



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 08:33 PM EDT

PDB ID : 3LW5
Title : Improved model of plant photosystem I
Authors : Nelson, N.; Toporik, H.
Deposited on : 2010-02-23
Resolution : 3.30 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 : 2.23.1
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) : 2.23.1

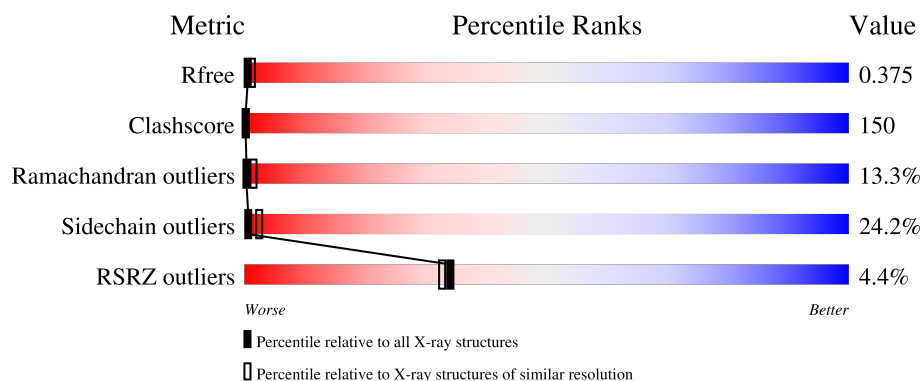
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	738	
2	B	733	
3	C	81	
4	D	138	
5	E	64	

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Mol	Chain	Length	Quality of chain
6	F	154	
7	G	95	
8	H	69	
9	I	30	
10	J	42	
11	K	84	
12	L	161	
13	N	85	
14	R	53	
15	1	170	
16	2	176	
17	3	172	
18	4	166	

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
19	CLA	1	1001	X	-	-	-
19	CLA	1	1002	X	-	-	-
19	CLA	1	1003	X	-	-	-
19	CLA	1	1005	X	-	-	-
19	CLA	1	1006	X	-	-	X
19	CLA	1	1007	X	-	-	-
19	CLA	1	1008	X	-	-	-
19	CLA	1	1010	X	-	-	-
19	CLA	1	1011	X	-	-	-
19	CLA	1	1012	X	-	-	-
19	CLA	1	1013	X	-	-	X
19	CLA	1	1014	X	-	-	-
19	CLA	1	1015	X	-	-	-
19	CLA	1	1303	X	-	-	-
19	CLA	1	1310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	1307	X	-	-	X
19	CLA	2	2001	X	-	-	-
19	CLA	2	2002	X	-	-	-
19	CLA	2	2003	X	-	-	-
19	CLA	2	2004	X	-	-	-
19	CLA	2	2005	X	-	-	-
19	CLA	2	2006	X	-	-	-
19	CLA	2	2007	X	-	-	-
19	CLA	2	2008	X	-	-	-
19	CLA	2	2010	X	-	-	-
19	CLA	2	2011	X	-	-	-
19	CLA	2	2012	X	-	-	-
19	CLA	2	2013	X	-	-	-
19	CLA	2	2014	X	-	X	-
19	CLA	2	4009	X	-	-	-
19	CLA	3	1118	X	-	-	-
19	CLA	3	1147	X	-	-	-
19	CLA	3	2009	X	-	X	-
19	CLA	3	3001	X	-	-	-
19	CLA	3	3002	X	-	-	-
19	CLA	3	3003	X	-	-	-
19	CLA	3	3004	X	-	-	-
19	CLA	3	3005	X	-	-	-
19	CLA	3	3006	X	-	-	-
19	CLA	3	3007	X	-	-	-
19	CLA	3	3008	X	-	-	-
19	CLA	3	3010	X	-	-	-
19	CLA	3	3011	X	-	-	-
19	CLA	3	3012	X	-	-	-
19	CLA	3	3013	X	-	-	-
19	CLA	3	3014	X	-	-	X
19	CLA	3	3015	X	-	-	X
19	CLA	3	3016	X	-	-	X
19	CLA	3	3017	X	-	-	-
19	CLA	4	1004	X	-	X	-
19	CLA	4	1009	X	-	-	-
19	CLA	4	1304	X	-	X	-
19	CLA	4	1306	X	-	-	-
19	CLA	4	4001	X	-	-	X
19	CLA	4	4002	X	-	X	-
19	CLA	4	4003	X	-	-	-
19	CLA	4	4004	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	4005	X	-	-	-
19	CLA	4	4006	X	-	-	-
19	CLA	4	4007	X	-	-	-
19	CLA	4	4010	X	-	-	-
19	CLA	4	4011	X	-	-	-
19	CLA	4	4012	X	-	-	-
19	CLA	4	4013	X	-	-	-
19	CLA	4	4014	X	-	-	-
19	CLA	4	4015	X	-	-	-
19	CLA	A	1101	X	-	-	-
19	CLA	A	1102	X	-	-	-
19	CLA	A	1103	X	-	-	-
19	CLA	A	1104	X	-	-	-
19	CLA	A	1105	X	-	X	-
19	CLA	A	1106	X	-	X	-
19	CLA	A	1107	X	-	X	-
19	CLA	A	1108	X	-	-	-
19	CLA	A	1109	X	-	-	-
19	CLA	A	1110	X	-	-	-
19	CLA	A	1111	X	-	X	-
19	CLA	A	1112	X	-	X	X
19	CLA	A	1113	X	-	-	-
19	CLA	A	1115	X	-	X	-
19	CLA	A	1116	X	-	-	-
19	CLA	A	1117	X	-	X	-
19	CLA	A	1119	X	-	X	-
19	CLA	A	1120	X	-	-	-
19	CLA	A	1121	X	-	-	-
19	CLA	A	1122	X	-	X	-
19	CLA	A	1123	X	-	X	-
19	CLA	A	1124	X	-	X	-
19	CLA	A	1125	X	-	X	-
19	CLA	A	1126	X	-	X	-
19	CLA	A	1127	X	-	-	-
19	CLA	A	1128	X	-	X	-
19	CLA	A	1129	X	-	-	-
19	CLA	A	1131	X	-	X	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1133	X	-	X	-
19	CLA	A	1134	X	-	-	-
19	CLA	A	1135	X	-	X	-
19	CLA	A	1136	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1137	X	-	-	-
19	CLA	A	1138	X	-	X	-
19	CLA	A	1139	X	-	X	-
19	CLA	A	1140	X	-	X	-
19	CLA	A	1141	X	-	X	-
19	CLA	A	1149	X	-	-	-
19	CLA	A	1151	X	-	-	-
19	CLA	A	1237	X	-	X	-
19	CLA	A	1309	X	-	-	X
19	CLA	A	9011	X	-	-	-
19	CLA	A	9012	X	-	X	-
19	CLA	A	9013	X	-	X	-
19	CLA	A	9022	X	-	X	-
19	CLA	A	9023	X	-	X	-
19	CLA	B	1201	X	-	-	-
19	CLA	B	1202	X	-	X	-
19	CLA	B	1203	X	-	-	-
19	CLA	B	1205	X	-	X	-
19	CLA	B	1206	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1209	X	-	-	-
19	CLA	B	1210	X	-	X	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1212	X	-	-	-
19	CLA	B	1213	X	-	-	-
19	CLA	B	1214	X	-	X	-
19	CLA	B	1215	X	-	-	-
19	CLA	B	1216	X	-	-	-
19	CLA	B	1217	X	-	-	-
19	CLA	B	1218	X	-	-	-
19	CLA	B	1219	X	-	-	-
19	CLA	B	1220	X	-	X	-
19	CLA	B	1221	X	-	X	-
19	CLA	B	1222	X	-	X	-
19	CLA	B	1223	X	-	X	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	X	-
19	CLA	B	1226	X	-	X	-
19	CLA	B	1227	X	-	-	-
19	CLA	B	1228	X	-	-	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1230	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1231	X	-	-	-
19	CLA	B	1232	X	-	-	X
19	CLA	B	1233	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	X	-
19	CLA	B	1236	X	-	X	-
19	CLA	B	1238	X	-	X	-
19	CLA	B	1239	X	-	X	-
19	CLA	B	1301	X	-	-	-
19	CLA	B	9010	X	-	-	-
19	CLA	F	1240	X	-	-	-
19	CLA	F	1302	X	-	-	-
19	CLA	F	1305	X	-	-	-
19	CLA	G	1242	X	-	-	-
19	CLA	H	1145	X	-	X	-
19	CLA	H	1207	X	-	X	-
19	CLA	H	1241	X	-	-	-
19	CLA	H	1505	X	-	-	-
19	CLA	I	1204	X	-	-	-
19	CLA	J	1308	X	-	X	-
19	CLA	J	1311	X	-	-	-
19	CLA	K	1142	X	-	-	-
19	CLA	K	1143	X	-	X	-
19	CLA	K	1146	X	-	-	-
19	CLA	K	3009	X	-	-	-
19	CLA	L	1130	X	-	X	-
19	CLA	L	1148	X	-	X	-
19	CLA	L	1501	X	-	-	-
19	CLA	L	1502	X	-	X	-
19	CLA	L	1503	X	-	-	-
19	CLA	L	1504	X	-	X	X
19	CLA	R	1144	X	-	-	-
19	CLA	R	1150	X	-	-	-
20	PQN	A	5001	X	-	-	-
20	PQN	B	5002	X	-	X	-
21	BCR	1	6023	-	-	-	X
21	BCR	A	6002	-	-	X	-
21	BCR	A	6007	-	-	X	-
21	BCR	A	6008	-	-	X	-
21	BCR	A	6011	-	-	X	-
21	BCR	B	6010	-	-	X	-
21	BCR	B	6017	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	BCR	B	6020	-	-	X	-
21	BCR	F	6014	-	-	X	-
21	BCR	F	6016	-	-	X	-
21	BCR	I	6021	-	-	X	-
21	BCR	J	6012	-	-	X	-
21	BCR	L	6019	-	-	X	-
22	LMU	1	7004	-	-	-	X
22	LMU	3	7005	-	-	X	-
22	LMU	4	7034	-	-	X	-
22	LMU	4	7052	-	-	X	-
22	LMU	B	7038	-	-	-	X
22	LMU	D	7050	-	-	X	-
23	SF4	A	8001	-	-	X	-
23	SF4	C	8002	-	-	X	-
23	SF4	C	8003	-	-	X	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 36370 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
1	A	730	Total	C	N	O	S	0	0	0
			5739	3762	974	985	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5844	3841	997	993	13			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 4 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1097	704	191	199	3			

- Molecule 5 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	64	Total	C	N	O	0	0	0
			513	327	90	96			

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	0	0	0
			738	481	120	137			

- Molecule 8 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	69	Total	C	N	O	0	0	0
			517	334	80	103			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			334	228	51	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	84	Total	C	N	O	S	0	0	0
			592	377	102	110	3			

- Molecule 12 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	161	Total	C	N	O	S	0	0	0
			1209	797	192	219	1			

- Molecule 13 is a protein called Photosystem I-N subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 14 is a protein called CHAIN R.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 15 is a protein called AT3g54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1	165	Total	C	N	O	S	0	0	0
			1257	816	208	229	4			

- Molecule 16 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	2	176	Total	C	N	O	S	0	0	0
			1367	895	223	245	4			

- Molecule 17 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	3	156	Total	C	N	O	S	0	0	0
			1197	784	199	209	5			

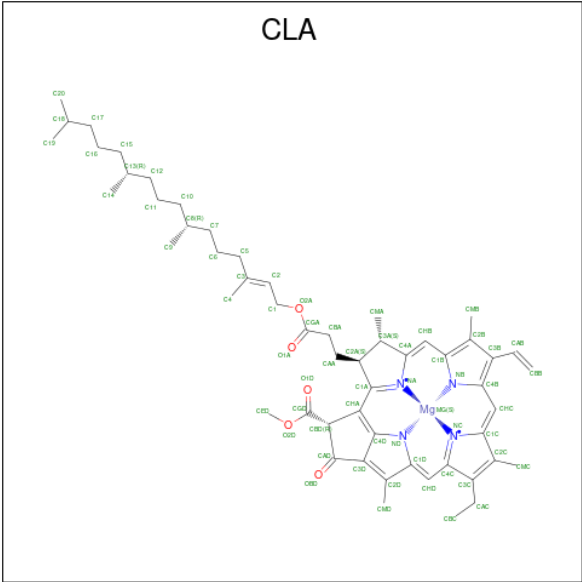
- Molecule 18 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	4	166	Total	C	N	O	S	0	0	0
			1309	856	216	234	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	SEE REMARK 999	UNP Q9SQL2

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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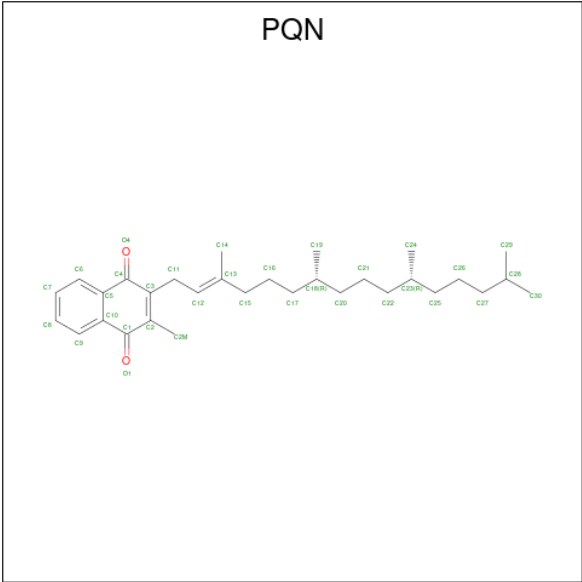
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	3	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
19	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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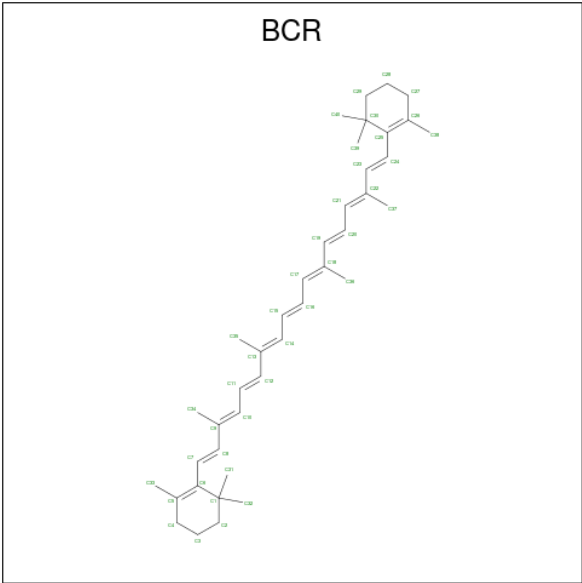
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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



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

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



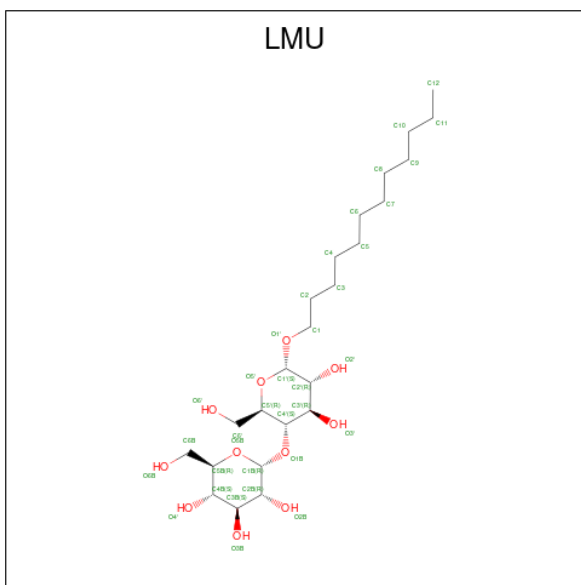
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	C		0
			40	40		
21	A	1	Total	C		0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	J	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	1	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0

- Molecule 22 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total 35	C 24	O 11	0	0
22	A	1	Total 35	C 24	O 11	0	0
22	A	1	Total 35	C 24	O 11	0	0
22	A	1	Total 35	C 24	O 11	0	0
22	A	1	Total 35	C 24	O 11	0	0
22	A	1	Total 35	C 24	O 11	0	0
22	B	1	Total 25	C 14	O 11	0	0
22	B	1	Total 35	C 24	O 11	0	0
22	B	1	Total 35	C 24	O 11	0	0
22	C	1	Total 35	C 24	O 11	0	0
22	D	1	Total 35	C 24	O 11	0	0
22	E	1	Total 35	C 24	O 11	0	0
22	E	1	Total 35	C 24	O 11	0	0
22	F	1	Total 34	C 23	O 11	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	G	1	Total	C	O	0	0
			35	24	11		
22	G	1	Total	C	O	0	0
			35	24	11		
22	G	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	L	1	Total	C	O	0	0
			35	24	11		
22	N	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		

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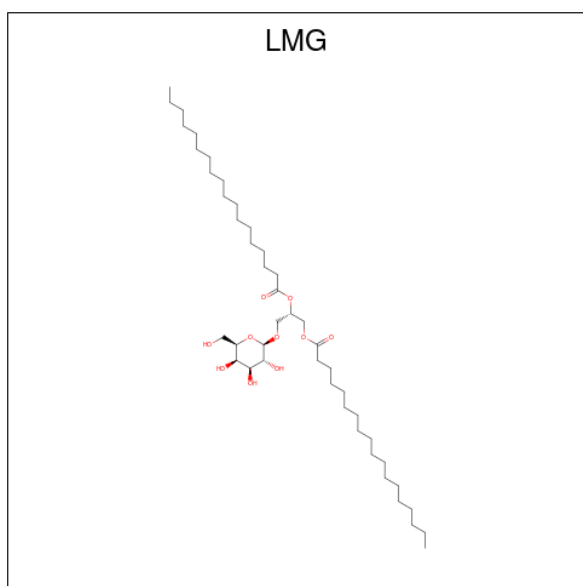
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	1	1	Total	C	O	0	0
			35	24	11		
22	1	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	3	1	Total	C	O	0	0
			35	24	11		
22	3	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			34	23	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			34	23	11		

- Molecule 23 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

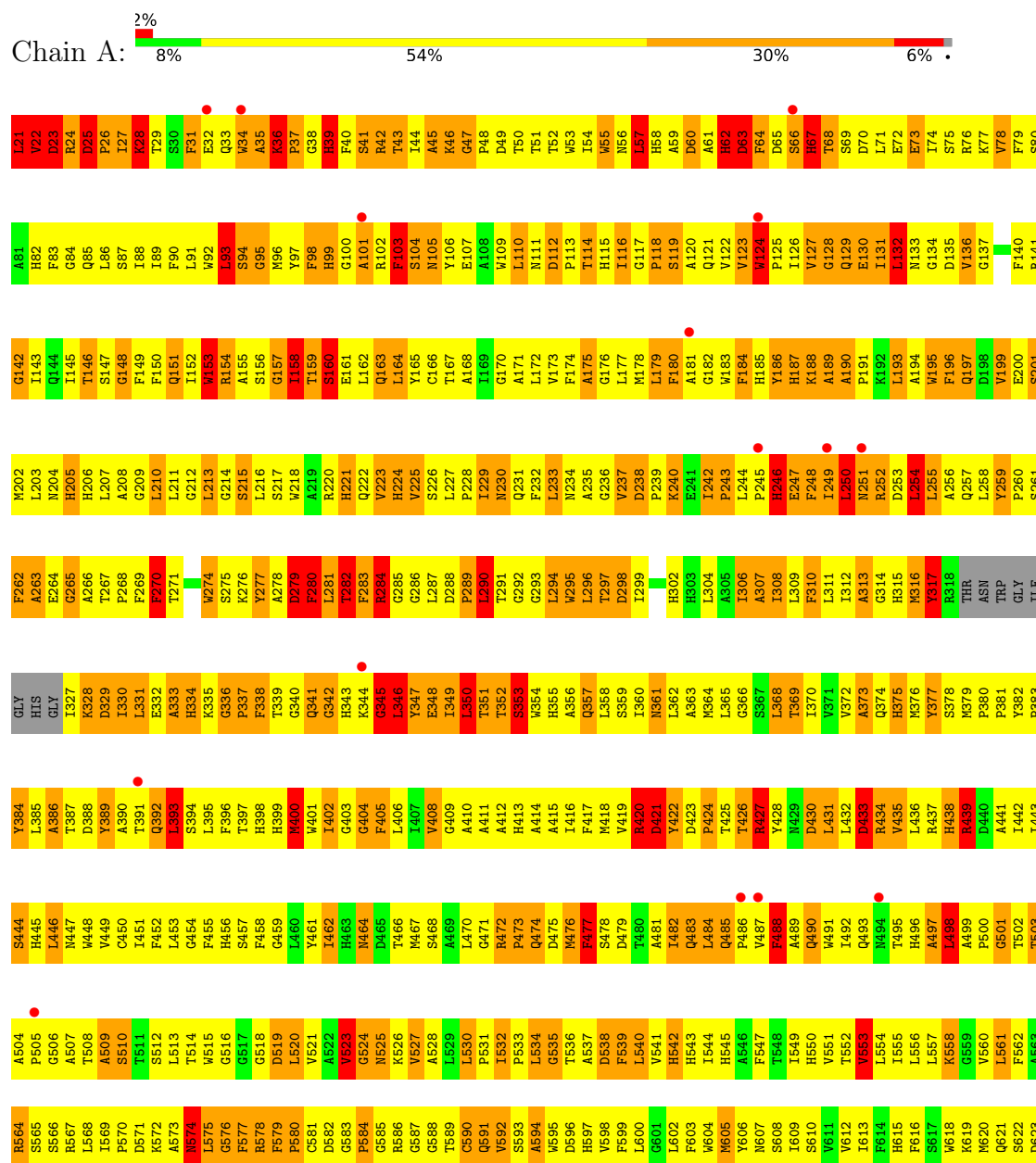


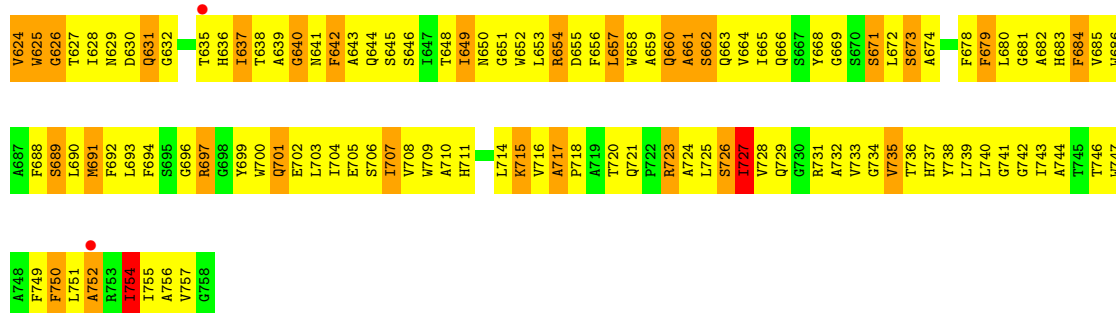
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			49	39	10		

3 Residue-property plots

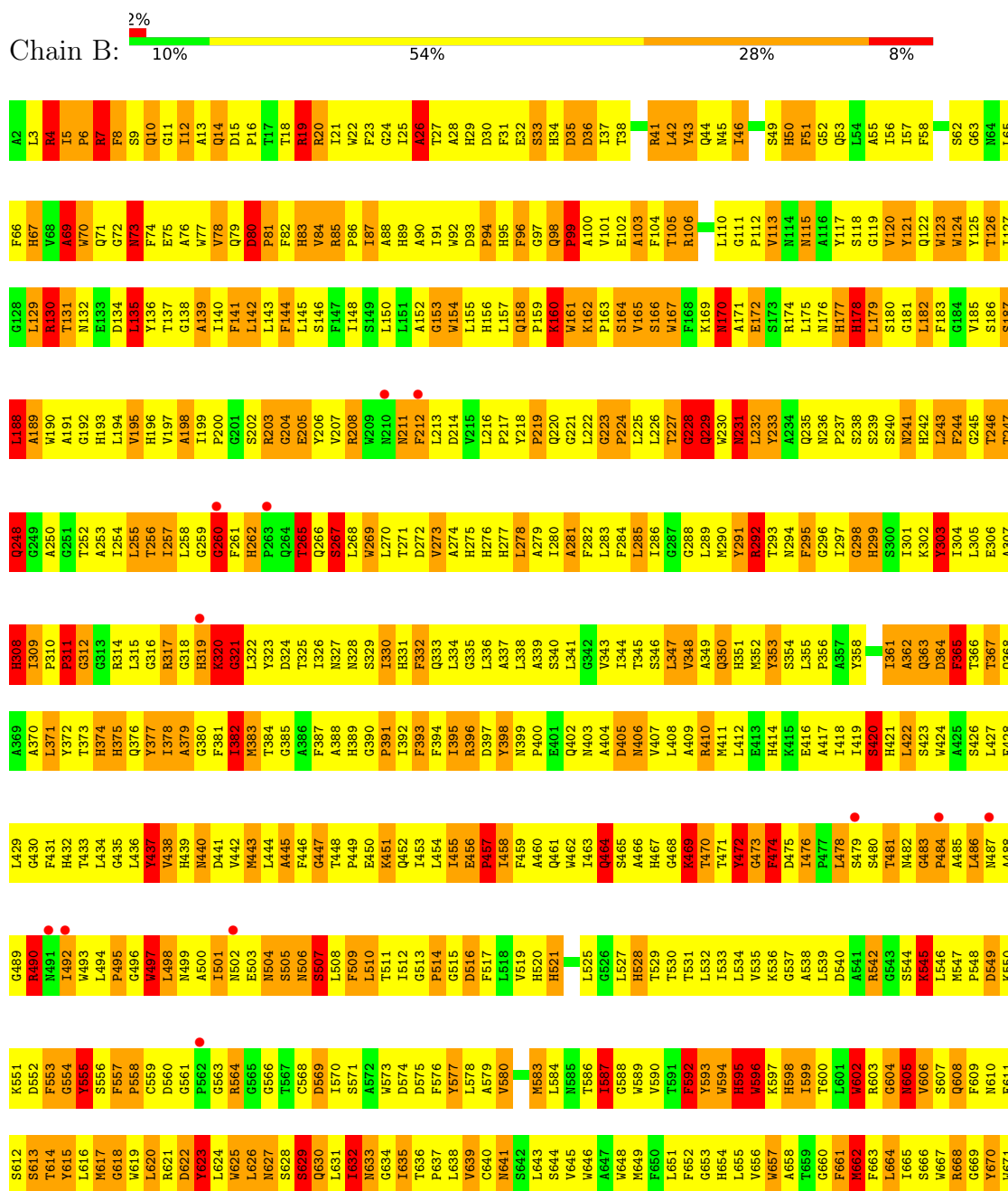
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

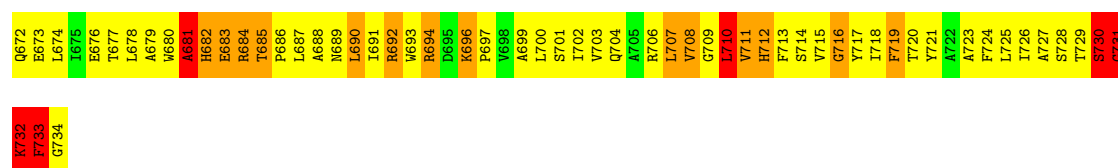
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



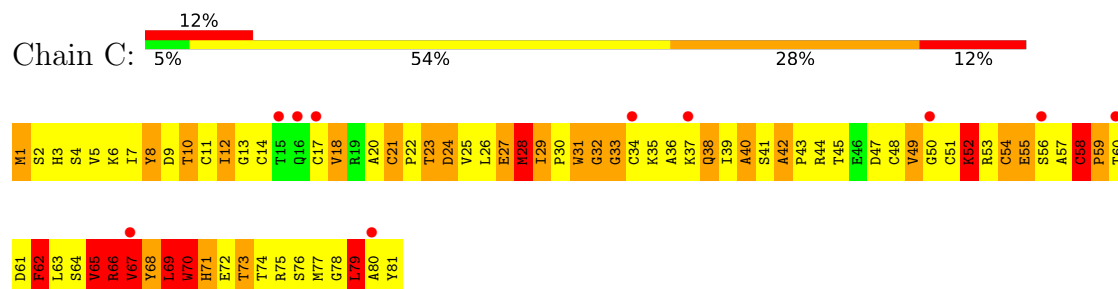


● Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

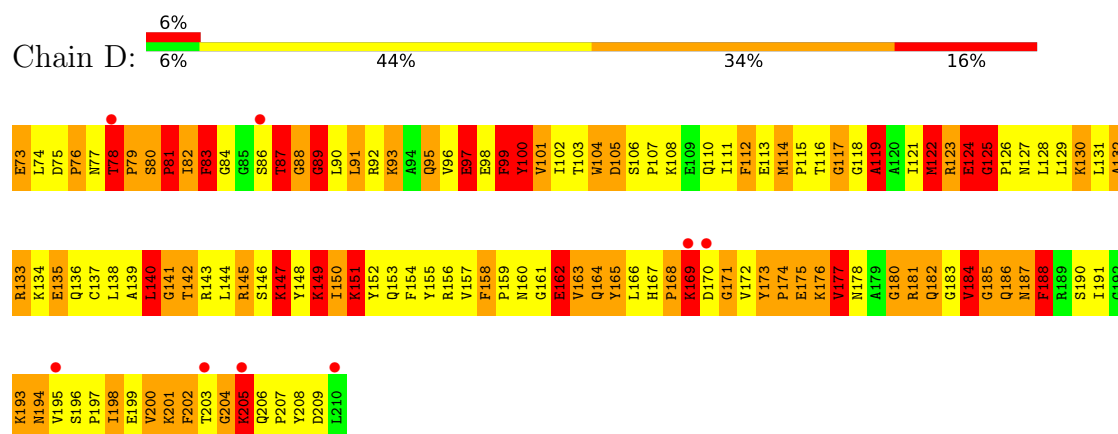




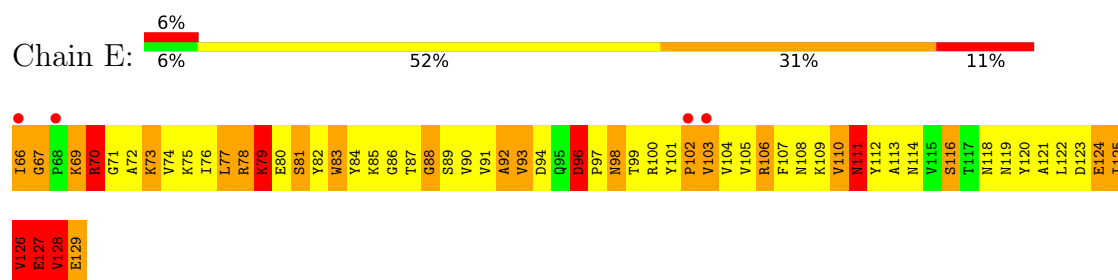
• Molecule 3: Photosystem I iron-sulfur center



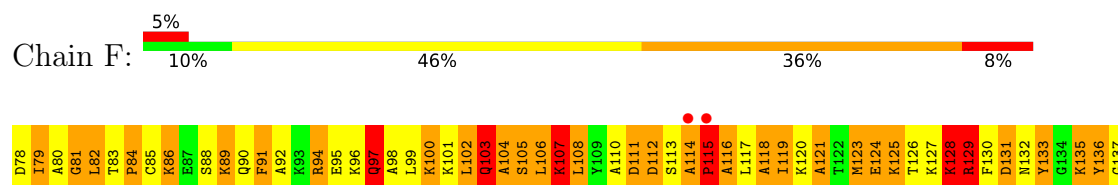
• Molecule 4: Putative uncharacterized protein

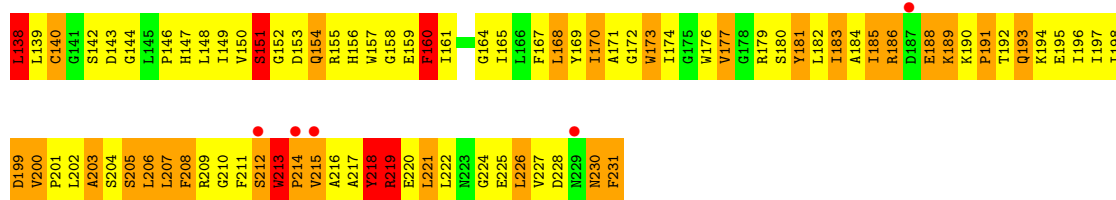


• Molecule 5: Putative uncharacterized protein

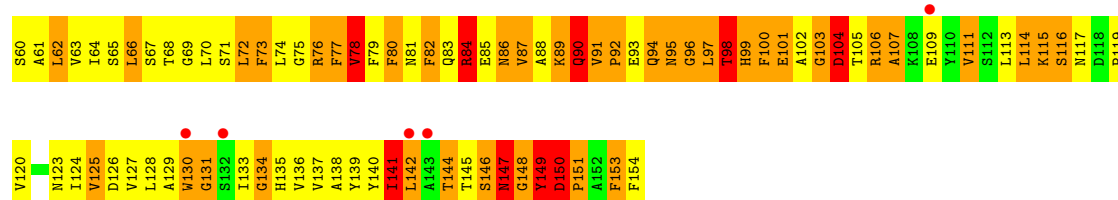


• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

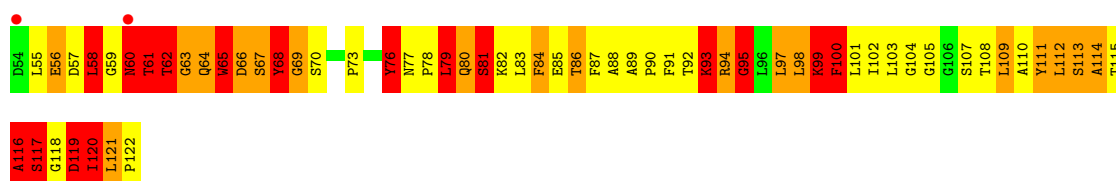




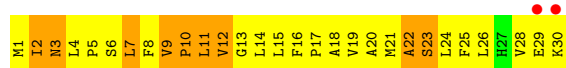
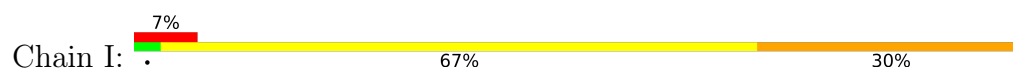
• Molecule 7: Putative uncharacterized protein



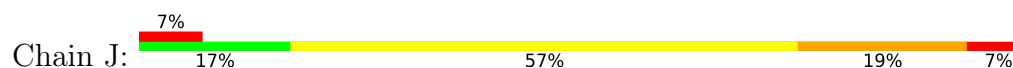
• Molecule 8: Putative uncharacterized protein



• Molecule 9: Photosystem I reaction center subunit VIII



• Molecule 10: Photosystem I reaction center subunit IX



• Molecule 11: Photosystem I reaction center subunit X psaK





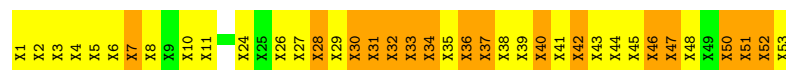
• Molecule 12: Putative uncharacterized protein



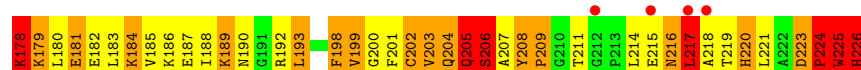
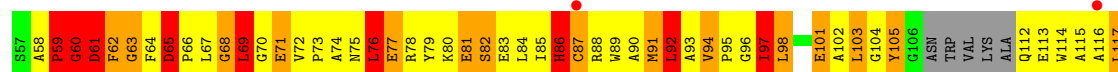
• Molecule 13: Photosystem I-N subunit



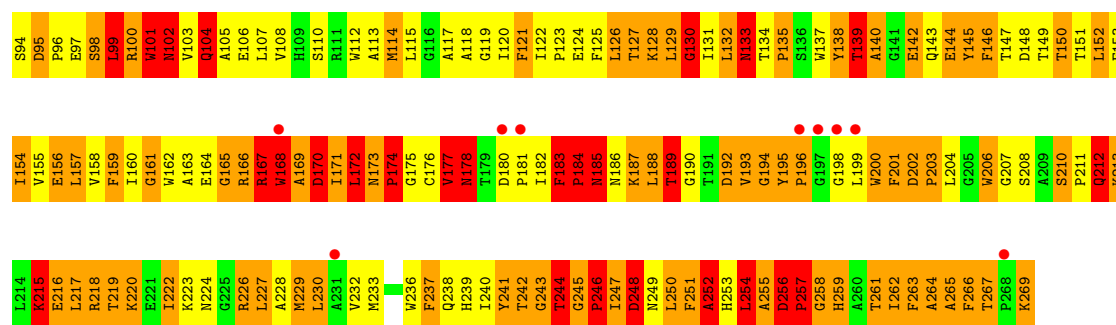
• Molecule 14: CHAIN R



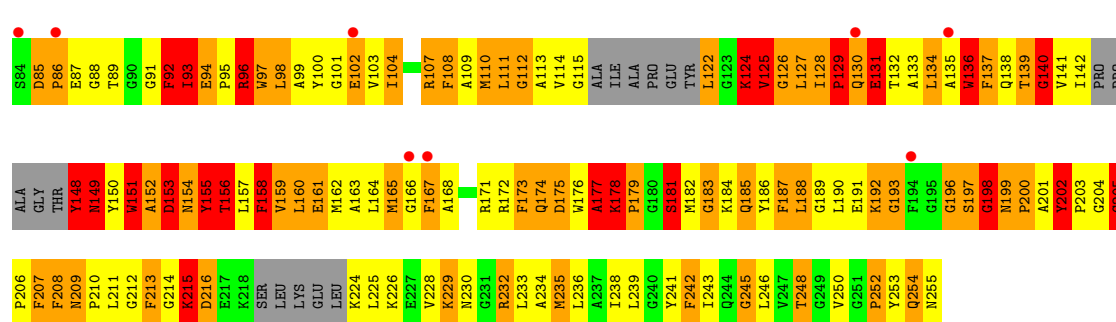
• Molecule 15: AT3g54890



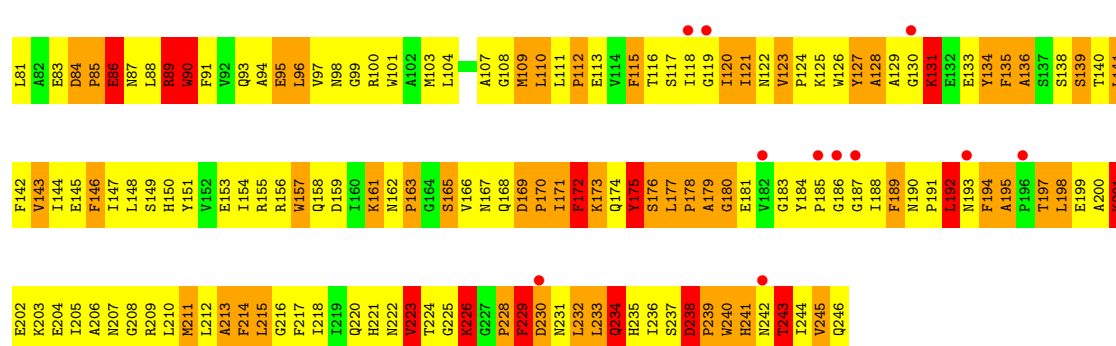
• Molecule 16: Type II chlorophyll a/b binding protein from photosystem I



• Molecule 17: Chlorophyll a-b binding protein 3, chloroplastic



• Molecule 18: Chlorophyll a-b binding protein P4, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 49.14 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 99.0 (49.14-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.349 , 0.383 0.353 , 0.375	Depositor DCC
R_{free} test set	4705 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 93.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	36370	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: PQN, SF4, CLA, BCR, LMG, LMU

