-C2-C3	-3.72	119.60	126.04
22	A	6017	BCR	C3-C4-C5	-3.72	107.44	114.08
18	A	1129	CLA	C1-C2-C3	-3.72	120.74	126.75
27	4	4502	LUT	C21-C26-C27	3.71	117.40	112.70
27	I	6018	LUT	C18-C5-C4	3.71	121.23	114.36
22	K	2011	BCR	C3-C4-C5	-3.71	107.45	114.08
18	3	3003	CLA	O2D-CGD-CBD	3.71	117.86	111.27
22	J	6012	BCR	C2-C1-C6	3.71	116.19	110.48
18	3	3017	CLA	C4D-C3D-CAD	3.70	110.54	108.47
18	2	2019	CLA	C2B-C1B-NB	3.70	113.35	110.11
18	B	1213	CLA	O2A-CGA-CBA	3.70	123.50	111.91
18	2	2002	CLA	O2A-CGA-O1A	-3.69	111.56	123.14
18	A	1139	CLA	O2A-CGA-CBA	3.69	123.49	111.91
18	1	1008	CLA	O2D-CGD-CBD	3.68	117.81	111.27
18	2	2005	CLA	O2A-CGA-CBA	3.68	123.46	111.91
22	F	6014	BCR	C37-C22-C21	-3.68	117.77	122.92
18	3	3003	CLA	O2A-CGA-O1A	-3.68	114.31	123.59
18	B	1216	CLA	O2A-CGA-CBA	3.68	123.45	111.91
18	4	4003	CLA	O2A-CGA-CBA	3.67	123.44	111.91
18	B	1224	CLA	C1-C2-C3	-3.67	119.69	126.04
22	K	2011	BCR	C7-C8-C9	-3.67	120.68	126.23
22	J	6012	BCR	C37-C22-C21	-3.67	117.78	122.92
18	B	1204	CLA	O2A-CGA-CBA	3.67	123.44	111.91
18	G	1002	CLA	O2A-CGA-O1A	-3.67	111.63	123.14
18	3	3010	CLA	CAC-C3C-C4C	3.67	129.57	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1205	CLA	O2D-CGD-CBD	3.67	117.78	111.27
29	4	4505	ZEX	C23-C24-C25	3.67	114.55	109.33
18	L	1502	CLA	O2A-CGA-CBA	3.66	123.40	111.91
22	B	6006	BCR	C34-C9-C10	-3.66	117.80	122.92
22	3	3503	BCR	C15-C14-C13	-3.66	122.09	127.31
27	3	3501	LUT	C21-C26-C25	3.66	117.97	111.42
18	A	1151	CLA	C1-C2-C3	-3.65	120.84	126.75
18	2	2012	CLA	C4-C3-C5	3.65	121.41	115.27
22	L	6019	BCR	C19-C18-C17	3.65	124.54	118.94
18	3	3005	CLA	CMC-C2C-C1C	3.65	130.59	125.04
28	4	4011	CHL	C2C-C3C-C4C	3.65	109.09	106.49
18	B	1231	CLA	O2A-CGA-CBA	3.64	123.35	111.91
18	B	1021	CLA	C1-C2-C3	-3.64	119.74	126.04
22	J	6013	BCR	C39-C30-C25	-3.64	104.39	110.30
18	A	1106	CLA	C1-C2-C3	-3.64	119.75	126.04
22	I	6020	BCR	C33-C5-C6	-3.63	120.45	124.53
18	2	2016	CLA	C3C-C4C-NC	3.63	114.64	110.57
18	1	1007	CLA	O2A-CGA-O1A	-3.63	111.76	123.14
22	B	6004	BCR	C28-C27-C26	-3.63	107.59	114.08
22	J	6012	BCR	C4-C5-C6	-3.63	117.46	122.73
18	1	1011	CLA	O2A-CGA-CBA	3.63	123.30	111.91
27	4	4501	LUT	C15-C14-C13	-3.62	122.14	127.31
29	4	4505	ZEX	C27-C26-C25	-3.62	116.98	122.84
27	I	6018	LUT	C10-C11-C12	-3.62	111.92	123.22
22	F	6014	BCR	C23-C22-C21	3.62	124.49	118.94
18	A	1102	CLA	O2A-CGA-CBA	3.62	123.26	111.91
18	2	2012	CLA	O2A-C1-C2	3.62	118.14	108.64
18	4	4012	CLA	O2A-CGA-CBA	3.61	123.24	111.91
18	A	1103	CLA	C1-C2-C3	-3.61	119.80	126.04
22	F	6014	BCR	C31-C1-C6	-3.61	104.44	110.30
18	L	1503	CLA	CMC-C2C-C1C	3.61	130.53	125.04
18	4	4008	CLA	O2D-CGD-O1D	-3.61	116.79	123.84
22	B	6006	BCR	C3-C4-C5	-3.60	107.65	114.08
18	G	1001	CLA	C4-C3-C5	3.60	121.32	115.27
18	A	1138	CLA	O2A-CGA-CBA	3.60	123.19	111.91
18	B	1023	CLA	CAC-C3C-C4C	3.59	129.47	124.81
21	A	7001	LHG	O8-C23-C24	3.59	123.17	111.91
18	2	2019	CLA	CAD-C3D-C2D	3.59	141.45	132.79
27	2	2501	LUT	C15-C35-C34	-3.59	116.13	123.47
27	4	4501	LUT	C2-C3-C4	-3.59	105.39	110.30
18	A	1122	CLA	C4-C3-C5	3.59	121.30	115.27
27	4	4502	LUT	C35-C34-C33	-3.58	122.20	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	1014	CLA	O2A-CGA-CBA	3.58	126.39	112.23
22	L	6019	BCR	C30-C25-C26	-3.58	117.57	122.61
27	2	2502	LUT	C18-C5-C6	-3.58	120.51	124.53
18	L	1501	CLA	O2A-CGA-CBA	3.57	123.11	111.91
23	G	2021	LMG	O7-C10-C11	3.57	119.19	111.50
18	B	1012	CLA	OBD-CAD-C3D	-3.57	122.06	127.98
22	A	6017	BCR	C33-C5-C6	-3.57	120.52	124.53
18	1	1012	CLA	CAA-CBA-CGA	-3.56	102.84	113.25
18	4	4012	CLA	CAC-C3C-C4C	3.56	129.43	124.81
22	A	6011	BCR	C35-C13-C12	3.56	123.69	118.08
22	I	6020	BCR	C38-C26-C25	-3.56	120.53	124.53
18	1	1005	CLA	OBD-CAD-C3D	-3.56	122.08	127.98
22	J	6012	BCR	C19-C18-C17	3.56	124.40	118.94
22	A	6003	BCR	C36-C18-C17	-3.55	117.95	122.92
18	A	1013	CLA	O2A-CGA-CBA	3.55	123.05	111.91
22	L	6019	BCR	C39-C30-C25	-3.55	104.54	110.30
18	B	1221	CLA	O2A-CGA-CBA	3.55	123.04	111.91
18	A	1135	CLA	C4-C3-C5	3.55	120.04	115.98
23	F	5001	LMG	C8-O7-C10	-3.54	111.29	117.90
18	B	1218	CLA	C4-C3-C5	3.54	121.23	115.27
28	2	2013	CHL	C3C-C4C-NC	-3.53	106.61	110.57
22	B	6004	BCR	C3-C4-C5	-3.53	107.77	114.08
22	A	6017	BCR	C28-C27-C26	-3.53	107.78	114.08
18	1	1013	CLA	O2A-CGA-O1A	-3.52	112.09	123.14
18	1	1012	CLA	O2A-C1-C2	3.52	117.89	108.64
18	1	1014	CLA	O2A-CGA-O1A	-3.52	112.11	123.14
18	3	3004	CLA	OBD-CAD-C3D	-3.52	122.14	127.98
18	A	1117	CLA	O2A-CGA-CBA	3.51	122.93	111.91
18	3	3006	CLA	CMB-C2B-C3B	3.51	131.24	124.68
22	L	6020	BCR	C15-C14-C13	-3.51	122.30	127.31
28	1	1009	CHL	C2C-C3C-C4C	3.51	108.99	106.49
18	B	1209	CLA	CMB-C2B-C3B	3.51	131.24	124.68
28	2	2011	CHL	C2C-C3C-C4C	3.51	108.99	106.49
18	A	1103	CLA	O2A-CGA-CBA	3.51	122.91	111.91
22	L	6020	BCR	C7-C8-C9	-3.50	120.94	126.23
22	L	6019	BCR	C37-C22-C21	-3.50	118.02	122.92
22	A	6008	BCR	C3-C4-C5	-3.50	107.82	114.08
18	1	1012	CLA	O2A-CGA-O1A	-3.50	114.76	123.59
18	A	1104	CLA	C1-C2-C3	-3.50	119.99	126.04
22	B	6004	BCR	C15-C14-C13	-3.50	122.32	127.31
18	A	1130	CLA	CMB-C2B-C3B	3.50	131.22	124.68
22	F	6014	BCR	C34-C9-C10	-3.50	118.03	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	6020	BCR	C33-C5-C6	-3.50	120.60	124.53
21	2	2801	LHG	O7-C7-C8	3.49	120.55	110.80
18	1	1011	CLA	CAA-CBA-CGA	-3.49	103.05	113.25
28	2	2010	CHL	C3B-C4B-NB	-3.49	104.70	109.21
18	4	4008	CLA	C3C-C4C-NC	3.49	114.48	110.57
22	J	6012	BCR	C29-C30-C25	3.49	115.85	110.48
27	4	4503	LUT	C22-C23-C24	-3.48	107.78	111.74
28	4	4010	CHL	C3B-C4B-NB	-3.48	104.71	109.21
18	3	3002	CLA	CAC-C3C-C4C	3.48	129.32	124.81
23	F	5002	LMG	O8-C28-C29	3.48	122.83	111.91
18	B	1207	CLA	O2A-CGA-CBA	3.48	122.82	111.91
18	A	1138	CLA	O2A-C1-C2	3.48	117.77	108.64
18	A	1127	CLA	C1-C2-C3	-3.48	120.03	126.04
18	B	1221	CLA	C1-O2A-CGA	3.47	125.56	116.44
18	B	1201	CLA	C1-C2-C3	-3.46	121.15	126.75
18	A	1128	CLA	C4D-C3D-CAD	3.46	110.40	108.47
18	3	3010	CLA	C4-C3-C5	3.46	121.10	115.27
22	B	6004	BCR	C37-C22-C21	-3.46	118.07	122.92
18	B	1227	CLA	C1-C2-C3	-3.46	120.06	126.04
18	B	1213	CLA	CMB-C2B-C3B	3.46	131.15	124.68
22	B	6006	BCR	C29-C30-C25	-3.46	105.16	110.48
18	B	1227	CLA	O2A-CGA-CBA	3.45	122.75	111.91
18	A	1022	CLA	OBD-CAD-CBD	-3.45	120.97	125.89
28	1	1010	CHL	C3C-C4C-NC	-3.45	106.70	110.57
27	4	4501	LUT	C10-C11-C12	-3.45	112.46	123.22
18	3	3012	CLA	OBD-CAD-C3D	-3.45	122.26	127.98
21	B	5004	LHG	C5-O7-C7	-3.44	111.48	117.90
27	3	3501	LUT	C15-C14-C13	-3.44	122.40	127.31
18	4	4017	CLA	C1-C2-C3	-3.44	120.09	126.04
23	J	5001	LMG	O8-C28-C29	3.43	122.69	111.91
22	A	6007	BCR	C19-C18-C17	3.43	124.20	118.94
18	G	1001	CLA	CAC-C3C-C4C	3.43	129.26	124.81
18	1	1011	CLA	CMC-C2C-C1C	3.43	130.26	125.04
27	I	6018	LUT	C18-C5-C6	-3.42	120.68	124.53
18	B	1216	CLA	CMB-C2B-C3B	3.42	131.09	124.68
22	F	6016	BCR	C36-C18-C17	-3.42	118.13	122.92
18	3	3002	CLA	O2A-CGA-O1A	-3.42	112.42	123.14
18	1	1006	CLA	C1-C2-C3	-3.42	121.22	126.75
22	J	6013	BCR	C8-C9-C10	3.42	124.19	118.94
18	4	4001	CLA	CAA-C2A-C3A	-3.42	103.42	112.78
28	2	2010	CHL	C2C-C3C-C4C	3.42	108.93	106.49
18	B	1223	CLA	C1-C2-C3	-3.42	120.13	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6007	BCR	C36-C18-C17	-3.41	118.14	122.92
18	B	1210	CLA	C1-C2-C3	-3.41	120.14	126.04
22	B	6010	BCR	C1-C6-C5	-3.41	117.81	122.61
18	A	1132	CLA	C4D-C3D-CAD	3.40	110.37	108.47
18	B	1207	CLA	CMC-C2C-C1C	3.40	130.21	125.04
28	1	1010	CHL	C3B-C4B-NB	-3.39	104.82	109.21
18	3	3001	CLA	CAA-C2A-C3A	-3.39	103.49	112.78
18	A	1117	CLA	C1-C2-C3	-3.39	120.18	126.04
22	B	6005	BCR	C38-C26-C27	3.39	120.12	113.62
18	B	1225	CLA	C4-C3-C5	3.39	120.97	115.27
27	4	4502	LUT	C15-C14-C13	-3.39	122.48	127.31
22	B	6010	BCR	C1-C6-C7	3.37	125.32	115.78
18	2	2001	CLA	O2D-CGD-CBD	3.37	117.26	111.27
18	B	1232	CLA	C1-C2-C3	-3.37	120.22	126.04
18	2	2003	CLA	CMC-C2C-C1C	3.37	130.16	125.04
22	A	6002	BCR	C37-C22-C21	-3.36	118.21	122.92
18	4	4006	CLA	O2A-CGA-CBA	3.36	122.46	111.91
18	A	1135	CLA	C1-C2-C3	-3.36	120.23	126.04
27	1	1501	LUT	C18-C5-C6	-3.36	120.75	124.53
26	B	8002	LMU	C1B-O1B-C4'	-3.36	109.64	117.96
18	B	1211	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
28	2	2013	CHL	C1B-CHB-C4A	-3.36	123.46	130.12
22	A	6017	BCR	C37-C22-C21	-3.36	118.22	122.92
22	B	6009	BCR	C36-C18-C17	-3.36	118.22	122.92
18	B	1226	CLA	CMB-C2B-C3B	3.36	130.96	124.68
22	A	6008	BCR	C36-C18-C17	-3.35	118.22	122.92
22	A	6011	BCR	C34-C9-C10	-3.35	118.23	122.92
27	1	1502	LUT	C11-C10-C9	-3.35	122.53	127.31
18	A	1128	CLA	CMB-C2B-C3B	3.35	130.95	124.68
29	4	4505	ZEX	C15-C14-C13	-3.35	122.53	127.31
27	I	6018	LUT	C31-C30-C29	-3.34	122.54	127.31
22	J	6013	BCR	C28-C27-C26	-3.34	108.11	114.08
22	F	6014	BCR	C36-C18-C17	-3.34	118.25	122.92
27	1	1501	LUT	C31-C32-C33	-3.33	117.05	126.42
18	3	3019	CLA	CAD-C3D-C2D	3.33	140.83	132.79
27	4	4501	LUT	C31-C30-C29	-3.33	122.56	127.31
22	J	6012	BCR	C33-C5-C4	3.33	120.01	113.62
22	I	6020	BCR	C7-C8-C9	-3.33	121.20	126.23
18	A	1119	CLA	C1-C2-C3	-3.33	120.28	126.04
18	1	1001	CLA	C3C-C4C-NC	3.33	114.30	110.57
18	A	1101	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
18	4	4009	CLA	CMC-C2C-C1C	3.33	130.10	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3017	CLA	CMC-C2C-C1C	3.32	130.10	125.04
18	A	1124	CLA	C1-C2-C3	-3.32	120.30	126.04
22	A	6011	BCR	C12-C13-C14	-3.32	113.85	118.94
18	3	3017	CLA	O2A-CGA-CBA	3.32	125.34	112.23
22	K	2011	BCR	C37-C22-C21	-3.32	118.28	122.92
18	4	4008	CLA	CMC-C2C-C1C	3.31	130.09	125.04
22	J	6012	BCR	C36-C18-C17	-3.31	118.28	122.92
18	B	1201	CLA	CMC-C2C-C1C	3.31	130.08	125.04
18	2	2004	CLA	O1D-CGD-CBD	-3.31	117.71	124.48
22	A	6003	BCR	C19-C18-C17	3.31	124.02	118.94
22	F	6014	BCR	C33-C5-C6	-3.31	120.81	124.53
18	B	1204	CLA	C1-O2A-CGA	3.31	125.12	116.44
22	A	6002	BCR	C38-C26-C27	3.30	119.97	113.62
18	B	1228	CLA	C1-C2-C3	-3.30	120.33	126.04
22	G	2011	BCR	C24-C23-C22	-3.30	121.25	126.23
18	B	1212	CLA	C1-C2-C3	-3.30	120.34	126.04
18	4	4003	CLA	C1-C2-C3	-3.29	120.35	126.04
18	A	1013	CLA	CMB-C2B-C3B	3.29	130.83	124.68
18	4	4009	CLA	C1-C2-C3	-3.29	121.43	126.75
18	1	1005	CLA	C3C-C4C-NC	3.28	114.25	110.57
18	1	1013	CLA	CAC-C3C-C4C	3.28	129.06	124.81
18	4	4002	CLA	C1-C2-C3	-3.28	121.45	126.75
18	B	1221	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
18	1	1002	CLA	CMC-C2C-C1C	3.27	130.02	125.04
22	L	6020	BCR	C23-C22-C21	3.27	123.95	118.94
18	L	1502	CLA	CMC-C2C-C1C	3.27	130.01	125.04
27	2	2502	LUT	C35-C34-C33	-3.26	122.66	127.31
27	4	4503	LUT	C17-C1-C6	-3.26	105.01	110.30
27	2	2502	LUT	C21-C26-C27	3.25	116.81	112.70
18	B	1211	CLA	C1-C2-C3	-3.25	120.42	126.04
22	J	6013	BCR	C29-C30-C25	3.24	115.47	110.48
18	G	1002	CLA	CAC-C3C-C4C	3.24	129.01	124.81
18	H	1000	CLA	O2A-CGA-CBA	3.24	125.03	112.23
18	B	1021	CLA	CMC-C2C-C1C	3.24	129.97	125.04
18	B	1227	CLA	CMC-C2C-C1C	3.23	129.97	125.04
18	3	3012	CLA	C1-C2-C3	-3.23	121.52	126.75
18	2	2006	CLA	C1-C2-C3	-3.23	120.46	126.04
18	A	1140	CLA	C4-C3-C5	3.23	120.70	115.27
18	2	2001	CLA	CBA-CAA-C2A	3.22	123.36	113.86
22	B	6009	BCR	C37-C22-C21	-3.22	118.42	122.92
18	3	3003	CLA	OBD-CAD-C3D	-3.22	122.64	127.98
18	A	1139	CLA	CMC-C2C-C1C	3.22	129.94	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1240	CLA	O2A-CGA-CBA	3.21	121.99	111.91
18	3	3008	CLA	OBD-CAD-CBD	-3.21	121.31	125.89
22	A	6011	BCR	C33-C5-C6	-3.21	120.93	124.53
23	G	2021	LMG	O8-C28-C29	3.21	121.97	111.91
18	2	2007	CLA	C1-C2-C3	-3.21	120.50	126.04
18	L	1501	CLA	CMC-C2C-C1C	3.21	129.92	125.04
18	A	1101	CLA	CMB-C2B-C3B	3.20	130.67	124.68
22	B	6010	BCR	C19-C18-C17	3.20	123.85	118.94
22	F	6016	BCR	C34-C9-C8	3.20	123.12	118.08
22	J	6013	BCR	C33-C5-C6	-3.20	120.94	124.53
22	J	6012	BCR	C1-C6-C5	-3.20	118.11	122.61
18	A	1112	CLA	C1-C2-C3	-3.20	120.52	126.04
18	G	1001	CLA	O2A-C1-C2	3.19	117.03	108.64
18	B	1215	CLA	CMB-C2B-C3B	3.19	130.65	124.68
18	1	1008	CLA	CAC-C3C-C4C	3.19	128.95	124.81
18	3	3018	CLA	C1-C2-C3	-3.19	121.59	126.75
22	B	6006	BCR	C30-C25-C26	-3.19	118.12	122.61
18	3	3017	CLA	CMB-C2B-C3B	3.19	130.64	124.68
27	3	3502	LUT	C1-C6-C5	-3.19	118.13	122.61
18	4	4002	CLA	O2D-CGD-CBD	3.19	116.93	111.27
18	B	1213	CLA	C4-C3-C5	3.18	120.63	115.27
18	1	1008	CLA	O2A-CGA-CBA	3.18	124.80	112.23
28	3	3011	CHL	C1B-CHB-C4A	-3.18	123.82	130.12
22	J	6013	BCR	C3-C4-C5	-3.18	108.40	114.08
27	4	4502	LUT	C18-C5-C6	-3.18	120.96	124.53
18	3	3013	CLA	OBD-CAD-C3D	-3.18	122.71	127.98
18	B	1236	CLA	CMC-C2C-C1C	3.18	129.88	125.04
18	4	4001	CLA	C1-O2A-CGA	3.17	124.77	116.44
18	3	3013	CLA	O2A-CGA-CBA	3.17	124.77	112.23
18	B	1228	CLA	CMB-C2B-C3B	3.17	130.61	124.68
18	G	1003	CLA	OBD-CAD-C3D	-3.17	122.72	127.98
27	4	4501	LUT	C8-C7-C6	-3.17	118.30	127.20
23	J	5001	LMG	O8-C28-O10	-3.17	115.60	123.59
18	B	1021	CLA	CMB-C2B-C3B	3.17	130.60	124.68
18	B	1215	CLA	C1-C2-C3	-3.17	120.57	126.04
18	B	1235	CLA	CMC-C2C-C1C	3.17	129.86	125.04
29	4	4505	ZEX	C38-C24-C25	-3.16	105.83	110.87
22	B	6004	BCR	C33-C5-C4	3.16	119.69	113.62
18	B	1231	CLA	C4-C3-C5	3.16	120.59	115.27
25	B	7101	DGD	O3G-C3G-C2G	-3.16	103.27	110.90
18	1	1002	CLA	O2A-CGA-O1A	-3.16	113.23	123.14
18	A	1106	CLA	CMB-C2B-C3B	3.16	130.59	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	5001	LMG	C12-C11-C10	-3.16	102.13	113.62
18	B	1231	CLA	C1-C2-C3	-3.15	120.59	126.04
22	F	6016	BCR	C23-C24-C25	-3.15	118.35	127.20
22	A	6007	BCR	C37-C22-C21	-3.15	118.51	122.92
18	3	3005	CLA	C4-C3-C5	3.15	120.57	115.27
18	4	4008	CLA	OBD-CAD-C3D	-3.15	122.75	127.98
22	3	3503	BCR	C38-C26-C25	-3.15	120.99	124.53
27	4	4503	LUT	C18-C5-C6	-3.15	121.00	124.53
18	L	1502	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
18	A	1102	CLA	C1-C2-C3	-3.14	121.67	126.75
25	B	7101	DGD	O6D-C1D-O3G	-3.14	102.55	109.97
18	2	2002	CLA	CMC-C2C-C1C	3.14	129.81	125.04
22	A	6002	BCR	C33-C5-C6	-3.14	121.01	124.53
18	A	1108	CLA	CMB-C2B-C3B	3.13	130.54	124.68
18	2	2016	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
18	2	2004	CLA	C1-C2-C3	-3.13	120.62	126.04
18	1	1004	CLA	C1-C2-C3	-3.13	120.62	126.04
27	4	4501	LUT	C18-C5-C4	3.13	120.16	114.36
22	I	6020	BCR	C24-C23-C22	-3.12	121.52	126.23
22	J	6012	BCR	C38-C26-C25	-3.12	121.02	124.53
18	A	1134	CLA	C1-C2-C3	-3.12	120.64	126.04
29	4	4505	ZEX	C31-C30-C29	-3.12	122.86	127.31
18	A	1113	CLA	O2A-CGA-CBA	3.12	124.56	112.23
18	B	1222	CLA	C4-C3-C5	3.12	120.52	115.27
22	B	6004	BCR	C30-C25-C26	-3.12	118.22	122.61
18	B	1230	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
18	B	1238	CLA	CMB-C2B-C3B	3.11	130.50	124.68
22	J	6013	BCR	C4-C5-C6	-3.11	118.21	122.73
23	4	4801	LMG	C8-O7-C10	-3.11	110.13	117.79
22	L	6020	BCR	C38-C26-C27	3.11	119.59	113.62
22	F	6014	BCR	C7-C8-C9	-3.11	121.53	126.23
18	A	1120	CLA	C1-C2-C3	-3.11	120.66	126.04
18	A	1112	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
18	A	1118	CLA	O2A-CGA-CBA	3.11	124.51	112.23
22	L	6020	BCR	C8-C9-C10	3.11	123.71	118.94
18	1	1012	CLA	O2A-CGA-CBA	3.11	121.65	111.91
18	4	4017	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
18	B	1217	CLA	O2A-CGA-CBA	3.10	124.49	112.23
18	B	1229	CLA	C3C-C4C-NC	3.10	114.05	110.57
18	L	1501	CLA	C1-O2A-CGA	3.10	124.58	116.44
27	3	3501	LUT	C8-C7-C6	-3.10	118.49	127.20
22	B	6010	BCR	C36-C18-C17	-3.10	118.58	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	2011	BCR	C33-C5-C6	-3.10	121.05	124.53
18	A	1128	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	L	6019	BCR	C8-C9-C10	3.09	123.69	118.94
18	A	1105	CLA	C1-C2-C3	-3.09	120.70	126.04
18	1	1002	CLA	O2A-CGA-CBA	3.09	124.45	112.23
18	B	1209	CLA	O2A-CGA-CBA	3.09	124.44	112.23
18	A	1121	CLA	C4-C3-C5	3.09	120.47	115.27
28	3	3011	CHL	C3B-C4B-NB	-3.09	105.22	109.21
18	G	1003	CLA	C1-C2-C3	-3.09	120.70	126.04
18	4	4016	CLA	O2A-CGA-CBA	3.09	124.43	112.23
18	A	1125	CLA	C3C-C4C-NC	3.09	114.03	110.57
18	A	1103	CLA	CMC-C2C-C1C	3.08	129.73	125.04
28	4	4011	CHL	CHD-C4C-C3C	3.08	129.37	124.84
18	1	1003	CLA	C1-C2-C3	-3.08	120.72	126.04
18	A	1013	CLA	C1-C2-C3	-3.08	120.72	126.04
18	B	1240	CLA	CMC-C2C-C1C	3.08	129.72	125.04
28	1	1010	CHL	C1B-CHB-C4A	-3.07	124.03	130.12
27	I	6018	LUT	C7-C8-C9	-3.07	121.59	126.23
22	J	6013	BCR	C38-C26-C25	-3.07	121.08	124.53
18	A	1108	CLA	O2A-CGA-CBA	3.07	124.37	112.23
18	A	1132	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
18	A	1107	CLA	CMC-C2C-C1C	3.07	129.71	125.04
27	1	1502	LUT	C35-C34-C33	-3.07	122.93	127.31
18	A	1101	CLA	C1-C2-C3	-3.07	120.74	126.04
18	4	4001	CLA	CBC-CAC-C3C	-3.06	103.98	112.43
22	K	2011	BCR	C34-C9-C10	-3.06	118.63	122.92
28	4	4010	CHL	CHB-C4A-NA	3.06	128.75	124.51
18	A	1123	CLA	CMC-C2C-C1C	3.06	129.70	125.04
18	2	2016	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
27	3	3501	LUT	C35-C15-C14	-3.06	117.20	123.47
18	A	1120	CLA	C4-C3-C5	3.06	120.42	115.27
29	4	4505	ZEX	C11-C10-C9	-3.06	122.94	127.31
18	1	1007	CLA	O2A-CGA-CBA	3.06	124.33	112.23
18	K	1001	CLA	O2A-CGA-CBA	3.06	124.32	112.23
22	A	6002	BCR	C23-C22-C21	3.06	123.63	118.94
18	B	1216	CLA	CMC-C2C-C1C	3.06	129.69	125.04
18	2	2016	CLA	O1D-CGD-CBD	-3.06	118.23	124.48
18	2	2005	CLA	C4-C3-C5	3.05	120.41	115.27
29	4	4505	ZEX	C15-C35-C34	-3.05	117.22	123.47
18	B	1223	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
18	A	1114	CLA	O2A-CGA-CBA	3.05	124.29	112.23
22	A	6002	BCR	C3-C4-C5	-3.05	108.63	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4009	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
18	B	1239	CLA	C1-C2-C3	-3.05	120.77	126.04
18	3	3001	CLA	CMD-C2D-C3D	-3.05	118.98	124.68
18	A	1112	CLA	C4-C3-C5	3.04	120.39	115.27
18	1	1006	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
28	4	4010	CHL	CHA-C1A-NA	-3.04	119.43	126.40
17	A	1011	CL0	CMC-C2C-C1C	3.04	129.67	125.04
18	1	1001	CLA	C6-C5-C3	-3.04	105.49	113.45
18	L	1502	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
18	A	1117	CLA	CMB-C2B-C3B	3.04	130.36	124.68
18	B	1023	CLA	C1-C2-C3	-3.03	120.79	126.04
18	B	1210	CLA	CAC-C3C-C4C	3.03	128.75	124.81
18	3	3018	CLA	CAC-C3C-C4C	3.03	128.75	124.81
18	B	1235	CLA	C1-C2-C3	-3.03	120.80	126.04
27	3	3502	LUT	C35-C34-C33	-3.03	122.99	127.31
18	2	2012	CLA	CMA-C3A-C4A	-3.03	103.63	111.77
18	2	2003	CLA	C1-C2-C3	-3.03	120.81	126.04
22	I	6020	BCR	C36-C18-C17	-3.03	118.68	122.92
18	4	4001	CLA	CMA-C3A-C4A	-3.03	103.64	111.77
18	B	1012	CLA	C3C-C4C-NC	3.03	113.96	110.57
18	G	1002	CLA	CMC-C2C-C1C	3.03	129.65	125.04
18	B	1231	CLA	CMC-C2C-C1C	3.02	129.65	125.04
18	B	1012	CLA	C1-C2-C3	-3.02	120.81	126.04
18	1	1013	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
23	J	5001	LMG	O6-C5-C4	-3.02	104.21	109.69
18	1	1005	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
18	A	1115	CLA	O2A-CGA-CBA	3.02	124.16	112.23
18	A	1102	CLA	CMB-C2B-C3B	3.02	130.32	124.68
25	B	7101	DGD	O5D-C6D-C5D	-3.02	103.47	109.05
18	B	1012	CLA	C4-C3-C5	3.02	120.34	115.27
18	3	3002	CLA	O2A-CGA-CBA	3.01	124.14	112.23
18	L	1502	CLA	C1-C2-C3	-3.01	120.83	126.04
18	3	3008	CLA	C3C-C4C-NC	3.01	113.95	110.57
18	4	4008	CLA	O2A-CGA-CBA	3.01	124.12	112.23
18	3	3005	CLA	C3C-C4C-NC	3.01	113.94	110.57
18	A	1137	CLA	CMC-C2C-C1C	3.00	129.62	125.04
18	B	1222	CLA	CMB-C2B-C3B	3.00	130.30	124.68
18	3	3008	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
28	4	4013	CHL	CHD-C4C-C3C	3.00	129.25	124.84
18	1	1013	CLA	O2A-CGA-CBA	3.00	124.09	112.23
18	A	1136	CLA	C1-C2-C3	-3.00	120.86	126.04
18	G	1002	CLA	O2A-CGA-CBA	3.00	124.08	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	1001	CLA	CAA-C2A-C1A	-3.00	102.15	111.97
18	1	1008	CLA	CMC-C2C-C1C	3.00	129.60	125.04
18	B	1213	CLA	CMC-C2C-C1C	3.00	129.60	125.04
20	A	5001	PQN	C11-C12-C13	-2.99	121.81	126.79
18	4	4006	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
18	A	1022	CLA	C4-C3-C5	2.99	120.30	115.27
18	4	4008	CLA	CAC-C3C-C4C	2.99	128.69	124.81
22	K	2011	BCR	C38-C26-C25	-2.99	121.18	124.53
18	B	1219	CLA	C1-C2-C3	-2.98	120.88	126.04
18	B	1230	CLA	CMC-C2C-C1C	2.98	129.58	125.04
18	B	1230	CLA	C1-C2-C3	-2.98	120.89	126.04
18	G	1001	CLA	CMC-C2C-C1C	2.98	129.57	125.04
18	B	1216	CLA	C4-C3-C5	2.98	120.28	115.27
22	B	6009	BCR	C34-C9-C10	-2.98	118.75	122.92
18	B	1207	CLA	CAC-C3C-C4C	2.97	128.67	124.81
18	4	4006	CLA	CMC-C2C-C1C	2.97	129.57	125.04
18	B	1223	CLA	C3C-C4C-NC	2.97	113.90	110.57
27	1	1502	LUT	C15-C35-C34	-2.97	117.39	123.47
22	A	6007	BCR	C38-C26-C27	2.97	119.32	113.62
21	1	1801	LHG	C6-C5-C4	-2.97	104.77	111.79
27	1	1502	LUT	C10-C11-C12	-2.97	113.96	123.22
18	A	1123	CLA	CMB-C2B-C3B	2.96	130.22	124.68
18	2	2002	CLA	O2A-CGA-CBA	2.96	123.94	112.23
18	B	1207	CLA	C1-O2A-CGA	2.96	124.22	116.44
18	3	3008	CLA	CMB-C2B-C3B	2.96	130.22	124.68
18	B	1227	CLA	C4-C3-C5	2.96	120.25	115.27
22	B	6005	BCR	C1-C6-C5	-2.96	118.44	122.61
18	B	1221	CLA	CMC-C2C-C1C	2.96	129.55	125.04
18	A	1123	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
18	A	1237	CLA	CMC-C2C-C1C	2.96	129.54	125.04
18	4	4005	CLA	C3C-C4C-NC	2.96	113.89	110.57
22	L	6020	BCR	C38-C26-C25	-2.95	121.21	124.53
18	A	1138	CLA	CED-O2D-CGD	2.95	122.62	115.94
18	B	1222	CLA	CMC-C2C-C1C	2.95	129.53	125.04
18	B	1218	CLA	CMC-C2C-C1C	2.95	129.53	125.04
27	1	1502	LUT	C18-C5-C6	-2.95	121.22	124.53
22	3	3503	BCR	C3-C4-C5	-2.95	108.81	114.08
27	3	3502	LUT	C11-C10-C9	-2.95	123.11	127.31
22	3	3503	BCR	C23-C22-C21	2.94	123.45	118.94
18	B	1202	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
29	4	4505	ZEX	C19-C9-C10	-2.94	118.81	122.92
28	2	2011	CHL	CHD-C4C-C3C	2.94	129.16	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3001	CLA	C1-C2-C3	-2.94	122.00	126.75
18	3	3005	CLA	C1-C2-C3	-2.93	120.97	126.04
18	A	1127	CLA	CMB-C2B-C3B	2.93	130.16	124.68
18	1	1007	CLA	CMC-C2C-C1C	2.93	129.50	125.04
28	3	3011	CHL	C1-O2A-CGA	2.93	124.13	116.44
18	B	1238	CLA	CMC-C2C-C1C	2.93	129.50	125.04
27	3	3502	LUT	C19-C9-C10	-2.93	118.82	122.92
18	B	1212	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	A	6008	BCR	C38-C26-C27	2.93	119.24	113.62
18	A	1109	CLA	C4-C3-C5	2.92	120.19	115.27
22	A	6017	BCR	C12-C13-C14	2.92	123.43	118.94
18	A	1104	CLA	C4-C3-C5	2.92	120.19	115.27
18	A	1120	CLA	CMC-C2C-C1C	2.92	129.49	125.04
22	B	6005	BCR	C37-C22-C21	-2.92	118.83	122.92
18	G	1003	CLA	CMC-C2C-C1C	2.92	129.49	125.04
18	3	3003	CLA	O2A-CGA-CBA	2.92	121.06	111.91
18	3	3013	CLA	CMC-C2C-C1C	2.91	129.48	125.04
22	A	6017	BCR	C8-C9-C10	2.91	123.41	118.94
18	B	1224	CLA	C4-C3-C5	2.91	120.17	115.27
18	L	1501	CLA	OBD-CAD-CBD	-2.91	121.73	125.89
22	I	6020	BCR	C3-C4-C5	-2.91	108.88	114.08
18	A	1119	CLA	CMB-C2B-C3B	2.91	130.12	124.68
18	A	1138	CLA	CMB-C2B-C3B	2.91	130.12	124.68
18	2	2004	CLA	CMC-C2C-C1C	2.91	129.47	125.04
18	B	1208	CLA	CMC-C2C-C1C	2.91	129.47	125.04
18	B	1239	CLA	CMC-C2C-C1C	2.91	129.47	125.04
18	L	1501	CLA	O1D-CGD-CBD	-2.91	118.53	124.48
22	F	6014	BCR	C19-C18-C17	2.91	123.40	118.94
27	I	6018	LUT	C8-C7-C6	-2.91	119.04	127.20
18	A	1104	CLA	CAA-C2A-C3A	-2.91	104.82	112.78
18	A	1102	CLA	CMC-C2C-C1C	2.91	129.47	125.04
18	B	1215	CLA	CMC-C2C-C1C	2.91	129.46	125.04
18	B	1021	CLA	CMA-C3A-C4A	-2.90	103.97	111.77
18	A	1133	CLA	CMC-C2C-C1C	2.90	129.46	125.04
17	A	1011	CL0	C3C-C4C-NC	2.90	113.82	110.57
18	1	1014	CLA	C3C-C4C-NC	2.90	113.82	110.57
18	A	1106	CLA	CMC-C2C-C1C	2.90	129.45	125.04
18	A	1132	CLA	CMB-C2B-C3B	2.90	130.10	124.68
18	2	2002	CLA	CAC-C3C-C4C	2.90	128.57	124.81
18	2	2008	CLA	CMC-C2C-C1C	2.90	129.45	125.04
18	A	1130	CLA	C1-C2-C3	-2.89	122.07	126.75
18	A	1103	CLA	O2D-CGD-O1D	-2.89	118.18	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	1009	CHL	C3B-C4B-NB	-2.89	105.47	109.21
18	A	1110	CLA	CMB-C2B-C3B	2.89	130.08	124.68
18	B	1201	CLA	CMB-C2B-C3B	2.89	130.08	124.68
18	3	3012	CLA	CAA-C2A-C3A	-2.88	104.88	112.78
18	B	1209	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
18	B	1232	CLA	C4-C3-C5	2.88	120.12	115.27
18	B	1207	CLA	C1-C2-C3	-2.88	121.06	126.04
22	A	6011	BCR	C33-C5-C4	2.88	119.15	113.62
18	B	1226	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
18	A	1125	CLA	C1-C2-C3	-2.88	121.07	126.04
18	2	2019	CLA	C3A-C4A-CHB	-2.88	120.39	123.91
18	A	1151	CLA	C3C-C4C-NC	2.87	113.79	110.57
18	B	1225	CLA	CMC-C2C-C1C	2.87	129.41	125.04
18	A	1104	CLA	CMC-C2C-C1C	2.87	129.41	125.04
18	3	3006	CLA	CMC-C2C-C1C	2.87	129.41	125.04
28	2	2013	CHL	CHD-C4C-C3C	2.87	129.06	124.84
28	4	4011	CHL	C1B-CHB-C4A	-2.87	124.43	130.12
22	A	6008	BCR	C34-C9-C10	-2.87	118.90	122.92
18	A	1131	CLA	CMC-C2C-C1C	2.87	129.41	125.04
18	A	1106	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
28	2	2011	CHL	C3B-C4B-NB	-2.87	105.50	109.21
18	3	3012	CLA	CMA-C3A-C4A	-2.87	104.07	111.77
18	A	1108	CLA	CMC-C2C-C1C	2.87	129.41	125.04
22	A	6008	BCR	C37-C22-C21	-2.86	118.91	122.92
18	A	1102	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	B	6004	BCR	C38-C26-C27	2.86	119.11	113.62
18	B	1202	CLA	CMB-C2B-C3B	2.86	130.03	124.68
18	A	1130	CLA	CMC-C2C-C1C	2.86	129.40	125.04
18	B	1227	CLA	CMB-C2B-C3B	2.86	130.03	124.68
18	B	1219	CLA	CMB-C2B-C3B	2.86	130.03	124.68
18	A	1132	CLA	C1-C2-C3	-2.86	121.10	126.04
18	4	4007	CLA	C1-O2A-CGA	2.86	123.94	116.44
18	2	2001	CLA	CMA-C3A-C4A	-2.86	104.09	111.77
18	A	1129	CLA	CMC-C2C-C1C	2.86	129.39	125.04
18	B	1203	CLA	CMC-C2C-C1C	2.86	129.39	125.04
18	B	1218	CLA	C1-C2-C3	-2.86	121.10	126.04
18	A	1131	CLA	C1-C2-C3	-2.86	121.10	126.04
22	F	6016	BCR	C38-C26-C25	-2.86	121.32	124.53
18	A	1126	CLA	CMB-C2B-C3B	2.85	130.02	124.68
23	F	5001	LMG	O7-C10-O9	-2.85	117.30	122.96
18	3	3001	CLA	CMC-C2C-C1C	2.85	129.38	125.04
18	1	1011	CLA	CAC-C3C-C4C	2.85	128.51	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4012	CLA	C1-C2-C3	-2.85	121.11	126.04
18	2	2003	CLA	CAC-C3C-C4C	2.85	128.51	124.81
18	1	1005	CLA	C1-C2-C3	-2.85	121.12	126.04
18	G	1002	CLA	O1D-CGD-CBD	-2.85	118.66	124.48
27	3	3501	LUT	C17-C1-C6	-2.85	105.68	110.30
22	B	6006	BCR	C36-C18-C17	-2.85	118.94	122.92
27	4	4502	LUT	C1-C2-C3	-2.84	107.22	113.64
18	4	4016	CLA	CAC-C3C-C4C	2.84	128.50	124.81
27	3	3501	LUT	C18-C5-C4	2.84	119.62	114.36
18	2	2003	CLA	C3C-C4C-NC	2.84	113.76	110.57
18	3	3007	CLA	CAC-C3C-C4C	2.84	128.50	124.81
22	B	6005	BCR	C23-C24-C25	-2.84	119.23	127.20
22	I	6020	BCR	C38-C26-C27	2.84	119.07	113.62
18	B	1203	CLA	C4-C3-C5	2.84	120.04	115.27
28	3	3011	CHL	C1-C2-C3	-2.84	121.14	126.04
27	2	2501	LUT	C38-C25-C24	-2.84	117.49	123.56
18	B	1230	CLA	O1D-CGD-CBD	-2.83	118.69	124.48
18	F	1301	CLA	CMC-C2C-C1C	2.83	129.35	125.04
18	A	1131	CLA	C4-C3-C5	2.83	120.04	115.27
28	4	4013	CHL	C3B-C4B-NB	-2.83	105.55	109.21
18	4	4003	CLA	CMC-C2C-C1C	2.83	129.34	125.04
27	1	1502	LUT	C3-C4-C5	-2.83	106.23	111.85
18	2	2004	CLA	CMB-C2B-C3B	2.82	129.96	124.68
18	1	1002	CLA	OBD-CAD-C3D	-2.82	123.30	127.98
18	2	2019	CLA	C3C-C4C-NC	2.82	112.57	109.97
18	J	1302	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	B	1215	CLA	C4-C3-C5	2.82	120.01	115.27
18	A	1105	CLA	C1-O2A-CGA	2.82	123.83	116.44
22	3	3503	BCR	C23-C24-C25	-2.82	119.29	127.20
18	2	2006	CLA	CAA-C2A-C3A	-2.82	105.07	112.78
17	A	1011	CL0	CMA-C3A-C4A	-2.82	104.21	111.77
29	4	4505	ZEX	C17-C1-C6	-2.81	105.73	110.30
18	1	1011	CLA	C5-C3-C4	2.81	120.82	114.60
28	4	4013	CHL	C1B-CHB-C4A	-2.81	124.54	130.12
18	A	1132	CLA	CMC-C2C-C1C	2.81	129.32	125.04
18	J	1302	CLA	CMC-C2C-C1C	2.81	129.32	125.04
18	A	1129	CLA	C3C-C4C-NC	2.81	113.72	110.57
18	4	4007	CLA	CMC-C2C-C1C	2.81	129.32	125.04
18	4	4004	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
18	B	1238	CLA	C4-C3-C5	2.81	120.00	115.27
18	4	4012	CLA	CMC-C2C-C1C	2.81	129.32	125.04
18	A	1116	CLA	CMC-C2C-C1C	2.81	129.32	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4001	CLA	C4-C3-C5	2.81	120.00	115.27
18	A	1116	CLA	C4-C3-C5	2.81	120.00	115.27
18	F	1302	CLA	CMC-C2C-C1C	2.81	129.32	125.04
18	B	1023	CLA	CMB-C2B-C3B	2.81	129.93	124.68
18	A	1128	CLA	C4-C3-C5	2.81	119.99	115.27
18	B	1222	CLA	C3C-C4C-NC	2.81	113.72	110.57
18	B	1234	CLA	CMB-C2B-C3B	2.81	129.93	124.68
18	3	3018	CLA	CMC-C2C-C1C	2.81	129.31	125.04
18	2	2003	CLA	C4-C3-C5	2.81	119.99	115.27
18	A	1013	CLA	C4-C3-C5	2.81	119.99	115.27
18	B	1012	CLA	CMC-C2C-C1C	2.80	129.31	125.04
18	4	4005	CLA	OBD-CAD-CBD	-2.80	121.89	125.89
22	L	6020	BCR	C35-C13-C14	-2.80	119.00	122.92
18	A	1101	CLA	C4-C3-C5	2.80	119.98	115.27
18	3	3010	CLA	C1-C2-C3	-2.80	121.20	126.04
18	2	2012	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
27	3	3502	LUT	C18-C5-C4	2.80	119.53	114.36
18	A	1121	CLA	CMC-C2C-C1C	2.79	129.29	125.04
18	B	1216	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
18	2	2007	CLA	C4-C3-C5	2.79	119.97	115.27
18	A	1124	CLA	CMC-C2C-C1C	2.79	129.29	125.04
22	K	2011	BCR	C38-C26-C27	2.79	118.97	113.62
18	B	1226	CLA	C1-C2-C3	-2.79	121.22	126.04
18	1	1014	CLA	O1D-CGD-CBD	-2.79	118.78	124.48
18	A	1102	CLA	C3C-C4C-NC	2.78	113.69	110.57
18	B	1222	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
18	B	1224	CLA	CMB-C2B-C3B	2.78	129.88	124.68
27	1	1502	LUT	C40-C33-C32	2.78	122.46	118.08
18	B	1208	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
18	B	1223	CLA	OBD-CAD-C3D	-2.78	123.36	127.98
18	2	2005	CLA	CMC-C2C-C1C	2.78	129.27	125.04
18	4	4002	CLA	CBC-CAC-C3C	-2.78	104.77	112.43
28	4	4010	CHL	CAA-C2A-C1A	2.78	121.08	111.97
18	A	1140	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
18	A	1127	CLA	C4-C3-C5	2.78	119.94	115.27
18	A	1022	CLA	C3C-C4C-NC	2.78	113.69	110.57
18	B	1219	CLA	CMC-C2C-C1C	2.78	129.27	125.04
21	A	5003	LHG	O8-C23-C24	2.78	120.62	111.91
22	A	6007	BCR	C23-C22-C21	2.77	123.19	118.94
23	B	5005	LMG	O8-C28-C29	2.77	120.60	111.91
22	J	6012	BCR	C31-C1-C6	-2.77	105.81	110.30
22	F	6016	BCR	C37-C22-C21	-2.77	119.04	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1111	CLA	CMC-C2C-C1C	2.77	129.25	125.04
18	B	1023	CLA	C4-C3-C5	2.77	119.93	115.27
18	1	1013	CLA	CMC-C2C-C1C	2.77	129.25	125.04
18	F	1302	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	F	6014	BCR	C34-C9-C8	2.76	122.43	118.08
18	A	1137	CLA	C4-C3-C5	2.76	119.92	115.27
18	B	1235	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	3	3503	BCR	C31-C1-C6	-2.76	105.82	110.30
18	1	1005	CLA	CMC-C2C-C1C	2.76	129.25	125.04
18	A	1111	CLA	CMB-C2B-C3B	2.76	129.85	124.68
18	4	4001	CLA	O2D-CGD-CBD	2.76	116.18	111.27
27	4	4502	LUT	C8-C7-C6	-2.76	119.44	127.20
18	B	1206	CLA	CMC-C2C-C1C	2.76	129.24	125.04
18	A	1105	CLA	CMC-C2C-C1C	2.76	129.24	125.04
18	A	1124	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
28	4	4010	CHL	CAA-CBA-CGA	2.76	121.32	113.25
22	F	6016	BCR	C19-C18-C17	2.76	123.18	118.94
18	A	1103	CLA	C4-C3-C5	2.76	119.91	115.27
22	A	6011	BCR	C23-C24-C25	-2.76	119.45	127.20
18	A	1125	CLA	CMC-C2C-C1C	2.76	129.24	125.04
26	B	8002	LMU	C1-O1'-C1'	-2.76	109.27	113.84
18	A	1125	CLA	C4-C3-C5	2.76	119.91	115.27
18	B	1206	CLA	C4-C3-C5	2.76	119.91	115.27
21	1	1801	LHG	O8-C23-C24	2.76	120.56	111.91
18	2	2008	CLA	C3C-C4C-NC	2.76	113.66	110.57
18	B	1206	CLA	CMB-C2B-C3B	2.75	129.83	124.68
22	J	6012	BCR	C35-C13-C12	2.75	122.42	118.08
27	2	2502	LUT	C8-C7-C6	-2.75	119.47	127.20
18	2	2003	CLA	CMB-C2B-C3B	2.75	129.83	124.68
18	A	1126	CLA	CMC-C2C-C1C	2.75	129.23	125.04
18	A	1135	CLA	CMC-C2C-C1C	2.75	129.23	125.04
18	B	1212	CLA	CMC-C2C-C1C	2.75	129.23	125.04
18	A	1135	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	2	2802	LMG	C9-C8-C7	-2.75	105.29	111.79
18	A	1118	CLA	CMC-C2C-C1C	2.75	129.22	125.04
18	B	1217	CLA	CMC-C2C-C1C	2.75	129.22	125.04
23	F	5001	LMG	O6-C5-C4	-2.75	104.70	109.69
18	B	1218	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
18	4	4002	CLA	OBD-CAD-CBD	-2.75	121.97	125.89
18	2	2009	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
18	A	1133	CLA	C4-C3-C5	2.74	119.89	115.27
27	1	1501	LUT	C10-C11-C12	-2.74	114.66	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	1002	CLA	CBA-CAA-C2A	-2.74	105.77	113.86
29	4	4505	ZEX	O23-C23-C22	-2.74	103.52	109.91
18	A	1107	CLA	C1-O2A-CGA	2.74	123.64	116.44
18	A	1139	CLA	C1-C2-C3	-2.74	121.31	126.04
18	3	3007	CLA	CMC-C2C-C1C	2.74	129.21	125.04
23	2	2802	LMG	O6-C1-C2	-2.74	104.55	110.35
18	A	1115	CLA	CMC-C2C-C1C	2.73	129.20	125.04
18	A	1135	CLA	CMB-C2B-C3B	2.73	129.79	124.68
22	F	6016	BCR	C33-C5-C6	-2.73	121.46	124.53
18	A	1013	CLA	CMC-C2C-C1C	2.73	129.20	125.04
18	G	1001	CLA	CMB-C2B-C3B	2.73	129.79	124.68
18	A	1140	CLA	C1-C2-C3	-2.73	121.32	126.04
18	A	1123	CLA	C1-C2-C3	-2.73	121.32	126.04
18	3	3003	CLA	C1-C2-C3	-2.73	121.32	126.04
18	A	1104	CLA	C3C-C4C-NC	2.73	113.63	110.57
18	2	2009	CLA	CMC-C2C-C1C	2.73	129.19	125.04
18	4	4006	CLA	CAC-C3C-C4C	2.73	128.35	124.81
18	A	1117	CLA	C4-C3-C5	2.72	119.86	115.27
22	G	2011	BCR	C15-C14-C13	-2.72	123.42	127.31
18	B	1240	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
27	4	4501	LUT	C38-C25-C24	-2.72	117.74	123.56
18	2	2001	CLA	C4-C3-C5	2.72	119.85	115.27
22	B	6009	BCR	C33-C5-C4	2.72	118.84	113.62
21	A	5003	LHG	C5-O7-C7	-2.72	111.10	117.79
22	B	6004	BCR	C34-C9-C10	-2.72	119.12	122.92
18	L	1501	CLA	CMB-C2B-C3B	2.72	129.76	124.68
18	4	4003	CLA	C4-C3-C5	2.72	119.84	115.27
18	A	1125	CLA	OBD-CAD-C3D	-2.71	123.47	127.98
22	B	6006	BCR	C38-C26-C25	-2.71	121.48	124.53
18	2	2007	CLA	CMC-C2C-C1C	2.71	129.17	125.04
22	L	6020	BCR	C39-C30-C25	-2.71	105.90	110.30
18	A	1117	CLA	CMC-C2C-C1C	2.71	129.17	125.04
22	B	6005	BCR	C33-C5-C6	-2.71	121.48	124.53
18	B	1235	CLA	C4-C3-C5	2.71	119.83	115.27
27	3	3502	LUT	C10-C11-C12	-2.71	114.77	123.22
28	2	2010	CHL	C1-O2A-CGA	2.71	125.02	116.11
18	A	1107	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
28	2	2010	CHL	CHB-C4A-NA	2.70	128.25	124.51
18	4	4004	CLA	C1-C2-C3	-2.70	121.37	126.04
18	4	4008	CLA	CAA-C2A-C1A	-2.70	103.11	111.97
18	4	4006	CLA	OBD-CAD-CBD	-2.70	122.03	125.89
18	B	1230	CLA	C3C-C4C-NC	2.70	113.60	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1207	CLA	CMB-C2B-C3B	2.70	129.73	124.68
27	2	2501	LUT	C31-C30-C29	-2.70	123.45	127.31
22	B	6009	BCR	C38-C26-C27	2.70	118.80	113.62
18	A	1116	CLA	C4-C3-C2	-2.70	116.76	123.68
18	B	1229	CLA	CMC-C2C-C1C	2.70	129.15	125.04
28	4	4013	CHL	C2C-C3C-C4C	2.70	108.41	106.49
18	1	1005	CLA	CAC-C3C-C4C	2.69	128.30	124.81
18	2	2001	CLA	CMB-C2B-C3B	2.69	129.72	124.68
18	A	1134	CLA	CMC-C2C-C1C	2.69	129.14	125.04
18	B	1214	CLA	CMC-C2C-C1C	2.69	129.13	125.04
18	4	4017	CLA	CMC-C2C-C1C	2.69	129.13	125.04
18	3	3007	CLA	OBD-CAD-C3D	-2.69	123.52	127.98
22	J	6013	BCR	C1-C6-C7	2.68	123.37	115.78
18	A	1109	CLA	CMC-C2C-C1C	2.68	129.13	125.04
18	2	2008	CLA	CMA-C3A-C4A	-2.68	104.57	111.77
18	1	1012	CLA	CBC-CAC-C3C	-2.68	105.04	112.43
28	1	1009	CHL	C1-C2-C3	-2.68	121.41	126.04
18	B	1216	CLA	C3C-C4C-NC	2.68	113.57	110.57
18	2	2008	CLA	CMB-C2B-C3B	2.68	129.69	124.68
18	B	1210	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
18	G	1003	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
22	L	6019	BCR	C29-C28-C27	2.67	117.35	111.38
18	2	2006	CLA	CMC-C2C-C1C	2.67	129.10	125.04
18	A	1121	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
18	B	1240	CLA	C1-C2-C3	-2.67	121.43	126.04
18	A	1119	CLA	CMC-C2C-C1C	2.67	129.10	125.04
18	B	1236	CLA	C3C-C4C-NC	2.67	113.56	110.57
18	4	4004	CLA	C4-C3-C5	2.67	119.75	115.27
18	A	1123	CLA	C3C-C4C-NC	2.67	113.56	110.57
18	2	2006	CLA	C4-C3-C5	2.66	119.75	115.27
18	B	1212	CLA	C3C-C4C-NC	2.66	113.56	110.57
18	B	1219	CLA	C4-C3-C5	2.66	119.75	115.27
18	4	4002	CLA	C3C-C4C-NC	2.66	113.56	110.57
18	B	1209	CLA	CMC-C2C-C1C	2.66	129.09	125.04
22	A	6008	BCR	C19-C18-C17	2.66	123.03	118.94
18	B	1229	CLA	CMB-C2B-C3B	2.66	129.66	124.68
18	3	3017	CLA	CED-O2D-CGD	2.66	121.95	115.94
18	3	3013	CLA	OBD-CAD-CBD	-2.66	122.09	125.89
18	B	1229	CLA	C4-C3-C5	2.66	119.75	115.27
18	B	1226	CLA	C4-C3-C5	2.66	119.74	115.27
18	B	1232	CLA	CMC-C2C-C1C	2.66	129.09	125.04
18	2	2003	CLA	CMA-C3A-C4A	-2.66	104.64	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1011	CL0	O2D-CGD-O1D	-2.66	118.65	123.84
22	A	6007	BCR	C3-C4-C5	-2.66	109.34	114.08
18	3	3017	CLA	CAC-C3C-C4C	2.66	128.25	124.81
18	L	1502	CLA	C3C-C4C-NC	2.65	113.55	110.57
18	A	1013	CLA	CAA-C2A-C3A	-2.65	105.51	112.78
18	B	1219	CLA	C3C-C4C-NC	2.65	113.55	110.57
18	A	1138	CLA	CMC-C2C-C1C	2.65	129.08	125.04
28	4	4010	CHL	C2A-C3A-C4A	2.65	106.15	101.87
18	L	1503	CLA	CMB-C2B-C3B	2.65	129.64	124.68
18	A	1114	CLA	CMC-C2C-C1C	2.65	129.08	125.04
22	B	6006	BCR	C35-C13-C12	2.65	122.25	118.08
18	A	1138	CLA	C4-C3-C5	2.65	119.73	115.27
18	B	1206	CLA	C1-C2-C3	-2.65	121.46	126.04
18	B	1211	CLA	OBD-CAD-C3D	-2.65	123.58	127.98
18	3	3003	CLA	C4-C3-C5	2.65	119.72	115.27
18	A	1124	CLA	C4-C3-C5	2.65	119.72	115.27
23	4	4801	LMG	O2-C2-C3	-2.65	104.23	110.35
23	4	4801	LMG	O8-C28-O10	-2.65	116.91	123.59
18	1	1003	CLA	CAC-C3C-C4C	2.65	128.24	124.81
18	B	1225	CLA	C3C-C4C-NC	2.65	113.54	110.57
18	1	1003	CLA	C4-C3-C5	2.65	119.72	115.27
28	3	3011	CHL	C2C-C3C-C4C	2.64	108.37	106.49
27	2	2502	LUT	C37-C21-C36	2.64	111.79	107.89
18	B	1227	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
18	A	1140	CLA	CMC-C2C-C1C	2.64	129.06	125.04
18	A	1111	CLA	CAC-C3C-C4C	2.64	128.24	124.81
18	3	3003	CLA	C3C-C4C-NC	2.64	113.53	110.57
22	A	6003	BCR	C37-C22-C21	-2.64	119.23	122.92
22	B	6010	BCR	C33-C5-C4	2.64	118.69	113.62
18	A	1113	CLA	CAC-C3C-C4C	2.64	128.23	124.81
18	A	1101	CLA	CMC-C2C-C1C	2.64	129.06	125.04
27	3	3501	LUT	C38-C25-C24	-2.64	117.92	123.56
18	3	3003	CLA	C1-O2A-CGA	2.64	123.36	116.44
22	B	6004	BCR	C23-C22-C21	2.64	122.99	118.94
18	B	1205	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
18	A	1137	CLA	C3C-C4C-NC	2.63	113.53	110.57
18	B	1211	CLA	C4-C3-C5	2.63	119.70	115.27
18	A	1112	CLA	CMC-C2C-C1C	2.63	129.05	125.04
18	B	1235	CLA	C3C-C4C-NC	2.63	113.52	110.57
23	G	2021	LMG	O8-C28-O10	-2.63	116.96	123.59
23	4	4801	LMG	O7-C10-O9	-2.63	117.35	123.70
26	B	8002	LMU	C1'-O5'-C5'	2.63	118.85	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6008	BCR	C35-C13-C14	-2.63	119.24	122.92
18	B	1204	CLA	CMB-C2B-C3B	2.63	129.59	124.68
18	4	4008	CLA	CMA-C3A-C4A	-2.63	104.72	111.77
18	A	1022	CLA	CMC-C2C-C1C	2.62	129.04	125.04
22	L	6020	BCR	C31-C1-C6	-2.62	106.04	110.30
18	B	1221	CLA	CMB-C2B-C3B	2.62	129.59	124.68
18	3	3007	CLA	CMB-C2B-C3B	2.62	129.59	124.68
18	A	1125	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	G	2011	BCR	C29-C28-C27	2.62	117.23	111.38
27	2	2502	LUT	C15-C35-C34	-2.62	118.11	123.47
18	2	2004	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
27	1	1502	LUT	C38-C25-C24	-2.62	117.96	123.56
18	A	1118	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
18	1	1008	CLA	OBD-CAD-C3D	-2.62	123.64	127.98
18	4	4005	CLA	CMC-C2C-C1C	2.62	129.02	125.04
18	3	3003	CLA	CHC-C1C-C2C	-2.61	119.49	126.72
18	1	1004	CLA	CMC-C2C-C1C	2.61	129.01	125.04
22	A	6017	BCR	C38-C26-C27	2.61	118.63	113.62
27	2	2502	LUT	C37-C21-C26	-2.61	105.59	109.55
18	1	1007	CLA	OBD-CAD-C3D	-2.61	123.65	127.98
18	B	1212	CLA	C4-C3-C5	2.61	119.66	115.27
27	1	1501	LUT	C7-C8-C9	-2.61	122.30	126.23
18	4	4004	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
18	2	2016	CLA	C1-O2A-CGA	2.61	123.28	116.44
22	3	3503	BCR	C1-C6-C7	2.61	123.15	115.78
22	J	6012	BCR	C35-C13-C14	-2.60	119.27	122.92
18	B	1215	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
18	4	4012	CLA	CAA-C2A-C3A	-2.60	105.65	112.78
18	H	1000	CLA	CMC-C2C-C1C	2.60	129.00	125.04
18	B	1236	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
18	A	1115	CLA	CMB-C2B-C3B	2.60	129.55	124.68
18	1	1001	CLA	CMC-C2C-C1C	2.60	129.00	125.04
22	K	2011	BCR	C23-C22-C21	2.60	122.93	118.94
18	A	1151	CLA	CMB-C2B-C3B	2.60	129.54	124.68
18	B	1206	CLA	C3C-C4C-NC	2.60	113.49	110.57
27	I	6018	LUT	C30-C31-C32	-2.60	115.11	123.22
18	B	1021	CLA	C4-C3-C5	2.60	119.64	115.27
18	1	1013	CLA	CMD-C2D-C3D	-2.60	119.82	124.68
18	3	3010	CLA	CMC-C2C-C1C	2.60	128.99	125.04
18	A	1122	CLA	CMC-C2C-C1C	2.60	128.99	125.04
18	B	1207	CLA	C3C-C4C-NC	2.59	113.48	110.57
18	A	1139	CLA	O2D-CGD-O1D	-2.59	118.77	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6017	BCR	C24-C23-C22	-2.59	122.32	126.23
18	4	4003	CLA	CMB-C2B-C3B	2.59	129.53	124.68
18	B	1240	CLA	C4-C3-C5	2.59	119.63	115.27
18	A	1123	CLA	C4-C3-C5	2.59	119.63	115.27
28	4	4011	CHL	C3B-C4B-NB	-2.59	105.86	109.21
18	A	1109	CLA	CMB-C2B-C3B	2.59	129.52	124.68
18	B	1239	CLA	C4-C3-C5	2.59	119.63	115.27
23	F	5002	LMG	O8-C28-O10	-2.59	117.06	123.59
18	A	1111	CLA	C4-C3-C5	2.59	119.62	115.27
18	A	1136	CLA	CMC-C2C-C1C	2.58	128.97	125.04
22	F	6016	BCR	C2-C1-C6	2.58	114.46	110.48
18	B	1234	CLA	C4-C3-C5	2.58	119.61	115.27
18	B	1231	CLA	CMB-C2B-C3B	2.58	129.51	124.68
18	A	1136	CLA	C1-O2A-CGA	2.58	123.22	116.44
27	3	3502	LUT	C1-C6-C7	2.58	123.08	115.78
18	L	1503	CLA	CAC-C3C-C4C	2.58	128.16	124.81
18	A	1113	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
18	A	1104	CLA	CMB-C2B-C3B	2.58	129.50	124.68
18	4	4005	CLA	C4-C3-C5	2.58	119.61	115.27
18	A	1140	CLA	C3C-C4C-NC	2.58	113.46	110.57
18	A	1110	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
18	A	1132	CLA	C4-C3-C5	2.58	119.61	115.27
18	A	1237	CLA	C4-C3-C5	2.58	119.61	115.27
18	B	1228	CLA	C4-C3-C5	2.58	119.61	115.27
18	A	1119	CLA	C4-C3-C5	2.58	119.61	115.27
25	B	7101	DGD	CDB-CCB-CBB	-2.58	101.35	114.42
18	A	1111	CLA	C1-C2-C3	-2.57	121.59	126.04
22	B	6010	BCR	C24-C23-C22	-2.57	122.35	126.23
18	B	1205	CLA	CMC-C2C-C1C	2.57	128.95	125.04
18	A	1124	CLA	CMB-C2B-C3B	2.57	129.49	124.68
27	4	4501	LUT	C39-C29-C30	-2.57	119.32	122.92
18	B	1216	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
18	A	1134	CLA	C4-C3-C5	2.57	119.59	115.27
18	A	1136	CLA	C4-C3-C5	2.57	119.59	115.27
18	B	1211	CLA	CMB-C2B-C3B	2.57	129.48	124.68
18	3	3002	CLA	CMC-C2C-C1C	2.57	128.95	125.04
18	B	1240	CLA	C3C-C4C-NC	2.56	113.45	110.57
17	A	1011	CL0	CAA-C2A-C3A	-2.56	105.76	112.78
18	B	1220	CLA	CMC-C2C-C1C	2.56	128.94	125.04
18	B	1023	CLA	C3C-C4C-NC	2.56	113.44	110.57
18	A	1127	CLA	C3C-C4C-NC	2.56	113.44	110.57
18	B	1226	CLA	CAC-C3C-C4C	2.56	128.13	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	2002	CLA	CBC-CAC-C3C	-2.56	105.37	112.43
22	L	6020	BCR	C29-C28-C27	2.56	117.09	111.38
18	2	2016	CLA	CGD-CBD-CAD	-2.56	102.45	110.73
18	A	1116	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
18	A	1103	CLA	CAA-C2A-C3A	-2.56	105.78	112.78
18	B	1207	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
18	A	1123	CLA	CAC-C3C-C4C	2.56	128.13	124.81
23	F	5002	LMG	O7-C10-O9	-2.56	117.53	123.70
18	A	1105	CLA	C3C-C4C-NC	2.55	113.44	110.57
18	3	3005	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
22	B	6004	BCR	C38-C26-C25	-2.55	121.66	124.53
18	A	1121	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
18	A	1110	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
18	3	3008	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
18	B	1215	CLA	C3C-C4C-NC	2.55	113.43	110.57
18	A	1109	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
28	2	2013	CHL	C2C-C3C-C4C	2.55	108.31	106.49
18	B	1204	CLA	CMC-C2C-C1C	2.55	128.92	125.04
22	B	6006	BCR	C7-C6-C5	-2.55	115.28	121.46
18	A	1114	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
18	A	1136	CLA	C3C-C4C-NC	2.55	113.43	110.57
18	A	1127	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
29	4	4505	ZEX	C18-C5-C4	2.55	119.08	114.36
28	2	2013	CHL	C3B-C4B-NB	-2.55	105.92	109.21
18	B	1023	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
18	B	1225	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
18	B	1234	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
18	2	2004	CLA	C4-C3-C5	2.55	119.55	115.27
18	4	4016	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
18	A	1135	CLA	C3C-C4C-NC	2.54	113.42	110.57
18	2	2012	CLA	CAC-C3C-C4C	2.54	128.11	124.81
22	J	6012	BCR	C8-C9-C10	2.54	122.84	118.94
18	A	1127	CLA	CMC-C2C-C1C	2.54	128.91	125.04
18	B	1207	CLA	C4-C3-C5	2.54	119.55	115.27
18	4	4006	CLA	C3C-C4C-NC	2.54	113.42	110.57
22	L	6019	BCR	C33-C5-C4	2.54	118.50	113.62
18	B	1204	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
18	A	1122	CLA	C4-C3-C2	-2.54	117.17	123.68
18	K	1001	CLA	CMC-C2C-C1C	2.54	128.90	125.04
18	2	2004	CLA	C1-O2A-CGA	2.54	123.10	116.44
18	2	2016	CLA	C5-C3-C4	2.54	120.21	114.60
18	A	1121	CLA	CMB-C2B-C3B	2.54	129.42	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1214	CLA	CMB-C2B-C3B	2.54	129.42	124.68
18	B	1201	CLA	C1-O2A-CGA	2.54	123.10	116.44
18	B	1217	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
18	B	1021	CLA	CMA-C3A-C2A	-2.54	103.60	113.83
18	A	1103	CLA	CMB-C2B-C3B	2.54	129.42	124.68
18	A	1133	CLA	C3C-C4C-NC	2.54	113.41	110.57
18	L	1503	CLA	C3C-C4C-NC	2.53	113.41	110.57
22	G	2011	BCR	C8-C7-C6	-2.53	120.08	127.20
18	B	1236	CLA	CMB-C2B-C3B	2.53	129.42	124.68
18	4	4006	CLA	CMB-C2B-C3B	2.53	129.42	124.68
27	2	2502	LUT	C36-C21-C26	-2.53	105.71	109.55
18	A	1013	CLA	CAA-C2A-C1A	-2.53	103.67	111.97
18	1	1008	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
27	1	1501	LUT	C35-C34-C33	-2.53	123.70	127.31
18	3	3012	CLA	CMC-C2C-C1C	2.53	128.90	125.04
28	4	4011	CHL	C4A-NA-C1A	-2.53	105.57	106.71
18	3	3005	CLA	OBD-CAD-C3D	-2.53	123.78	127.98
18	3	3004	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
18	B	1201	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
18	B	1240	CLA	CMB-C2B-C3B	2.53	129.41	124.68
18	A	1101	CLA	CAC-C3C-C4C	2.53	128.09	124.81
18	A	1137	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
18	1	1006	CLA	CMD-C2D-C3D	-2.52	119.95	124.68
18	A	1120	CLA	C3C-C4C-NC	2.52	113.40	110.57
18	3	3002	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
18	B	1023	CLA	CED-O2D-CGD	2.52	121.64	115.94
22	K	2011	BCR	C33-C5-C4	2.52	118.46	113.62
18	J	1302	CLA	C3C-C4C-NC	2.52	113.40	110.57
18	1	1004	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
29	4	4505	ZEX	C16-C1-C6	-2.52	106.21	110.30
27	2	2502	LUT	C10-C11-C12	-2.52	115.36	123.22
18	3	3012	CLA	C5-C3-C4	2.52	120.17	114.60
18	B	1217	CLA	CMB-C2B-C3B	2.52	129.39	124.68
18	4	4005	CLA	C4-C3-C2	-2.52	117.22	123.68
18	B	1201	CLA	CAC-C3C-C4C	2.52	128.07	124.81
18	A	1119	CLA	C3C-C4C-NC	2.52	113.39	110.57
18	1	1003	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
18	G	1003	CLA	CMB-C2B-C3B	2.52	129.38	124.68
18	L	1501	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
18	A	1116	CLA	CMB-C2B-C3B	2.51	129.38	124.68
18	A	1126	CLA	CAC-C3C-C4C	2.51	128.07	124.81
18	L	1501	CLA	OBD-CAD-C3D	-2.51	123.81	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1110	CLA	CMC-C2C-C1C	2.51	128.87	125.04
18	B	1203	CLA	C3C-C4C-NC	2.51	113.39	110.57
27	I	6018	LUT	C38-C25-C24	-2.51	118.18	123.56
18	B	1238	CLA	C3C-C4C-NC	2.51	113.39	110.57
18	G	1001	CLA	C1-C2-C3	-2.51	121.70	126.04
18	A	1138	CLA	C1-C2-C3	-2.51	121.70	126.04
27	2	2501	LUT	C11-C10-C9	-2.51	123.73	127.31
18	2	2006	CLA	CMB-C2B-C3B	2.51	129.37	124.68
18	A	1129	CLA	CMB-C2B-C3B	2.51	129.37	124.68
22	A	6017	BCR	C33-C5-C4	2.51	118.43	113.62
18	4	4009	CLA	C3C-C4C-NC	2.50	113.38	110.57
18	B	1214	CLA	C4-C3-C5	2.50	119.48	115.27
17	A	1011	CL0	C4-C3-C5	2.50	119.48	115.27
18	B	1223	CLA	CMC-C2C-C1C	2.50	128.85	125.04
18	B	1232	CLA	C3C-C4C-NC	2.50	113.38	110.57
18	G	1001	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
18	A	1106	CLA	C4-C3-C5	2.50	119.48	115.27
18	4	4003	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
18	A	1114	CLA	CAC-C3C-C4C	2.50	128.05	124.81
18	B	1210	CLA	C4-C3-C5	2.50	119.47	115.27
18	A	1114	CLA	C3C-C4C-NC	2.50	113.37	110.57
18	A	1124	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
18	4	4003	CLA	CAC-C3C-C4C	2.50	128.05	124.81
18	B	1210	CLA	CMC-C2C-C1C	2.50	128.84	125.04
18	A	1118	CLA	CMB-C2B-C3B	2.49	129.35	124.68
18	4	4017	CLA	C3C-C4C-NC	2.49	113.37	110.57
18	3	3010	CLA	C1-O2A-CGA	2.49	122.99	116.44
18	2	2009	CLA	CMA-C3A-C4A	-2.49	105.07	111.77
18	B	1206	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
18	A	1136	CLA	CMB-C2B-C3B	2.49	129.34	124.68
22	A	6002	BCR	C34-C9-C10	-2.49	119.43	122.92
18	A	1126	CLA	C4-C3-C5	2.49	119.46	115.27
18	1	1006	CLA	C5-C3-C4	2.49	120.11	114.60
18	B	1202	CLA	C3C-C4C-NC	2.49	113.36	110.57
28	4	4010	CHL	C1-O2A-CGA	2.49	124.32	116.11
18	4	4002	CLA	CMC-C2C-C1C	2.49	128.83	125.04
18	A	1117	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
18	B	1021	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
28	3	3011	CHL	C4A-NA-C1A	-2.49	105.59	106.71
18	A	1108	CLA	CED-O2D-CGD	2.49	121.56	115.94
22	A	6011	BCR	C8-C9-C10	2.49	122.76	118.94
22	G	2011	BCR	C4-C5-C6	-2.49	119.12	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1001	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
18	L	1501	CLA	CAA-C2A-C3A	-2.49	105.97	112.78
18	B	1235	CLA	CMB-C2B-C3B	2.49	129.33	124.68
27	I	6018	LUT	C12-C13-C14	-2.49	115.12	118.94
18	4	4016	CLA	CMC-C2C-C1C	2.49	128.82	125.04
18	1	1002	CLA	C3C-C4C-NC	2.49	113.36	110.57
18	3	3010	CLA	CHC-C1C-C2C	-2.48	119.85	126.72
27	4	4501	LUT	C37-C21-C26	-2.48	105.78	109.55
18	B	1209	CLA	CAC-C3C-C4C	2.48	128.03	124.81
18	B	1227	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
18	4	4012	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
18	3	3003	CLA	OBD-CAD-CBD	-2.48	122.35	125.89
22	B	6010	BCR	C38-C26-C27	2.48	118.38	113.62
18	A	1131	CLA	C3C-C4C-NC	2.48	113.35	110.57
18	4	4009	CLA	C5-C3-C4	2.48	120.08	114.60
18	A	1107	CLA	CMB-C2B-C3B	2.48	129.31	124.68
18	A	1126	CLA	C3C-C4C-NC	2.48	113.35	110.57
18	1	1011	CLA	O1D-CGD-CBD	-2.48	119.42	124.48
18	3	3002	CLA	CAA-CBA-CGA	-2.48	106.02	113.25
22	A	6011	BCR	C37-C22-C21	-2.48	119.46	122.92
18	A	1125	CLA	CMB-C2B-C3B	2.47	129.31	124.68
18	A	1113	CLA	CMB-C2B-C3B	2.47	129.31	124.68
22	I	6020	BCR	C23-C24-C25	-2.47	120.25	127.20
18	1	1012	CLA	CMC-C2C-C1C	2.47	128.81	125.04
18	B	1226	CLA	CMC-C2C-C1C	2.47	128.81	125.04
18	A	1120	CLA	CMB-C2B-C3B	2.47	129.30	124.68
18	B	1220	CLA	C1-C2-C3	-2.47	121.77	126.04
28	4	4013	CHL	CHC-C1C-NC	2.47	127.95	124.20
18	B	1012	CLA	CMB-C2B-C3B	2.47	129.30	124.68
18	L	1502	CLA	C1-O2A-CGA	2.47	122.92	116.44
18	A	1112	CLA	C3C-C4C-NC	2.47	113.34	110.57
27	4	4501	LUT	C19-C9-C8	2.47	121.97	118.08
18	A	1133	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
18	2	2001	CLA	CBC-CAC-C3C	-2.47	105.63	112.43
18	4	4001	CLA	CMB-C2B-C3B	2.47	129.29	124.68
18	B	1202	CLA	CMC-C2C-C1C	2.47	128.80	125.04
18	1	1008	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
18	3	3018	CLA	C5-C3-C4	2.46	120.05	114.60
18	J	1302	CLA	CBA-CAA-C2A	-2.46	106.59	113.86
18	B	1205	CLA	CMB-C2B-C3B	2.46	129.29	124.68
18	4	4007	CLA	CHC-C1C-C2C	-2.46	119.91	126.72
18	3	3019	CLA	C3A-C2A-C1A	-2.46	101.31	104.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1223	CLA	CMB-C2B-C3B	2.46	129.28	124.68
18	A	1111	CLA	C3C-C4C-NC	2.46	113.33	110.57
18	3	3012	CLA	C3C-C4C-NC	2.46	113.33	110.57
27	2	2501	LUT	C35-C34-C33	-2.46	123.80	127.31
22	K	2011	BCR	C1-C6-C7	2.46	122.73	115.78
18	2	2012	CLA	C3C-C4C-NC	2.46	113.33	110.57
18	B	1228	CLA	CED-O2D-CGD	2.46	121.49	115.94
18	A	1112	CLA	CMB-C2B-C3B	2.46	129.27	124.68
18	1	1002	CLA	CMB-C2B-C3B	2.46	129.27	124.68
22	L	6019	BCR	C38-C26-C25	-2.46	121.77	124.53
18	A	1107	CLA	C4-C3-C5	2.46	119.40	115.27
28	2	2011	CHL	C1B-CHB-C4A	-2.45	125.25	130.12
18	3	3006	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
18	A	1140	CLA	CMB-C2B-C3B	2.45	129.27	124.68
27	1	1502	LUT	C40-C33-C34	-2.45	119.49	122.92
18	4	4002	CLA	C1-O2A-CGA	2.45	122.88	116.44
22	3	3503	BCR	C30-C25-C26	-2.45	119.16	122.61
22	G	2011	BCR	C38-C26-C27	2.45	118.32	113.62
18	J	1302	CLA	OBD-CAD-C3D	-2.45	123.91	127.98
18	3	3006	CLA	C5-C3-C4	2.45	120.02	114.60
27	I	6018	LUT	C20-C13-C12	2.45	121.94	118.08
18	1	1003	CLA	CMC-C2C-C1C	2.45	128.77	125.04
22	B	6006	BCR	C24-C23-C22	-2.45	122.54	126.23
18	B	1234	CLA	C3C-C4C-NC	2.45	113.32	110.57
18	3	3018	CLA	CGD-CBD-CAD	-2.45	102.81	110.73
18	4	4016	CLA	CMD-C2D-C3D	-2.45	120.10	124.68
28	1	1009	CHL	C1B-CHB-C4A	-2.45	125.27	130.12
18	B	1230	CLA	CAA-CBA-CGA	-2.45	106.10	113.25
18	F	1302	CLA	CMB-C2B-C3B	2.45	129.25	124.68
18	3	3001	CLA	C1-O2A-CGA	2.44	122.86	116.44
18	H	1000	CLA	C3C-C4C-NC	2.44	113.31	110.57
18	4	4005	CLA	CHC-C1C-C2C	-2.44	119.97	126.72
18	2	2009	CLA	CMB-C2B-C3B	2.44	129.24	124.68
18	1	1013	CLA	CHC-C1C-C2C	-2.44	119.97	126.72
18	B	1021	CLA	C3C-C4C-NC	2.44	113.31	110.57
23	4	4801	LMG	O6-C1-C2	-2.44	105.19	110.35
18	B	1205	CLA	C4-C3-C5	2.44	119.37	115.27
18	A	1139	CLA	CMB-C2B-C3B	2.44	129.24	124.68
22	L	6020	BCR	C27-C26-C25	-2.44	119.19	122.73
18	B	1228	CLA	C3C-C4C-NC	2.44	113.30	110.57
18	A	1022	CLA	C1-C2-C3	-2.44	121.83	126.04
18	B	1023	CLA	CAA-C2A-C3A	-2.44	106.11	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	2019	CLA	C2B-C3B-C4B	2.44	108.37	106.29
18	1	1008	CLA	C3C-C4C-NC	2.44	113.30	110.57
18	2	2012	CLA	C1-C2-C3	-2.43	121.83	126.04
18	B	1236	CLA	C1-O2A-CGA	2.43	122.83	116.44
18	A	1113	CLA	C3C-C4C-NC	2.43	113.30	110.57
18	A	1140	CLA	C1-O2A-CGA	2.43	122.83	116.44
18	A	1129	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
18	4	4008	CLA	OBD-CAD-CBD	-2.43	122.42	125.89
22	3	3503	BCR	C1-C6-C5	-2.43	119.19	122.61
18	G	1001	CLA	CHC-C1C-C2C	-2.43	120.00	126.72
18	B	1238	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
18	A	1105	CLA	CMB-C2B-C3B	2.43	129.22	124.68
22	F	6016	BCR	C8-C7-C6	-2.43	120.39	127.20
18	A	1013	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
18	1	1012	CLA	CMB-C2B-C3B	2.42	129.22	124.68
18	B	1211	CLA	OBD-CAD-CBD	-2.42	122.43	125.89
18	A	1022	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
18	A	1117	CLA	C3C-C4C-NC	2.42	113.29	110.57
18	4	4005	CLA	CAC-C3C-C4C	2.42	127.95	124.81
18	A	1130	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
18	4	4016	CLA	CMB-C2B-C3B	2.42	129.21	124.68
18	A	1130	CLA	C3C-C4C-NC	2.42	113.28	110.57
27	4	4501	LUT	C35-C15-C14	-2.42	118.52	123.47
18	A	1131	CLA	CMB-C2B-C3B	2.42	129.20	124.68
22	B	6004	BCR	C27-C26-C25	-2.42	119.22	122.73
22	3	3503	BCR	C29-C28-C27	2.42	116.78	111.38
18	B	1213	CLA	C3C-C4C-NC	2.42	113.28	110.57
21	2	2801	LHG	O8-C23-C24	2.42	119.49	111.91
29	4	4505	ZEX	C20-C13-C12	2.41	121.88	118.08
18	B	1229	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
18	B	1239	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
18	H	1000	CLA	CAC-C3C-C4C	2.41	127.94	124.81
18	A	1113	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
18	2	2004	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
18	B	1222	CLA	CED-O2D-CGD	2.41	121.39	115.94
18	B	1203	CLA	CMB-C2B-C3B	2.41	129.19	124.68
18	A	1134	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	F	6016	BCR	C38-C26-C27	2.41	118.25	113.62
18	4	4008	CLA	CHC-C1C-C2C	-2.41	120.05	126.72
18	A	1116	CLA	C3C-C4C-NC	2.41	113.27	110.57
18	A	1138	CLA	C1-O2A-CGA	2.41	122.77	116.44
18	B	1218	CLA	OBD-CAD-C3D	-2.41	123.98	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	6019	BCR	C40-C30-C25	2.41	114.20	110.30
18	L	1502	CLA	OBD-CAD-C3D	-2.41	123.98	127.98
18	G	1003	CLA	C4-C3-C5	2.41	119.32	115.27
18	B	1232	CLA	CMB-C2B-C3B	2.41	129.18	124.68
18	4	4012	CLA	OBD-CAD-C3D	-2.41	123.99	127.98
18	B	1222	CLA	O2D-CGD-O1D	-2.41	119.14	123.84
23	J	5001	LMG	O4-C4-C5	-2.41	103.33	109.30
18	4	4002	CLA	CHC-C1C-C2C	-2.40	120.07	126.72
18	3	3004	CLA	CMC-C2C-C1C	2.40	128.70	125.04
18	1	1006	CLA	CMB-C2B-C3B	2.40	129.18	124.68
22	A	6008	BCR	C28-C27-C26	-2.40	109.78	114.08
18	A	1139	CLA	C3C-C4C-NC	2.40	113.27	110.57
18	2	2001	CLA	CHC-C1C-C2C	-2.40	120.07	126.72
18	B	1023	CLA	CMC-C2C-C1C	2.40	128.70	125.04
27	3	3501	LUT	C2-C3-C4	-2.40	107.02	110.30
18	B	1223	CLA	C4-C3-C5	2.40	119.31	115.27
18	4	4008	CLA	CMB-C2B-C3B	2.40	129.17	124.68
18	A	1138	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
18	B	1221	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
18	B	1221	CLA	C3C-C4C-NC	2.40	113.26	110.57
18	B	1210	CLA	C3C-C4C-NC	2.40	113.26	110.57
18	3	3002	CLA	CHC-C1C-C2C	-2.40	120.09	126.72
18	B	1211	CLA	CMC-C2C-C1C	2.40	128.69	125.04
18	B	1225	CLA	CMB-C2B-C3B	2.40	129.16	124.68
23	G	2021	LMG	O4-C4-C3	-2.39	104.81	110.35
18	4	4002	CLA	CMB-C2B-C3B	2.39	129.16	124.68
18	B	1208	CLA	C3C-C4C-NC	2.39	113.25	110.57
18	2	2005	CLA	C1-C2-C3	-2.39	121.90	126.04
22	B	6005	BCR	C30-C25-C26	-2.39	119.24	122.61
22	A	6008	BCR	C33-C5-C4	2.39	118.21	113.62
18	1	1003	CLA	C1-O2A-CGA	2.39	122.71	116.44
18	J	1302	CLA	CMB-C2B-C3B	2.39	129.15	124.68
18	A	1134	CLA	C3C-C4C-NC	2.39	113.25	110.57
18	1	1007	CLA	C3C-C4C-NC	2.39	113.25	110.57
18	4	4006	CLA	C5-C3-C4	2.39	119.88	114.60
18	A	1103	CLA	CAC-C3C-C4C	2.39	127.91	124.81
18	A	1106	CLA	C3C-C4C-NC	2.39	113.25	110.57
18	A	1103	CLA	C3C-C4C-NC	2.39	113.25	110.57
21	A	7001	LHG	C5-O7-C7	-2.39	111.92	117.79
28	4	4010	CHL	C2A-C1A-CHA	2.39	128.03	123.86
18	3	3002	CLA	OBD-CAD-CBD	-2.39	122.49	125.89
18	F	1301	CLA	C3C-C4C-NC	2.39	113.25	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1139	CLA	C4-C3-C5	2.38	119.28	115.27
21	A	7001	LHG	O8-C23-O10	-2.38	117.57	123.59
18	A	1137	CLA	CMB-C2B-C3B	2.38	129.14	124.68
18	B	1230	CLA	CMB-C2B-C3B	2.38	129.14	124.68
18	G	1003	CLA	C1-O2A-CGA	2.38	122.70	116.44
23	2	2802	LMG	O1-C7-C8	-2.38	105.15	110.90
18	A	1136	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
18	A	1124	CLA	C3C-C4C-NC	2.38	113.24	110.57
18	2	2019	CLA	C2A-C3A-C4A	-2.38	100.86	103.59
22	L	6019	BCR	C23-C22-C21	2.38	122.59	118.94
18	B	1220	CLA	CED-O2D-CGD	2.38	121.32	115.94
18	A	1237	CLA	CAC-C3C-C4C	2.38	127.90	124.81
18	A	1237	CLA	C3C-C4C-NC	2.38	113.24	110.57
27	4	4502	LUT	C28-C29-C30	2.38	122.59	118.94
18	1	1014	CLA	CAA-CBA-CGA	-2.38	106.31	113.25
18	B	1218	CLA	CMB-C2B-C3B	2.38	129.12	124.68
18	B	1209	CLA	C3C-C4C-NC	2.38	113.23	110.57
18	B	1021	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
18	4	4001	CLA	CMD-C2D-C3D	-2.37	120.24	124.68
18	A	1126	CLA	CAA-CBA-CGA	-2.37	106.32	113.25
18	4	4017	CLA	CMB-C2B-C3B	2.37	129.12	124.68
18	1	1007	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
18	4	4012	CLA	CMA-C3A-C4A	-2.37	105.40	111.77
18	A	1110	CLA	C3C-C4C-NC	2.37	113.23	110.57
18	A	1118	CLA	C3C-C4C-NC	2.37	113.23	110.57
18	B	1220	CLA	CAC-C3C-C4C	2.37	127.89	124.81
18	B	1224	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
18	A	1132	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
18	2	2005	CLA	CMB-C2B-C3B	2.37	129.11	124.68
27	4	4503	LUT	C36-C21-C26	-2.37	105.96	109.55
22	B	6010	BCR	C28-C27-C26	-2.37	109.85	114.08
18	B	1212	CLA	CMB-C2B-C3B	2.37	129.11	124.68
22	B	6006	BCR	C19-C18-C17	2.37	122.57	118.94
22	F	6014	BCR	C29-C28-C27	2.37	116.66	111.38
18	3	3007	CLA	C1-O2A-CGA	2.36	122.65	116.44
18	A	1117	CLA	CAC-C3C-C4C	2.36	127.88	124.81
18	A	1104	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
18	A	1237	CLA	C4-C3-C2	-2.36	117.62	123.68
22	B	6005	BCR	C34-C9-C10	-2.36	119.61	122.92
18	A	1108	CLA	C3C-C4C-NC	2.36	113.22	110.57
18	A	1121	CLA	C3C-C4C-NC	2.36	113.22	110.57
18	F	1302	CLA	C5-C3-C4	2.36	119.82	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4001	CLA	CHC-C1C-C2C	-2.36	120.19	126.72
22	B	6006	BCR	C28-C27-C26	-2.36	109.86	114.08
22	J	6012	BCR	C39-C30-C25	-2.36	106.47	110.30
18	3	3008	CLA	C1-O2A-CGA	2.36	122.63	116.44
18	B	1239	CLA	C3C-C4C-NC	2.36	113.22	110.57
18	A	1128	CLA	C3C-C4C-NC	2.36	113.22	110.57
18	B	1203	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
18	4	4005	CLA	CHA-C1A-NA	-2.36	121.00	126.40
18	3	3008	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
18	A	1119	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
18	A	1128	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
28	4	4011	CHL	C1-C2-C3	-2.35	122.94	126.75
18	A	1013	CLA	C3C-C4C-NC	2.35	113.21	110.57
22	B	6005	BCR	C24-C23-C22	-2.35	122.68	126.23
18	B	1228	CLA	CMC-C2C-C1C	2.35	128.62	125.04
18	2	2002	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
18	A	1133	CLA	CAC-C3C-C4C	2.35	127.86	124.81
18	1	1003	CLA	CMB-C2B-C3B	2.35	129.07	124.68
18	B	1211	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
18	A	1122	CLA	C3C-C4C-NC	2.35	113.20	110.57
22	B	6005	BCR	C23-C22-C21	2.35	122.54	118.94
18	A	1151	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
18	A	1131	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
18	B	1220	CLA	CMB-C2B-C3B	2.35	129.07	124.68
18	B	1221	CLA	C1-C2-C3	-2.35	121.99	126.04
18	L	1501	CLA	C5-C3-C4	2.35	119.78	114.60
18	B	1234	CLA	CMC-C2C-C1C	2.35	128.61	125.04
22	J	6013	BCR	C31-C1-C6	-2.35	106.50	110.30
18	B	1239	CLA	CMB-C2B-C3B	2.34	129.06	124.68
27	I	6018	LUT	C40-C33-C32	2.34	121.77	118.08
18	4	4017	CLA	CAC-C3C-C4C	2.34	127.85	124.81
18	1	1011	CLA	CMA-C3A-C4A	-2.34	105.47	111.77
18	L	1503	CLA	OBD-CAD-C3D	-2.34	124.09	127.98
18	4	4017	CLA	C4-C3-C5	2.34	119.21	115.27
18	A	1151	CLA	C5-C3-C4	2.34	119.77	114.60
18	B	1224	CLA	CAC-C3C-C4C	2.34	127.85	124.81
18	B	1201	CLA	C3C-C4C-NC	2.34	113.19	110.57
18	3	3017	CLA	CHA-C1A-NA	-2.34	121.04	126.40
18	B	1221	CLA	CAC-C3C-C4C	2.34	127.84	124.81
18	B	1212	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
18	A	1125	CLA	C1-O2A-CGA	2.34	122.58	116.44
18	B	1220	CLA	C3C-C4C-NC	2.34	113.19	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	2001	CLA	OBD-CAD-CBD	-2.34	122.56	125.89
22	A	6008	BCR	C30-C25-C26	-2.34	119.32	122.61
18	B	1224	CLA	CMC-C2C-C1C	2.34	128.60	125.04
18	1	1004	CLA	CMB-C2B-C3B	2.33	129.05	124.68
18	B	1217	CLA	C3C-C4C-NC	2.33	113.19	110.57
18	1	1008	CLA	CMB-C2B-C3B	2.33	129.04	124.68
18	3	3013	CLA	CMB-C2B-C3B	2.33	129.04	124.68
18	B	1208	CLA	CMB-C2B-C3B	2.33	129.04	124.68
22	B	6010	BCR	C34-C9-C10	-2.33	119.66	122.92
18	2	2009	CLA	C5-C3-C4	2.33	119.75	114.60
22	A	6002	BCR	C30-C25-C26	-2.33	119.33	122.61
18	A	1138	CLA	CAC-C3C-C4C	2.33	127.83	124.81
18	A	1111	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
27	4	4502	LUT	C39-C29-C30	-2.33	119.66	122.92
18	2	2004	CLA	OBD-CAD-CBD	-2.33	122.57	125.89
22	3	3503	BCR	C35-C13-C14	-2.33	119.66	122.92
18	B	1202	CLA	CAC-C3C-C4C	2.33	127.83	124.81
18	A	1120	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
18	B	1012	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
18	B	1234	CLA	OBD-CAD-C3D	-2.33	124.12	127.98
18	A	1237	CLA	CMB-C2B-C3B	2.33	129.03	124.68
28	2	2010	CHL	CMD-C2D-C3D	2.33	129.03	124.68
18	4	4005	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
18	A	1134	CLA	CMB-C2B-C3B	2.32	129.03	124.68
18	B	1219	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
18	K	1001	CLA	CMD-C2D-C3D	-2.32	120.33	124.68
18	2	2008	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
18	B	1202	CLA	C4-C3-C5	2.32	119.17	115.27
22	K	2011	BCR	C35-C13-C12	2.32	121.73	118.08
18	3	3006	CLA	CMD-C2D-C3D	-2.32	120.34	124.68
18	F	1301	CLA	OBD-CAD-C3D	-2.32	124.13	127.98
18	B	1221	CLA	C4-C3-C5	2.32	119.17	115.27
18	A	1107	CLA	C3C-C4C-NC	2.32	113.17	110.57
22	B	6006	BCR	C33-C5-C4	2.32	118.06	113.62
18	2	2007	CLA	CMB-C2B-C3B	2.31	129.01	124.68
27	3	3501	LUT	C31-C30-C29	-2.31	124.01	127.31
22	A	6011	BCR	C8-C7-C6	-2.31	120.71	127.20
23	4	4801	LMG	O4-C4-C5	-2.31	103.56	109.30
18	J	1302	CLA	CAC-C3C-C4C	2.31	127.81	124.81
18	B	1210	CLA	CMB-C2B-C3B	2.31	129.00	124.68
18	4	4012	CLA	C1-O2A-CGA	2.31	122.50	116.44
18	A	1108	CLA	O2D-CGD-O1D	-2.31	119.33	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4005	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
18	1	1006	CLA	C1-O2A-CGA	2.31	122.50	116.44
18	1	1014	CLA	CMB-C2B-C3B	2.31	128.99	124.68
18	A	1115	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
18	A	1135	CLA	CAC-C3C-C4C	2.30	127.80	124.81
18	A	1130	CLA	C5-C3-C4	2.30	119.69	114.60
18	B	1204	CLA	C3C-C4C-NC	2.30	113.15	110.57
18	4	4001	CLA	CMC-C2C-C1C	2.30	128.54	125.04
18	3	3013	CLA	C3C-C4C-NC	2.30	113.15	110.57
27	2	2501	LUT	C8-C7-C6	-2.30	120.74	127.20
18	A	1122	CLA	CAC-C3C-C4C	2.30	127.80	124.81
18	A	1129	CLA	C5-C3-C4	2.30	119.68	114.60
22	B	6010	BCR	C23-C24-C25	-2.30	120.75	127.20
18	L	1501	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
18	A	1118	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
18	2	2008	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
23	G	2021	LMG	C7-O1-C1	-2.30	109.25	113.74
18	B	1206	CLA	CAC-C3C-C4C	2.30	127.79	124.81
18	B	1201	CLA	C5-C3-C4	2.30	119.68	114.60
18	A	1128	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
27	3	3502	LUT	C31-C30-C29	-2.30	124.03	127.31
18	4	4004	CLA	O1D-CGD-CBD	-2.30	119.79	124.48
18	1	1002	CLA	CHD-C4C-C3C	-2.29	121.47	124.84
18	3	3007	CLA	OBD-CAD-CBD	-2.29	122.62	125.89
27	4	4502	LUT	C38-C25-C24	-2.29	118.66	123.56
18	2	2001	CLA	CMC-C2C-C1C	2.29	128.53	125.04
22	A	6011	BCR	C24-C23-C22	-2.29	122.77	126.23
18	3	3010	CLA	OBD-CAD-C3D	-2.29	124.18	127.98
18	G	1002	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
28	1	1009	CHL	CMD-C2D-C3D	2.29	128.96	124.68
18	4	4004	CLA	CMB-C2B-C3B	2.29	128.96	124.68
18	A	1129	CLA	CAC-C3C-C4C	2.29	127.78	124.81
22	A	6003	BCR	C33-C5-C4	2.29	118.01	113.62
18	B	1227	CLA	C3C-C4C-NC	2.29	113.14	110.57
18	B	1228	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
18	2	2001	CLA	CAA-CBA-CGA	2.29	119.94	113.25
18	2	2007	CLA	CAC-C3C-C4C	2.29	127.78	124.81
18	2	2008	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
18	2	2001	CLA	CAC-C3C-C4C	2.29	127.78	124.81
18	2	2008	CLA	CGD-CBD-CAD	-2.28	103.33	110.73
18	1	1011	CLA	CMB-C2B-C3B	2.28	128.95	124.68
18	4	4004	CLA	CMC-C2C-C1C	2.28	128.52	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1134	CLA	CAC-C3C-C4C	2.28	127.77	124.81
20	A	5001	PQN	C2M-C2-C3	-2.28	120.68	124.40
27	4	4503	LUT	C15-C35-C34	-2.28	118.80	123.47
22	B	6004	BCR	C30-C25-C24	2.28	122.23	115.78
18	A	1115	CLA	CAC-C3C-C4C	2.28	127.77	124.81
18	1	1007	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
18	B	1240	CLA	CAA-CBA-CGA	-2.28	106.60	113.25
18	B	1240	CLA	C4-C3-C2	-2.28	117.84	123.68
18	2	2007	CLA	C3C-C4C-NC	2.28	113.12	110.57
18	3	3003	CLA	CAC-C3C-C4C	2.28	127.76	124.81
18	A	1136	CLA	CAC-C3C-C4C	2.27	127.76	124.81
18	4	4009	CLA	CMB-C2B-C3B	2.27	128.93	124.68
18	B	1220	CLA	CAA-CBA-CGA	-2.27	106.61	113.25
18	B	1213	CLA	CAC-C3C-C4C	2.27	127.76	124.81
27	4	4502	LUT	C40-C33-C34	-2.27	119.74	122.92
18	A	1118	CLA	O1D-CGD-CBD	-2.27	119.83	124.48
18	4	4007	CLA	CMD-C2D-C3D	-2.27	120.43	124.68
22	B	6004	BCR	C1-C6-C7	2.27	122.20	115.78
18	J	1302	CLA	C5-C3-C4	2.27	119.62	114.60
18	3	3008	CLA	CHD-C4C-C3C	-2.27	121.50	124.84
18	B	1216	CLA	CAC-C3C-C4C	2.27	127.76	124.81
18	1	1003	CLA	CHC-C1C-C2C	-2.27	120.44	126.72
18	A	1109	CLA	C3C-C4C-NC	2.27	113.12	110.57
18	L	1503	CLA	C5-C3-C4	2.27	119.62	114.60
18	2	2016	CLA	CAA-CBA-CGA	-2.27	106.62	113.25
18	A	1106	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
18	A	1137	CLA	CAC-C3C-C4C	2.27	127.75	124.81
18	B	1210	CLA	OBD-CAD-C3D	-2.27	124.22	127.98
18	1	1002	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
18	A	1127	CLA	CAC-C3C-C4C	2.27	127.75	124.81
22	A	6007	BCR	C33-C5-C4	2.26	117.97	113.62
18	H	1000	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
18	2	2019	CLA	C2C-C1C-CHC	-2.26	120.25	125.67
18	4	4005	CLA	C6-C5-C3	-2.26	107.52	113.45
18	1	1014	CLA	C1-O2A-CGA	2.26	123.57	116.11
18	2	2012	CLA	CMC-C2C-C1C	2.26	128.49	125.04
18	B	1221	CLA	C6-C5-C3	-2.26	107.52	113.45
18	2	2006	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
21	1	1801	LHG	O7-C7-O9	-2.26	118.23	123.70
18	B	1211	CLA	CAC-C3C-C4C	2.26	127.75	124.81
18	4	4012	CLA	CMB-C2B-C3B	2.26	128.91	124.68
28	4	4011	CHL	C3A-C2A-C1A	2.26	104.72	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	2002	CLA	CMB-C2B-C3B	2.26	128.90	124.68
23	4	4801	LMG	O8-C28-C29	2.26	119.00	111.91
18	A	1124	CLA	CAC-C3C-C4C	2.26	127.74	124.81
28	2	2011	CHL	CHC-C1C-NC	2.26	127.63	124.20
22	J	6012	BCR	C23-C22-C21	2.26	122.40	118.94
18	A	1140	CLA	CAC-C3C-C4C	2.26	127.74	124.81
27	4	4502	LUT	C10-C11-C12	-2.25	116.18	123.22
18	4	4007	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
27	1	1501	LUT	C20-C13-C14	-2.25	119.77	122.92
18	B	1224	CLA	C3C-C4C-NC	2.25	113.10	110.57
18	A	1105	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
18	B	1222	CLA	CAA-C2A-C1A	-2.25	104.60	111.97
22	F	6014	BCR	C30-C25-C26	-2.25	119.44	122.61
22	G	2011	BCR	C30-C25-C24	2.25	122.14	115.78
18	G	1003	CLA	CAA-C2A-C1A	-2.25	104.61	111.97
21	A	5003	LHG	O8-C23-O10	-2.25	117.92	123.59
22	F	6016	BCR	C23-C22-C21	2.25	122.39	118.94
18	A	1107	CLA	C1-C2-C3	-2.25	122.16	126.04
18	3	3018	CLA	CMB-C2B-C3B	2.25	128.88	124.68
18	A	1108	CLA	CAC-C3C-C4C	2.25	127.72	124.81
18	1	1007	CLA	CAC-C3C-C4C	2.25	127.72	124.81
18	B	1226	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
18	1	1004	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
22	B	6006	BCR	C1-C6-C7	2.24	122.12	115.78
18	B	1214	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
27	I	6018	LUT	C1-C6-C7	2.24	122.12	115.78
23	2	2802	LMG	O8-C28-C29	2.24	118.94	111.91
28	1	1009	CHL	C1-O2A-CGA	2.24	122.32	116.44
22	F	6016	BCR	C31-C1-C6	-2.24	106.67	110.30
28	2	2011	CHL	C4A-NA-C1A	-2.24	105.70	106.71
18	A	1103	CLA	CAA-C2A-C1A	-2.23	104.65	111.97
18	B	1205	CLA	C3C-C4C-NC	2.23	113.08	110.57
18	2	2003	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
18	3	3018	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
18	1	1004	CLA	C4-C3-C5	2.23	119.03	115.27
18	A	1115	CLA	C3C-C4C-NC	2.23	113.08	110.57
18	B	1231	CLA	CAC-C3C-C4C	2.23	127.71	124.81
18	2	2003	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
18	A	1112	CLA	OBD-CAD-C3D	-2.23	124.28	127.98
18	A	1132	CLA	C3C-C4C-NC	2.23	113.07	110.57
18	B	1235	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
18	A	1105	CLA	CAC-C3C-C4C	2.23	127.70	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1229	CLA	C6-C7-C8	-2.23	108.72	115.92
22	K	2011	BCR	C15-C14-C13	-2.23	124.13	127.31
18	B	1204	CLA	CAC-C3C-C4C	2.23	127.70	124.81
28	2	2013	CHL	CMD-C2D-C3D	2.23	128.84	124.68
18	B	1205	CLA	CAC-C3C-C4C	2.22	127.69	124.81
18	L	1503	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
18	2	2019	CLA	C3A-C2A-C1A	-2.22	101.64	104.74
22	B	6004	BCR	C35-C13-C14	-2.22	119.81	122.92
22	L	6020	BCR	C12-C13-C14	2.22	122.35	118.94
28	1	1010	CHL	CMD-C2D-C3D	2.22	128.84	124.68
27	3	3502	LUT	C30-C31-C32	-2.22	116.28	123.22
18	B	1231	CLA	C3C-C4C-NC	2.22	113.06	110.57
18	2	2002	CLA	CBA-CAA-C2A	-2.22	107.31	113.86
18	B	1206	CLA	C1-O2A-CGA	2.22	122.27	116.44
22	G	2011	BCR	C1-C6-C7	2.22	122.06	115.78
18	1	1005	CLA	C4C-C3C-C2C	-2.22	103.67	106.90
18	4	4002	CLA	CHA-C1A-NA	-2.22	121.32	126.40
18	4	4016	CLA	CED-O2D-CGD	2.22	120.95	115.94
18	B	1218	CLA	C3C-C4C-NC	2.22	113.06	110.57
18	B	1227	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
18	A	1022	CLA	CAC-C3C-C4C	2.21	127.68	124.81
18	B	1214	CLA	C3C-C4C-NC	2.21	113.05	110.57
28	3	3011	CHL	CMD-C2D-C3D	2.21	128.82	124.68
18	4	4004	CLA	C3C-C4C-NC	2.21	113.05	110.57
18	A	1126	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
18	3	3019	CLA	CAD-CBD-CHA	-2.21	102.66	105.67
18	F	1302	CLA	C3C-C4C-NC	2.21	113.05	110.57
18	B	1220	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
18	1	1005	CLA	CAA-CBA-CGA	-2.21	106.80	113.25
18	A	1102	CLA	C5-C3-C4	2.21	119.48	114.60
22	A	6017	BCR	C2-C1-C6	2.21	113.88	110.48
18	B	1227	CLA	CAC-C3C-C4C	2.21	127.67	124.81
22	G	2011	BCR	C27-C26-C25	-2.21	119.53	122.73
22	A	6008	BCR	C31-C1-C6	-2.21	106.72	110.30
18	2	2008	CLA	CAA-C2A-C1A	-2.21	104.75	111.97
18	2	2016	CLA	CHD-C4C-C3C	-2.20	121.60	124.84
18	4	4004	CLA	CMA-C3A-C4A	-2.20	105.85	111.77
25	B	7101	DGD	CFB-CEB-CDB	-2.20	103.24	114.42
18	A	1108	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
21	2	2801	LHG	C5-O7-C7	-2.20	112.37	117.79
22	K	2011	BCR	C29-C28-C27	2.20	116.30	111.38
18	4	4006	CLA	OBD-CAD-C3D	-2.20	124.33	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	1501	LUT	C15-C35-C34	-2.20	118.97	123.47
18	3	3019	CLA	C2B-C3B-C4B	2.20	108.17	106.29
27	1	1502	LUT	C17-C1-C6	-2.20	106.73	110.30
18	A	1107	CLA	CAC-C3C-C4C	2.20	127.66	124.81
18	B	1232	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
18	4	4016	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
18	3	3006	CLA	CAC-C3C-C4C	2.19	127.66	124.81
18	L	1502	CLA	CMB-C2B-C3B	2.19	128.78	124.68
18	2	2002	CLA	C1-O2A-CGA	2.19	123.33	116.11
18	A	1111	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
26	B	8001	LMU	C1B-C2B-C3B	2.19	114.56	110.00
18	A	1111	CLA	C1-O2A-CGA	2.19	122.20	116.44
18	B	1218	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
22	A	6003	BCR	C3-C4-C5	-2.19	110.17	114.08
18	3	3001	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
28	1	1010	CHL	CMB-C2B-C1B	-2.19	125.10	128.46
18	1	1003	CLA	CAA-CBA-CGA	-2.19	106.86	113.25
18	4	4001	CLA	CED-O2D-CGD	2.19	120.89	115.94
18	3	3001	CLA	CMB-C2B-C3B	2.19	128.77	124.68
18	B	1229	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
18	1	1003	CLA	C6-C5-C3	-2.19	107.72	113.45
28	4	4013	CHL	CMD-C2D-C3D	2.18	128.76	124.68
28	4	4010	CHL	CMD-C2D-C3D	2.18	128.76	124.68
18	B	1208	CLA	C4-C3-C5	2.18	118.94	115.27
18	F	1301	CLA	CAC-C3C-C4C	2.18	127.64	124.81
28	4	4011	CHL	CMD-C2D-C3D	2.18	128.76	124.68
18	3	3004	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
22	A	6008	BCR	C30-C25-C24	2.18	121.95	115.78
27	3	3502	LUT	C15-C14-C13	-2.18	124.20	127.31
28	3	3011	CHL	CHD-C4C-C3C	2.18	128.04	124.84
27	3	3502	LUT	C38-C25-C24	-2.18	118.90	123.56
18	4	4016	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
18	3	3002	CLA	CMB-C2B-C3B	2.18	128.75	124.68
18	A	1122	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
26	B	8001	LMU	O1B-C4'-C3'	2.18	113.07	107.28
18	3	3002	CLA	CBA-CAA-C2A	-2.18	107.44	113.86
18	1	1014	CLA	CMC-C2C-C1C	2.17	128.35	125.04
18	2	2006	CLA	C3C-C4C-NC	2.17	113.01	110.57
18	A	1119	CLA	CAC-C3C-C4C	2.17	127.63	124.81
22	F	6016	BCR	C35-C13-C12	2.17	121.50	118.08
18	2	2012	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
18	A	1105	CLA	CED-O2D-CGD	2.17	120.85	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	1502	CLA	C4-C3-C5	2.17	118.92	115.27
22	A	6011	BCR	C27-C26-C25	-2.17	119.58	122.73
22	3	3503	BCR	C39-C30-C25	-2.17	106.78	110.30
18	3	3005	CLA	CMB-C2B-C3B	2.17	128.74	124.68
18	A	1133	CLA	CMB-C2B-C3B	2.17	128.74	124.68
22	I	6020	BCR	C15-C14-C13	-2.17	124.22	127.31
18	1	1001	CLA	CMB-C2B-C3B	2.17	128.73	124.68
18	A	1237	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
23	2	2802	LMG	C3-C4-C5	2.17	114.10	110.24
18	4	4007	CLA	C3C-C4C-NC	2.17	113.00	110.57
28	2	2011	CHL	CMB-C2B-C1B	-2.17	125.14	128.46
18	3	3003	CLA	O2D-CGD-O1D	-2.17	119.61	123.84
18	A	1105	CLA	CAA-CBA-CGA	-2.16	106.93	113.25
18	A	1112	CLA	CAC-C3C-C4C	2.16	127.61	124.81
18	H	1000	CLA	CED-O2D-CGD	2.16	120.82	115.94
18	3	3017	CLA	C3C-C4C-NC	2.16	112.99	110.57
22	L	6019	BCR	C2-C1-C6	2.16	113.80	110.48
27	2	2502	LUT	C39-C29-C30	-2.16	119.90	122.92
18	G	1003	CLA	CMD-C2D-C3D	-2.16	120.65	124.68
22	B	6006	BCR	C38-C26-C27	2.15	117.75	113.62
18	4	4002	CLA	CED-O2D-CGD	2.15	120.81	115.94
25	B	7101	DGD	O3E-C3E-C2E	-2.15	105.37	110.35
27	1	1501	LUT	C11-C10-C9	-2.15	124.24	127.31
18	A	1101	CLA	C3C-C4C-NC	2.15	112.99	110.57
22	A	6003	BCR	C34-C9-C10	-2.15	119.91	122.92
18	A	1123	CLA	OBD-CAD-C3D	-2.15	124.41	127.98
18	4	4016	CLA	OBD-CAD-C3D	-2.15	124.41	127.98
18	B	1206	CLA	OBD-CAD-C3D	-2.15	124.41	127.98
27	4	4503	LUT	C35-C15-C14	-2.15	119.07	123.47
18	3	3018	CLA	CMD-C2D-C3D	-2.15	120.66	124.68
18	3	3004	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
22	B	6009	BCR	C19-C18-C17	2.15	122.24	118.94
18	B	1211	CLA	C3C-C4C-NC	2.15	112.98	110.57
27	4	4502	LUT	C7-C8-C9	-2.15	122.99	126.23
18	1	1012	CLA	C5-C3-C4	2.15	119.34	114.60
23	F	5001	LMG	C7-O1-C1	-2.15	109.55	113.74
18	B	1214	CLA	CAC-C3C-C4C	2.14	127.59	124.81
22	A	6011	BCR	C38-C26-C27	2.14	117.74	113.62
18	B	1208	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
27	3	3502	LUT	C39-C29-C30	-2.14	119.92	122.92
18	3	3013	CLA	CMA-C3A-C4A	-2.14	106.01	111.77
18	3	3005	CLA	CAC-C3C-C4C	2.14	127.59	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	6013	BCR	C38-C26-C27	2.14	117.73	113.62
18	1	1011	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
18	A	1128	CLA	CAC-C3C-C4C	2.14	127.59	124.81
18	1	1004	CLA	C3C-C4C-NC	2.14	112.97	110.57
18	2	2001	CLA	CGD-CBD-CAD	2.14	117.67	110.73
18	A	1128	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
18	A	1129	CLA	CMA-C3A-C4A	-2.14	106.03	111.77
18	B	1205	CLA	OBD-CAD-C3D	-2.14	124.43	127.98
18	G	1001	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
27	2	2502	LUT	C38-C25-C24	-2.14	118.98	123.56
28	2	2010	CHL	C1D-CHD-C4C	2.14	125.38	122.56
27	1	1502	LUT	C37-C21-C26	-2.14	106.31	109.55
22	B	6010	BCR	C39-C30-C25	-2.14	106.83	110.30
27	3	3501	LUT	C39-C29-C28	2.14	121.44	118.08
18	3	3008	CLA	CMC-C2C-C1C	2.13	128.29	125.04
18	A	1123	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
18	L	1503	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
18	2	2005	CLA	C1-O2A-CGA	2.13	122.04	116.44
18	B	1023	CLA	C4C-C3C-C2C	-2.13	103.79	106.90
18	A	1139	CLA	CAC-C3C-C4C	2.13	127.57	124.81
18	B	1214	CLA	C6-C5-C3	-2.13	107.87	113.45
28	1	1009	CHL	CHD-C4C-C3C	2.13	127.97	124.84
25	B	7101	DGD	C3G-C2G-C1G	-2.13	106.75	111.79
22	G	2011	BCR	C39-C30-C25	-2.13	106.85	110.30
28	1	1009	CHL	CMB-C2B-C1B	-2.13	125.20	128.46
18	L	1501	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
18	2	2002	CLA	C3C-C4C-NC	2.12	112.95	110.57
18	G	1003	CLA	CAC-C3C-C4C	2.12	127.56	124.81
25	B	7101	DGD	CBB-CAB-C9B	-2.12	103.65	114.42
22	G	2011	BCR	C38-C26-C25	-2.12	122.15	124.53
27	I	6018	LUT	C7-C6-C5	-2.12	116.32	121.46
28	4	4013	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
18	B	1212	CLA	CAC-C3C-C4C	2.12	127.56	124.81
22	B	6009	BCR	C23-C22-C21	2.12	122.19	118.94
18	1	1014	CLA	CHC-C1C-C2C	-2.12	120.86	126.72
18	2	2008	CLA	C5-C3-C4	2.12	119.28	114.60
18	A	1110	CLA	CAC-C3C-C4C	2.12	127.56	124.81
29	4	4505	ZEX	C21-C26-C27	2.12	121.76	115.78
18	3	3013	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
28	4	4011	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
18	A	1013	CLA	C6-C5-C3	-2.11	107.91	113.45
18	B	1239	CLA	C1-O2A-CGA	2.11	121.99	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	1002	CLA	CHC-C1C-C2C	-2.11	120.88	126.72
18	2	2007	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
22	L	6020	BCR	C2-C1-C6	2.11	113.73	110.48
27	1	1502	LUT	C1-C6-C5	-2.11	119.64	122.61
18	1	1003	CLA	OBD-CAD-C3D	-2.11	124.48	127.98
22	L	6020	BCR	C33-C5-C4	2.11	117.67	113.62
18	1	1003	CLA	OBD-CAD-CBD	-2.11	122.88	125.89
18	A	1121	CLA	CAC-C3C-C4C	2.11	127.54	124.81
25	B	7101	DGD	O6E-C1E-O5D	-2.11	104.98	109.97
18	3	3007	CLA	C5-C3-C4	2.11	119.25	114.60
18	4	4003	CLA	C6-C5-C3	-2.11	107.93	113.45
18	B	1205	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
18	2	2008	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
18	A	1114	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
18	F	1301	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
27	2	2501	LUT	C10-C11-C12	-2.10	116.66	123.22
18	A	1132	CLA	C1-O2A-CGA	2.10	121.96	116.44
23	B	5005	LMG	O7-C10-O9	-2.10	118.62	123.70
27	3	3501	LUT	C37-C21-C26	-2.10	106.36	109.55
22	J	6012	BCR	C40-C30-C25	-2.10	106.89	110.30
22	F	6014	BCR	C30-C25-C24	2.10	121.72	115.78
18	K	1001	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
18	A	1119	CLA	CED-O2D-CGD	2.10	120.68	115.94
25	B	7101	DGD	O2D-C2D-C1D	-2.10	104.95	110.05
28	4	4010	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
18	3	3002	CLA	CMD-C2D-C3D	-2.10	120.75	124.68
18	4	4008	CLA	CHA-C1A-NA	-2.10	121.60	126.40
18	A	1133	CLA	C1-O2A-CGA	2.10	121.94	116.44
21	2	2801	LHG	O7-C7-O9	-2.09	118.64	123.70
18	B	1236	CLA	C4-C3-C5	2.09	118.79	115.27
27	4	4503	LUT	C11-C12-C13	-2.09	120.54	126.42
22	B	6009	BCR	C15-C14-C13	-2.09	124.32	127.31
18	1	1008	CLA	CHA-C1A-NA	-2.09	121.61	126.40
18	B	1012	CLA	C6-C7-C8	-2.09	109.16	115.92
18	2	2016	CLA	CMB-C2B-C1B	2.09	131.68	128.46
20	B	5002	PQN	C12-C11-C3	-2.09	106.41	112.05
27	3	3501	LUT	C39-C29-C30	-2.09	120.00	122.92
22	B	6004	BCR	C1-C6-C5	-2.09	119.67	122.61
18	2	2012	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
18	4	4007	CLA	C1-C2-C3	-2.09	122.43	126.04
18	K	1001	CLA	CMB-C2B-C3B	2.09	128.58	124.68
18	A	1137	CLA	C1-C2-C3	-2.09	122.43	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1223	CLA	CAC-C3C-C4C	2.09	127.52	124.81
28	2	2010	CHL	CHA-C1A-NA	-2.09	121.62	126.40
18	B	1240	CLA	CAC-C3C-C4C	2.08	127.52	124.81
18	1	1004	CLA	CBC-CAC-C3C	-2.08	106.69	112.43
18	F	1301	CLA	CAA-CBA-CGA	-2.08	109.11	113.59
18	A	1113	CLA	CMC-C2C-C1C	2.08	128.21	125.04
18	A	1121	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
18	B	1224	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
27	2	2501	LUT	C2-C3-C4	-2.08	107.46	110.30
21	B	5004	LHG	O7-C7-O9	-2.08	118.83	122.96
18	B	1234	CLA	CAC-C3C-C4C	2.08	127.51	124.81
18	4	4017	CLA	CHA-C1A-NA	-2.08	121.64	126.40
22	A	6007	BCR	C31-C1-C6	-2.08	106.93	110.30
18	B	1203	CLA	C1-O2A-CGA	2.08	121.89	116.44
22	G	2011	BCR	C3-C4-C5	-2.08	110.37	114.08
18	2	2009	CLA	C3C-C4C-NC	2.08	112.90	110.57
27	1	1502	LUT	C30-C31-C32	-2.08	116.74	123.22
18	B	1238	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
18	B	1231	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
18	B	1023	CLA	OBD-CAD-C3D	-2.07	124.54	127.98
18	2	2016	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
18	3	3002	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
18	B	1215	CLA	CAC-C3C-C4C	2.07	127.50	124.81
28	2	2010	CHL	CMB-C2B-C1B	-2.07	125.28	128.46
18	G	1001	CLA	C4-C3-C2	-2.07	118.37	123.68
18	A	1109	CLA	CAC-C3C-C4C	2.07	127.50	124.81
18	3	3007	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
18	B	1206	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
18	B	1234	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
23	F	5001	LMG	C3-C4-C5	-2.07	106.55	110.24
18	G	1002	CLA	C3C-C4C-NC	2.07	112.89	110.57
25	B	7101	DGD	C5B-C4B-C3B	-2.07	103.93	114.42
18	4	4012	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
18	4	4012	CLA	CBC-CAC-C3C	-2.06	106.74	112.43
18	B	1217	CLA	CAC-C3C-C4C	2.06	127.49	124.81
18	2	2012	CLA	OBD-CAD-C3D	-2.06	124.56	127.98
18	1	1012	CLA	C1-O2A-CGA	2.06	121.86	116.44
18	B	1231	CLA	CED-O2D-CGD	2.06	120.60	115.94
18	1	1007	CLA	CHC-C1C-C2C	-2.06	121.02	126.72
18	4	4003	CLA	C3C-C4C-NC	2.06	112.88	110.57
22	J	6013	BCR	C35-C13-C14	-2.06	120.04	122.92
22	B	6005	BCR	C30-C25-C24	2.06	121.61	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	2005	CLA	C3C-C4C-NC	2.06	112.88	110.57
28	3	3011	CHL	CMB-C2B-C1B	-2.06	125.30	128.46
27	3	3501	LUT	C30-C31-C32	-2.06	116.79	123.22
18	2	2019	CLA	CAD-CBD-CHA	-2.06	102.87	105.67
18	2	2008	CLA	CHD-C4C-C3C	-2.06	121.81	124.84
27	2	2502	LUT	C19-C9-C8	2.06	121.32	118.08
18	A	1132	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
22	B	6006	BCR	C30-C25-C24	2.06	121.59	115.78
22	I	6020	BCR	C33-C5-C4	2.05	117.56	113.62
22	K	2011	BCR	C31-C1-C6	-2.05	106.97	110.30
17	A	1011	CL0	C1-O2A-CGA	2.05	121.83	116.44
22	J	6012	BCR	C38-C26-C27	2.05	117.56	113.62
18	A	1237	CLA	CMD-C2D-C3D	-2.05	120.84	124.68
18	G	1002	CLA	CMB-C2B-C3B	2.05	128.52	124.68
18	B	1229	CLA	CAC-C3C-C4C	2.05	127.47	124.81
18	B	1229	CLA	C4C-C3C-C2C	-2.05	103.91	106.90
18	B	1240	CLA	C1-O2A-CGA	2.05	121.83	116.44
18	B	1234	CLA	C4-C3-C2	-2.05	118.42	123.68
22	A	6007	BCR	C34-C9-C10	-2.05	120.05	122.92
28	2	2013	CHL	CMB-C2B-C1B	-2.05	125.31	128.46
23	2	2802	LMG	O1-C1-C2	2.05	111.50	108.30
18	A	1127	CLA	CED-O2D-CGD	2.05	120.57	115.94
18	3	3018	CLA	CHC-C1C-C2C	-2.05	121.06	126.72
18	B	1214	CLA	OBD-CAD-C3D	-2.04	124.59	127.98
28	2	2013	CHL	CHC-C1C-NC	2.04	127.31	124.20
18	B	1202	CLA	CHB-C4A-NA	2.04	127.34	124.51
18	B	1222	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
18	3	3008	CLA	CMC-C2C-C3C	2.04	131.66	126.12
18	B	1210	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
28	2	2011	CHL	CMD-C2D-C3D	2.04	128.50	124.68
18	A	1110	CLA	C1-C2-C3	-2.04	122.51	126.04
18	A	1138	CLA	C3C-C4C-NC	2.04	112.86	110.57
18	A	1110	CLA	CBA-CAA-C2A	2.04	119.89	113.86
18	A	1114	CLA	CMB-C2B-C3B	2.04	128.49	124.68
28	4	4013	CHL	OBD-CAD-CBD	-2.04	122.98	125.89
18	A	1122	CLA	CMB-C2B-C3B	2.04	128.49	124.68
18	1	1005	CLA	CHC-C1C-C2C	-2.04	121.08	126.72
23	4	4801	LMG	C7-O1-C1	-2.04	109.76	113.74
18	4	4001	CLA	CHB-C4A-NA	2.04	127.33	124.51
18	A	1113	CLA	CAA-CBA-CGA	-2.03	107.31	113.25
18	1	1008	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
23	J	5001	LMG	C8-O7-C10	2.03	122.80	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	1003	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
28	4	4010	CHL	C1D-CHD-C4C	2.03	125.24	122.56
18	4	4016	CLA	C3C-C4C-NC	2.03	112.85	110.57
18	1	1005	CLA	CMB-C2B-C3B	2.03	128.48	124.68
18	2	2005	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
18	A	1120	CLA	OBD-CAD-C3D	-2.03	124.61	127.98
27	1	1501	LUT	C8-C7-C6	-2.03	121.50	127.20
18	2	2005	CLA	CED-O2D-CGD	2.03	120.52	115.94
27	1	1501	LUT	C39-C29-C30	-2.03	120.08	122.92
22	B	6009	BCR	C8-C9-C10	2.03	122.05	118.94
18	1	1012	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
18	4	4006	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
18	3	3012	CLA	CMB-C2B-C3B	2.03	128.47	124.68
18	2	2005	CLA	CAA-C2A-C1A	-2.03	105.33	111.97
21	1	1801	LHG	O8-C23-O10	-2.03	118.48	123.59
18	3	3019	CLA	C2A-C3A-C4A	-2.03	101.27	103.59
28	1	1010	CHL	C1-O2A-CGA	2.03	122.78	116.11
18	3	3005	CLA	CHA-C1A-NA	-2.03	121.76	126.40
18	A	1136	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
18	A	1133	CLA	OBD-CAD-CBD	-2.02	123.00	125.89
18	G	1003	CLA	C3C-C4C-NC	2.02	112.84	110.57
18	B	1213	CLA	CED-O2D-CGD	2.02	120.51	115.94
18	2	2008	CLA	CHC-C1C-C2C	-2.02	121.13	126.72
18	A	1106	CLA	C6-C5-C3	-2.02	108.16	113.45
18	1	1001	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
18	1	1006	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
18	B	1211	CLA	CHB-C4A-NA	2.02	127.30	124.51
18	1	1014	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
18	1	1005	CLA	CHA-C1A-NA	-2.02	121.78	126.40
18	B	1205	CLA	C1-C2-C3	-2.02	122.55	126.04
18	B	1201	CLA	CED-O2D-CGD	2.02	120.50	115.94
27	3	3501	LUT	C40-C33-C34	-2.02	120.10	122.92
28	1	1009	CHL	CHB-C4A-NA	2.01	127.30	124.51
22	3	3503	BCR	C38-C26-C27	2.01	117.49	113.62
18	3	3019	CLA	C3A-C4A-CHB	-2.01	121.44	123.91
29	4	4505	ZEX	C21-C22-C23	-2.01	109.33	113.69
26	B	8001	LMU	C3'-C4'-C5'	-2.01	106.31	110.93
23	F	5002	LMG	O6-C1-C2	-2.01	106.09	110.35
18	1	1007	CLA	CMD-C2D-C3D	-2.01	120.92	124.68
18	3	3001	CLA	CED-O2D-CGD	2.01	120.48	115.94
27	4	4501	LUT	C40-C33-C32	2.01	121.24	118.08
18	4	4017	CLA	CHC-C1C-C2C	-2.01	121.17	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	2011	BCR	C7-C6-C5	-2.01	116.60	121.46
18	G	1001	CLA	C3C-C4C-NC	2.01	112.82	110.57
22	A	6003	BCR	C38-C26-C27	2.01	117.47	113.62
23	4	4801	LMG	O1-C1-C2	2.01	111.44	108.30
18	B	1225	CLA	CED-O2D-CGD	2.01	120.48	115.94
18	B	1225	CLA	CAC-C3C-C4C	2.01	127.41	124.81
18	A	1139	CLA	C1-O2A-CGA	2.01	121.71	116.44
18	2	2009	CLA	OBD-CAD-C3D	-2.00	124.65	127.98
22	A	6002	BCR	C30-C25-C24	2.00	121.45	115.78
18	A	1136	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
18	2	2002	CLA	CHC-C1C-C2C	-2.00	121.18	126.72
18	B	1212	CLA	C1-O2A-CGA	2.00	121.70	116.44
18	4	4003	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
26	B	8001	LMU	O5'-C1'-C2'	2.00	114.59	110.35
20	B	5002	PQN	C11-C12-C13	-2.00	123.46	126.79
28	4	4013	CHL	C1-O2A-CGA	2.00	122.70	116.11
18	A	1022	CLA	C1-O2A-CGA	2.00	121.69	116.44

All (454) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	1132	CLA	NC
18	A	1132	CLA	ND
18	A	1132	CLA	NA
18	B	1220	CLA	NC
18	B	1220	CLA	NA
18	B	1201	CLA	NC
18	B	1201	CLA	ND
18	B	1201	CLA	NA
18	4	4001	CLA	NC
18	4	4001	CLA	ND
18	4	4001	CLA	NA
18	1	1005	CLA	NC
18	1	1005	CLA	ND
18	1	1005	CLA	NA
18	3	3004	CLA	NC
18	3	3004	CLA	ND
18	3	3004	CLA	NA
18	B	1222	CLA	NC
18	B	1222	CLA	ND
18	B	1222	CLA	NA
18	B	1240	CLA	ND

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Mol	Chain	Res	Type	Atom
18	B	1240	CLA	NA
18	B	1225	CLA	NC
18	B	1225	CLA	ND
18	B	1225	CLA	NA
18	1	1003	CLA	NC
18	1	1003	CLA	ND
18	1	1003	CLA	NA
18	4	4009	CLA	NC
18	4	4009	CLA	ND
18	4	4009	CLA	NA
18	A	1013	CLA	NC
18	A	1013	CLA	ND
18	A	1013	CLA	NA
18	J	1302	CLA	NC
18	J	1302	CLA	ND
18	J	1302	CLA	NA
18	A	1126	CLA	NC
18	A	1126	CLA	ND
18	A	1126	CLA	NA
18	A	1111	CLA	ND
18	A	1111	CLA	NA
28	4	4011	CHL	NC
28	4	4011	CHL	ND
28	4	4011	CHL	NA
18	1	1013	CLA	NC
18	1	1013	CLA	ND
18	1	1013	CLA	NA
18	A	1114	CLA	NC
18	A	1114	CLA	ND
18	A	1114	CLA	NA
18	2	2001	CLA	NC
18	2	2001	CLA	ND
18	2	2001	CLA	NA
18	A	1237	CLA	NC
18	A	1237	CLA	ND
18	A	1237	CLA	NA
18	A	1121	CLA	NC
18	A	1121	CLA	ND
18	A	1121	CLA	NA
18	2	2004	CLA	NC
18	2	2004	CLA	ND
18	2	2004	CLA	NA

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Mol	Chain	Res	Type	Atom
18	3	3008	CLA	NC
18	3	3008	CLA	ND
18	3	3008	CLA	NA
18	G	1003	CLA	NC
18	G	1003	CLA	ND
18	G	1003	CLA	NA
27	2	2502	LUT	C26
27	2	2501	LUT	C26
18	3	3002	CLA	NC
18	3	3002	CLA	ND
18	3	3002	CLA	NA
28	2	2010	CHL	NC
28	2	2010	CHL	ND
28	2	2010	CHL	NA
18	A	1137	CLA	NC
18	A	1137	CLA	ND
18	A	1137	CLA	NA
18	3	3013	CLA	NC
18	3	3013	CLA	ND
18	3	3013	CLA	NA
18	2	2009	CLA	NC
18	2	2009	CLA	ND
18	2	2009	CLA	NA
18	2	2008	CLA	NC
18	2	2008	CLA	ND
18	2	2008	CLA	NA
18	B	1228	CLA	NC
18	B	1228	CLA	ND
18	B	1228	CLA	NA
18	A	1112	CLA	ND
18	A	1112	CLA	NA
18	A	1118	CLA	NC
18	A	1118	CLA	ND
18	A	1118	CLA	NA
18	A	1139	CLA	NC
18	A	1139	CLA	ND
18	A	1139	CLA	NA
27	3	3502	LUT	C26
18	A	1130	CLA	NC
18	A	1130	CLA	NA
18	4	4003	CLA	NC
18	4	4003	CLA	ND

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Mol	Chain	Res	Type	Atom
18	4	4003	CLA	NA
18	A	1107	CLA	NC
18	A	1107	CLA	ND
18	A	1107	CLA	NA
18	2	2019	CLA	NC
18	2	2019	CLA	ND
18	2	2019	CLA	NA
18	B	1221	CLA	NC
18	B	1221	CLA	ND
18	B	1221	CLA	NA
18	4	4016	CLA	NC
18	4	4016	CLA	ND
18	4	4016	CLA	NA
27	1	1502	LUT	C26
18	B	1208	CLA	NC
18	B	1208	CLA	ND
18	B	1208	CLA	NA
18	A	1116	CLA	NC
18	A	1116	CLA	ND
18	A	1116	CLA	NA
18	B	1204	CLA	ND
18	B	1204	CLA	NA
18	2	2006	CLA	NC
18	2	2006	CLA	ND
18	2	2006	CLA	NA
18	2	2012	CLA	NC
18	2	2012	CLA	ND
18	2	2012	CLA	NA
27	4	4502	LUT	C26
18	2	2003	CLA	NC
18	2	2003	CLA	ND
18	2	2003	CLA	NA
18	1	1001	CLA	NC
18	1	1001	CLA	ND
18	1	1001	CLA	NA
18	4	4007	CLA	NC
18	4	4007	CLA	ND
18	4	4007	CLA	NA
18	A	1123	CLA	ND
18	A	1123	CLA	NA
18	A	1115	CLA	NC
18	A	1115	CLA	ND

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Mol	Chain	Res	Type	Atom
18	A	1115	CLA	NA
18	H	1000	CLA	NC
18	H	1000	CLA	ND
18	H	1000	CLA	NA
18	A	1134	CLA	ND
18	A	1134	CLA	NA
18	3	3010	CLA	NC
18	3	3010	CLA	ND
18	3	3010	CLA	NA
27	4	4503	LUT	C26
18	1	1006	CLA	NC
18	1	1006	CLA	ND
18	1	1006	CLA	NA
18	2	2005	CLA	NC
18	2	2005	CLA	ND
18	2	2005	CLA	NA
18	A	1022	CLA	ND
18	A	1022	CLA	NA
18	B	1232	CLA	NC
18	B	1232	CLA	ND
18	B	1232	CLA	NA
18	A	1129	CLA	ND
18	A	1129	CLA	NA
28	1	1010	CHL	NC
28	1	1010	CHL	ND
28	1	1010	CHL	NA
18	F	1301	CLA	NC
18	F	1301	CLA	ND
18	F	1301	CLA	NA
18	L	1502	CLA	NC
18	L	1502	CLA	ND
18	L	1502	CLA	NA
27	1	1501	LUT	C26
18	2	2007	CLA	NC
18	2	2007	CLA	ND
18	2	2007	CLA	NA
18	3	3007	CLA	NC
18	3	3007	CLA	ND
18	3	3007	CLA	NA
18	2	2002	CLA	NC
18	2	2002	CLA	ND
18	2	2002	CLA	NA

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Mol	Chain	Res	Type	Atom
18	B	1223	CLA	NC
18	B	1223	CLA	NA
18	A	1133	CLA	NC
18	A	1133	CLA	NA
28	1	1009	CHL	C8
28	1	1009	CHL	NC
28	1	1009	CHL	ND
28	1	1009	CHL	NA
18	A	1151	CLA	NC
18	A	1151	CLA	ND
18	A	1151	CLA	NA
18	B	1238	CLA	NC
18	B	1238	CLA	ND
18	B	1238	CLA	NA
18	A	1104	CLA	NC
18	A	1104	CLA	ND
18	A	1104	CLA	NA
18	B	1023	CLA	NC
18	B	1023	CLA	ND
18	B	1023	CLA	NA
18	3	3018	CLA	NC
18	3	3018	CLA	ND
18	3	3018	CLA	NA
18	3	3019	CLA	NC
18	3	3019	CLA	ND
18	3	3019	CLA	NA
18	B	1202	CLA	ND
18	B	1202	CLA	NA
18	B	1229	CLA	NC
18	B	1229	CLA	ND
18	B	1229	CLA	NA
18	A	1135	CLA	ND
18	A	1135	CLA	NA
18	A	1102	CLA	NC
18	A	1102	CLA	ND
18	A	1102	CLA	NA
18	A	1127	CLA	NC
18	A	1127	CLA	ND
18	A	1127	CLA	NA
18	3	3017	CLA	NC
18	3	3017	CLA	ND
18	3	3017	CLA	NA

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Mol	Chain	Res	Type	Atom
18	4	4005	CLA	NC
18	4	4005	CLA	ND
18	4	4005	CLA	NA
17	A	1011	CL0	NC
17	A	1011	CL0	ND
17	A	1011	CL0	NA
18	4	4008	CLA	NC
18	4	4008	CLA	ND
18	4	4008	CLA	NA
18	4	4004	CLA	NC
18	4	4004	CLA	ND
18	4	4004	CLA	NA
18	B	1227	CLA	NC
18	B	1227	CLA	ND
18	B	1227	CLA	NA
18	B	1230	CLA	NC
18	B	1230	CLA	ND
18	B	1230	CLA	NA
18	A	1120	CLA	NC
18	A	1120	CLA	ND
18	A	1120	CLA	NA
28	4	4013	CHL	NC
28	4	4013	CHL	ND
28	4	4013	CHL	NA
18	A	1108	CLA	NC
18	A	1108	CLA	ND
18	A	1108	CLA	NA
28	4	4010	CHL	NC
28	4	4010	CHL	ND
28	4	4010	CHL	NA
18	4	4002	CLA	NC
18	4	4002	CLA	ND
18	4	4002	CLA	NA
18	A	1125	CLA	NC
18	A	1125	CLA	ND
18	A	1125	CLA	NA
18	B	1206	CLA	ND
18	B	1206	CLA	NA
18	A	1117	CLA	ND
18	A	1117	CLA	NA
18	B	1207	CLA	NC
18	B	1207	CLA	NA

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Mol	Chain	Res	Type	Atom
18	B	1235	CLA	ND
18	B	1235	CLA	NA
18	A	1140	CLA	NC
18	A	1140	CLA	ND
18	A	1140	CLA	NA
18	1	1004	CLA	NC
18	1	1004	CLA	ND
18	1	1004	CLA	NA
18	A	1110	CLA	NC
18	A	1110	CLA	ND
18	A	1110	CLA	NA
18	B	1211	CLA	NC
18	B	1211	CLA	ND
18	B	1211	CLA	NA
18	2	2016	CLA	NC
18	2	2016	CLA	ND
18	2	2016	CLA	NA
27	4	4501	LUT	C26
18	3	3005	CLA	NC
18	3	3005	CLA	ND
18	3	3005	CLA	NA
18	B	1214	CLA	NC
18	B	1214	CLA	ND
18	B	1214	CLA	NA
18	L	1503	CLA	NC
18	L	1503	CLA	ND
18	L	1503	CLA	NA
18	A	1131	CLA	NC
18	A	1131	CLA	ND
18	A	1131	CLA	NA
18	B	1231	CLA	NC
18	B	1231	CLA	ND
18	B	1231	CLA	NA
18	B	1234	CLA	NC
18	B	1234	CLA	ND
18	B	1234	CLA	NA
27	I	6018	LUT	C26
18	3	3006	CLA	NC
18	3	3006	CLA	ND
18	3	3006	CLA	NA
18	3	3003	CLA	NC
18	3	3003	CLA	ND

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Mol	Chain	Res	Type	Atom
18	3	3003	CLA	NA
18	B	1209	CLA	NC
18	B	1209	CLA	ND
18	B	1209	CLA	NA
18	1	1014	CLA	NC
18	1	1014	CLA	ND
18	1	1014	CLA	NA
18	B	1236	CLA	ND
18	B	1236	CLA	NA
18	3	3012	CLA	NC
18	3	3012	CLA	ND
18	3	3012	CLA	NA
18	1	1011	CLA	NC
18	1	1011	CLA	ND
18	1	1011	CLA	NA
18	B	1219	CLA	NC
18	B	1219	CLA	ND
18	B	1219	CLA	NA
18	B	1218	CLA	NC
18	B	1218	CLA	ND
18	B	1218	CLA	NA
18	A	1109	CLA	NC
18	A	1109	CLA	ND
18	A	1109	CLA	NA
18	B	1203	CLA	ND
18	B	1203	CLA	NA
18	1	1012	CLA	NC
18	1	1012	CLA	ND
18	1	1012	CLA	NA
18	A	1106	CLA	NC
18	A	1106	CLA	ND
18	A	1106	CLA	NA
18	G	1002	CLA	NC
18	G	1002	CLA	ND
18	G	1002	CLA	NA
28	3	3011	CHL	C8
28	3	3011	CHL	NC
28	3	3011	CHL	ND
28	3	3011	CHL	NA
18	A	1103	CLA	ND
18	A	1103	CLA	NA
18	B	1224	CLA	NC

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Mol	Chain	Res	Type	Atom
18	B	1224	CLA	ND
18	B	1224	CLA	NA
18	4	4006	CLA	NC
18	4	4006	CLA	ND
18	4	4006	CLA	NA
18	F	1302	CLA	NC
18	F	1302	CLA	ND
18	F	1302	CLA	NA
28	2	2013	CHL	NC
28	2	2013	CHL	ND
28	2	2013	CHL	NA
18	4	4017	CLA	NC
18	4	4017	CLA	ND
18	4	4017	CLA	NA
18	A	1122	CLA	NC
18	A	1122	CLA	ND
18	A	1122	CLA	NA
27	3	3501	LUT	C26
18	B	1239	CLA	NC
18	B	1239	CLA	ND
18	B	1239	CLA	NA
28	2	2011	CHL	NC
28	2	2011	CHL	ND
28	2	2011	CHL	NA
18	B	1216	CLA	NC
18	B	1216	CLA	ND
18	B	1216	CLA	NA
18	1	1007	CLA	NC
18	1	1007	CLA	ND
18	1	1007	CLA	NA
18	A	1124	CLA	NC
18	A	1124	CLA	ND
18	A	1124	CLA	NA
18	1	1008	CLA	NC
18	1	1008	CLA	ND
18	1	1008	CLA	NA
18	A	1113	CLA	ND
18	A	1113	CLA	NA
18	1	1002	CLA	NC
18	1	1002	CLA	ND
18	1	1002	CLA	NA
18	B	1213	CLA	NC

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Mol	Chain	Res	Type	Atom
18	B	1213	CLA	NA
18	A	1105	CLA	NC
18	A	1105	CLA	ND
18	A	1105	CLA	NA
18	L	1501	CLA	NC
18	L	1501	CLA	ND
18	L	1501	CLA	NA
18	A	1136	CLA	NC
18	A	1136	CLA	ND
18	A	1136	CLA	NA
18	B	1021	CLA	NC
18	B	1021	CLA	ND
18	B	1021	CLA	NA
18	B	1215	CLA	ND
18	B	1215	CLA	NA
18	A	1128	CLA	NC
18	A	1128	CLA	ND
18	A	1128	CLA	NA
18	3	3001	CLA	NC
18	3	3001	CLA	ND
18	3	3001	CLA	NA
18	4	4012	CLA	NC
18	4	4012	CLA	ND
18	4	4012	CLA	NA
18	A	1119	CLA	NC
18	A	1119	CLA	ND
18	A	1119	CLA	NA
18	B	1217	CLA	NC
18	B	1217	CLA	ND
18	B	1217	CLA	NA
18	A	1101	CLA	ND
18	A	1101	CLA	NA
18	A	1138	CLA	NC
18	A	1138	CLA	ND
18	A	1138	CLA	NA
18	B	1212	CLA	NC
18	B	1212	CLA	ND
18	B	1212	CLA	NA
18	K	1001	CLA	NC
18	K	1001	CLA	ND
18	K	1001	CLA	NA
18	B	1012	CLA	ND

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Mol	Chain	Res	Type	Atom
18	B	1012	CLA	NA
18	G	1001	CLA	NC
18	G	1001	CLA	ND
18	G	1001	CLA	NA
18	B	1205	CLA	NC
18	B	1205	CLA	ND
18	B	1205	CLA	NA
18	B	1210	CLA	NC
18	B	1210	CLA	ND
18	B	1210	CLA	NA
18	B	1226	CLA	NC
18	B	1226	CLA	ND
18	B	1226	CLA	NA

All (2378) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	B	5004	LHG	C3-O3-P-O4
21	B	5004	LHG	C4-O6-P-O4
21	B	5004	LHG	C8-C7-O7-C5
21	1	1801	LHG	C3-O3-P-O4
21	1	1801	LHG	C3-O3-P-O5
21	1	1801	LHG	C4-O6-P-O5
21	1	1801	LHG	O9-C7-O7-C5
21	1	1801	LHG	C8-C7-O7-C5
18	B	1201	CLA	C1A-C2A-CAA-CBA
18	B	1201	CLA	C3A-C2A-CAA-CBA
18	B	1201	CLA	CBD-CGD-O2D-CED
22	I	6020	BCR	C11-C10-C9-C8
22	I	6020	BCR	C11-C10-C9-C34
22	I	6020	BCR	C10-C11-C12-C13
22	A	6003	BCR	C11-C10-C9-C8
22	A	6003	BCR	C11-C10-C9-C34
22	A	6003	BCR	C17-C18-C19-C20
22	A	6003	BCR	C36-C18-C19-C20
22	A	6003	BCR	C21-C22-C23-C24
22	A	6003	BCR	C37-C22-C23-C24
18	1	1005	CLA	CHA-CBD-CGD-O1D
18	1	1005	CLA	CHA-CBD-CGD-O2D
18	B	1222	CLA	C1A-C2A-CAA-CBA
18	B	1240	CLA	CBD-CGD-O2D-CED
18	B	1225	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	1225	CLA	C3A-C2A-CAA-CBA
18	B	1225	CLA	CHA-CBD-CGD-O1D
18	B	1225	CLA	CHA-CBD-CGD-O2D
18	1	1003	CLA	CBA-CGA-O2A-C1
18	1	1003	CLA	O1A-CGA-O2A-C1
18	1	1003	CLA	CBD-CGD-O2D-CED
18	A	1013	CLA	CHA-CBD-CGD-O1D
18	J	1302	CLA	CAD-CBD-CGD-O1D
18	J	1302	CLA	CAD-CBD-CGD-O2D
18	J	1302	CLA	CBD-CGD-O2D-CED
28	4	4011	CHL	C4C-C3C-CAC-CBC
22	B	6004	BCR	C7-C8-C9-C10
22	B	6004	BCR	C7-C8-C9-C34
18	1	1013	CLA	CBD-CGD-O2D-CED
18	A	1114	CLA	CBA-CGA-O2A-C1
18	A	1114	CLA	O1A-CGA-O2A-C1
18	A	1114	CLA	CBD-CGD-O2D-CED
18	2	2001	CLA	C1A-C2A-CAA-CBA
18	2	2001	CLA	C3A-C2A-CAA-CBA
18	2	2001	CLA	CBD-CGD-O2D-CED
18	2	2001	CLA	C2-C3-C5-C6
18	2	2001	CLA	C4-C3-C5-C6
18	2	2004	CLA	C3A-C2A-CAA-CBA
18	2	2004	CLA	CHA-CBD-CGD-O1D
18	2	2004	CLA	CHA-CBD-CGD-O2D
18	2	2004	CLA	C2-C3-C5-C6
18	2	2004	CLA	C4-C3-C5-C6
26	B	8001	LMU	C2'-C1'-O1'-C1
18	3	3008	CLA	C1A-C2A-CAA-CBA
18	3	3008	CLA	C3A-C2A-CAA-CBA
18	3	3008	CLA	CHA-CBD-CGD-O1D
18	3	3008	CLA	CHA-CBD-CGD-O2D
18	3	3008	CLA	CBD-CGD-O2D-CED
18	G	1003	CLA	C3A-C2A-CAA-CBA
27	2	2502	LUT	C21-C26-C27-C28
27	2	2502	LUT	C27-C28-C29-C30
27	2	2502	LUT	C27-C28-C29-C39
27	2	2501	LUT	C21-C26-C27-C28
18	3	3002	CLA	CBD-CGD-O2D-CED
18	A	1137	CLA	CBD-CGD-O2D-CED
18	A	1137	CLA	C2-C3-C5-C6
18	A	1137	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	3	3013	CLA	C3A-C2A-CAA-CBA
18	2	2009	CLA	C1A-C2A-CAA-CBA
18	2	2009	CLA	C3A-C2A-CAA-CBA
18	2	2009	CLA	CBD-CGD-O2D-CED
18	2	2008	CLA	C2-C1-O2A-CGA
18	2	2008	CLA	CBD-CGD-O2D-CED
18	B	1228	CLA	C1A-C2A-CAA-CBA
18	B	1228	CLA	C3A-C2A-CAA-CBA
18	B	1228	CLA	CBD-CGD-O2D-CED
22	B	6006	BCR	C1-C6-C7-C8
22	B	6006	BCR	C5-C6-C7-C8
22	B	6006	BCR	C21-C22-C23-C24
22	B	6006	BCR	C37-C22-C23-C24
22	L	6020	BCR	C7-C8-C9-C10
22	L	6020	BCR	C7-C8-C9-C34
22	L	6020	BCR	C11-C10-C9-C8
22	L	6020	BCR	C11-C10-C9-C34
22	L	6020	BCR	C9-C10-C11-C12
22	L	6020	BCR	C10-C11-C12-C13
18	A	1112	CLA	C1A-C2A-CAA-CBA
18	A	1112	CLA	C3A-C2A-CAA-CBA
18	A	1118	CLA	CBA-CGA-O2A-C1
18	A	1139	CLA	CBD-CGD-O2D-CED
18	A	1139	CLA	C2-C3-C5-C6
18	A	1139	CLA	C4-C3-C5-C6
27	3	3502	LUT	C21-C26-C27-C28
27	3	3502	LUT	C25-C26-C27-C28
18	A	1130	CLA	CBD-CGD-O2D-CED
18	A	1107	CLA	C1A-C2A-CAA-CBA
18	A	1107	CLA	CBD-CGD-O2D-CED
22	J	6013	BCR	C7-C8-C9-C10
22	J	6013	BCR	C7-C8-C9-C34
22	J	6013	BCR	C11-C10-C9-C8
22	J	6013	BCR	C11-C10-C9-C34
22	J	6013	BCR	C10-C11-C12-C13
22	J	6013	BCR	C21-C22-C23-C24
22	J	6013	BCR	C37-C22-C23-C24
21	A	7001	LHG	C3-O3-P-O5
21	A	7001	LHG	C3-O3-P-O6
21	A	7001	LHG	C4-O6-P-O3
21	A	7001	LHG	C4-O6-P-O4
21	A	7001	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
18	B	1221	CLA	C2-C1-O2A-CGA
18	4	4016	CLA	C1A-C2A-CAA-CBA
18	4	4016	CLA	CBA-CGA-O2A-C1
18	4	4016	CLA	CBD-CGD-O2D-CED
27	1	1502	LUT	C21-C26-C27-C28
26	B	8002	LMU	C2'-C1'-O1'-C1
26	B	8002	LMU	C2-C1-O1'-C1'
21	2	2801	LHG	O1-C1-C2-C3
21	2	2801	LHG	C4-O6-P-O3
21	2	2801	LHG	C4-O6-P-O4
21	2	2801	LHG	C4-O6-P-O5
18	B	1208	CLA	C1A-C2A-CAA-CBA
18	B	1208	CLA	C3A-C2A-CAA-CBA
18	A	1116	CLA	C3A-C2A-CAA-CBA
18	A	1116	CLA	CBD-CGD-O2D-CED
18	2	2006	CLA	O1A-CGA-O2A-C1
18	2	2006	CLA	C2-C1-O2A-CGA
18	2	2006	CLA	CBD-CGD-O2D-CED
25	B	7101	DGD	C2B-C1B-O2G-C2G
25	B	7101	DGD	O1B-C1B-O2G-C2G
18	2	2012	CLA	C2-C1-O2A-CGA
22	F	6014	BCR	C7-C8-C9-C10
22	F	6014	BCR	C7-C8-C9-C34
22	F	6014	BCR	C11-C10-C9-C8
22	F	6014	BCR	C11-C10-C9-C34
22	F	6014	BCR	C23-C24-C25-C30
27	4	4502	LUT	C1-C6-C7-C8
27	4	4502	LUT	C5-C6-C7-C8
27	4	4502	LUT	C21-C26-C27-C28
18	2	2003	CLA	CBD-CGD-O2D-CED
22	A	6017	BCR	C11-C10-C9-C8
22	A	6017	BCR	C11-C10-C9-C34
22	A	6017	BCR	C10-C11-C12-C13
22	A	6017	BCR	C21-C22-C23-C24
22	A	6017	BCR	C37-C22-C23-C24
22	A	6017	BCR	C23-C24-C25-C26
22	A	6017	BCR	C23-C24-C25-C30
22	L	6019	BCR	C5-C6-C7-C8
22	L	6019	BCR	C11-C10-C9-C8
22	L	6019	BCR	C11-C10-C9-C34
22	L	6019	BCR	C10-C11-C12-C13
18	1	1001	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	4	4505	ZEX	C25-C26-C27-C28
18	A	1123	CLA	C2-C1-O2A-CGA
18	A	1123	CLA	C11-C12-C13-C14
18	A	1115	CLA	C2A-CAA-CBA-CGA
18	H	1000	CLA	C3A-C2A-CAA-CBA
18	H	1000	CLA	CHA-CBD-CGD-O1D
18	H	1000	CLA	CHA-CBD-CGD-O2D
18	A	1134	CLA	CHA-CBD-CGD-O1D
18	A	1134	CLA	CHA-CBD-CGD-O2D
18	3	3010	CLA	CBA-CGA-O2A-C1
18	3	3010	CLA	O1A-CGA-O2A-C1
18	3	3010	CLA	C4-C3-C5-C6
27	4	4503	LUT	C21-C26-C27-C28
27	4	4503	LUT	C27-C28-C29-C39
27	4	4503	LUT	C31-C32-C33-C34
27	4	4503	LUT	C31-C32-C33-C40
18	1	1006	CLA	CHA-CBD-CGD-O1D
18	1	1006	CLA	CHA-CBD-CGD-O2D
18	1	1006	CLA	CBD-CGD-O2D-CED
18	2	2005	CLA	C2-C1-O2A-CGA
18	2	2005	CLA	CBD-CGD-O2D-CED
18	2	2005	CLA	C2-C3-C5-C6
18	2	2005	CLA	C4-C3-C5-C6
18	A	1022	CLA	CBD-CGD-O2D-CED
18	B	1232	CLA	CBD-CGD-O2D-CED
18	L	1502	CLA	C1A-C2A-CAA-CBA
18	L	1502	CLA	C3A-C2A-CAA-CBA
18	L	1502	CLA	CHA-CBD-CGD-O1D
27	1	1501	LUT	C7-C8-C9-C10
27	1	1501	LUT	C7-C8-C9-C19
27	1	1501	LUT	C21-C26-C27-C28
27	1	1501	LUT	C27-C28-C29-C30
27	1	1501	LUT	C27-C28-C29-C39
27	1	1501	LUT	C31-C32-C33-C34
27	1	1501	LUT	C31-C32-C33-C40
18	2	2007	CLA	CBD-CGD-O2D-CED
18	2	2007	CLA	C2-C3-C5-C6
18	2	2007	CLA	C4-C3-C5-C6
18	3	3007	CLA	CHA-CBD-CGD-O2D
18	2	2002	CLA	CBD-CGD-O2D-CED
18	B	1223	CLA	C1A-C2A-CAA-CBA
18	A	1133	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	4	4801	LMG	O6-C1-O1-C7
28	1	1009	CHL	C1A-C2A-CAA-CBA
28	1	1009	CHL	CHA-CBD-CGD-O1D
18	A	1151	CLA	CHA-CBD-CGD-O1D
18	A	1151	CLA	CHA-CBD-CGD-O2D
18	A	1151	CLA	CBD-CGD-O2D-CED
18	B	1238	CLA	C2-C1-O2A-CGA
18	A	1104	CLA	CBD-CGD-O2D-CED
18	B	1023	CLA	CHA-CBD-CGD-O1D
18	B	1023	CLA	CHA-CBD-CGD-O2D
18	3	3018	CLA	C2-C1-O2A-CGA
18	B	1202	CLA	C3A-C2A-CAA-CBA
18	B	1202	CLA	CHA-CBD-CGD-O1D
18	B	1202	CLA	CHA-CBD-CGD-O2D
18	B	1202	CLA	CAD-CBD-CGD-O1D
18	B	1202	CLA	CAD-CBD-CGD-O2D
18	B	1229	CLA	C2-C1-O2A-CGA
18	A	1135	CLA	C4-C3-C5-C6
22	B	6005	BCR	C1-C6-C7-C8
22	B	6005	BCR	C11-C10-C9-C8
22	B	6005	BCR	C11-C10-C9-C34
18	3	3017	CLA	CBD-CGD-O2D-CED
18	4	4005	CLA	C3A-C2A-CAA-CBA
23	F	5001	LMG	C11-C10-O7-C8
22	3	3503	BCR	C1-C6-C7-C8
22	3	3503	BCR	C5-C6-C7-C8
22	3	3503	BCR	C7-C8-C9-C10
22	3	3503	BCR	C7-C8-C9-C34
22	3	3503	BCR	C11-C10-C9-C8
22	3	3503	BCR	C11-C10-C9-C34
22	3	3503	BCR	C10-C11-C12-C13
22	3	3503	BCR	C15-C16-C17-C18
22	3	3503	BCR	C23-C24-C25-C26
22	3	3503	BCR	C23-C24-C25-C30
18	4	4008	CLA	C1A-C2A-CAA-CBA
18	4	4008	CLA	C3A-C2A-CAA-CBA
18	4	4008	CLA	C2A-CAA-CBA-CGA
18	4	4008	CLA	CBA-CGA-O2A-C1
18	4	4008	CLA	CHA-CBD-CGD-O1D
18	4	4004	CLA	CHA-CBD-CGD-O1D
18	4	4004	CLA	CHA-CBD-CGD-O2D
18	B	1230	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	1230	CLA	C3A-C2A-CAA-CBA
18	B	1230	CLA	CHA-CBD-CGD-O1D
18	B	1230	CLA	CHA-CBD-CGD-O2D
18	B	1230	CLA	C2-C3-C5-C6
18	B	1230	CLA	C4-C3-C5-C6
18	A	1120	CLA	C2-C3-C5-C6
18	A	1120	CLA	C4-C3-C5-C6
28	4	4013	CHL	C2C-C3C-CAC-CBC
28	4	4013	CHL	C4C-C3C-CAC-CBC
18	A	1108	CLA	CHA-CBD-CGD-O1D
18	A	1108	CLA	CHA-CBD-CGD-O2D
28	4	4010	CHL	C2A-CAA-CBA-CGA
18	B	1206	CLA	C2-C1-O2A-CGA
18	A	1117	CLA	C1A-C2A-CAA-CBA
18	A	1117	CLA	C3A-C2A-CAA-CBA
18	B	1207	CLA	C2-C1-O2A-CGA
23	J	5001	LMG	O9-C10-O7-C8
18	B	1235	CLA	CHA-CBD-CGD-O1D
18	B	1235	CLA	CHA-CBD-CGD-O2D
18	A	1140	CLA	C1A-C2A-CAA-CBA
18	A	1140	CLA	C4-C3-C5-C6
18	1	1004	CLA	C11-C12-C13-C14
18	A	1110	CLA	C1A-C2A-CAA-CBA
18	A	1110	CLA	C3A-C2A-CAA-CBA
22	J	6012	BCR	C7-C8-C9-C10
22	J	6012	BCR	C7-C8-C9-C34
22	J	6012	BCR	C11-C10-C9-C8
22	J	6012	BCR	C11-C10-C9-C34
22	J	6012	BCR	C10-C11-C12-C13
22	J	6012	BCR	C11-C12-C13-C14
22	J	6012	BCR	C11-C12-C13-C35
18	2	2016	CLA	C2-C1-O2A-CGA
18	2	2016	CLA	CAD-CBD-CGD-O1D
18	2	2016	CLA	CBD-CGD-O2D-CED
27	4	4501	LUT	C5-C6-C7-C8
27	4	4501	LUT	C21-C26-C27-C28
22	G	2011	BCR	C1-C6-C7-C8
22	G	2011	BCR	C5-C6-C7-C8
22	G	2011	BCR	C10-C11-C12-C13
18	3	3005	CLA	CHA-CBD-CGD-O1D
18	3	3005	CLA	CHA-CBD-CGD-O2D
18	B	1214	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	B	1214	CLA	CBD-CGD-O2D-CED
18	L	1503	CLA	CBD-CGD-O2D-CED
18	A	1131	CLA	CBD-CGD-O2D-CED
27	I	6018	LUT	C25-C26-C27-C28
18	3	3006	CLA	CBD-CGD-O2D-CED
18	3	3003	CLA	CBD-CGD-O2D-CED
18	B	1209	CLA	CBA-CGA-O2A-C1
18	1	1014	CLA	CBA-CGA-O2A-C1
18	1	1014	CLA	CBD-CGD-O2D-CED
18	3	3012	CLA	C2-C1-O2A-CGA
18	3	3012	CLA	CBD-CGD-O2D-CED
18	1	1011	CLA	C1A-C2A-CAA-CBA
18	B	1219	CLA	CHA-CBD-CGD-O1D
18	B	1219	CLA	CHA-CBD-CGD-O2D
23	B	5005	LMG	C2-C1-O1-C7
23	B	5005	LMG	O6-C1-O1-C7
23	B	5005	LMG	C11-C10-O7-C8
18	B	1218	CLA	C2-C1-O2A-CGA
18	B	1218	CLA	CHA-CBD-CGD-O1D
18	B	1218	CLA	CHA-CBD-CGD-O2D
18	B	1218	CLA	C2-C3-C5-C6
18	B	1218	CLA	C4-C3-C5-C6
18	A	1109	CLA	C1A-C2A-CAA-CBA
18	A	1109	CLA	C3A-C2A-CAA-CBA
18	A	1109	CLA	C2-C3-C5-C6
18	A	1109	CLA	C4-C3-C5-C6
18	B	1203	CLA	C6-C7-C8-C9
18	1	1012	CLA	C3A-C2A-CAA-CBA
18	A	1106	CLA	C3A-C2A-CAA-CBA
28	3	3011	CHL	C2-C1-O2A-CGA
22	A	6008	BCR	C11-C10-C9-C8
22	A	6008	BCR	C11-C10-C9-C34
22	A	6008	BCR	C10-C11-C12-C13
18	A	1103	CLA	C1A-C2A-CAA-CBA
18	A	1103	CLA	CHA-CBD-CGD-O1D
18	A	1103	CLA	CHA-CBD-CGD-O2D
18	A	1103	CLA	CAD-CBD-CGD-O1D
18	A	1103	CLA	CAD-CBD-CGD-O2D
18	B	1224	CLA	C1A-C2A-CAA-CBA
18	B	1224	CLA	C3A-C2A-CAA-CBA
18	B	1224	CLA	CBD-CGD-O2D-CED
18	4	4006	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	4	4006	CLA	CHA-CBD-CGD-O2D
18	4	4006	CLA	CBD-CGD-O2D-CED
18	F	1302	CLA	CHA-CBD-CGD-O1D
18	F	1302	CLA	CHA-CBD-CGD-O2D
18	F	1302	CLA	CBD-CGD-O2D-CED
18	4	4017	CLA	C2-C1-O2A-CGA
18	A	1122	CLA	C1A-C2A-CAA-CBA
18	A	1122	CLA	CHA-CBD-CGD-O1D
18	A	1122	CLA	CHA-CBD-CGD-O2D
27	3	3501	LUT	C21-C26-C27-C28
27	3	3501	LUT	C27-C28-C29-C30
27	3	3501	LUT	C27-C28-C29-C39
22	B	6010	BCR	C11-C10-C9-C8
22	B	6010	BCR	C11-C10-C9-C34
22	B	6010	BCR	C17-C18-C19-C20
22	B	6010	BCR	C36-C18-C19-C20
18	B	1239	CLA	C1A-C2A-CAA-CBA
18	B	1239	CLA	C3A-C2A-CAA-CBA
18	B	1239	CLA	CBD-CGD-O2D-CED
18	1	1007	CLA	CBD-CGD-O2D-CED
18	A	1124	CLA	C2-C1-O2A-CGA
18	1	1008	CLA	CBD-CGD-O2D-CED
18	1	1002	CLA	CBA-CGA-O2A-C1
18	B	1213	CLA	CBD-CGD-O2D-CED
18	B	1213	CLA	C2-C3-C5-C6
18	B	1213	CLA	C4-C3-C5-C6
18	A	1105	CLA	C1A-C2A-CAA-CBA
18	A	1105	CLA	C3A-C2A-CAA-CBA
18	A	1105	CLA	C2A-CAA-CBA-CGA
18	A	1105	CLA	C2-C1-O2A-CGA
18	A	1105	CLA	CBD-CGD-O2D-CED
18	A	1105	CLA	C2-C3-C5-C6
18	A	1105	CLA	C4-C3-C5-C6
22	B	6009	BCR	C1-C6-C7-C8
22	B	6009	BCR	C5-C6-C7-C8
22	B	6009	BCR	C7-C8-C9-C10
22	B	6009	BCR	C7-C8-C9-C34
22	K	2011	BCR	C7-C8-C9-C10
22	K	2011	BCR	C7-C8-C9-C34
22	A	6002	BCR	C7-C8-C9-C10
22	A	6002	BCR	C7-C8-C9-C34
22	A	6002	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	A	6002	BCR	C11-C10-C9-C34
22	A	6002	BCR	C10-C11-C12-C13
22	A	6002	BCR	C21-C22-C23-C24
22	A	6002	BCR	C37-C22-C23-C24
18	L	1501	CLA	C1A-C2A-CAA-CBA
18	B	1021	CLA	CHA-CBD-CGD-O1D
18	B	1021	CLA	CHA-CBD-CGD-O2D
18	B	1215	CLA	C3A-C2A-CAA-CBA
18	B	1215	CLA	CBD-CGD-O2D-CED
18	B	1215	CLA	C2-C3-C5-C6
18	B	1215	CLA	C4-C3-C5-C6
18	A	1128	CLA	CHA-CBD-CGD-O2D
20	B	5002	PQN	C12-C13-C15-C16
20	B	5002	PQN	C14-C13-C15-C16
21	A	5003	LHG	O2-C2-C3-O3
21	A	5003	LHG	C3-O3-P-O5
21	A	5003	LHG	C3-O3-P-O6
22	A	6011	BCR	C11-C12-C13-C14
22	A	6011	BCR	C11-C12-C13-C35
22	A	6011	BCR	C21-C22-C23-C24
22	A	6011	BCR	C37-C22-C23-C24
18	A	1119	CLA	C1A-C2A-CAA-CBA
22	F	6016	BCR	C11-C10-C9-C8
22	F	6016	BCR	C11-C10-C9-C34
22	F	6016	BCR	C10-C11-C12-C13
18	A	1101	CLA	C2-C1-O2A-CGA
18	A	1138	CLA	CHA-CBD-CGD-O1D
18	A	1138	CLA	CHA-CBD-CGD-O2D
18	K	1001	CLA	CBA-CGA-O2A-C1
18	B	1012	CLA	CBD-CGD-O2D-CED
18	G	1001	CLA	C2-C1-O2A-CGA
18	G	1001	CLA	CBD-CGD-O2D-CED
18	G	1001	CLA	O1D-CGD-O2D-CED
18	B	1205	CLA	CBD-CGD-O2D-CED
18	B	1210	CLA	CHA-CBD-CGD-O1D
18	B	1210	CLA	CHA-CBD-CGD-O2D
18	B	1210	CLA	CBD-CGD-O2D-CED
22	A	6007	BCR	C11-C10-C9-C8
22	A	6007	BCR	C11-C10-C9-C34
22	A	6007	BCR	C10-C11-C12-C13
18	B	1226	CLA	C11-C12-C13-C14
28	4	4011	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	4	4010	CHL	C2C-C3C-CAC-CBC
18	B	1201	CLA	O1D-CGD-O2D-CED
18	2	2001	CLA	O1D-CGD-O2D-CED
18	4	4003	CLA	O1D-CGD-O2D-CED
18	B	1232	CLA	O1D-CGD-O2D-CED
18	2	2002	CLA	O1D-CGD-O2D-CED
18	A	1151	CLA	O1D-CGD-O2D-CED
18	B	1023	CLA	O1D-CGD-O2D-CED
18	3	3018	CLA	O1D-CGD-O2D-CED
18	4	4002	CLA	O1D-CGD-O2D-CED
18	L	1503	CLA	O1D-CGD-O2D-CED
18	1	1011	CLA	O1D-CGD-O2D-CED
18	B	1219	CLA	O1D-CGD-O2D-CED
18	B	1203	CLA	O1D-CGD-O2D-CED
18	1	1012	CLA	O1D-CGD-O2D-CED
18	4	4006	CLA	O1D-CGD-O2D-CED
18	1	1008	CLA	O1D-CGD-O2D-CED
18	A	1113	CLA	O1D-CGD-O2D-CED
21	B	5004	LHG	O9-C7-O7-C5
18	2	2002	CLA	C2C-C3C-CAC-CBC
18	F	1302	CLA	C2C-C3C-CAC-CBC
18	B	1240	CLA	O1D-CGD-O2D-CED
18	1	1003	CLA	O1D-CGD-O2D-CED
18	A	1126	CLA	O1D-CGD-O2D-CED
18	1	1013	CLA	O1D-CGD-O2D-CED
18	2	2009	CLA	O1D-CGD-O2D-CED
18	4	4016	CLA	O1D-CGD-O2D-CED
18	4	4007	CLA	O1D-CGD-O2D-CED
18	A	1115	CLA	O1D-CGD-O2D-CED
18	H	1000	CLA	O1D-CGD-O2D-CED
18	F	1301	CLA	O1D-CGD-O2D-CED
18	2	2007	CLA	O1D-CGD-O2D-CED
18	A	1104	CLA	O1D-CGD-O2D-CED
18	2	2016	CLA	O1D-CGD-O2D-CED
18	3	3006	CLA	O1D-CGD-O2D-CED
18	3	3003	CLA	O1D-CGD-O2D-CED
18	3	3012	CLA	O1D-CGD-O2D-CED
18	1	1007	CLA	O1D-CGD-O2D-CED
18	B	1213	CLA	O1D-CGD-O2D-CED
18	K	1001	CLA	O1D-CGD-O2D-CED
18	B	1210	CLA	O1D-CGD-O2D-CED
18	B	1226	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	F	5001	LMG	C29-C28-O8-C9
18	3	3004	CLA	CBD-CGD-O2D-CED
18	B	1222	CLA	CBD-CGD-O2D-CED
18	A	1013	CLA	CBD-CGD-O2D-CED
18	A	1126	CLA	CBD-CGD-O2D-CED
18	A	1237	CLA	CBD-CGD-O2D-CED
18	A	1121	CLA	CBD-CGD-O2D-CED
18	A	1112	CLA	CBD-CGD-O2D-CED
18	A	1118	CLA	CBD-CGD-O2D-CED
18	4	4003	CLA	CBD-CGD-O2D-CED
18	B	1208	CLA	CBD-CGD-O2D-CED
18	B	1204	CLA	CBD-CGD-O2D-CED
18	2	2012	CLA	CBD-CGD-O2D-CED
18	4	4007	CLA	CBD-CGD-O2D-CED
18	A	1115	CLA	CBD-CGD-O2D-CED
18	H	1000	CLA	CBD-CGD-O2D-CED
18	A	1129	CLA	CBD-CGD-O2D-CED
18	F	1301	CLA	CBD-CGD-O2D-CED
18	L	1502	CLA	CBD-CGD-O2D-CED
18	B	1023	CLA	CBD-CGD-O2D-CED
18	3	3018	CLA	CBD-CGD-O2D-CED
18	B	1202	CLA	CBD-CGD-O2D-CED
18	B	1229	CLA	CBD-CGD-O2D-CED
18	A	1135	CLA	CBD-CGD-O2D-CED
18	A	1127	CLA	CBD-CGD-O2D-CED
18	4	4005	CLA	CBD-CGD-O2D-CED
18	B	1230	CLA	CBD-CGD-O2D-CED
18	A	1120	CLA	CBD-CGD-O2D-CED
18	A	1108	CLA	CBD-CGD-O2D-CED
18	4	4002	CLA	CBD-CGD-O2D-CED
18	A	1125	CLA	CBD-CGD-O2D-CED
18	B	1206	CLA	CBD-CGD-O2D-CED
18	A	1117	CLA	CBD-CGD-O2D-CED
18	B	1207	CLA	CBD-CGD-O2D-CED
18	B	1235	CLA	CBD-CGD-O2D-CED
18	A	1140	CLA	CBD-CGD-O2D-CED
18	1	1004	CLA	CBD-CGD-O2D-CED
18	3	3005	CLA	CBD-CGD-O2D-CED
18	B	1231	CLA	CBD-CGD-O2D-CED
18	B	1234	CLA	CBD-CGD-O2D-CED
18	B	1209	CLA	CBD-CGD-O2D-CED
18	1	1011	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	B	1219	CLA	CBD-CGD-O2D-CED
18	A	1109	CLA	CBD-CGD-O2D-CED
18	B	1203	CLA	CBD-CGD-O2D-CED
18	1	1012	CLA	CBD-CGD-O2D-CED
18	A	1106	CLA	CBD-CGD-O2D-CED
18	G	1002	CLA	CBD-CGD-O2D-CED
18	A	1122	CLA	CBD-CGD-O2D-CED
18	A	1124	CLA	CBD-CGD-O2D-CED
18	A	1113	CLA	CBD-CGD-O2D-CED
18	B	1021	CLA	CBD-CGD-O2D-CED
18	A	1128	CLA	CBD-CGD-O2D-CED
18	3	3001	CLA	CBD-CGD-O2D-CED
18	A	1119	CLA	CBD-CGD-O2D-CED
18	B	1217	CLA	CBD-CGD-O2D-CED
18	A	1138	CLA	CBD-CGD-O2D-CED
18	B	1212	CLA	CBD-CGD-O2D-CED
18	K	1001	CLA	CBD-CGD-O2D-CED
18	B	1226	CLA	CBD-CGD-O2D-CED
18	B	1222	CLA	O1A-CGA-O2A-C1
18	A	1237	CLA	O1A-CGA-O2A-C1
18	A	1133	CLA	O1A-CGA-O2A-C1
18	B	1234	CLA	O1A-CGA-O2A-C1
18	3	3013	CLA	O1A-CGA-O2A-C1
18	4	4016	CLA	O1A-CGA-O2A-C1
18	4	4008	CLA	O1A-CGA-O2A-C1
18	1	1014	CLA	O1A-CGA-O2A-C1
18	2	2002	CLA	C4C-C3C-CAC-CBC
18	A	1151	CLA	C4C-C3C-CAC-CBC
28	4	4010	CHL	C4C-C3C-CAC-CBC
18	A	1237	CLA	O1D-CGD-O2D-CED
18	1	1001	CLA	O1D-CGD-O2D-CED
18	3	3017	CLA	O1D-CGD-O2D-CED
18	A	1120	CLA	O1D-CGD-O2D-CED
18	B	1206	CLA	O1D-CGD-O2D-CED
18	3	3005	CLA	O1D-CGD-O2D-CED
18	A	1131	CLA	O1D-CGD-O2D-CED
18	B	1231	CLA	O1D-CGD-O2D-CED
18	A	1109	CLA	O1D-CGD-O2D-CED
18	F	1302	CLA	O1D-CGD-O2D-CED
18	A	1105	CLA	O1D-CGD-O2D-CED
18	B	1021	CLA	O1D-CGD-O2D-CED
18	B	1205	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	1126	CLA	C10-C11-C12-C13
18	3	3013	CLA	CBA-CGA-O2A-C1
18	G	1002	CLA	CBA-CGA-O2A-C1
18	B	1217	CLA	CBA-CGA-O2A-C1
18	2	2007	CLA	C4C-C3C-CAC-CBC
18	F	1302	CLA	C4C-C3C-CAC-CBC
18	A	1114	CLA	O1D-CGD-O2D-CED
18	3	3002	CLA	O1D-CGD-O2D-CED
18	A	1137	CLA	O1D-CGD-O2D-CED
18	2	2008	CLA	O1D-CGD-O2D-CED
18	B	1228	CLA	O1D-CGD-O2D-CED
18	A	1116	CLA	O1D-CGD-O2D-CED
18	2	2006	CLA	O1D-CGD-O2D-CED
18	2	2012	CLA	O1D-CGD-O2D-CED
18	1	1006	CLA	O1D-CGD-O2D-CED
18	2	2005	CLA	O1D-CGD-O2D-CED
18	B	1207	CLA	O1D-CGD-O2D-CED
18	B	1214	CLA	O1D-CGD-O2D-CED
18	1	1014	CLA	O1D-CGD-O2D-CED
18	B	1215	CLA	O1D-CGD-O2D-CED
18	B	1012	CLA	O1D-CGD-O2D-CED
18	B	1222	CLA	CBA-CGA-O2A-C1
18	A	1237	CLA	CBA-CGA-O2A-C1
18	B	1232	CLA	CBA-CGA-O2A-C1
18	A	1133	CLA	CBA-CGA-O2A-C1
18	A	1120	CLA	CBA-CGA-O2A-C1
18	B	1225	CLA	CBD-CGD-O2D-CED
18	G	1003	CLA	CBD-CGD-O2D-CED
18	3	3013	CLA	CBD-CGD-O2D-CED
18	B	1238	CLA	CBD-CGD-O2D-CED
18	4	4008	CLA	CBD-CGD-O2D-CED
18	A	1103	CLA	CBD-CGD-O2D-CED
18	4	4017	CLA	CBD-CGD-O2D-CED
18	B	1216	CLA	CBD-CGD-O2D-CED
18	L	1501	CLA	CBD-CGD-O2D-CED
18	4	4012	CLA	CBD-CGD-O2D-CED
18	A	1151	CLA	C2C-C3C-CAC-CBC
18	2	2009	CLA	O1A-CGA-O2A-C1
18	4	4003	CLA	O1A-CGA-O2A-C1
18	4	4007	CLA	O1A-CGA-O2A-C1
18	B	1232	CLA	O1A-CGA-O2A-C1
18	3	3018	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	1102	CLA	O1A-CGA-O2A-C1
18	A	1120	CLA	O1A-CGA-O2A-C1
18	4	4002	CLA	O1A-CGA-O2A-C1
18	F	1302	CLA	O1A-CGA-O2A-C1
18	4	4012	CLA	O1A-CGA-O2A-C1
18	1	1013	CLA	O1A-CGA-O2A-C1
18	A	1115	CLA	O1A-CGA-O2A-C1
18	B	1209	CLA	O1A-CGA-O2A-C1
18	G	1002	CLA	O1A-CGA-O2A-C1
18	K	1001	CLA	O1A-CGA-O2A-C1
18	3	3008	CLA	O1D-CGD-O2D-CED
18	A	1139	CLA	O1D-CGD-O2D-CED
18	A	1107	CLA	O1D-CGD-O2D-CED
18	2	2003	CLA	O1D-CGD-O2D-CED
18	A	1022	CLA	O1D-CGD-O2D-CED
18	A	1133	CLA	O1D-CGD-O2D-CED
18	B	1224	CLA	O1D-CGD-O2D-CED
18	4	4007	CLA	C2C-C3C-CAC-CBC
18	2	2007	CLA	C2C-C3C-CAC-CBC
18	J	1302	CLA	O1D-CGD-O2D-CED
18	B	1204	CLA	O1D-CGD-O2D-CED
18	3	3018	CLA	C4C-C3C-CAC-CBC
18	A	1102	CLA	CBD-CGD-O2D-CED
18	A	1110	CLA	CBD-CGD-O2D-CED
18	A	1013	CLA	O1D-CGD-O2D-CED
18	A	1130	CLA	O1D-CGD-O2D-CED
18	A	1140	CLA	O1D-CGD-O2D-CED
18	B	1239	CLA	O1D-CGD-O2D-CED
23	B	5005	LMG	O9-C10-O7-C8
23	J	5001	LMG	C4-C5-C6-O5
18	A	1135	CLA	O1A-CGA-O2A-C1
18	3	3005	CLA	O1A-CGA-O2A-C1
18	A	1124	CLA	O1A-CGA-O2A-C1
18	1	1013	CLA	CBA-CGA-O2A-C1
18	A	1115	CLA	CBA-CGA-O2A-C1
18	A	1108	CLA	CBA-CGA-O2A-C1
18	1	1007	CLA	CBA-CGA-O2A-C1
18	A	1113	CLA	CBA-CGA-O2A-C1
18	4	4007	CLA	C4C-C3C-CAC-CBC
18	3	3018	CLA	C2C-C3C-CAC-CBC
18	A	1108	CLA	O1A-CGA-O2A-C1
18	B	1212	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	1013	CLA	C3-C5-C6-C7
18	2	2001	CLA	C3-C5-C6-C7
18	G	1003	CLA	C3-C5-C6-C7
18	4	4003	CLA	C3-C5-C6-C7
18	A	1107	CLA	C3-C5-C6-C7
18	L	1502	CLA	C3-C5-C6-C7
18	A	1131	CLA	C3-C5-C6-C7
18	B	1203	CLA	C3-C5-C6-C7
18	A	1103	CLA	C3-C5-C6-C7
18	G	1001	CLA	C3-C5-C6-C7
18	B	1226	CLA	C3-C5-C6-C7
18	4	4001	CLA	CBA-CGA-O2A-C1
18	2	2009	CLA	CBA-CGA-O2A-C1
18	4	4003	CLA	CBA-CGA-O2A-C1
18	A	1116	CLA	CBA-CGA-O2A-C1
18	B	1204	CLA	CBA-CGA-O2A-C1
18	2	2006	CLA	CBA-CGA-O2A-C1
18	4	4007	CLA	CBA-CGA-O2A-C1
18	3	3018	CLA	CBA-CGA-O2A-C1
18	A	1102	CLA	CBA-CGA-O2A-C1
18	B	1234	CLA	CBA-CGA-O2A-C1
18	F	1302	CLA	CBA-CGA-O2A-C1
18	3	3002	CLA	C2C-C3C-CAC-CBC
23	F	5001	LMG	O10-C28-O8-C9
23	J	5001	LMG	C11-C10-O7-C8
18	A	1121	CLA	O1D-CGD-O2D-CED
18	A	1124	CLA	O1D-CGD-O2D-CED
18	A	1111	CLA	CBD-CGD-O2D-CED
18	B	1236	CLA	CBD-CGD-O2D-CED
18	4	4016	CLA	C2C-C3C-CAC-CBC
18	2	2012	CLA	O1A-CGA-O2A-C1
18	1	1006	CLA	O1A-CGA-O2A-C1
18	A	1118	CLA	O1A-CGA-O2A-C1
18	A	1113	CLA	O1A-CGA-O2A-C1
18	1	1002	CLA	O1A-CGA-O2A-C1
18	B	1217	CLA	O1A-CGA-O2A-C1
18	2	2008	CLA	C2C-C3C-CAC-CBC
28	1	1010	CHL	C2C-C3C-CAC-CBC
23	F	5001	LMG	O9-C10-O7-C8
23	J	5001	LMG	O6-C5-C6-O5
18	B	1208	CLA	C4-C3-C5-C6
18	A	1116	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	2	2006	CLA	C4-C3-C5-C6
18	B	1207	CLA	C4-C3-C5-C6
18	A	1122	CLA	C4-C3-C5-C6
18	A	1101	CLA	C4-C3-C5-C6
18	B	1208	CLA	C2-C3-C5-C6
18	B	1207	CLA	C2-C3-C5-C6
18	A	1140	CLA	C2-C3-C5-C6
18	A	1122	CLA	C2-C3-C5-C6
18	G	1003	CLA	C2A-CAA-CBA-CGA
18	3	3013	CLA	C2A-CAA-CBA-CGA
18	B	1208	CLA	C2A-CAA-CBA-CGA
18	H	1000	CLA	C2A-CAA-CBA-CGA
18	A	1129	CLA	C2A-CAA-CBA-CGA
18	L	1502	CLA	C2A-CAA-CBA-CGA
18	1	1014	CLA	C2A-CAA-CBA-CGA
28	3	3011	CHL	C2A-CAA-CBA-CGA
18	B	1239	CLA	C2A-CAA-CBA-CGA
18	G	1001	CLA	C2A-CAA-CBA-CGA
18	A	1104	CLA	O1A-CGA-O2A-C1
18	B	1222	CLA	O1D-CGD-O2D-CED
18	A	1108	CLA	O1D-CGD-O2D-CED
18	B	1234	CLA	O1D-CGD-O2D-CED
18	1	1007	CLA	O1A-CGA-O2A-C1
18	B	1220	CLA	C3-C5-C6-C7
18	1	1003	CLA	C3-C5-C6-C7
18	2	2004	CLA	C3-C5-C6-C7
18	B	1204	CLA	C3-C5-C6-C7
18	A	1134	CLA	C3-C5-C6-C7
18	A	1120	CLA	C3-C5-C6-C7
18	A	1106	CLA	C3-C5-C6-C7
21	1	1801	LHG	C24-C23-O8-C6
18	A	1112	CLA	CBA-CGA-O2A-C1
18	A	1130	CLA	CBA-CGA-O2A-C1
18	A	1104	CLA	CBA-CGA-O2A-C1
18	A	1135	CLA	CBA-CGA-O2A-C1
18	B	1230	CLA	CBA-CGA-O2A-C1
18	4	4002	CLA	CBA-CGA-O2A-C1
18	B	1211	CLA	CBA-CGA-O2A-C1
18	3	3005	CLA	CBA-CGA-O2A-C1
18	3	3012	CLA	CBA-CGA-O2A-C1
18	A	1124	CLA	CBA-CGA-O2A-C1
18	4	4012	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	B	8001	LMU	O5B-C5B-C6B-O6B
23	F	5001	LMG	O6-C5-C6-O5
18	A	1129	CLA	O1D-CGD-O2D-CED
18	B	1202	CLA	O1D-CGD-O2D-CED
18	A	1117	CLA	O1D-CGD-O2D-CED
18	A	1106	CLA	O1D-CGD-O2D-CED
18	3	3007	CLA	C2C-C3C-CAC-CBC
18	L	1502	CLA	O1D-CGD-O2D-CED
18	A	1127	CLA	O1D-CGD-O2D-CED
18	4	4005	CLA	O1D-CGD-O2D-CED
18	B	1209	CLA	O1D-CGD-O2D-CED
18	G	1002	CLA	O1D-CGD-O2D-CED
18	3	3001	CLA	O1D-CGD-O2D-CED
18	B	1217	CLA	O1D-CGD-O2D-CED
26	B	8002	LMU	O5B-C5B-C6B-O6B
18	4	4009	CLA	O1A-CGA-O2A-C1
18	A	1112	CLA	O1A-CGA-O2A-C1
18	B	1204	CLA	O1A-CGA-O2A-C1
18	B	1227	CLA	O1A-CGA-O2A-C1
18	B	1230	CLA	O1A-CGA-O2A-C1
18	B	1211	CLA	O1A-CGA-O2A-C1
18	B	1208	CLA	O1D-CGD-O2D-CED
18	A	1135	CLA	O1D-CGD-O2D-CED
18	B	1230	CLA	O1D-CGD-O2D-CED
18	1	1004	CLA	O1D-CGD-O2D-CED
18	A	1138	CLA	O1D-CGD-O2D-CED
22	A	6003	BCR	C9-C10-C11-C12
22	L	6020	BCR	C19-C20-C21-C22
22	3	3503	BCR	C9-C10-C11-C12
23	F	5001	LMG	C4-C5-C6-O5
18	3	3008	CLA	C2C-C3C-CAC-CBC
18	4	4016	CLA	C4C-C3C-CAC-CBC
18	4	4008	CLA	C2C-C3C-CAC-CBC
18	A	1119	CLA	O1D-CGD-O2D-CED
21	B	5004	LHG	O2-C2-C3-O3
21	2	2801	LHG	O2-C2-C3-O3
18	B	1218	CLA	C3-C5-C6-C7
18	A	1124	CLA	C3-C5-C6-C7
18	A	1138	CLA	C3-C5-C6-C7
18	B	1205	CLA	C3-C5-C6-C7
18	4	4009	CLA	CBA-CGA-O2A-C1
18	2	2012	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	2	2005	CLA	CBA-CGA-O2A-C1
18	B	1227	CLA	CBA-CGA-O2A-C1
23	B	5005	LMG	C29-C28-O8-C9
18	4	4006	CLA	CBA-CGA-O2A-C1
18	A	1101	CLA	CBA-CGA-O2A-C1
18	1	1002	CLA	C2C-C3C-CAC-CBC
21	B	5004	LHG	C24-C23-O8-C6
18	4	4001	CLA	O1A-CGA-O2A-C1
18	A	1116	CLA	O1A-CGA-O2A-C1
18	3	3004	CLA	O1D-CGD-O2D-CED
18	A	1118	CLA	O1D-CGD-O2D-CED
18	A	1128	CLA	O1D-CGD-O2D-CED
18	3	3002	CLA	C4C-C3C-CAC-CBC
18	1	1008	CLA	CBA-CGA-O2A-C1
18	B	1220	CLA	CBD-CGD-O2D-CED
18	1	1007	CLA	C2C-C3C-CAC-CBC
23	F	5002	LMG	O6-C5-C6-O5
18	A	1112	CLA	O1D-CGD-O2D-CED
18	B	1234	CLA	C3-C5-C6-C7
18	B	1219	CLA	C3-C5-C6-C7
18	1	1006	CLA	CBA-CGA-O2A-C1
18	2	2007	CLA	CBA-CGA-O2A-C1
23	J	5001	LMG	C29-C28-O8-C9
18	2	2008	CLA	C4C-C3C-CAC-CBC
21	2	2801	LHG	C2-C3-O3-P
21	1	1801	LHG	O10-C23-O8-C6
18	A	1130	CLA	O1A-CGA-O2A-C1
18	2	2005	CLA	O1A-CGA-O2A-C1
23	B	5005	LMG	O6-C5-C6-O5
18	4	4001	CLA	C4-C3-C5-C6
18	B	1222	CLA	C4-C3-C5-C6
18	B	1225	CLA	C4-C3-C5-C6
18	A	1121	CLA	C4-C3-C5-C6
20	A	5001	PQN	C14-C13-C15-C16
18	3	3005	CLA	C4-C3-C5-C6
18	4	4001	CLA	C2-C3-C5-C6
18	B	1222	CLA	C2-C3-C5-C6
18	B	1225	CLA	C2-C3-C5-C6
18	A	1121	CLA	C2-C3-C5-C6
18	2	2006	CLA	C2-C3-C5-C6
18	3	3010	CLA	C2-C3-C5-C6
20	A	5001	PQN	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	3	3005	CLA	C2-C3-C5-C6
18	B	1225	CLA	C2A-CAA-CBA-CGA
18	A	1151	CLA	C2A-CAA-CBA-CGA
18	A	1125	CLA	O1D-CGD-O2D-CED
18	A	1122	CLA	O1D-CGD-O2D-CED
18	K	1001	CLA	C2C-C3C-CAC-CBC
18	2	2007	CLA	O1A-CGA-O2A-C1
23	J	5001	LMG	O10-C28-O8-C9
18	L	1503	CLA	O1A-CGA-O2A-C1
18	3	3012	CLA	O1A-CGA-O2A-C1
23	B	5005	LMG	O10-C28-O8-C9
18	4	4006	CLA	O1A-CGA-O2A-C1
18	A	1101	CLA	O1A-CGA-O2A-C1
18	A	1137	CLA	CBA-CGA-O2A-C1
18	B	1235	CLA	CBA-CGA-O2A-C1
18	L	1503	CLA	CBA-CGA-O2A-C1
18	A	1136	CLA	CBA-CGA-O2A-C1
18	B	1226	CLA	CBA-CGA-O2A-C1
18	1	1001	CLA	C2C-C3C-CAC-CBC
18	3	3002	CLA	CBA-CGA-O2A-C1
28	1	1010	CHL	C4C-C3C-CAC-CBC
18	B	1229	CLA	O1D-CGD-O2D-CED
18	B	1235	CLA	O1D-CGD-O2D-CED
23	F	5002	LMG	C4-C5-C6-O5
18	B	1225	CLA	O1D-CGD-O2D-CED
18	3	3013	CLA	O1D-CGD-O2D-CED
18	3	3012	CLA	C2C-C3C-CAC-CBC
21	B	5004	LHG	C1-C2-C3-O3
26	B	8002	LMU	C4B-C5B-C6B-O6B
18	3	3008	CLA	O1A-CGA-O2A-C1
18	A	1137	CLA	O1A-CGA-O2A-C1
18	B	1226	CLA	O1A-CGA-O2A-C1
18	4	4001	CLA	C3-C5-C6-C7
18	B	1207	CLA	C3-C5-C6-C7
18	4	4012	CLA	O1D-CGD-O2D-CED
18	A	1132	CLA	CBA-CGA-O2A-C1
18	1	1005	CLA	CBA-CGA-O2A-C1
18	B	1240	CLA	CBA-CGA-O2A-C1
18	J	1302	CLA	CBA-CGA-O2A-C1
18	2	2004	CLA	CBA-CGA-O2A-C1
18	3	3008	CLA	CBA-CGA-O2A-C1
18	2	2008	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	1123	CLA	CBA-CGA-O2A-C1
18	A	1129	CLA	CBA-CGA-O2A-C1
23	4	4801	LMG	C29-C28-O8-C9
18	B	1202	CLA	CBA-CGA-O2A-C1
18	A	1125	CLA	CBA-CGA-O2A-C1
18	A	1117	CLA	CBA-CGA-O2A-C1
18	1	1004	CLA	CBA-CGA-O2A-C1
18	B	1231	CLA	CBA-CGA-O2A-C1
18	3	3006	CLA	CBA-CGA-O2A-C1
23	G	2021	LMG	C29-C28-O8-C9
18	B	1219	CLA	CBA-CGA-O2A-C1
18	4	4017	CLA	CBA-CGA-O2A-C1
18	B	1215	CLA	CBA-CGA-O2A-C1
18	A	1128	CLA	CBA-CGA-O2A-C1
18	G	1001	CLA	CBA-CGA-O2A-C1
18	B	1210	CLA	CBA-CGA-O2A-C1
23	G	2021	LMG	O6-C5-C6-O5
18	3	3010	CLA	CBD-CGD-O2D-CED
22	A	6008	BCR	C15-C16-C17-C18
22	K	2011	BCR	C19-C20-C21-C22
21	A	5003	LHG	C23-C24-C25-C26
18	A	1107	CLA	C13-C15-C16-C17
18	B	1203	CLA	C8-C10-C11-C12
18	B	1216	CLA	O1D-CGD-O2D-CED
18	1	1008	CLA	O1A-CGA-O2A-C1
18	3	3013	CLA	C2C-C3C-CAC-CBC
26	B	8001	LMU	C4B-C5B-C6B-O6B
23	B	5005	LMG	C4-C5-C6-O5
18	A	1132	CLA	C13-C15-C16-C17
18	B	1220	CLA	C8-C10-C11-C12
18	B	1220	CLA	C10-C11-C12-C13
18	B	1240	CLA	C15-C16-C17-C18
18	A	1123	CLA	C10-C11-C12-C13
18	B	1229	CLA	C13-C15-C16-C17
21	1	1801	LHG	C23-C24-C25-C26
21	A	7001	LHG	C23-C24-C25-C26
18	G	1002	CLA	C2C-C3C-CAC-CBC
18	A	1129	CLA	O1A-CGA-O2A-C1
18	3	3006	CLA	O1A-CGA-O2A-C1
18	A	1116	CLA	C2-C3-C5-C6
18	A	1101	CLA	C2-C3-C5-C6
18	B	1220	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	4	4001	CLA	C6-C7-C8-C9
18	B	1222	CLA	C6-C7-C8-C9
18	2	2001	CLA	C6-C7-C8-C9
18	A	1237	CLA	C11-C10-C8-C9
18	A	1112	CLA	C11-C10-C8-C9
18	A	1139	CLA	C11-C12-C13-C14
18	4	4003	CLA	C6-C7-C8-C9
18	B	1221	CLA	C11-C12-C13-C14
18	1	1001	CLA	C11-C10-C8-C9
18	A	1120	CLA	C11-C10-C8-C9
18	A	1125	CLA	C6-C7-C8-C9
18	B	1207	CLA	C6-C7-C8-C9
18	A	1140	CLA	C11-C10-C8-C9
18	A	1103	CLA	C14-C13-C15-C16
18	A	1122	CLA	C11-C12-C13-C14
18	A	1119	CLA	C11-C12-C13-C14
18	B	1226	CLA	C14-C13-C15-C16
18	4	4008	CLA	O1D-CGD-O2D-CED
18	A	1139	CLA	C15-C16-C17-C18
18	B	1216	CLA	C8-C10-C11-C12
18	A	1116	CLA	C2A-CAA-CBA-CGA
18	A	1109	CLA	C2A-CAA-CBA-CGA
18	L	1501	CLA	C2A-CAA-CBA-CGA
22	A	6003	BCR	C7-C8-C9-C34
22	B	6006	BCR	C7-C8-C9-C34
27	3	3502	LUT	C7-C8-C9-C19
22	F	6014	BCR	C36-C18-C19-C20
22	F	6014	BCR	C37-C22-C23-C24
27	4	4502	LUT	C27-C28-C29-C39
22	L	6019	BCR	C7-C8-C9-C34
27	4	4503	LUT	C7-C8-C9-C19
22	3	3503	BCR	C36-C18-C19-C20
22	G	2011	BCR	C37-C22-C23-C24
27	3	3501	LUT	C7-C8-C9-C19
22	B	6010	BCR	C7-C8-C9-C34
22	A	6011	BCR	C7-C8-C9-C34
22	F	6016	BCR	C11-C12-C13-C35
22	A	6003	BCR	C7-C8-C9-C10
22	B	6006	BCR	C7-C8-C9-C10
27	3	3502	LUT	C7-C8-C9-C10
22	F	6014	BCR	C21-C22-C23-C24
27	4	4502	LUT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
22	L	6019	BCR	C7-C8-C9-C10
27	4	4503	LUT	C7-C8-C9-C10
27	4	4503	LUT	C27-C28-C29-C30
22	G	2011	BCR	C21-C22-C23-C24
27	3	3501	LUT	C7-C8-C9-C10
22	B	6010	BCR	C7-C8-C9-C10
22	A	6011	BCR	C7-C8-C9-C10
23	G	2021	LMG	C4-C5-C6-O5
18	J	1302	CLA	O1A-CGA-O2A-C1
18	2	2008	CLA	O1A-CGA-O2A-C1
18	B	1202	CLA	O1A-CGA-O2A-C1
18	1	1004	CLA	O1A-CGA-O2A-C1
18	B	1219	CLA	O1A-CGA-O2A-C1
18	A	1128	CLA	O1A-CGA-O2A-C1
18	B	1210	CLA	O1A-CGA-O2A-C1
18	3	3010	CLA	C10-C11-C12-C13
18	A	1022	CLA	C10-C11-C12-C13
18	B	1227	CLA	C13-C15-C16-C17
18	A	1120	CLA	C8-C10-C11-C12
18	B	1214	CLA	C5-C6-C7-C8
18	A	1131	CLA	C8-C10-C11-C12
20	B	5002	PQN	C23-C25-C26-C27
20	B	5002	PQN	C25-C26-C27-C28
18	4	4012	CLA	C8-C10-C11-C12
18	B	1238	CLA	O1D-CGD-O2D-CED
18	2	2016	CLA	C2C-C3C-CAC-CBC
18	3	3008	CLA	C4C-C3C-CAC-CBC
18	3	3007	CLA	C4C-C3C-CAC-CBC
18	2	2012	CLA	C3-C5-C6-C7
18	B	1206	CLA	C3-C5-C6-C7
18	B	1012	CLA	C3-C5-C6-C7
18	B	1201	CLA	CBA-CGA-O2A-C1
18	B	1207	CLA	CBA-CGA-O2A-C1
18	1	1011	CLA	CBA-CGA-O2A-C1
18	A	1119	CLA	CBA-CGA-O2A-C1
21	B	5004	LHG	O10-C23-O8-C6
18	A	1132	CLA	C8-C10-C11-C12
18	B	1225	CLA	C15-C16-C17-C18
18	B	1228	CLA	C10-C11-C12-C13
18	A	1112	CLA	C13-C15-C16-C17
18	4	4003	CLA	C15-C16-C17-C18
18	B	1221	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	B	1221	CLA	C15-C16-C17-C18
18	2	2012	CLA	C5-C6-C7-C8
18	A	1123	CLA	C13-C15-C16-C17
18	B	1232	CLA	C5-C6-C7-C8
18	B	1223	CLA	C15-C16-C17-C18
18	A	1104	CLA	C15-C16-C17-C18
18	A	1127	CLA	C5-C6-C7-C8
18	B	1230	CLA	C5-C6-C7-C8
18	B	1203	CLA	C13-C15-C16-C17
18	A	1106	CLA	C13-C15-C16-C17
18	B	1224	CLA	C10-C11-C12-C13
18	A	1128	CLA	C5-C6-C7-C8
18	B	1226	CLA	C8-C10-C11-C12
18	B	1240	CLA	O1A-CGA-O2A-C1
18	B	1225	CLA	C5-C6-C7-C8
18	2	2001	CLA	C10-C11-C12-C13
18	A	1112	CLA	C10-C11-C12-C13
18	B	1221	CLA	C8-C10-C11-C12
18	B	1204	CLA	C5-C6-C7-C8
18	L	1502	CLA	C10-C11-C12-C13
18	2	2007	CLA	C10-C11-C12-C13
18	4	4005	CLA	C8-C10-C11-C12
18	B	1207	CLA	C8-C10-C11-C12
18	1	1004	CLA	C13-C15-C16-C17
18	B	1218	CLA	C8-C10-C11-C12
18	B	1203	CLA	C5-C6-C7-C8
18	A	1122	CLA	C13-C15-C16-C17
18	B	1021	CLA	C13-C15-C16-C17
18	B	1012	CLA	C13-C15-C16-C17
18	B	1205	CLA	C10-C11-C12-C13
18	4	4008	CLA	C4C-C3C-CAC-CBC
18	A	1103	CLA	O1D-CGD-O2D-CED
18	4	4017	CLA	O1D-CGD-O2D-CED
18	L	1501	CLA	O1D-CGD-O2D-CED
21	B	5004	LHG	O1-C1-C2-O2
21	A	5003	LHG	O1-C1-C2-O2
23	4	4801	LMG	O10-C28-O8-C9
18	A	1117	CLA	O1A-CGA-O2A-C1
21	1	1801	LHG	C7-C8-C9-C10
23	G	2021	LMG	C28-C29-C30-C31
18	A	1132	CLA	C10-C11-C12-C13
18	2	2004	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
18	B	1021	CLA	C15-C16-C17-C18
18	A	1119	CLA	C10-C11-C12-C13
18	A	1119	CLA	C13-C15-C16-C17
18	B	1210	CLA	C15-C16-C17-C18
18	G	1003	CLA	O1D-CGD-O2D-CED
18	J	1302	CLA	C2-C1-O2A-CGA
18	A	1137	CLA	C2-C1-O2A-CGA
18	A	1112	CLA	C2-C1-O2A-CGA
18	A	1139	CLA	C2-C1-O2A-CGA
18	A	1022	CLA	C2-C1-O2A-CGA
18	A	1104	CLA	C2-C1-O2A-CGA
18	B	1230	CLA	C2-C1-O2A-CGA
18	A	1120	CLA	C2-C1-O2A-CGA
18	A	1140	CLA	C2-C1-O2A-CGA
18	1	1011	CLA	C2-C1-O2A-CGA
18	B	1203	CLA	C2-C1-O2A-CGA
18	A	1103	CLA	C2-C1-O2A-CGA
18	A	1119	CLA	C2-C1-O2A-CGA
18	B	1012	CLA	C2-C1-O2A-CGA
23	2	2802	LMG	C4-C5-C6-O5
18	A	1107	CLA	C15-C16-C17-C18
18	A	1104	CLA	C5-C6-C7-C8
18	4	4004	CLA	C8-C10-C11-C12
18	B	1215	CLA	C10-C11-C12-C13
21	A	7001	LHG	C7-C8-C9-C10
18	1	1011	CLA	C2C-C3C-CAC-CBC
18	4	4003	CLA	C2C-C3C-CAC-CBC
18	G	1003	CLA	C5-C6-C7-C8
18	A	1124	CLA	C5-C6-C7-C8
18	4	4001	CLA	C6-C7-C8-C10
18	B	1223	CLA	C11-C10-C8-C7
18	A	1104	CLA	C12-C13-C15-C16
18	B	1230	CLA	C11-C10-C8-C7
18	B	1234	CLA	C6-C7-C8-C10
18	A	1103	CLA	C12-C13-C15-C16
18	A	1122	CLA	C11-C10-C8-C7
18	B	1201	CLA	O1A-CGA-O2A-C1
18	1	1005	CLA	O1A-CGA-O2A-C1
18	A	1123	CLA	O1A-CGA-O2A-C1
18	B	1235	CLA	O1A-CGA-O2A-C1
18	B	1231	CLA	O1A-CGA-O2A-C1
18	1	1011	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	1136	CLA	O1A-CGA-O2A-C1
27	1	1502	LUT	C13-C14-C15-C35
22	A	6017	BCR	C9-C10-C11-C12
27	1	1501	LUT	C29-C30-C31-C32
27	I	6018	LUT	C13-C14-C15-C35
18	A	1151	CLA	CBA-CGA-O2A-C1
18	B	1228	CLA	C2A-CAA-CBA-CGA
18	1	1011	CLA	C2A-CAA-CBA-CGA
18	A	1110	CLA	O1D-CGD-O2D-CED
18	A	1126	CLA	C15-C16-C17-C18
18	B	1207	CLA	C5-C6-C7-C8
18	B	1235	CLA	C13-C15-C16-C17
18	B	1234	CLA	C8-C10-C11-C12
18	A	1122	CLA	C5-C6-C7-C8
20	B	5002	PQN	C15-C16-C17-C18
18	G	1001	CLA	C5-C6-C7-C8
18	2	2004	CLA	O1A-CGA-O2A-C1
18	A	1125	CLA	O1A-CGA-O2A-C1
18	B	1207	CLA	O1A-CGA-O2A-C1
18	4	4017	CLA	O1A-CGA-O2A-C1
26	B	8001	LMU	O5'-C1'-O1'-C1
18	B	1222	CLA	C5-C6-C7-C8
20	A	5001	PQN	C23-C25-C26-C27
18	A	1117	CLA	C15-C16-C17-C18
18	1	1004	CLA	C5-C6-C7-C8
18	B	1216	CLA	C13-C15-C16-C17
18	A	1119	CLA	C8-C10-C11-C12
22	F	6014	BCR	C10-C11-C12-C13
22	B	6010	BCR	C10-C11-C12-C13
22	K	2011	BCR	C10-C11-C12-C13
22	A	6011	BCR	C10-C11-C12-C13
18	1	1005	CLA	C3-C5-C6-C7
18	1	1001	CLA	C5-C6-C7-C8
18	B	1238	CLA	C5-C6-C7-C8
18	B	1202	CLA	C15-C16-C17-C18
18	B	1219	CLA	C5-C6-C7-C8
23	F	5002	LMG	C29-C28-O8-C9
18	L	1502	CLA	CBA-CGA-O2A-C1
18	A	1134	CLA	CBD-CGD-O2D-CED
18	A	1132	CLA	O1A-CGA-O2A-C1
18	B	1215	CLA	O1A-CGA-O2A-C1
18	G	1001	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	3	3017	CLA	CBA-CGA-O2A-C1
18	A	1123	CLA	C15-C16-C17-C18
18	A	1140	CLA	C5-C6-C7-C8
18	3	3005	CLA	C5-C6-C7-C8
18	A	1138	CLA	C8-C10-C11-C12
18	3	3005	CLA	C2C-C3C-CAC-CBC
21	A	5003	LHG	C28-C29-C30-C31
18	K	1001	CLA	C4C-C3C-CAC-CBC
23	G	2021	LMG	O10-C28-O8-C9
18	A	1105	CLA	O1A-CGA-O2A-C1
23	4	4801	LMG	C11-C10-O7-C8
18	1	1007	CLA	C4C-C3C-CAC-CBC
18	A	1102	CLA	O1D-CGD-O2D-CED
18	4	4001	CLA	C8-C10-C11-C12
18	B	1222	CLA	C15-C16-C17-C18
18	A	1126	CLA	C13-C15-C16-C17
18	A	1107	CLA	C8-C10-C11-C12
18	4	4004	CLA	C10-C11-C12-C13
18	B	1207	CLA	C13-C15-C16-C17
18	B	1224	CLA	C15-C16-C17-C18
18	B	1012	CLA	C5-C6-C7-C8
18	B	1210	CLA	C8-C10-C11-C12
21	B	5004	LHG	C3-O3-P-O6
21	1	1801	LHG	C3-O3-P-O6
18	B	1208	CLA	CBA-CGA-O2A-C1
18	B	1218	CLA	CBA-CGA-O2A-C1
18	B	1216	CLA	CBA-CGA-O2A-C1
18	B	1208	CLA	C5-C6-C7-C8
18	B	1218	CLA	C13-C15-C16-C17
18	A	1109	CLA	C13-C15-C16-C17
18	A	1119	CLA	O1A-CGA-O2A-C1
18	1	1002	CLA	C4C-C3C-CAC-CBC
18	A	1111	CLA	O1D-CGD-O2D-CED
18	B	1236	CLA	O1D-CGD-O2D-CED
21	2	2801	LHG	C1-C2-C3-O3
21	A	5003	LHG	C1-C2-C3-O3
23	4	4801	LMG	O9-C10-O7-C8
18	3	3010	CLA	C5-C6-C7-C8
28	1	1010	CHL	C2A-CAA-CBA-CGA
18	A	1106	CLA	C2A-CAA-CBA-CGA
18	2	2003	CLA	C6-C7-C8-C9
18	B	1229	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	B	1219	CLA	C11-C12-C13-C15
18	A	1139	CLA	C3-C5-C6-C7
18	A	1022	CLA	C3-C5-C6-C7
18	3	3004	CLA	CBA-CGA-O2A-C1
18	B	1229	CLA	CBA-CGA-O2A-C1
18	A	1105	CLA	CBA-CGA-O2A-C1
18	A	1132	CLA	C15-C16-C17-C18
20	A	5001	PQN	C18-C20-C21-C22
22	G	2011	BCR	C11-C10-C9-C34
22	K	2011	BCR	C11-C10-C9-C34
21	A	7001	LHG	C13-C14-C15-C16
26	B	8002	LMU	O1'-C1-C2-C3
23	4	4801	LMG	C11-C12-C13-C14
23	4	4801	LMG	C32-C33-C34-C35
23	J	5001	LMG	C29-C30-C31-C32
23	J	5001	LMG	C40-C41-C42-C43
18	4	4012	CLA	C2C-C3C-CAC-CBC
18	A	1137	CLA	C6-C7-C8-C10
18	2	2012	CLA	C6-C7-C8-C9
18	A	1133	CLA	C6-C7-C8-C9
18	A	1122	CLA	C16-C17-C18-C19
18	4	4012	CLA	C16-C17-C18-C19
17	A	1011	CL0	CBA-CGA-O2A-C1
23	F	5002	LMG	C19-C20-C21-C22
25	B	7101	DGD	C8A-C9A-CAA-CBA
23	J	5001	LMG	C16-C17-C18-C19
23	J	5001	LMG	C41-C42-C43-C44
23	G	2021	LMG	C13-C14-C15-C16
23	2	2802	LMG	C31-C32-C33-C34
21	A	5003	LHG	C31-C32-C33-C34
23	J	5001	LMG	C9-C8-O7-C10
18	B	1238	CLA	C8-C10-C11-C12
18	A	1117	CLA	C5-C6-C7-C8
18	A	1109	CLA	C10-C11-C12-C13
18	B	1226	CLA	C10-C11-C12-C13
21	1	1801	LHG	C10-C11-C12-C13
25	B	7101	DGD	C5A-C6A-C7A-C8A
21	A	7001	LHG	C28-C29-C30-C31
25	B	7101	DGD	CAB-CBB-CCB-CDB
23	G	2021	LMG	C29-C30-C31-C32
18	B	1221	CLA	C5-C6-C7-C8
18	A	1137	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	4	4007	CLA	C3-C5-C6-C7
23	J	5001	LMG	C28-C29-C30-C31
22	K	2011	BCR	C11-C10-C9-C8
18	A	1107	CLA	CBA-CGA-O2A-C1
18	B	1206	CLA	CBA-CGA-O2A-C1
18	1	1004	CLA	C15-C16-C17-C18
18	B	1229	CLA	O1A-CGA-O2A-C1
18	B	1218	CLA	O1A-CGA-O2A-C1
18	B	1216	CLA	O1A-CGA-O2A-C1
18	A	1111	CLA	C11-C12-C13-C14
18	B	1223	CLA	C16-C17-C18-C19
18	A	1127	CLA	C16-C17-C18-C20
17	A	1011	CL0	C16-C17-C18-C19
18	B	1211	CLA	C16-C17-C18-C19
18	3	3003	CLA	C4-C3-C5-C6
18	A	1119	CLA	C4-C3-C5-C6
25	B	7101	DGD	CCB-CDB-CEB-CFB
18	1	1001	CLA	C4C-C3C-CAC-CBC
23	J	5001	LMG	C21-C22-C23-C24
21	A	5003	LHG	C33-C34-C35-C36
18	A	1119	CLA	C2-C3-C5-C6
18	A	1123	CLA	C11-C10-C8-C9
18	L	1502	CLA	C6-C7-C8-C9
18	A	1131	CLA	C14-C13-C15-C16
18	B	1215	CLA	C6-C7-C8-C9
18	B	1226	CLA	C6-C7-C8-C9
21	1	1801	LHG	C26-C27-C28-C29
18	B	1214	CLA	C10-C11-C12-C13
18	B	1201	CLA	C2A-CAA-CBA-CGA
18	A	1127	CLA	C2A-CAA-CBA-CGA
23	F	5002	LMG	O10-C28-O8-C9
18	A	1151	CLA	O1A-CGA-O2A-C1
22	B	6005	BCR	C7-C8-C9-C34
22	B	6005	BCR	C37-C22-C23-C24
22	A	6008	BCR	C36-C18-C19-C20
21	A	5003	LHG	C26-C27-C28-C29
21	B	5004	LHG	O1-C1-C2-C3
21	A	5003	LHG	O1-C1-C2-C3
22	B	6005	BCR	C7-C8-C9-C10
22	B	6005	BCR	C21-C22-C23-C24
18	A	1123	CLA	C3-C5-C6-C7
18	B	1223	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	B	1229	CLA	C3-C5-C6-C7
18	3	3003	CLA	C3-C5-C6-C7
28	3	3011	CHL	C3-C5-C6-C7
21	1	1801	LHG	C34-C35-C36-C37
23	F	5002	LMG	C13-C14-C15-C16
25	B	7101	DGD	C2B-C3B-C4B-C5B
23	B	5005	LMG	C14-C15-C16-C17
23	G	2021	LMG	C11-C12-C13-C14
23	G	2021	LMG	C33-C34-C35-C36
18	2	2012	CLA	C6-C7-C8-C10
18	2	2003	CLA	C6-C7-C8-C10
18	A	1123	CLA	C16-C17-C18-C20
18	L	1502	CLA	C11-C12-C13-C14
18	A	1133	CLA	C6-C7-C8-C10
18	B	1219	CLA	C11-C12-C13-C14
26	B	8002	LMU	O5'-C1'-O1'-C1
23	J	5001	LMG	O6-C1-O1-C7
18	B	1240	CLA	C13-C15-C16-C17
18	A	1111	CLA	C8-C10-C11-C12
18	B	1239	CLA	C15-C16-C17-C18
21	A	7001	LHG	C31-C32-C33-C34
23	J	5001	LMG	C18-C19-C20-C21
23	B	5005	LMG	C11-C12-C13-C14
21	A	5003	LHG	C24-C25-C26-C27
18	B	1220	CLA	O1D-CGD-O2D-CED
26	B	8001	LMU	C5-C6-C7-C8
18	B	1208	CLA	O1A-CGA-O2A-C1
23	G	2021	LMG	C31-C32-C33-C34
18	2	2001	CLA	CBA-CGA-O2A-C1
18	4	4004	CLA	CBA-CGA-O2A-C1
18	B	1213	CLA	CBA-CGA-O2A-C1
18	J	1302	CLA	C3A-C2A-CAA-CBA
18	A	1107	CLA	C3A-C2A-CAA-CBA
18	B	1221	CLA	C3A-C2A-CAA-CBA
18	4	4016	CLA	C3A-C2A-CAA-CBA
18	B	1223	CLA	C3A-C2A-CAA-CBA
28	1	1009	CHL	C3A-C2A-CAA-CBA
18	A	1104	CLA	C3A-C2A-CAA-CBA
18	A	1140	CLA	C3A-C2A-CAA-CBA
18	3	3005	CLA	C3A-C2A-CAA-CBA
18	1	1014	CLA	C3A-C2A-CAA-CBA
18	1	1011	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	G	1002	CLA	C3A-C2A-CAA-CBA
18	A	1103	CLA	C3A-C2A-CAA-CBA
18	A	1113	CLA	C3A-C2A-CAA-CBA
18	L	1501	CLA	C3A-C2A-CAA-CBA
18	A	1119	CLA	C3A-C2A-CAA-CBA
18	A	1101	CLA	C3A-C2A-CAA-CBA
18	B	1210	CLA	C3A-C2A-CAA-CBA
18	2	2016	CLA	C4C-C3C-CAC-CBC
18	3	3004	CLA	O1A-CGA-O2A-C1
18	3	3002	CLA	O1A-CGA-O2A-C1
18	A	1111	CLA	C11-C12-C13-C15
18	A	1137	CLA	C6-C7-C8-C9
18	B	1223	CLA	C16-C17-C18-C20
18	A	1127	CLA	C16-C17-C18-C19
18	A	1122	CLA	C16-C17-C18-C20
23	F	5002	LMG	C14-C15-C16-C17
18	3	3012	CLA	C4C-C3C-CAC-CBC
23	B	5005	LMG	C29-C30-C31-C32
18	A	1121	CLA	C3-C5-C6-C7
23	2	2802	LMG	O6-C5-C6-O5
23	J	5001	LMG	C10-C11-C12-C13
18	1	1005	CLA	C2-C3-C5-C6
18	3	3003	CLA	C2-C3-C5-C6
23	F	5002	LMG	C11-C10-O7-C8
18	1	1006	CLA	C2C-C3C-CAC-CBC
23	J	5001	LMG	C39-C40-C41-C42
23	B	5005	LMG	C15-C16-C17-C18
17	A	1011	CL0	O1A-CGA-O2A-C1
18	B	1206	CLA	O1A-CGA-O2A-C1
18	B	1211	CLA	C16-C17-C18-C20
18	B	1213	CLA	C11-C12-C13-C15
18	3	3010	CLA	C3-C5-C6-C7
20	A	5001	PQN	C13-C15-C16-C17
26	B	8002	LMU	C1-C2-C3-C4
18	3	3013	CLA	C4C-C3C-CAC-CBC
23	F	5002	LMG	C17-C18-C19-C20
25	B	7101	DGD	C5B-C6B-C7B-C8B
18	G	1002	CLA	C4C-C3C-CAC-CBC
18	A	1107	CLA	O1A-CGA-O2A-C1
18	L	1502	CLA	O1A-CGA-O2A-C1
25	B	7101	DGD	C2A-C3A-C4A-C5A
25	B	7101	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
25	B	7101	DGD	C4B-C5B-C6B-C7B
23	F	5002	LMG	O9-C10-O7-C8
18	B	1201	CLA	C2-C1-O2A-CGA
18	4	4009	CLA	C2-C1-O2A-CGA
18	A	1126	CLA	C2-C1-O2A-CGA
18	2	2001	CLA	C2-C1-O2A-CGA
18	G	1003	CLA	C2-C1-O2A-CGA
18	A	1130	CLA	C2-C1-O2A-CGA
18	A	1107	CLA	C2-C1-O2A-CGA
18	B	1232	CLA	C2-C1-O2A-CGA
18	A	1151	CLA	C2-C1-O2A-CGA
18	A	1127	CLA	C2-C1-O2A-CGA
18	A	1125	CLA	C2-C1-O2A-CGA
18	3	3005	CLA	C2-C1-O2A-CGA
18	B	1239	CLA	C2-C1-O2A-CGA
18	B	1215	CLA	C2-C1-O2A-CGA
18	B	1212	CLA	C2-C1-O2A-CGA
18	A	1103	CLA	C8-C10-C11-C12
18	4	4004	CLA	O1A-CGA-O2A-C1
18	B	1213	CLA	O1A-CGA-O2A-C1
18	3	3010	CLA	C11-C12-C13-C14
22	A	6003	BCR	C1-C6-C7-C8
22	A	6003	BCR	C5-C6-C7-C8
22	B	6004	BCR	C1-C6-C7-C8
22	B	6004	BCR	C5-C6-C7-C8
22	B	6004	BCR	C23-C24-C25-C26
22	B	6004	BCR	C23-C24-C25-C30
18	A	1237	CLA	C3-C5-C6-C7
18	A	1116	CLA	C3-C5-C6-C7
22	F	6014	BCR	C23-C24-C25-C26
22	L	6019	BCR	C1-C6-C7-C8
22	L	6019	BCR	C23-C24-C25-C26
27	4	4503	LUT	C5-C6-C7-C8
22	B	6005	BCR	C5-C6-C7-C8
22	J	6012	BCR	C23-C24-C25-C26
22	J	6012	BCR	C23-C24-C25-C30
27	4	4501	LUT	C1-C6-C7-C8
22	A	6008	BCR	C23-C24-C25-C26
22	A	6008	BCR	C23-C24-C25-C30
22	B	6010	BCR	C23-C24-C25-C26
22	B	6010	BCR	C23-C24-C25-C30
22	A	6011	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	A	6011	BCR	C5-C6-C7-C8
23	4	4801	LMG	C30-C31-C32-C33
18	B	1238	CLA	CBA-CGA-O2A-C1
18	A	1127	CLA	CBA-CGA-O2A-C1
18	4	4005	CLA	CBA-CGA-O2A-C1
18	A	1106	CLA	CBA-CGA-O2A-C1
18	B	1219	CLA	C8-C10-C11-C12
18	4	4012	CLA	C10-C11-C12-C13
18	A	1101	CLA	C10-C11-C12-C13
21	1	1801	LHG	C28-C29-C30-C31
23	J	5001	LMG	C15-C16-C17-C18
18	1	1003	CLA	C5-C6-C7-C8
18	B	1223	CLA	C8-C10-C11-C12
21	1	1801	LHG	C25-C26-C27-C28
18	4	4017	CLA	C4-C3-C5-C6
18	A	1237	CLA	C11-C10-C8-C7
18	1	1001	CLA	C11-C10-C8-C7
18	B	1238	CLA	C11-C12-C13-C15
18	B	1227	CLA	C6-C7-C8-C10
18	A	1131	CLA	C12-C13-C15-C16
18	A	1109	CLA	C6-C7-C8-C10
18	A	1122	CLA	C11-C12-C13-C15
18	B	1215	CLA	C6-C7-C8-C10
20	B	5002	PQN	C17-C18-C20-C21
18	A	1119	CLA	C11-C12-C13-C15
18	B	1226	CLA	C6-C7-C8-C10
18	2	2001	CLA	O1A-CGA-O2A-C1
18	B	1222	CLA	C13-C15-C16-C17
18	B	1225	CLA	C8-C10-C11-C12
18	A	1116	CLA	C5-C6-C7-C8
18	B	1206	CLA	C15-C16-C17-C18
22	B	6005	BCR	C19-C20-C21-C22
18	B	1236	CLA	C6-C7-C8-C9
21	A	7001	LHG	O9-C7-O7-C5
21	2	2801	LHG	O9-C7-O7-C5
23	2	2802	LMG	C28-C29-C30-C31
18	2	2003	CLA	CBA-CGA-O2A-C1
18	1	1001	CLA	CBA-CGA-O2A-C1
23	2	2802	LMG	C29-C28-O8-C9
18	B	1021	CLA	CBA-CGA-O2A-C1
18	4	4003	CLA	C2A-CAA-CBA-CGA
18	1	1012	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	B	1230	CLA	C8-C10-C11-C12
18	B	1234	CLA	C10-C11-C12-C13
18	B	1021	CLA	C8-C10-C11-C12
26	B	8002	LMU	C9-C10-C11-C12
28	3	3011	CHL	C2C-C3C-CAC-CBC
18	B	1023	CLA	C10-C11-C12-C13
18	1	1004	CLA	C3-C5-C6-C7
18	A	1237	CLA	C11-C12-C13-C14
18	A	1110	CLA	C6-C7-C8-C9
18	A	1134	CLA	C5-C6-C7-C8
21	A	7001	LHG	C26-C27-C28-C29
23	2	2802	LMG	C11-C12-C13-C14
21	A	7001	LHG	C8-C7-O7-C5
21	2	2801	LHG	C8-C7-O7-C5
21	A	5003	LHG	C8-C7-O7-C5
23	G	2021	LMG	C30-C31-C32-C33
18	B	1240	CLA	C10-C11-C12-C13
18	A	1123	CLA	C5-C6-C7-C8
28	1	1009	CHL	CBD-CGD-O2D-CED
18	2	2002	CLA	CBA-CGA-O2A-C1
18	A	1127	CLA	O1A-CGA-O2A-C1
23	4	4801	LMG	C2-C1-O1-C7
23	4	4801	LMG	O7-C8-C9-O8
23	F	5001	LMG	O1-C7-C8-O7
21	A	7001	LHG	C10-C11-C12-C13
21	A	7001	LHG	C33-C34-C35-C36
25	B	7101	DGD	C8B-C9B-CAB-CBB
18	1	1005	CLA	C4-C3-C5-C6
18	A	1138	CLA	C2-C3-C5-C6
21	A	7001	LHG	C25-C26-C27-C28
23	J	5001	LMG	C31-C32-C33-C34
18	A	1107	CLA	C11-C12-C13-C14
18	B	1238	CLA	C11-C12-C13-C14
18	B	1230	CLA	C11-C10-C8-C9
18	B	1234	CLA	C6-C7-C8-C9
18	A	1109	CLA	C6-C7-C8-C9
18	B	1224	CLA	C11-C10-C8-C9
18	B	1239	CLA	C14-C13-C15-C16
18	A	1138	CLA	C11-C10-C8-C9
18	B	1211	CLA	CBD-CGD-O2D-CED
18	A	1111	CLA	C3-C5-C6-C7
18	A	1127	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	A	1126	CLA	C2A-CAA-CBA-CGA
26	B	8002	LMU	O5'-C5'-C6'-O6'
18	B	1225	CLA	C13-C15-C16-C17
18	A	1103	CLA	C5-C6-C7-C8
23	J	5001	LMG	C14-C15-C16-C17
26	B	8001	LMU	C1-C2-C3-C4
18	2	2003	CLA	O1A-CGA-O2A-C1
18	4	4005	CLA	O1A-CGA-O2A-C1
18	A	1106	CLA	O1A-CGA-O2A-C1
18	B	1021	CLA	O1A-CGA-O2A-C1
18	B	1220	CLA	C1A-C2A-CAA-CBA
18	J	1302	CLA	C1A-C2A-CAA-CBA
18	A	1121	CLA	C1A-C2A-CAA-CBA
18	2	2004	CLA	C1A-C2A-CAA-CBA
18	G	1003	CLA	C1A-C2A-CAA-CBA
18	3	3013	CLA	C1A-C2A-CAA-CBA
18	B	1221	CLA	C1A-C2A-CAA-CBA
18	A	1116	CLA	C1A-C2A-CAA-CBA
18	A	1115	CLA	C1A-C2A-CAA-CBA
18	H	1000	CLA	C1A-C2A-CAA-CBA
18	A	1104	CLA	C1A-C2A-CAA-CBA
18	B	1202	CLA	C1A-C2A-CAA-CBA
18	B	1229	CLA	C1A-C2A-CAA-CBA
18	4	4005	CLA	C1A-C2A-CAA-CBA
18	3	3005	CLA	C1A-C2A-CAA-CBA
18	B	1214	CLA	C1A-C2A-CAA-CBA
18	1	1014	CLA	C1A-C2A-CAA-CBA
18	B	1219	CLA	C1A-C2A-CAA-CBA
18	1	1012	CLA	C1A-C2A-CAA-CBA
18	A	1106	CLA	C1A-C2A-CAA-CBA
18	G	1002	CLA	C1A-C2A-CAA-CBA
28	3	3011	CHL	C1A-C2A-CAA-CBA
28	2	2011	CHL	C1A-C2A-CAA-CBA
18	B	1216	CLA	C1A-C2A-CAA-CBA
18	A	1113	CLA	C1A-C2A-CAA-CBA
18	B	1215	CLA	C1A-C2A-CAA-CBA
18	A	1128	CLA	C1A-C2A-CAA-CBA
18	3	3001	CLA	C1A-C2A-CAA-CBA
18	A	1101	CLA	C1A-C2A-CAA-CBA
18	B	1210	CLA	C1A-C2A-CAA-CBA
18	A	1237	CLA	C11-C12-C13-C15
18	A	1123	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	3	3010	CLA	C11-C12-C13-C15
18	B	1229	CLA	C16-C17-C18-C20
17	A	1011	CL0	C16-C17-C18-C20
18	B	1236	CLA	C6-C7-C8-C10
18	B	1213	CLA	C11-C12-C13-C14
18	4	4012	CLA	C16-C17-C18-C20
26	B	8001	LMU	O1'-C1-C2-C3
22	B	6004	BCR	C19-C20-C21-C22
22	J	6012	BCR	C9-C10-C11-C12
22	F	6016	BCR	C9-C10-C11-C12
18	B	1218	CLA	C15-C16-C17-C18
20	B	5002	PQN	C20-C21-C22-C23
18	A	1101	CLA	CBD-CGD-O2D-CED
18	B	1208	CLA	C3-C5-C6-C7
18	A	1120	CLA	C10-C11-C12-C13
18	B	1224	CLA	C13-C15-C16-C17
18	A	1134	CLA	CBA-CGA-O2A-C1
21	B	5004	LHG	O6-C4-C5-C6
23	2	2802	LMG	C29-C30-C31-C32
23	J	5001	LMG	C8-C9-O8-C28
18	A	1134	CLA	C6-C7-C8-C10
18	L	1502	CLA	C11-C12-C13-C15
18	4	4017	CLA	C16-C17-C18-C19
25	B	7101	DGD	CEB-CFB-CGB-CHB
23	G	2021	LMG	C14-C15-C16-C17
18	A	1138	CLA	C4-C3-C5-C6
25	B	7101	DGD	C4A-C5A-C6A-C7A
18	B	1238	CLA	O1A-CGA-O2A-C1
23	2	2802	LMG	O10-C28-O8-C9
18	F	1302	CLA	C2A-CAA-CBA-CGA
18	A	1119	CLA	C16-C17-C18-C19
18	A	1140	CLA	C3-C5-C6-C7
23	4	4801	LMG	C7-C8-C9-O8
18	A	1133	CLA	C5-C6-C7-C8
18	A	1122	CLA	C10-C11-C12-C13
28	2	2013	CHL	C2C-C3C-CAC-CBC
18	3	3005	CLA	C4C-C3C-CAC-CBC
18	4	4003	CLA	C4C-C3C-CAC-CBC
21	2	2801	LHG	O1-C1-C2-O2
23	J	5001	LMG	C36-C37-C38-C39
21	1	1801	LHG	C30-C31-C32-C33
18	B	1202	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
18	B	1219	CLA	C10-C11-C12-C13
18	3	3017	CLA	O1A-CGA-O2A-C1
23	2	2802	LMG	C10-C11-C12-C13
18	A	1121	CLA	CBA-CGA-O2A-C1
18	B	1212	CLA	C5-C6-C7-C8
21	A	7001	LHG	C11-C10-C9-C8
23	4	4801	LMG	C29-C30-C31-C32
18	1	1011	CLA	C4C-C3C-CAC-CBC
18	1	1003	CLA	C2A-CAA-CBA-CGA
18	A	1130	CLA	C2A-CAA-CBA-CGA
18	A	1133	CLA	C2A-CAA-CBA-CGA
18	B	1225	CLA	C2-C1-O2A-CGA
18	3	3008	CLA	C2-C1-O2A-CGA
18	A	1116	CLA	C2-C1-O2A-CGA
18	A	1110	CLA	C2-C1-O2A-CGA
18	A	1131	CLA	C2-C1-O2A-CGA
21	1	1801	LHG	C13-C14-C15-C16
18	A	1125	CLA	C5-C6-C7-C8
21	A	7001	LHG	C24-C25-C26-C27
18	A	1134	CLA	CAA-CBA-CGA-O2A
18	A	1134	CLA	C6-C7-C8-C9
18	G	1001	CLA	C2C-C3C-CAC-CBC
18	1	1001	CLA	O1A-CGA-O2A-C1
18	A	1127	CLA	C15-C16-C17-C18
18	A	1134	CLA	O1D-CGD-O2D-CED
23	J	5001	LMG	C2-C1-O1-C7
18	2	2004	CLA	C2C-C3C-CAC-CBC
21	A	7001	LHG	O7-C5-C6-O8
23	F	5002	LMG	O7-C8-C9-O8
18	1	1004	CLA	C10-C11-C12-C13
18	A	1134	CLA	O1A-CGA-O2A-C1
18	1	1005	CLA	C6-C7-C8-C9
18	A	1110	CLA	C6-C7-C8-C10
18	4	4012	CLA	C4C-C3C-CAC-CBC
18	B	1223	CLA	C5-C6-C7-C8
18	B	1236	CLA	C5-C6-C7-C8
18	B	1220	CLA	C12-C13-C15-C16
18	A	1107	CLA	C11-C12-C13-C15
18	A	1116	CLA	C6-C7-C8-C10
18	B	1202	CLA	C12-C13-C15-C16
18	B	1229	CLA	C12-C13-C15-C16
18	A	1127	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	A	1125	CLA	C11-C10-C8-C7
18	B	1211	CLA	C12-C13-C15-C16
18	B	1231	CLA	C6-C7-C8-C10
18	B	1218	CLA	C12-C13-C15-C16
18	B	1224	CLA	C11-C10-C8-C7
18	B	1224	CLA	C11-C12-C13-C15
18	4	4017	CLA	C6-C7-C8-C10
18	4	4017	CLA	C11-C12-C13-C15
18	B	1239	CLA	C11-C12-C13-C15
18	B	1239	CLA	C12-C13-C15-C16
18	B	1216	CLA	C6-C7-C8-C10
18	B	1213	CLA	C6-C7-C8-C10
18	A	1128	CLA	C12-C13-C15-C16
18	A	1101	CLA	C11-C10-C8-C7
18	A	1138	CLA	C11-C10-C8-C7
18	B	1240	CLA	CAA-CBA-CGA-O2A
18	A	1132	CLA	C11-C12-C13-C14
18	A	1126	CLA	C11-C10-C8-C9
18	A	1126	CLA	C14-C13-C15-C16
18	A	1139	CLA	C14-C13-C15-C16
18	1	1001	CLA	C6-C7-C8-C9
18	3	3010	CLA	C6-C7-C8-C9
18	A	1104	CLA	C11-C12-C13-C14
18	B	1202	CLA	C14-C13-C15-C16
18	A	1127	CLA	C14-C13-C15-C16
18	4	4004	CLA	C6-C7-C8-C9
18	A	1125	CLA	C11-C10-C8-C9
18	B	1235	CLA	C14-C13-C15-C16
18	B	1231	CLA	C6-C7-C8-C9
18	B	1219	CLA	C6-C7-C8-C9
18	B	1218	CLA	C14-C13-C15-C16
18	A	1103	CLA	C11-C12-C13-C14
18	4	4017	CLA	C6-C7-C8-C9
18	4	4017	CLA	C11-C12-C13-C14
18	B	1239	CLA	C11-C12-C13-C14
18	B	1216	CLA	C6-C7-C8-C9
18	B	1216	CLA	C11-C10-C8-C9
18	B	1213	CLA	C6-C7-C8-C9
18	4	4012	CLA	C6-C7-C8-C9
18	4	4012	CLA	C14-C13-C15-C16
18	A	1101	CLA	C11-C10-C8-C9
22	F	6014	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
22	G	2011	BCR	C7-C8-C9-C34
18	4	4017	CLA	C16-C17-C18-C20
21	1	1801	LHG	C16-C17-C18-C19
21	1	1801	LHG	O1-C1-C2-C3
26	B	8002	LMU	C2-C3-C4-C5
18	4	4005	CLA	C3-C5-C6-C7
18	B	1231	CLA	C3-C5-C6-C7
21	A	5003	LHG	O9-C7-O7-C5
18	B	1231	CLA	C10-C11-C12-C13
18	A	1103	CLA	C10-C11-C12-C13
21	A	5003	LHG	C9-C10-C11-C12
18	B	1212	CLA	CBA-CGA-O2A-C1
23	J	5001	LMG	C34-C35-C36-C37
18	B	1213	CLA	C8-C10-C11-C12
18	B	1226	CLA	C13-C15-C16-C17
23	2	2802	LMG	C33-C34-C35-C36
18	3	3010	CLA	O1D-CGD-O2D-CED
18	A	1237	CLA	C10-C11-C12-C13
18	4	4012	CLA	C15-C16-C17-C18
18	A	1123	CLA	C4-C3-C5-C6
18	4	4017	CLA	C2-C3-C5-C6
25	B	7101	DGD	CBB-CCB-CDB-CEB
18	B	1230	CLA	C3-C5-C6-C7
18	1	1005	CLA	C6-C7-C8-C10
18	B	1239	CLA	C16-C17-C18-C20
18	2	2016	CLA	CAA-CBA-CGA-O2A
18	A	1121	CLA	O1A-CGA-O2A-C1
18	B	1222	CLA	C3A-C2A-CAA-CBA
28	1	1010	CHL	C3A-C2A-CAA-CBA
18	A	1120	CLA	C3A-C2A-CAA-CBA
18	B	1214	CLA	C3A-C2A-CAA-CBA
28	2	2011	CHL	C3A-C2A-CAA-CBA
18	B	1023	CLA	C2C-C3C-CAC-CBC
22	L	6020	BCR	C13-C14-C15-C16
27	4	4503	LUT	C33-C34-C35-C15
25	B	7101	DGD	C6A-C7A-C8A-C9A
18	B	1223	CLA	CBA-CGA-O2A-C1
18	B	1229	CLA	C15-C16-C17-C18
21	A	7001	LHG	C4-C5-C6-O8
25	B	7101	DGD	O1G-C1G-C2G-C3G
23	J	5001	LMG	C7-C8-C9-O8
23	G	2021	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	B	5005	LMG	C7-C8-C9-O8
21	1	1801	LHG	C35-C36-C37-C38
18	A	1128	CLA	C13-C15-C16-C17
18	B	1220	CLA	C4-C3-C5-C6
18	B	1240	CLA	C4-C3-C5-C6
18	4	4003	CLA	C4-C3-C5-C6
18	A	1128	CLA	C4-C3-C5-C6
18	A	1119	CLA	C16-C17-C18-C20
18	A	1101	CLA	C8-C10-C11-C12
21	B	5004	LHG	C4-O6-P-O3
18	A	1119	CLA	C2A-CAA-CBA-CGA
18	A	1106	CLA	C15-C16-C17-C18
21	A	7001	LHG	C11-C12-C13-C14
21	B	5004	LHG	O6-C4-C5-O7
21	A	7001	LHG	O6-C4-C5-O7
18	B	1238	CLA	C16-C17-C18-C20
23	4	4801	LMG	C33-C34-C35-C36
25	B	7101	DGD	O2G-C2G-C3G-O3G
23	B	5005	LMG	O7-C8-C9-O8
18	A	1132	CLA	C16-C17-C18-C19
18	B	1021	CLA	C16-C17-C18-C20
18	A	1237	CLA	C8-C10-C11-C12
18	B	1202	CLA	C4-C3-C5-C6
18	B	1205	CLA	C4-C3-C5-C6
18	3	3004	CLA	C2-C1-O2A-CGA
18	A	1136	CLA	C2-C1-O2A-CGA
18	A	1123	CLA	C2-C3-C5-C6
18	B	1210	CLA	C10-C11-C12-C13
18	A	1132	CLA	C14-C13-C15-C16
18	B	1240	CLA	C11-C12-C13-C14
18	B	1225	CLA	C14-C13-C15-C16
18	G	1003	CLA	C6-C7-C8-C9
18	B	1229	CLA	C14-C13-C15-C16
18	B	1206	CLA	C6-C7-C8-C9
18	A	1117	CLA	C14-C13-C15-C16
18	B	1235	CLA	C6-C7-C8-C9
18	1	1004	CLA	C14-C13-C15-C16
20	B	5002	PQN	C24-C23-C25-C26
18	A	1119	CLA	C11-C10-C8-C9
18	B	1205	CLA	C11-C10-C8-C9
18	4	4005	CLA	C5-C6-C7-C8
18	B	1215	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	A	5003	LHG	C2-C3-O3-P
22	A	6003	BCR	C23-C24-C25-C26
22	A	6003	BCR	C23-C24-C25-C30
27	2	2501	LUT	C1-C6-C7-C8
27	2	2501	LUT	C5-C6-C7-C8
22	J	6013	BCR	C5-C6-C7-C8
22	J	6013	BCR	C23-C24-C25-C26
22	L	6019	BCR	C23-C24-C25-C30
22	B	6005	BCR	C23-C24-C25-C26
22	B	6005	BCR	C23-C24-C25-C30
18	B	1227	CLA	C3-C5-C6-C7
22	A	6002	BCR	C23-C24-C25-C26
22	A	6011	BCR	C23-C24-C25-C26
22	A	6011	BCR	C23-C24-C25-C30
22	A	6007	BCR	C23-C24-C25-C26
22	A	6007	BCR	C23-C24-C25-C30
18	A	1013	CLA	C15-C16-C17-C18
18	B	1227	CLA	C5-C6-C7-C8
22	F	6016	BCR	C11-C12-C13-C14
18	A	1140	CLA	C10-C11-C12-C13
28	2	2013	CHL	C4C-C3C-CAC-CBC
21	A	5003	LHG	O6-C4-C5-C6
18	B	1222	CLA	C11-C10-C8-C7
18	B	1240	CLA	C11-C12-C13-C15
18	B	1225	CLA	C12-C13-C15-C16
18	A	1126	CLA	C11-C10-C8-C7
18	A	1126	CLA	C11-C12-C13-C15
18	A	1139	CLA	C12-C13-C15-C16
18	A	1123	CLA	C11-C12-C13-C15
18	3	3010	CLA	C6-C7-C8-C10
18	A	1022	CLA	C6-C7-C8-C10
18	A	1022	CLA	C11-C10-C8-C7
18	A	1104	CLA	C11-C12-C13-C15
18	B	1202	CLA	C2-C3-C5-C6
20	A	5001	PQN	C16-C17-C18-C20
20	A	5001	PQN	C21-C22-C23-C25
18	4	4004	CLA	C6-C7-C8-C10
18	A	1120	CLA	C11-C10-C8-C7
18	B	1206	CLA	C6-C7-C8-C10
18	A	1117	CLA	C12-C13-C15-C16
18	B	1235	CLA	C6-C7-C8-C10
18	1	1004	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	1	1004	CLA	C12-C13-C15-C16
18	B	1214	CLA	C11-C10-C8-C7
18	B	1219	CLA	C6-C7-C8-C10
18	B	1218	CLA	C11-C12-C13-C15
18	B	1203	CLA	C6-C7-C8-C10
18	A	1103	CLA	C11-C12-C13-C15
18	B	1224	CLA	C6-C7-C8-C10
18	B	1239	CLA	C11-C10-C8-C7
18	B	1213	CLA	C11-C10-C8-C7
18	4	4012	CLA	C6-C7-C8-C10
18	4	4012	CLA	C11-C12-C13-C15
18	A	1119	CLA	C11-C10-C8-C7
18	B	1205	CLA	C2-C3-C5-C6
18	B	1205	CLA	C11-C10-C8-C7
18	B	1226	CLA	C11-C12-C13-C15
18	A	1101	CLA	C3-C5-C6-C7
18	A	1110	CLA	C5-C6-C7-C8
22	J	6013	BCR	C9-C10-C11-C12
22	J	6013	BCR	C19-C20-C21-C22
29	4	4505	ZEX	C29-C30-C31-C32
18	A	1013	CLA	CBA-CGA-O2A-C1
18	1	1006	CLA	C4C-C3C-CAC-CBC
18	4	4001	CLA	C10-C11-C12-C13
18	3	3005	CLA	C3-C5-C6-C7
18	B	1210	CLA	C3-C5-C6-C7
18	1	1005	CLA	C5-C6-C7-C8
18	B	1234	CLA	C5-C6-C7-C8
18	B	1205	CLA	C8-C10-C11-C12
18	B	1236	CLA	CBA-CGA-O2A-C1
18	B	1222	CLA	C8-C10-C11-C12
18	4	4001	CLA	CAD-CBD-CGD-O2D
18	B	1240	CLA	CAD-CBD-CGD-O2D
18	4	4016	CLA	CAD-CBD-CGD-O2D
18	A	1135	CLA	CAD-CBD-CGD-O2D
18	B	1227	CLA	CAD-CBD-CGD-O2D
18	2	2016	CLA	CAD-CBD-CGD-O2D
18	3	3006	CLA	CAD-CBD-CGD-O2D
18	A	1101	CLA	CAD-CBD-CGD-O2D
18	B	1220	CLA	C5-C6-C7-C8
18	A	1139	CLA	C13-C15-C16-C17
18	2	2005	CLA	C5-C6-C7-C8
18	B	1012	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	A	1122	CLA	CBA-CGA-O2A-C1
18	B	1012	CLA	CBA-CGA-O2A-C1
18	4	4007	CLA	C11-C12-C13-C14
18	G	1001	CLA	C6-C7-C8-C10
18	B	1224	CLA	C8-C10-C11-C12
23	F	5002	LMG	C7-C8-C9-O8
18	B	1212	CLA	O1A-CGA-O2A-C1
21	A	5003	LHG	O6-C4-C5-O7
21	A	7001	LHG	C14-C15-C16-C17
18	B	1204	CLA	C2A-CAA-CBA-CGA
23	J	5001	LMG	C23-C24-C25-C26
18	4	4004	CLA	C11-C12-C13-C14
18	B	1239	CLA	C16-C17-C18-C19
18	B	1240	CLA	CHA-CBD-CGD-O1D
18	A	1013	CLA	CHA-CBD-CGD-O2D
18	A	1121	CLA	CHA-CBD-CGD-O1D
18	A	1121	CLA	CHA-CBD-CGD-O2D
18	3	3013	CLA	CHA-CBD-CGD-O1D
18	3	3013	CLA	CHA-CBD-CGD-O2D
18	B	1221	CLA	CHA-CBD-CGD-O1D
18	B	1221	CLA	CHA-CBD-CGD-O2D
18	B	1208	CLA	CHA-CBD-CGD-O1D
18	B	1208	CLA	CHA-CBD-CGD-O2D
18	2	2006	CLA	CHA-CBD-CGD-O1D
18	2	2006	CLA	CHA-CBD-CGD-O2D
18	3	3010	CLA	CHA-CBD-CGD-O1D
18	3	3010	CLA	CHA-CBD-CGD-O2D
18	L	1502	CLA	CHA-CBD-CGD-O2D
18	3	3007	CLA	CHA-CBD-CGD-O1D
18	2	2002	CLA	CHA-CBD-CGD-O1D
18	2	2002	CLA	CHA-CBD-CGD-O2D
28	1	1009	CHL	CHA-CBD-CGD-O2D
18	3	3017	CLA	CHA-CBD-CGD-O1D
18	3	3017	CLA	CHA-CBD-CGD-O2D
18	A	1125	CLA	CHA-CBD-CGD-O1D
18	A	1125	CLA	CHA-CBD-CGD-O2D
18	A	1106	CLA	CHA-CBD-CGD-O1D
18	A	1106	CLA	CHA-CBD-CGD-O2D
18	1	1008	CLA	CHA-CBD-CGD-O1D
18	1	1002	CLA	CHA-CBD-CGD-O1D
18	1	1002	CLA	CHA-CBD-CGD-O2D
18	A	1128	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	B	1217	CLA	CHA-CBD-CGD-O1D
18	B	1217	CLA	CHA-CBD-CGD-O2D
18	K	1001	CLA	CHA-CBD-CGD-O1D
18	G	1001	CLA	CHA-CBD-CGD-O1D
18	1	1001	CLA	C3-C5-C6-C7
18	A	1013	CLA	O1A-CGA-O2A-C1
18	B	1012	CLA	O1A-CGA-O2A-C1
22	G	2011	BCR	C11-C10-C9-C8
25	B	7101	DGD	O1G-C1G-C2G-O2G
23	J	5001	LMG	O7-C8-C9-O8
23	G	2021	LMG	O1-C7-C8-O7
18	B	1223	CLA	O1A-CGA-O2A-C1
18	B	1236	CLA	O1A-CGA-O2A-C1
21	A	7001	LHG	O1-C1-C2-O2
18	A	1101	CLA	O1D-CGD-O2D-CED
18	A	1120	CLA	C5-C6-C7-C8
18	B	1228	CLA	C5-C6-C7-C8
18	A	1122	CLA	C11-C10-C8-C9
18	B	1012	CLA	C14-C13-C15-C16
23	J	5001	LMG	C13-C14-C15-C16
18	1	1008	CLA	C2A-CAA-CBA-CGA
18	A	1122	CLA	O1A-CGA-O2A-C1
27	3	3502	LUT	C11-C12-C13-C20
27	4	4502	LUT	C11-C12-C13-C20
22	A	6011	BCR	C36-C18-C19-C20
25	B	7101	DGD	C9A-CAA-CBA-CCA
22	F	6014	BCR	C17-C18-C19-C20
22	3	3503	BCR	C17-C18-C19-C20
22	G	2011	BCR	C7-C8-C9-C10
18	3	3007	CLA	C1A-C2A-CAA-CBA
18	A	1120	CLA	C1A-C2A-CAA-CBA
18	B	1215	CLA	C11-C12-C13-C14
23	G	2021	LMG	C12-C13-C14-C15
18	A	1129	CLA	C2-C1-O2A-CGA
18	B	1231	CLA	C2-C1-O2A-CGA
18	3	3006	CLA	C2-C1-O2A-CGA
18	1	1012	CLA	C2-C1-O2A-CGA
23	B	5005	LMG	C13-C14-C15-C16
21	1	1801	LHG	C4-O6-P-O3
18	B	1204	CLA	C4-C3-C5-C6
21	B	5004	LHG	C4-O6-P-O5
25	B	7101	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
18	A	1013	CLA	C8-C10-C11-C12
18	4	4017	CLA	C15-C16-C17-C18
21	A	7001	LHG	O6-C4-C5-C6
18	B	1214	CLA	C3-C5-C6-C7
18	B	1211	CLA	O1D-CGD-O2D-CED
18	3	3008	CLA	O2A-C1-C2-C3
18	B	1238	CLA	C16-C17-C18-C19
18	3	3005	CLA	C6-C7-C8-C10
18	A	1138	CLA	C16-C17-C18-C19
18	A	1111	CLA	CAD-CBD-CGD-O1D
18	2	2006	CLA	CAD-CBD-CGD-O1D
18	2	2007	CLA	CAD-CBD-CGD-O1D
18	A	1125	CLA	CAD-CBD-CGD-O1D
18	B	1211	CLA	CAD-CBD-CGD-O1D
18	1	1008	CLA	CAD-CBD-CGD-O1D
18	B	1217	CLA	CAD-CBD-CGD-O1D
18	H	1000	CLA	CBA-CGA-O2A-C1
18	A	1112	CLA	C8-C10-C11-C12
18	B	1238	CLA	C15-C16-C17-C18
18	A	1119	CLA	C5-C6-C7-C8
23	G	2021	LMG	C15-C16-C17-C18
28	3	3011	CHL	C4C-C3C-CAC-CBC
23	J	5001	LMG	C33-C34-C35-C36
18	1	1001	CLA	C11-C12-C13-C14
18	B	1222	CLA	C6-C7-C8-C10
18	2	2001	CLA	C6-C7-C8-C10
18	A	1112	CLA	C11-C10-C8-C7
18	A	1130	CLA	C3A-C2A-CAA-CBA
18	4	4003	CLA	C11-C10-C8-C7
18	B	1221	CLA	C6-C7-C8-C10
18	B	1221	CLA	C11-C12-C13-C15
18	4	4007	CLA	C6-C7-C8-C10
18	A	1102	CLA	C3A-C2A-CAA-CBA
18	A	1125	CLA	C3A-C2A-CAA-CBA
18	B	1235	CLA	C11-C12-C13-C15
18	A	1140	CLA	C6-C7-C8-C10
18	B	1231	CLA	C11-C10-C8-C7
18	A	1122	CLA	C3A-C2A-CAA-CBA
18	A	1122	CLA	C6-C7-C8-C10
18	A	1138	CLA	C11-C12-C13-C15
18	B	1012	CLA	C12-C13-C15-C16
18	G	1001	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	1226	CLA	C11-C10-C8-C7
18	A	1237	CLA	C5-C6-C7-C8
23	B	5005	LMG	C10-C11-C12-C13
18	4	4007	CLA	C10-C11-C12-C13
18	A	1121	CLA	C2A-CAA-CBA-CGA
18	B	1218	CLA	C16-C17-C18-C20
23	G	2021	LMG	C34-C35-C36-C37
23	F	5002	LMG	C15-C16-C17-C18
18	3	3005	CLA	C6-C7-C8-C9
18	G	1001	CLA	C6-C7-C8-C9
18	B	1240	CLA	C5-C6-C7-C8
18	B	1224	CLA	CBA-CGA-O2A-C1
18	B	1207	CLA	C10-C11-C12-C13
18	B	1222	CLA	C11-C10-C8-C9
18	A	1022	CLA	C6-C7-C8-C9
18	A	1022	CLA	C11-C10-C8-C9
18	B	1223	CLA	C11-C10-C8-C9
18	A	1104	CLA	C14-C13-C15-C16
20	A	5001	PQN	C16-C17-C18-C19
20	A	5001	PQN	C21-C22-C23-C24
18	B	1207	CLA	C11-C10-C8-C9
18	A	1140	CLA	C6-C7-C8-C9
18	A	1131	CLA	C11-C12-C13-C14
18	B	1218	CLA	C11-C12-C13-C14
18	B	1224	CLA	C6-C7-C8-C9
18	B	1213	CLA	C11-C10-C8-C9
18	A	1128	CLA	C6-C7-C8-C9
18	4	4012	CLA	C11-C10-C8-C9
18	4	4012	CLA	C11-C12-C13-C14
18	A	1138	CLA	C6-C7-C8-C9
18	A	1111	CLA	O1A-CGA-O2A-C1
18	A	1139	CLA	O1A-CGA-O2A-C1
22	B	6006	BCR	C18-C19-C20-C21
22	K	2011	BCR	C18-C19-C20-C21
18	B	1216	CLA	C15-C16-C17-C18
18	2	2005	CLA	C6-C7-C8-C9
18	A	1104	CLA	C16-C17-C18-C19
23	B	5005	LMG	C12-C13-C14-C15
22	B	6009	BCR	C11-C10-C9-C34
23	J	5001	LMG	C17-C18-C19-C20
18	2	2003	CLA	C4-C3-C5-C6
18	4	4007	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	F	5002	LMG	C11-C12-C13-C14
23	G	2021	LMG	C9-C8-O7-C10
23	2	2802	LMG	C9-C8-O7-C10
18	A	1111	CLA	CBA-CGA-O2A-C1
18	4	4004	CLA	C2-C1-O2A-CGA
18	1	1004	CLA	C2-C1-O2A-CGA
18	B	1224	CLA	C2-C1-O2A-CGA
18	L	1501	CLA	C2-C1-O2A-CGA
18	B	1226	CLA	C2-C1-O2A-CGA
18	2	2002	CLA	O1A-CGA-O2A-C1
18	G	1001	CLA	C4C-C3C-CAC-CBC
18	A	1122	CLA	C3-C5-C6-C7
18	A	1103	CLA	C4-C3-C5-C6
18	B	1227	CLA	O1D-CGD-O2D-CED
22	A	6002	BCR	C23-C24-C25-C30
18	A	1139	CLA	CBA-CGA-O2A-C1
18	A	1127	CLA	CAA-CBA-CGA-O2A
23	4	4801	LMG	C13-C14-C15-C16
18	4	4003	CLA	C16-C17-C18-C20
18	A	1117	CLA	C16-C17-C18-C20
18	4	4003	CLA	C8-C10-C11-C12
18	2	2001	CLA	C2A-CAA-CBA-CGA
22	A	6017	BCR	C16-C17-C18-C19
21	2	2801	LHG	C3-O3-P-O6
21	A	5003	LHG	C4-O6-P-O3
18	1	1004	CLA	C8-C10-C11-C12
23	F	5001	LMG	O1-C7-C8-C9
18	3	3004	CLA	C6-C7-C8-C10
18	A	1126	CLA	C12-C13-C15-C16
18	4	4005	CLA	C6-C7-C8-C10
18	A	1125	CLA	C6-C7-C8-C10
18	B	1206	CLA	C11-C12-C13-C15
18	A	1128	CLA	C2-C3-C5-C6
21	A	7001	LHG	O8-C23-C24-C25
17	A	1011	CL0	CAA-CBA-CGA-O2A
18	A	1126	CLA	C11-C12-C13-C14
18	B	1221	CLA	C6-C7-C8-C9
18	A	1116	CLA	C6-C7-C8-C9
18	B	1211	CLA	C14-C13-C15-C16
18	B	1231	CLA	C11-C10-C8-C9
18	B	1224	CLA	C11-C12-C13-C14
18	A	1122	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	A	1138	CLA	C11-C12-C13-C14
18	B	1226	CLA	C11-C10-C8-C9
27	3	3502	LUT	C9-C10-C11-C12
27	4	4501	LUT	C33-C34-C35-C15
22	B	6009	BCR	C19-C20-C21-C22
18	A	1132	CLA	C16-C17-C18-C20
18	B	1215	CLA	C11-C12-C13-C15
18	A	1116	CLA	C8-C10-C11-C12
18	B	1224	CLA	O1A-CGA-O2A-C1
18	B	1203	CLA	C16-C17-C18-C19
18	A	1138	CLA	C16-C17-C18-C20
18	A	1132	CLA	C5-C6-C7-C8
26	B	8001	LMU	C4'-C5'-C6'-O6'
23	F	5002	LMG	C28-C29-C30-C31
18	B	1227	CLA	CBD-CGD-O2D-CED
18	A	1151	CLA	CAA-CBA-CGA-O2A
18	2	2005	CLA	C2A-CAA-CBA-CGA
18	A	1104	CLA	C16-C17-C18-C20
22	I	6020	BCR	C19-C20-C21-C22
22	B	6006	BCR	C19-C20-C21-C22
22	L	6019	BCR	C9-C10-C11-C12
22	B	6010	BCR	C19-C20-C21-C22
22	K	2011	BCR	C13-C14-C15-C16
22	A	6002	BCR	C9-C10-C11-C12
22	A	6002	BCR	C19-C20-C21-C22
18	B	1220	CLA	C13-C15-C16-C17
26	B	8002	LMU	C3-C4-C5-C6
18	A	1121	CLA	C6-C7-C8-C10
18	1	1013	CLA	C2C-C3C-CAC-CBC
18	A	1110	CLA	O1A-CGA-O2A-C1
18	A	1134	CLA	C2-C1-O2A-CGA
18	3	3003	CLA	C2-C1-O2A-CGA
18	4	4001	CLA	C2C-C3C-CAC-CBC
18	B	1235	CLA	C3-C5-C6-C7
26	B	8002	LMU	C5-C6-C7-C8
18	B	1223	CLA	C2A-CAA-CBA-CGA
18	B	1214	CLA	CAA-CBA-CGA-O2A
20	A	5001	PQN	C15-C16-C17-C18
18	A	1133	CLA	C3A-C2A-CAA-CBA
18	A	1127	CLA	C3A-C2A-CAA-CBA
17	A	1011	CL0	C3A-C2A-CAA-CBA
28	4	4013	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	A	1106	CLA	C5-C6-C7-C8
18	A	1125	CLA	C11-C12-C13-C15
26	B	8002	LMU	C6-C7-C8-C9
18	H	1000	CLA	CAA-CBA-CGA-O2A
18	4	4008	CLA	CAA-CBA-CGA-O2A
18	3	3004	CLA	C11-C10-C8-C9
18	A	1112	CLA	C14-C13-C15-C16
18	A	1107	CLA	C6-C7-C8-C9
18	L	1502	CLA	C11-C10-C8-C9
20	B	5002	PQN	C19-C18-C20-C21
26	B	8002	LMU	C7-C8-C9-C10
18	A	1112	CLA	C5-C6-C7-C8
22	I	6020	BCR	C16-C17-C18-C36
22	I	6020	BCR	C20-C21-C22-C37
22	B	6004	BCR	C16-C17-C18-C36
22	B	6006	BCR	C11-C10-C9-C34
22	A	6017	BCR	C16-C17-C18-C36
22	B	6005	BCR	C16-C17-C18-C36
22	G	2011	BCR	C16-C17-C18-C36
22	K	2011	BCR	C16-C17-C18-C36
22	A	6011	BCR	C16-C17-C18-C36
22	F	6016	BCR	C16-C17-C18-C36
18	B	1221	CLA	C3-C5-C6-C7
18	B	1209	CLA	C2A-CAA-CBA-CGA
18	2	2005	CLA	C6-C7-C8-C10
18	B	1206	CLA	C8-C10-C11-C12
18	4	4001	CLA	C1A-C2A-CAA-CBA
18	A	1114	CLA	C1A-C2A-CAA-CBA
18	2	2005	CLA	C1A-C2A-CAA-CBA
28	1	1010	CHL	C1A-C2A-CAA-CBA
17	A	1011	CL0	C1A-C2A-CAA-CBA
18	A	1125	CLA	C1A-C2A-CAA-CBA
18	4	4017	CLA	C1A-C2A-CAA-CBA
23	J	5001	LMG	C32-C33-C34-C35
18	A	1132	CLA	C11-C12-C13-C15
18	B	1228	CLA	C6-C7-C8-C10
18	B	1202	CLA	C11-C10-C8-C7
18	A	1140	CLA	C11-C10-C8-C7
18	B	1203	CLA	C11-C12-C13-C15
18	B	1021	CLA	C12-C13-C15-C16
18	A	1119	CLA	C3-C5-C6-C7
18	A	1110	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	3	3003	CLA	C8-C10-C11-C12
18	B	1012	CLA	C16-C17-C18-C20
18	A	1237	CLA	C2A-CAA-CBA-CGA
18	B	1224	CLA	C2A-CAA-CBA-CGA
18	B	1210	CLA	C13-C15-C16-C17
18	3	3003	CLA	C10-C11-C12-C13
18	A	1134	CLA	CAA-CBA-CGA-O1A
22	I	6020	BCR	C16-C17-C18-C19
22	I	6020	BCR	C20-C21-C22-C23
22	B	6004	BCR	C16-C17-C18-C19
22	B	6006	BCR	C11-C10-C9-C8
22	B	6005	BCR	C16-C17-C18-C19
22	G	2011	BCR	C16-C17-C18-C19
22	K	2011	BCR	C16-C17-C18-C19
22	A	6011	BCR	C16-C17-C18-C19
22	F	6016	BCR	C16-C17-C18-C19
23	J	5001	LMG	C35-C36-C37-C38
21	2	2801	LHG	O7-C5-C6-O8
18	B	1238	CLA	C2A-CAA-CBA-CGA
18	2	2004	CLA	C4C-C3C-CAC-CBC
22	L	6019	BCR	C15-C16-C17-C18
22	3	3503	BCR	C13-C14-C15-C16
18	B	1021	CLA	C16-C17-C18-C19
18	B	1224	CLA	C4-C3-C5-C6
18	A	1132	CLA	C2-C1-O2A-CGA
18	A	1111	CLA	C2-C1-O2A-CGA
18	2	2009	CLA	C2-C1-O2A-CGA
18	B	1228	CLA	C2-C1-O2A-CGA
18	2	2003	CLA	C2-C1-O2A-CGA
18	A	1102	CLA	C2-C1-O2A-CGA
18	2	2003	CLA	C2-C3-C5-C6
18	B	1221	CLA	O1A-CGA-O2A-C1
18	B	1203	CLA	O1A-CGA-O2A-C1
18	4	4017	CLA	C11-C10-C8-C9
20	B	5002	PQN	C21-C22-C23-C24
18	A	1117	CLA	C8-C10-C11-C12
18	A	1131	CLA	C5-C6-C7-C8
18	2	2001	CLA	C5-C6-C7-C8
18	A	1118	CLA	C2A-CAA-CBA-CGA
18	B	1207	CLA	C2A-CAA-CBA-CGA
18	A	1113	CLA	C2A-CAA-CBA-CGA
18	B	1023	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	J	5001	LMG	C38-C39-C40-C41
18	L	1501	CLA	O1A-CGA-O2A-C1
22	J	6013	BCR	C1-C6-C7-C8
22	J	6013	BCR	C23-C24-C25-C30
27	4	4503	LUT	C1-C6-C7-C8
22	J	6012	BCR	C1-C6-C7-C8
27	I	6018	LUT	C1-C6-C7-C8
22	A	6008	BCR	C1-C6-C7-C8
22	K	2011	BCR	C23-C24-C25-C30
21	1	1801	LHG	C11-C12-C13-C14
18	B	1228	CLA	O1A-CGA-O2A-C1
22	I	6020	BCR	C9-C10-C11-C12
27	2	2502	LUT	C29-C30-C31-C32
22	A	6011	BCR	C19-C20-C21-C22
22	A	6007	BCR	C19-C20-C21-C22
25	B	7101	DGD	C9B-CAB-CBB-CCB
28	1	1009	CHL	C4-C3-C5-C6
18	B	1206	CLA	C4-C3-C5-C6
18	A	1131	CLA	C4-C3-C5-C6
22	I	6020	BCR	C21-C22-C23-C24
18	A	1121	CLA	C6-C7-C8-C9
18	B	1229	CLA	C2-C3-C5-C6
18	A	1103	CLA	C2-C3-C5-C6
18	A	1120	CLA	CAA-CBA-CGA-O2A
18	A	1117	CLA	C16-C17-C18-C19
18	B	1217	CLA	C2A-CAA-CBA-CGA
18	B	1023	CLA	C13-C15-C16-C17
18	1	1013	CLA	C4C-C3C-CAC-CBC
18	3	3004	CLA	C3-C5-C6-C7
18	1	1004	CLA	C16-C17-C18-C19
18	B	1235	CLA	C8-C10-C11-C12
21	A	7001	LHG	C19-C20-C21-C22
21	1	1801	LHG	O6-C4-C5-C6
18	A	1104	CLA	C4-C3-C5-C6
18	B	1240	CLA	C2-C3-C5-C6
18	1	1001	CLA	C6-C7-C8-C10
28	1	1009	CHL	C2-C3-C5-C6
18	4	4017	CLA	C11-C10-C8-C7
18	B	1203	CLA	CBA-CGA-O2A-C1
18	4	4017	CLA	C8-C10-C11-C12
23	F	5001	LMG	O7-C8-C9-O8
18	B	1221	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	4	4801	LMG	C31-C32-C33-C34
18	A	1118	CLA	C2C-C3C-CAC-CBC
21	A	7001	LHG	C27-C28-C29-C30
18	1	1007	CLA	CAA-CBA-CGA-O2A
18	B	1021	CLA	CAA-CBA-CGA-O2A
18	B	1221	CLA	C2A-CAA-CBA-CGA
18	4	4003	CLA	C16-C17-C18-C19
18	B	1023	CLA	C15-C16-C17-C18
22	A	6011	BCR	C11-C10-C9-C34
23	G	2021	LMG	C10-C11-C12-C13
18	A	1134	CLA	C4-C3-C5-C6
18	B	1216	CLA	C4-C3-C5-C6
18	B	1220	CLA	C2-C3-C5-C6
18	4	4003	CLA	C2-C3-C5-C6
18	B	1204	CLA	C2-C3-C5-C6
18	B	1220	CLA	CAA-CBA-CGA-O2A
21	2	2801	LHG	O8-C23-C24-C25
18	A	1113	CLA	CAA-CBA-CGA-O2A
18	A	1136	CLA	C11-C10-C8-C7
18	B	1228	CLA	C6-C7-C8-C9
18	4	4007	CLA	C6-C7-C8-C9
18	B	1202	CLA	C11-C10-C8-C9
18	B	1206	CLA	C11-C12-C13-C14
18	B	1207	CLA	C11-C12-C13-C14
18	B	1235	CLA	C11-C12-C13-C14
18	1	1004	CLA	C11-C10-C8-C9
18	B	1203	CLA	C11-C12-C13-C14
18	B	1239	CLA	C11-C10-C8-C9
18	B	1021	CLA	C14-C13-C15-C16
18	A	1140	CLA	CAA-CBA-CGA-O2A
18	2	2001	CLA	CAD-CBD-CGD-O2D
18	A	1118	CLA	CAD-CBD-CGD-O2D
18	A	1129	CLA	CAD-CBD-CGD-O2D
18	B	1223	CLA	CAD-CBD-CGD-O2D
18	B	1207	CLA	CAD-CBD-CGD-O2D
18	3	3001	CLA	CAD-CBD-CGD-O2D
18	K	1001	CLA	CAD-CBD-CGD-O2D
18	A	1125	CLA	C11-C12-C13-C14
21	A	5003	LHG	C35-C36-C37-C38
18	2	2004	CLA	C13-C15-C16-C17
23	J	5001	LMG	C11-C12-C13-C14
18	B	1201	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	2	2001	CLA	CAA-CBA-CGA-O2A
18	B	1228	CLA	CAA-CBA-CGA-O2A
18	1	1012	CLA	CAA-CBA-CGA-O2A
18	A	1105	CLA	CAA-CBA-CGA-O2A
18	B	1240	CLA	CAA-CBA-CGA-O1A
18	A	1013	CLA	C4-C3-C5-C6
18	B	1236	CLA	C4-C3-C5-C6
18	A	1134	CLA	C2-C3-C5-C6
18	B	1224	CLA	C2-C3-C5-C6
18	2	2008	CLA	CAA-CBA-CGA-O2A
18	2	2003	CLA	CAA-CBA-CGA-O2A
23	G	2021	LMG	O7-C10-C11-C12
23	G	2021	LMG	O8-C28-C29-C30
18	B	1236	CLA	CAA-CBA-CGA-O2A
18	A	1122	CLA	CAA-CBA-CGA-O2A
22	B	6004	BCR	C21-C22-C23-C24
27	4	4502	LUT	C11-C12-C13-C14
22	A	6008	BCR	C17-C18-C19-C20
22	A	6011	BCR	C17-C18-C19-C20
18	A	1136	CLA	C11-C10-C8-C9
25	B	7101	DGD	C1G-C2G-C3G-O3G
18	A	1138	CLA	O1A-CGA-O2A-C1
18	2	2007	CLA	CAA-CBA-CGA-O2A
18	A	1125	CLA	CAA-CBA-CGA-O2A
18	B	1235	CLA	CAA-CBA-CGA-O2A
18	B	1224	CLA	CAA-CBA-CGA-O2A
18	K	1001	CLA	CAA-CBA-CGA-O2A
18	B	1210	CLA	CAA-CBA-CGA-O2A
18	A	1022	CLA	C16-C17-C18-C20
18	A	1124	CLA	C2A-CAA-CBA-CGA
18	G	1001	CLA	CAA-CBA-CGA-O2A
18	2	2016	CLA	CAA-CBA-CGA-O1A
18	B	1220	CLA	CHA-CBD-CGD-O2D
18	3	3004	CLA	CHA-CBD-CGD-O1D
18	B	1240	CLA	CHA-CBD-CGD-O2D
18	J	1302	CLA	CHA-CBD-CGD-O1D
18	J	1302	CLA	CHA-CBD-CGD-O2D
18	A	1126	CLA	CHA-CBD-CGD-O1D
18	A	1126	CLA	CHA-CBD-CGD-O2D
18	A	1111	CLA	CHA-CBD-CGD-O1D
18	1	1013	CLA	CHA-CBD-CGD-O1D
18	1	1013	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	A	1114	CLA	CHA-CBD-CGD-O1D
18	G	1003	CLA	CHA-CBD-CGD-O1D
18	G	1003	CLA	CHA-CBD-CGD-O2D
28	2	2010	CHL	CHA-CBD-CGD-O2D
18	A	1137	CLA	CHA-CBD-CGD-O1D
18	A	1137	CLA	CHA-CBD-CGD-O2D
18	B	1204	CLA	CHA-CBD-CGD-O1D
18	B	1204	CLA	CHA-CBD-CGD-O2D
18	4	4007	CLA	CHA-CBD-CGD-O1D
18	4	4007	CLA	CHA-CBD-CGD-O2D
18	A	1123	CLA	CHA-CBD-CGD-O2D
18	2	2005	CLA	CHA-CBD-CGD-O1D
18	2	2005	CLA	CHA-CBD-CGD-O2D
18	A	1127	CLA	CHA-CBD-CGD-O1D
18	A	1127	CLA	CHA-CBD-CGD-O2D
18	4	4005	CLA	CHA-CBD-CGD-O1D
18	4	4005	CLA	CHA-CBD-CGD-O2D
18	4	4008	CLA	CHA-CBD-CGD-O2D
18	4	4002	CLA	CHA-CBD-CGD-O1D
18	4	4002	CLA	CHA-CBD-CGD-O2D
18	1	1004	CLA	CHA-CBD-CGD-O2D
18	B	1211	CLA	CHA-CBD-CGD-O1D
18	1	1014	CLA	CHA-CBD-CGD-O1D
18	1	1014	CLA	CHA-CBD-CGD-O2D
18	1	1008	CLA	CHA-CBD-CGD-O2D
18	A	1113	CLA	CHA-CBD-CGD-O1D
18	A	1113	CLA	CHA-CBD-CGD-O2D
18	A	1119	CLA	CHA-CBD-CGD-O1D
18	A	1119	CLA	CHA-CBD-CGD-O2D
18	B	1212	CLA	CHA-CBD-CGD-O2D
18	K	1001	CLA	CHA-CBD-CGD-O2D
18	B	1012	CLA	CHA-CBD-CGD-O1D
18	B	1226	CLA	CHA-CBD-CGD-O1D
18	B	1226	CLA	CHA-CBD-CGD-O2D
18	4	4016	CLA	CAA-CBA-CGA-O2A
18	B	1208	CLA	CAA-CBA-CGA-O2A
18	A	1136	CLA	CAA-CBA-CGA-O2A
21	A	7001	LHG	C30-C31-C32-C33
22	A	6011	BCR	C11-C10-C9-C8
18	3	3010	CLA	CAA-CBA-CGA-O2A
18	B	1238	CLA	CAA-CBA-CGA-O2A
18	2	2007	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	3	3003	CLA	CAA-CBA-CGA-O2A
18	B	1239	CLA	CAA-CBA-CGA-O2A
18	A	1138	CLA	C5-C6-C7-C8
18	B	1205	CLA	CAA-CBA-CGA-O2A
18	G	1001	CLA	C4-C3-C5-C6
18	B	1220	CLA	CAA-CBA-CGA-O1A
18	A	1013	CLA	C2-C3-C5-C6
18	A	1140	CLA	C12-C13-C15-C16
20	B	5002	PQN	C22-C23-C25-C26
18	B	1219	CLA	CAA-CBA-CGA-O2A
18	3	3004	CLA	C6-C7-C8-C9
18	A	1127	CLA	C11-C12-C13-C14
18	1	1007	CLA	CAA-CBA-CGA-O1A
18	B	1216	CLA	C16-C17-C18-C19
18	A	1103	CLA	O1A-CGA-O2A-C1
18	B	1023	CLA	C8-C10-C11-C12
18	B	1228	CLA	CBA-CGA-O2A-C1
21	2	2801	LHG	O10-C23-C24-C25
18	A	1125	CLA	CAA-CBA-CGA-O1A
18	A	1113	CLA	CAA-CBA-CGA-O1A
18	B	1227	CLA	C4-C3-C5-C6
21	A	7001	LHG	O1-C1-C2-C3
18	A	1122	CLA	CAA-CBA-CGA-O1A
22	B	6009	BCR	C21-C22-C23-C24
23	G	2021	LMG	C17-C18-C19-C20
28	4	4011	CHL	C1A-C2A-CAA-CBA
18	1	1001	CLA	C1A-C2A-CAA-CBA
18	A	1022	CLA	C1A-C2A-CAA-CBA
18	A	1133	CLA	C1A-C2A-CAA-CBA
18	A	1102	CLA	C1A-C2A-CAA-CBA
18	3	3017	CLA	C1A-C2A-CAA-CBA
28	4	4013	CHL	C1A-C2A-CAA-CBA
28	4	4010	CHL	C1A-C2A-CAA-CBA
18	B	1206	CLA	C1A-C2A-CAA-CBA
18	F	1302	CLA	C1A-C2A-CAA-CBA
18	G	1001	CLA	C1A-C2A-CAA-CBA
23	J	5001	LMG	C19-C20-C21-C22
18	B	1204	CLA	C6-C7-C8-C10
18	2	2007	CLA	CAA-CBA-CGA-O1A
18	B	1228	CLA	CAA-CBA-CGA-O1A
18	K	1001	CLA	CAA-CBA-CGA-O1A
18	G	1001	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	A	1013	CLA	C16-C17-C18-C20
20	B	5002	PQN	C26-C27-C28-C29
18	2	2008	CLA	CAA-CBA-CGA-O1A
23	G	2021	LMG	O9-C10-C11-C12
18	H	1000	CLA	O1A-CGA-O2A-C1
18	B	1229	CLA	C4-C3-C5-C6
18	A	1106	CLA	CAA-CBA-CGA-O2A
18	B	1201	CLA	CAA-CBA-CGA-O1A
18	2	2001	CLA	CAA-CBA-CGA-O1A
18	B	1208	CLA	CAA-CBA-CGA-O1A
18	B	1238	CLA	CAA-CBA-CGA-O1A
18	A	1136	CLA	CAA-CBA-CGA-O1A
18	B	1210	CLA	CAA-CBA-CGA-O1A
21	2	2801	LHG	C3-O3-P-O5
21	A	5003	LHG	C4-O6-P-O5
18	1	1012	CLA	CAA-CBA-CGA-O1A
18	B	1239	CLA	CAA-CBA-CGA-O1A
23	4	4801	LMG	O8-C28-C29-C30
27	3	3502	LUT	C5-C6-C7-C8
18	2	2003	CLA	CAA-CBA-CGA-O1A
18	3	3010	CLA	CAA-CBA-CGA-O1A
18	B	1235	CLA	CAA-CBA-CGA-O1A
18	A	1105	CLA	CAA-CBA-CGA-O1A
18	4	4016	CLA	CAA-CBA-CGA-O1A
23	G	2021	LMG	O10-C28-C29-C30
18	B	1220	CLA	CAD-CBD-CGD-O1D
18	B	1228	CLA	CAD-CBD-CGD-O1D
18	4	4003	CLA	CAD-CBD-CGD-O1D
18	4	4002	CLA	CAD-CBD-CGD-O1D
18	B	1234	CLA	CAD-CBD-CGD-O1D
18	4	4017	CLA	CAD-CBD-CGD-O1D
18	B	1239	CLA	CAD-CBD-CGD-O1D
23	2	2802	LMG	C7-C8-O7-C10
18	A	1136	CLA	CAD-CBD-CGD-O1D
18	A	1119	CLA	CAD-CBD-CGD-O1D
18	B	1012	CLA	CAD-CBD-CGD-O1D
18	3	3007	CLA	O1A-CGA-O2A-C1
18	3	3003	CLA	CAA-CBA-CGA-O1A
18	B	1236	CLA	CAA-CBA-CGA-O1A
18	B	1221	CLA	C11-C10-C8-C9
18	B	1207	CLA	C14-C13-C15-C16
18	A	1103	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	A	1118	CLA	C4C-C3C-CAC-CBC
18	A	1116	CLA	CAA-CBA-CGA-O2A
18	A	1129	CLA	CAA-CBA-CGA-O2A
23	J	5001	LMG	O7-C10-C11-C12
18	A	1131	CLA	CAA-CBA-CGA-O2A
18	A	1124	CLA	CAA-CBA-CGA-O2A
18	B	1226	CLA	CAA-CBA-CGA-O2A
21	1	1801	LHG	C1-C2-C3-O3
18	B	1235	CLA	C5-C6-C7-C8
18	B	1012	CLA	C16-C17-C18-C19
18	B	1211	CLA	C4-C3-C5-C6
18	A	1136	CLA	C5-C6-C7-C8
18	B	1221	CLA	C11-C10-C8-C7
27	4	4502	LUT	C25-C26-C27-C28
18	A	1022	CLA	C3A-C2A-CAA-CBA
18	A	1127	CLA	C11-C12-C13-C15
18	B	1227	CLA	C11-C10-C8-C7
18	B	1206	CLA	C3A-C2A-CAA-CBA
18	A	1131	CLA	C11-C12-C13-C15
20	B	5002	PQN	C21-C22-C23-C25
18	B	1219	CLA	CAA-CBA-CGA-O1A
18	A	1121	CLA	CAA-CBA-CGA-O2A
18	L	1503	CLA	CAA-CBA-CGA-O2A
18	A	1138	CLA	CAA-CBA-CGA-O2A
22	L	6020	BCR	C21-C22-C23-C24
27	3	3502	LUT	C11-C12-C13-C14
27	1	1502	LUT	C7-C8-C9-C10
18	3	3017	CLA	CAA-CBA-CGA-O1A
18	4	4001	CLA	CAA-CBA-CGA-O2A
18	3	3017	CLA	CAA-CBA-CGA-O2A
18	G	1003	CLA	O1A-CGA-O2A-C1
18	A	1124	CLA	CAA-CBA-CGA-O1A
18	A	1139	CLA	C8-C10-C11-C12
17	A	1011	CL0	C5-C6-C7-C8
18	A	1116	CLA	CAA-CBA-CGA-O1A
18	4	4009	CLA	C2A-CAA-CBA-CGA
28	2	2010	CHL	C2A-CAA-CBA-CGA
18	G	1003	CLA	C10-C11-C12-C13
18	A	1138	CLA	CBA-CGA-O2A-C1
18	A	1121	CLA	CAA-CBA-CGA-O1A
18	A	1129	CLA	CAA-CBA-CGA-O1A
18	1	1008	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	1	1009	CHL	O1D-CGD-O2D-CED

There are no ring outliers.

205 monomers are involved in 1953 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	5004	LHG	1	0
21	1	1801	LHG	15	0
18	A	1132	CLA	7	0
18	B	1220	CLA	11	0
18	B	1201	CLA	2	0
22	I	6020	BCR	3	0
22	A	6003	BCR	2	0
18	4	4001	CLA	25	0
18	1	1005	CLA	15	0
18	3	3004	CLA	20	0
18	B	1222	CLA	8	0
18	B	1240	CLA	10	0
18	B	1225	CLA	4	0
18	1	1003	CLA	32	0
18	4	4009	CLA	9	0
18	A	1013	CLA	8	0
18	J	1302	CLA	7	0
18	B	1211	CLA	7	0
18	A	1126	CLA	10	0
18	A	1111	CLA	8	0
28	4	4011	CHL	20	0
22	B	6004	BCR	10	0
18	1	1013	CLA	16	0
18	A	1114	CLA	3	0
18	2	2001	CLA	33	0
18	A	1237	CLA	5	0
18	A	1121	CLA	4	0
18	2	2004	CLA	23	0
26	B	8001	LMU	1	0
18	3	3008	CLA	19	0
18	G	1003	CLA	30	0
27	2	2502	LUT	32	0
27	2	2501	LUT	23	0
18	3	3002	CLA	10	0
18	3	3013	CLA	23	0
18	2	2009	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	2008	CLA	16	0
18	B	1228	CLA	1	0
22	B	6006	BCR	5	0
18	A	1112	CLA	13	0
18	A	1118	CLA	3	0
18	A	1139	CLA	5	0
27	3	3502	LUT	24	0
18	A	1130	CLA	4	0
18	4	4003	CLA	13	0
18	A	1107	CLA	3	0
22	J	6013	BCR	8	0
21	A	7001	LHG	7	0
18	B	1221	CLA	14	0
18	4	4016	CLA	24	0
27	1	1502	LUT	17	0
26	B	8002	LMU	3	0
21	2	2801	LHG	6	0
18	B	1208	CLA	7	0
23	F	5002	LMG	6	0
18	A	1116	CLA	7	0
18	B	1204	CLA	10	0
18	2	2006	CLA	22	0
25	B	7101	DGD	4	0
22	F	6014	BCR	8	0
18	A	1137	CLA	3	0
18	2	2003	CLA	30	0
22	J	6012	BCR	7	0
22	L	6019	BCR	22	0
18	1	1001	CLA	48	0
29	4	4505	ZEX	12	0
18	4	4007	CLA	20	0
18	A	1123	CLA	4	0
18	A	1115	CLA	3	0
18	H	1000	CLA	4	0
18	A	1134	CLA	2	0
18	3	3010	CLA	34	0
27	4	4503	LUT	32	0
18	1	1006	CLA	11	0
18	2	2005	CLA	24	0
18	A	1022	CLA	7	0
18	B	1232	CLA	3	0
18	A	1129	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	1	1010	CHL	8	0
18	F	1301	CLA	6	0
18	L	1502	CLA	13	0
27	1	1501	LUT	31	0
18	2	2007	CLA	26	0
18	3	3007	CLA	8	0
18	2	2002	CLA	38	0
18	B	1223	CLA	4	0
18	A	1133	CLA	3	0
23	4	4801	LMG	6	0
28	1	1009	CHL	27	0
18	A	1151	CLA	4	0
18	A	1104	CLA	4	0
18	B	1023	CLA	5	0
18	3	3018	CLA	19	0
18	3	3019	CLA	1	0
18	2	2012	CLA	24	0
18	B	1238	CLA	9	0
18	A	1135	CLA	4	0
20	A	5001	PQN	3	0
22	B	6005	BCR	2	0
18	A	1102	CLA	4	0
18	A	1127	CLA	6	0
18	3	3017	CLA	11	0
18	4	4005	CLA	16	0
17	A	1011	CL0	6	0
22	A	6017	BCR	5	0
23	F	5001	LMG	7	0
27	4	4502	LUT	31	0
18	4	4004	CLA	19	0
18	B	1202	CLA	7	0
18	B	1227	CLA	8	0
18	B	1230	CLA	8	0
18	A	1120	CLA	3	0
28	4	4013	CHL	19	0
18	A	1108	CLA	3	0
28	4	4010	CHL	8	0
18	4	4002	CLA	11	0
18	A	1125	CLA	3	0
18	B	1206	CLA	6	0
18	A	1117	CLA	4	0
18	B	1207	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	J	5001	LMG	9	0
18	3	3012	CLA	32	0
18	A	1140	CLA	5	0
18	1	1004	CLA	26	0
18	4	4008	CLA	15	0
22	L	6020	BCR	6	0
18	2	2016	CLA	36	0
27	4	4501	LUT	21	0
28	2	2010	CHL	18	0
18	3	3005	CLA	18	0
18	B	1214	CLA	3	0
18	A	1110	CLA	10	0
18	L	1503	CLA	11	0
18	A	1131	CLA	3	0
18	B	1231	CLA	3	0
18	B	1234	CLA	8	0
27	I	6018	LUT	14	0
18	3	3006	CLA	36	0
18	3	3003	CLA	51	0
18	B	1209	CLA	3	0
23	G	2021	LMG	20	0
18	1	1014	CLA	14	0
18	B	1236	CLA	5	0
18	B	1235	CLA	5	0
18	1	1011	CLA	18	0
18	B	1219	CLA	2	0
23	B	5005	LMG	3	0
18	B	1218	CLA	11	0
18	A	1109	CLA	8	0
18	B	1203	CLA	3	0
18	1	1012	CLA	16	0
18	A	1106	CLA	9	0
18	G	1002	CLA	26	0
28	3	3011	CHL	22	0
22	A	6008	BCR	2	0
18	A	1103	CLA	6	0
18	B	1224	CLA	7	0
18	4	4006	CLA	21	0
18	F	1302	CLA	14	0
28	2	2013	CHL	18	0
18	4	4017	CLA	11	0
18	A	1122	CLA	6	0

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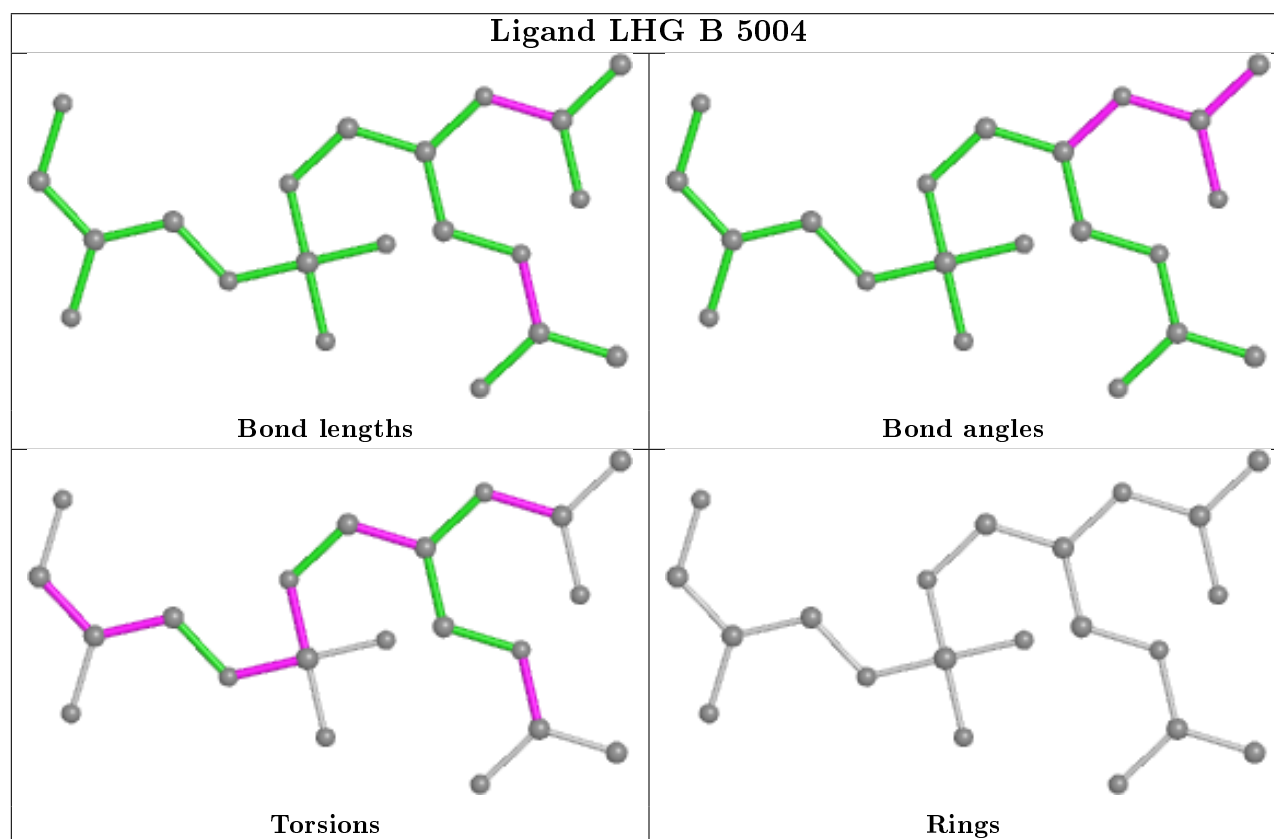
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	3	3501	LUT	38	0
22	B	6010	BCR	1	0
18	B	1239	CLA	5	0
28	2	2011	CHL	6	0
18	B	1216	CLA	7	0
23	2	2802	LMG	9	0
18	1	1007	CLA	10	0
18	A	1124	CLA	4	0
18	1	1008	CLA	34	0
18	A	1113	CLA	2	0
18	1	1002	CLA	21	0
18	B	1213	CLA	6	0
19	A	3001	SF4	1	0
18	A	1105	CLA	3	0
22	B	6009	BCR	6	0
22	K	2011	BCR	17	0
22	A	6002	BCR	4	0
18	L	1501	CLA	15	0
18	A	1136	CLA	7	0
18	B	1021	CLA	9	0
18	B	1215	CLA	4	0
18	A	1128	CLA	11	0
20	B	5002	PQN	5	0
18	3	3001	CLA	24	0
22	3	3503	BCR	21	0
18	4	4012	CLA	28	0
21	A	5003	LHG	5	0
22	A	6011	BCR	5	0
18	A	1119	CLA	7	0
22	F	6016	BCR	11	0
18	B	1217	CLA	1	0
18	A	1101	CLA	6	0
18	A	1138	CLA	4	0
22	G	2011	BCR	29	0
18	K	1001	CLA	12	0
18	B	1212	CLA	5	0
18	B	1012	CLA	6	0
18	G	1001	CLA	36	0
18	B	1205	CLA	8	0
18	B	1210	CLA	9	0
22	A	6007	BCR	3	0
18	B	1229	CLA	6	0

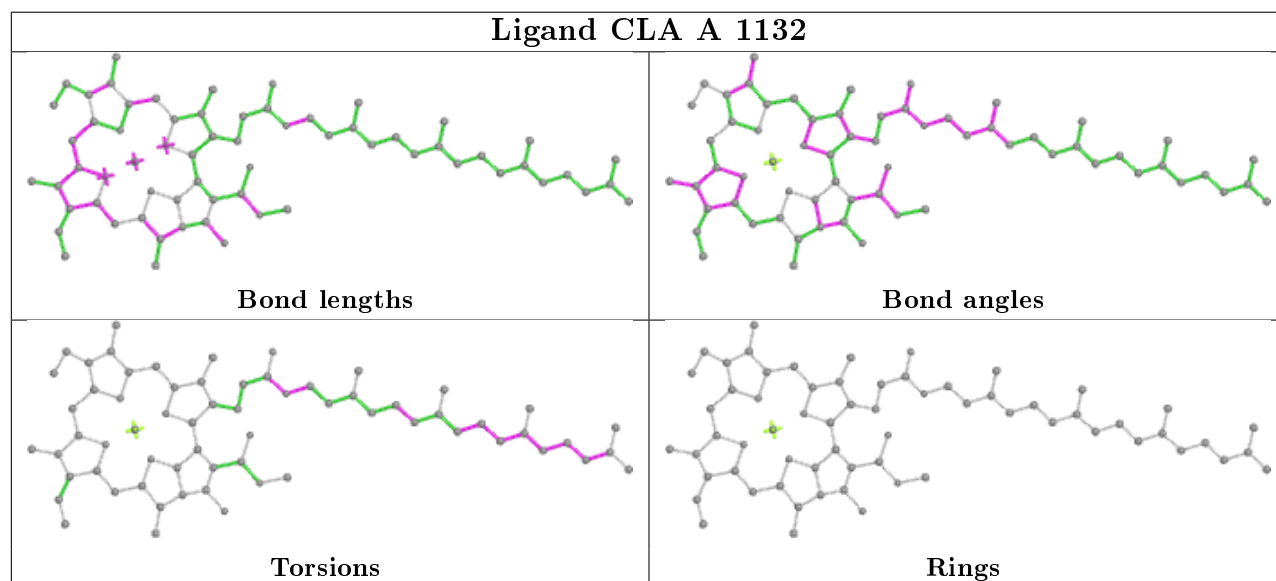
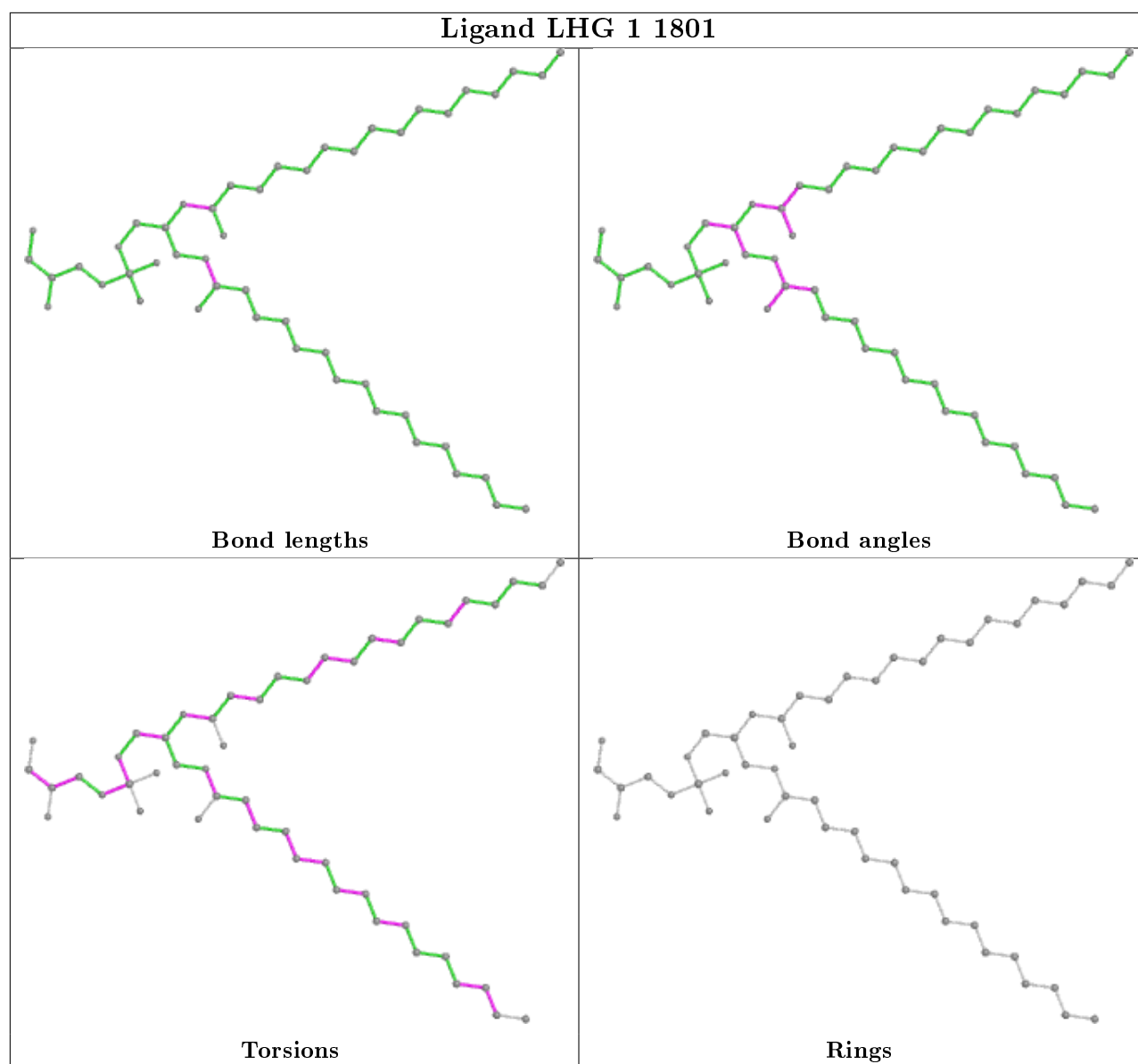
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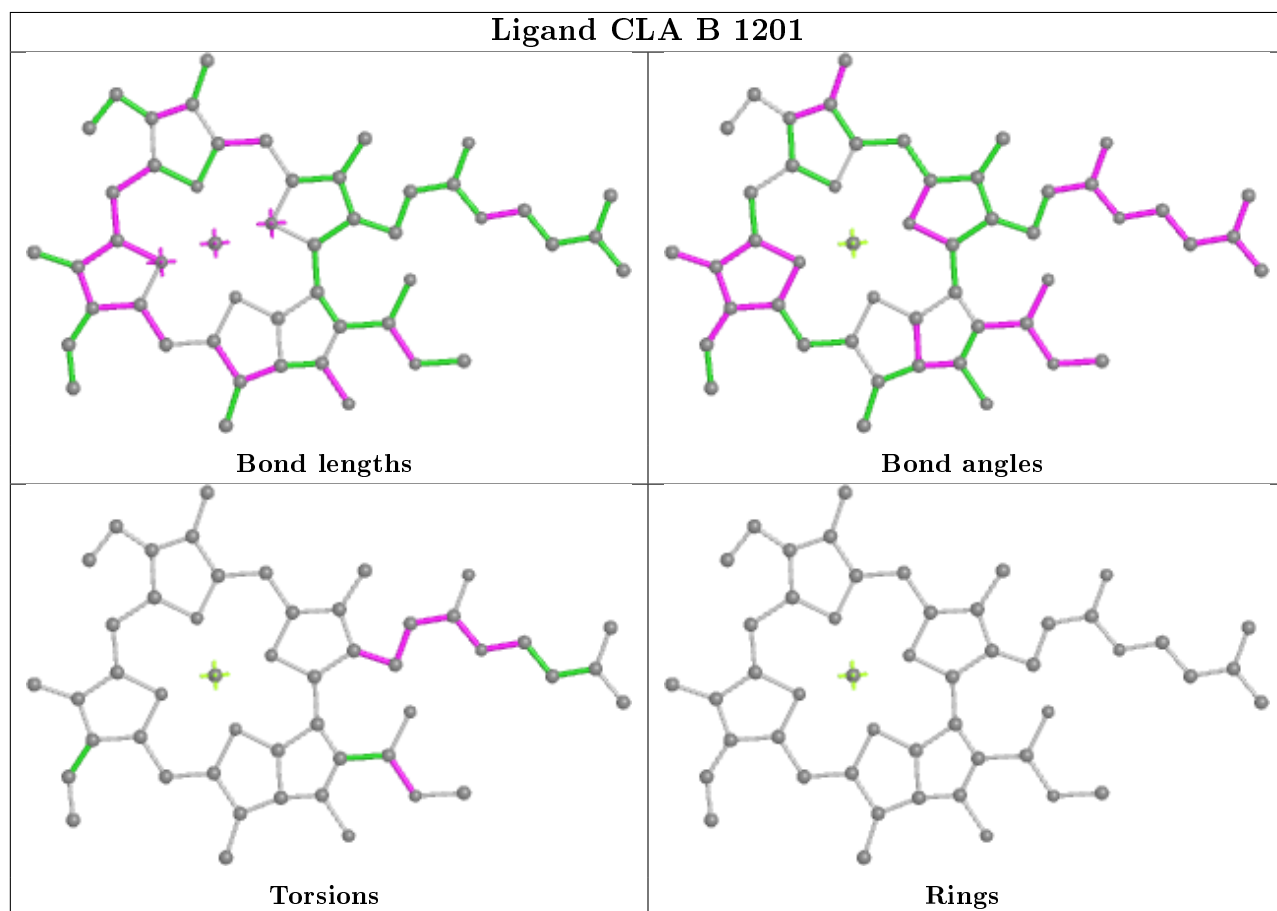
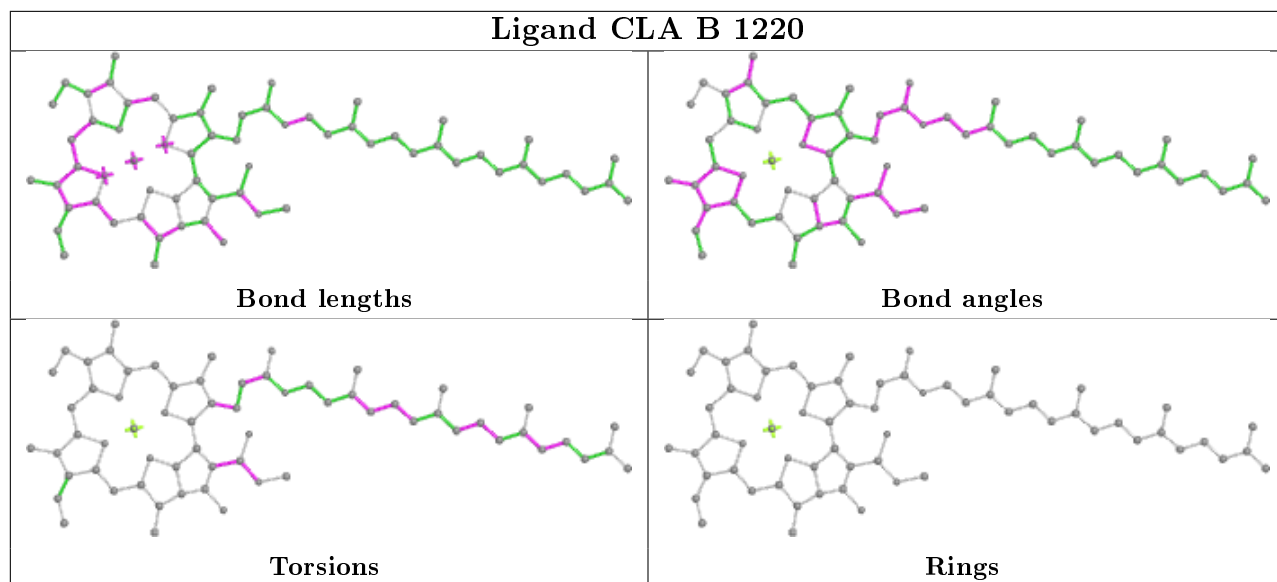
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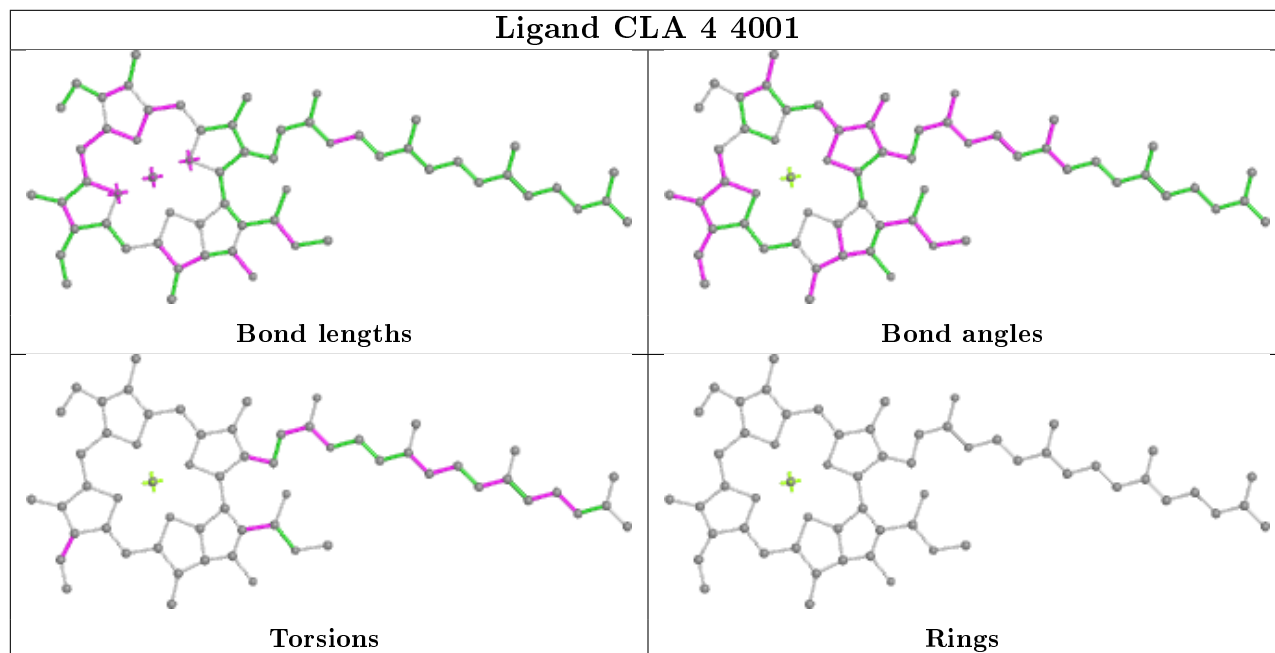
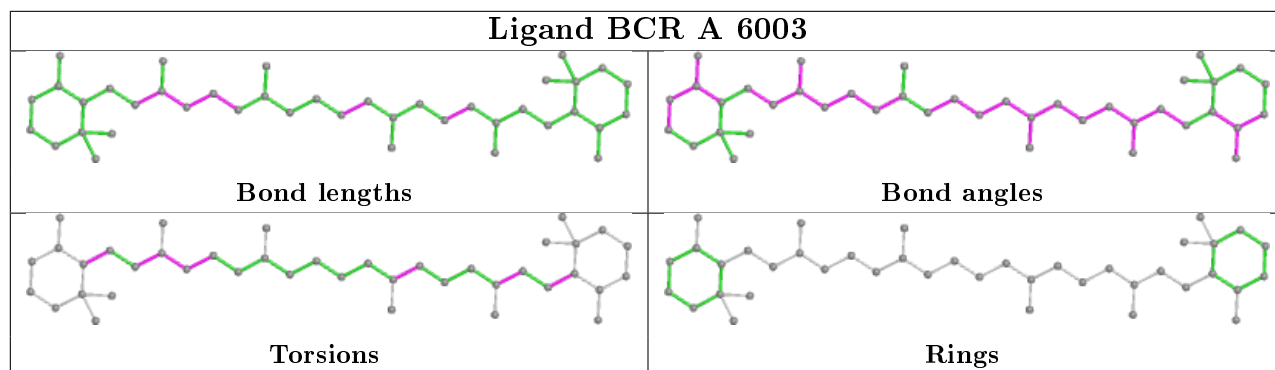
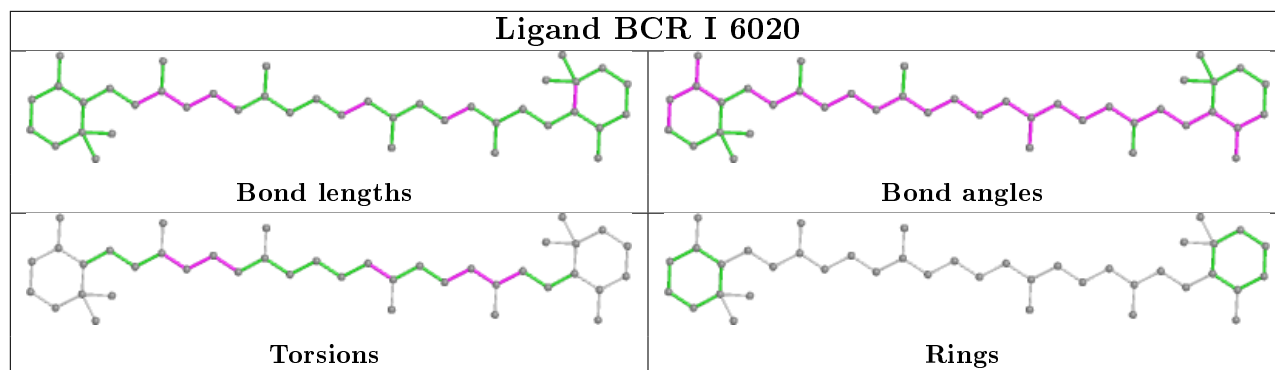
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	1226	CLA	7	0