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	0.88	5/5932 (0.1%)	1.20	49/8096 (0.6%)
2	B	0.96	8/6054 (0.1%)	1.16	35/8273 (0.4%)
3	C	1.10	1/632 (0.2%)	1.35	5/856 (0.6%)
4	D	1.13	2/1124 (0.2%)	1.49	15/1516 (1.0%)
5	E	1.26	2/523 (0.4%)	1.38	7/710 (1.0%)
6	F	0.98	0/1250	1.29	10/1687 (0.6%)
7	G	1.00	3/757 (0.4%)	1.41	5/1031 (0.5%)
8	H	1.12	3/530 (0.6%)	1.58	11/722 (1.5%)
9	I	0.82	0/235	0.88	0/320
10	J	0.83	0/344	0.99	0/469
11	K	1.14	4/599 (0.7%)	1.50	8/811 (1.0%)
12	L	1.07	3/1244 (0.2%)	1.32	10/1703 (0.6%)
13	N	1.11	3/699 (0.4%)	1.51	10/936 (1.1%)
15	1	1.50	20/1295 (1.5%)	1.51	21/1763 (1.2%)
16	2	1.16	9/1413 (0.6%)	1.51	30/1934 (1.6%)
17	3	1.09	9/1231 (0.7%)	1.37	18/1658 (1.1%)
18	4	1.13	6/1349 (0.4%)	1.56	13/1839 (0.7%)
All	All	1.04	78/25211 (0.3%)	1.32	247/34324 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	81
2	B	0	83
3	C	0	14
4	D	0	37
5	E	0	10
6	F	0	27

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	1	24
8	H	2	22
11	K	0	21
12	L	0	23
13	N	0	40
14	R	0	17
15	1	0	37
16	2	0	45
17	3	0	35
18	4	0	28
All	All	3	544

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	119	GLY	N-CA	13.83	1.66	1.46
15	1	172	GLY	C-O	12.76	1.44	1.23
15	1	63	GLY	C-O	11.60	1.42	1.23
15	1	225	TRP	C-N	10.48	1.58	1.34
2	B	94	PRO	N-CD	-10.34	1.33	1.47
15	1	60	GLY	CA-C	-9.76	1.36	1.51
16	2	194	GLY	N-CA	8.95	1.59	1.46
1	A	337	PRO	N-CD	-8.94	1.35	1.47
15	1	225	TRP	C-O	8.79	1.40	1.23
15	1	171	LEU	C-O	8.58	1.39	1.23
15	1	63	GLY	CA-C	8.39	1.65	1.51
15	1	166	GLY	N-CA	8.32	1.58	1.46
16	2	133	ASN	C-O	8.31	1.39	1.23
2	B	99	PRO	N-CD	-8.30	1.36	1.47
12	L	64	PRO	N-CD	-8.29	1.36	1.47
15	1	60	GLY	N-CA	7.95	1.57	1.46
2	B	219	PRO	N-CD	-7.88	1.36	1.47
11	K	123	GLY	C-N	7.83	1.52	1.34
17	3	198	GLY	N-CA	7.75	1.57	1.46
18	4	239	PRO	N-CD	-7.30	1.37	1.47
15	1	172	GLY	CA-C	7.23	1.63	1.51
15	1	225	TRP	CB-CG	7.21	1.63	1.50
17	3	158	PHE	C-O	7.20	1.37	1.23
2	B	457	PRO	N-CD	-7.19	1.37	1.47
13	N	157	LYS	C-N	6.90	1.50	1.34
16	2	167	ARG	CZ-NH1	6.75	1.41	1.33
16	2	184	PRO	C-N	6.71	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	172	GLY	N-CA	6.67	1.56	1.46
15	1	173	TYR	CD2-CE2	-6.47	1.29	1.39
17	3	129	PRO	N-CD	-6.38	1.39	1.47
16	2	165	GLY	C-O	6.38	1.33	1.23
13	N	157	LYS	C-O	6.33	1.35	1.23
4	D	188	PHE	CB-CG	-6.25	1.40	1.51
1	A	21	LEU	C-O	6.15	1.35	1.23
18	4	129	ALA	N-CA	6.14	1.58	1.46
2	B	229	GLN	C-O	6.03	1.34	1.23
17	3	196	GLY	C-O	6.02	1.33	1.23
16	2	130	GLY	C-O	-6.00	1.14	1.23
1	A	153	TRP	CB-CG	-5.96	1.39	1.50
13	N	146	LEU	N-CA	5.96	1.58	1.46
5	E	127	GLU	CG-CD	-5.96	1.43	1.51
16	2	177	VAL	CB-CG1	5.96	1.65	1.52
15	1	61	ASP	N-CA	-5.94	1.34	1.46
7	G	149	TYR	C-N	5.89	1.47	1.34
18	4	176	SER	CB-OG	5.80	1.49	1.42
8	H	95	GLY	N-CA	5.79	1.54	1.46
7	G	107	ALA	N-CA	5.73	1.57	1.46
1	A	137	GLY	N-CA	5.71	1.54	1.46
2	B	167	TRP	CB-CG	-5.71	1.40	1.50
18	4	234	GLN	N-CA	5.70	1.57	1.46
15	1	215	GLU	CB-CG	5.65	1.62	1.52
17	3	158	PHE	C-N	5.65	1.47	1.34
16	2	175	GLY	N-CA	5.62	1.54	1.46
7	G	151	PRO	N-CD	-5.60	1.40	1.47
16	2	178	ASN	CG-OD1	5.56	1.36	1.24
11	K	92	GLY	N-CA	5.55	1.54	1.46
3	C	31	TRP	CB-CG	5.53	1.60	1.50
2	B	497	TRP	CB-CG	-5.47	1.40	1.50
11	K	96	GLY	CA-C	5.46	1.60	1.51
12	L	62	GLY	N-CA	5.43	1.54	1.46
15	1	226	HIS	N-CA	5.42	1.57	1.46
8	H	65	TRP	C-N	5.38	1.46	1.34
4	D	185	GLY	N-CA	5.36	1.54	1.46
15	1	226	HIS	CA-C	5.32	1.66	1.52
17	3	102	GLU	CB-CG	5.29	1.62	1.52
2	B	205	GLU	CB-CG	5.28	1.62	1.52
5	E	81	SER	CB-OG	5.22	1.49	1.42
17	3	124	LYS	CD-CE	5.22	1.64	1.51
1	A	55	TRP	CB-CG	-5.21	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	148	TYR	CG-CD2	5.20	1.46	1.39
17	3	126	GLY	N-CA	5.15	1.53	1.46
18	4	229	PHE	C-O	5.08	1.33	1.23
12	L	172	GLU	CG-CD	-5.05	1.44	1.51
15	1	173	TYR	C-O	-5.04	1.13	1.23
18	4	90	TRP	CB-CG	-5.04	1.41	1.50
11	K	128	GLY	C-O	5.03	1.31	1.23
15	1	209	PRO	N-CD	5.02	1.54	1.47
8	H	116	ALA	C-N	5.01	1.45	1.34

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	84	ASP	C-N-CD	-31.95	50.30	120.60
16	2	184	PRO	O-C-N	11.36	140.88	122.70
16	2	258	GLY	N-CA-C	10.50	139.35	113.10
4	D	123	ARG	NE-CZ-NH2	-10.44	115.08	120.30
18	4	186	GLY	N-CA-C	10.00	138.11	113.10
12	L	84	SER	N-CA-C	9.30	136.11	111.00
11	K	113	GLY	N-CA-C	-9.14	90.24	113.10
11	K	114	HIS	N-CA-C	-9.09	86.47	111.00
16	2	184	PRO	CA-C-O	-8.94	98.75	120.20
1	A	524	GLY	N-CA-C	8.71	134.87	113.10
1	A	47	GLY	N-CA-C	-8.64	91.49	113.10
16	2	132	LEU	CA-CB-CG	8.59	135.06	115.30
1	A	284	ARG	N-CA-C	8.51	133.98	111.00
18	4	169	ASP	N-CA-C	8.15	133.01	111.00
15	1	225	TRP	C-N-CA	-7.99	101.72	121.70
6	F	103	GLN	O-C-N	-7.92	110.03	122.70
4	D	141	GLY	N-CA-C	-7.83	93.53	113.10
2	B	602	TRP	N-CA-C	7.78	132.00	111.00
4	D	169	LYS	N-CA-C	7.72	131.84	111.00
11	K	97	ASP	N-CA-C	7.65	131.64	111.00
13	N	134	CYS	N-CA-C	-7.63	90.40	111.00
13	N	159	LYS	N-CA-C	7.60	131.53	111.00
1	A	238	ASP	N-CA-C	-7.51	90.73	111.00
4	D	125	GLY	N-CA-C	7.46	131.76	113.10
17	3	131	GLU	N-CA-C	-7.46	90.86	111.00
17	3	158	PHE	N-CA-C	-7.45	90.89	111.00
16	2	126	LEU	N-CA-C	-7.41	90.99	111.00
5	E	128	VAL	N-CA-C	-7.30	91.29	111.00
18	4	234	GLN	N-CA-C	7.27	130.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ILE	N-CA-C	7.18	130.39	111.00
17	3	154	ASN	N-CA-C	7.12	130.22	111.00
12	L	132	LEU	CA-CB-CG	7.05	131.53	115.30
1	A	346	LEU	CA-CB-CG	-7.05	99.09	115.30
4	D	122	MET	N-CA-C	7.04	130.01	111.00
2	B	72	GLY	N-CA-C	-7.03	95.53	113.10
15	1	202	CYS	CA-CB-SG	-6.98	101.43	114.00
1	A	350	LEU	CA-CB-CG	-6.98	99.24	115.30
16	2	252	ALA	N-CA-C	-6.97	92.18	111.00
15	1	65	ASP	C-N-CD	-6.95	105.31	120.60
1	A	336	GLY	C-N-CD	-6.94	105.33	120.60
16	2	102	ASN	N-CA-C	-6.93	92.28	111.00
1	A	534	LEU	N-CA-C	6.83	129.44	111.00
8	H	60	ASN	N-CA-C	6.80	129.37	111.00
7	G	72	LEU	CA-CB-CG	6.79	130.91	115.30
13	N	149	ASP	N-CA-C	-6.77	92.73	111.00
2	B	632	ILE	C-N-CA	-6.76	104.81	121.70
16	2	185	ASN	N-CA-C	6.75	129.21	111.00
5	E	98	ASN	N-CA-C	6.73	129.17	111.00
4	D	99	PHE	N-CA-C	6.72	129.15	111.00
15	1	143	LEU	CA-CB-CG	-6.72	99.85	115.30
5	E	127	GLU	N-CA-CB	-6.67	98.59	110.60
5	E	127	GLU	N-CA-C	6.66	128.99	111.00
18	4	175	TYR	N-CA-C	-6.65	93.06	111.00
1	A	348	GLU	N-CA-C	-6.59	93.20	111.00
4	D	100	TYR	N-CA-C	6.59	128.79	111.00
4	D	205	LYS	N-CA-C	6.56	128.72	111.00
1	A	295	TRP	O-C-N	6.55	133.18	122.70
1	A	28	LYS	N-CA-C	6.55	128.68	111.00
2	B	99	PRO	CA-N-CD	-6.51	102.38	111.50
1	A	345	GLY	N-CA-C	-6.47	96.92	113.10
16	2	127	THR	CB-CA-C	-6.47	94.12	111.60
18	4	194	PHE	N-CA-C	6.46	128.45	111.00
16	2	253	HIS	CB-CA-C	6.46	123.32	110.40
17	3	183	GLY	N-CA-C	-6.44	97.01	113.10
2	B	625	TRP	N-CA-C	6.42	128.33	111.00
3	C	67	VAL	CB-CA-C	-6.41	99.23	111.40
18	4	215	LEU	C-N-CA	-6.36	108.95	122.30
1	A	116	ILE	N-CA-C	6.35	128.15	111.00
5	E	70	ARG	N-CA-C	6.34	128.12	111.00
15	1	168	PHE	N-CA-C	6.34	128.11	111.00
3	C	79	LEU	CA-CB-CG	6.33	129.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	SER	N-CA-C	6.31	128.03	111.00
4	D	180	GLY	N-CA-C	6.29	128.82	113.10
4	D	177	VAL	CB-CA-C	-6.28	99.48	111.40
16	2	130	GLY	CA-C-N	-6.27	103.40	117.20
13	N	145	PHE	C-N-CA	-6.27	106.02	121.70
13	N	126	LYS	N-CA-C	6.25	127.86	111.00
13	N	166	VAL	N-CA-C	-6.24	94.16	111.00
15	1	69	LEU	O-C-N	-6.23	112.61	123.20
1	A	246	HIS	N-CA-C	6.22	127.81	111.00
15	1	165	GLY	C-N-CA	-6.20	109.28	122.30
18	4	180	GLY	N-CA-C	-6.20	97.61	113.10
1	A	290	LEU	CA-CB-CG	6.19	129.54	115.30
2	B	243	LEU	CA-CB-CG	6.17	129.49	115.30
16	2	183	PHE	N-CA-C	6.16	127.64	111.00
2	B	710	LEU	N-CA-C	-6.13	94.44	111.00
5	E	126	VAL	CB-CA-C	-6.11	99.78	111.40
15	1	63	GLY	CA-C-O	6.11	131.59	120.60
12	L	64	PRO	CA-N-CD	-6.09	102.97	111.50
11	K	94	GLN	N-CA-C	6.09	127.45	111.00
1	A	295	TRP	CA-C-N	-6.08	103.83	117.20
1	A	503	THR	N-CA-C	-6.08	94.59	111.00
17	3	104	ILE	CB-CA-C	-6.08	99.44	111.60
2	B	321	GLY	N-CA-C	6.07	128.28	113.10
2	B	19	ARG	N-CA-C	-6.07	94.62	111.00
1	A	158	ILE	N-CA-C	-6.06	94.64	111.00
16	2	129	LEU	N-CA-C	-6.04	94.69	111.00
1	A	265	GLY	N-CA-C	6.03	128.17	113.10
17	3	155	TYR	N-CA-C	6.03	127.27	111.00
17	3	125	VAL	C-N-CA	-6.01	109.68	122.30
18	4	215	LEU	N-CA-C	-6.01	94.78	111.00
1	A	530	LEU	CA-CB-CG	6.01	129.12	115.30
15	1	163	TYR	N-CA-C	-6.00	94.80	111.00
2	B	553	PHE	N-CA-C	-5.98	94.84	111.00
8	H	61	THR	CA-C-N	-5.96	104.10	117.20
1	A	337	PRO	CA-N-CD	-5.94	103.19	111.50
2	B	483	GLY	N-CA-C	-5.93	98.26	113.10
2	B	14	GLN	N-CA-C	5.91	126.95	111.00
15	1	92	LEU	CA-CB-CG	5.90	128.86	115.30
8	H	58	LEU	CA-CB-CG	5.89	128.86	115.30
8	H	68	TYR	N-CA-C	5.89	126.92	111.00
2	B	228	GLY	N-CA-C	-5.89	98.37	113.10
6	F	226	LEU	N-CA-C	-5.89	95.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	159	VAL	CB-CA-C	-5.89	100.21	111.40
16	2	161	GLY	N-CA-C	-5.88	98.39	113.10
2	B	469	LYS	C-N-CA	-5.86	107.05	121.70
1	A	62	HIS	N-CA-C	-5.85	95.21	111.00
2	B	303	TYR	CB-CA-C	-5.84	98.71	110.40
17	3	196	GLY	N-CA-C	5.84	127.71	113.10
16	2	130	GLY	N-CA-C	-5.82	98.56	113.10
2	B	626	LEU	CA-CB-CG	5.79	128.62	115.30
17	3	166	GLY	N-CA-C	-5.77	98.67	113.10
16	2	171	ILE	CB-CA-C	-5.77	100.06	111.60
6	F	219	ARG	N-CA-C	5.76	126.56	111.00
18	4	230	ASP	N-CA-C	5.76	126.55	111.00
17	3	205	GLY	N-CA-C	-5.72	98.79	113.10
6	F	114	ALA	N-CA-C	5.71	126.41	111.00
15	1	171	LEU	O-C-N	5.70	132.89	123.20
1	A	101	ALA	C-N-CA	-5.70	107.46	121.70
15	1	172	GLY	CA-C-N	-5.70	104.67	117.20
15	1	82	SER	N-CA-C	-5.69	95.63	111.00
13	N	157	LYS	C-N-CA	-5.69	107.47	121.70
6	F	206	LEU	CA-CB-CG	-5.69	102.22	115.30
6	F	82	LEU	CA-CB-CG	-5.68	102.23	115.30
17	3	151	TRP	N-CA-C	-5.68	95.67	111.00
16	2	216	GLU	N-CA-C	-5.67	95.69	111.00
7	G	150	ASP	N-CA-C	5.63	126.21	111.00
16	2	194	GLY	N-CA-C	5.62	127.14	113.10
2	B	456	GLU	N-CA-C	-5.61	95.84	111.00
11	K	52	PRO	N-CA-C	-5.61	97.51	112.10
1	A	43	THR	N-CA-C	-5.61	95.86	111.00
2	B	219	PRO	CA-N-CD	-5.60	103.67	111.50
7	G	96	GLY	N-CA-C	-5.60	99.11	113.10
16	2	99	LEU	CA-CB-CG	-5.57	102.48	115.30
4	D	87	THR	N-CA-C	5.57	126.03	111.00
6	F	103	GLN	CA-C-N	5.56	129.44	117.20
4	D	140	LEU	CB-CG-CD2	-5.56	101.55	111.00
17	3	128	ILE	N-CA-C	5.56	126.00	111.00
2	B	255	LEU	CA-CB-CG	5.56	128.08	115.30
16	2	169	ALA	N-CA-C	-5.55	96.01	111.00
1	A	254	LEU	CA-CB-CG	-5.54	102.56	115.30
1	A	353	SER	CB-CA-C	-5.53	99.59	110.10
1	A	501	GLY	N-CA-C	-5.52	99.30	113.10
13	N	101	LEU	N-CA-C	-5.51	96.11	111.00
1	A	157	GLY	N-CA-C	-5.50	99.34	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	123	GLY	C-N-CA	-5.50	107.95	121.70
2	B	94	PRO	CA-N-CD	-5.50	103.80	111.50
2	B	623	TYR	N-CA-C	-5.50	96.16	111.00
15	1	86	HIS	N-CA-CB	-5.50	100.71	110.60
16	2	227	LEU	CA-CB-CG	5.49	127.93	115.30
4	D	188	PHE	CB-CG-CD1	-5.49	116.96	120.80
16	2	171	ILE	N-CA-C	-5.49	96.18	111.00
15	1	157	ASP	N-CA-C	5.46	125.74	111.00
16	2	254	LEU	CB-CG-CD1	5.45	120.27	111.00
4	D	142	THR	N-CA-C	-5.44	96.31	111.00
17	3	177	ALA	N-CA-C	-5.43	96.34	111.00
8	H	99	LYS	CA-C-O	-5.43	108.70	120.10
2	B	553	PHE	C-N-CA	-5.41	110.94	122.30
2	B	120	VAL	CB-CA-C	-5.41	101.13	111.40
15	1	172	GLY	CA-C-O	5.41	130.34	120.60
12	L	164	LEU	N-CA-C	5.40	125.58	111.00
12	L	93	VAL	N-CA-C	-5.39	96.43	111.00
1	A	22	VAL	N-CA-C	5.39	125.55	111.00
18	4	238	ASP	C-N-CD	-5.38	108.75	120.60
8	H	117	SER	N-CA-C	5.38	125.53	111.00
16	2	130	GLY	O-C-N	5.37	131.29	122.70
1	A	528	ALA	N-CA-C	5.36	125.48	111.00
8	H	84	PHE	N-CA-C	5.36	125.47	111.00
1	A	131	ILE	N-CA-C	-5.35	96.55	111.00
18	4	211	MET	CB-CA-C	5.35	121.10	110.40
2	B	312	GLY	N-CA-C	5.34	126.46	113.10
17	3	129	PRO	CA-N-CD	-5.33	104.04	111.50
2	B	731	GLY	N-CA-C	-5.33	99.79	113.10
12	L	159	SER	N-CA-C	5.32	125.35	111.00
2	B	605	ASN	N-CA-C	-5.31	96.66	111.00
11	K	57	MET	N-CA-C	-5.31	96.66	111.00
2	B	260	GLY	N-CA-C	5.30	126.36	113.10
16	2	127	THR	N-CA-CB	5.30	120.37	110.30
1	A	353	SER	N-CA-CB	-5.29	102.56	110.50
3	C	69	LEU	N-CA-C	5.29	125.29	111.00
12	L	146	THR	N-CA-CB	5.29	120.35	110.30
1	A	330	ILE	CB-CA-C	-5.29	101.03	111.60
12	L	89	TYR	N-CA-C	5.28	125.25	111.00
5	E	96	ASP	CB-CG-OD1	-5.26	113.56	118.30
13	N	102	ASN	N-CA-C	5.26	125.20	111.00
1	A	118	PRO	N-CA-C	5.25	125.76	112.10
2	B	683	GLU	N-CA-C	-5.25	96.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	SER	C-N-CA	-5.24	111.29	122.30
1	A	23	ASP	N-CA-C	-5.24	96.87	111.00
7	G	77	PHE	N-CA-C	5.24	125.14	111.00
1	A	281	LEU	CB-CG-CD2	-5.23	102.11	111.00
16	2	257	PRO	CA-C-N	5.23	126.66	116.20
17	3	149	ASN	CA-C-N	-5.23	105.70	117.20
3	C	70	TRP	N-CA-C	-5.22	96.91	111.00
15	1	69	LEU	CA-CB-CG	-5.21	103.31	115.30
16	2	172	LEU	N-CA-C	5.21	125.08	111.00
12	L	181	GLY	N-CA-C	-5.21	100.08	113.10
6	F	115	PRO	N-CA-C	5.21	125.64	112.10
2	B	69	ALA	N-CA-C	5.21	125.05	111.00
4	D	185	GLY	N-CA-C	-5.20	100.10	113.10
16	2	256	ASP	C-N-CD	-5.19	109.19	120.60
17	3	216	ASP	N-CA-C	-5.19	96.99	111.00
6	F	81	GLY	N-CA-C	-5.18	100.15	113.10
2	B	507	SER	N-CA-C	5.18	124.98	111.00
2	B	227	THR	N-CA-C	-5.16	97.06	111.00
7	G	131	GLY	N-CA-C	5.16	125.99	113.10
1	A	280	PHE	N-CA-C	5.14	124.88	111.00
1	A	282	THR	N-CA-C	-5.13	97.14	111.00
2	B	498	LEU	N-CA-C	-5.13	97.14	111.00
1	A	342	GLY	N-CA-C	-5.12	100.30	113.10
2	B	681	ALA	N-CA-C	-5.12	97.19	111.00
3	C	62	PHE	N-CA-C	-5.12	97.18	111.00
12	L	74	THR	CB-CA-C	-5.12	97.79	111.60
1	A	540	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	63	ASP	N-CA-C	5.11	124.79	111.00
2	B	486	LEU	CA-CB-CG	5.09	127.02	115.30
2	B	684	ARG	N-CA-C	5.09	124.73	111.00
6	F	97	GLN	N-CA-C	-5.07	97.31	111.00
8	H	76	TYR	N-CA-C	5.07	124.68	111.00
15	1	76	LEU	N-CA-C	-5.07	97.32	111.00
15	1	129	VAL	N-CA-C	5.07	124.68	111.00
17	3	86	PRO	N-CA-C	5.07	125.28	112.10
8	H	121	LEU	CA-CB-CG	5.06	126.94	115.30
16	2	170	ASP	N-CA-C	5.06	124.66	111.00
8	H	81	SER	N-CA-C	-5.05	97.37	111.00
1	A	42	ARG	N-CA-C	5.04	124.61	111.00
16	2	246	PRO	N-CD-CG	-5.04	95.64	103.20
1	A	94	SER	N-CA-C	-5.04	97.40	111.00
11	K	98	PRO	CA-N-CD	-5.04	104.45	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	121	ILE	N-CA-C	-5.03	97.41	111.00
15	1	69	LEU	CA-C-N	5.02	126.25	116.20
8	H	99	LYS	CA-C-N	5.02	128.25	117.20
1	A	95	GLY	C-N-CA	-5.02	109.15	121.70
1	A	154	ARG	NE-CZ-NH2	-5.02	117.79	120.30
15	1	156	LYS	CA-C-N	5.02	128.24	117.20
13	N	143	VAL	C-N-CD	-5.02	109.56	120.60
1	A	193	LEU	CA-CB-CG	5.01	126.81	115.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	77	PHE	CA
8	H	60	ASN	CA
8	H	68	TYR	CA

All (544) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	1	105	TYR	Peptide
15	1	118	PRO	Peptide
15	1	121	GLN	Peptide
15	1	122	ALA	Peptide
15	1	125	LEU	Peptide
15	1	130	PRO	Peptide
15	1	155	GLU	Peptide
15	1	156	LYS	Peptide
15	1	157	ASP	Peptide
15	1	170	PRO	Peptide
15	1	171	LEU	Peptide
15	1	172	GLY	Peptide
15	1	174	SER	Peptide
15	1	176	ASP	Peptide
15	1	178	LYS	Peptide
15	1	179	LYS	Peptide
15	1	184	LYS	Peptide
15	1	185	VAL	Peptide
15	1	204	GLN	Peptide
15	1	205	GLN	Peptide
15	1	206	SER	Peptide
15	1	208	TYR	Peptide
15	1	216	ASN	Peptide

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Mol	Chain	Res	Type	Group
15	1	217	LEU	Peptide
15	1	224	PRO	Peptide,Mainchain
15	1	225	TRP	Peptide
15	1	59	PRO	Peptide
15	1	60	GLY	Peptide
15	1	61	ASP	Peptide
15	1	62	PHE	Peptide
15	1	63	GLY	Peptide,Mainchain
15	1	65	ASP	Peptide
15	1	68	GLY	Mainchain
15	1	69	LEU	Mainchain
15	1	97	ILE	Peptide
16	2	100	ARG	Peptide
16	2	101	TRP	Peptide
16	2	102	ASN	Peptide
16	2	130	GLY	Peptide
16	2	133	ASN	Peptide
16	2	138	TYR	Peptide
16	2	139	THR	Peptide
16	2	140	ALA	Peptide
16	2	142	GLU	Peptide
16	2	166	ARG	Peptide
16	2	170	ASP	Peptide
16	2	172	LEU	Peptide
16	2	174	PRO	Peptide
16	2	177	VAL	Peptide
16	2	178	ASN	Peptide
16	2	181	PRO	Peptide
16	2	184	PRO	Peptide
16	2	189	THR	Peptide
16	2	193	VAL	Peptide
16	2	199	LEU	Peptide
16	2	210	SER	Peptide
16	2	212	GLN	Peptide
16	2	213	LYS	Peptide
16	2	215	LYS	Peptide
16	2	216	GLU	Peptide
16	2	218	ARG	Peptide
16	2	243	GLY	Peptide
16	2	244	THR	Peptide
16	2	245	GLY	Peptide
16	2	246	PRO	Peptide

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Mol	Chain	Res	Type	Group
16	2	247	ILE	Peptide
16	2	248	ASP	Peptide
16	2	250	LEU	Peptide
16	2	252	ALA	Peptide
16	2	255	ALA	Peptide
16	2	256	ASP	Peptide
16	2	257	PRO	Peptide
16	2	261	THR	Peptide
16	2	262	ILE	Peptide
16	2	263	PHE	Peptide
16	2	264	ALA	Peptide
16	2	266	PHE	Peptide
16	2	267	THR	Peptide
16	2	98	SER	Peptide
16	2	99	LEU	Peptide
17	3	110	MET	Peptide
17	3	122	LEU	Peptide
17	3	125	VAL	Peptide
17	3	127	LEU	Peptide
17	3	128	ILE	Peptide
17	3	129	PRO	Peptide
17	3	130	GLN	Peptide
17	3	131	GLU	Peptide
17	3	136	TRP	Peptide
17	3	139	THR	Peptide
17	3	140	GLY	Peptide
17	3	148	TYR	Peptide
17	3	149	ASN	Peptide
17	3	153	ASP	Peptide
17	3	158	PHE	Peptide
17	3	177	ALA	Peptide
17	3	178	LYS	Peptide
17	3	179	PRO	Peptide
17	3	181	SER	Peptide
17	3	188	LEU	Peptide
17	3	189	GLY	Peptide
17	3	193	GLY	Peptide
17	3	196	GLY	Peptide
17	3	197	SER	Peptide
17	3	198	GLY	Peptide
17	3	199	ASN	Peptide
17	3	200	PRO	Peptide

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Mol	Chain	Res	Type	Group
17	3	205	GLY	Peptide
17	3	212	GLY	Peptide
17	3	213	PHE	Peptide
17	3	215	LYS	Peptide
17	3	85	ASP	Peptide
17	3	93	ILE	Peptide
17	3	96	ARG	Peptide
17	3	98	LEU	Peptide
18	4	110	LEU	Peptide
18	4	112	PRO	Peptide
18	4	119	GLY	Peptide
18	4	123	VAL	Peptide
18	4	127	TYR	Peptide
18	4	128	ALA	Peptide
18	4	130	GLY	Peptide
18	4	131	LYS	Peptide
18	4	135	PHE	Peptide
18	4	136	ALA	Peptide
18	4	170	PRO	Peptide
18	4	171	ILE	Peptide
18	4	172	PHE	Peptide
18	4	175	TYR	Peptide,Mainchain
18	4	178	PRO	Peptide
18	4	189	PHE	Peptide
18	4	197	THR	Peptide
18	4	198	LEU	Peptide
18	4	213	ALA	Peptide
18	4	223	VAL	Peptide
18	4	226	LYS	Peptide
18	4	229	PHE	Peptide
18	4	232	LEU	Peptide
18	4	233	LEU	Peptide
18	4	243	THR	Peptide
18	4	86	GLU	Peptide
18	4	89	ARG	Peptide
1	A	103	PHE	Peptide
1	A	114	THR	Peptide
1	A	117	GLY	Peptide
1	A	119	SER	Peptide
1	A	123	VAL	Peptide
1	A	128	GLY	Peptide
1	A	132	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	134	GLY	Peptide
1	A	136	VAL	Peptide
1	A	142	GLY	Peptide
1	A	146	THR	Peptide
1	A	148	GLY	Peptide
1	A	189	ALA	Peptide
1	A	197	GLN	Peptide
1	A	199	VAL	Peptide
1	A	201	SER	Peptide
1	A	21	LEU	Peptide
1	A	22	VAL	Peptide
1	A	23	ASP	Peptide
1	A	240	LYS	Peptide
1	A	246	HIS	Peptide
1	A	25	ASP	Peptide
1	A	250	LEU	Peptide
1	A	251	ASN	Peptide
1	A	257	GLN	Peptide
1	A	26	PRO	Peptide
1	A	262	PHE	Peptide
1	A	263	ALA	Peptide
1	A	27	ILE	Peptide
1	A	270	PHE	Peptide
1	A	274	TRP	Peptide
1	A	275	SER	Peptide
1	A	276	LYS	Peptide
1	A	279	ASP	Peptide
1	A	28	LYS	Peptide
1	A	280	PHE	Peptide
1	A	282	THR	Peptide
1	A	290	LEU	Peptide
1	A	316	MET	Peptide
1	A	345	GLY	Peptide
1	A	346	LEU	Peptide
1	A	349	ILE	Peptide
1	A	352	THR	Peptide
1	A	36	LYS	Peptide
1	A	37	PRO	Peptide
1	A	38	GLY	Peptide
1	A	39	HIS	Peptide
1	A	393	LEU	Peptide
1	A	420	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	427	ARG	Peptide
1	A	430	ASP	Peptide
1	A	45	ALA	Peptide
1	A	46	LYS	Peptide
1	A	47	GLY	Peptide
1	A	482	ILE	Peptide
1	A	483	GLN	Peptide
1	A	486	PRO	Peptide
1	A	488	PHE	Peptide
1	A	497	ALA	Peptide
1	A	501	GLY	Peptide
1	A	505	PRO	Peptide
1	A	506	GLY	Peptide
1	A	510	SER	Peptide
1	A	518	GLY	Peptide
1	A	519	ASP	Peptide
1	A	520	LEU	Peptide
1	A	525	ASN	Peptide
1	A	527	VAL	Peptide
1	A	535	GLY	Peptide
1	A	574	ASN	Peptide
1	A	575	LEU	Peptide
1	A	576	GLY	Peptide
1	A	62	HIS	Peptide
1	A	625	TRP	Peptide
1	A	626	GLY	Peptide
1	A	631	GLN	Peptide
1	A	64	PHE	Peptide
1	A	66	SER	Peptide
1	A	67	HIS	Peptide
1	A	73	GLU	Peptide
1	A	93	LEU	Peptide
2	B	103	ALA	Peptide
2	B	126	THR	Peptide
2	B	130	ARG	Peptide
2	B	135	LEU	Peptide
2	B	139	ALA	Peptide
2	B	162	LYS	Peptide
2	B	166	SER	Peptide
2	B	170	ASN	Peptide
2	B	203	ARG	Peptide
2	B	204	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	B	211	ASN	Peptide
2	B	223	GLY	Peptide
2	B	224	PRO	Peptide
2	B	228	GLY	Peptide
2	B	229	GLN	Peptide
2	B	231	ASN	Peptide
2	B	232	LEU	Peptide
2	B	238	SER	Peptide
2	B	246	THR	Peptide
2	B	248	GLN	Peptide
2	B	256	THR	Peptide
2	B	257	ILE	Peptide
2	B	259	GLY	Peptide
2	B	26	ALA	Peptide
2	B	260	GLY	Peptide
2	B	265	THR	Peptide
2	B	267	SER	Peptide
2	B	292	ARG	Peptide
2	B	298	GLY	Peptide
2	B	303	TYR	Peptide
2	B	308	HIS	Peptide
2	B	311	PRO	Peptide
2	B	320	LYS	Peptide
2	B	33	SER	Peptide
2	B	36	ASP	Peptide
2	B	363	GLN	Peptide
2	B	364	ASP	Peptide
2	B	365	PHE	Peptide
2	B	377	TYR	Peptide
2	B	4	ARG	Peptide
2	B	405	ASP	Peptide
2	B	406	ASN	Peptide
2	B	445	ALA	Peptide
2	B	447	GLY	Peptide
2	B	458	ILE	Peptide
2	B	464	GLN	Peptide
2	B	468	GLY	Peptide
2	B	469	LYS	Peptide
2	B	472	TYR	Peptide
2	B	473	GLY	Peptide
2	B	474	PHE	Peptide
2	B	478	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	B	481	THR	Peptide
2	B	483	GLY	Peptide
2	B	484	PRO	Peptide
2	B	5	ILE	Peptide
2	B	504	ASN	Peptide
2	B	507	SER	Peptide
2	B	510	LEU	Peptide
2	B	540	ASP	Peptide
2	B	549	ASP	Peptide
2	B	563	GLY	Peptide
2	B	595	HIS	Peptide
2	B	602	TRP	Peptide
2	B	603	ARG	Peptide
2	B	604	GLY	Peptide
2	B	605	ASN	Peptide
2	B	606	VAL	Peptide
2	B	618	GLY	Peptide
2	B	627	ASN	Peptide
2	B	632	ILE	Peptide
2	B	633	ASN	Peptide
2	B	635	ILE	Peptide
2	B	641	ASN	Peptide
2	B	69	ALA	Peptide
2	B	690	LEU	Peptide
2	B	7	ARG	Peptide
2	B	73	ASN	Peptide
2	B	730	SER	Peptide
2	B	732	LYS	Peptide
2	B	80	ASP	Peptide
2	B	84	VAL	Peptide
2	B	9	SER	Peptide
3	C	1	MET	Peptide
3	C	27	GLU	Peptide
3	C	28	MET	Peptide
3	C	29	ILE	Peptide
3	C	33	GLY	Peptide
3	C	42	ALA	Peptide
3	C	54	CYS	Peptide
3	C	65	VAL	Peptide
3	C	67	VAL	Peptide
3	C	68	TYR	Peptide
3	C	69	LEU	Peptide

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Mol	Chain	Res	Type	Group
3	C	70	TRP	Peptide
3	C	73	THR	Peptide
3	C	79	LEU	Peptide
4	D	108	LYS	Peptide
4	D	114	MET	Peptide
4	D	117	GLY	Peptide
4	D	118	GLY	Peptide
4	D	119	ALA	Peptide
4	D	124	GLU	Peptide
4	D	125	GLY	Peptide
4	D	145	ARG	Peptide
4	D	147	LYS	Peptide
4	D	150	ILE	Peptide
4	D	151	LYS	Peptide
4	D	158	PHE	Peptide
4	D	161	GLY	Peptide
4	D	162	GLU	Peptide
4	D	163	VAL	Peptide
4	D	168	PRO	Peptide
4	D	171	GLY	Peptide
4	D	174	PRO	Peptide
4	D	177	VAL	Peptide
4	D	181	ARG	Peptide
4	D	182	GLN	Peptide
4	D	184	VAL	Peptide
4	D	190	SER	Peptide
4	D	193	LYS	Peptide
4	D	194	ASN	Peptide
4	D	204	GLY	Peptide
4	D	209	ASP	Peptide
4	D	73	GLU	Peptide
4	D	78	THR	Peptide
4	D	79	PRO	Peptide
4	D	81	PRO	Peptide
4	D	83	PHE	Peptide
4	D	87	THR	Peptide
4	D	89	GLY	Peptide
4	D	91	LEU	Peptide
4	D	93	LYS	Peptide
4	D	97	GLU	Peptide
5	E	116	SER	Peptide
5	E	124	GLU	Peptide

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Mol	Chain	Res	Type	Group
5	E	125	ILE	Peptide
5	E	126	VAL	Mainchain
5	E	127	GLU	Peptide
5	E	67	GLY	Peptide
5	E	79	LYS	Peptide
5	E	88	GLY	Peptide
5	E	96	ASP	Peptide
5	E	97	PRO	Peptide
6	F	103	GLN	Mainchain
6	F	104	ALA	Peptide
6	F	105	SER	Peptide
6	F	107	LYS	Peptide
6	F	108	LEU	Peptide
6	F	111	ASP	Peptide
6	F	112	ASP	Peptide
6	F	115	PRO	Peptide
6	F	116	ALA	Peptide
6	F	118	ALA	Peptide
6	F	129	ARG	Peptide
6	F	133	TYR	Peptide
6	F	135	LYS	Peptide
6	F	137	GLY	Peptide
6	F	138	LEU	Peptide
6	F	151	SER	Peptide
6	F	185	ILE	Peptide
6	F	189	LYS	Peptide
6	F	196	ILE	Peptide
6	F	199	ASP	Peptide
6	F	203	ALA	Peptide
6	F	212	SER	Peptide
6	F	213	TRP	Peptide
6	F	218	TYR	Peptide
6	F	230	ASN	Peptide
6	F	79	ILE	Peptide
6	F	97	GLN	Mainchain
7	G	100	PHE	Peptide
7	G	103	GLY	Peptide
7	G	104	ASP	Peptide
7	G	106	ARG	Peptide
7	G	111	VAL	Peptide
7	G	114	LEU	Peptide
7	G	115	LYS	Peptide

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Mol	Chain	Res	Type	Group
7	G	134	GLY	Peptide
7	G	141	ILE	Peptide
7	G	146	SER	Peptide
7	G	147	ASN	Peptide
7	G	148	GLY	Peptide
7	G	149	TYR	Peptide
7	G	153	PHE	Peptide
7	G	71	SER	Peptide
7	G	78	VAL	Peptide
7	G	82	PHE	Peptide
7	G	84	ARG	Peptide
7	G	86	ASN	Peptide
7	G	90	GLN	Peptide
7	G	91	VAL	Peptide
7	G	95	ASN	Peptide
7	G	98	THR	Peptide
7	G	99	HIS	Peptide
8	H	114	ALA	Peptide
8	H	116	ALA	Peptide
8	H	118	GLY	Peptide
8	H	119	ASP	Peptide
8	H	120	ILE	Peptide
8	H	56	GLU	Peptide
8	H	58	LEU	Peptide
8	H	60	ASN	Peptide
8	H	61	THR	Peptide
8	H	62	THR	Peptide
8	H	63	GLY	Peptide
8	H	65	TRP	Peptide
8	H	67	SER	Peptide
8	H	68	TYR	Peptide
8	H	69	GLY	Peptide
8	H	79	LEU	Peptide
8	H	81	SER	Peptide
8	H	84	PHE	Peptide
8	H	86	THR	Peptide
8	H	93	LYS	Peptide
8	H	95	GLY	Peptide
8	H	97	LEU	Peptide
11	K	113	GLY	Peptide
11	K	118	VAL	Peptide
11	K	119	GLY	Peptide

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Mol	Chain	Res	Type	Group
11	K	120	VAL	Peptide
11	K	122	LEU	Peptide
11	K	123	GLY	Peptide
11	K	125	LYS	Peptide
11	K	126	ASN	Peptide
11	K	128	GLY	Peptide
11	K	129	ALA	Peptide
11	K	73	ALA	Peptide
11	K	76	ALA	Peptide
11	K	80	ALA	Peptide
11	K	86	LEU	Peptide
11	K	88	VAL	Peptide
11	K	89	ARG	Peptide
11	K	91	SER	Peptide
11	K	93	LEU	Peptide
11	K	94	GLN	Peptide
11	K	96	GLY	Peptide
11	K	97	ASP	Peptide
12	L	128	GLN	Peptide
12	L	129	ALA	Peptide
12	L	143	LEU	Peptide
12	L	152	SER	Peptide
12	L	154	ASN	Peptide
12	L	156	GLY	Peptide
12	L	157	ALA	Peptide
12	L	160	THR	Peptide
12	L	165	THR	Peptide
12	L	166	LEU	Peptide
12	L	168	GLY	Peptide
12	L	169	ARG	Peptide
12	L	174	ASP	Peptide
12	L	176	LEU	Peptide
12	L	206	VAL	Peptide
12	L	52	PRO	Peptide
12	L	61	ASN	Peptide
12	L	67	GLY	Peptide
12	L	68	SER	Peptide
12	L	73	VAL	Peptide
12	L	79	ILE	Peptide
12	L	88	ALA	Peptide
12	L	95	PRO	Peptide
13	N	100	GLU	Peptide

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Mol	Chain	Res	Type	Group
13	N	102	ASN	Peptide
13	N	108	ALA	Peptide
13	N	111	GLY	Peptide
13	N	112	ALA	Peptide
13	N	113	ASN	Peptide
13	N	118	TYR	Peptide
13	N	119	THR	Peptide
13	N	120	VAL	Peptide
13	N	123	GLY	Peptide
13	N	125	CYS	Peptide
13	N	126	LYS	Peptide
13	N	127	PHE	Peptide
13	N	129	GLU	Peptide
13	N	131	PHE	Peptide
13	N	133	GLY	Peptide
13	N	135	GLN	Peptide
13	N	136	ASP	Peptide
13	N	137	LEU	Peptide
13	N	142	LYS	Peptide
13	N	145	PHE	Peptide
13	N	147	SER	Peptide
13	N	148	ASP	Peptide
13	N	150	LEU	Peptide
13	N	151	ASP	Peptide
13	N	152	LEU	Peptide
13	N	155	GLU	Peptide
13	N	156	GLY	Peptide
13	N	157	LYS	Peptide
13	N	158	ASP	Peptide
13	N	160	TYR	Peptide
13	N	162	CYS	Peptide
13	N	164	SER	Peptide
13	N	166	VAL	Peptide
13	N	168	TRP	Peptide
13	N	169	LYS	Peptide
13	N	90	GLU	Peptide
13	N	92	LEU	Peptide
13	N	96	LYS	Peptide
13	N	97	THR	Peptide
14	R	28	UNK	Peptide
14	R	30	UNK	Peptide
14	R	31	UNK	Peptide

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Mol	Chain	Res	Type	Group
14	R	32	UNK	Peptide
14	R	33	UNK	Peptide
14	R	34	UNK	Peptide
14	R	36	UNK	Peptide
14	R	37	UNK	Peptide
14	R	40	UNK	Peptide
14	R	42	UNK	Peptide
14	R	46	UNK	Peptide
14	R	47	UNK	Peptide
14	R	48	UNK	Peptide
14	R	50	UNK	Peptide
14	R	51	UNK	Peptide
14	R	52	UNK	Peptide
14	R	7	UNK	Peptide

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	5739	0	5574	1922	6
2	B	5844	0	5648	1926	14
3	C	619	0	605	325	0
4	D	1097	0	1101	436	4
5	E	513	0	514	252	0
6	F	1221	0	1247	373	28
7	G	738	0	709	337	6
8	H	517	0	503	208	2
9	I	229	0	252	53	1
10	J	334	0	344	84	0
11	K	592	0	618	270	5
12	L	1209	0	1220	435	64
13	N	685	0	667	344	0
14	R	265	0	67	79	0
15	1	1257	0	1220	592	37
16	2	1367	0	1312	644	35
17	3	1197	0	1137	516	2
18	4	1309	0	1264	532	45
19	1	665	0	453	123	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2	663	0	494	142	0
19	3	736	0	453	158	0
19	4	729	0	496	154	0
19	A	2676	0	2544	1037	0
19	B	2177	0	2072	680	0
19	F	130	0	85	21	0
19	G	51	0	40	9	0
19	H	240	0	237	61	0
19	I	60	0	58	7	0
19	J	116	0	107	51	0
19	K	210	0	179	40	8
19	L	322	0	275	118	0
19	R	122	0	123	13	0
20	A	33	0	45	9	0
20	B	33	0	46	22	0
21	1	40	0	54	6	0
21	3	40	0	54	6	0
21	A	200	0	271	162	0
21	B	240	0	323	116	0
21	F	80	0	107	61	0
21	I	80	0	111	46	0
21	J	40	0	52	32	0
21	L	40	0	53	34	0
22	1	70	0	92	10	0
22	2	140	0	184	14	0
22	3	70	0	90	38	0
22	4	278	0	357	69	0
22	A	210	0	275	27	0
22	B	95	0	115	11	0
22	C	35	0	46	0	0
22	D	35	0	45	21	0
22	E	70	0	92	24	0
22	F	34	0	41	12	0
22	G	105	0	138	14	0
22	H	245	0	322	40	0
22	K	140	0	184	37	2
22	L	35	0	46	11	0
22	N	35	0	46	9	0
22	R	245	0	322	34	0
23	A	8	0	0	2	0
23	C	16	0	0	9	0
24	B	49	0	71	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	36370	0	35200	10756	130

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 150.