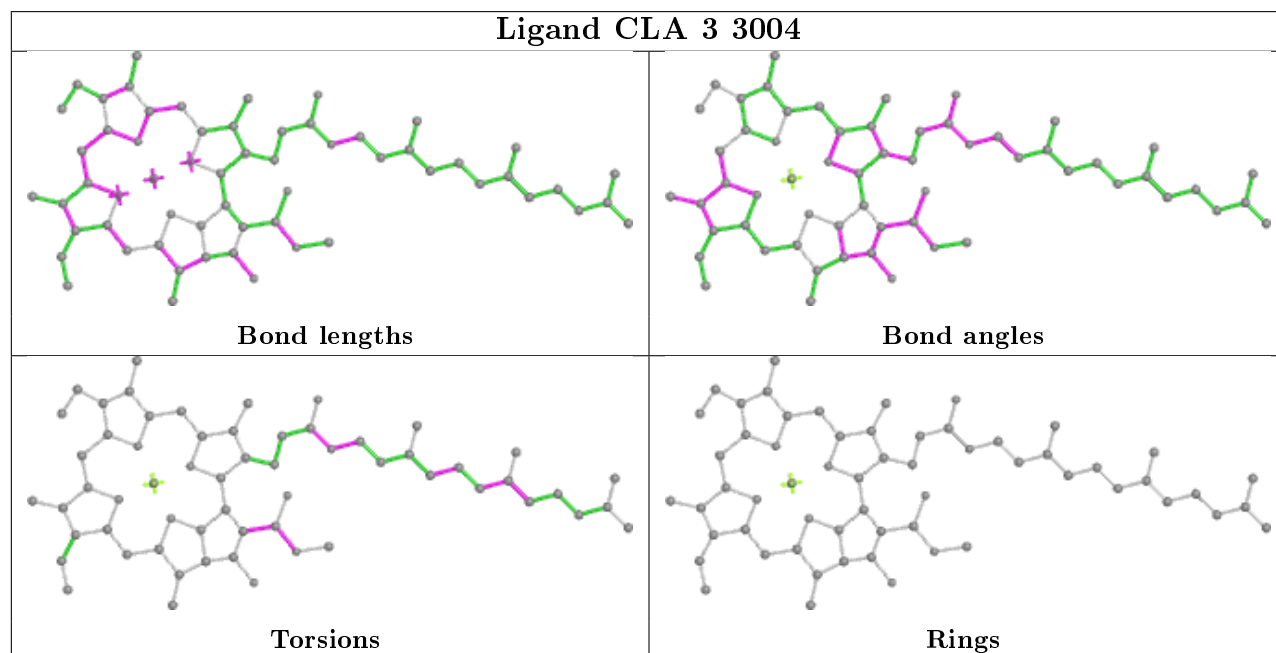
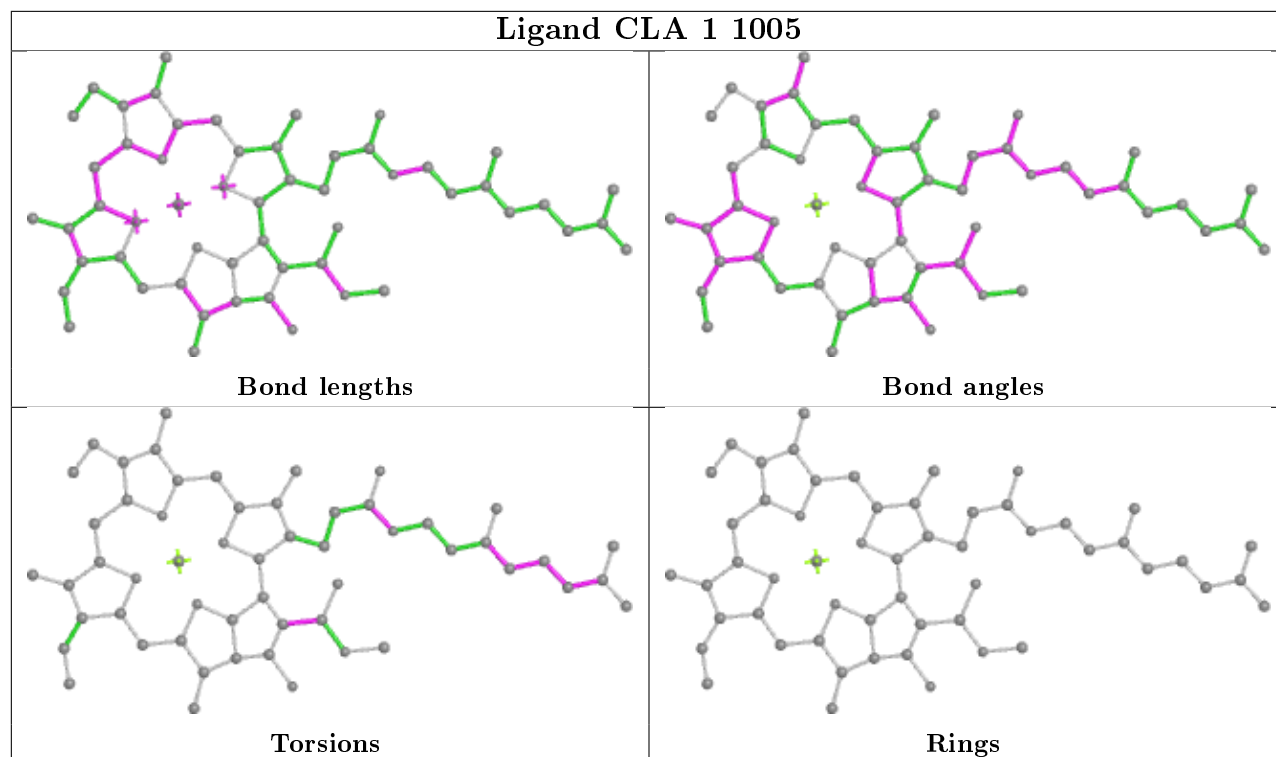
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

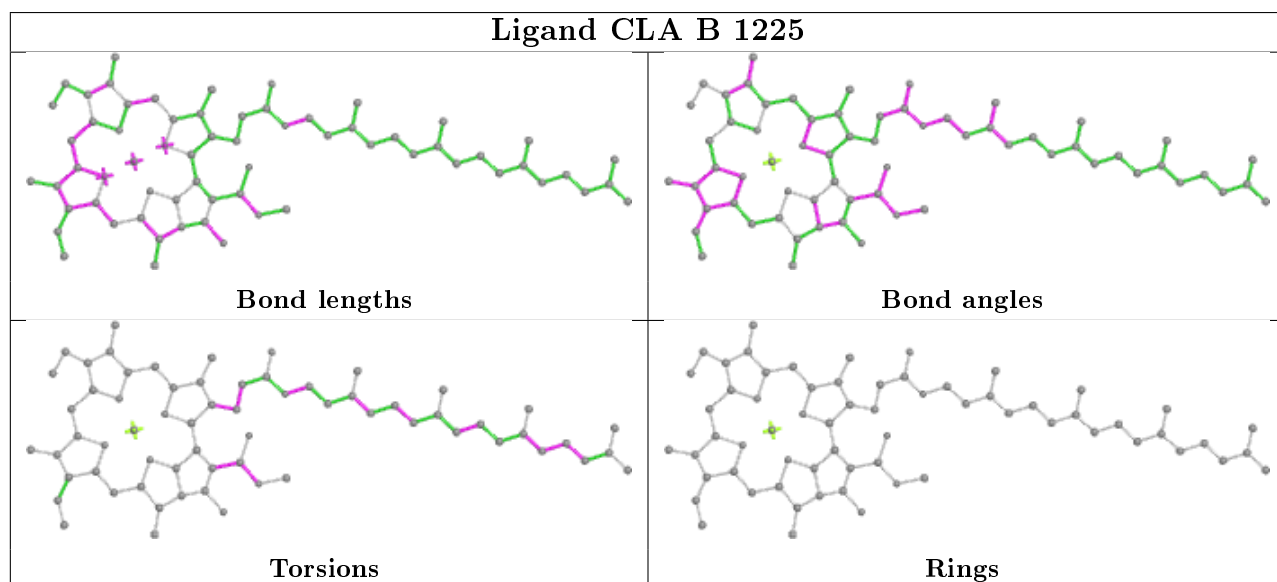
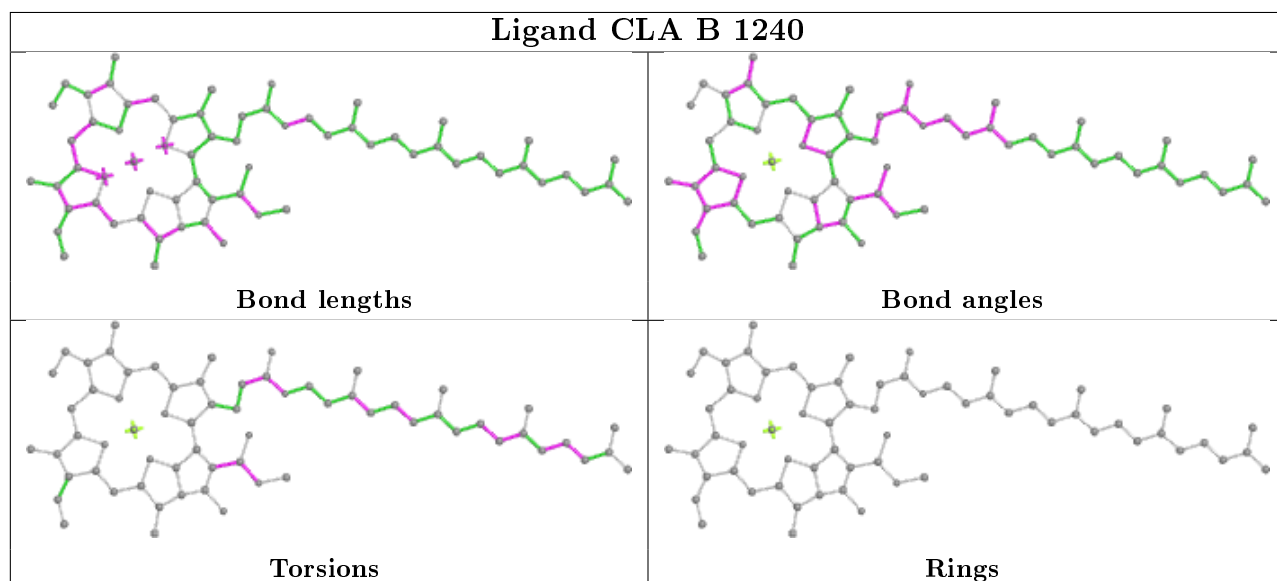
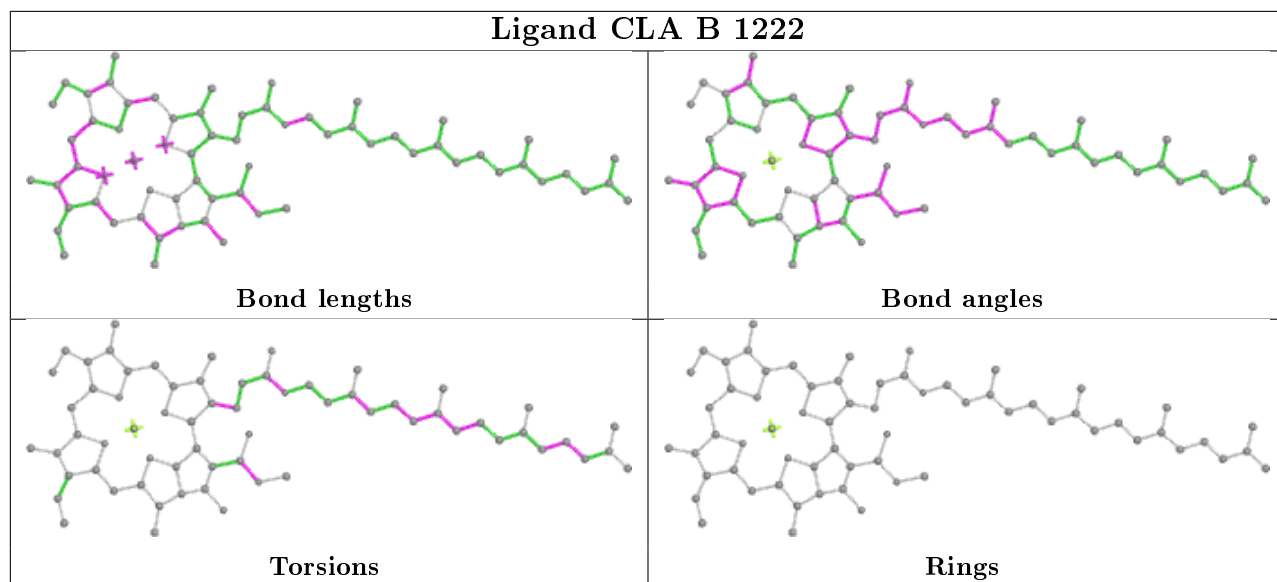


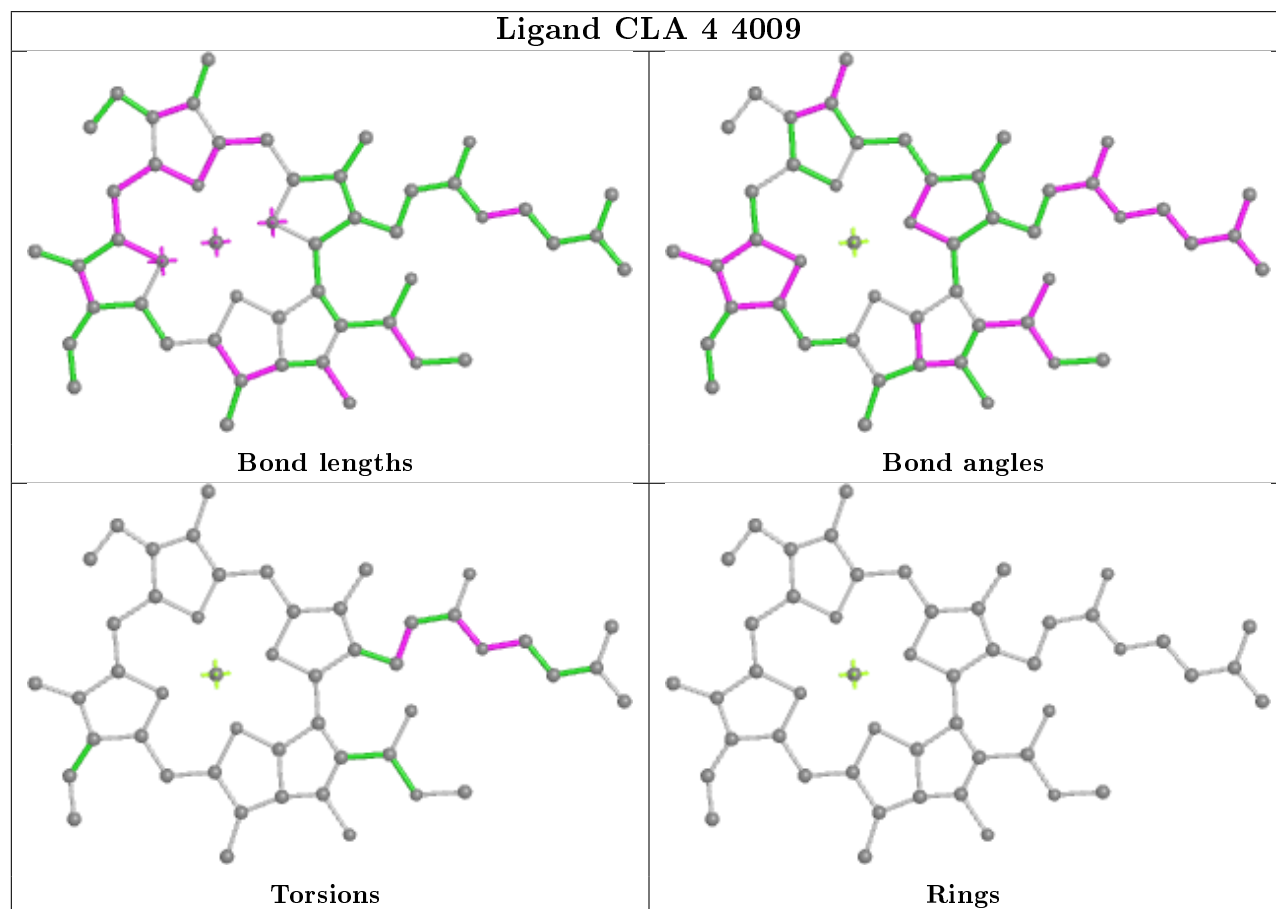
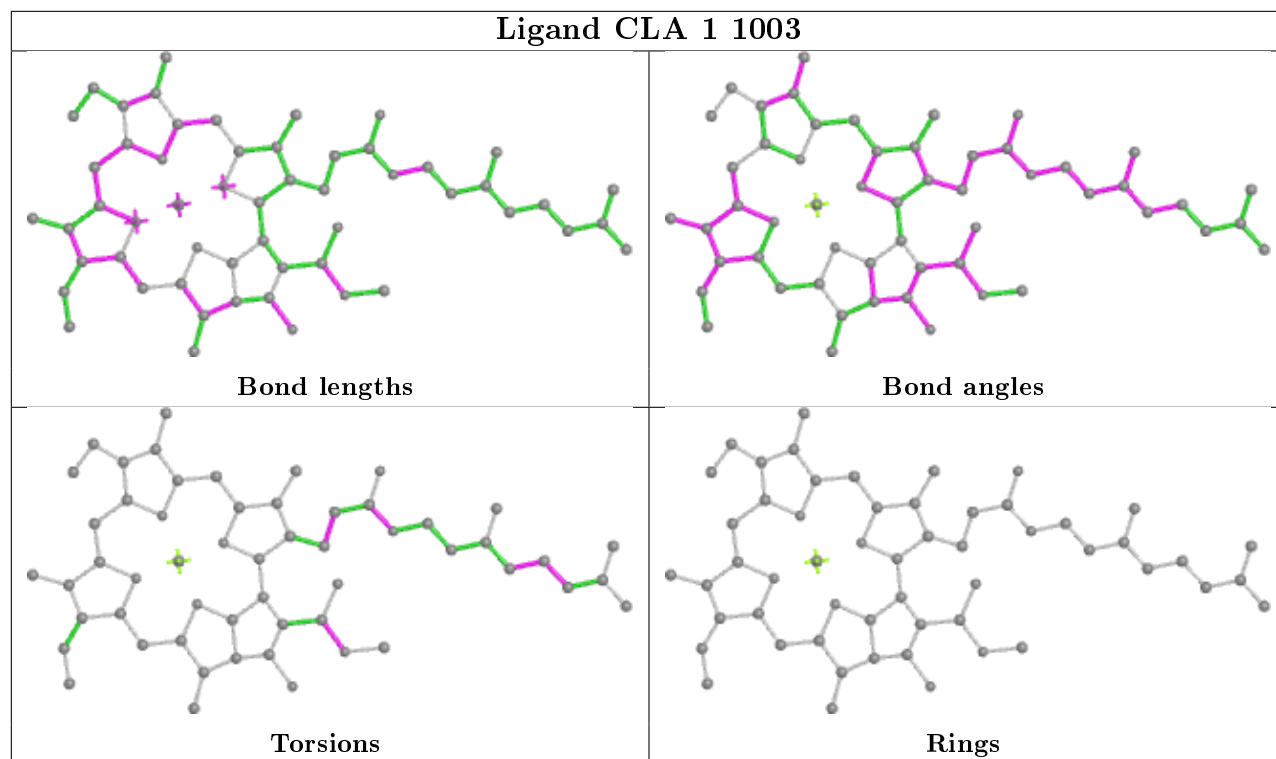


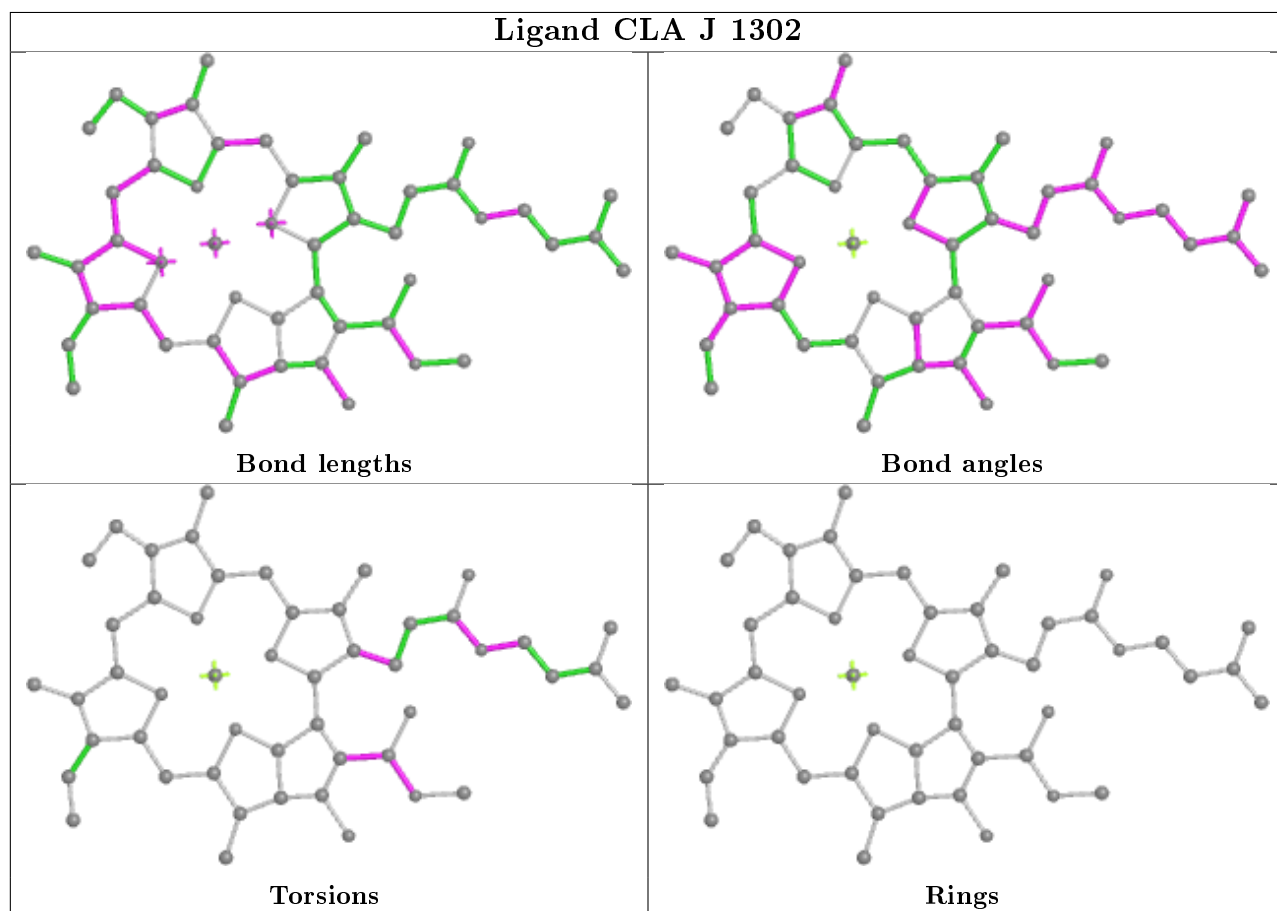
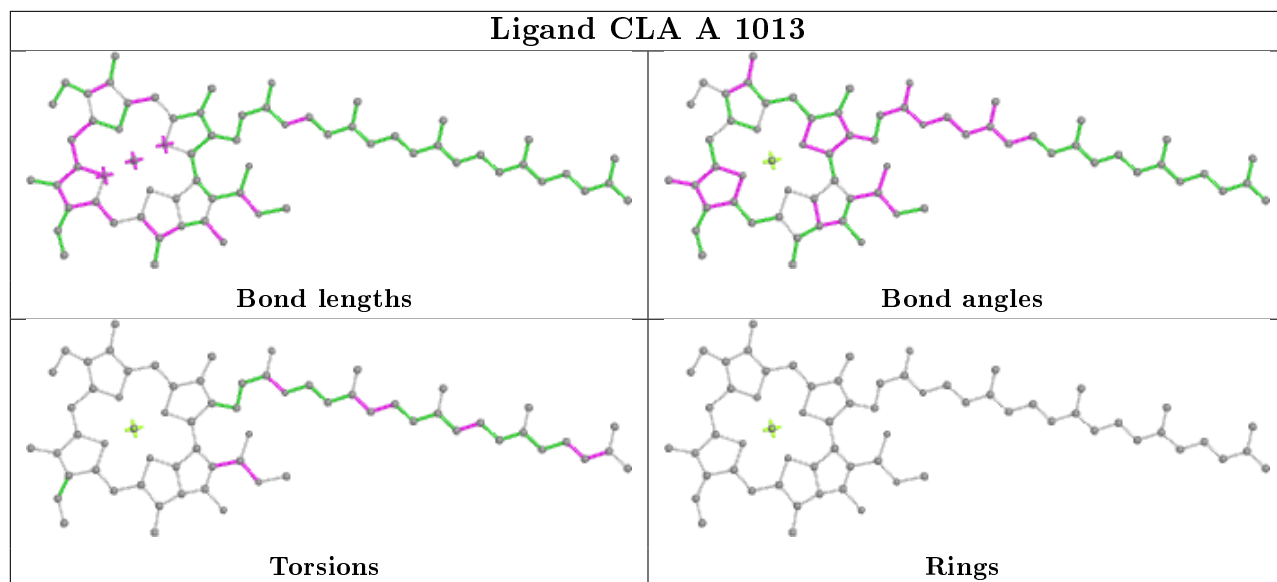


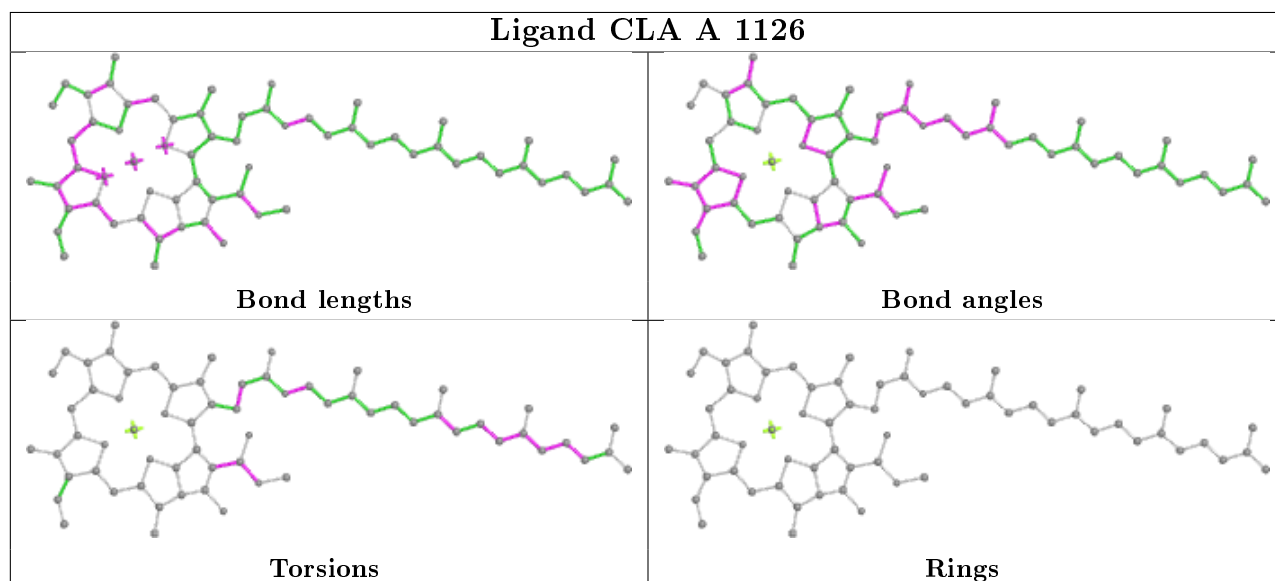
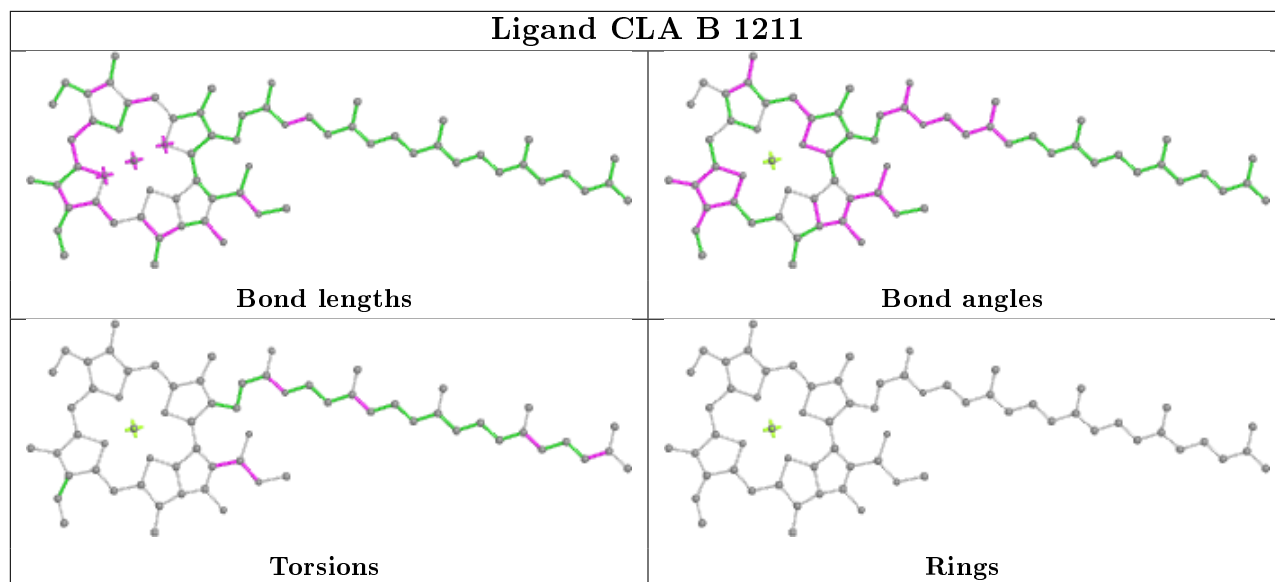


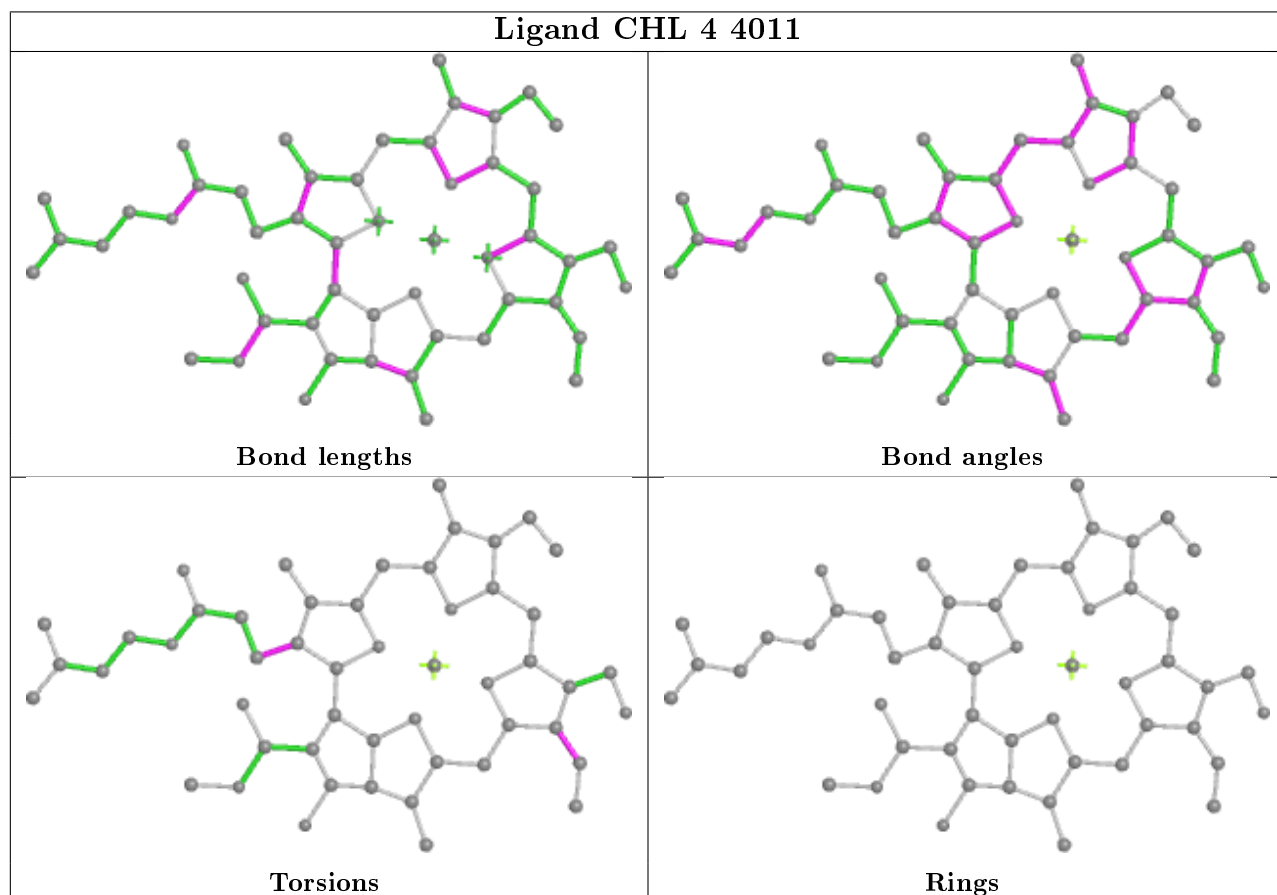
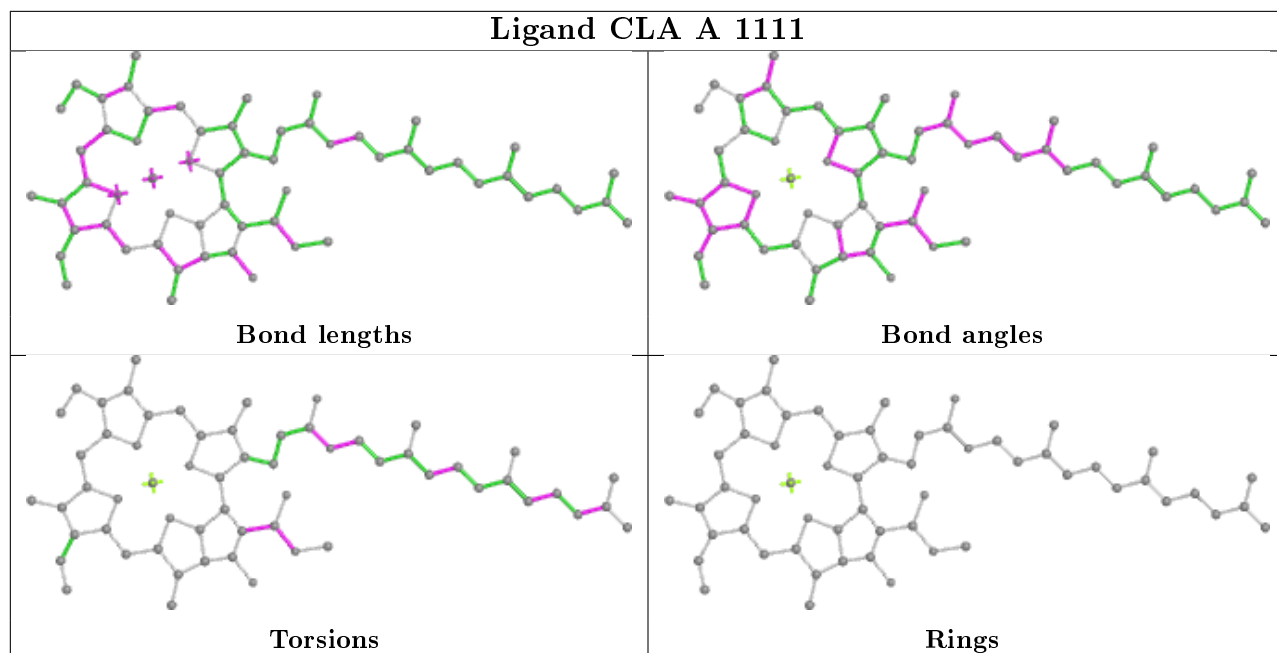


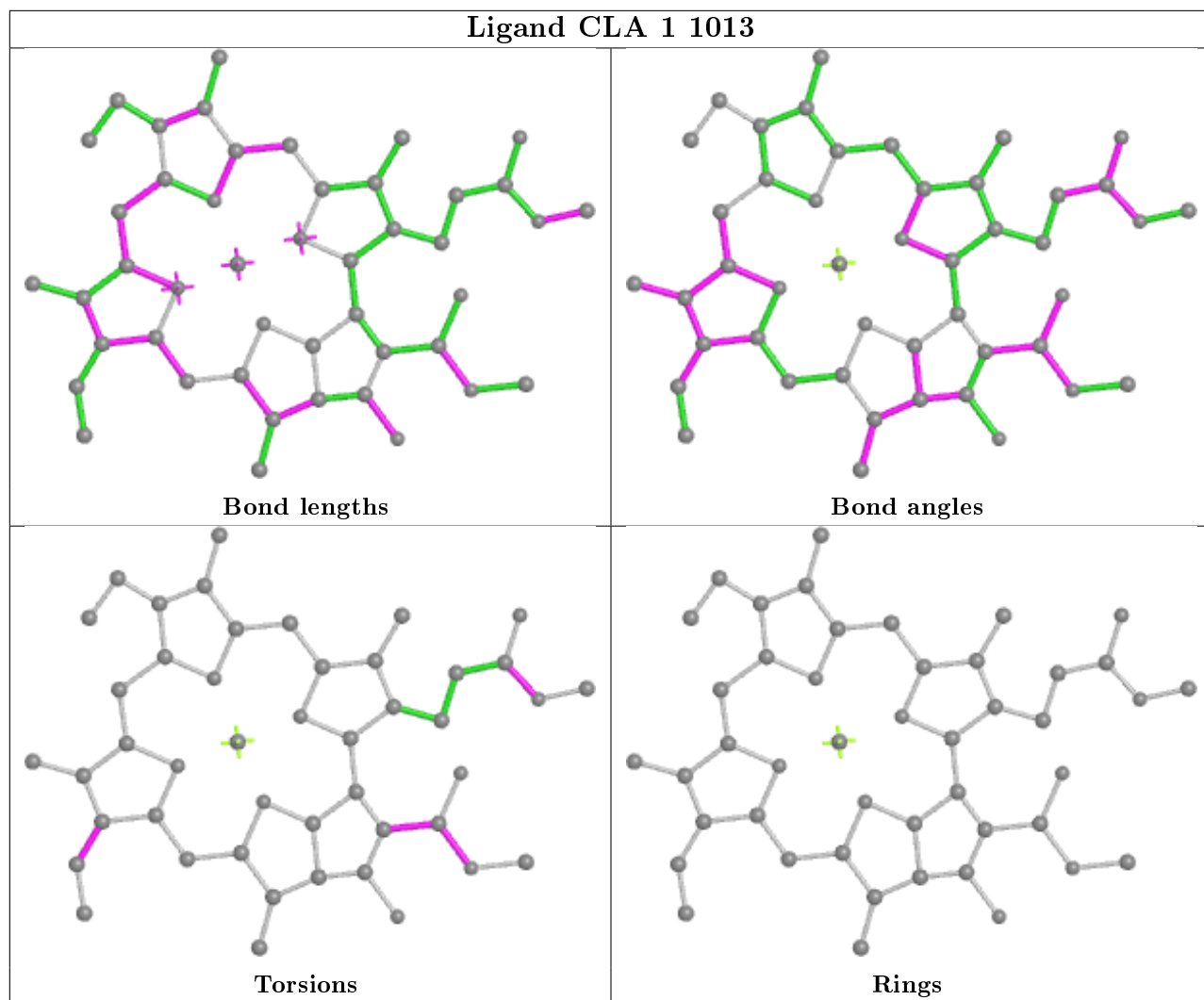
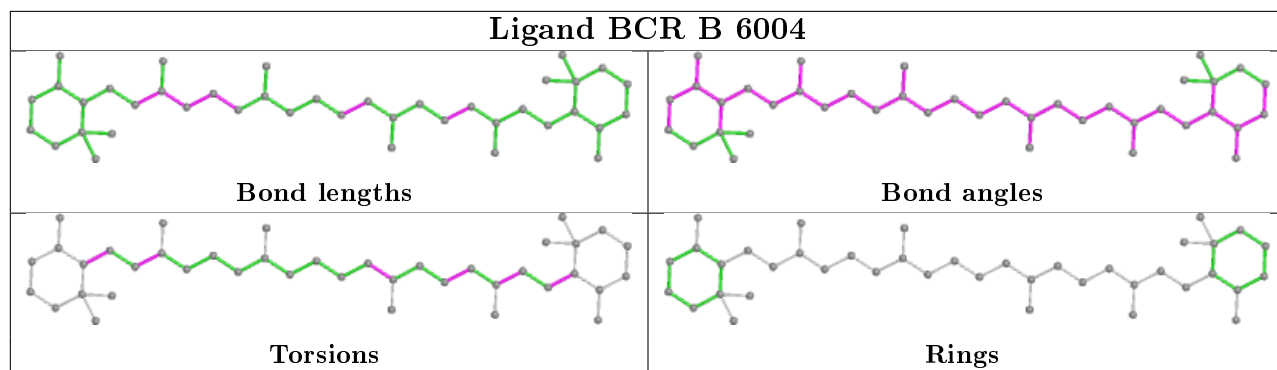


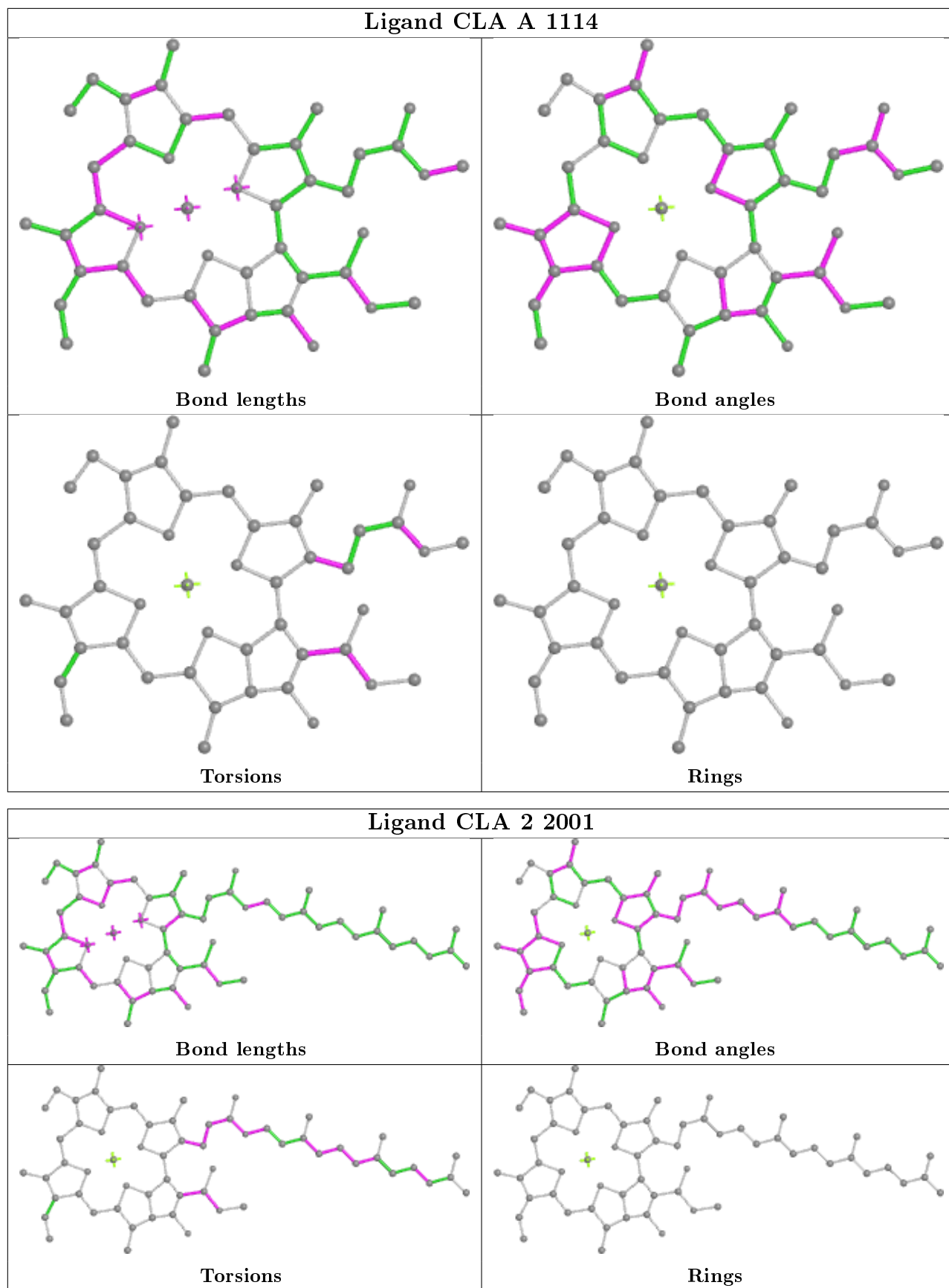


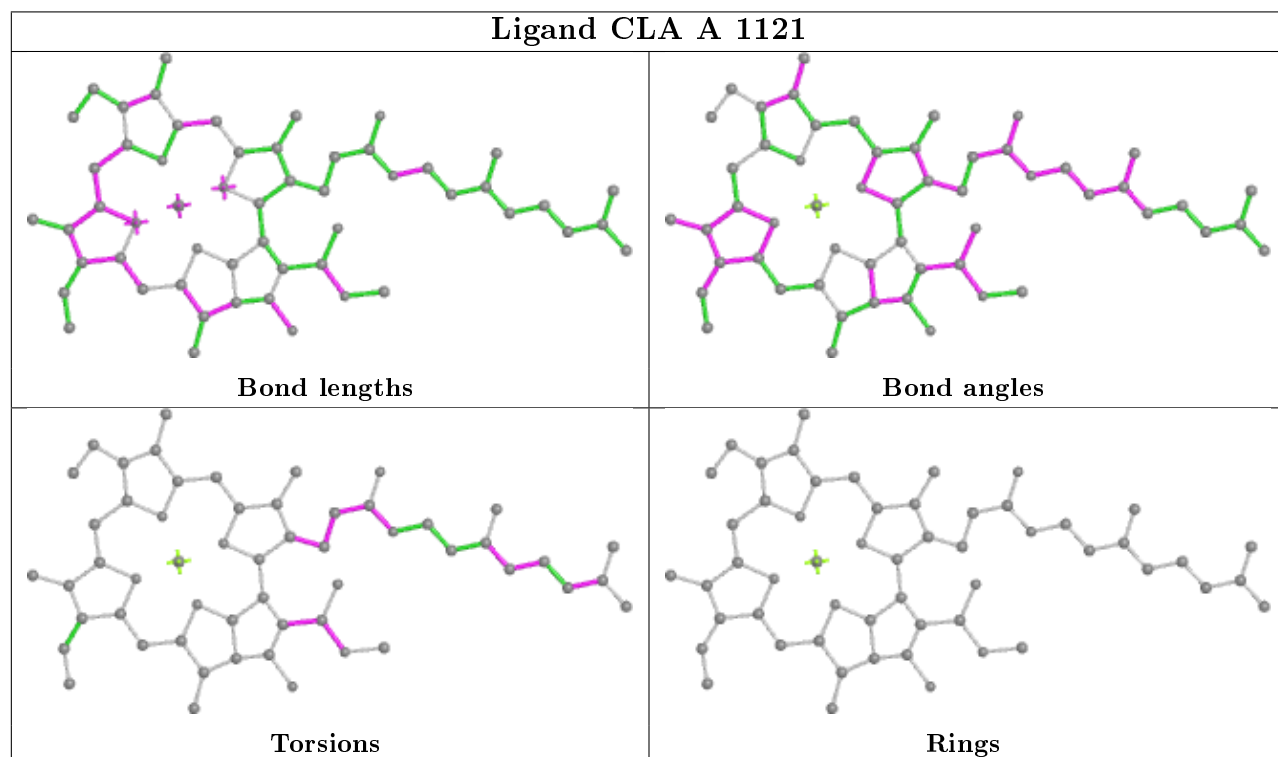
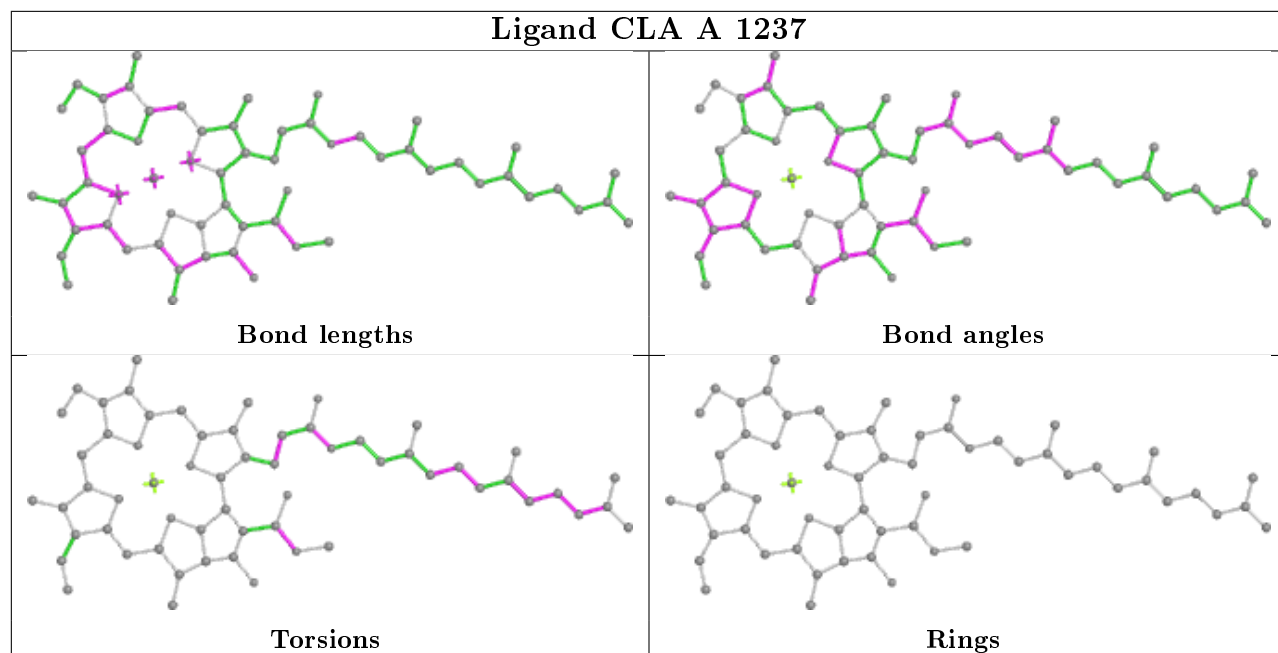


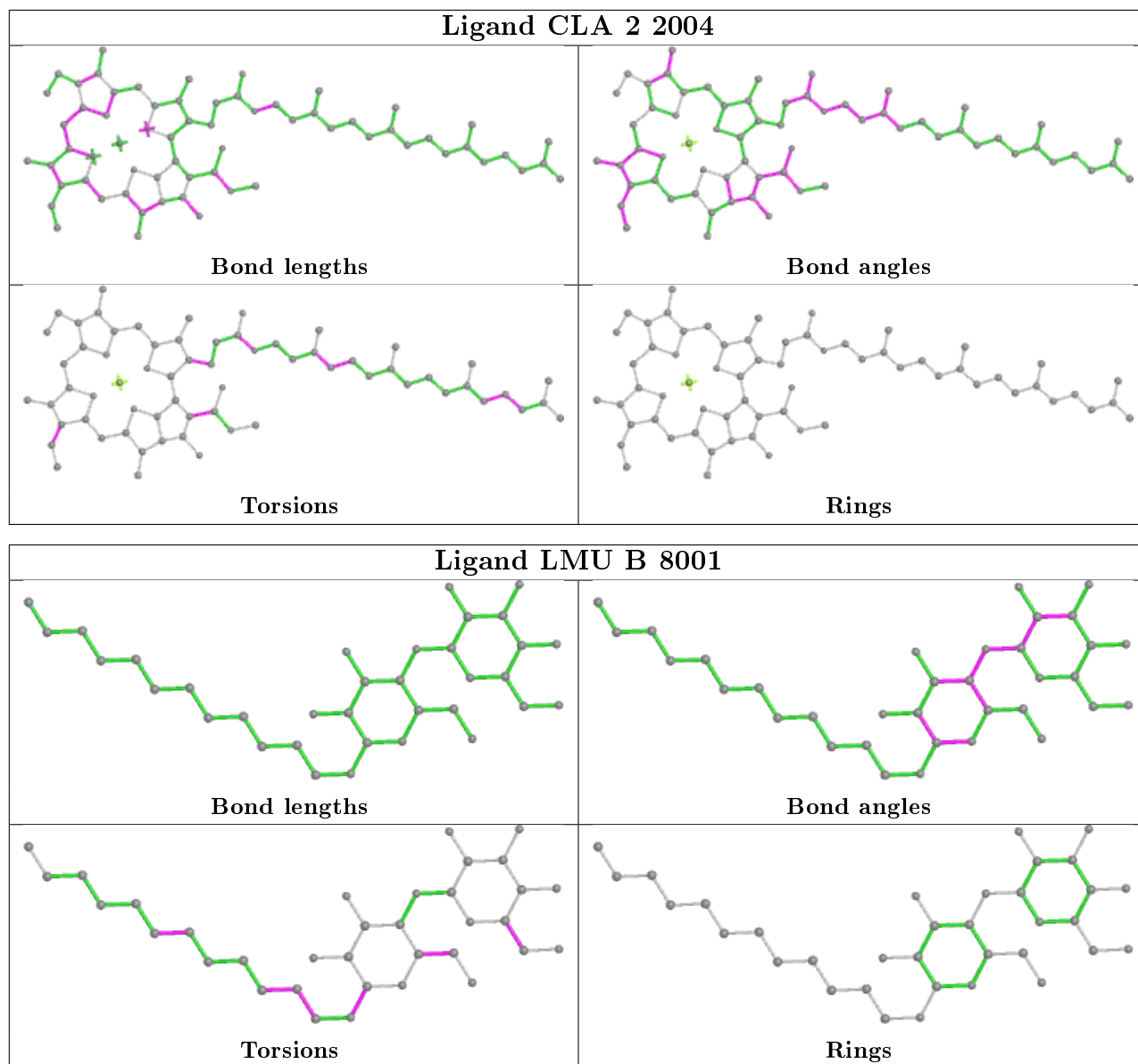


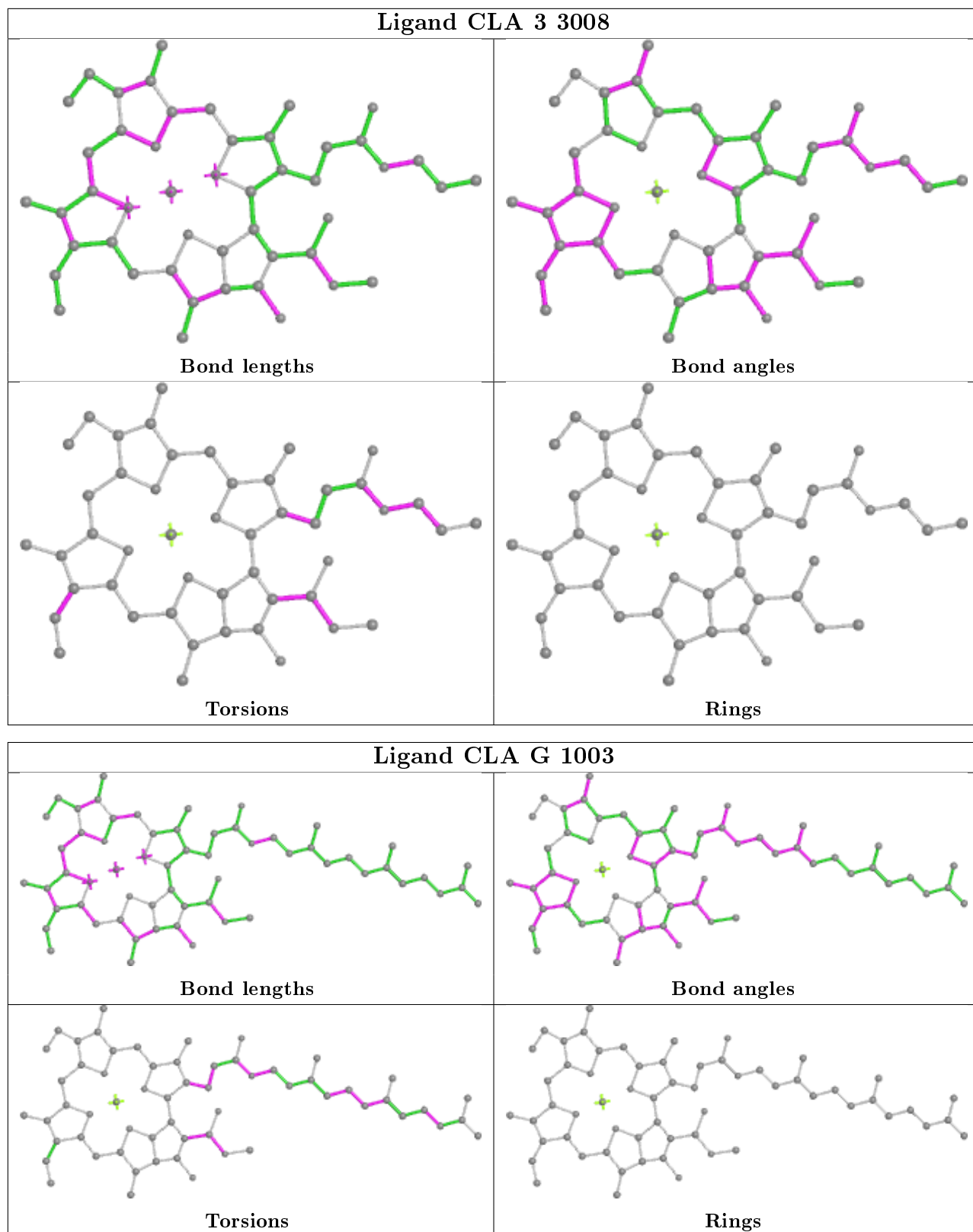


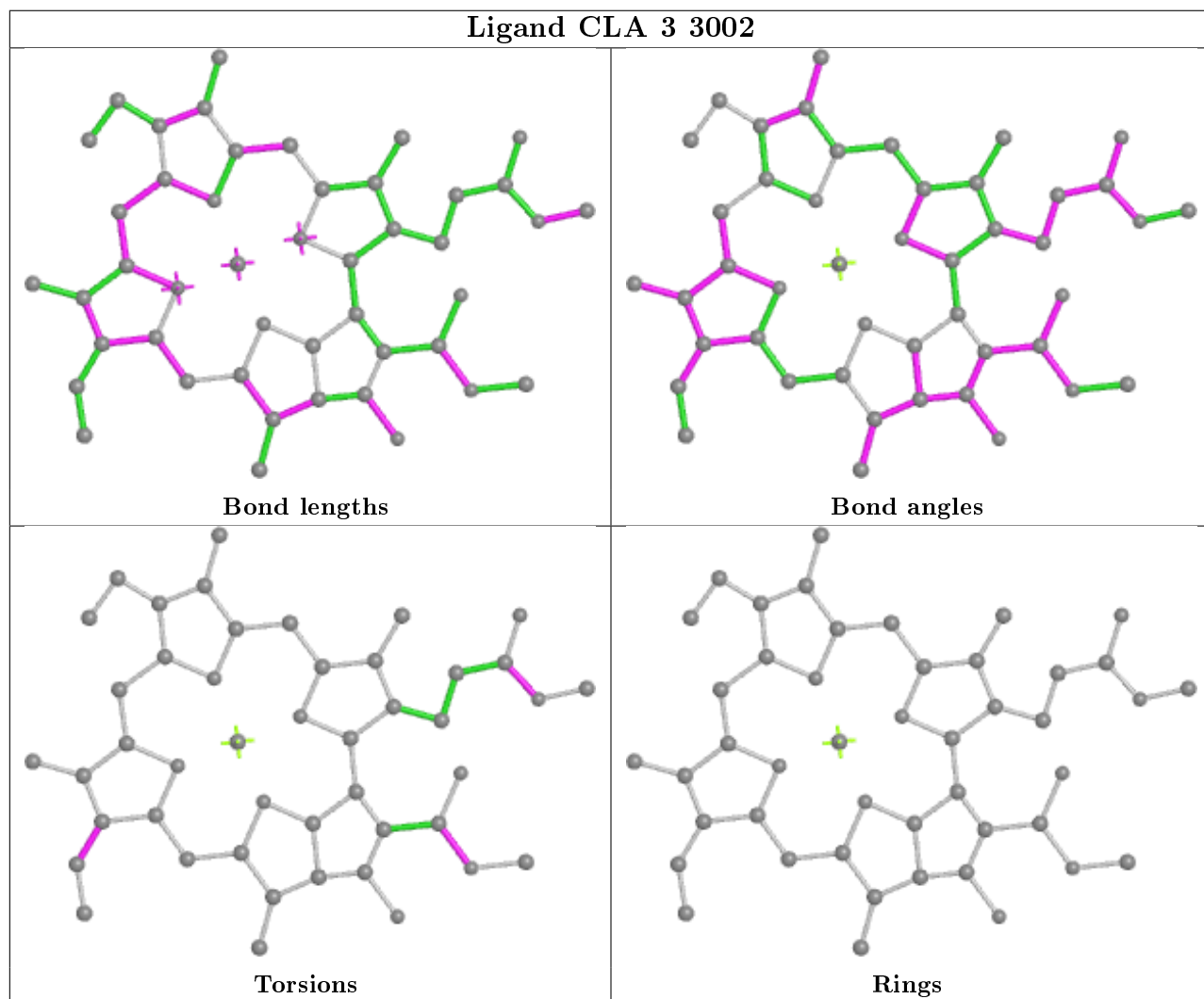
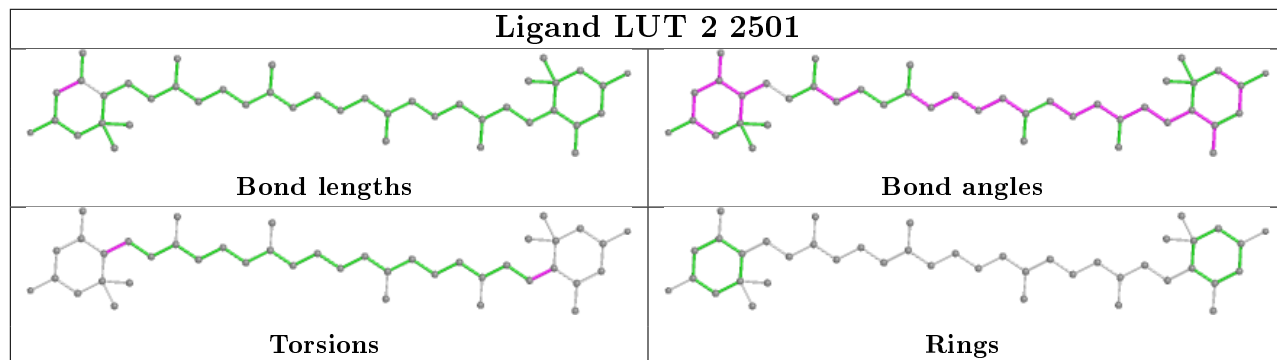
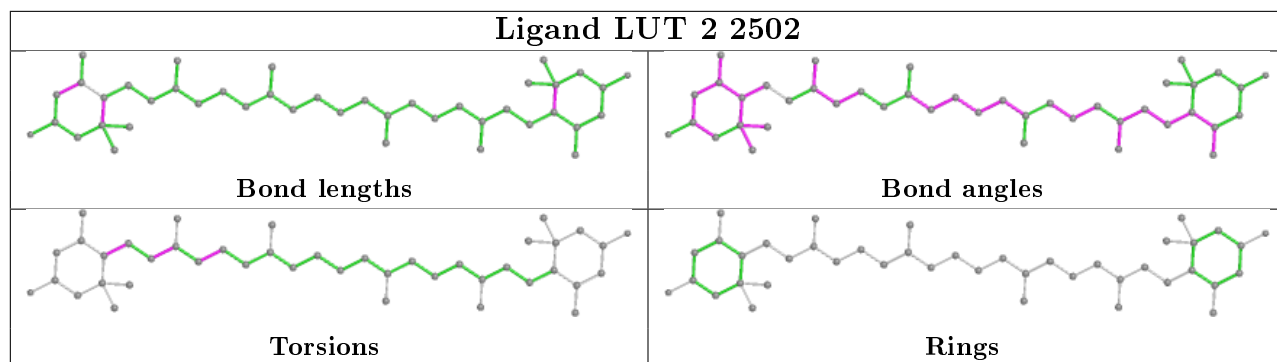


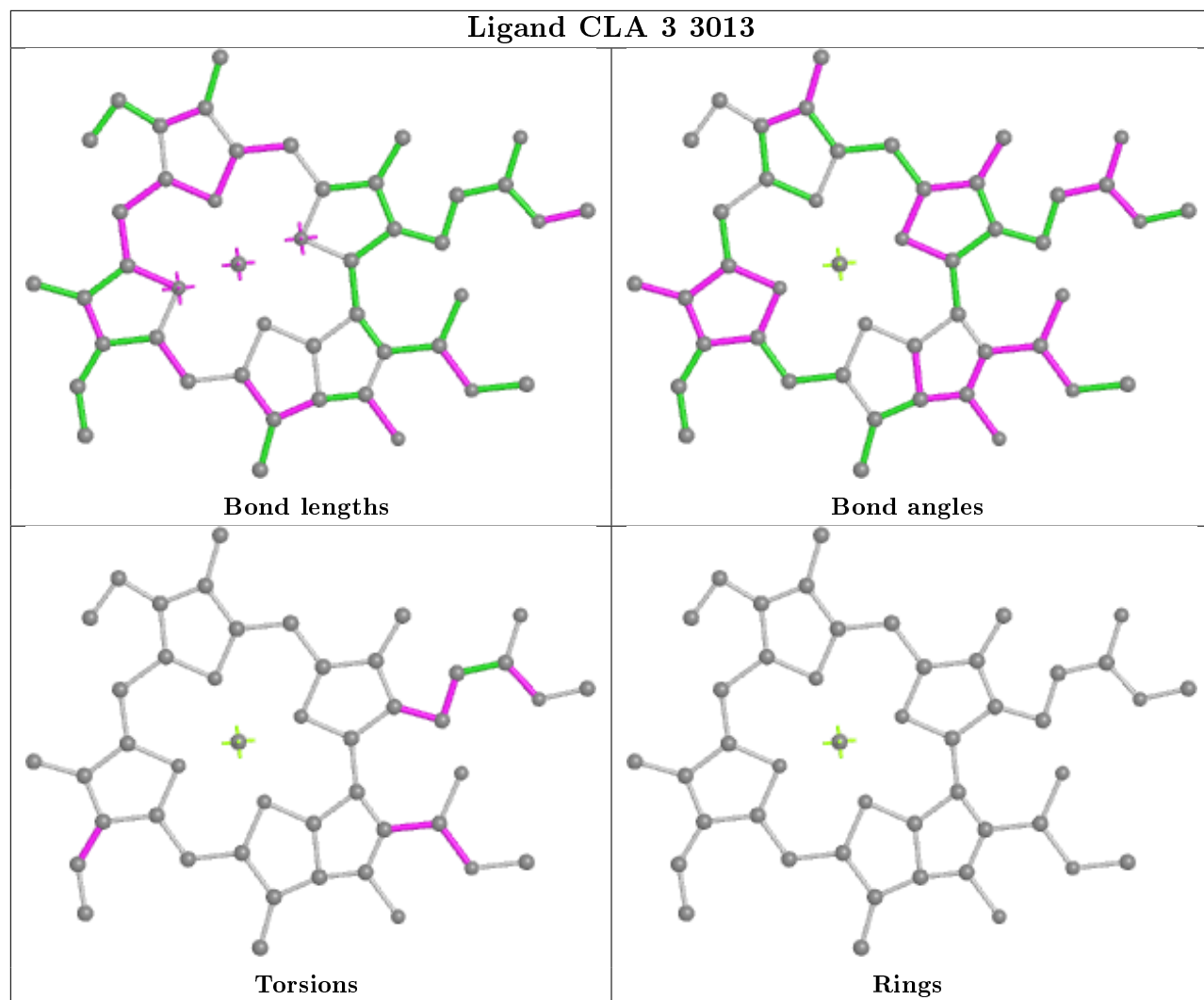


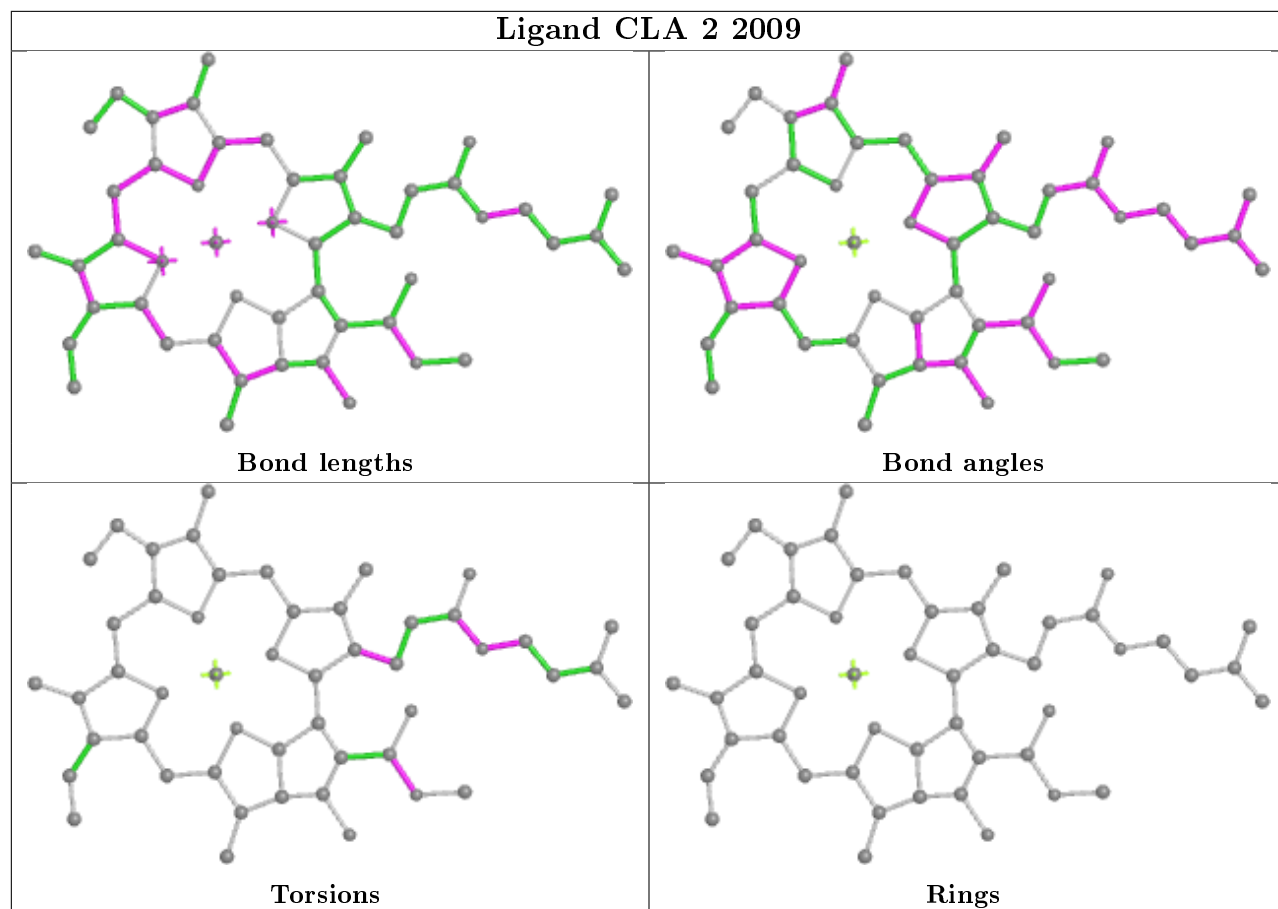


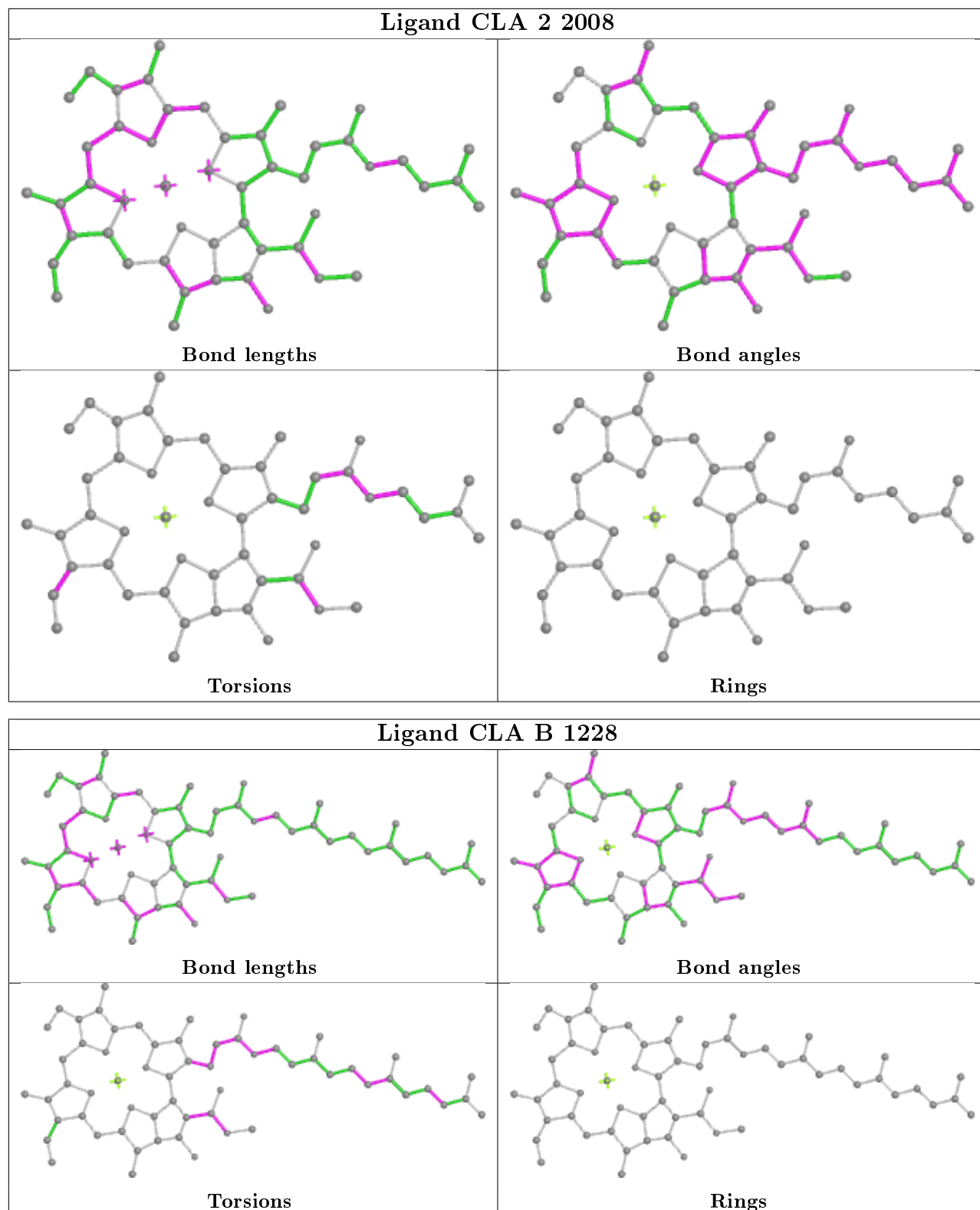


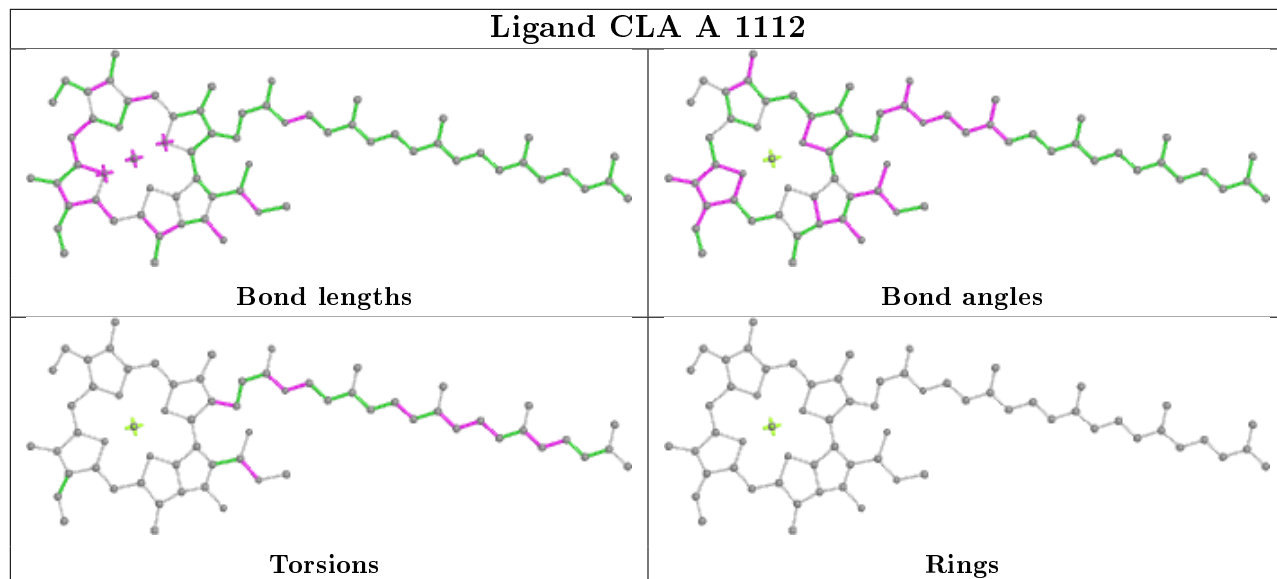
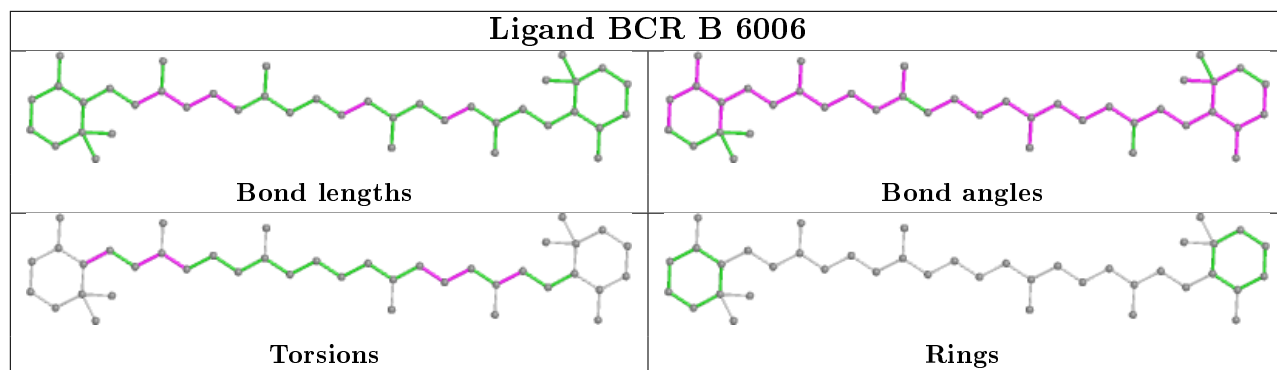


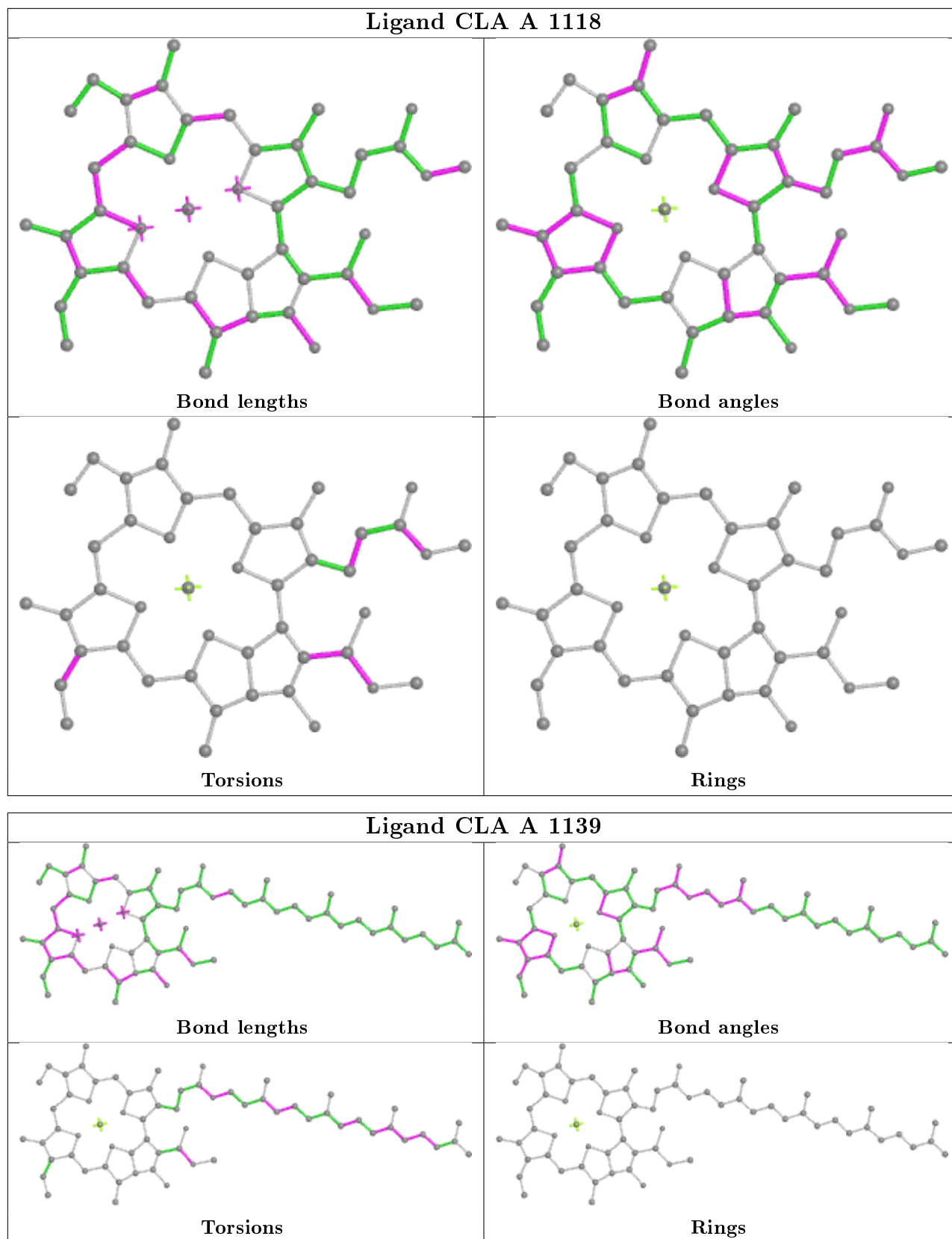


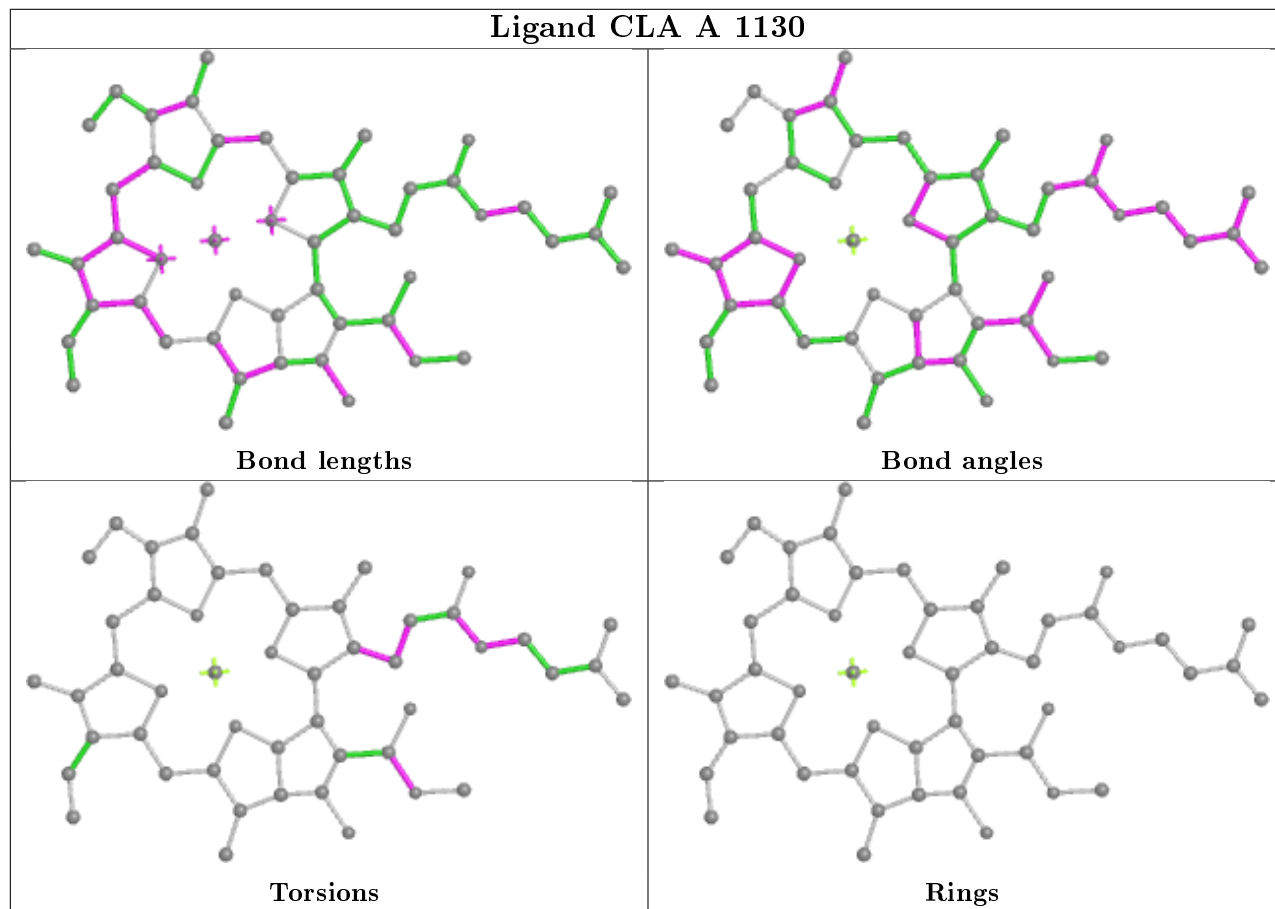
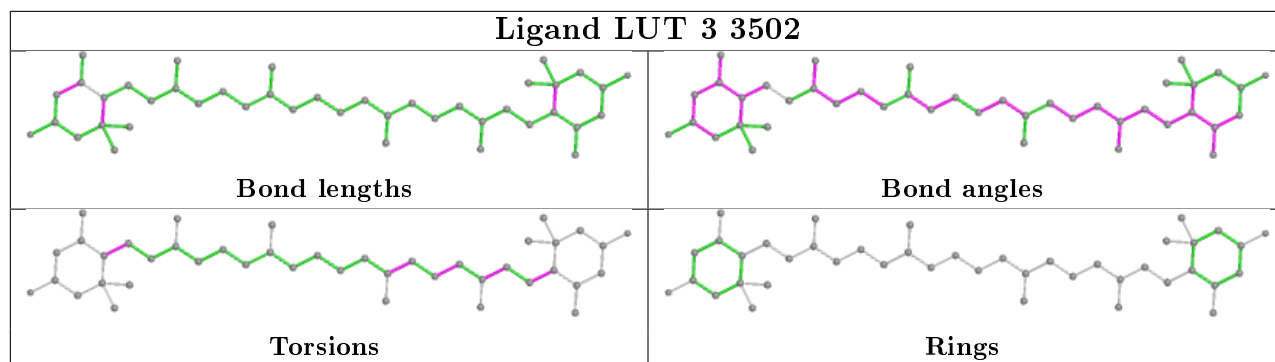


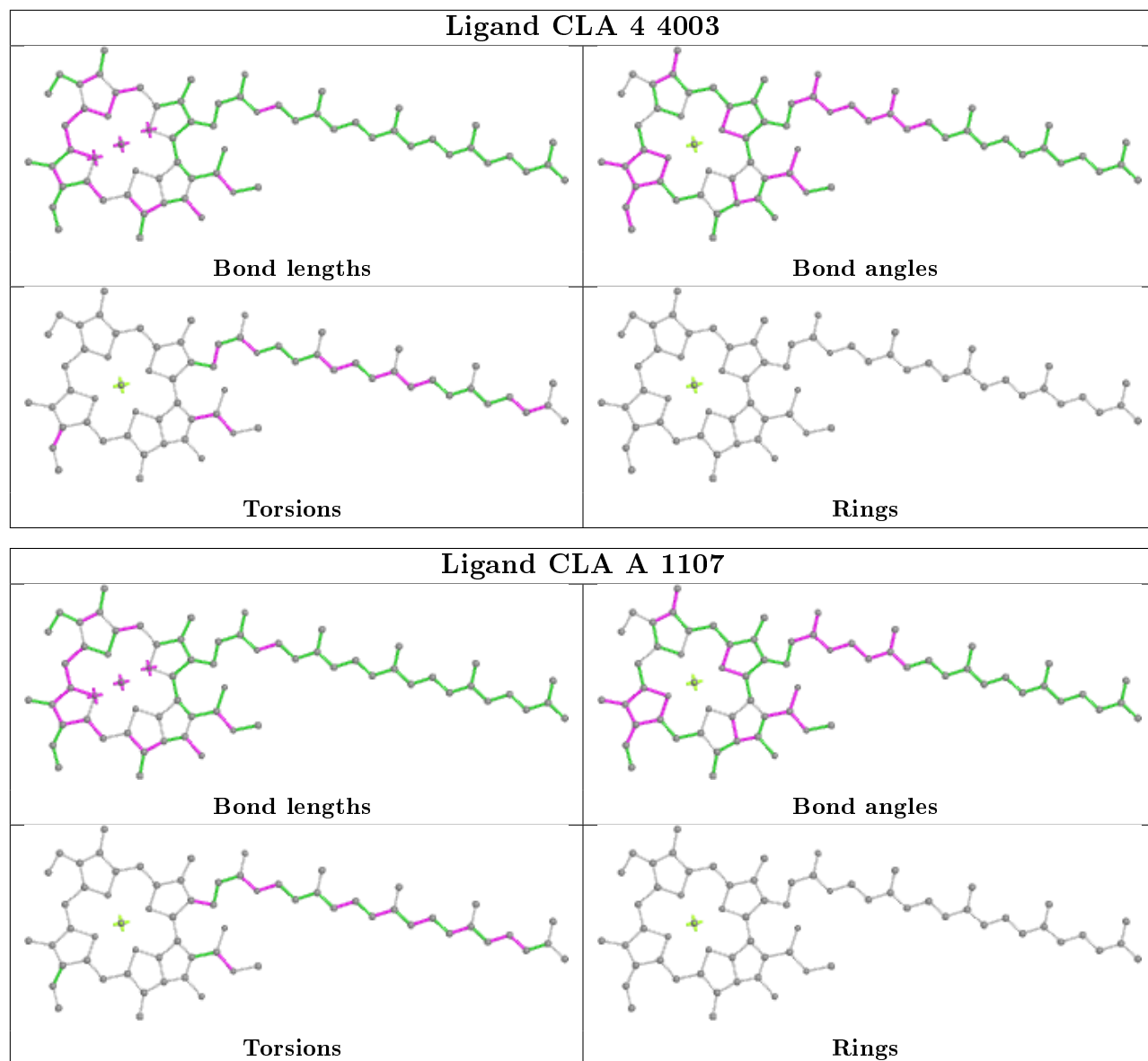


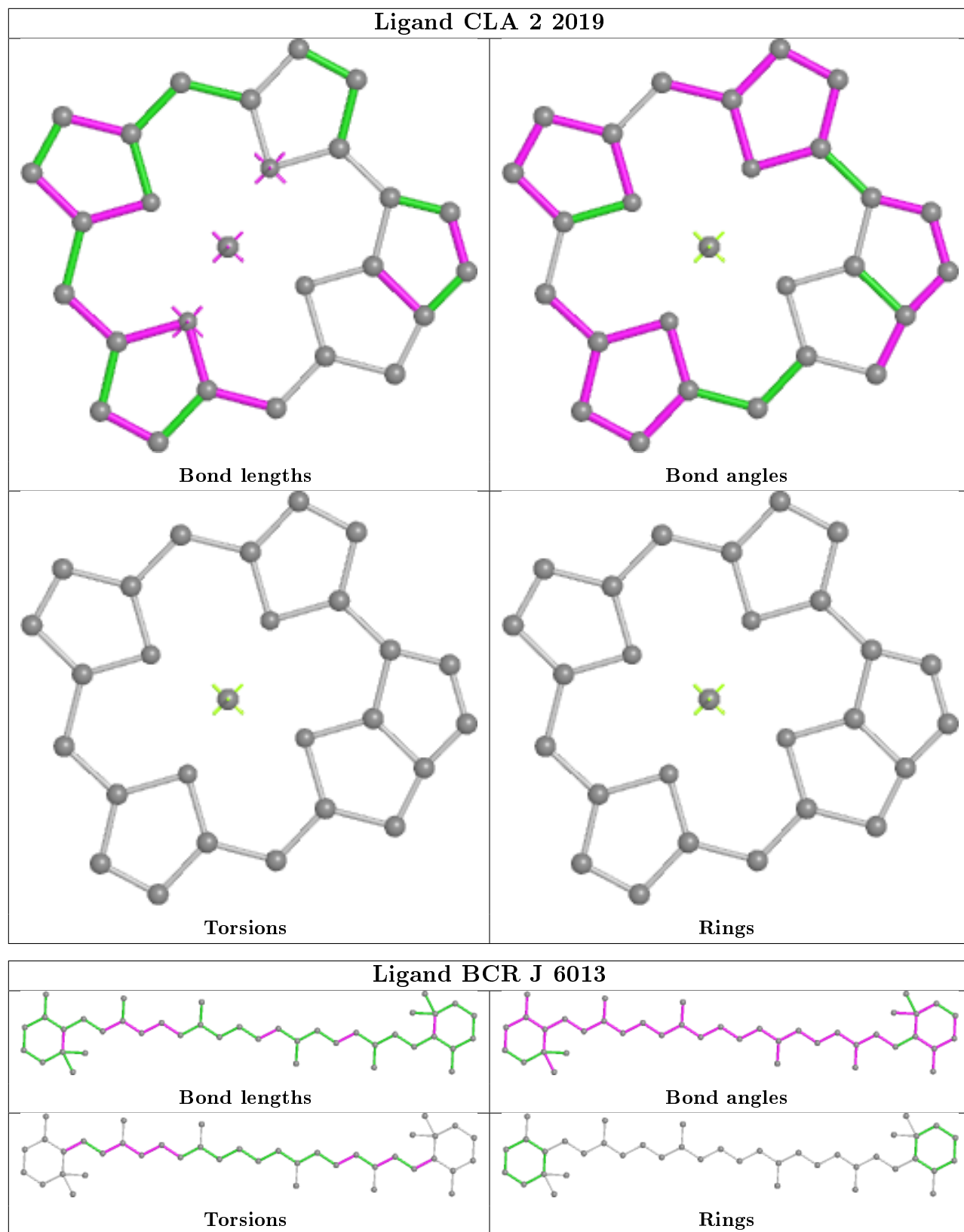


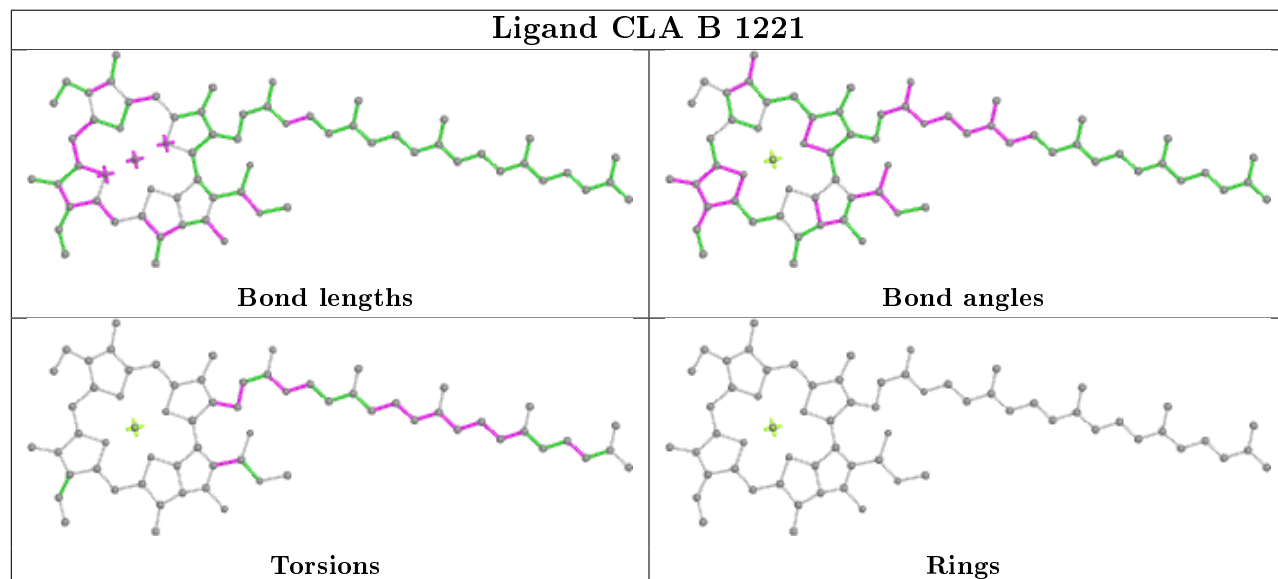
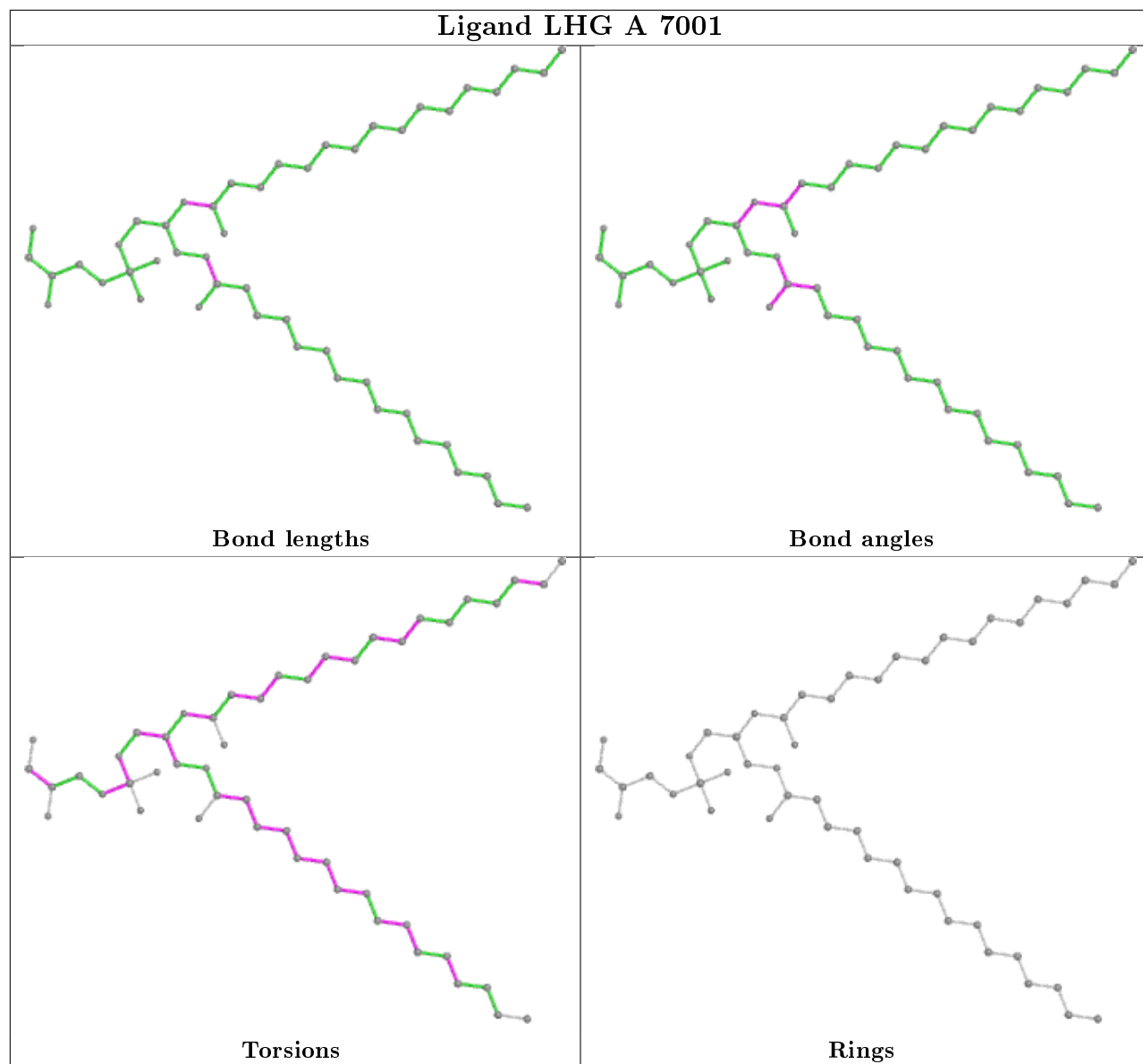


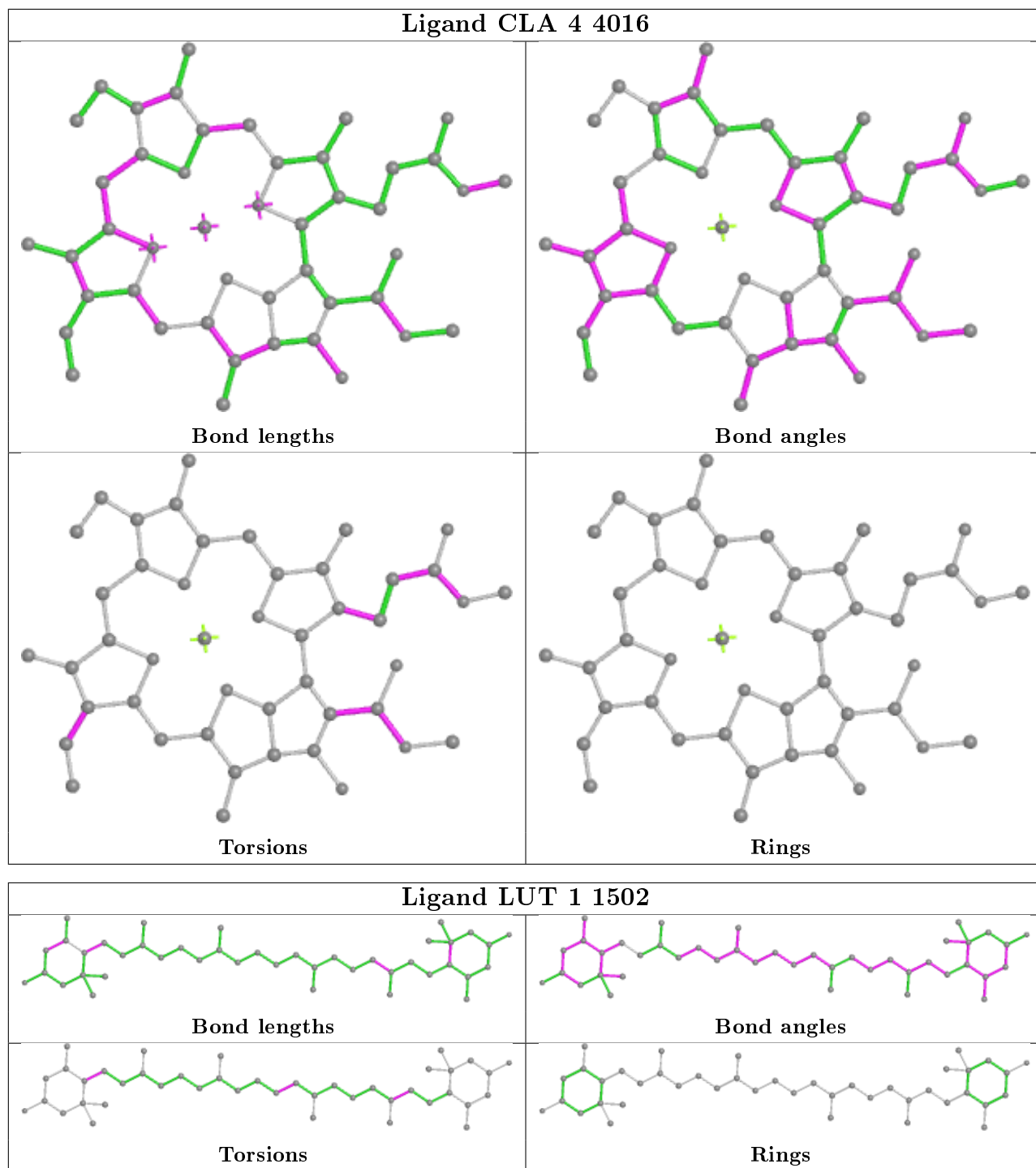


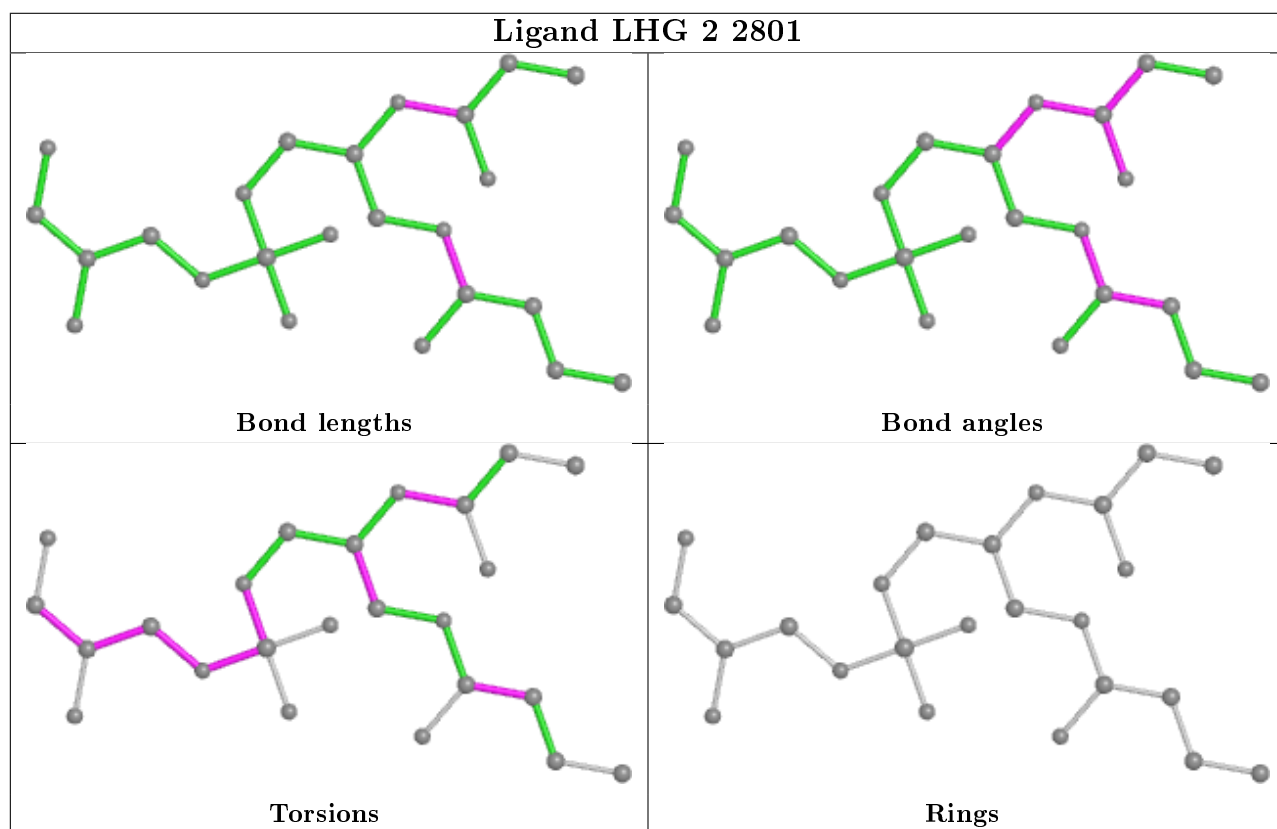
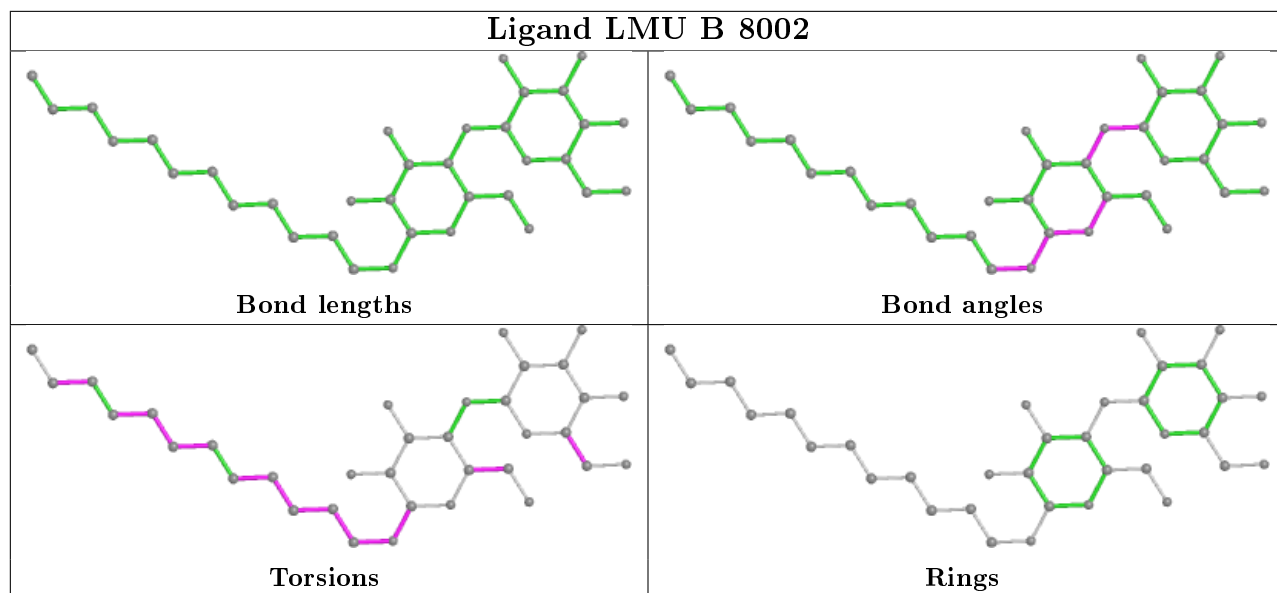


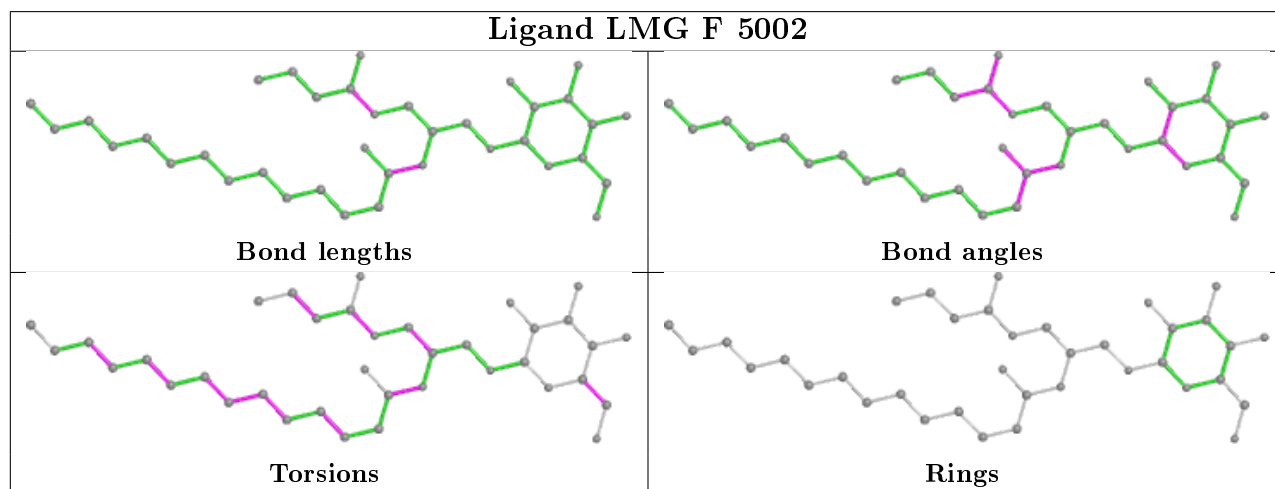
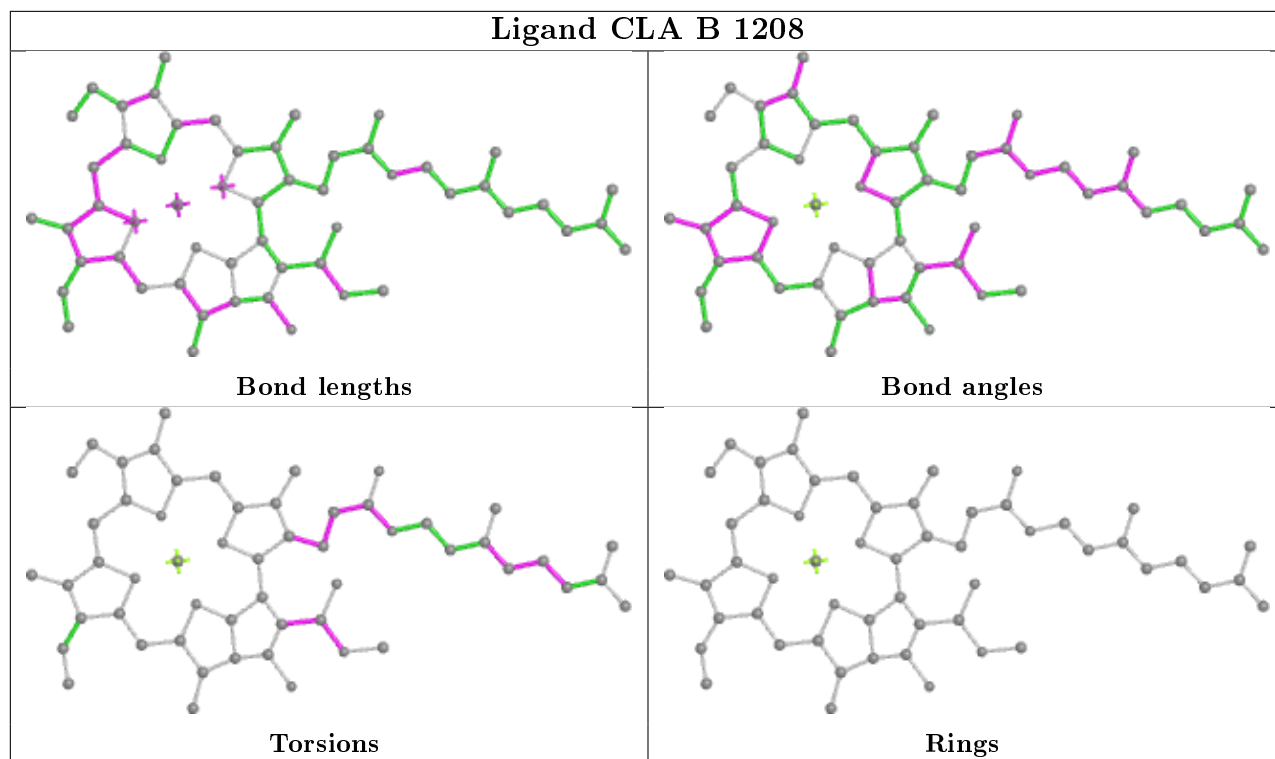


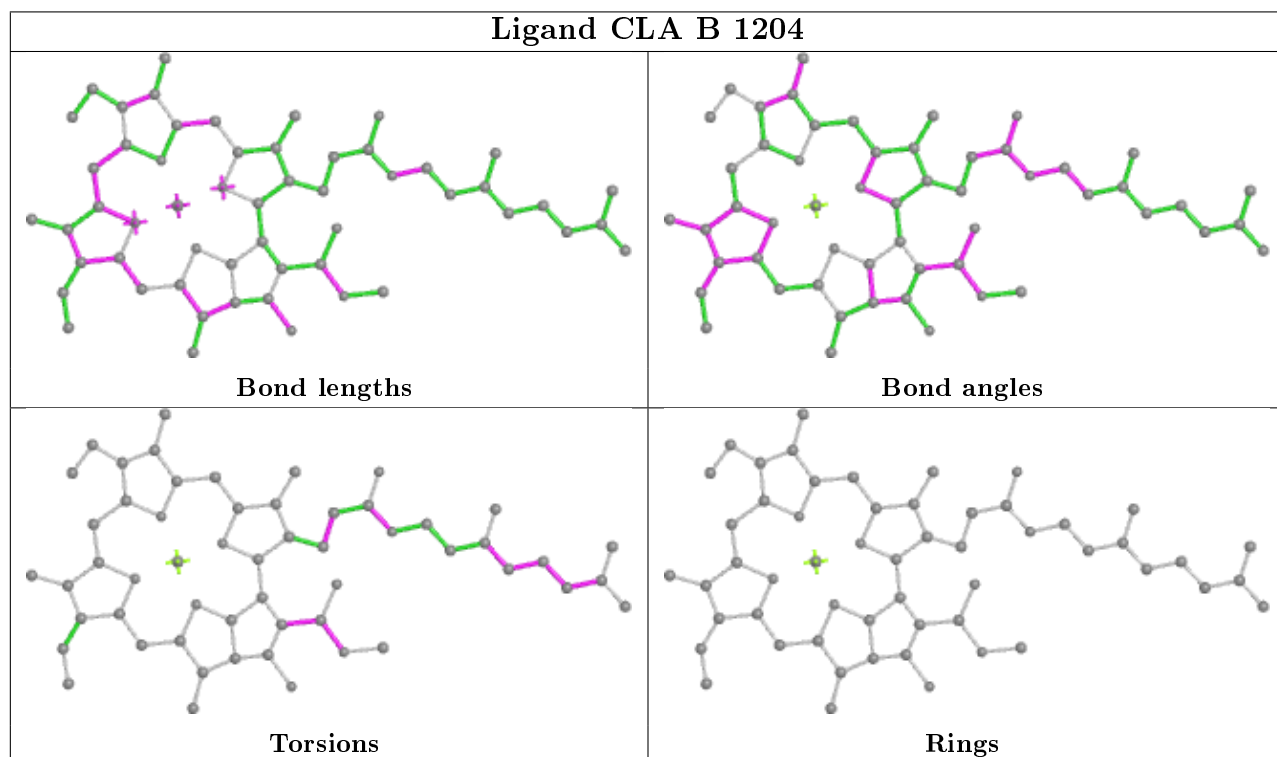
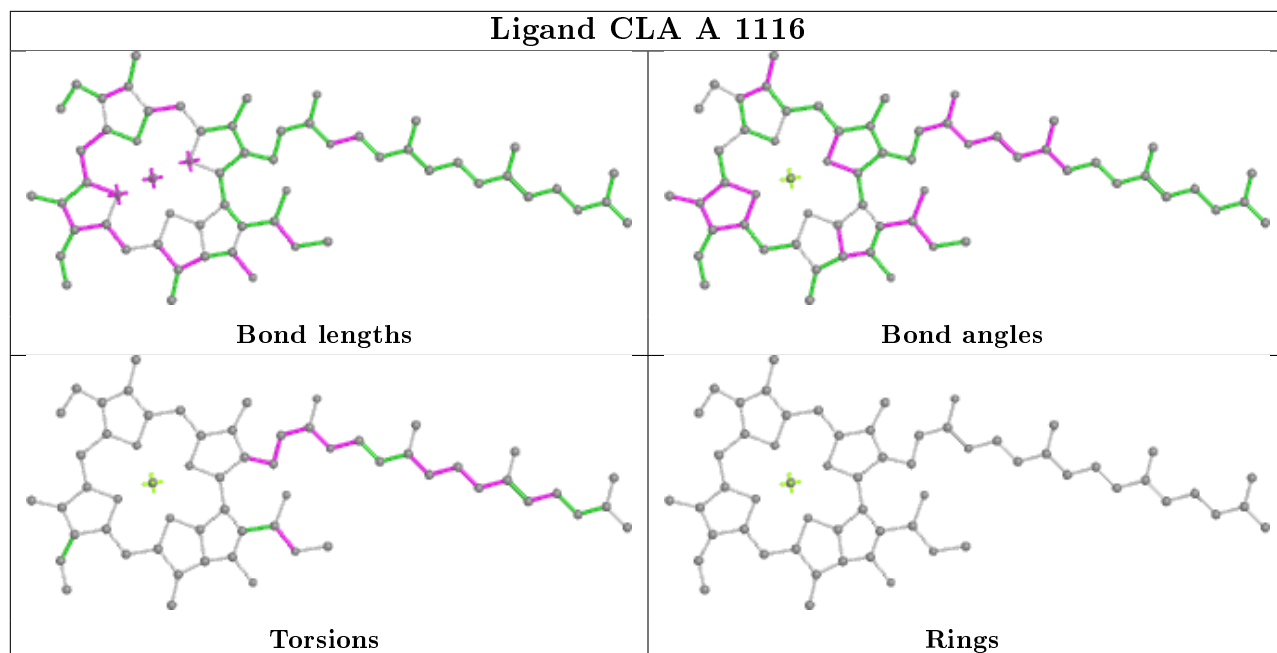


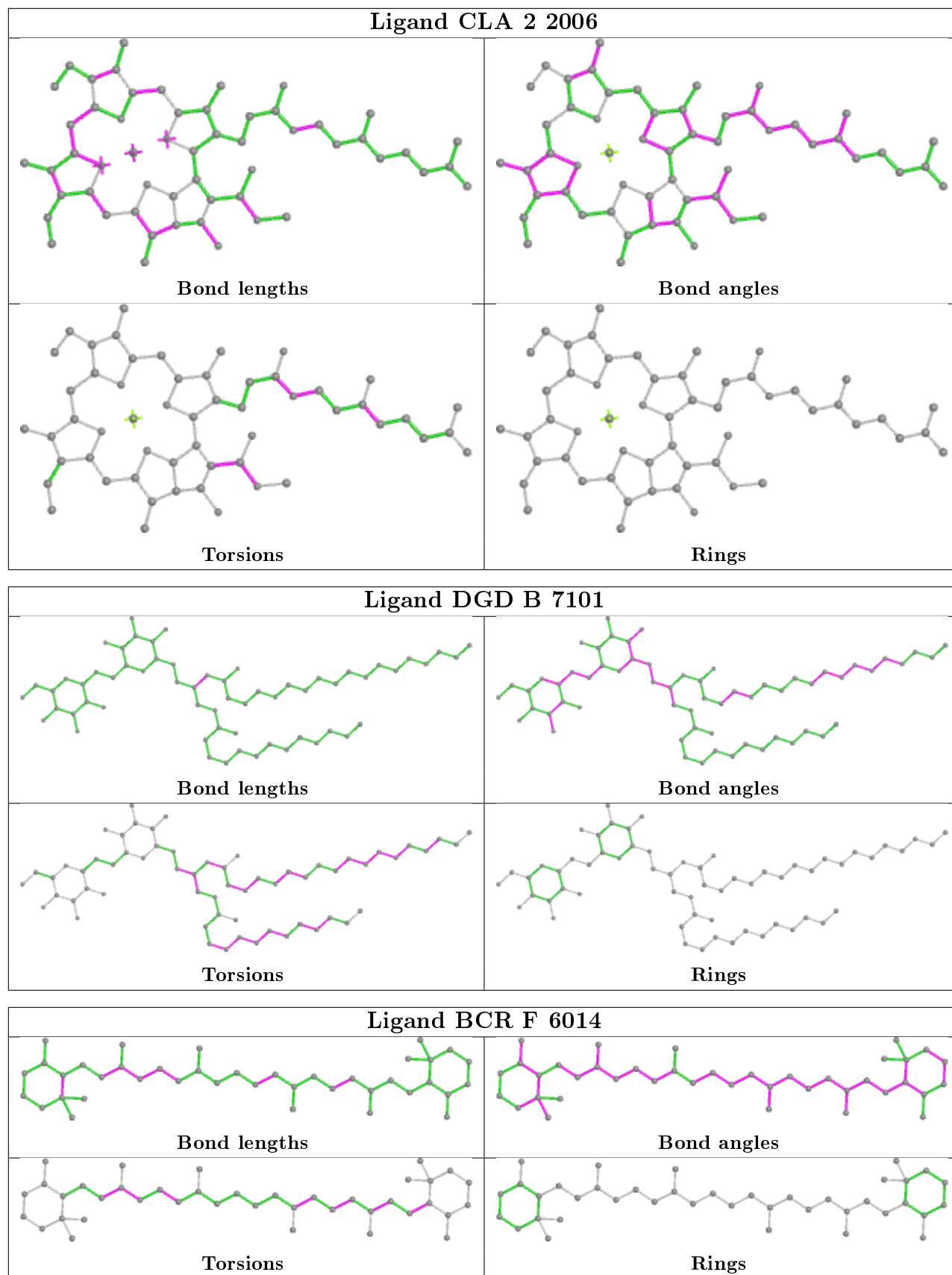


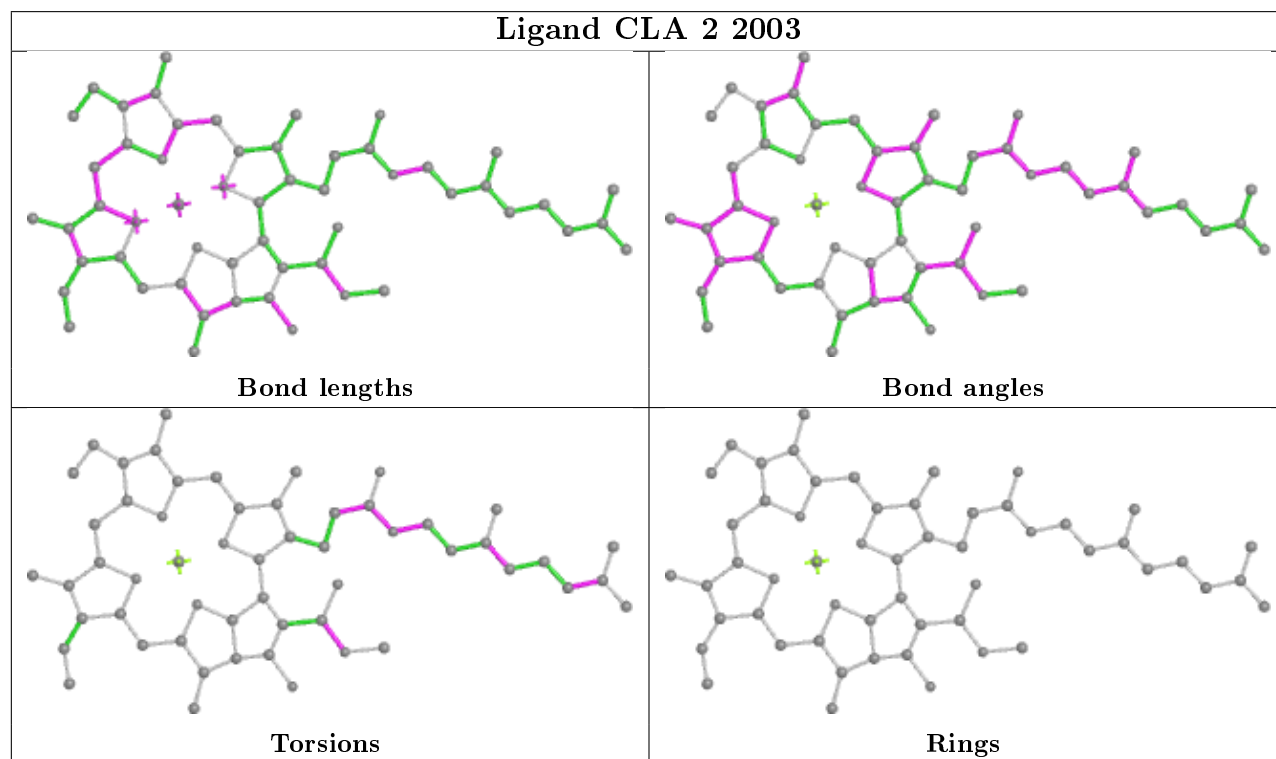
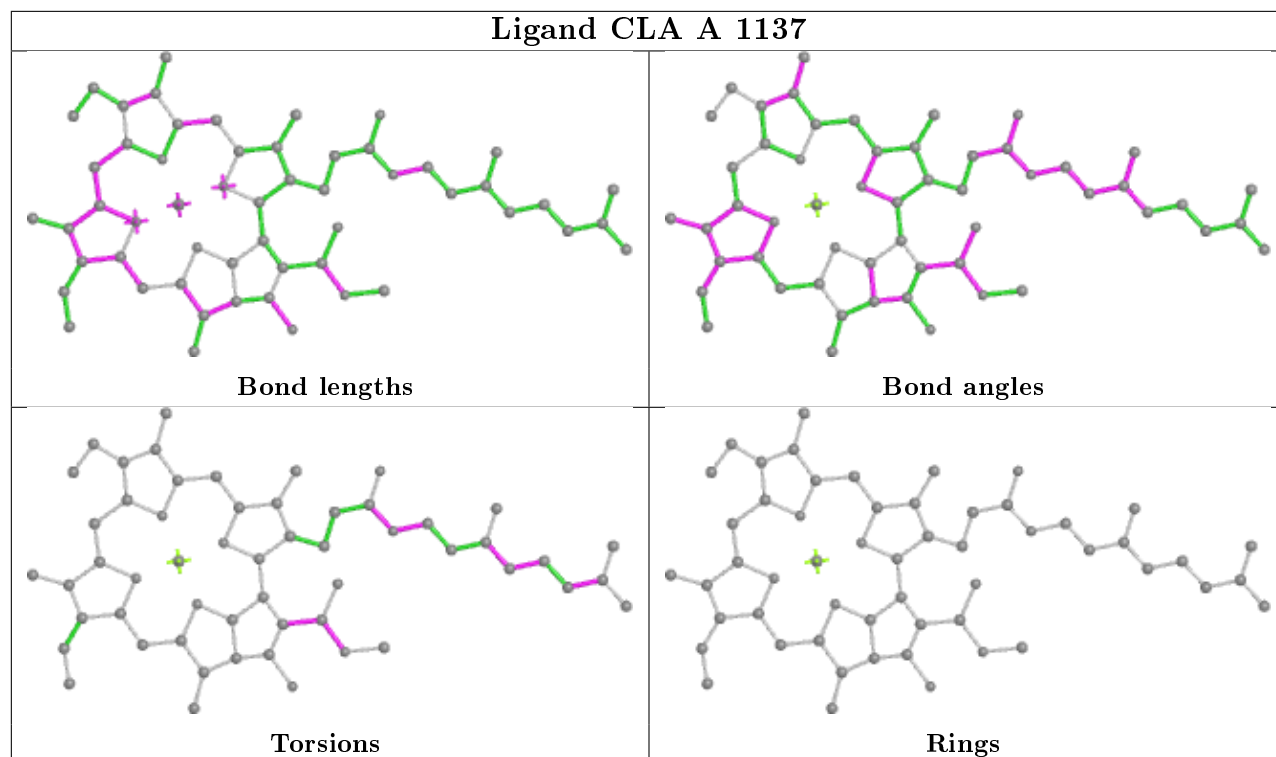


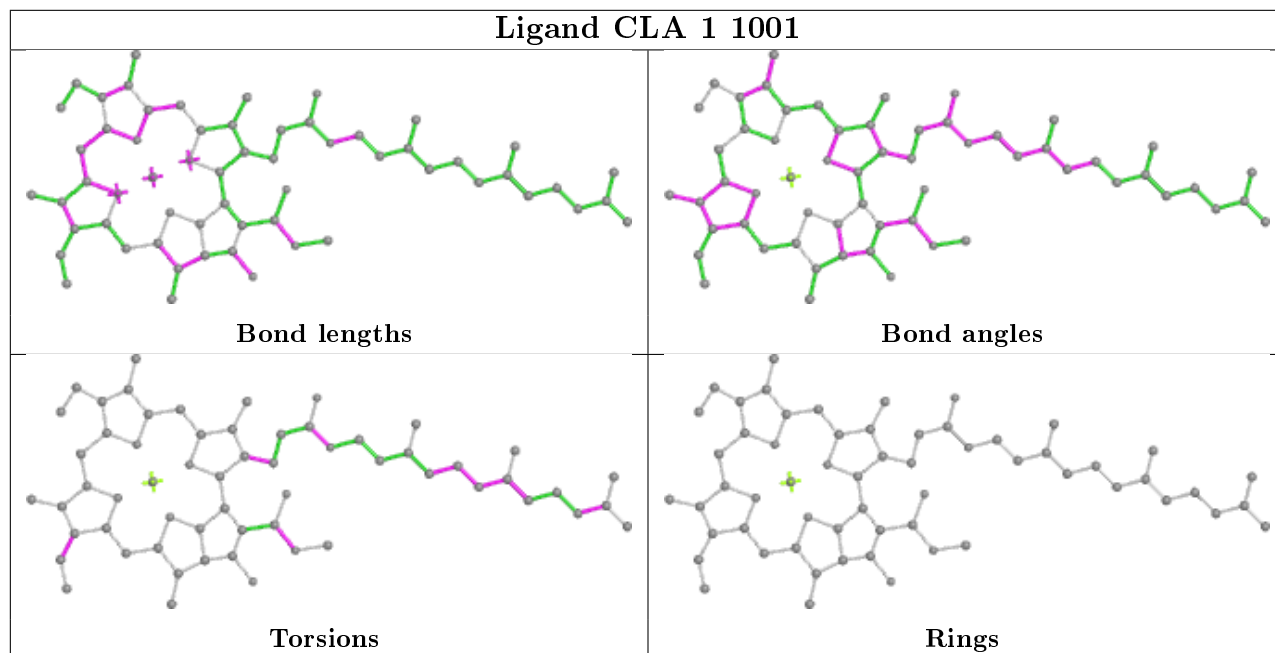
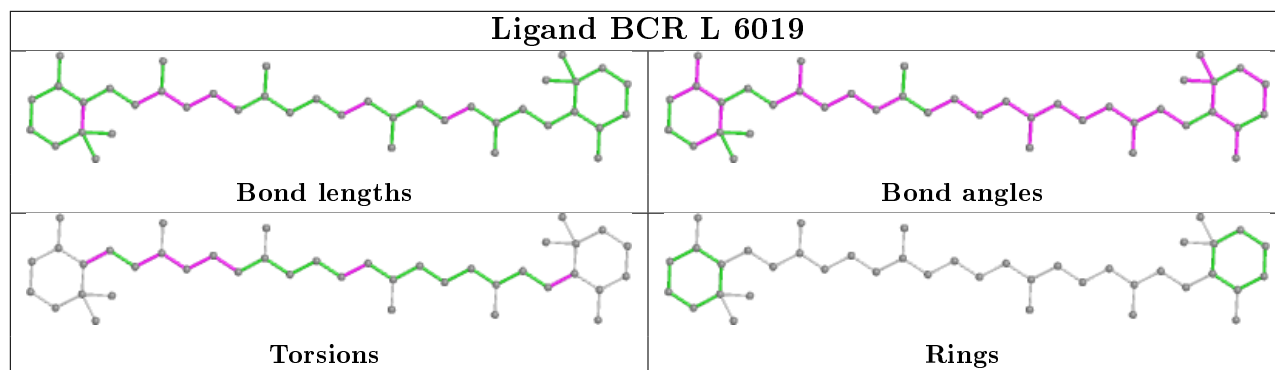
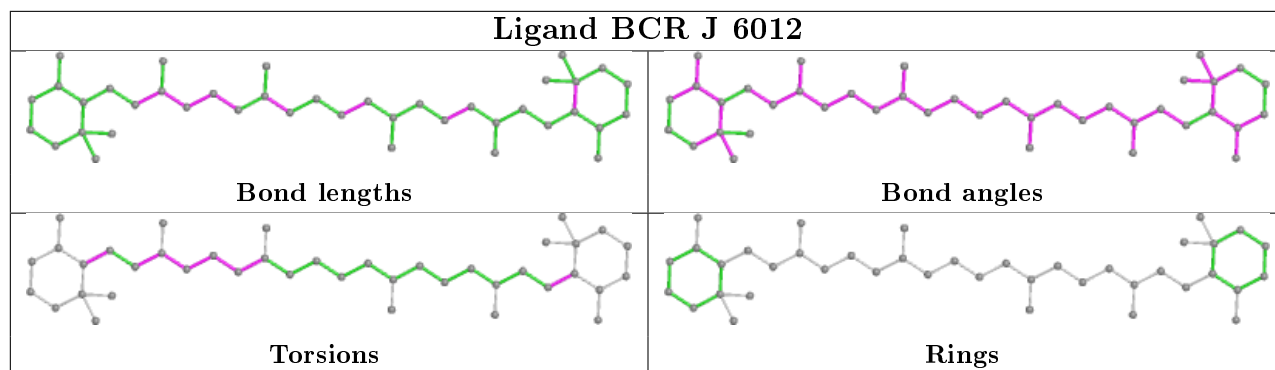


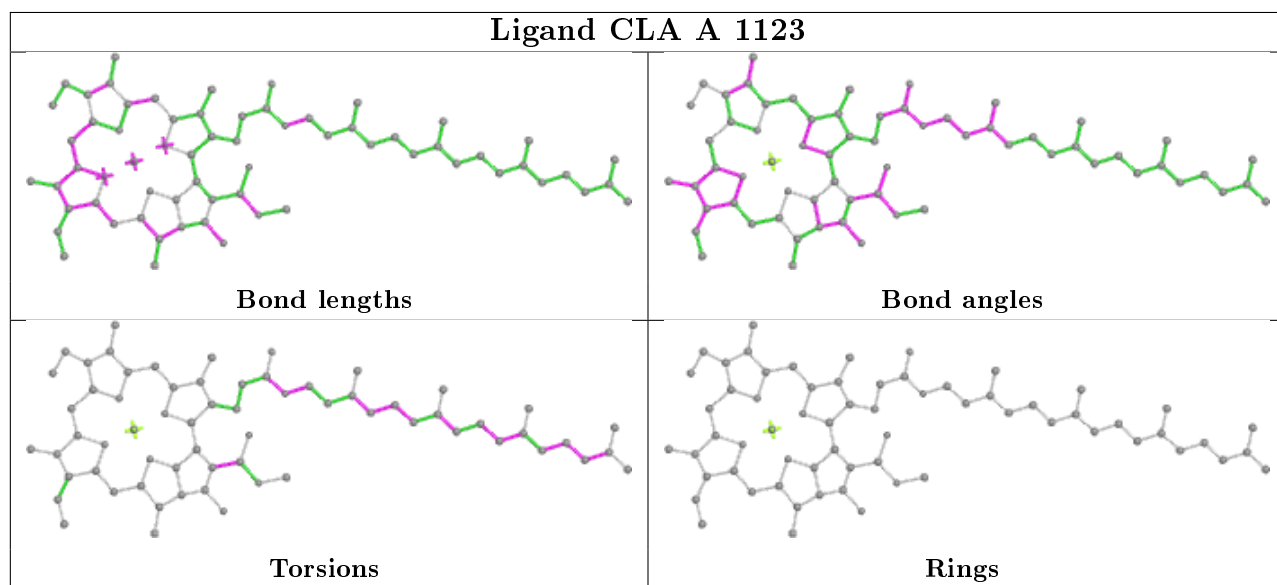
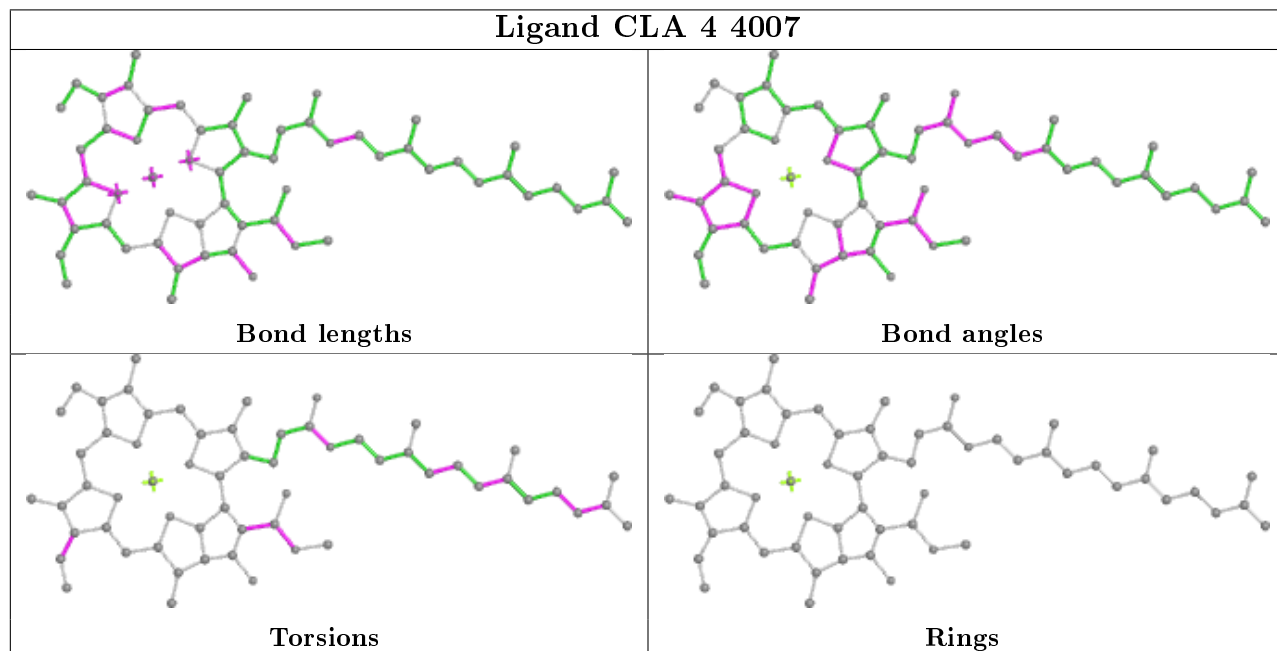
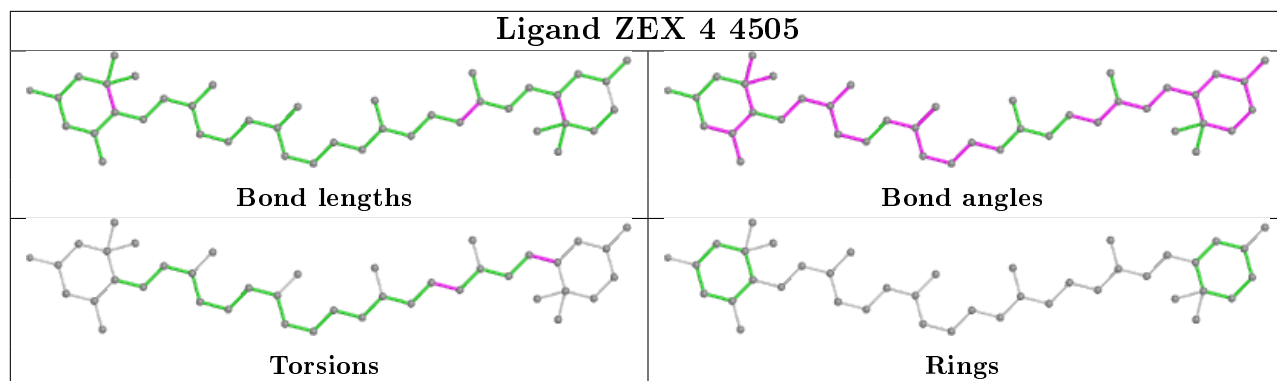


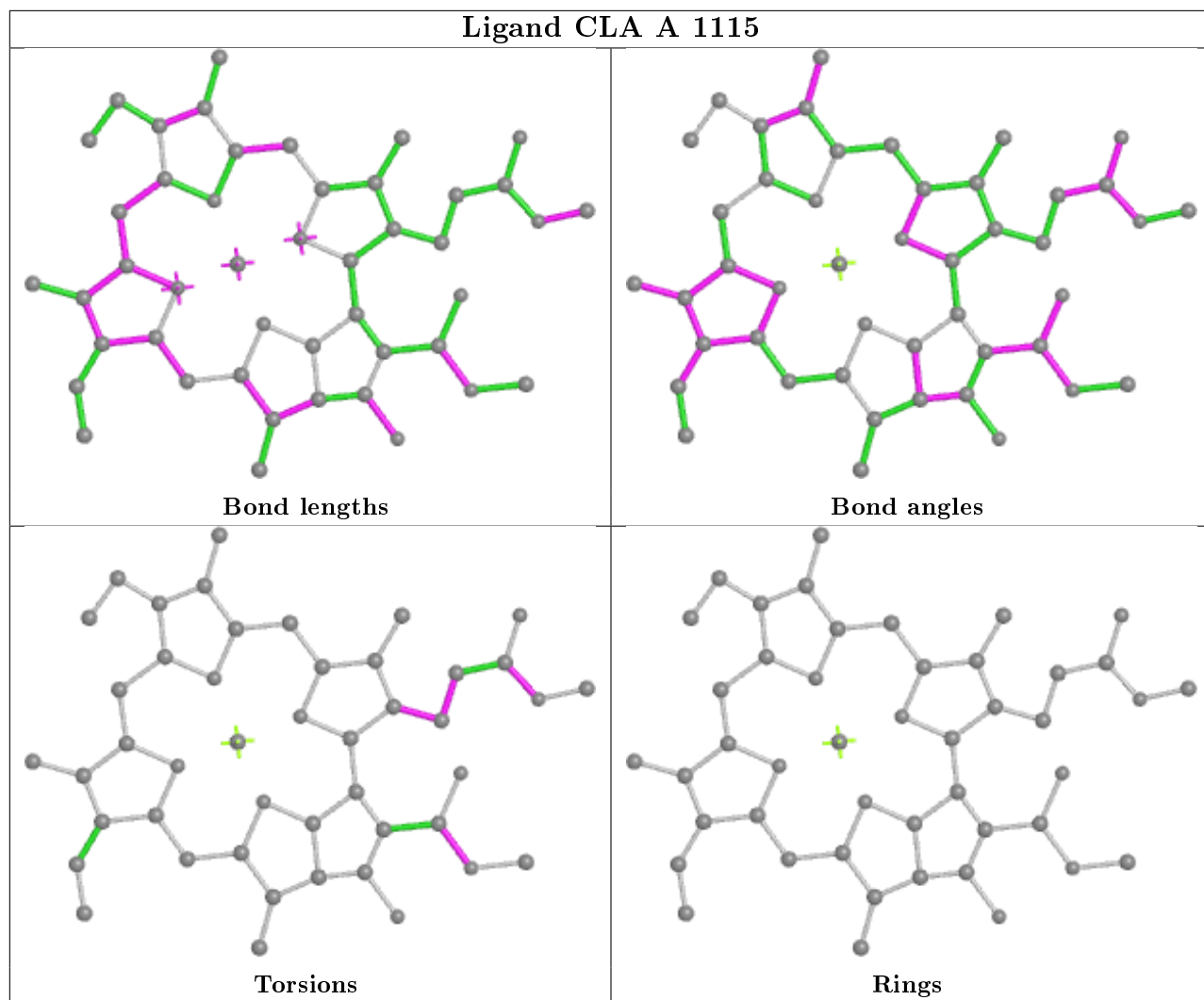


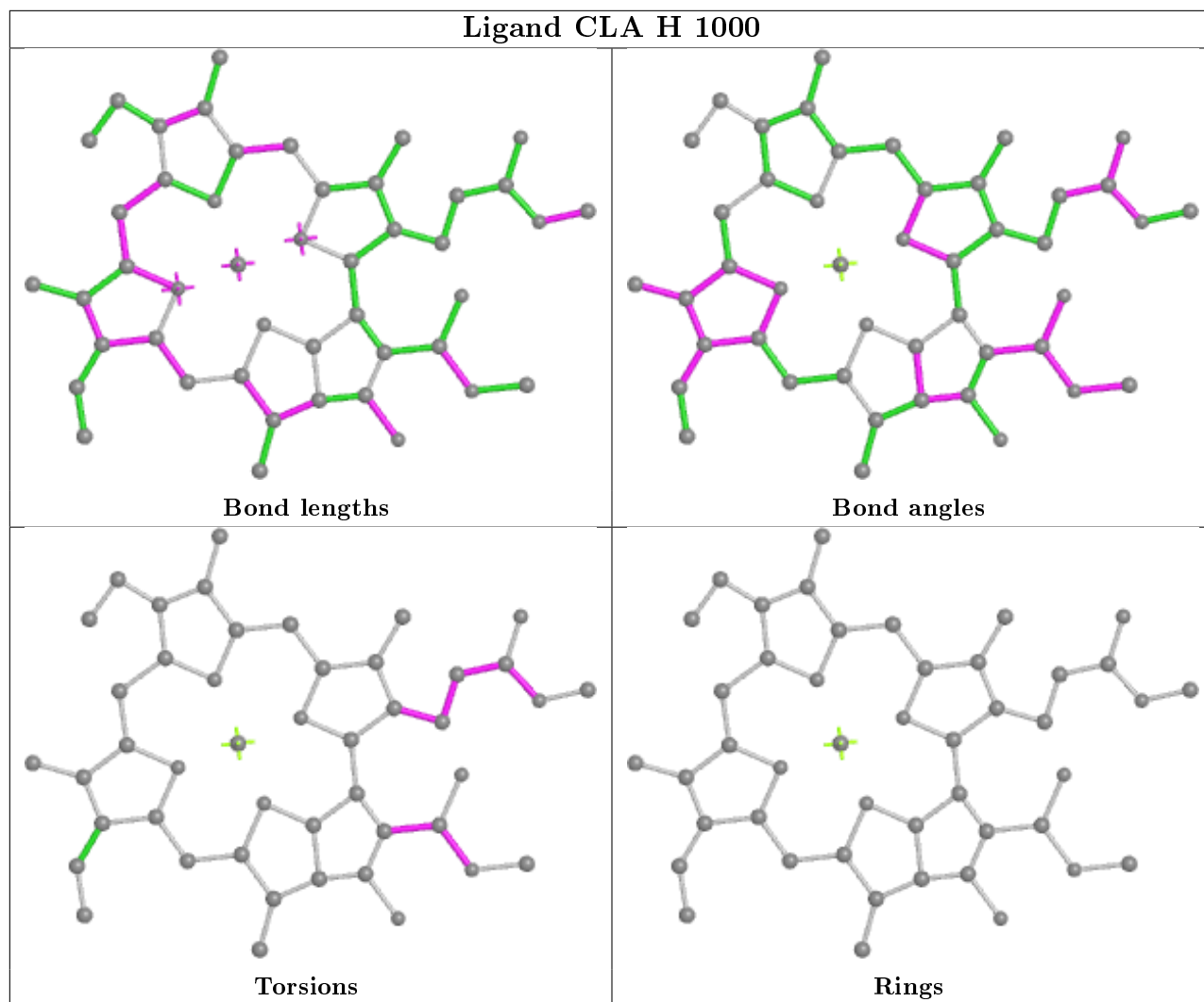


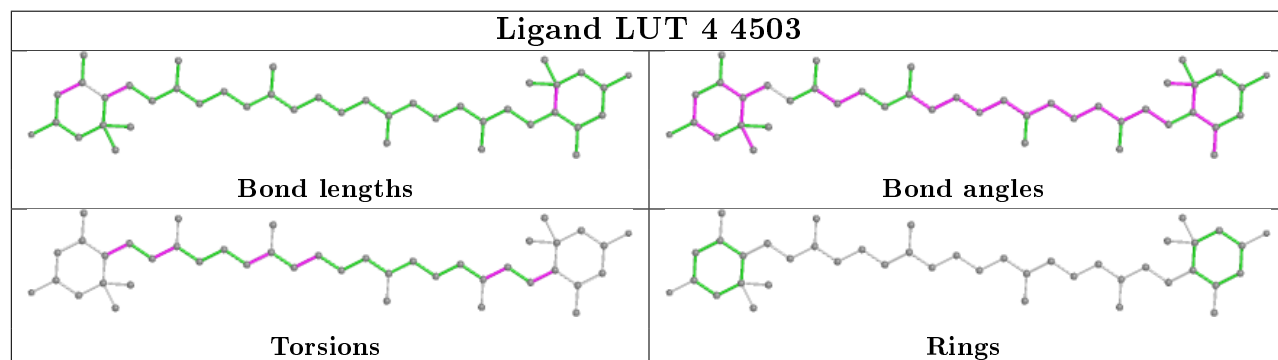
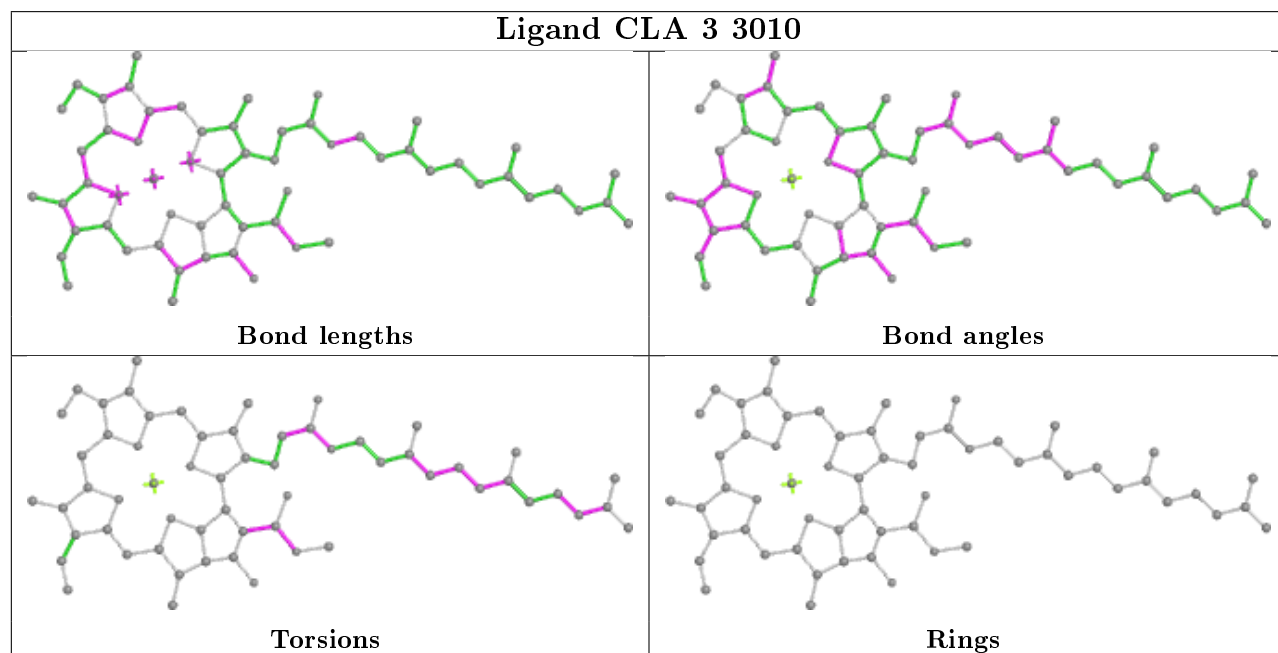
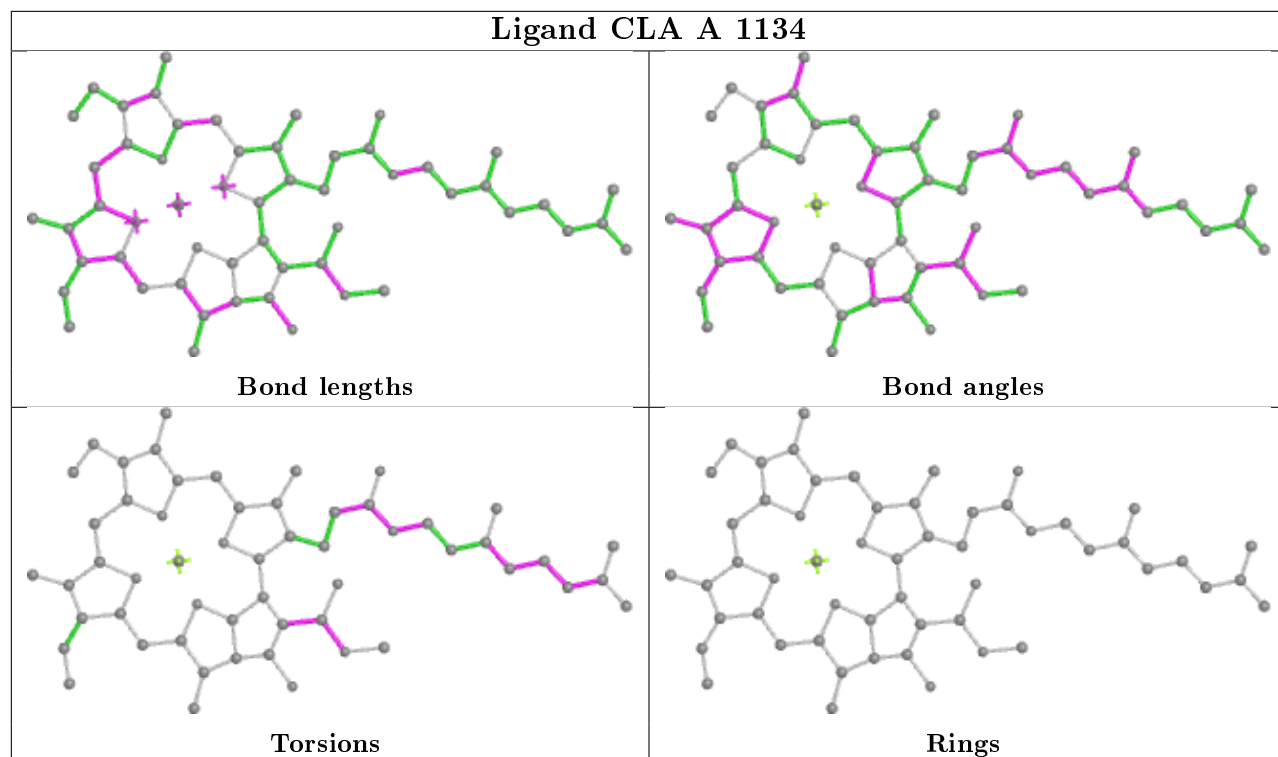


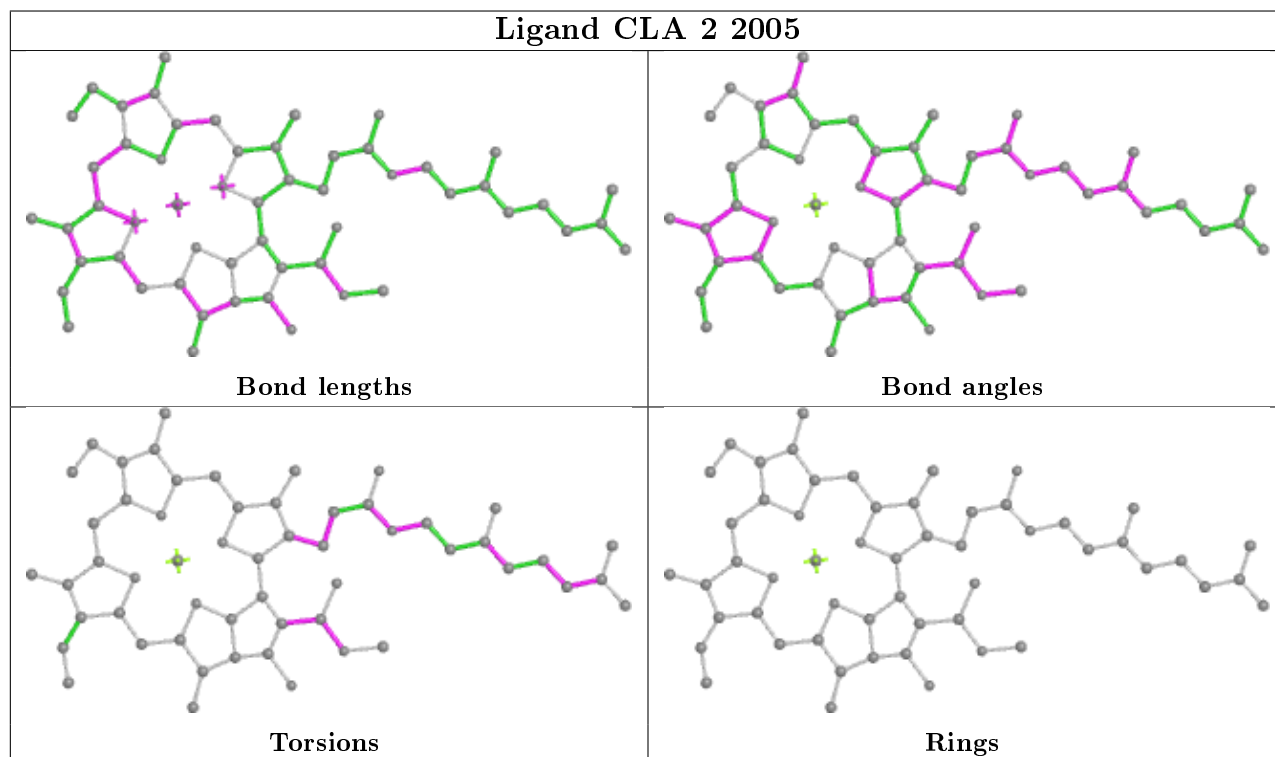
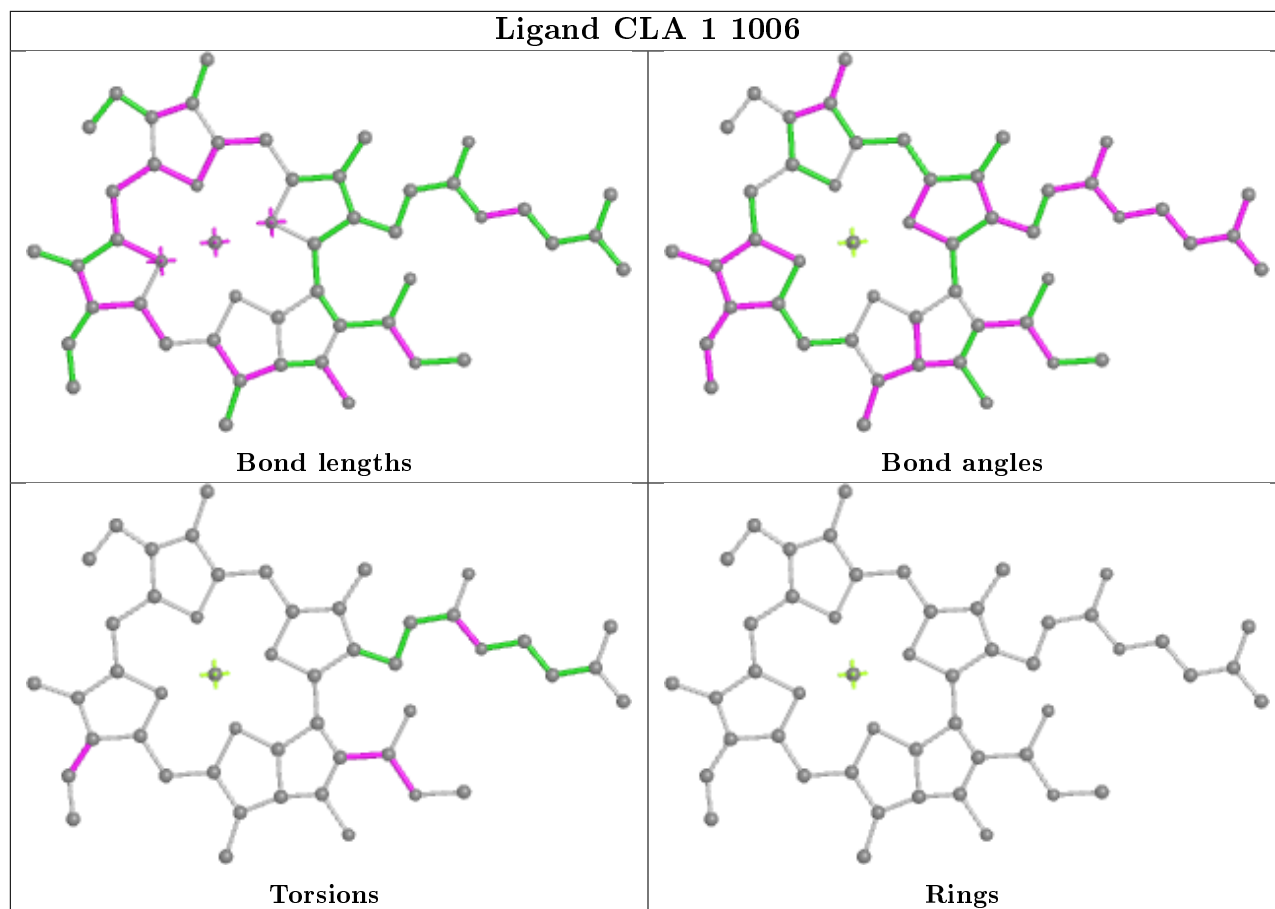


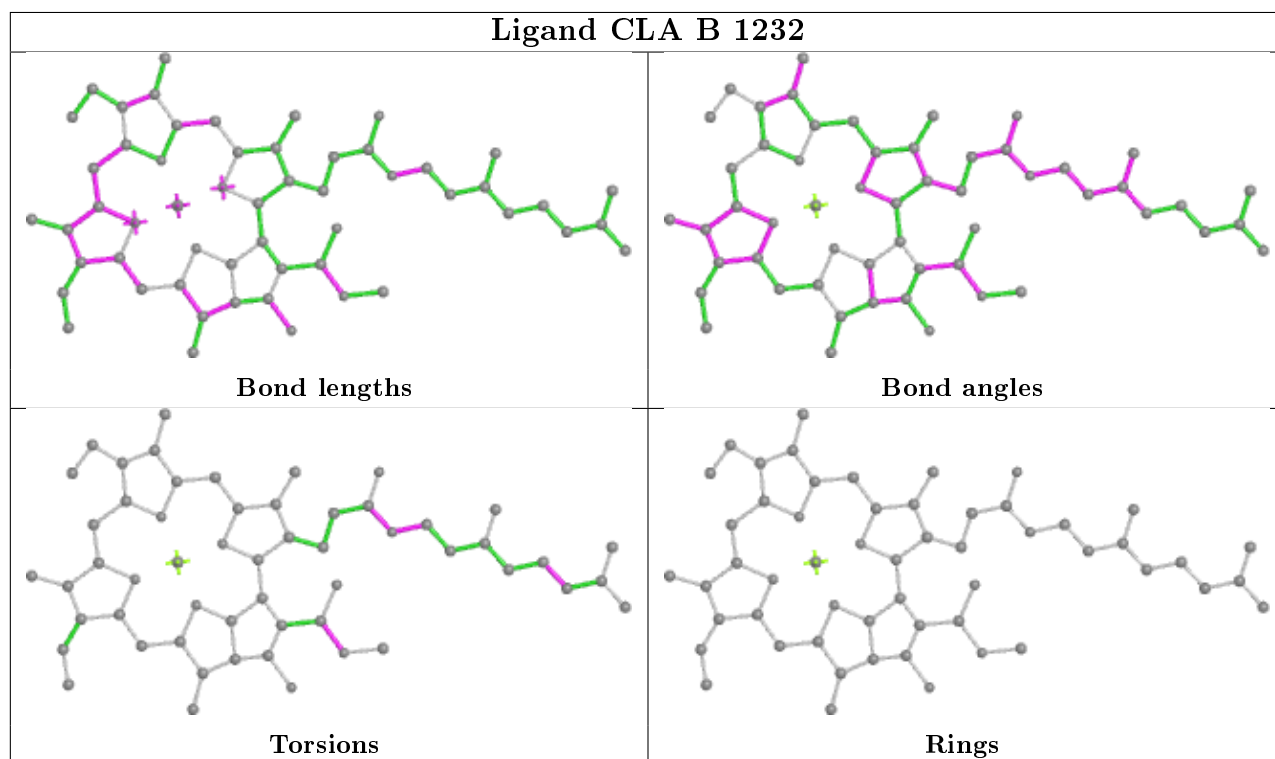
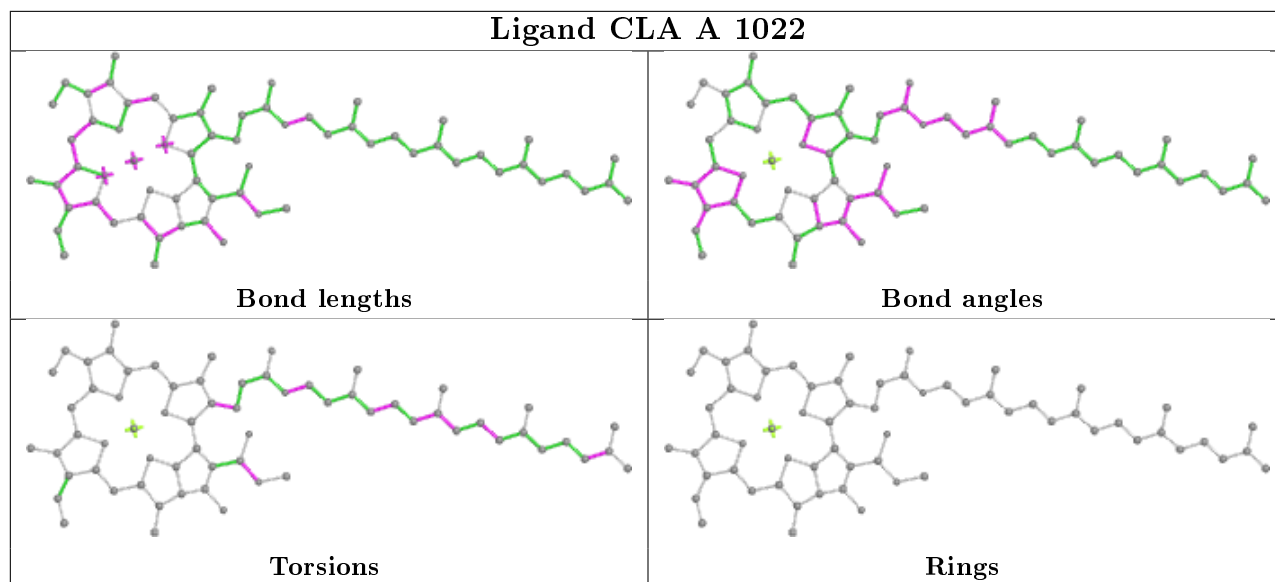


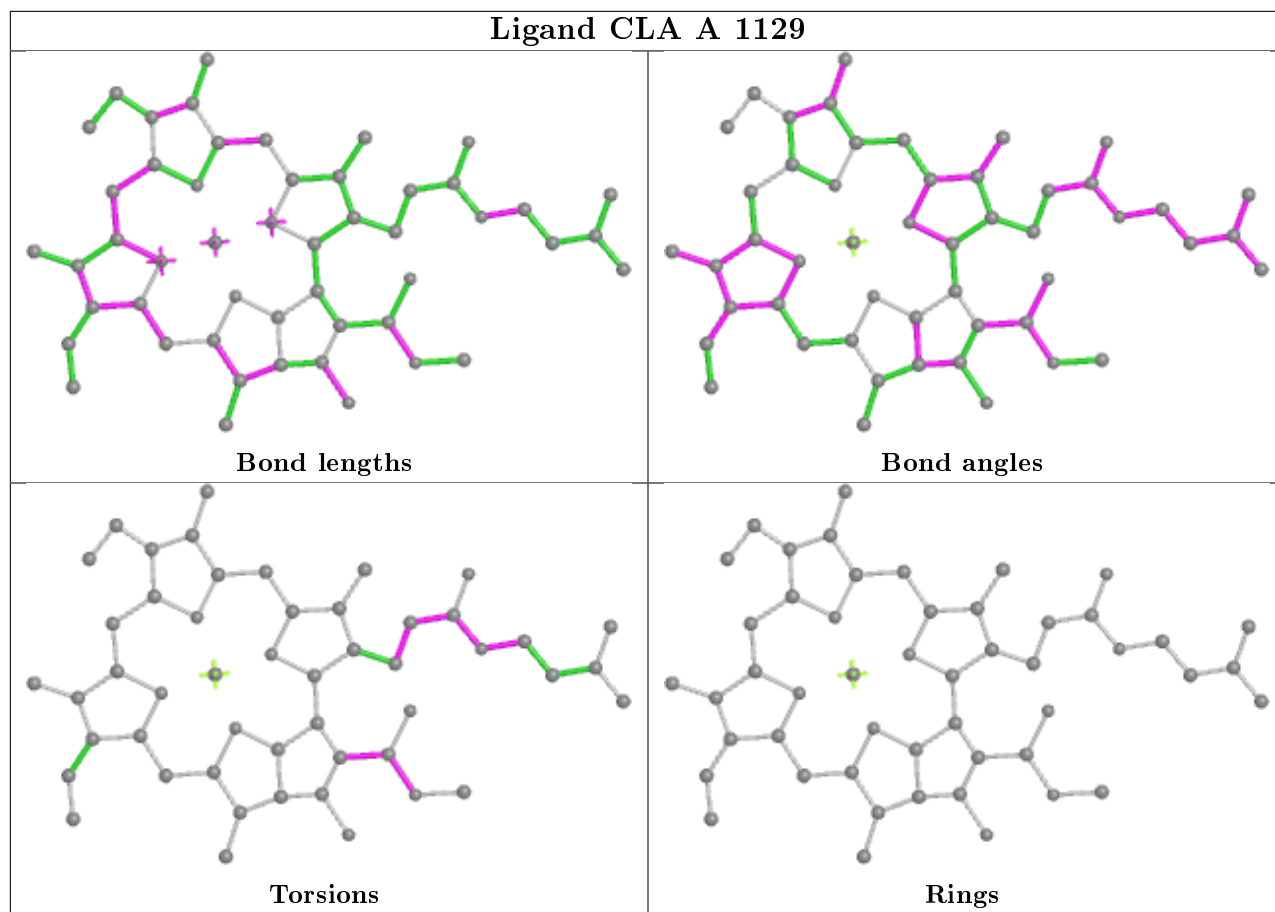


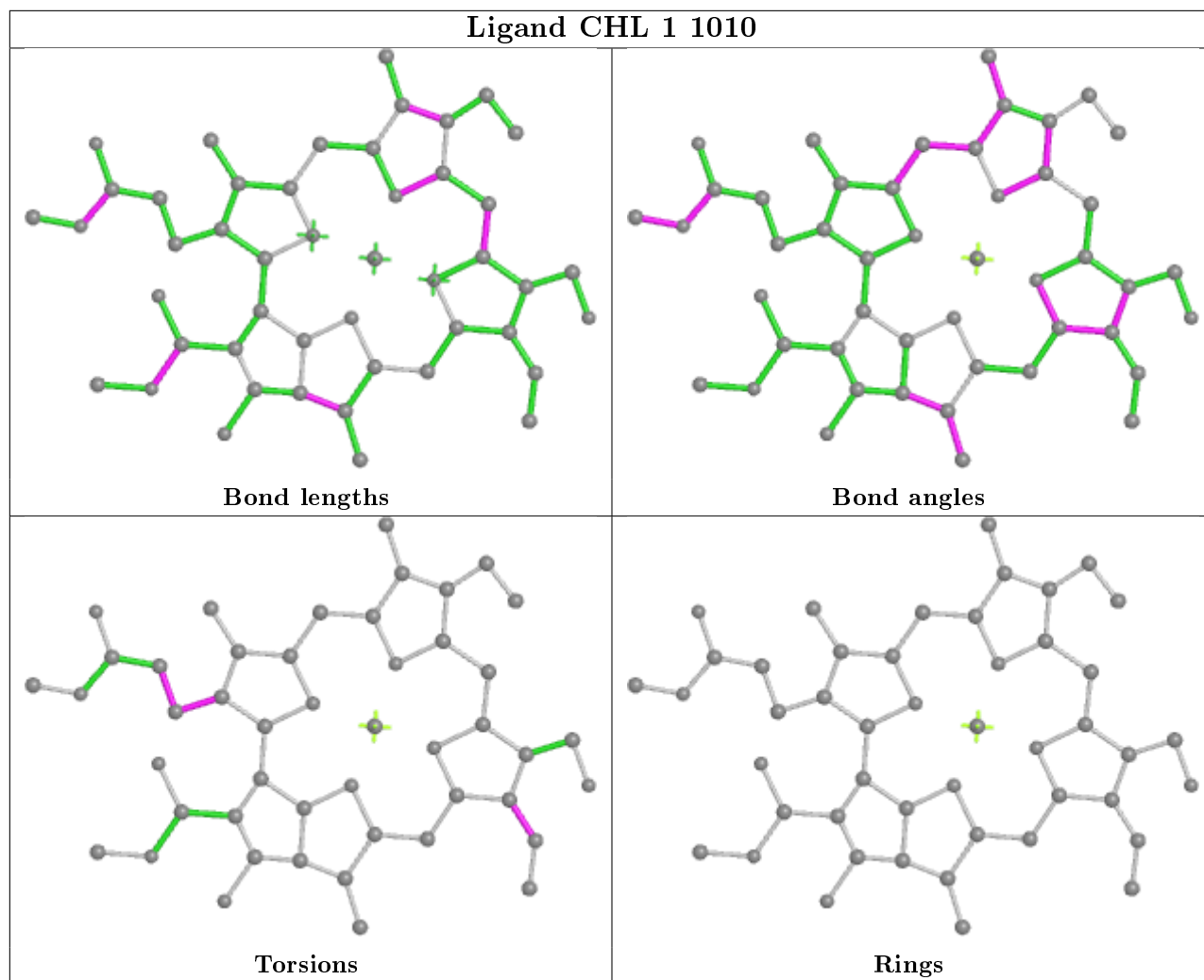


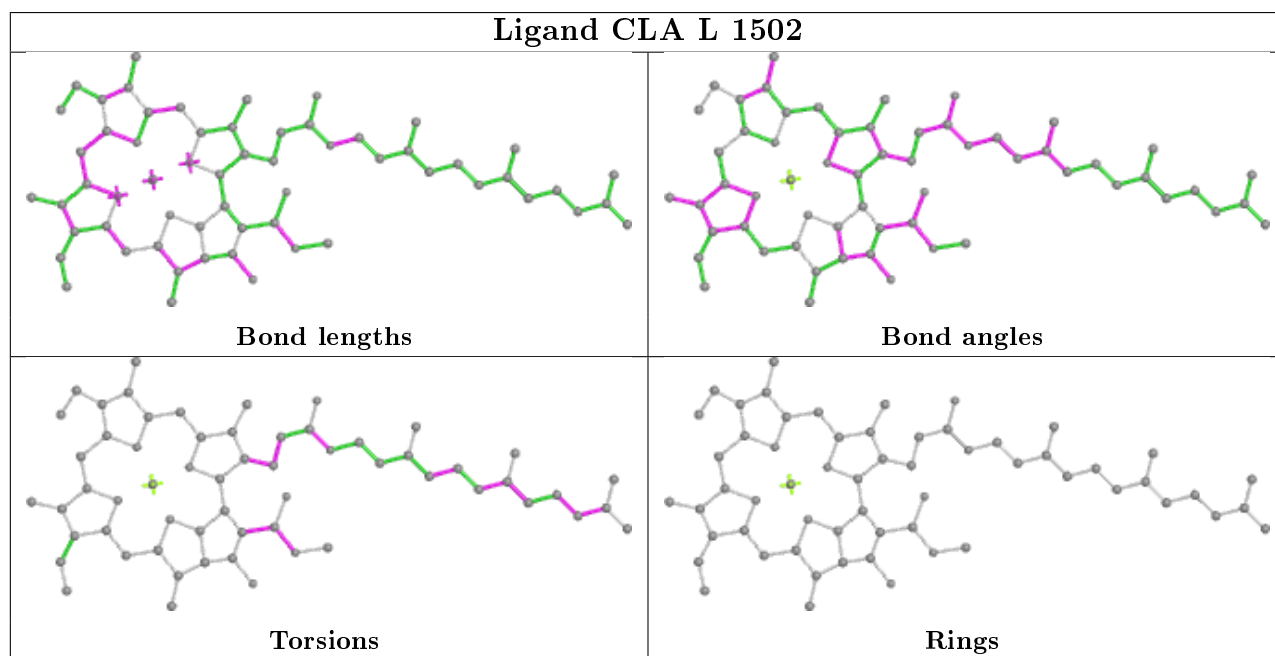
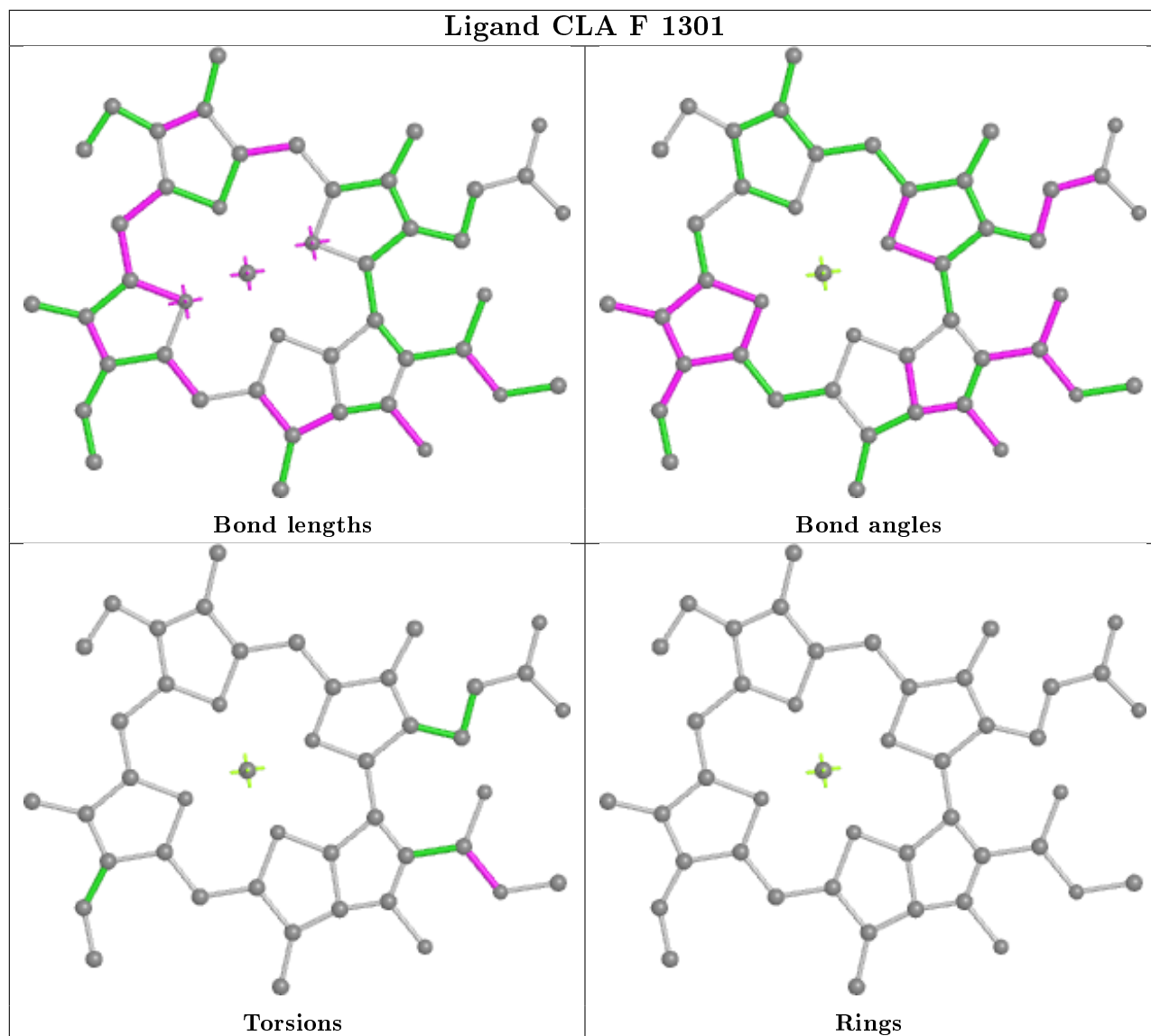


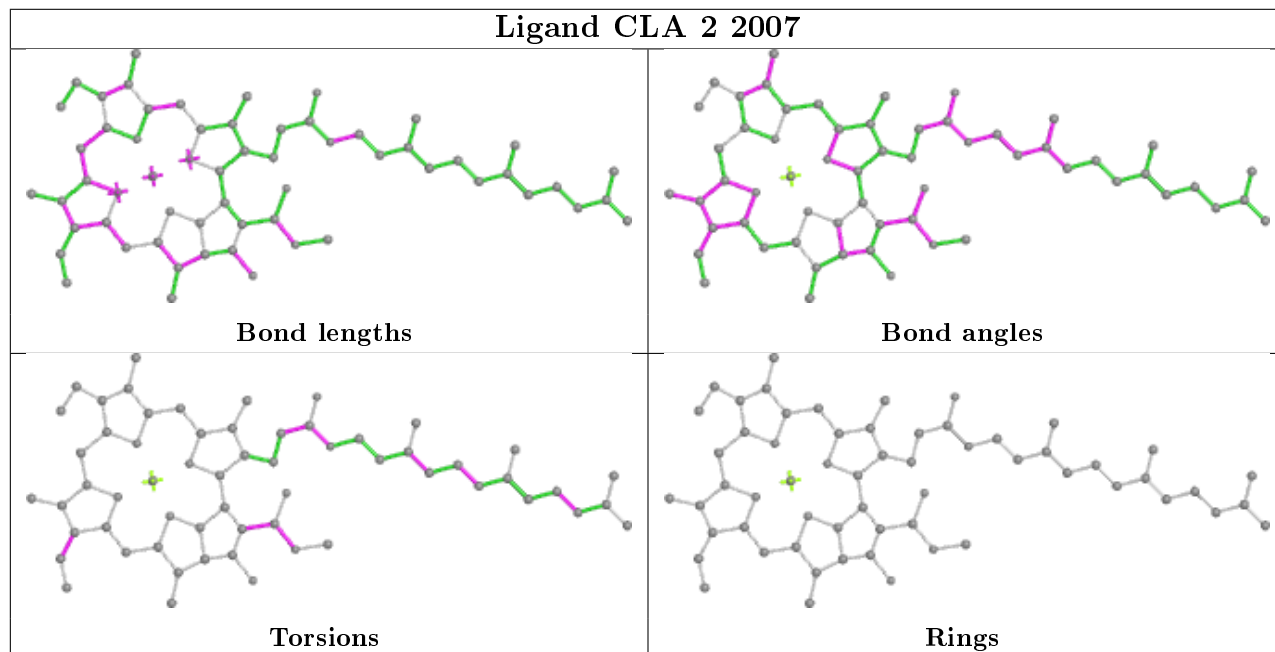
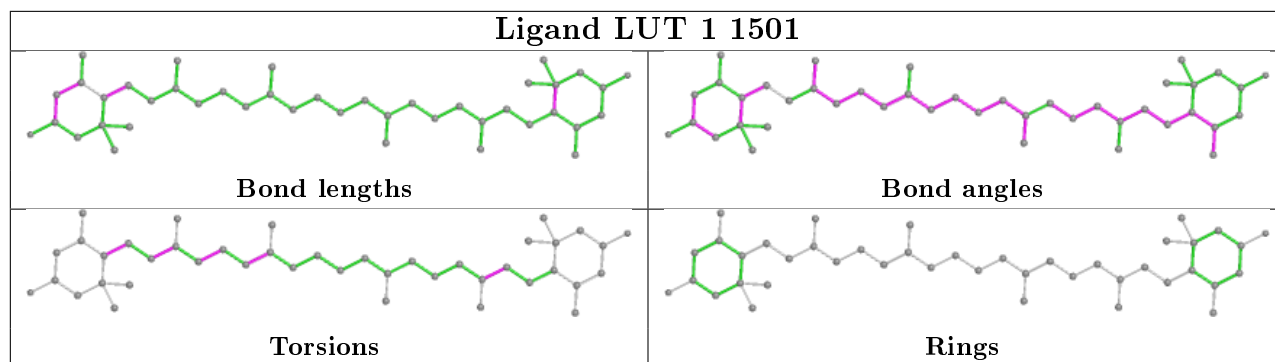


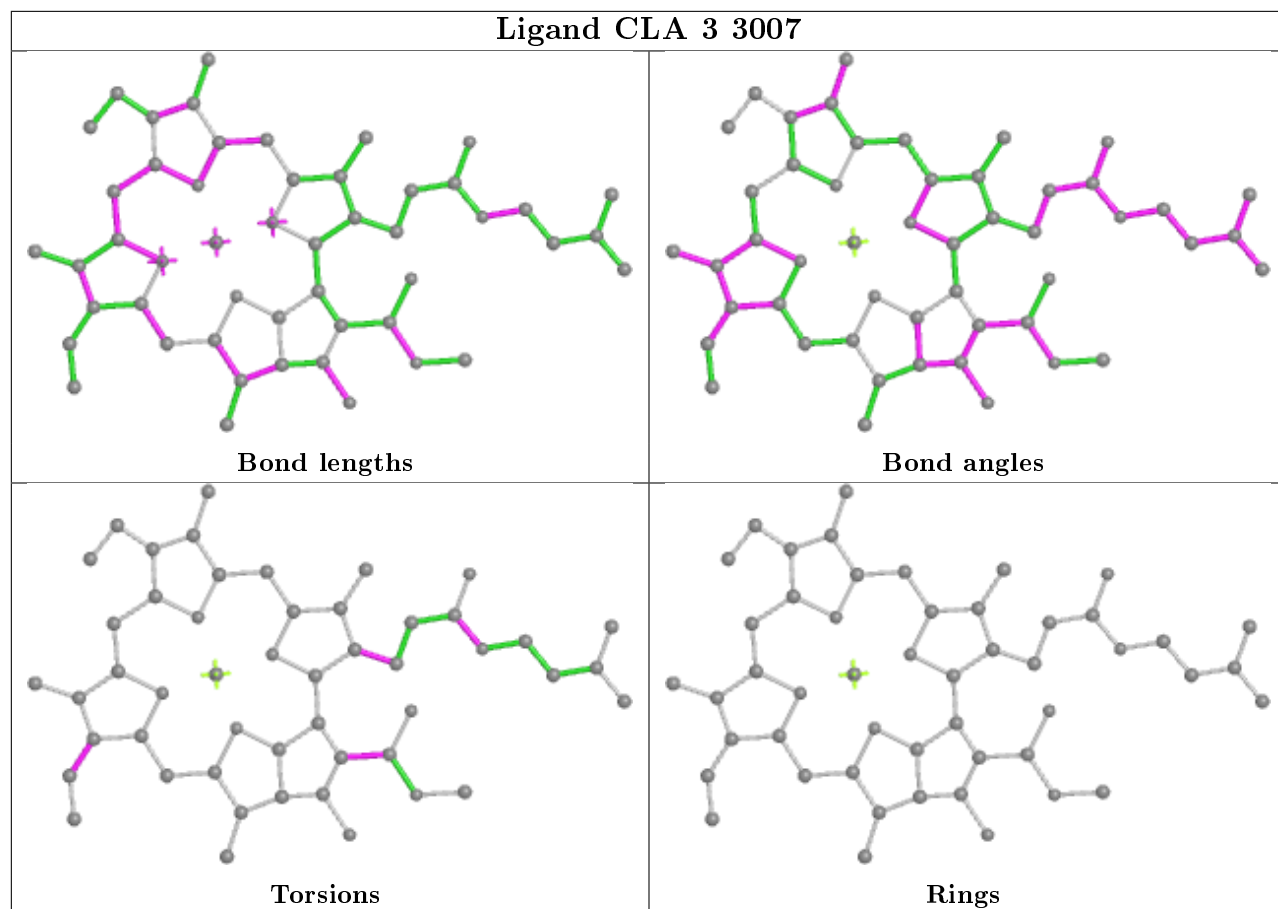


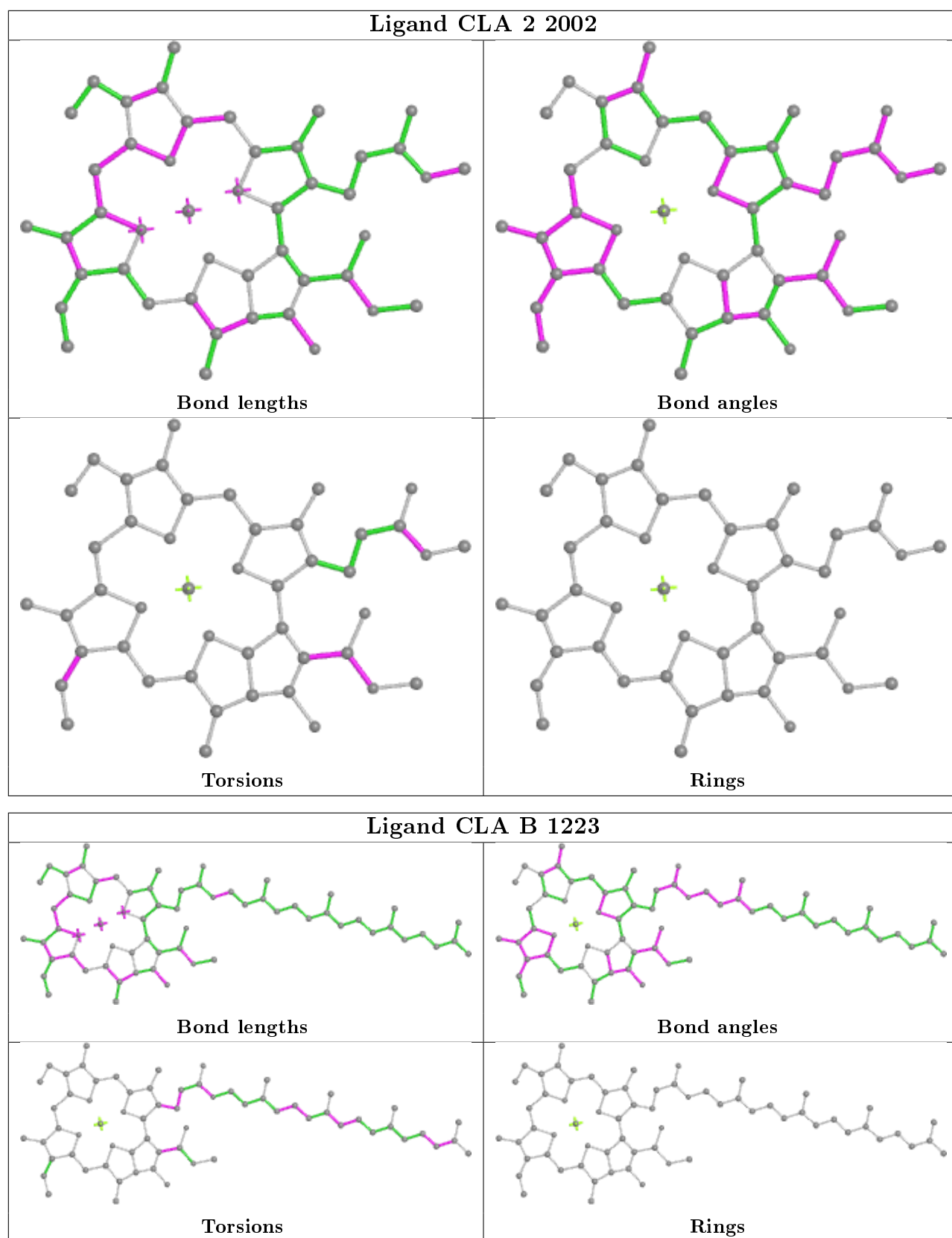


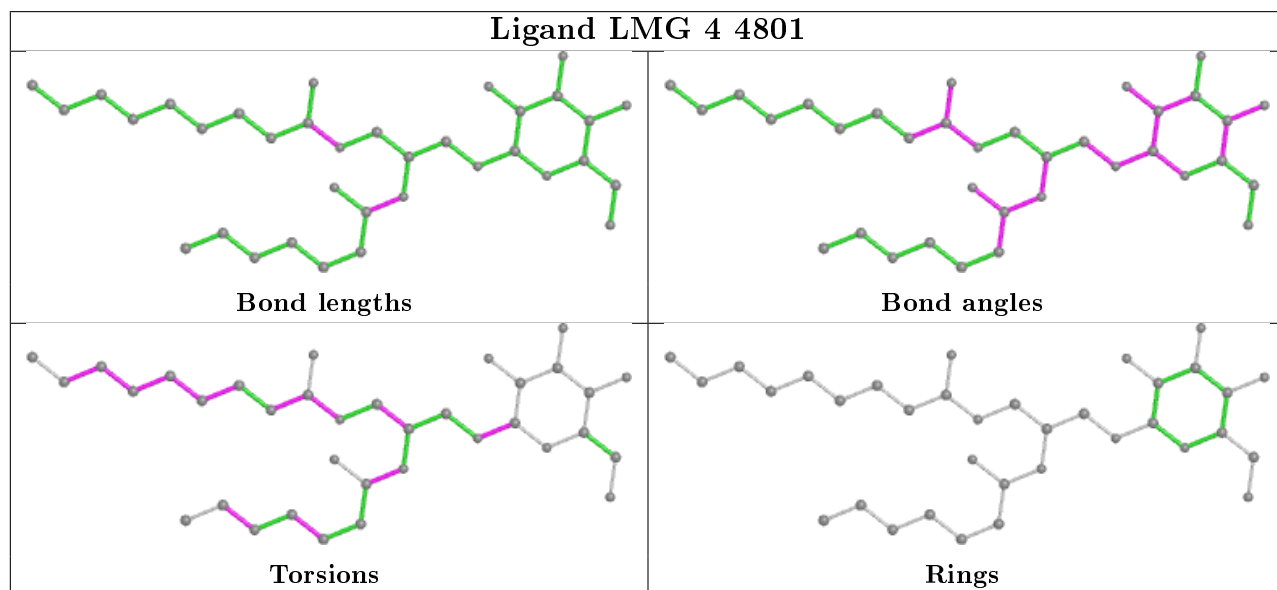
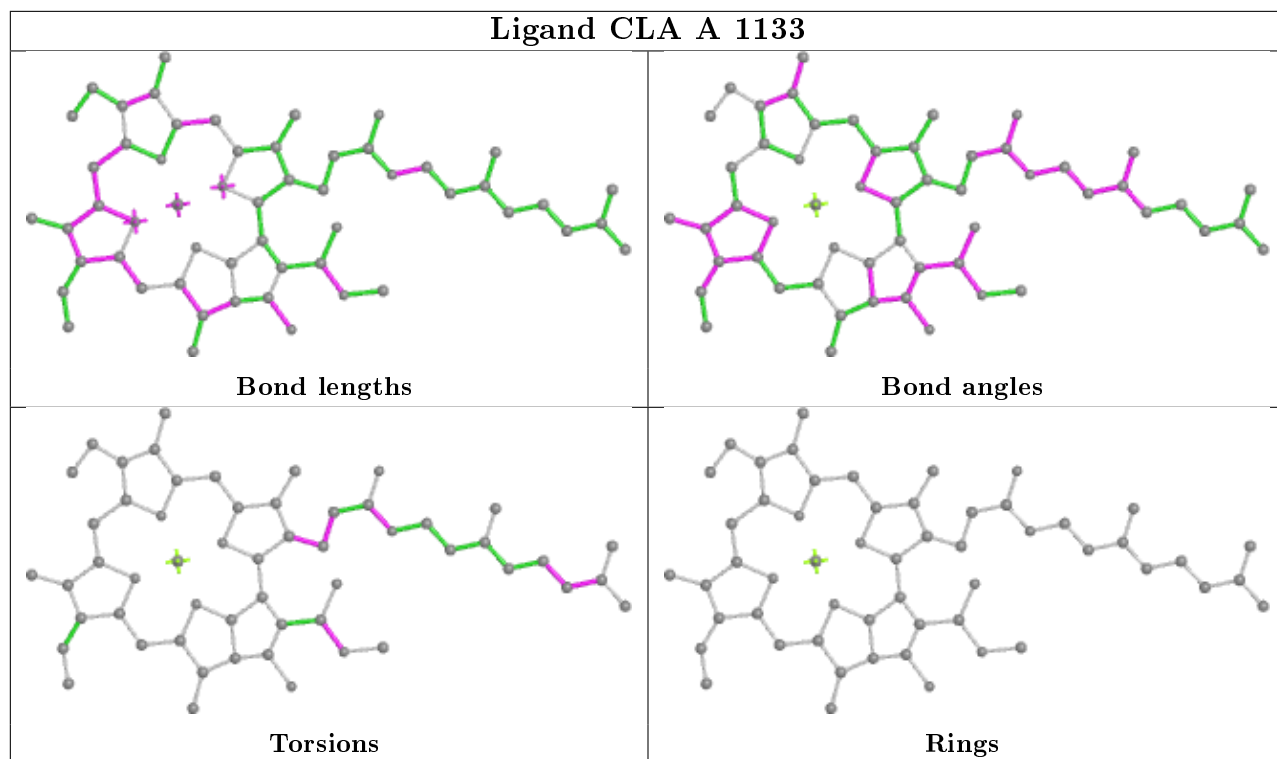


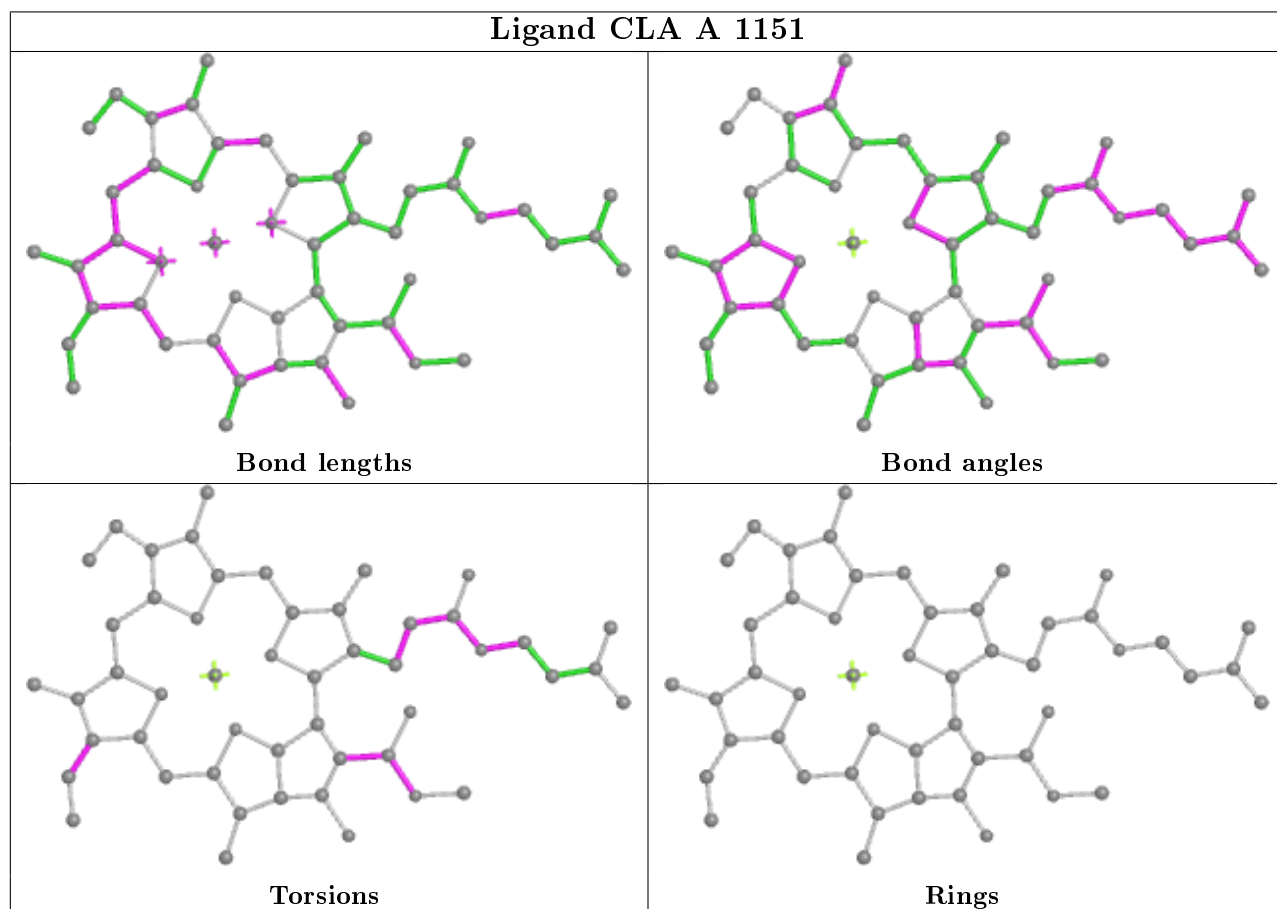
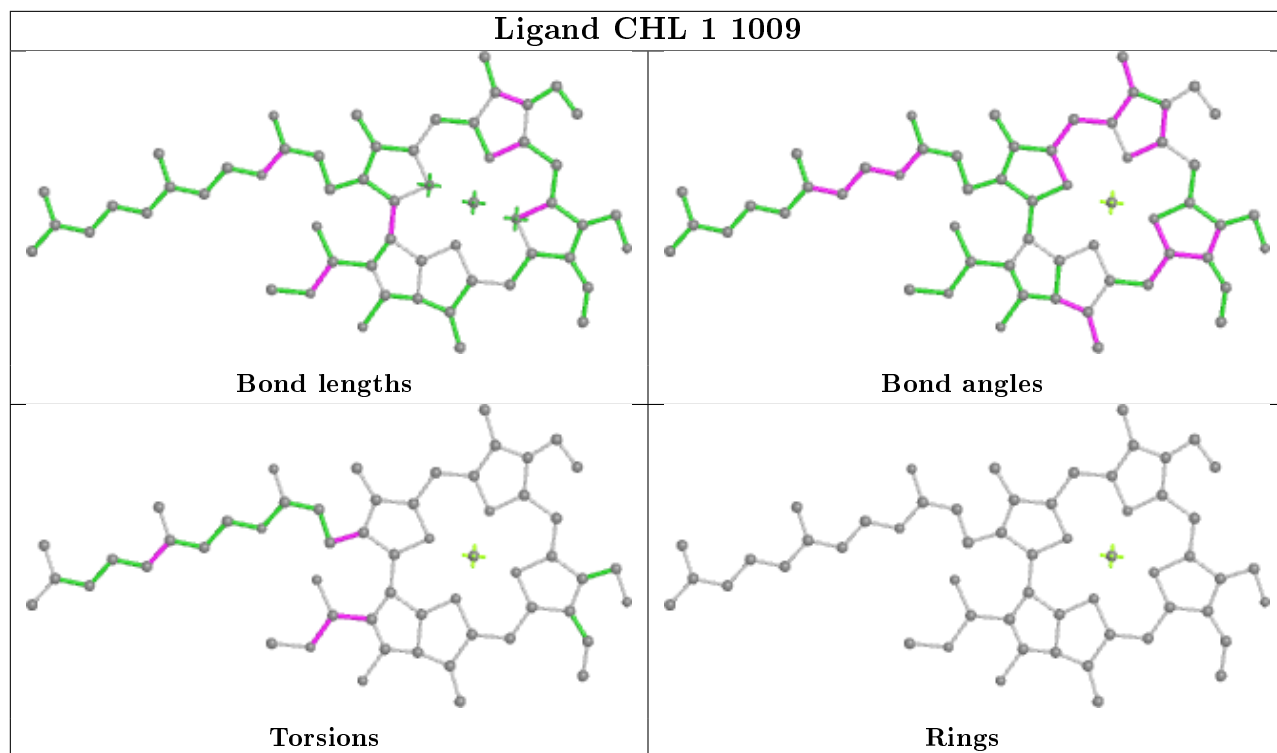


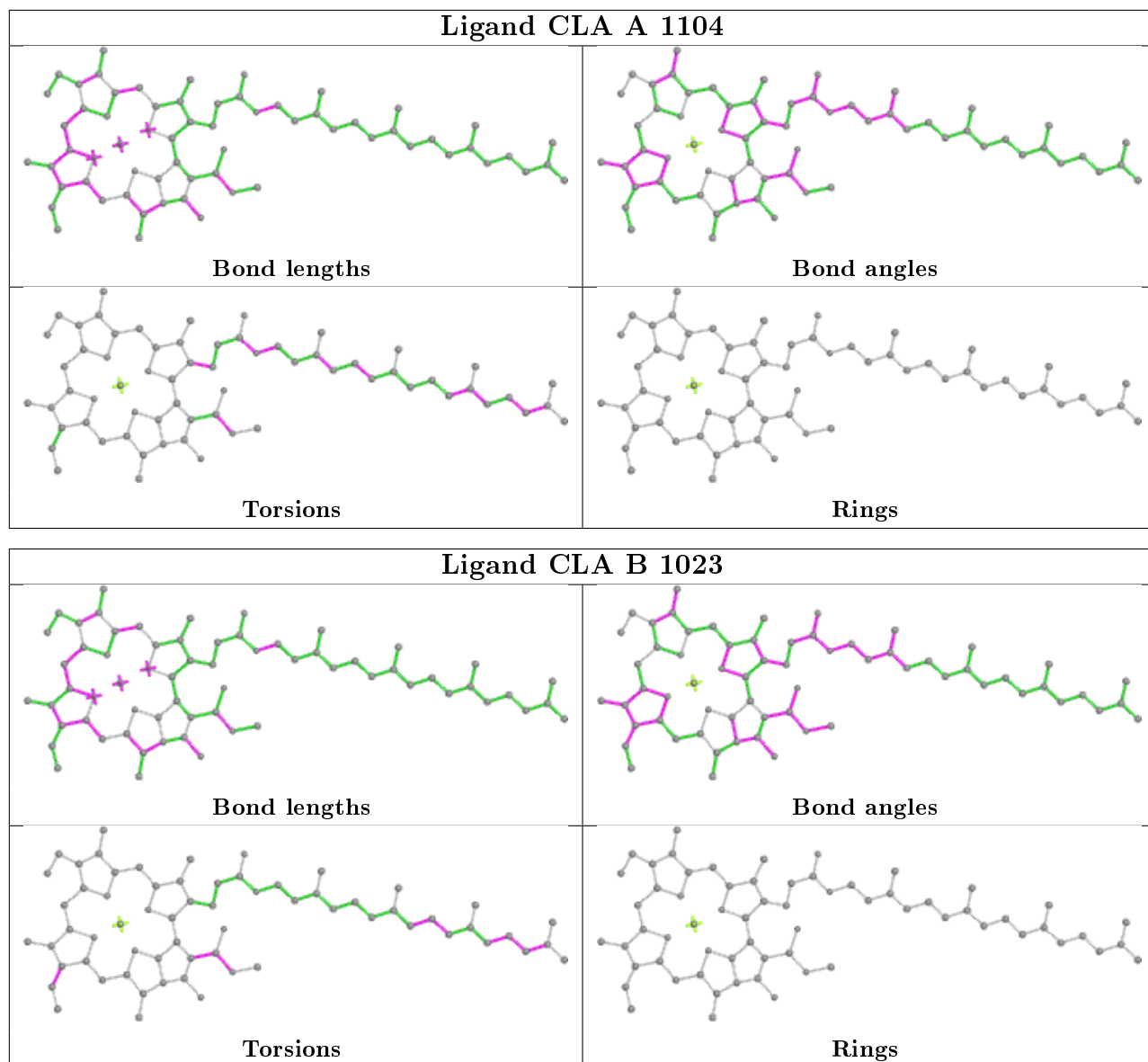


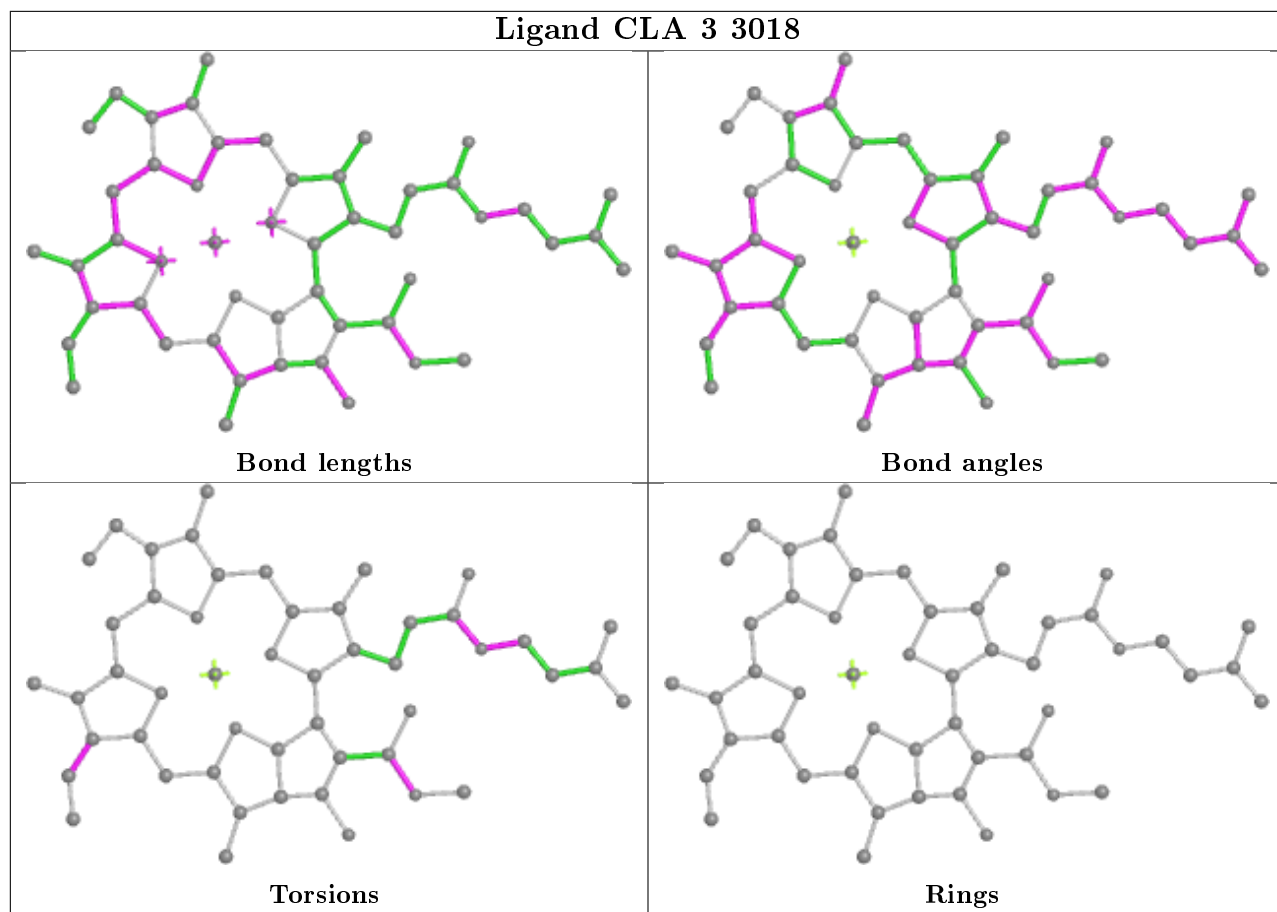


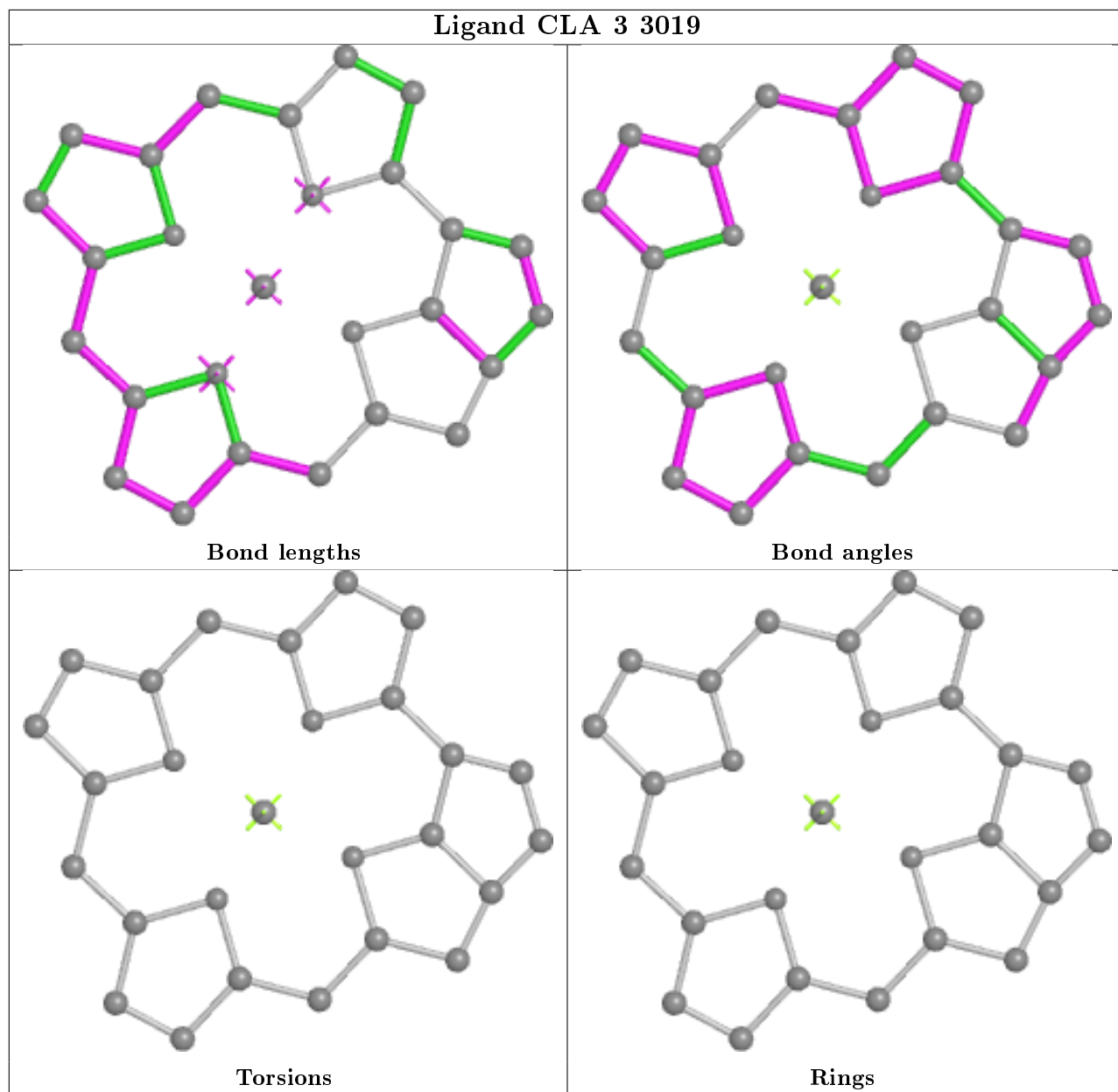


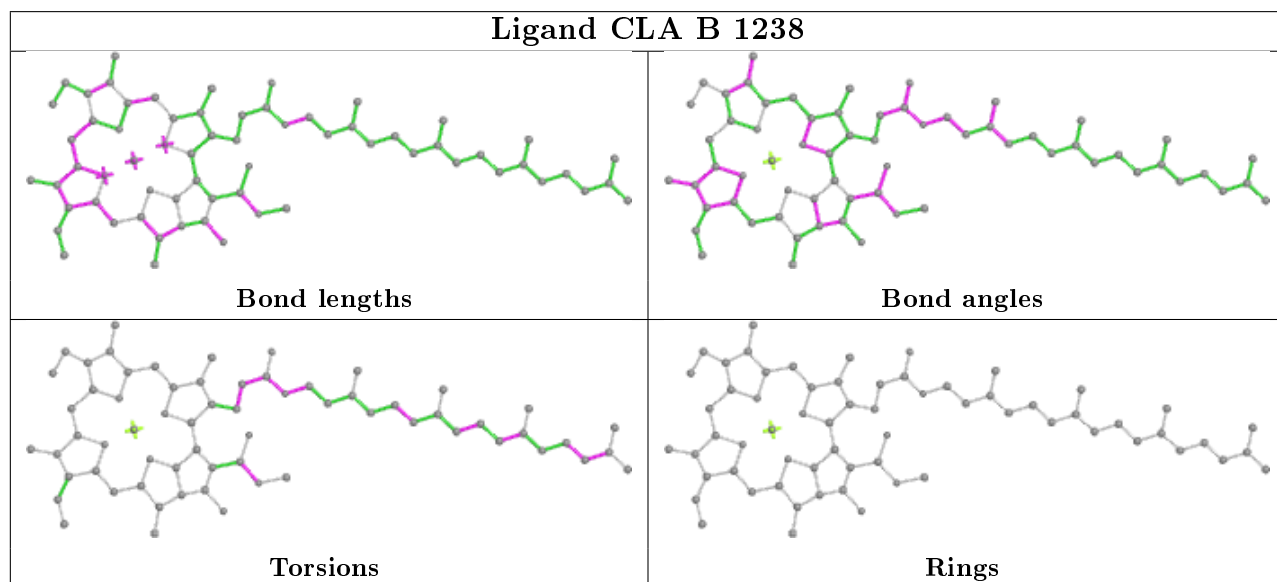
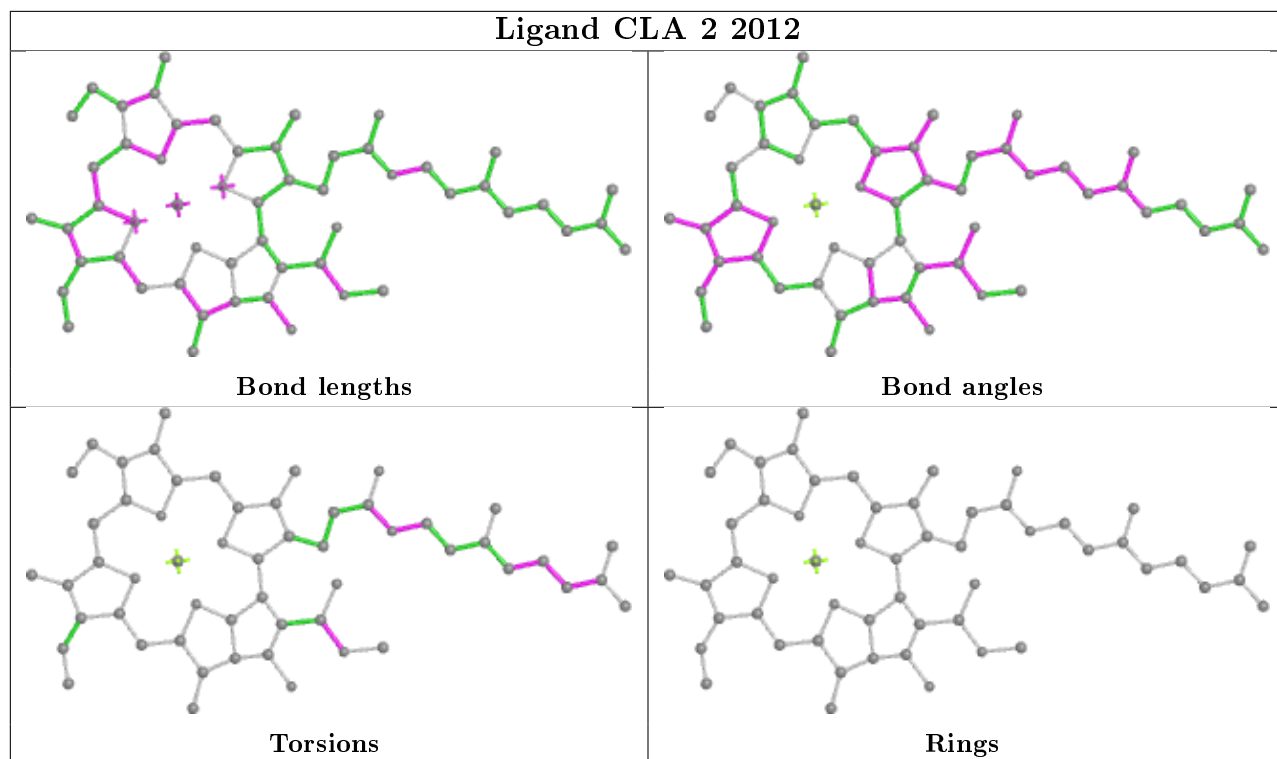


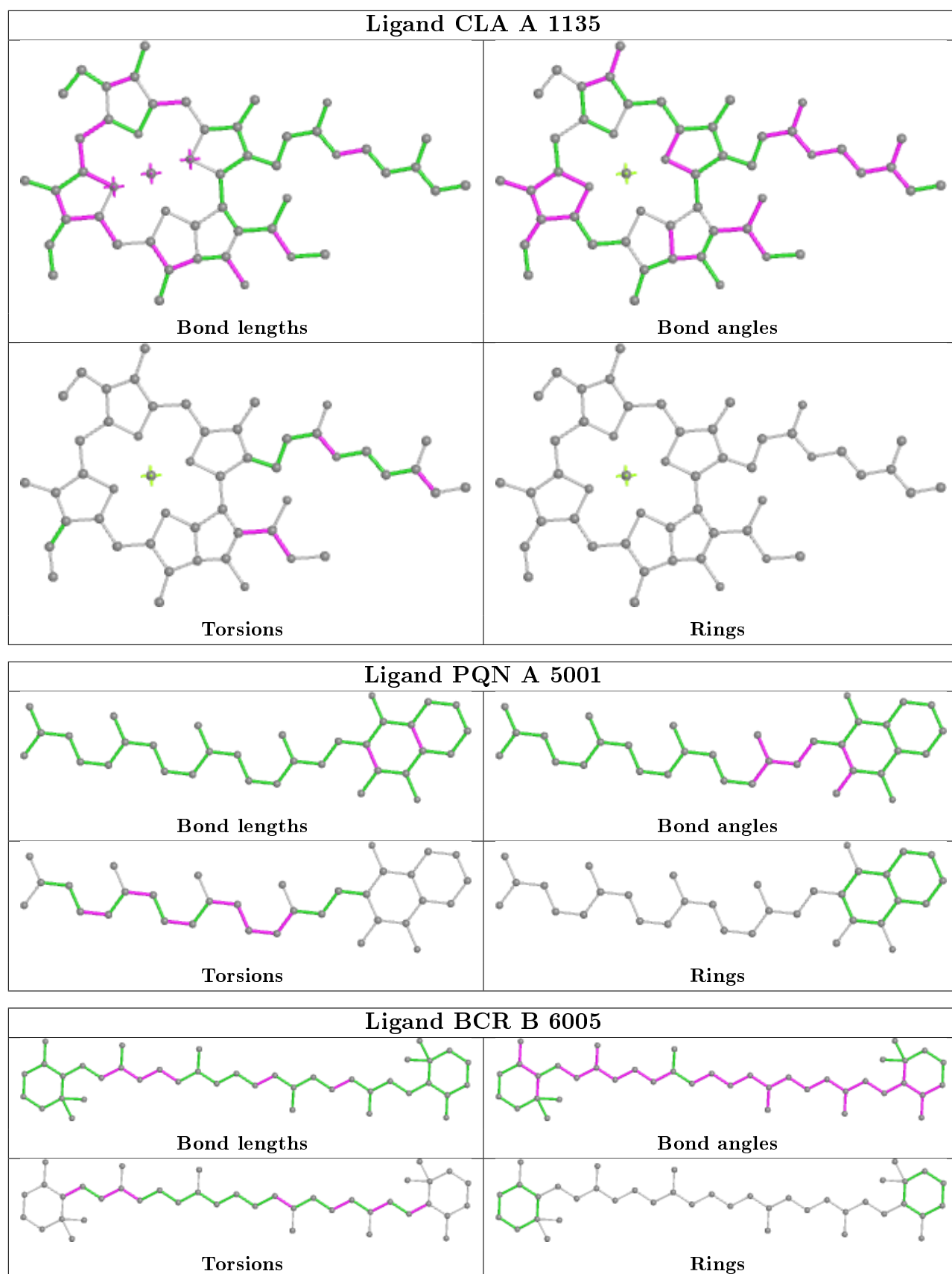


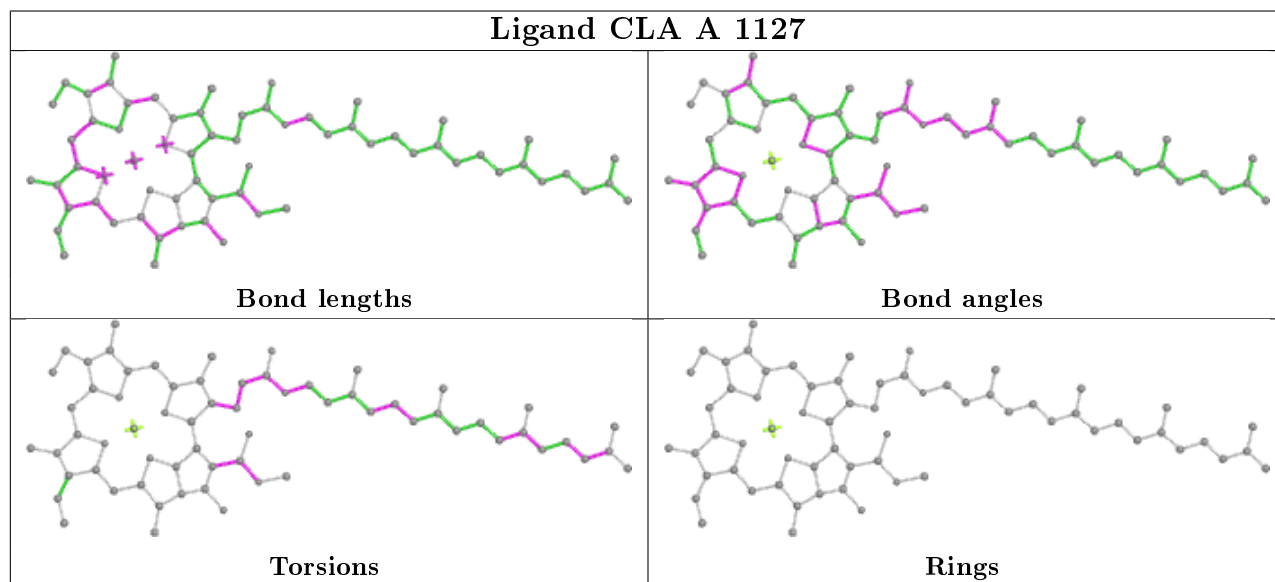
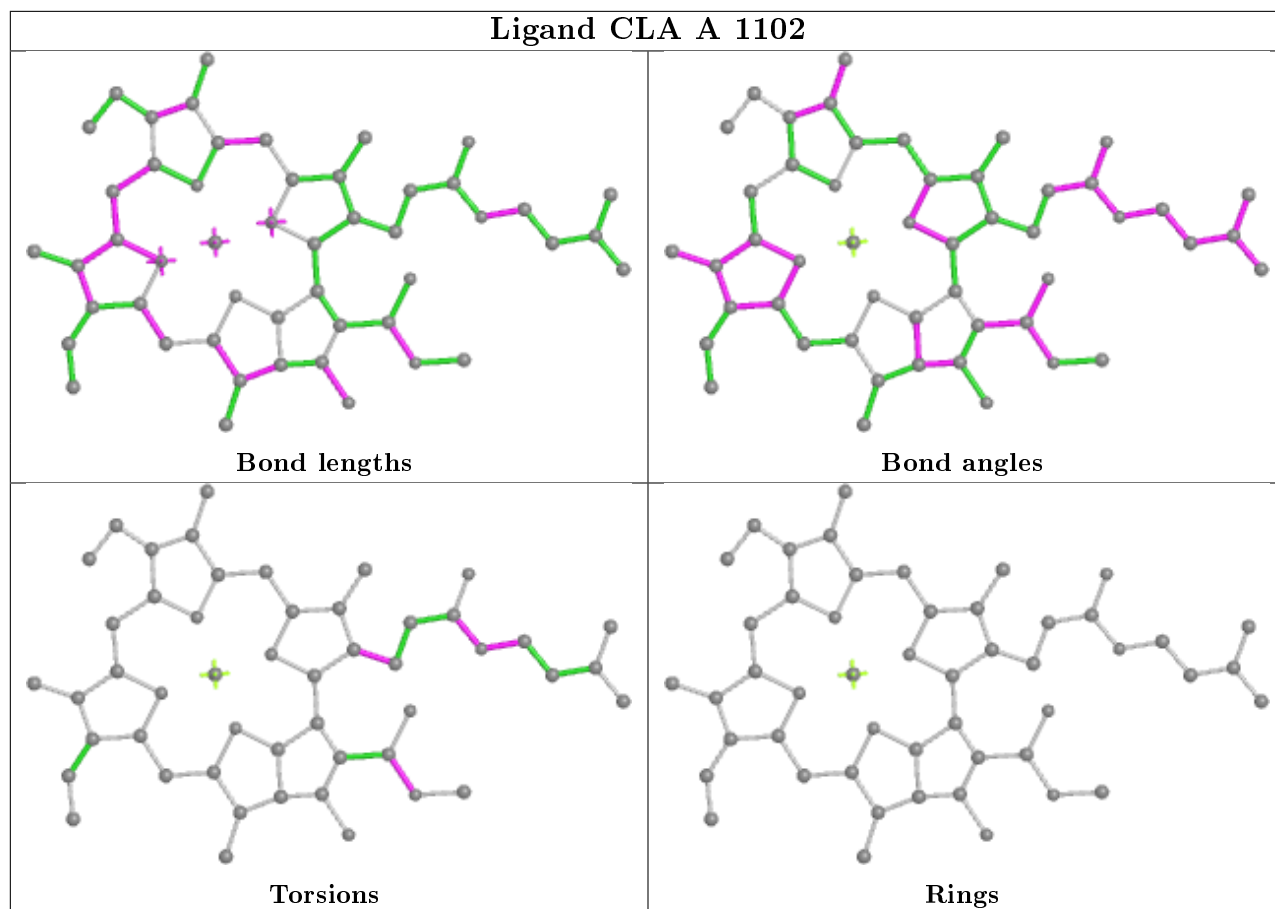


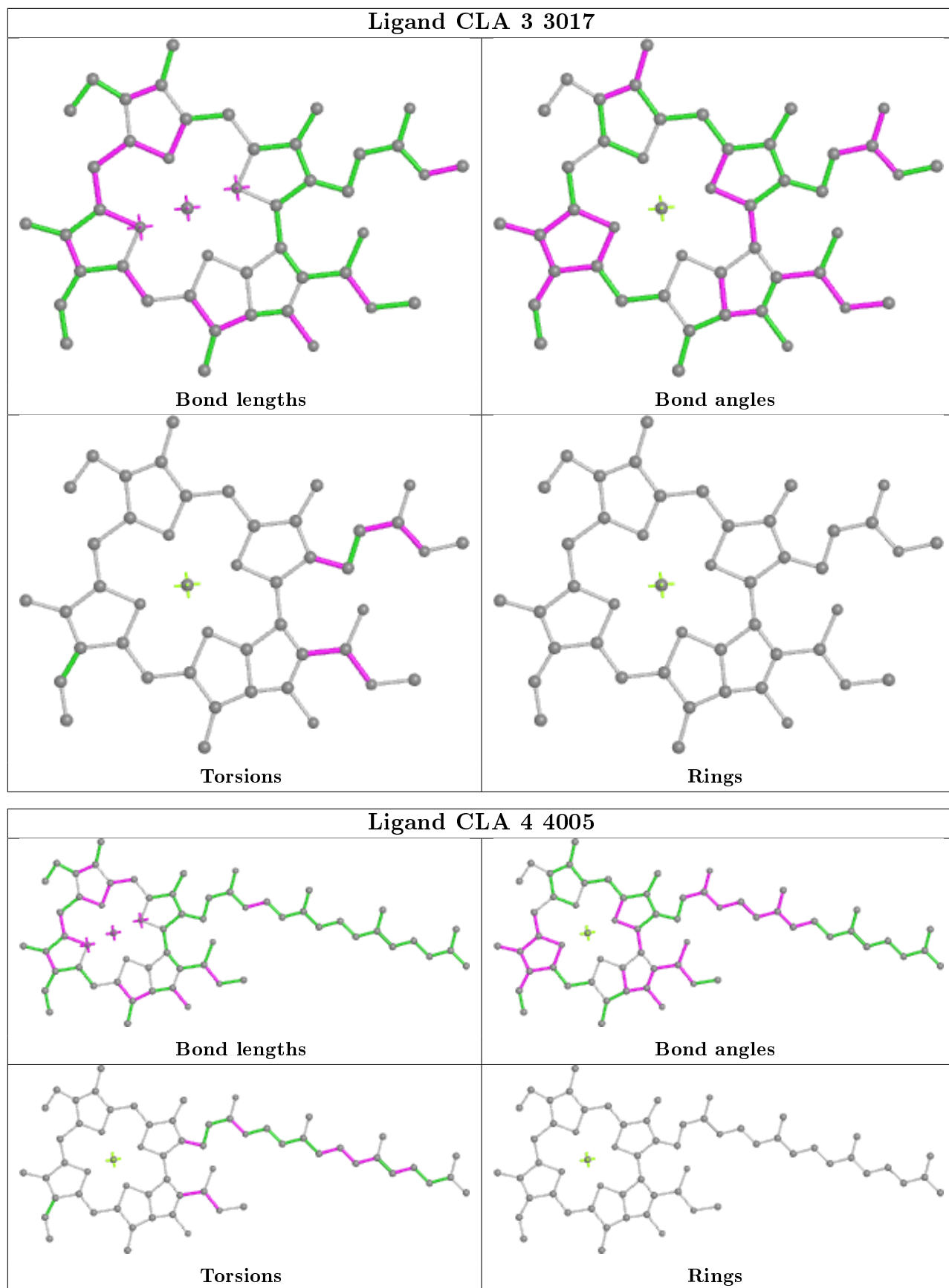


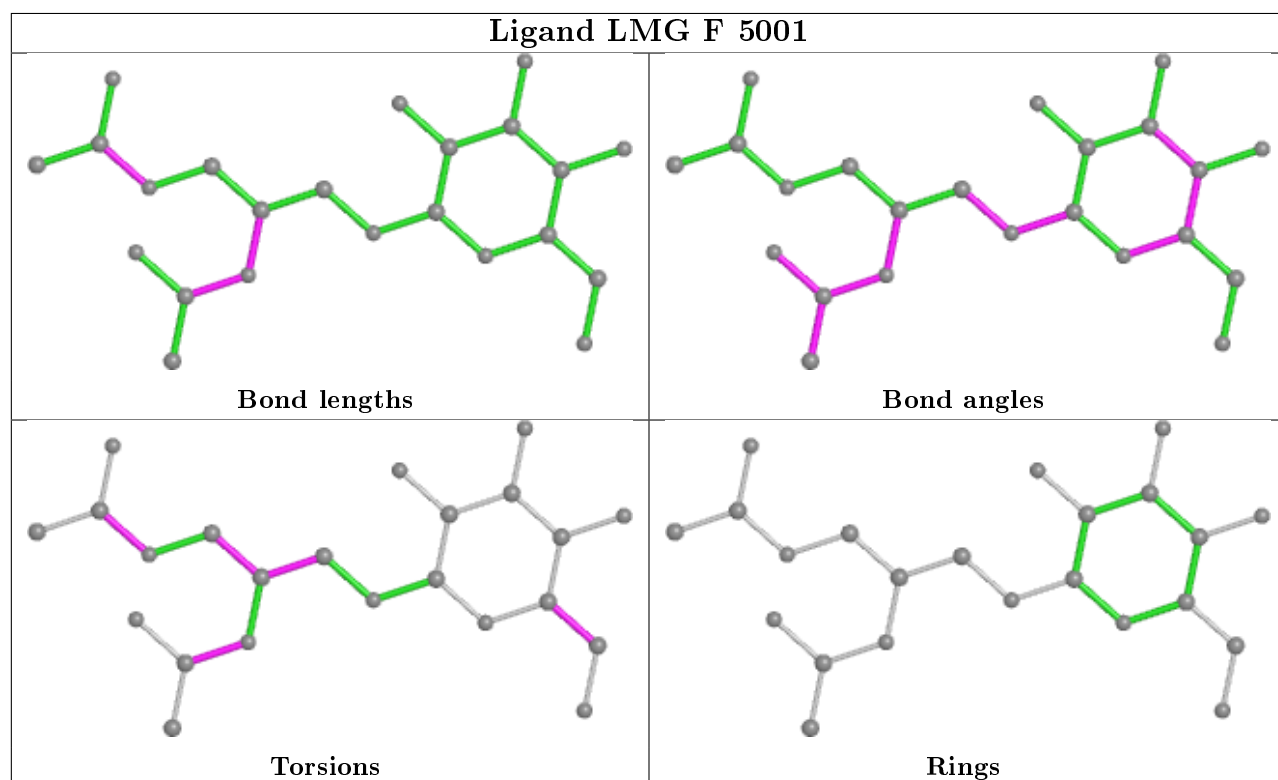
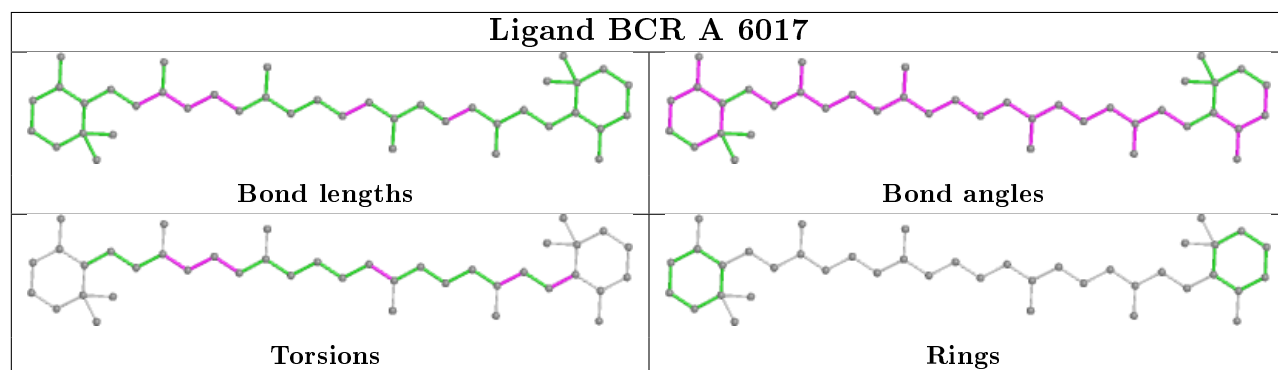
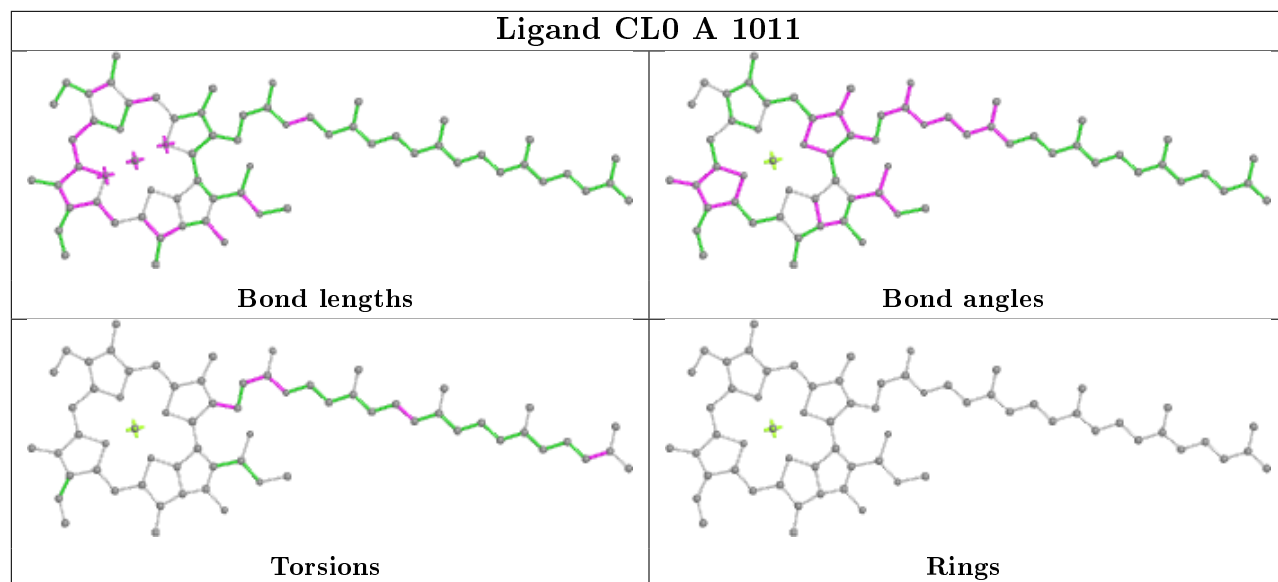


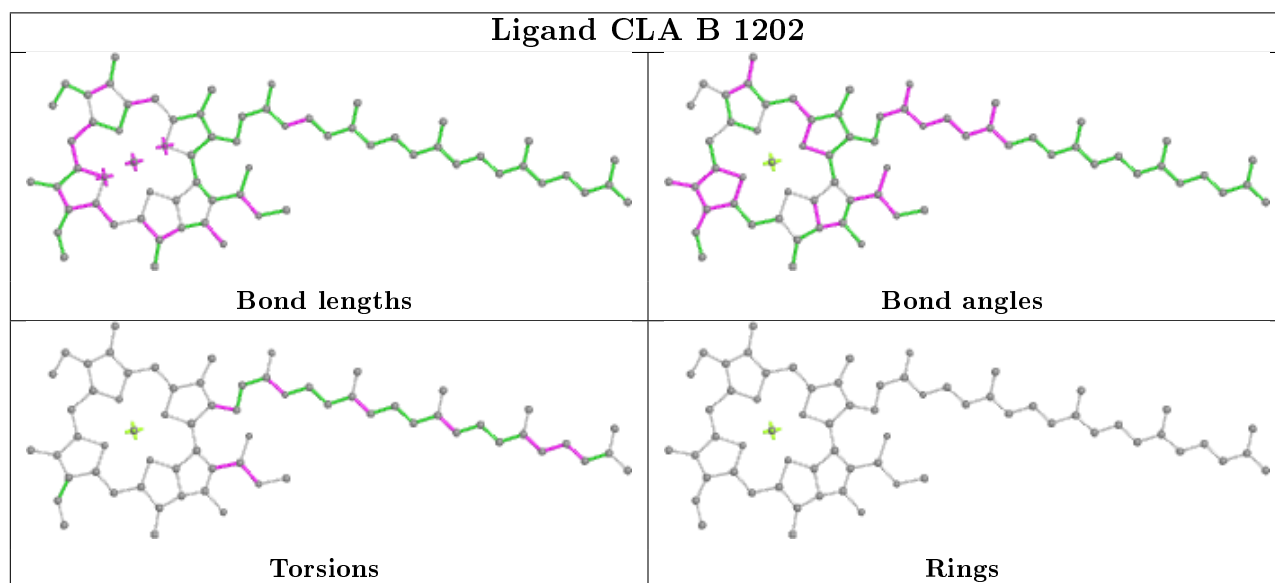
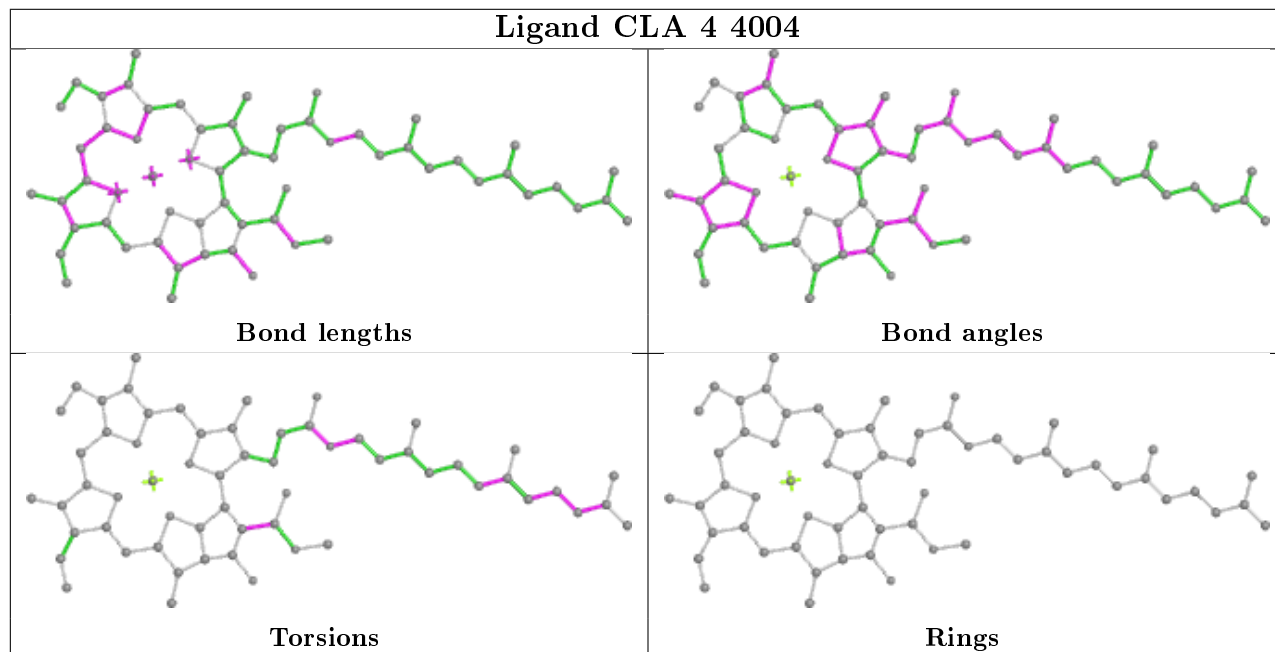
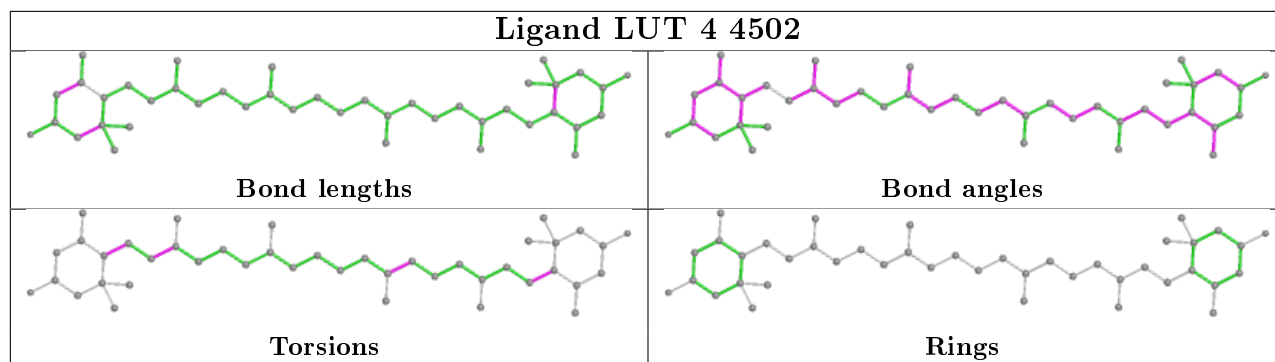


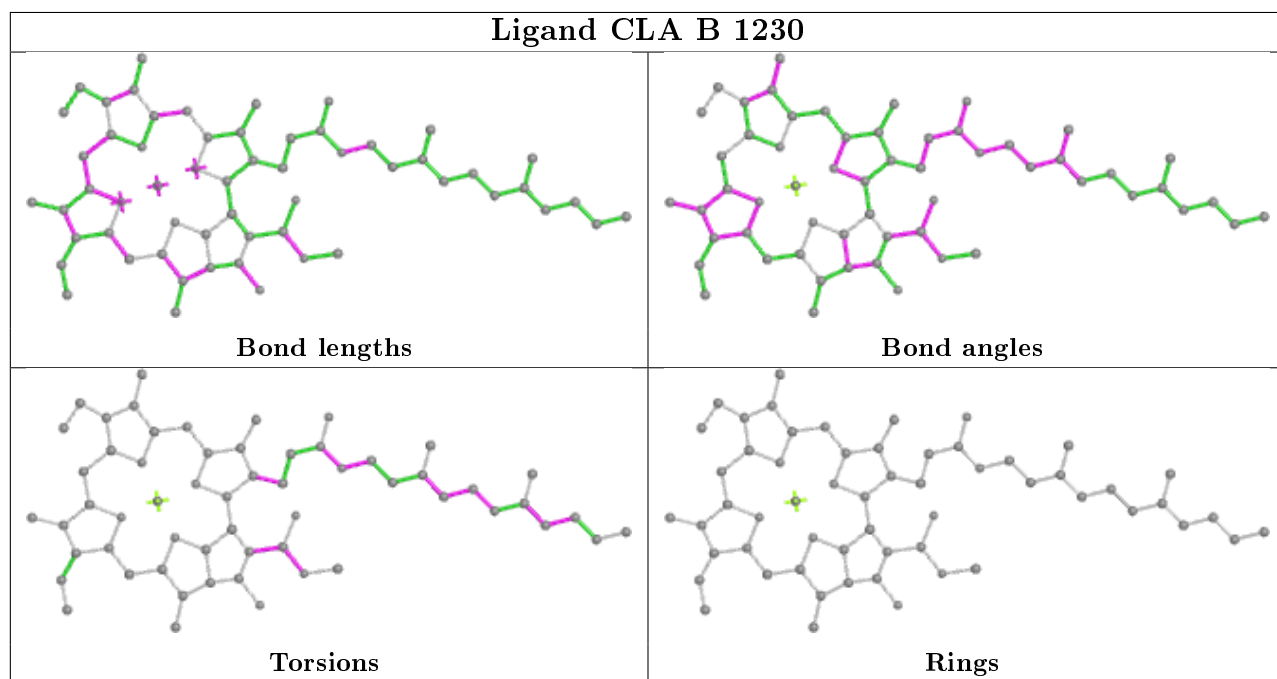
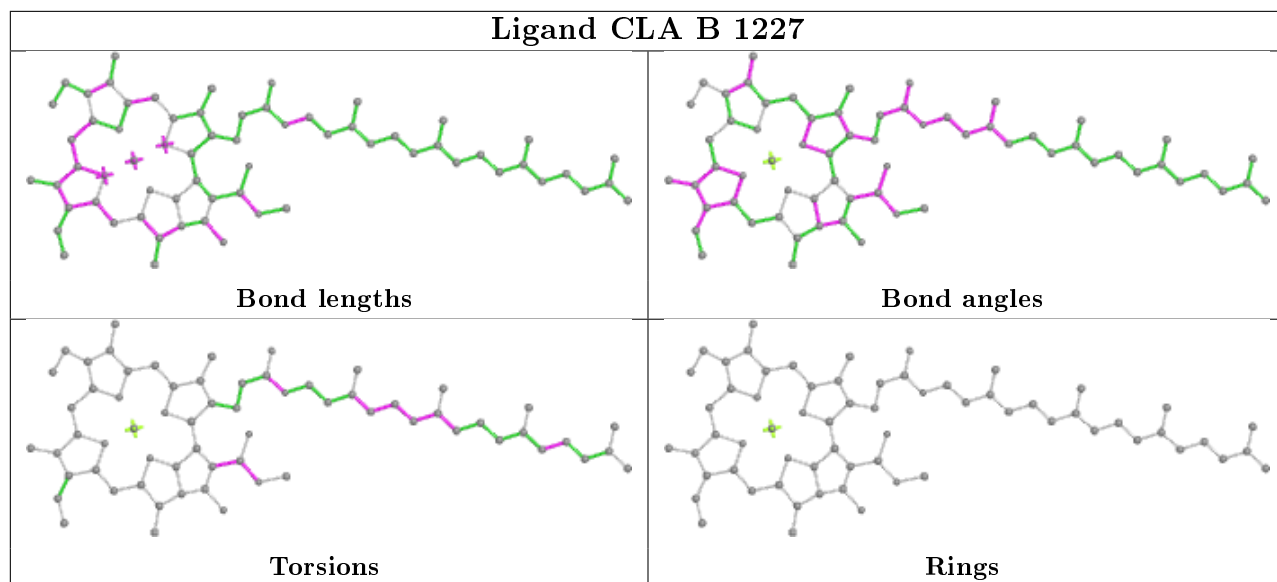


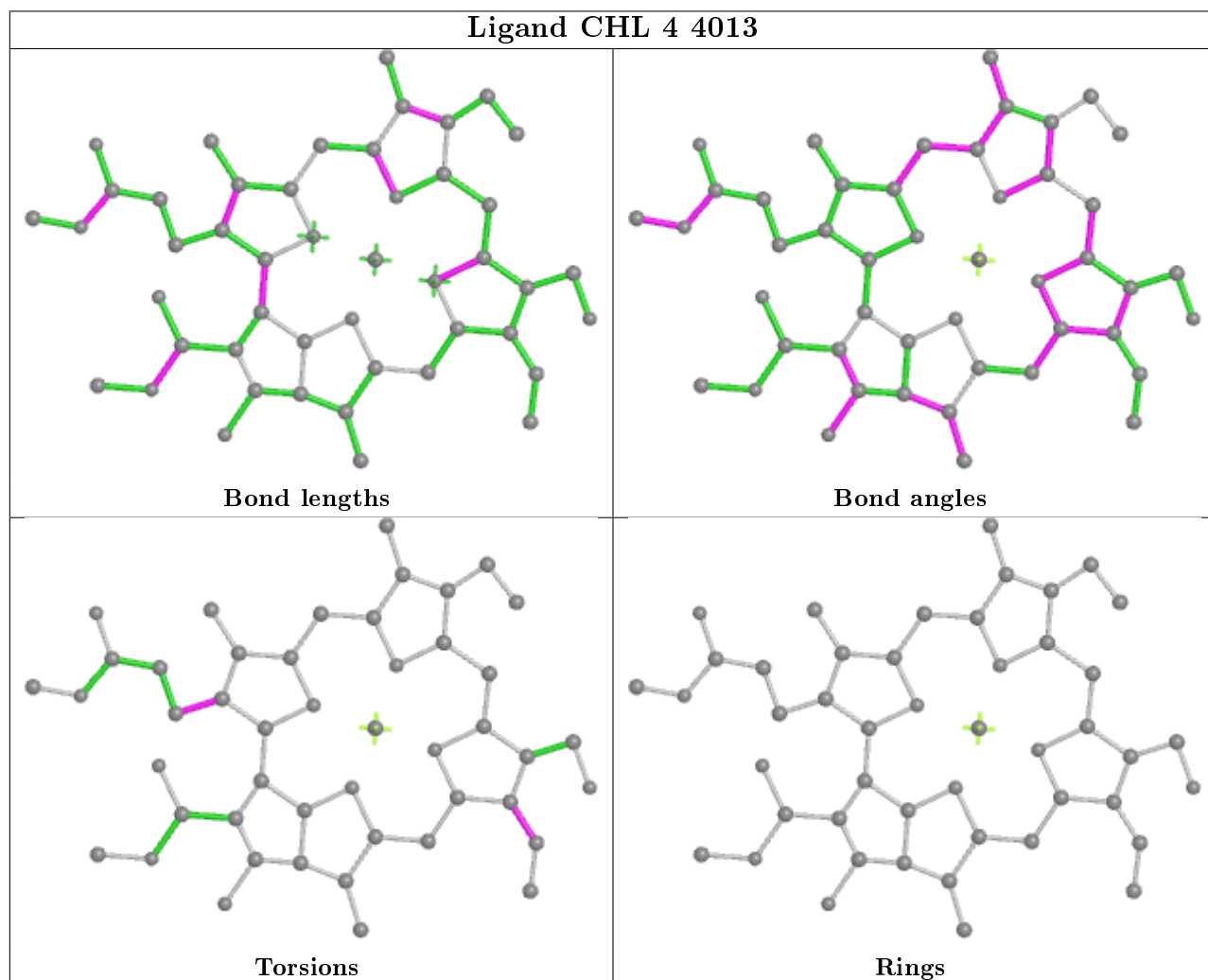
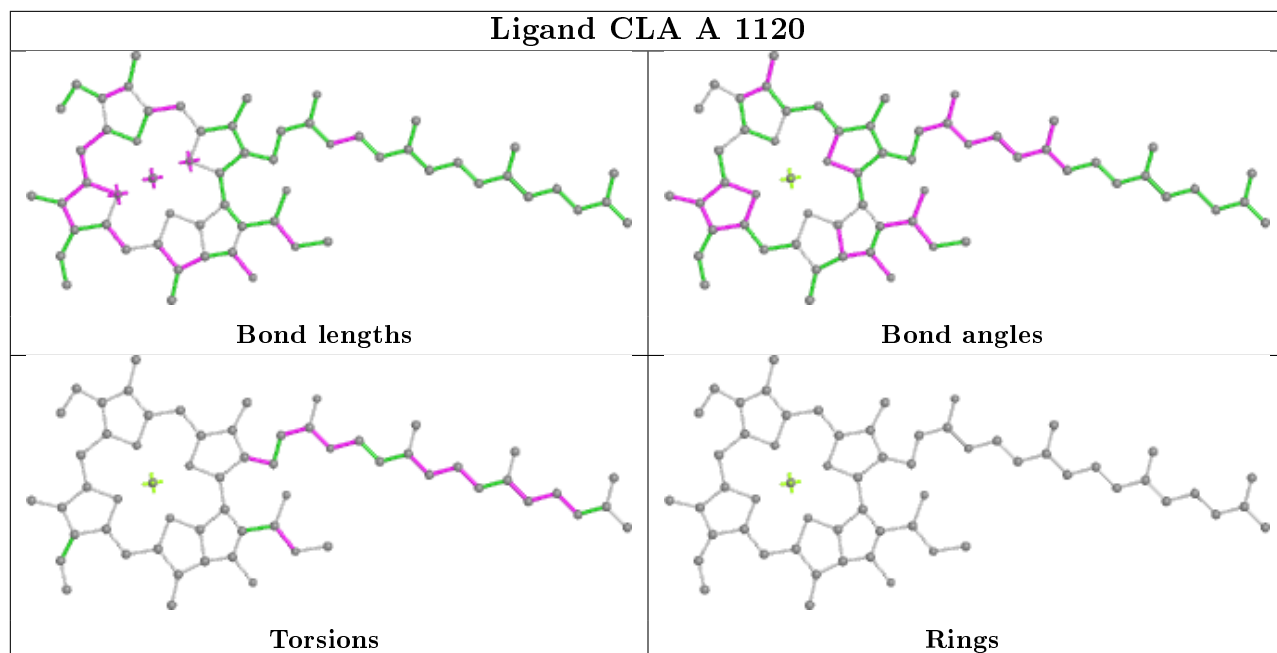


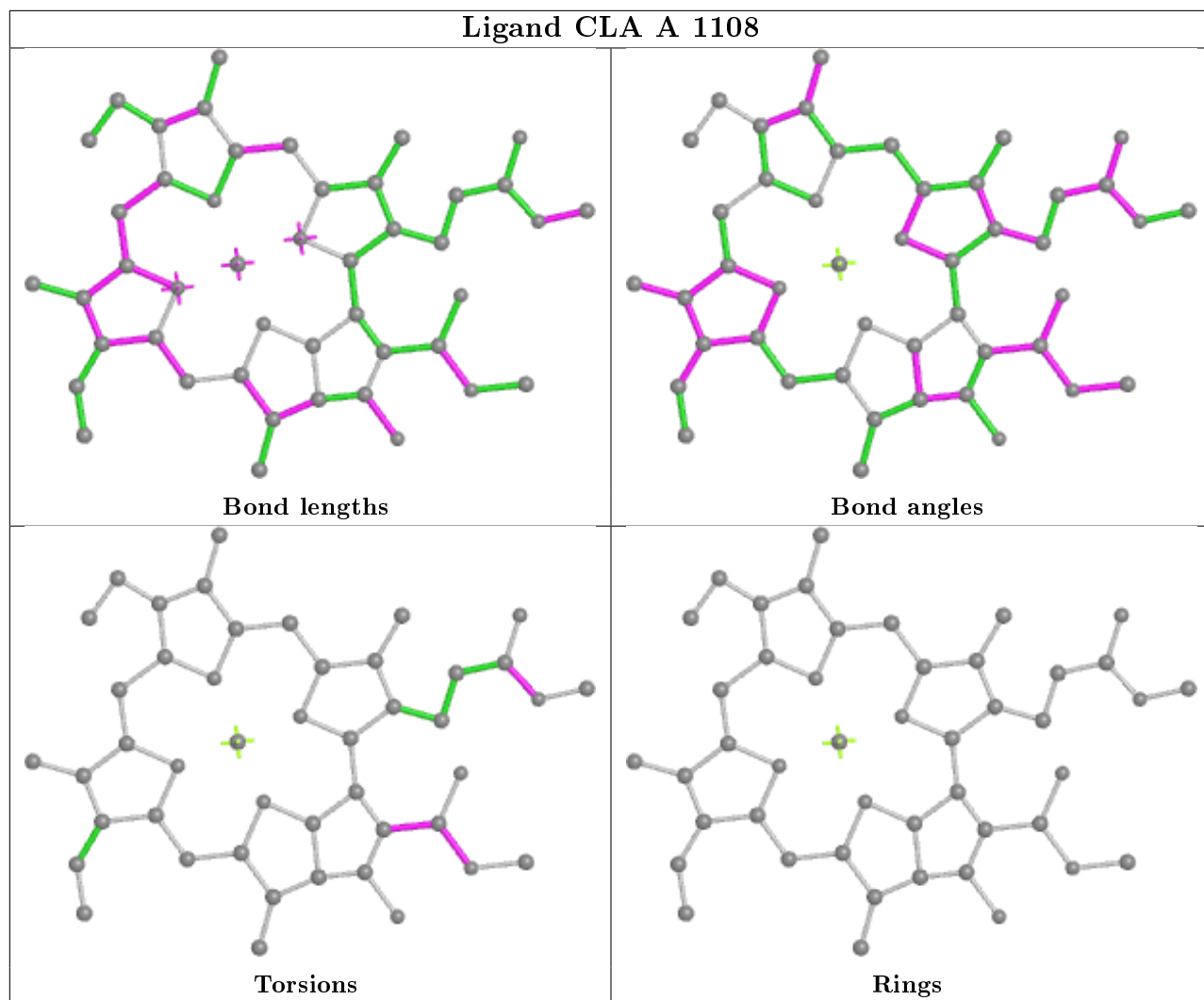


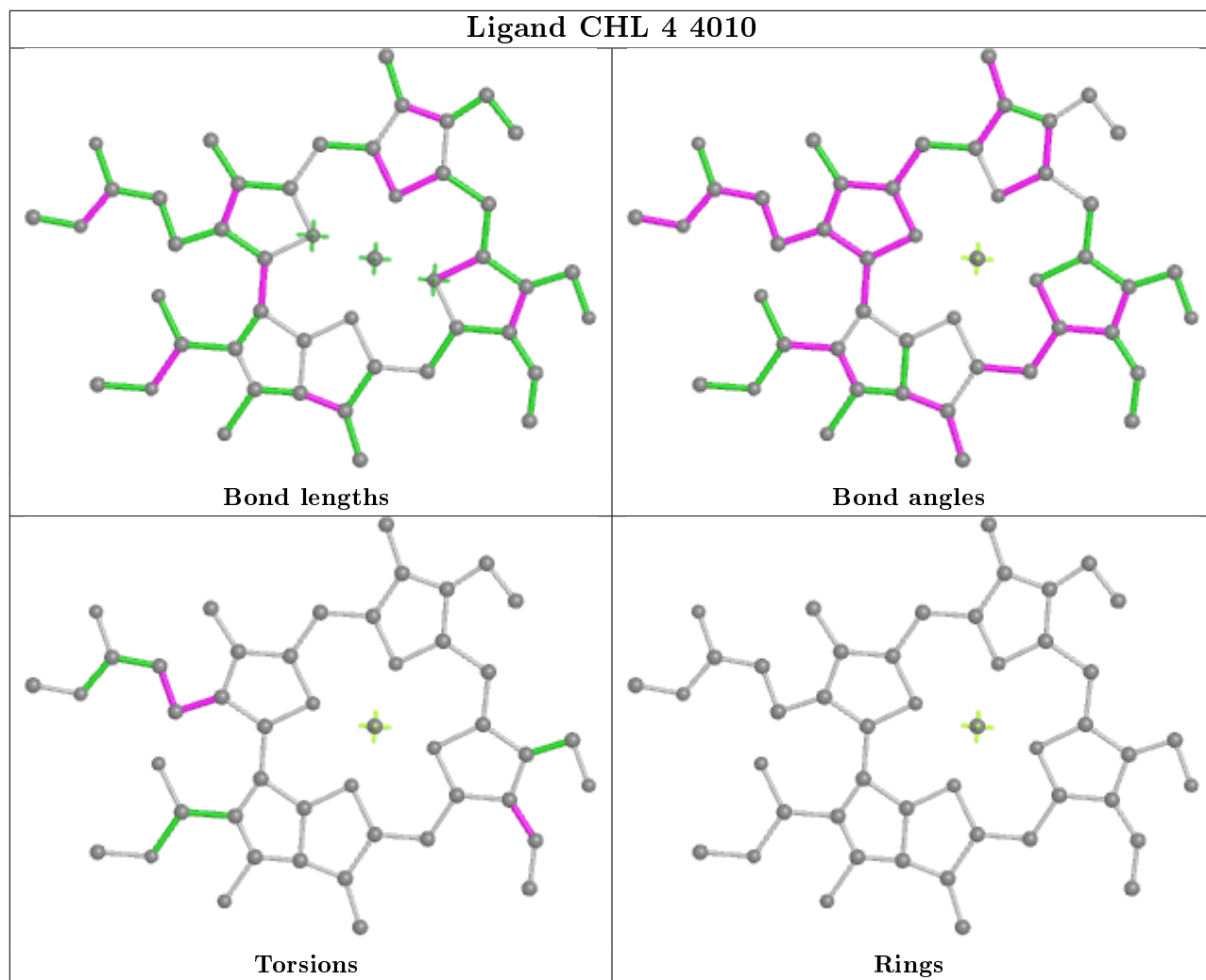


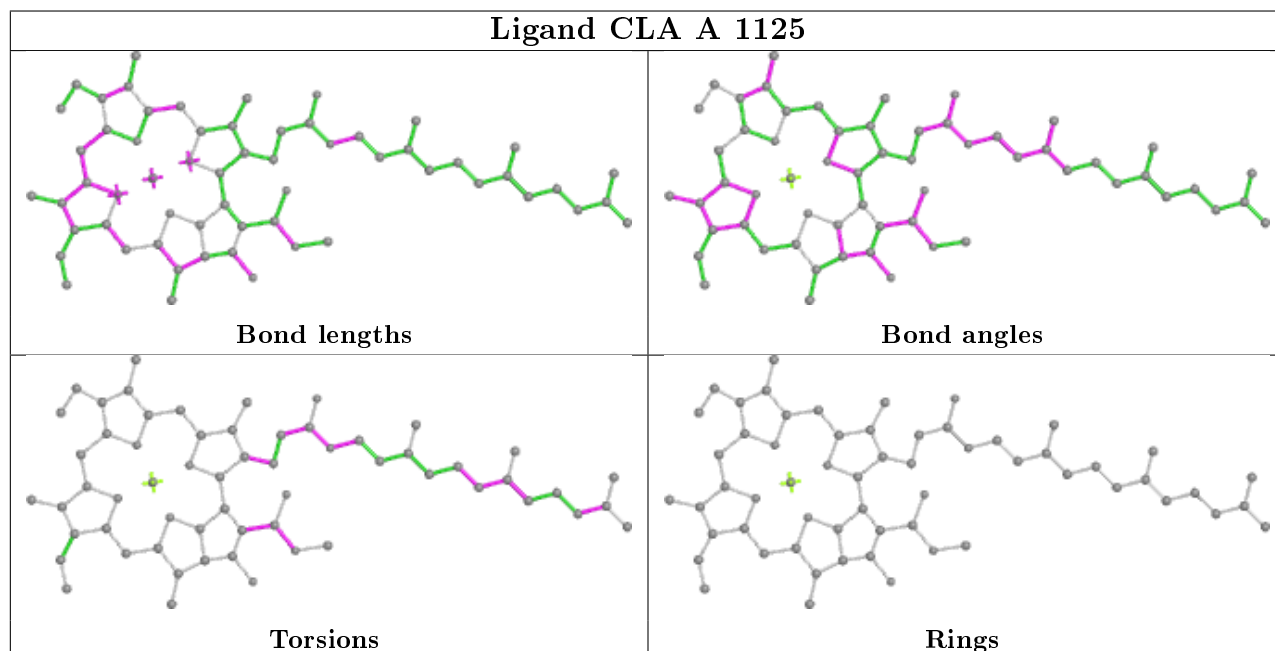
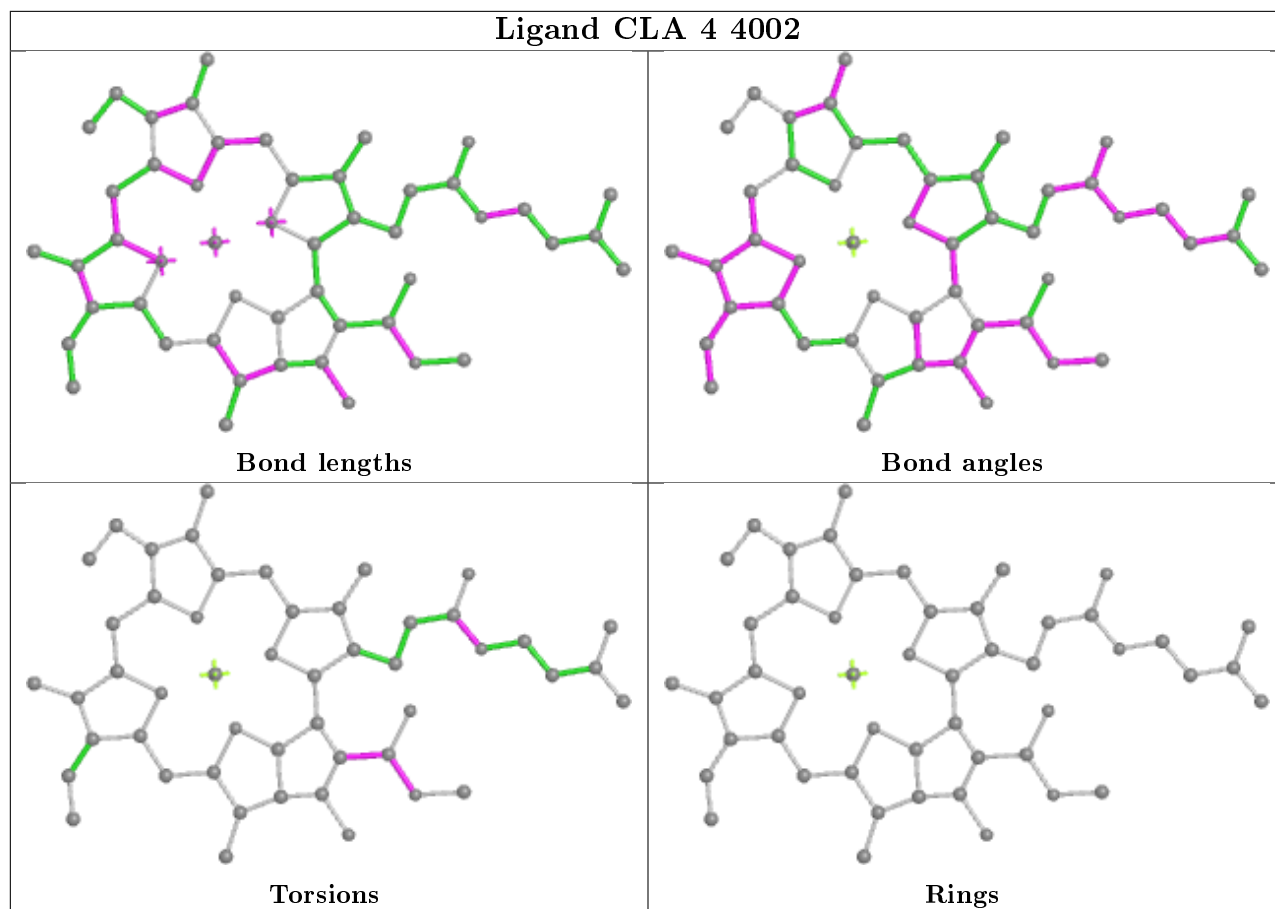


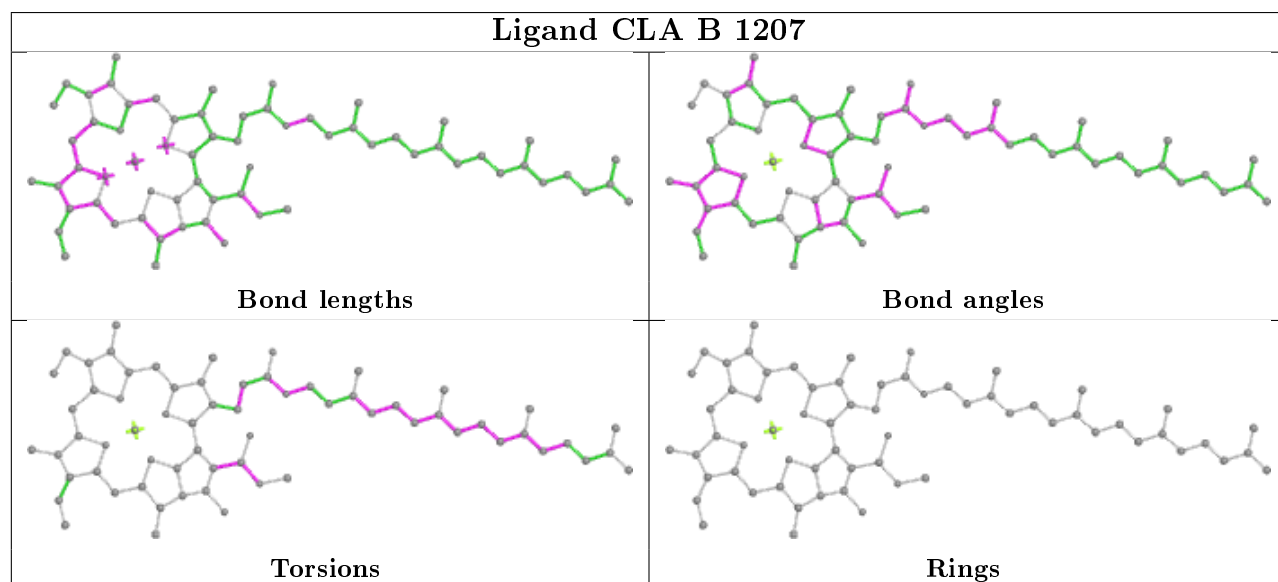
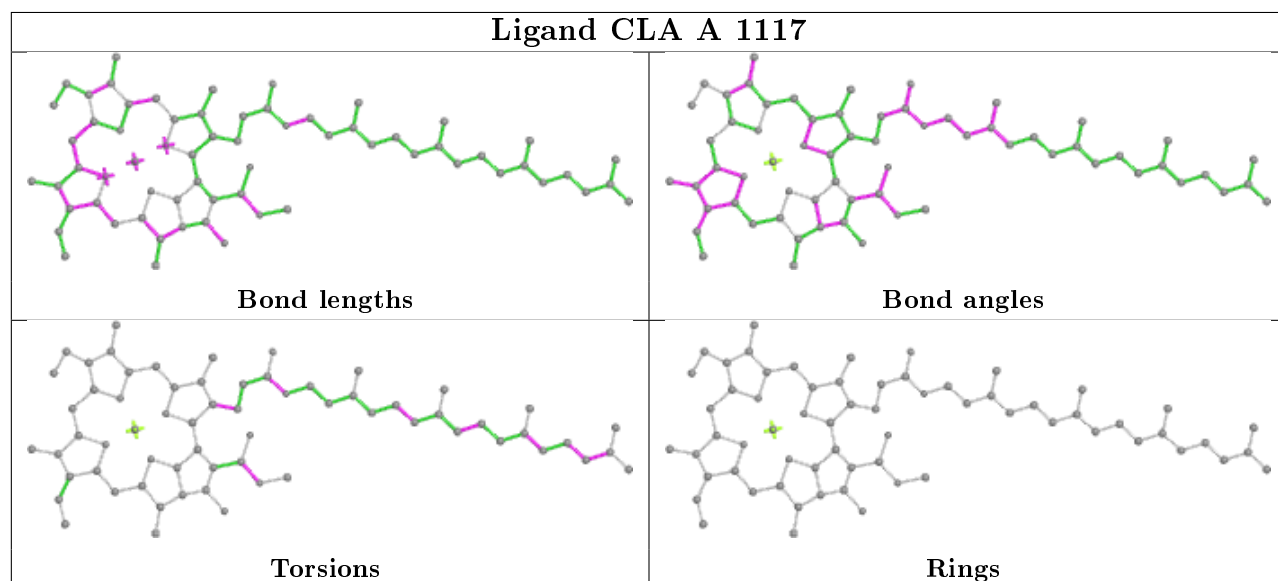
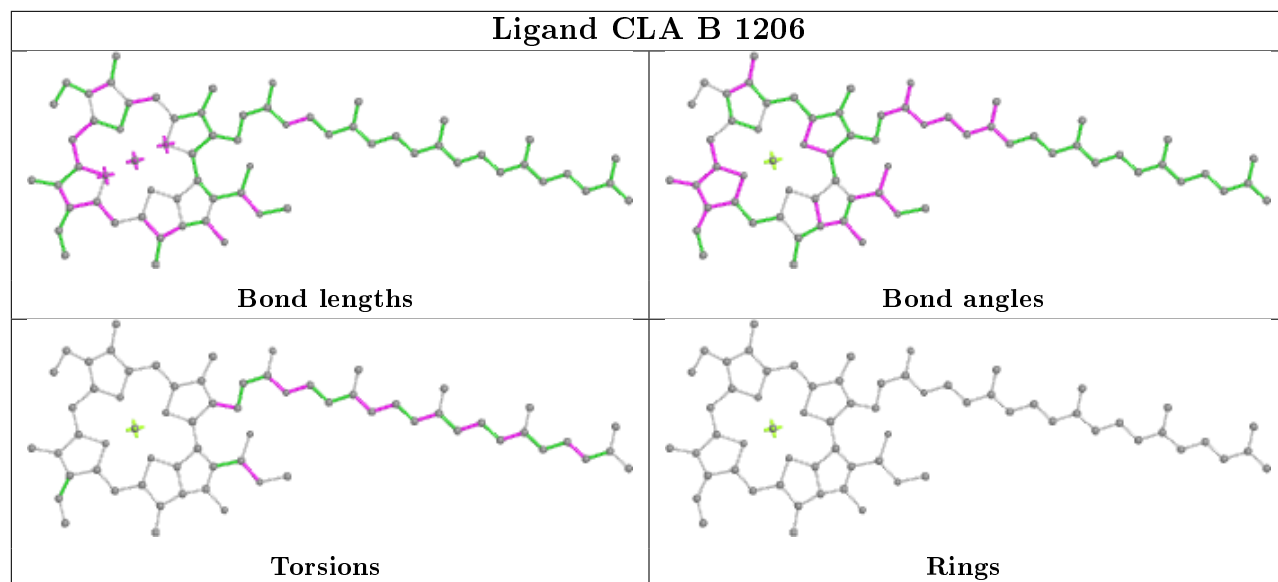


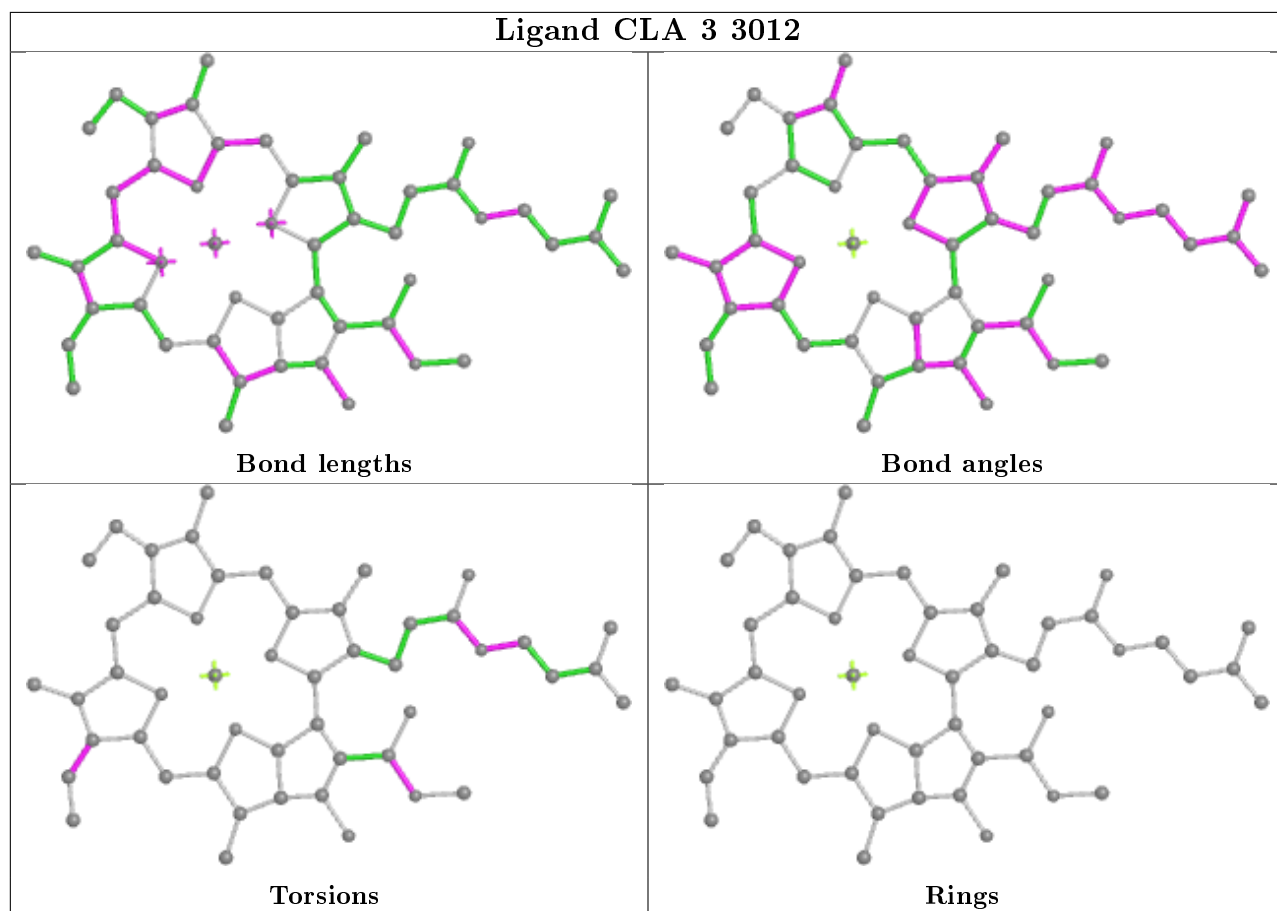
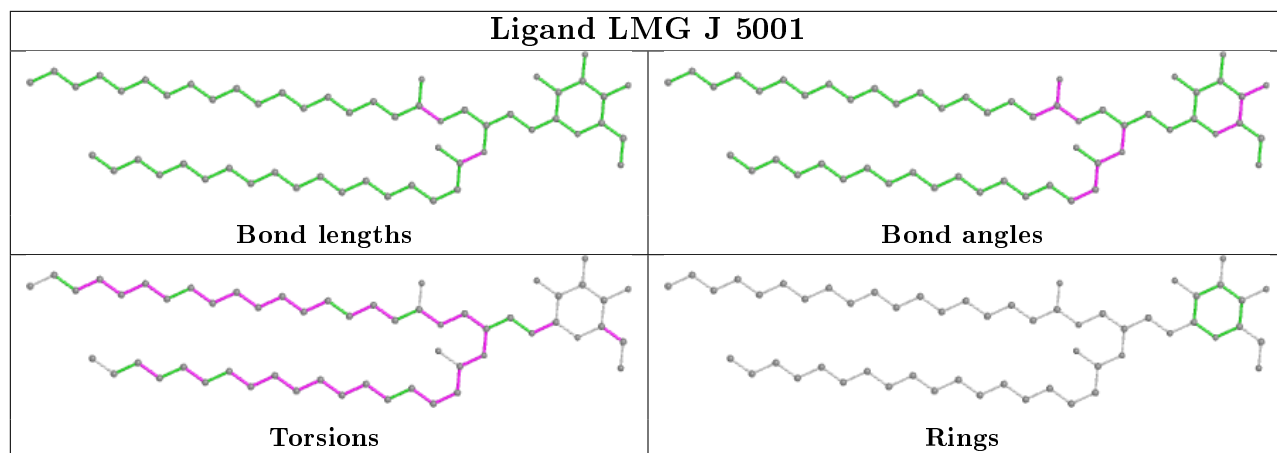


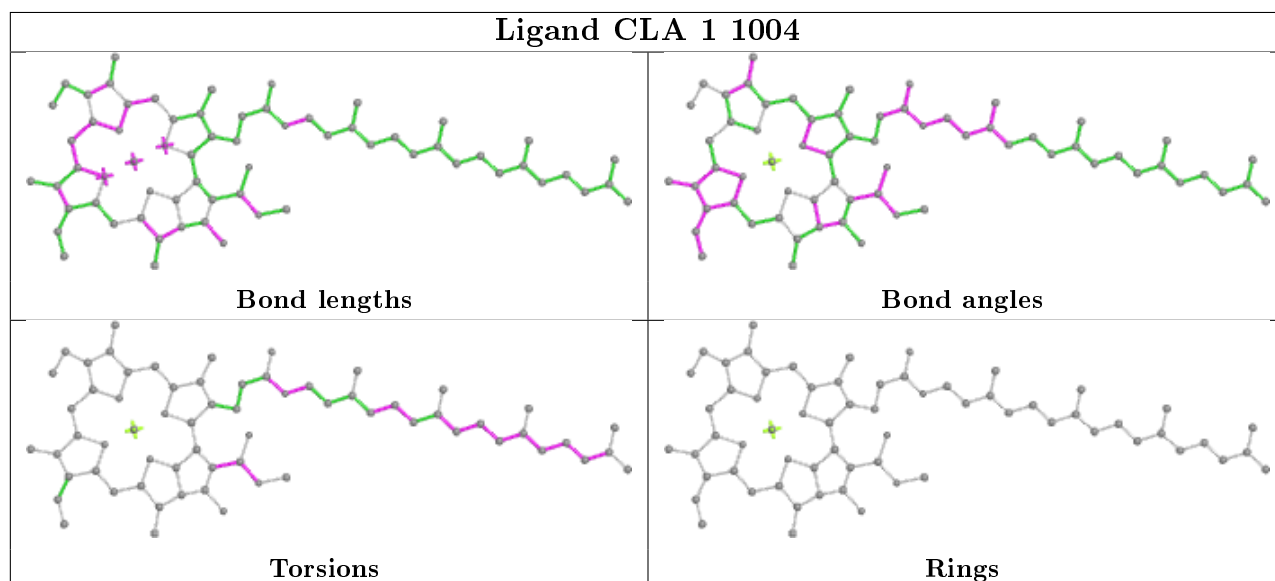
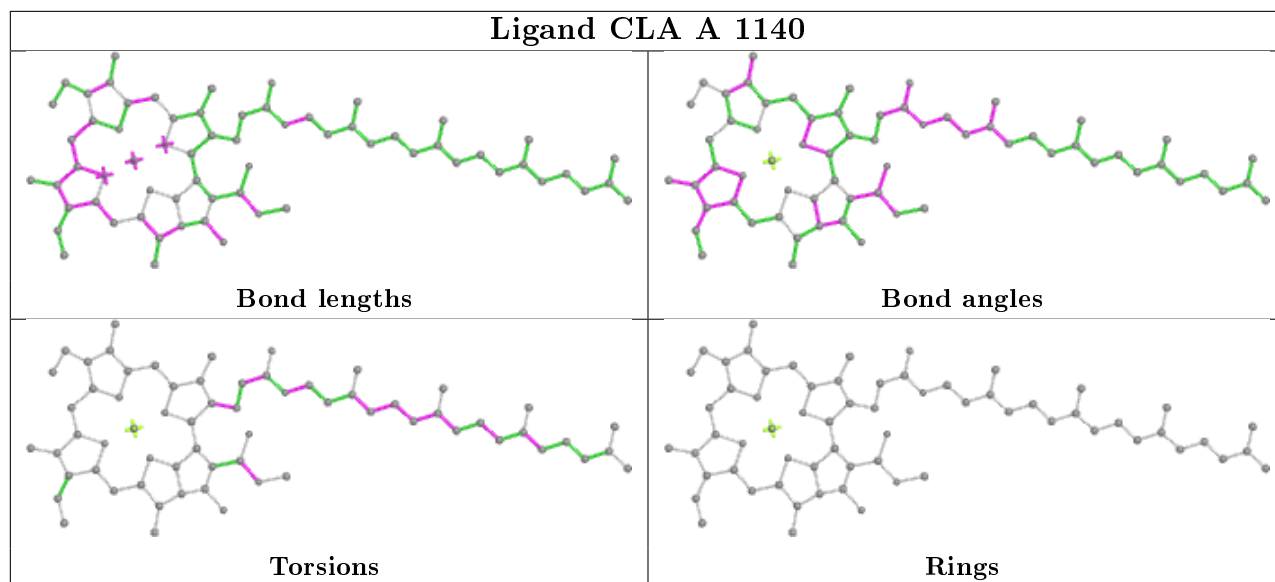


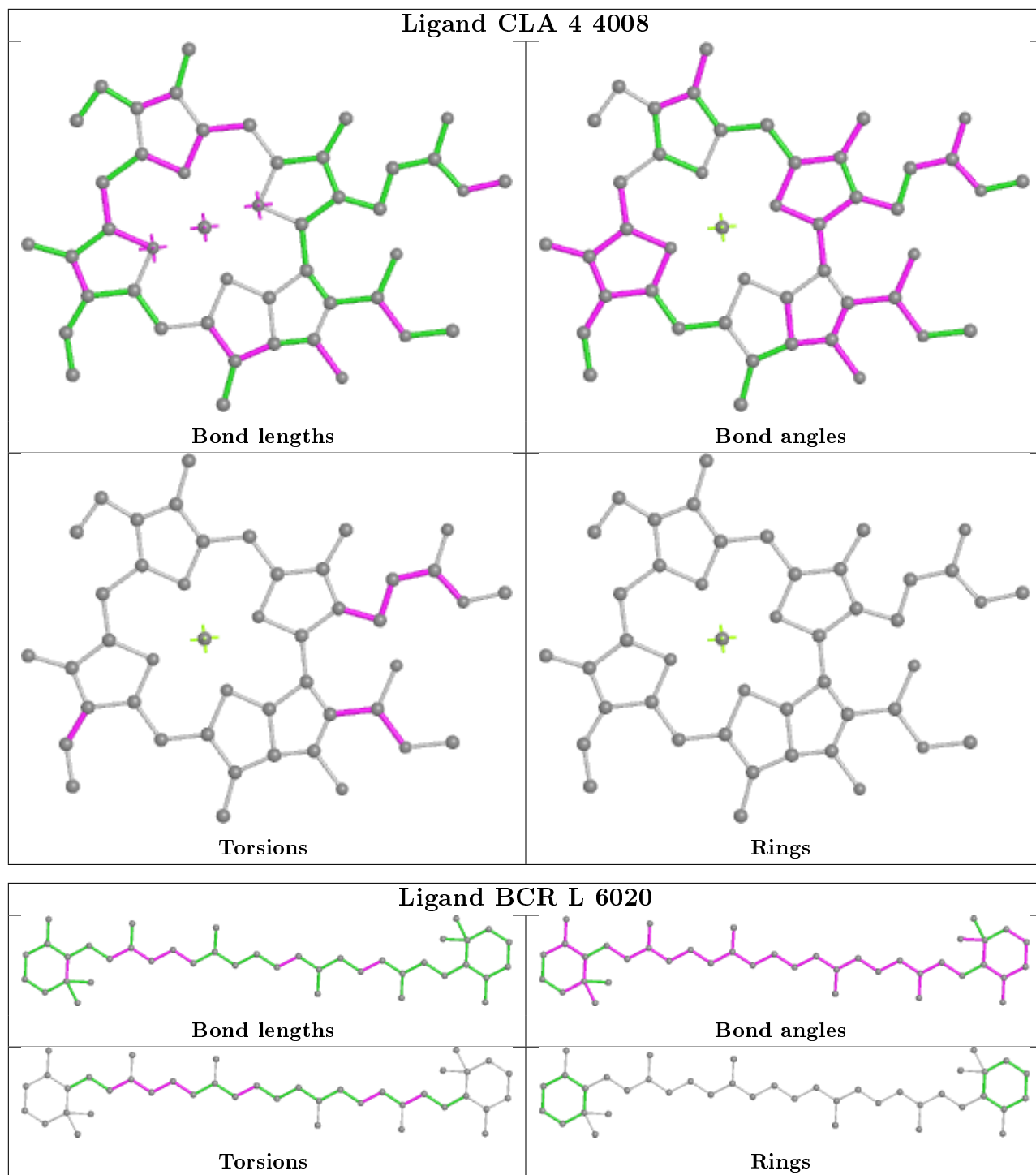


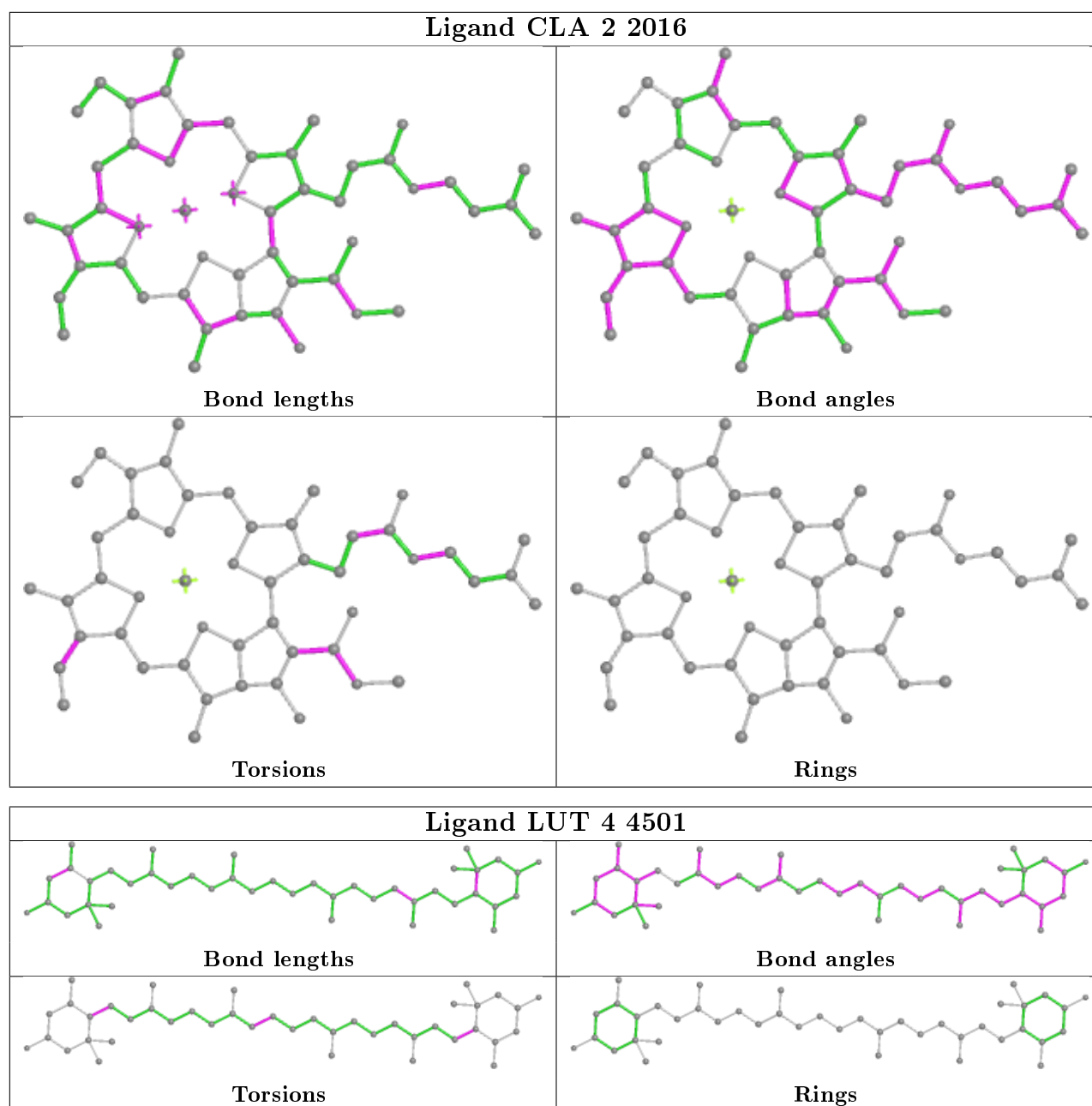


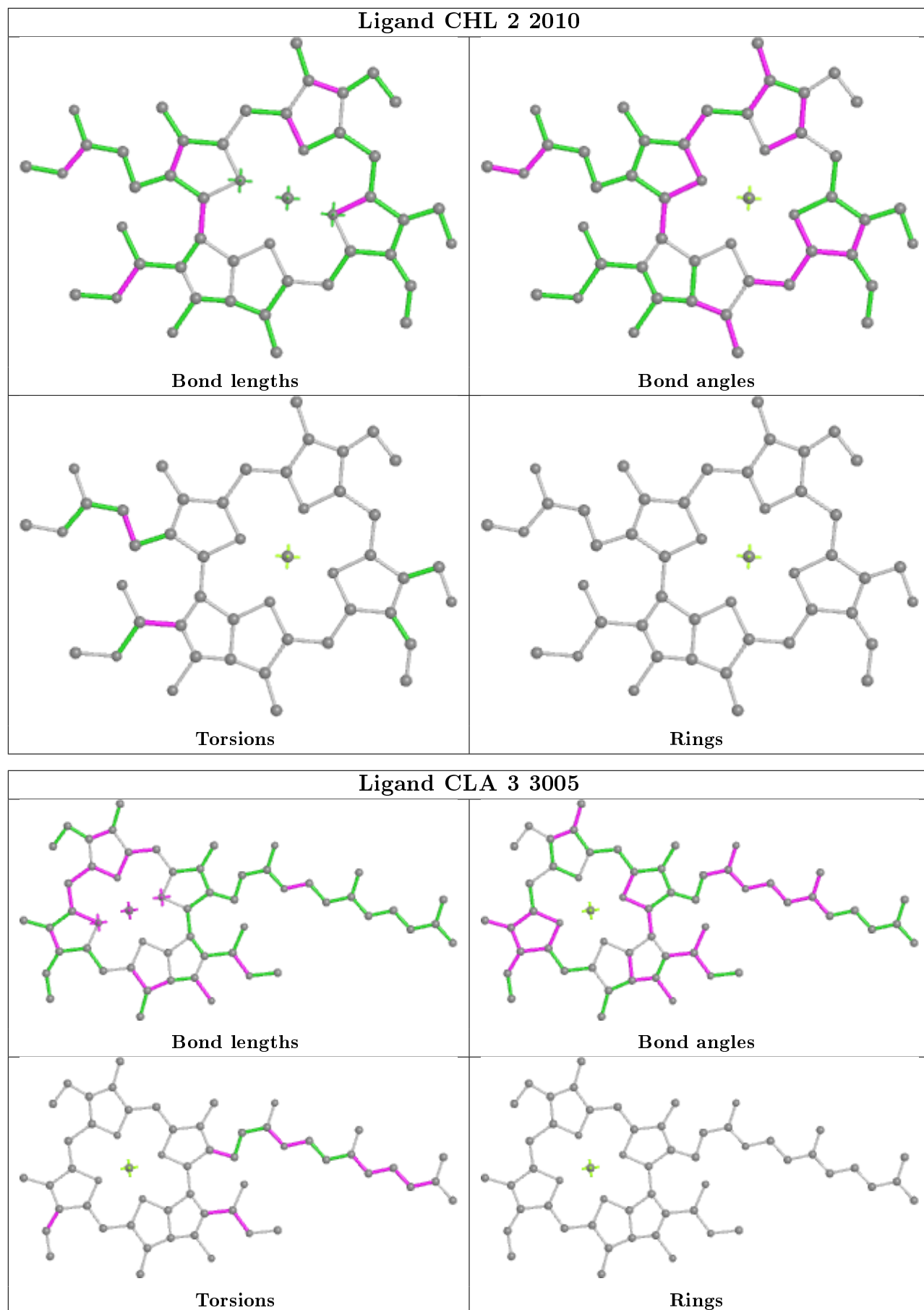


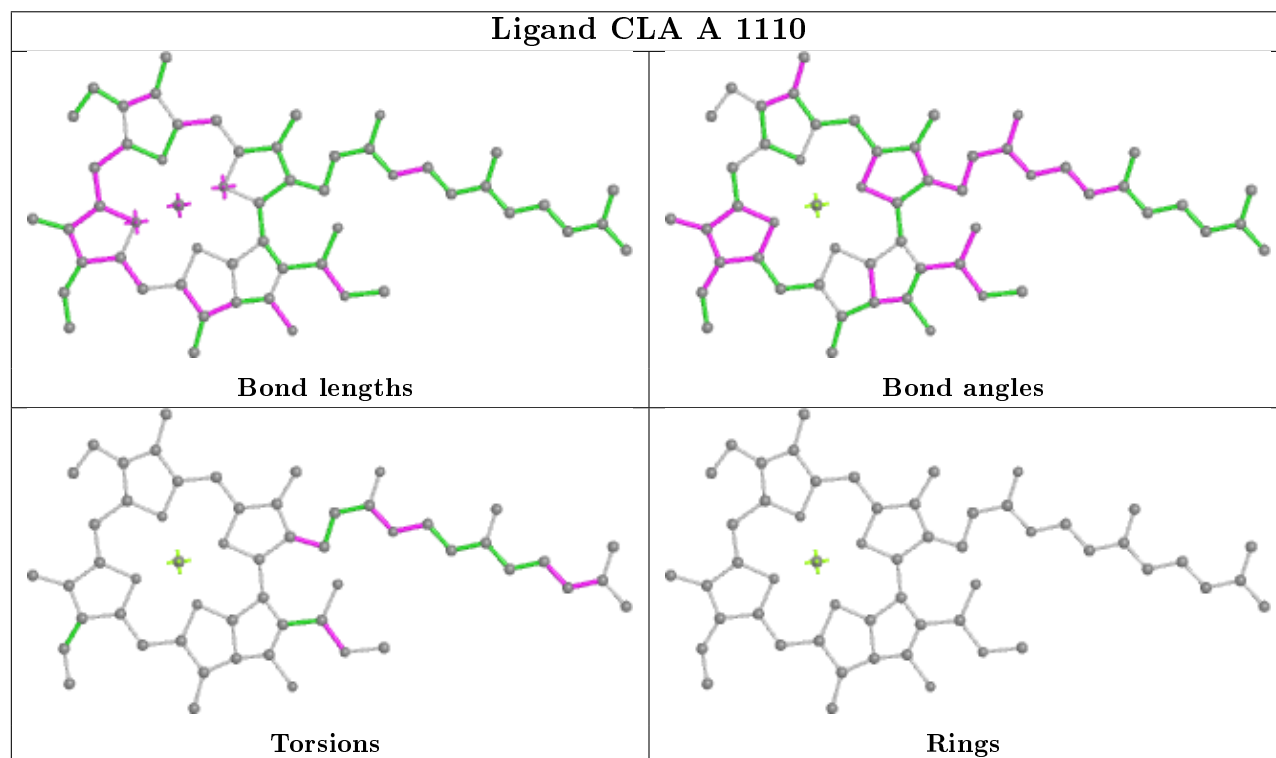
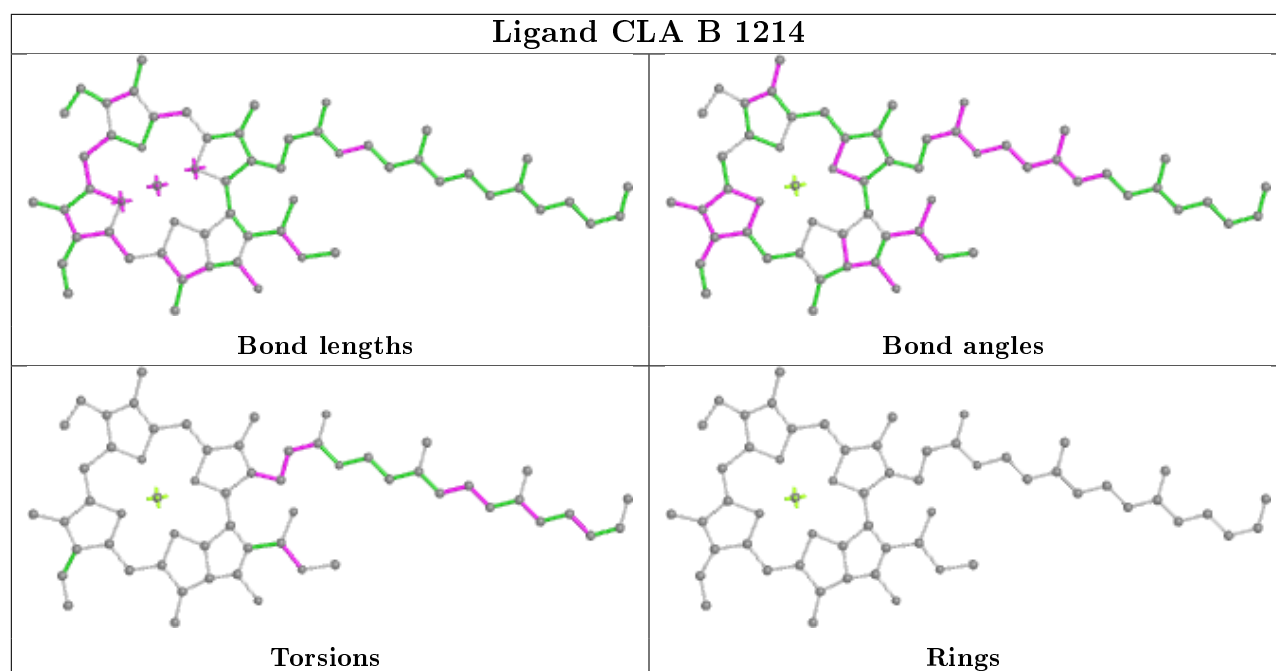