All (10756) 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)
22:4:7034:LMU:C9	22:4:7052:LMU:H1'	1.24	1.64
2:B:459:PHE:CE2	19:B:1235:CLA:C2D	1.76	1.63
19:A:1125:CLA:HBB2	19:A:1133:CLA:CMA	1.18	1.60
1:A:244:LEU:CB	1:A:247:GLU:HG3	1.25	1.60
16:2:130:GLY:CA	16:2:131:ILE:HG13	1.29	1.60
2:B:459:PHE:CD2	19:B:1235:CLA:C3D	1.79	1.59
1:A:21:LEU:CA	1:A:22:VAL:HG12	1.16	1.59
15:1:177:PRO:HD2	15:1:180:LEU:CG	1.13	1.58
1:A:281:LEU:HD13	19:A:1115:CLA:CED	1.24	1.57
19:2:2007:CLA:CBC	19:3:2009:CLA:HED2	1.11	1.57
5:E:89:SER:HB2	5:E:106:ARG:CZ	1.28	1.56
16:2:130:GLY:HA2	16:2:131:ILE:CG1	1.29	1.56
22:4:7034:LMU:C8	22:4:7052:LMU:H2'	1.09	1.56
18:4:158:GLN:HB3	19:4:1004:CLA:CMA	1.12	1.56
2:B:459:PHE:HD2	19:B:1235:CLA:C3D	0.91	1.56
22:4:7034:LMU:H81	22:4:7052:LMU:C2'	1.23	1.56
8:H:61:THR:CA	8:H:62:THR:HG23	1.36	1.55
13:N:130:ASN:CB	13:N:139:LYS:HG2	1.36	1.55
15:1:177:PRO:CD	15:1:180:LEU:HG	1.08	1.55
15:1:93:ALA:HB1	19:1:1006:CLA:CHC	1.34	1.54
18:4:120:ILE:CD1	18:4:226:LYS:HG3	1.12	1.54
3:C:44:ARG:NH2	4:D:181:ARG:CD	1.68	1.54
18:4:120:ILE:HD11	18:4:226:LYS:CG	1.24	1.54
13:N:103:ASP:HB2	13:N:107:LEU:CD1	1.35	1.52
18:4:103:MET:CE	18:4:208:GLY:N	1.71	1.52
18:4:103:MET:HE2	18:4:208:GLY:CA	1.38	1.52
19:A:1125:CLA:CBB	19:A:1133:CLA:HMA2	1.04	1.52
17:3:103:VAL:HG13	17:3:107:ARG:CD	1.36	1.51
2:B:459:PHE:CD2	19:B:1235:CLA:C2D	1.82	1.51
8:H:58:LEU:CD1	8:H:62:THR:HG21	1.38	1.51
14:R:32:UNK:CB	14:R:33:UNK:CB	1.85	1.51
15:1:97:ILE:HD13	15:1:98:LEU:CA	1.10	1.51
17:3:113:ALA:CB	17:3:239:LEU:HD11	1.34	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:103:MET:CE	18:4:208:GLY:CA	1.88	1.51
2:B:314:ARG:NH1	15:1:67:LEU:HD21	1.22	1.50
18:4:172:PHE:CB	18:4:194:PHE:HE2	0.89	1.50
18:4:158:GLN:CB	19:4:1004:CLA:HMA3	1.37	1.50
8:H:61:THR:HA	8:H:62:THR:CG2	1.37	1.50
1:A:244:LEU:HB2	1:A:247:GLU:CG	1.40	1.49
18:4:172:PHE:HB2	18:4:194:PHE:CE2	1.00	1.49
6:F:190:LYS:NZ	6:F:192:THR:HG21	1.18	1.49
1:A:250:LEU:HB2	17:3:136:TRP:CH2	1.47	1.49
15:1:97:ILE:CD1	15:1:98:LEU:N	1.69	1.49
15:1:97:ILE:CD1	15:1:98:LEU:CA	1.85	1.49
19:1:1013:CLA:C6	19:1:1014:CLA:HED3	1.41	1.48
1:A:281:LEU:CD1	19:A:1115:CLA:HED1	1.41	1.47
3:C:62:PHE:CZ	5:E:80:GLU:CD	1.88	1.47
19:L:1148:CLA:HED1	19:L:1148:CLA:C2	1.38	1.47
13:N:103:ASP:CB	13:N:107:LEU:HD12	1.43	1.47
1:A:443:ILE:HD11	1:A:557:LEU:CD2	1.41	1.46
13:N:155:GLU:HB3	13:N:157:LYS:N	1.21	1.46
17:3:135:ALA:HB1	17:3:139:THR:CB	1.44	1.46
17:3:127:LEU:CB	19:3:1147:CLA:HED3	1.45	1.45
4:D:156:ARG:NH1	4:D:158:PHE:HE1	0.97	1.45
1:A:249:ILE:CG2	17:3:136:TRP:HZ3	1.25	1.45
22:4:7034:LMU:H92	22:4:7052:LMU:C1'	1.42	1.45
2:B:123:TRP:HA	2:B:126:THR:CG2	1.44	1.44
2:B:596:TRP:CH2	2:B:612:SER:O	1.68	1.44
2:B:89:HIS:C	2:B:113:VAL:HG11	1.10	1.44
2:B:294:ASN:ND2	7:G:94:GLN:HG3	1.25	1.44
8:H:58:LEU:CD1	8:H:62:THR:CG2	1.91	1.44
17:3:122:LEU:CD2	19:3:3006:CLA:CHA	1.94	1.44
18:4:87:ASN:HB2	18:4:90:TRP:CE3	1.51	1.44
19:4:4006:CLA:C10	22:4:7034:LMU:H121	1.47	1.44
1:A:308:ILE:CD1	19:A:1115:CLA:HHC	1.47	1.43
15:1:176:ASP:HB3	15:1:180:LEU:CD1	1.46	1.43
16:2:160:ILE:CG2	19:2:2012:CLA:CBB	1.95	1.43
2:B:633:ASN:CB	2:B:636:THR:HB	1.48	1.43
21:B:6020:BCR:C33	19:L:1502:CLA:C4B	1.95	1.43
13:N:146:LEU:CD1	17:3:142:ILE:O	1.66	1.43
16:2:133:ASN:ND2	16:2:134:THR:HB	1.28	1.43
17:3:103:VAL:CG1	17:3:107:ARG:HD3	1.47	1.42
18:4:175:TYR:O	18:4:194:PHE:CE1	1.69	1.42
22:3:7003:LMU:H3B	22:3:7005:LMU:C5B	1.46	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:CYS:HA	3:C:17:CYS:SG	1.58	1.41
4:D:167:HIS:NE2	4:D:172:VAL:HG11	1.12	1.41
6:F:190:LYS:NZ	6:F:192:THR:CG2	1.82	1.41
16:2:133:ASN:HD22	16:2:134:THR:CB	1.33	1.41
19:2:2007:CLA:CBC	19:3:2009:CLA:CED	1.95	1.40
4:D:167:HIS:NE2	4:D:172:VAL:CG1	1.84	1.40
16:2:168:TRP:HD1	16:2:171:ILE:CG2	1.35	1.40
1:A:154:ARG:NE	1:A:384:TYR:HE1	1.19	1.40
19:A:1115:CLA:CED	19:A:1115:CLA:H2A	1.49	1.39
11:K:92:GLY:O	11:K:93:LEU:HG	1.22	1.39
13:N:139:LYS:CB	13:N:142:LYS:HD3	1.50	1.39
17:3:150:TYR:CG	17:3:151:TRP:CD1	2.10	1.39
1:A:338:PHE:CE1	19:A:1151:CLA:CBB	2.06	1.39
1:A:478:SER:CB	1:A:644:GLN:HE22	1.35	1.39
16:2:122:ILE:HD11	19:2:2002:CLA:CAB	1.51	1.39
16:2:166:ARG:N	16:2:167:ARG:HB2	1.21	1.39
1:A:342:GLY:CA	1:A:430:ASP:HB2	1.48	1.39
2:B:257:ILE:O	2:B:497:TRP:CE3	1.75	1.39
2:B:247:THR:HA	2:B:250:ALA:CB	1.52	1.39
13:N:155:GLU:C	13:N:157:LYS:CE	1.90	1.39
1:A:21:LEU:N	1:A:22:VAL:CG1	1.83	1.38
22:4:7034:LMU:H111	22:4:7052:LMU:C4'	1.38	1.38
16:2:160:ILE:HG22	19:2:2012:CLA:CBB	1.52	1.38
17:3:127:LEU:CB	19:3:1147:CLA:CED	2.01	1.38
1:A:534:LEU:HD12	1:A:535:GLY:N	1.31	1.38
13:N:155:GLU:CB	13:N:157:LYS:H	1.37	1.38
1:A:21:LEU:CA	1:A:22:VAL:CG1	1.98	1.37
15:1:176:ASP:CB	15:1:180:LEU:HD12	1.54	1.37
1:A:21:LEU:HA	1:A:22:VAL:CG1	1.54	1.37
1:A:249:ILE:HG23	17:3:136:TRP:CZ3	1.60	1.37
13:N:130:ASN:HB2	13:N:139:LYS:CG	1.51	1.37
16:2:168:TRP:CD1	16:2:171:ILE:HG21	1.59	1.37
18:4:158:GLN:NE2	19:4:1004:CLA:C1A	1.87	1.37
16:2:118:ALA:HA	16:2:121:PHE:CE2	1.60	1.36
1:A:279:ASP:O	1:A:281:LEU:HG	1.24	1.36
2:B:459:PHE:HE2	19:B:1235:CLA:C1D	1.39	1.36
2:B:732:LYS:HG2	2:B:734:GLY:N	1.34	1.36
12:L:205:TYR:CD1	12:L:207:LEU:HD12	1.61	1.36
13:N:132:THR:CG2	13:N:139:LYS:HD3	1.55	1.36
19:3:1147:CLA:CBC	19:3:1147:CLA:HMC1	1.46	1.36
22:3:7003:LMU:H3B	22:3:7005:LMU:C4B	1.52	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:VAL:HA	2:B:123:TRP:CD1	1.61	1.35
17:3:150:TYR:N	17:3:152:ALA:HB2	1.40	1.35
19:3:2009:CLA:HBD	19:3:2009:CLA:CGA	1.56	1.35
7:G:98:THR:CB	7:G:101:GLU:CD	1.95	1.34
19:3:2009:CLA:H92	19:3:2009:CLA:C5	1.45	1.34
3:C:44:ARG:NH2	4:D:181:ARG:HD3	1.04	1.34
1:A:308:ILE:HD11	19:A:1115:CLA:CAB	1.56	1.34
4:D:114:MET:CG	4:D:115:PRO:O	1.76	1.34
15:1:67:LEU:HD12	15:1:68:GLY:N	1.41	1.34
18:4:103:MET:CE	18:4:208:GLY:HA2	1.49	1.34
7:G:89:LYS:HA	7:G:89:LYS:CE	1.55	1.33
20:B:5002:PQN:H162	21:B:6017:BCR:C33	1.54	1.33
13:N:114:PHE:CD1	13:N:117:ALA:HB2	1.62	1.33
16:2:118:ALA:CA	16:2:121:PHE:HE2	1.40	1.33
16:2:134:THR:OG1	16:2:135:PRO:HD2	1.22	1.33
1:A:744:ALA:CB	21:A:6011:BCR:H391	1.59	1.32
3:C:64:SER:O	3:C:65:VAL:HG12	1.16	1.32
18:4:145:GLU:HG3	18:4:146:PHE:CD1	1.62	1.32
19:A:1119:CLA:H92	21:A:6007:BCR:C37	1.57	1.32
4:D:140:LEU:CD1	4:D:141:GLY:N	1.92	1.32
5:E:89:SER:OG	5:E:106:ARG:CD	1.78	1.32
19:L:1148:CLA:CED	19:L:1148:CLA:H2	1.57	1.32
2:B:304:ILE:CD1	19:B:1216:CLA:HED2	1.59	1.31
17:3:150:TYR:CD2	17:3:151:TRP:CD1	2.18	1.31
5:E:89:SER:OG	5:E:106:ARG:HD3	1.28	1.31
7:G:98:THR:HG21	7:G:101:GLU:OE2	1.18	1.31
19:L:1148:CLA:HAA1	19:L:1148:CLA:CGD	1.60	1.31
15:1:91:MET:O	15:1:95:PRO:HD3	1.20	1.31
16:2:186:ASN:OD1	16:2:188:LEU:HD11	1.27	1.31
2:B:36:ASP:O	2:B:41:ARG:NH1	1.63	1.31
3:C:62:PHE:CE2	5:E:80:GLU:HG3	1.65	1.31
16:2:117:ALA:CB	16:2:230:LEU:HG	1.58	1.31
1:A:120:ALA:H	1:A:145:ILE:CD1	1.41	1.30
19:A:1115:CLA:HED3	19:A:1115:CLA:C2A	1.61	1.30
2:B:257:ILE:O	2:B:497:TRP:CZ3	1.84	1.30
8:H:78:PRO:HD3	19:L:1501:CLA:CMD	1.61	1.30
17:3:113:ALA:HB2	17:3:239:LEU:CD1	1.62	1.30
15:1:189:LYS:CG	19:1:1007:CLA:HMC2	1.62	1.30
16:2:165:GLY:C	16:2:167:ARG:HB2	1.50	1.30
17:3:111:LEU:O	17:3:114:VAL:N	1.65	1.30
1:A:338:PHE:CE1	19:A:1151:CLA:HBB1	1.65	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:155:GLU:C	13:N:157:LYS:HE2	1.49	1.29
21:B:6020:BCR:H333	19:L:1502:CLA:C4B	1.56	1.29
15:1:88:ARG:O	15:1:92:LEU:HB2	1.28	1.29
2:B:732:LYS:HG2	2:B:733:PHE:C	1.52	1.29
1:A:281:LEU:CD2	19:A:1115:CLA:CMA	2.07	1.29
19:K:1143:CLA:CAC	22:K:7001:LMU:O3B	1.79	1.29
17:3:150:TYR:CD2	17:3:151:TRP:NE1	2.01	1.29
16:2:96:PRO:HD2	17:3:85:ASP:OD2	1.30	1.29
1:A:21:LEU:N	1:A:22:VAL:HG12	0.99	1.28
7:G:98:THR:CG2	7:G:101:GLU:OE2	1.77	1.28
8:H:119:ASP:O	8:H:120:ILE:HG22	1.24	1.28
12:L:154:ASN:O	12:L:178:THR:HG23	1.18	1.28
13:N:132:THR:HG21	13:N:139:LYS:CD	1.62	1.28
1:A:246:HIS:HA	1:A:248:PHE:CE2	1.67	1.28
19:3:2009:CLA:H52	19:3:2009:CLA:C9	1.54	1.28
1:A:157:GLY:HA3	1:A:229:ILE:CG2	1.60	1.28
1:A:668:TYR:CD1	2:B:445:ALA:HB2	1.68	1.28
2:B:122:GLN:O	2:B:126:THR:CB	1.80	1.28
16:2:134:THR:OG1	16:2:135:PRO:CD	1.80	1.28
19:2:2007:CLA:HAC2	19:3:2009:CLA:CED	1.62	1.28
4:D:140:LEU:HD12	4:D:141:GLY:N	0.95	1.27
18:4:167:ASN:OD1	19:4:4014:CLA:C2	1.80	1.27
2:B:229:GLN:C	7:G:63:VAL:HG21	1.55	1.27
11:K:49:ILE:O	11:K:52:PRO:CG	1.80	1.27
11:K:49:ILE:O	11:K:52:PRO:HG2	1.14	1.27
22:4:7034:LMU:C11	22:4:7052:LMU:C4'	2.12	1.27
1:A:157:GLY:O	1:A:158:ILE:CG2	1.79	1.27
1:A:162:LEU:O	1:A:165:TYR:HB3	1.34	1.27
1:A:368:LEU:HD21	19:A:1117:CLA:C9	1.63	1.27
4:D:123:ARG:NH2	22:D:7050:LMU:C4B	1.98	1.27
4:D:156:ARG:NH1	4:D:158:PHE:CE1	1.74	1.27
5:E:89:SER:CB	5:E:106:ARG:CZ	2.11	1.27
15:1:95:PRO:O	15:1:98:LEU:HB3	1.30	1.27
19:2:2007:CLA:CAC	19:3:2009:CLA:CED	2.11	1.27
2:B:317:ARG:NH1	2:B:405:ASP:O	1.68	1.27
7:G:72:LEU:HD23	7:G:124:ILE:CD1	1.65	1.27
12:L:129:ALA:O	12:L:201:TYR:HB3	1.35	1.27
15:1:77:GLU:HA	15:1:80:LYS:CG	1.65	1.27
15:1:97:ILE:HD13	15:1:98:LEU:N	0.94	1.27
1:A:744:ALA:HB2	21:A:6011:BCR:C39	1.64	1.26
5:E:107:PHE:CE2	5:E:109:LYS:HG3	1.69	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:209:LEU:CD1	12:L:210:PRO:HD2	1.64	1.26
17:3:109:ALA:C	17:3:111:LEU:HB3	1.55	1.26
12:L:60:ILE:CG2	12:L:61:ASN:H	1.43	1.26
1:A:242:ILE:HG13	1:A:243:PRO:CD	1.65	1.26
4:D:123:ARG:NH2	22:D:7050:LMU:O4'	1.67	1.26
15:1:95:PRO:O	15:1:98:LEU:CB	1.83	1.26
16:2:130:GLY:CA	16:2:131:ILE:CG1	1.97	1.26
4:D:167:HIS:CD2	4:D:172:VAL:HG21	1.68	1.26
6:F:200:VAL:CG1	10:J:7:TYR:HB2	1.65	1.26
7:G:98:THR:HB	7:G:101:GLU:CD	1.54	1.26
2:B:232:LEU:CD1	2:B:235:GLN:HG3	1.66	1.26
2:B:317:ARG:NH2	2:B:410:ARG:HG2	1.49	1.26
2:B:459:PHE:CE2	19:B:1235:CLA:CMD	2.18	1.26
4:D:200:VAL:HG21	4:D:206:GLN:NE2	1.48	1.26
13:N:155:GLU:O	13:N:157:LYS:HE3	1.22	1.26
1:A:242:ILE:CG1	1:A:243:PRO:HD3	1.64	1.25
2:B:160:LYS:HD3	2:B:161:TRP:CE2	1.70	1.25
16:2:226:ARG:HD2	16:2:230:LEU:CD2	1.67	1.25
17:3:103:VAL:HG13	17:3:107:ARG:NE	1.49	1.25
2:B:403:ASN:O	2:B:406:ASN:HB3	1.34	1.25
3:C:5:VAL:CG2	3:C:65:VAL:HG23	1.66	1.25
11:K:127:ILE:C	11:K:129:ALA:HA	1.56	1.25
19:B:1209:CLA:HAC2	19:B:1210:CLA:CBB	1.65	1.25
19:B:1209:CLA:CAC	19:B:1210:CLA:HBB2	1.65	1.25
8:H:76:TYR:OH	12:L:90:ARG:NE	1.68	1.25
13:N:139:LYS:CG	13:N:142:LYS:HD3	1.66	1.24
1:A:281:LEU:CD1	19:A:1115:CLA:CED	2.00	1.24
4:D:156:ARG:CZ	4:D:158:PHE:HE1	1.48	1.24
2:B:5:ILE:HG22	2:B:6:PRO:CD	1.67	1.24
16:2:254:LEU:HD22	16:2:255:ALA:N	1.49	1.24
11:K:49:ILE:C	11:K:52:PRO:CG	2.05	1.24
18:4:146:PHE:HZ	19:4:4013:CLA:C4C	1.50	1.24
19:A:9012:CLA:H11	2:B:616:LEU:CD1	1.66	1.24
7:G:98:THR:HB	7:G:101:GLU:OE1	1.15	1.23
1:A:284:ARG:HA	1:A:284:ARG:NH1	1.50	1.23
2:B:36:ASP:O	2:B:41:ARG:CZ	1.86	1.23
2:B:225:LEU:HD13	2:B:233:TYR:OH	1.33	1.23
7:G:72:LEU:CD2	7:G:124:ILE:CD1	2.15	1.23
8:H:76:TYR:OH	12:L:90:ARG:CD	1.84	1.23
19:A:1119:CLA:C9	21:A:6007:BCR:H373	1.67	1.23
16:2:148:ASP:CB	16:2:152:LEU:HB3	1.64	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:7034:LMU:C11	22:4:7052:LMU:H4'	1.67	1.23
4:D:114:MET:HG3	4:D:115:PRO:O	1.30	1.22
17:3:96:ARG:HA	17:3:99:ALA:CB	1.67	1.22
1:A:154:ARG:NE	1:A:384:TYR:CE1	2.08	1.22
4:D:80:SER:OG	4:D:126:PRO:HD2	1.06	1.22
5:E:106:ARG:NH2	5:E:107:PHE:HA	1.51	1.22
7:G:98:THR:CB	7:G:101:GLU:OE1	1.86	1.22
15:1:157:ASP:HB2	15:1:178:LYS:CA	1.69	1.22
6:F:190:LYS:HZ2	6:F:192:THR:CG2	1.42	1.22
7:G:149:TYR:HA	7:G:150:ASP:OD1	1.36	1.22
16:2:122:ILE:CD1	19:2:2002:CLA:C3B	2.16	1.22
22:3:7003:LMU:C3B	22:3:7005:LMU:H4B	1.68	1.22
19:A:1237:CLA:H141	12:L:141:LEU:CD2	1.68	1.22
6:F:107:LYS:O	6:F:108:LEU:HD12	1.05	1.22
15:1:78:ARG:HH21	15:1:179:LYS:CD	1.52	1.22
17:3:122:LEU:HD22	19:3:3006:CLA:CHA	1.60	1.22
2:B:469:LYS:CD	2:B:470:THR:HA	1.70	1.21
2:B:558:PRO:CB	2:B:703:VAL:HG22	1.69	1.21
12:L:72:PRO:O	12:L:73:VAL:HG22	1.36	1.21
16:2:133:ASN:ND2	16:2:134:THR:CB	1.94	1.21
19:A:1122:CLA:CHD	21:A:6007:BCR:H19C	1.68	1.21
6:F:100:LYS:O	6:F:103:GLN:HB3	1.38	1.21
19:1:1006:CLA:CAB	19:1:1013:CLA:HBC2	1.70	1.21
16:2:165:GLY:C	16:2:167:ARG:CB	2.09	1.21
18:4:103:MET:CE	18:4:207:ASN:C	2.09	1.21
18:4:169:ASP:O	18:4:173:LYS:HG2	1.36	1.21
2:B:73:ASN:O	2:B:121:TYR:OH	1.55	1.21
2:B:294:ASN:ND2	7:G:94:GLN:CG	2.02	1.21
4:D:162:GLU:O	4:D:163:VAL:HG23	1.37	1.21
19:A:1140:CLA:H141	21:A:6011:BCR:C2	1.71	1.21
2:B:398:TYR:O	4:D:197:PRO:HG2	1.37	1.21
15:1:95:PRO:HA	15:1:98:LEU:HG	1.22	1.21
1:A:250:LEU:HB2	17:3:136:TRP:CZ2	1.73	1.21
2:B:315:LEU:CD1	2:B:317:ARG:HG2	1.71	1.21
2:B:429:LEU:O	2:B:525:LEU:HD12	1.36	1.21
21:I:6021:BCR:H313	21:I:6021:BCR:C8	1.51	1.21
22:4:7034:LMU:C9	22:4:7052:LMU:C1'	2.07	1.21
2:B:123:TRP:CA	2:B:126:THR:HG22	1.68	1.20
16:2:240:ILE:CG2	16:2:263:PHE:HB3	1.70	1.20
17:3:111:LEU:CG	17:3:112:GLY:H	1.38	1.20
17:3:130:GLN:HB3	17:3:132:THR:N	1.56	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:130:GLN:CB	17:3:132:THR:H	1.55	1.20
17:3:197:SER:CB	17:3:206:PRO:HD3	1.70	1.20
19:A:1105:CLA:C3B	21:J:6012:BCR:H331	1.71	1.20
11:K:115:ILE:HG12	11:K:122:LEU:N	1.55	1.20
17:3:113:ALA:CB	17:3:239:LEU:CD1	2.15	1.20
17:3:150:TYR:CB	17:3:151:TRP:CD1	2.22	1.20
18:4:159:ASP:OD1	18:4:171:ILE:HD11	1.04	1.20
22:4:7034:LMU:H111	22:4:7052:LMU:C3'	1.70	1.20
1:A:702:GLU:OE2	2:B:550:LYS:NZ	1.74	1.20
6:F:99:LEU:O	6:F:102:LEU:HG	1.35	1.20
15:1:190:ASN:HD21	19:1:1002:CLA:C1A	1.53	1.20
18:4:103:MET:HE1	18:4:207:ASN:C	1.58	1.20
2:B:596:TRP:HH2	2:B:612:SER:O	0.94	1.20
11:K:84:LEU:HG	11:K:85:LYS:HG2	1.24	1.20
16:2:96:PRO:CD	17:3:85:ASP:OD2	1.90	1.20
18:4:172:PHE:CB	18:4:194:PHE:CE2	1.76	1.20
1:A:223:VAL:HG23	1:A:227:LEU:CD1	1.70	1.20
11:K:113:GLY:O	11:K:116:ILE:HG22	1.41	1.20
18:4:89:ARG:HD3	18:4:90:TRP:N	1.54	1.20
18:4:158:GLN:OE1	19:4:1004:CLA:O1D	1.55	1.20
18:4:165:SER:O	18:4:168:GLN:HG3	1.06	1.20
4:D:123:ARG:NH2	22:D:7050:LMU:C6B	2.00	1.19
19:B:1235:CLA:H93	19:B:1235:CLA:CBB	1.72	1.19
5:E:89:SER:CB	5:E:106:ARG:NE	2.06	1.19
11:K:127:ILE:CA	11:K:130:LEU:HG	1.71	1.19
16:2:118:ALA:O	16:2:121:PHE:CE2	1.96	1.19
1:A:575:LEU:HD12	1:A:576:GLY:N	1.56	1.19
3:C:17:CYS:HB2	3:C:58:CYS:SG	1.83	1.19
11:K:115:ILE:HA	11:K:118:VAL:CG2	1.72	1.19
2:B:294:ASN:HB2	7:G:94:GLN:CD	1.62	1.19
14:R:41:UNK:CB	14:R:42:UNK:HA	1.70	1.19
17:3:185:GLN:HG2	17:3:186:TYR:N	1.45	1.19
18:4:177:LEU:CD1	18:4:178:PRO:HD3	1.69	1.19
2:B:459:PHE:CE2	19:B:1235:CLA:C1D	2.17	1.19
15:1:157:ASP:HB2	15:1:178:LYS:CB	1.73	1.19
17:3:135:ALA:HB1	17:3:139:THR:OG1	1.40	1.19
12:L:92:ALA:H	12:L:98:ARG:NH1	1.39	1.18
15:1:150:HIS:CD2	15:1:151:GLN:HE22	1.61	1.18
17:3:95:PRO:O	17:3:96:ARG:HG2	1.36	1.18
17:3:192:LYS:CE	17:3:192:LYS:HA	1.66	1.18
1:A:668:TYR:CG	2:B:445:ALA:HB2	1.77	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:LEU:HD12	8:H:61:THR:CB	1.73	1.18
14:R:52:UNK:HA	14:R:53:UNK:CB	1.68	1.18
15:1:149:GLU:HG2	15:1:152:ARG:NH1	1.55	1.18
17:3:150:TYR:H	17:3:152:ALA:CB	1.56	1.18
1:A:425:THR:CB	1:A:428:TYR:HE1	1.55	1.18
1:A:715:LYS:HD2	6:F:230:ASN:ND2	1.58	1.18
3:C:69:LEU:HD13	3:C:70:TRP:O	1.44	1.18
6:F:185:ILE:O	6:F:186:ARG:HG2	1.44	1.18
1:A:113:PRO:O	1:A:114:THR:HG22	1.43	1.18
21:B:6020:BCR:C33	19:L:1502:CLA:CHC	2.22	1.18
15:1:177:PRO:HD2	15:1:180:LEU:CB	1.73	1.18
1:A:21:LEU:HD12	1:A:21:LEU:O	1.39	1.18
1:A:545:HIS:CG	19:A:1135:CLA:HBB2	1.79	1.18
2:B:440:ASN:OD1	2:B:614:THR:CG2	1.91	1.18
4:D:86:SER:O	12:L:67:GLY:HA3	1.42	1.18
12:L:205:TYR:CD1	12:L:207:LEU:CD1	2.25	1.18
13:N:142:LYS:HA	13:N:142:LYS:HE3	1.18	1.18
15:1:78:ARG:HD3	19:1:1011:CLA:HMC2	1.25	1.18
1:A:281:LEU:HD13	19:A:1115:CLA:HED2	1.22	1.17
2:B:123:TRP:CA	2:B:126:THR:CG2	2.21	1.17
19:B:1220:CLA:H151	19:B:1220:CLA:H102	1.24	1.17
11:K:81:THR:HG23	11:K:83:GLY:H	1.02	1.17
19:L:1503:CLA:HBC3	19:L:1503:CLA:HHD	1.18	1.17
13:N:99:LYS:HA	13:N:102:ASN:OD1	1.44	1.17
13:N:103:ASP:CB	13:N:107:LEU:CD1	2.07	1.17
16:2:184:PRO:HD3	16:2:187:LYS:CB	1.74	1.17
1:A:223:VAL:CG2	1:A:227:LEU:HD12	1.71	1.17
1:A:281:LEU:CD2	19:A:1115:CLA:HMA2	1.69	1.17
1:A:351:THR:O	19:A:1123:CLA:H191	1.43	1.17
2:B:247:THR:CG2	2:B:248:GLN:H	1.56	1.17
8:H:58:LEU:CD1	8:H:61:THR:HB	1.74	1.17
11:K:49:ILE:C	11:K:52:PRO:CD	2.12	1.17
12:L:153:PHE:HA	12:L:179:ALA:HB2	1.24	1.17
16:2:182:ILE:HB	16:2:187:LYS:CB	1.72	1.17
17:3:98:LEU:HD11	19:3:3012:CLA:C2D	1.75	1.17
22:A:7016:LMU:H21	22:A:7016:LMU:H81	1.24	1.17
6:F:127:LYS:C	6:F:129:ARG:H	1.39	1.17
1:A:342:GLY:HA3	1:A:430:ASP:CB	1.75	1.17
19:A:1115:CLA:HMC1	19:A:1115:CLA:HBC3	1.25	1.17
4:D:140:LEU:HD21	4:D:144:LEU:HD12	1.26	1.17
19:K:1143:CLA:HAC2	22:K:7001:LMU:O3B	1.39	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:229:MET:SD	16:2:230:LEU:HD22	1.85	1.17
19:3:3008:CLA:HBA2	19:3:3008:CLA:CBD	1.75	1.17
18:4:159:ASP:OD1	18:4:171:ILE:CD1	1.92	1.17
18:4:158:GLN:CB	19:4:1004:CLA:CMA	2.03	1.16
1:A:24:ARG:HD2	1:A:24:ARG:N	1.60	1.16
19:B:1218:CLA:HBC2	19:B:1218:CLA:HHD	1.27	1.16
11:K:49:ILE:CA	11:K:52:PRO:HG3	1.73	1.16
15:1:92:LEU:O	15:1:95:PRO:HD2	1.41	1.16
19:4:4002:CLA:HMA2	19:4:4002:CLA:HBA1	1.20	1.16
19:A:1122:CLA:C4C	21:A:6007:BCR:H19C	1.75	1.16
19:A:1124:CLA:H72	19:A:1125:CLA:CED	1.76	1.16
3:C:44:ARG:NH2	4:D:181:ARG:CG	2.08	1.16
6:F:127:LYS:O	6:F:129:ARG:N	1.77	1.16
9:I:7:LEU:HD12	21:I:6021:BCR:H333	1.17	1.16
15:1:93:ALA:CB	19:1:1006:CLA:CHC	2.22	1.16
16:2:226:ARG:HD2	16:2:230:LEU:HD21	1.19	1.16
1:A:423:ASP:HB3	1:A:424:PRO:HG3	1.20	1.16
2:B:633:ASN:HB2	2:B:636:THR:CB	1.76	1.16
4:D:111:ILE:HG12	4:D:121:ILE:HG22	1.22	1.16
22:E:7048:LMU:C4B	22:F:7036:LMU:H6E	1.74	1.16
6:F:200:VAL:HG12	10:J:7:TYR:HB2	1.17	1.16
12:L:92:ALA:H	12:L:98:ARG:CZ	1.58	1.16
16:2:195:TYR:CD1	16:2:196:PRO:HD2	1.81	1.16
17:3:197:SER:OG	17:3:205:GLY:HA3	1.46	1.16
18:4:158:GLN:HE22	19:4:1004:CLA:C1A	1.51	1.16
18:4:228:PRO:HB2	18:4:229:PHE:CD1	1.80	1.16
1:A:217:SER:OG	21:A:6002:BCR:H15C	1.42	1.16
2:B:216:LEU:HD23	2:B:218:TYR:O	1.44	1.16
2:B:293:THR:HG22	7:G:94:GLN:CD	1.64	1.16
6:F:99:LEU:HA	6:F:102:LEU:HD23	1.28	1.16
19:J:1308:CLA:HHD	19:J:1308:CLA:CBC	1.74	1.16
13:N:114:PHE:CG	13:N:117:ALA:HB2	1.80	1.16
15:1:189:LYS:CB	19:1:1007:CLA:HMC2	1.75	1.16
19:3:3011:CLA:HMA2	19:3:3011:CLA:H12	1.24	1.16
15:1:171:LEU:HA	15:1:173:TYR:CE2	1.80	1.15
16:2:125:PHE:CA	16:2:127:THR:HG23	1.76	1.15
16:2:177:VAL:HG12	16:2:178:ASN:HB2	1.18	1.15
16:2:269:LYS:HA	16:2:269:LYS:NZ	1.59	1.15
4:D:114:MET:HG3	4:D:115:PRO:C	1.67	1.15
21:I:6021:BCR:HC8	21:I:6021:BCR:C31	1.74	1.15
11:K:127:ILE:HA	11:K:130:LEU:HG	1.22	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:1143:CLA:CBC	22:K:7001:LMU:O3B	1.95	1.15
13:N:139:LYS:HA	13:N:142:LYS:NZ	1.62	1.15
17:3:122:LEU:HD21	19:3:3006:CLA:CHA	1.65	1.15
18:4:169:ASP:C	18:4:173:LYS:HA	1.67	1.15
18:4:177:LEU:CG	18:4:178:PRO:HD3	1.75	1.15
1:A:249:ILE:CG2	17:3:136:TRP:CZ3	2.18	1.15
1:A:342:GLY:CA	1:A:430:ASP:CB	2.23	1.15
2:B:470:THR:N	2:B:501:ILE:HB	1.32	1.15
3:C:10:THR:HG23	5:E:101:TYR:CD2	1.82	1.15
6:F:124:GLU:HG3	6:F:128:LYS:HD3	1.21	1.15
8:H:58:LEU:HD12	8:H:62:THR:CG2	1.66	1.15
8:H:116:ALA:HB1	8:H:117:SER:HA	1.26	1.15
16:2:156:GLU:CG	16:2:157:LEU:HD13	1.75	1.15
1:A:451:ILE:HD12	19:A:1131:CLA:HED3	1.28	1.15
4:D:132:ALA:O	4:D:133:ARG:HD3	1.44	1.15
4:D:140:LEU:HD11	4:D:144:LEU:HB2	1.22	1.15
5:E:82:TYR:HB3	5:E:83:TRP:CZ3	1.81	1.15
15:1:77:GLU:HA	15:1:80:LYS:HG2	1.23	1.15
2:B:620:LEU:HD12	2:B:624:LEU:HD23	1.23	1.15
2:B:628:SER:O	2:B:631:LEU:HD23	1.45	1.15
4:D:201:LYS:H	4:D:201:LYS:HD2	1.02	1.15
13:N:139:LYS:HA	13:N:142:LYS:HZ3	0.98	1.15
13:N:139:LYS:HE3	13:N:142:LYS:CE	1.76	1.15
16:2:184:PRO:HD3	16:2:187:LYS:CG	1.74	1.15
18:4:174:GLN:O	18:4:194:PHE:CG	1.99	1.15
1:A:336:GLY:CA	1:A:339:THR:OG1	1.94	1.14
2:B:255:LEU:HA	2:B:271:THR:HB	1.16	1.14
8:H:58:LEU:HB3	8:H:61:THR:CG2	1.76	1.14
8:H:97:LEU:HG	8:H:98:LEU:HA	1.29	1.14
19:L:1148:CLA:HBC3	19:L:1148:CLA:HHD	1.26	1.14
16:2:182:ILE:CG2	16:2:187:LYS:HG3	1.76	1.14
17:3:111:LEU:HG	17:3:112:GLY:N	1.48	1.14
18:4:168:GLN:HB3	18:4:172:PHE:HE1	1.06	1.14
1:A:150:PHE:O	1:A:151:GLN:HG3	1.46	1.14
19:A:1119:CLA:CMD	19:A:1121:CLA:HBB2	1.75	1.14
16:2:112:TRP:CZ2	16:2:167:ARG:NH2	2.04	1.14
16:2:182:ILE:HG22	16:2:187:LYS:HG3	1.26	1.14
17:3:150:TYR:HB3	17:3:151:TRP:CD1	1.81	1.14
11:K:118:VAL:HG23	11:K:121:VAL:HG22	1.25	1.14
14:R:26:UNK:O	14:R:28:UNK:CB	1.96	1.14
2:B:75:GLU:CB	2:B:132:ASN:ND2	2.09	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:79:LYS:HG3	5:E:84:TYR:CZ	1.82	1.14
1:A:443:ILE:CD1	1:A:557:LEU:HD22	1.77	1.14
1:A:575:LEU:HD12	1:A:576:GLY:CA	1.78	1.14
17:3:141:VAL:HG23	17:3:142:ILE:HG12	1.30	1.14
18:4:175:TYR:HD2	18:4:195:ALA:O	1.26	1.14
1:A:267:THR:HG22	1:A:269:PHE:CE2	1.83	1.13
1:A:499:ALA:HB1	19:A:1133:CLA:HED1	1.24	1.13
2:B:329:SER:O	2:B:330:ILE:HG22	1.48	1.13
2:B:569:ASP:OD1	2:B:706:ARG:CZ	1.95	1.13
7:G:149:TYR:HA	7:G:150:ASP:CG	1.66	1.13
16:2:171:ILE:HG13	16:2:172:LEU:N	1.60	1.13
16:2:187:LYS:HA	16:2:187:LYS:HE3	1.28	1.13
1:A:281:LEU:CD2	19:A:1115:CLA:HMA3	1.74	1.13
1:A:397:THR:CG2	1:A:613:ILE:HG13	1.78	1.13
22:R:7020:LMU:H5B	22:R:7020:LMU:H6E	1.30	1.13
2:B:469:LYS:HD2	2:B:470:THR:CA	1.77	1.13
11:K:111:VAL:O	11:K:114:HIS:HB2	1.46	1.13
15:1:177:PRO:CD	15:1:180:LEU:CG	1.86	1.13
19:1:1303:CLA:HMC1	19:1:1303:CLA:HBC2	1.30	1.13
16:2:246:PRO:HB3	16:2:247:ILE:HD13	1.13	1.13
17:3:103:VAL:HG12	17:3:107:ARG:HD3	1.30	1.13
18:4:87:ASN:HB2	18:4:90:TRP:CZ3	1.82	1.13
18:4:173:LYS:NZ	18:4:201:LYS:HG3	1.64	1.13
1:A:152:ILE:HD11	19:A:1127:CLA:O1D	1.45	1.13
2:B:22:TRP:HE1	19:B:1238:CLA:CBB	1.62	1.13
2:B:310:PRO:CB	2:B:311:PRO:HD3	1.71	1.13
22:D:7050:LMU:H6E	22:D:7050:LMU:C2B	1.78	1.13
19:H:1145:CLA:HBC2	19:H:1145:CLA:HMC1	1.30	1.13
17:3:109:ALA:CA	17:3:111:LEU:HB3	1.78	1.13
17:3:159:VAL:O	17:3:161:GLU:N	1.81	1.13
22:3:7003:LMU:C3B	22:3:7005:LMU:C4B	2.25	1.13
19:A:1124:CLA:HBC2	19:A:1124:CLA:HHD	1.29	1.12
19:A:9022:CLA:H93	19:A:9023:CLA:H91	1.28	1.12
2:B:247:THR:HA	2:B:250:ALA:HB2	1.25	1.12
2:B:294:ASN:HD22	7:G:94:GLN:CA	1.60	1.12
3:C:66:ARG:HG2	3:C:66:ARG:HH21	1.12	1.12
7:G:89:LYS:HA	7:G:89:LYS:NZ	1.63	1.12
7:G:100:PHE:N	7:G:101:GLU:HB2	1.64	1.13
11:K:78:ARG:NE	11:K:78:ARG:HA	1.60	1.12
12:L:60:ILE:HG22	12:L:61:ASN:N	1.52	1.12
12:L:141:LEU:HD11	21:L:6019:BCR:H312	1.24	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:7029:LMU:H1'	22:L:7029:LMU:H31	1.31	1.12
13:N:139:LYS:HB3	13:N:142:LYS:HD3	1.18	1.12
15:1:92:LEU:C	15:1:95:PRO:HD2	1.68	1.13
15:1:189:LYS:HG3	19:1:1007:CLA:HMC2	1.19	1.13
19:1:1014:CLA:HBC3	19:1:1014:CLA:HHD	1.25	1.13
16:2:148:ASP:HB3	16:2:152:LEU:CB	1.79	1.12
17:3:201:ALA:HB1	17:3:202:TYR:CE2	1.83	1.12
19:A:1141:CLA:H12	19:A:1141:CLA:HMA2	1.23	1.12
2:B:553:PHE:O	2:B:554:GLY:C	1.85	1.12
7:G:72:LEU:CD2	7:G:124:ILE:HD11	1.78	1.12
22:N:7049:LMU:H61	22:N:7049:LMU:H12	1.19	1.12
19:1:1010:CLA:HBC3	19:1:1010:CLA:HHD	1.26	1.12
18:4:175:TYR:CD2	18:4:195:ALA:O	2.00	1.12
1:A:217:SER:OG	21:A:6002:BCR:C15	1.98	1.12
2:B:304:ILE:HD11	19:B:1216:CLA:CED	1.79	1.12
2:B:382:ILE:HG22	2:B:383:MET:H	1.09	1.12
19:J:1308:CLA:HBA2	19:J:1308:CLA:HBD	1.28	1.12
18:4:193:ASN:O	18:4:194:PHE:CG	2.03	1.12
1:A:281:LEU:HD22	19:A:1115:CLA:CED	1.80	1.12
1:A:502:THR:HG22	1:A:504:ALA:H	1.09	1.12
2:B:310:PRO:HB2	2:B:311:PRO:HD3	1.21	1.12
2:B:314:ARG:HH12	15:1:67:LEU:CD2	1.61	1.12
19:B:1235:CLA:H152	21:F:6016:BCR:C31	1.78	1.12
11:K:125:LYS:HB2	11:K:128:GLY:CA	1.80	1.12
22:L:7029:LMU:H4'	22:L:7029:LMU:H5B	1.27	1.12
19:1:1014:CLA:H71	19:1:1014:CLA:H41	1.31	1.12
1:A:158:ILE:CG1	1:A:159:THR:H	1.62	1.12
1:A:669:GLY:N	2:B:445:ALA:HA	1.63	1.12
4:D:167:HIS:CE1	4:D:172:VAL:HG11	1.85	1.12
13:N:103:ASP:HB3	13:N:107:LEU:HD12	1.15	1.12
15:1:97:ILE:HD13	15:1:98:LEU:CB	1.80	1.12
17:3:98:LEU:O	17:3:101:GLY:N	1.81	1.12
17:3:103:VAL:CG1	17:3:107:ARG:CD	2.14	1.12
1:A:244:LEU:CB	1:A:247:GLU:CG	2.11	1.11
1:A:487:VAL:HG13	1:A:489:ALA:N	1.63	1.11
19:A:1115:CLA:H141	19:A:1115:CLA:H172	1.26	1.11
3:C:62:PHE:CE2	5:E:80:GLU:CG	2.33	1.11
11:K:125:LYS:CA	11:K:126:ASN:HB3	1.79	1.11
12:L:96:LEU:HD23	12:L:96:LEU:H	1.13	1.11
19:1:1014:CLA:H52	19:1:1014:CLA:H102	1.28	1.11
16:2:125:PHE:HA	16:2:127:THR:HG23	1.14	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HD21	1:A:296:LEU:O	1.48	1.11
2:B:230:TRP:N	7:G:63:VAL:HG21	1.62	1.11
2:B:315:LEU:HD12	2:B:317:ARG:HG2	1.13	1.11
6:F:173:TRP:CZ3	6:F:211:PHE:HB2	1.84	1.11
13:N:103:ASP:HB2	13:N:107:LEU:HD11	1.22	1.11
13:N:139:LYS:CE	13:N:142:LYS:HE2	1.78	1.11
15:1:97:ILE:CD1	15:1:98:LEU:HA	1.66	1.11
17:3:243:ILE:HD11	19:3:3005:CLA:C2C	1.80	1.11
1:A:167:THR:HG22	19:A:1112:CLA:HAA2	1.32	1.11
1:A:472:ARG:NH1	12:L:120:LEU:HD22	1.64	1.11
1:A:492:ILE:HD11	19:A:1133:CLA:HMC3	1.13	1.11
19:A:1124:CLA:HED1	19:A:1125:CLA:C2D	1.80	1.11
2:B:89:HIS:O	2:B:113:VAL:HG13	1.45	1.11
2:B:90:ALA:HA	2:B:113:VAL:HG13	1.33	1.11
2:B:123:TRP:HA	2:B:126:THR:CB	1.79	1.11
3:C:44:ARG:HB3	4:D:182:GLN:NE2	1.65	1.11
13:N:132:THR:HB	13:N:139:LYS:NZ	1.65	1.11
13:N:135:GLN:HA	13:N:136:ASP:O	1.47	1.11
16:2:176:CYS:O	16:2:177:VAL:HG23	1.50	1.11
19:3:1147:CLA:HBC3	19:3:1147:CLA:CMC	1.77	1.11
2:B:53:GLN:NE2	19:B:1201:CLA:HBB1	1.63	1.11
2:B:89:HIS:C	2:B:113:VAL:CG1	1.81	1.11
2:B:174:ARG:HB2	19:B:1210:CLA:HBC2	1.32	1.11
19:B:1202:CLA:O1A	19:B:1202:CLA:H2	1.30	1.11
19:B:1235:CLA:H152	21:F:6016:BCR:H312	1.18	1.11
5:E:96:ASP:HB3	5:E:98:ASN:H	1.03	1.11
12:L:128:GLN:HA	12:L:130:GLY:HA3	1.27	1.11
15:1:157:ASP:CB	15:1:178:LYS:HA	1.79	1.11
16:2:166:ARG:N	16:2:167:ARG:CB	2.14	1.11
16:2:186:ASN:CG	16:2:188:LEU:HD11	1.54	1.11
17:3:135:ALA:CB	17:3:139:THR:HB	1.80	1.11
5:E:125:ILE:O	5:E:125:ILE:HG13	1.40	1.11
13:N:146:LEU:HD11	17:3:142:ILE:O	1.22	1.11
19:4:1304:CLA:HAA2	19:4:1304:CLA:CED	1.79	1.11
1:A:308:ILE:HD12	19:A:1115:CLA:HHC	1.20	1.10
1:A:478:SER:HB2	1:A:644:GLN:NE2	1.65	1.10
2:B:314:ARG:NH1	15:1:67:LEU:CD2	2.14	1.10
1:A:73:GLU:O	1:A:76:ARG:N	1.85	1.10
1:A:478:SER:HB2	1:A:644:GLN:HE22	1.06	1.10
19:A:1134:CLA:CGA	19:A:1141:CLA:HBB1	1.80	1.10
21:A:6002:BCR:H311	21:A:6002:BCR:HC8	1.15	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:VAL:HG22	2:B:123:TRP:HE1	0.93	1.10
6:F:207:LEU:HD13	6:F:208:PHE:H	1.03	1.10
8:H:58:LEU:HD12	8:H:61:THR:HB	1.17	1.10
13:N:155:GLU:CA	13:N:157:LYS:HE2	1.81	1.10
15:1:157:ASP:HB2	15:1:178:LYS:HA	1.24	1.10
2:B:25:ILE:HG13	2:B:25:ILE:O	1.50	1.10
2:B:620:LEU:HD12	2:B:624:LEU:CD2	1.81	1.10
4:D:140:LEU:HD13	4:D:144:LEU:HG	1.19	1.10
6:F:107:LYS:O	6:F:108:LEU:CD1	1.99	1.10
6:F:130:PHE:N	6:F:133:TYR:HE1	1.50	1.10
6:F:173:TRP:HZ3	6:F:211:PHE:HB2	1.07	1.10
7:G:113:LEU:O	7:G:117:ASN:ND2	1.85	1.10
15:1:177:PRO:HD3	15:1:180:LEU:HG	1.32	1.10
16:2:184:PRO:CB	16:2:187:LYS:HD2	1.81	1.10
22:3:7003:LMU:C4B	22:3:7005:LMU:H4B	1.81	1.10
1:A:157:GLY:HA3	1:A:229:ILE:HG21	1.22	1.10
1:A:158:ILE:HG13	1:A:159:THR:N	1.56	1.10
19:B:1220:CLA:HMC1	19:B:1220:CLA:HBC3	1.17	1.10
4:D:84:GLY:O	12:L:64:PRO:HB3	1.50	1.10
5:E:111:ASN:ND2	5:E:113:ALA:H	1.50	1.10
8:H:58:LEU:HD11	8:H:62:THR:HG21	1.13	1.10
15:1:85:ILE:HG12	15:1:88:ARG:CZ	1.82	1.10
15:1:168:PHE:O	15:1:169:ASP:HB2	1.52	1.10
17:3:108:PHE:HB3	19:3:3013:CLA:C4	1.82	1.10
18:4:141:LEU:H	18:4:141:LEU:CD2	1.64	1.10
1:A:316:MET:HB3	1:A:317:TYR:HB2	1.34	1.10
1:A:423:ASP:HB3	1:A:424:PRO:CG	1.82	1.10
2:B:20:ARG:HG3	2:B:20:ARG:HH11	1.02	1.10
2:B:140:ILE:HG13	2:B:141:PHE:N	1.59	1.10
2:B:317:ARG:NH2	2:B:410:ARG:CG	2.14	1.10
2:B:429:LEU:C	2:B:525:LEU:HD12	1.70	1.10
2:B:459:PHE:HD2	19:B:1235:CLA:CAD	1.63	1.10
4:D:158:PHE:HB3	4:D:159:PRO:HD2	1.34	1.10
8:H:58:LEU:HB3	8:H:61:THR:CB	1.81	1.10
8:H:78:PRO:HD3	19:L:1501:CLA:HMD3	1.14	1.10
14:R:38:UNK:O	14:R:42:UNK:HA	1.48	1.10
19:A:1124:CLA:HED1	19:A:1125:CLA:C3D	1.81	1.09
2:B:131:THR:HG22	2:B:134:ASP:H	1.01	1.09
6:F:82:LEU:HG	6:F:83:THR:H	1.12	1.09
6:F:119:ILE:HG13	6:F:120:LYS:H	1.07	1.09
21:F:6016:BCR:C8	21:F:6016:BCR:H321	1.62	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:89:LYS:HA	7:G:89:LYS:HE3	1.32	1.09
16:2:122:ILE:HD13	19:2:2002:CLA:C3B	1.78	1.09
17:3:135:ALA:CB	17:3:139:THR:CB	2.28	1.09
22:4:7034:LMU:H112	22:4:7052:LMU:H4'	1.29	1.09
1:A:435:VAL:O	1:A:438:HIS:O	1.70	1.09
2:B:98:GLN:O	2:B:100:ALA:N	1.86	1.09
19:B:1235:CLA:H161	21:F:6016:BCR:H313	1.30	1.09
4:D:140:LEU:HD12	4:D:140:LEU:C	1.60	1.09
5:E:82:TYR:HB3	5:E:83:TRP:CE3	1.86	1.09
5:E:106:ARG:HH21	5:E:107:PHE:CA	1.63	1.09
5:E:127:GLU:HB3	5:E:129:GLU:O	1.49	1.09
8:H:56:GLU:HG3	8:H:57:ASP:N	1.65	1.09
12:L:131:SER:HB3	12:L:201:TYR:CE2	1.67	1.09
16:2:168:TRP:CD1	16:2:171:ILE:CG2	2.26	1.09
16:2:184:PRO:HD2	16:2:185:ASN:C	1.72	1.09
1:A:56:ASN:O	1:A:57:LEU:HB3	1.37	1.09
19:A:1125:CLA:CBB	19:A:1133:CLA:CMA	1.89	1.09
4:D:80:SER:OG	4:D:126:PRO:CD	1.99	1.09
14:R:46:UNK:CB	14:R:47:UNK:CB	2.30	1.09
19:2:2007:CLA:HBC2	19:3:2009:CLA:HED2	1.13	1.09
17:3:210:PRO:HG2	17:3:211:LEU:HD12	1.30	1.09
19:3:3008:CLA:HBA2	19:3:3008:CLA:HBD	1.15	1.09
19:4:1306:CLA:HMC1	19:4:1306:CLA:HBC3	1.21	1.09
1:A:331:LEU:HD11	1:A:346:LEU:HB3	1.10	1.09
1:A:669:GLY:H	2:B:445:ALA:HA	1.15	1.09
2:B:89:HIS:O	2:B:113:VAL:CB	2.00	1.09
2:B:545:LYS:HD3	2:B:546:LEU:H	1.01	1.09
3:C:44:ARG:CZ	4:D:181:ARG:HD3	1.83	1.09
10:J:11:ALA:HB1	10:J:12:PRO:HD2	1.29	1.09
12:L:73:VAL:O	19:L:1130:CLA:O2A	1.71	1.09
14:R:34:UNK:CB	14:R:35:UNK:CB	2.30	1.09
15:1:78:ARG:NH2	15:1:179:LYS:HB3	1.67	1.09
16:2:122:ILE:HD11	19:2:2002:CLA:C3B	1.81	1.09
16:2:182:ILE:CB	16:2:187:LYS:HG3	1.81	1.09
21:3:6022:BCR:H23C	21:3:6022:BCR:C39	1.82	1.09
18:4:158:GLN:NE2	19:4:1004:CLA:NA	2.00	1.09
1:A:24:ARG:HD2	1:A:24:ARG:H	0.92	1.09
1:A:145:ILE:HG23	19:A:1106:CLA:OBD	1.50	1.09
1:A:158:ILE:HG13	1:A:159:THR:H	1.03	1.09
1:A:331:LEU:HD21	1:A:343:HIS:O	1.53	1.09
1:A:338:PHE:HE1	19:A:1151:CLA:HBB1	0.93	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:6020:BCR:H331	19:L:1502:CLA:CHC	1.83	1.09
19:K:1142:CLA:CED	19:K:1143:CLA:HMB2	1.82	1.09
12:L:141:LEU:HD11	21:L:6019:BCR:C31	1.81	1.09
14:R:41:UNK:CB	14:R:42:UNK:CA	2.30	1.09
17:3:185:GLN:CG	17:3:186:TYR:H	1.65	1.09
19:A:1101:CLA:H42	19:A:1140:CLA:H61	1.12	1.08
19:A:1102:CLA:H12	19:A:1109:CLA:H61	1.28	1.08
21:A:6011:BCR:H23C	21:A:6011:BCR:H393	1.27	1.08
2:B:475:ASP:HB3	2:B:480:SER:HA	1.33	1.08
4:D:87:THR:HG23	12:L:69:LEU:HD12	1.11	1.08
22:E:7048:LMU:H4B	22:F:7036:LMU:H6E	1.15	1.08
19:J:1308:CLA:HHD	19:J:1308:CLA:HBC2	1.33	1.08
12:L:171:LYS:C	12:L:173:PRO:CD	2.21	1.08
16:2:130:GLY:HA2	16:2:131:ILE:HG12	1.21	1.08
16:2:152:LEU:HD13	16:2:153:PHE:H	0.99	1.08
17:3:150:TYR:CD2	17:3:151:TRP:CE2	2.41	1.08
18:4:96:LEU:C	18:4:96:LEU:HD12	1.73	1.08
2:B:225:LEU:CD1	2:B:233:TYR:OH	2.00	1.08
2:B:247:THR:HG23	2:B:248:GLN:H	1.16	1.08
19:B:1222:CLA:HHD	19:B:1222:CLA:HBC2	1.31	1.08
3:C:14:CYS:CA	3:C:17:CYS:SG	2.41	1.08
7:G:62:LEU:HB3	7:G:65:SER:HB3	1.24	1.08
12:L:115:VAL:HG11	12:L:130:GLY:H	1.14	1.08
13:N:143:VAL:HB	13:N:144:PRO:HD2	1.15	1.08
13:N:147:SER:HB3	13:N:151:ASP:HA	1.19	1.08
13:N:155:GLU:C	13:N:157:LYS:HE3	1.60	1.08
16:2:125:PHE:HA	16:2:127:THR:CG2	1.80	1.08
17:3:96:ARG:HA	17:3:99:ALA:HB3	1.30	1.08
18:4:103:MET:HE3	18:4:208:GLY:CA	1.71	1.08
1:A:86:LEU:HD13	1:A:178:MET:HE1	1.25	1.08
1:A:425:THR:HB	1:A:428:TYR:HE1	1.04	1.08
2:B:255:LEU:HA	2:B:271:THR:CB	1.82	1.08
2:B:558:PRO:HB2	2:B:703:VAL:HG22	1.16	1.08
3:C:24:ASP:HB2	23:C:8002:SF4:S2	1.92	1.08
6:F:179:ARG:HG2	6:F:183:ILE:HD11	1.25	1.08
6:F:224:GLY:C	6:F:227:VAL:HG12	1.72	1.08
8:H:121:LEU:HB3	8:H:122:PRO:HD2	1.13	1.08
22:H:7030:LMU:H91	22:H:7030:LMU:H52	1.32	1.08
22:R:7022:LMU:H21	22:R:7022:LMU:H2'	1.27	1.08
15:1:70:GLY:O	15:1:73:PRO:HD2	1.51	1.08
15:1:177:PRO:CD	15:1:180:LEU:CD2	2.30	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:89:ARG:HD3	18:4:90:TRP:H	1.08	1.08
1:A:361:ASN:ND2	19:A:1103:CLA:OBD	1.84	1.08
19:A:1140:CLA:H141	21:A:6011:BCR:HC22	1.20	1.08
6:F:221:LEU:HD23	6:F:222:LEU:CD2	1.82	1.08
21:I:6021:BCR:C8	21:I:6021:BCR:C31	2.28	1.08
16:2:117:ALA:HB3	16:2:230:LEU:HG	1.28	1.08
19:2:2001:CLA:H42	19:2:2001:CLA:O1A	1.53	1.08
1:A:71:LEU:HG	1:A:72:GLU:H	1.14	1.08
1:A:492:ILE:HD11	19:A:1133:CLA:CMC	1.83	1.08
1:A:567:ARG:NH1	4:D:89:GLY:HA2	1.68	1.08
2:B:247:THR:HA	2:B:250:ALA:HB3	1.27	1.08
2:B:302:LYS:O	2:B:303:TYR:HB2	1.52	1.08
2:B:459:PHE:CE2	19:B:1235:CLA:HMD2	1.87	1.08
11:K:97:ASP:HB2	11:K:101:PHE:HE2	1.12	1.08
14:R:39:UNK:C	14:R:41:UNK:CB	2.30	1.08
17:3:96:ARG:HH11	17:3:96:ARG:CG	1.67	1.08
18:4:146:PHE:CZ	19:4:4013:CLA:C1C	2.36	1.08
1:A:443:ILE:HD11	1:A:557:LEU:HD22	1.14	1.07
1:A:479:ASP:HA	1:A:536:THR:HG21	1.32	1.07
1:A:567:ARG:NH2	4:D:136:GLN:OE1	1.85	1.07
19:A:1124:CLA:HED1	19:A:1125:CLA:CMD	1.84	1.07
19:A:1141:CLA:H71	19:A:1141:CLA:H121	1.33	1.07
2:B:25:ILE:HG21	21:L:6019:BCR:H292	1.28	1.07
2:B:493:TRP:CH2	19:B:1232:CLA:HMA2	1.89	1.07
2:B:551:LYS:O	2:B:552:ASP:OD1	1.72	1.07
4:D:140:LEU:HD13	4:D:144:LEU:CG	1.84	1.07
16:2:118:ALA:O	16:2:121:PHE:CD2	2.06	1.07
16:2:227:LEU:HD21	19:2:2004:CLA:C1C	1.84	1.07
19:3:3008:CLA:HMC1	19:3:3008:CLA:HBC2	1.30	1.07
18:4:146:PHE:CZ	19:4:4013:CLA:C2C	2.37	1.07
1:A:163:GLN:HA	1:A:166:CYS:SG	1.93	1.07
2:B:119:GLY:HA3	19:B:1225:CLA:HED1	1.22	1.07
2:B:131:THR:HG22	2:B:134:ASP:N	1.70	1.07
2:B:294:ASN:ND2	7:G:94:GLN:CA	2.17	1.07
2:B:527:LEU:HD13	19:B:1236:CLA:HMA2	1.28	1.07
3:C:62:PHE:CZ	5:E:80:GLU:CG	2.37	1.07
4:D:87:THR:HG23	12:L:69:LEU:CD1	1.83	1.07
5:E:99:THR:HG22	5:E:100:ARG:N	1.65	1.07
6:F:213:TRP:HB2	6:F:216:ALA:HB2	1.36	1.07
11:K:52:PRO:HD2	11:K:53:THR:H	1.19	1.07
12:L:131:SER:CB	12:L:201:TYR:CE2	2.31	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:148:ASP:N	13:N:149:ASP:HB2	1.68	1.07
15:1:77:GLU:O	15:1:80:LYS:HG3	1.55	1.07
16:2:195:TYR:HD1	16:2:196:PRO:HD2	1.04	1.07
19:3:3016:CLA:HMC1	19:3:3016:CLA:HBC3	1.35	1.07
18:4:173:LYS:HZ3	18:4:201:LYS:HG3	1.09	1.07
19:A:1122:CLA:HBB2	21:A:6007:BCR:C35	1.85	1.07
19:A:1125:CLA:CAB	19:A:1133:CLA:CMA	2.32	1.07
2:B:89:HIS:O	2:B:113:VAL:HG12	1.34	1.07
2:B:500:ALA:O	2:B:501:ILE:HG12	1.55	1.07
2:B:551:LYS:HG2	2:B:552:ASP:H	1.17	1.07
15:1:80:LYS:O	15:1:83:GLU:HB3	1.52	1.07
1:A:51:THR:HG21	19:A:1139:CLA:HBB2	1.37	1.07
1:A:328:LYS:HD2	1:A:332:GLU:HB2	1.33	1.07
2:B:11:GLY:HA3	3:C:71:HIS:HD2	1.03	1.07
5:E:107:PHE:CE2	5:E:109:LYS:HE3	1.88	1.07
11:K:81:THR:HG23	11:K:83:GLY:N	1.68	1.07
16:2:148:ASP:HB3	16:2:152:LEU:HB3	1.15	1.07
17:3:139:THR:HG22	17:3:140:GLY:H	0.90	1.07
17:3:139:THR:HG22	17:3:140:GLY:N	1.65	1.07
12:L:164:LEU:HB2	12:L:165:THR:HG23	1.36	1.07
12:L:209:LEU:HD12	12:L:210:PRO:CD	1.83	1.07
13:N:139:LYS:HG3	13:N:142:LYS:CD	1.85	1.07
16:2:152:LEU:HD13	16:2:153:PHE:N	1.70	1.07
16:2:184:PRO:HB3	16:2:187:LYS:HD2	1.33	1.07
18:4:146:PHE:CZ	19:4:4013:CLA:C3C	2.38	1.07
18:4:165:SER:O	18:4:168:GLN:CG	2.02	1.07
1:A:281:LEU:HD21	19:A:1115:CLA:HMA2	1.08	1.06
2:B:110:LEU:HD12	2:B:111:GLY:N	1.71	1.06
6:F:207:LEU:HD22	6:F:208:PHE:CA	1.85	1.06
7:G:84:ARG:HG3	7:G:85:GLU:CB	1.83	1.06
11:K:49:ILE:CA	11:K:52:PRO:CG	2.31	1.06
11:K:49:ILE:HA	11:K:52:PRO:HG3	1.11	1.06
11:K:127:ILE:HA	11:K:130:LEU:CG	1.85	1.06
16:2:168:TRP:HA	16:2:171:ILE:HG23	1.28	1.06
17:3:192:LYS:HA	17:3:192:LYS:HE2	1.27	1.06
1:A:157:GLY:O	1:A:158:ILE:HG23	0.89	1.06
1:A:478:SER:HB3	1:A:644:GLN:HE22	1.16	1.06
1:A:499:ALA:HB1	19:A:1133:CLA:CED	1.85	1.06
19:A:1105:CLA:C3B	21:J:6012:BCR:C33	2.33	1.06
2:B:123:TRP:HA	2:B:126:THR:HG22	1.13	1.06
3:C:65:VAL:HG22	3:C:66:ARG:H	1.17	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:ARG:HG3	7:G:85:GLU:N	1.65	1.06
7:G:96:GLY:C	7:G:97:LEU:HG	1.76	1.06
15:1:134:LEU:HA	15:1:137:ILE:HD11	1.10	1.06
16:2:246:PRO:HB3	16:2:247:ILE:CD1	1.84	1.06
17:3:109:ALA:CA	17:3:111:LEU:CB	2.33	1.06
17:3:113:ALA:HB1	17:3:239:LEU:HD11	1.12	1.06
18:4:242:ASN:O	18:4:243:THR:HG22	1.55	1.06
1:A:316:MET:HG2	1:A:317:TYR:CD1	1.89	1.06
1:A:478:SER:CB	1:A:644:GLN:NE2	2.18	1.06
19:A:1122:CLA:HBB2	21:A:6007:BCR:H351	1.35	1.06
19:A:1134:CLA:H3A	19:A:1141:CLA:HBB2	1.31	1.06
2:B:475:ASP:CB	2:B:480:SER:HA	1.84	1.06
2:B:696:LYS:HG2	3:C:80:ALA:HA	1.38	1.06
19:J:1308:CLA:CAD	19:J:1308:CLA:HED3	1.86	1.06
11:K:125:LYS:HA	11:K:126:ASN:CB	1.84	1.06
16:2:118:ALA:CA	16:2:121:PHE:CE2	2.25	1.06
17:3:93:ILE:HG13	17:3:95:PRO:O	1.55	1.06
17:3:197:SER:OG	17:3:206:PRO:HD3	1.55	1.06
17:3:201:ALA:C	17:3:202:TYR:HD2	1.59	1.06
18:4:146:PHE:CZ	19:4:4013:CLA:C4C	2.37	1.06
18:4:209:ARG:O	18:4:212:LEU:O	1.72	1.06
19:A:9012:CLA:H11	2:B:616:LEU:HD13	1.35	1.06
19:A:9012:CLA:C1	2:B:616:LEU:HD13	1.85	1.06
2:B:475:ASP:O	2:B:476:ILE:HG22	1.54	1.06
4:D:163:VAL:O	4:D:164:GLN:HG3	1.53	1.06
5:E:78:ARG:HH22	5:E:125:ILE:HG21	1.14	1.06
12:L:143:LEU:HD22	12:L:146:THR:HG22	1.31	1.06
17:3:110:MET:O	17:3:113:ALA:HB3	1.54	1.06
1:A:21:LEU:HA	1:A:22:VAL:HG13	1.33	1.06
1:A:365:LEU:HD23	19:A:1103:CLA:HED3	1.31	1.06
1:A:578:ARG:HB2	1:A:578:ARG:CZ	1.81	1.06
1:A:707:ILE:HG22	1:A:711:HIS:NE2	1.71	1.06
2:B:122:GLN:O	2:B:126:THR:HB	0.89	1.06
2:B:317:ARG:CZ	2:B:410:ARG:HG2	1.85	1.06
19:B:1235:CLA:HBB2	19:B:1235:CLA:C9	1.85	1.06
7:G:64:ILE:O	7:G:68:THR:HG23	1.53	1.06
9:I:11:LEU:HD12	21:I:6021:BCR:H10C	1.34	1.06
13:N:130:ASN:C	13:N:132:THR:HG22	1.75	1.06
13:N:139:LYS:HG3	13:N:142:LYS:HD3	1.37	1.06
15:1:162:LYS:C	15:1:164:PRO:HD3	1.75	1.06
19:1:1014:CLA:H52	19:1:1014:CLA:C10	1.86	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:117:ALA:HB1	16:2:230:LEU:HG	1.37	1.06
16:2:119:GLY:O	16:2:123:PRO:CG	2.02	1.06
19:4:1004:CLA:HBC2	19:4:1004:CLA:HHD	1.30	1.06
1:A:163:GLN:HG3	1:A:164:LEU:H	1.18	1.05
1:A:188:LYS:O	1:A:190:ALA:HB2	1.56	1.05
1:A:397:THR:HG22	1:A:613:ILE:HG13	1.11	1.05
2:B:89:HIS:O	2:B:113:VAL:CG1	0.76	1.05
5:E:78:ARG:NH2	5:E:125:ILE:HG21	1.68	1.05
8:H:76:TYR:OH	12:L:90:ARG:HD2	1.53	1.05
18:4:172:PHE:HB3	18:4:194:PHE:CE2	1.88	1.05
1:A:439:ARG:NH1	1:A:565:SER:O	1.90	1.05
1:A:483:GLN:HB3	1:A:485:GLN:NE2	1.71	1.05
2:B:70:TRP:HB3	2:B:136:TYR:OH	1.56	1.05
6:F:132:ASN:O	6:F:133:TYR:HD1	1.38	1.05
6:F:219:ARG:HG2	6:F:219:ARG:HH11	0.93	1.05
8:H:98:LEU:CD2	12:L:146:THR:HG21	1.86	1.05
12:L:60:ILE:HG22	12:L:61:ASN:H	1.02	1.05
19:2:2007:CLA:HAC2	19:3:2009:CLA:HED3	1.38	1.05
19:2:2014:CLA:C10	19:2:2014:CLA:H152	1.75	1.05
1:A:281:LEU:CD2	19:A:1115:CLA:CED	2.33	1.05
1:A:425:THR:HB	1:A:428:TYR:CE1	1.90	1.05
4:D:102:ILE:HD12	4:D:137:CYS:HB3	1.39	1.05
7:G:65:SER:O	7:G:68:THR:OG1	1.74	1.05
8:H:58:LEU:HB3	8:H:61:THR:HG21	1.36	1.05
10:J:31:ARG:HH22	19:J:1311:CLA:C4B	1.69	1.05
15:1:189:LYS:CB	19:1:1007:CLA:CMC	2.33	1.05
16:2:182:ILE:HB	16:2:187:LYS:HB3	1.05	1.05
22:3:7003:LMU:H3B	22:3:7005:LMU:O5B	1.55	1.05
1:A:259:TYR:HB3	1:A:260:PRO:HD2	1.37	1.05
1:A:279:ASP:O	1:A:281:LEU:CG	2.03	1.05
2:B:11:GLY:CA	3:C:71:HIS:HD2	1.68	1.05
2:B:87:ILE:HA	2:B:115:ASN:HA	1.38	1.05
7:G:98:THR:CB	7:G:101:GLU:OE2	2.01	1.05
10:J:37:LEU:O	10:J:38:ILE:HG13	1.56	1.05
15:1:78:ARG:HG3	15:1:81:GLU:OE1	1.55	1.05
19:1:1013:CLA:O1D	19:1:1013:CLA:HAA2	1.53	1.05
19:2:2014:CLA:H41	19:2:2014:CLA:H72	1.39	1.05
1:A:51:THR:CG2	19:A:1139:CLA:HBB2	1.85	1.05
1:A:250:LEU:CB	17:3:136:TRP:CH2	2.39	1.05
1:A:581:CYS:HB2	1:A:590:CYS:HA	1.38	1.05
1:A:715:LYS:CD	6:F:230:ASN:HD21	1.69	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:GLY:HA3	3:C:71:HIS:CD2	1.91	1.05
2:B:517:PHE:CD2	2:B:517:PHE:O	2.09	1.05
4:D:114:MET:SD	4:D:115:PRO:O	2.15	1.05
5:E:127:GLU:O	5:E:128:VAL:HG23	1.55	1.05
6:F:190:LYS:HZ3	6:F:192:THR:HG22	1.17	1.05
7:G:131:GLY:HA2	7:G:136:VAL:HG23	1.35	1.05
16:2:103:VAL:HG13	16:2:104:GLN:OE1	1.56	1.05
16:2:160:ILE:HG21	19:2:2012:CLA:CBB	1.81	1.05
1:A:451:ILE:CD1	19:A:1131:CLA:CED	2.35	1.04
1:A:588:GLY:CA	2:B:668:ARG:HD3	1.86	1.04
3:C:54:CYS:SG	23:C:8002:SF4:S1	2.54	1.04
8:H:85:GLU:HG3	8:H:86:THR:H	1.10	1.04
15:1:97:ILE:CD1	15:1:98:LEU:CB	2.34	1.04
16:2:174:PRO:HB2	16:2:194:GLY:HA3	1.37	1.04
19:3:2009:CLA:HBD	19:3:2009:CLA:O1A	1.52	1.04
22:4:7034:LMU:C9	22:4:7052:LMU:H2'	1.86	1.04
1:A:120:ALA:H	1:A:145:ILE:HD11	1.15	1.04
1:A:443:ILE:CD1	1:A:557:LEU:CD2	2.33	1.04
2:B:319:HIS:CE1	2:B:322:LEU:HD12	1.92	1.04
3:C:5:VAL:CB	3:C:65:VAL:HG23	1.88	1.04
22:D:7050:LMU:H6E	22:D:7050:LMU:H2B	1.05	1.04
6:F:190:LYS:HZ3	6:F:192:THR:CG2	1.57	1.04
12:L:153:PHE:HB2	12:L:155:GLU:OE1	1.55	1.04
15:1:78:ARG:HH21	15:1:179:LYS:HD2	1.14	1.04
19:1:1001:CLA:HMC1	19:1:1001:CLA:HBC3	1.34	1.04
17:3:150:TYR:C	17:3:152:ALA:N	1.99	1.04
22:4:7034:LMU:C8	22:4:7052:LMU:C2'	2.01	1.04
2:B:213:LEU:HD12	2:B:214:ASP:N	1.72	1.04
2:B:694:ARG:HG2	2:B:694:ARG:HH21	0.90	1.04
21:B:6020:BCR:H333	19:L:1502:CLA:CHC	1.87	1.04
15:1:162:LYS:H	15:1:164:PRO:HG3	1.18	1.04
17:3:201:ALA:HB1	17:3:202:TYR:CD2	1.92	1.04
1:A:308:ILE:CD1	19:A:1115:CLA:CHC	2.34	1.04
2:B:315:LEU:C	2:B:315:LEU:HD13	1.78	1.04
12:L:131:SER:N	12:L:201:TYR:CE2	2.25	1.04
16:2:226:ARG:CD	16:2:230:LEU:CD2	2.35	1.04
17:3:113:ALA:HB2	17:3:239:LEU:HD11	1.11	1.04
18:4:169:ASP:HA	18:4:173:LYS:HA	1.35	1.04
19:A:9022:CLA:H151	21:B:6017:BCR:H20C	1.36	1.04
2:B:202:SER:OG	2:B:270:LEU:HD22	1.57	1.04
19:B:1220:CLA:NA	19:B:1220:CLA:C4	2.21	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:SER:O	3:C:65:VAL:CG1	2.06	1.04
6:F:127:LYS:C	6:F:129:ARG:N	2.07	1.04
22:R:7014:LMU:H62	22:R:7014:LMU:H11	1.34	1.04
16:2:165:GLY:O	16:2:167:ARG:HB3	1.55	1.04
17:3:238:ILE:CD1	19:3:3003:CLA:HMC2	1.88	1.04
19:3:3011:CLA:HAC2	19:3:3012:CLA:C2A	1.88	1.04
1:A:86:LEU:HD13	1:A:178:MET:CE	1.87	1.03
1:A:126:ILE:O	1:A:127:VAL:HG22	1.54	1.03
1:A:575:LEU:HD12	1:A:576:GLY:HA3	1.40	1.03
2:B:294:ASN:HD22	7:G:94:GLN:CB	1.71	1.03
2:B:469:LYS:HG3	2:B:470:THR:HG23	1.35	1.03
6:F:170:ILE:HG21	21:F:6014:BCR:C37	1.88	1.03
12:L:145:LEU:HD11	21:L:6019:BCR:H313	1.39	1.03
13:N:139:LYS:HD2	13:N:142:LYS:HZ3	1.17	1.03
17:3:150:TYR:O	17:3:152:ALA:N	1.91	1.03
22:3:7003:LMU:C3B	22:3:7005:LMU:C5B	2.35	1.03
1:A:343:HIS:O	1:A:346:LEU:HB2	1.56	1.03
2:B:120:VAL:CA	2:B:123:TRP:CD1	2.39	1.03
2:B:459:PHE:CD2	19:B:1235:CLA:CMD	2.38	1.03
21:F:6016:BCR:H321	21:F:6016:BCR:HC8	1.05	1.03
11:K:97:ASP:CB	11:K:101:PHE:HE2	1.72	1.03
16:2:156:GLU:HG2	16:2:157:LEU:HD13	1.08	1.03
17:3:122:LEU:HD21	19:3:3006:CLA:C4D	1.87	1.03
17:3:150:TYR:O	17:3:151:TRP:C	1.95	1.03
18:4:158:GLN:HE22	19:4:1004:CLA:CHA	1.72	1.03
1:A:98:PHE:O	1:A:100:GLY:N	1.90	1.03
1:A:525:ASN:HB3	1:A:526:LYS:HG3	1.40	1.03
12:L:154:ASN:C	12:L:178:THR:HG23	1.79	1.03
13:N:130:ASN:O	13:N:132:THR:CG2	2.06	1.03
16:2:120:ILE:HG13	16:2:121:PHE:N	1.69	1.03
16:2:124:GLU:O	16:2:127:THR:HA	1.59	1.03
16:2:195:TYR:HD1	16:2:196:PRO:CD	1.70	1.03
21:3:6022:BCR:H23C	21:3:6022:BCR:H393	1.04	1.03
1:A:484:LEU:H	1:A:484:LEU:CD2	1.71	1.03
2:B:199:ILE:HG23	2:B:270:LEU:HD13	1.05	1.03