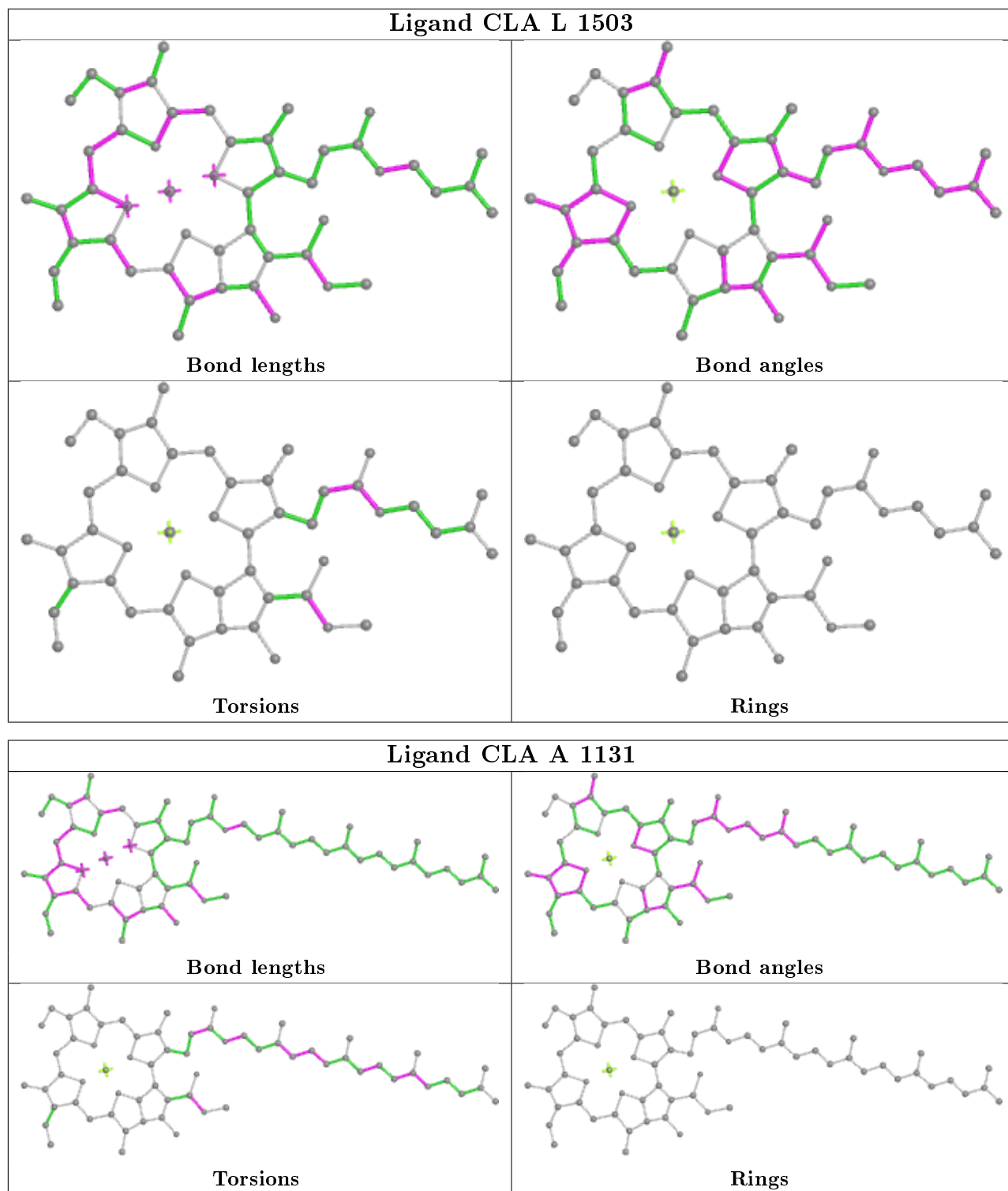


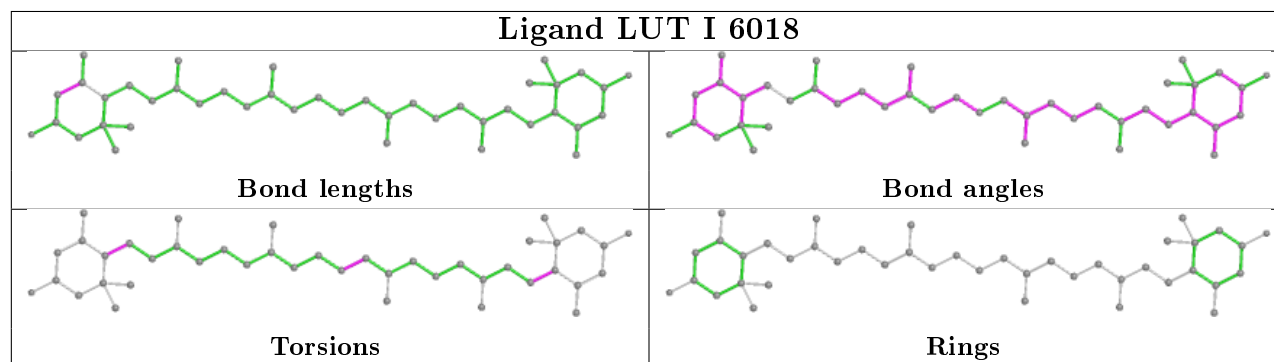
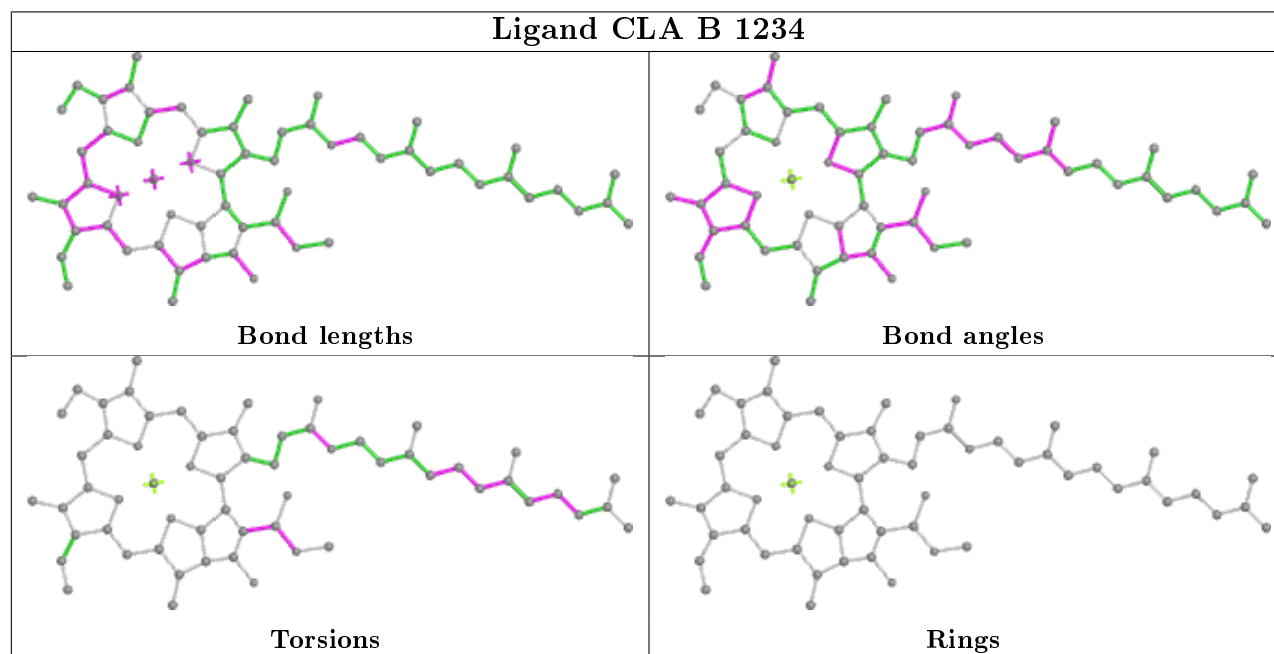
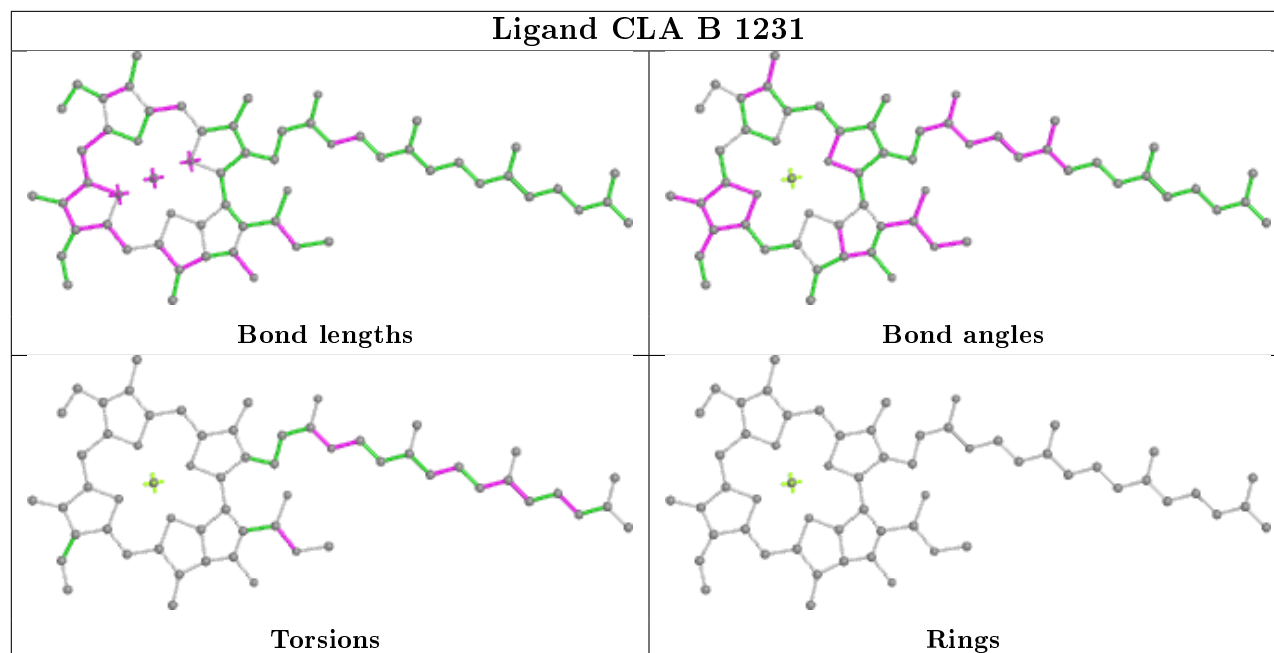


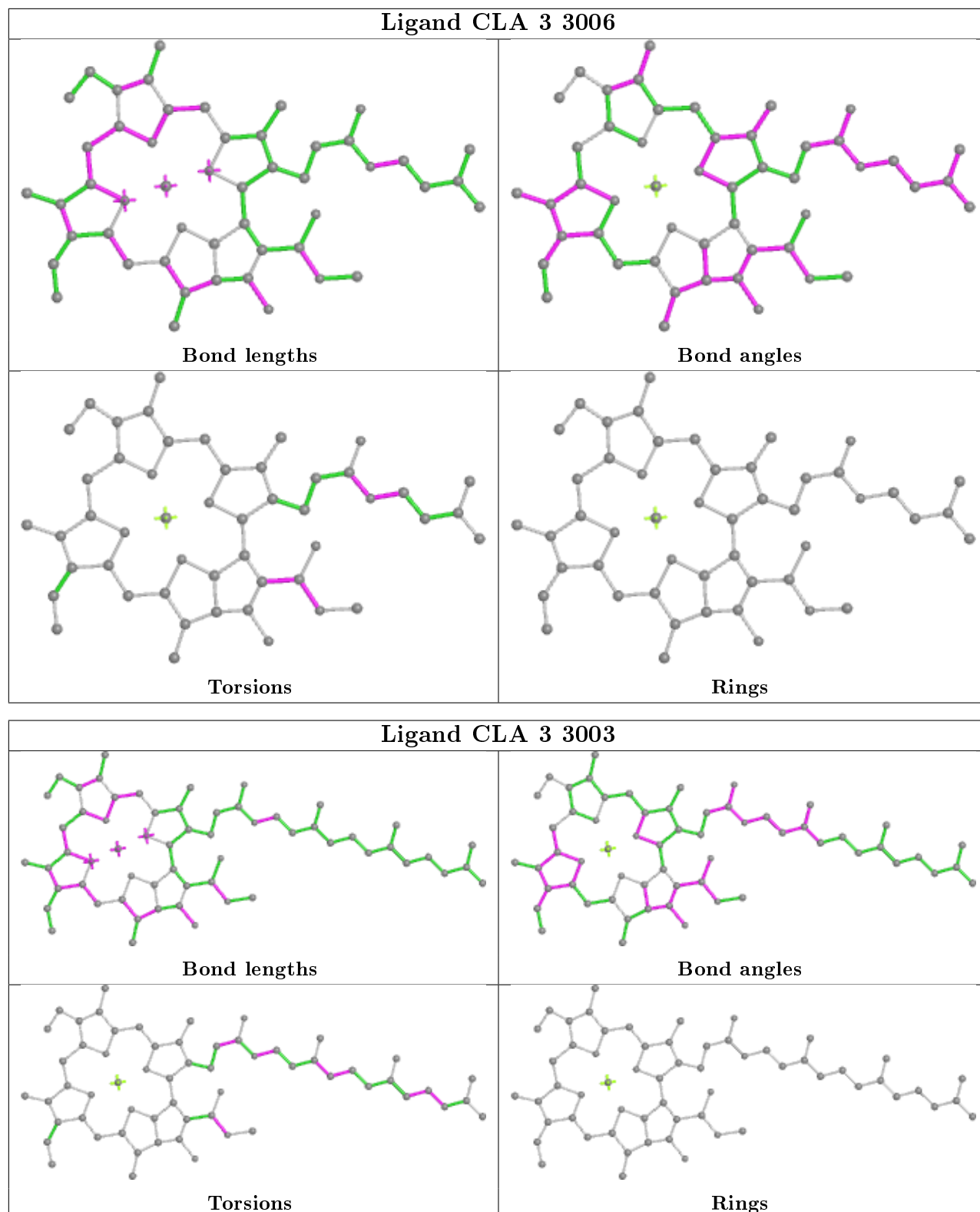


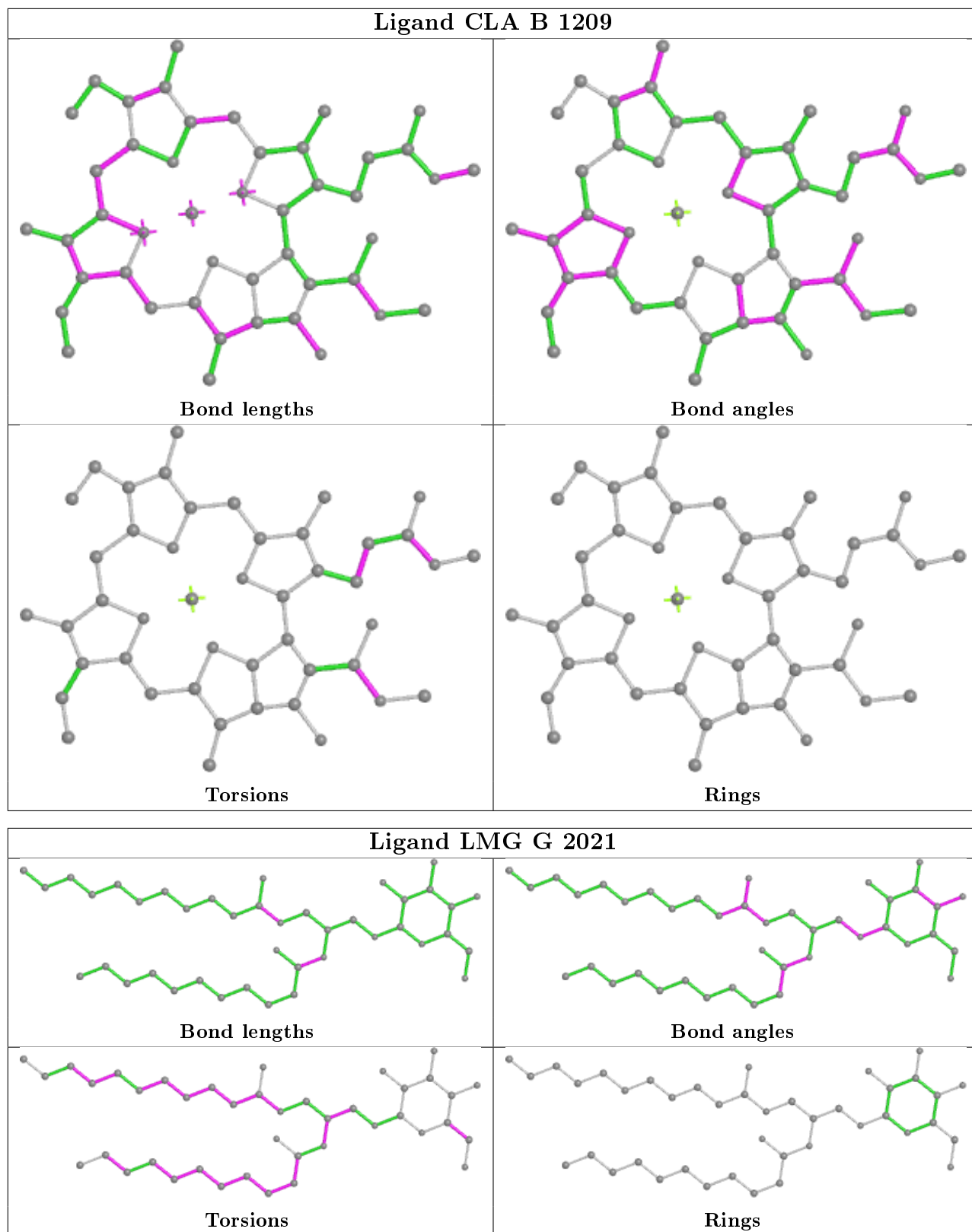


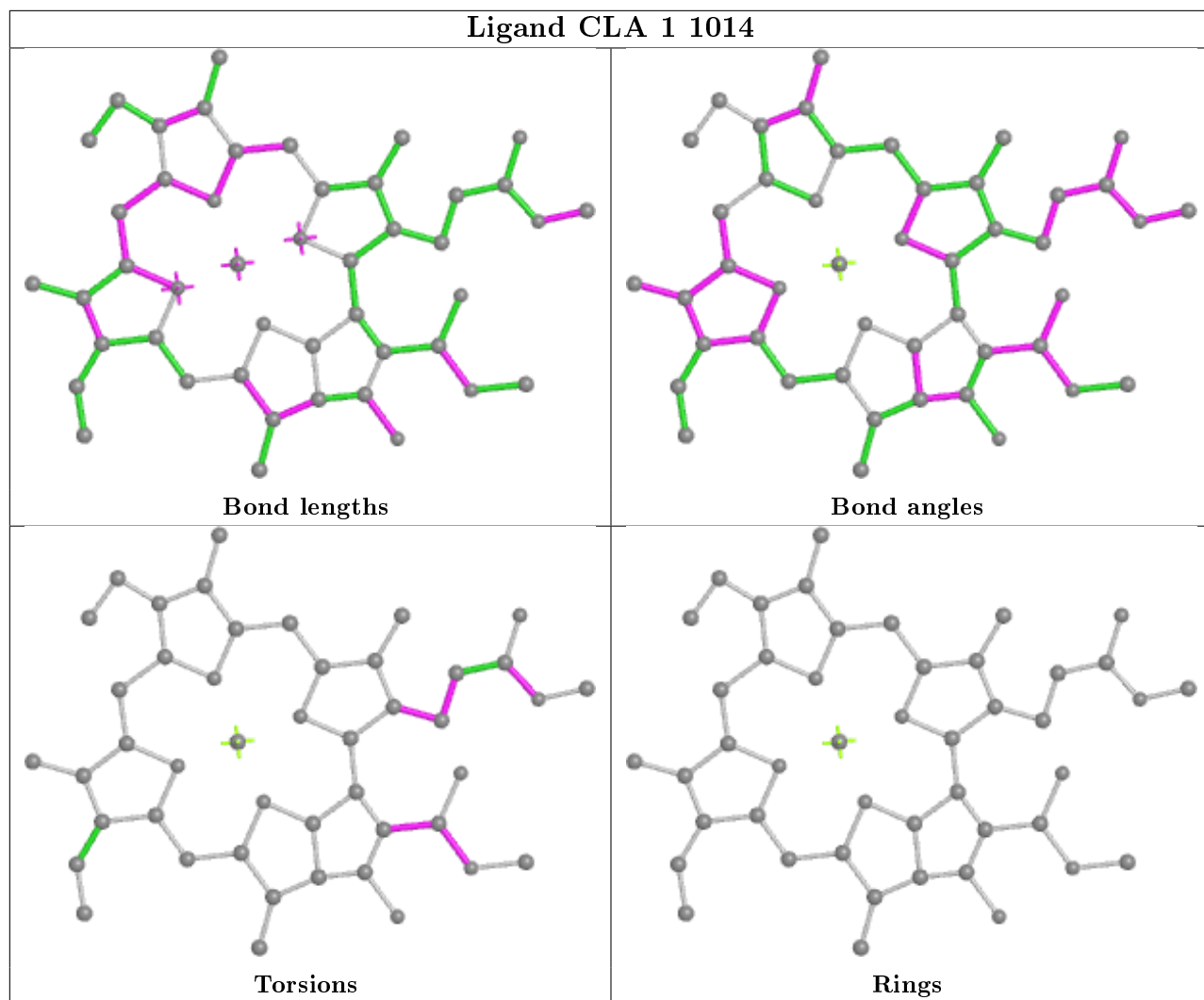


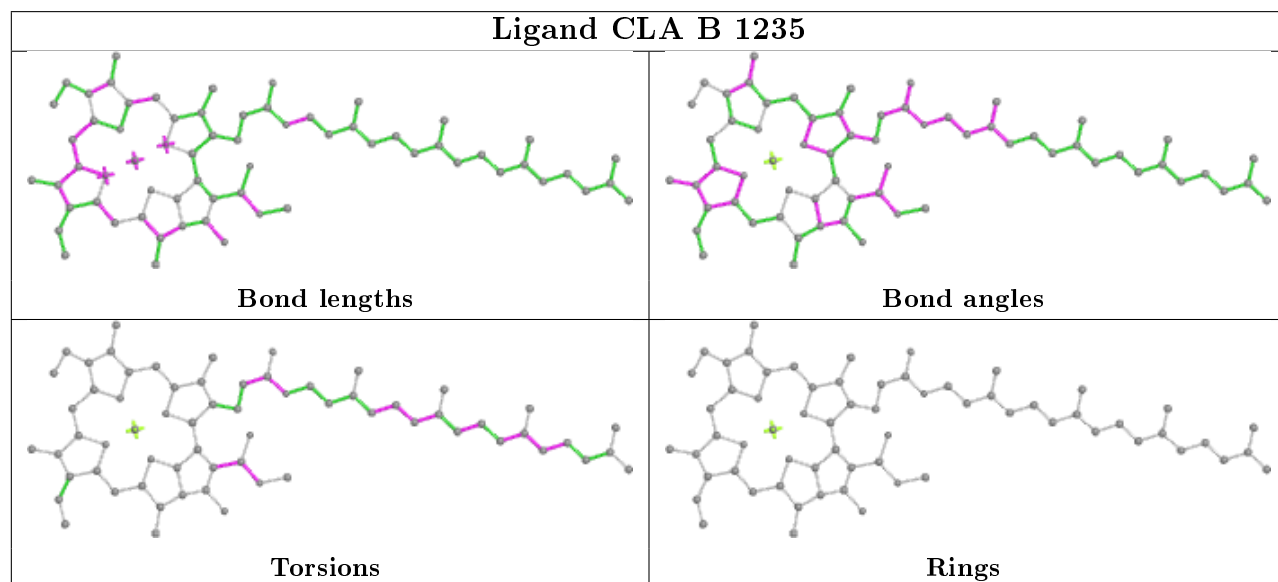
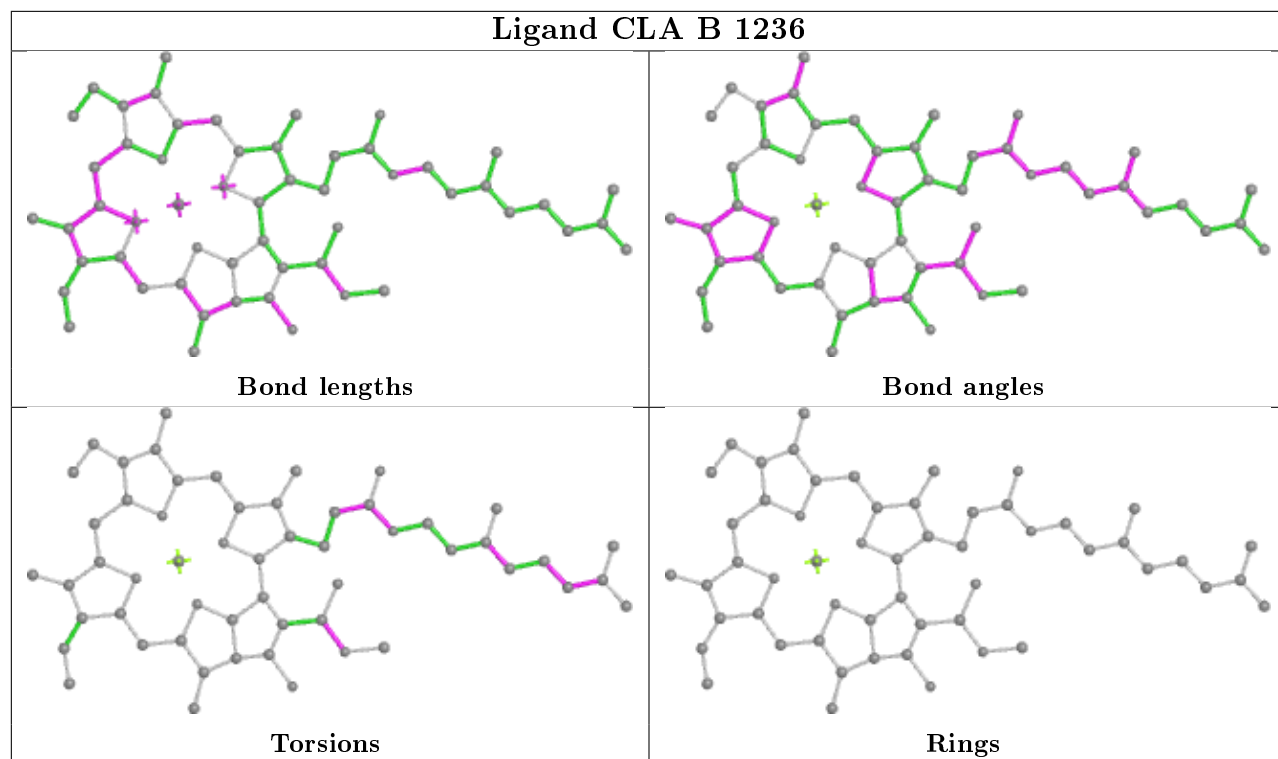


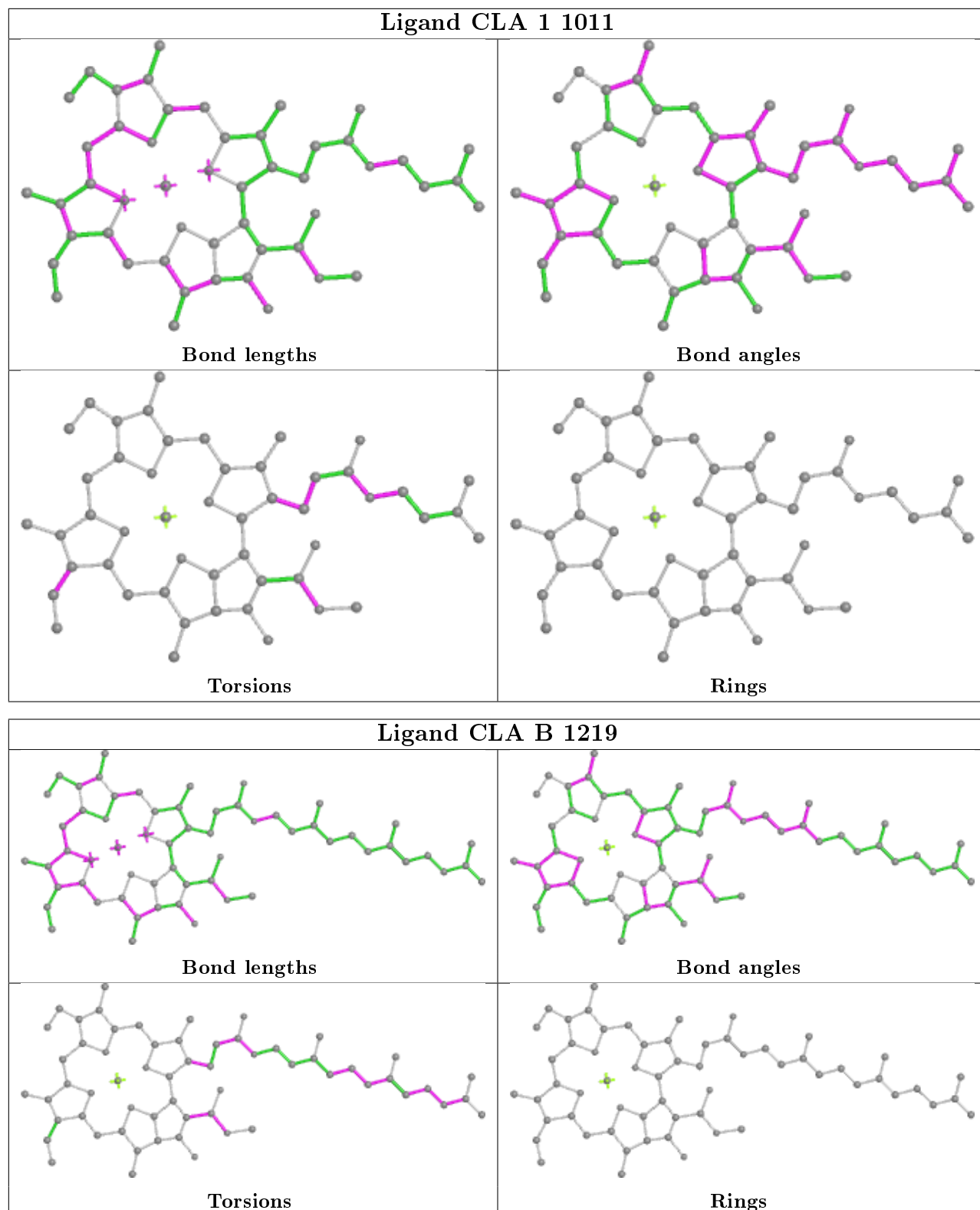


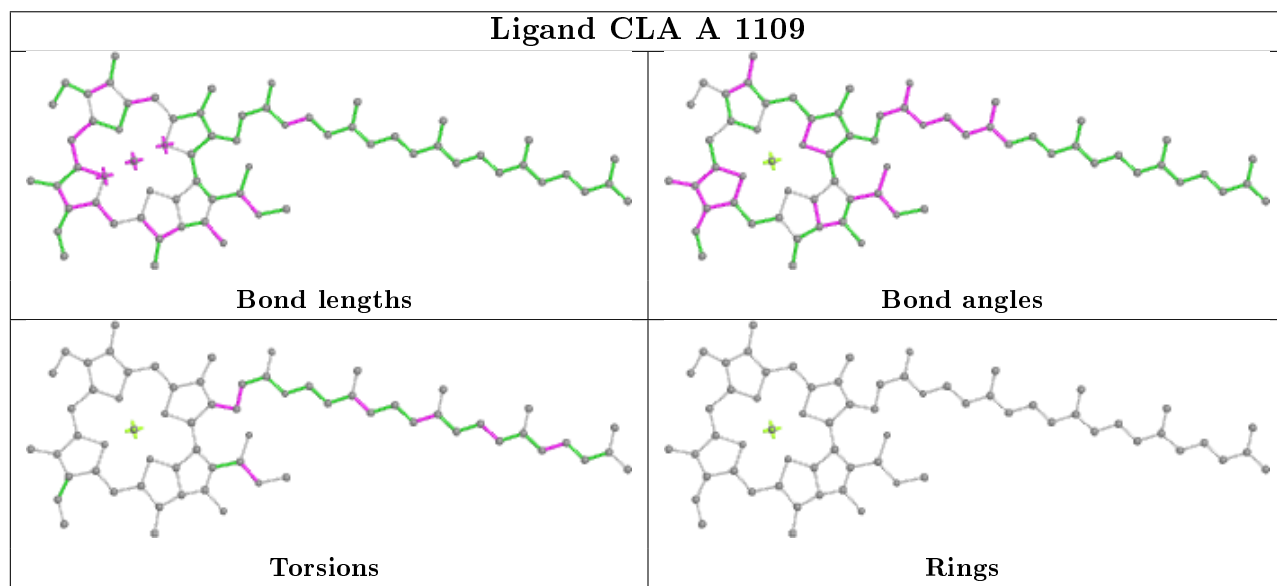
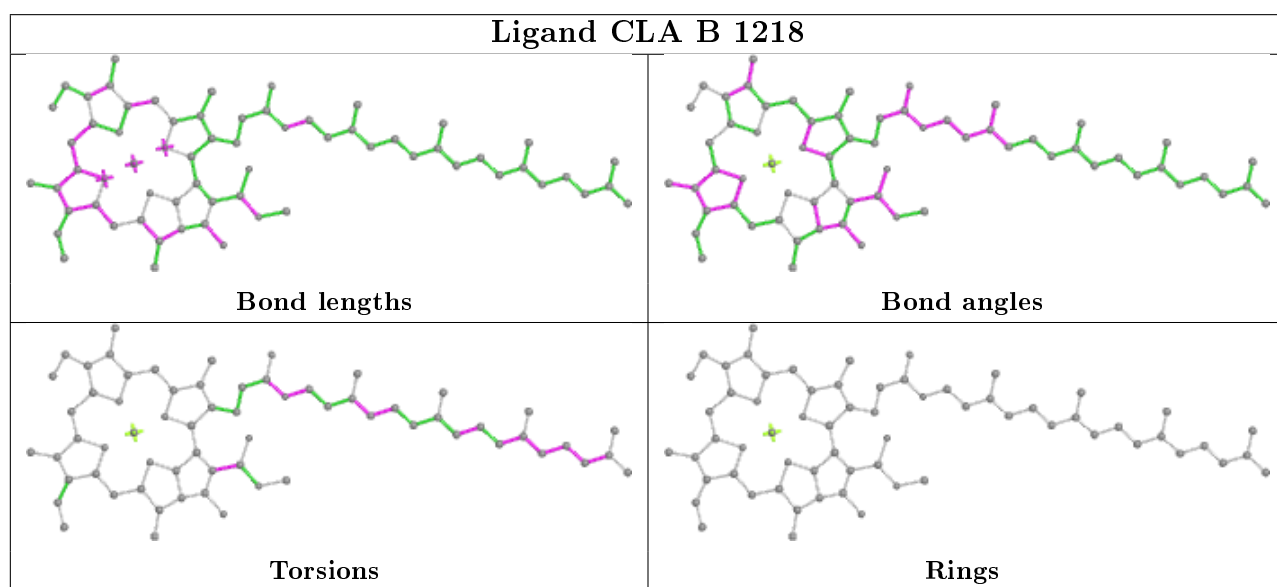
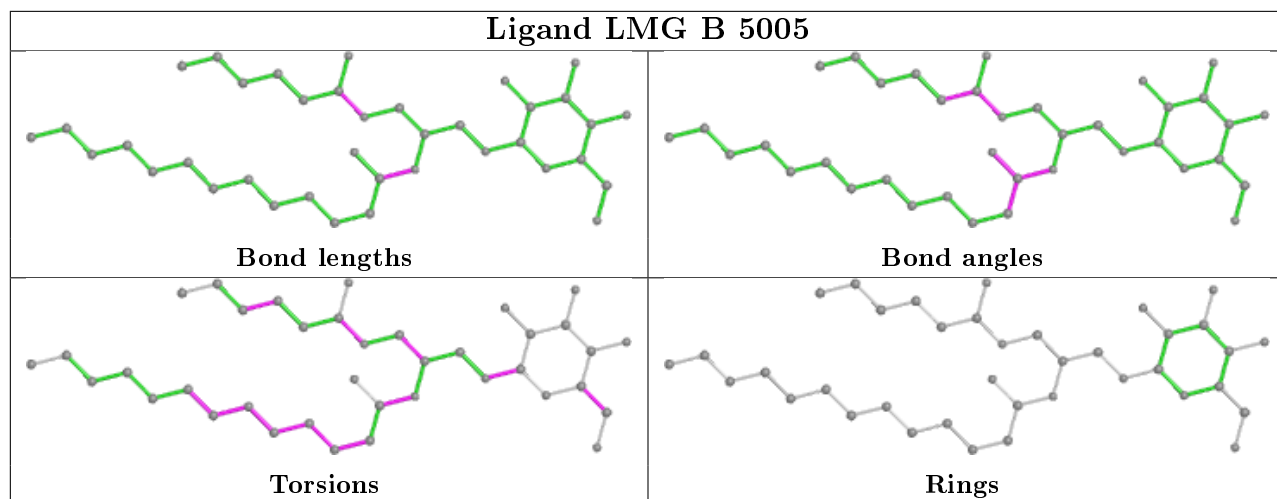


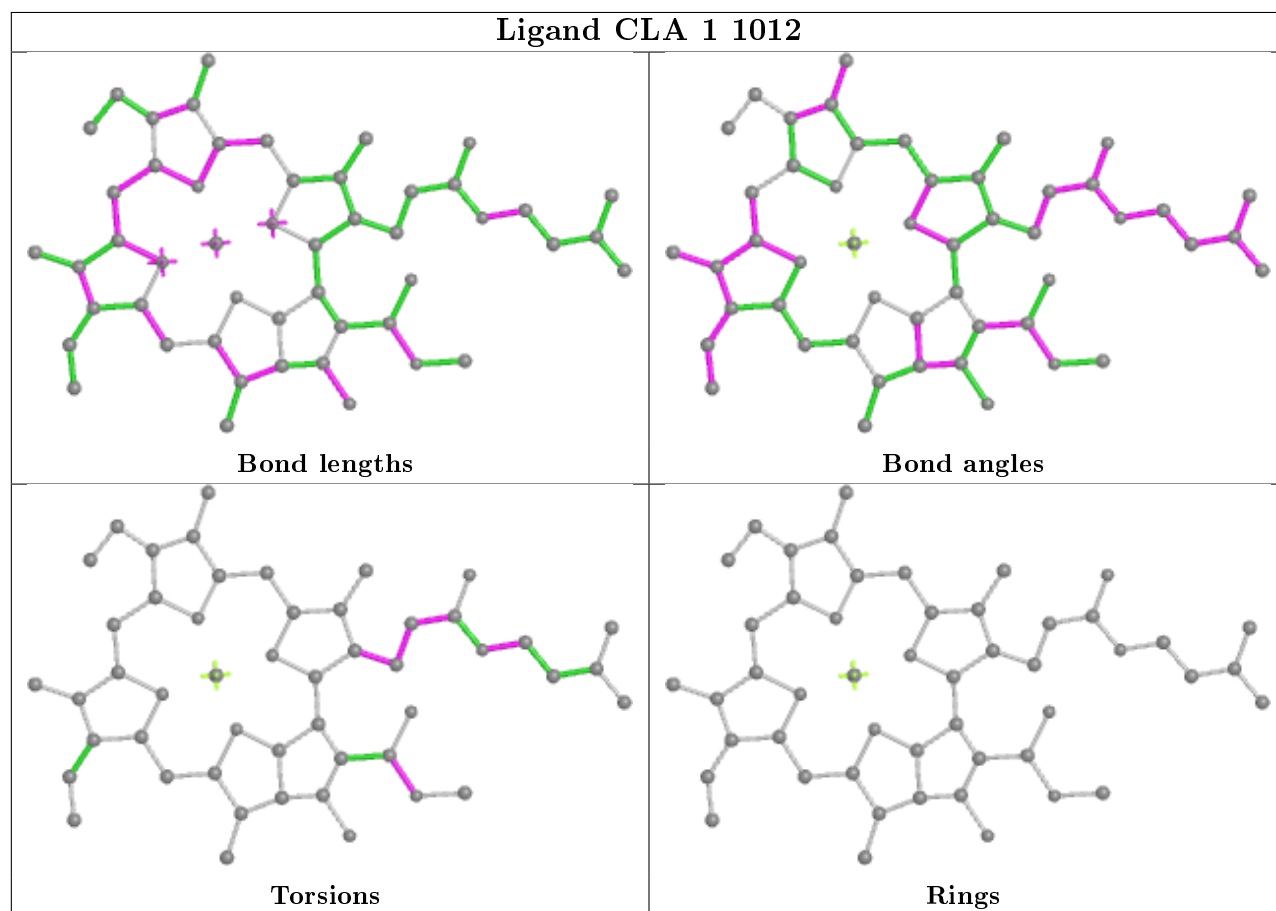
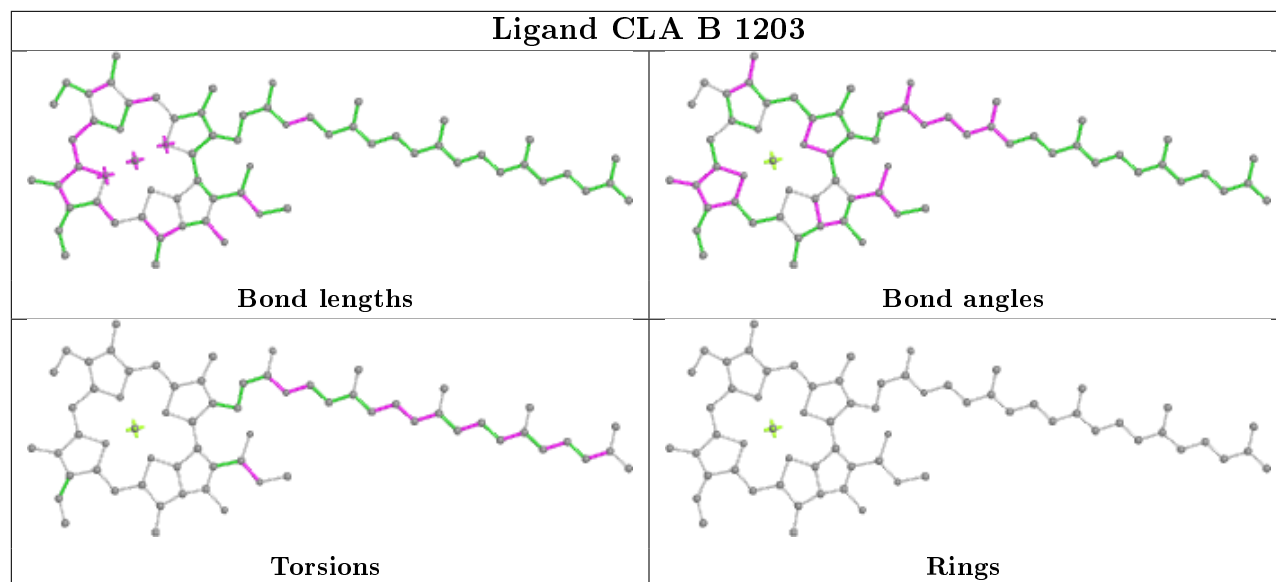


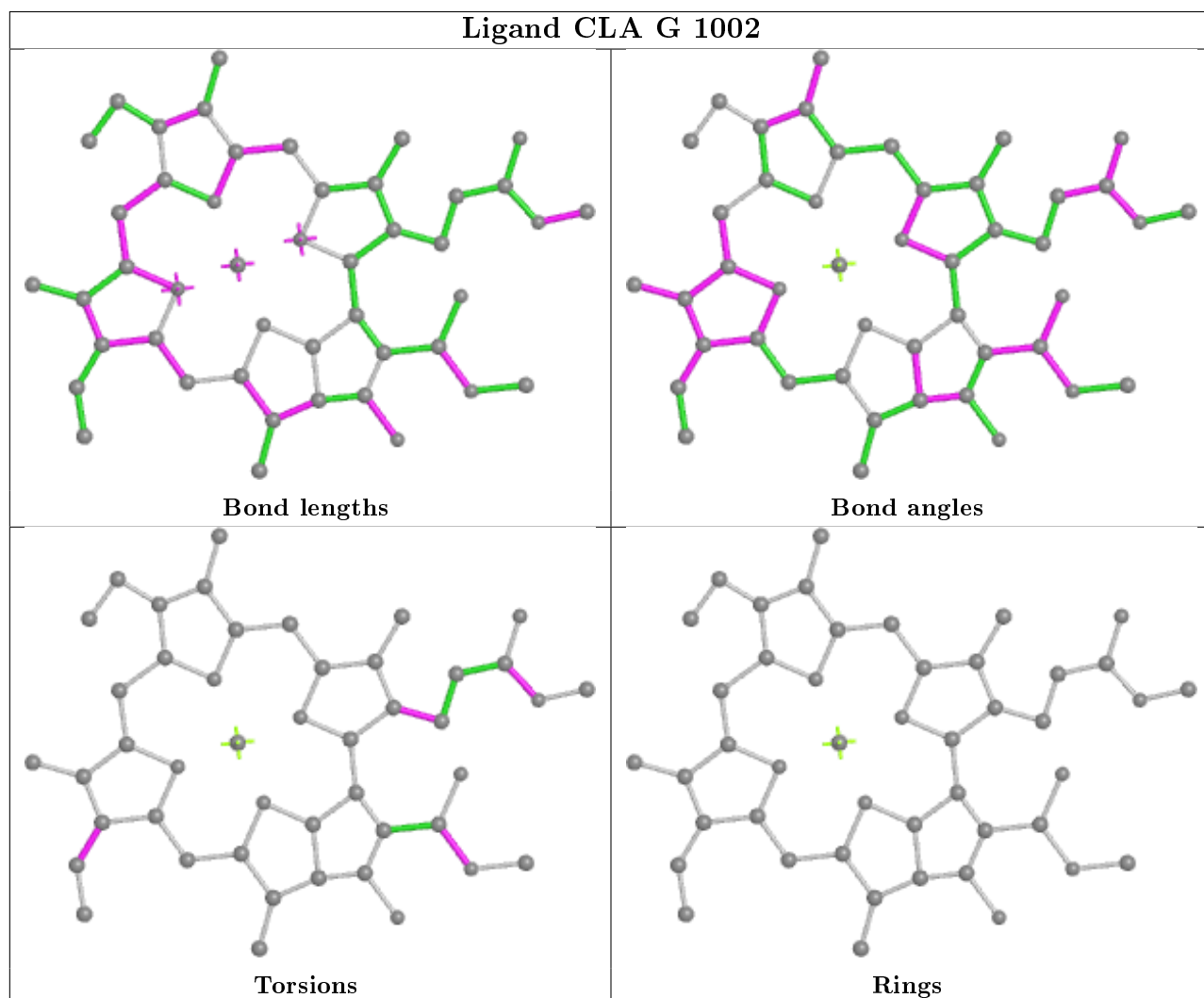
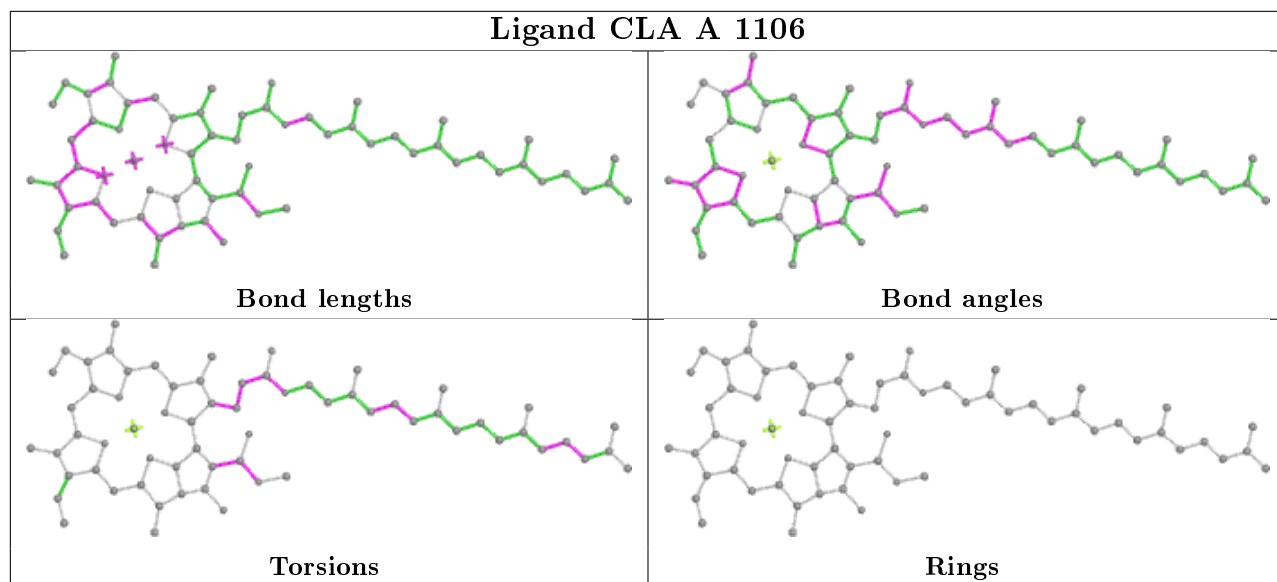


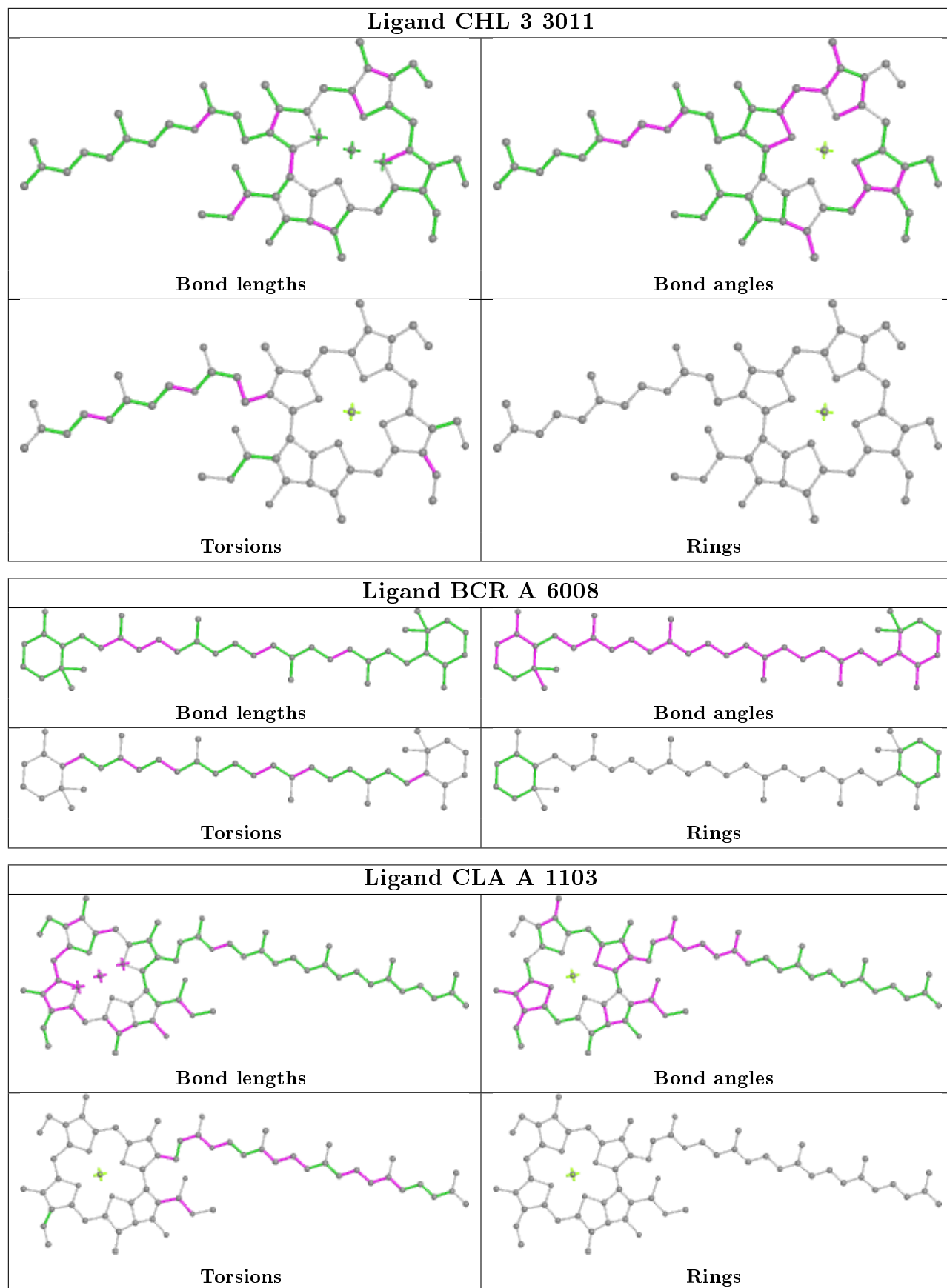


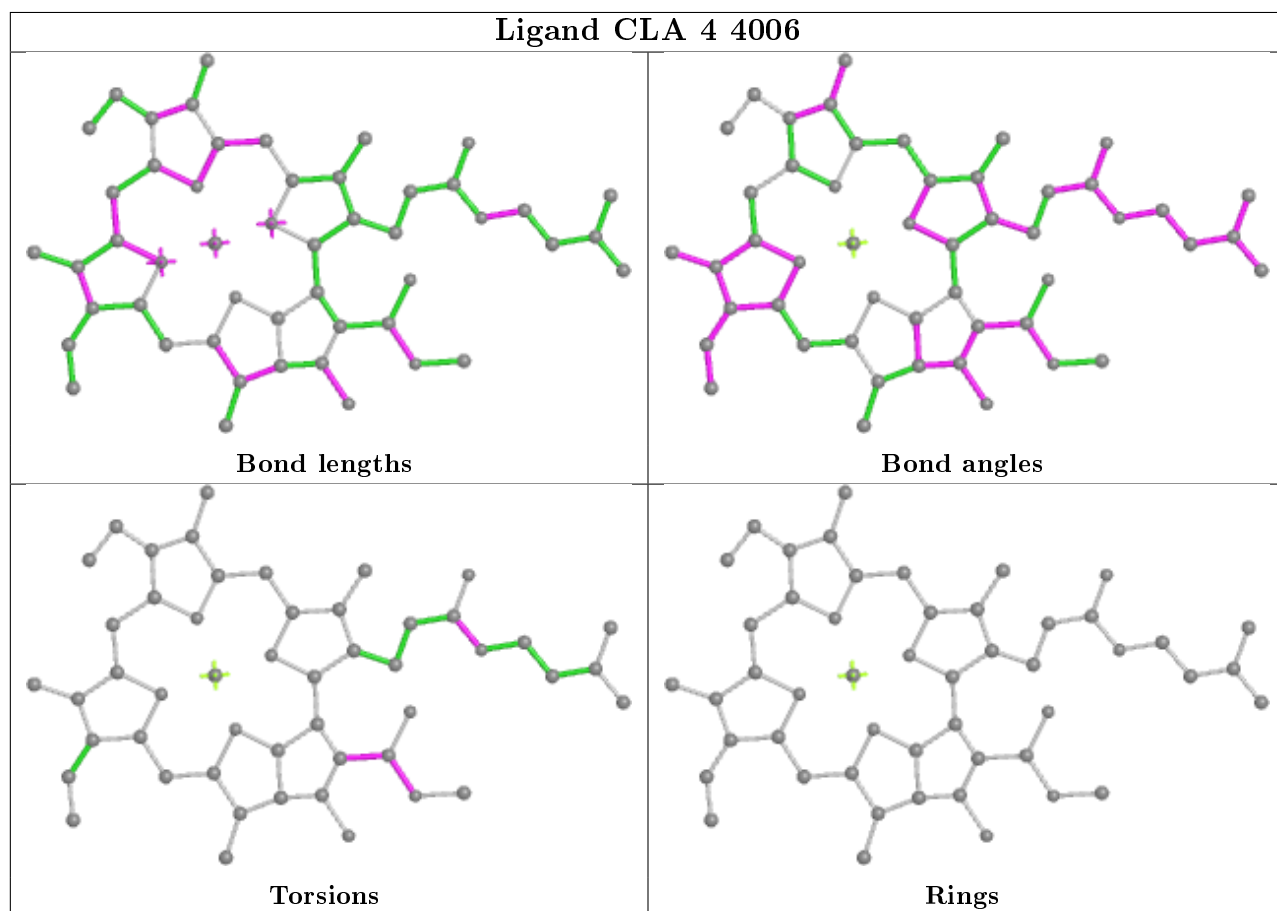
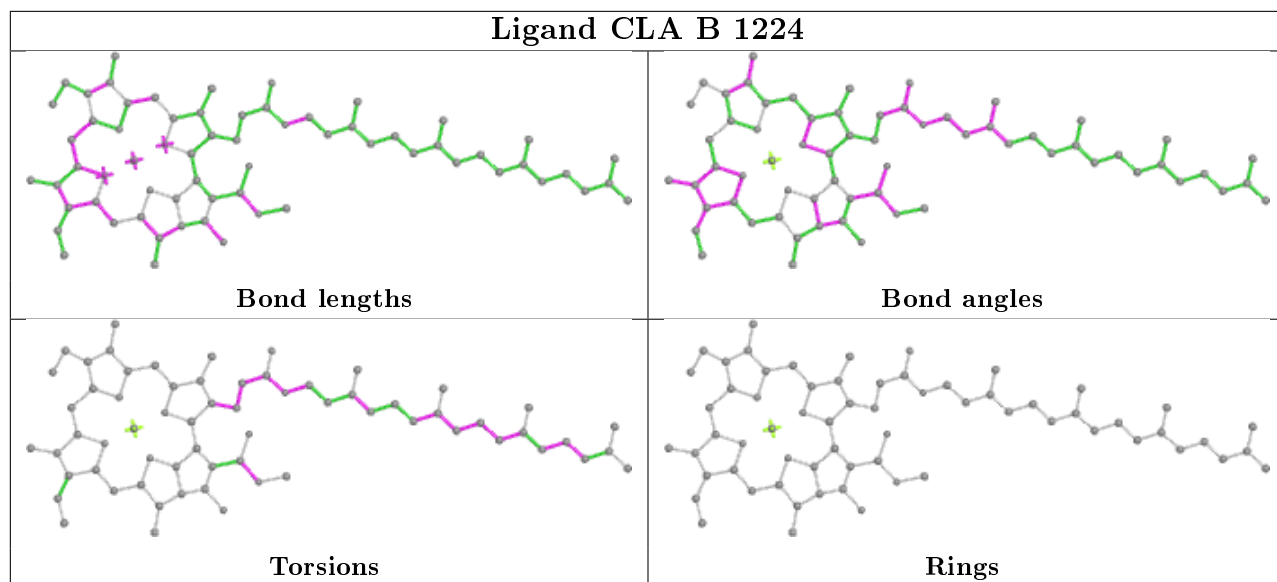


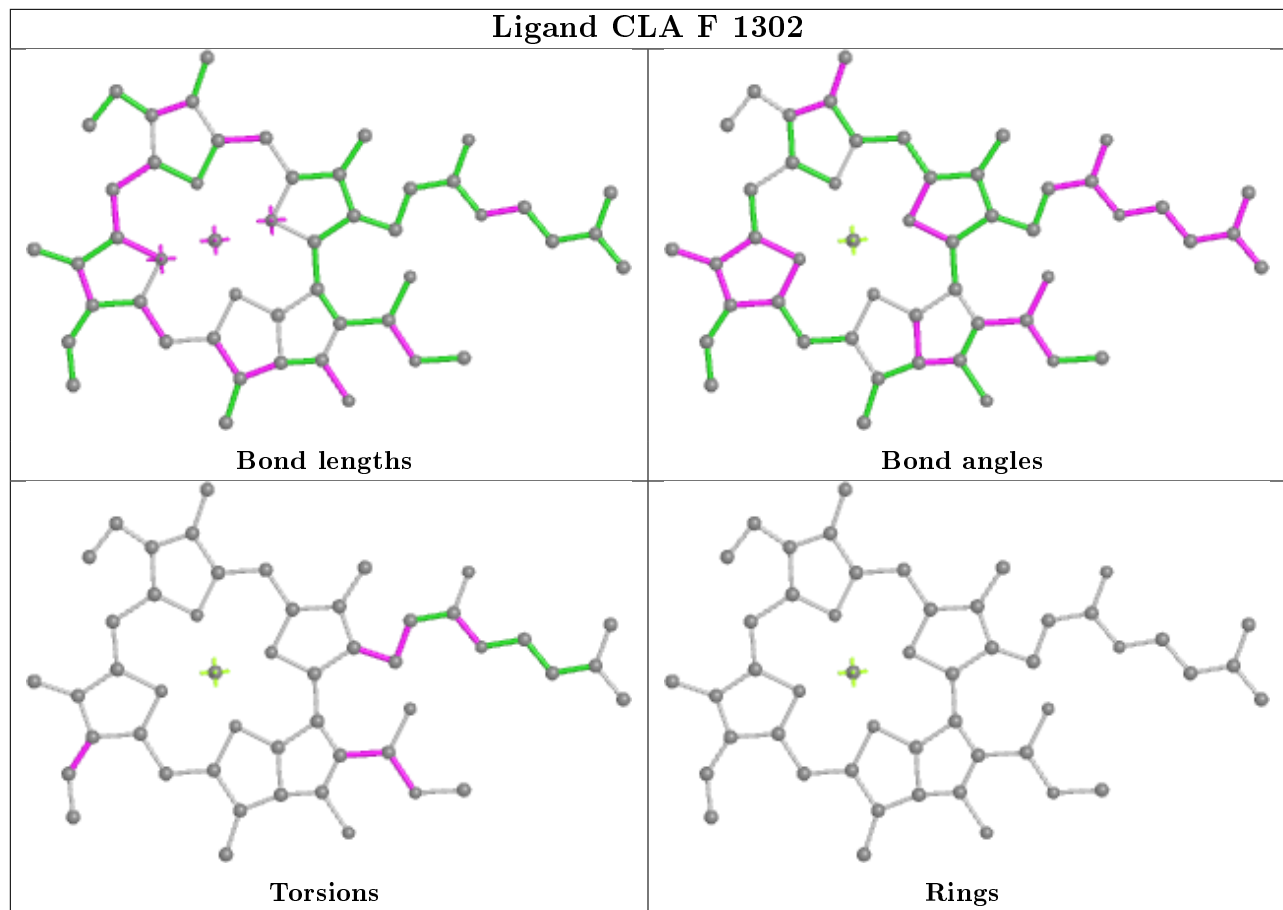


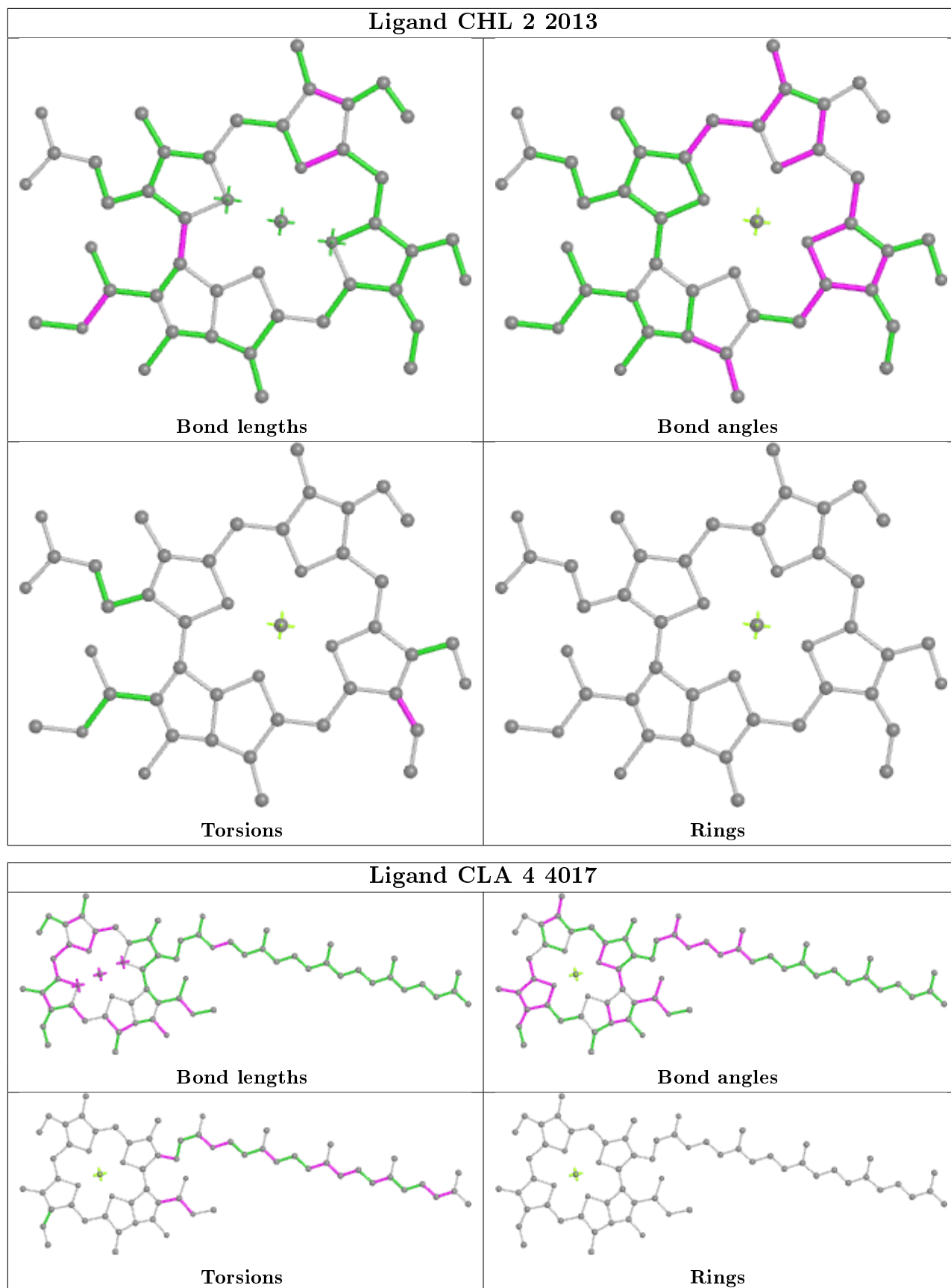


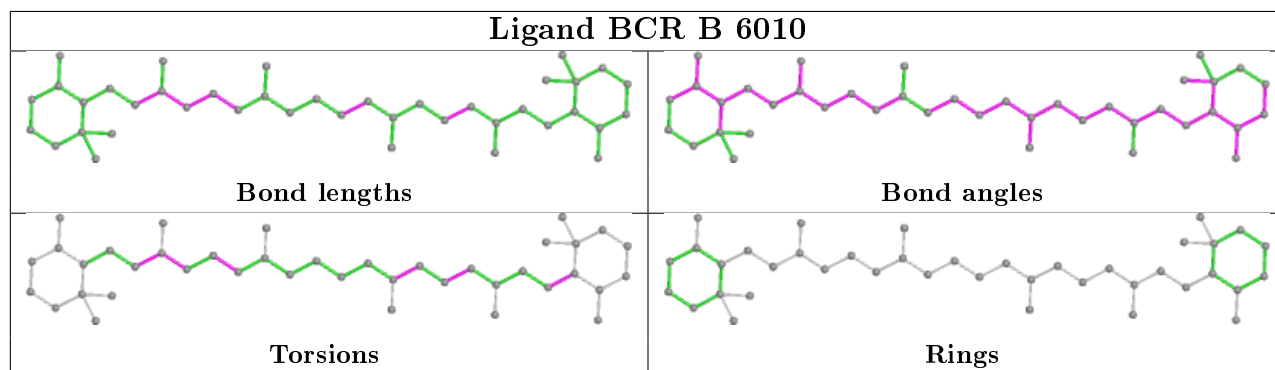
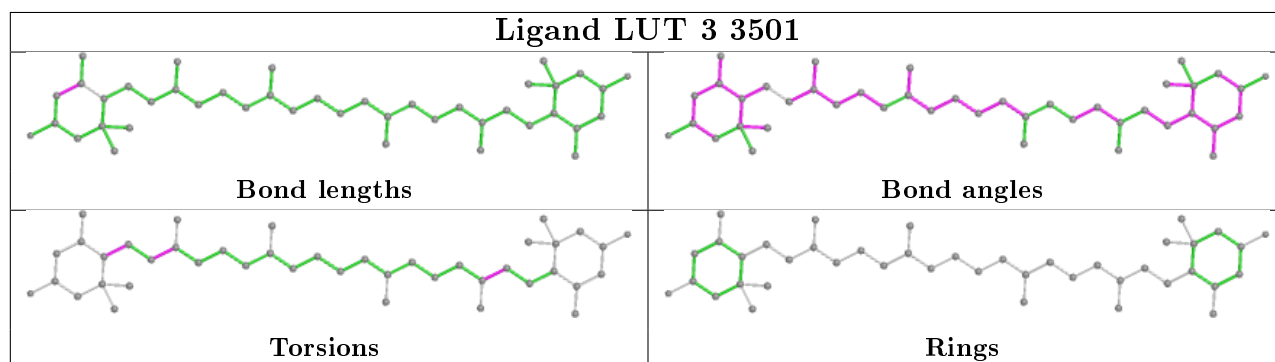
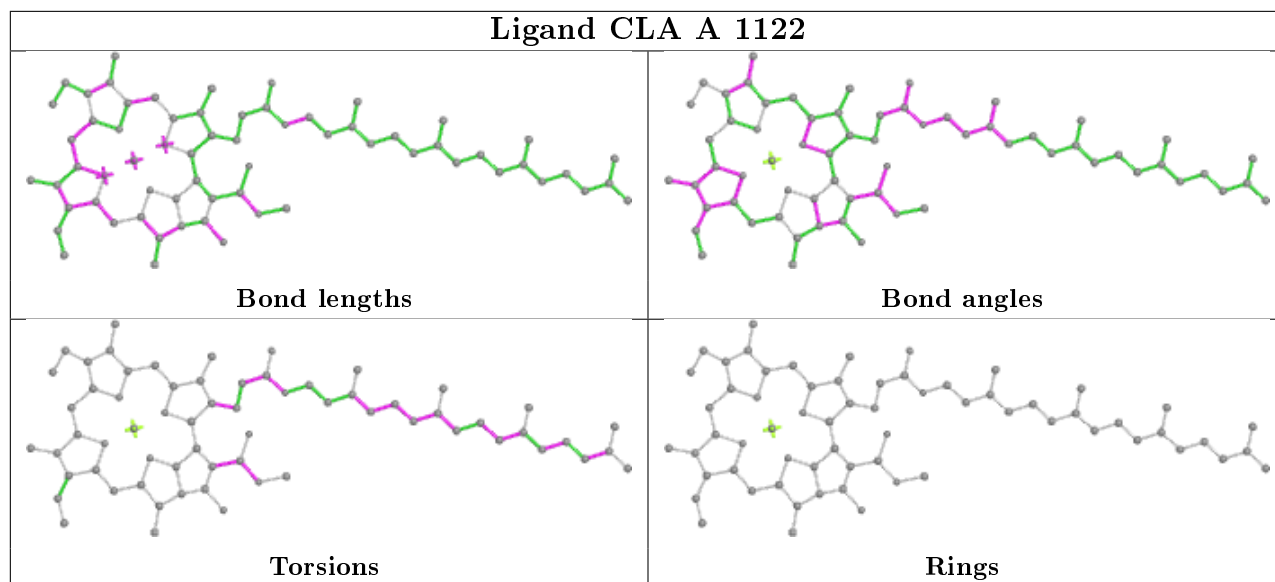


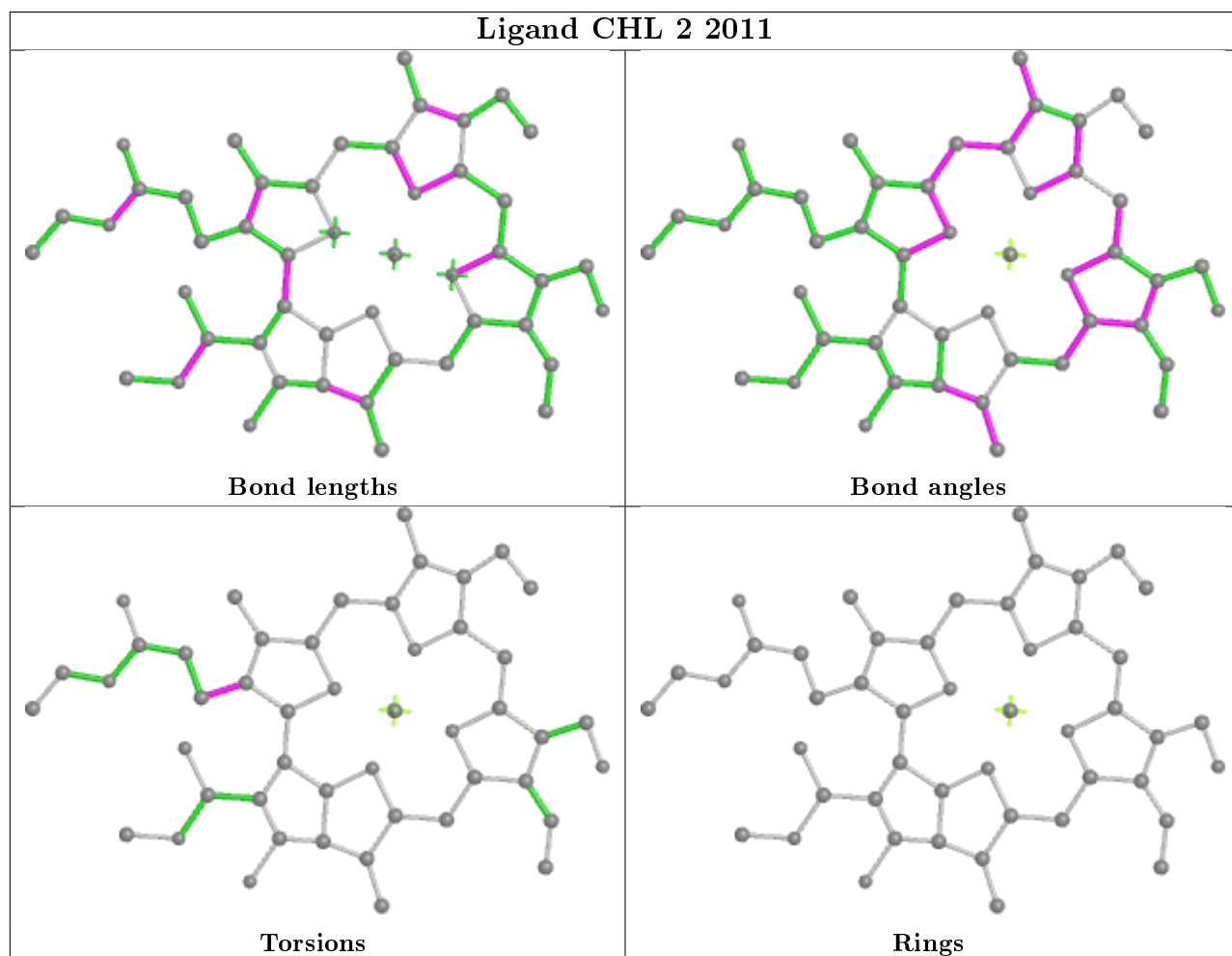
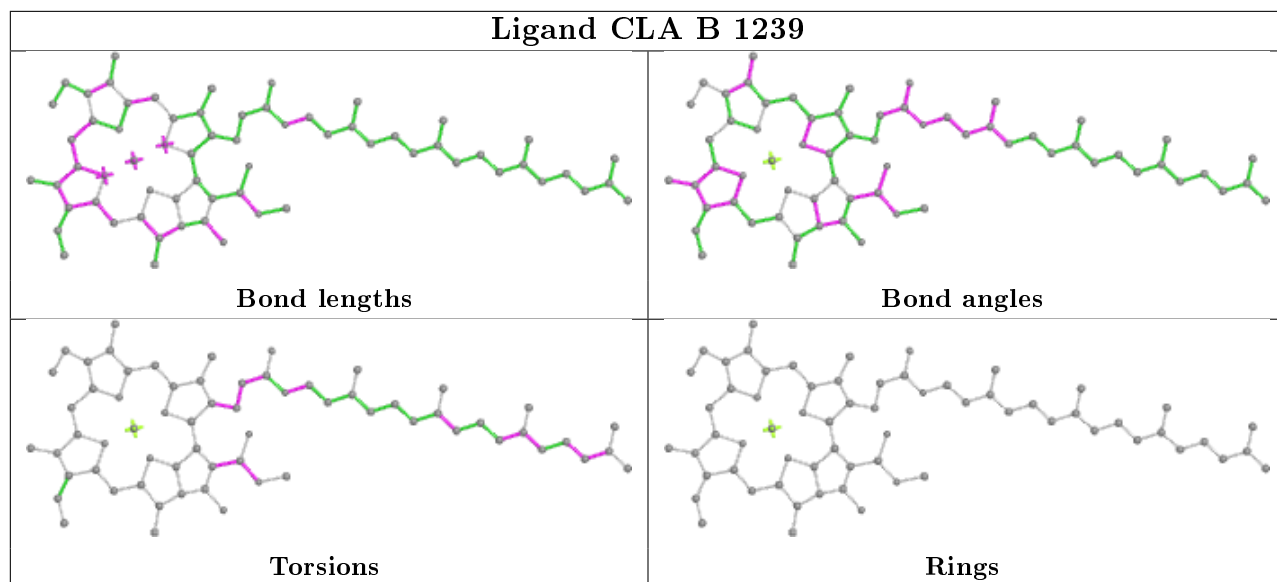


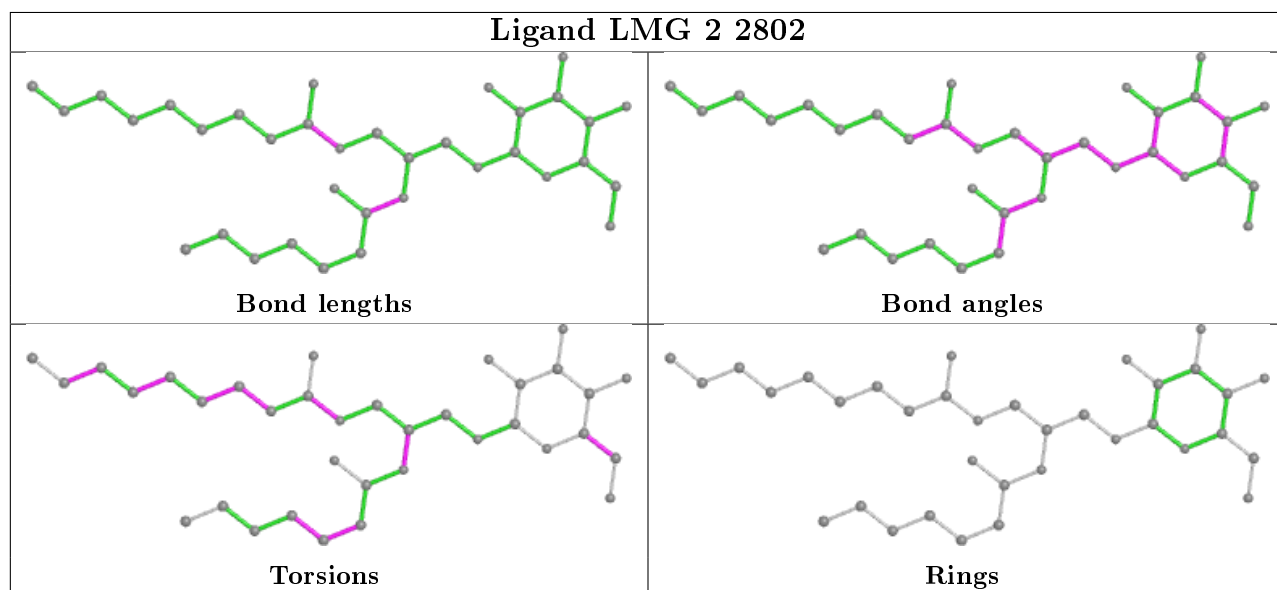
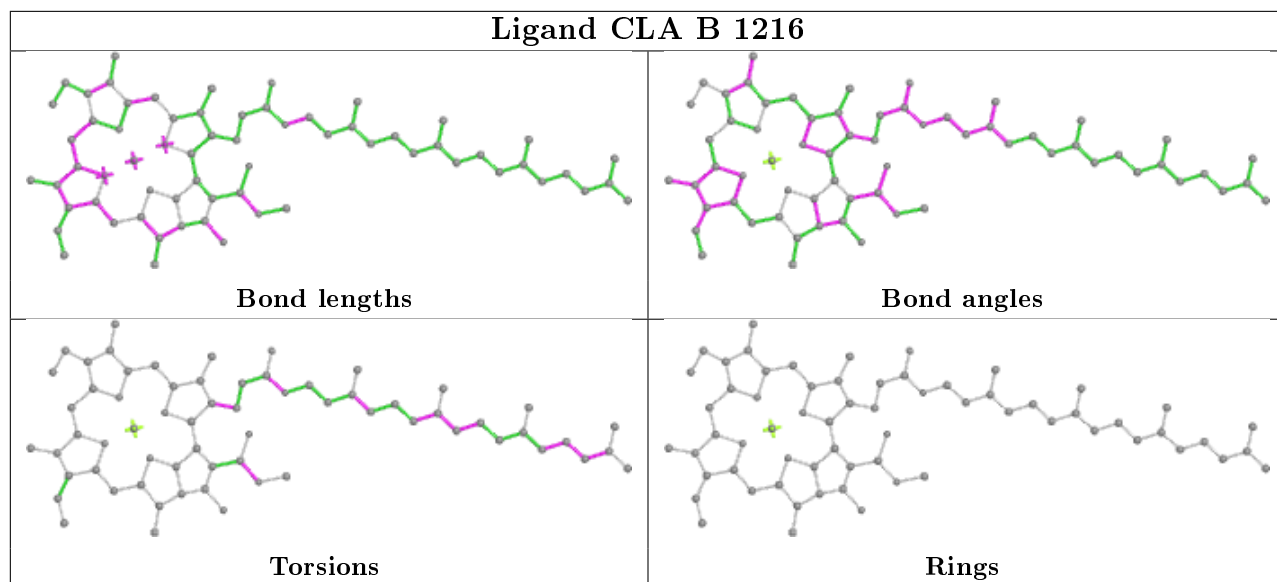


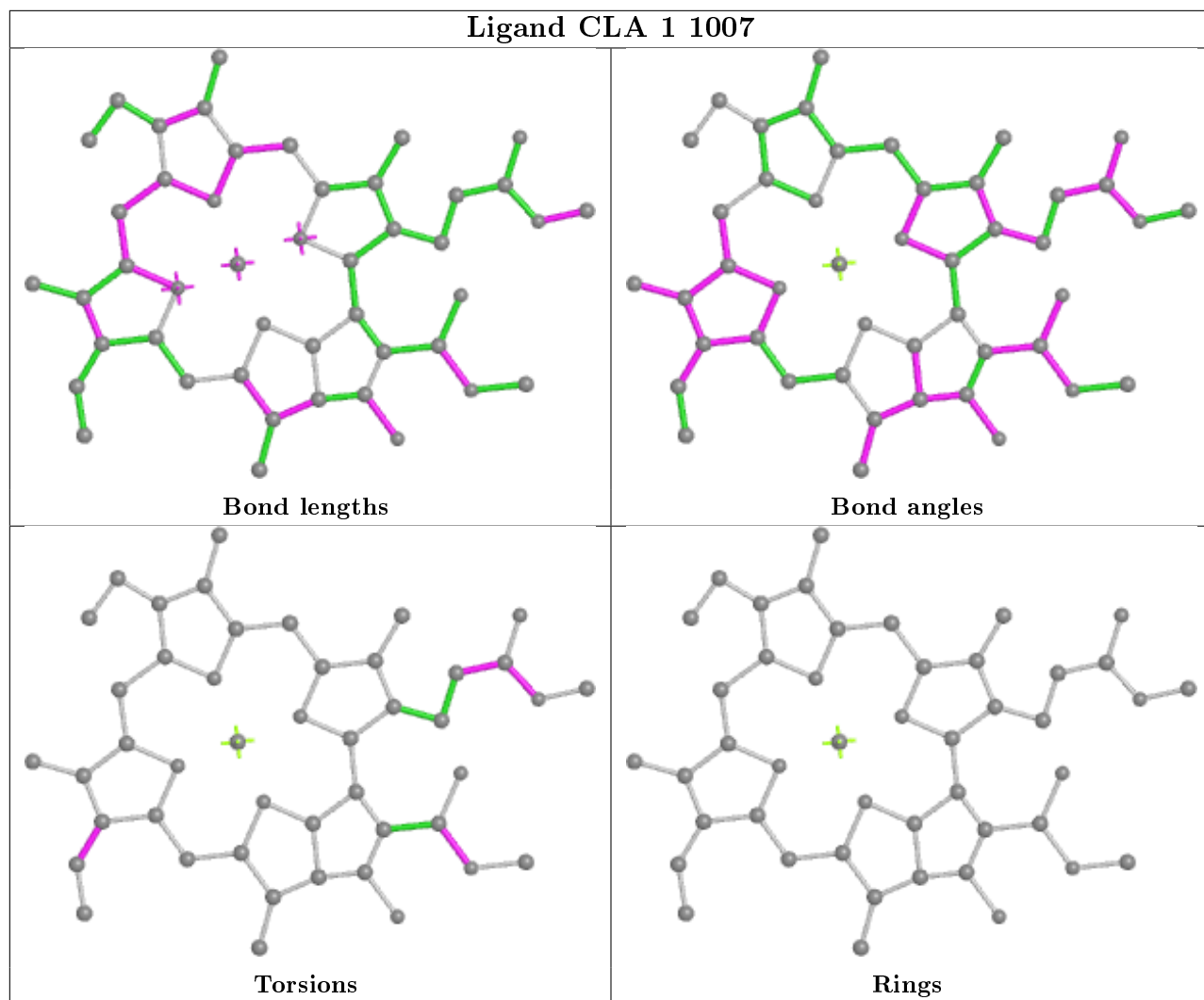


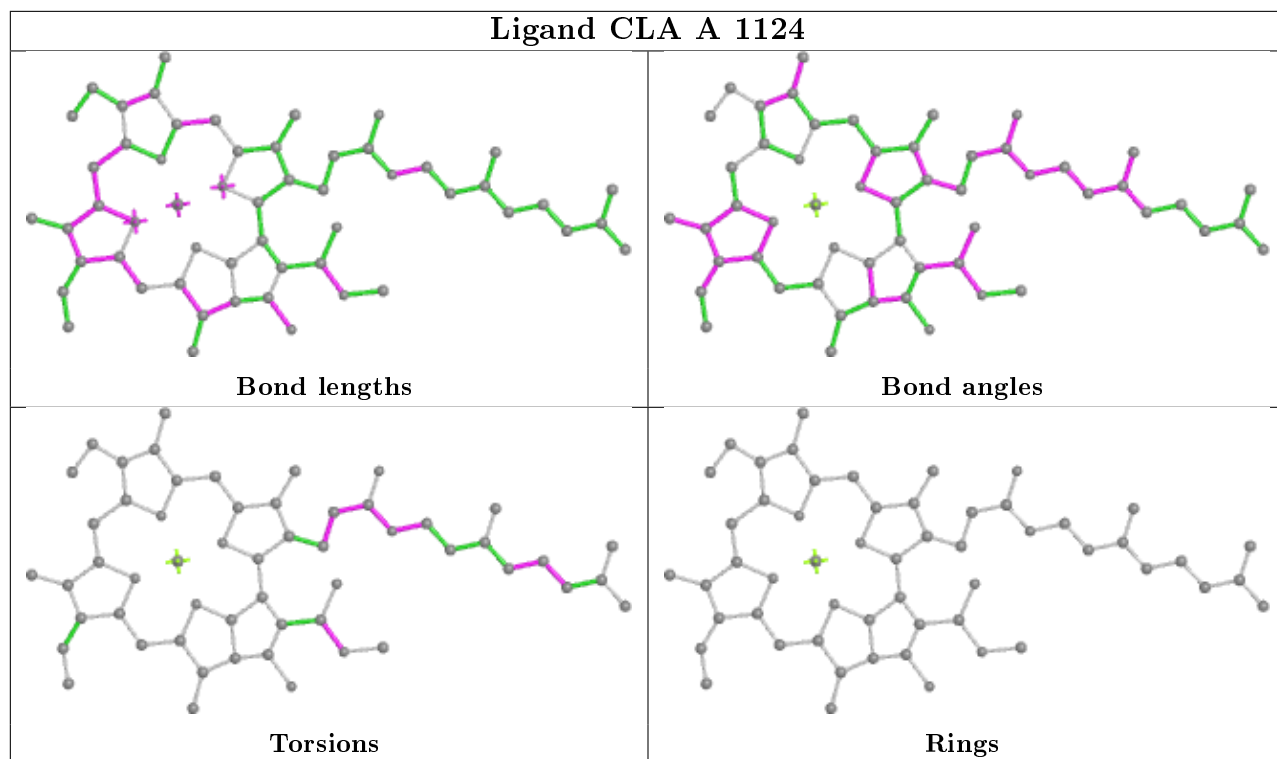


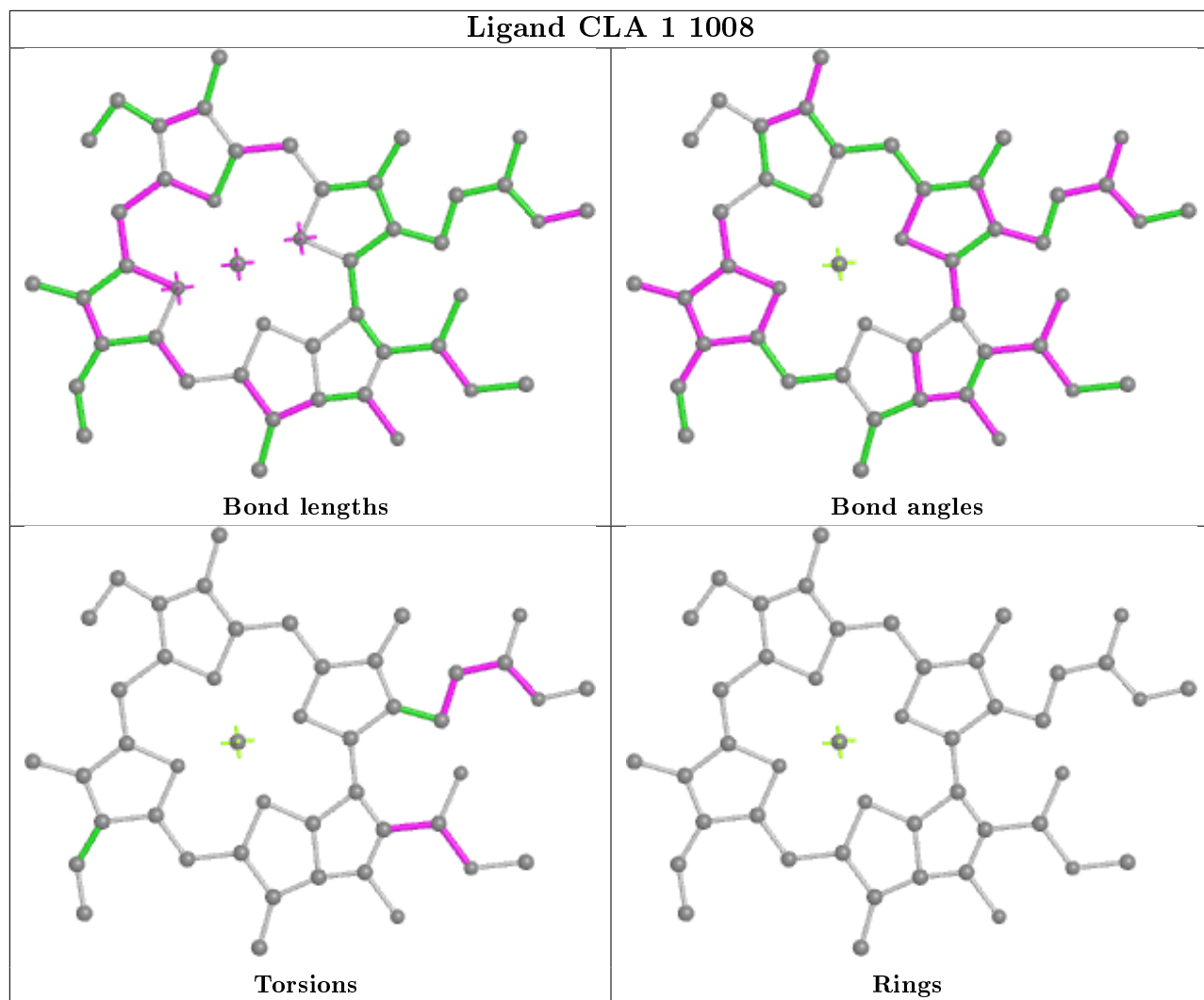


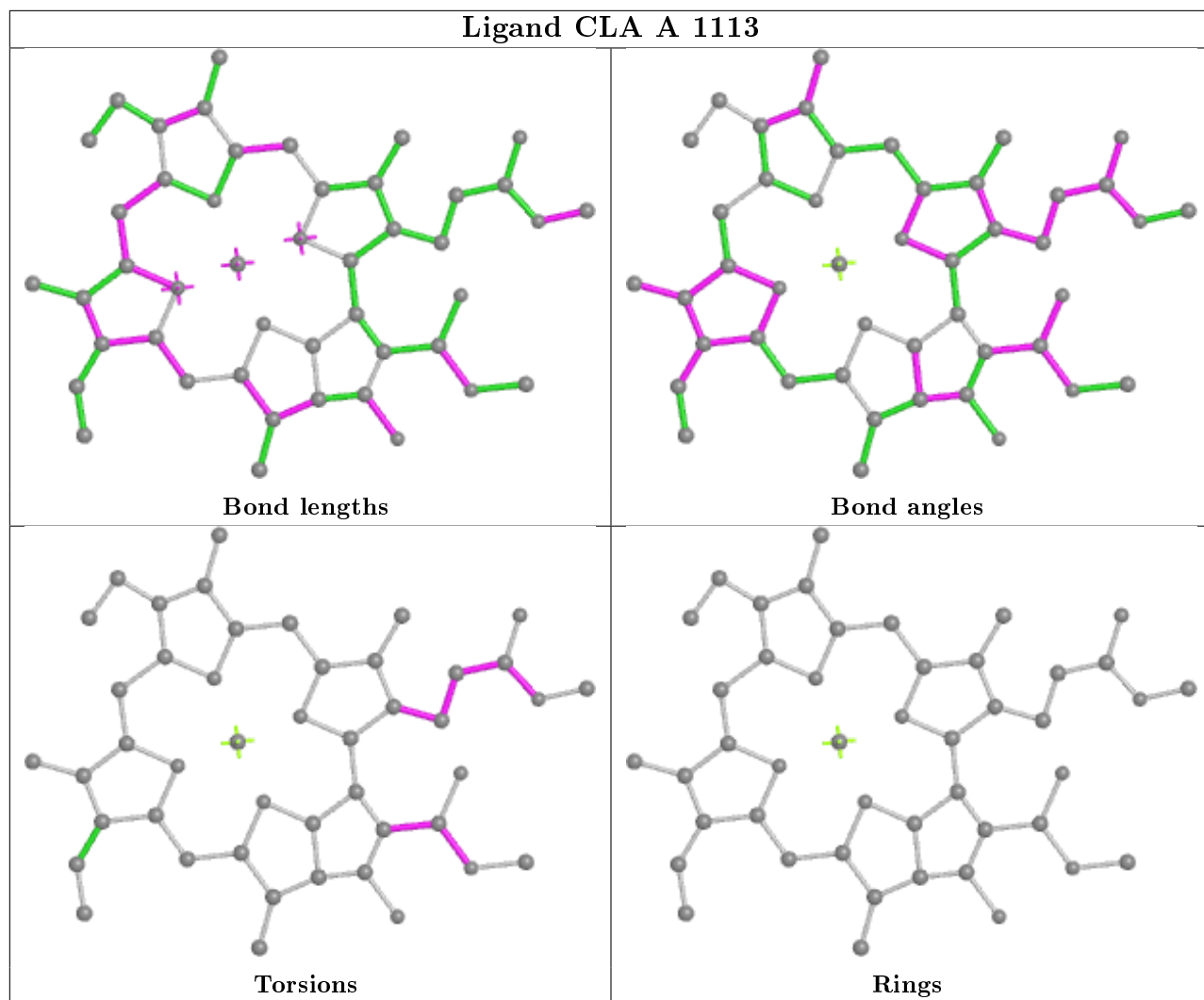


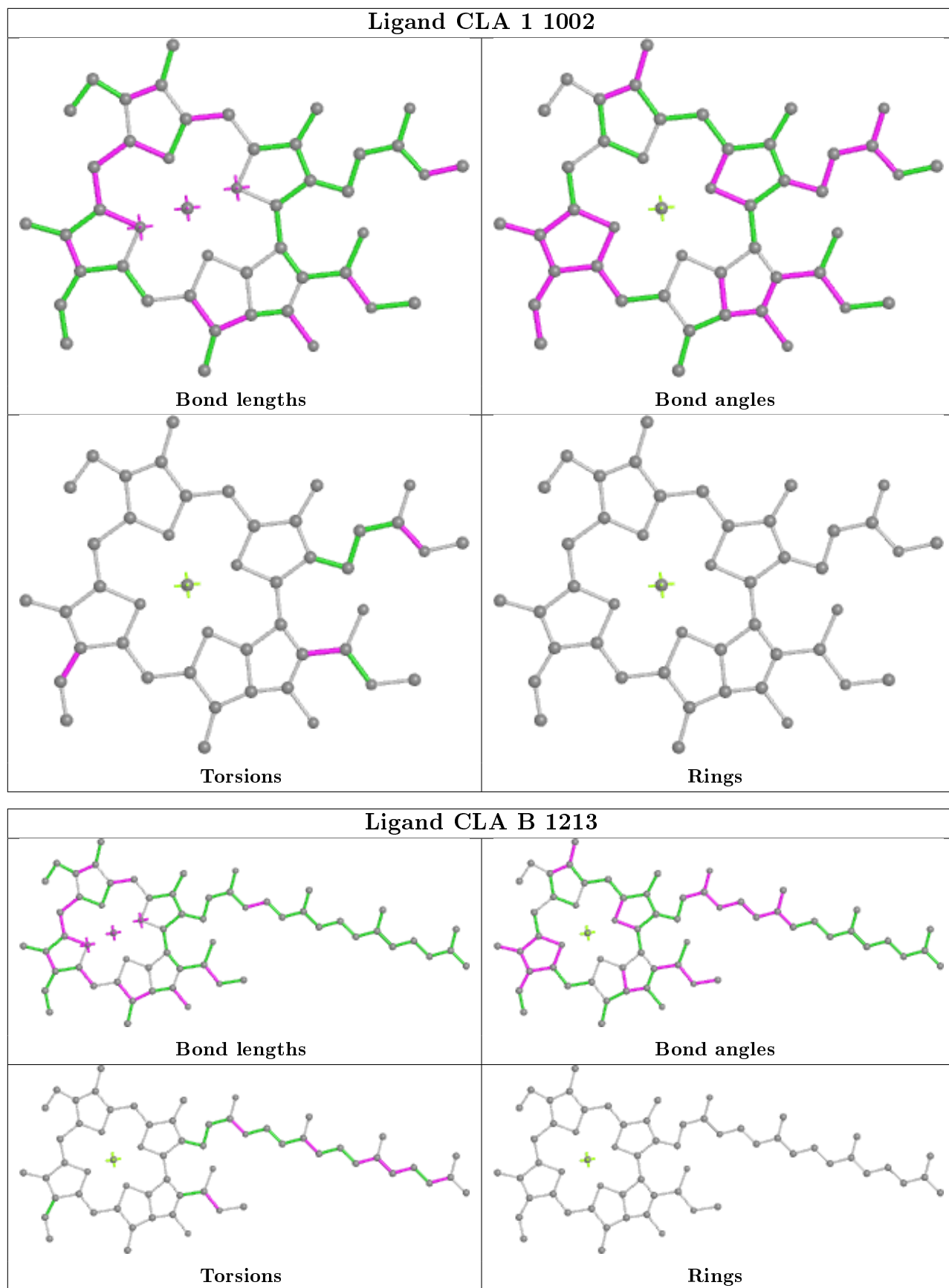


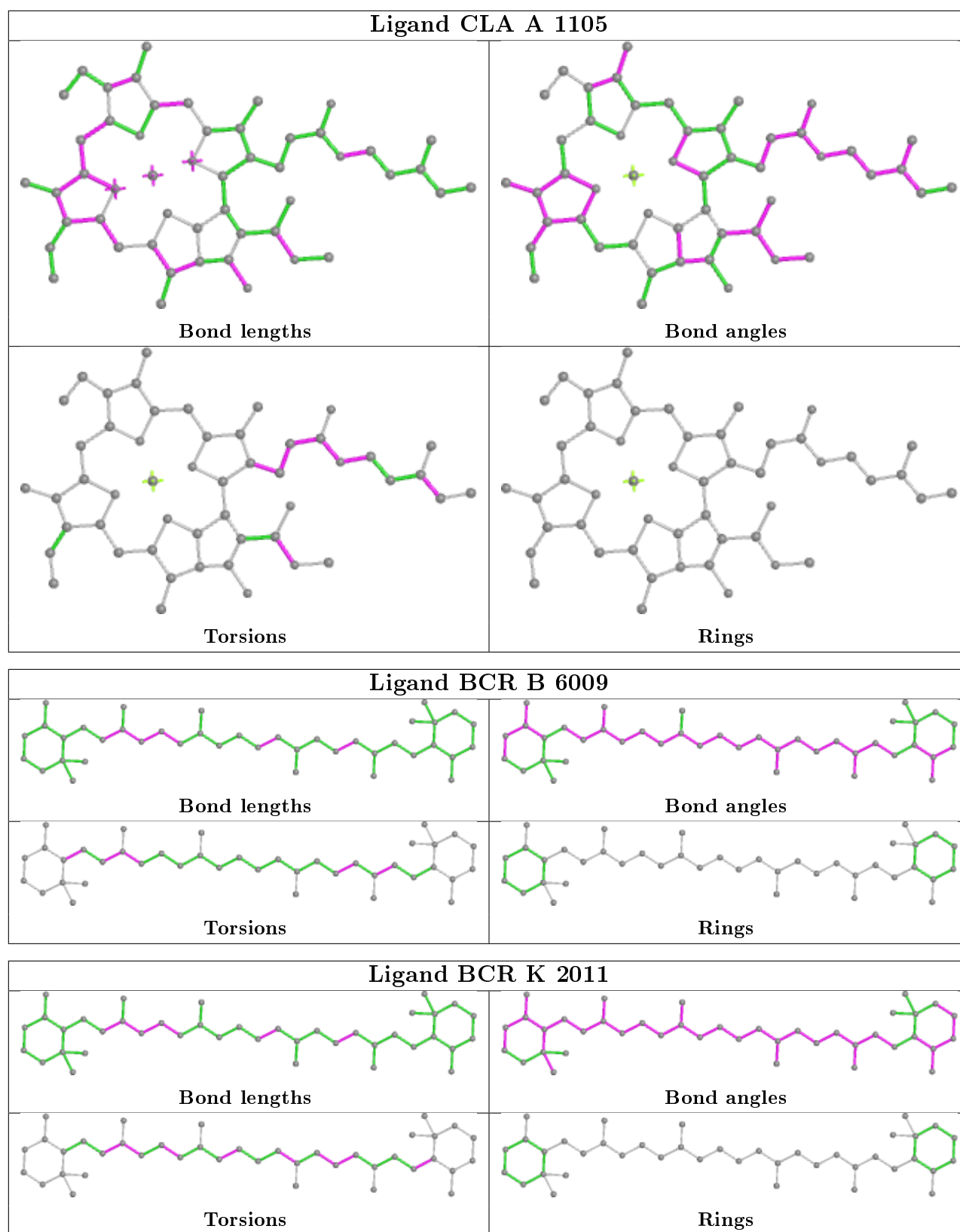


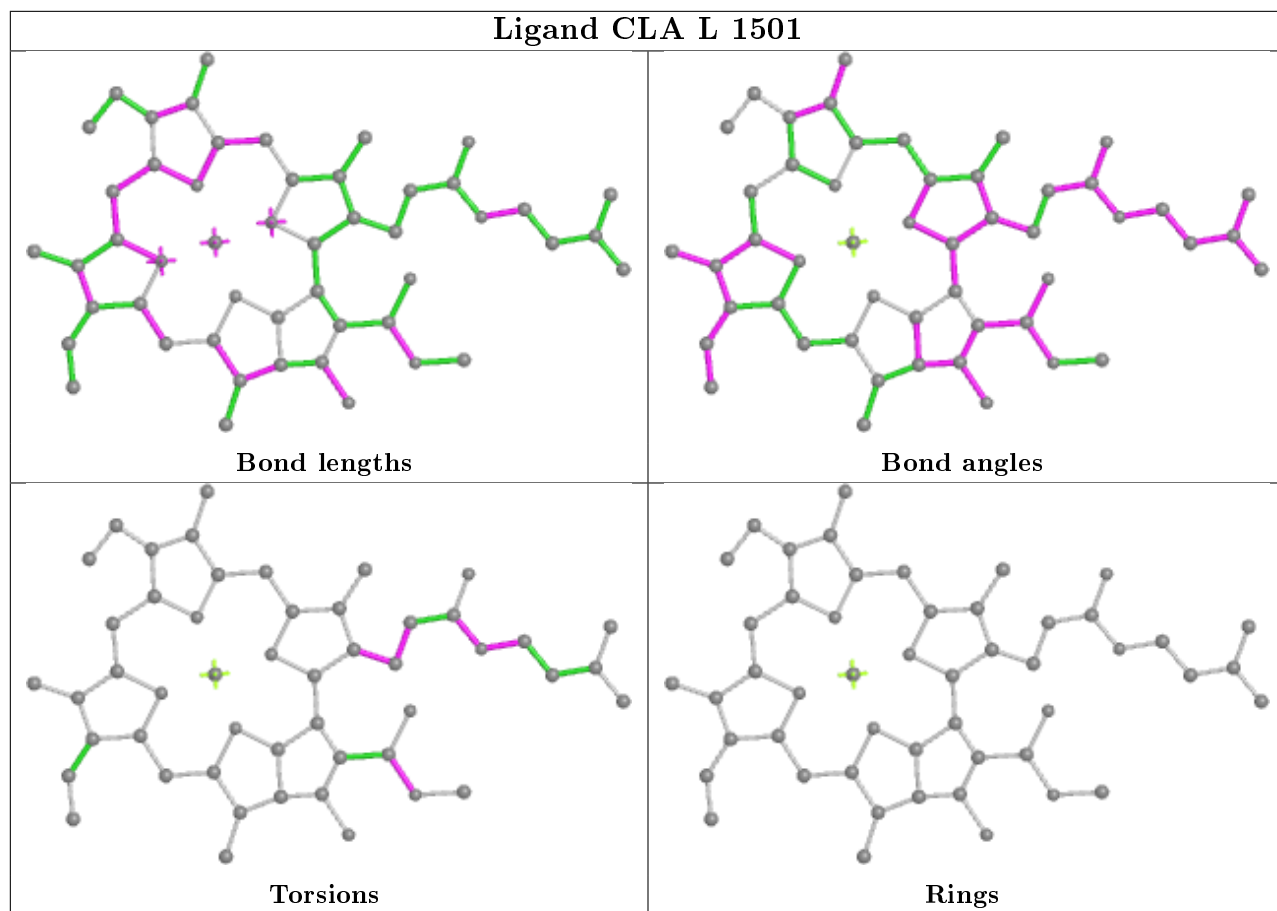
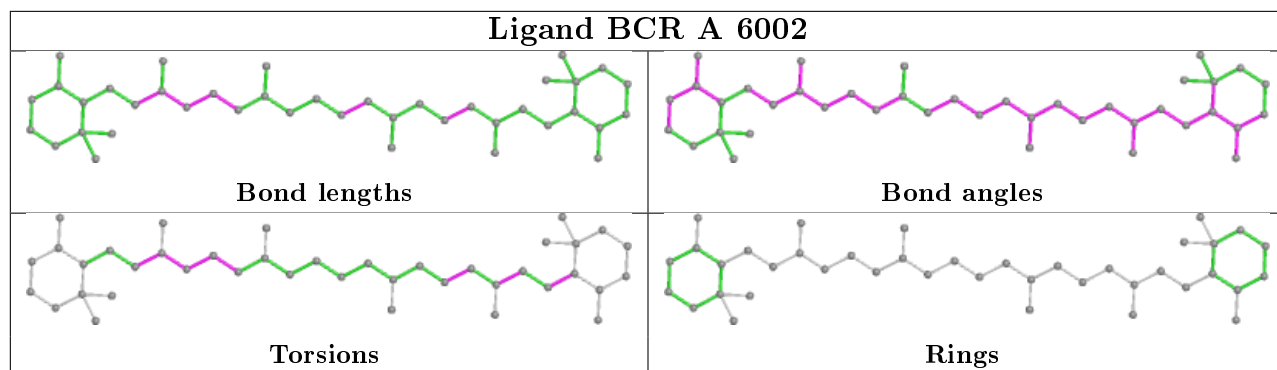


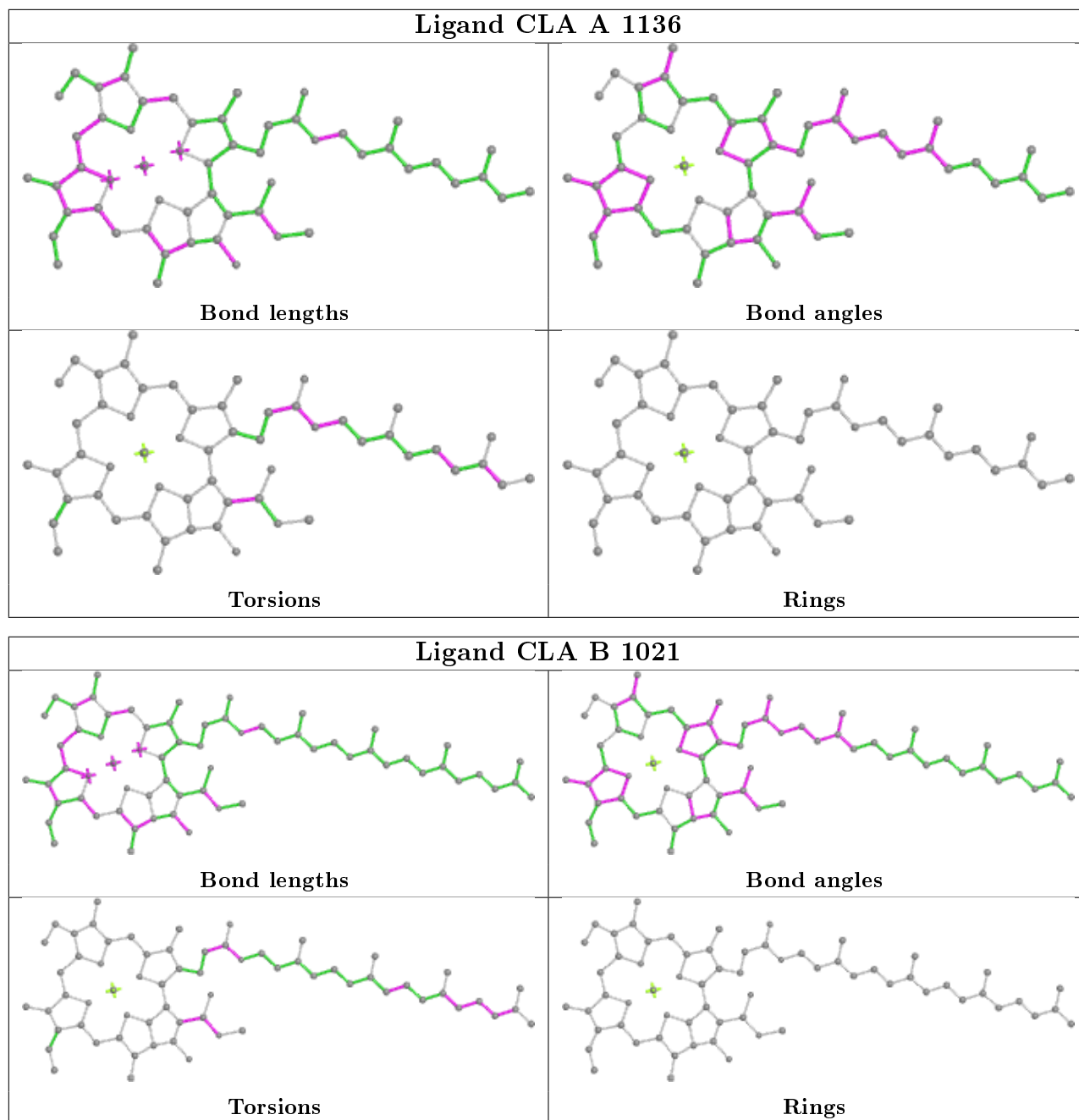


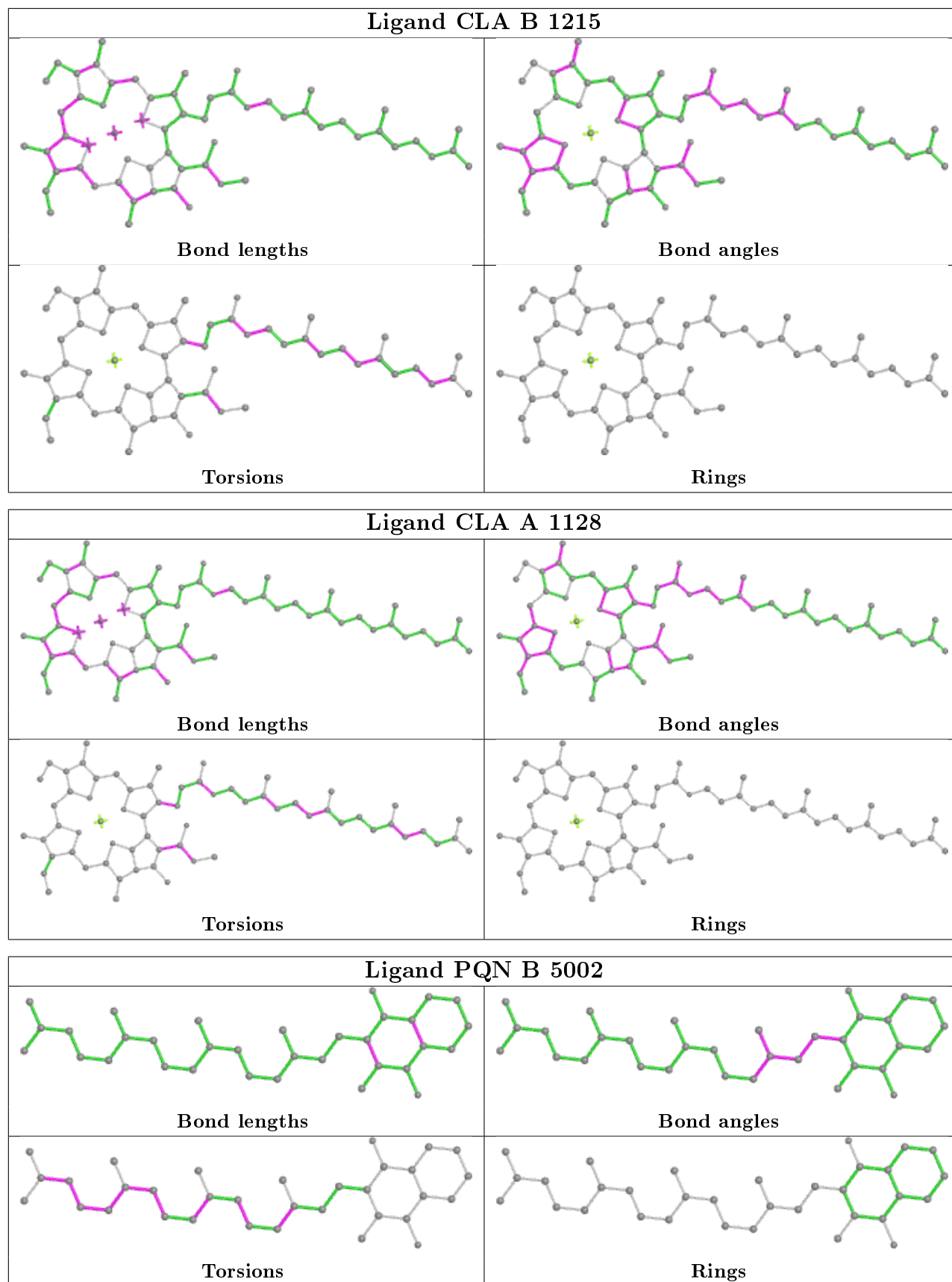


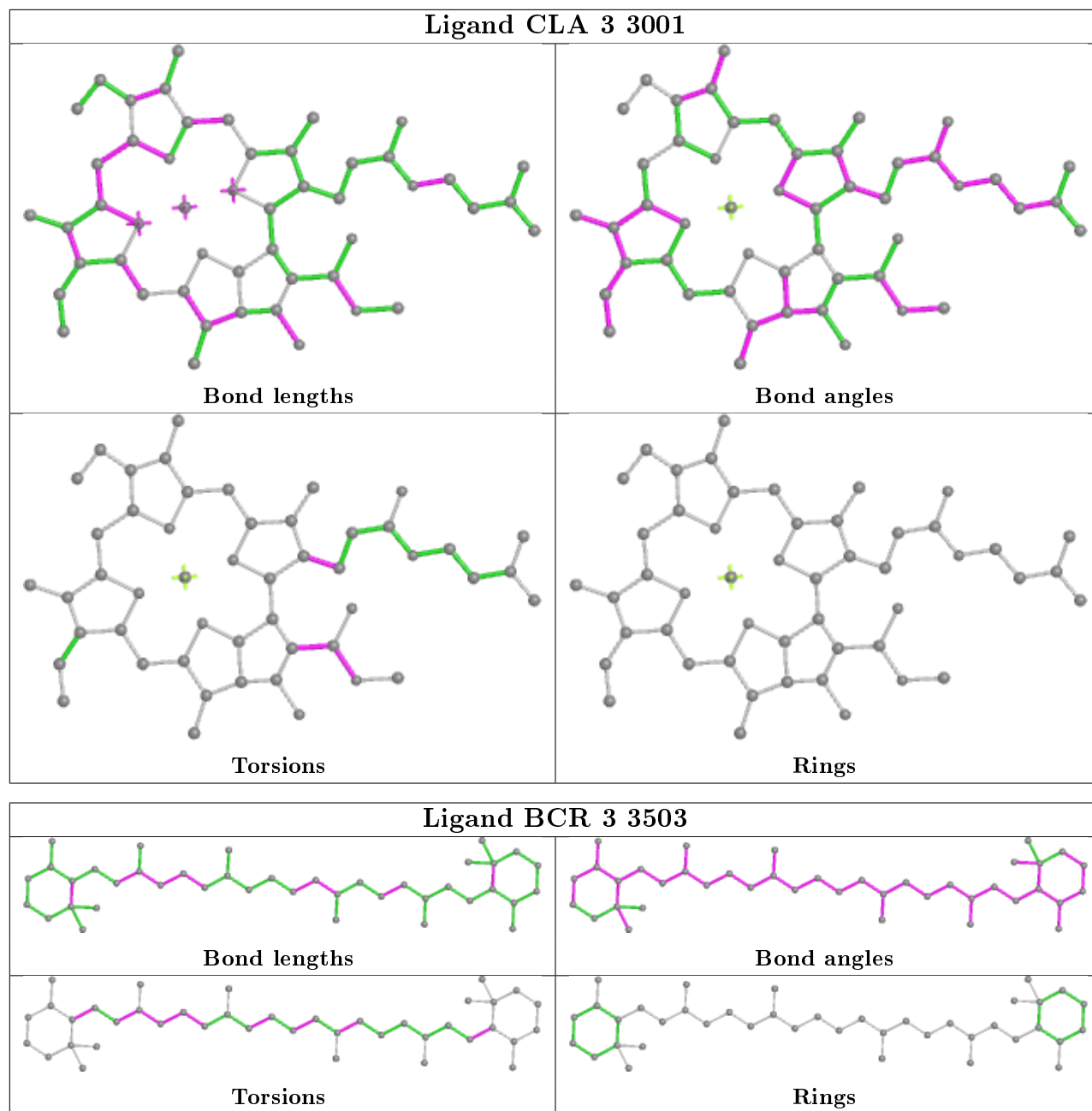


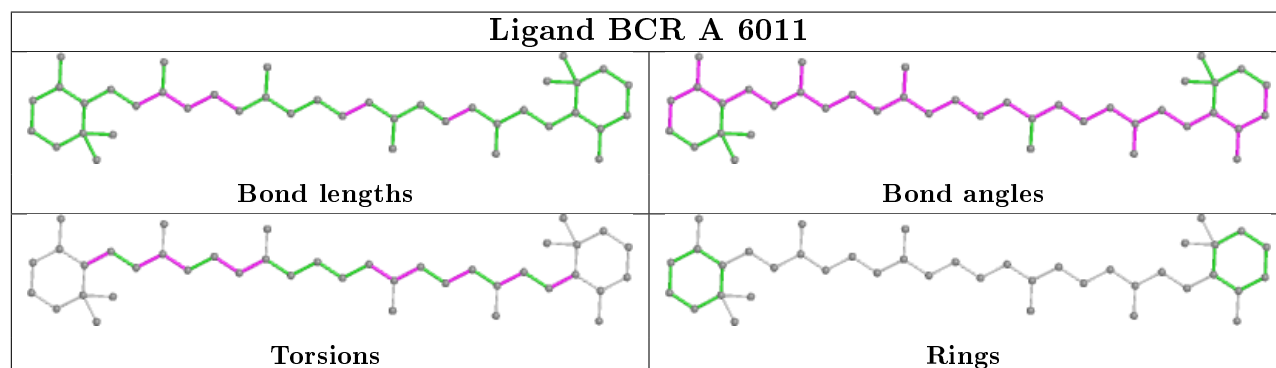
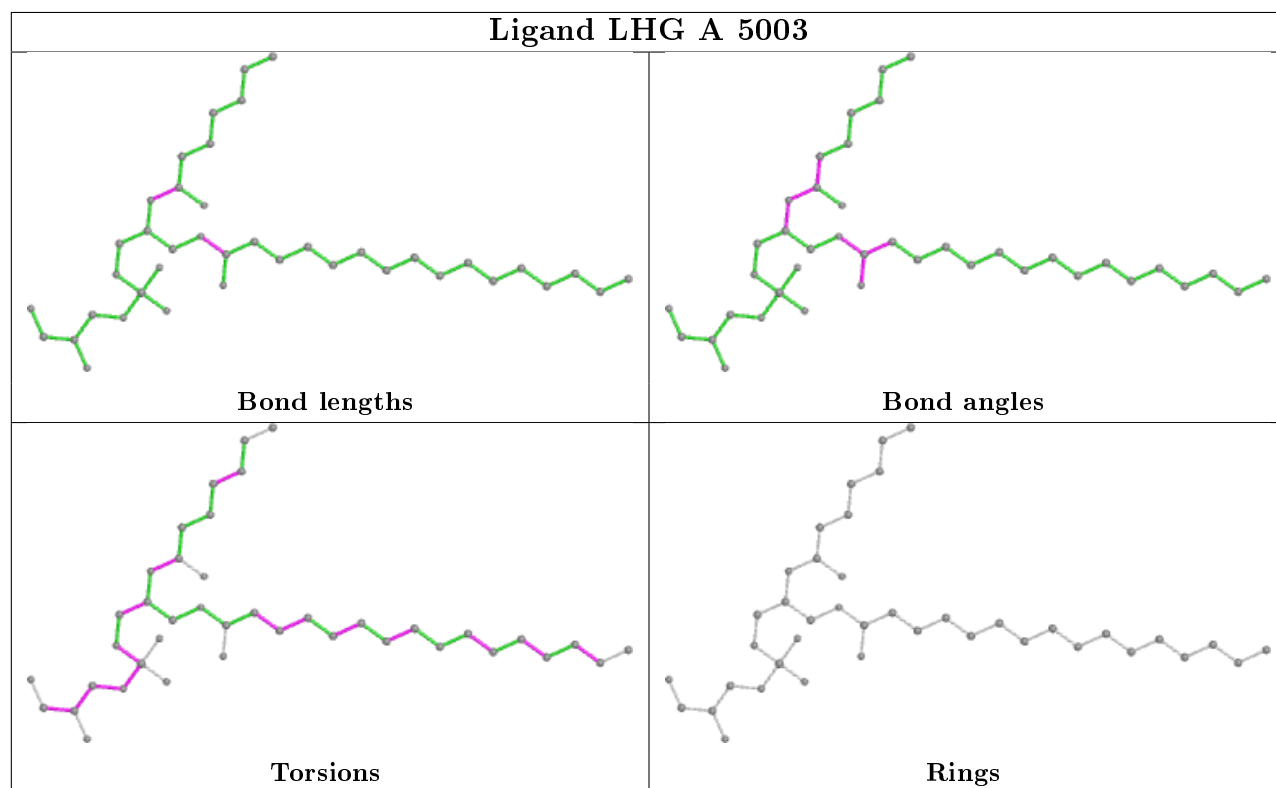
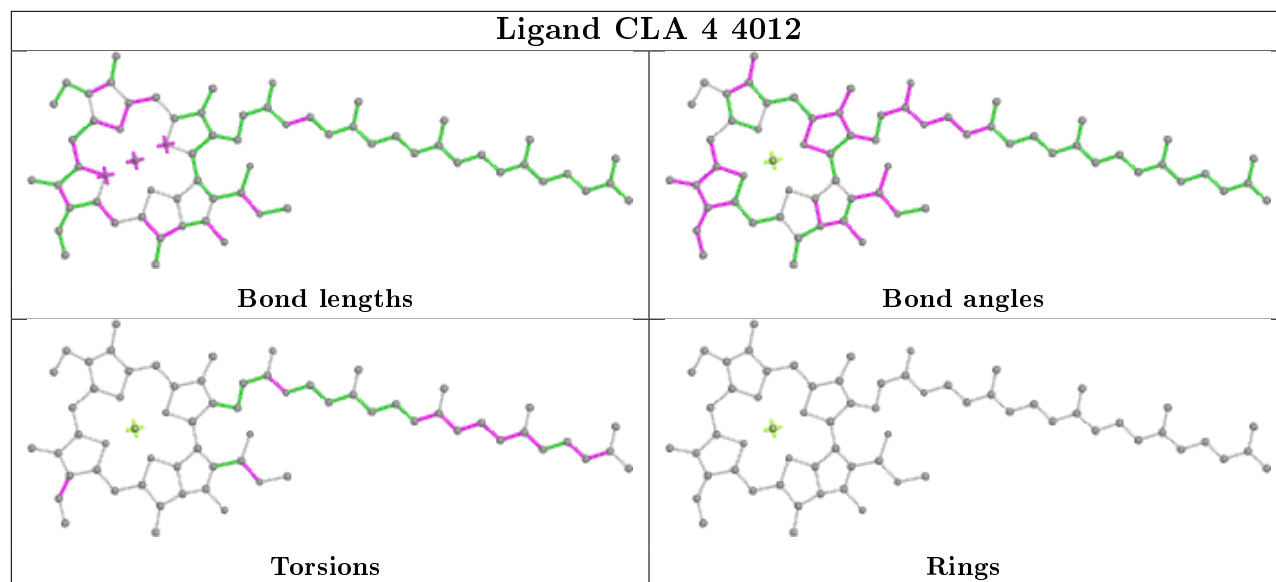


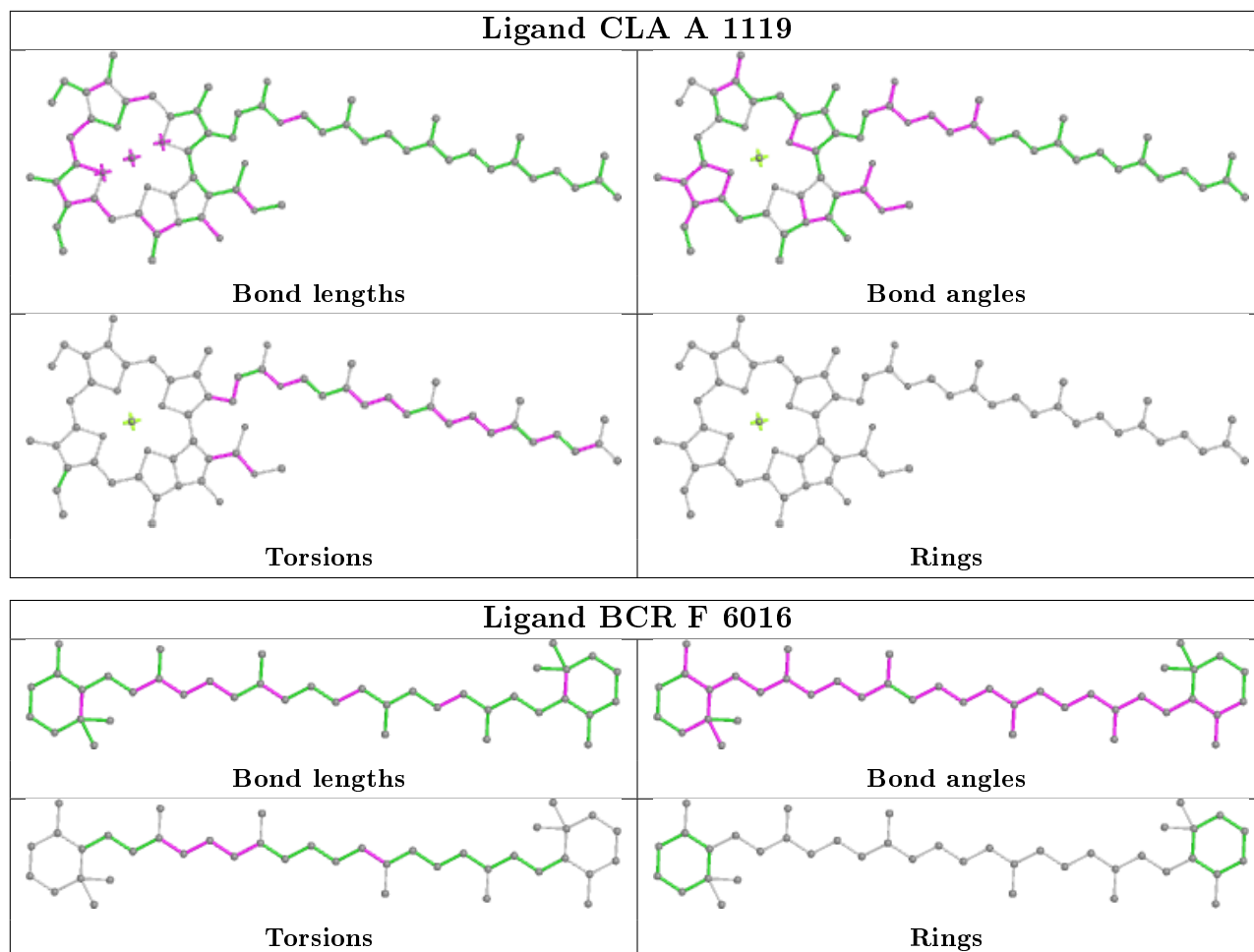


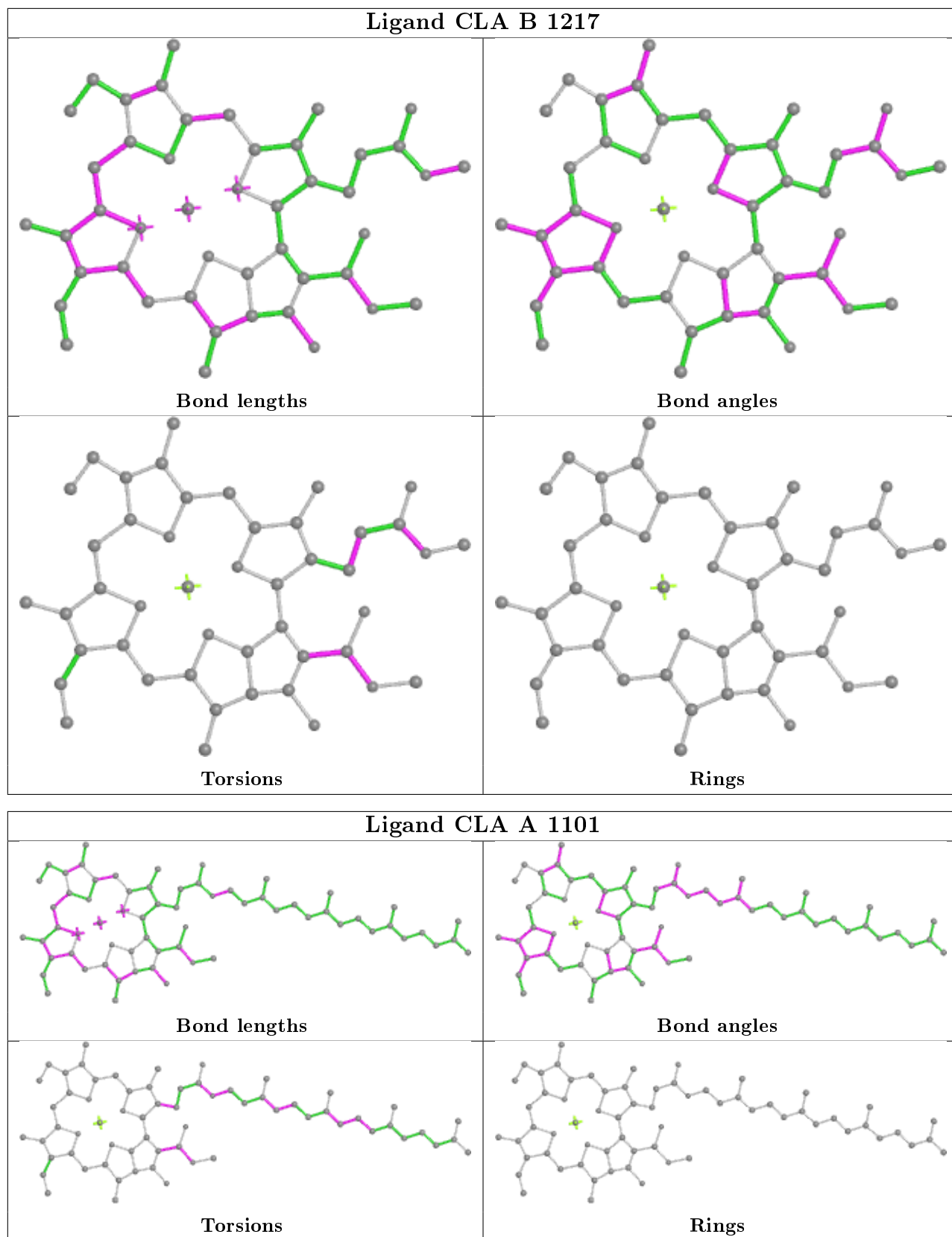


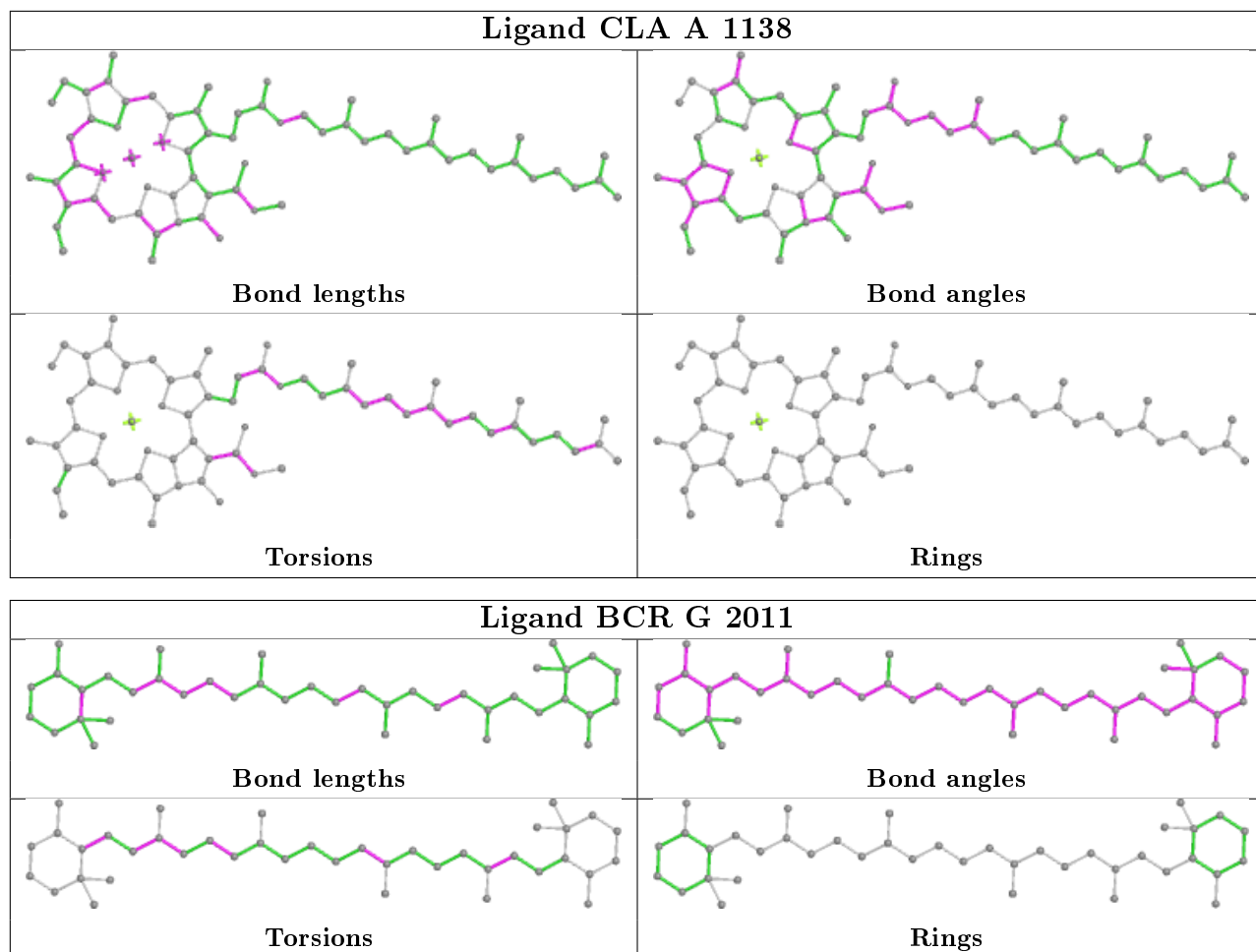


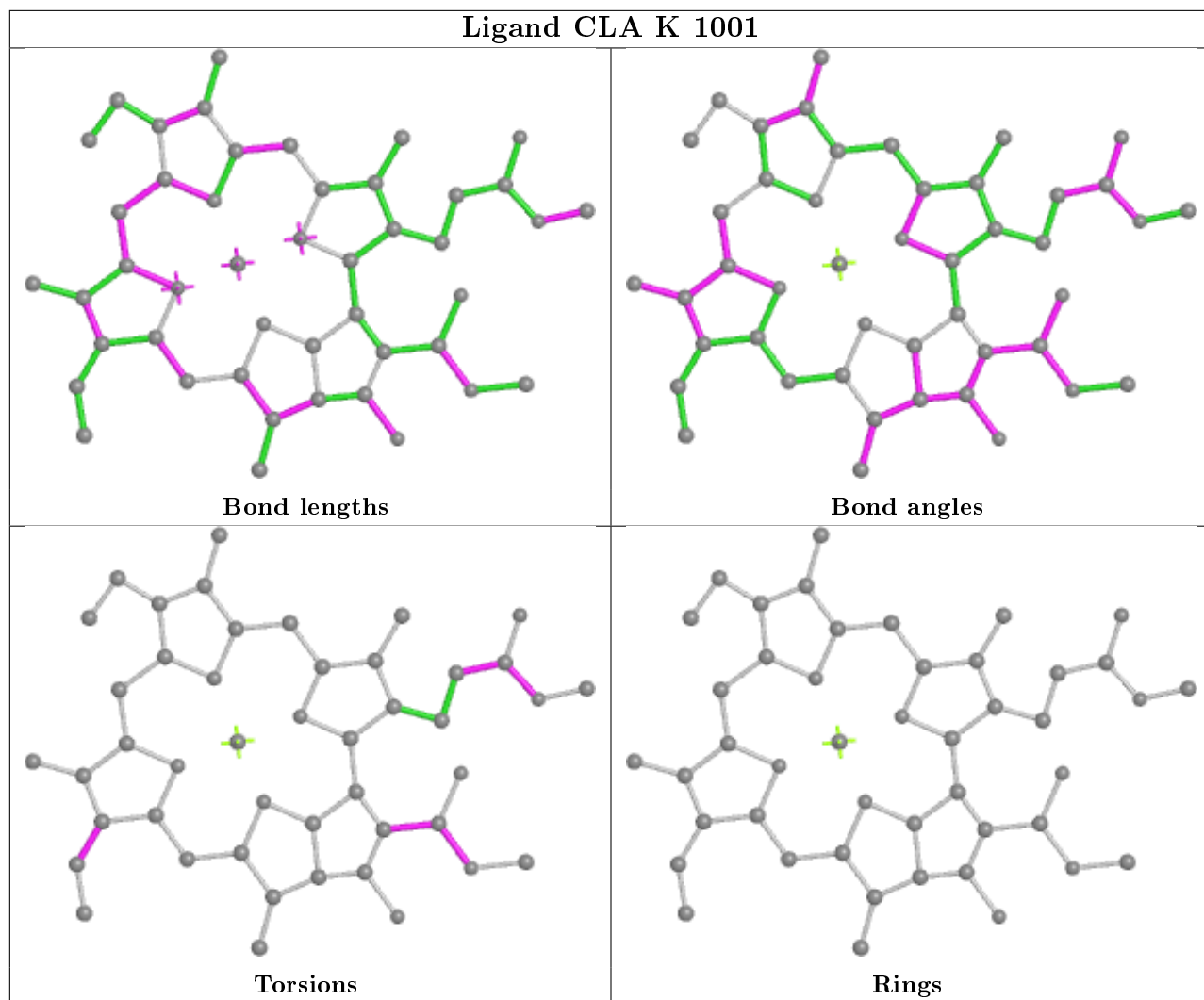


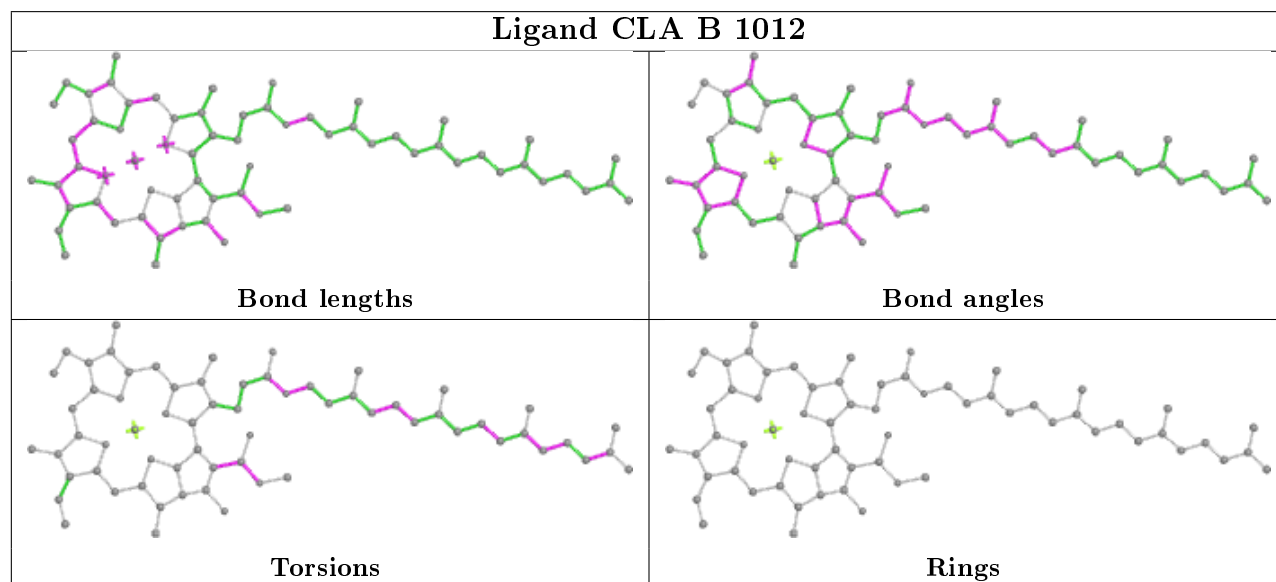
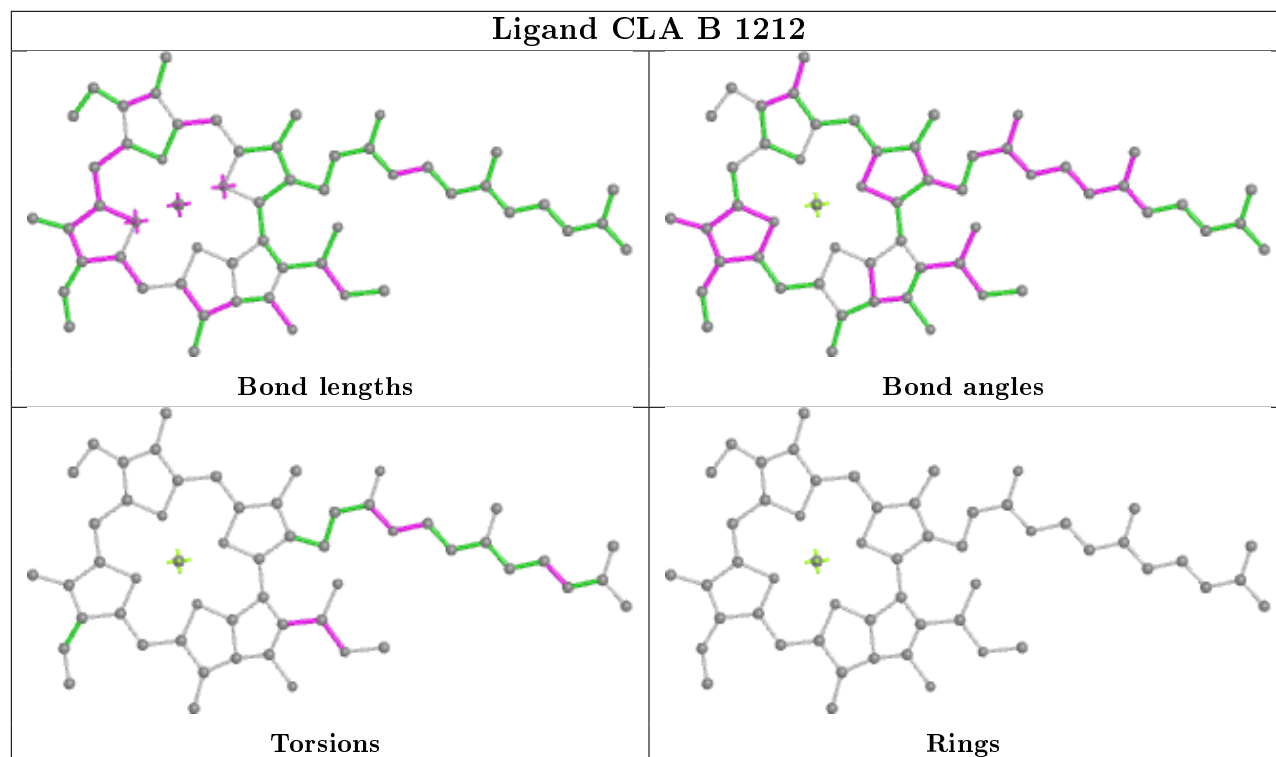


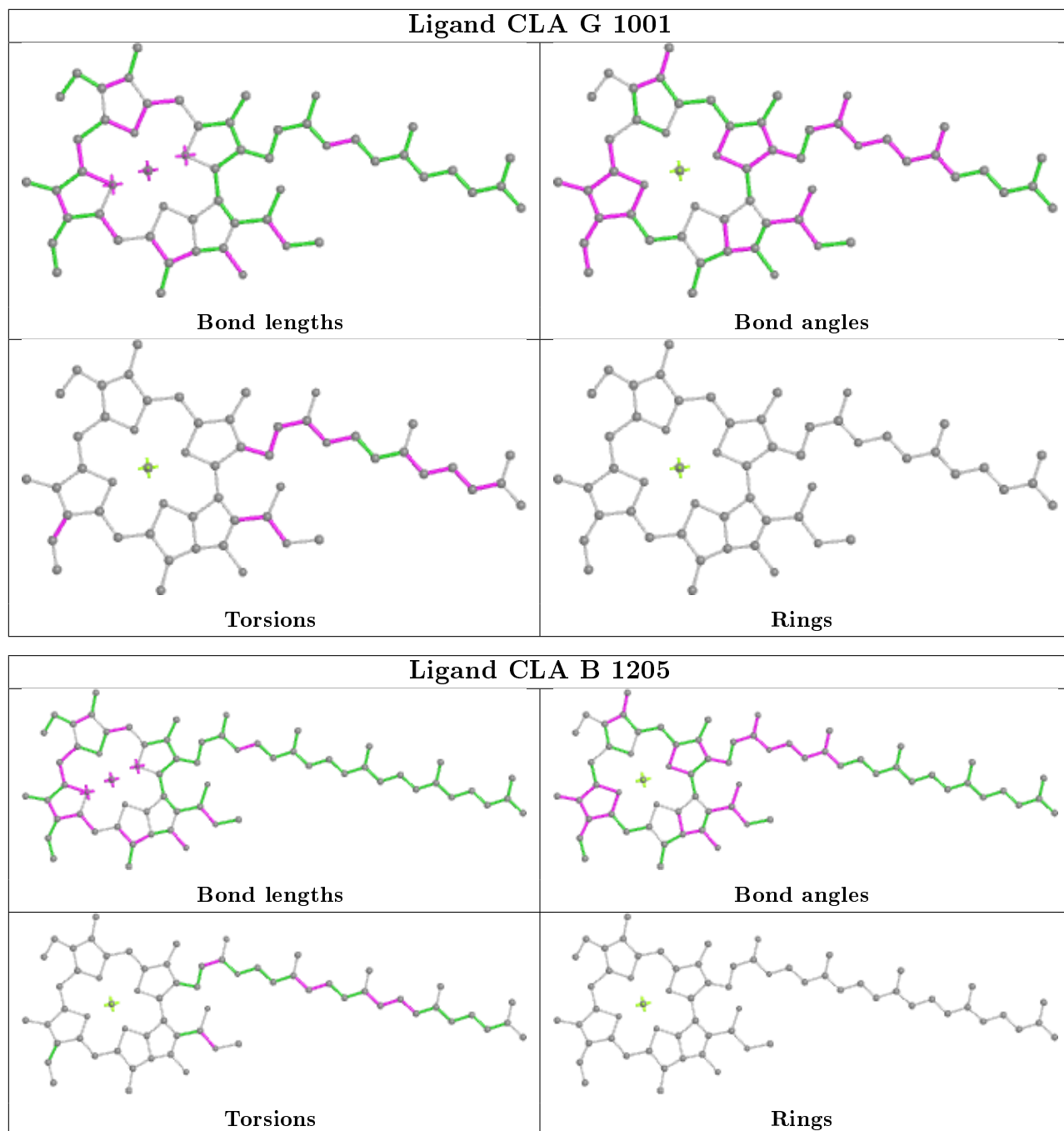


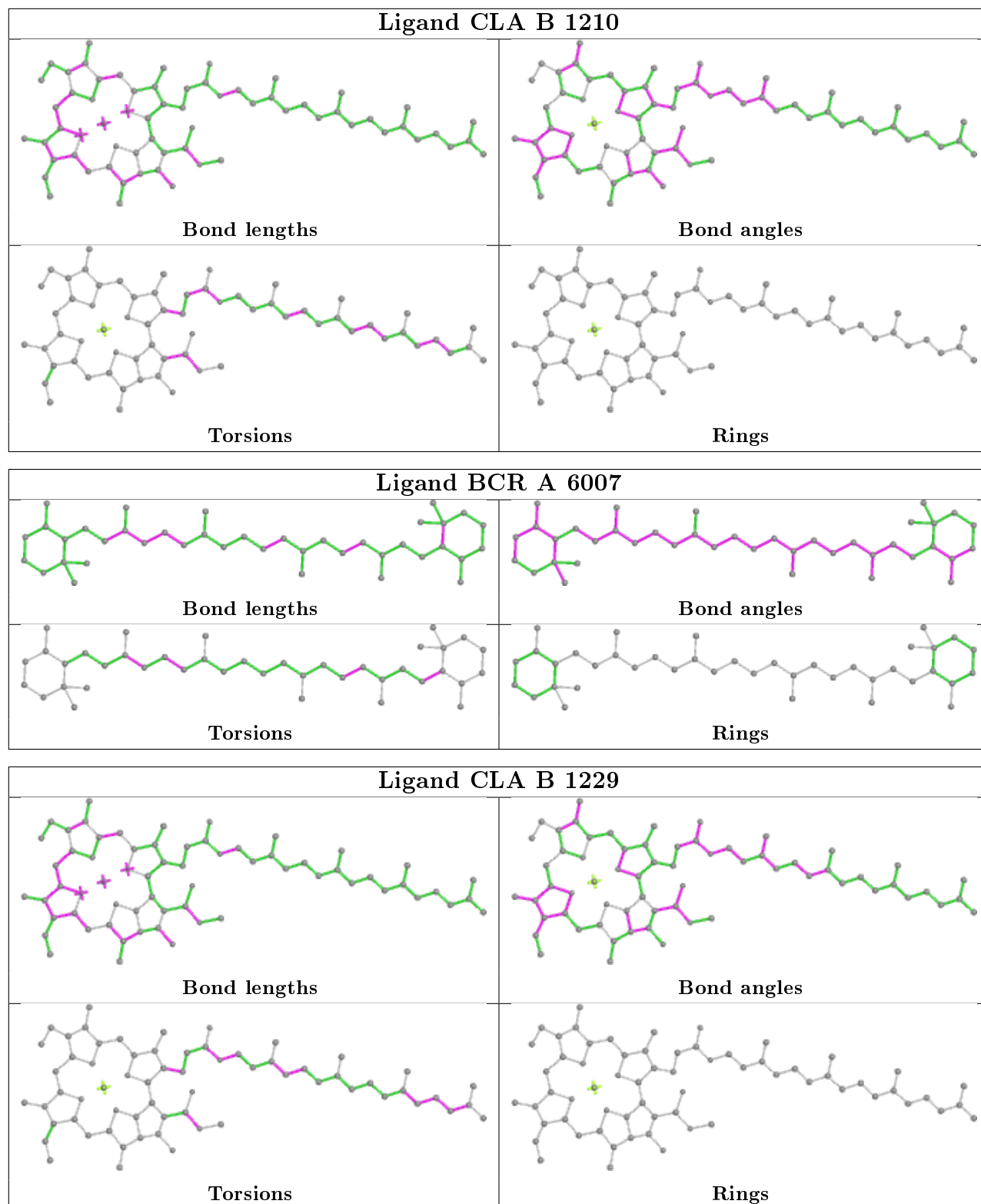


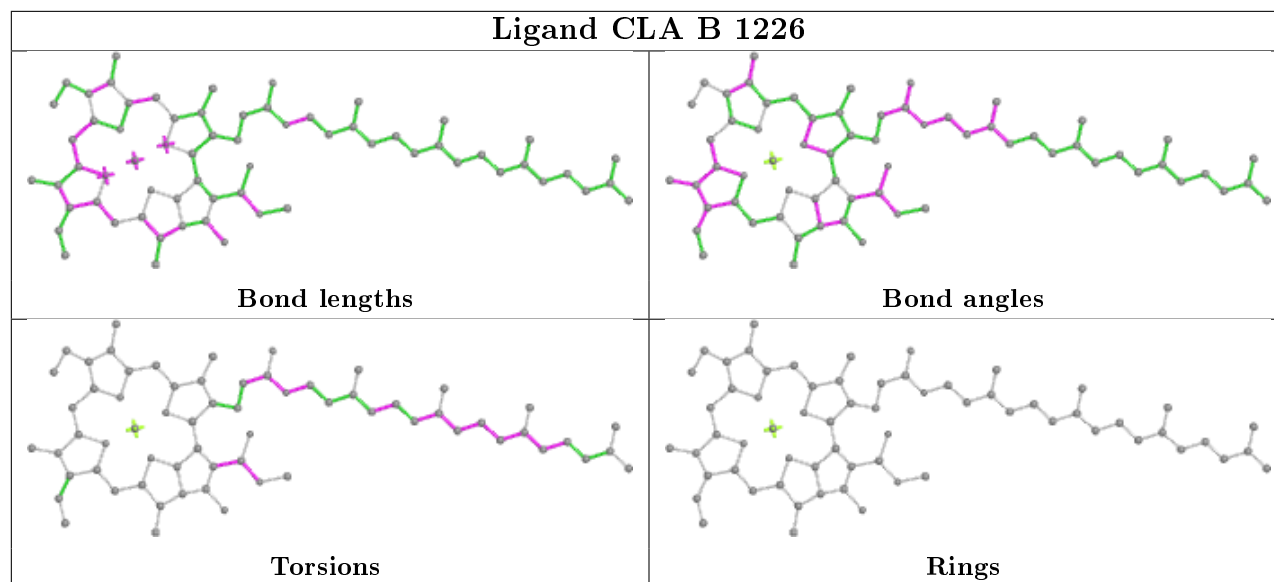












5.7 Other polymers [i](#)

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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	742/758 (97%)	0.36	49 (6%) 18 11	56, 92, 150, 244	0
2	B	732/733 (99%)	0.30	43 (5%) 22 14	61, 89, 126, 157	0
3	I	29/30 (96%)	0.52	4 (13%) 2 1	89, 114, 148, 153	0
4	J	41/42 (97%)	0.18	3 (7%) 15 8	70, 80, 116, 164	0
5	F	150/154 (97%)	0.08	6 (4%) 38 28	66, 90, 122, 157	0
6	G	91/97 (93%)	0.50	11 (12%) 4 2	98, 129, 174, 184	0
7	L	160/167 (95%)	0.68	24 (15%) 2 1	86, 123, 172, 197	0
8	C	80/81 (98%)	0.11	4 (5%) 28 19	66, 81, 96, 106	0
9	D	141/147 (95%)	0.56	20 (14%) 2 1	77, 97, 120, 139	0
10	E	66/66 (100%)	0.35	8 (12%) 4 2	65, 91, 136, 183	0
11	H	84/90 (93%)	0.33	11 (13%) 3 2	103, 138, 178, 234	0
12	K	57/129 (44%)	1.59	20 (35%) 0 0	147, 215, 286, 324	0
13	2	207/269 (76%)	0.60	30 (14%) 2 1	85, 130, 180, 270	0
14	4	198/252 (78%)	0.60	26 (13%) 3 2	84, 121, 193, 274	0
15	1	194/202 (96%)	0.85	39 (20%) 1 0	95, 147, 225, 289	0
16	3	215/275 (78%)	0.74	34 (15%) 2 1	111, 179, 317, 368	0
All	All	3187/3492 (91%)	0.46	332 (10%) 6 3	56, 106, 205, 368	0