6:F:200:VAL:HG12	10:J:7:TYR:CB	1.89	1.03
7:G:72:LEU:HD22	7:G:124:ILE:HD12	1.37	1.03
8:H:58:LEU:HD12	8:H:62:THR:HG23	1.06	1.03
12:L:171:LYS:C	12:L:173:PRO:HD2	1.79	1.03
15:1:206:SER:O	15:1:209:PRO:HG3	1.59	1.03
16:2:229:MET:SD	16:2:230:LEU:HD13	1.98	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:111:LEU:HD12	18:4:112:PRO:CD	1.88	1.03
18:4:141:LEU:H	18:4:141:LEU:HD22	1.19	1.03
19:4:4002:CLA:CGD	19:4:4002:CLA:HAA2	1.86	1.03
19:A:1112:CLA:C3B	21:A:6002:BCR:H19C	1.89	1.03
2:B:224:PRO:HB2	2:B:227:THR:HB	1.36	1.03
2:B:490:ARG:HG3	2:B:490:ARG:NH1	1.61	1.03
3:C:5:VAL:CG2	3:C:65:VAL:CG2	2.36	1.03
5:E:99:THR:CG2	5:E:100:ARG:H	1.69	1.03
8:H:58:LEU:CG	8:H:61:THR:HB	1.88	1.03
8:H:58:LEU:HD13	8:H:62:THR:HG21	1.41	1.03
10:J:2:ARG:HH12	10:J:8:LEU:HD13	1.21	1.03
15:1:85:ILE:HA	15:1:88:ARG:CG	1.89	1.03
19:1:1013:CLA:C6	19:1:1014:CLA:CED	2.35	1.03
19:3:3016:CLA:H142	19:3:3016:CLA:C10	1.89	1.03
18:4:103:MET:HE1	18:4:208:GLY:N	1.66	1.03
18:4:210:LEU:O	18:4:214:PHE:HB2	1.59	1.03
1:A:370:ILE:HG23	1:A:403:GLY:HA3	1.36	1.02
1:A:555:ILE:HD11	19:A:9023:CLA:OBD	1.59	1.02
2:B:558:PRO:CG	2:B:703:VAL:HG22	1.88	1.02
7:G:64:ILE:O	7:G:68:THR:CG2	2.06	1.02
7:G:90:GLN:HB3	7:G:91:VAL:O	1.58	1.02
19:K:1143:CLA:O1A	19:K:1143:CLA:H3A	1.59	1.02
19:R:1150:CLA:HBA2	19:R:1150:CLA:HBD	1.35	1.02
15:1:170:PRO:HD2	15:1:173:TYR:CE2	1.93	1.02
18:4:193:ASN:O	18:4:194:PHE:CD1	2.12	1.02
1:A:64:PHE:CE2	1:A:74:ILE:CG2	2.42	1.02
2:B:199:ILE:HG23	2:B:270:LEU:CD1	1.88	1.02
2:B:459:PHE:CD2	19:B:1235:CLA:CAD	2.40	1.02
2:B:504:ASN:OD1	2:B:504:ASN:O	1.77	1.02
19:B:1235:CLA:HBC1	6:F:160:PHE:CZ	1.93	1.02
8:H:97:LEU:CD1	8:H:100:PHE:HB2	1.88	1.02
11:K:125:LYS:HB2	11:K:128:GLY:HA2	1.38	1.02
15:1:97:ILE:HD11	15:1:98:LEU:HA	1.34	1.02
15:1:162:LYS:N	15:1:164:PRO:HG3	1.73	1.02
16:2:130:GLY:HA3	16:2:131:ILE:HG13	1.03	1.02
18:4:175:TYR:O	18:4:194:PHE:CZ	2.12	1.02
1:A:541:VAL:HG11	1:A:615:HIS:CD2	1.93	1.02
2:B:122:GLN:C	2:B:126:THR:HB	1.79	1.02
4:D:140:LEU:HA	4:D:143:ARG:HB2	1.03	1.02
7:G:124:ILE:HG12	7:G:128:LEU:CD1	1.89	1.02
8:H:58:LEU:HD12	8:H:61:THR:CA	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:152:LEU:C	13:N:153:GLU:HG3	1.78	1.02
16:2:133:ASN:HD22	16:2:134:THR:CA	1.71	1.02
16:2:246:PRO:CB	16:2:247:ILE:HD13	1.89	1.02
1:A:249:ILE:C	1:A:251:ASN:H	1.60	1.02
1:A:255:LEU:HD13	1:A:280:PHE:HZ	1.20	1.02
2:B:5:ILE:HG22	2:B:6:PRO:HD3	1.05	1.02
2:B:90:ALA:CA	2:B:113:VAL:HG13	1.88	1.02
2:B:160:LYS:HD3	2:B:161:TRP:CD2	1.94	1.02
20:B:5002:PQN:C16	21:B:6017:BCR:C33	2.37	1.02
4:D:111:ILE:HG12	4:D:121:ILE:CG2	1.88	1.02
7:G:98:THR:OG1	7:G:101:GLU:CD	1.98	1.02
19:H:1241:CLA:CAC	21:I:6021:BCR:HC31	1.88	1.02
22:R:7020:LMU:H6E	22:R:7020:LMU:C5B	1.89	1.02
16:2:122:ILE:O	16:2:126:LEU:HG	1.60	1.02
17:3:150:TYR:HD2	17:3:151:TRP:NE1	1.45	1.02
1:A:107:GLU:OE2	1:A:161:GLU:HG3	1.58	1.02
1:A:249:ILE:O	1:A:251:ASN:N	1.93	1.02
19:A:1104:CLA:H43	19:A:1128:CLA:H11	1.38	1.02
2:B:310:PRO:O	19:B:1301:CLA:CHD	2.07	1.02
22:E:7048:LMU:C6B	22:E:7048:LMU:H3'	1.89	1.02
12:L:96:LEU:H	12:L:96:LEU:CD2	1.67	1.02
12:L:112:GLY:HA3	19:L:1503:CLA:CHC	1.90	1.02
12:L:171:LYS:O	12:L:173:PRO:HD2	1.59	1.02
16:2:122:ILE:CD1	19:2:2002:CLA:CAB	2.36	1.02
17:3:135:ALA:HB1	17:3:139:THR:HB	1.34	1.02
1:A:149:PHE:O	1:A:150:PHE:HB2	1.54	1.01
1:A:351:THR:O	19:A:1123:CLA:C19	2.07	1.01
1:A:370:ILE:HG22	1:A:400:MET:HA	1.41	1.01
2:B:542:ARG:HH11	2:B:542:ARG:CG	1.71	1.01
6:F:88:SER:OG	6:F:91:PHE:HB3	1.58	1.01
19:L:1148:CLA:HED1	19:L:1148:CLA:C1	1.90	1.01
16:2:117:ALA:O	16:2:120:ILE:HG12	1.58	1.01
1:A:21:LEU:O	1:A:21:LEU:CD1	2.08	1.01
1:A:157:GLY:HA3	1:A:229:ILE:HG22	1.40	1.01
1:A:340:GLY:O	1:A:343:HIS:HB2	1.58	1.01
2:B:120:VAL:CG2	2:B:123:TRP:HE1	1.74	1.01
4:D:95:GLN:NE2	4:D:96:VAL:HA	1.76	1.01
6:F:200:VAL:HG13	10:J:7:TYR:H	1.25	1.01
7:G:123:ASN:HA	7:G:126:ASP:OD2	1.58	1.01
19:H:1241:CLA:HAC2	21:I:6021:BCR:HC31	1.42	1.01
12:L:92:ALA:N	12:L:98:ARG:NH1	2.06	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:157:LYS:HB3	13:N:159:LYS:N	1.73	1.01
19:3:1147:CLA:CBC	19:3:1147:CLA:CMC	2.30	1.01
18:4:120:ILE:HD12	18:4:226:LYS:HG3	1.40	1.01
18:4:170:PRO:HG3	19:4:4011:CLA:C2D	1.90	1.01
19:4:1304:CLA:HAA2	19:4:1304:CLA:HED3	1.03	1.01
1:A:157:GLY:CA	1:A:229:ILE:HG21	1.89	1.01
19:A:1124:CLA:HED2	19:A:1125:CLA:CAD	1.91	1.01
19:A:1134:CLA:CBC	21:A:6008:BCR:HC31	1.90	1.01
2:B:120:VAL:HA	2:B:123:TRP:HD1	1.23	1.01
3:C:44:ARG:CA	4:D:182:GLN:OE1	2.08	1.01
15:1:64:PHE:O	15:1:69:LEU:HD13	1.60	1.01
15:1:84:LEU:O	15:1:88:ARG:HG3	1.60	1.01
15:1:112:GLN:HG2	15:1:113:GLU:H	1.20	1.01
17:3:243:ILE:HG12	19:3:3005:CLA:C4C	1.88	1.01
22:3:7005:LMU:C1	22:3:7005:LMU:H51	1.88	1.01
1:A:132:LEU:HD11	1:A:674:ALA:HB2	1.41	1.01
1:A:328:LYS:CD	1:A:332:GLU:HB2	1.88	1.01
1:A:368:LEU:HD21	19:A:1117:CLA:H93	1.42	1.01
2:B:294:ASN:CG	7:G:94:GLN:HG3	1.81	1.01
4:D:140:LEU:CD1	4:D:144:LEU:HB2	1.89	1.01
11:K:81:THR:CG2	11:K:83:GLY:H	1.71	1.01
15:1:97:ILE:CG1	15:1:98:LEU:N	2.22	1.01
19:1:1010:CLA:HBC3	19:1:1010:CLA:CHD	1.89	1.01
16:2:184:PRO:HG3	16:2:187:LYS:H	1.24	1.01
17:3:150:TYR:CB	17:3:151:TRP:HD1	1.71	1.01
1:A:227:LEU:CD2	1:A:296:LEU:O	2.09	1.01
1:A:249:ILE:HG23	17:3:136:TRP:HZ3	0.85	1.01
1:A:426:THR:HG22	1:A:428:TYR:CE2	1.96	1.01
1:A:575:LEU:CD1	1:A:576:GLY:HA3	1.90	1.01
19:A:9012:CLA:C1	2:B:616:LEU:CD1	2.39	1.01
2:B:732:LYS:CG	2:B:733:PHE:C	2.29	1.01
19:B:1223:CLA:HED1	19:B:1231:CLA:HBB2	1.41	1.01
15:1:78:ARG:HD3	19:1:1011:CLA:CMC	1.91	1.01
15:1:102:ALA:C	15:1:103:LEU:HD23	1.81	1.01
15:1:136:THR:O	15:1:140:ILE:HG12	1.61	1.01
15:1:170:PRO:HD2	15:1:173:TYR:CD2	1.96	1.01
1:A:487:VAL:HG13	1:A:489:ALA:H	0.89	1.00
19:A:1124:CLA:HBA2	19:A:1137:CLA:HED1	1.38	1.00
2:B:457:PRO:HB3	2:B:517:PHE:HB2	1.44	1.00
2:B:545:LYS:CD	2:B:546:LEU:H	1.74	1.00
19:B:1205:CLA:HBB2	19:B:1205:CLA:H92	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:5002:PQN:H162	21:B:6017:BCR:H333	1.05	1.00
11:K:49:ILE:O	11:K:52:PRO:CD	2.08	1.00
12:L:92:ALA:HB2	12:L:98:ARG:NH2	1.75	1.00
15:1:77:GLU:HG3	15:1:80:LYS:HD2	1.42	1.00
15:1:189:LYS:HE2	15:1:189:LYS:CA	1.86	1.00
16:2:125:PHE:C	16:2:127:THR:HG23	1.82	1.00
17:3:95:PRO:O	17:3:96:ARG:CG	2.09	1.00
17:3:122:LEU:HD22	19:3:3006:CLA:C1A	1.90	1.00
2:B:409:ALA:O	2:B:410:ARG:HB2	1.56	1.00
7:G:96:GLY:O	7:G:97:LEU:HG	1.62	1.00
13:N:147:SER:HB3	13:N:151:ASP:CA	1.91	1.00
15:1:162:LYS:H	15:1:164:PRO:CG	1.73	1.00
22:1:7004:LMU:H12	22:1:7004:LMU:H3'	1.43	1.00
16:2:254:LEU:C	16:2:254:LEU:CD2	2.30	1.00
18:4:96:LEU:HD11	18:4:100:ARG:CZ	1.90	1.00
1:A:342:GLY:HA2	1:A:430:ASP:CB	1.91	1.00
2:B:120:VAL:HG22	2:B:123:TRP:NE1	1.77	1.00
19:B:1222:CLA:HBB1	19:B:1236:CLA:HBB	1.40	1.00
19:B:1228:CLA:HHD	19:B:1228:CLA:CBC	1.91	1.00
3:C:44:ARG:HB3	4:D:182:GLN:CD	1.80	1.00
3:C:69:LEU:CD1	3:C:70:TRP:O	2.09	1.00
6:F:200:VAL:CG1	10:J:7:TYR:CB	2.39	1.00
7:G:84:ARG:CG	7:G:85:GLU:N	2.24	1.00
8:H:56:GLU:HG3	8:H:57:ASP:CA	1.92	1.00
12:L:79:ILE:HD11	19:L:1130:CLA:C4	1.90	1.00
15:1:77:GLU:HA	15:1:80:LYS:CD	1.91	1.00
15:1:134:LEU:CA	15:1:137:ILE:HD11	1.91	1.00
16:2:147:THR:HG22	16:2:148:ASP:OD2	1.61	1.00
1:A:267:THR:CG2	1:A:269:PHE:HE2	1.74	1.00
2:B:638:LEU:O	2:B:639:VAL:HG12	1.60	1.00
2:B:732:LYS:CG	2:B:734:GLY:N	2.23	1.00
4:D:140:LEU:HD21	4:D:144:LEU:CD1	1.90	1.00
4:D:187:ASN:HD22	4:D:187:ASN:N	1.60	1.00
11:K:99:ALA:O	11:K:103:LEU:HD11	1.60	1.00
15:1:93:ALA:HB1	19:1:1006:CLA:HHC	1.42	1.00
15:1:157:ASP:HB2	15:1:178:LYS:HB2	1.40	1.00
16:2:160:ILE:CG2	19:2:2012:CLA:HBB1	1.91	1.00
19:A:1125:CLA:CAB	19:A:1133:CLA:HMA2	1.89	1.00
2:B:50:HIS:HD2	19:B:1202:CLA:HAA2	1.24	1.00
2:B:247:THR:CA	2:B:250:ALA:HB2	1.92	1.00
5:E:107:PHE:CD2	5:E:109:LYS:HG3	1.97	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:164:LEU:HD12	12:L:165:THR:N	1.75	1.00
15:1:95:PRO:HA	15:1:98:LEU:CG	1.92	1.00
16:2:165:GLY:O	16:2:167:ARG:CB	2.07	1.00
17:3:176:TRP:O	17:3:178:LYS:HB2	1.62	1.00
1:A:116:ILE:O	1:A:136:VAL:O	1.77	1.00
2:B:353:TYR:CG	2:B:594:TRP:HZ3	1.79	1.00
2:B:560:ASP:HB2	3:C:66:ARG:HE	1.27	1.00
4:D:140:LEU:CA	4:D:143:ARG:HB2	1.90	1.00
22:E:7048:LMU:H3'	22:E:7048:LMU:H6'2	1.44	1.00
12:L:52:PRO:HB2	12:L:55:GLN:O	1.60	1.00
1:A:304:LEU:HG	19:A:1115:CLA:CBB	1.91	1.00
4:D:167:HIS:CD2	4:D:172:VAL:CG2	2.44	1.00
3:C:27:GLU:OE1	3:C:39:ILE:O	1.78	0.99
4:D:200:VAL:CG2	4:D:206:GLN:HE21	1.74	0.99
5:E:79:LYS:HA	5:E:84:TYR:CE1	1.97	0.99
22:N:7049:LMU:H61	22:N:7049:LMU:C1	1.91	0.99
22:R:7020:LMU:H5B	22:R:7020:LMU:C6'	1.90	0.99
15:1:68:GLY:O	15:1:72:VAL:HB	1.61	0.99
15:1:83:GLU:C	15:1:86:HIS:HD2	1.64	0.99
16:2:218:ARG:HB2	16:2:219:THR:CG2	1.91	0.99
18:4:177:LEU:HD13	18:4:178:PRO:HD3	1.42	0.99
19:4:4006:CLA:HMA1	22:4:7034:LMU:H62	1.40	0.99
1:A:328:LYS:CG	1:A:332:GLU:HB2	1.92	0.99
1:A:531:PRO:O	1:A:532:ILE:HG22	1.63	0.99
19:A:1124:CLA:CED	19:A:1125:CLA:CAD	2.40	0.99
22:A:7016:LMU:H22	22:A:7016:LMU:H61	1.42	0.99
19:A:9022:CLA:HBB2	19:A:9023:CLA:C1B	1.92	0.99
2:B:58:PHE:CD2	2:B:145:LEU:HD22	1.97	0.99
2:B:352:MET:HE1	19:B:1225:CLA:OBD	1.62	0.99
2:B:430:GLY:HA2	2:B:525:LEU:HD11	1.41	0.99
13:N:114:PHE:HB3	13:N:117:ALA:HB3	1.41	0.99
16:2:104:GLN:O	16:2:107:LEU:HG	1.62	0.99
16:2:171:ILE:CG1	16:2:172:LEU:N	2.25	0.99
16:2:172:LEU:HB3	16:2:173:ASN:ND2	1.77	0.99
18:4:88:LEU:C	18:4:90:TRP:HB3	1.82	0.99
1:A:246:HIS:CA	1:A:248:PHE:HE2	1.75	0.99
1:A:336:GLY:HA3	1:A:339:THR:OG1	1.62	0.99
2:B:131:THR:HG22	2:B:134:ASP:HB2	1.44	0.99
19:B:1213:CLA:HHD	19:B:1213:CLA:HBC2	1.44	0.99
4:D:201:LYS:H	4:D:201:LYS:CD	1.66	0.99
19:K:1146:CLA:HMA2	19:K:1146:CLA:O1A	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:186:ASN:CG	16:2:188:LEU:CD1	2.25	0.99
1:A:208:ALA:HA	1:A:310:PHE:O	1.62	0.99
1:A:451:ILE:CD1	19:A:1131:CLA:HED3	1.92	0.99
19:A:1138:CLA:H191	6:F:181:TYR:HB3	1.41	0.99
19:A:1141:CLA:HMA2	19:A:1141:CLA:C1	1.90	0.99
2:B:7:ARG:HH11	2:B:7:ARG:CG	1.75	0.99
2:B:58:PHE:CE2	2:B:145:LEU:CD2	2.44	0.99
2:B:58:PHE:HB2	2:B:146:SER:HB3	1.41	0.99
2:B:73:ASN:O	2:B:121:TYR:CZ	2.16	0.99
17:3:127:LEU:CB	19:3:1147:CLA:HED1	1.88	0.99
18:4:232:LEU:HB2	18:4:236:ILE:HD12	1.41	0.99
1:A:22:VAL:HG22	1:A:22:VAL:O	1.59	0.99
1:A:51:THR:HG21	19:A:1139:CLA:CBB	1.92	0.99
1:A:422:TYR:N	1:A:422:TYR:HD1	1.58	0.99
13:N:130:ASN:HB3	13:N:139:LYS:HG2	1.40	0.99
15:1:66:PRO:HD2	15:1:67:LEU:H	1.23	0.99
17:3:173:PHE:HD1	17:3:174:GLN:N	1.59	0.99
19:4:4006:CLA:C10	22:4:7034:LMU:C12	2.40	0.99
2:B:294:ASN:ND2	7:G:94:GLN:N	2.11	0.99
2:B:531:THR:HG22	19:B:1222:CLA:HMC2	1.44	0.99
3:C:80:ALA:O	3:C:81:TYR:HB3	1.62	0.99
15:1:137:ILE:O	15:1:141:GLU:HG2	1.63	0.99
16:2:139:THR:HG23	16:2:140:ALA:H	1.21	0.99
17:3:109:ALA:HA	17:3:111:LEU:CB	1.91	0.99
1:A:249:ILE:O	1:A:252:ARG:HG3	1.62	0.99
1:A:534:LEU:CD1	1:A:535:GLY:N	2.25	0.99
2:B:694:ARG:HG2	2:B:694:ARG:NH2	1.62	0.99
4:D:103:THR:HG22	4:D:128:LEU:HG	1.42	0.99
14:R:52:UNK:CA	14:R:53:UNK:CB	2.36	0.99
19:2:2002:CLA:HBC2	19:2:2002:CLA:HHD	1.43	0.99
22:4:7052:LMU:H61	22:4:7052:LMU:O1'	1.61	0.99
2:B:199:ILE:CG2	2:B:270:LEU:HD13	1.92	0.99
19:B:1205:CLA:H92	19:B:1205:CLA:CBB	1.93	0.99
4:D:200:VAL:HG21	4:D:206:GLN:HE21	0.84	0.99
17:3:96:ARG:NH1	17:3:96:ARG:HB2	1.77	0.99
19:A:1124:CLA:CED	19:A:1125:CLA:HMD1	1.92	0.99
19:A:1141:CLA:H121	19:A:1141:CLA:C7	1.91	0.99
2:B:85:ARG:HG2	2:B:85:ARG:HH11	1.24	0.99
2:B:268:LEU:HD21	19:B:1214:CLA:CMA	1.91	0.99
19:B:1202:CLA:O1A	19:B:1202:CLA:H62	1.63	0.99
8:H:97:LEU:CD1	8:H:100:PHE:CB	2.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:178:LYS:HG3	15:1:179:LYS:H	1.23	0.99
15:1:189:LYS:HB2	19:1:1007:CLA:CMC	1.93	0.99
16:2:237:PHE:HA	16:2:240:ILE:CD1	1.92	0.99
1:A:368:LEU:CD2	19:A:1117:CLA:C9	2.41	0.99
1:A:699:TYR:OH	2:B:533:ILE:HG22	1.61	0.99
2:B:490:ARG:HH11	2:B:490:ARG:CG	1.75	0.99
21:F:6016:BCR:HC8	21:F:6016:BCR:C32	1.89	0.99
7:G:102:ALA:HA	7:G:104:ASP:CG	1.82	0.99
8:H:77:ASN:CG	8:H:78:PRO:HD2	1.81	0.99
12:L:79:ILE:CD1	19:L:1130:CLA:H42	1.92	0.99
18:4:158:GLN:C	19:4:1004:CLA:HMA2	1.84	0.99
1:A:163:GLN:CG	1:A:164:LEU:H	1.74	0.98
1:A:365:LEU:CD2	19:A:1103:CLA:HED3	1.92	0.98
1:A:715:LYS:NZ	6:F:230:ASN:OD1	1.95	0.98
2:B:58:PHE:CB	2:B:146:SER:HB3	1.93	0.98
7:G:90:GLN:HB2	7:G:92:PRO:HD3	1.43	0.98
12:L:60:ILE:CG2	12:L:61:ASN:N	2.12	0.98
12:L:96:LEU:HD23	12:L:96:LEU:N	1.77	0.98
15:1:129:VAL:HG12	15:1:130:PRO:HD3	1.41	0.98
15:1:161:LYS:HE2	15:1:162:LYS:HB2	1.45	0.98
15:1:190:ASN:HD21	19:1:1002:CLA:CHA	1.76	0.98
16:2:177:VAL:HG12	16:2:178:ASN:CB	1.93	0.98
18:4:223:VAL:O	18:4:223:VAL:HG12	1.63	0.98
1:A:567:ARG:HH12	4:D:89:GLY:HA2	1.21	0.98
11:K:63:LEU:HD13	11:K:63:LEU:N	1.75	0.98
17:3:159:VAL:HG13	17:3:160:LEU:N	1.72	0.98
1:A:106:TYR:O	1:A:110:LEU:HD23	1.61	0.98
1:A:120:ALA:N	1:A:145:ILE:CD1	2.26	0.98
1:A:397:THR:HG22	1:A:613:ILE:CG1	1.92	0.98
7:G:84:ARG:HA	19:G:1242:CLA:HMA3	1.41	0.98
15:1:198:PHE:O	15:1:202:CYS:HB3	1.63	0.98
1:A:90:PHE:CE1	19:A:1103:CLA:H91	1.99	0.98
2:B:476:ILE:CG2	2:B:479:SER:OG	2.11	0.98
4:D:158:PHE:HB3	4:D:159:PRO:O	1.60	0.98
8:H:63:GLY:O	8:H:66:ASP:OD1	1.81	0.98
19:J:1308:CLA:C9	19:2:2014:CLA:O1D	2.11	0.98
13:N:146:LEU:CD1	17:3:142:ILE:C	2.31	0.98
17:3:150:TYR:HD2	17:3:151:TRP:CE2	1.80	0.98
19:4:4003:CLA:HBC2	19:4:4003:CLA:HMC1	1.38	0.98
1:A:605:MET:HA	1:A:608:SER:OG	1.63	0.98
1:A:711:HIS:CD2	19:A:1139:CLA:HBC1	1.98	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1125:CLA:HMC1	19:A:1125:CLA:HBC2	1.43	0.98
2:B:622:ASP:HB2	2:B:626:LEU:HD12	1.42	0.98
3:C:1:MET:HG2	3:C:4:SER:OG	1.62	0.98
8:H:78:PRO:CD	19:L:1501:CLA:CMD	2.40	0.98
19:4:1304:CLA:C20	19:4:1304:CLA:H151	1.93	0.98
1:A:132:LEU:O	1:A:671:SER:O	1.80	0.98
2:B:189:ALA:HB2	19:B:1225:CLA:H203	1.46	0.98
2:B:429:LEU:O	2:B:525:LEU:CD1	2.11	0.98
6:F:97:GLN:CD	6:F:98:ALA:H	1.67	0.98
13:N:146:LEU:CD2	17:3:142:ILE:O	2.10	0.98
1:A:249:ILE:HG21	17:3:136:TRP:HZ3	1.24	0.98
2:B:303:TYR:HA	2:B:306:GLU:HB2	1.45	0.98
22:E:7048:LMU:H72	22:E:7048:LMU:H111	1.45	0.98
8:H:58:LEU:HD13	8:H:62:THR:CG2	1.92	0.98
8:H:89:ALA:HA	8:H:92:THR:HB	1.45	0.98
19:L:1148:CLA:HHD	19:L:1148:CLA:CBC	1.93	0.98
16:2:237:PHE:CA	16:2:240:ILE:HD12	1.92	0.98
16:2:269:LYS:HA	16:2:269:LYS:HZ2	1.22	0.98
1:A:64:PHE:HZ	1:A:77:LYS:HE2	1.29	0.98
1:A:267:THR:HG22	1:A:269:PHE:HE2	1.18	0.98
19:A:1119:CLA:HMD3	19:A:1121:CLA:CBB	1.93	0.98
2:B:304:ILE:CD1	19:B:1216:CLA:CED	2.39	0.98
13:N:132:THR:OG1	13:N:137:LEU:O	1.82	0.98
16:2:113:ALA:C	16:2:114:MET:HE3	1.84	0.98
1:A:68:THR:CG2	1:A:70:ASP:H	1.76	0.98
1:A:193:LEU:HA	1:A:196:PHE:HE2	1.27	0.98
13:N:139:LYS:CB	13:N:142:LYS:CD	2.41	0.98
19:A:1119:CLA:HMD3	19:A:1121:CLA:HBB2	0.98	0.98
19:A:9022:CLA:C15	21:B:6017:BCR:H20C	1.93	0.98
6:F:219:ARG:HH11	6:F:219:ARG:CG	1.75	0.98
21:J:6012:BCR:H23C	21:J:6012:BCR:H393	1.46	0.98
18:4:96:LEU:HD11	18:4:100:ARG:NH1	1.77	0.98
1:A:51:THR:OG1	19:A:1139:CLA:HBB2	1.62	0.97
1:A:89:ILE:O	1:A:92:TRP:O	1.82	0.97
1:A:217:SER:HG	21:A:6002:BCR:H15C	1.24	0.97
7:G:102:ALA:HA	7:G:104:ASP:OD1	1.63	0.97
8:H:97:LEU:HD11	8:H:100:PHE:CB	1.94	0.97
12:L:154:ASN:O	12:L:178:THR:CG2	2.11	0.97
1:A:454:GLY:H	1:A:457:SER:HB3	1.23	0.97
2:B:268:LEU:CD2	19:B:1214:CLA:HMA2	1.93	0.97
7:G:99:HIS:C	7:G:101:GLU:HB2	1.84	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:155:GLU:HA	12:L:178:THR:CG2	1.93	0.97
16:2:119:GLY:O	16:2:123:PRO:HG2	1.63	0.97
18:4:87:ASN:CB	18:4:90:TRP:CE3	2.46	0.97
18:4:172:PHE:HB2	18:4:194:PHE:CD2	1.97	0.97
2:B:486:LEU:HB2	19:B:1232:CLA:HMD3	1.44	0.97
2:B:732:LYS:HB3	2:B:733:PHE:HA	1.45	0.97
7:G:99:HIS:HA	7:G:100:PHE:HB3	1.46	0.97
22:H:7032:LMU:H31	22:H:7032:LMU:C1B	1.92	0.97
12:L:79:ILE:HD11	19:L:1130:CLA:H42	1.00	0.97
16:2:103:VAL:CG1	16:2:104:GLN:OE1	2.12	0.97
19:2:2007:CLA:HBC1	19:3:2009:CLA:HED2	1.00	0.97
19:4:1304:CLA:H151	19:4:1304:CLA:H203	1.45	0.97
1:A:129:GLN:O	1:A:130:GLU:HB3	1.62	0.97
2:B:353:TYR:CD2	2:B:594:TRP:CZ3	2.51	0.97
11:K:127:ILE:HB	11:K:129:ALA:HB1	1.45	0.97
12:L:73:VAL:HA	19:L:1504:CLA:CMA	1.92	0.97
15:1:149:GLU:HG2	15:1:152:ARG:HH12	1.16	0.97
18:4:158:GLN:HB3	19:4:1004:CLA:HMA2	1.43	0.97
11:K:92:GLY:O	11:K:93:LEU:CG	2.11	0.97
1:A:491:TRP:HE1	19:A:1135:CLA:H12	1.27	0.97
1:A:564:ARG:HB3	1:A:564:ARG:HH21	1.29	0.97
15:1:158:PRO:HA	15:1:175:LYS:HG3	1.46	0.97
2:B:172:GLU:O	2:B:176:ASN:HB2	1.64	0.97
2:B:310:PRO:HG3	19:B:1220:CLA:HMA1	1.47	0.97
2:B:708:VAL:O	2:B:712:HIS:HB2	1.62	0.97
8:H:99:LYS:O	8:H:101:LEU:N	1.97	0.97
11:K:125:LYS:HA	11:K:126:ASN:HB3	0.97	0.97
13:N:139:LYS:HE3	13:N:142:LYS:HE2	0.98	0.97
15:1:171:LEU:HA	15:1:173:TYR:CZ	2.00	0.97
1:A:296:LEU:HD12	1:A:297:THR:HG22	1.47	0.97
19:A:1122:CLA:C1D	21:A:6007:BCR:H19C	1.93	0.97
2:B:213:LEU:HD12	2:B:214:ASP:H	1.29	0.97
2:B:527:LEU:HD13	19:B:1236:CLA:CMA	1.94	0.97
4:D:140:LEU:HA	4:D:143:ARG:CB	1.93	0.97
6:F:139:LEU:HD13	6:F:149:ILE:CD1	1.93	0.97
8:H:109:LEU:O	8:H:113:SER:HB2	1.63	0.97
18:4:169:ASP:CA	18:4:173:LYS:HA	1.94	0.97
1:A:64:PHE:CE2	1:A:74:ILE:HG21	2.00	0.97
6:F:221:LEU:HD23	6:F:222:LEU:HD23	1.46	0.97
22:H:7030:LMU:H91	22:H:7030:LMU:C5	1.93	0.97
11:K:49:ILE:HA	11:K:52:PRO:CG	1.92	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:122:PHE:N	13:N:122:PHE:HD2	1.60	0.97
15:1:67:LEU:CD1	15:1:68:GLY:N	2.27	0.97
15:1:78:ARG:NH2	15:1:179:LYS:HD2	1.80	0.97
16:2:126:LEU:HB3	19:2:2006:CLA:H192	1.45	0.97
16:2:237:PHE:HA	16:2:240:ILE:HD12	0.98	0.97
2:B:666:SER:HB3	2:B:671:TRP:HE1	1.27	0.96
5:E:99:THR:HG22	5:E:100:ARG:H	0.81	0.96
8:H:113:SER:OG	19:H:1207:CLA:H61	1.65	0.96
11:K:98:PRO:HD2	11:K:99:ALA:H	1.28	0.96
13:N:136:ASP:O	13:N:137:LEU:HD22	1.64	0.96
2:B:594:TRP:O	2:B:595:HIS:HB3	1.61	0.96
8:H:86:THR:HG22	8:H:87:PHE:O	1.65	0.96
8:H:121:LEU:HB3	8:H:122:PRO:CD	1.95	0.96
22:R:7021:LMU:H1'	22:R:7021:LMU:H31	1.45	0.96
16:2:160:ILE:HG21	19:2:2012:CLA:HBB1	1.44	0.96
1:A:426:THR:HA	1:A:428:TYR:CZ	2.00	0.96
2:B:98:GLN:C	2:B:100:ALA:H	1.63	0.96
2:B:256:THR:O	2:B:272:ASP:OD1	1.83	0.96
21:F:6016:BCR:C8	21:F:6016:BCR:C32	2.38	0.96
15:1:85:ILE:HA	15:1:88:ARG:HG3	1.47	0.96
17:3:254:GLN:HG3	17:3:255:ASN:H	1.27	0.96
18:4:145:GLU:HG3	18:4:146:PHE:HD1	1.20	0.96
2:B:189:ALA:CB	19:B:1225:CLA:H203	1.96	0.96
3:C:44:ARG:H	4:D:182:GLN:HG3	1.27	0.96
11:K:49:ILE:C	11:K:52:PRO:HG2	1.77	0.96
16:2:118:ALA:C	16:2:121:PHE:CE2	2.37	0.96
17:3:176:TRP:CH2	17:3:199:ASN:OD1	2.15	0.96
2:B:225:LEU:HD13	2:B:233:TYR:HH	1.29	0.96
2:B:621:ARG:O	2:B:625:TRP:HB3	1.66	0.96
3:C:72:GLU:HG2	3:C:77:MET:HE2	1.48	0.96
16:2:172:LEU:O	16:2:174:PRO:HD3	1.63	0.96
17:3:176:TRP:O	17:3:178:LYS:CB	2.13	0.96
18:4:173:LYS:NZ	18:4:201:LYS:CG	2.27	0.96
19:4:4002:CLA:HMA2	19:4:4002:CLA:CBA	1.94	0.96
3:C:44:ARG:H	4:D:182:GLN:CG	1.77	0.96
5:E:127:GLU:HB3	5:E:128:VAL:O	1.65	0.96
6:F:130:PHE:H	6:F:133:TYR:HE1	1.01	0.96
13:N:157:LYS:N	13:N:157:LYS:HE2	1.80	0.96
18:4:159:ASP:CG	18:4:171:ILE:HD11	1.85	0.96
1:A:281:LEU:HD22	19:A:1115:CLA:HED3	1.45	0.96
1:A:491:TRP:NE1	19:A:1135:CLA:H12	1.79	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:ARG:CZ	15:1:67:LEU:HD21	1.94	0.96
5:E:93:VAL:HG23	5:E:103:VAL:HB	1.46	0.96
16:2:167:ARG:HA	16:2:167:ARG:NE	1.77	0.96
18:4:111:LEU:HD12	18:4:112:PRO:N	1.80	0.96
1:A:308:ILE:HD13	19:A:1115:CLA:H102	1.48	0.96
1:A:430:ASP:O	1:A:432:LEU:N	1.98	0.96
2:B:480:SER:O	2:B:481:THR:HG22	1.63	0.96
2:B:527:LEU:HD22	19:B:1222:CLA:ND	1.80	0.96
8:H:111:TYR:C	8:H:112:LEU:HD23	1.86	0.96
16:2:118:ALA:C	16:2:121:PHE:HE2	1.68	0.96
1:A:24:ARG:H	1:A:24:ARG:CD	1.75	0.96
1:A:308:ILE:HD13	19:A:1115:CLA:HHC	1.46	0.96
2:B:422:LEU:HD13	2:B:535:VAL:HG11	1.47	0.96
12:L:138:VAL:O	12:L:142:SER:OG	1.84	0.96
13:N:146:LEU:HD13	17:3:142:ILE:C	1.85	0.96
17:3:96:ARG:HH11	17:3:96:ARG:HG3	1.25	0.96
17:3:197:SER:HB3	17:3:206:PRO:HD3	1.46	0.96
1:A:252:ARG:H	1:A:252:ARG:HD3	1.30	0.96
1:A:394:SER:HB2	19:A:1126:CLA:HMA1	1.45	0.96
19:B:1219:CLA:HBB2	19:B:1219:CLA:H72	1.47	0.96
21:B:6020:BCR:H333	19:L:1502:CLA:NB	1.81	0.96
4:D:87:THR:CG2	12:L:69:LEU:HD12	1.95	0.96
19:F:1305:CLA:H42	19:4:1306:CLA:HAA1	1.45	0.96
19:H:1145:CLA:C2	19:H:1145:CLA:HMA2	1.95	0.96
18:4:168:GLN:HB3	18:4:172:PHE:CE1	1.99	0.96
2:B:131:THR:CG2	2:B:134:ASP:HB2	1.94	0.95
2:B:569:ASP:OD1	2:B:706:ARG:NH1	1.99	0.95
4:D:124:GLU:OE1	4:D:125:GLY:HA3	1.66	0.95
4:D:140:LEU:CD1	4:D:144:LEU:CB	2.44	0.95
6:F:207:LEU:HD21	6:F:208:PHE:CD1	2.00	0.95
12:L:141:LEU:CD1	12:L:145:LEU:CD1	2.44	0.95
13:N:133:GLY:C	13:N:134:CYS:SG	2.44	0.95
13:N:143:VAL:CB	13:N:144:PRO:HD2	1.95	0.95
15:1:177:PRO:HD2	15:1:180:LEU:CD2	1.92	0.95
16:2:103:VAL:O	16:2:106:GLU:N	1.99	0.95
17:3:130:GLN:HB3	17:3:132:THR:H	0.79	0.95
18:4:175:TYR:HB3	18:4:194:PHE:CD1	2.00	0.95
1:A:412:ALA:HB2	1:A:598:VAL:HG11	1.47	0.95
2:B:282:PHE:HZ	19:B:1213:CLA:C1	1.79	0.95
2:B:292:ARG:NH1	2:B:296:GLY:H	1.63	0.95
5:E:111:ASN:HD21	5:E:113:ALA:H	0.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:148:LEU:HD12	6:F:148:LEU:O	1.65	0.95
11:K:62:SER:OG	11:K:63:LEU:HD13	1.64	0.95
15:1:200:GLY:O	15:1:203:VAL:HG12	1.66	0.95
18:4:228:PRO:HB2	18:4:229:PHE:CE1	2.00	0.95
1:A:425:THR:O	1:A:427:ARG:HD3	1.66	0.95
2:B:459:PHE:HD2	19:B:1235:CLA:C4D	1.77	0.95
5:E:107:PHE:CE2	5:E:109:LYS:CG	2.48	0.95
18:4:145:GLU:HG3	18:4:146:PHE:CE1	2.00	0.95
3:C:44:ARG:N	4:D:182:GLN:OE1	2.00	0.95
8:H:78:PRO:CG	19:L:1501:CLA:HMD1	1.95	0.95
8:H:119:ASP:O	8:H:120:ILE:CG2	2.13	0.95
15:1:76:LEU:HB3	15:1:77:GLU:OE1	1.66	0.95
16:2:183:PHE:N	16:2:187:LYS:HG2	1.81	0.95
19:3:3008:CLA:HBA2	19:3:3008:CLA:CGD	1.95	0.95
21:A:6007:BCR:H382	21:A:6007:BCR:H23C	1.44	0.95
2:B:180:SER:HB3	2:B:288:GLY:HA3	1.47	0.95
2:B:382:ILE:CG2	2:B:383:MET:H	1.80	0.95
5:E:89:SER:HB2	5:E:106:ARG:NH1	1.81	0.95
19:J:1311:CLA:HED3	19:J:1311:CLA:C1A	1.97	0.95
15:1:94:VAL:O	15:1:97:ILE:HG23	1.64	0.95
16:2:240:ILE:HG23	16:2:263:PHE:HB3	1.46	0.95
17:3:181:SER:CB	19:3:2009:CLA:C11	2.40	0.95
2:B:103:ALA:HB1	2:B:106:ARG:HD2	1.49	0.95
2:B:478:LEU:O	2:B:478:LEU:HD23	1.65	0.95
3:C:62:PHE:CE2	5:E:80:GLU:CD	2.40	0.95
6:F:204:SER:O	6:F:207:LEU:HD12	1.65	0.95
7:G:89:LYS:NZ	7:G:89:LYS:CA	2.29	0.95
22:R:7022:LMU:H21	22:R:7022:LMU:C2'	1.95	0.95
16:2:218:ARG:HB2	16:2:219:THR:HG22	1.45	0.95
18:4:187:GLY:O	18:4:188:ILE:HB	1.64	0.95
15:1:91:MET:O	15:1:95:PRO:CD	2.13	0.95
1:A:302:HIS:O	1:A:306:ILE:HG12	1.67	0.95
1:A:714:LEU:HD13	21:F:6016:BCR:H393	1.48	0.95
19:B:1226:CLA:CB	19:B:1226:CLA:HMC1	1.97	0.95
17:3:139:THR:CG2	17:3:140:GLY:H	1.79	0.95
18:4:172:PHE:CB	18:4:194:PHE:CZ	2.49	0.95
1:A:281:LEU:HD11	19:A:1115:CLA:HED1	1.46	0.95
19:A:9022:CLA:C9	19:A:9023:CLA:H91	1.97	0.95
22:H:7011:LMU:H2B	22:H:7011:LMU:H6E	1.46	0.95
19:L:1503:CLA:HHD	19:L:1503:CLA:CB	1.96	0.95
15:1:128:PRO:HG2	15:1:131:TRP:CH2	2.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:124:PRO:HB2	18:4:126:TRP:H	1.31	0.95
2:B:294:ASN:HD22	7:G:94:GLN:N	1.64	0.95
3:C:5:VAL:HB	3:C:65:VAL:HG23	1.47	0.95
3:C:5:VAL:HG21	3:C:65:VAL:CG2	1.97	0.95
3:C:34:CYS:H	3:C:37:LYS:HB3	1.30	0.95
4:D:156:ARG:NH2	4:D:158:PHE:CE1	2.35	0.95
6:F:204:SER:O	6:F:207:LEU:N	2.00	0.95
6:F:207:LEU:CD1	6:F:208:PHE:H	1.78	0.95
7:G:72:LEU:CD2	7:G:124:ILE:HD12	1.90	0.95
8:H:78:PRO:CD	19:L:1501:CLA:HMD3	1.96	0.95
19:K:1143:CLA:HBC1	22:K:7001:LMU:O3B	1.63	0.95
14:R:40:UNK:N	14:R:41:UNK:CB	2.30	0.95
19:2:2001:CLA:CBC	19:2:2001:CLA:HMC1	1.97	0.95
1:A:190:ALA:HB1	1:A:191:PRO:CD	1.97	0.94
1:A:586:ARG:HG3	3:C:49:VAL:HG21	1.48	0.94
2:B:622:ASP:CB	2:B:626:LEU:CD1	2.44	0.94
12:L:128:GLN:HA	12:L:130:GLY:CA	1.96	0.94
12:L:131:SER:CA	12:L:201:TYR:CE2	2.50	0.94
14:R:34:UNK:N	14:R:36:UNK:CB	2.30	0.94
1:A:26:PRO:HB2	1:A:27:ILE:HG13	1.49	0.94
1:A:73:GLU:HG3	1:A:74:ILE:N	1.82	0.94
2:B:298:GLY:HA2	19:B:1218:CLA:HMD3	1.49	0.94
6:F:150:VAL:HG21	6:F:160:PHE:HB2	1.48	0.94
7:G:99:HIS:CA	7:G:100:PHE:HB3	1.97	0.94
17:3:150:TYR:HB3	17:3:151:TRP:NE1	1.82	0.94
17:3:207:PHE:HD1	17:3:207:PHE:O	1.50	0.94
1:A:102:ARG:C	1:A:103:PHE:HD2	1.70	0.94
19:A:1112:CLA:HMB2	21:A:6002:BCR:C38	1.98	0.94
2:B:20:ARG:HH11	2:B:20:ARG:CG	1.78	0.94
2:B:293:THR:HG21	19:B:1209:CLA:HMA2	1.49	0.94
2:B:315:LEU:HD13	2:B:315:LEU:O	1.68	0.94
2:B:490:ARG:HG3	2:B:490:ARG:HH11	0.82	0.94
19:B:1220:CLA:HAA1	19:B:1220:CLA:H43	1.48	0.94
5:E:76:ILE:HB	5:E:84:TYR:O	1.67	0.94
6:F:119:ILE:HG13	6:F:120:LYS:N	1.77	0.94
17:3:103:VAL:O	17:3:107:ARG:HD2	1.67	0.94
19:A:1126:CLA:H203	21:J:6012:BCR:H17C	1.46	0.94
2:B:294:ASN:HD22	7:G:94:GLN:CG	1.74	0.94
22:D:7050:LMU:H2B	22:D:7050:LMU:C6'	1.97	0.94
2:B:247:THR:CA	2:B:250:ALA:CB	2.45	0.94
2:B:542:ARG:HH11	2:B:542:ARG:HG3	1.29	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:213:TRP:HB2	6:F:216:ALA:CB	1.97	0.94
8:H:76:TYR:HH	12:L:90:ARG:CD	1.69	0.94
11:K:97:ASP:HB2	11:K:101:PHE:CE2	2.02	0.94
16:2:168:TRP:HD1	16:2:171:ILE:HG23	1.32	0.94
1:A:248:PHE:H	1:A:248:PHE:HD2	1.11	0.94
1:A:502:THR:HB	1:A:504:ALA:HB3	1.46	0.94
1:A:588:GLY:HA3	2:B:668:ARG:HD3	1.46	0.94
19:A:1124:CLA:C7	19:A:1125:CLA:HED1	1.97	0.94
2:B:7:ARG:HH11	2:B:7:ARG:HG3	1.30	0.94
5:E:75:LYS:HA	5:E:87:THR:HG22	1.50	0.94
15:1:85:ILE:O	15:1:88:ARG:HB2	1.67	0.94
16:2:160:ILE:HG22	19:2:2012:CLA:HBB2	1.47	0.94
16:2:189:THR:O	16:2:192:ASP:O	1.86	0.94
17:3:96:ARG:CA	17:3:99:ALA:H	1.79	0.94
1:A:338:PHE:HE1	19:A:1151:CLA:CBB	1.61	0.94
2:B:317:ARG:HH22	2:B:410:ARG:CG	1.76	0.94
8:H:112:LEU:HD23	8:H:112:LEU:N	1.78	0.94
11:K:127:ILE:HG12	11:K:130:LEU:HD12	1.46	0.94
15:1:80:LYS:O	15:1:83:GLU:CB	2.15	0.94
1:A:331:LEU:CD1	1:A:346:LEU:HB3	1.97	0.94
1:A:523:VAL:HG13	1:A:524:GLY:N	1.80	0.94
19:A:1237:CLA:H141	12:L:141:LEU:HD23	1.47	0.94
2:B:73:ASN:O	2:B:121:TYR:CE1	2.21	0.94
2:B:454:LEU:HD11	6:F:147:HIS:HA	1.47	0.94
3:C:72:GLU:CG	3:C:77:MET:HE2	1.98	0.94
4:D:141:GLY:H	4:D:144:LEU:H	1.01	0.94
11:K:63:LEU:HD22	11:K:63:LEU:H	1.31	0.94
11:K:70:PHE:C	11:K:70:PHE:HD1	1.71	0.94
15:1:95:PRO:O	15:1:98:LEU:HB2	1.66	0.94
16:2:182:ILE:CB	16:2:187:LYS:HB3	1.97	0.94
16:2:187:LYS:HE3	16:2:187:LYS:CA	1.97	0.94
19:2:2014:CLA:H41	19:2:2014:CLA:C7	1.98	0.94
17:3:96:ARG:HH11	17:3:96:ARG:CB	1.79	0.94
17:3:150:TYR:O	17:3:152:ALA:CB	2.15	0.94
18:4:89:ARG:CD	18:4:90:TRP:H	1.79	0.94
18:4:120:ILE:HD11	18:4:226:LYS:CB	1.96	0.94
18:4:226:LYS:CE	18:4:226:LYS:H	1.80	0.94
19:A:1122:CLA:CBB	21:A:6007:BCR:H351	1.98	0.94
2:B:394:PHE:O	2:B:542:ARG:NE	2.01	0.94
4:D:123:ARG:HH21	22:D:7050:LMU:C4B	1.71	0.94
4:D:140:LEU:CD2	4:D:144:LEU:CD1	2.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:76:ALA:H	11:K:78:ARG:HH12	1.02	0.94
11:K:115:ILE:HA	11:K:118:VAL:HG22	1.46	0.94
15:1:78:ARG:NH2	15:1:179:LYS:CB	2.30	0.94
15:1:130:PRO:O	15:1:131:TRP:HE3	1.49	0.94
16:2:229:MET:SD	16:2:230:LEU:HA	2.06	0.94
18:4:87:ASN:HB2	18:4:90:TRP:CD2	2.02	0.94
1:A:157:GLY:CA	1:A:229:ILE:CG2	2.45	0.94
1:A:248:PHE:CD2	1:A:248:PHE:N	2.36	0.94
2:B:58:PHE:HB2	2:B:146:SER:CB	1.97	0.94
2:B:493:TRP:CH2	19:B:1214:CLA:H122	2.02	0.94
2:B:622:ASP:HB2	2:B:626:LEU:CD1	1.96	0.94
3:C:62:PHE:HZ	5:E:80:GLU:CD	1.60	0.94
6:F:82:LEU:HG	6:F:83:THR:N	1.72	0.94
13:N:96:LYS:HG3	13:N:97:THR:OG1	1.67	0.94
16:2:254:LEU:CD2	16:2:255:ALA:N	2.30	0.94
18:4:169:ASP:O	18:4:173:LYS:CG	2.15	0.94
2:B:268:LEU:HD21	19:B:1214:CLA:HMA2	0.98	0.93
2:B:493:TRP:HE1	19:B:1213:CLA:HAC2	1.30	0.93
2:B:685:THR:OG1	19:L:1130:CLA:H3A	1.68	0.93
4:D:100:TYR:CE1	4:D:134:LYS:HG3	2.02	0.93
5:E:78:ARG:NH2	5:E:125:ILE:CG2	2.29	0.93
7:G:84:ARG:NE	7:G:85:GLU:HB3	1.83	0.93
11:K:60:SER:HA	11:K:63:LEU:HD21	1.49	0.93
16:2:237:PHE:HE1	16:2:241:TYR:CZ	1.86	0.93
1:A:249:ILE:HG12	1:A:250:LEU:N	1.81	0.93
19:A:9012:CLA:H11	2:B:616:LEU:HD12	1.45	0.93
2:B:130:ARG:HH11	2:B:130:ARG:HG3	1.32	0.93
2:B:294:ASN:CB	7:G:94:GLN:CD	2.37	0.93
3:C:1:MET:N	3:C:4:SER:OG	2.01	0.93
11:K:115:ILE:HG12	11:K:122:LEU:H	1.24	0.93
11:K:118:VAL:O	11:K:121:VAL:HG23	1.69	0.93
17:3:173:PHE:HD1	17:3:173:PHE:C	1.70	0.93
1:A:382:TYR:OH	19:A:1127:CLA:H42	1.67	0.93
2:B:340:SER:HA	19:B:1223:CLA:H51	1.49	0.93
2:B:560:ASP:HB2	3:C:66:ARG:NE	1.82	0.93
11:K:99:ALA:O	11:K:103:LEU:CD1	2.15	0.93
1:A:462:ILE:HD11	19:A:9022:CLA:H51	1.50	0.93
19:A:1124:CLA:CED	19:A:1125:CLA:CMD	2.45	0.93
2:B:131:THR:CG2	2:B:134:ASP:H	1.81	0.93
3:C:66:ARG:HH21	3:C:66:ARG:CG	1.81	0.93
7:G:124:ILE:HG12	7:G:128:LEU:HD12	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:85:GLU:HG3	8:H:86:THR:N	1.73	0.93
1:A:127:VAL:HG23	1:A:128:GLY:N	1.83	0.93
1:A:259:TYR:CB	1:A:260:PRO:HD2	1.87	0.93
1:A:426:THR:HA	1:A:428:TYR:CE2	2.04	0.93
1:A:514:THR:O	1:A:531:PRO:HA	1.69	0.93
2:B:620:LEU:HA	2:B:624:LEU:HD23	1.47	0.93
17:3:201:ALA:C	17:3:202:TYR:CD2	2.42	0.93
19:A:1138:CLA:HED3	19:A:1138:CLA:H2A	1.48	0.93
2:B:3:LEU:HD13	9:I:29:GLU:OE1	1.66	0.93
9:I:26:LEU:HA	9:I:29:GLU:O	1.67	0.93
16:2:101:TRP:H	16:2:103:VAL:HB	1.32	0.93
1:A:127:VAL:HG21	19:A:1107:CLA:CBB	1.99	0.93
1:A:606:TYR:O	1:A:610:SER:HB2	1.68	0.93
2:B:25:ILE:HG22	21:L:6019:BCR:H282	1.51	0.93
2:B:633:ASN:HB2	2:B:636:THR:HB	0.94	0.93
19:B:1235:CLA:C15	21:F:6016:BCR:C31	2.46	0.93
21:B:6017:BCR:H382	21:B:6017:BCR:H23C	1.49	0.93
8:H:58:LEU:CD1	8:H:62:THR:HG23	1.76	0.93
13:N:139:LYS:CG	13:N:142:LYS:CD	2.42	0.93
18:4:177:LEU:HD22	18:4:178:PRO:N	1.84	0.93
21:A:6011:BCR:C31	19:A:9013:CLA:H143	1.98	0.93
4:D:115:PRO:O	4:D:116:THR:OG1	1.87	0.93
1:A:57:LEU:HD23	1:A:57:LEU:C	1.88	0.93
4:D:201:LYS:HD2	4:D:201:LYS:N	1.78	0.93
15:1:91:MET:C	15:1:95:PRO:HD3	1.87	0.93
16:2:212:GLN:HG2	16:2:213:LYS:H	1.31	0.93
18:4:153:GLU:OE2	19:4:4012:CLA:C3B	2.16	0.93
19:4:4015:CLA:HBD	19:4:4015:CLA:HBA1	1.50	0.93
2:B:361:ILE:HG23	2:B:368:GLN:OE1	1.69	0.93
19:B:1220:CLA:H43	19:B:1220:CLA:C1A	1.99	0.93
4:D:140:LEU:CD1	4:D:144:LEU:CG	2.47	0.93
4:D:140:LEU:HD11	4:D:144:LEU:CB	1.99	0.93
6:F:207:LEU:HD22	6:F:208:PHE:N	1.84	0.93
17:3:156:THR:O	17:3:158:PHE:C	2.08	0.93
1:A:250:LEU:CB	17:3:136:TRP:CZ2	2.50	0.92
19:A:1237:CLA:C14	12:L:141:LEU:CD2	2.46	0.92
21:A:6002:BCR:H341	21:A:6002:BCR:H12C	1.50	0.92
5:E:126:VAL:C	5:E:127:GLU:HG3	1.88	0.92
7:G:125:VAL:HG13	7:G:129:ALA:HB3	1.49	0.92
12:L:73:VAL:HG12	19:L:1504:CLA:HMA3	1.50	0.92
12:L:205:TYR:HD1	12:L:207:LEU:HD12	1.18	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:187:LYS:HA	16:2:187:LYS:CE	1.83	0.92
17:3:109:ALA:HA	17:3:111:LEU:HD22	1.49	0.92
1:A:648:THR:HG23	1:A:651:GLY:H	1.32	0.92
2:B:8:PHE:N	2:B:8:PHE:CD1	2.37	0.92
2:B:558:PRO:HB2	2:B:703:VAL:CG2	1.99	0.92
15:1:133:THR:O	15:1:137:ILE:HD13	1.68	0.92
16:2:156:GLU:HG2	16:2:157:LEU:CD1	1.97	0.92
19:3:3016:CLA:C14	19:3:3016:CLA:H102	1.97	0.92
18:4:158:GLN:OE1	19:4:1004:CLA:CGD	2.15	0.92
1:A:668:TYR:CD1	2:B:445:ALA:CB	2.51	0.92
2:B:419:ILE:O	2:B:420:SER:OG	1.87	0.92
2:B:696:LYS:HE3	3:C:80:ALA:HB1	1.48	0.92
4:D:140:LEU:CD2	4:D:144:LEU:HD12	1.99	0.92
5:E:79:LYS:HG3	5:E:84:TYR:CE1	2.02	0.92
6:F:139:LEU:HD13	6:F:149:ILE:HD13	1.49	0.92
15:1:89:TRP:O	15:1:92:LEU:HB3	1.69	0.92
18:4:158:GLN:CB	19:4:1004:CLA:HMA2	1.98	0.92
1:A:267:THR:O	1:A:269:PHE:CD2	2.22	0.92
1:A:388:ASP:OD1	1:A:391:THR:OG1	1.87	0.92
2:B:188:LEU:HD11	19:B:1212:CLA:HBB2	1.51	0.92
19:B:1220:CLA:O2D	19:B:1220:CLA:H2A	1.70	0.92
19:B:1232:CLA:HMB1	21:B:6010:BCR:H292	1.50	0.92
6:F:219:ARG:HG2	6:F:219:ARG:NH1	1.62	0.92
16:2:114:MET:HG2	16:2:227:LEU:HA	1.51	0.92
1:A:120:ALA:H	1:A:145:ILE:HD12	1.34	0.92
1:A:351:THR:O	19:A:1123:CLA:C18	2.17	0.92
3:C:54:CYS:HB2	23:C:8002:SF4:S1	2.08	0.92
4:D:123:ARG:NH2	22:D:7050:LMU:C5B	2.32	0.92
5:E:78:ARG:N	5:E:78:ARG:HD2	1.83	0.92
19:H:1241:CLA:C4C	21:I:6021:BCR:HC22	2.00	0.92
19:R:1144:CLA:HED3	19:R:1144:CLA:CHA	2.00	0.92
16:2:173:ASN:HD22	16:2:173:ASN:N	1.65	0.92
19:2:2007:CLA:HAC2	19:3:2009:CLA:HED1	1.48	0.92
21:A:6011:BCR:C31	19:A:9013:CLA:C14	2.47	0.92
19:L:1148:CLA:HAA1	19:L:1148:CLA:O2D	1.69	0.92
17:3:185:GLN:HG2	17:3:186:TYR:H	0.79	0.92
1:A:281:LEU:HD23	19:A:1115:CLA:CMA	1.98	0.92
1:A:358:LEU:HD11	1:A:413:HIS:CG	2.05	0.92
1:A:451:ILE:CD1	19:A:1131:CLA:HED1	2.00	0.92
1:A:672:LEU:O	1:A:674:ALA:N	2.02	0.92
2:B:694:ARG:HH21	2:B:694:ARG:CG	1.81	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1224:CLA:O1D	19:B:1225:CLA:HMA1	1.69	0.92
11:K:115:ILE:CG1	11:K:122:LEU:N	2.32	0.92
1:A:246:HIS:HA	1:A:248:PHE:HE2	0.79	0.92
19:A:1124:CLA:H72	19:A:1125:CLA:HED2	1.51	0.92
2:B:453:ILE:HG23	2:B:453:ILE:O	1.68	0.92
5:E:126:VAL:O	5:E:127:GLU:HG3	1.69	0.92
18:4:120:ILE:HG22	18:4:121:ILE:H	1.33	0.92
1:A:51:THR:CB	19:A:1139:CLA:HBB2	1.99	0.92
1:A:390:ALA:HB2	1:A:754:ILE:HB	1.52	0.92
7:G:72:LEU:HD23	7:G:124:ILE:CG1	2.00	0.92
17:3:197:SER:OG	17:3:205:GLY:CA	2.17	0.92
19:3:3016:CLA:H142	19:3:3016:CLA:H102	1.50	0.92
18:4:146:PHE:CE2	19:4:4013:CLA:C3C	2.52	0.92
18:4:173:LYS:HZ3	18:4:201:LYS:CG	1.81	0.92
1:A:236:GLY:O	1:A:237:VAL:HG13	1.71	0.92
19:A:9023:CLA:HHB	19:A:9023:CLA:H43	1.52	0.92
2:B:317:ARG:HH22	2:B:410:ARG:HG2	1.18	0.92
24:B:7101:LMG:O3	3:C:70:TRP:CZ2	2.23	0.92
3:C:39:ILE:HG23	3:C:40:ALA:N	1.85	0.92
4:D:167:HIS:HD2	4:D:172:VAL:HG21	1.20	0.92
7:G:84:ARG:HE	7:G:89:LYS:HE2	1.34	0.92
7:G:99:HIS:HA	7:G:100:PHE:CB	1.99	0.92
11:K:125:LYS:HB2	11:K:128:GLY:N	1.84	0.92
21:1:6023:BCR:C8	21:1:6023:BCR:H313	1.74	0.92
16:2:226:ARG:CB	16:2:226:ARG:HH11	1.82	0.92
17:3:109:ALA:HA	17:3:111:LEU:CG	1.99	0.92
18:4:222:ASN:O	18:4:223:VAL:HB	1.66	0.92
1:A:281:LEU:HD23	19:A:1115:CLA:HMA3	1.49	0.91
19:B:1235:CLA:C16	21:F:6016:BCR:H313	2.00	0.91
6:F:173:TRP:HZ3	6:F:211:PHE:CB	1.83	0.91
8:H:97:LEU:HD11	8:H:100:PHE:HB3	1.50	0.91
9:I:12:VAL:O	9:I:17:PRO:HD3	1.69	0.91
19:L:1148:CLA:HED1	19:L:1148:CLA:H2	0.92	0.91
15:1:189:LYS:HG3	19:1:1007:CLA:CMC	1.99	0.91
18:4:174:GLN:O	18:4:194:PHE:CB	2.18	0.91
1:A:628:ILE:HD12	1:A:629:ASN:H	1.34	0.91
19:B:1220:CLA:C2	19:B:1220:CLA:H71	1.99	0.91
15:1:77:GLU:CG	15:1:80:LYS:HD2	1.99	0.91
15:1:190:ASN:ND2	19:1:1002:CLA:C1A	2.33	0.91
17:3:133:ALA:HB3	17:3:134:LEU:CD1	1.99	0.91
18:4:134:TYR:HB3	18:4:136:ALA:HB2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1107:CLA:HBB2	19:B:1230:CLA:CMD	2.00	0.91
2:B:5:ILE:CG2	2:B:6:PRO:HD3	1.98	0.91
2:B:457:PRO:HB3	2:B:517:PHE:CD1	2.04	0.91
3:C:14:CYS:HA	3:C:17:CYS:HG	1.13	0.91
6:F:207:LEU:HD13	6:F:208:PHE:N	1.85	0.91
21:I:6021:BCR:H391	21:L:6019:BCR:H401	1.47	0.91
19:K:1142:CLA:HED1	19:K:1143:CLA:HMB2	1.50	0.91
15:1:129:VAL:HG12	15:1:130:PRO:CD	1.99	0.91
15:1:129:VAL:CG1	15:1:130:PRO:HD3	2.00	0.91
16:2:182:ILE:HD13	16:2:190:GLY:HA3	1.51	0.91
16:2:184:PRO:CD	16:2:187:LYS:HD2	2.00	0.91
1:A:336:GLY:N	1:A:339:THR:OG1	2.02	0.91
1:A:368:LEU:HD11	19:A:1125:CLA:H61	1.52	0.91
1:A:425:THR:CB	1:A:428:TYR:CE1	2.48	0.91
1:A:483:GLN:C	1:A:485:GLN:HE22	1.73	0.91
2:B:443:MET:O	2:B:446:PHE:HB2	1.69	0.91
7:G:116:SER:HA	7:G:119:PRO:HG2	1.52	0.91
11:K:51:SER:N	11:K:52:PRO:CD	2.34	0.91
12:L:102:VAL:HA	19:L:1502:CLA:HED2	1.50	0.91
18:4:226:LYS:H	18:4:226:LYS:CD	1.81	0.91
1:A:328:LYS:NZ	1:A:345:GLY:CA	2.33	0.91
1:A:411:ALA:HB2	21:A:6008:BCR:H392	1.53	0.91
1:A:564:ARG:HB3	1:A:564:ARG:NH2	1.85	0.91
19:A:1107:CLA:HBB2	19:B:1230:CLA:HMD2	1.51	0.91
19:A:1149:CLA:O1D	19:A:1149:CLA:HAA1	1.71	0.91
3:C:6:LYS:HE2	4:D:191:ILE:HG13	1.49	0.91
5:E:96:ASP:OD2	5:E:98:ASN:OD1	1.87	0.91
7:G:131:GLY:O	7:G:136:VAL:HB	1.68	0.91
19:H:1145:CLA:HMC1	19:H:1145:CLA:CBC	1.99	0.91
12:L:110:LEU:HB3	12:L:114:PHE:HE1	1.32	0.91
12:L:142:SER:O	12:L:143:LEU:HG	1.70	0.91
15:1:142:PHE:HA	15:1:145:ILE:CD1	2.00	0.91
16:2:101:TRP:CA	16:2:103:VAL:H	1.82	0.91
19:3:2009:CLA:HBA2	19:3:2009:CLA:CHA	2.00	0.91
1:A:365:LEU:HD23	19:A:1103:CLA:CED	1.99	0.91
1:A:484:LEU:H	1:A:484:LEU:HD22	1.36	0.91
11:K:118:VAL:CG2	11:K:121:VAL:HG22	2.00	0.91
19:A:1112:CLA:HHC	21:A:6002:BCR:H17C	1.50	0.91
19:A:1125:CLA:O1D	19:A:1125:CLA:HBA1	1.69	0.91
2:B:103:ALA:HA	2:B:105:THR:N	1.85	0.91
2:B:310:PRO:CG	2:B:311:PRO:HD3	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:95:GLN:HE21	4:D:96:VAL:HA	1.30	0.91
5:E:89:SER:O	5:E:106:ARG:N	2.03	0.91
7:G:124:ILE:O	7:G:128:LEU:HB2	1.71	0.91
17:3:133:ALA:HB3	17:3:134:LEU:HD11	1.53	0.91
1:A:338:PHE:CE1	19:A:1151:CLA:HBB2	2.03	0.91
19:A:1113:CLA:CBB	21:A:6002:BCR:H352	2.01	0.91
4:D:83:PHE:HB3	4:D:84:GLY:O	1.71	0.91
4:D:100:TYR:CD1	4:D:134:LYS:HG3	2.06	0.91
6:F:132:ASN:O	6:F:133:TYR:CD1	2.23	0.91
7:G:63:VAL:CG2	7:G:64:ILE:H	1.84	0.91
7:G:94:GLN:O	7:G:97:LEU:HD23	1.70	0.91
7:G:125:VAL:HG13	7:G:129:ALA:CB	2.01	0.91
12:L:137:LEU:HD23	12:L:137:LEU:C	1.91	0.91
15:1:157:ASP:CG	15:1:178:LYS:HA	1.89	0.91
15:1:177:PRO:HD3	15:1:180:LEU:CD2	2.00	0.91
22:4:7034:LMU:H71	22:4:7052:LMU:H11	1.53	0.91
1:A:105:ASN:OD1	1:A:118:PRO:HA	1.70	0.91
2:B:270:LEU:HD12	2:B:271:THR:N	1.86	0.91
2:B:574:ASP:HA	2:B:577:TYR:HB3	1.50	0.91
8:H:120:ILE:HG13	8:H:120:ILE:O	1.68	0.91
12:L:174:ASP:OD2	12:L:175:GLN:HG3	1.70	0.91
19:A:1126:CLA:H203	21:J:6012:BCR:C17	2.01	0.91
19:A:1141:CLA:C7	19:A:1141:CLA:C12	2.48	0.91
2:B:110:LEU:HD12	2:B:111:GLY:CA	2.01	0.91
2:B:403:ASN:O	2:B:406:ASN:CB	2.19	0.91
2:B:672:GLN:HE22	3:C:79:LEU:HD12	1.35	0.91
4:D:133:ARG:H	4:D:136:GLN:NE2	1.66	0.91
4:D:186:GLN:C	4:D:187:ASN:HD22	1.74	0.91
15:1:177:PRO:HG2	15:1:179:LYS:O	1.70	0.91
2:B:257:ILE:O	2:B:497:TRP:HE3	1.38	0.90
2:B:306:GLU:HG3	2:B:307:ALA:H	1.31	0.90
3:C:52:LYS:O	3:C:52:LYS:HG3	1.71	0.90
3:C:62:PHE:CD2	5:E:80:GLU:HG3	2.07	0.90
8:H:56:GLU:CG	8:H:57:ASP:N	2.34	0.90
19:H:1145:CLA:HMA2	19:H:1145:CLA:C1	2.01	0.90
16:2:117:ALA:HB1	16:2:230:LEU:CG	2.02	0.90
17:3:150:TYR:H	17:3:152:ALA:HB2	0.75	0.90
18:4:177:LEU:CD2	18:4:178:PRO:HD3	2.01	0.90
1:A:188:LYS:HD2	1:A:188:LYS:C	1.92	0.90
21:A:6002:BCR:HC8	21:A:6002:BCR:C31	2.01	0.90
2:B:560:ASP:OD1	2:B:561:GLY:N	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:LEU:HB3	8:H:61:THR:HB	1.48	0.90
19:J:1308:CLA:CAD	19:J:1308:CLA:CED	2.50	0.90
14:R:33:UNK:C	14:R:36:UNK:CB	2.50	0.90
19:1:1014:CLA:HBC3	19:1:1014:CLA:CHD	2.01	0.90
4:D:137:CYS:O	4:D:140:LEU:O	1.89	0.90
5:E:111:ASN:HB3	5:E:116:SER:OG	1.71	0.90
13:N:155:GLU:HB3	13:N:157:LYS:CA	2.01	0.90
16:2:156:GLU:OE2	19:2:2013:CLA:CHD	2.18	0.90
1:A:129:GLN:NE2	19:A:1107:CLA:NA	2.19	0.90
2:B:558:PRO:HG2	2:B:703:VAL:CG2	2.02	0.90
19:B:1210:CLA:H151	19:B:1225:CLA:HMD2	1.50	0.90
3:C:5:VAL:HG21	3:C:65:VAL:HG23	1.52	0.90
5:E:79:LYS:HA	5:E:84:TYR:CD1	2.06	0.90
5:E:103:VAL:HG13	5:E:120:TYR:O	1.72	0.90
11:K:128:GLY:N	11:K:129:ALA:HA	1.80	0.90
15:1:65:ASP:CG	15:1:66:PRO:N	2.24	0.90
19:3:3011:CLA:H122	19:3:3011:CLA:H172	1.52	0.90
1:A:733:VAL:O	1:A:733:VAL:HG12	1.72	0.90
2:B:75:GLU:HB2	2:B:132:ASN:ND2	1.83	0.90
19:B:1234:CLA:HMC1	19:B:1234:CLA:HBC3	1.53	0.90
21:B:6006:BCR:H331	21:B:6006:BCR:C8	2.00	0.90
6:F:130:PHE:N	6:F:133:TYR:CE1	2.37	0.90
12:L:74:THR:HG22	12:L:75:SER:OG	1.71	0.90
13:N:133:GLY:C	13:N:134:CYS:HG	1.74	0.90
13:N:165:ASN:C	13:N:167:PHE:H	1.75	0.90
16:2:137:TRP:O	16:2:139:THR:HG22	1.72	0.90
17:3:173:PHE:C	17:3:173:PHE:CD1	2.40	0.90
17:3:206:PRO:HG2	17:3:208:PHE:CE2	2.06	0.90
19:4:4014:CLA:HHD	19:4:4014:CLA:HBC2	1.51	0.90
1:A:62:HIS:O	19:A:1128:CLA:HAA2	1.71	0.90
1:A:64:PHE:CD2	1:A:74:ILE:HG21	2.05	0.90
2:B:459:PHE:HB2	19:B:1235:CLA:CAD	2.01	0.90
8:H:58:LEU:HD12	8:H:61:THR:HA	1.52	0.90
8:H:58:LEU:CB	8:H:61:THR:HB	2.00	0.90
13:N:120:VAL:O	13:N:120:VAL:HG12	1.69	0.90
15:1:221:LEU:HD13	19:1:1003:CLA:HAC1	1.51	0.90
1:A:96:MET:HE3	19:A:1106:CLA:HED2	1.54	0.90
2:B:370:ALA:O	19:B:1224:CLA:HMA1	1.71	0.90
2:B:457:PRO:HB3	2:B:517:PHE:HD1	1.37	0.90
2:B:459:PHE:HE2	19:B:1235:CLA:C2D	1.42	0.90
21:3:6022:BCR:H393	21:3:6022:BCR:C23	1.95	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HD11	19:A:1107:CLA:CMA	2.02	0.90
1:A:342:GLY:HA2	1:A:430:ASP:HB3	1.52	0.90
1:A:345:GLY:C	1:A:347:TYR:H	1.73	0.90
19:A:1141:CLA:H12	19:A:1141:CLA:CMA	2.01	0.90
2:B:224:PRO:HB2	2:B:227:THR:CB	2.01	0.90
2:B:229:GLN:O	7:G:63:VAL:HG21	1.70	0.90
2:B:352:MET:CE	19:B:1225:CLA:OBD	2.20	0.90
19:J:1308:CLA:CBC	19:J:1308:CLA:CHD	2.48	0.90
11:K:70:PHE:HB3	11:K:98:PRO:HB3	1.52	0.90
12:L:131:SER:HB3	12:L:201:TYR:HE2	1.34	0.90
16:2:131:ILE:O	16:2:131:ILE:HG22	1.71	0.90
17:3:159:VAL:CG1	17:3:160:LEU:N	2.31	0.90
17:3:205:GLY:N	17:3:206:PRO:HD2	1.85	0.90
21:B:6020:BCR:H332	19:L:1502:CLA:C4B	2.00	0.90
4:D:140:LEU:CD1	4:D:144:LEU:HG	2.00	0.90
15:1:64:PHE:CD1	15:1:65:ASP:N	2.40	0.90
17:3:109:ALA:HA	17:3:111:LEU:CD2	2.02	0.90
18:4:169:ASP:OD2	18:4:174:GLN:HB2	1.70	0.90
7:G:69:GLY:O	7:G:72:LEU:HG	1.71	0.90
7:G:77:PHE:O	7:G:79:PHE:CB	2.19	0.90
1:A:71:LEU:CG	1:A:72:GLU:H	1.84	0.89
2:B:120:VAL:CA	2:B:123:TRP:HD1	1.79	0.89
2:B:269:TRP:HB2	2:B:497:TRP:HH2	1.38	0.89
2:B:312:GLY:HA3	2:B:315:LEU:CB	2.03	0.89
2:B:545:LYS:HD3	2:B:546:LEU:N	1.87	0.89
2:B:558:PRO:HG2	2:B:703:VAL:HG22	1.53	0.89
2:B:655:LEU:HD21	19:B:1239:CLA:HBB1	1.53	0.89
19:B:1222:CLA:CAD	19:B:1234:CLA:HBB1	2.03	0.89
6:F:170:ILE:HG21	21:F:6014:BCR:H371	1.52	0.89
13:N:143:VAL:HB	13:N:144:PRO:CD	1.99	0.89
15:1:69:LEU:C	15:1:73:PRO:HD3	1.93	0.89
16:2:184:PRO:HD3	16:2:187:LYS:CA	2.02	0.89
18:4:146:PHE:CZ	19:4:4013:CLA:NC	2.39	0.89
1:A:281:LEU:HD21	19:A:1115:CLA:CMA	1.85	0.89
2:B:232:LEU:HD13	2:B:235:GLN:HG3	1.50	0.89
18:4:146:PHE:CE2	19:4:4013:CLA:C2C	2.53	0.89
22:4:7034:LMU:C11	22:4:7052:LMU:C3'	2.47	0.89
1:A:331:LEU:CD2	1:A:343:HIS:O	2.21	0.89
1:A:499:ALA:CB	19:A:1133:CLA:HED1	2.02	0.89
1:A:740:LEU:HD21	19:A:1140:CLA:CMA	2.01	0.89
21:A:6011:BCR:C39	21:A:6011:BCR:H23C	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:9022:CLA:H112	21:B:6017:BCR:H19C	1.53	0.89
4:D:82:ILE:O	4:D:82:ILE:HG13	1.69	0.89
11:K:48:PHE:O	11:K:52:PRO:HD3	1.72	0.89
12:L:171:LYS:C	12:L:173:PRO:HD3	1.92	0.89
15:1:170:PRO:HG2	15:1:171:LEU:CA	2.02	0.89
16:2:119:GLY:O	16:2:123:PRO:CD	2.20	0.89
18:4:96:LEU:CD1	18:4:100:ARG:CZ	2.50	0.89
18:4:110:LEU:O	18:4:113:GLU:HG3	1.71	0.89
18:4:175:TYR:O	18:4:194:PHE:CD1	2.25	0.89
19:A:1237:CLA:H201	12:L:110:LEU:HD21	1.52	0.89
2:B:244:PHE:C	2:B:244:PHE:CD2	2.46	0.89
4:D:140:LEU:HD12	4:D:141:GLY:CA	2.02	0.89
6:F:221:LEU:HD23	6:F:222:LEU:HD21	1.52	0.89
12:L:143:LEU:HA	12:L:146:THR:H	1.36	0.89
13:N:169:LYS:HB3	13:N:170:TRP:CD1	2.06	0.89
15:1:134:LEU:HA	15:1:137:ILE:CD1	2.01	0.89
1:A:78:VAL:O	1:A:82:HIS:CD2	2.26	0.89
1:A:83:PHE:CE1	19:A:1111:CLA:HED1	2.08	0.89
1:A:250:LEU:HB2	17:3:136:TRP:HH2	1.36	0.89
1:A:381:PRO:HB2	19:A:1117:CLA:HAA2	1.54	0.89
5:E:79:LYS:CA	5:E:84:TYR:CE1	2.54	0.89
19:H:1145:CLA:H101	19:H:1145:CLA:H142	1.50	0.89
13:N:130:ASN:HB2	13:N:139:LYS:CD	2.02	0.89
16:2:237:PHE:HE1	16:2:241:TYR:CE1	1.90	0.89
1:A:163:GLN:HG3	1:A:164:LEU:N	1.86	0.89
1:A:547:PHE:O	1:A:551:VAL:HG13	1.73	0.89
19:A:1134:CLA:C3A	19:A:1141:CLA:HBB2	2.01	0.89