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	1	103	GLY	12.4
16	3	145	ALA	10.8
15	1	172	LYS	9.5
2	B	82	PHE	8.1
9	D	206	LYS	7.5

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Mol	Chain	Res	Type	RSRZ
7	L	211	TYR	7.5
16	3	132	THR	7.3
9	D	196	VAL	7.2
2	B	491	ASN	7.1
1	A	250	LEU	6.9
16	3	87	GLU	6.9
11	H	132	PRO	6.5
16	3	217	GLU	6.3
15	1	162	GLY	6.2
16	3	121	TYR	6.1
15	1	176	LYS	6.1
12	K	77	MET	6.0
16	3	125	VAL	5.8
2	B	490	ARG	5.8
3	I	4	LEU	5.8
2	B	214	ASP	5.7
1	A	115	HIS	5.7
12	K	122	THR	5.7
15	1	100	LEU	5.6
7	L	123	THR	5.6
7	L	212	TYR	5.5
6	G	108	ALA	5.5
1	A	257	GLN	5.5
1	A	277	TYR	5.5
1	A	502	THR	5.4
9	D	208	PRO	5.4
2	B	159	PRO	5.4
15	1	54	SER	5.3
2	B	161	TRP	5.3
1	A	263	ALA	5.3
9	D	207	GLN	5.2
1	A	517	GLY	5.2
15	1	60	GLY	5.2
15	1	219	ALA	5.1
9	D	200	GLU	5.0
13	2	127	THR	5.0
6	G	147	ASP	4.9
14	4	118	ILE	4.8
6	G	109	LYS	4.8
1	A	264	GLU	4.8
14	4	133	GLU	4.8
10	E	91	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
15	1	102	LEU	4.7
16	3	144	PRO	4.7
1	A	260	PRO	4.6
13	2	185	ASN	4.5
16	3	253	TYR	4.5
14	4	195	ALA	4.5
1	A	518	GLY	4.5
15	1	175	LYS	4.5
2	B	482	ASN	4.4
1	A	276	LYS	4.4
16	3	124	LYS	4.4
15	1	123	GLY	4.4
14	4	178	PRO	4.3
7	L	205	TYR	4.3
12	K	88	SER	4.3
7	L	172	GLN	4.3
16	3	89	THR	4.3
15	1	99	ALA	4.3
9	D	76	ASP	4.3
15	1	174	PRO	4.2
16	3	96	ARG	4.2
7	L	171	LYS	4.2
15	1	173	ASP	4.2
1	A	259	TYR	4.2
9	D	211	LEU	4.2
11	H	117	THR	4.2
15	1	161	PRO	4.1
2	B	552	ASP	4.1
15	1	125	PRO	4.1
9	D	197	SER	4.0
15	1	171	SER	4.0
12	K	140	LEU	3.9
1	A	23	ASP	3.9
7	L	131	SER	3.9
12	K	125	CYS	3.9
6	G	110	GLU	3.9
6	G	107	ARG	3.9
12	K	87	PRO	3.9
16	3	77	GLY	3.8
3	I	5	PRO	3.8
1	A	279	ASP	3.8
2	B	210	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
16	3	184	LYS	3.8
12	K	136	VAL	3.8
4	J	7	TYR	3.8
1	A	271	THR	3.8
13	2	264	ALA	3.7
15	1	218	LEU	3.7
14	4	225	THR	3.7
1	A	42	ARG	3.7
11	H	113	TYR	3.7
16	3	129	PRO	3.7
14	4	198	LEU	3.7
2	B	487	ASN	3.7
11	H	75	PRO	3.7
14	4	52	LYS	3.7
2	B	295	PHE	3.7
3	I	32	LEU	3.7
15	1	96	VAL	3.7
1	A	261	SER	3.6
14	4	120	ILE	3.6
12	K	134	VAL	3.6
7	L	174	ASP	3.6
10	E	71	GLY	3.6
5	F	189	LYS	3.5
8	C	32	GLY	3.5
7	L	173	PRO	3.5
14	4	119	GLY	3.5
1	A	46	LYS	3.5
14	4	238	SER	3.4
13	2	78	ASP	3.4
13	2	178	ASN	3.4
11	H	131	LEU	3.4
1	A	525	ASN	3.4
9	D	190	ARG	3.4
14	4	121	ILE	3.4
2	B	212	PHE	3.3
2	B	360	PHE	3.3
7	L	116	LYS	3.3
13	2	184	PRO	3.3
15	1	233	PRO	3.3
9	D	72	PRO	3.3
15	1	157	LYS	3.3
11	H	135	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	280	PHE	3.3
13	2	77	LEU	3.3
12	K	121	ASP	3.3
7	L	170	LYS	3.2
12	K	61	PHE	3.2
1	A	240	LYS	3.2
2	B	430	GLY	3.2
16	3	134	LEU	3.2
7	L	115	VAL	3.2
10	E	98	ASN	3.2
1	A	25	ASP	3.2
13	2	134	THR	3.2
9	D	199	ILE	3.1
2	B	232	LEU	3.1
6	G	144	ASN	3.1
2	B	229	GLN	3.1
16	3	146	GLY	3.1
13	2	133	LEU	3.1
2	B	475	ASP	3.1
7	L	208	ASP	3.1
12	K	78	LEU	3.1
14	4	68	GLY	3.1
7	L	210	PRO	3.0
15	1	50	TYR	3.0
13	2	251	PHE	3.0
12	K	89	ALA	3.0
13	2	80	SER	3.0
1	A	17	GLU	3.0
14	4	131	LYS	3.0
7	L	54	TYR	3.0
2	B	157	LEU	2.9
13	2	145	TYR	2.9
14	4	53	LYS	2.9
13	2	186	ASN	2.9
16	3	86	PRO	2.9
9	D	210	ASP	2.9
13	2	59	VAL	2.9
15	1	59	PHE	2.9
15	1	151	MET	2.9
7	L	169	ARG	2.8
16	3	263	PRO	2.8
7	L	121	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
12	K	79	PHE	2.8
16	3	189	GLY	2.8
10	E	128	VAL	2.8
16	3	58	TRP	2.8
14	4	237	ILE	2.8
9	D	204	THR	2.8
12	K	76	LEU	2.8
14	4	199	GLU	2.7
11	H	73	ASP	2.7
11	H	77	PRO	2.7
14	4	115	PHE	2.7
13	2	204	LEU	2.7
7	L	92	ALA	2.7
13	2	128	LYS	2.7
1	A	26	PRO	2.7
15	1	51	LEU	2.7
15	1	110	GLU	2.7
16	3	118	ALA	2.7
10	E	92	THR	2.7
1	A	251	ASN	2.7
2	B	486	LEU	2.7
5	F	109	TYR	2.6
1	A	366	GLY	2.6
6	G	88	ALA	2.6
13	2	248	ASP	2.6
1	A	107	GLU	2.6
8	C	35	LYS	2.6
16	3	94	GLU	2.6
1	A	140	PHE	2.6
15	1	165	PHE	2.6
2	B	294	ASN	2.6
2	B	374	HIS	2.6
8	C	34	CYS	2.6
12	K	83	PHE	2.6
15	1	134	ILE	2.6
15	1	178	HIS	2.6
14	4	188	ILE	2.5
9	D	201	VAL	2.5
2	B	70	TRP	2.5
6	G	145	GLY	2.5
1	A	520	LEU	2.5
2	B	160	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
16	3	185	GLN	2.5
10	E	106	ARG	2.5
4	J	3	ASP	2.5
15	1	47	ARG	2.5
2	B	277	HIS	2.5
6	G	111	TYR	2.5
11	H	78	TYR	2.5
12	K	75	THR	2.5
13	2	79	GLY	2.5
15	1	152	GLU	2.5
16	3	149	ASN	2.5
1	A	138	GLY	2.4
1	A	165	TYR	2.4
15	1	115	PRO	2.4
9	D	100	PHE	2.4
2	B	219	PRO	2.4
1	A	241	GLU	2.4
10	E	129	LYS	2.4
13	2	126	LEU	2.4
9	D	195	ASN	2.4
7	L	156	GLY	2.4
16	3	61	SER	2.4
9	D	156	TYR	2.4
13	2	123	PRO	2.4
2	B	220	GLN	2.4
5	F	225	GLU	2.4
2	B	276	HIS	2.4
13	2	138	TYR	2.4
13	2	265	ALA	2.4
1	A	258	LEU	2.4
13	2	125	PHE	2.4
1	A	108	ALA	2.4
12	K	80	ALA	2.4
14	4	82	ALA	2.4
1	A	456	HIS	2.3
1	A	142	GLY	2.3
15	1	57	GLY	2.3
6	G	146	TYR	2.3
2	B	349	ALA	2.3
13	2	142	GLU	2.3
14	4	192	LEU	2.3
14	4	197	THR	2.3

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Mol	Chain	Res	Type	RSRZ
7	L	108	PHE	2.3
12	K	133	GLY	2.3
7	L	62	GLY	2.3
1	A	247	GLU	2.3
13	2	65	PRO	2.3
16	3	99	ALA	2.3
2	B	244	PHE	2.3
16	3	147	THR	2.3
2	B	549	ASP	2.3
13	2	73	PRO	2.3
11	H	89	PHE	2.3
15	1	158	LYS	2.3
2	B	345	THR	2.2
12	K	137	VAL	2.2
16	3	260	VAL	2.2
9	D	209	TYR	2.2
14	4	59	GLY	2.2
13	2	183	PHE	2.2
14	4	224	VAL	2.2
14	4	122	ASN	2.2
7	L	111	VAL	2.2
2	B	426	SER	2.2
3	I	8	PHE	2.2
2	B	158	GLN	2.2
13	2	239	HIS	2.2
15	1	97	PRO	2.2
2	B	211	ASN	2.2
2	B	83	HIS	2.2
13	2	72	THR	2.2
5	F	188	GLU	2.2
8	C	13	GLY	2.2
1	A	273	ASN	2.2
11	H	72	SER	2.2
14	4	179	ALA	2.1
2	B	433	THR	2.1
1	A	139	GLY	2.1
1	A	633	VAL	2.1
16	3	250	VAL	2.1
15	1	114	LEU	2.1
1	A	278	ALA	2.1
16	3	178	LYS	2.1
7	L	78	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	281	ALA	2.1
9	D	73	PRO	2.1
2	B	84	VAL	2.1
2	B	434	LEU	2.1
5	F	187	ASP	2.1
15	1	101	GLY	2.1
12	K	91	ARG	2.1
1	A	116	ILE	2.1
4	J	2	ARG	2.1
1	A	282	THR	2.1
16	3	272	LEU	2.1
9	D	166	TYR	2.1
1	A	122	VAL	2.1
14	4	117	SER	2.1
16	3	92	PHE	2.1
1	A	628	ILE	2.1
2	B	605	ASN	2.1
1	A	455	PHE	2.1
2	B	66	PHE	2.1
2	B	154	TRP	2.0
1	A	513	LEU	2.0
15	1	148	GLN	2.0
1	A	69	SER	2.0
2	B	688	ALA	2.0
16	3	148	TYR	2.0
6	G	62	LEU	2.0
13	2	199	LEU	2.0
1	A	141	ARG	2.0
15	1	61	PHE	2.0
5	F	113	SER	2.0
10	E	89	SER	2.0
16	3	187	PHE	2.0
7	L	209	LEU	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 monosaccharides 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
18	CLA	3	3019	27/65	0.29	0.59	158,174,188,189	1
23	LMG	B	5005	38/55	0.61	0.31	76,120,141,143	0
18	CLA	2	2016	50/65	0.67	0.30	114,164,207,211	0
22	BCR	G	2011	40/40	0.68	0.29	112,132,172,174	0
27	LUT	3	3501	42/42	0.68	0.63	202,209,216,218	0
27	LUT	2	2501	42/42	0.71	0.35	121,137,141,143	0
22	BCR	B	6005	40/40	0.72	0.41	87,103,182,184	0
27	LUT	3	3502	42/42	0.74	0.34	133,142,164,166	0
22	BCR	J	6013	40/40	0.75	0.34	74,94,112,116	0
22	BCR	3	3503	40/40	0.76	0.31	119,136,175,177	0
23	LMG	G	2021	41/55	0.76	0.29	138,156,175,176	0
22	BCR	B	6004	40/40	0.77	0.36	105,112,138,144	0
18	CLA	1	1013	46/65	0.77	0.34	127,154,181,185	0
18	CLA	2	2019	27/65	0.77	0.18	148,159,174,174	1
22	BCR	B	6006	40/40	0.78	0.35	94,115,164,164	0
18	CLA	4	4016	46/65	0.79	0.30	126,166,177,183	0
27	LUT	1	1501	42/42	0.79	0.32	115,142,189,197	0
22	BCR	K	2011	40/40	0.79	0.37	125,136,144,147	0
28	CHL	3	3011	56/66	0.80	0.34	144,156,197,200	0
18	CLA	4	4006	50/65	0.80	0.24	110,127,148,156	0
26	LMU	B	8001	35/35	0.80	0.28	104,158,168,172	0
18	CLA	1	1008	46/65	0.80	0.25	112,129,142,150	0
18	CLA	3	3003	60/65	0.80	0.25	137,170,188,190	0
18	CLA	K	1001	46/65	0.80	0.35	147,173,200,209	0
18	CLA	3	3007	50/65	0.81	0.23	175,193,239,246	0
27	LUT	4	4501	42/42	0.81	0.25	107,121,142,149	0
18	CLA	3	3018	50/65	0.81	0.31	173,190,207,213	0
23	LMG	2	2802	35/55	0.81	0.41	108,127,149,152	0
21	LHG	2	2801	24/49	0.81	0.25	109,123,148,152	0
22	BCR	L	6019	40/40	0.81	0.40	88,105,132,135	0
18	CLA	3	3004	60/65	0.81	0.26	125,139,154,155	0
18	CLA	4	4002	50/65	0.82	0.24	107,141,171,211	0
18	CLA	3	3006	50/65	0.82	0.25	125,157,167,170	0
18	CLA	3	3010	60/65	0.82	0.29	122,158,181,196	0
18	CLA	2	2002	46/65	0.82	0.21	137,154,171,183	0
18	CLA	3	3008	48/65	0.83	0.46	180,199,214,217	0
22	BCR	A	6008	40/40	0.83	0.31	76,97,137,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	1	1006	50/65	0.83	0.24	125,138,144,148	0
18	CLA	L	1503	50/65	0.83	0.37	106,114,143,149	0
28	CHL	4	4010	47/66	0.83	0.28	105,125,180,187	0
26	LMU	B	8002	35/35	0.83	0.23	162,173,189,191	0
22	BCR	J	6012	40/40	0.83	0.31	67,80,89,91	0
18	CLA	2	2007	60/65	0.83	0.30	116,142,189,195	0
18	CLA	B	1214	59/65	0.84	0.30	71,91,100,108	0
18	CLA	1	1001	60/65	0.84	0.20	122,151,165,171	0
18	CLA	J	1302	50/65	0.84	0.35	137,152,189,196	0
27	LUT	4	4503	42/42	0.84	0.38	110,135,158,160	0
18	CLA	G	1003	60/65	0.84	0.24	97,121,149,153	0
18	CLA	4	4001	60/65	0.84	0.27	113,129,158,160	0
18	CLA	B	1212	55/65	0.84	0.26	109,129,146,154	0
28	CHL	2	2010	47/66	0.84	0.25	111,134,142,143	0
18	CLA	3	3012	50/65	0.85	0.22	117,135,142,144	0
18	CLA	1	1011	50/65	0.85	0.29	126,153,175,185	0
18	CLA	H	1000	46/65	0.85	0.31	119,150,170,176	0
18	CLA	B	1222	65/65	0.85	0.30	58,74,103,110	0
27	LUT	2	2502	42/42	0.85	0.36	102,115,124,131	0
23	LMG	F	5002	37/55	0.85	0.39	84,107,120,126	0
22	BCR	A	6003	40/40	0.85	0.34	79,94,139,140	0
22	BCR	B	6010	40/40	0.85	0.28	64,73,96,100	0
18	CLA	4	4008	46/65	0.85	0.25	93,112,129,137	0
18	CLA	B	1234	60/65	0.85	0.30	64,77,106,108	0
18	CLA	A	1113	46/65	0.85	0.27	119,135,172,187	0
22	BCR	B	6009	40/40	0.85	0.28	63,78,94,95	0
27	LUT	1	1502	42/42	0.85	0.27	85,116,128,129	0
18	CLA	4	4007	60/65	0.85	0.29	110,130,179,183	0
23	LMG	J	5001	55/55	0.85	0.22	62,96,110,122	0
18	CLA	2	2006	55/65	0.86	0.23	105,132,173,174	0
27	LUT	I	6018	42/42	0.86	0.28	101,109,116,121	0
18	CLA	A	1134	55/65	0.86	0.27	112,124,168,172	0
27	LUT	4	4502	42/42	0.86	0.26	88,106,117,121	0
18	CLA	3	3013	46/65	0.86	0.19	127,157,166,176	0
18	CLA	A	1107	65/65	0.86	0.29	60,77,94,105	0
18	CLA	B	1213	60/65	0.86	0.23	85,105,118,126	0
28	CHL	1	1010	47/66	0.86	0.17	125,137,152,155	0
18	CLA	A	1112	65/65	0.86	0.25	101,118,138,140	0
18	CLA	L	1501	50/65	0.86	0.22	106,129,153,159	0
18	CLA	A	1123	65/65	0.86	0.31	70,88,93,96	0
18	CLA	B	1231	60/65	0.86	0.23	65,81,101,104	0
22	BCR	A	6007	40/40	0.86	0.30	77,90,147,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
28	CHL	1	1009	56/66	0.87	0.25	92,105,113,130	0
18	CLA	A	1151	50/65	0.87	0.24	99,113,187,189	0
18	CLA	A	1110	55/65	0.87	0.27	97,114,138,143	0
18	CLA	B	1228	60/65	0.87	0.26	63,73,111,114	0
25	DGD	B	7101	61/66	0.87	0.24	62,79,104,113	0
18	CLA	1	1014	46/65	0.87	0.17	83,110,123,143	0
22	BCR	F	6014	40/40	0.87	0.27	54,64,73,74	0
23	LMG	F	5001	23/55	0.87	0.27	86,94,106,109	0
18	CLA	3	3005	55/65	0.87	0.25	107,131,144,157	0
18	CLA	3	3001	50/65	0.87	0.31	147,169,201,206	0
18	CLA	1	1005	55/65	0.87	0.21	84,113,122,124	0
18	CLA	A	1115	46/65	0.87	0.24	107,141,170,178	0
23	LMG	4	4801	35/55	0.87	0.25	104,117,128,132	0
18	CLA	A	1105	51/65	0.88	0.25	66,88,97,100	0
18	CLA	3	3017	46/65	0.88	0.24	101,119,134,145	0
28	CHL	2	2011	48/66	0.88	0.24	108,124,129,136	0
21	LHG	1	1801	49/49	0.88	0.26	94,113,164,170	0
18	CLA	4	4004	60/65	0.88	0.24	76,99,112,118	0
18	CLA	4	4017	65/65	0.88	0.27	93,103,120,121	0
18	CLA	1	1002	46/65	0.88	0.19	120,155,171,194	0
18	CLA	G	1001	55/65	0.88	0.17	119,145,181,184	0
18	CLA	A	1109	65/65	0.88	0.22	71,85,94,101	0
18	CLA	A	1104	65/65	0.89	0.28	55,73,81,85	0
18	CLA	B	1023	65/65	0.89	0.24	57,70,94,105	0
18	CLA	1	1004	65/65	0.89	0.23	98,114,122,125	0
18	CLA	F	1301	45/65	0.89	0.23	61,73,86,101	0
18	CLA	L	1502	60/65	0.89	0.23	86,116,125,130	0
22	BCR	L	6020	40/40	0.89	0.37	98,131,157,164	0
18	CLA	2	2003	55/65	0.89	0.16	103,127,135,158	0
18	CLA	A	1114	46/65	0.89	0.29	107,117,124,136	0
18	CLA	B	1218	65/65	0.89	0.25	86,100,155,160	0
18	CLA	A	1118	46/65	0.89	0.23	99,108,127,131	0
29	ZEX	4	4505	42/42	0.89	0.25	85,96,107,114	0
18	CLA	3	3002	46/65	0.89	0.24	173,188,195,222	0
18	CLA	A	1103	65/65	0.89	0.25	66,83,104,107	0
18	CLA	B	1227	65/65	0.89	0.23	60,74,99,105	0
24	CA	B	6000	1/1	0.89	0.06	100,100,100,100	0
18	CLA	2	2001	60/65	0.89	0.29	114,134,167,169	0
18	CLA	4	4003	65/65	0.90	0.23	84,106,135,143	0
18	CLA	A	1106	65/65	0.90	0.28	59,74,90,106	0
18	CLA	A	1111	60/65	0.90	0.24	75,91,112,118	0
18	CLA	2	2012	55/65	0.90	0.29	86,104,149,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	2	2009	50/65	0.90	0.18	100,117,138,139	0
18	CLA	A	1120	60/65	0.90	0.18	95,118,178,182	0
28	CHL	2	2013	46/66	0.90	0.23	110,125,130,135	0
18	CLA	A	1130	50/65	0.90	0.23	83,100,123,127	0
18	CLA	A	1022	65/65	0.90	0.24	58,76,88,99	0
22	BCR	F	6016	40/40	0.90	0.21	66,75,91,94	0
18	CLA	B	1232	55/65	0.90	0.22	80,97,118,122	0
18	CLA	A	1140	65/65	0.90	0.28	58,66,78,106	0
18	CLA	B	1216	65/65	0.90	0.24	73,86,105,108	0
21	LHG	A	7001	49/49	0.90	0.23	56,72,84,92	0
28	CHL	4	4013	47/66	0.91	0.20	98,118,130,134	0
18	CLA	A	1108	46/65	0.91	0.29	85,101,121,126	0
18	CLA	2	2004	65/65	0.91	0.22	84,105,117,125	0
18	CLA	A	1116	60/65	0.91	0.25	89,119,137,142	0
18	CLA	B	1204	55/65	0.91	0.20	80,103,118,124	0
18	CLA	1	1007	46/65	0.91	0.19	112,131,162,181	0
18	CLA	B	1229	65/65	0.91	0.26	60,72,82,84	0
18	CLA	B	1236	55/65	0.91	0.24	56,69,117,124	0
18	CLA	A	1135	51/65	0.91	0.28	72,92,114,117	0
18	CLA	2	2008	50/65	0.91	0.20	109,138,148,156	0
18	CLA	2	2005	55/65	0.91	0.25	93,103,129,135	0
18	CLA	B	1211	65/65	0.91	0.23	93,107,131,136	0
18	CLA	4	4005	60/65	0.91	0.21	84,97,106,120	0
22	BCR	A	6002	40/40	0.91	0.28	82,115,168,169	0
18	CLA	B	1223	65/65	0.91	0.22	59,78,90,96	0
18	CLA	B	1021	65/65	0.91	0.25	61,72,80,83	0
18	CLA	A	1133	55/65	0.91	0.23	83,109,120,126	0
18	CLA	1	1003	55/65	0.91	0.19	100,122,134,142	0
18	CLA	A	1101	65/65	0.91	0.23	58,72,90,113	0
18	CLA	A	1139	65/65	0.91	0.25	56,70,98,104	0
28	CHL	4	4011	51/66	0.91	0.23	117,131,149,154	0
18	CLA	B	1012	65/65	0.91	0.27	51,69,85,92	0
18	CLA	B	1230	58/65	0.91	0.20	58,74,83,86	0
18	CLA	B	1210	65/65	0.91	0.28	81,94,107,113	0
18	CLA	B	1208	55/65	0.91	0.19	82,114,133,137	0
18	CLA	A	1124	55/65	0.92	0.23	59,77,104,116	0
18	CLA	B	1225	65/65	0.92	0.30	66,81,98,105	0
18	CLA	A	1102	50/65	0.92	0.20	58,69,95,104	0
18	CLA	A	1127	65/65	0.92	0.33	69,83,95,99	0
22	BCR	A	6017	40/40	0.92	0.25	71,86,105,122	0
18	CLA	A	1125	60/65	0.92	0.22	79,94,102,114	0
18	CLA	B	1207	65/65	0.92	0.23	78,102,122,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	A	1132	65/65	0.92	0.28	79,94,120,129	0
18	CLA	B	1224	65/65	0.92	0.30	65,83,100,107	0
18	CLA	B	1235	65/65	0.92	0.22	54,68,78,92	0
18	CLA	A	1136	56/65	0.92	0.17	84,98,115,119	0
18	CLA	B	1220	65/65	0.92	0.23	61,76,114,118	0
18	CLA	B	1215	60/65	0.92	0.30	82,91,102,109	0
18	CLA	A	1128	65/65	0.92	0.21	56,66,74,85	0
18	CLA	A	1126	65/65	0.92	0.28	65,79,87,97	0
18	CLA	4	4012	65/65	0.92	0.21	92,104,117,120	0
21	LHG	A	5003	40/49	0.92	0.21	101,117,132,134	0
22	BCR	A	6011	40/40	0.92	0.36	61,73,88,96	0
18	CLA	A	1119	65/65	0.92	0.23	78,95,107,115	0
18	CLA	A	1122	65/65	0.92	0.23	76,96,122,139	0
18	CLA	B	1217	46/65	0.92	0.27	96,109,124,127	0
18	CLA	A	1121	55/65	0.92	0.17	104,123,209,211	0
18	CLA	A	1138	65/65	0.92	0.26	55,65,75,82	0
22	BCR	I	6020	40/40	0.92	0.26	85,97,110,111	0
18	CLA	B	1239	65/65	0.92	0.24	69,82,111,116	0
21	LHG	B	5004	21/49	0.92	0.16	86,102,116,119	0
18	CLA	A	1129	50/65	0.92	0.24	71,93,115,126	0
20	PQN	A	5001	33/33	0.92	0.24	53,63,76,85	0
18	CLA	B	1219	60/65	0.92	0.20	82,97,134,135	0
18	CLA	A	1117	65/65	0.93	0.36	85,98,110,114	0
18	CLA	A	1131	65/65	0.93	0.30	79,93,103,112	0
18	CLA	B	1238	65/65	0.93	0.22	70,85,96,116	0
18	CLA	4	4009	50/65	0.93	0.20	85,94,116,131	0
18	CLA	A	1137	55/65	0.93	0.22	71,85,125,126	0
18	CLA	A	1013	65/65	0.93	0.32	49,62,74,90	0
18	CLA	B	1240	65/65	0.93	0.19	66,84,103,108	0
18	CLA	B	1206	65/65	0.93	0.21	86,104,112,127	0
18	CLA	B	1209	46/65	0.93	0.22	100,109,118,145	0
18	CLA	B	1226	65/65	0.93	0.23	65,76,97,103	0
18	CLA	A	1237	60/65	0.94	0.29	75,94,113,116	0
18	CLA	1	1012	50/65	0.94	0.16	103,125,130,132	0
18	CLA	B	1221	65/65	0.94	0.24	66,78,115,122	0
18	CLA	F	1302	50/65	0.94	0.16	67,84,114,124	0
18	CLA	G	1002	46/65	0.94	0.19	142,160,173,181	0
18	CLA	B	1205	65/65	0.94	0.26	90,103,116,152	0
18	CLA	B	1201	50/65	0.94	0.18	80,93,131,134	0
17	CL0	A	1011	65/65	0.94	0.24	52,70,82,84	0
20	PQN	B	5002	33/33	0.94	0.23	54,72,91,93	0
18	CLA	B	1202	65/65	0.95	0.22	71,82,91,104	0

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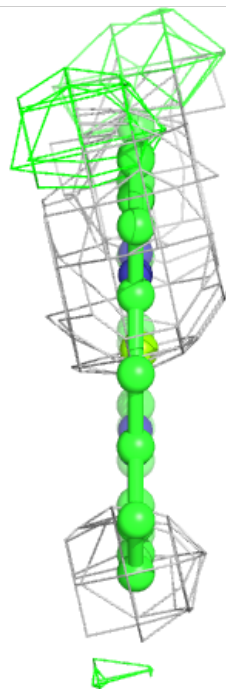
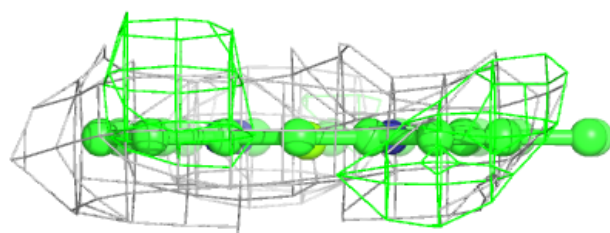
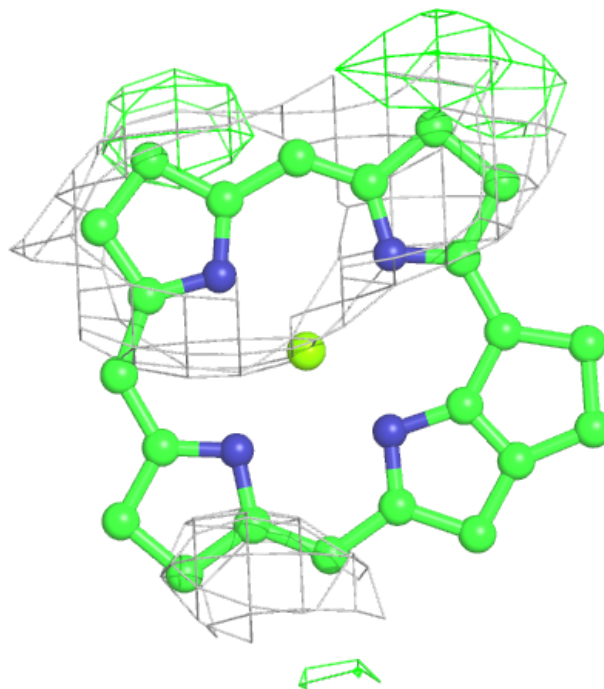
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	SF4	C	3002	8/8	0.95	0.12	73,103,107,107	0
18	CLA	B	1203	65/65	0.96	0.22	68,82,97,104	0
19	SF4	C	3003	8/8	0.97	0.07	89,106,119,126	0
19	SF4	A	3001	8/8	0.98	0.10	69,95,97,99	0

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.

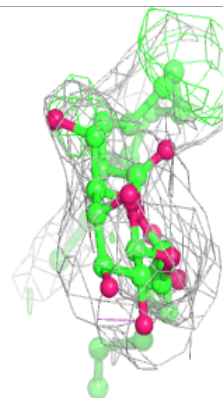
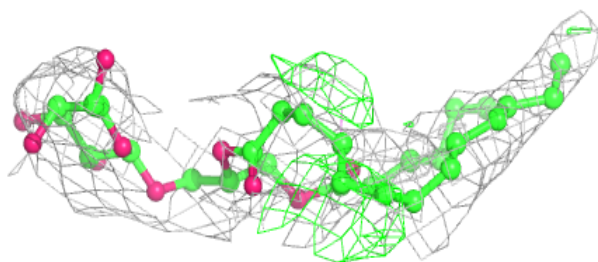
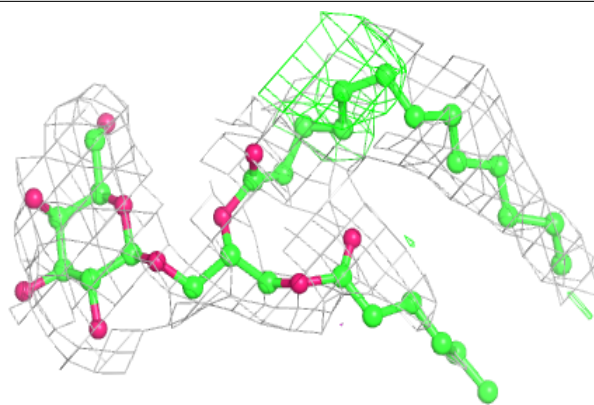
Electron density around CLA 3 3019:

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

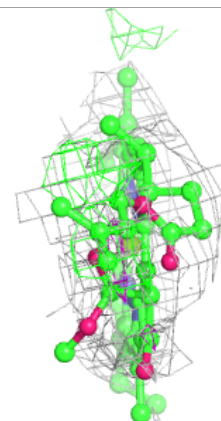
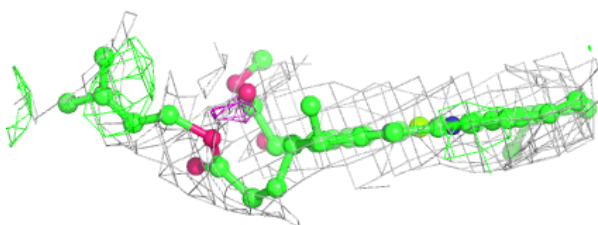
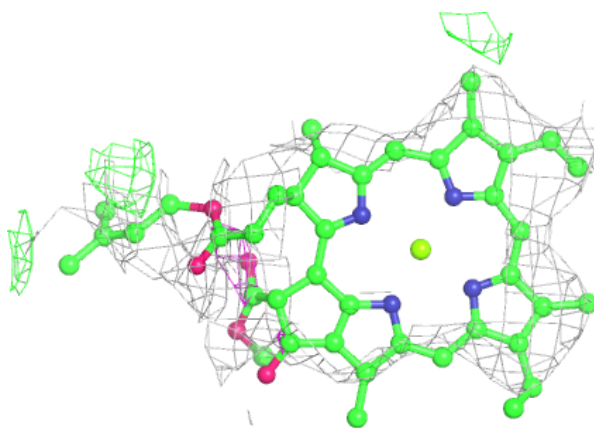


Electron density around LMG B 5005:

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

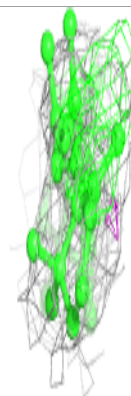
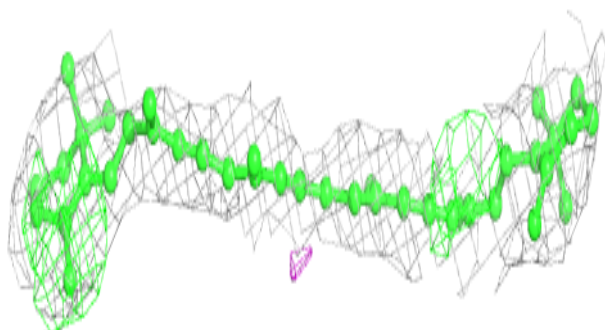
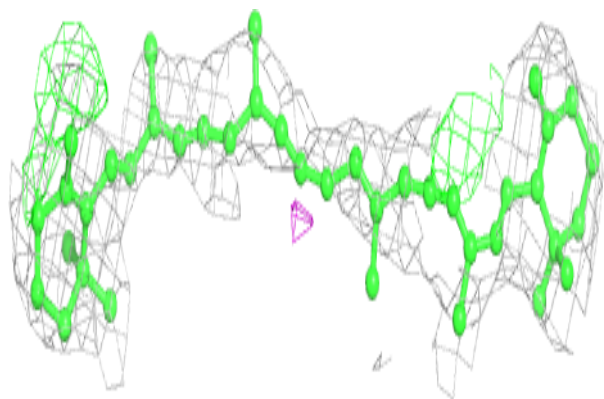
**Electron density around CLA 2 2016:**

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

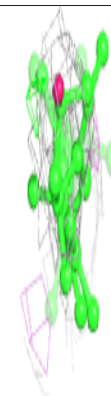
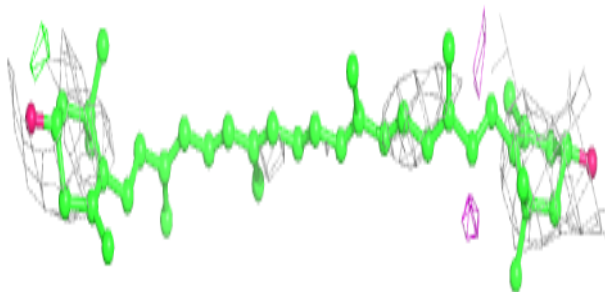
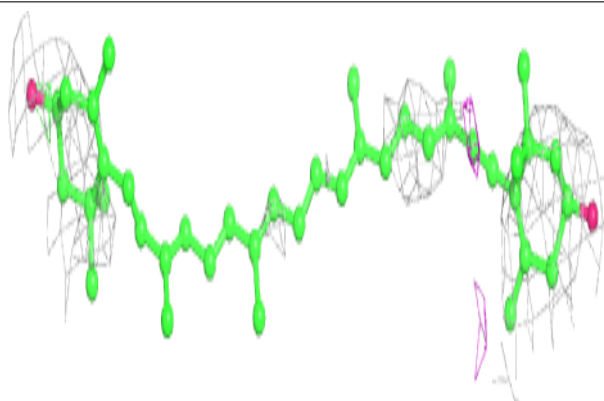


Electron density around BCR G 2011:

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

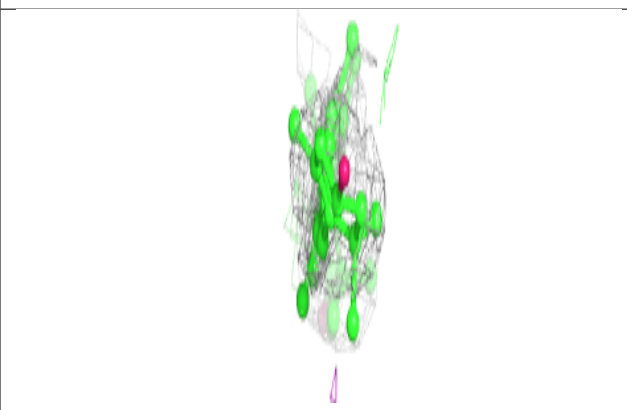
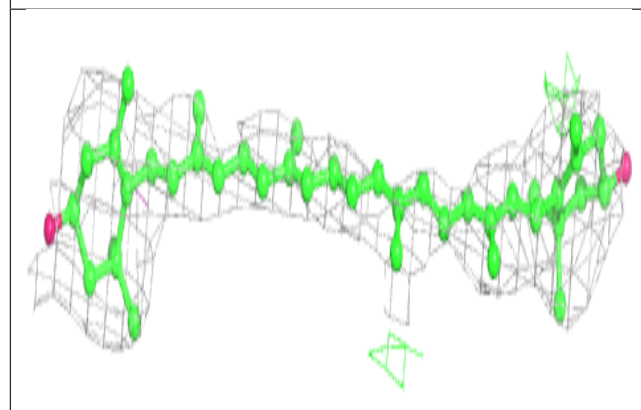
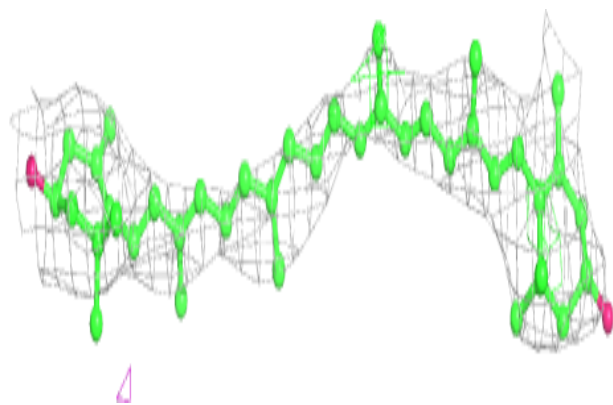
**Electron density around LUT 3 3501:**

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

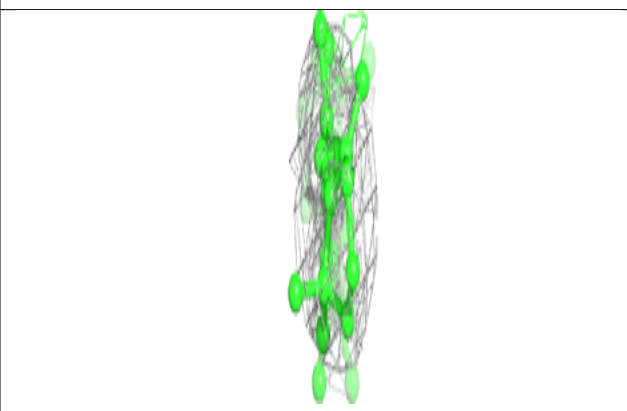
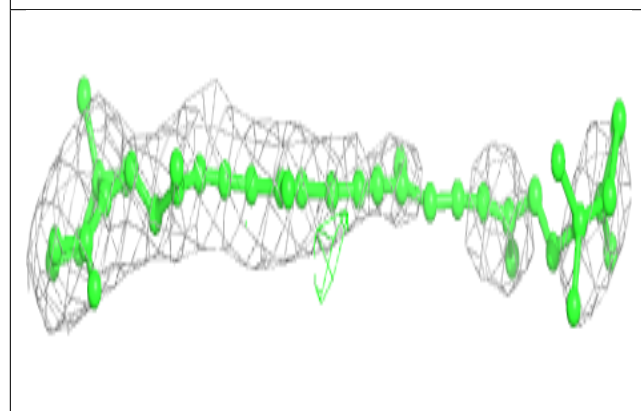
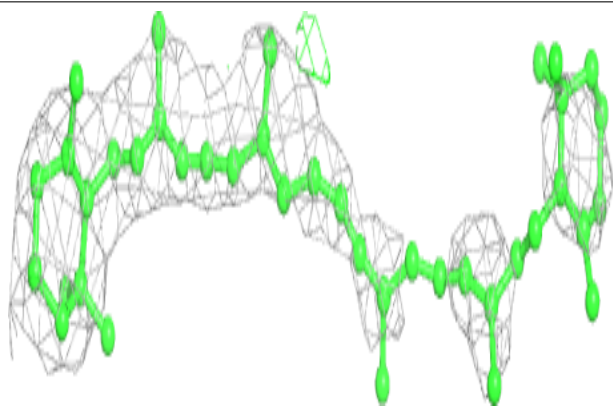


Electron density around LUT 2 2501:

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

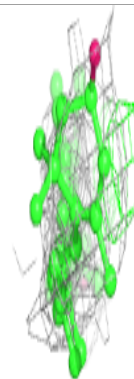
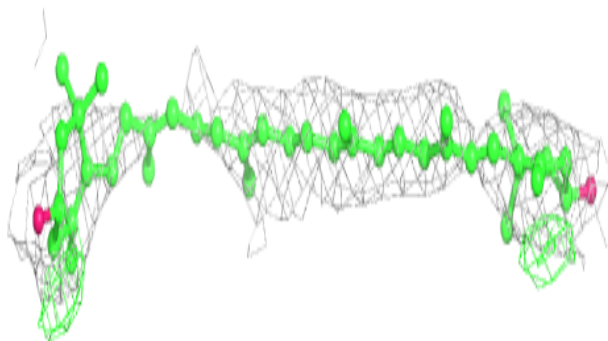
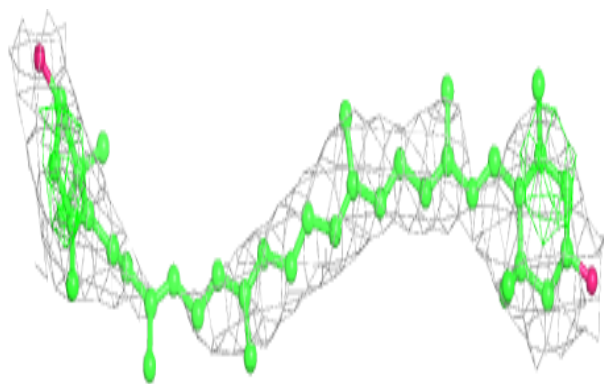
**Electron density around BCR B 6005:**

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

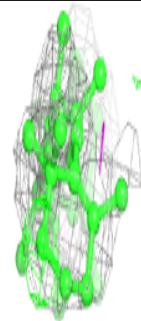
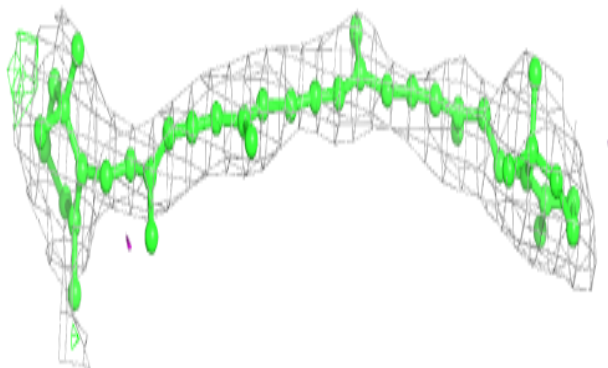
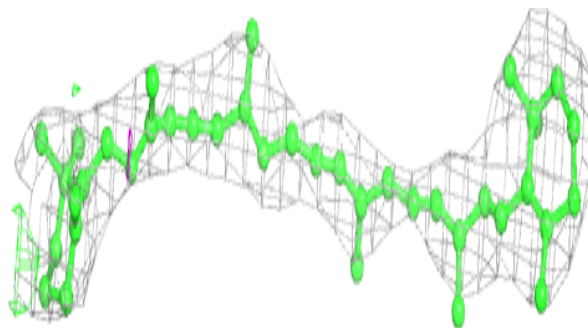


Electron density around LUT 3 3502:

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

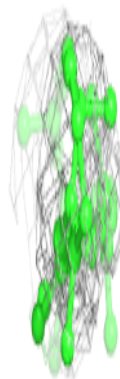
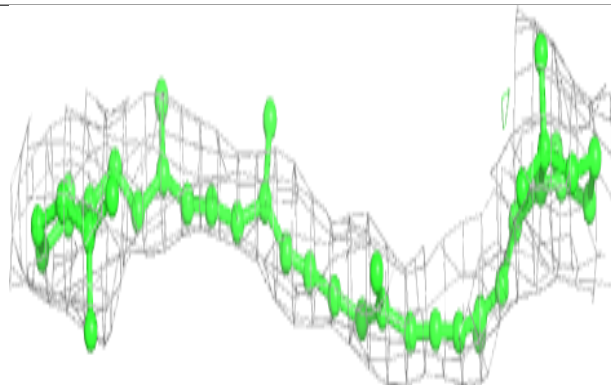
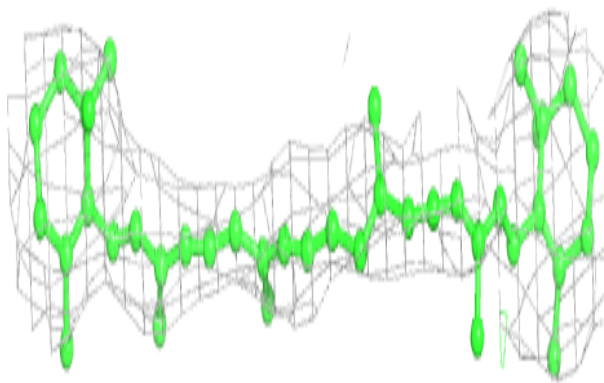
**Electron density around BCR J 6013:**

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

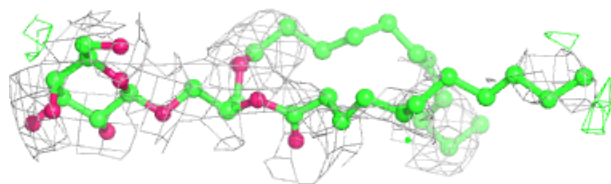
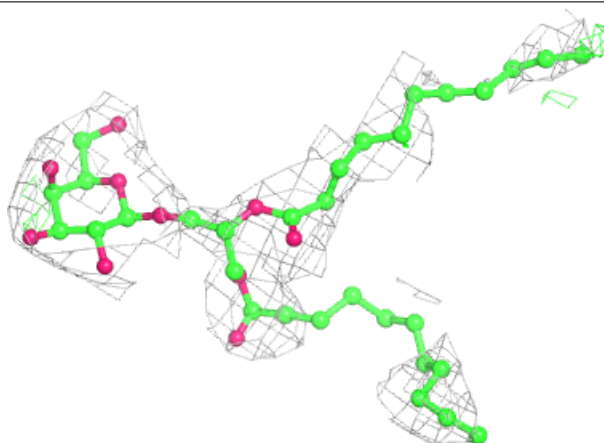


Electron density around BCR 3 3503:

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

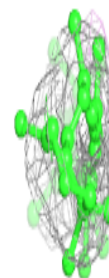
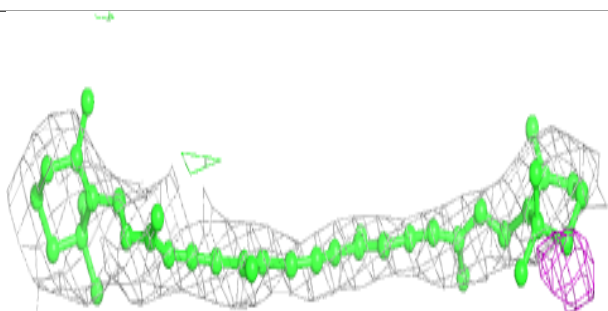
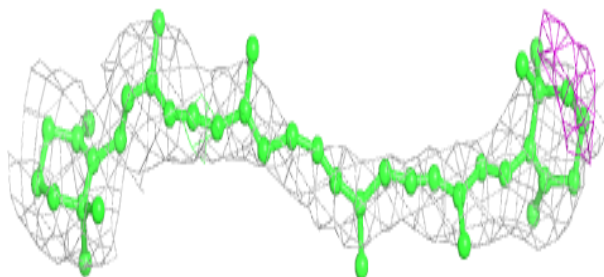
**Electron density around LMG G 2021:**

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

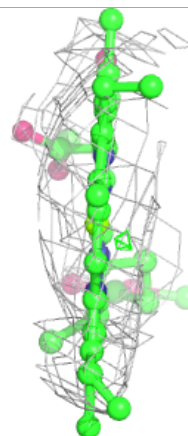
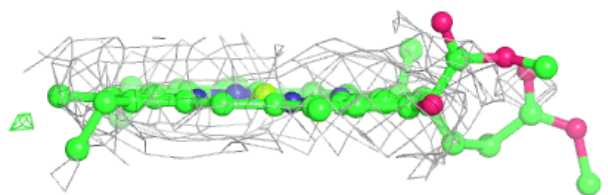
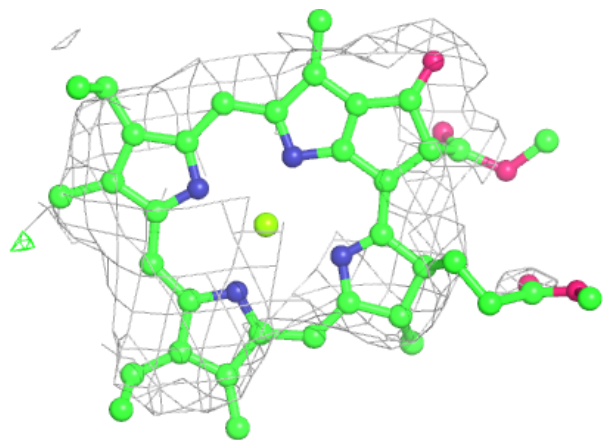


Electron density around BCR B 6004:

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

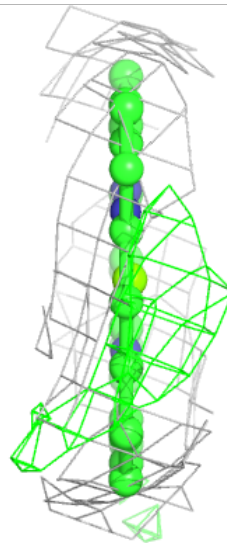
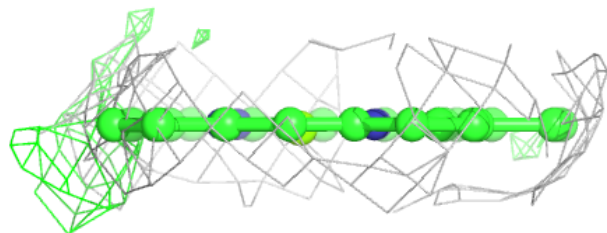
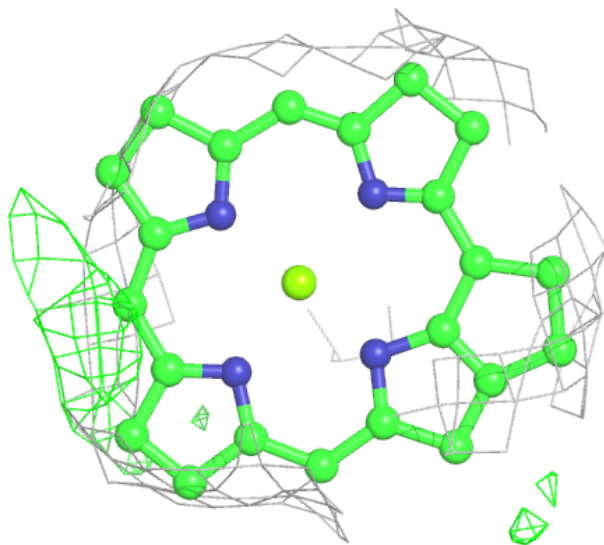
**Electron density around CLA 1 1013:**

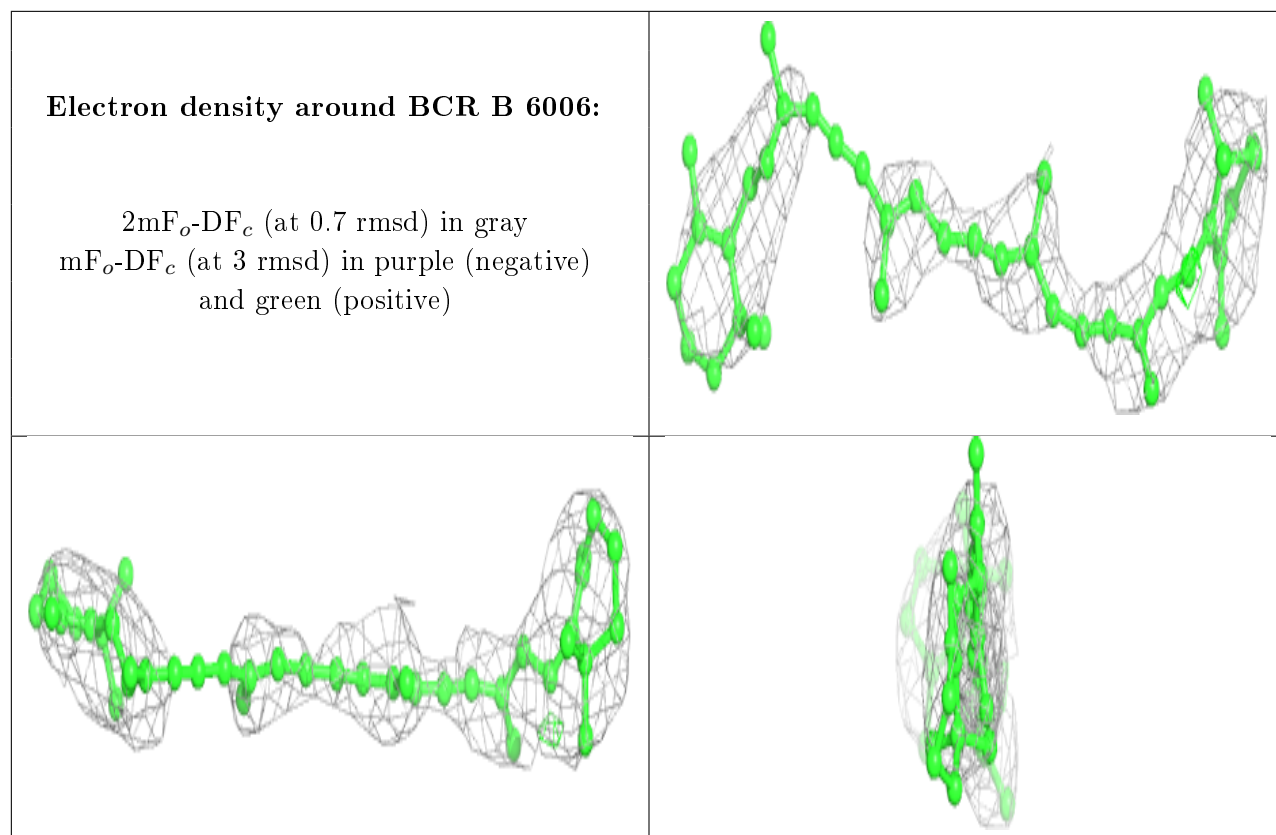
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 2019:

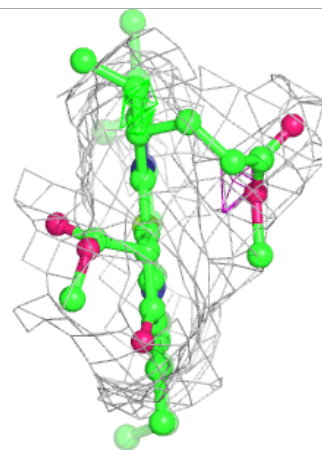
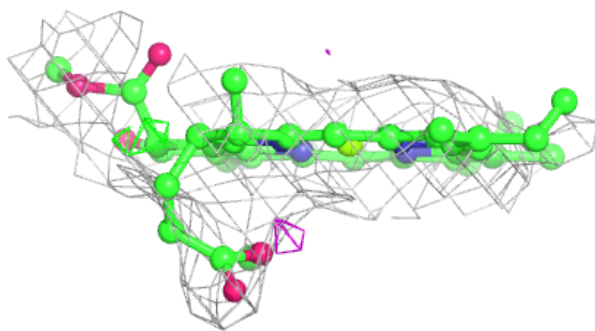
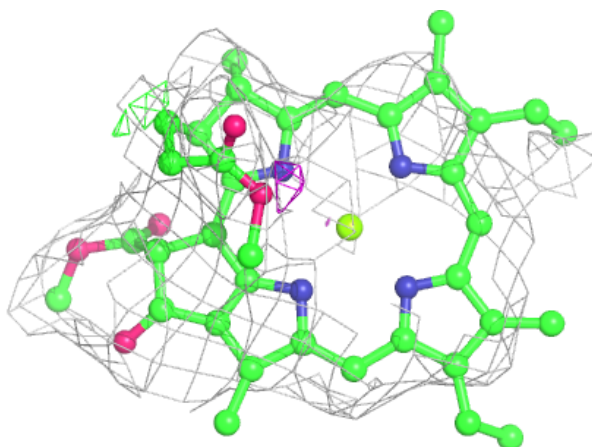
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





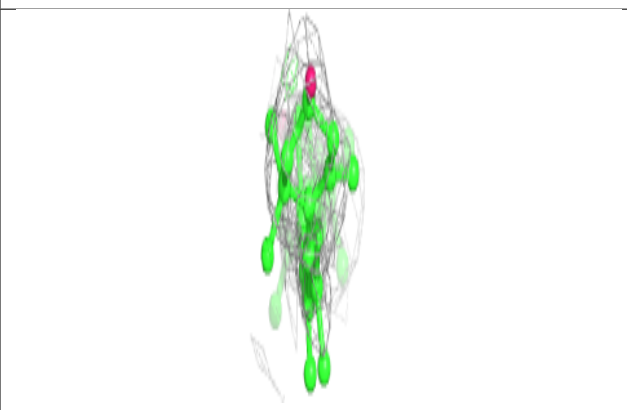
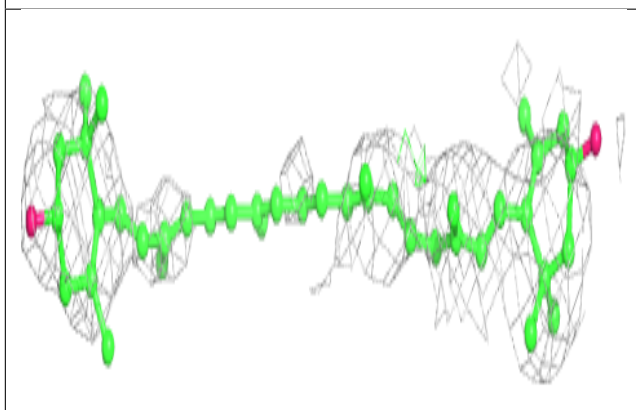
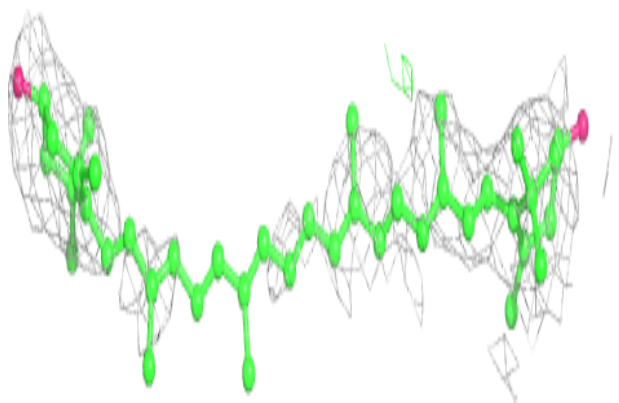
Electron density around CLA 4 4016:

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

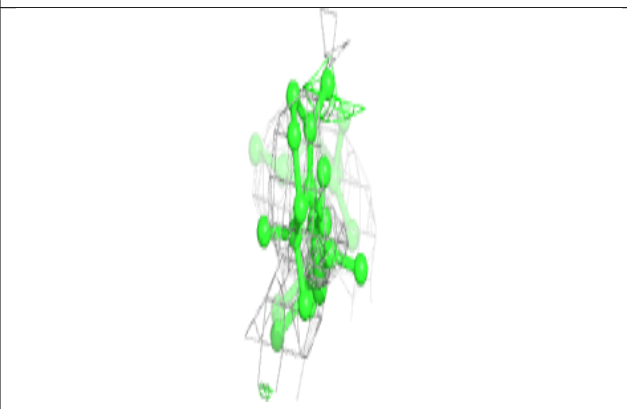
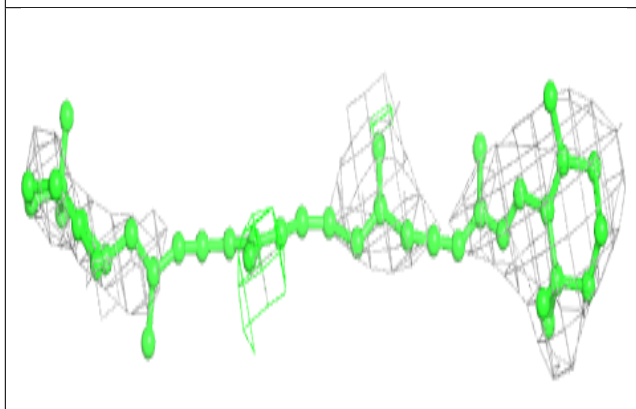
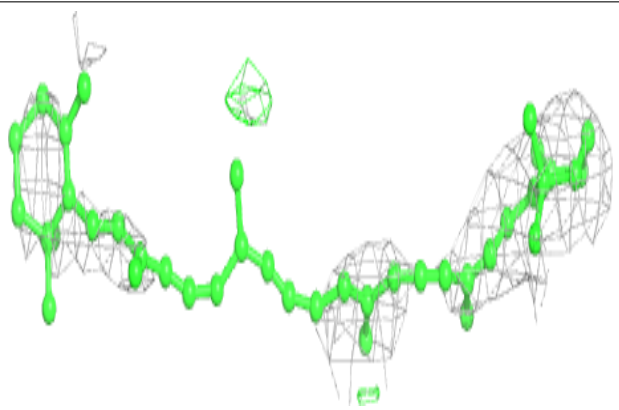


Electron density around LUT 1 1501:

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

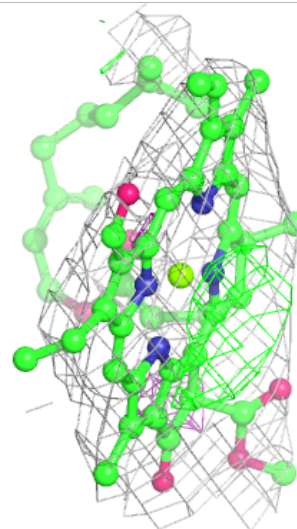
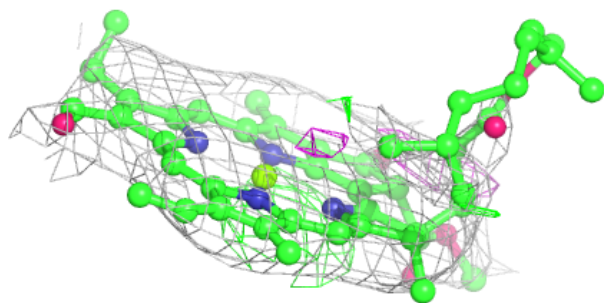
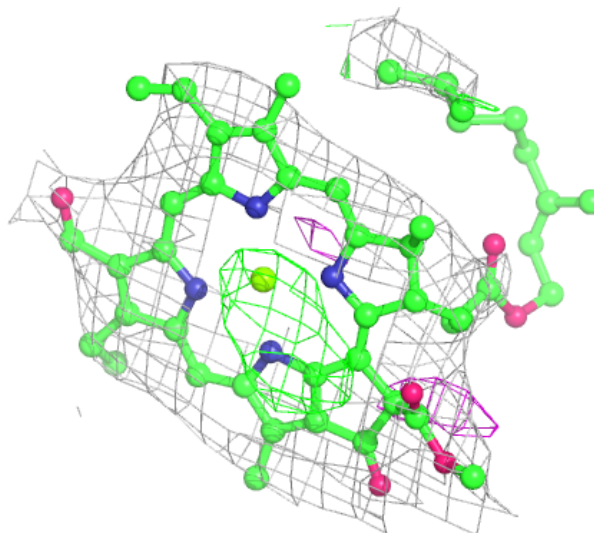
**Electron density around BCR K 2011:**

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



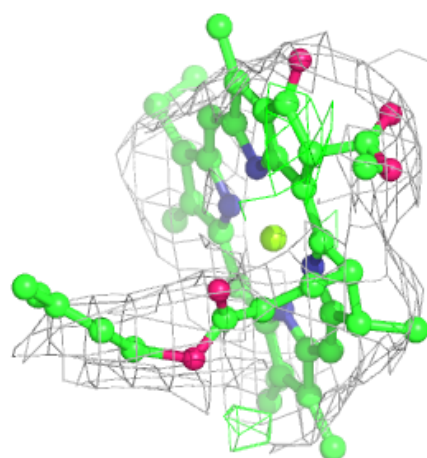
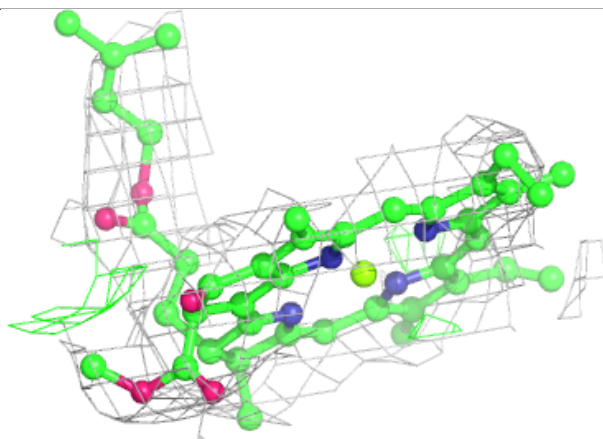
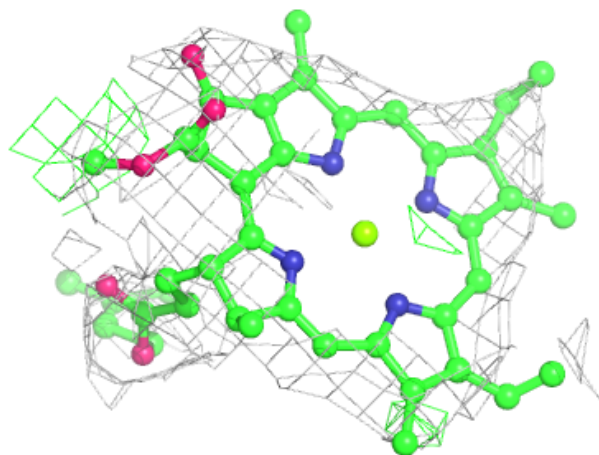
Electron density around CHL 3 3011:

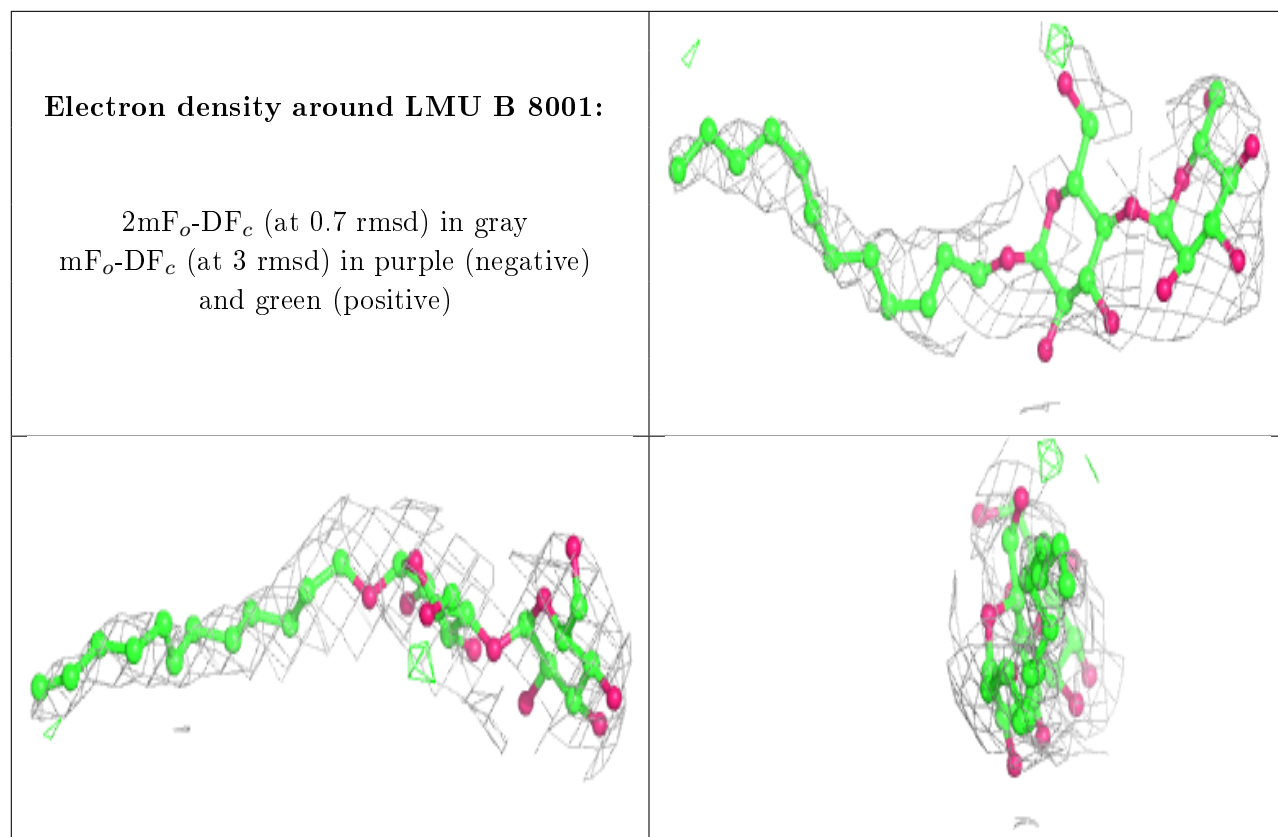
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 4 4006:

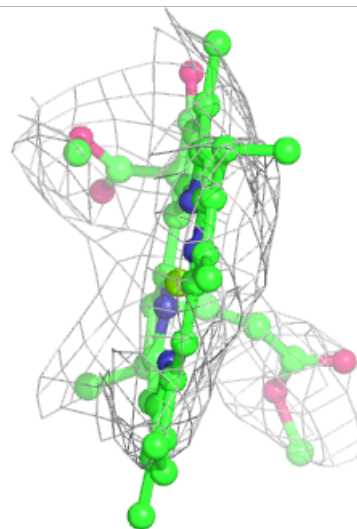
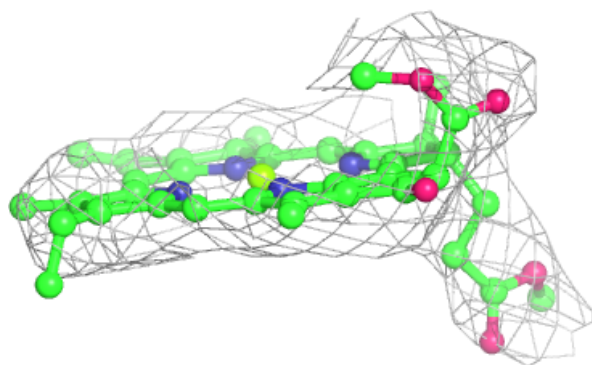
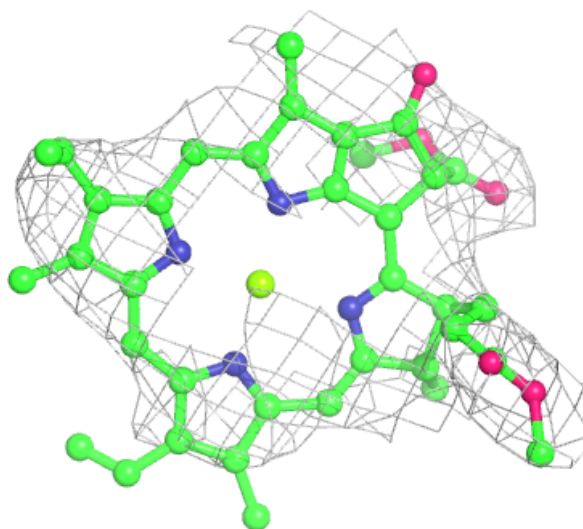
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





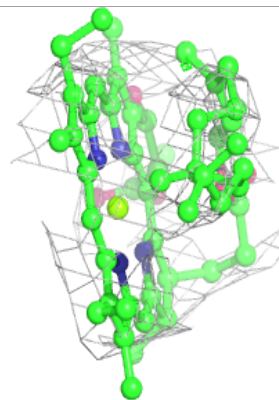
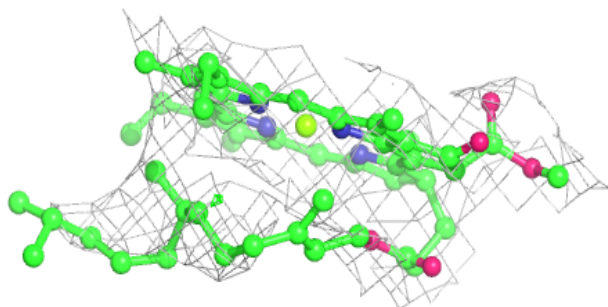
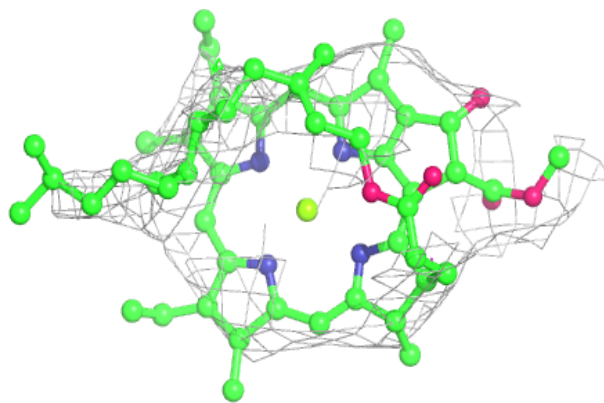
Electron density around CLA 1 1008:

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



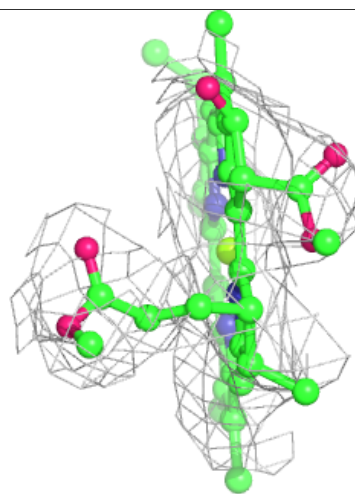
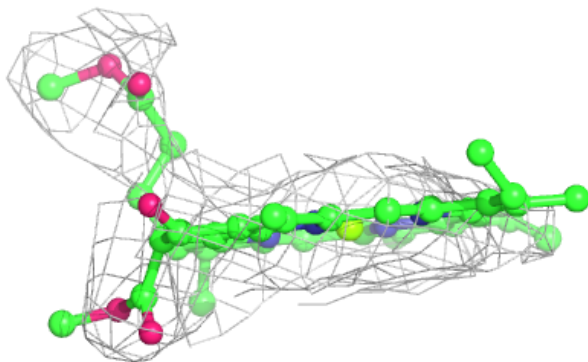
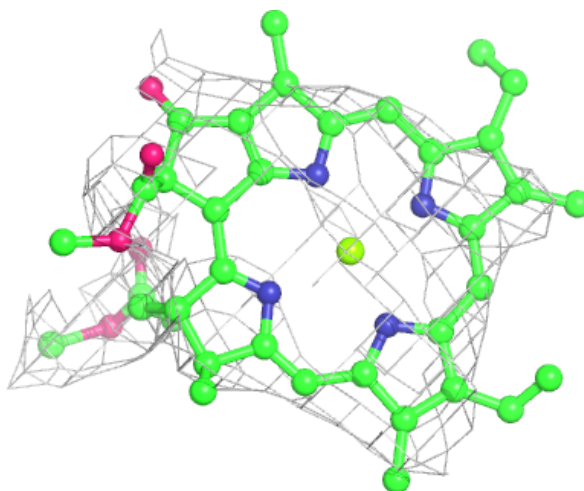
Electron density around CLA 3 3003:

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



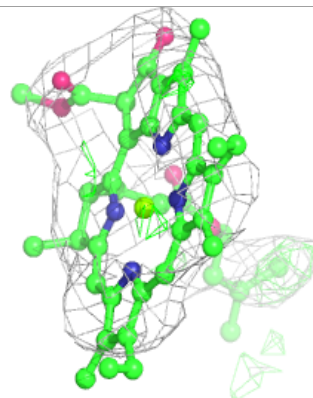
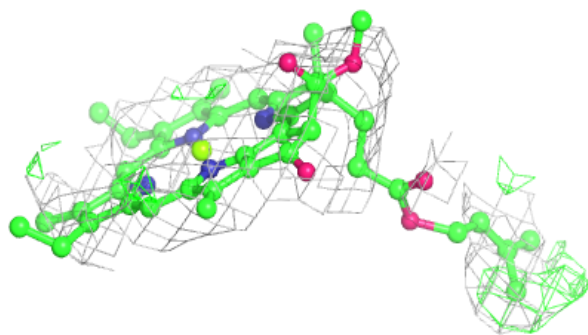
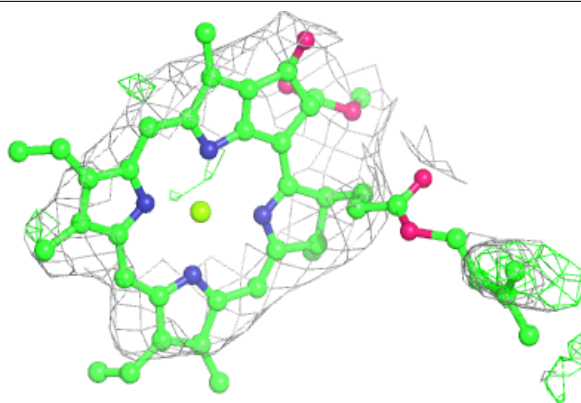
Electron density around CLA K 1001:

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

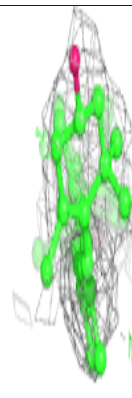
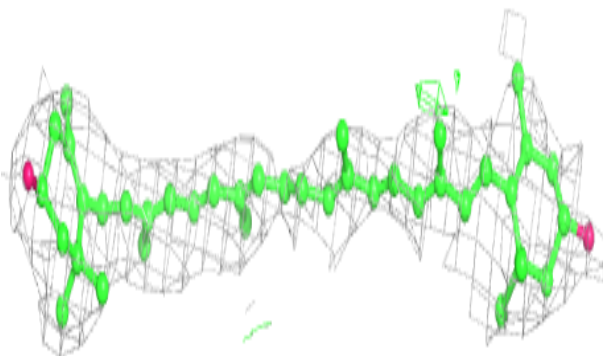
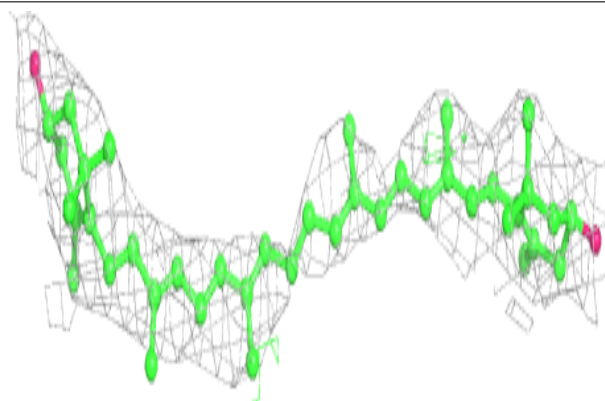


Electron density around CLA 3 3007:

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

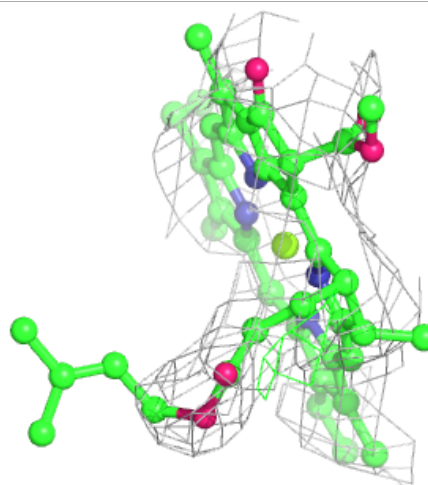
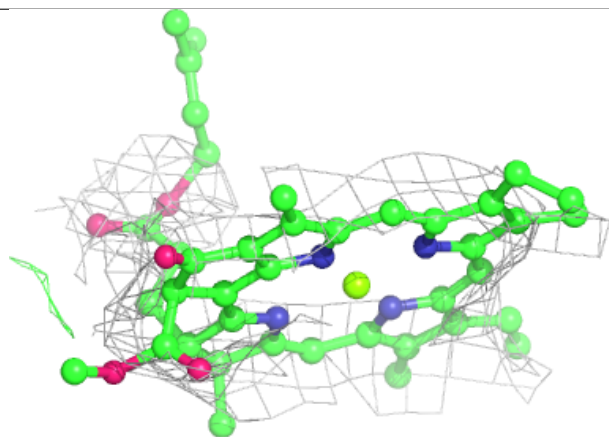
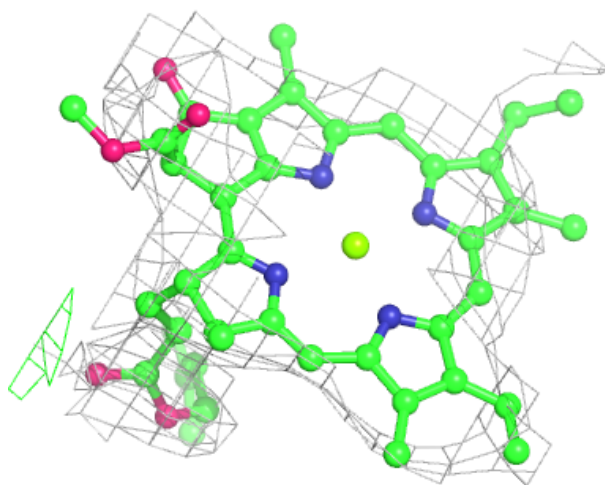
**Electron density around LUT 4 4501:**

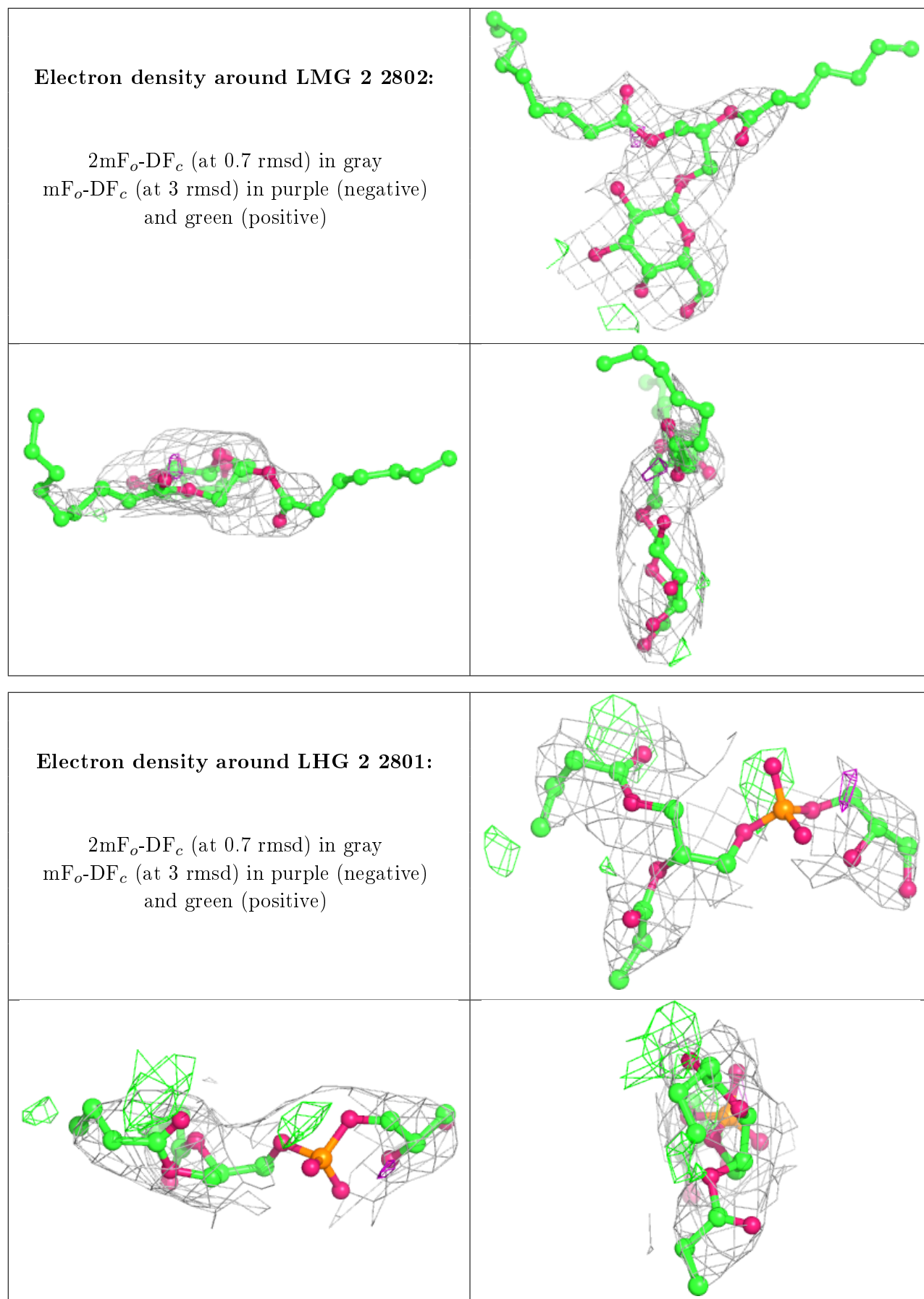
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

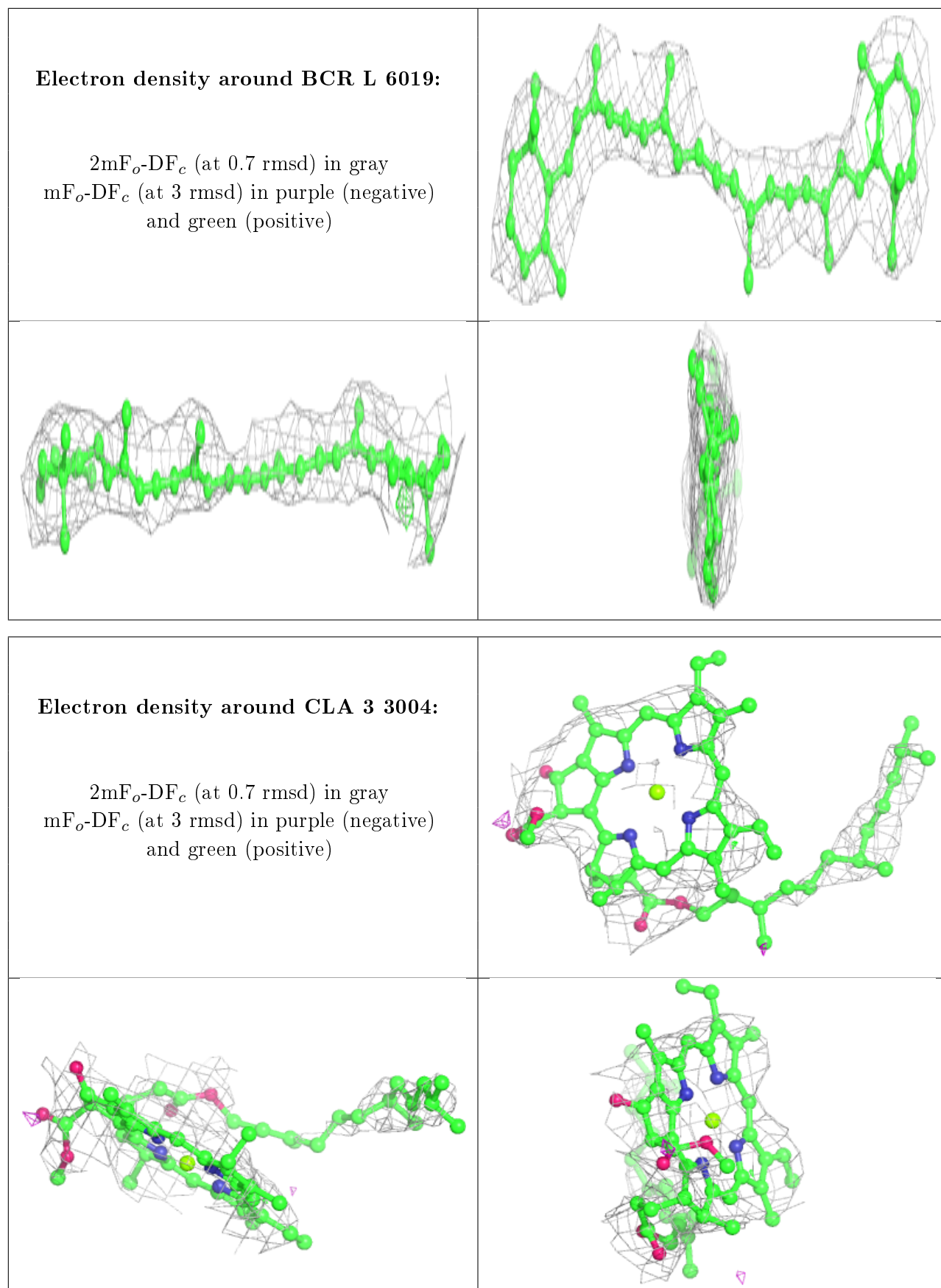


Electron density around CLA 3 3018:

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

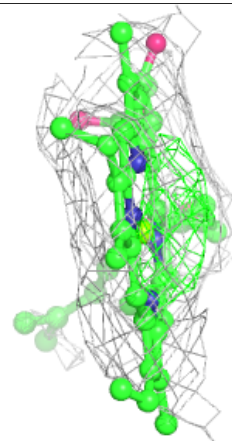
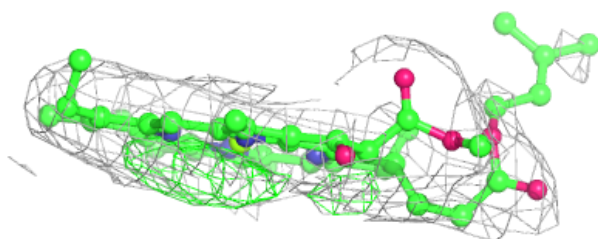
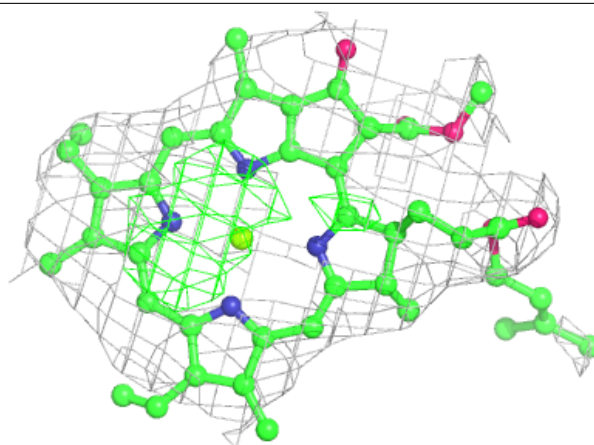






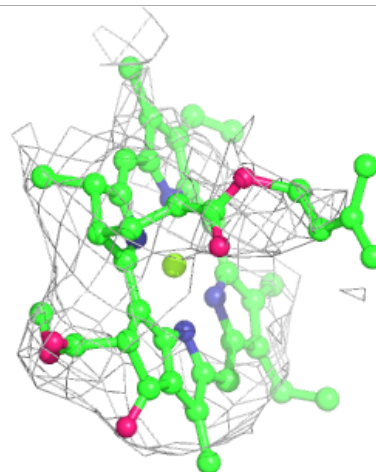
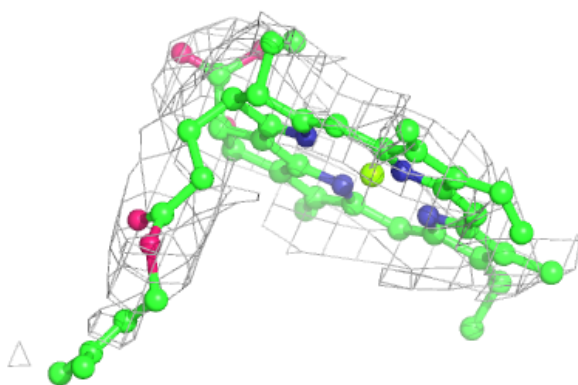
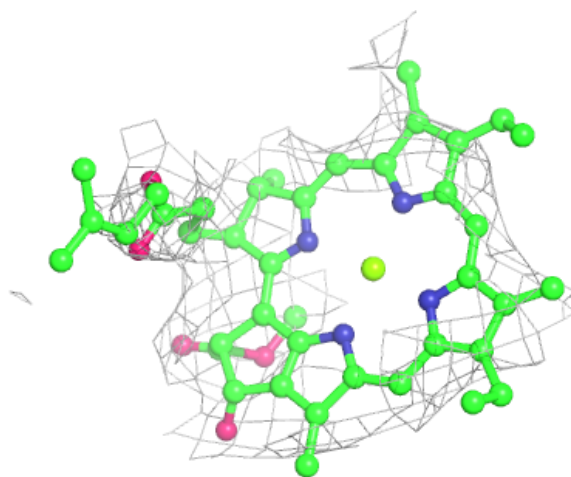
Electron density around CLA 4 4002:

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



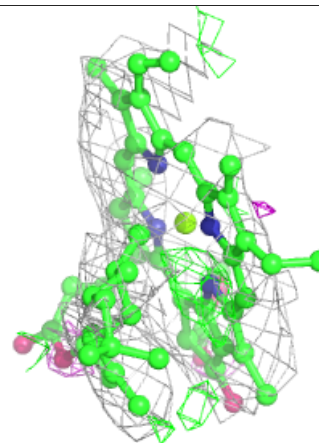
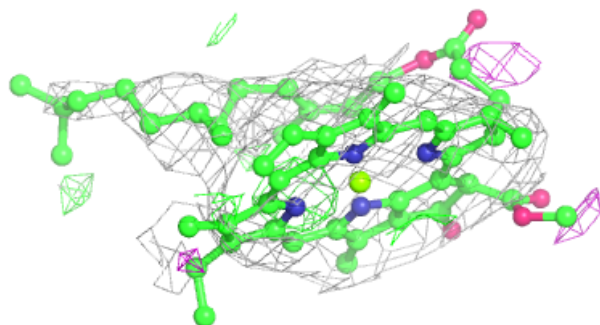
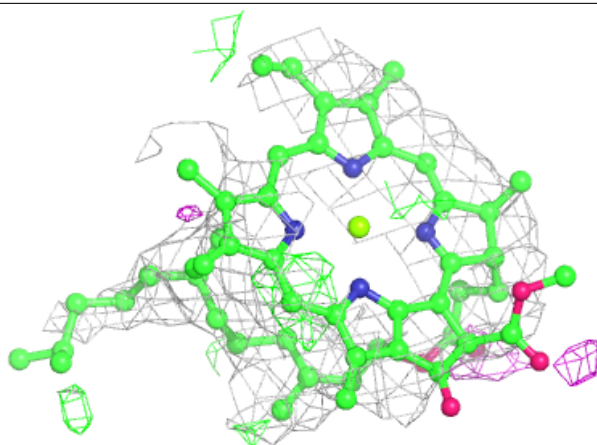
Electron density around CLA 3 3006:

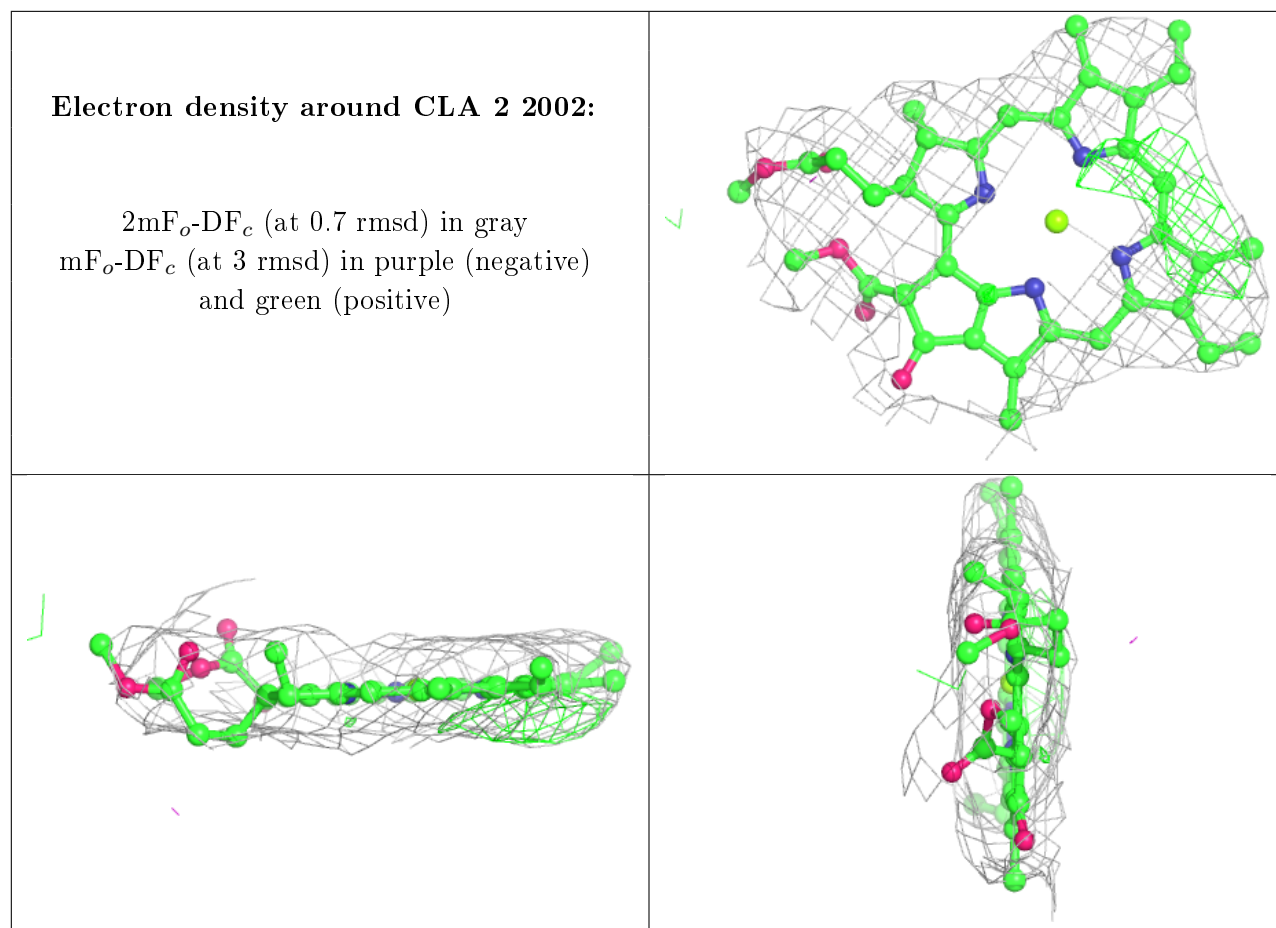
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 3 3010:

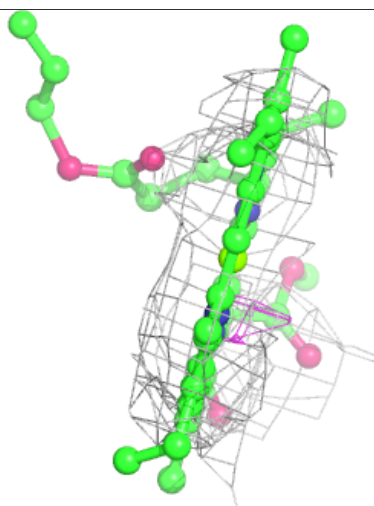
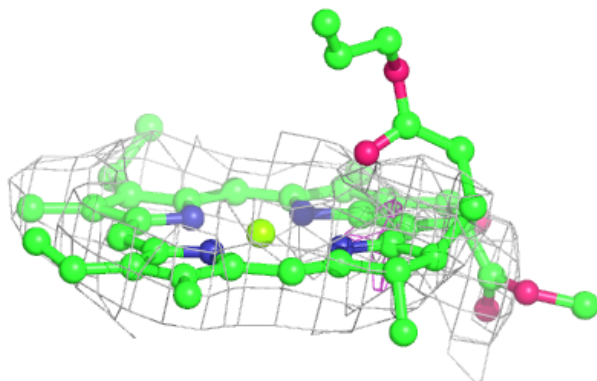
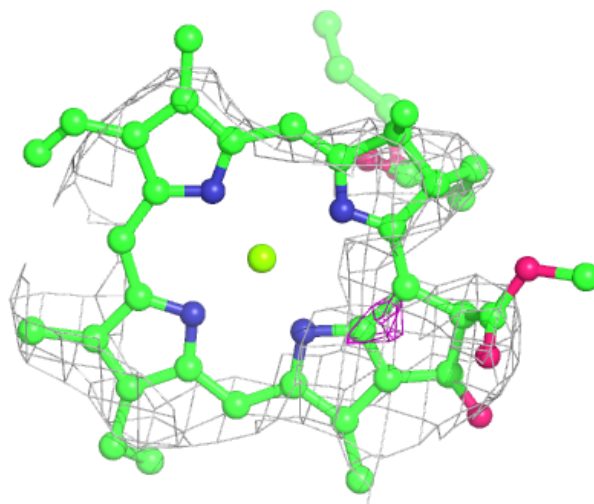
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

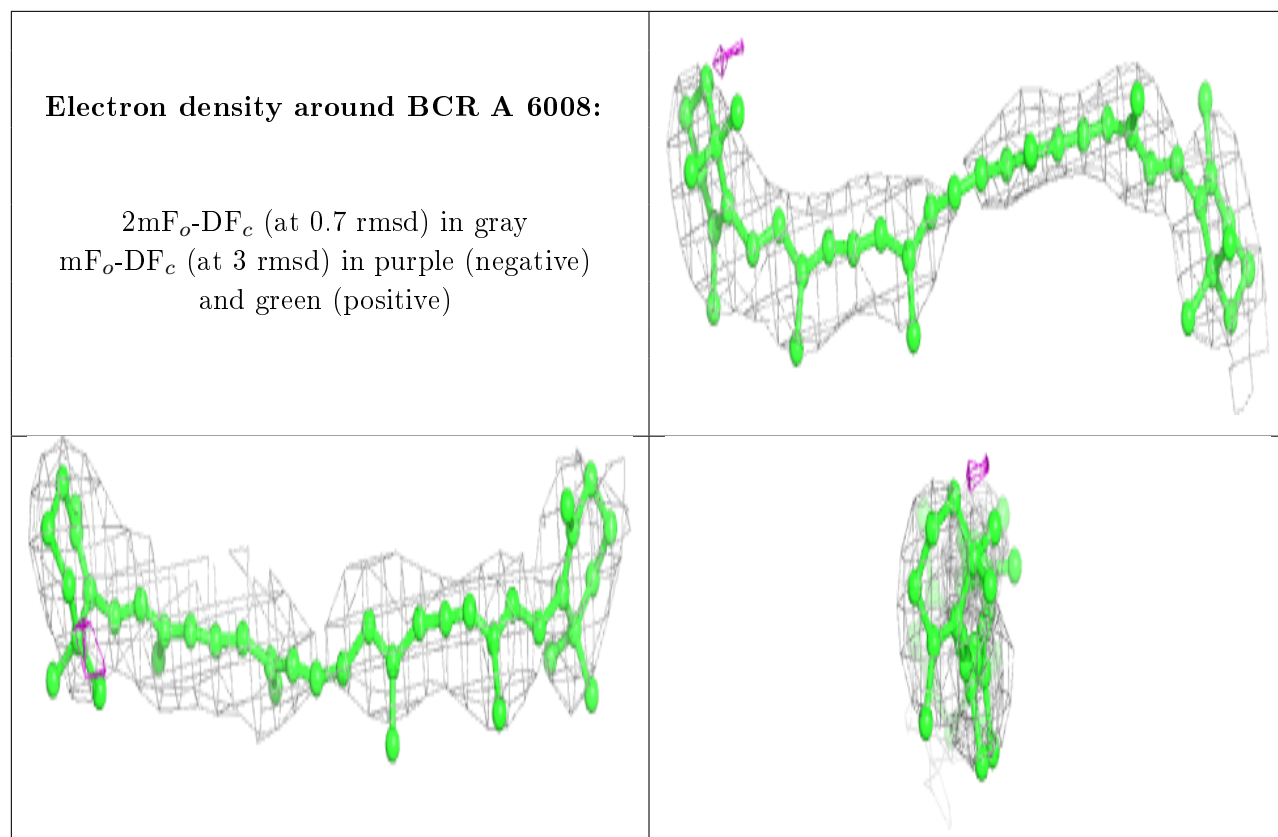




Electron density around CLA 3 3008:

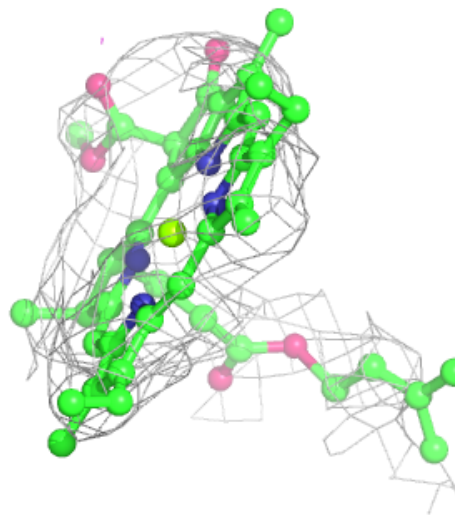
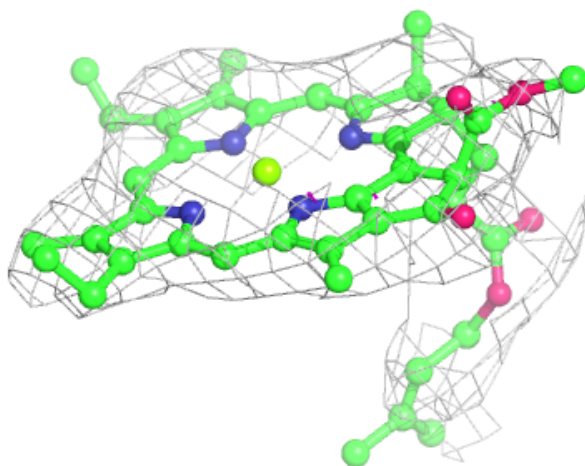
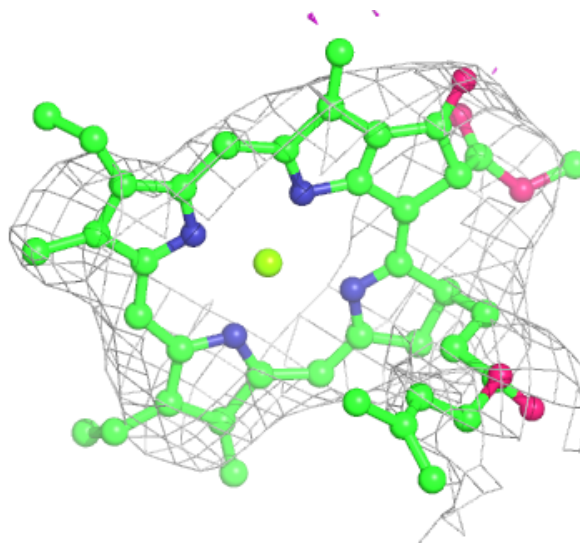
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





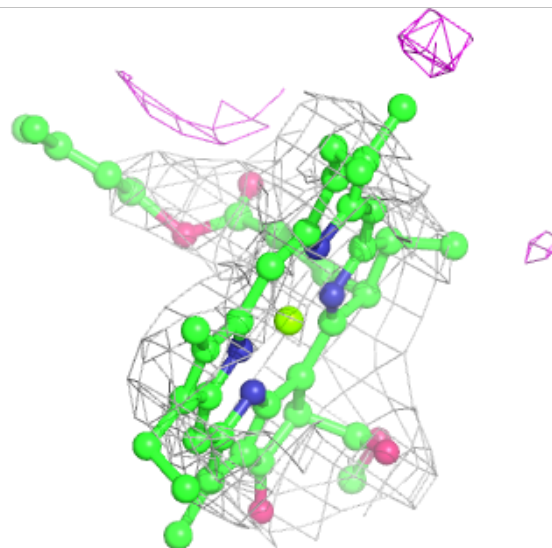
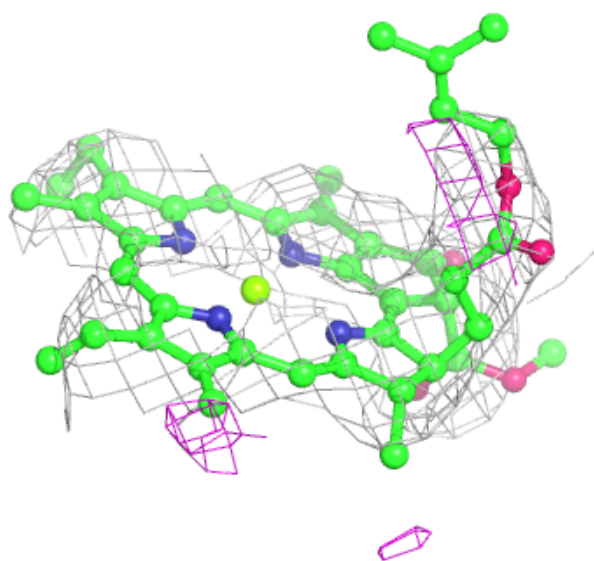
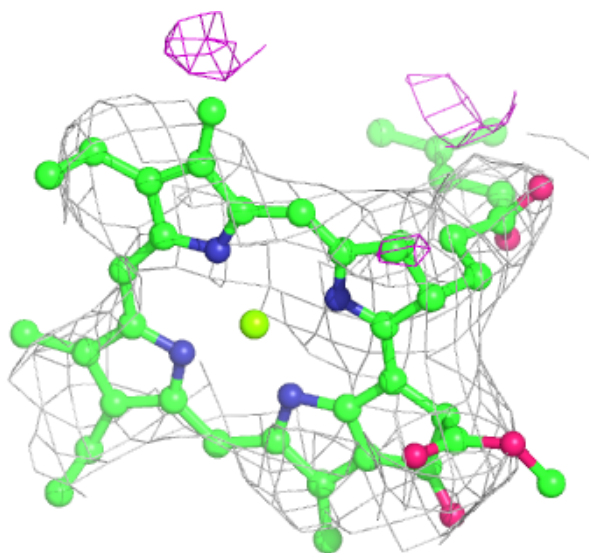
Electron density around CLA 1 1006:

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



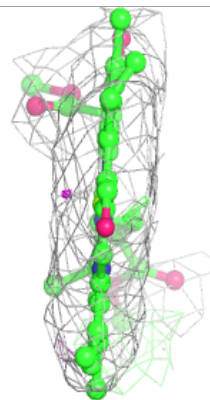
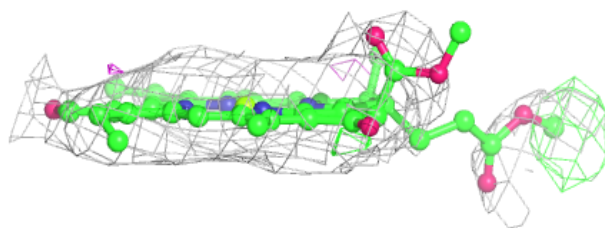
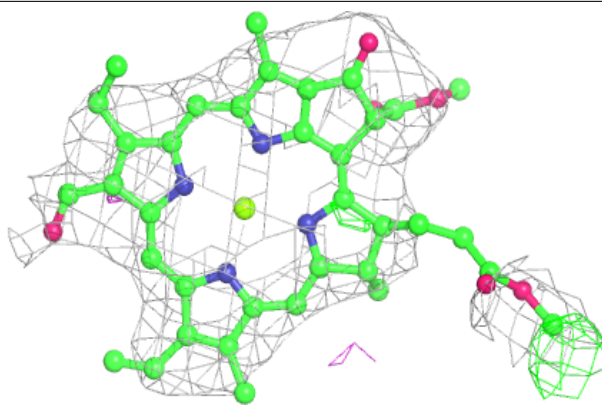
Electron density around CLA L 1503:

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

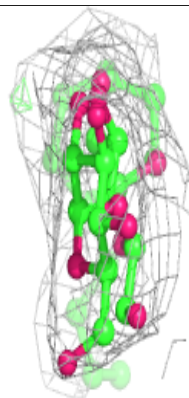
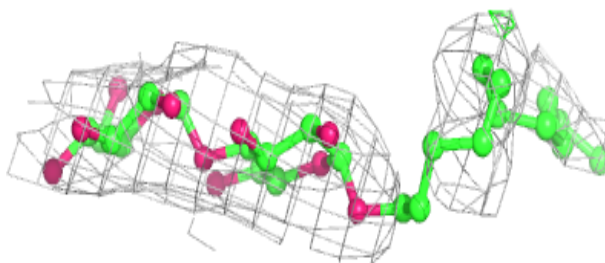
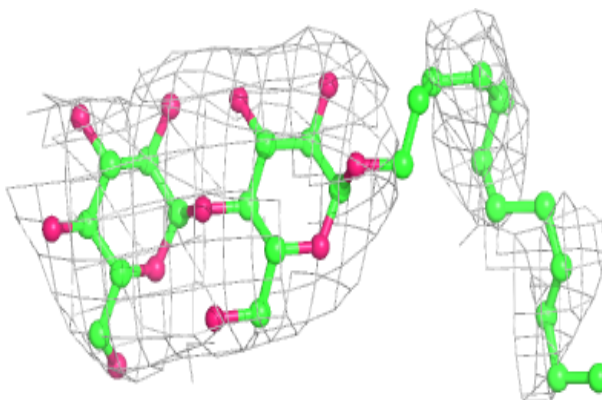


Electron density around CHL 4 4010:

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

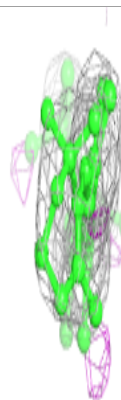
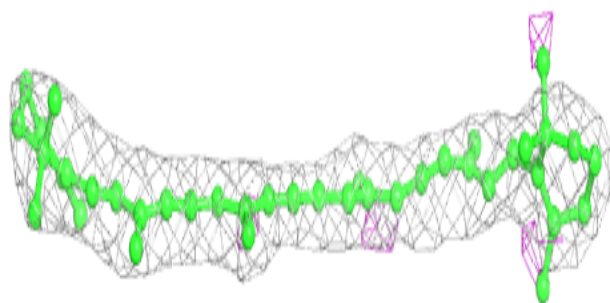
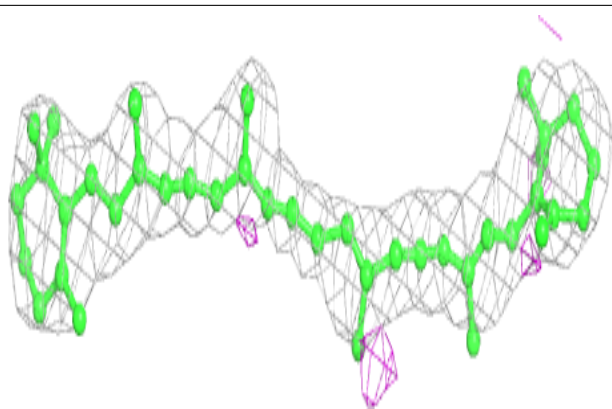
**Electron density around LMU B 8002:**

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

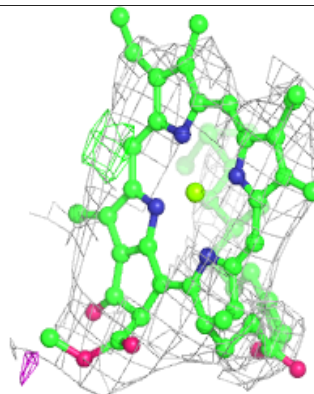
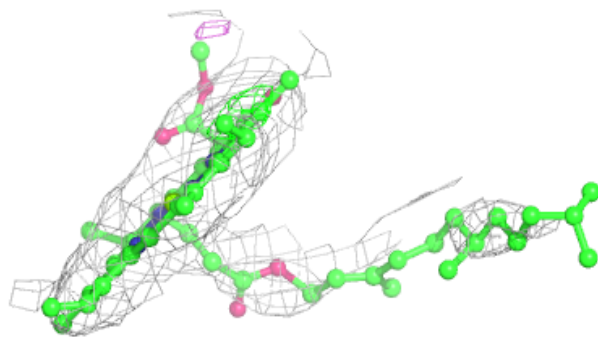
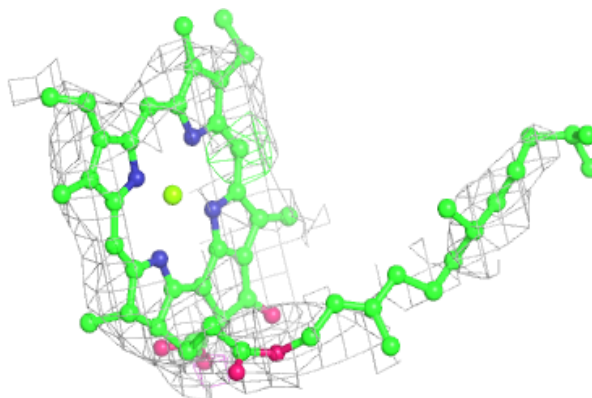


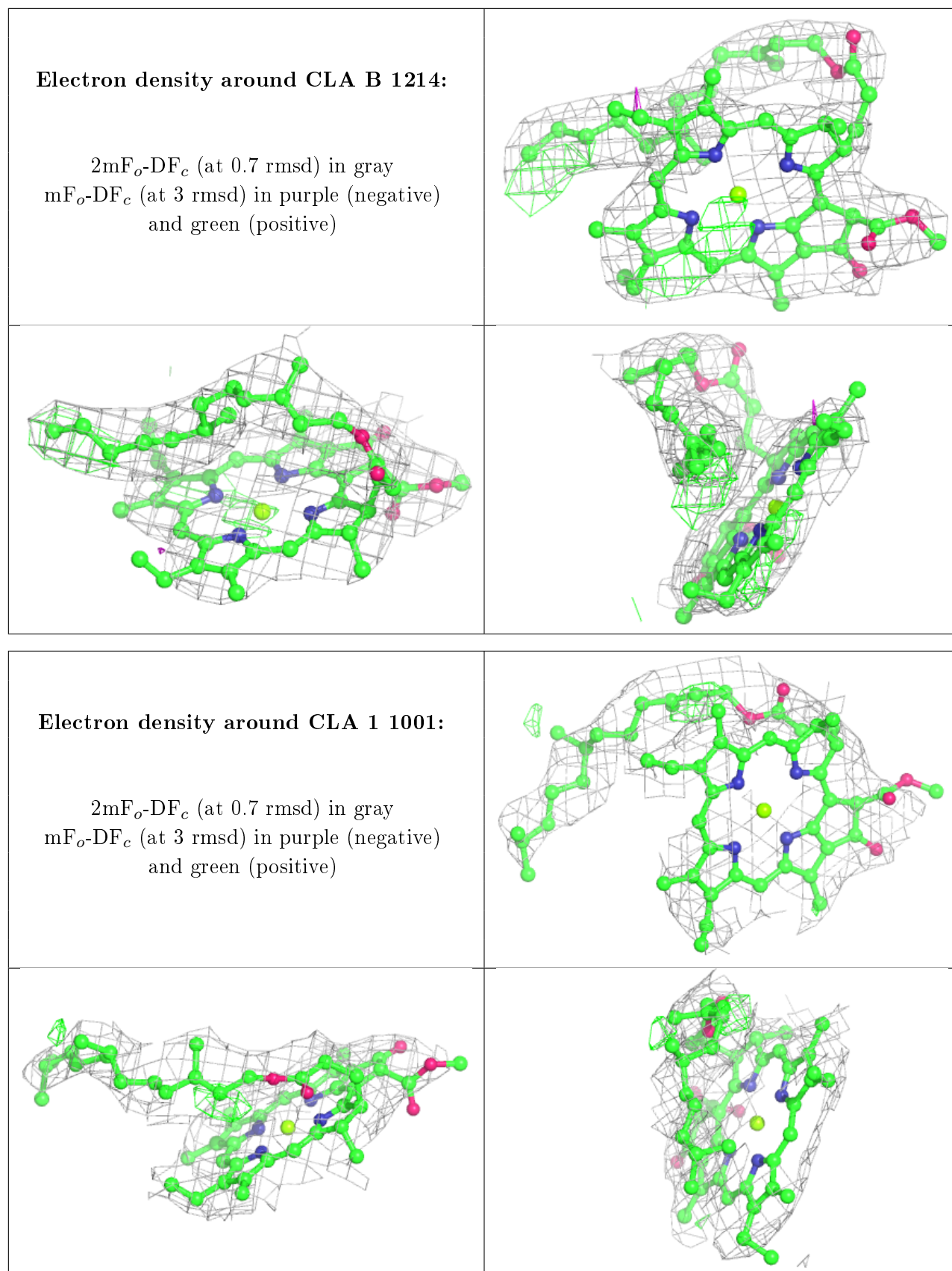
Electron density around BCR J 6012:

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

**Electron density around CLA 2 2007:**

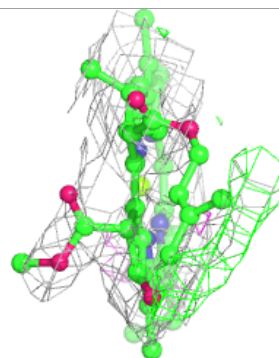
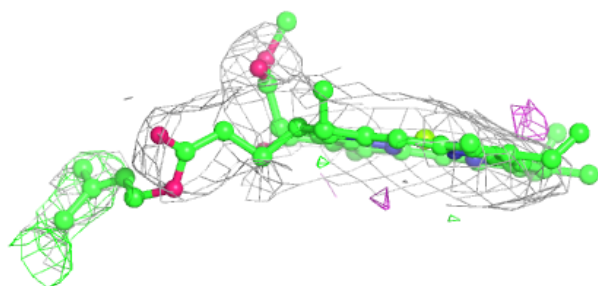
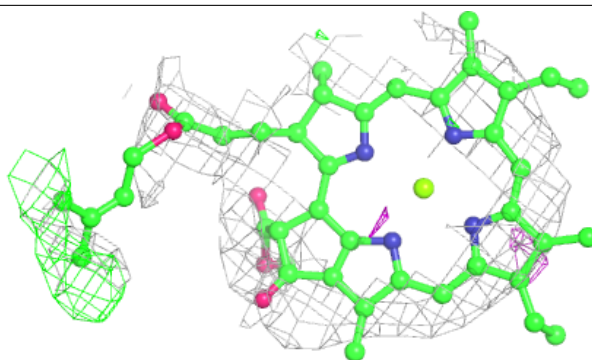
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



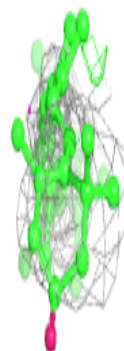
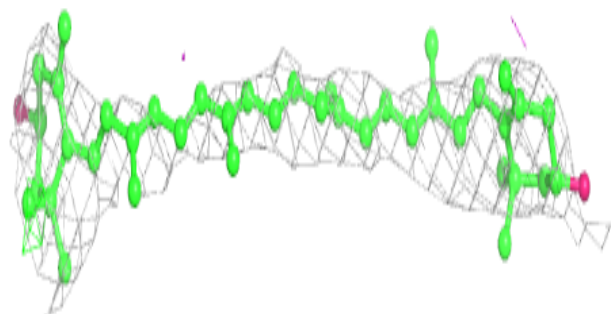
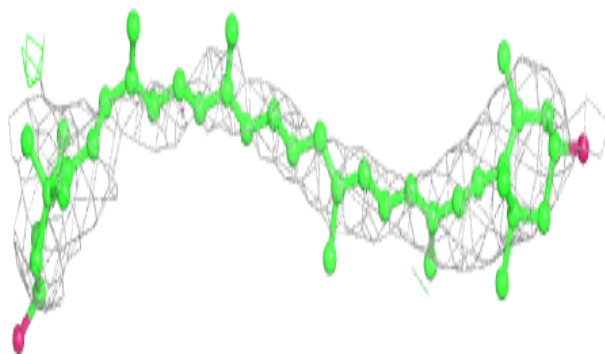


Electron density around CLA J 1302:

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

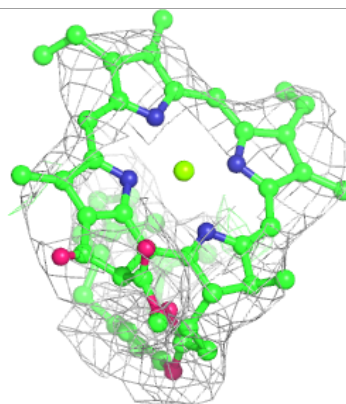
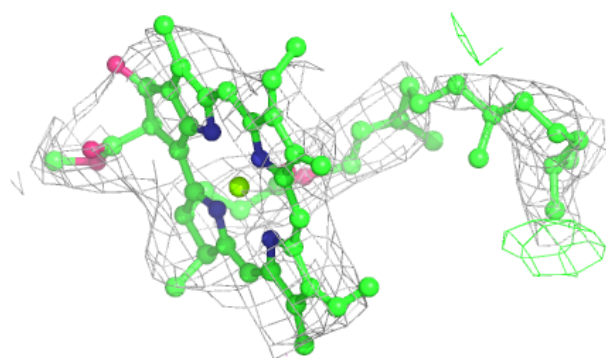
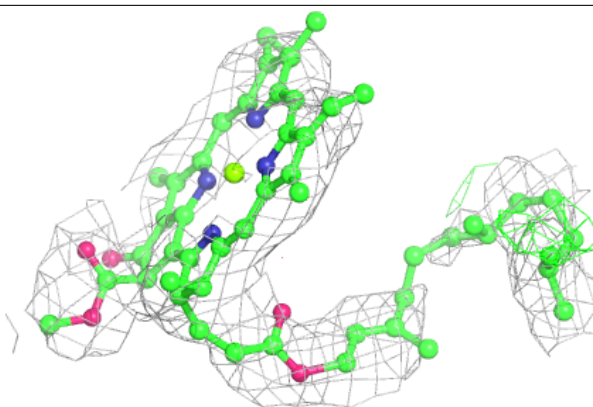
**Electron density around LUT 4 4503:**

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

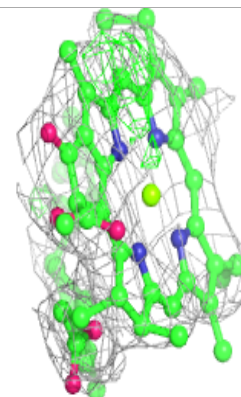
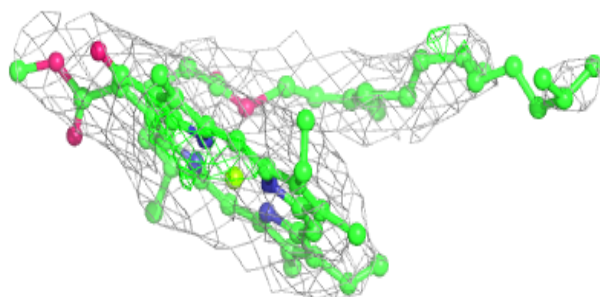
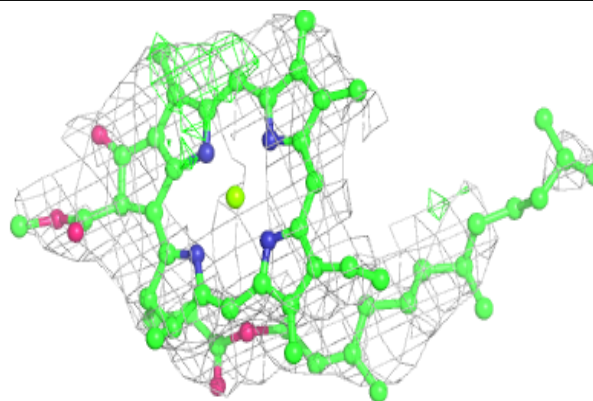


Electron density around CLA G 1003:

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

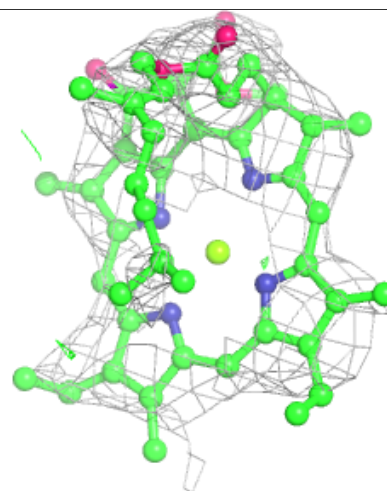
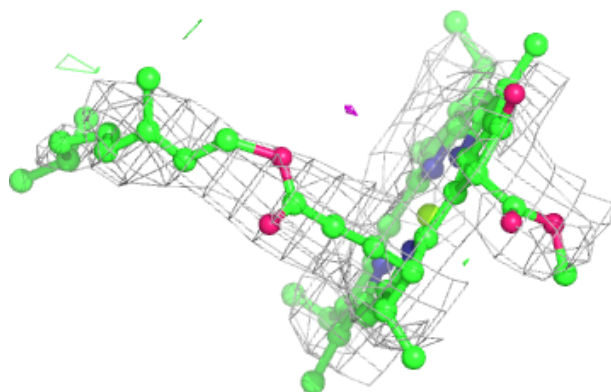
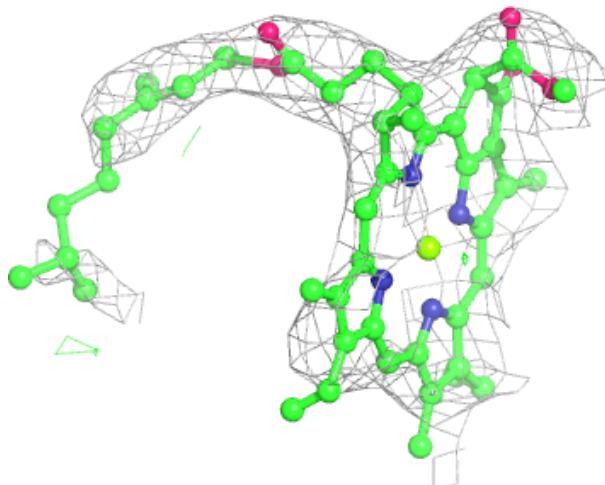
**Electron density around CLA 4 4001:**

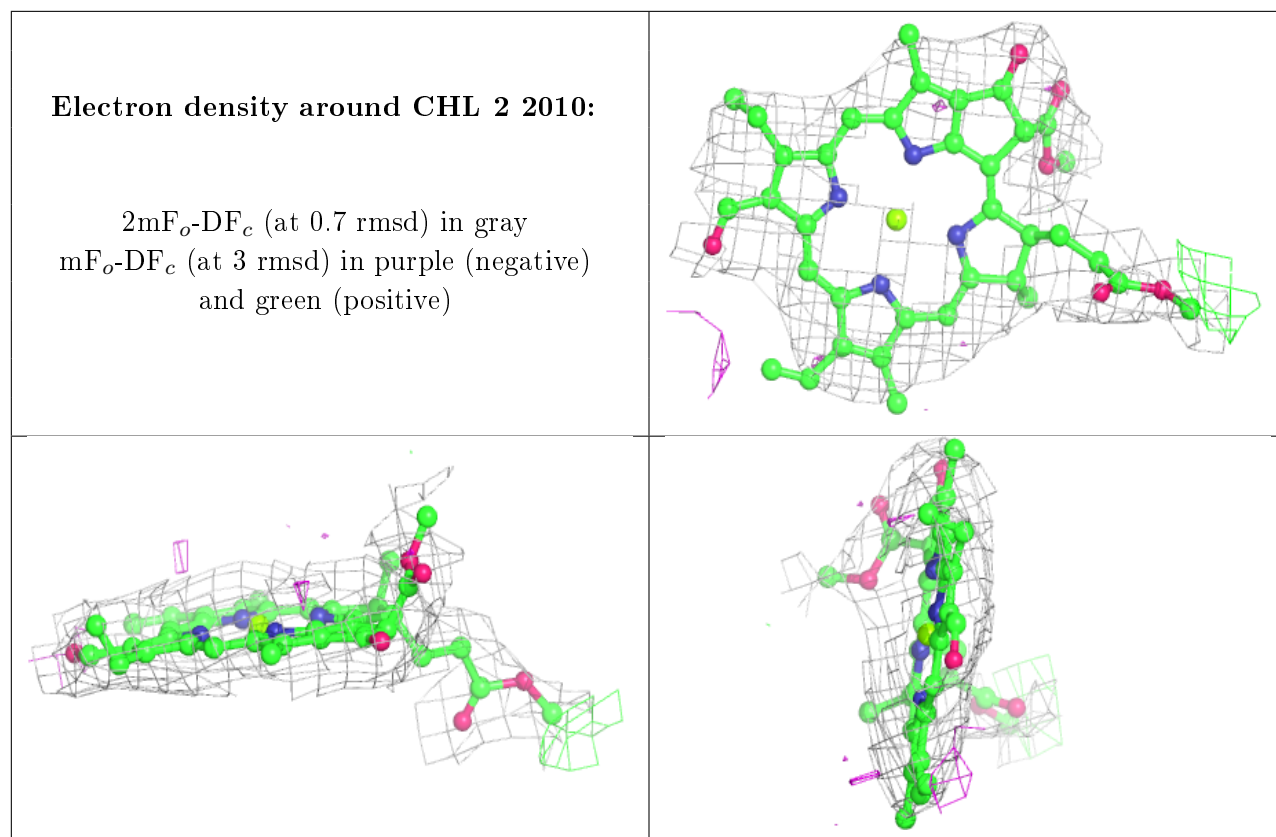
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1212:

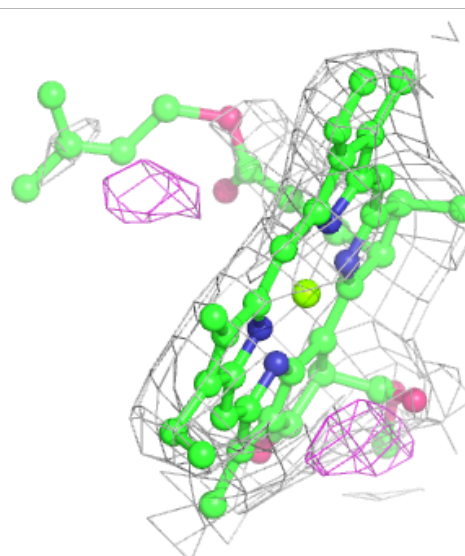
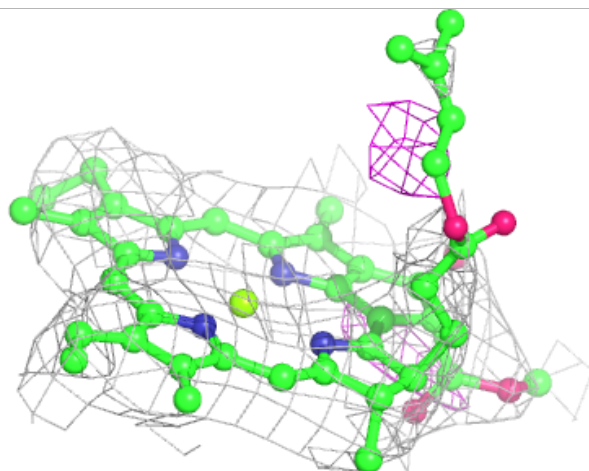
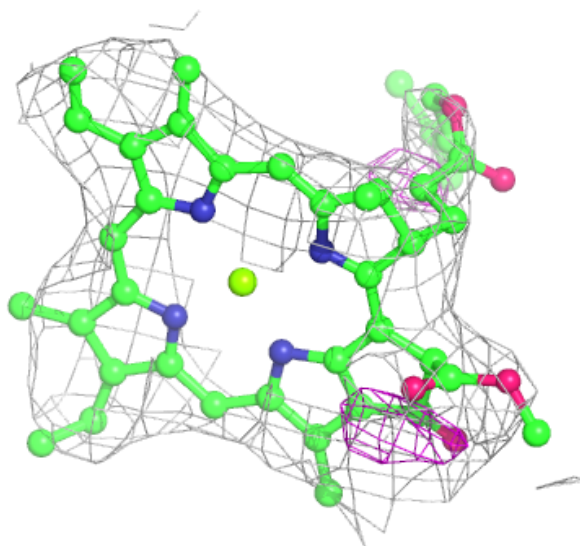
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





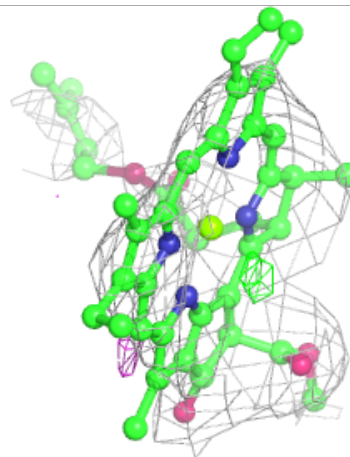
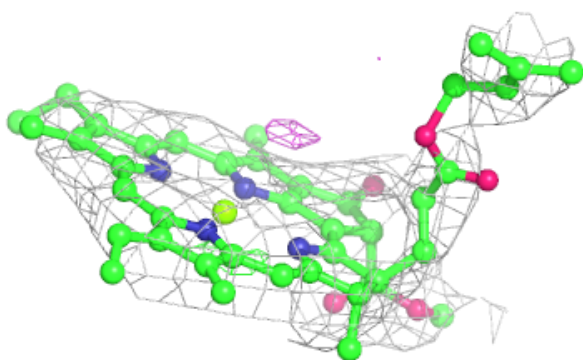
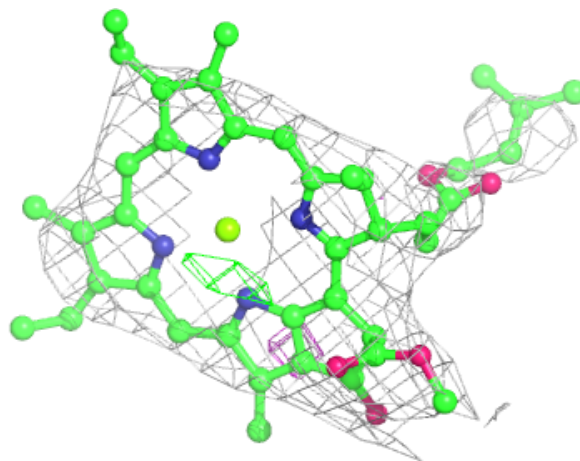
Electron density around CLA 3 3012:

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



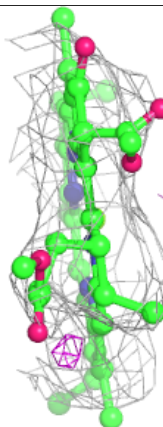
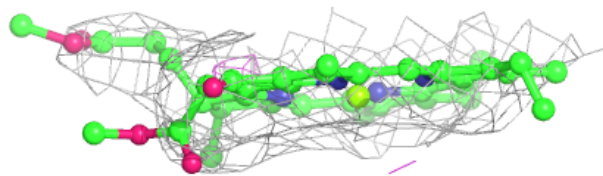
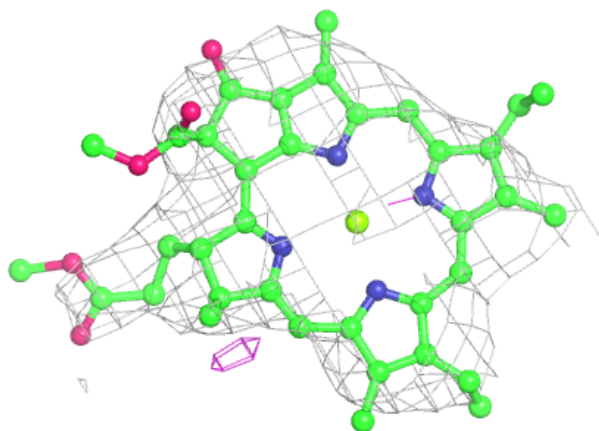
Electron density around CLA 1 1011:

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

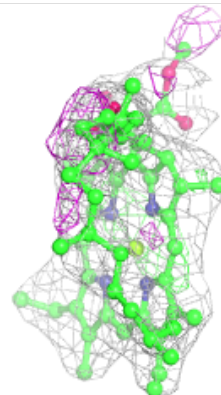
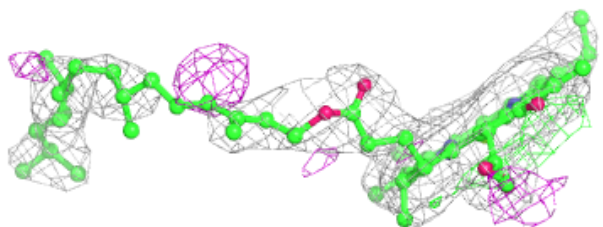
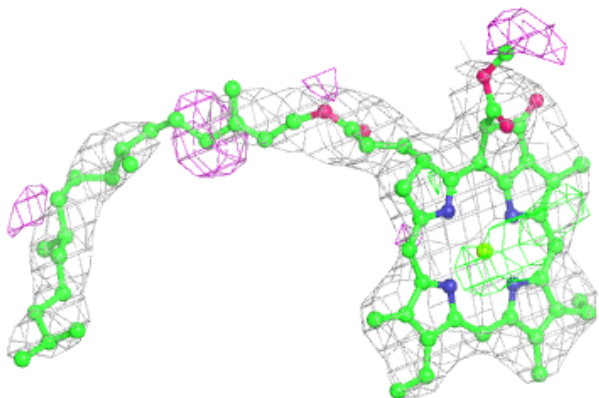


Electron density around CLA H 1000:

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

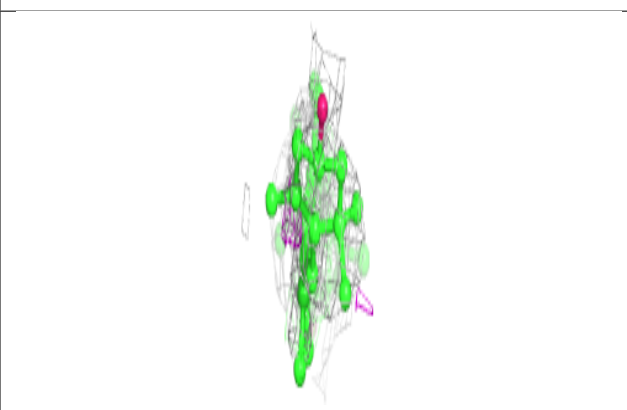
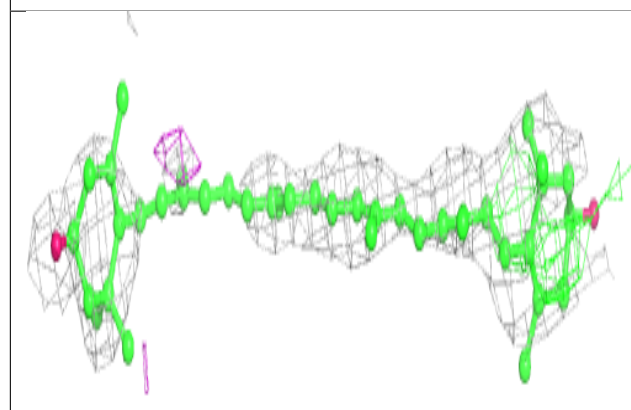
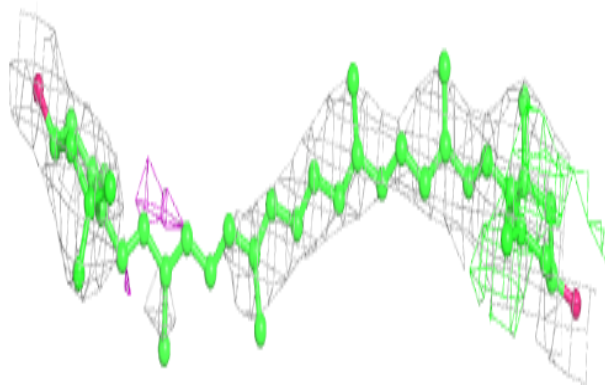
**Electron density around CLA B 1222:**

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

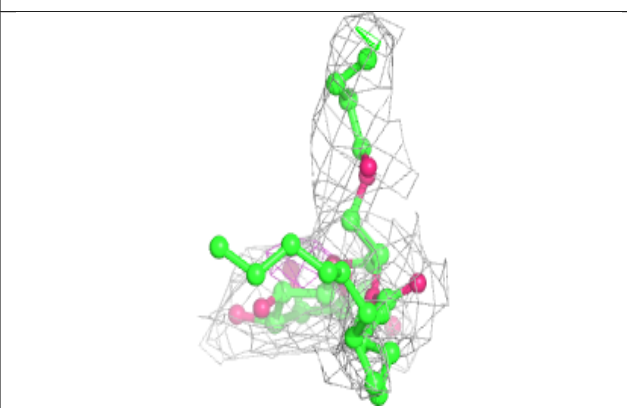
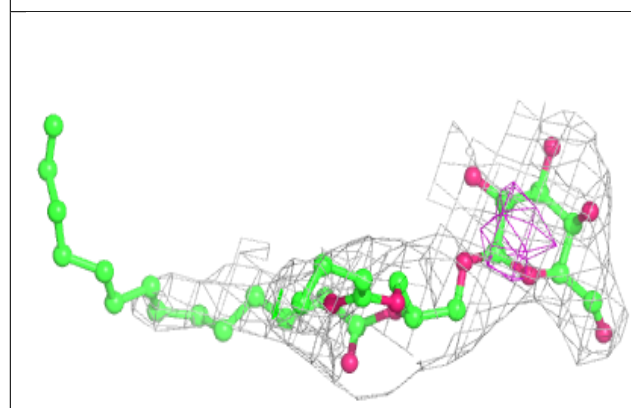


Electron density around LUT 2 2502:

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

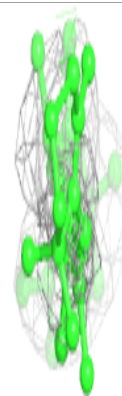
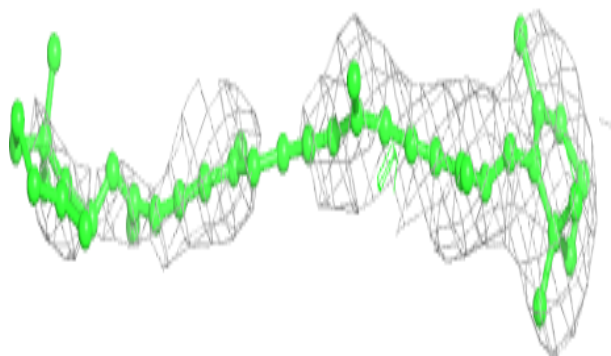
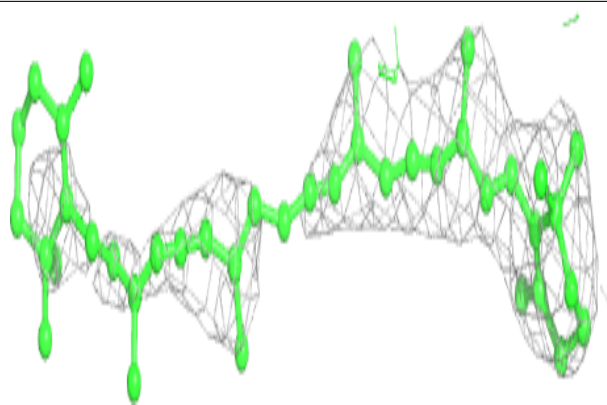
**Electron density around LMG F 5002:**

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

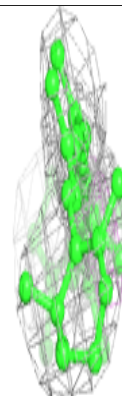
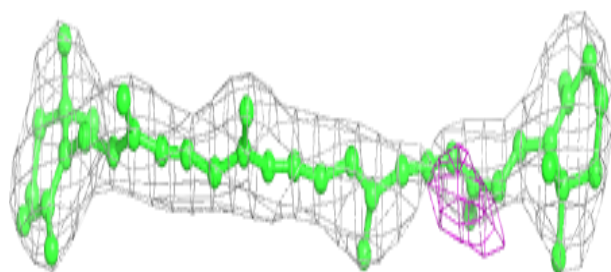
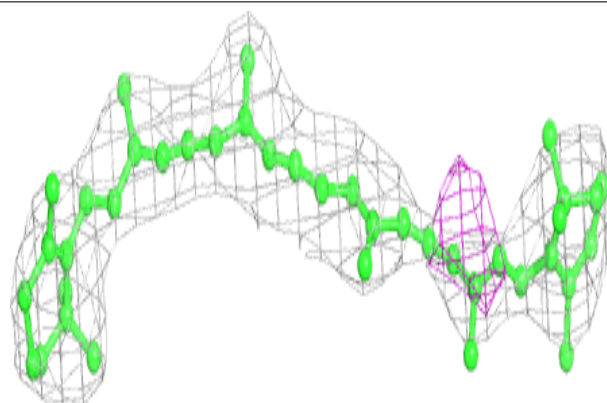


Electron density around BCR A 6003:

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

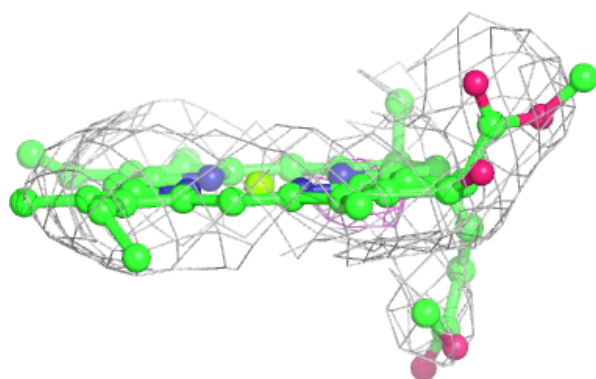
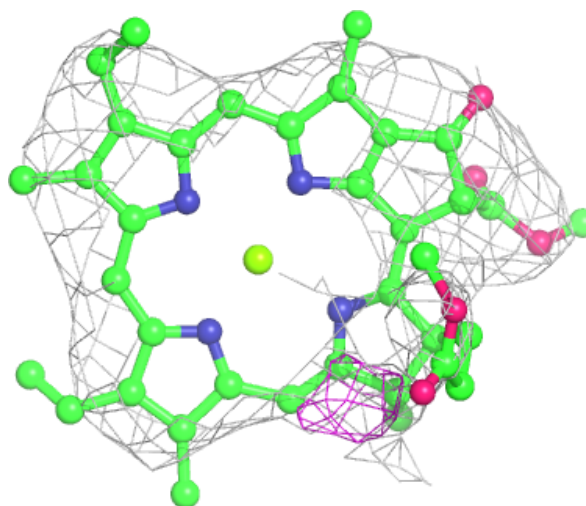
**Electron density around BCR B 6010:**

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



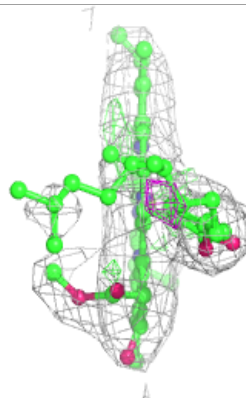
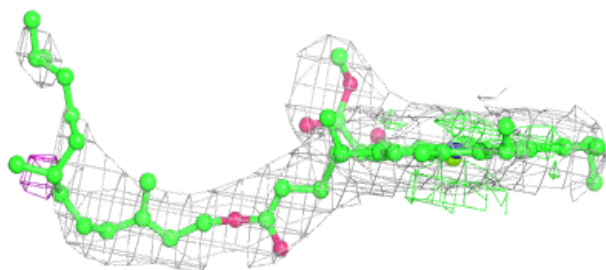
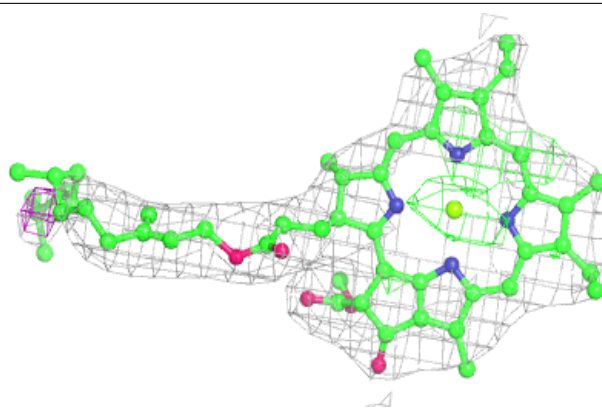
Electron density around CLA 4 4008:

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

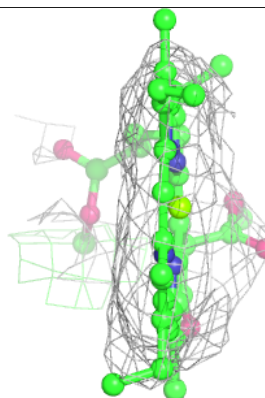
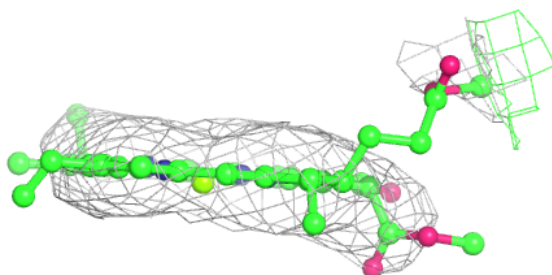
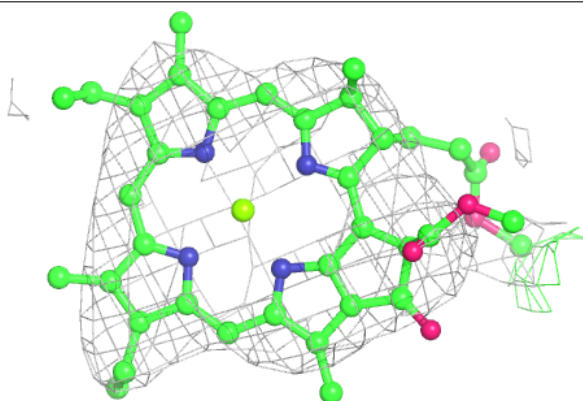