2:B:140:ILE:CG1	2:B:141:PHE:N	2.34	0.89
19:B:1211:CLA:HMA1	21:B:6006:BCR:H313	1.53	0.89
7:G:145:THR:HG23	7:G:146:SER:N	1.87	0.89
11:K:118:VAL:O	11:K:121:VAL:CG2	2.20	0.89
11:K:127:ILE:HG23	11:K:130:LEU:CG	1.95	0.89
13:N:139:LYS:HB3	13:N:142:LYS:CD	1.99	0.89
16:2:112:TRP:HZ2	16:2:167:ARG:NH2	1.30	0.89
16:2:117:ALA:CB	16:2:230:LEU:CG	2.49	0.89
18:4:173:LYS:HD2	18:4:201:LYS:HE3	1.52	0.89
1:A:24:ARG:N	1:A:24:ARG:CD	2.33	0.89
1:A:426:THR:CG2	1:A:428:TYR:CE2	2.55	0.89
1:A:715:LYS:HD2	6:F:230:ASN:HD21	0.76	0.89
5:E:78:ARG:HH22	5:E:125:ILE:CG2	1.86	0.89
13:N:130:ASN:O	13:N:132:THR:HG23	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:142:LYS:O	13:N:145:PHE:N	2.06	0.89
15:1:177:PRO:HD3	15:1:180:LEU:CG	1.92	0.89
15:1:189:LYS:HB2	19:1:1007:CLA:HMC1	1.53	0.89
17:3:197:SER:HG	17:3:205:GLY:HA3	1.30	0.89
1:A:316:MET:HB3	1:A:317:TYR:CB	2.02	0.89
1:A:423:ASP:HB3	1:A:424:PRO:CD	2.02	0.89
2:B:391:PRO:HB3	2:B:538:ALA:HA	1.51	0.89
8:H:57:ASP:O	8:H:59:GLY:N	2.06	0.89
15:1:171:LEU:CA	15:1:173:TYR:CE2	2.55	0.89
17:3:96:ARG:HA	17:3:99:ALA:N	1.87	0.89
1:A:103:PHE:HE1	19:A:1105:CLA:O1D	1.55	0.89
1:A:244:LEU:HD12	1:A:247:GLU:CD	1.93	0.89
2:B:244:PHE:C	2:B:244:PHE:HD2	1.76	0.89
4:D:123:ARG:HH22	22:D:7050:LMU:C4B	1.85	0.89
5:E:70:ARG:HG2	5:E:71:GLY:N	1.88	0.89
5:E:83:TRP:N	5:E:83:TRP:HE3	1.71	0.89
11:K:49:ILE:O	11:K:52:PRO:HD2	1.73	0.89
15:1:133:THR:O	15:1:136:THR:HG23	1.73	0.89
1:A:204:ASN:O	1:A:205:HIS:HB2	1.73	0.89
19:A:1112:CLA:HMB2	21:A:6002:BCR:H382	1.55	0.89
2:B:459:PHE:CD2	19:B:1235:CLA:C4D	2.54	0.89
2:B:535:VAL:O	2:B:539:LEU:HD23	1.72	0.89
19:B:1235:CLA:C15	21:F:6016:BCR:H312	2.03	0.89
4:D:73:GLU:O	4:D:76:PRO:HD2	1.73	0.89
4:D:203:THR:HG22	4:D:205:LYS:H	1.37	0.89
12:L:92:ALA:N	12:L:98:ARG:HH12	1.71	0.89
13:N:139:LYS:O	13:N:142:LYS:HD2	1.72	0.89
15:1:97:ILE:HD13	15:1:97:ILE:C	1.94	0.89
16:2:148:ASP:CG	16:2:152:LEU:HB3	1.92	0.89
18:4:202:GLU:O	18:4:205:ILE:HG12	1.72	0.89
18:4:220:GLN:CG	19:4:1306:CLA:HAC2	2.03	0.89
1:A:71:LEU:CG	1:A:72:GLU:N	2.36	0.88
1:A:127:VAL:HG23	1:A:128:GLY:H	1.34	0.88
1:A:207:LEU:CD2	19:A:1119:CLA:HBB2	2.03	0.88
1:A:502:THR:CG2	1:A:504:ALA:H	1.86	0.88
1:A:599:PHE:CE2	1:A:731:ARG:HB3	2.06	0.88
2:B:232:LEU:CD1	2:B:235:GLN:CG	2.50	0.88
2:B:521:HIS:HE1	19:B:1235:CLA:NA	1.69	0.88
19:B:1202:CLA:O1A	19:B:1202:CLA:C2	2.20	0.88
7:G:98:THR:OG1	7:G:101:GLU:HB2	1.71	0.88
11:K:52:PRO:CD	11:K:53:THR:H	1.81	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:146:LEU:CG	17:3:142:ILE:O	2.21	0.88
17:3:96:ARG:CA	17:3:99:ALA:CB	2.50	0.88
17:3:157:LEU:O	17:3:160:LEU:N	2.06	0.88
18:4:90:TRP:CG	18:4:91:PHE:N	2.36	0.88
1:A:316:MET:CB	1:A:317:TYR:CD1	2.57	0.88
19:A:1123:CLA:H92	19:A:1123:CLA:OBD	1.72	0.88
2:B:319:HIS:HE1	2:B:322:LEU:CD1	1.85	0.88
13:N:114:PHE:HB3	13:N:117:ALA:CB	2.02	0.88
15:1:142:PHE:HA	15:1:145:ILE:HD11	1.54	0.88
16:2:211:PRO:HD2	16:2:212:GLN:H	1.36	0.88
1:A:453:LEU:HB3	1:A:547:PHE:HB2	1.55	0.88
19:A:1122:CLA:CBB	21:A:6007:BCR:C35	2.51	0.88
2:B:382:ILE:HG22	2:B:383:MET:N	1.89	0.88
19:B:1235:CLA:H93	19:B:1235:CLA:HBB2	0.92	0.88
4:D:146:SER:O	4:D:147:LYS:HG3	1.72	0.88
5:E:96:ASP:HB3	5:E:98:ASN:N	1.88	0.88
7:G:72:LEU:HD23	7:G:124:ILE:HD11	1.34	0.88
7:G:141:ILE:O	7:G:142:LEU:HB2	1.71	0.88
17:3:96:ARG:CA	17:3:99:ALA:HB3	2.04	0.88
17:3:108:PHE:HB3	19:3:3013:CLA:H42	1.54	0.88
19:A:1131:CLA:H161	21:L:6019:BCR:H361	1.53	0.88
19:A:1138:CLA:H61	21:F:6014:BCR:H12C	1.52	0.88
11:K:84:LEU:CG	11:K:85:LYS:HG2	2.03	0.88
14:R:39:UNK:HA	14:R:42:UNK:CB	2.04	0.88
15:1:88:ARG:O	15:1:92:LEU:CB	2.20	0.88
16:2:184:PRO:HG3	16:2:187:LYS:N	1.89	0.88
18:4:198:LEU:HG	18:4:199:GLU:N	1.88	0.88
1:A:23:ASP:CG	1:A:33:GLN:HG2	1.92	0.88
1:A:289:PRO:O	1:A:290:LEU:HB3	1.73	0.88
1:A:426:THR:HG22	1:A:428:TYR:HE2	1.32	0.88
19:B:1220:CLA:HMC1	19:B:1220:CLA:CBC	2.03	0.88
19:K:1142:CLA:HMD1	19:K:1143:CLA:NA	1.87	0.88
16:2:182:ILE:HB	16:2:187:LYS:CG	2.02	0.88
17:3:93:ILE:CG1	17:3:95:PRO:O	2.20	0.88
17:3:159:VAL:O	17:3:162:MET:N	2.05	0.88
2:B:222:LEU:HD12	2:B:223:GLY:O	1.74	0.88
2:B:268:LEU:HD22	2:B:273:VAL:HG12	1.54	0.88
2:B:398:TYR:O	4:D:197:PRO:CG	2.20	0.88
21:B:6010:BCR:H382	21:B:6010:BCR:H23C	1.53	0.88
3:C:65:VAL:O	3:C:66:ARG:HB3	1.71	0.88
4:D:95:GLN:HE21	4:D:96:VAL:CA	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:56:ILE:HA	11:K:59:THR:CG2	2.02	0.88
16:2:254:LEU:HD22	16:2:254:LEU:C	1.89	0.88
17:3:135:ALA:CB	17:3:139:THR:OG1	2.20	0.88
2:B:87:ILE:HA	2:B:115:ASN:CA	2.04	0.88
2:B:293:THR:HG21	19:B:1209:CLA:CMA	2.04	0.88
2:B:693:TRP:CD1	19:B:1238:CLA:C2D	2.56	0.88
19:B:1214:CLA:CB	19:B:1223:CLA:HBB2	2.04	0.88
20:B:5002:PQN:C16	21:B:6017:BCR:H333	2.00	0.88
3:C:62:PHE:CZ	5:E:80:GLU:OE2	2.24	0.88
5:E:129:GLU:C	5:E:129:GLU:CD	2.30	0.88
6:F:200:VAL:HG11	10:J:7:TYR:HB2	1.54	0.88
7:G:149:TYR:CA	7:G:150:ASP:OD1	2.20	0.88
12:L:51:LYS:HE2	12:L:51:LYS:HA	1.54	0.88
12:L:102:VAL:HA	19:L:1502:CLA:CED	2.04	0.88
17:3:238:ILE:HD11	19:3:3003:CLA:HMC2	1.55	0.88
18:4:143:VAL:O	18:4:147:ILE:HD12	1.73	0.88
21:A:6011:BCR:C8	21:A:6011:BCR:H311	2.04	0.88
19:B:1228:CLA:H12	19:B:1228:CLA:HMA2	1.54	0.88
3:C:31:TRP:HD1	3:C:32:GLY:N	1.72	0.88
19:2:4009:CLA:H152	19:2:4009:CLA:H192	1.54	0.88
17:3:122:LEU:HD21	19:3:3006:CLA:C3D	2.02	0.88
19:3:2009:CLA:CGA	19:3:2009:CLA:CB	2.49	0.88
19:A:9022:CLA:HBB2	19:A:9023:CLA:CHB	2.03	0.88
2:B:299:HIS:CE1	19:B:1219:CLA:HMD1	2.08	0.88
2:B:442:VAL:HG21	19:B:1230:CLA:HAC2	1.55	0.88
3:C:65:VAL:HG22	3:C:66:ARG:N	1.84	0.88
5:E:107:PHE:HE2	5:E:109:LYS:HG3	1.19	0.88
7:G:72:LEU:HD12	7:G:73:PHE:CE2	2.09	0.88
8:H:119:ASP:OD2	8:H:121:LEU:HG	1.72	0.88
16:2:195:TYR:CD2	16:2:198:GLY:HA3	2.08	0.88
16:2:261:THR:HG22	16:2:262:ILE:H	1.38	0.88
17:3:207:PHE:C	17:3:207:PHE:CD1	2.45	0.88
1:A:252:ARG:H	1:A:252:ARG:CD	1.82	0.88
2:B:469:LYS:HG3	2:B:470:THR:CG2	2.03	0.88
2:B:470:THR:H	2:B:501:ILE:HB	1.29	0.88
2:B:493:TRP:HH2	19:B:1214:CLA:H122	1.36	0.88
21:B:6020:BCR:H331	21:B:6020:BCR:HC8	1.55	0.88
5:E:81:SER:OG	5:E:120:TYR:OH	1.64	0.88
19:H:1145:CLA:H143	19:H:1145:CLA:H193	1.55	0.88
18:4:103:MET:HE3	18:4:208:GLY:N	1.71	0.88
1:A:71:LEU:HD12	1:A:72:GLU:N	1.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:HA	1:A:76:ARG:HD2	1.54	0.87
1:A:154:ARG:HE	1:A:384:TYR:HE1	0.92	0.87
2:B:294:ASN:ND2	7:G:94:GLN:HA	1.88	0.87
2:B:693:TRP:HD1	19:B:1238:CLA:C2D	1.87	0.87
19:B:1228:CLA:HHD	19:B:1228:CLA:HBC2	1.56	0.87
16:2:184:PRO:CD	16:2:187:LYS:CG	2.52	0.87
1:A:566:SER:OG	2:B:673:GLU:OE2	1.90	0.87
19:A:1133:CLA:HBC2	19:A:1133:CLA:HMC1	1.55	0.87
19:A:1136:CLA:H192	19:L:1130:CLA:HBB1	1.54	0.87
4:D:100:TYR:CE1	4:D:134:LYS:CG	2.57	0.87
12:L:141:LEU:HD13	12:L:145:LEU:HD12	1.57	0.87
12:L:142:SER:O	12:L:143:LEU:CG	2.23	0.87
12:L:209:LEU:HD12	12:L:210:PRO:HD2	0.89	0.87
16:2:120:ILE:O	16:2:123:PRO:HD2	1.73	0.87
1:A:207:LEU:HA	1:A:211:LEU:HG	1.55	0.87
1:A:368:LEU:CD2	19:A:1117:CLA:H92	2.03	0.87
1:A:668:TYR:CG	2:B:445:ALA:CB	2.58	0.87
21:A:6002:BCR:H311	21:A:6002:BCR:C8	2.01	0.87
2:B:475:ASP:OD1	2:B:480:SER:O	1.92	0.87
3:C:43:PRO:HA	4:D:182:GLN:HB3	1.56	0.87
3:C:44:ARG:N	4:D:182:GLN:CD	2.27	0.87
3:C:52:LYS:HZ1	3:C:64:SER:HB2	1.39	0.87
19:L:1148:CLA:C2	19:L:1148:CLA:CED	2.31	0.87
17:3:197:SER:CB	17:3:206:PRO:CD	2.52	0.87
19:3:1147:CLA:HMC1	19:3:1147:CLA:HBC3	0.87	0.87
18:4:172:PHE:HB3	18:4:194:PHE:CZ	2.09	0.87
1:A:150:PHE:H	1:A:153:TRP:HB2	1.39	0.87
19:A:9012:CLA:HMB3	19:B:9010:CLA:H18	1.55	0.87
2:B:319:HIS:HE1	2:B:322:LEU:HD12	1.32	0.87
4:D:100:TYR:CE1	4:D:134:LYS:HE3	2.09	0.87
15:1:85:ILE:HA	15:1:88:ARG:CD	2.03	0.87
16:2:103:VAL:O	16:2:105:ALA:N	2.08	0.87
1:A:71:LEU:HG	1:A:72:GLU:N	1.86	0.87
1:A:85:GLN:O	1:A:87:SER:O	1.91	0.87
1:A:92:TRP:O	1:A:93:LEU:CD2	2.23	0.87
1:A:160:SER:O	1:A:163:GLN:HG2	1.74	0.87
19:A:1124:CLA:C7	19:A:1125:CLA:CED	2.51	0.87
19:A:1140:CLA:H141	21:A:6011:BCR:HC21	1.55	0.87
2:B:303:TYR:CA	2:B:306:GLU:HB2	2.03	0.87
2:B:312:GLY:HA3	2:B:315:LEU:HB2	1.55	0.87
2:B:697:PRO:O	3:C:79:LEU:HD13	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:SER:HG	4:D:126:PRO:HD2	1.07	0.87
4:D:150:ILE:O	4:D:151:LYS:HG2	1.73	0.87
19:L:1503:CLA:HBC3	19:L:1503:CLA:CHD	2.05	0.87
13:N:155:GLU:CA	13:N:157:LYS:CE	2.31	0.87
15:1:141:GLU:O	15:1:145:ILE:HG13	1.74	0.87
17:3:96:ARG:HH11	17:3:96:ARG:HB2	1.36	0.87
19:3:1147:CLA:HMC1	19:3:1147:CLA:HBC2	1.55	0.87
1:A:261:SER:O	1:A:262:PHE:CD1	2.28	0.87
1:A:281:LEU:CG	19:A:1115:CLA:CED	2.53	0.87
1:A:316:MET:CG	1:A:317:TYR:CD1	2.58	0.87
1:A:470:LEU:CD1	2:B:95:HIS:HB3	2.03	0.87
19:B:1214:CLA:H52	19:B:1223:CLA:HMB1	1.53	0.87
21:B:6020:BCR:H331	21:B:6020:BCR:C8	2.03	0.87
5:E:96:ASP:OD2	5:E:98:ASN:CG	2.11	0.87
17:3:201:ALA:CB	17:3:202:TYR:CD2	2.58	0.87
22:4:7053:LMU:H11	22:4:7053:LMU:H5'	1.56	0.87
1:A:89:ILE:O	1:A:92:TRP:HB3	1.75	0.87
1:A:723:ARG:H	19:A:1139:CLA:HBB1	1.37	0.87
19:A:1237:CLA:H141	12:L:141:LEU:HD21	1.56	0.87
22:H:7043:LMU:H102	22:H:7043:LMU:H62	1.55	0.87
10:J:5:LYS:HG3	16:2:178:ASN:OD1	1.75	0.87
11:K:127:ILE:CG2	11:K:130:LEU:HG	2.04	0.87
12:L:143:LEU:HD22	12:L:146:THR:CG2	2.04	0.87
15:1:189:LYS:HE2	15:1:189:LYS:HA	1.56	0.87
2:B:482:ASN:OD1	2:B:485:ALA:HB2	1.75	0.87
2:B:622:ASP:CB	2:B:626:LEU:HD12	2.03	0.87
6:F:200:VAL:CG1	10:J:7:TYR:H	1.86	0.87
12:L:70:GLU:HG2	12:L:74:THR:HG21	1.57	0.87
12:L:153:PHE:O	12:L:179:ALA:N	2.08	0.87
17:3:205:GLY:N	17:3:206:PRO:CD	2.34	0.87
1:A:246:HIS:O	1:A:248:PHE:HD2	1.57	0.87
1:A:308:ILE:HD12	19:A:1115:CLA:CHC	2.03	0.87
1:A:491:TRP:HE1	19:A:1135:CLA:C1	1.87	0.87
1:A:659:ALA:O	1:A:662:SER:OG	1.93	0.87
19:A:1125:CLA:CAB	19:A:1133:CLA:HMA1	2.02	0.87
19:A:1134:CLA:HBC1	21:A:6008:BCR:HC31	1.54	0.87
2:B:50:HIS:CD2	19:B:1202:CLA:HAA2	2.09	0.87
8:H:109:LEU:CD2	19:H:1207:CLA:H52	2.05	0.87
13:N:114:PHE:CD1	13:N:117:ALA:CB	2.53	0.87
15:1:193:LEU:HD23	15:1:193:LEU:C	1.96	0.87
22:4:7053:LMU:H6E	22:4:7053:LMU:H1B	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:PHE:O	1:A:41:SER:O	1.93	0.86
1:A:387:THR:HG22	1:A:523:VAL:HG11	1.54	0.86
19:B:1214:CLA:CAD	19:B:1223:CLA:HBB2	2.05	0.86
22:H:7032:LMU:H31	22:H:7032:LMU:H1B	1.56	0.86
22:H:7032:LMU:H3'	22:H:7032:LMU:O5B	1.75	0.86
1:A:316:MET:HB3	1:A:317:TYR:CD1	2.10	0.86
1:A:502:THR:HG22	1:A:504:ALA:N	1.90	0.86
2:B:393:PHE:HD2	2:B:397:ASP:OD1	1.59	0.86
2:B:469:LYS:HE3	2:B:470:THR:HG23	1.56	0.86
3:C:62:PHE:CZ	5:E:80:GLU:OE1	2.28	0.86
4:D:100:TYR:CE1	4:D:134:LYS:CE	2.57	0.86
4:D:103:THR:HG22	4:D:128:LEU:CG	2.05	0.86
22:D:7050:LMU:H4'	22:D:7050:LMU:O2B	1.73	0.86
5:E:89:SER:HB2	5:E:106:ARG:NH2	1.90	0.86
16:2:184:PRO:CG	16:2:187:LYS:HD2	2.04	0.86
19:4:1304:CLA:HED3	19:4:1304:CLA:CAA	1.98	0.86
1:A:443:ILE:HD11	1:A:557:LEU:HD23	1.57	0.86
15:1:177:PRO:N	15:1:180:LEU:HG	1.89	0.86
15:1:190:ASN:ND2	19:1:1002:CLA:NA	2.23	0.86
17:3:202:TYR:HB3	17:3:203:PRO:CD	2.04	0.86
1:A:316:MET:CB	1:A:317:TYR:HB2	2.03	0.86
1:A:331:LEU:HD11	1:A:346:LEU:CB	2.03	0.86
19:A:1111:CLA:HBA1	19:A:1123:CLA:H41	1.55	0.86
2:B:353:TYR:CG	2:B:594:TRP:CZ3	2.63	0.86
3:C:14:CYS:SG	3:C:18:VAL:O	2.32	0.86
4:D:82:ILE:HG23	4:D:121:ILE:O	1.74	0.86
15:1:64:PHE:CG	15:1:65:ASP:N	2.44	0.86
15:1:66:PRO:HD2	15:1:67:LEU:N	1.91	0.86
19:1:1001:CLA:HBC3	19:1:1001:CLA:CMC	2.03	0.86
19:2:2001:CLA:H42	19:2:2001:CLA:CGA	2.04	0.86
19:2:2013:CLA:HBC3	19:2:2013:CLA:HMC1	1.57	0.86
17:3:151:TRP:CD1	17:3:152:ALA:N	2.41	0.86
22:4:7034:LMU:C9	22:4:7052:LMU:C2'	2.42	0.86
2:B:247:THR:CG2	2:B:248:GLN:N	2.33	0.86
2:B:254:ILE:HB	2:B:255:LEU:HD23	1.56	0.86
3:C:7:ILE:O	3:C:8:TYR:O	1.92	0.86
16:2:182:ILE:C	16:2:187:LYS:CG	2.44	0.86
2:B:58:PHE:CD2	2:B:145:LEU:CD2	2.57	0.86
2:B:140:ILE:HG13	2:B:141:PHE:H	1.36	0.86
2:B:382:ILE:O	2:B:384:THR:N	2.08	0.86
6:F:96:LYS:O	6:F:100:LYS:HB2	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:61:THR:CB	8:H:62:THR:HG23	2.05	0.86
17:3:103:VAL:O	17:3:107:ARG:HB2	1.74	0.86
17:3:150:TYR:O	17:3:152:ALA:HB3	1.73	0.86
1:A:402:ILE:HG13	19:A:1127:CLA:HBB2	1.56	0.86
19:A:1138:CLA:HMD3	21:F:6014:BCR:HC41	1.57	0.86
2:B:310:PRO:CB	2:B:311:PRO:CD	2.54	0.86
2:B:561:GLY:HA3	3:C:52:LYS:HG2	1.56	0.86
19:B:1222:CLA:CBB	19:B:1236:CLA:HMB3	2.05	0.86
7:G:84:ARG:HG3	7:G:85:GLU:CA	2.05	0.86
8:H:99:LYS:O	8:H:100:PHE:C	2.14	0.86
11:K:97:ASP:CB	11:K:101:PHE:CE2	2.50	0.86
12:L:150:ILE:C	12:L:150:ILE:HD12	1.95	0.86
13:N:114:PHE:CG	13:N:117:ALA:CB	2.59	0.86
16:2:237:PHE:CE1	16:2:241:TYR:CZ	2.64	0.86
18:4:169:ASP:CG	18:4:174:GLN:HB2	1.95	0.86
18:4:243:THR:HG23	18:4:244:ILE:O	1.74	0.86
1:A:23:ASP:HB3	1:A:33:GLN:CD	1.95	0.86
1:A:64:PHE:CE2	1:A:74:ILE:HG23	2.09	0.86
1:A:103:PHE:HD2	1:A:103:PHE:N	1.71	0.86
1:A:240:LYS:N	1:A:243:PRO:HD2	1.89	0.86
1:A:248:PHE:HD2	1:A:248:PHE:N	1.73	0.86
1:A:267:THR:O	1:A:269:PHE:HD2	1.56	0.86
1:A:308:ILE:HD11	19:A:1115:CLA:CBB	2.04	0.86
1:A:401:TRP:CD1	19:A:1126:CLA:HHC	2.11	0.86
19:A:1105:CLA:C2B	21:J:6012:BCR:H331	2.05	0.86
2:B:444:LEU:CD2	2:B:452:GLN:HE22	1.87	0.86
19:B:1223:CLA:H122	21:B:6010:BCR:C14	2.05	0.86
6:F:89:LYS:HG2	6:F:90:GLN:N	1.90	0.86
7:G:131:GLY:HA2	7:G:136:VAL:CG2	2.06	0.86
10:J:31:ARG:NH2	19:J:1311:CLA:C4B	2.39	0.86
16:2:148:ASP:HB3	16:2:152:LEU:CG	2.04	0.86
18:4:207:ASN:ND2	19:4:4002:CLA:NA	2.23	0.86
1:A:207:LEU:HD11	1:A:314:GLY:CA	2.05	0.86
2:B:123:TRP:CB	2:B:126:THR:HG21	2.06	0.86
2:B:304:ILE:O	2:B:308:HIS:HB2	1.76	0.86
2:B:421:HIS:NE2	19:B:1228:CLA:ND	2.23	0.86
19:B:1226:CLA:HMC1	19:B:1226:CLA:HBC2	1.56	0.86
21:B:6020:BCR:C33	19:L:1502:CLA:C3B	2.54	0.86
15:1:137:ILE:HG22	19:1:1013:CLA:HBB2	1.58	0.86
17:3:151:TRP:HD1	17:3:152:ALA:H	1.21	0.86
1:A:331:LEU:HD23	1:A:331:LEU:O	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:THR:CB	2:B:134:ASP:HB2	2.06	0.86
18:4:177:LEU:HD13	18:4:178:PRO:CD	2.05	0.86
1:A:120:ALA:N	1:A:145:ILE:HD11	1.89	0.85
1:A:472:ARG:HH12	12:L:120:LEU:HD22	1.37	0.85
19:A:1137:CLA:HMC1	19:A:1137:CLA:HBC3	1.55	0.85
5:E:78:ARG:CZ	5:E:125:ILE:HG21	2.05	0.85
12:L:85:ASN:O	12:L:92:ALA:HB2	1.76	0.85
12:L:104:LEU:HD21	12:L:199:TRP:HZ2	1.41	0.85
15:1:158:PRO:HG2	15:1:159:GLU:H	1.38	0.85
16:2:186:ASN:OD1	16:2:188:LEU:CD1	2.19	0.85
1:A:190:ALA:HB1	1:A:191:PRO:HD3	1.57	0.85
1:A:195:TRP:CZ2	19:A:1108:CLA:HMA1	2.10	0.85
19:A:1131:CLA:H52	21:B:6017:BCR:H343	1.58	0.85
4:D:140:LEU:HD12	4:D:141:GLY:H	1.06	0.85
4:D:159:PRO:HD2	4:D:159:PRO:O	1.75	0.85
12:L:78:LEU:HD12	12:L:79:ILE:N	1.91	0.85
22:R:7021:LMU:H22	22:R:7021:LMU:H62	1.57	0.85
15:1:150:HIS:CD2	15:1:151:GLN:NE2	2.43	0.85
16:2:139:THR:HG23	16:2:140:ALA:N	1.85	0.85
16:2:182:ILE:CB	16:2:187:LYS:CG	2.54	0.85
18:4:122:ASN:O	18:4:123:VAL:HG12	1.76	0.85
19:B:1239:CLA:HBC2	19:B:1239:CLA:HMC1	1.56	0.85
11:K:115:ILE:CA	11:K:118:VAL:HG22	2.05	0.85
19:2:2007:CLA:HBC1	19:3:2009:CLA:CED	1.81	0.85
17:3:154:ASN:C	17:3:155:TYR:CD2	2.49	0.85
18:4:103:MET:HE2	18:4:208:GLY:HA2	0.87	0.85
18:4:172:PHE:HD1	18:4:173:LYS:O	1.57	0.85
19:4:1306:CLA:HMC1	19:4:1306:CLA:CBC	2.04	0.85
1:A:207:LEU:HD11	1:A:314:GLY:N	1.91	0.85
2:B:329:SER:O	2:B:330:ILE:CG2	2.23	0.85
2:B:596:TRP:CZ3	2:B:612:SER:O	2.30	0.85
4:D:139:ALA:O	4:D:142:THR:HG22	1.76	0.85
22:E:7048:LMU:H111	22:E:7048:LMU:C7	2.04	0.85
6:F:124:GLU:HG3	6:F:128:LYS:CD	2.06	0.85
13:N:155:GLU:CB	13:N:157:LYS:HE2	2.06	0.85
15:1:67:LEU:HD12	15:1:68:GLY:CA	2.06	0.85
21:1:6023:BCR:C8	21:1:6023:BCR:C31	2.54	0.85
18:4:167:ASN:CG	19:4:4014:CLA:C2	2.45	0.85
1:A:64:PHE:CZ	1:A:77:LYS:HE2	2.11	0.85
2:B:551:LYS:HG2	2:B:552:ASP:N	1.91	0.85
19:B:1203:CLA:HHB	19:B:1226:CLA:HBB2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:5:LYS:HD2	16:2:178:ASN:HA	1.56	0.85
19:L:1503:CLA:HAA1	19:L:1503:CLA:CGD	2.05	0.85
13:N:142:LYS:HA	13:N:142:LYS:CE	2.00	0.85
16:2:168:TRP:HD1	16:2:171:ILE:HG21	0.91	0.85
16:2:251:PHE:O	16:2:251:PHE:CD1	2.29	0.85
17:3:101:GLY:HA2	17:3:104:ILE:HD12	1.57	0.85
2:B:471:THR:O	2:B:472:TYR:CD1	2.29	0.85
2:B:672:GLN:NE2	3:C:79:LEU:HD12	1.91	0.85
4:D:156:ARG:CZ	4:D:158:PHE:CE1	2.35	0.85
4:D:157:VAL:HG12	4:D:158:PHE:O	1.77	0.85
19:I:1204:CLA:H142	21:I:6018:BCR:H392	1.59	0.85
12:L:79:ILE:CG2	12:L:80:ALA:N	2.39	0.85
15:1:206:SER:O	15:1:209:PRO:CG	2.25	0.85
16:2:184:PRO:HB3	16:2:187:LYS:CD	2.06	0.85
1:A:308:ILE:CD1	19:A:1115:CLA:CAB	2.51	0.85
1:A:308:ILE:HD11	19:A:1115:CLA:C3B	2.06	0.85
1:A:723:ARG:CG	1:A:723:ARG:HH11	1.89	0.85
22:A:7023:LMU:H91	22:A:7023:LMU:H21	1.59	0.85
2:B:25:ILE:HG21	21:L:6019:BCR:C29	2.06	0.85
2:B:200:PRO:O	2:B:204:GLY:HA3	1.77	0.85
2:B:600:THR:O	2:B:604:GLY:CA	2.25	0.85
6:F:150:VAL:O	6:F:150:VAL:HG13	1.75	0.85
11:K:56:ILE:HG23	11:K:59:THR:HG23	1.58	0.85
12:L:125:ILE:HG21	12:L:128:GLN:OE1	1.77	0.85
13:N:130:ASN:C	13:N:132:THR:CG2	2.43	0.85
13:N:139:LYS:CD	13:N:142:LYS:HZ3	1.89	0.85
1:A:71:LEU:CD1	1:A:72:GLU:N	2.39	0.85
1:A:167:THR:CG2	19:A:1112:CLA:HAA2	2.04	0.85
1:A:259:TYR:HB3	1:A:260:PRO:CD	2.07	0.85
1:A:558:LYS:NZ	2:B:674:LEU:HB2	1.92	0.85
22:A:7016:LMU:H81	22:A:7016:LMU:C2	2.04	0.85
2:B:44:GLN:CD	2:B:163:PRO:HB2	1.97	0.85
2:B:58:PHE:HE2	2:B:145:LEU:HD21	1.42	0.85
2:B:351:HIS:HB3	19:B:1214:CLA:HED1	1.58	0.85
19:B:1220:CLA:C4	19:B:1220:CLA:C4A	2.55	0.85
7:G:77:PHE:O	7:G:79:PHE:HB2	1.76	0.85
7:G:84:ARG:HE	7:G:89:LYS:CE	1.87	0.85
19:J:1308:CLA:HHD	19:J:1308:CLA:HBC3	1.56	0.85
11:K:63:LEU:N	11:K:63:LEU:HD22	1.89	0.85
13:N:132:THR:HB	13:N:139:LYS:HZ2	1.35	0.85
1:A:157:GLY:C	1:A:158:ILE:HG23	1.96	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:H	17:3:137:PHE:HZ	1.24	0.85
1:A:600:LEU:HD21	2:B:665:ILE:O	1.76	0.85
19:A:1134:CLA:HBC2	21:A:6008:BCR:HC31	1.58	0.85
3:C:44:ARG:CB	4:D:182:GLN:CD	2.45	0.85
4:D:171:GLY:O	4:D:172:VAL:HG23	1.77	0.85
6:F:185:ILE:C	6:F:186:ARG:HG2	1.97	0.85
11:K:70:PHE:C	11:K:70:PHE:CD1	2.46	0.85
13:N:133:GLY:HA3	13:N:134:CYS:O	1.77	0.85
15:1:92:LEU:HA	15:1:95:PRO:HG2	1.59	0.85
18:4:173:LYS:HB2	18:4:194:PHE:HD2	1.40	0.85
1:A:661:ALA:O	1:A:664:VAL:HG22	1.77	0.85
2:B:98:GLN:O	2:B:101:VAL:N	2.08	0.85
4:D:103:THR:HG21	4:D:128:LEU:HD12	1.55	0.85
12:L:71:THR:O	12:L:74:THR:HB	1.76	0.85
12:L:92:ALA:H	12:L:98:ARG:NH2	1.72	0.85
12:L:94:SER:O	12:L:96:LEU:HD23	1.76	0.85
19:2:2014:CLA:H152	19:2:2014:CLA:H102	1.58	0.85
1:A:78:VAL:HG11	19:A:1103:CLA:HBC3	1.59	0.84
2:B:222:LEU:HA	19:B:1212:CLA:HMD1	1.59	0.84
2:B:469:LYS:CG	2:B:470:THR:HG23	2.07	0.84
4:D:191:ILE:H	4:D:191:ILE:HD12	1.40	0.84
6:F:170:ILE:O	6:F:173:TRP:HD1	1.60	0.84
8:H:78:PRO:CD	19:L:1501:CLA:HMD1	2.07	0.84
12:L:79:ILE:HG23	12:L:80:ALA:CA	2.07	0.84
22:L:7029:LMU:H6D	22:L:7029:LMU:H51	1.56	0.84
17:3:164:LEU:HD12	17:3:165:MET:N	1.90	0.84
1:A:51:THR:OG1	19:A:1139:CLA:CBB	2.24	0.84
2:B:542:ARG:HH11	2:B:542:ARG:CB	1.90	0.84
5:E:78:ARG:NH1	5:E:125:ILE:CG2	2.41	0.84
5:E:82:TYR:HB3	5:E:83:TRP:HZ3	1.40	0.84
9:I:11:LEU:CD1	21:I:6021:BCR:H10C	2.08	0.84
19:J:1308:CLA:HBD	19:J:1308:CLA:CBA	2.06	0.84
12:L:92:ALA:N	12:L:98:ARG:CZ	2.40	0.84
15:1:125:LEU:HD22	15:1:125:LEU:H	1.40	0.84
17:3:108:PHE:HB3	19:3:3013:CLA:H43	1.58	0.84
17:3:131:GLU:CB	17:3:148:TYR:CD2	2.60	0.84
1:A:244:LEU:CD1	1:A:247:GLU:CD	2.46	0.84
19:A:1115:CLA:H172	19:A:1115:CLA:C14	2.04	0.84
21:A:6011:BCR:H311	21:A:6011:BCR:HC8	1.58	0.84
19:A:9023:CLA:CMC	2:B:661:PHE:HB2	2.06	0.84
2:B:20:ARG:HG3	2:B:20:ARG:NH1	1.86	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:GLY:CA	19:B:1225:CLA:HED1	2.04	0.84
2:B:275:HIS:O	2:B:279:ALA:N	2.09	0.84
2:B:552:ASP:OD1	2:B:553:PHE:CD2	2.30	0.84
4:D:99:PHE:N	4:D:157:VAL:O	2.10	0.84
19:H:1241:CLA:CAC	21:I:6021:BCR:C3	2.55	0.84
19:2:2001:CLA:HMC1	19:2:2001:CLA:HBC3	1.57	0.84
1:A:397:THR:CG2	1:A:613:ILE:CG1	2.50	0.84
1:A:423:ASP:N	1:A:424:PRO:HD3	1.92	0.84
7:G:90:GLN:HB3	7:G:91:VAL:C	1.97	0.84
8:H:65:TRP:N	8:H:66:ASP:HA	1.92	0.84
19:J:1308:CLA:CMA	19:2:2014:CLA:HED2	2.06	0.84
11:K:78:ARG:NE	11:K:78:ARG:CA	2.39	0.84
19:L:1148:CLA:CGD	19:L:1148:CLA:CAA	2.51	0.84
15:1:85:ILE:CA	15:1:88:ARG:HG3	2.07	0.84
17:3:171:ARG:HG2	17:3:175:ASP:OD1	1.77	0.84
18:4:146:PHE:HZ	19:4:4013:CLA:NC	1.73	0.84
1:A:596:ASP:HA	1:A:599:PHE:HB3	1.60	0.84
19:A:1112:CLA:C4B	21:A:6002:BCR:C19	2.55	0.84
19:A:1126:CLA:HBA1	19:A:1126:CLA:H43	1.60	0.84
2:B:460:ALA:O	2:B:463:ILE:O	1.95	0.84
19:B:1202:CLA:H43	21:B:6005:BCR:H313	1.58	0.84
5:E:106:ARG:HH21	5:E:107:PHE:HA	0.72	0.84
15:1:170:PRO:C	15:1:173:TYR:HE2	1.80	0.84
15:1:183:LEU:C	15:1:184:LYS:HG2	1.96	0.84
16:2:246:PRO:CB	16:2:247:ILE:CD1	2.52	0.84
2:B:98:GLN:C	2:B:100:ALA:N	2.26	0.84
21:I:6021:BCR:C4	21:I:6021:BCR:H322	2.06	0.84
11:K:124:LEU:HD12	11:K:124:LEU:O	1.77	0.84
12:L:172:GLU:N	12:L:173:PRO:HD3	1.91	0.84
13:N:157:LYS:HB3	13:N:159:LYS:H	1.39	0.84
16:2:229:MET:SD	16:2:230:LEU:CD2	2.66	0.84
3:C:44:ARG:HE	4:D:182:GLN:HE21	1.21	0.84
6:F:170:ILE:CG2	21:F:6014:BCR:C37	2.56	0.84
8:H:70:SER:O	8:H:73:PRO:HD3	1.78	0.84
19:H:1241:CLA:C3C	21:I:6021:BCR:HC22	2.07	0.84
11:K:51:SER:N	11:K:52:PRO:HD3	1.92	0.84
15:1:77:GLU:CA	15:1:80:LYS:HG2	2.06	0.84
15:1:92:LEU:CA	15:1:95:PRO:CD	2.55	0.84
18:4:88:LEU:O	18:4:90:TRP:HB3	1.77	0.84
19:A:1149:CLA:HBC2	19:A:1149:CLA:HMC1	1.57	0.84
6:F:99:LEU:HA	6:F:102:LEU:CD2	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:153:PHE:N	12:L:153:PHE:CD2	2.45	0.84
18:4:205:ILE:CG1	18:4:206:ALA:N	2.40	0.84
1:A:527:VAL:HB	1:A:626:GLY:HA3	1.58	0.84