Electron density around CLA B 1234:

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

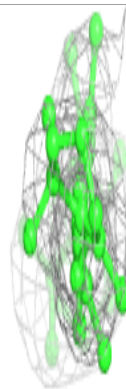
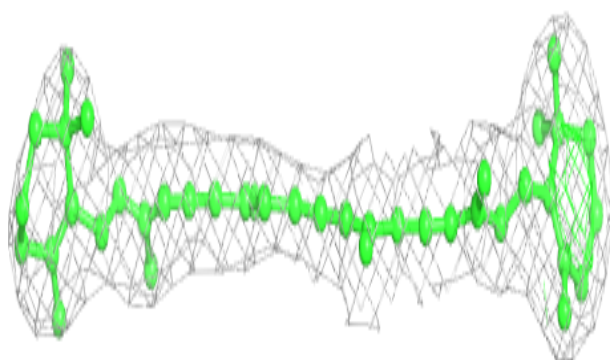
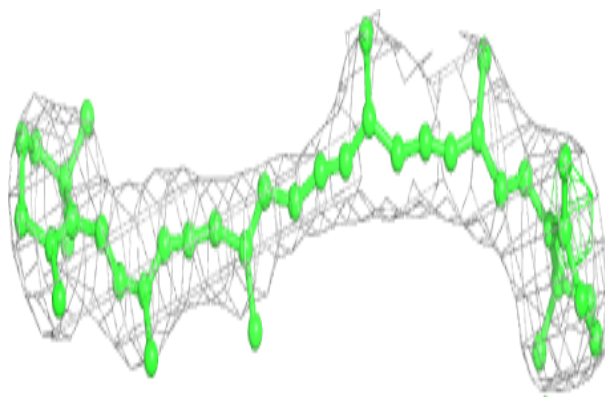
**Electron density around CLA A 1113:**

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

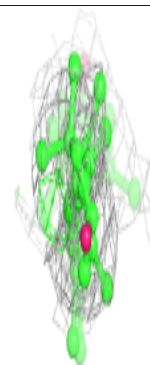
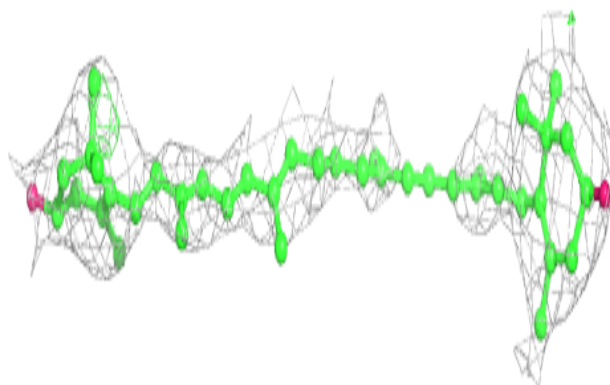
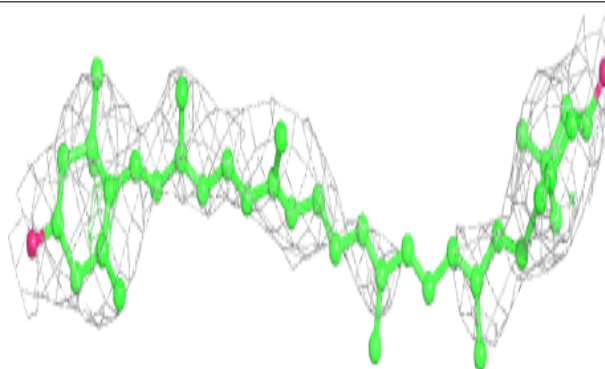


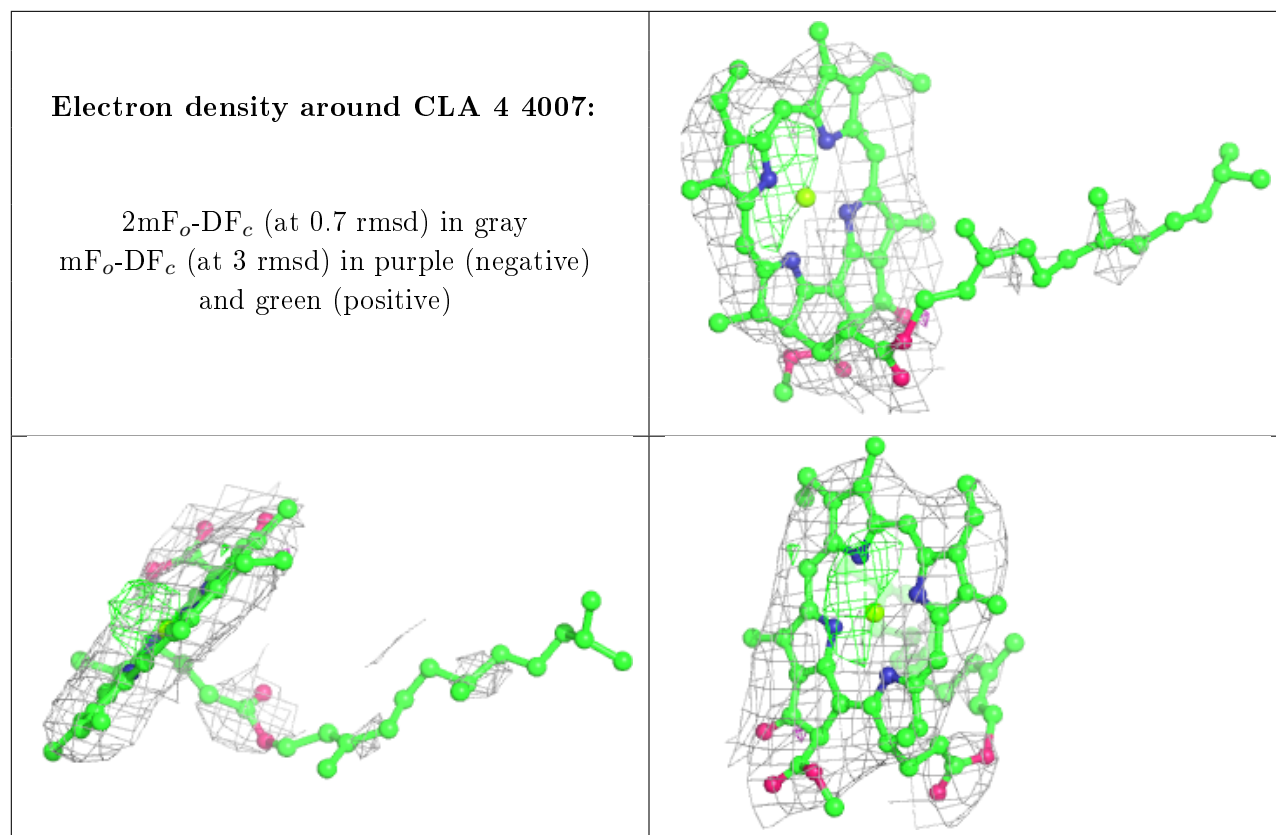
Electron density around BCR B 6009:

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

**Electron density around LUT 1 1502:**

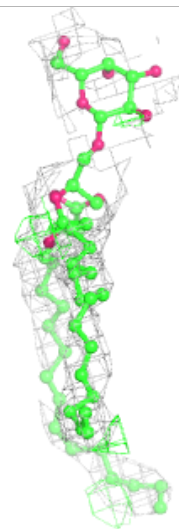
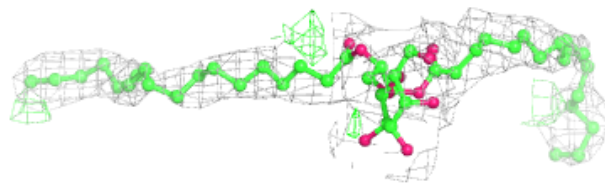
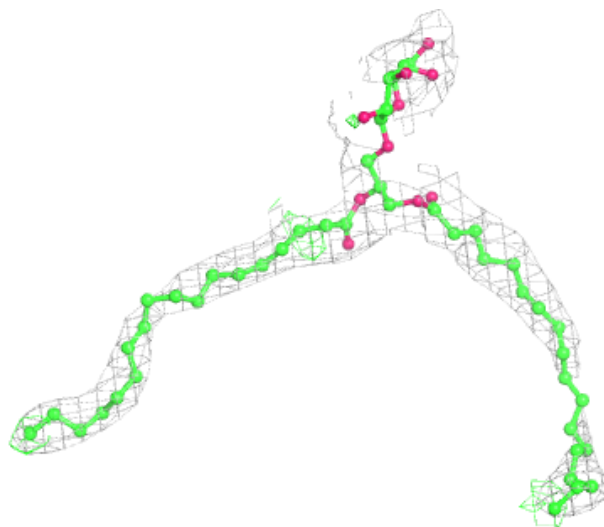
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





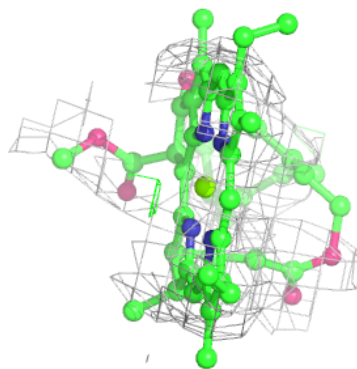
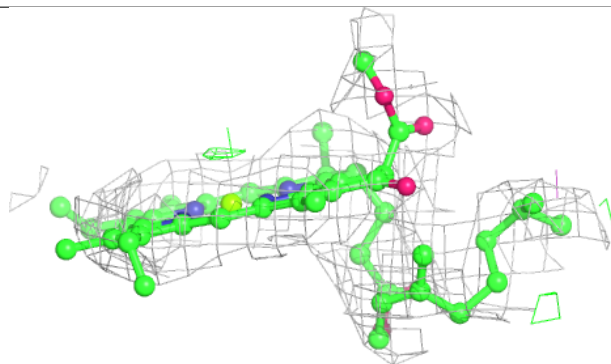
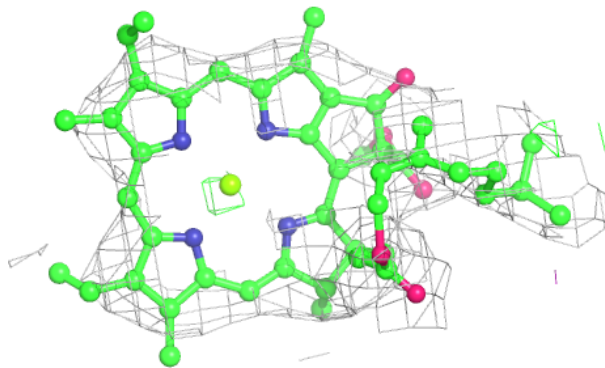
Electron density around LMG J 5001:

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

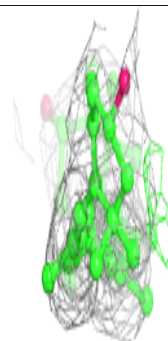
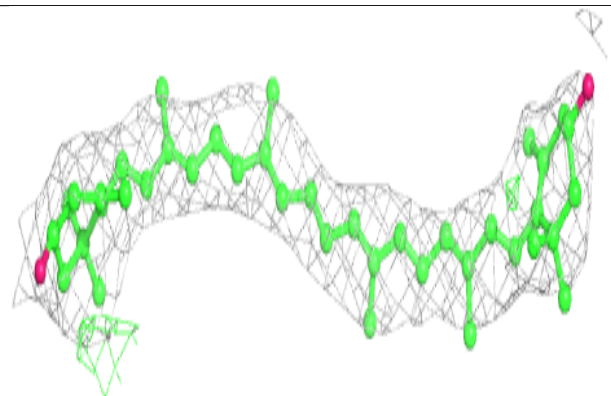
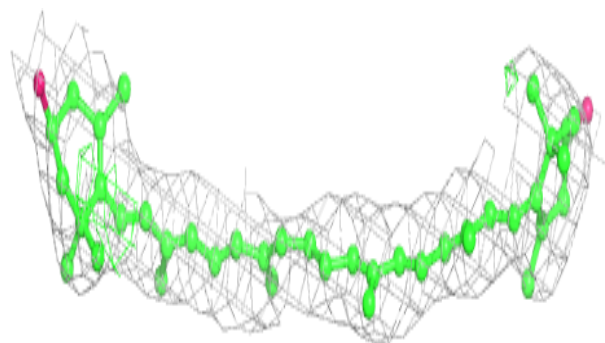


Electron density around CLA 2 2006:

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

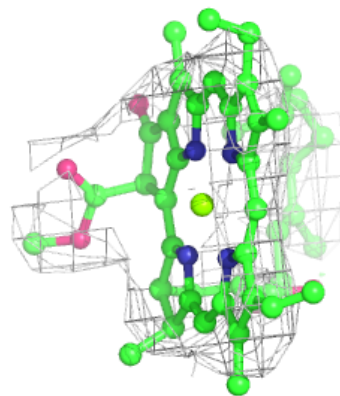
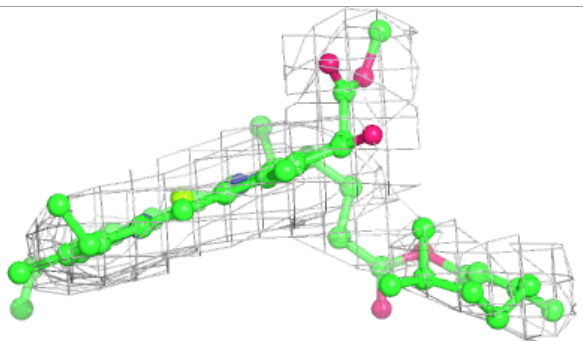
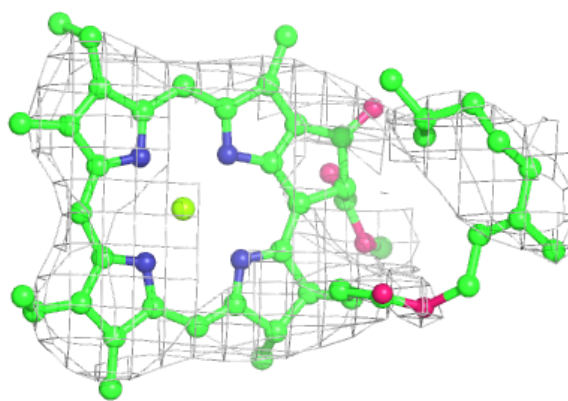
**Electron density around LUT I 6018:**

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

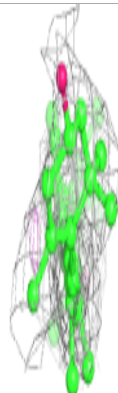
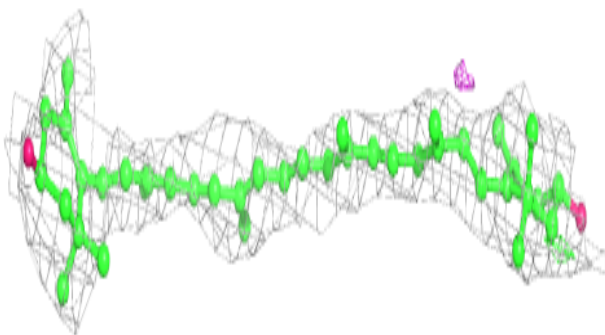
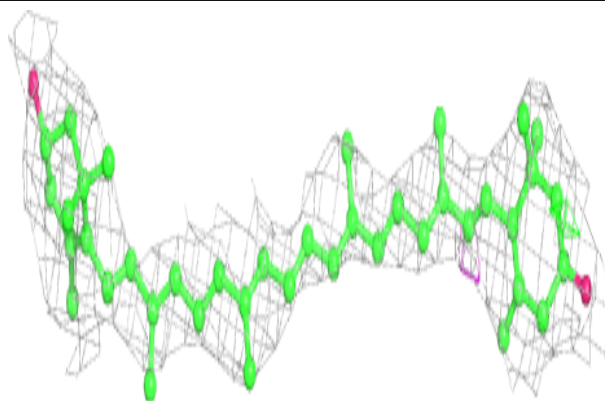


Electron density around CLA A 1134:

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

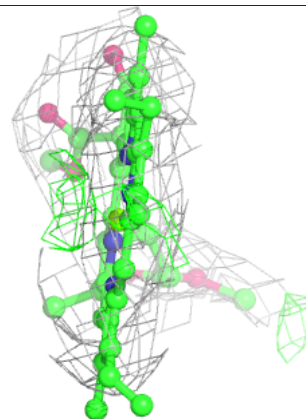
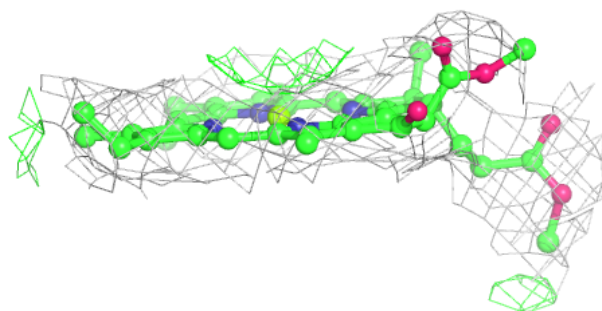
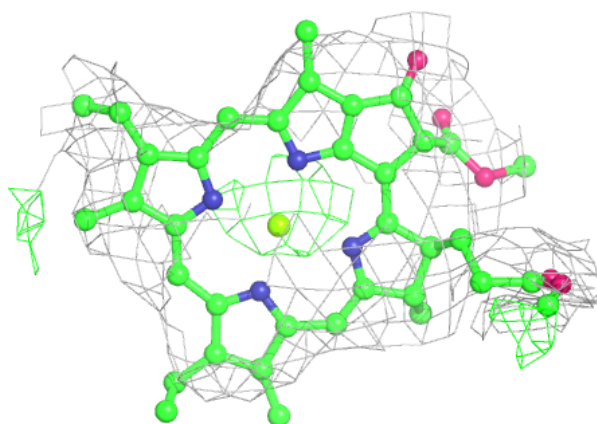
**Electron density around LUT 4 4502:**

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

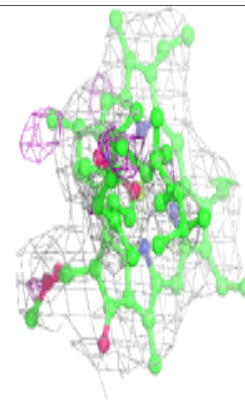
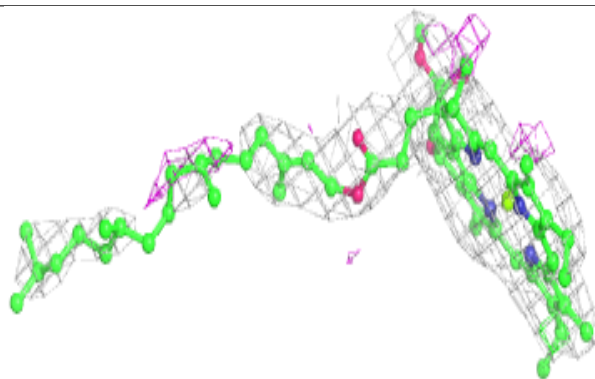
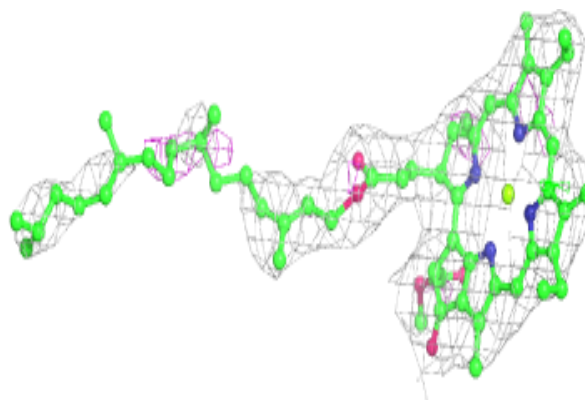


Electron density around CLA 3 3013:

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

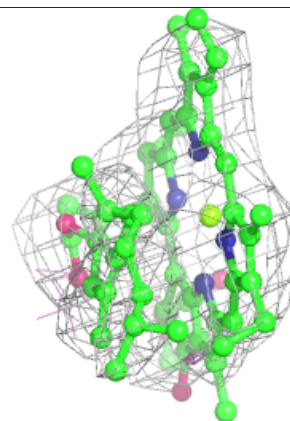
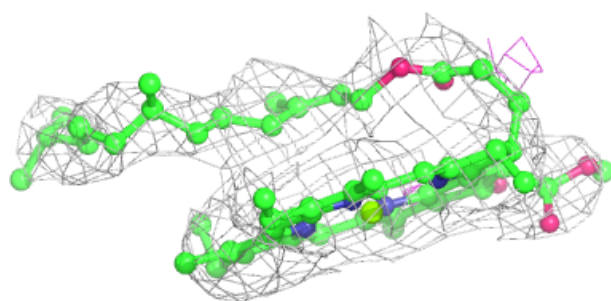
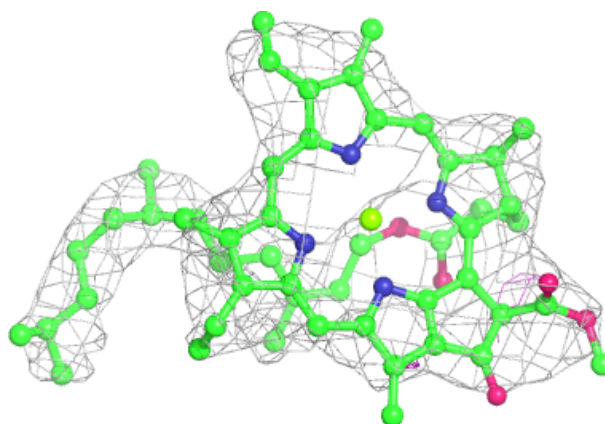
**Electron density around CLA A 1107:**

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



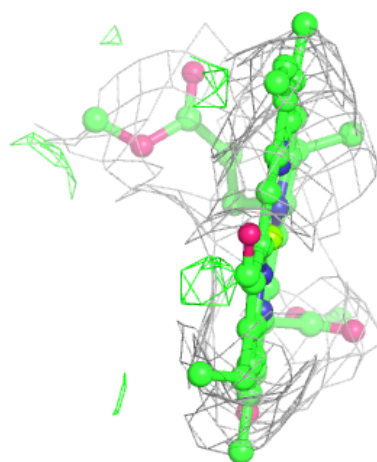
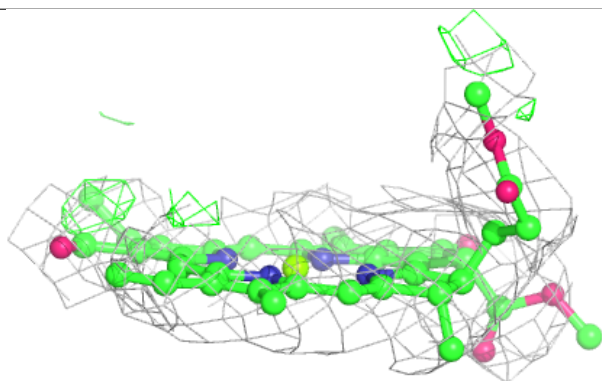
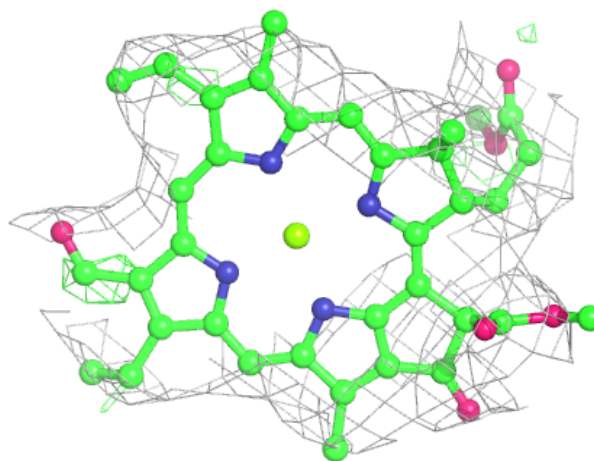
Electron density around CLA B 1213:

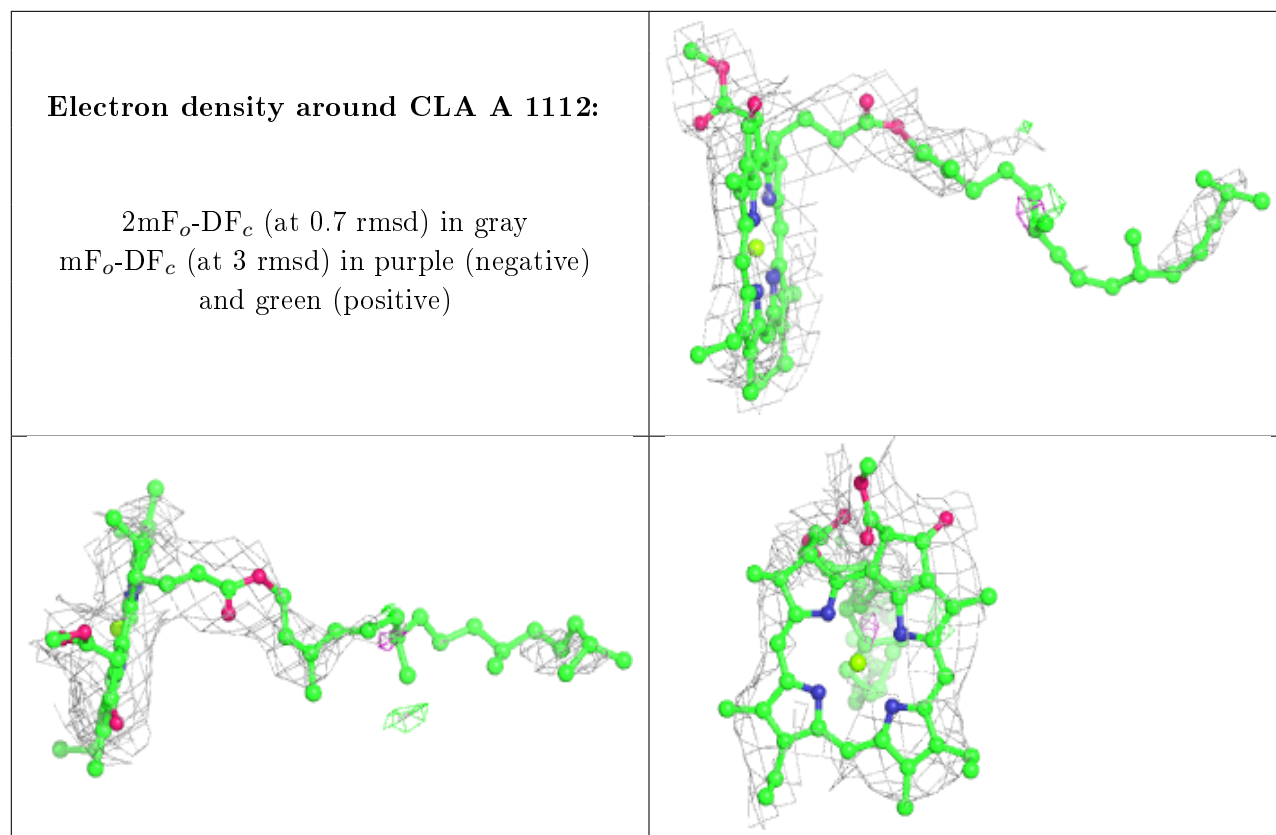
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CHL 1 1010:

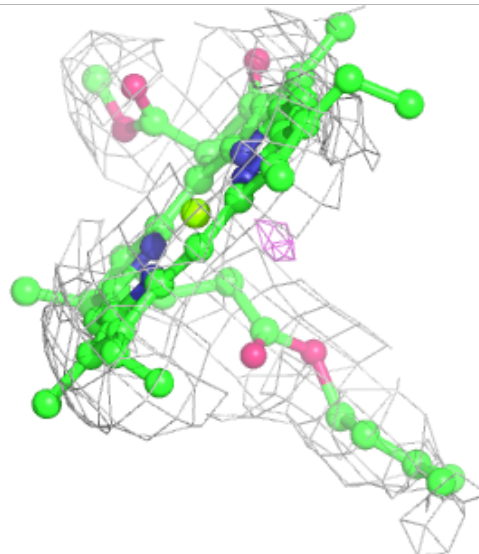
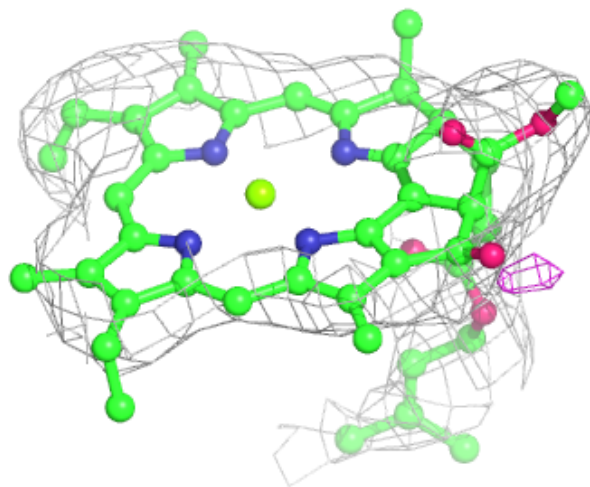
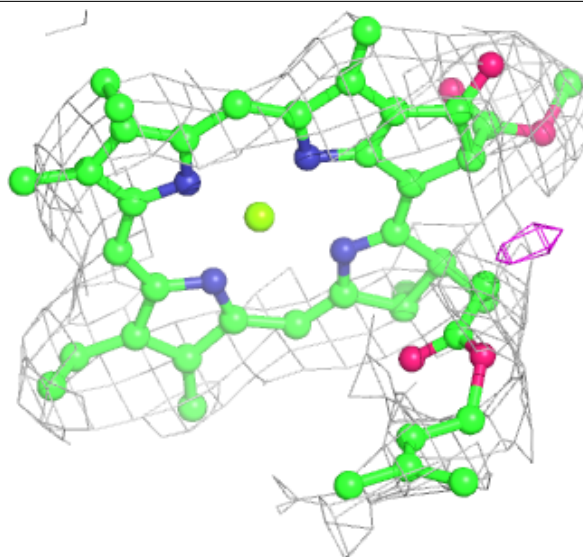
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





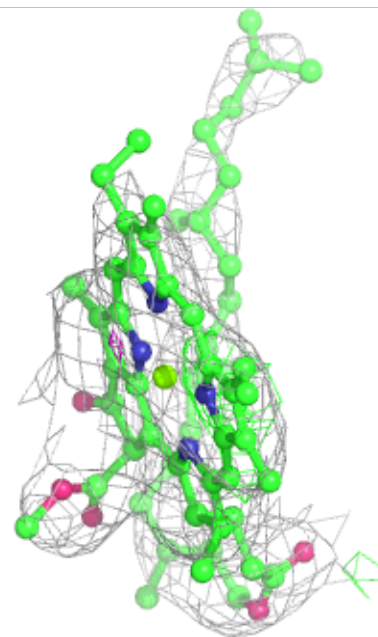
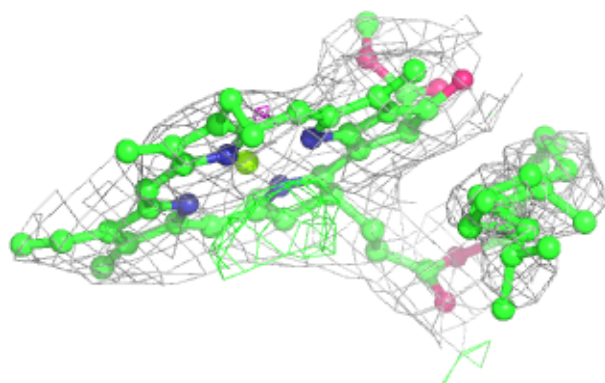
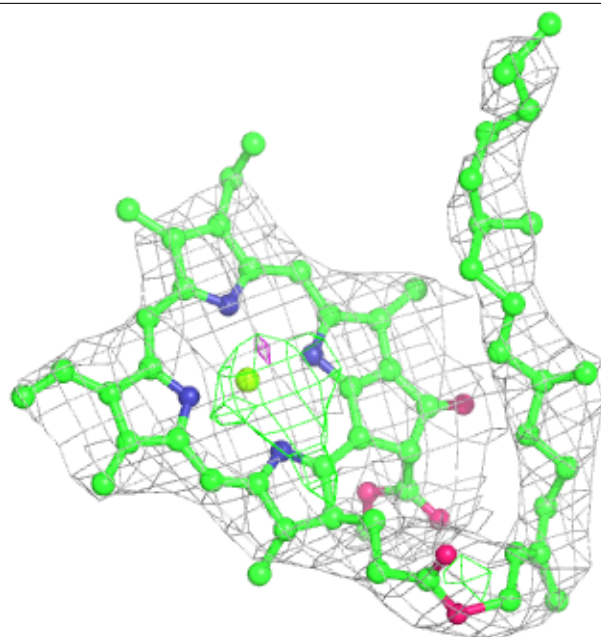
Electron density around CLA L 1501:

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



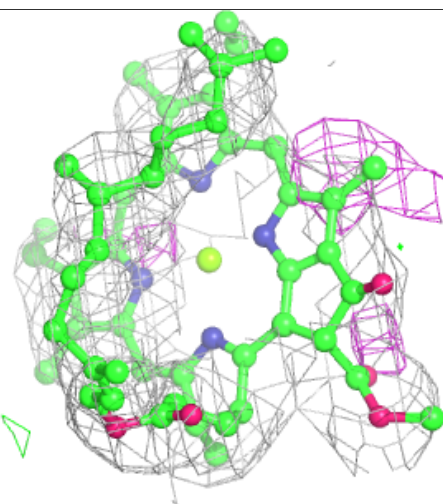
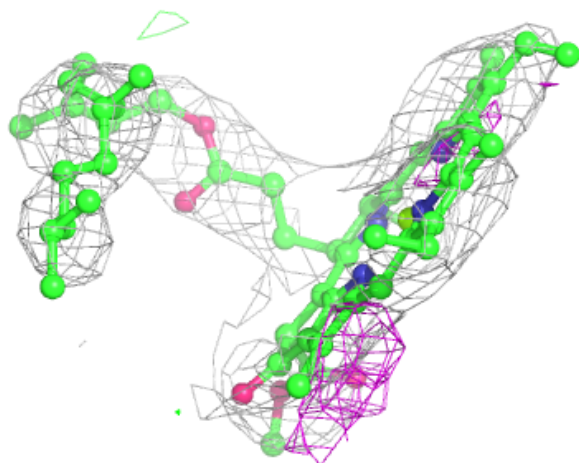
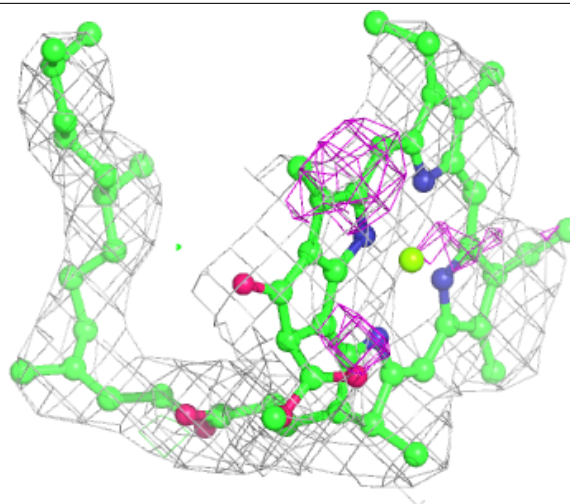
Electron density around CLA A 1123:

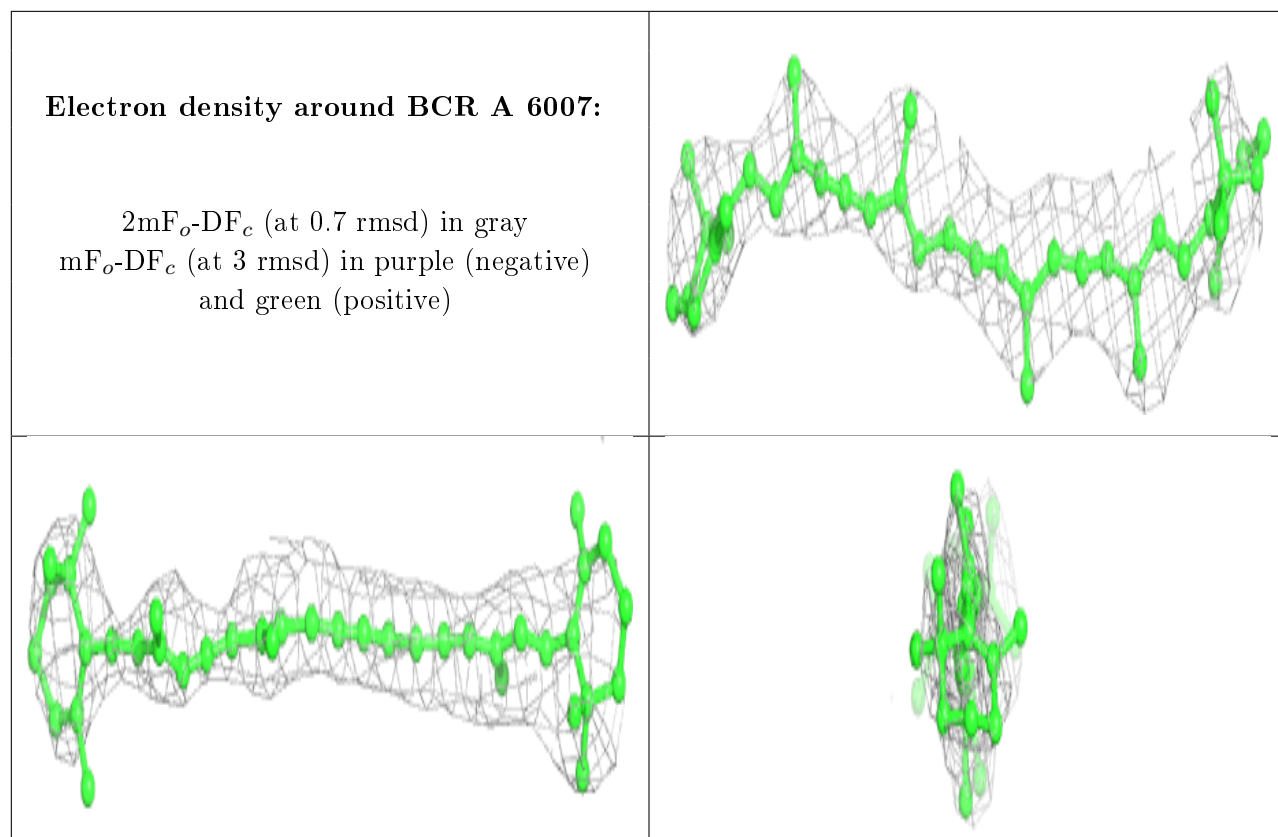
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1231:

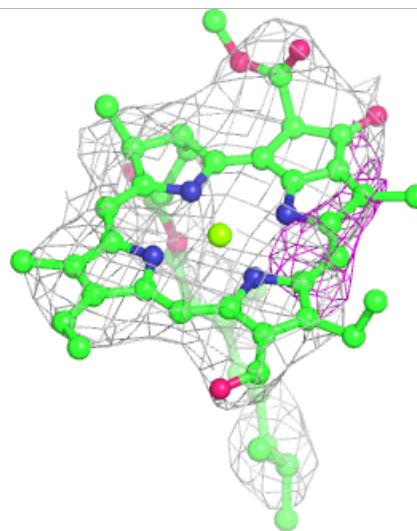
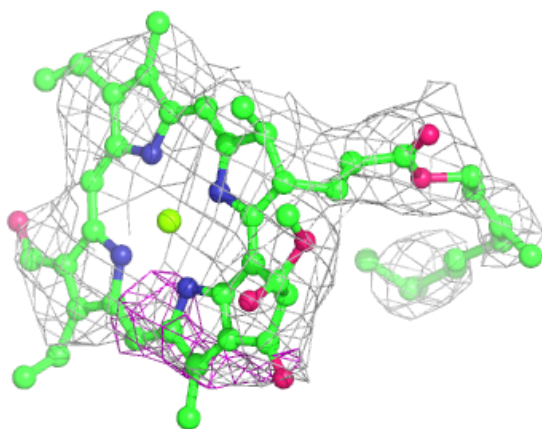
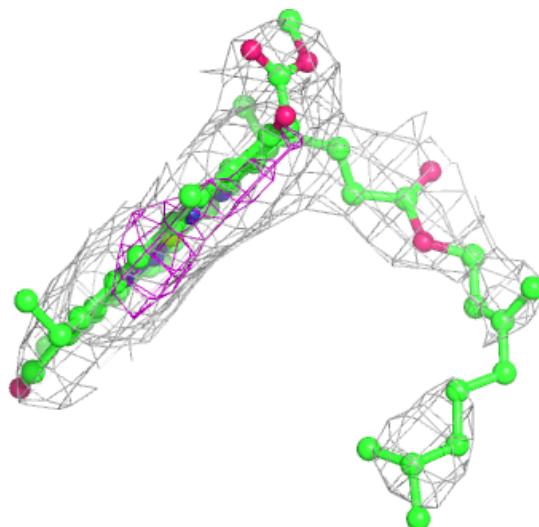
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

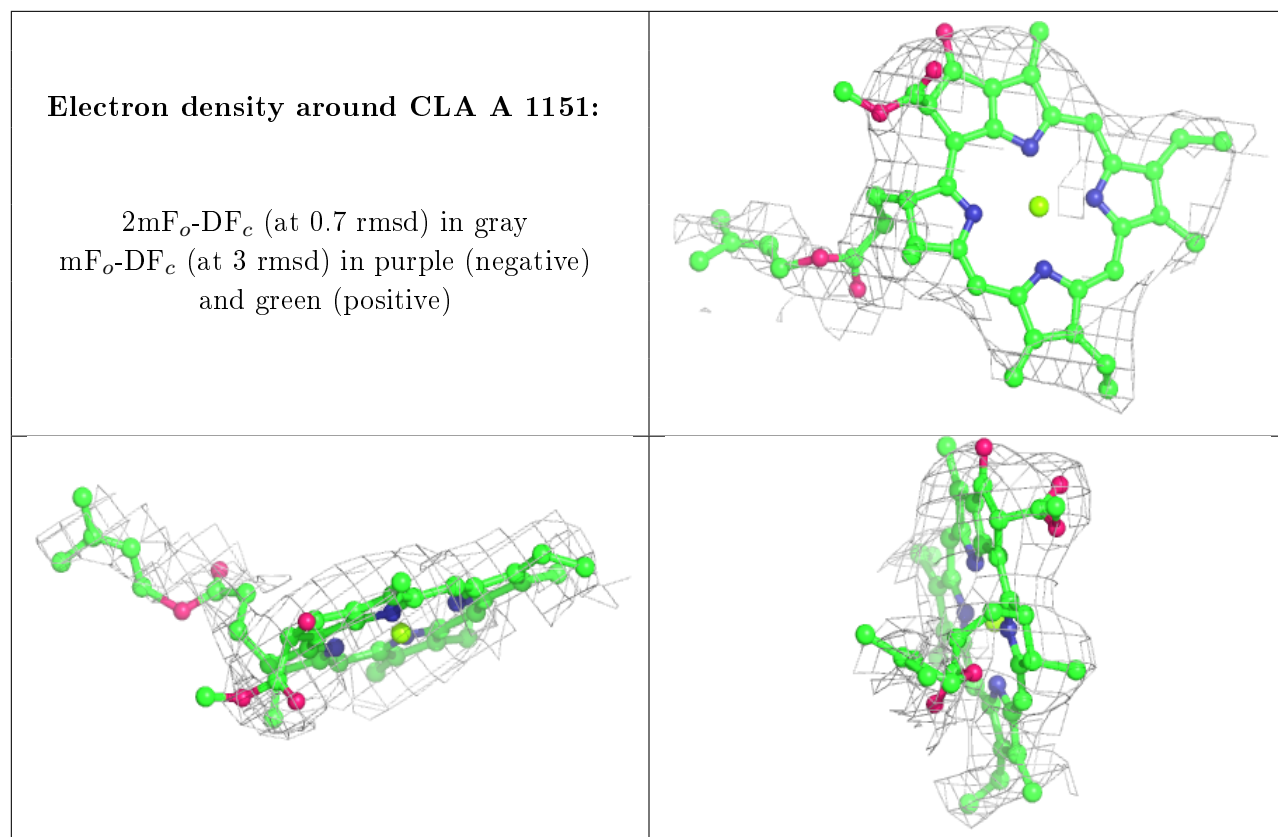




Electron density around CHL 1 1009:

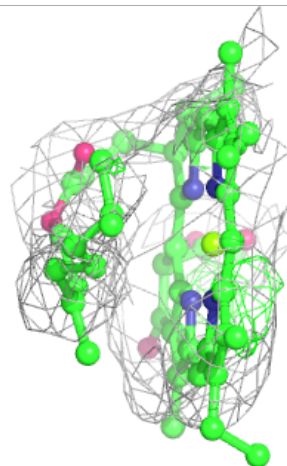
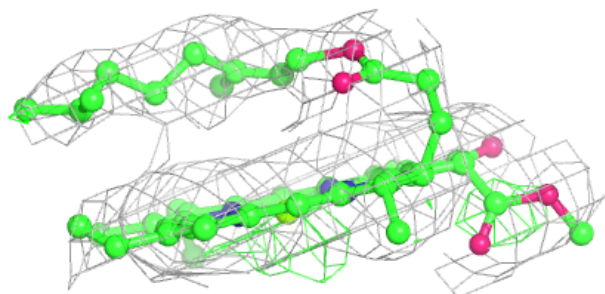
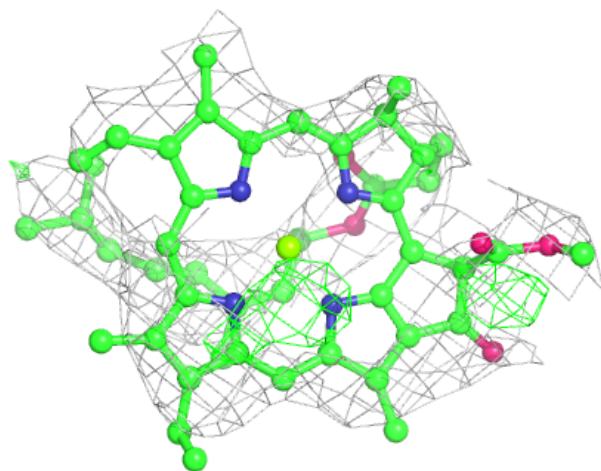
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





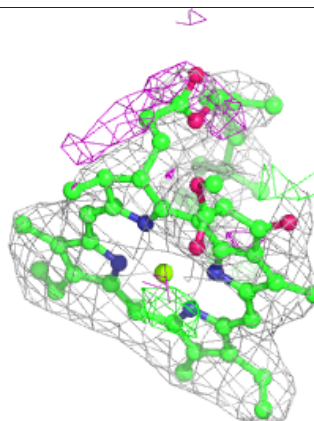
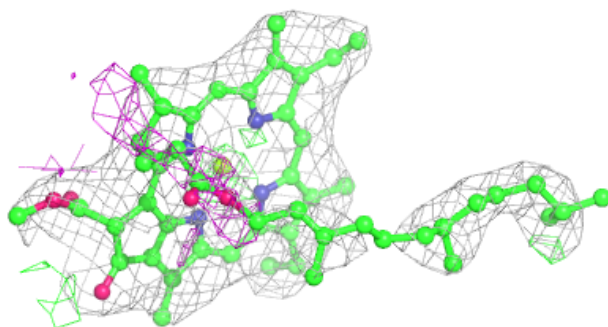
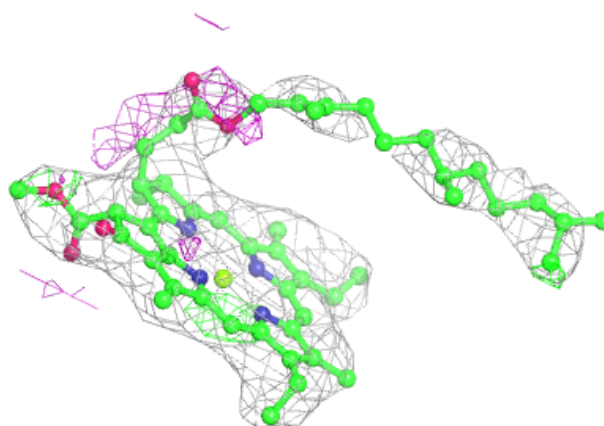
Electron density around CLA A 1110:

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

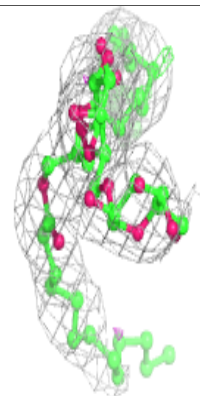
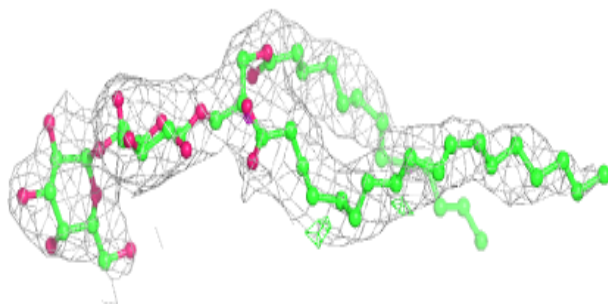
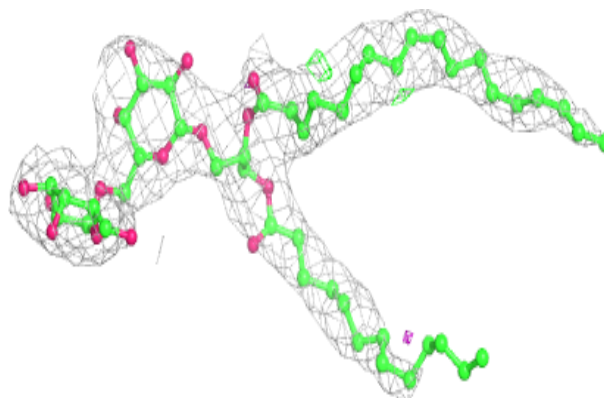


Electron density around CLA B 1228:

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

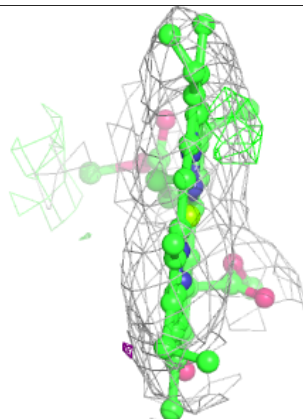
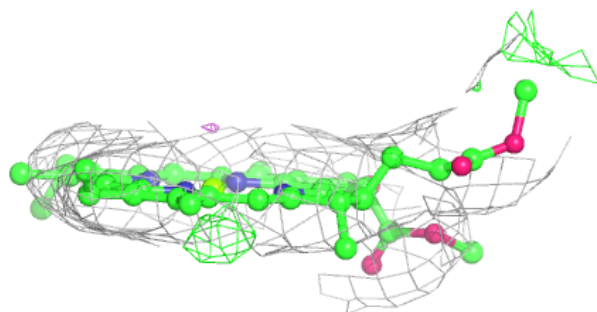
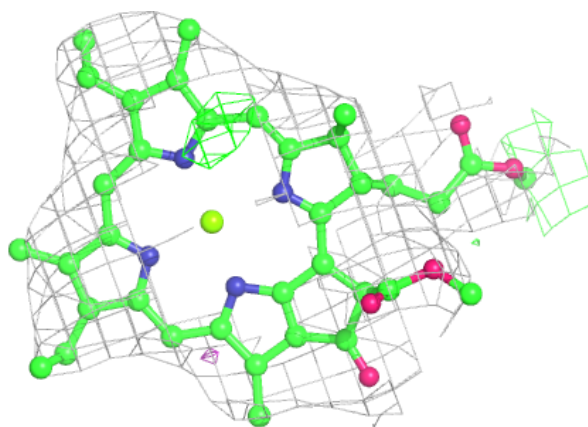
**Electron density around DGD B 7101:**

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

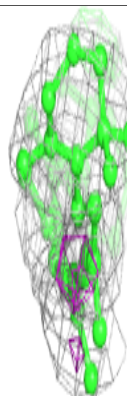
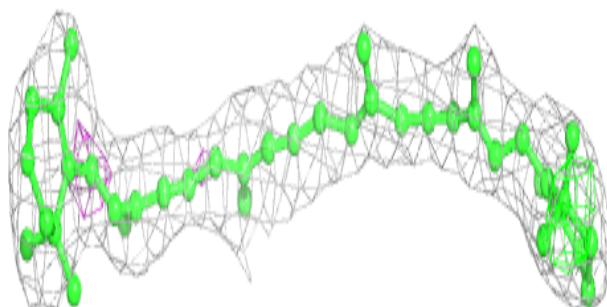
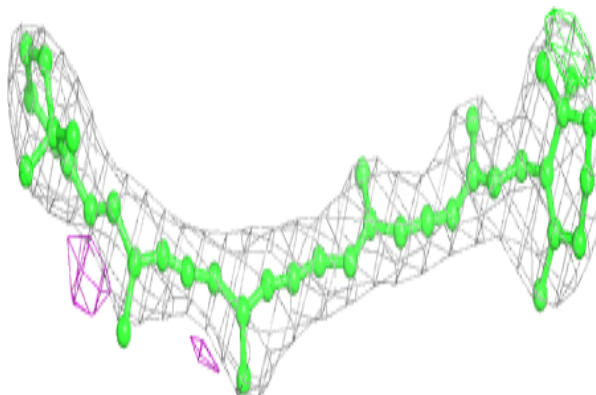


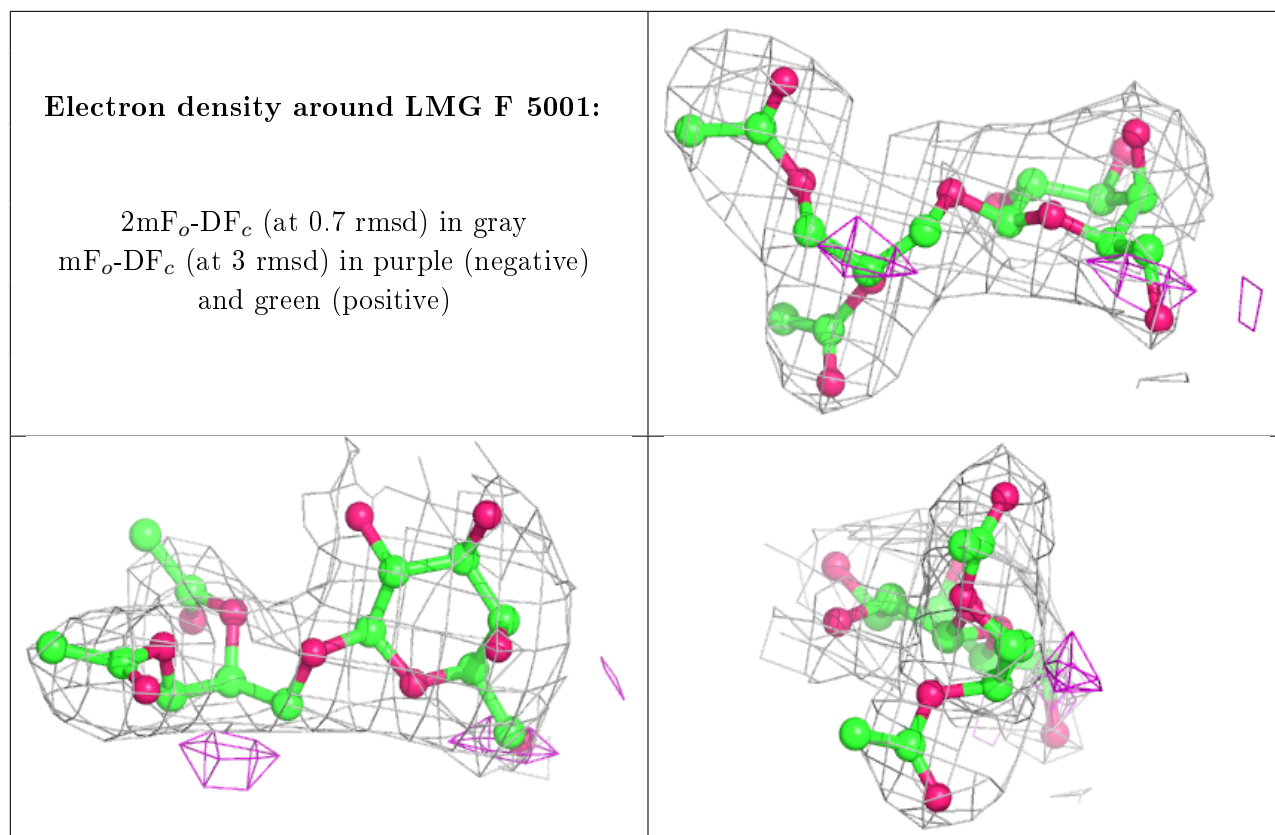
Electron density around CLA 1 1014:

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

**Electron density around BCR F 6014:**

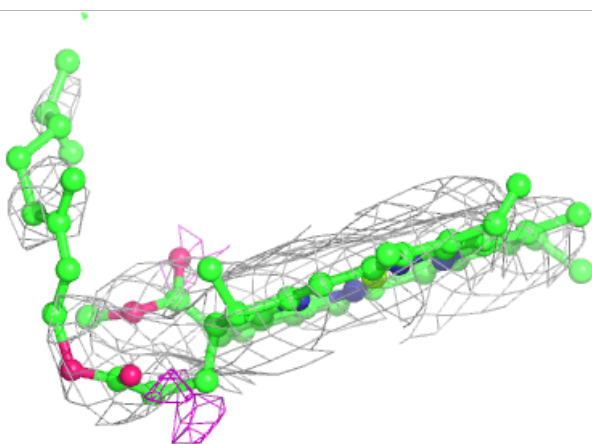
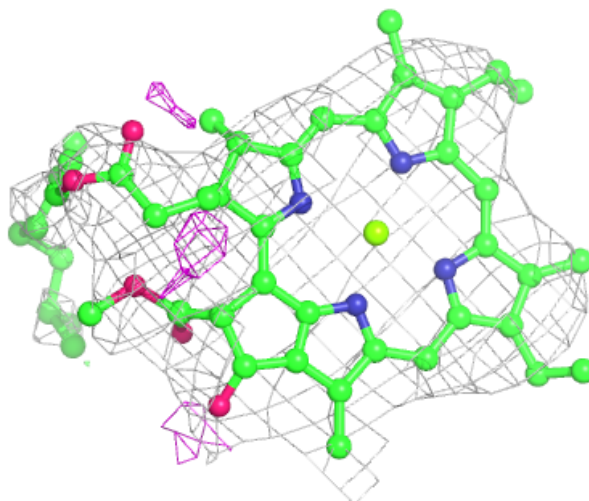
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





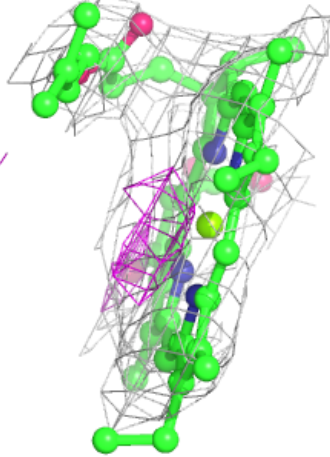
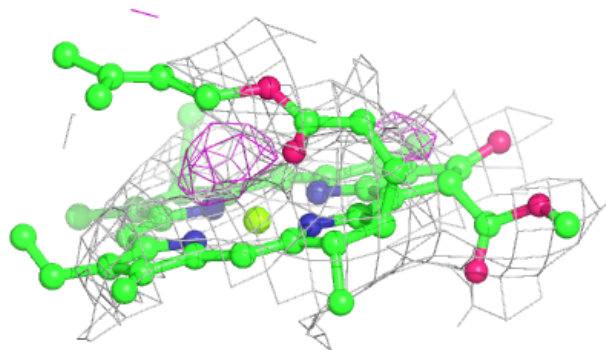
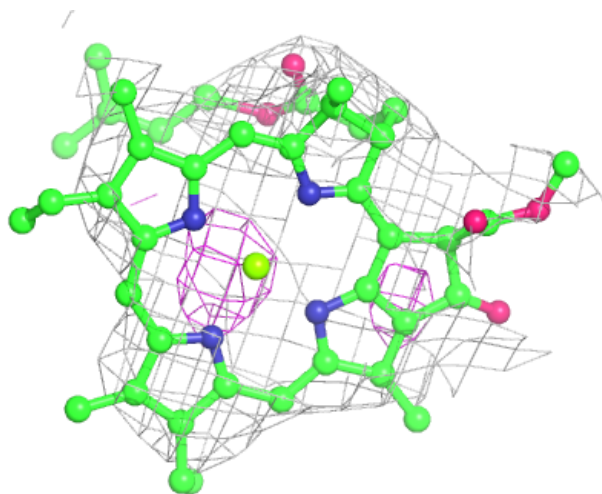
Electron density around CLA 3 3005:

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



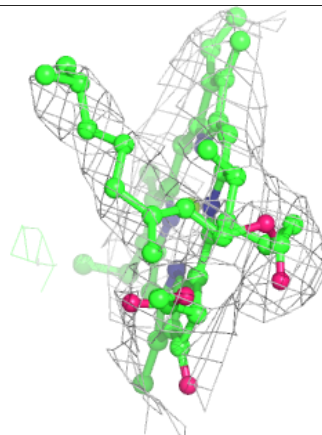
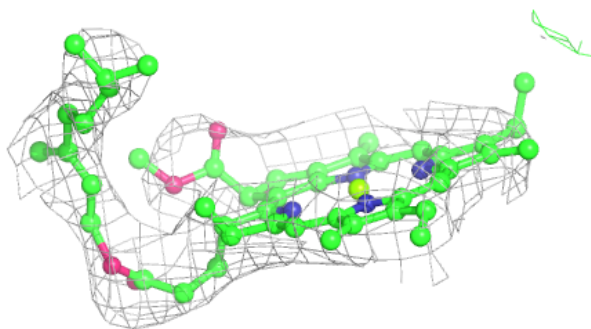
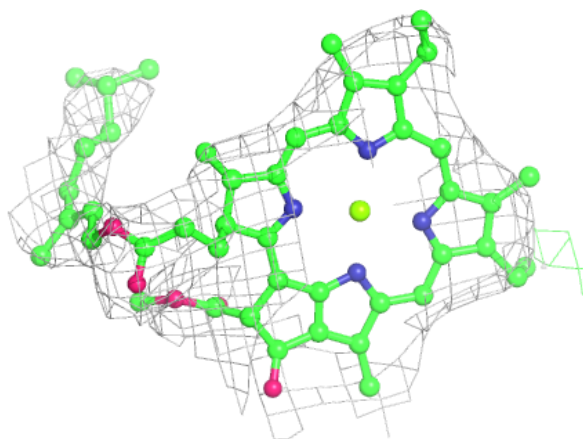
Electron density around CLA 3 3001:

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



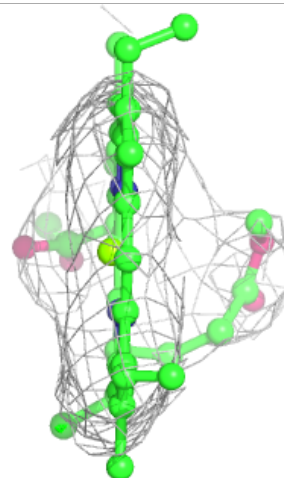
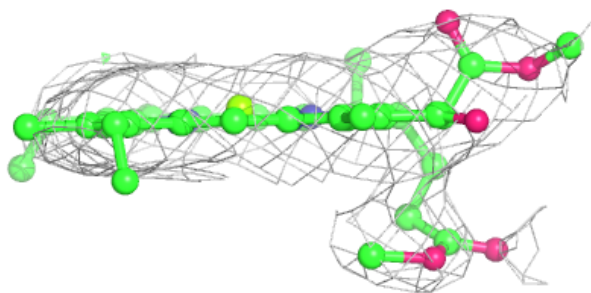
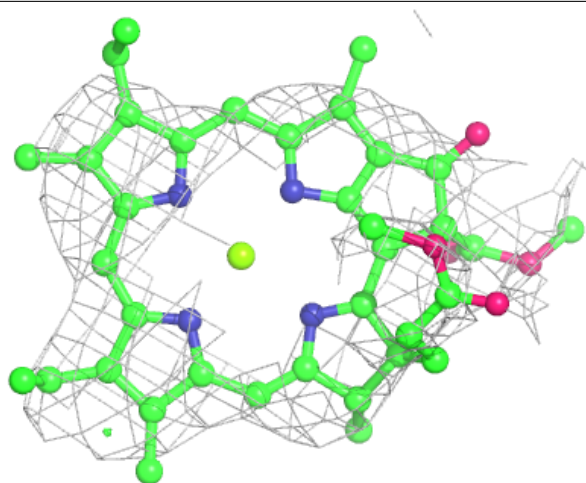
Electron density around CLA 1 1005:

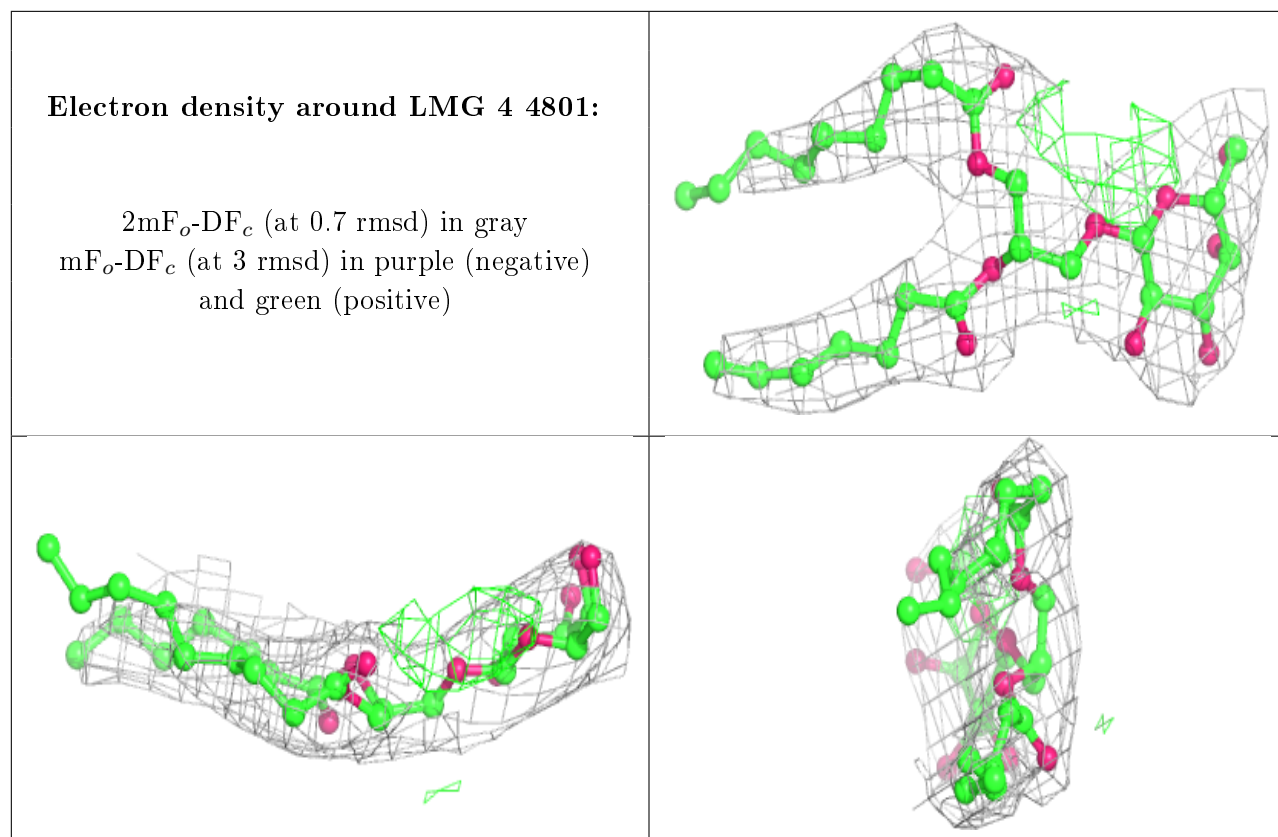
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 1115:

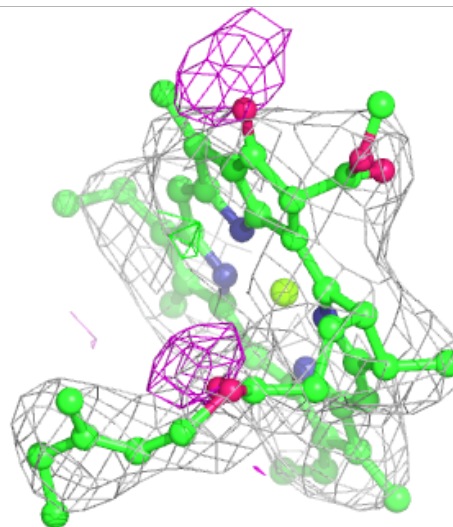
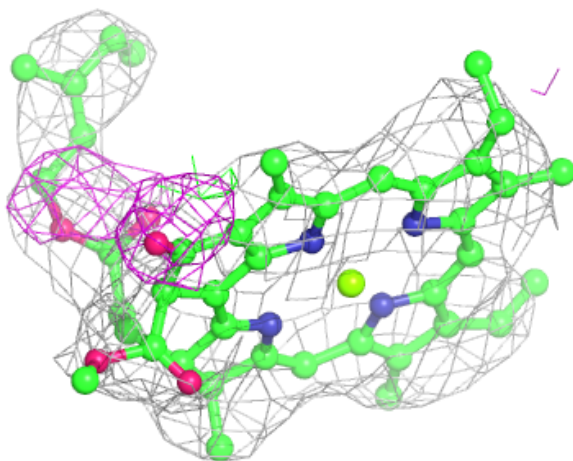
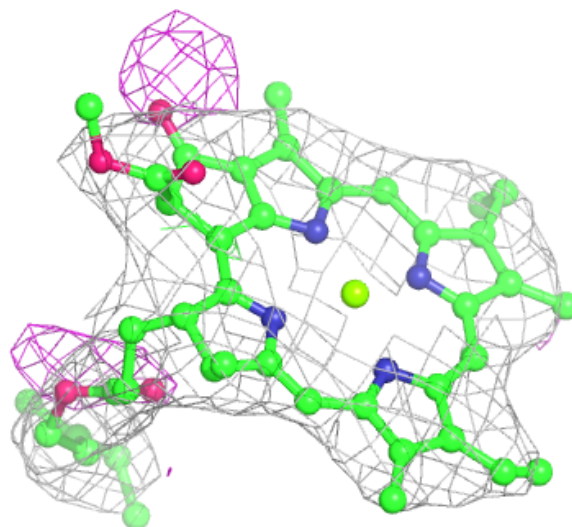
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





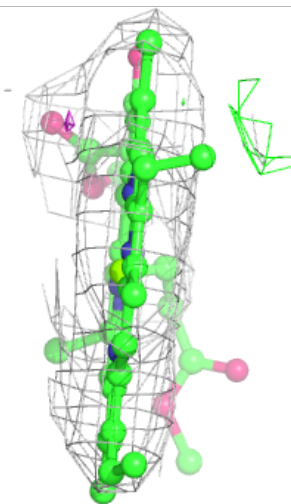
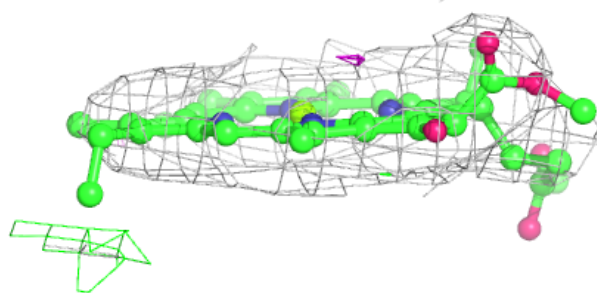
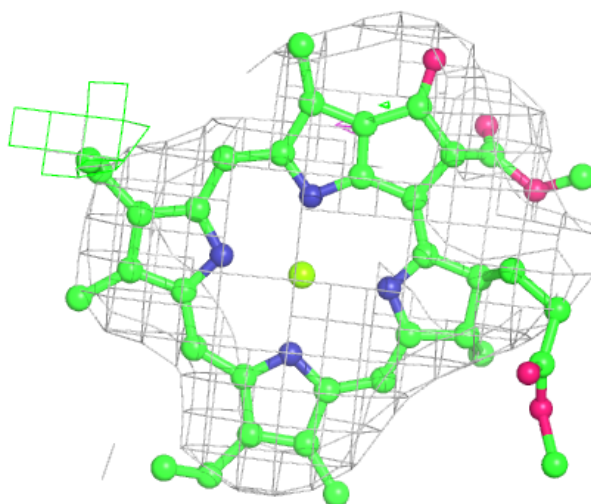
Electron density around CLA A 1105:

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



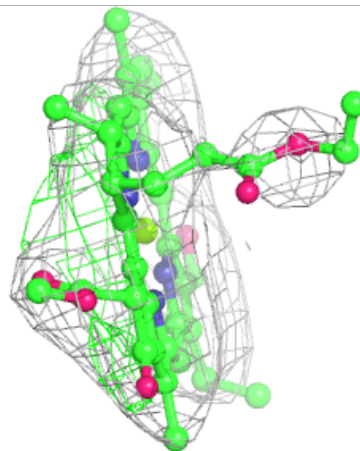
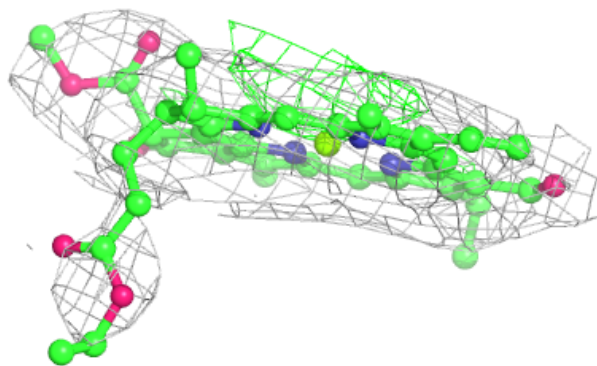
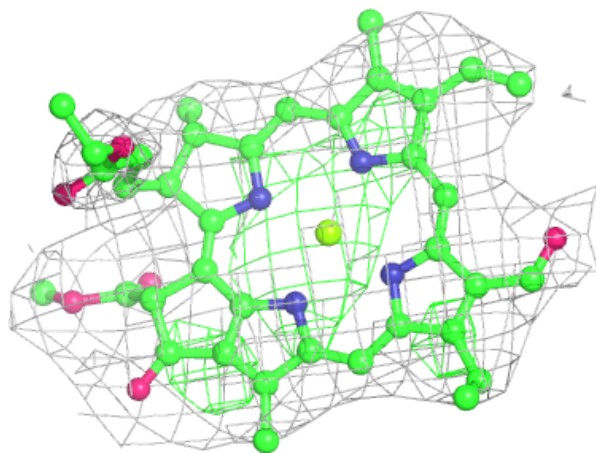
Electron density around CLA 3 3017:

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



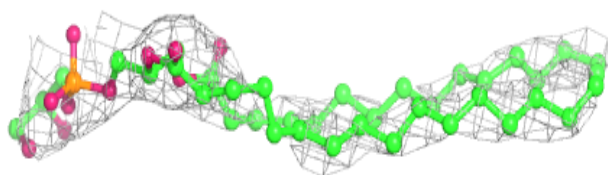
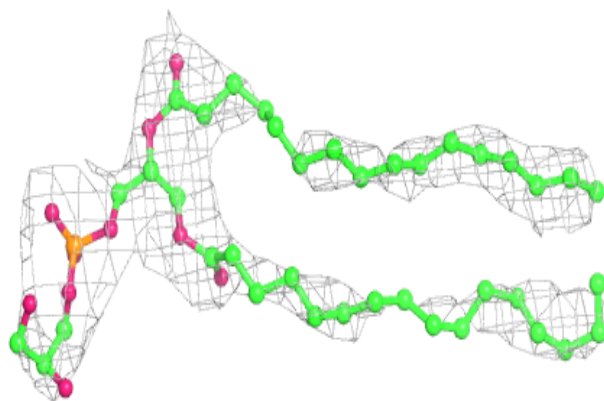
Electron density around CHL 2 2011:

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

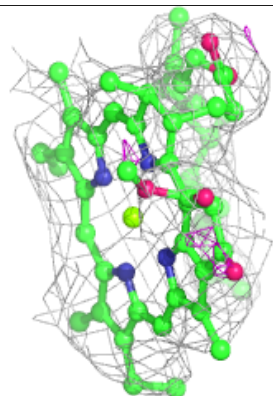
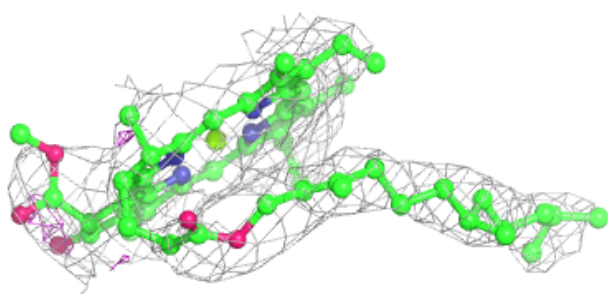
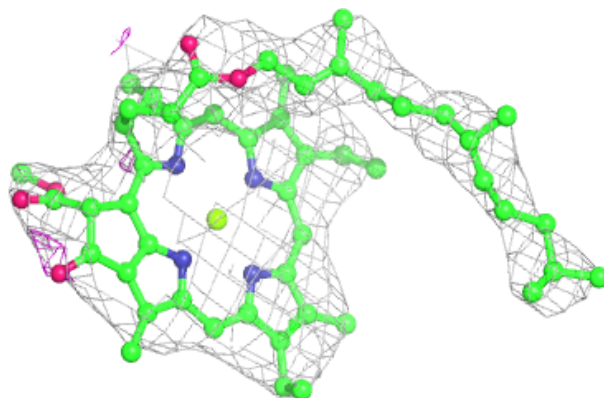


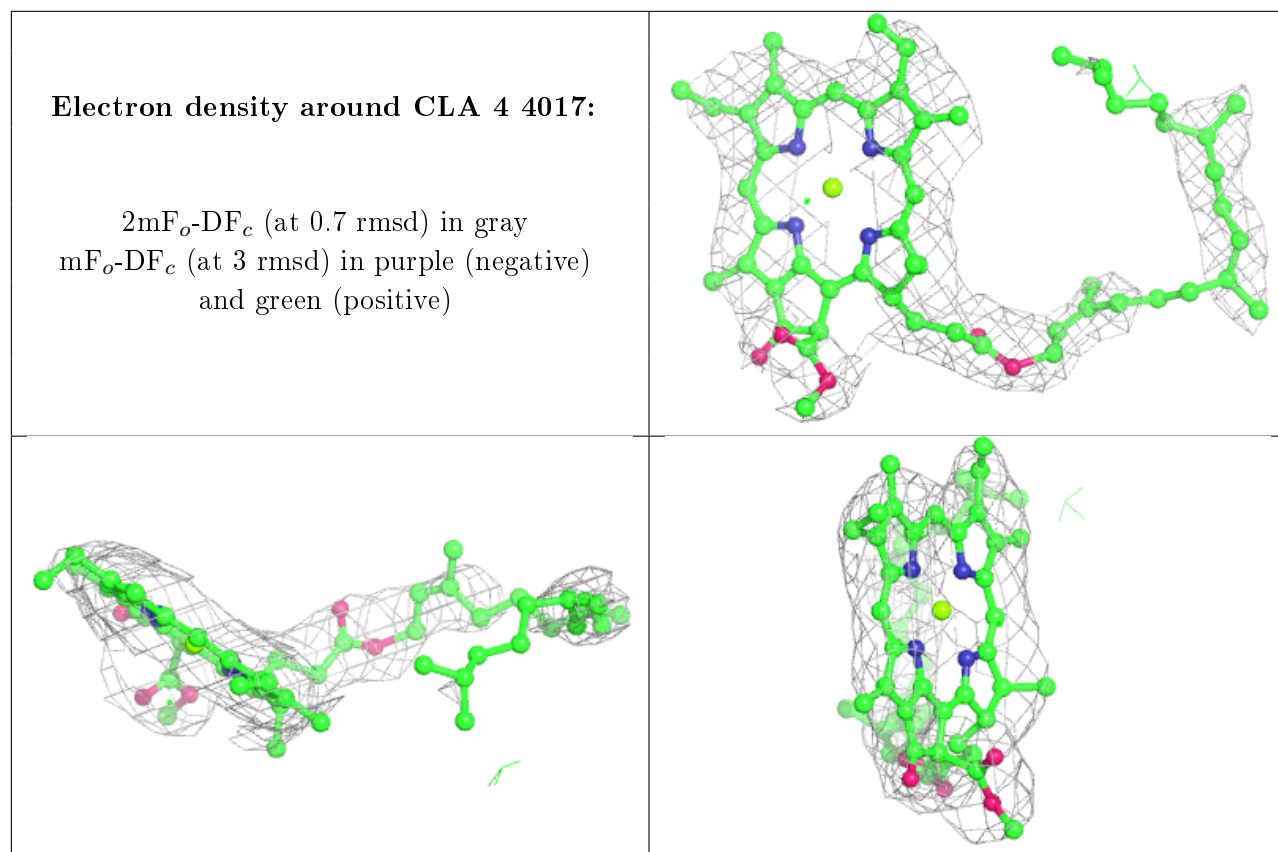
Electron density around LHG 1 1801:

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

**Electron density around CLA 4 4004:**

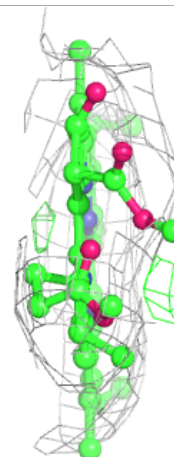
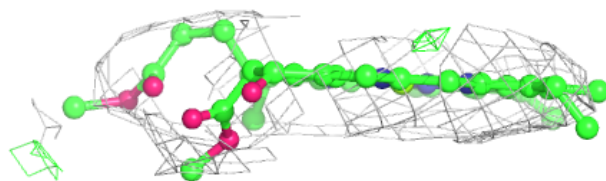
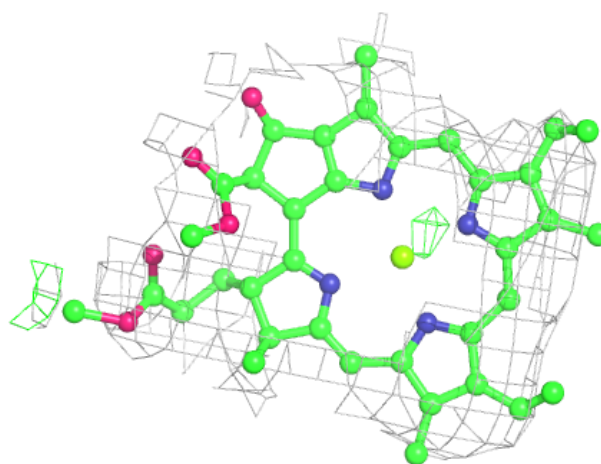
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





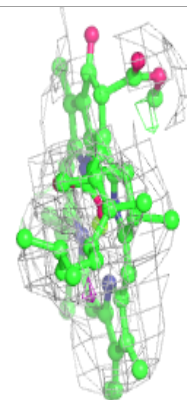
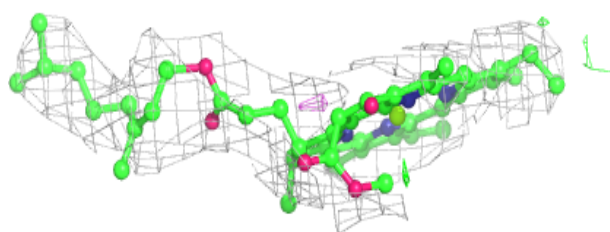
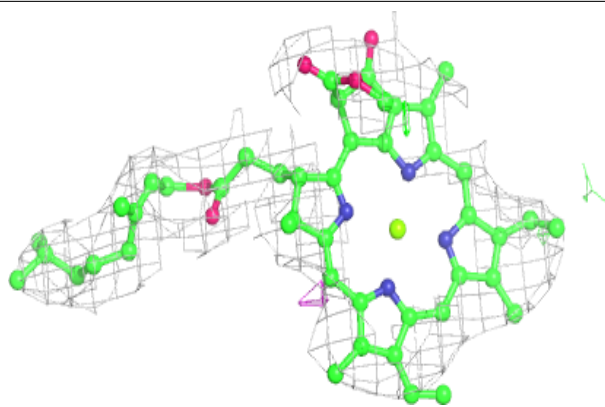
Electron density around CLA 1 1002:

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

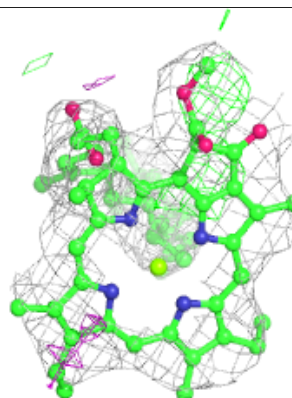
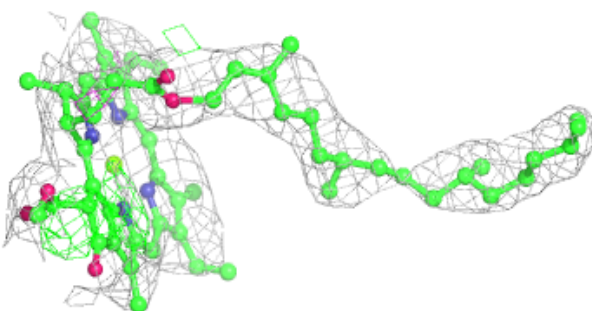
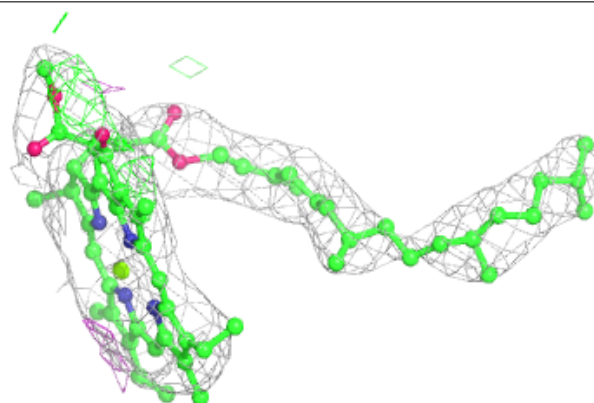


Electron density around CLA G 1001:

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

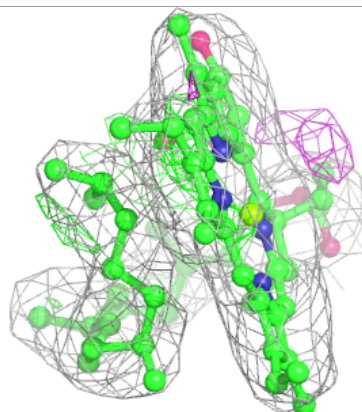
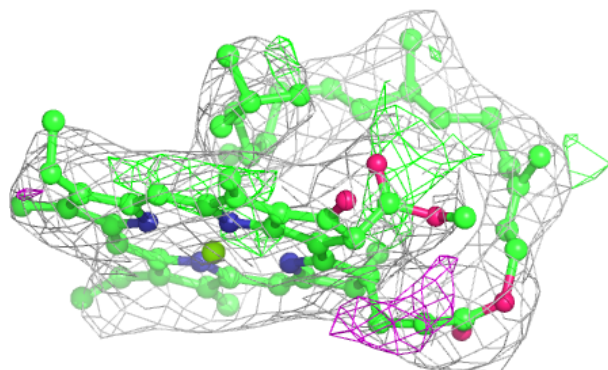
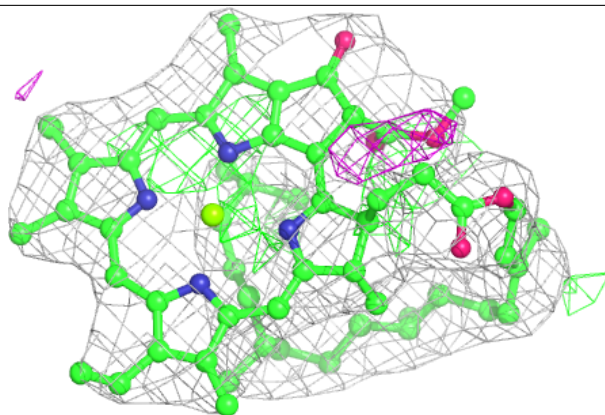
**Electron density around CLA A 1109:**

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

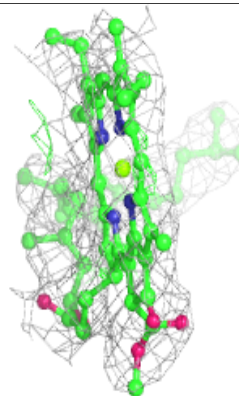
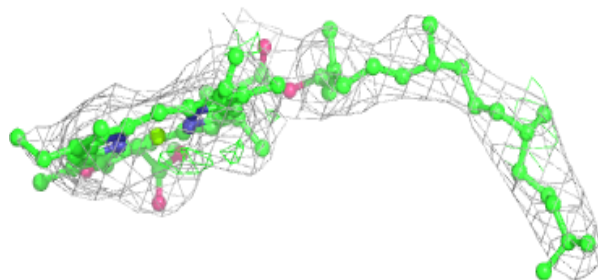
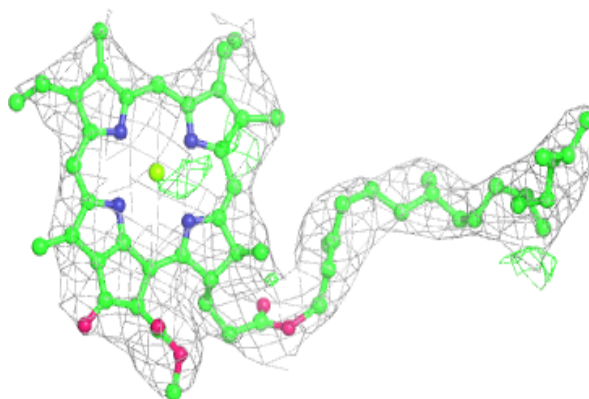


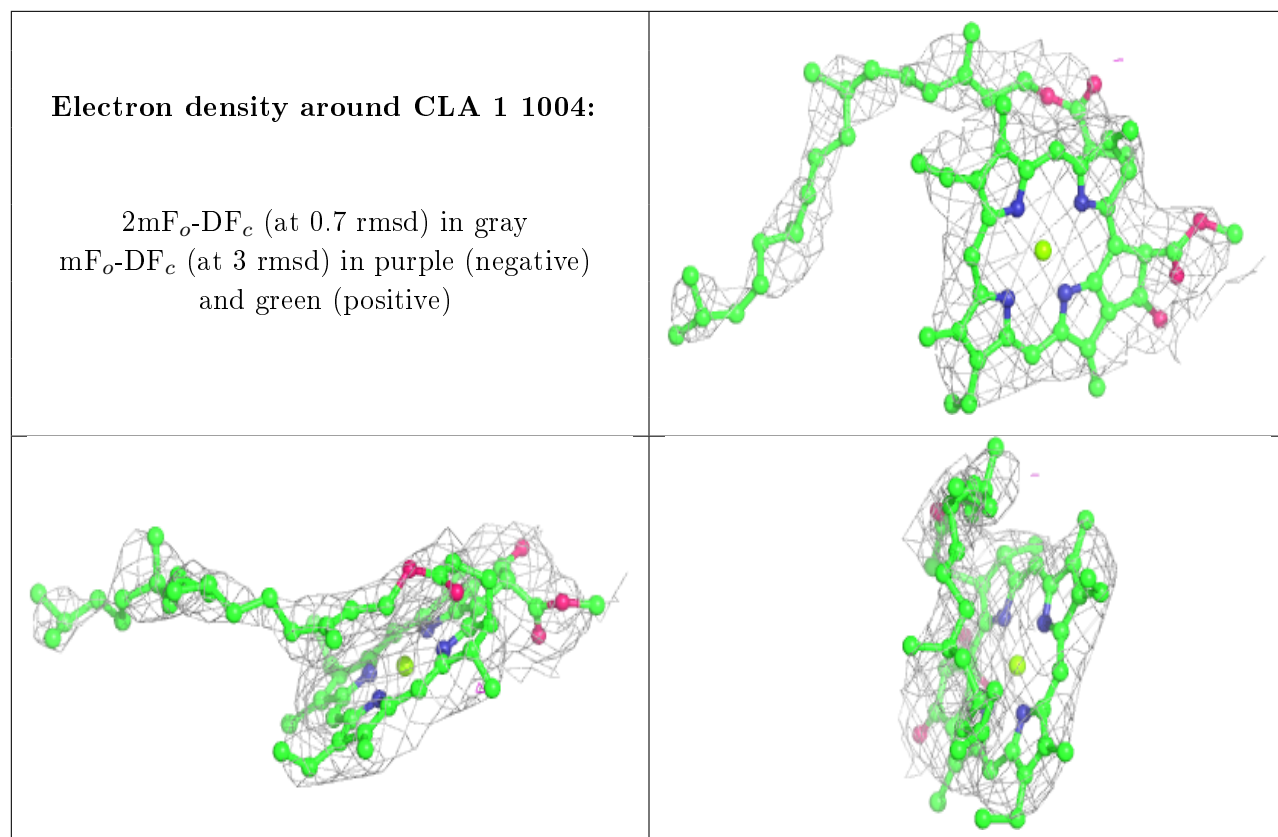
Electron density around CLA A 1104:

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

**Electron density around CLA B 1023:**

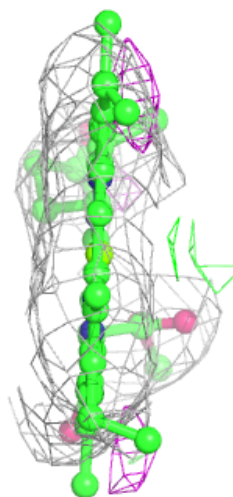
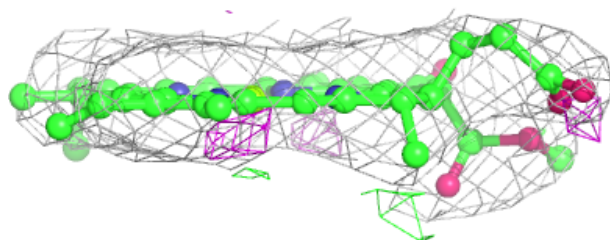
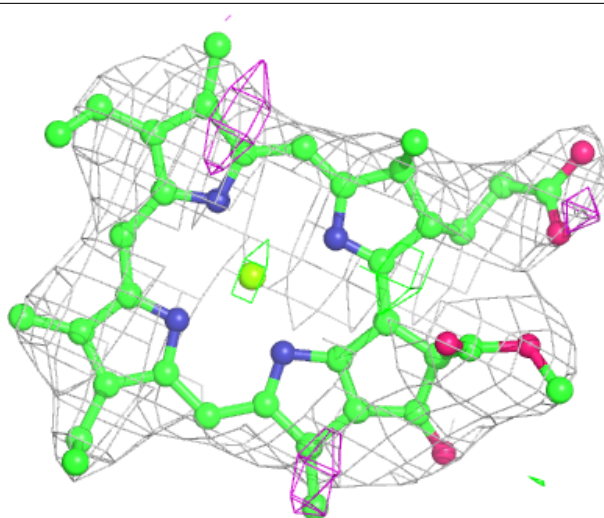
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





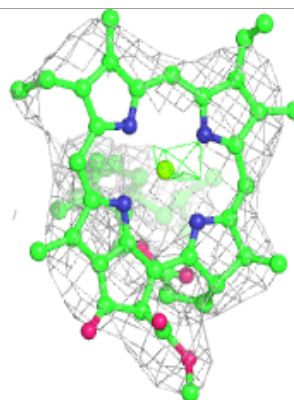
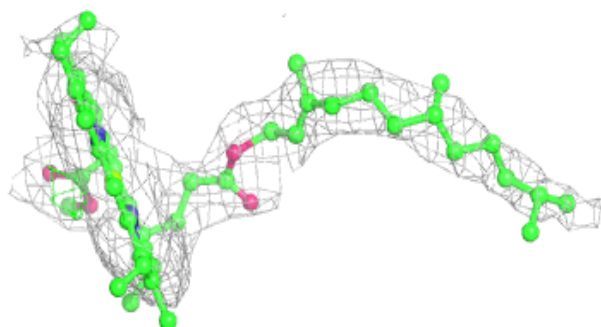
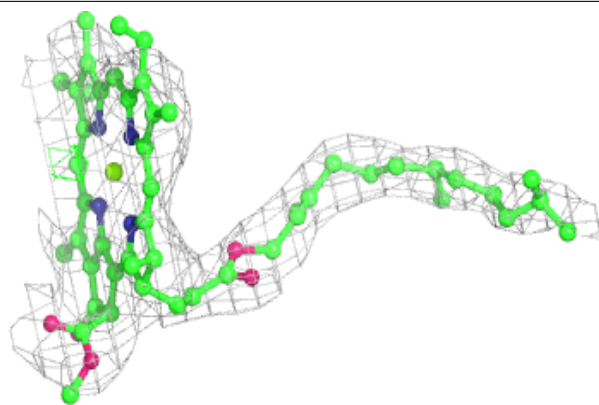
Electron density around CLA F 1301:

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

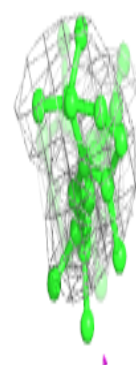
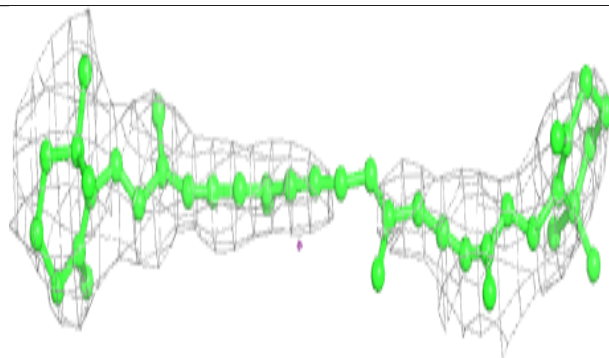
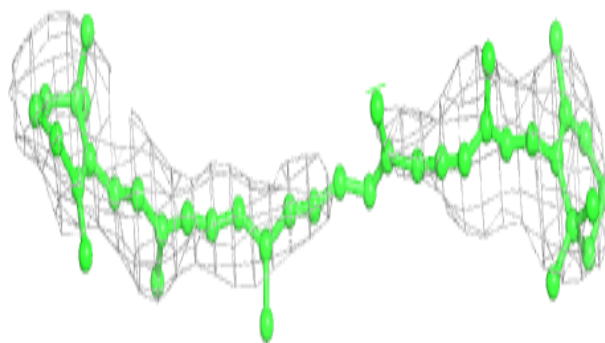


Electron density around CLA L 1502:

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

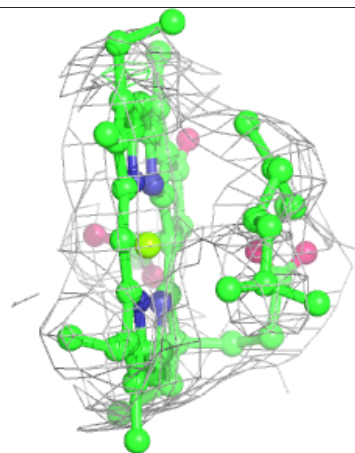
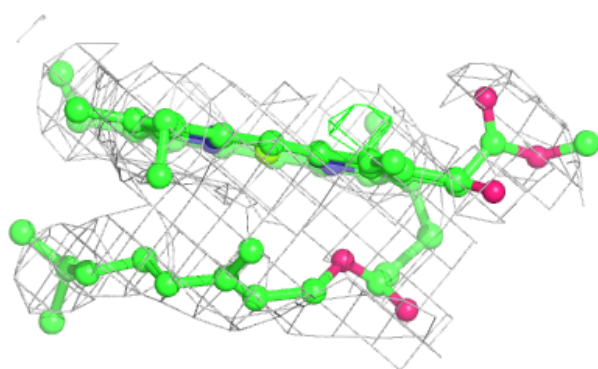
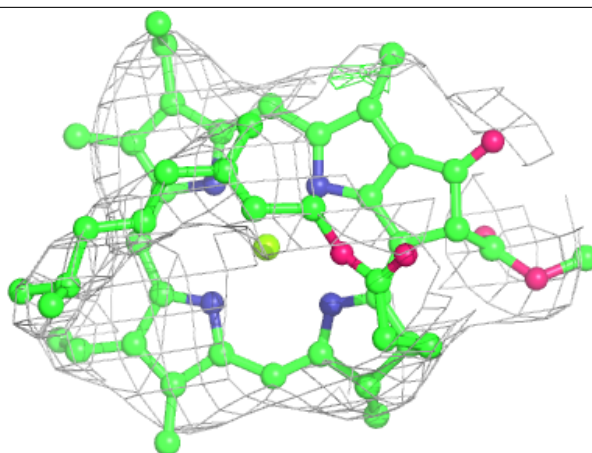
**Electron density around BCR L 6020:**

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



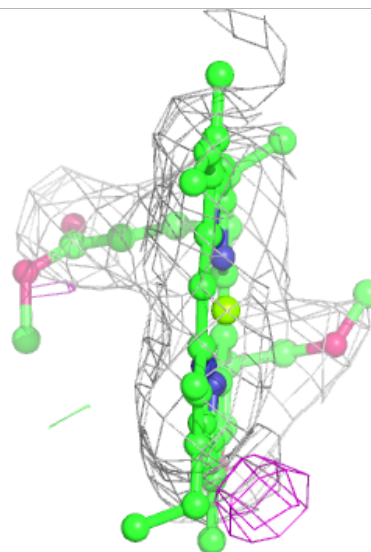
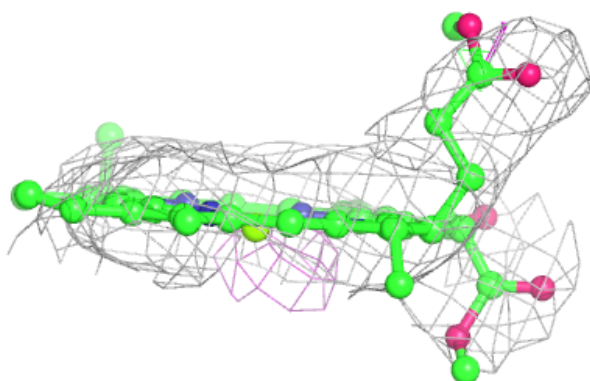
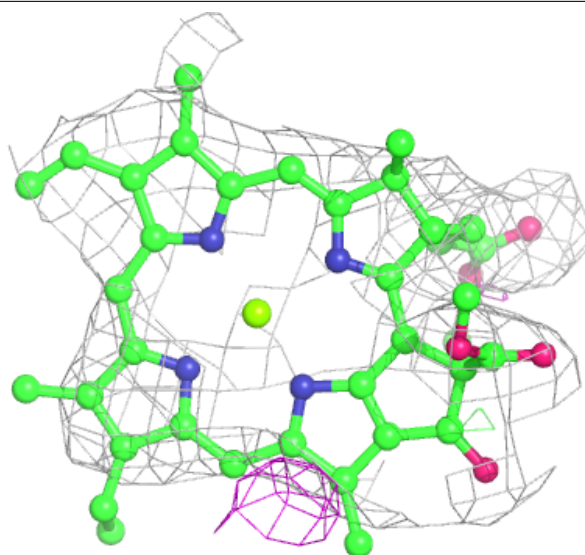
Electron density around CLA 2 2003:

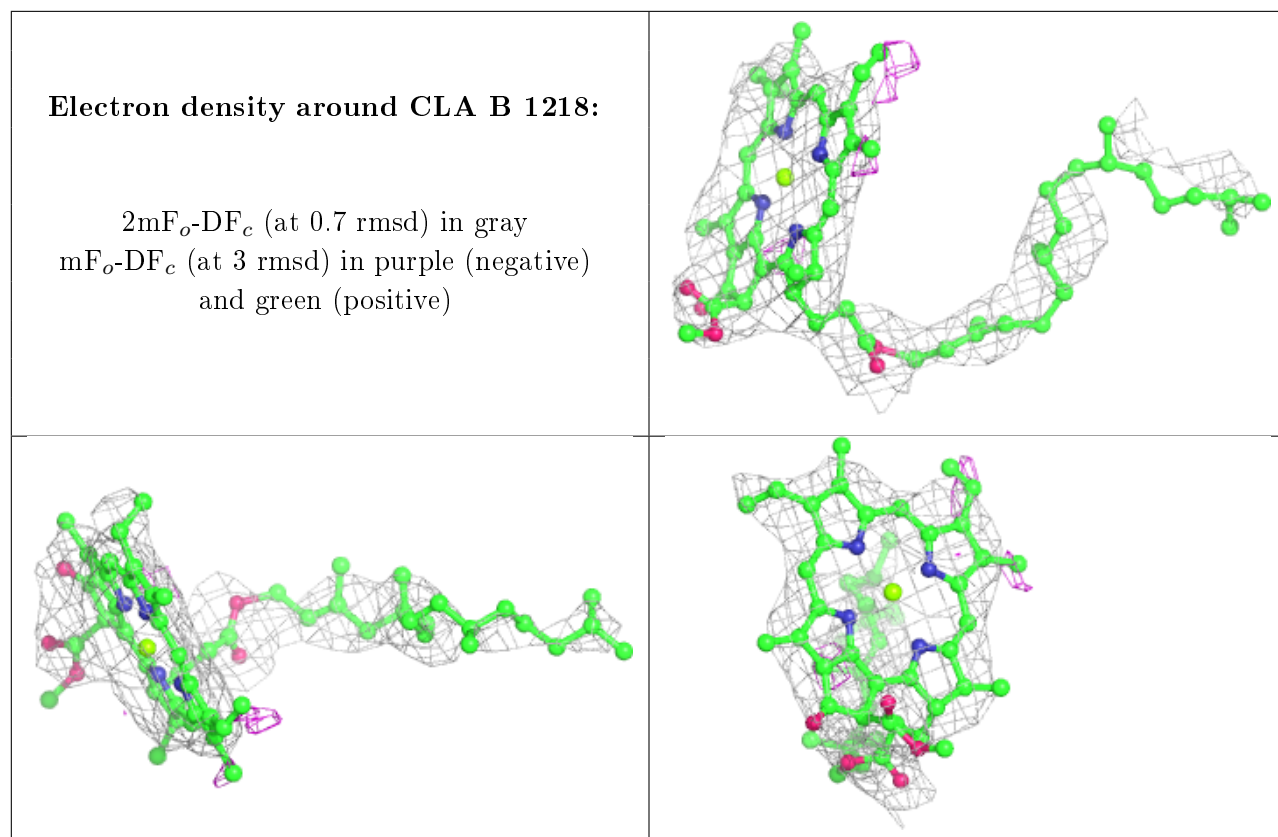
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 1114:

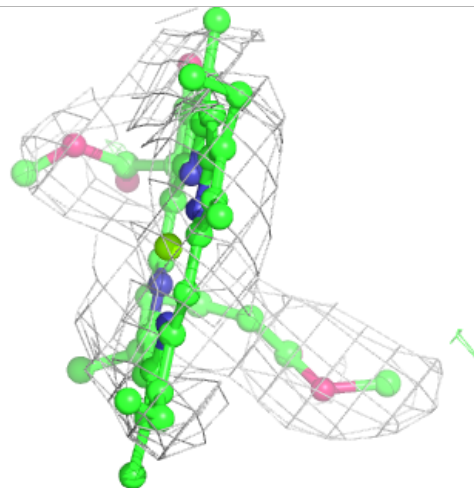
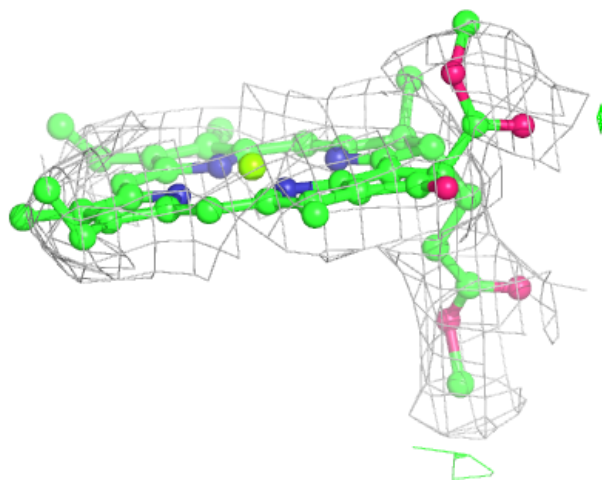
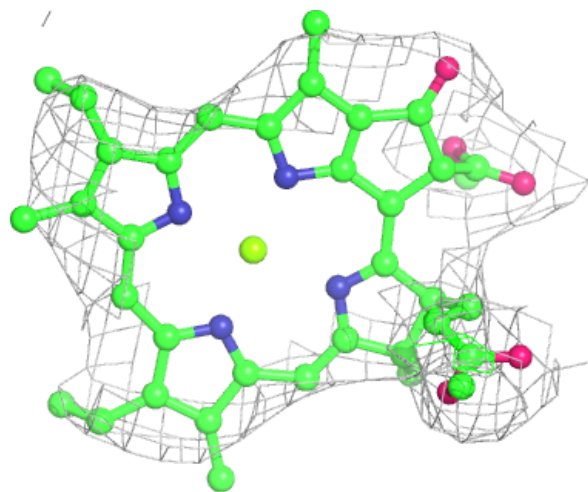
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

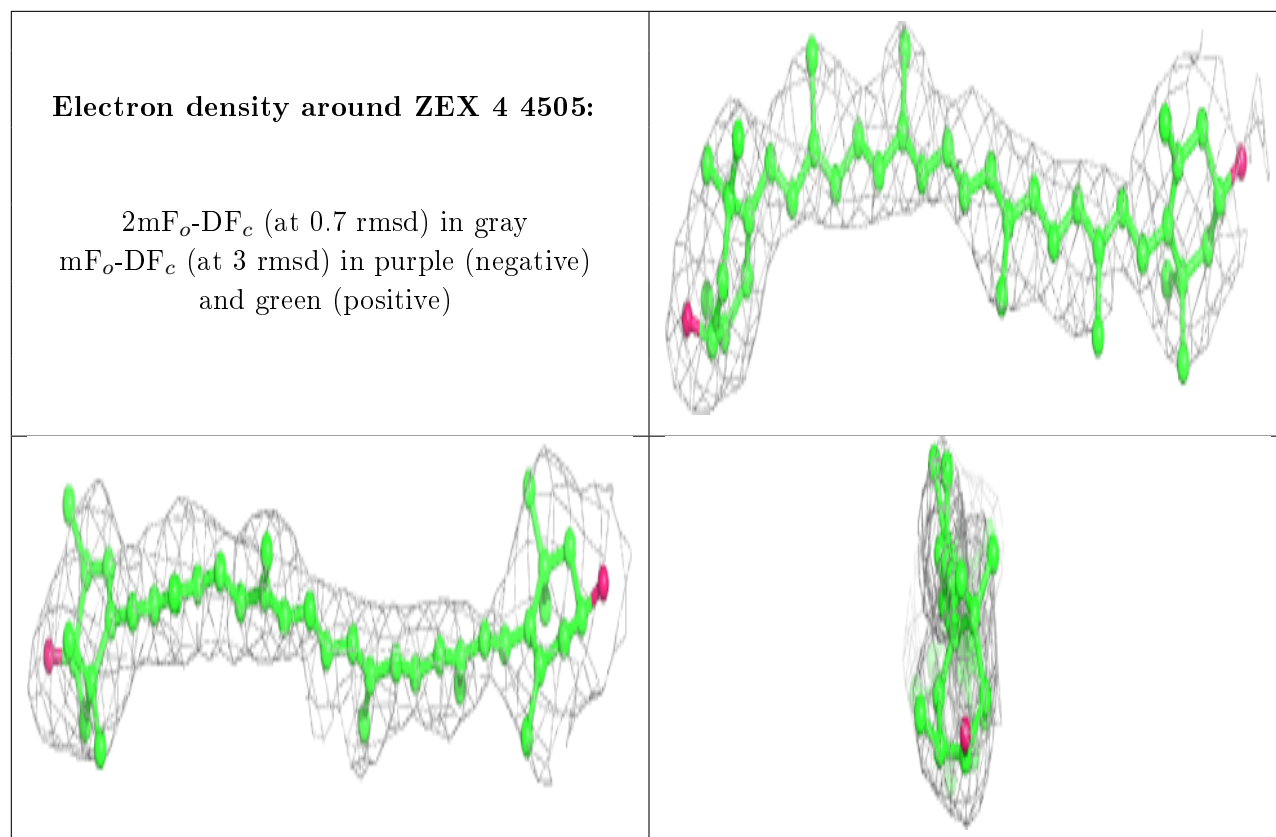




Electron density around CLA A 1118:

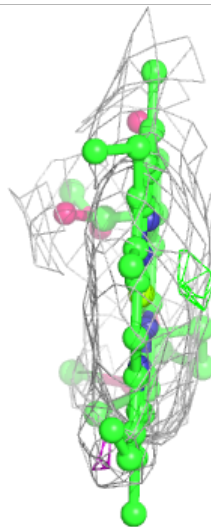
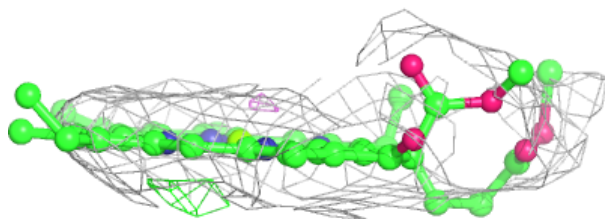
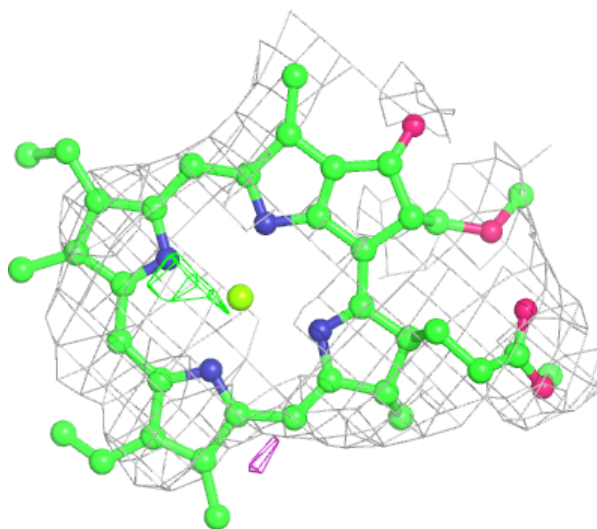
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

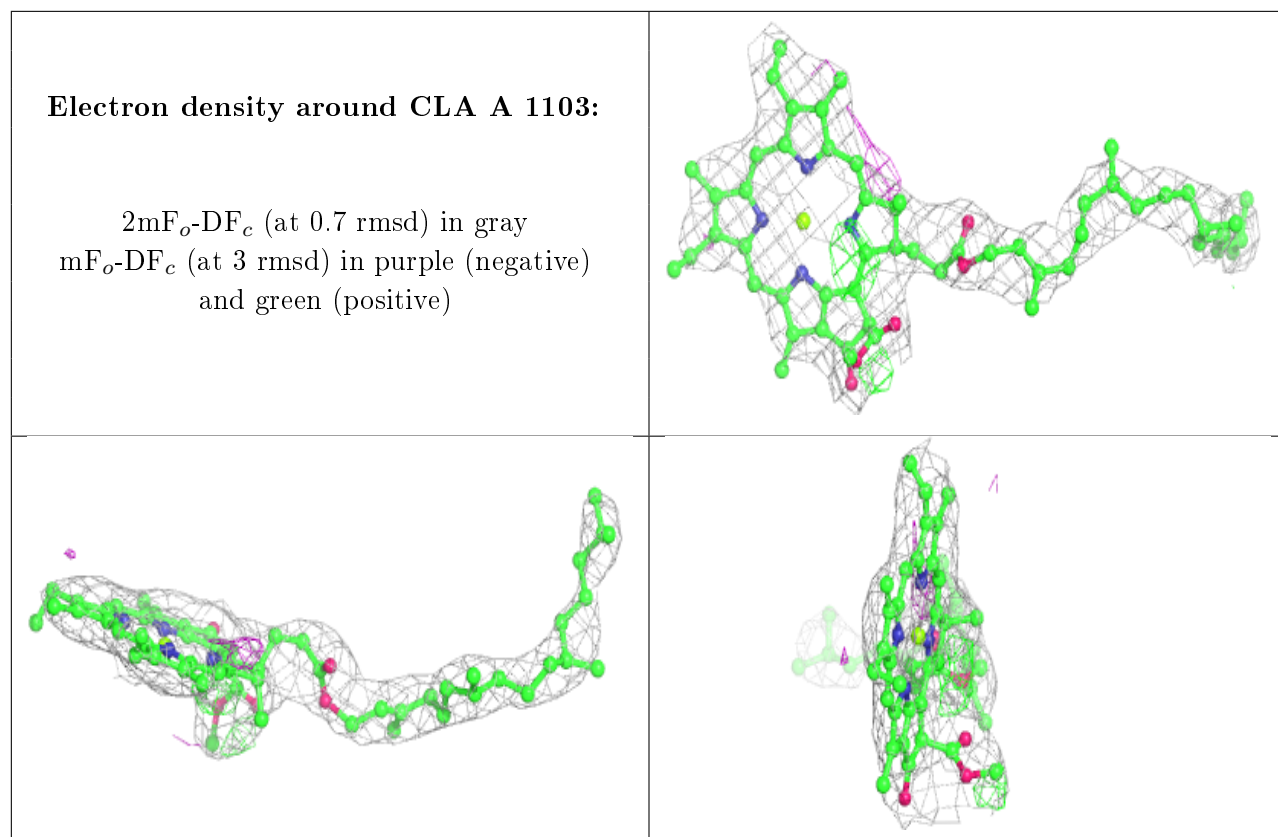




Electron density around CLA 3 3002:

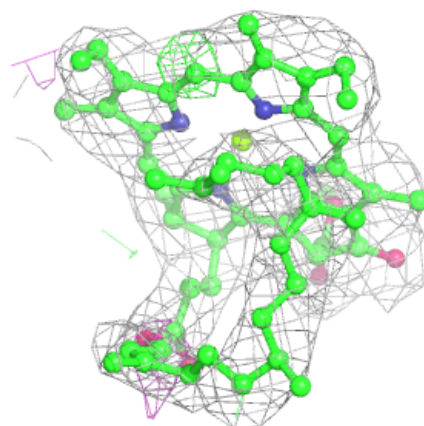
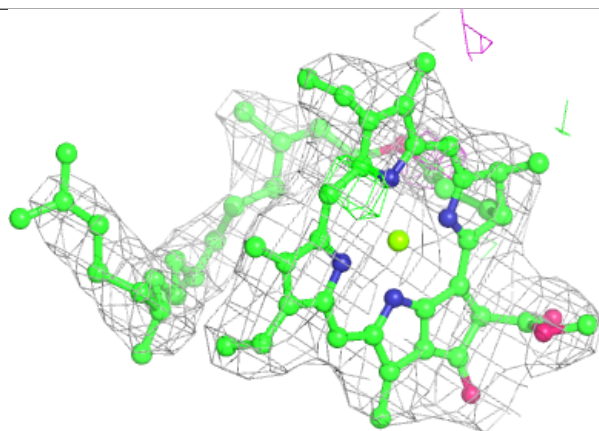
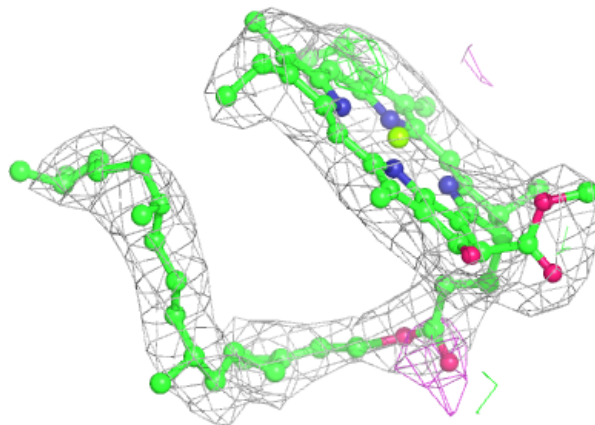
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





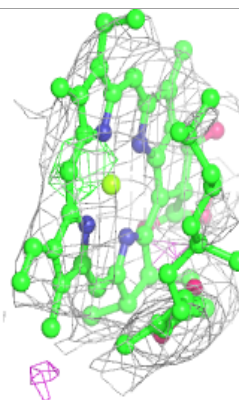
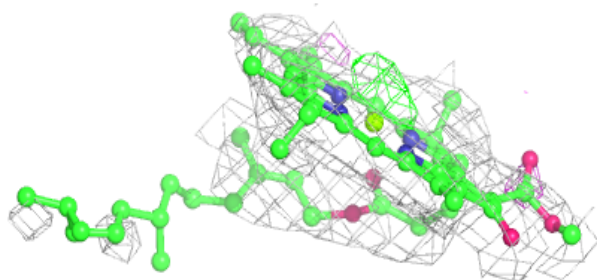
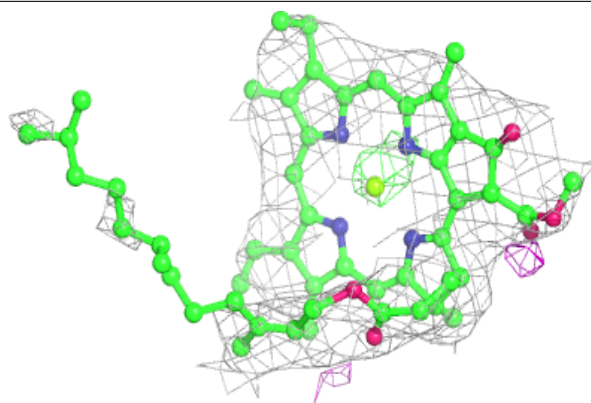
Electron density around CLA B 1227:

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

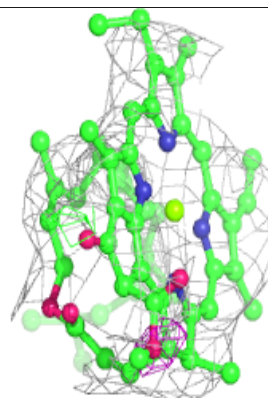
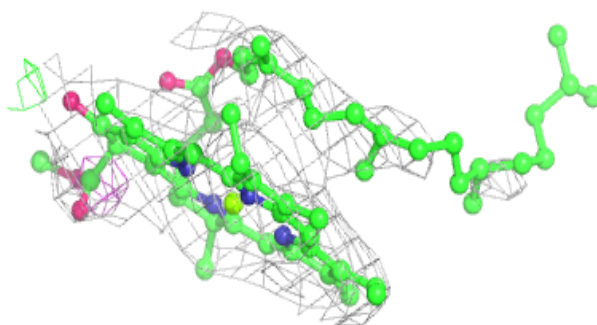
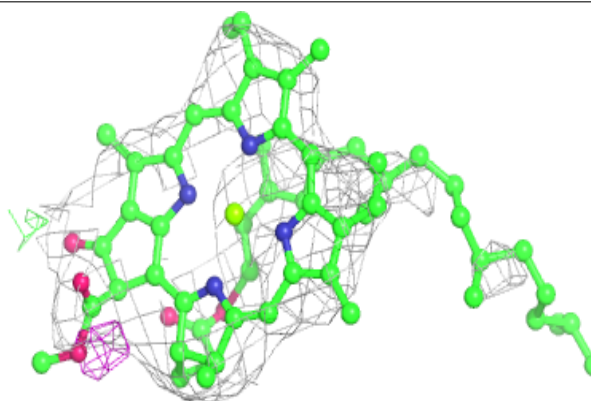


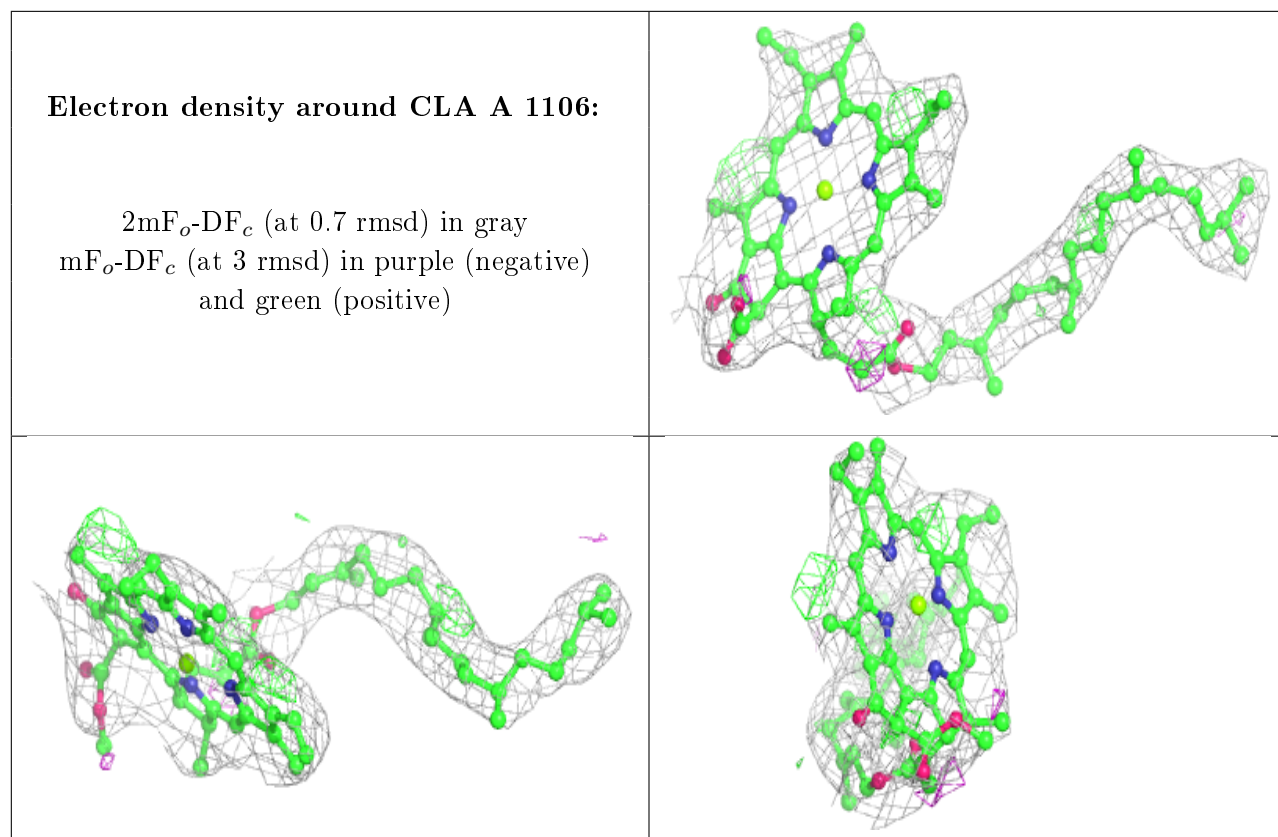
Electron density around CLA 2 2001:

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

**Electron density around CLA 4 4003:**

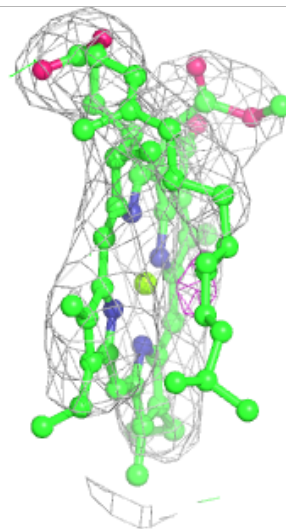
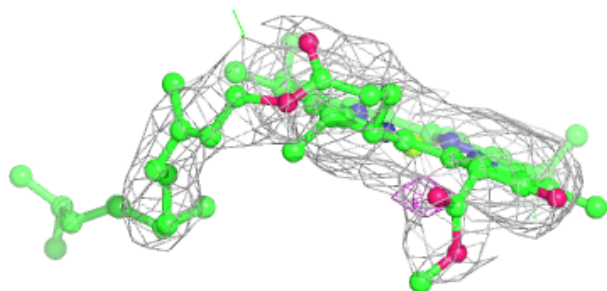
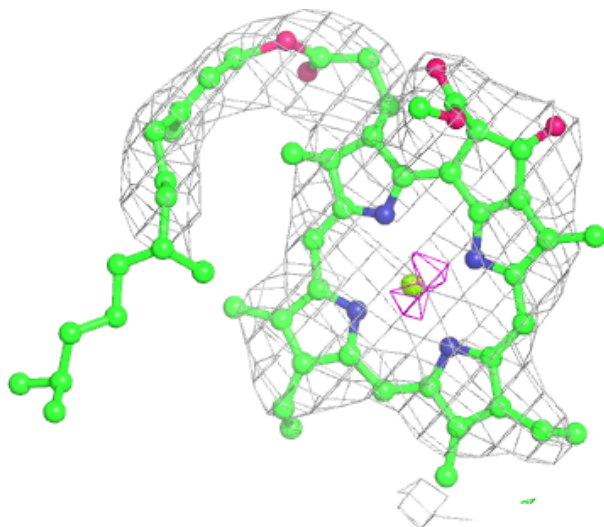
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





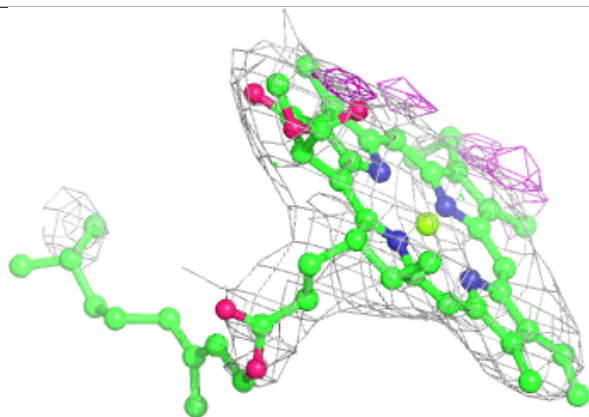
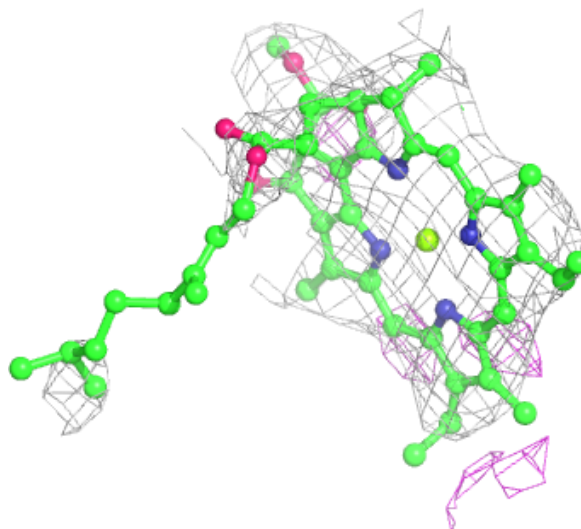
Electron density around CLA A 1111:

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



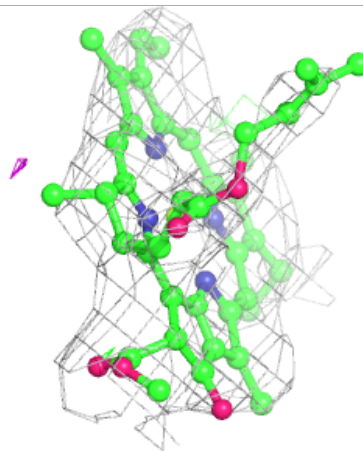
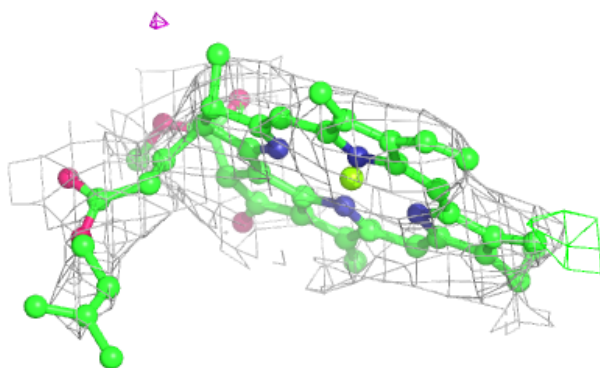
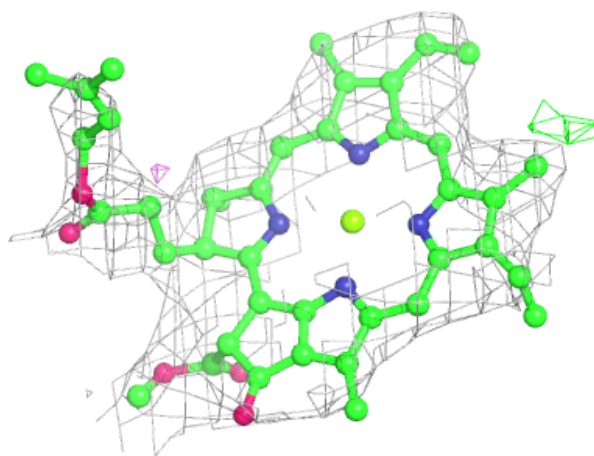
Electron density around CLA 2 2012:

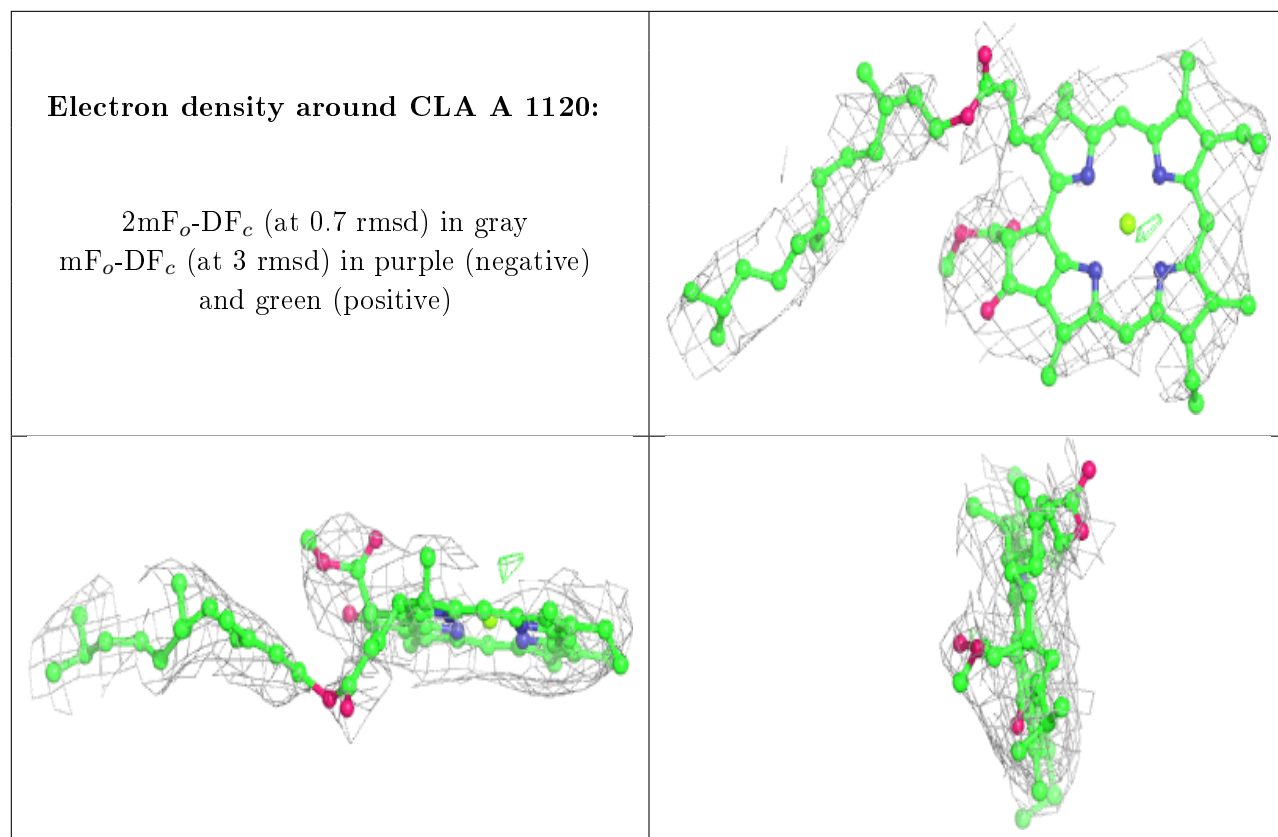
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 2009:

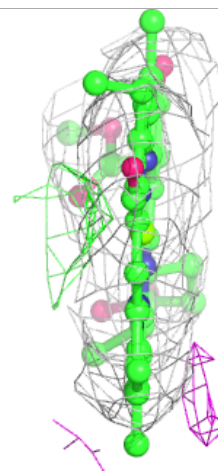
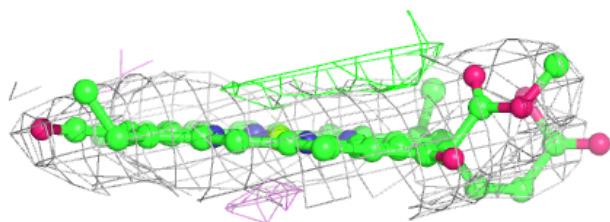
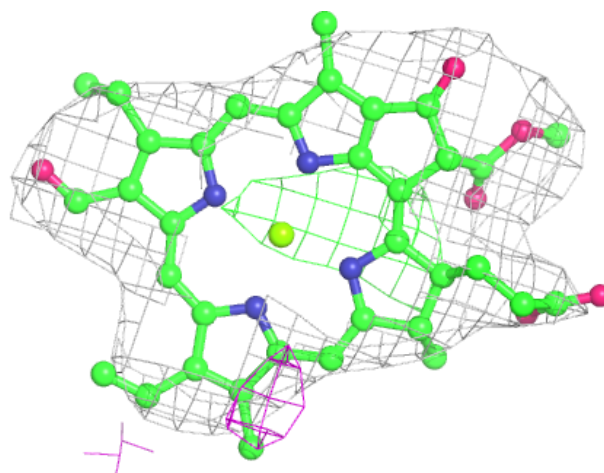
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





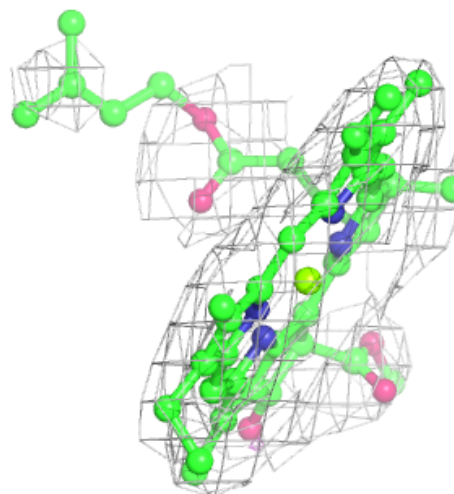
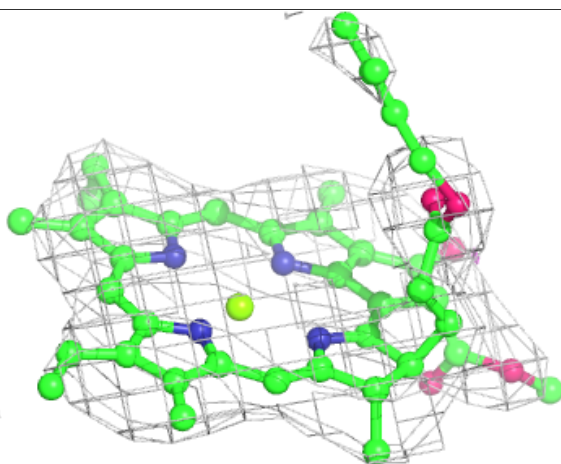
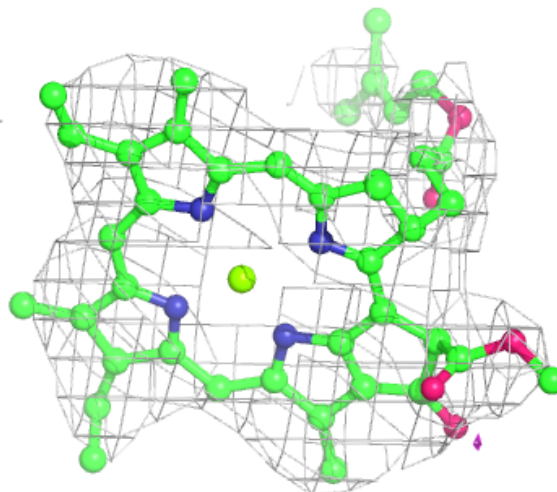
Electron density around CHL 2 2013:

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



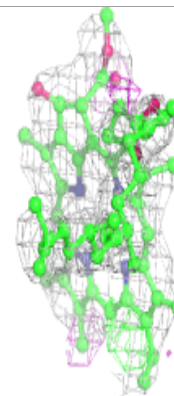
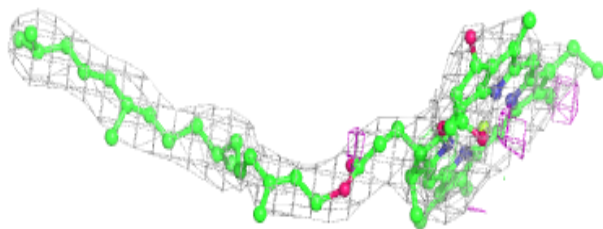
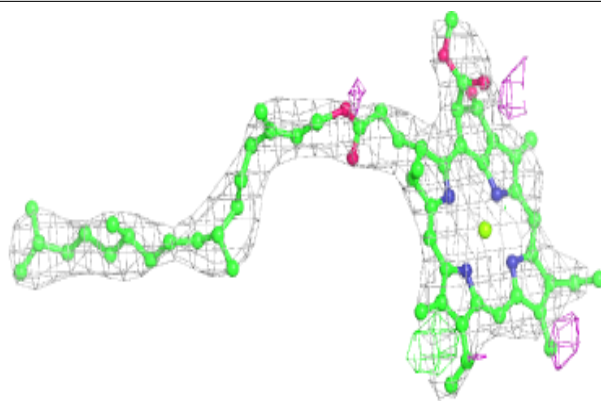
Electron density around CLA A 1130:

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

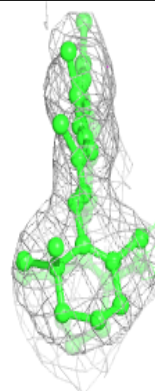
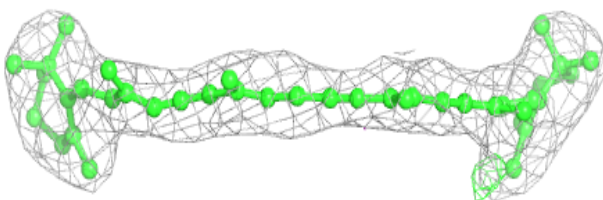
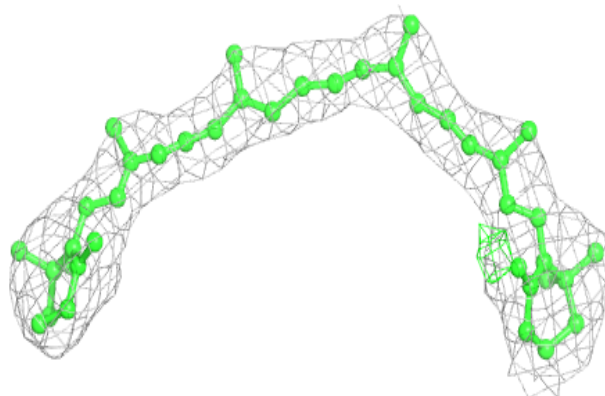


Electron density around CLA A 1022:

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

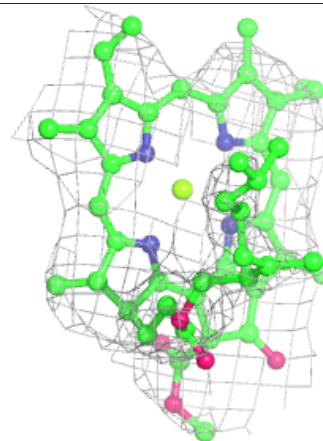
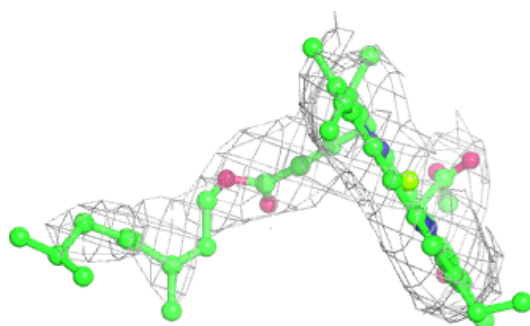
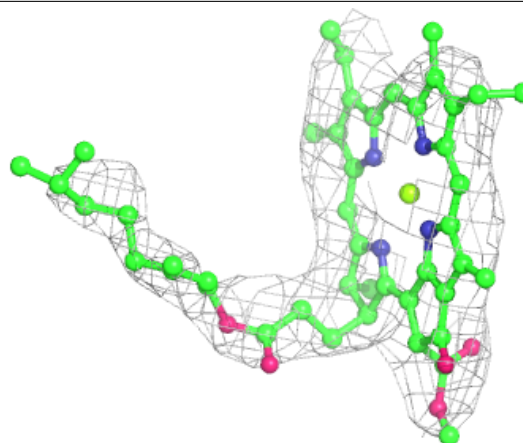
**Electron density around BCR F 6016:**

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

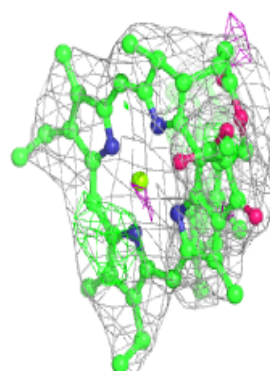
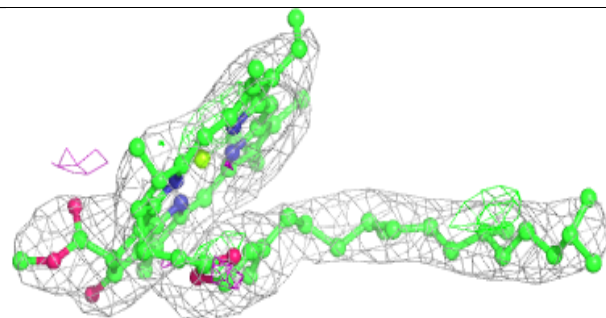
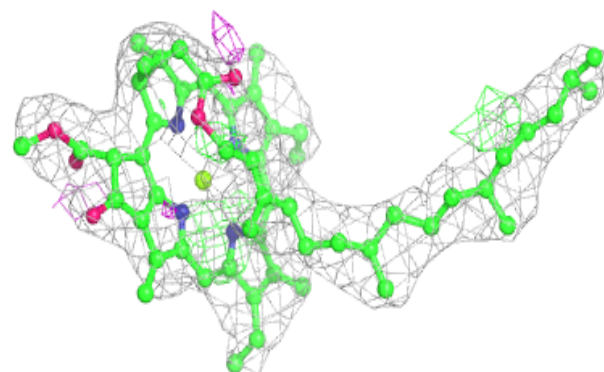


Electron density around CLA B 1232:

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

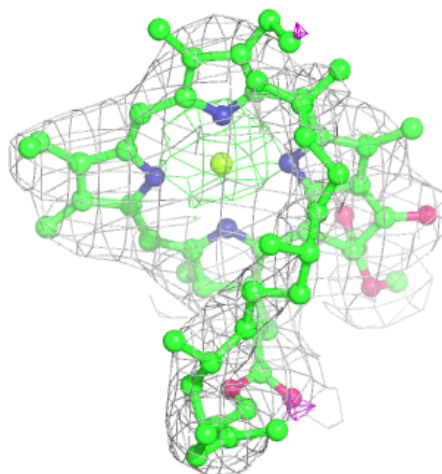
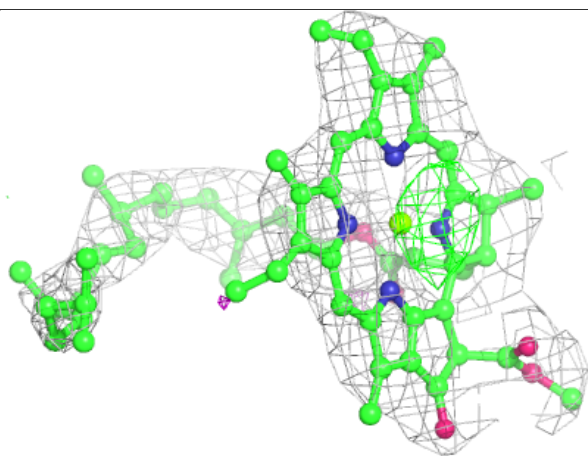
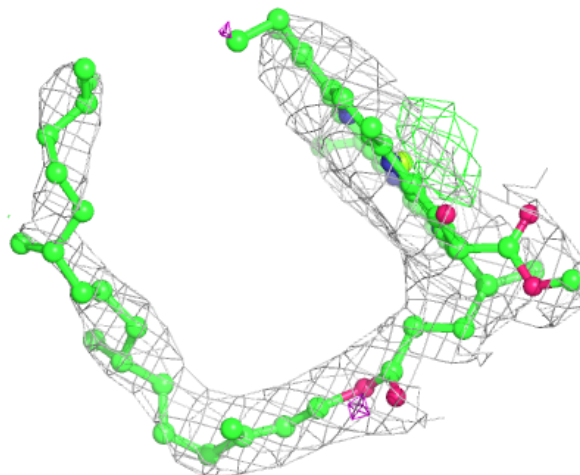
**Electron density around CLA A 1140:**

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



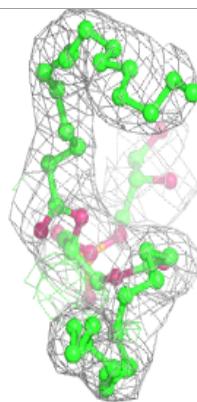
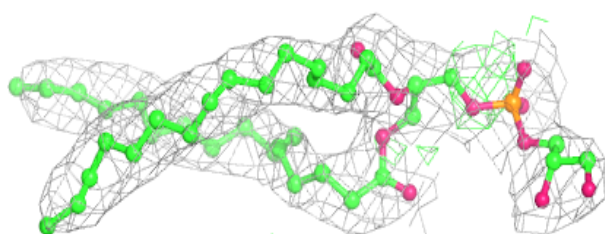
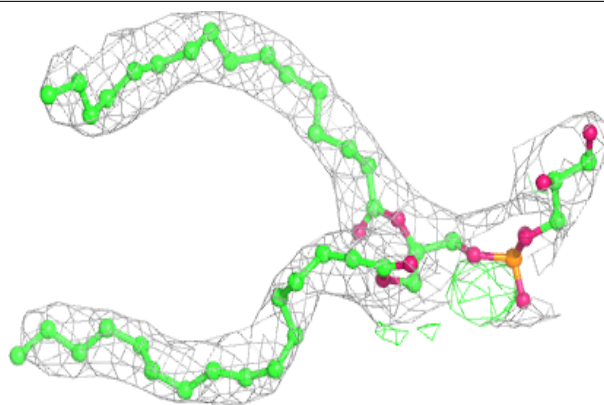
Electron density around CLA B 1216:

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

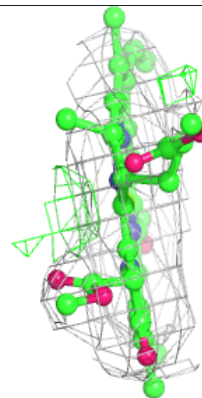
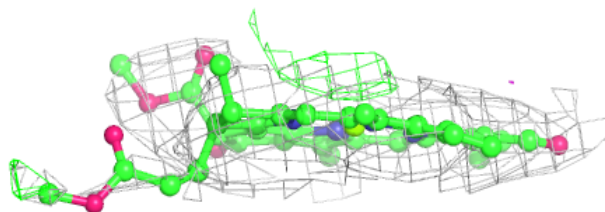
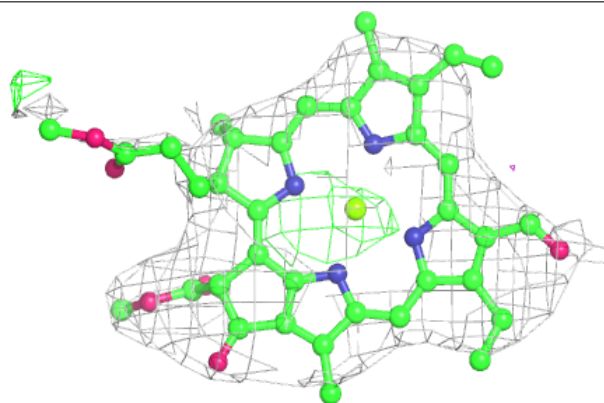


Electron density around LHG A 7001:

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

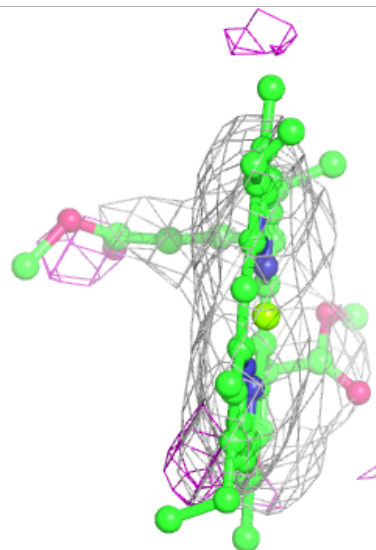
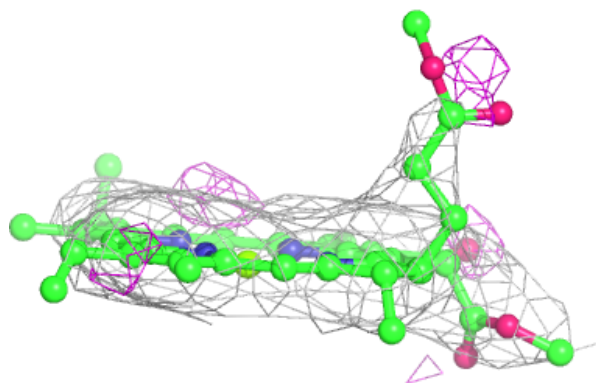
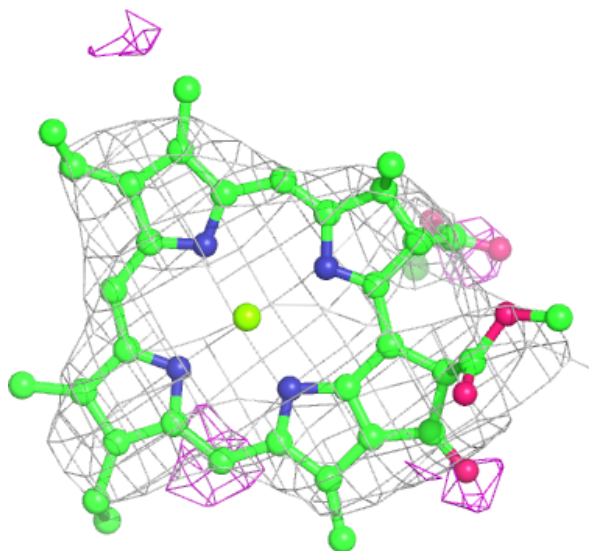
**Electron density around CHL 4 4013:**

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



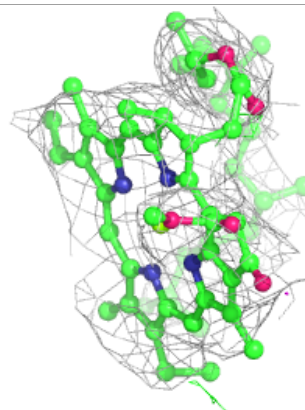
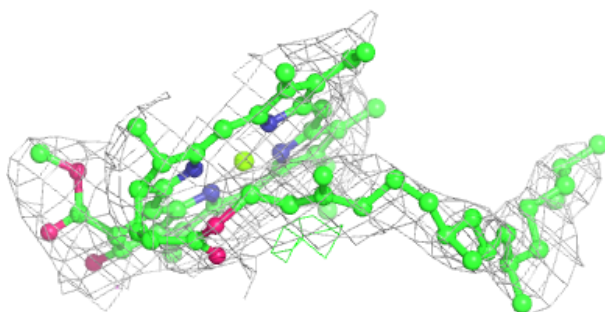
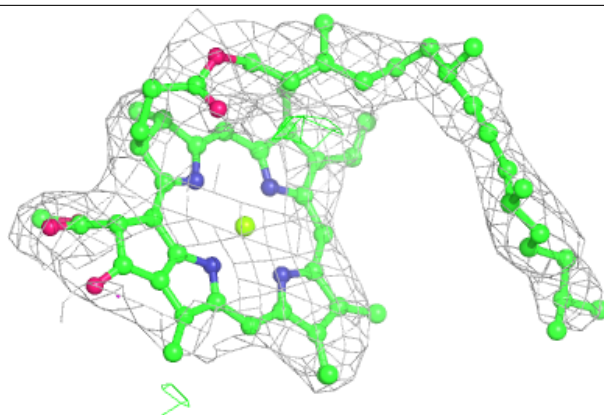
Electron density around CLA A 1108:

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

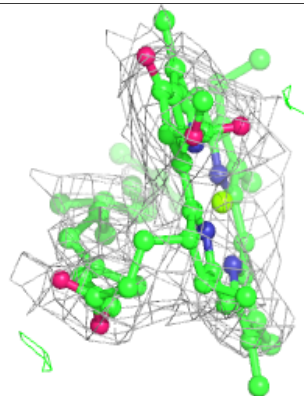
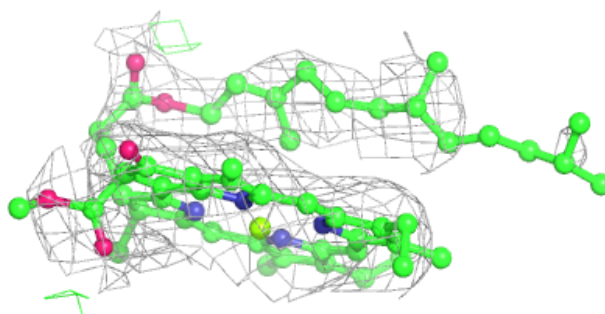
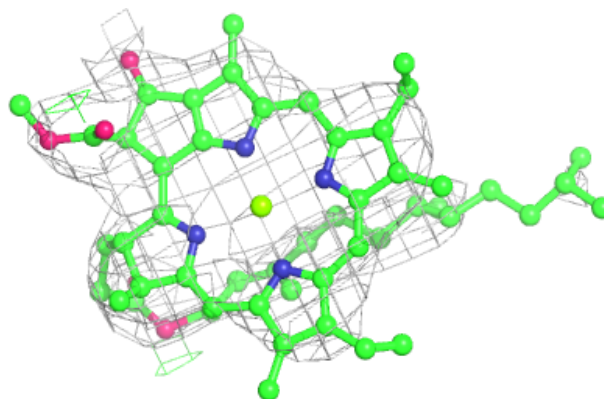


Electron density around CLA 2 2004:

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

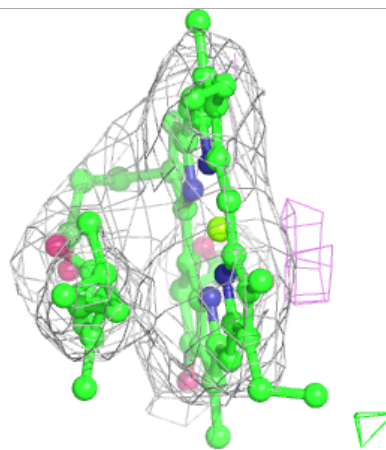
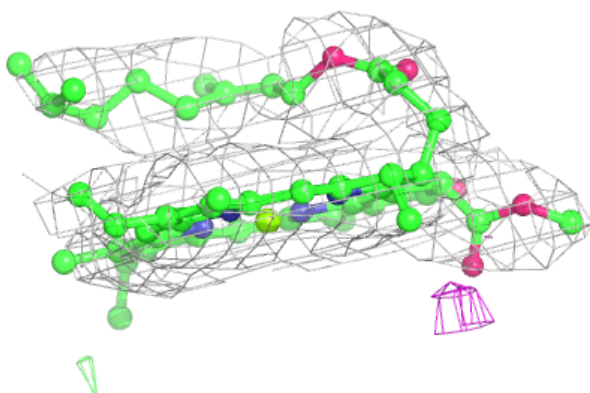
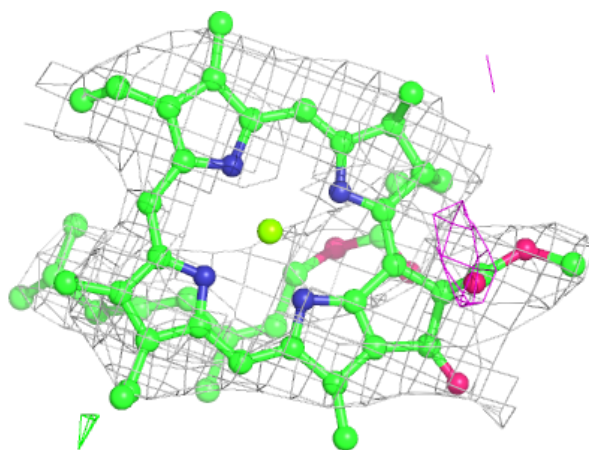
**Electron density around CLA A 1116:**

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



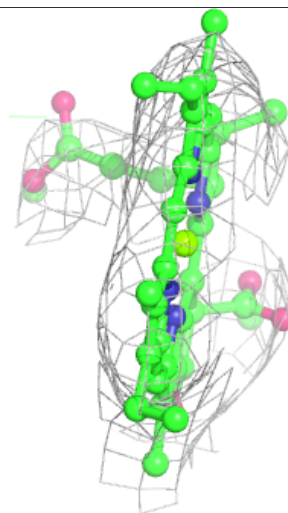
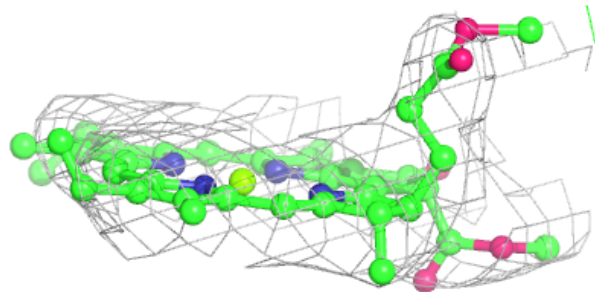
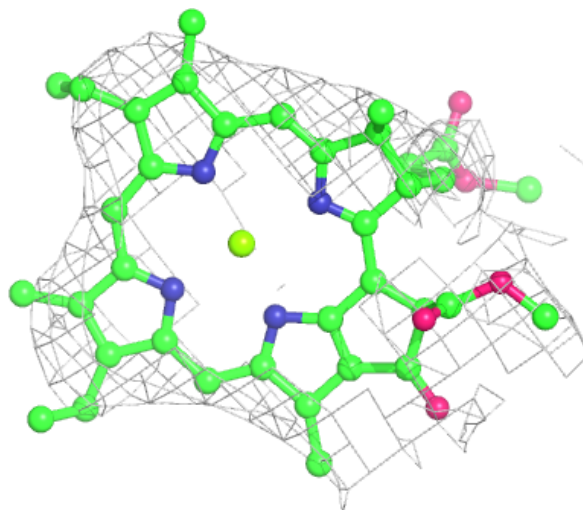
Electron density around CLA B 1204:

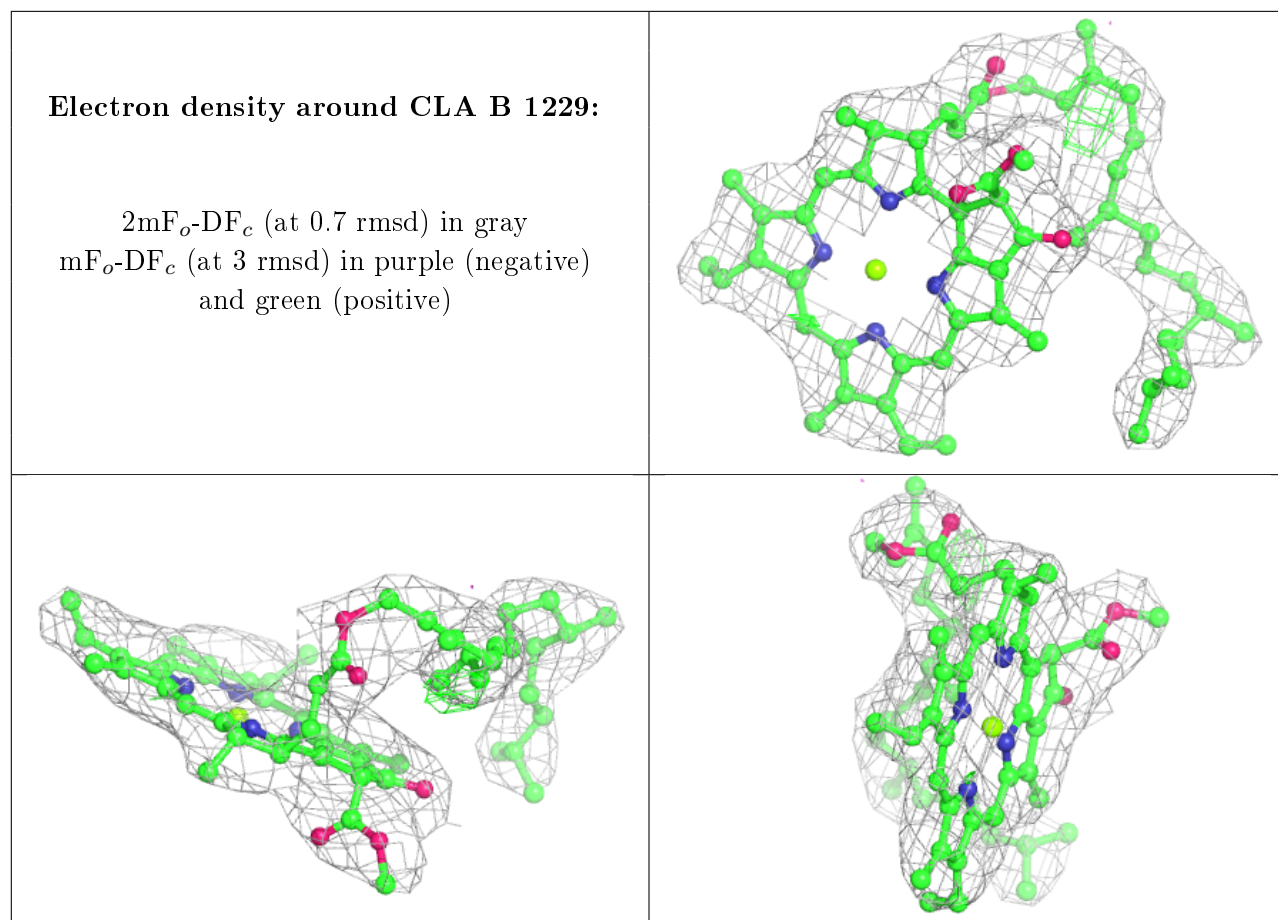
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 1 1007:

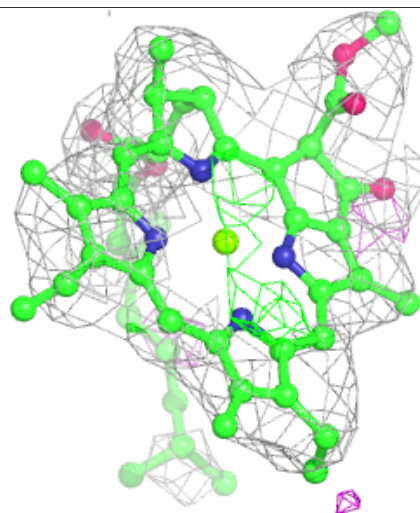
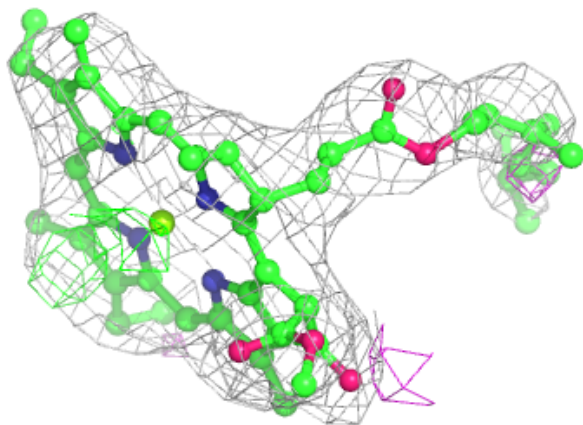
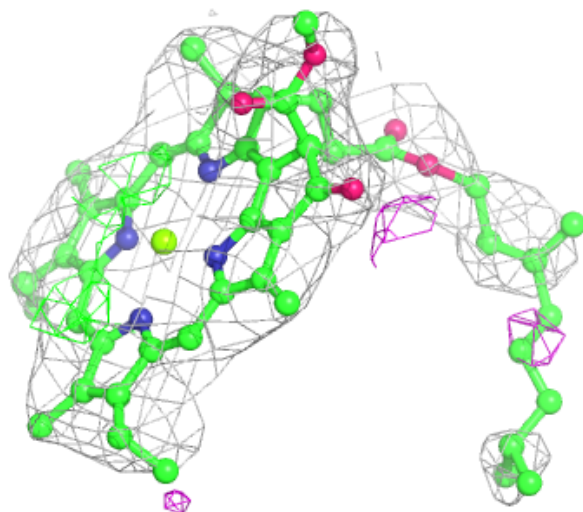
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

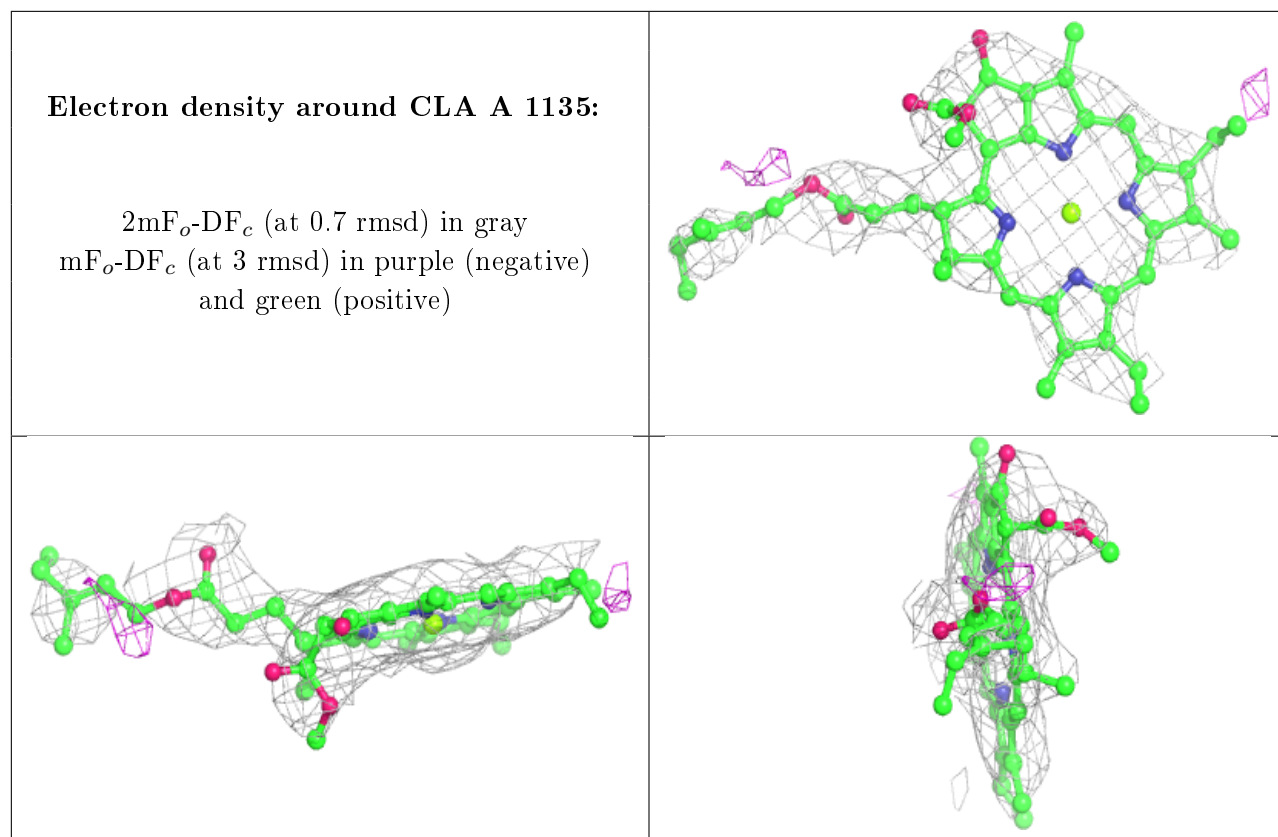




Electron density around CLA B 1236:

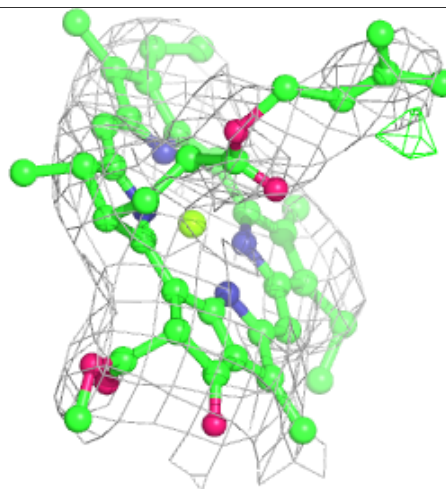
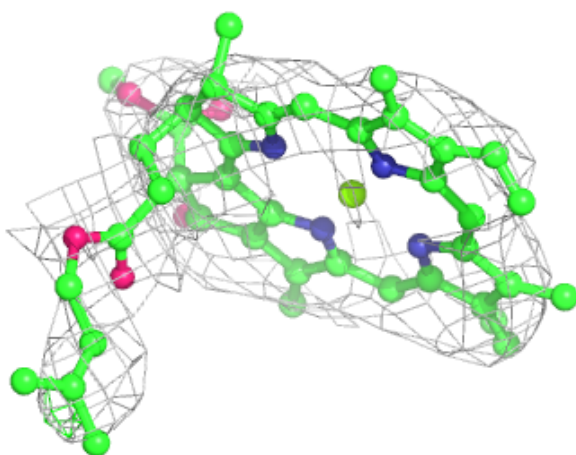
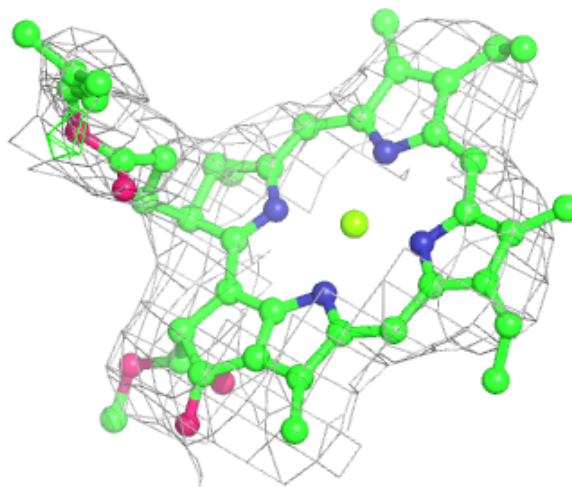
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





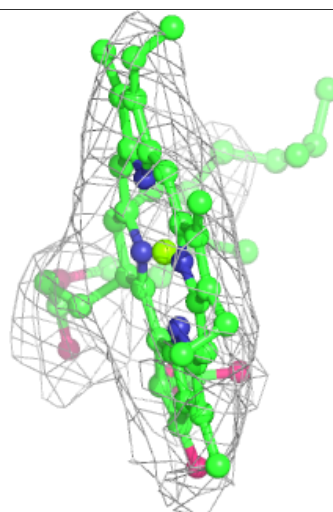
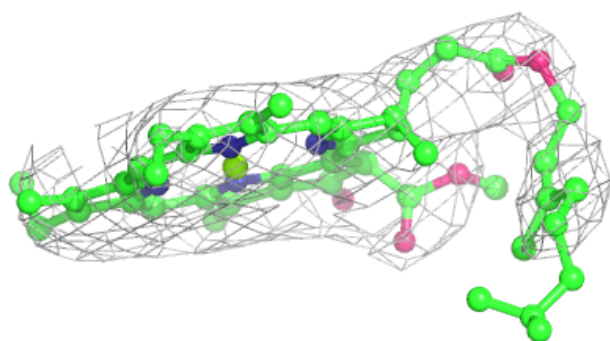
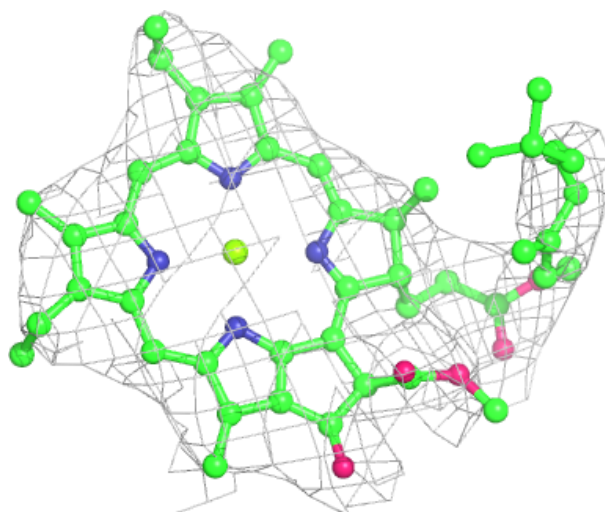
Electron density around CLA 2 2008:

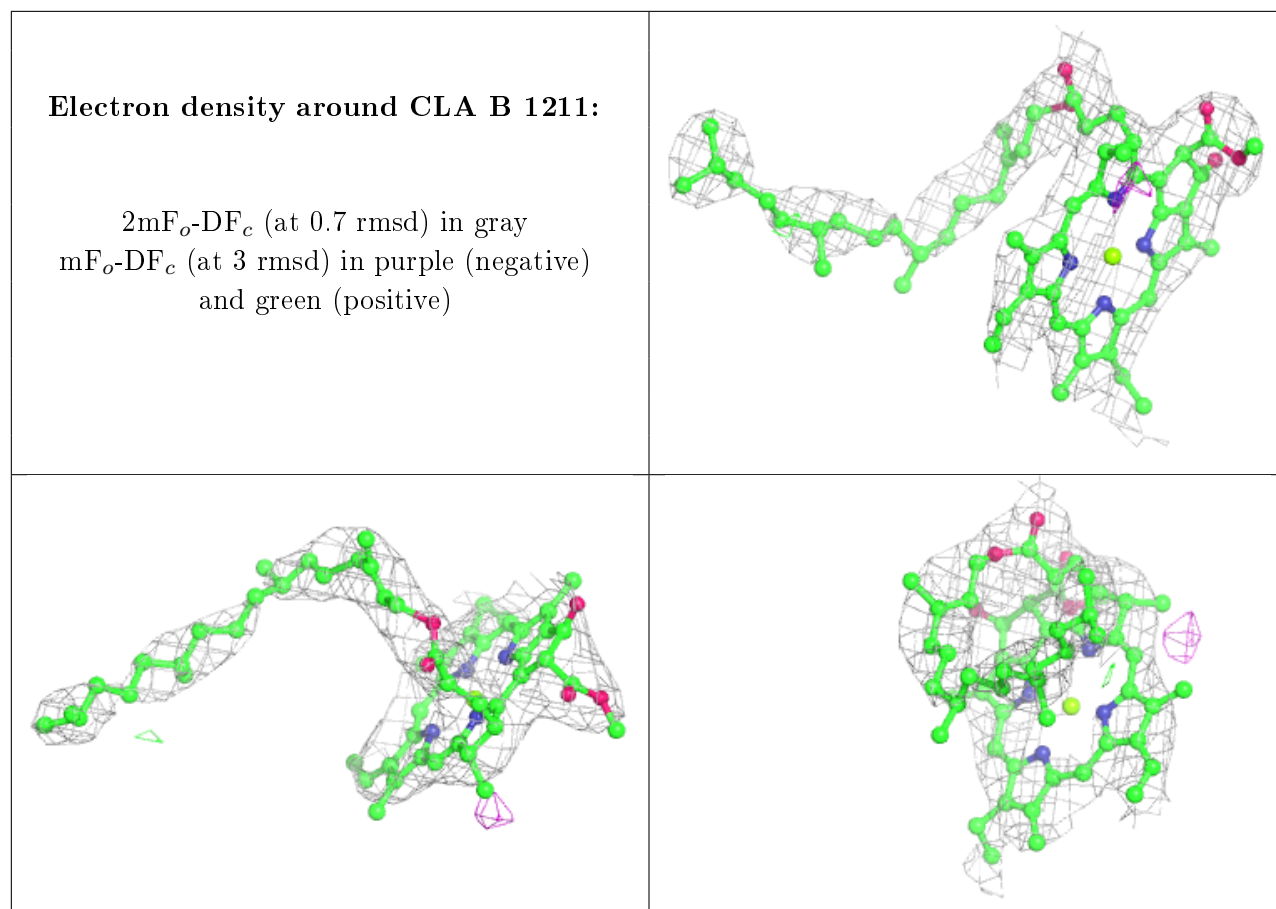
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 2005:

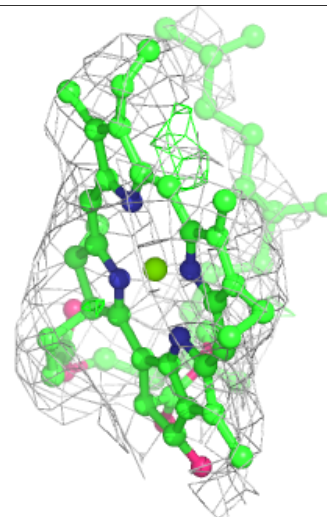
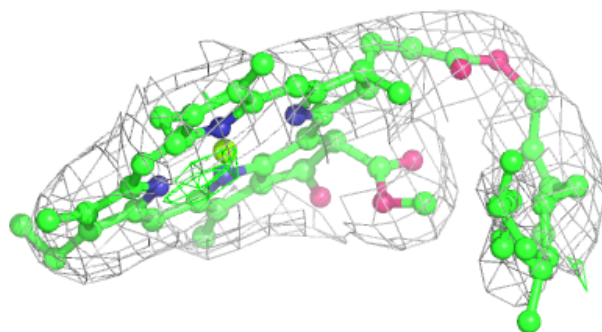
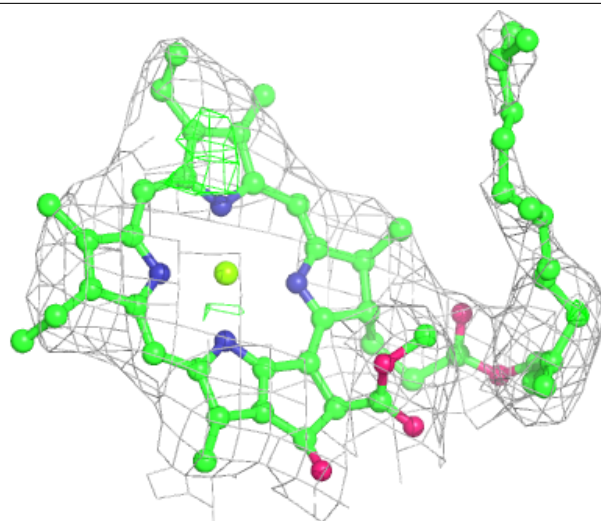
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





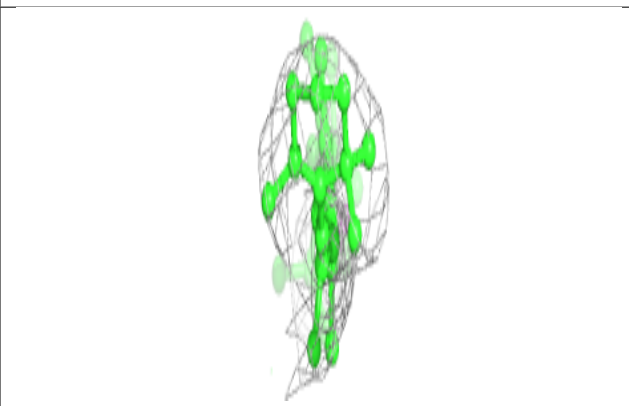
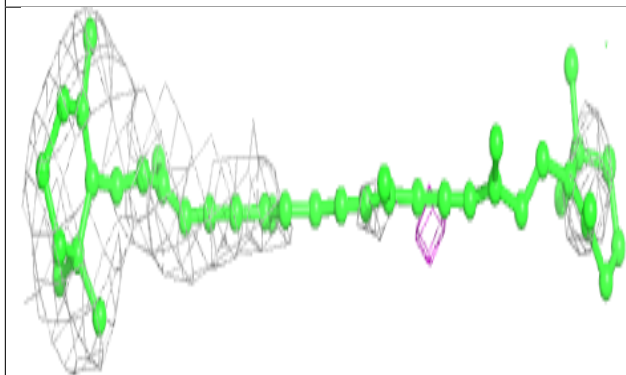
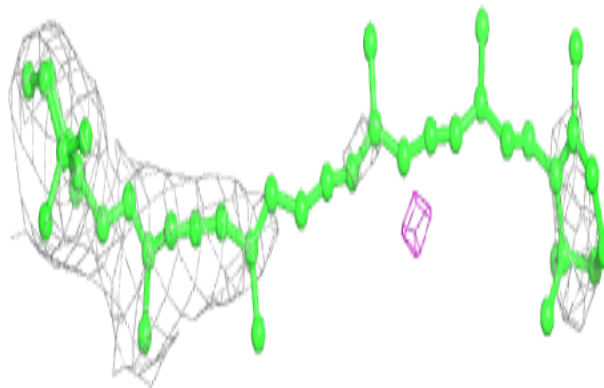
Electron density around CLA 4 4005:

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

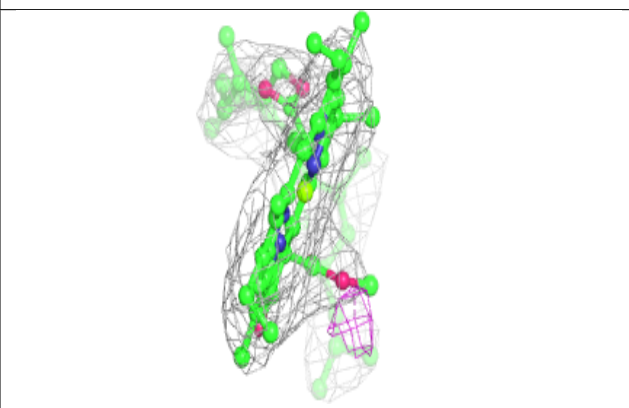
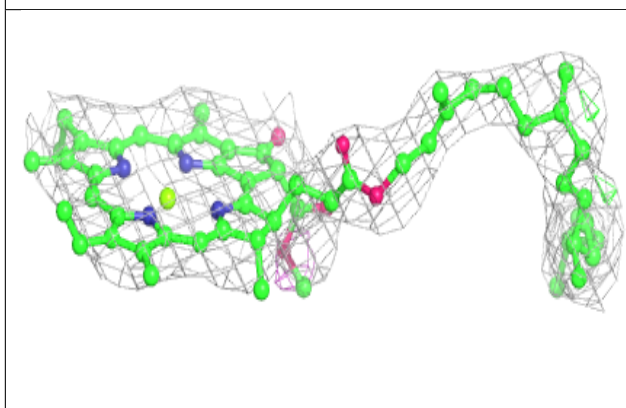
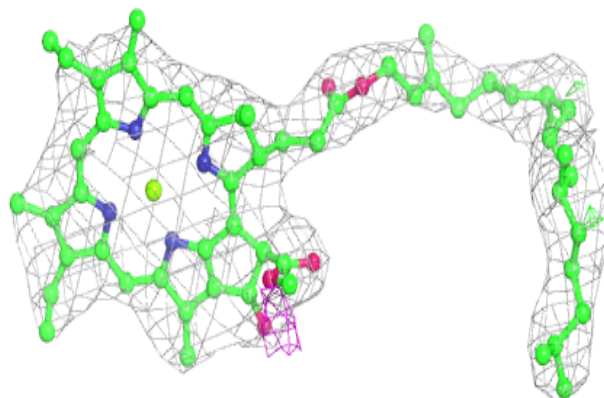


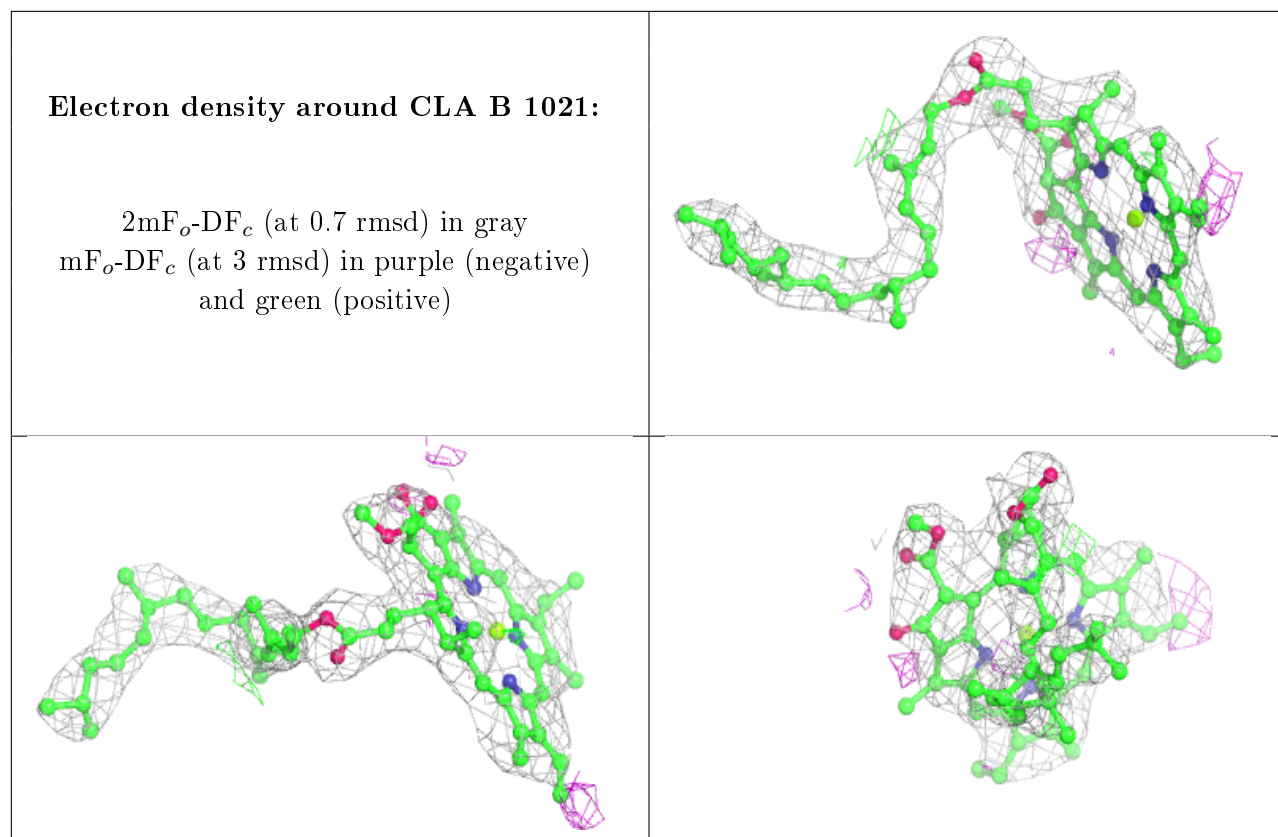
Electron density around BCR A 6002:

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

**Electron density around CLA B 1223:**

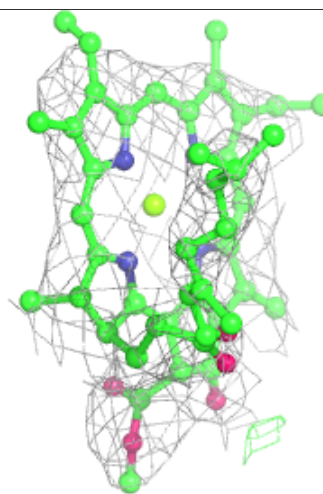
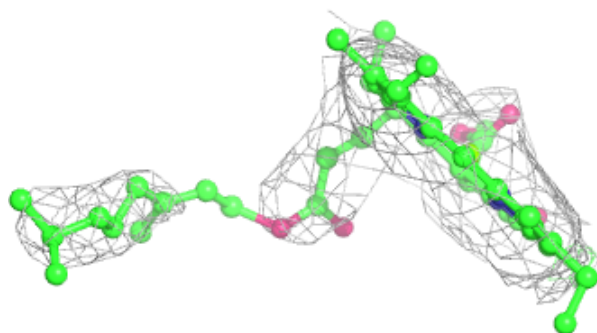
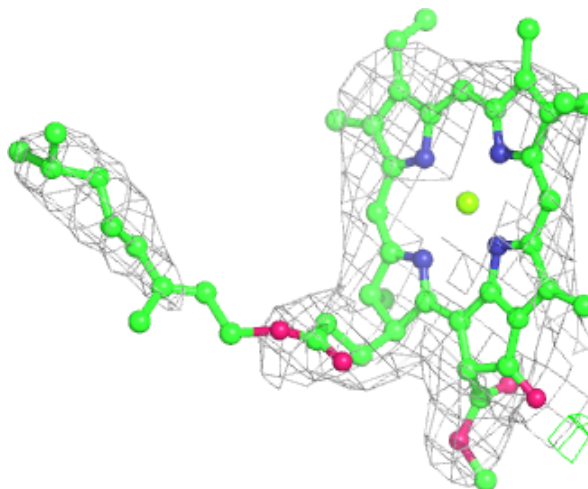
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





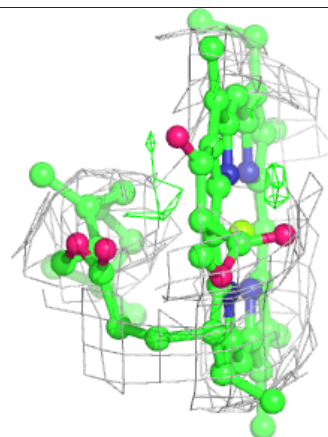
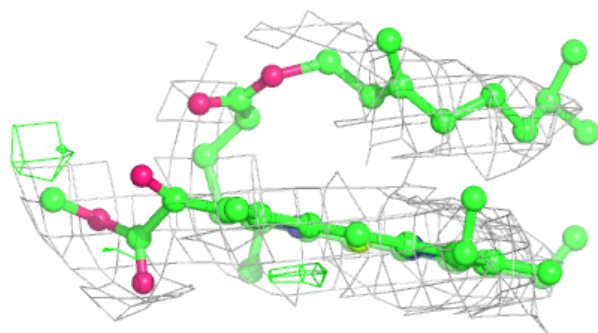
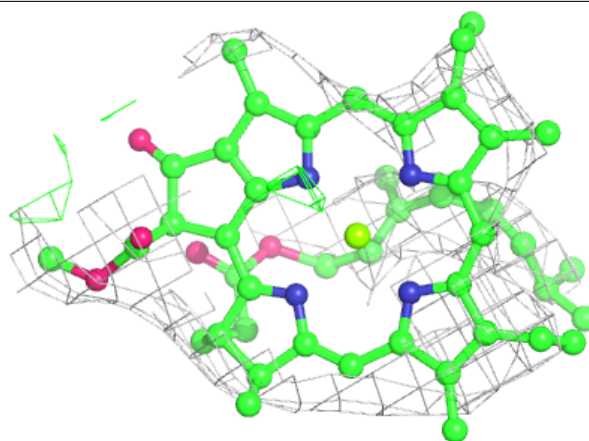
Electron density around CLA A 1133:

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

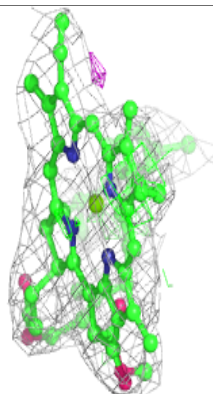
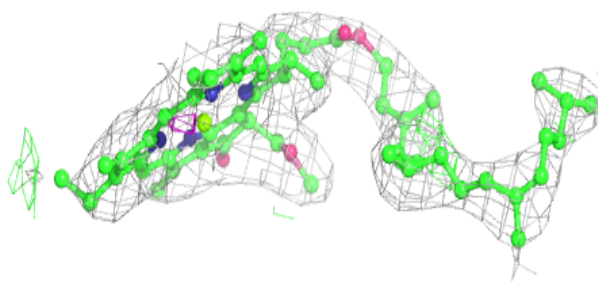
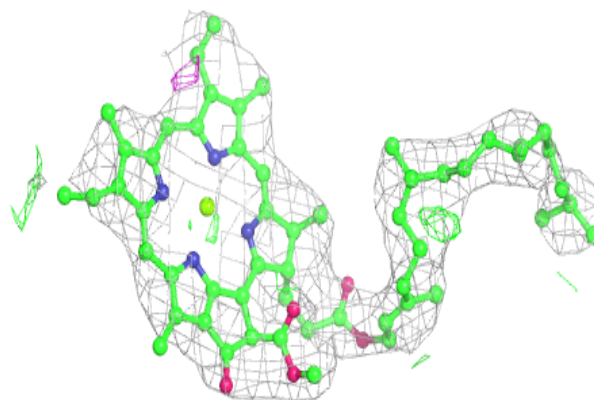


Electron density around CLA 1 1003:

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

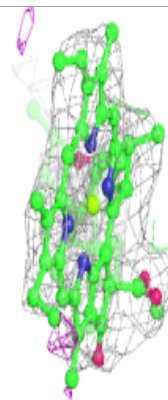
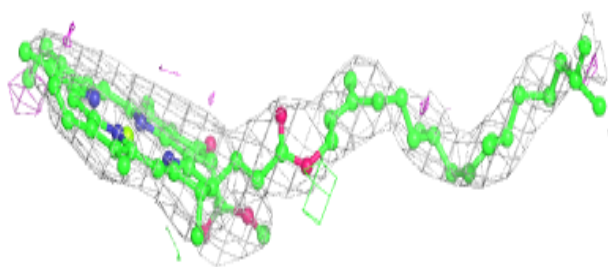
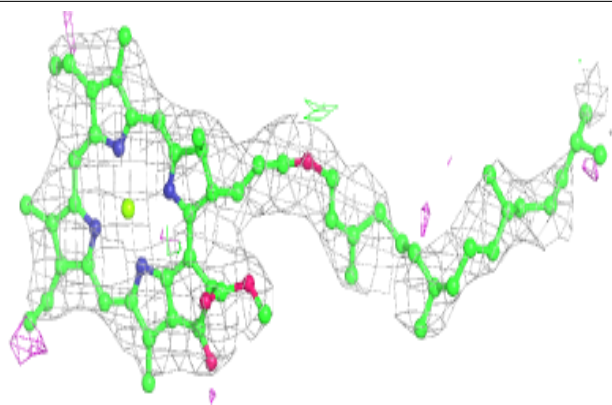
**Electron density around CLA A 1101:**

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

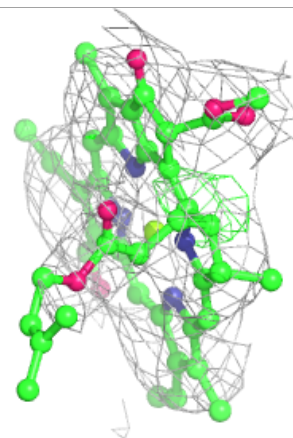
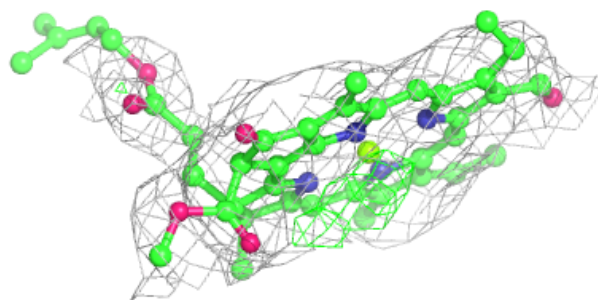
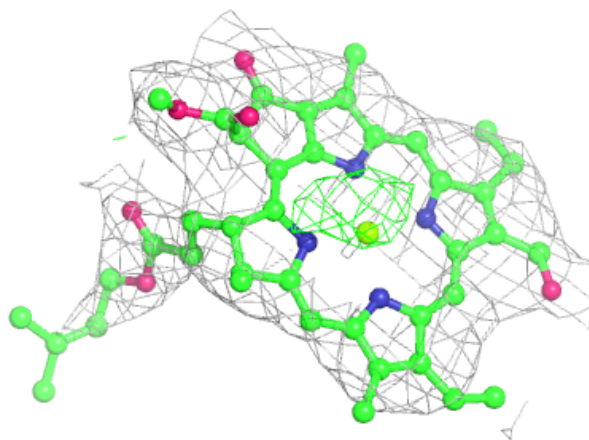


Electron density around CLA A 1139:

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

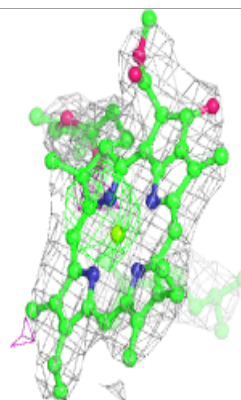
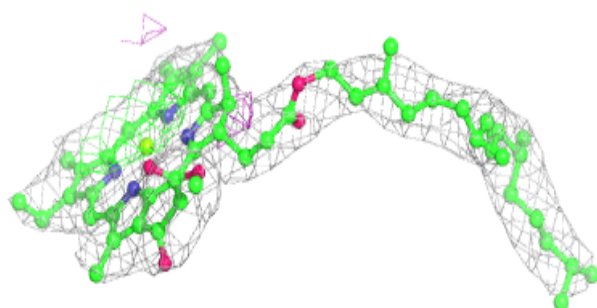
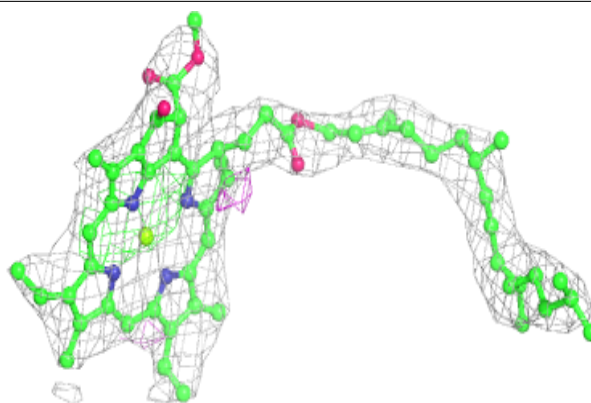
**Electron density around CHL 4 4011:**

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

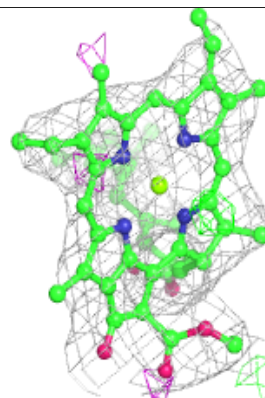
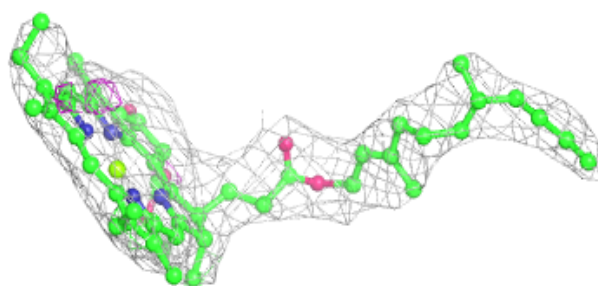
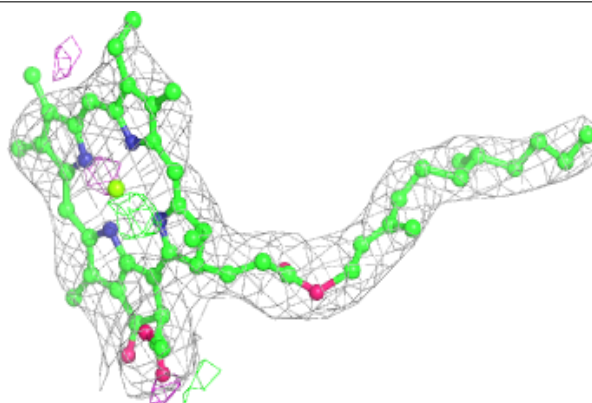


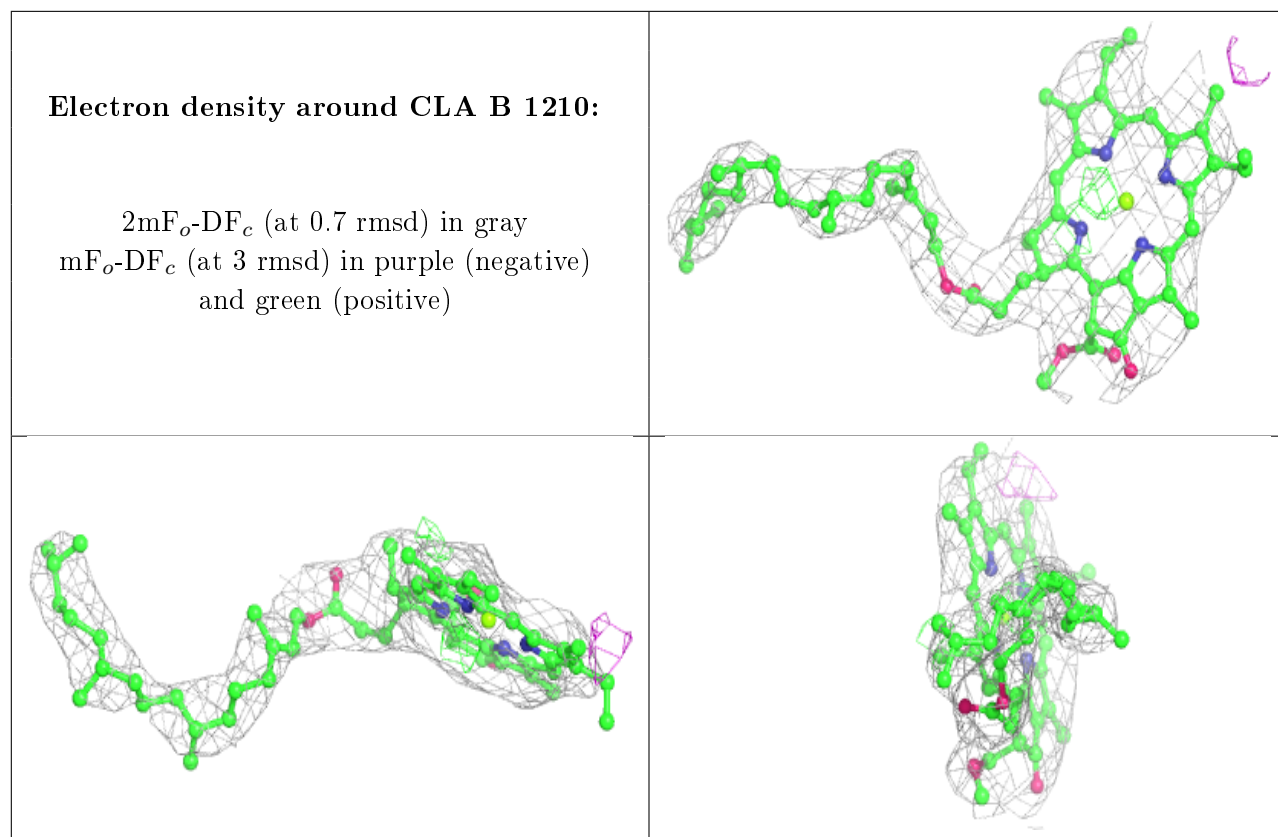
Electron density around CLA B 1012:

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

**Electron density around CLA B 1230:**

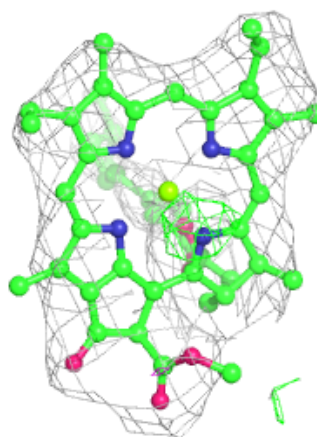
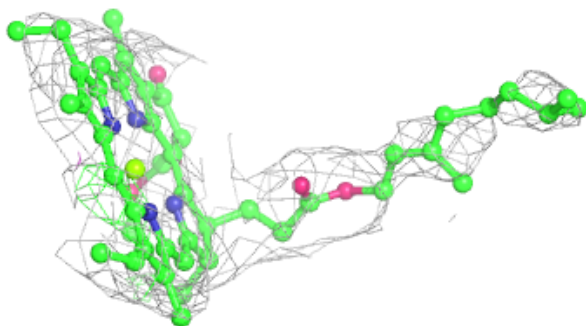
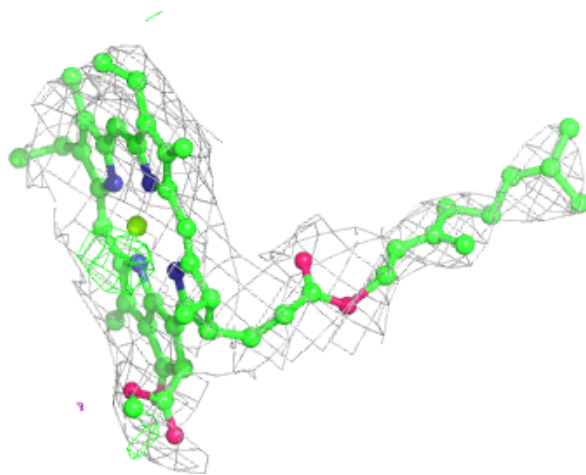
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





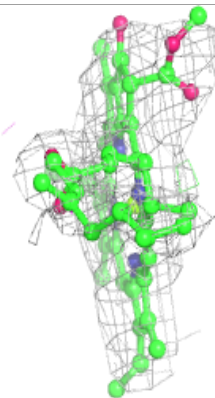
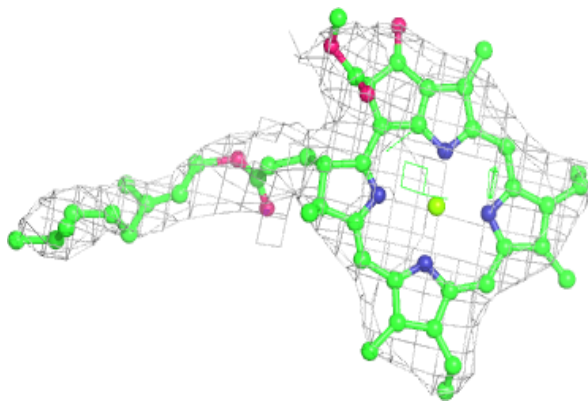
Electron density around CLA B 1208:

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

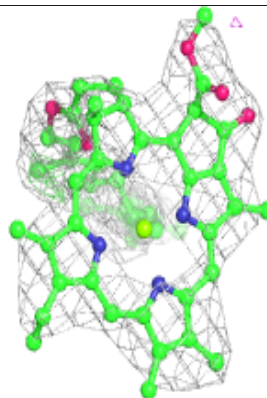
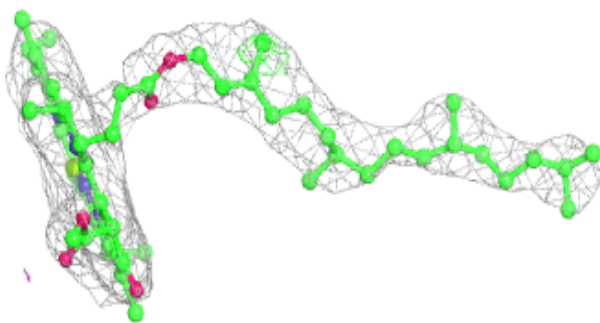
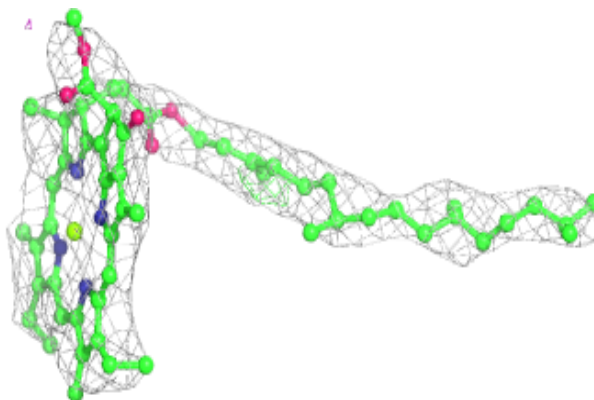


Electron density around CLA A 1124:

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

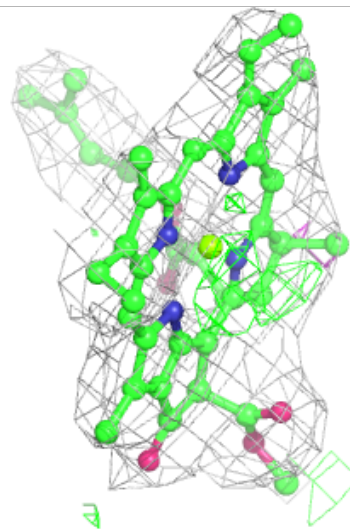
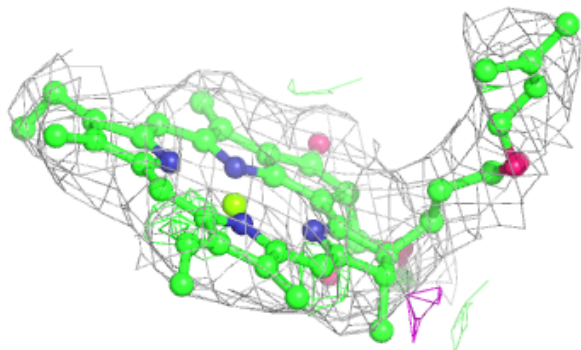
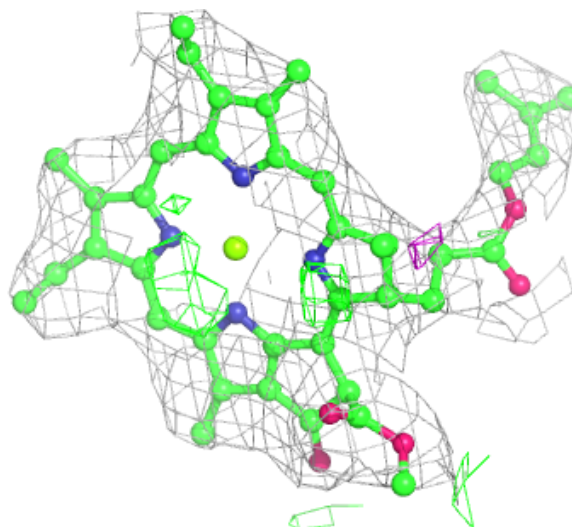
**Electron density around CLA B 1225:**

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



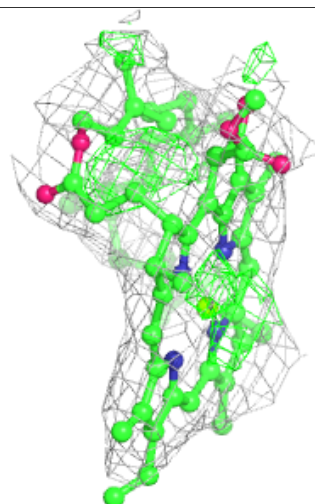
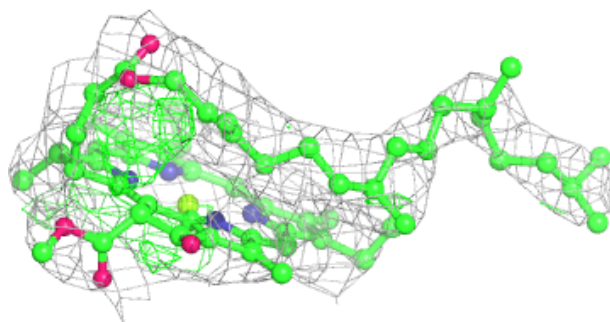
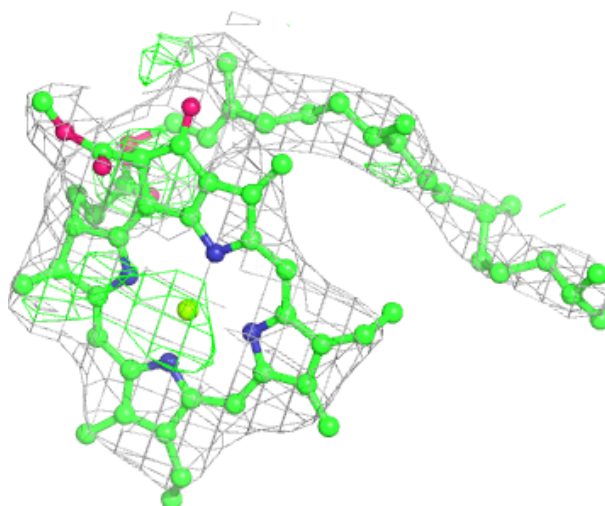
Electron density around CLA A 1102:

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



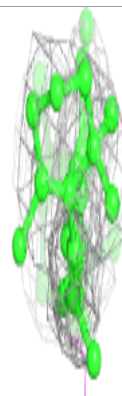
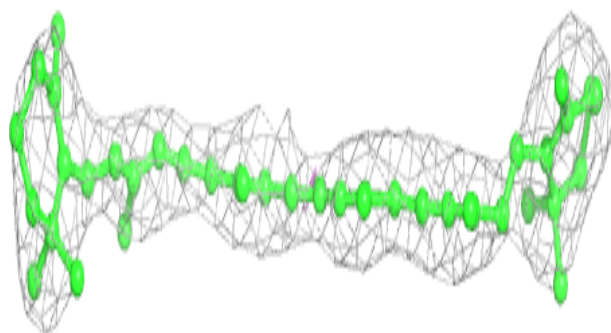
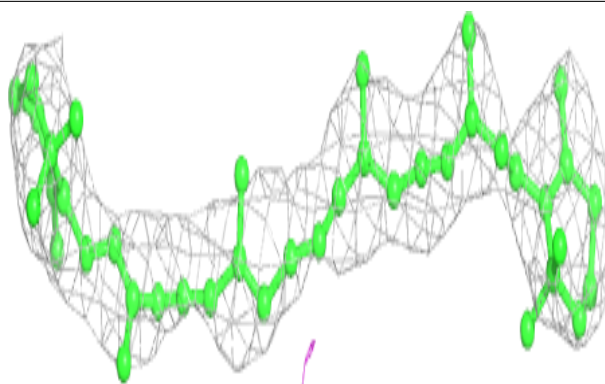
Electron density around CLA A 1127:

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

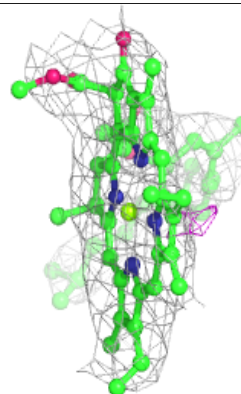
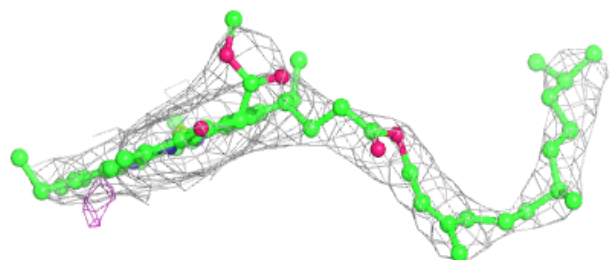
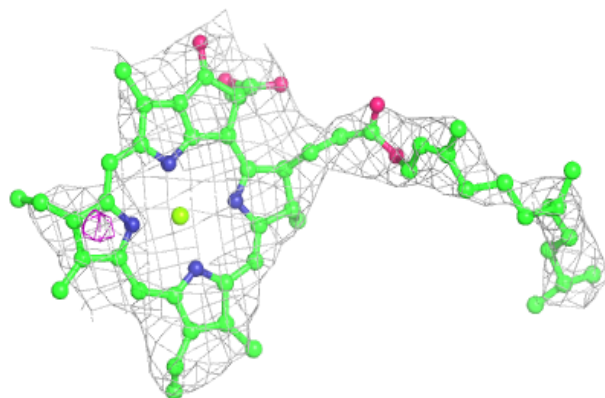


Electron density around BCR A 6017:

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

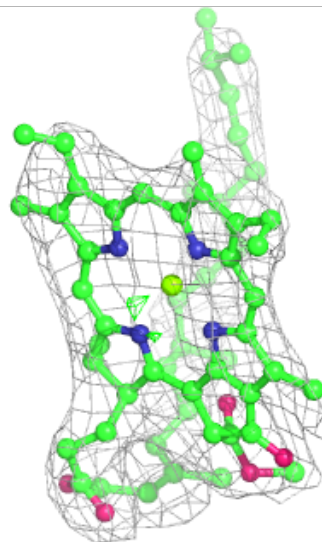
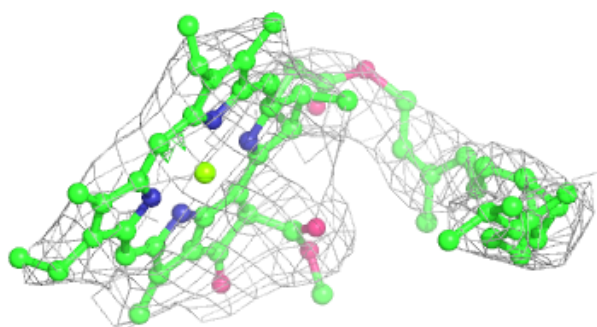
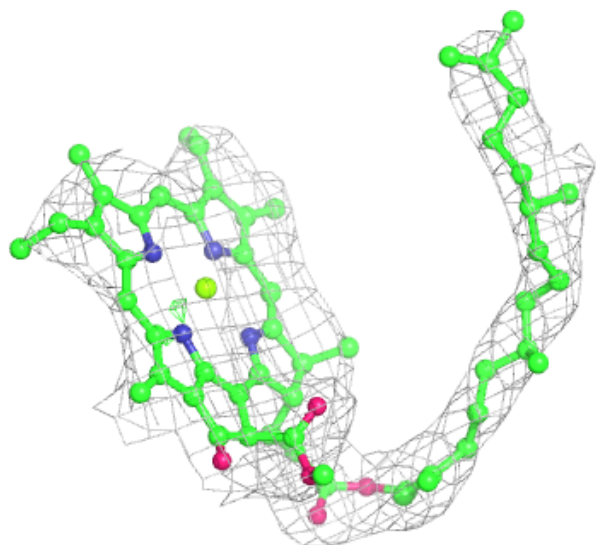
**Electron density around CLA A 1125:**

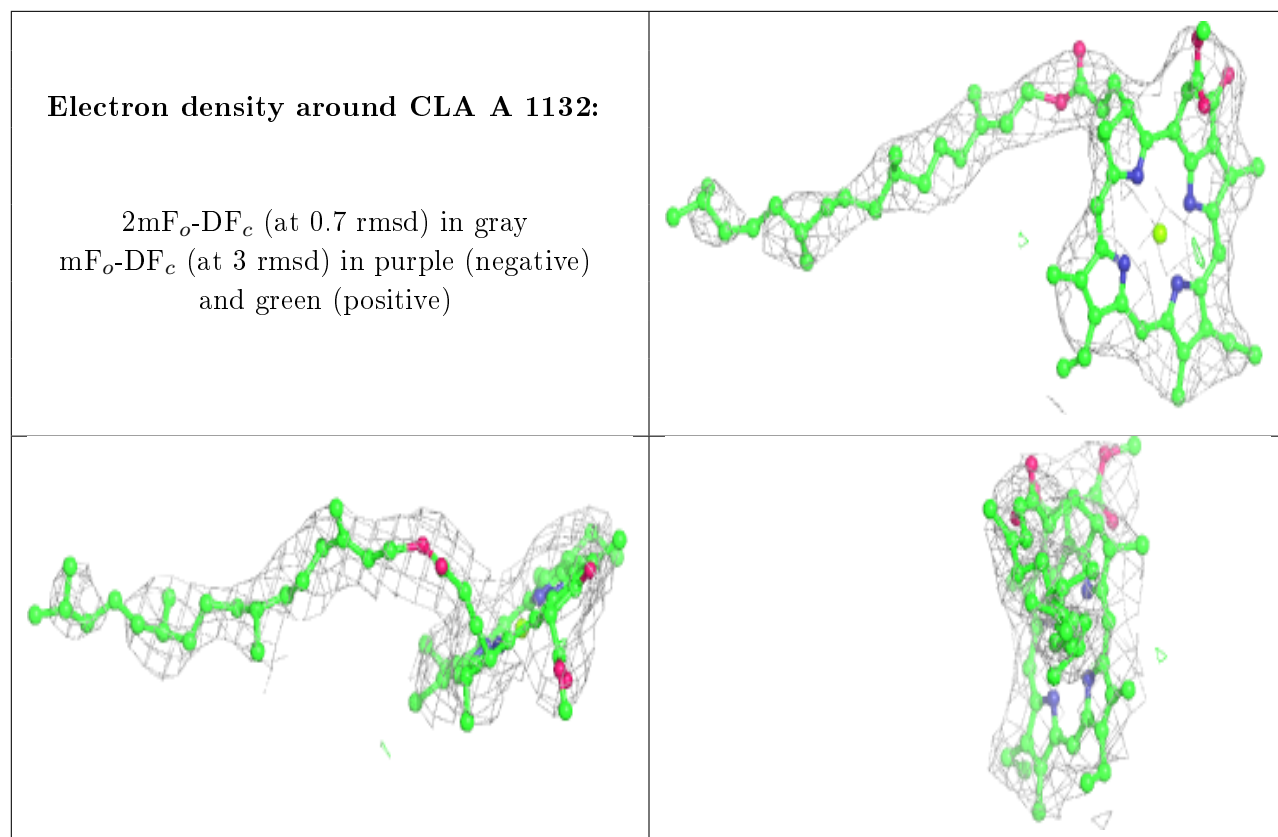
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1207:

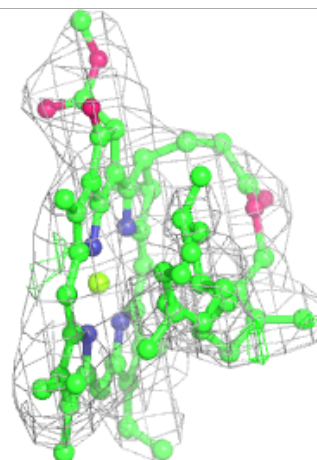
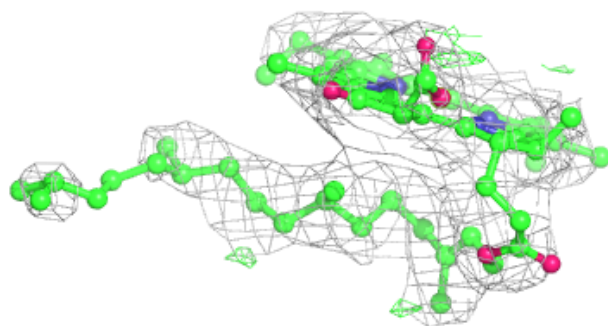
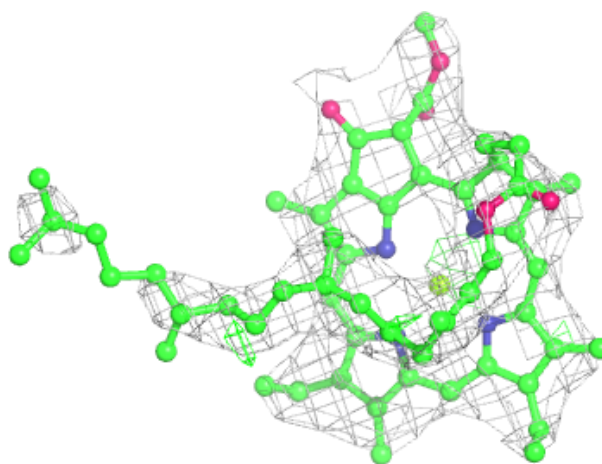
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





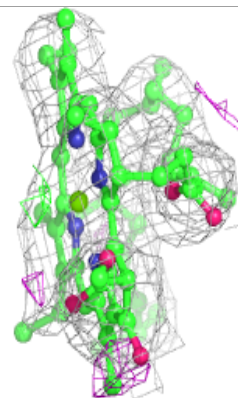
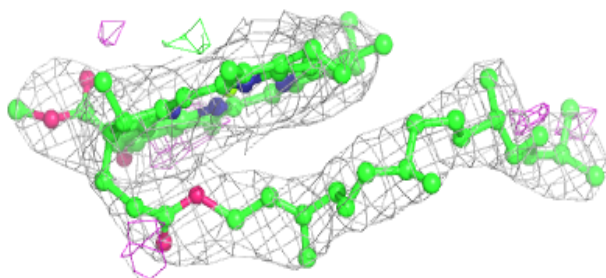
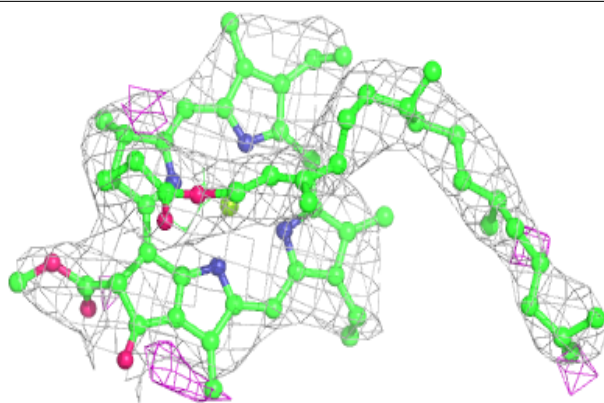
Electron density around CLA B 1224:

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

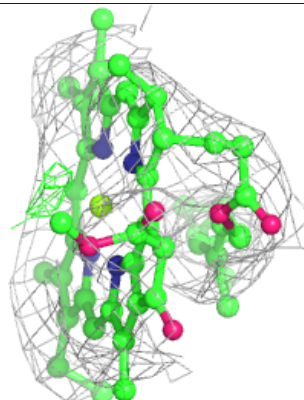
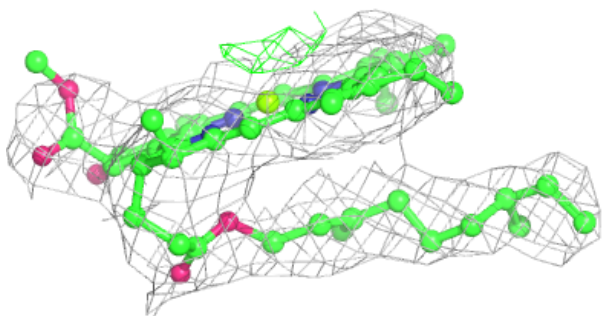
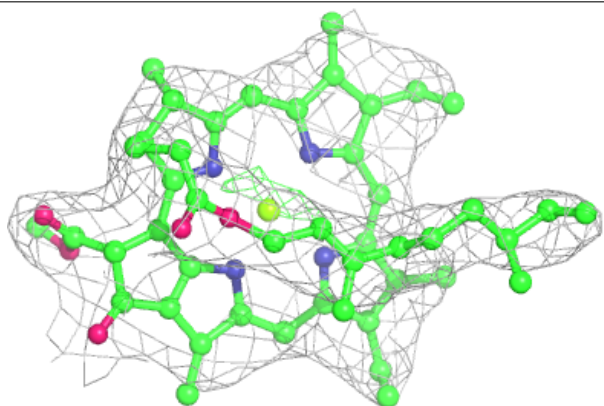


Electron density around CLA B 1235:

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

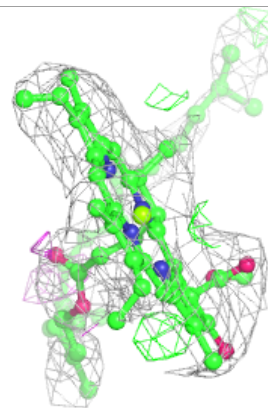
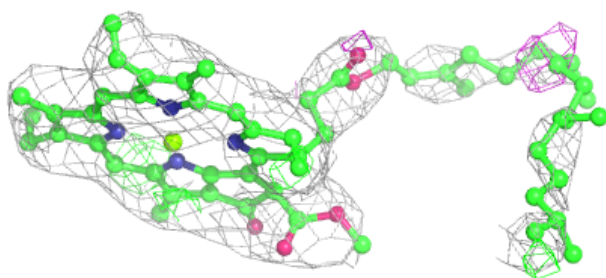
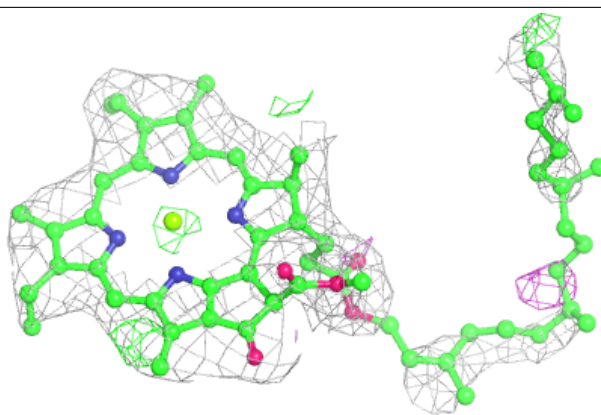
**Electron density around CLA A 1136:**

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

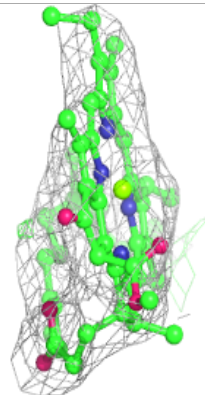
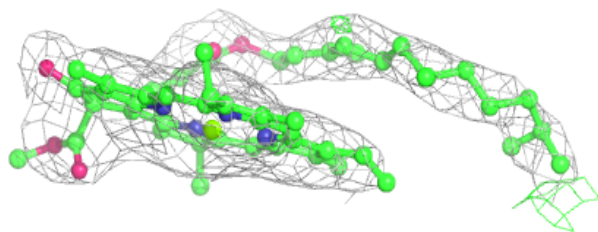
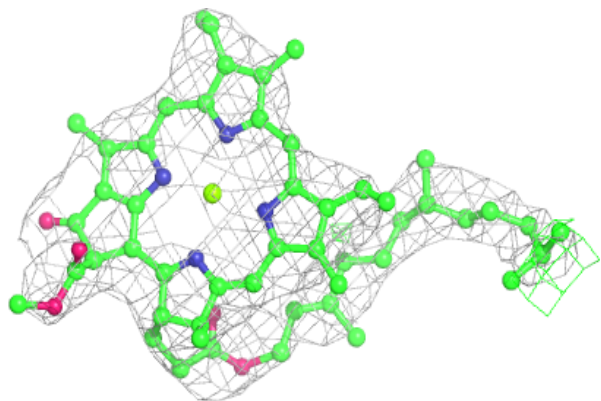


Electron density around CLA B 1220:

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

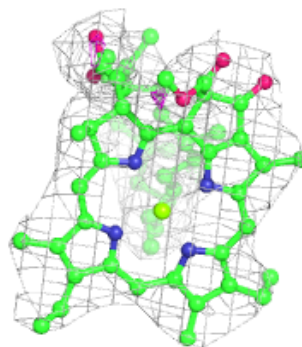
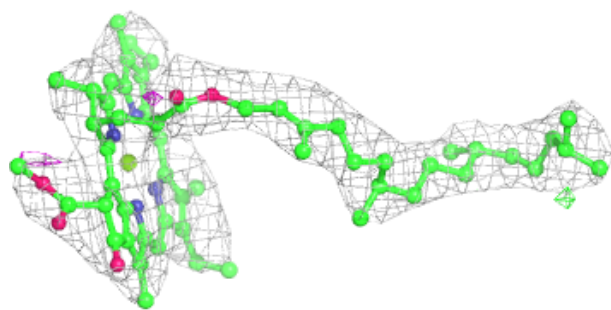
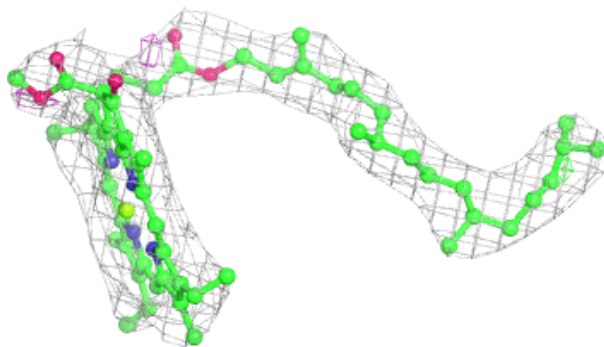
**Electron density around CLA B 1215:**

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

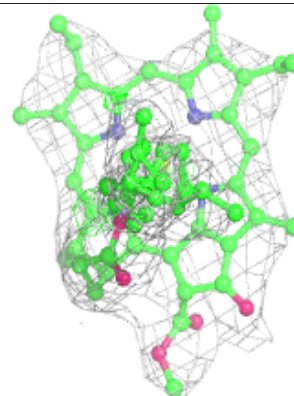
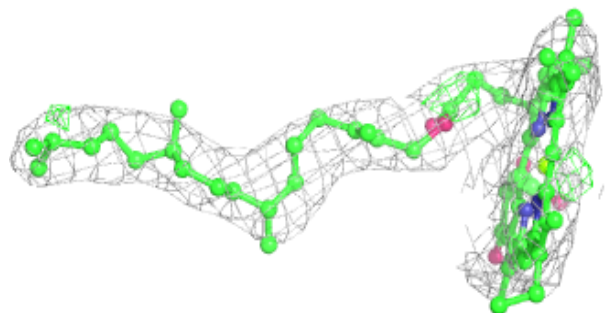
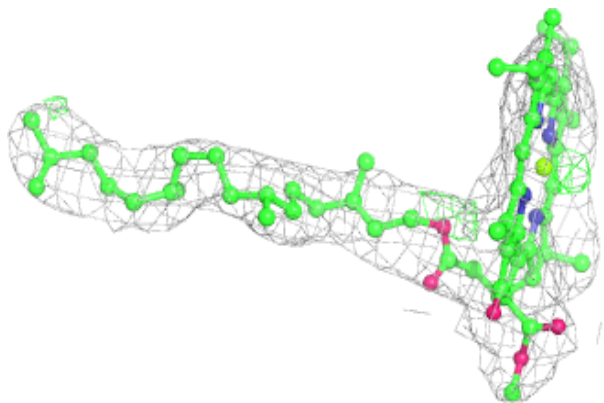


Electron density around CLA A 1128:

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

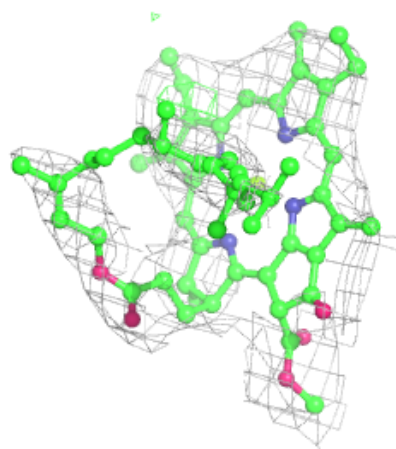
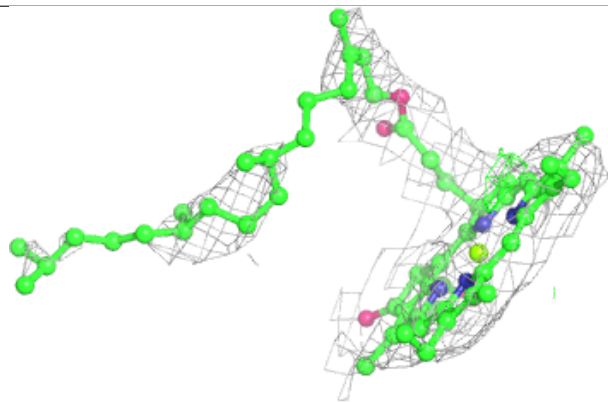
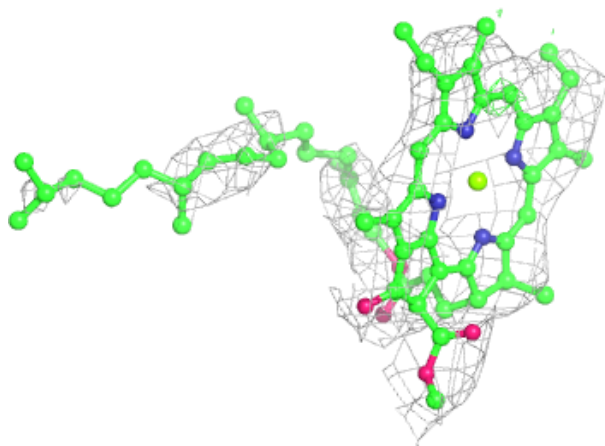
**Electron density around CLA A 1126:**

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



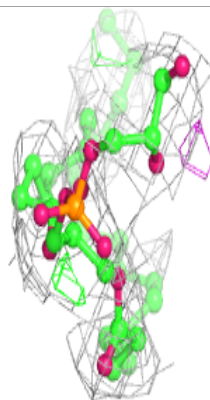
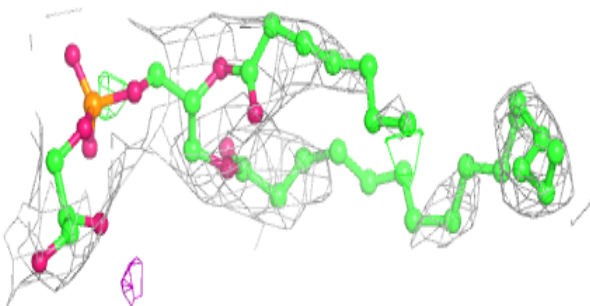
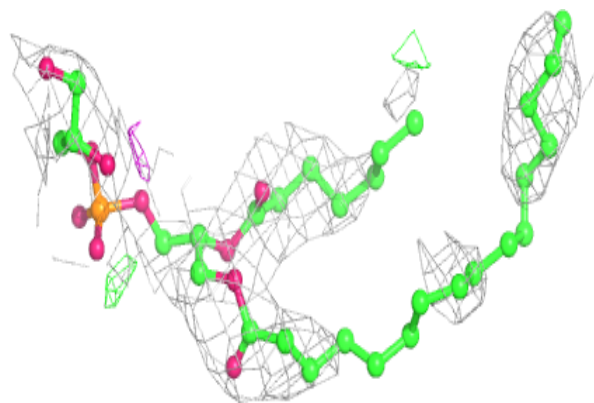
Electron density around CLA 4 4012:

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

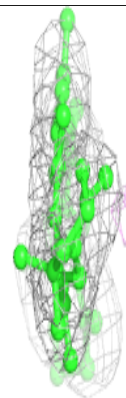
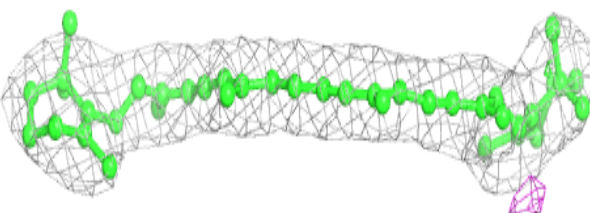
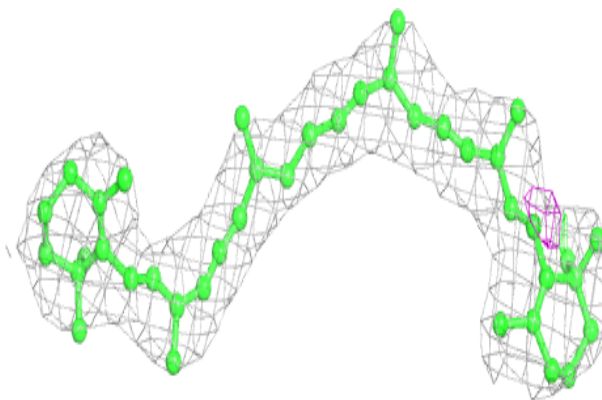


Electron density around LHG A 5003:

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

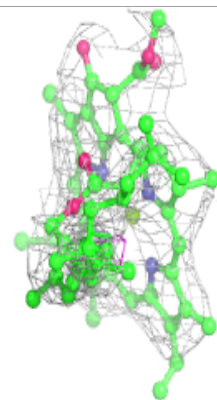
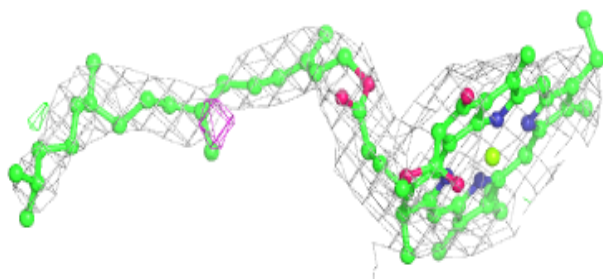
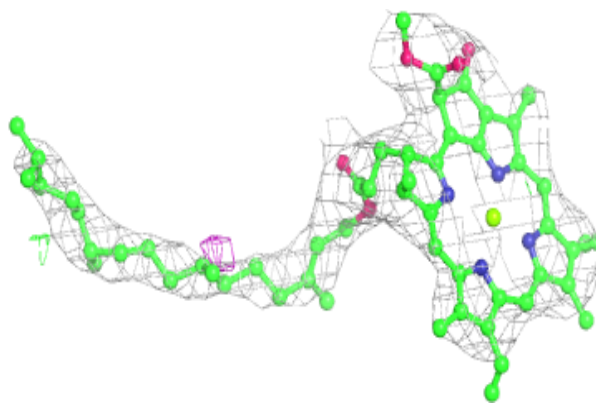
**Electron density around BCR A 6011:**

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

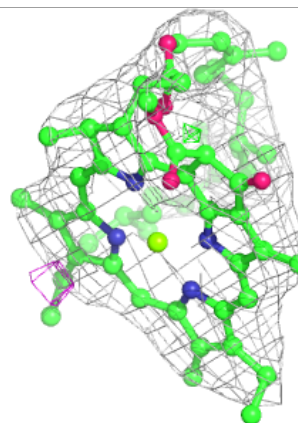
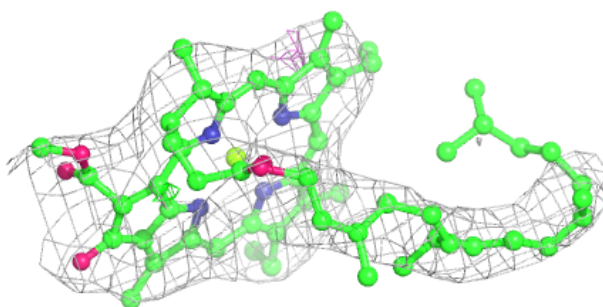
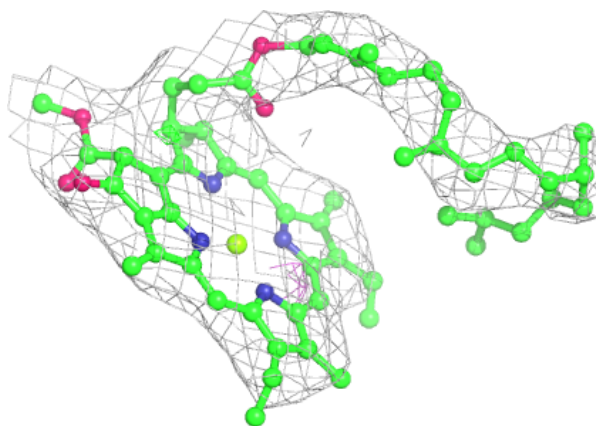


Electron density around CLA A 1119:

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

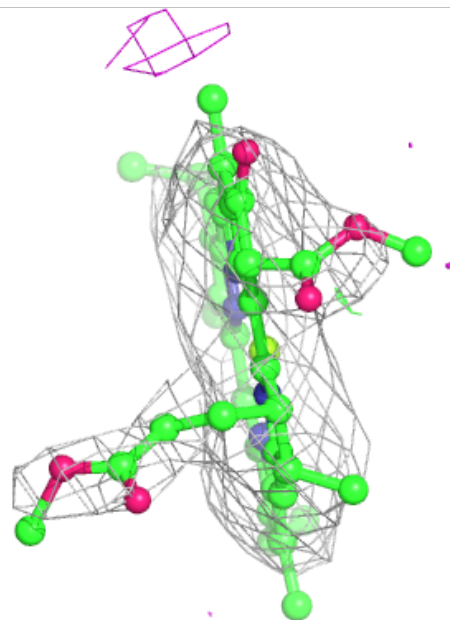
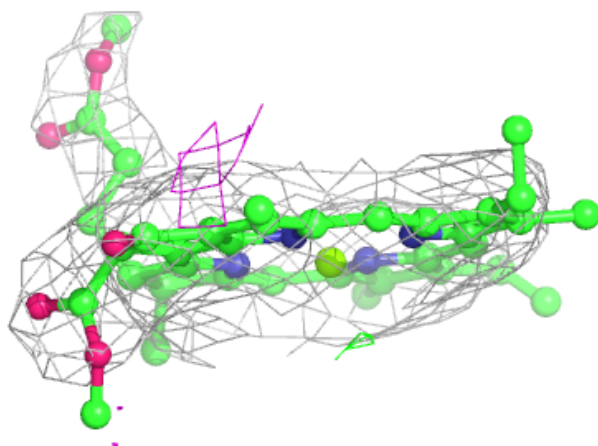
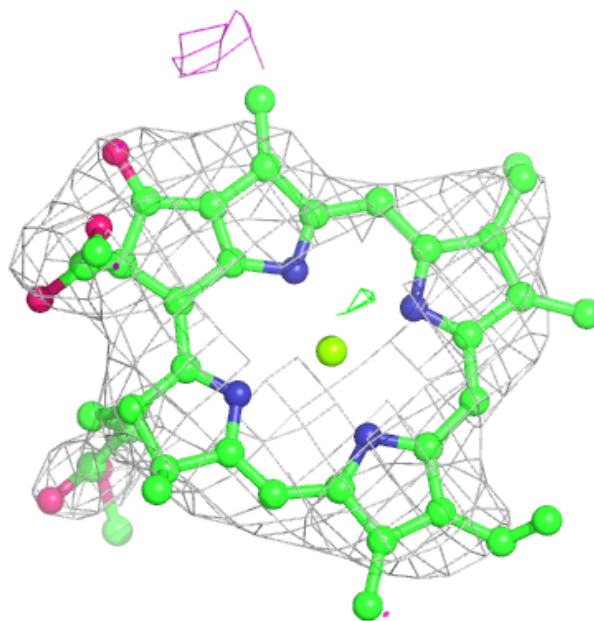
**Electron density around CLA A 1122:**

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



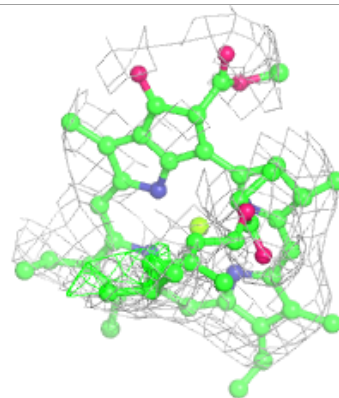
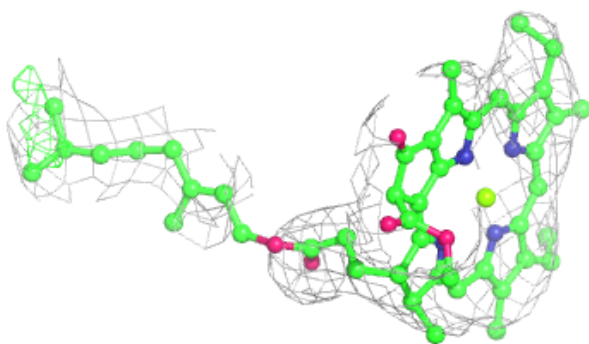
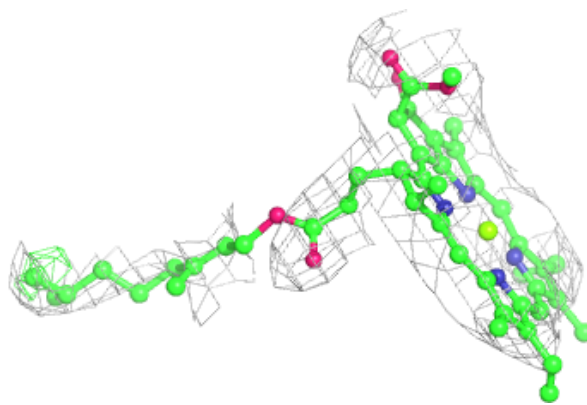
Electron density around CLA B 1217:

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

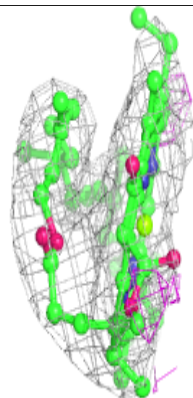
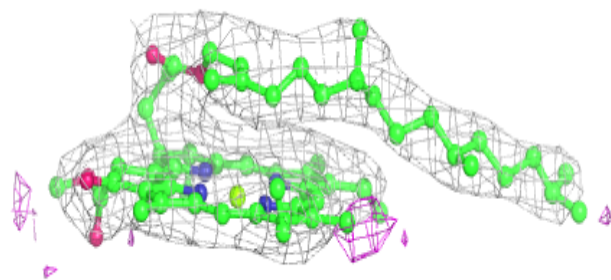
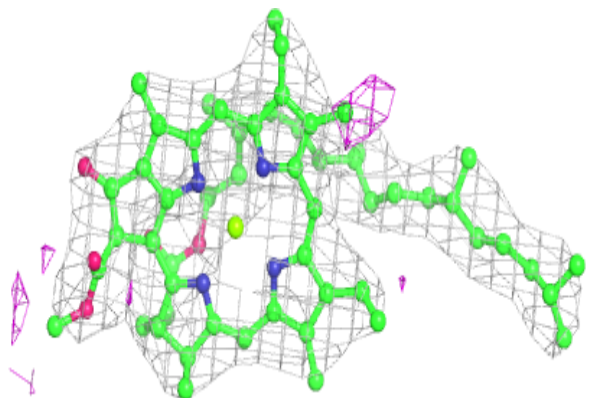


Electron density around CLA A 1121:

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

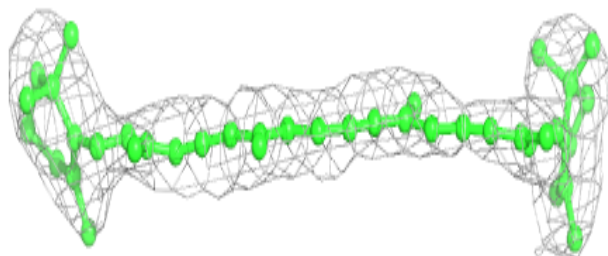
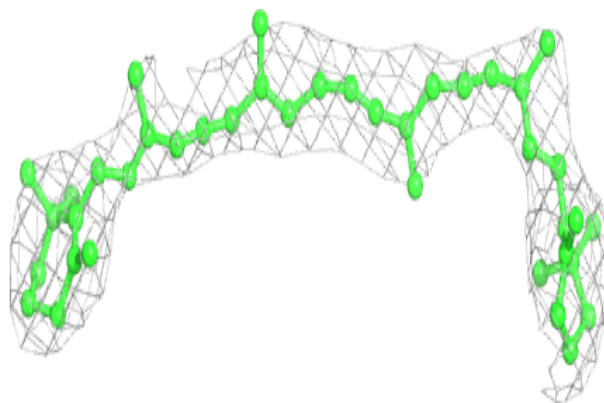
**Electron density around CLA A 1138:**

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

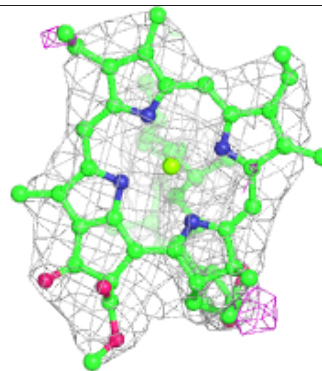
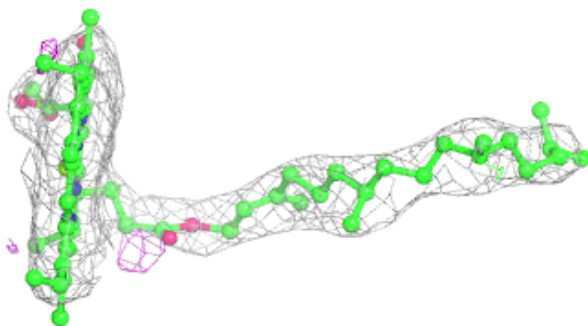
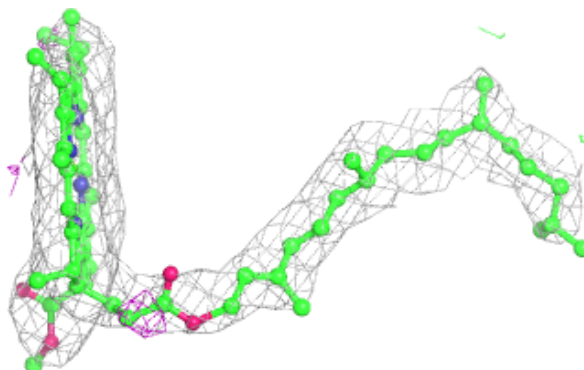


Electron density around BCR I 6020:

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

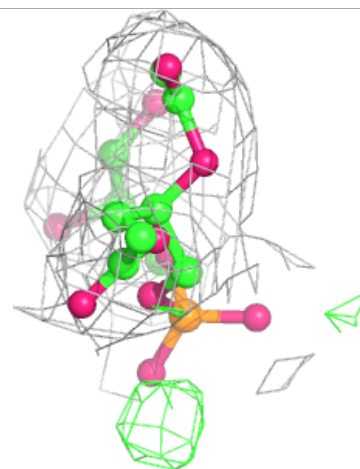
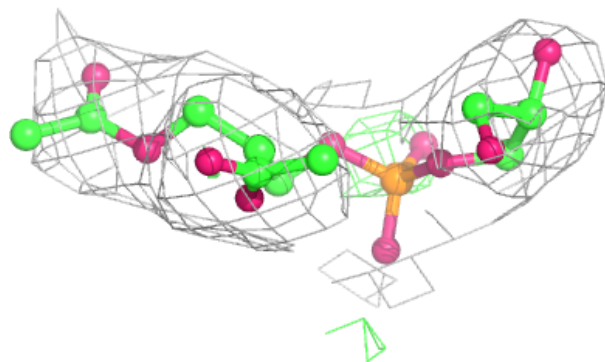
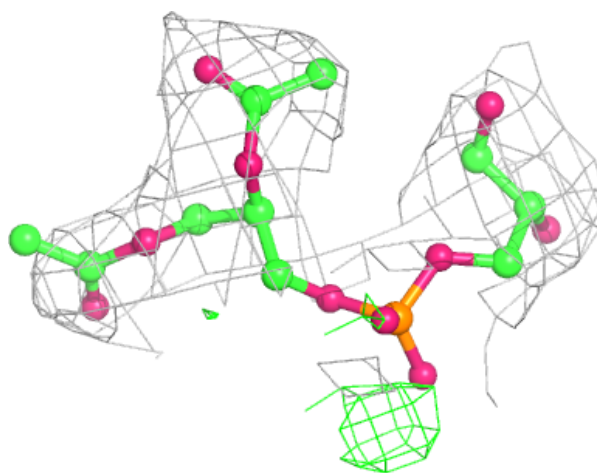
**Electron density around CLA B 1239:**

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



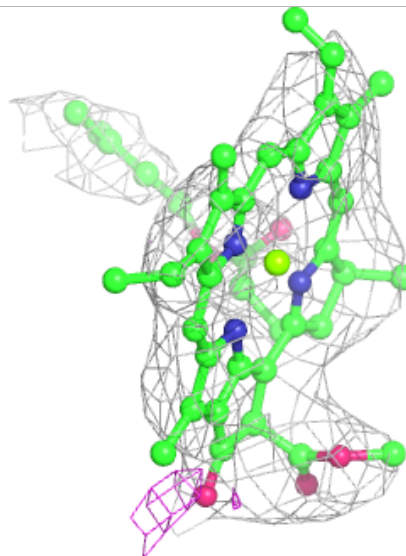
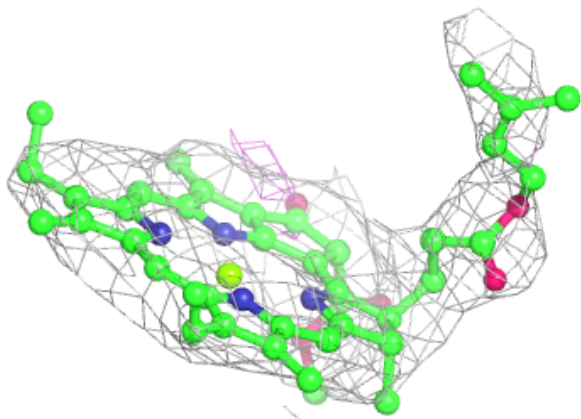
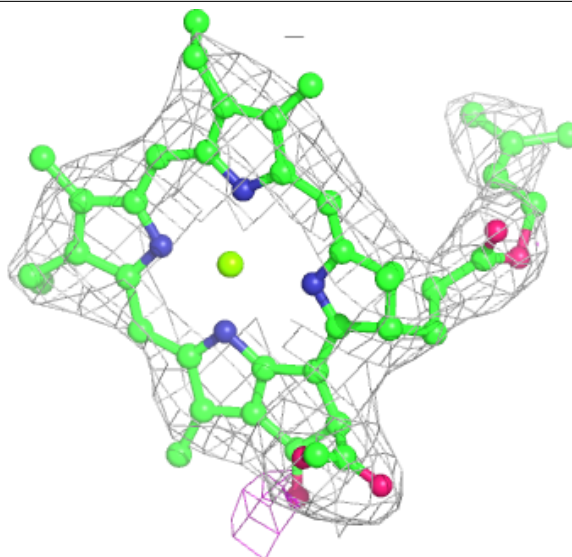
Electron density around LHG B 5004:

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



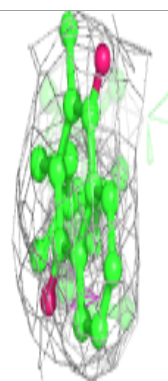
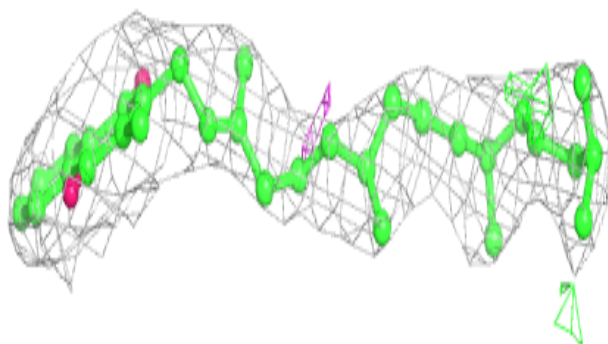
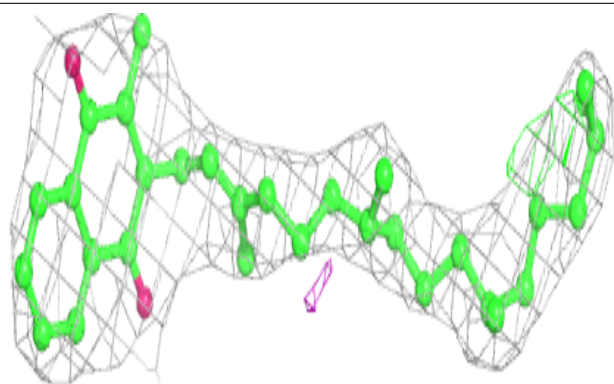
Electron density around CLA A 1129:

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

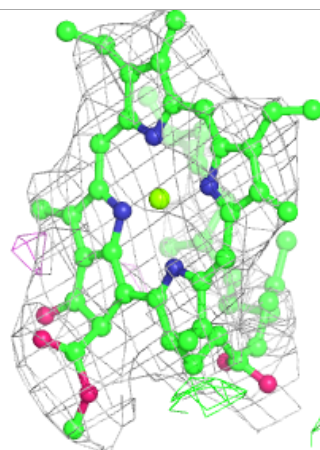
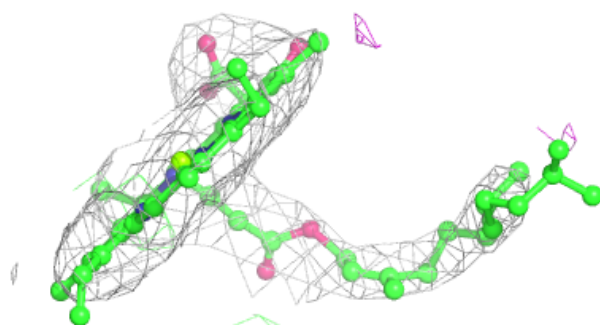
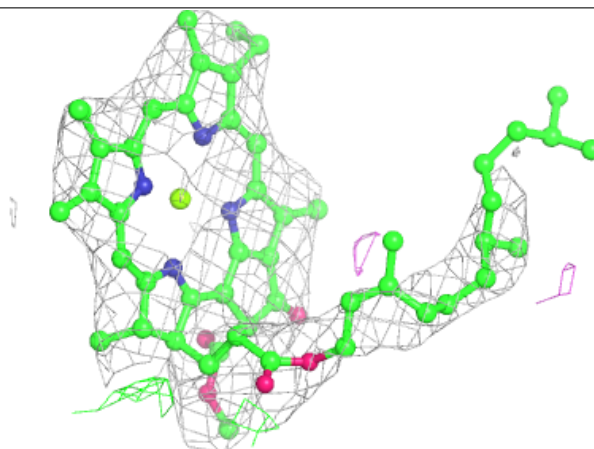


Electron density around PQN A 5001:

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

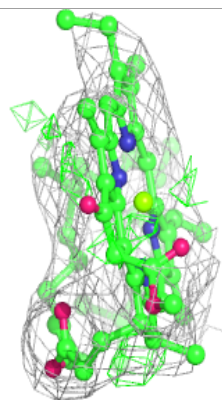
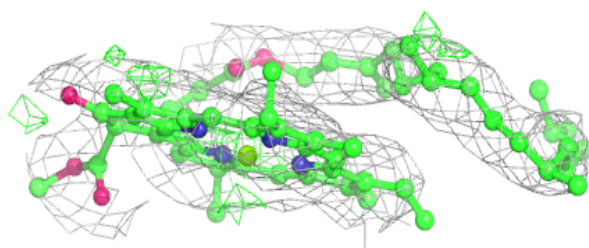
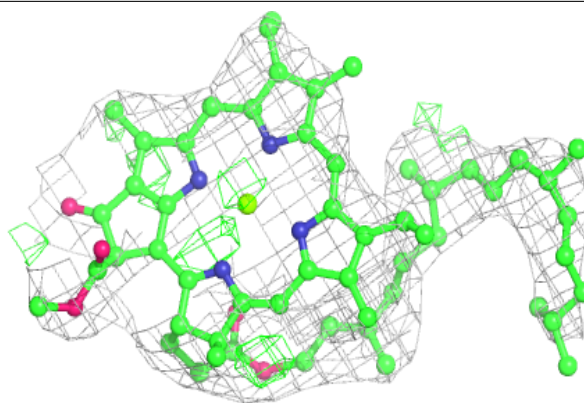
**Electron density around CLA B 1219:**

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

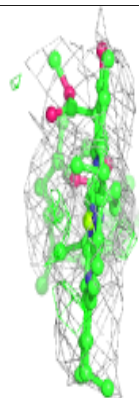
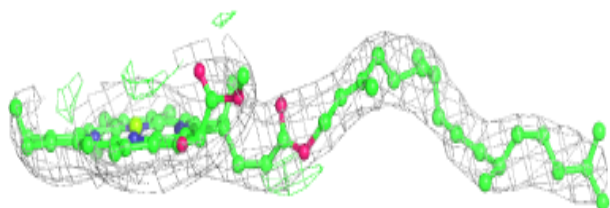
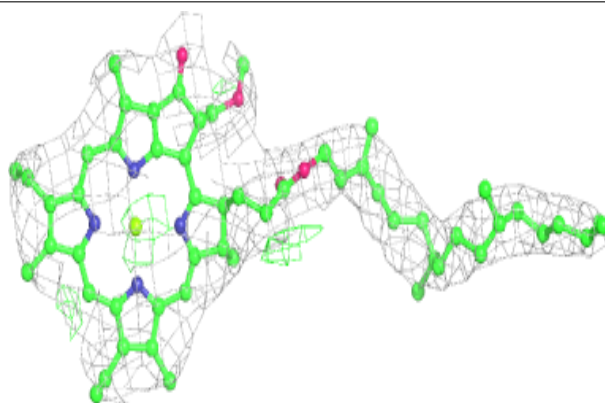


Electron density around CLA A 1117:

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

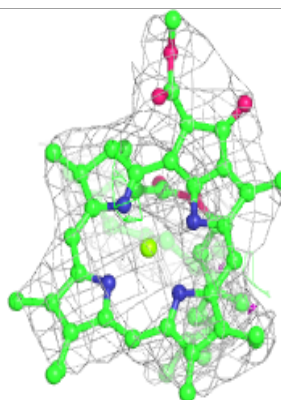
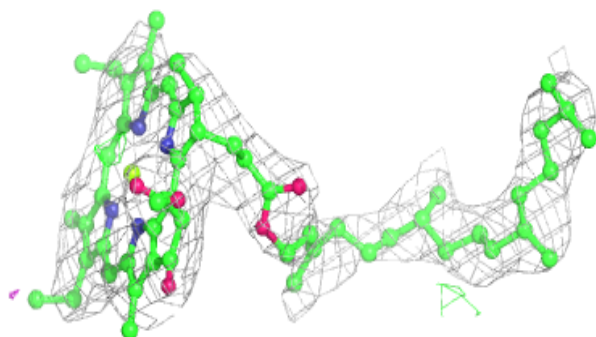
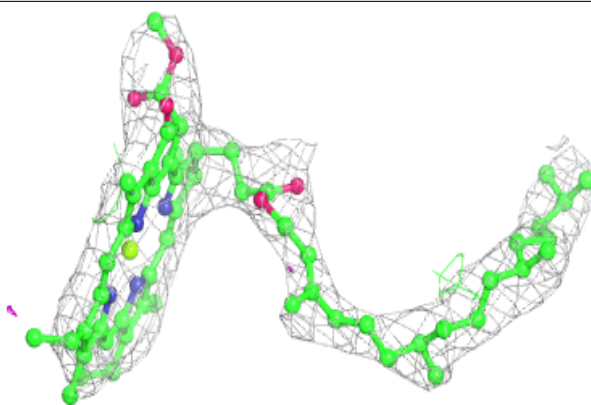
**Electron density around CLA A 1131:**

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

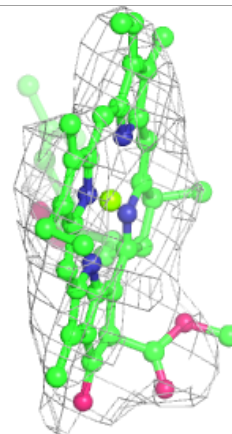
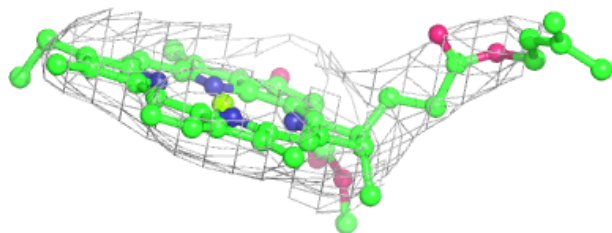
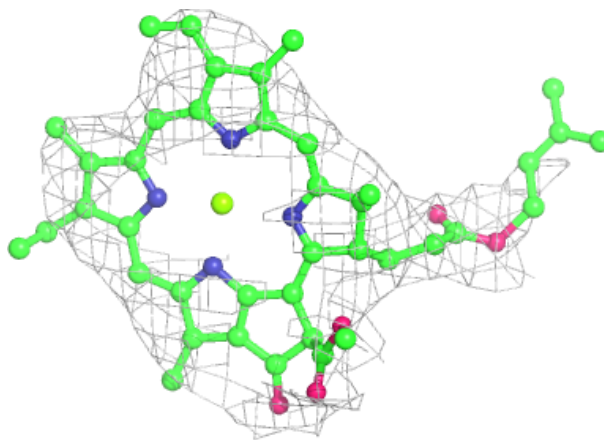


Electron density around CLA B 1238:

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

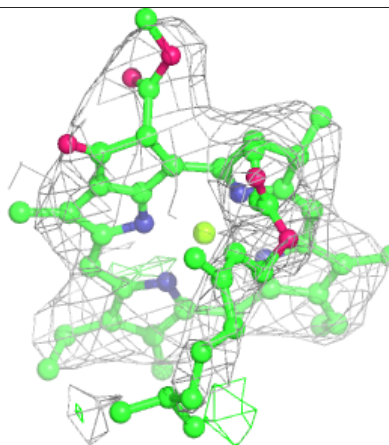
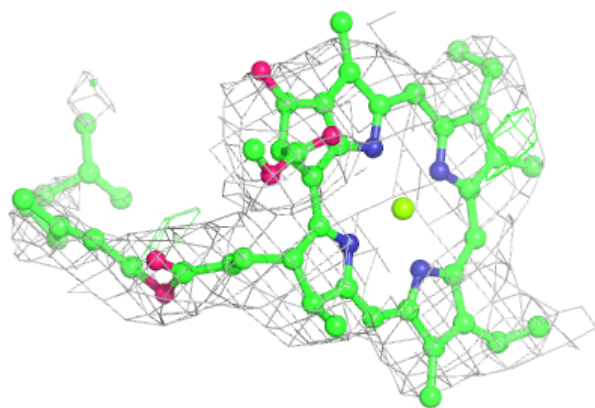
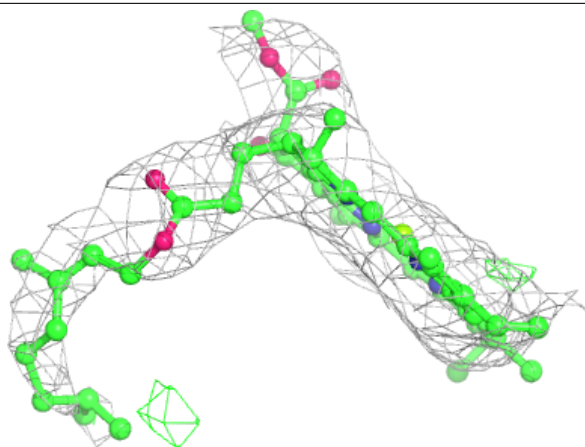
**Electron density around CLA 4 4009:**

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

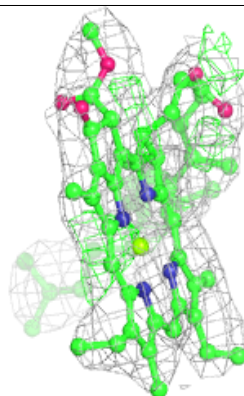
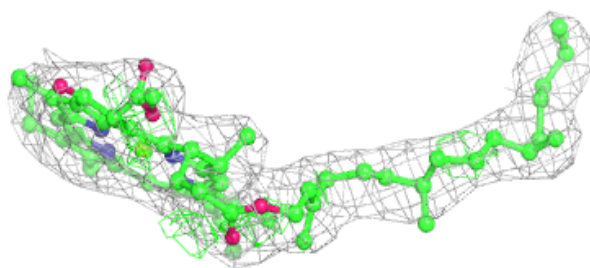
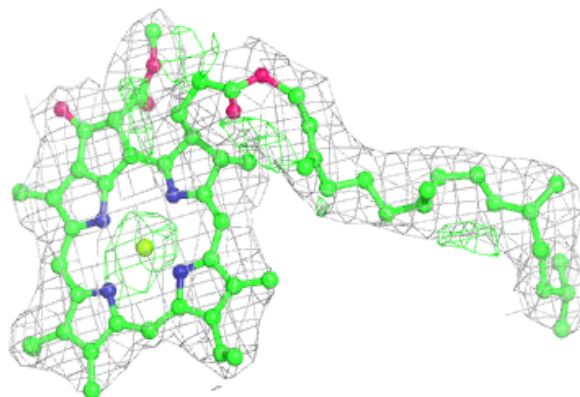


Electron density around CLA A 1137:

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

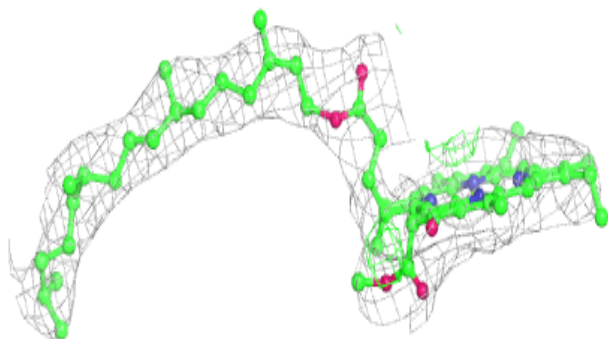
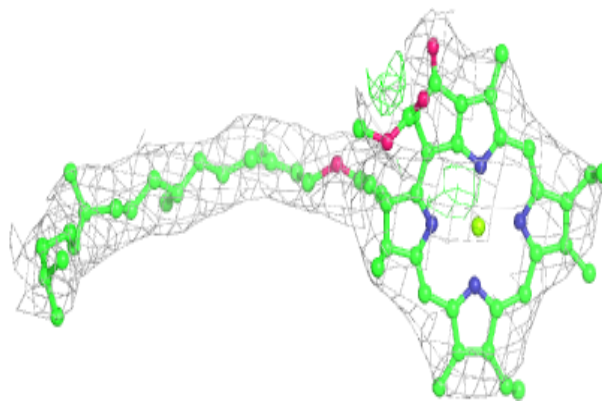
**Electron density around CLA A 1013:**

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

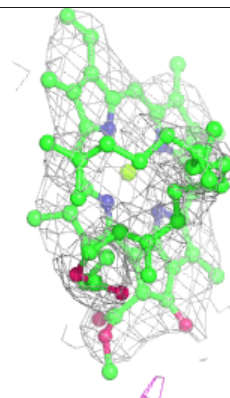
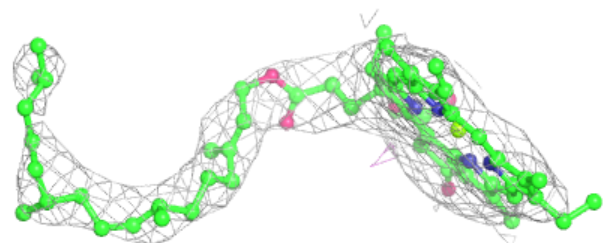
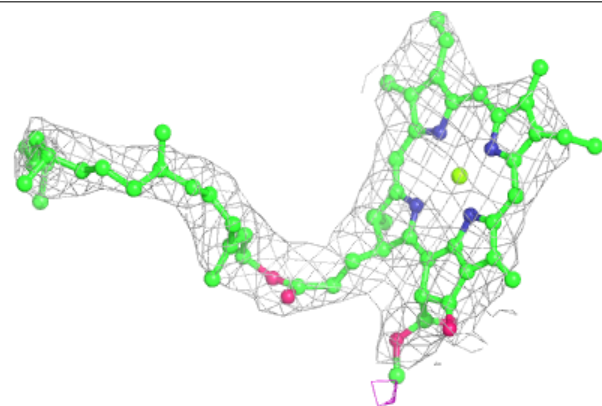


Electron density around CLA B 1240:

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

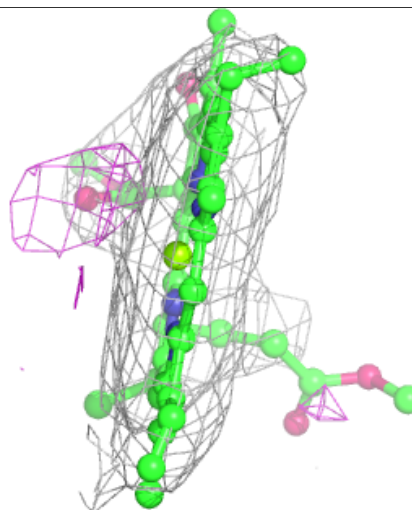
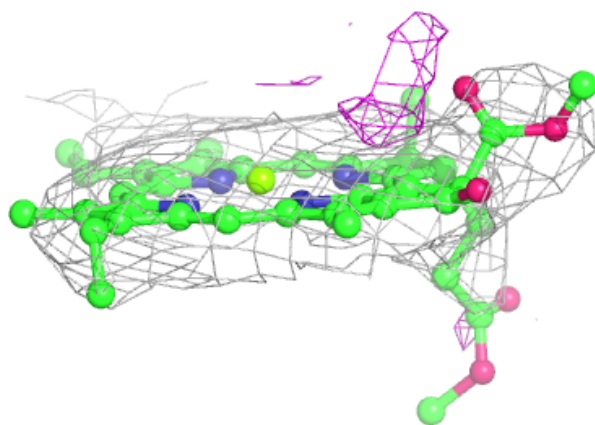
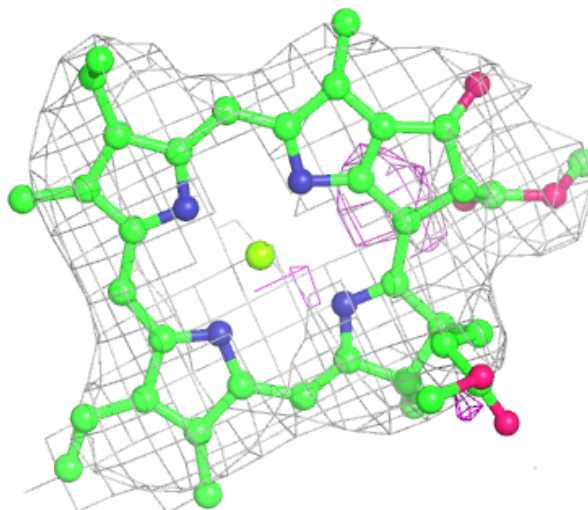
**Electron density around CLA B 1206:**

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



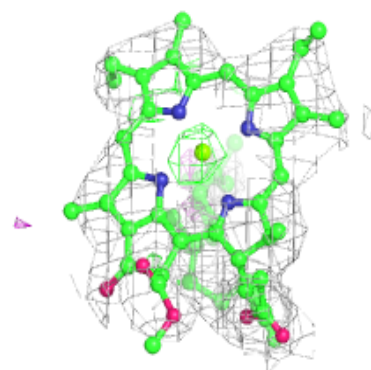
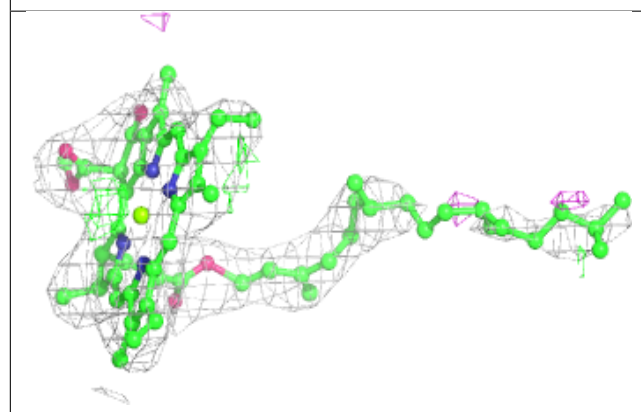
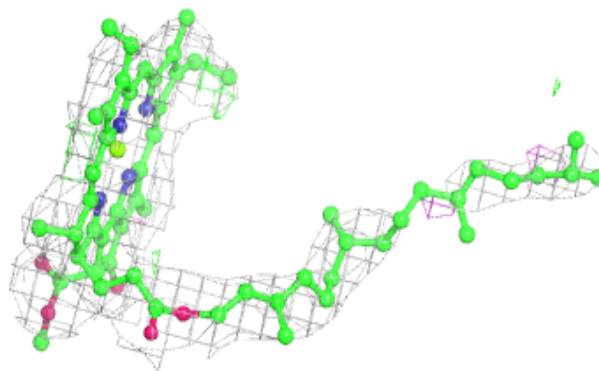
Electron density around CLA B 1209:

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

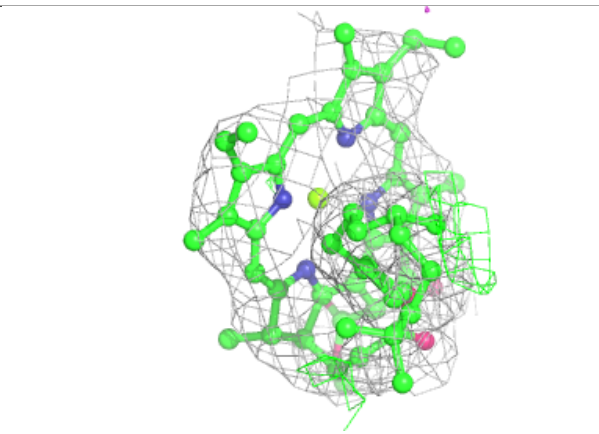
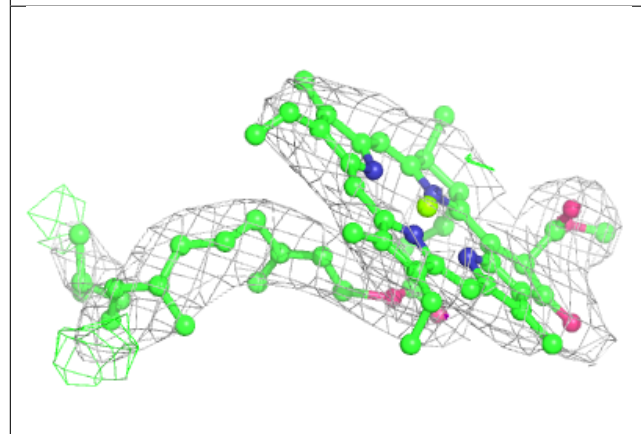
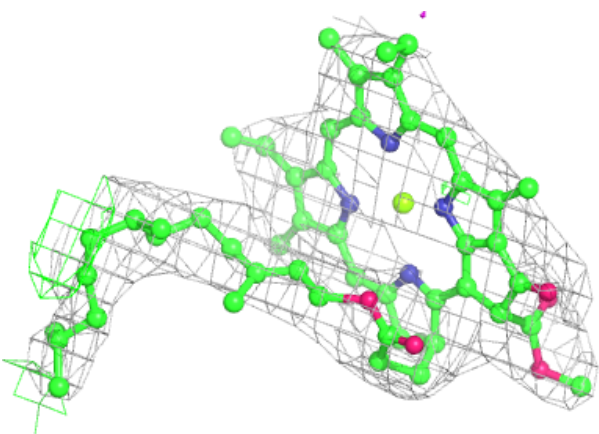


Electron density around CLA B 1226:

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

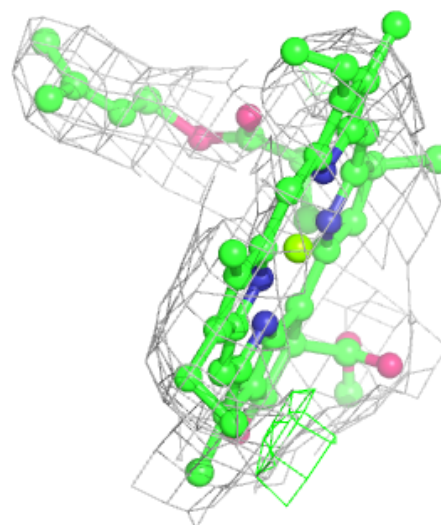
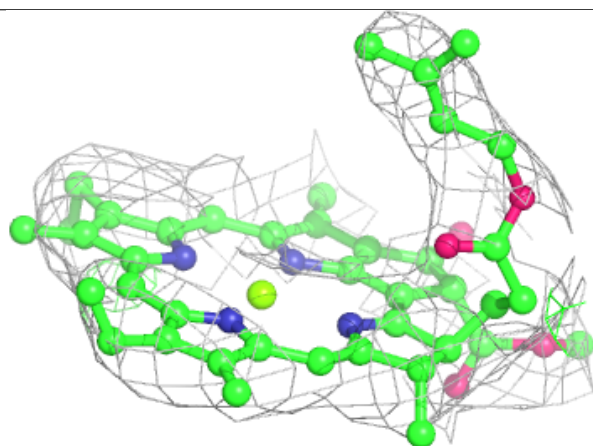
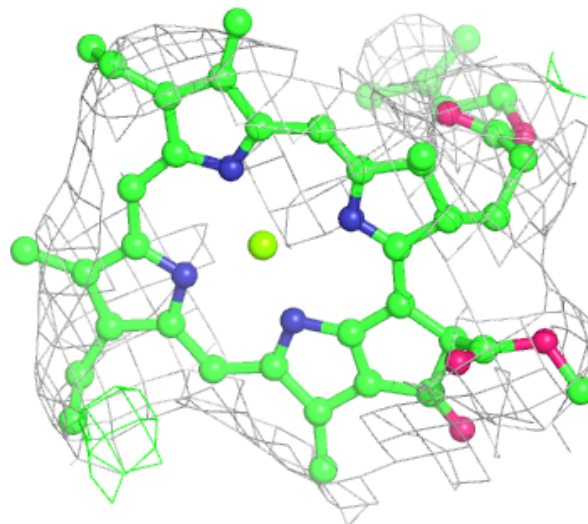
**Electron density around CLA A 1237:**

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



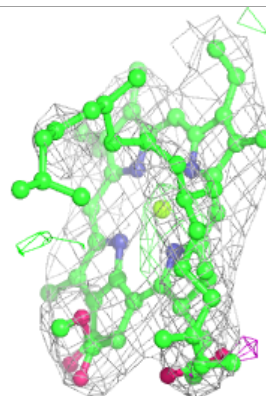
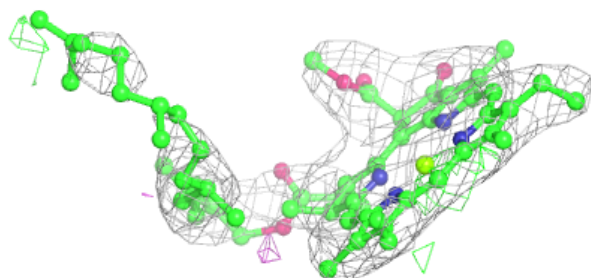
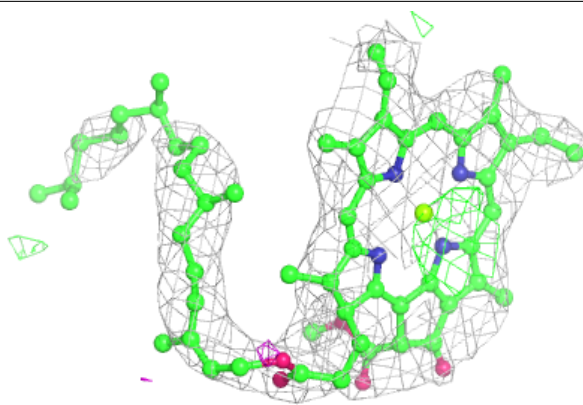
Electron density around CLA 1 1012:

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

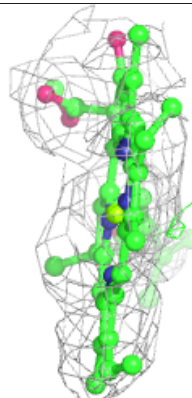
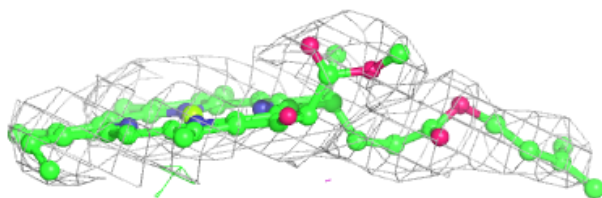
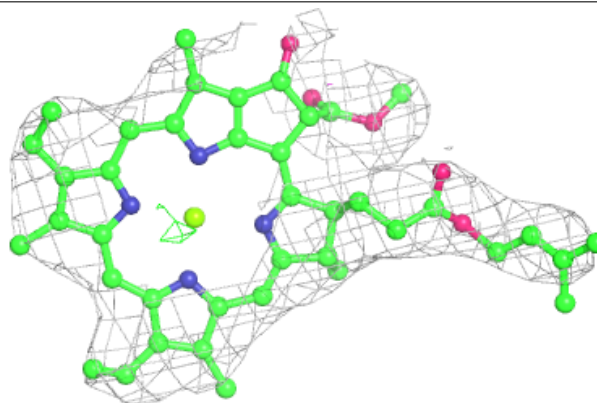


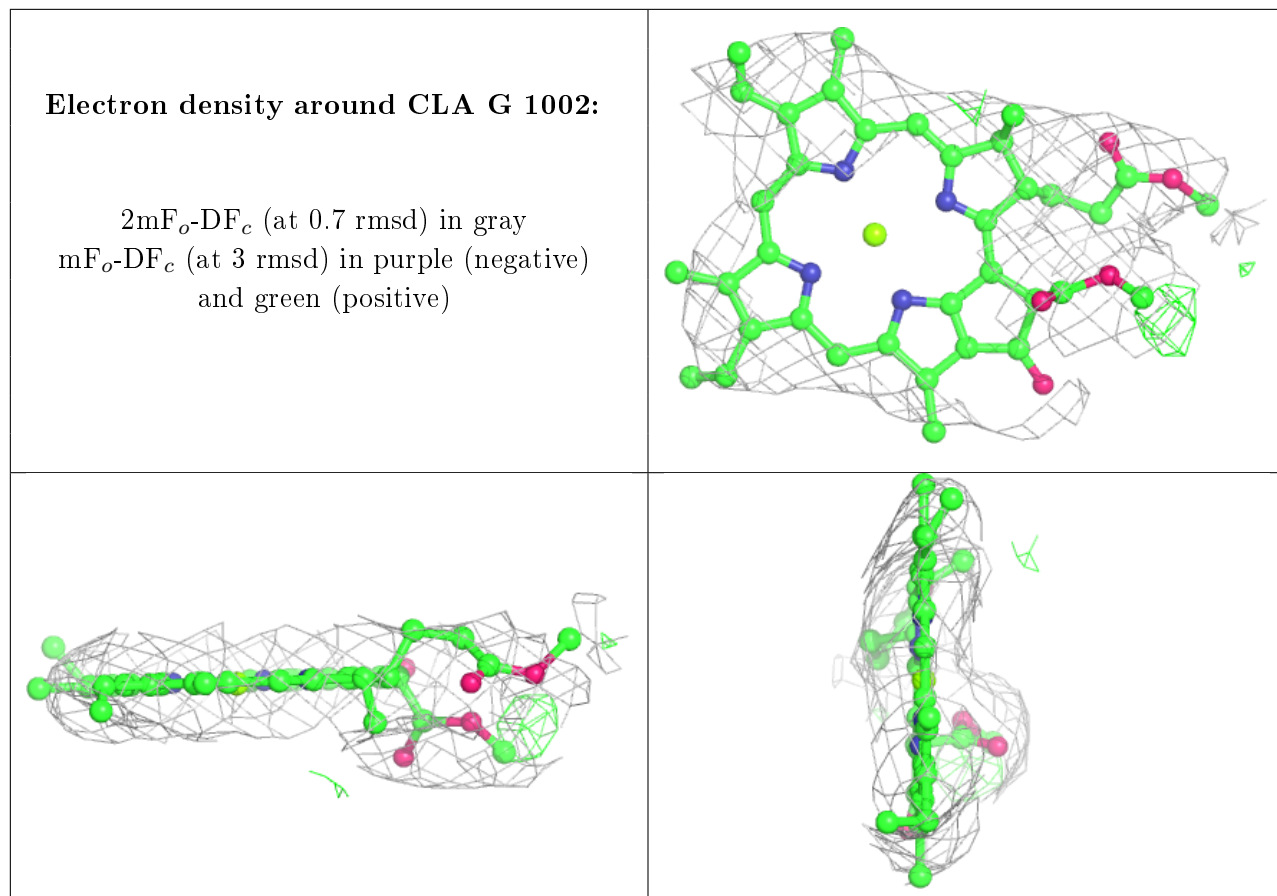
Electron density around CLA B 1221:

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

**Electron density around CLA F 1302:**

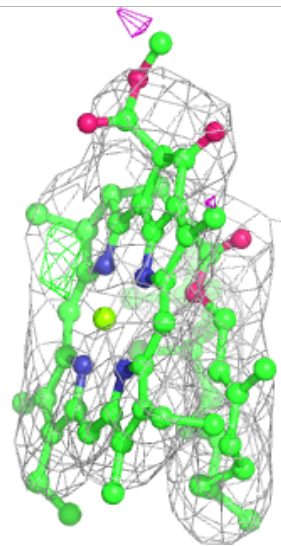
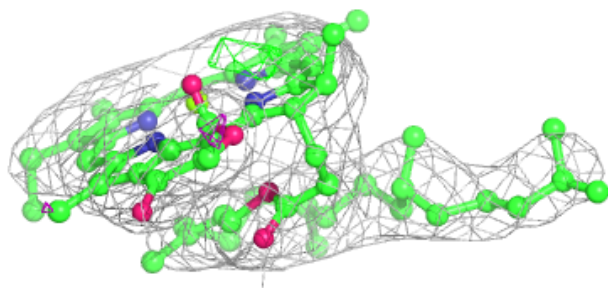
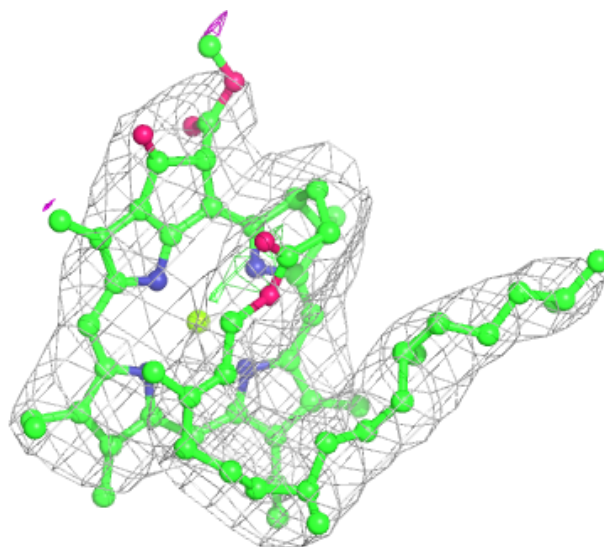
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





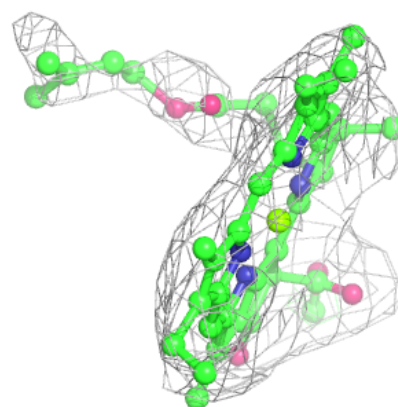
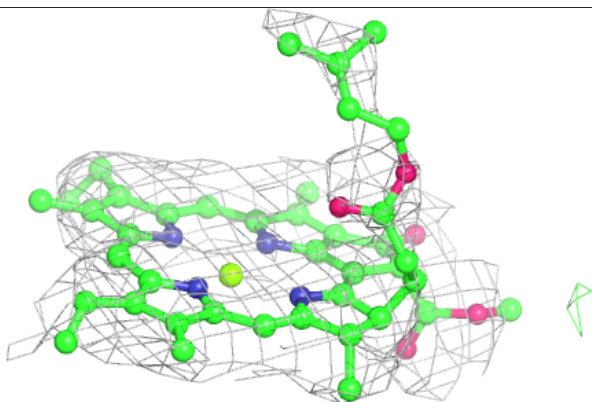
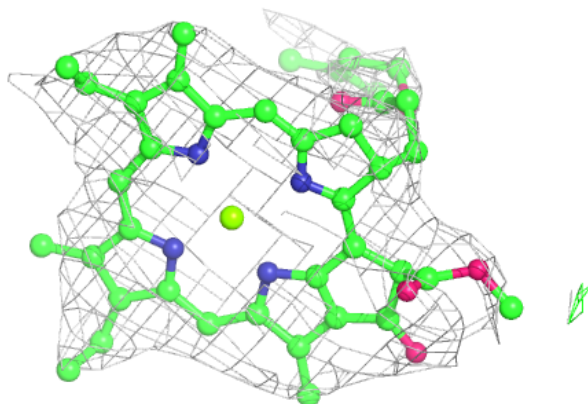
Electron density around CLA B 1205:

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

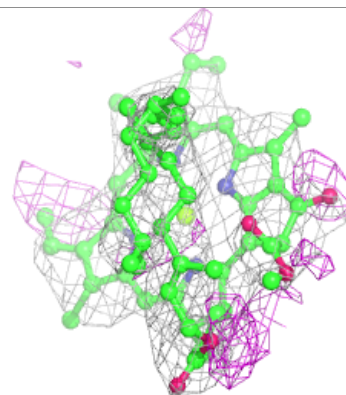
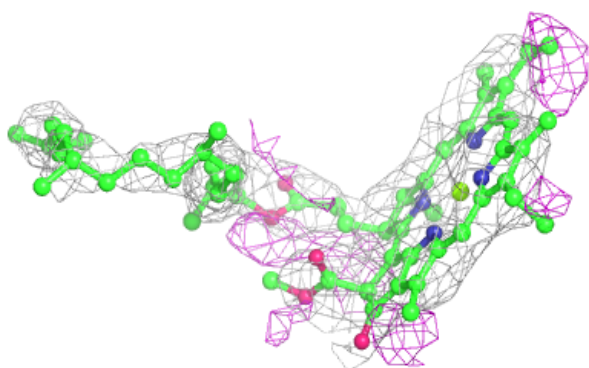
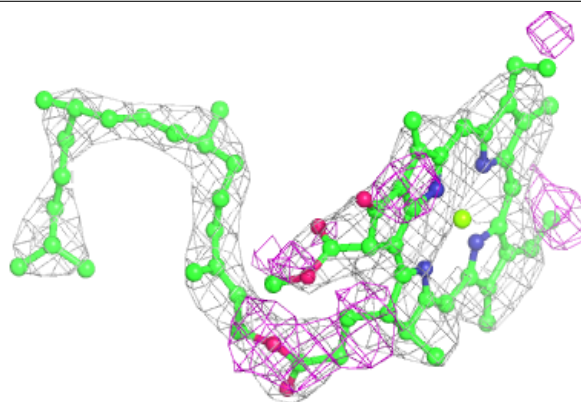


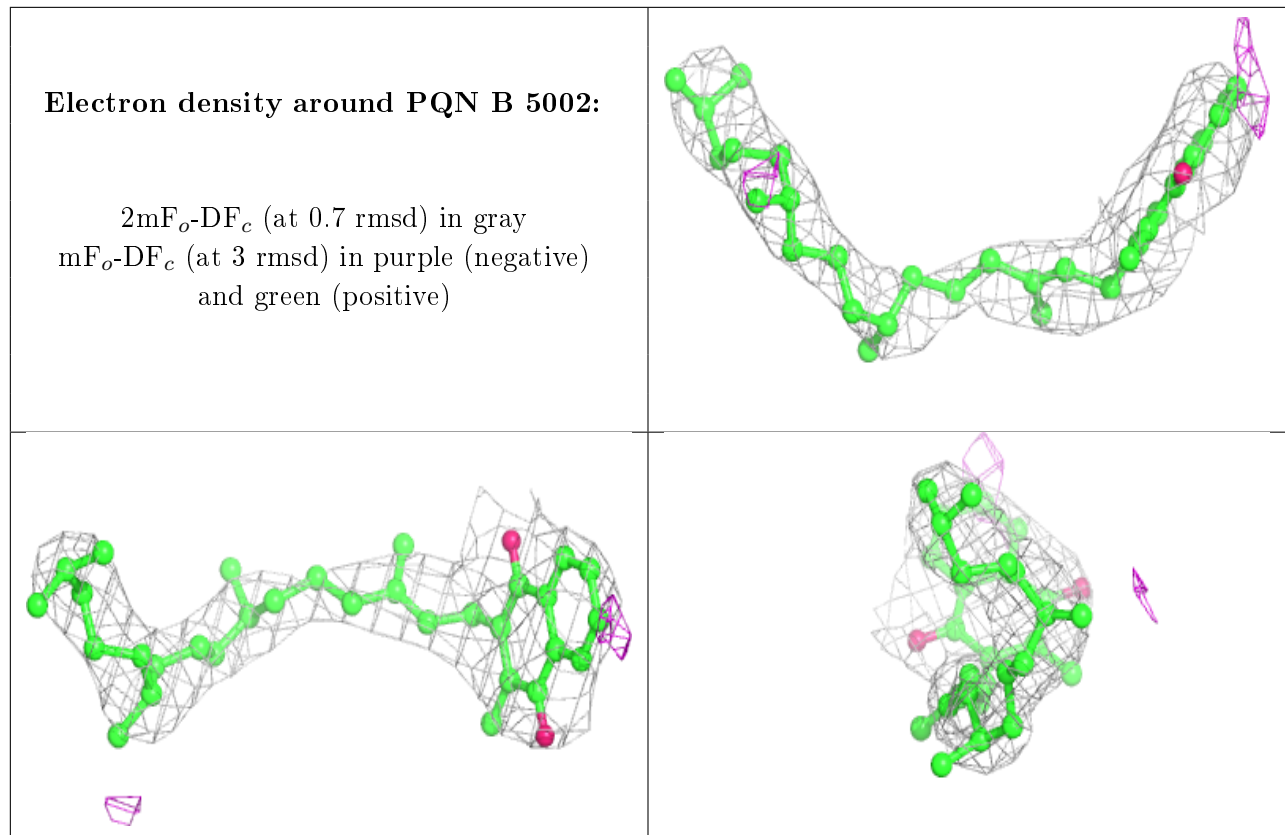
Electron density around CLA B 1201:

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

**Electron density around CL0 A 1011:**

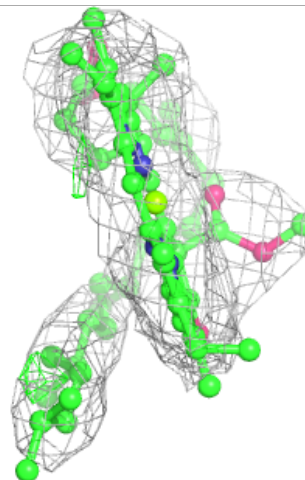
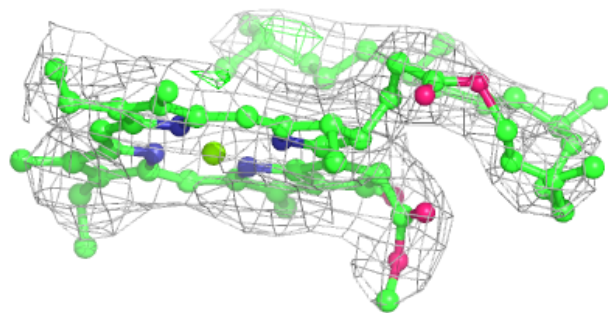
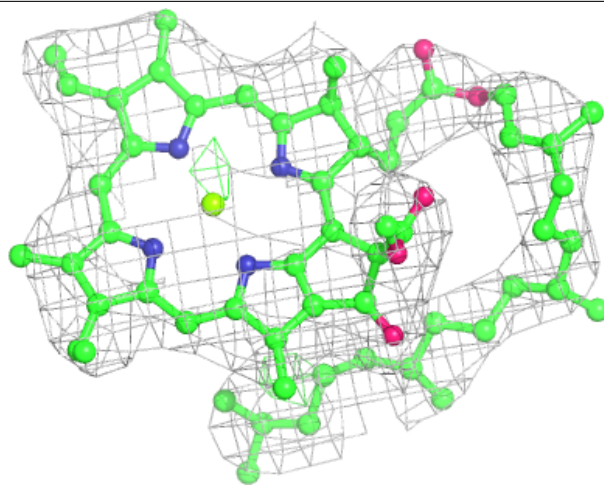
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

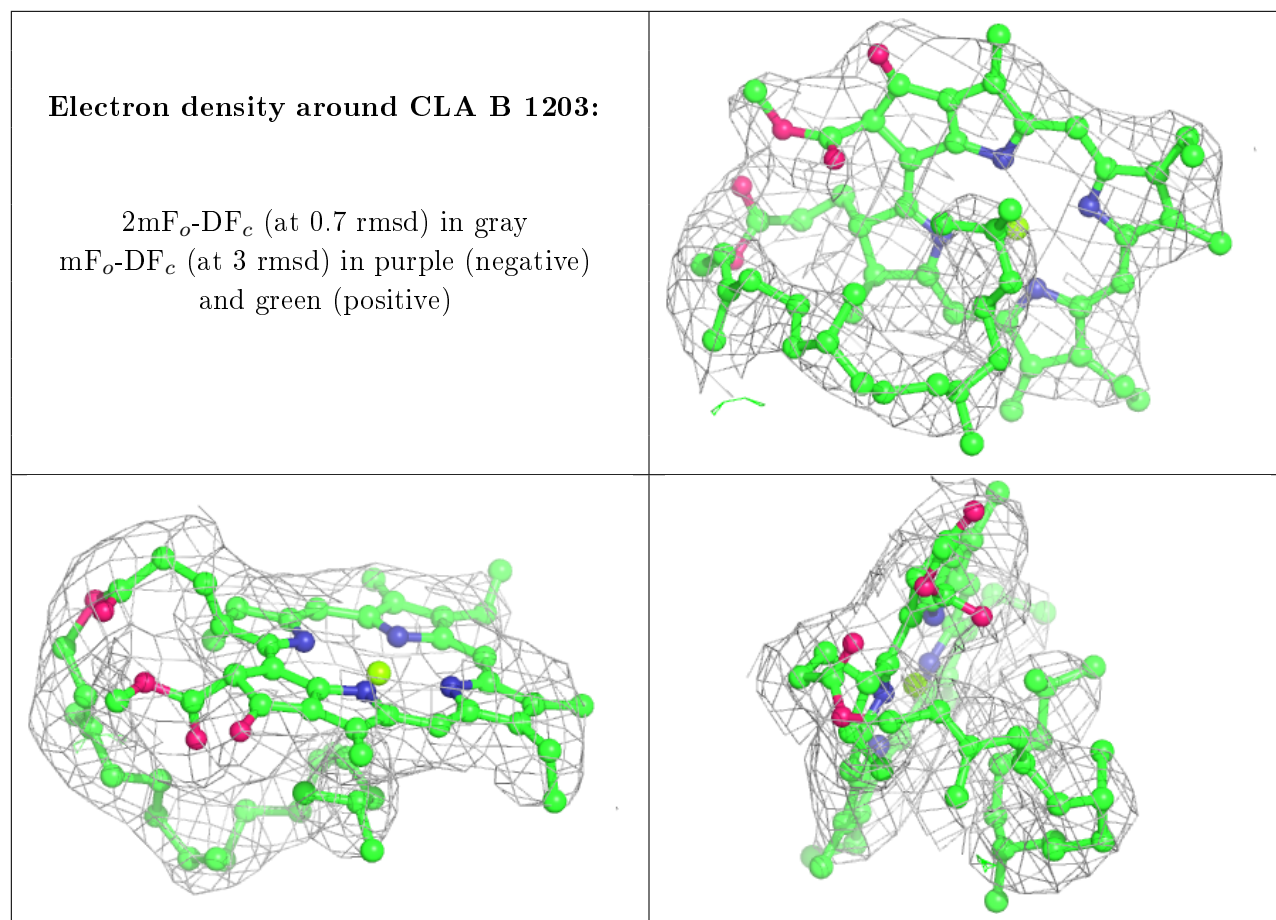




Electron density around CLA B 1202:

$2mF_o-DF_c$ (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.