12:L:60:ILE:HG23	12:L:61:ASN:H	1.39	0.84
15:1:64:PHE:O	15:1:69:LEU:CD1	2.25	0.84
1:A:284:ARG:HA	1:A:284:ARG:HH11	1.20	0.84
2:B:319:HIS:CE1	2:B:322:LEU:CD1	2.60	0.84
2:B:454:LEU:CD1	6:F:147:HIS:HA	2.07	0.84
2:B:542:ARG:HG3	2:B:542:ARG:NH1	1.86	0.84
19:B:1235:CLA:C20	21:F:6016:BCR:HC41	2.08	0.84
5:E:93:VAL:CG2	5:E:103:VAL:HB	2.08	0.84
7:G:124:ILE:CG1	7:G:128:LEU:HD12	2.06	0.84
15:1:90:ALA:O	15:1:94:VAL:HG23	1.77	0.84
15:1:93:ALA:HB1	19:1:1006:CLA:C1C	2.07	0.84
16:2:134:THR:HG1	16:2:135:PRO:HD2	0.99	0.84
2:B:75:GLU:CB	2:B:132:ASN:HD22	1.86	0.83
3:C:44:ARG:N	4:D:182:GLN:HG3	1.93	0.83
22:K:7042:LMU:H5'	22:K:7042:LMU:O2B	1.78	0.83
19:R:1144:CLA:HED3	19:R:1144:CLA:C1A	2.07	0.83
17:3:122:LEU:CD2	19:3:3006:CLA:C4D	2.52	0.83
1:A:733:VAL:HG21	19:A:1140:CLA:C2D	2.08	0.83
19:A:1112:CLA:HMC2	21:A:6002:BCR:C16	2.08	0.83
2:B:633:ASN:HB3	2:B:636:THR:HB	1.60	0.83
3:C:54:CYS:CB	23:C:8002:SF4:S1	2.66	0.83
8:H:78:PRO:CB	19:L:1501:CLA:HMD1	2.08	0.83
16:2:101:TRP:H	16:2:103:VAL:CB	1.90	0.83
18:4:158:GLN:CA	19:4:1004:CLA:HMA2	2.08	0.83
18:4:169:ASP:O	18:4:173:LYS:HA	1.77	0.83
1:A:356:ALA:O	1:A:360:ILE:HG22	1.77	0.83
19:A:9022:CLA:H151	21:B:6017:BCR:C20	2.09	0.83
2:B:308:HIS:CG	2:B:309:ILE:H	1.93	0.83
19:B:1220:CLA:HMD2	19:B:1221:CLA:CBB	2.09	0.83
3:C:67:VAL:HG13	3:C:68:TYR:CA	2.08	0.83
3:C:72:GLU:CD	3:C:77:MET:CE	2.46	0.83
11:K:49:ILE:C	11:K:52:PRO:HD2	1.98	0.83
13:N:164:SER:HA	13:N:165:ASN:C	1.98	0.83
17:3:96:ARG:HA	17:3:99:ALA:CA	2.08	0.83
1:A:281:LEU:HD22	19:A:1115:CLA:HMA3	1.59	0.83
22:A:7016:LMU:H1'	22:A:7016:LMU:H31	1.58	0.83
2:B:230:TRP:HB3	19:B:1213:CLA:HED3	1.57	0.83
2:B:302:LYS:HD3	7:G:105:THR:HA	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:HIS:HB2	19:B:1224:CLA:C1B	2.08	0.83
5:E:78:ARG:NH2	5:E:123:ASP:O	2.10	0.83
13:N:104:LYS:O	13:N:107:LEU:HB2	1.77	0.83
17:3:158:PHE:N	17:3:158:PHE:CD1	2.37	0.83
19:4:1004:CLA:HHD	19:4:1004:CLA:CBC	2.07	0.83
1:A:210:LEU:CD1	19:A:1111:CLA:HMB2	2.08	0.83
1:A:525:ASN:CB	1:A:526:LYS:HG3	2.08	0.83
19:B:1220:CLA:H151	19:B:1220:CLA:C10	1.97	0.83
4:D:111:ILE:CG1	4:D:121:ILE:HG22	2.07	0.83
5:E:83:TRP:HH2	5:E:116:SER:HB2	1.43	0.83
7:G:130:TRP:O	7:G:134:GLY:HA3	1.76	0.83
22:3:7003:LMU:C4B	22:3:7005:LMU:C4B	2.54	0.83
22:3:7003:LMU:H4B	22:3:7005:LMU:H4B	1.59	0.83
18:4:120:ILE:CD1	18:4:226:LYS:CG	2.07	0.83
1:A:203:LEU:HD22	19:A:1123:CLA:CED	2.07	0.83
1:A:249:ILE:HG21	17:3:136:TRP:CZ3	2.01	0.83
1:A:328:LYS:HG3	1:A:332:GLU:HB2	1.57	0.83
1:A:443:ILE:HD11	1:A:557:LEU:HD21	1.55	0.83
19:A:1133:CLA:OBD	19:A:1134:CLA:HAC1	1.79	0.83
2:B:586:THR:O	2:B:588:GLY:N	2.11	0.83
4:D:157:VAL:CG1	4:D:158:PHE:O	2.26	0.83
8:H:63:GLY:C	8:H:66:ASP:OD1	2.08	0.83
1:A:274:TRP:NE1	1:A:277:TYR:CE2	2.47	0.83
1:A:545:HIS:CB	19:A:1135:CLA:HBB2	2.08	0.83
1:A:628:ILE:CD1	1:A:632:GLY:HA2	2.08	0.83
2:B:269:TRP:HB2	2:B:497:TRP:CH2	2.14	0.83
5:E:107:PHE:HE2	5:E:109:LYS:CG	1.85	0.83
8:H:56:GLU:HG3	8:H:57:ASP:HA	1.59	0.83
8:H:113:SER:OG	19:H:1207:CLA:C6	2.26	0.83
12:L:100:ILE:HG22	12:L:191:PHE:O	1.79	0.83
13:N:132:THR:HB	13:N:139:LYS:HZ3	1.42	0.83
15:1:178:LYS:HG3	15:1:179:LYS:N	1.87	0.83
17:3:181:SER:HB2	19:3:2009:CLA:C11	2.07	0.83
18:4:122:ASN:HB3	18:4:124:PRO:HD3	1.59	0.83
22:4:7053:LMU:H11	22:4:7053:LMU:C5'	2.08	0.83
2:B:470:THR:N	2:B:501:ILE:CB	2.27	0.83
12:L:145:LEU:HD11	21:L:6019:BCR:C31	2.08	0.83
17:3:243:ILE:CD1	19:3:3005:CLA:C2C	2.57	0.83
1:A:92:TRP:O	1:A:93:LEU:HD23	1.76	0.83
1:A:244:LEU:HB3	1:A:247:GLU:CG	2.07	0.83
1:A:316:MET:CB	1:A:317:TYR:HD1	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1106:CLA:CHC	19:A:1107:CLA:HMD2	2.09	0.83
2:B:123:TRP:C	2:B:126:THR:HG22	1.99	0.83
19:B:1223:CLA:H8	21:B:6010:BCR:H12C	1.60	0.83
21:B:6020:BCR:H332	19:L:1502:CLA:C3B	2.08	0.83
3:C:44:ARG:H	4:D:182:GLN:CD	1.79	0.83
6:F:179:ARG:CG	6:F:183:ILE:HD11	2.09	0.83
11:K:125:LYS:CA	11:K:126:ASN:CB	2.51	0.83
12:L:79:ILE:HG23	12:L:80:ALA:N	1.92	0.83
16:2:158:VAL:HG22	16:2:159:PHE:N	1.92	0.83
17:3:156:THR:O	17:3:159:VAL:N	2.11	0.83
17:3:210:PRO:CG	17:3:211:LEU:HD12	2.07	0.83
2:B:7:ARG:HG3	2:B:7:ARG:NH1	1.89	0.83
2:B:131:THR:HG22	2:B:134:ASP:CB	2.09	0.83
2:B:174:ARG:HB2	19:B:1210:CLA:CBC	2.08	0.83
19:B:1222:CLA:CED	19:B:1223:CLA:HMD1	2.08	0.83
6:F:228:ASP:O	6:F:231:PHE:HB3	1.79	0.83
16:2:236:TRP:O	16:2:240:ILE:HG13	1.79	0.83
16:2:266:PHE:CD1	16:2:267:THR:N	2.47	0.83
17:3:108:PHE:CB	19:3:3013:CLA:C4	2.57	0.83
17:3:111:LEU:CG	17:3:112:GLY:N	2.19	0.83
18:4:173:LYS:C	18:4:194:PHE:CD2	2.52	0.83
1:A:207:LEU:O	1:A:310:PHE:HB3	1.77	0.82
1:A:249:ILE:HG12	1:A:250:LEU:H	1.41	0.82
19:A:1115:CLA:C19	11:K:64:MET:HE3	2.09	0.82
2:B:7:ARG:HH11	2:B:7:ARG:CB	1.91	0.82
2:B:257:ILE:O	2:B:497:TRP:HZ3	1.55	0.82
2:B:588:GLY:O	2:B:592:PHE:HB2	1.77	0.82
19:H:1145:CLA:HMA2	19:H:1145:CLA:O2A	1.79	0.82
13:N:99:LYS:HB3	13:N:102:ASN:HD21	1.41	0.82
13:N:132:THR:HG1	13:N:138:ALA:C	1.82	0.82
14:R:41:UNK:CB	14:R:42:UNK:CB	2.56	0.82
15:1:97:ILE:CD1	15:1:98:LEU:HD23	2.09	0.82
16:2:124:GLU:O	16:2:127:THR:CA	2.27	0.82
1:A:236:GLY:O	1:A:237:VAL:HG22	1.78	0.82
1:A:488:PHE:CE2	1:A:533:PRO:HB2	2.14	0.82
2:B:715:VAL:HG13	2:B:719:PHE:CD2	2.13	0.82
2:B:732:LYS:HB3	2:B:733:PHE:CA	2.08	0.82
3:C:20:ALA:O	3:C:21:CYS:HB2	1.76	0.82
8:H:64:GLN:HB2	8:H:67:SER:H	1.44	0.82
9:I:24:LEU:C	9:I:26:LEU:H	1.80	0.82
19:J:1308:CLA:HMA3	19:2:2014:CLA:HED2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:57:MET:SD	11:K:61:THR:OG1	2.36	0.82
19:K:1143:CLA:H3A	19:K:1143:CLA:CGA	2.09	0.82
12:L:83:LEU:O	12:L:83:LEU:HD12	1.78	0.82
12:L:92:ALA:CB	12:L:98:ARG:NH2	2.41	0.82
15:1:77:GLU:CA	15:1:80:LYS:CG	2.53	0.82
1:A:668:TYR:OH	2:B:441:ASP:OD1	1.96	0.82
23:A:8001:SF4:S4	2:B:560:ASP:O	2.37	0.82
2:B:515:GLY:HA3	2:B:613:SER:HB2	1.60	0.82
8:H:78:PRO:HD3	19:L:1501:CLA:HMD1	1.60	0.82
8:H:109:LEU:O	8:H:113:SER:CB	2.27	0.82
19:J:1308:CLA:H92	19:2:2014:CLA:CGD	2.10	0.82
12:L:51:LYS:HE2	12:L:51:LYS:CA	2.07	0.82
19:2:2014:CLA:H152	19:2:2014:CLA:C8	2.10	0.82
1:A:103:PHE:N	1:A:103:PHE:CD2	2.44	0.82
19:A:1113:CLA:HMC1	19:A:1113:CLA:HBC3	1.62	0.82
2:B:7:ARG:O	2:B:7:ARG:HG2	1.79	0.82
2:B:493:TRP:NE1	19:B:1213:CLA:HAC2	1.93	0.82
2:B:618:GLY:HA2	2:B:621:ARG:HB3	1.61	0.82
24:B:7101:LMG:O3	3:C:70:TRP:CE2	2.31	0.82
6:F:103:GLN:CG	6:F:104:ALA:H	1.91	0.82
6:F:200:VAL:CG1	10:J:7:TYR:N	2.42	0.82
13:N:157:LYS:H	13:N:157:LYS:HE2	1.42	0.82
16:2:177:VAL:CG1	16:2:178:ASN:HB2	2.05	0.82
1:A:207:LEU:HD22	19:A:1119:CLA:HBB2	1.59	0.82
19:A:1138:CLA:HBC2	19:A:1139:CLA:C1C	2.10	0.82
19:A:9023:CLA:HMC3	2:B:661:PHE:HB2	1.61	0.82
19:B:1210:CLA:H141	19:B:1215:CLA:H2	1.61	0.82
4:D:86:SER:O	12:L:67:GLY:CA	2.27	0.82
4:D:163:VAL:O	4:D:164:GLN:CG	2.27	0.82
4:D:185:GLY:O	4:D:186:GLN:HG3	1.79	0.82
15:1:208:TYR:N	15:1:209:PRO:HD3	1.94	0.82
19:3:3017:CLA:O1A	19:3:3017:CLA:HMA2	1.78	0.82
18:4:195:ALA:HB3	18:4:197:THR:O	1.79	0.82
1:A:93:LEU:CA	1:A:96:MET:H	1.91	0.82
2:B:268:LEU:HD22	2:B:273:VAL:CG1	2.10	0.82
19:B:1218:CLA:HBC2	19:B:1218:CLA:CHD	2.07	0.82
4:D:132:ALA:HB3	4:D:136:GLN:HE22	1.43	0.82
6:F:132:ASN:C	6:F:133:TYR:HD1	1.82	0.82
12:L:72:PRO:O	12:L:73:VAL:CG2	2.26	0.82
13:N:114:PHE:CB	13:N:117:ALA:HB3	2.09	0.82
16:2:229:MET:SD	16:2:230:LEU:CA	2.67	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:159:VAL:O	17:3:160:LEU:C	2.14	0.82
19:A:1134:CLA:CGA	19:A:1141:CLA:CBB	2.56	0.82
11:K:63:LEU:HD13	11:K:63:LEU:H	1.42	0.82
19:L:1130:CLA:H52	19:L:1504:CLA:HHB	1.61	0.82
18:4:96:LEU:HD12	18:4:97:VAL:N	1.95	0.82
2:B:279:ALA:O	19:B:1213:CLA:HMB3	1.80	0.82
2:B:315:LEU:HD12	2:B:317:ARG:CG	2.04	0.82
6:F:177:VAL:HA	6:F:180:SER:OG	1.78	0.82
16:2:128:LYS:HB3	16:2:131:ILE:HG12	1.59	0.82
19:2:2014:CLA:C15	19:2:2014:CLA:H91	2.09	0.82
17:3:150:TYR:CD2	17:3:151:TRP:CG	2.67	0.82
19:4:1306:CLA:HED1	19:4:1306:CLA:H2	1.60	0.82
5:E:90:VAL:HG12	5:E:91:VAL:N	1.95	0.82
7:G:124:ILE:HG12	7:G:128:LEU:HD13	1.62	0.82
15:1:92:LEU:C	15:1:95:PRO:CD	2.47	0.82
15:1:114:TRP:CH2	15:1:121:GLN:HG3	2.15	0.82
19:1:1007:CLA:CBC	19:1:1007:CLA:HHD	2.09	0.82
16:2:165:GLY:CA	16:2:167:ARG:HG2	2.08	0.82
17:3:156:THR:O	17:3:156:THR:CG2	2.26	0.82
1:A:246:HIS:CD2	19:3:1147:CLA:O1D	2.33	0.82
2:B:123:TRP:CB	2:B:126:THR:CG2	2.57	0.82
2:B:440:ASN:OD1	2:B:614:THR:HG22	1.76	0.82
2:B:440:ASN:OD1	2:B:614:THR:HG21	1.77	0.82
19:B:1220:CLA:HBC3	19:B:1220:CLA:CMC	2.04	0.82
19:B:1235:CLA:H161	21:F:6016:BCR:C31	2.08	0.82
3:C:63:LEU:CD2	3:C:65:VAL:H	1.92	0.82
11:K:78:ARG:HA	11:K:78:ARG:CZ	2.09	0.82
17:3:131:GLU:CB	17:3:148:TYR:CE2	2.62	0.82
17:3:187:PHE:C	17:3:187:PHE:CD1	2.54	0.82
1:A:162:LEU:O	1:A:165:TYR:CB	2.25	0.81
1:A:281:LEU:CG	19:A:1115:CLA:HED1	2.09	0.81
2:B:31:PHE:O	2:B:37:ILE:HG21	1.80	0.81
3:C:72:GLU:CD	3:C:77:MET:HE1	1.99	0.81
5:E:78:ARG:CZ	5:E:125:ILE:CG2	2.57	0.81
17:3:98:LEU:CD1	19:3:3012:CLA:C2D	2.57	0.81
18:4:111:LEU:HD12	18:4:112:PRO:CG	2.10	0.81
18:4:220:GLN:HG3	19:4:1306:CLA:HAC2	1.61	0.81
1:A:79:PHE:CD1	19:A:1111:CLA:HED3	2.16	0.81
19:A:1122:CLA:C4C	21:A:6007:BCR:C19	2.59	0.81
2:B:224:PRO:CB	2:B:227:THR:HB	2.10	0.81
2:B:679:ALA:O	2:B:683:GLU:OE1	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:100:PHE:N	7:G:101:GLU:CB	2.43	0.81
8:H:97:LEU:HG	8:H:98:LEU:CA	2.10	0.81
21:I:6021:BCR:C39	21:L:6019:BCR:H401	2.09	0.81
12:L:73:VAL:CG2	19:L:1130:CLA:OBD	2.28	0.81
12:L:115:VAL:CG1	12:L:130:GLY:H	1.91	0.81
19:2:2014:CLA:OBD	19:2:2014:CLA:HED3	1.79	0.81
1:A:129:GLN:NE2	19:A:1107:CLA:MG	1.36	0.81
1:A:284:ARG:NH2	1:A:507:ALA:O	2.11	0.81
1:A:426:THR:HG23	1:A:428:TYR:OH	1.79	0.81
2:B:79:GLN:O	2:B:80:ASP:HB3	1.79	0.81
2:B:293:THR:HG22	7:G:94:GLN:CG	2.10	0.81
2:B:556:SER:C	2:B:558:PRO:HD2	2.00	0.81
2:B:600:THR:O	2:B:604:GLY:HA3	1.81	0.81
2:B:633:ASN:CB	2:B:636:THR:CB	2.44	0.81
4:D:185:GLY:O	4:D:186:GLN:CG	2.28	0.81
5:E:107:PHE:CD2	5:E:109:LYS:CG	2.63	0.81
6:F:97:GLN:CD	6:F:98:ALA:N	2.33	0.81
8:H:98:LEU:HD23	12:L:146:THR:HG21	1.61	0.81
13:N:118:TYR:O	13:N:119:THR:HG23	1.80	0.81
15:1:149:GLU:CG	15:1:152:ARG:HH12	1.93	0.81
15:1:224:PRO:CA	15:1:225:TRP:HB2	2.10	0.81
17:3:161:GLU:HA	17:3:164:LEU:HG	1.61	0.81
17:3:204:GLY:HA3	17:3:206:PRO:O	1.80	0.81
22:3:7005:LMU:H51	22:3:7005:LMU:H11	1.61	0.81
18:4:96:LEU:C	18:4:96:LEU:CD1	2.48	0.81
18:4:169:ASP:HA	18:4:173:LYS:CA	2.10	0.81
19:B:1205:CLA:HMC2	21:B:6017:BCR:H281	1.61	0.81
3:C:52:LYS:HZ1	3:C:64:SER:CB	1.93	0.81
4:D:101:VAL:HG12	4:D:130:LYS:HB2	1.62	0.81
9:I:8:PHE:HB2	19:I:1204:CLA:OBD	1.80	0.81
11:K:56:ILE:HA	11:K:59:THR:HG22	1.62	0.81
11:K:76:ALA:H	11:K:78:ARG:NH1	1.78	0.81
12:L:141:LEU:HD13	12:L:145:LEU:CD1	2.09	0.81
15:1:77:GLU:CB	15:1:80:LYS:HD2	2.11	0.81
15:1:114:TRP:CH2	15:1:121:GLN:HA	2.14	0.81
15:1:172:GLY:HA2	15:1:173:TYR:CD2	2.14	0.81
17:3:96:ARG:NH1	17:3:96:ARG:CB	2.41	0.81
17:3:136:TRP:N	17:3:139:THR:OG1	2.13	0.81
18:4:131:LYS:H	18:4:131:LYS:HD2	1.45	0.81
1:A:158:ILE:HD13	19:A:1112:CLA:HED3	1.62	0.81
19:A:1112:CLA:C4B	21:A:6002:BCR:H19C	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:LEU:O	4:D:140:LEU:O	1.98	0.81
7:G:124:ILE:HG23	7:G:125:VAL:N	1.96	0.81
1:A:129:GLN:NE2	19:A:1107:CLA:ND	2.29	0.81
19:A:1105:CLA:HMB1	21:J:6012:BCR:HC7	1.62	0.81
19:A:1115:CLA:C19	11:K:64:MET:CE	2.59	0.81
23:A:8001:SF4:S2	2:B:702:ILE:HD11	2.21	0.81
2:B:172:GLU:O	2:B:176:ASN:CB	2.28	0.81
2:B:229:GLN:C	7:G:63:VAL:CG2	2.46	0.81
2:B:315:LEU:CD1	2:B:317:ARG:CG	2.57	0.81
2:B:353:TYR:CD2	2:B:594:TRP:HZ3	1.96	0.81
3:C:69:LEU:HD12	3:C:70:TRP:N	1.95	0.81
19:J:1308:CLA:HBC2	19:J:1308:CLA:CHD	2.10	0.81
12:L:141:LEU:CD1	12:L:145:LEU:HD11	2.08	0.81
15:1:117:LEU:HD13	15:1:117:LEU:N	1.96	0.81
16:2:184:PRO:CD	16:2:187:LYS:N	2.44	0.81
1:A:23:ASP:OD1	1:A:24:ARG:HD2	1.80	0.81
1:A:98:PHE:CZ	19:A:1105:CLA:HMD3	2.16	0.81
1:A:126:ILE:HD11	19:A:1107:CLA:HMA1	1.63	0.81
1:A:483:GLN:HB3	1:A:485:GLN:CD	2.01	0.81
19:A:1115:CLA:H193	11:K:64:MET:CE	2.10	0.81
2:B:140:ILE:CG1	2:B:141:PHE:H	1.92	0.81
2:B:232:LEU:HD11	2:B:235:GLN:HG3	1.59	0.81
4:D:93:LYS:HG3	4:D:96:VAL:CG1	2.10	0.81
5:E:127:GLU:CA	5:E:128:VAL:O	2.29	0.81
12:L:164:LEU:HD12	12:L:165:THR:H	1.42	0.81
12:L:210:PRO:C	12:L:211:TYR:CG	2.53	0.81
17:3:201:ALA:HB1	17:3:202:TYR:HE2	1.39	0.81
2:B:294:ASN:CB	7:G:94:GLN:OE1	2.25	0.81
5:E:127:GLU:CB	5:E:128:VAL:O	2.28	0.81
5:E:127:GLU:CB	5:E:129:GLU:O	2.29	0.81
8:H:116:ALA:HB1	8:H:117:SER:CA	2.06	0.81
15:1:97:ILE:HD12	15:1:98:LEU:HD23	1.63	0.81
15:1:137:ILE:HG12	15:1:138:LEU:N	1.96	0.81
15:1:158:PRO:CG	15:1:159:GLU:H	1.92	0.81
16:2:128:LYS:HB3	16:2:131:ILE:HG23	1.62	0.81
16:2:129:LEU:O	16:2:130:GLY:C	2.19	0.81
1:A:195:TRP:CZ2	19:A:1108:CLA:CMA	2.63	0.81
1:A:249:ILE:C	1:A:251:ASN:N	2.31	0.81
1:A:415:ALA:O	1:A:419:VAL:HG23	1.80	0.81
2:B:233:TYR:HD1	2:B:254:ILE:HG13	1.44	0.81
2:B:298:GLY:CA	19:B:1218:CLA:HMD3	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:ILE:O	4:D:198:ILE:HG13	1.75	0.81
5:E:107:PHE:CD2	5:E:109:LYS:CD	2.64	0.81
22:E:7048:LMU:H4B	22:F:7036:LMU:C6'	2.07	0.81
6:F:103:GLN:CG	6:F:104:ALA:N	2.44	0.81
7:G:69:GLY:O	7:G:72:LEU:CG	2.29	0.81
13:N:114:PHE:O	13:N:117:ALA:HB3	1.80	0.81
19:1:1007:CLA:HHD	19:1:1007:CLA:HBC2	1.63	0.81
16:2:124:GLU:O	16:2:127:THR:HG22	1.81	0.81
1:A:227:LEU:HD22	1:A:296:LEU:HD13	1.61	0.81
2:B:571:SER:OG	2:B:574:ASP:OD1	1.99	0.81
2:B:656:VAL:HG22	19:B:1239:CLA:HMB3	1.63	0.81
4:D:123:ARG:HH22	22:D:7050:LMU:H4B	1.45	0.81
5:E:78:ARG:NH1	5:E:125:ILE:HG21	1.95	0.81
6:F:200:VAL:HG23	6:F:204:SER:H	1.46	0.81
15:1:83:GLU:C	15:1:86:HIS:CD2	2.53	0.81
19:2:2014:CLA:C10	19:2:2014:CLA:C15	2.59	0.81
1:A:68:THR:HG22	1:A:70:ASP:H	1.42	0.80
2:B:314:ARG:HH12	15:1:67:LEU:HD21	0.98	0.80
2:B:388:ALA:C	2:B:391:PRO:HD2	2.00	0.80
2:B:542:ARG:NH2	4:D:195:VAL:O	2.14	0.80
19:B:1203:CLA:H2A	19:B:1203:CLA:O1D	1.81	0.80
7:G:73:PHE:O	7:G:76:ARG:HB2	1.80	0.80
12:L:174:ASP:CG	12:L:175:GLN:H	1.84	0.80
15:1:116:ALA:C	15:1:117:LEU:HD22	2.00	0.80
16:2:182:ILE:HG22	16:2:187:LYS:CG	2.09	0.80
17:3:125:VAL:HB	17:3:126:GLY:HA2	1.61	0.80
19:A:1126:CLA:H172	21:J:6012:BCR:H17C	1.62	0.80
2:B:58:PHE:CE2	2:B:145:LEU:HD21	2.14	0.80
2:B:224:PRO:CB	2:B:227:THR:CB	2.60	0.80
2:B:304:ILE:HD11	19:B:1216:CLA:HED2	0.83	0.80
2:B:625:TRP:CE3	2:B:625:TRP:C	2.55	0.80
19:B:1235:CLA:C16	21:F:6016:BCR:C31	2.59	0.80
7:G:79:PHE:CG	7:G:80:PHE:N	2.50	0.80
14:R:33:UNK:O	14:R:36:UNK:CB	2.30	0.80
15:1:137:ILE:HG12	15:1:138:LEU:H	1.46	0.80
18:4:174:GLN:O	18:4:194:PHE:HB3	1.80	0.80
18:4:215:LEU:O	18:4:216:GLY:C	2.17	0.80
1:A:352:THR:HA	19:A:1123:CLA:H201	1.61	0.80
19:A:1237:CLA:HMD3	21:B:6017:BCR:HC31	1.63	0.80
2:B:131:THR:O	2:B:135:LEU:HD23	1.82	0.80
2:B:378:ILE:O	2:B:380:GLY:N	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1235:CLA:HBC1	6:F:160:PHE:HZ	1.41	0.80
3:C:29:ILE:HG12	4:D:180:GLY:HA2	1.63	0.80
9:I:1:MET:O	9:I:2:ILE:HG22	1.80	0.80
15:1:85:ILE:HG12	15:1:88:ARG:NH2	1.97	0.80
15:1:170:PRO:C	15:1:173:TYR:CE2	2.54	0.80
17:3:113:ALA:HB1	17:3:239:LEU:CD1	1.98	0.80
1:A:279:ASP:O	1:A:281:LEU:CD1	2.29	0.80
1:A:370:ILE:CG2	1:A:400:MET:HA	2.11	0.80
1:A:445:HIS:O	1:A:446:LEU:HB3	1.80	0.80
2:B:58:PHE:CE2	2:B:145:LEU:HD22	2.09	0.80
6:F:103:GLN:HG3	6:F:104:ALA:H	1.47	0.80
7:G:62:LEU:CB	7:G:65:SER:HB3	2.09	0.80
11:K:47:ASP:HA	11:K:51:SER:HB2	1.64	0.80
11:K:115:ILE:CG1	11:K:122:LEU:H	1.92	0.80
12:L:73:VAL:HA	19:L:1504:CLA:HMA3	1.64	0.80
15:1:92:LEU:HA	15:1:95:PRO:CD	2.11	0.80
15:1:171:LEU:CA	15:1:173:TYR:CZ	2.63	0.80
16:2:177:VAL:CG1	16:2:178:ASN:CB	2.58	0.80
18:4:103:MET:HE2	18:4:208:GLY:N	1.62	0.80
18:4:211:MET:HG3	19:4:4002:CLA:CBB	2.12	0.80
1:A:255:LEU:CD1	1:A:280:PHE:HZ	1.93	0.80
1:A:281:LEU:CD2	19:A:1115:CLA:HED1	2.03	0.80
1:A:328:LYS:HZ3	1:A:345:GLY:HA2	1.44	0.80
1:A:356:ALA:HB2	1:A:417:PHE:CD2	2.17	0.80
1:A:423:ASP:CB	1:A:424:PRO:HD3	2.11	0.80
19:A:9013:CLA:HMD1	2:B:533:ILE:HG21	1.63	0.80
2:B:432:HIS:HE1	19:B:1229:CLA:NB	1.80	0.80
2:B:459:PHE:HE2	19:B:1235:CLA:CHD	1.95	0.80
2:B:628:SER:O	2:B:631:LEU:CD2	2.29	0.80
22:D:7050:LMU:C2B	22:D:7050:LMU:C6'	2.57	0.80
16:2:160:ILE:HG22	19:2:2012:CLA:CAB	2.12	0.80
1:A:76:ARG:NH1	1:A:193:LEU:HD22	1.96	0.80
1:A:123:VAL:O	19:A:1107:CLA:O1D	1.97	0.80
1:A:353:SER:O	1:A:354:TRP:HB2	1.82	0.80
2:B:119:GLY:HA3	19:B:1225:CLA:CED	2.09	0.80
2:B:457:PRO:CB	2:B:517:PHE:HB2	2.12	0.80
19:B:1213:CLA:HHH	19:B:1213:CLA:CBC	2.12	0.80
19:L:1148:CLA:HBC3	19:L:1148:CLA:CHD	2.09	0.80
13:N:110:THR:HG22	13:N:111:GLY:H	1.46	0.80
16:2:184:PRO:HD3	16:2:187:LYS:CD	2.12	0.80
16:2:237:PHE:C	16:2:237:PHE:CD1	2.54	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:131:LYS:H	18:4:131:LYS:CD	1.95	0.80
1:A:50:THR:CG2	1:A:51:THR:N	2.44	0.80
1:A:244:LEU:HD12	1:A:247:GLU:OE1	1.81	0.80
19:A:1131:CLA:H161	21:L:6019:BCR:C36	2.12	0.80
19:A:1138:CLA:C19	6:F:181:TYR:HB3	2.10	0.80
21:A:6011:BCR:H312	19:A:9013:CLA:H143	1.62	0.80
8:H:78:PRO:HB3	19:L:1501:CLA:HMD1	1.63	0.80
22:1:7004:LMU:O6B	22:1:7004:LMU:H1B	1.80	0.80
1:A:355:HIS:ND1	1:A:416:ILE:HG21	1.97	0.80
1:A:446:LEU:HD21	1:A:554:LEU:HA	1.62	0.80
2:B:282:PHE:CZ	19:B:1213:CLA:C1	2.64	0.80
2:B:462:TRP:CZ3	19:B:1231:CLA:CBC	2.65	0.80
4:D:102:ILE:HG13	4:D:154:PHE:HB3	1.64	0.80
5:E:126:VAL:O	5:E:127:GLU:CB	2.30	0.80
14:R:34:UNK:O	14:R:38:UNK:CB	2.30	0.80
18:4:112:PRO:HD2	18:4:113:GLU:HG3	1.62	0.80
1:A:442:ILE:HG23	19:A:1129:CLA:HMC3	1.64	0.80
19:A:1149:CLA:HAA1	19:A:1149:CLA:CGD	2.12	0.80
2:B:469:LYS:HD2	2:B:470:THR:HA	0.86	0.80
2:B:527:LEU:CD1	19:B:1236:CLA:CMA	2.60	0.80
19:B:1220:CLA:C4A	19:B:1220:CLA:H42	2.11	0.80
4:D:174:PRO:O	4:D:175:GLU:HG2	1.82	0.80
5:E:107:PHE:CE2	5:E:109:LYS:CE	2.65	0.80
22:H:7011:LMU:C10	22:H:7011:LMU:H61	2.12	0.80
19:J:1311:CLA:HED3	19:J:1311:CLA:CHA	2.10	0.80
13:N:132:THR:OG1	13:N:138:ALA:O	1.98	0.80
14:R:35:UNK:O	14:R:38:UNK:CB	2.29	0.80
16:2:120:ILE:HG13	16:2:121:PHE:H	1.47	0.80
16:2:134:THR:HG1	16:2:135:PRO:CD	1.74	0.80
16:2:156:GLU:CG	16:2:157:LEU:CD1	2.57	0.80
16:2:204:LEU:HD12	16:2:210:SER:O	1.82	0.80
17:3:104:ILE:HG21	19:3:3004:CLA:C1D	2.11	0.80
1:A:284:ARG:HG3	1:A:295:TRP:CD1	2.17	0.80
2:B:199:ILE:CG2	2:B:270:LEU:CD1	2.55	0.80
2:B:456:GLU:HA	2:B:514:PRO:HD3	1.62	0.80
19:B:1219:CLA:HBC2	19:B:1220:CLA:HBA1	1.62	0.80
5:E:126:VAL:O	5:E:127:GLU:CG	2.29	0.80
11:K:122:LEU:O	11:K:122:LEU:HD22	1.82	0.80
15:1:151:GLN:N	15:1:151:GLN:HE21	1.79	0.80
19:2:2007:CLA:CAC	19:3:2009:CLA:HED3	2.00	0.80
22:4:7034:LMU:H111	22:4:7052:LMU:C2'	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLY:HA3	1:A:430:ASP:HB2	0.81	0.79
1:A:389:TYR:CE1	1:A:625:TRP:CD1	2.70	0.79
2:B:102:GLU:O	2:B:104:PHE:HB2	1.82	0.79
2:B:293:THR:CG2	7:G:94:GLN:HG2	2.12	0.79
2:B:462:TRP:HZ3	19:B:1231:CLA:HBC2	1.47	0.79
6:F:214:PRO:O	6:F:215:VAL:HB	1.78	0.79
19:H:1207:CLA:HMA2	19:H:1207:CLA:O2A	1.82	0.79
22:H:7011:LMU:H61	22:H:7011:LMU:H101	1.61	0.79
21:I:6021:BCR:H313	21:I:6021:BCR:HC8	0.81	0.79
11:K:89:ARG:NH1	11:K:89:ARG:HG3	1.97	0.79
13:N:169:LYS:CB	13:N:170:TRP:HD1	1.95	0.79
14:R:36:UNK:O	14:R:38:UNK:CB	2.30	0.79
16:2:166:ARG:CA	16:2:167:ARG:HB2	2.11	0.79
22:2:7006:LMU:H5'	22:2:7006:LMU:O5B	1.79	0.79
17:3:141:VAL:HG23	17:3:142:ILE:CG1	2.10	0.79
17:3:153:ASP:HB2	17:3:154:ASN:OD1	1.81	0.79
18:4:177:LEU:HD22	18:4:178:PRO:CD	2.12	0.79
1:A:152:ILE:CD1	19:A:1127:CLA:O1D	2.29	0.79
1:A:316:MET:HG2	1:A:317:TYR:HD1	1.44	0.79
19:A:1105:CLA:CBA	19:A:1107:CLA:H12	2.12	0.79
19:A:1115:CLA:HMC1	19:A:1115:CLA:CBC	2.09	0.79
19:A:1124:CLA:HBC2	19:A:1124:CLA:CHD	2.10	0.79
2:B:306:GLU:HG3	2:B:307:ALA:N	1.97	0.79
19:B:1220:CLA:NA	19:B:1220:CLA:H41	1.95	0.79
3:C:44:ARG:N	4:D:182:GLN:CG	2.46	0.79
11:K:125:LYS:CB	11:K:128:GLY:HA2	2.13	0.79
12:L:78:LEU:HD22	19:L:1504:CLA:HED1	1.62	0.79
13:N:130:ASN:CB	13:N:139:LYS:CG	2.29	0.79
13:N:142:LYS:N	13:N:145:PHE:O	2.14	0.79
14:R:38:UNK:O	14:R:42:UNK:CA	2.29	0.79
15:1:190:ASN:ND2	19:1:1002:CLA:C4D	2.44	0.79
16:2:101:TRP:N	16:2:103:VAL:H	1.81	0.79
16:2:201:PHE:CD1	16:2:202:ASP:N	2.50	0.79
18:4:142:PHE:HA	18:4:145:GLU:OE1	1.82	0.79
2:B:626:LEU:O	2:B:627:ASN:HB2	1.82	0.79
6:F:100:LYS:O	6:F:100:LYS:HD2	1.81	0.79
7:G:128:LEU:HD23	7:G:128:LEU:C	2.03	0.79
12:L:145:LEU:HG	21:L:6019:BCR:HC7	1.62	0.79
13:N:130:ASN:HB2	13:N:139:LYS:HG2	0.80	0.79
13:N:148:ASP:HA	13:N:149:ASP:O	1.83	0.79
15:1:112:GLN:CG	15:1:113:GLU:H	1.92	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:111:LEU:O	17:3:114:VAL:CA	2.30	0.79
17:3:252:PRO:HB3	17:3:254:GLN:HE21	1.47	0.79
1:A:50:THR:HG22	1:A:51:THR:N	1.98	0.79
1:A:64:PHE:HZ	1:A:77:LYS:CE	1.95	0.79
1:A:162:LEU:C	1:A:165:TYR:HB3	2.03	0.79
1:A:267:THR:HG22	1:A:267:THR:O	1.81	0.79
22:E:7048:LMU:C4B	22:F:7036:LMU:C6'	2.60	0.79
18:4:87:ASN:CG	18:4:90:TRP:CE2	2.54	0.79
18:4:205:ILE:HG12	18:4:206:ALA:N	1.98	0.79
1:A:534:LEU:HD12	1:A:535:GLY:H	0.98	0.79
1:A:579:PHE:N	1:A:579:PHE:HD1	1.81	0.79
2:B:160:LYS:NZ	2:B:161:TRP:CE3	2.49	0.79
2:B:594:TRP:O	2:B:595:HIS:CB	2.31	0.79
3:C:12:ILE:HG13	23:C:8003:SF4:S1	2.23	0.79
6:F:200:VAL:HG23	6:F:204:SER:N	1.98	0.79
11:K:59:THR:O	11:K:63:LEU:HD21	1.83	0.79
11:K:127:ILE:C	11:K:130:LEU:HG	2.02	0.79
13:N:114:PHE:CB	13:N:117:ALA:CB	2.60	0.79
16:2:101:TRP:N	16:2:103:VAL:HB	1.96	0.79
16:2:131:ILE:O	16:2:132:LEU:HB2	1.82	0.79
16:2:227:LEU:HD21	19:2:2004:CLA:CHC	2.13	0.79
17:3:243:ILE:CD1	19:3:3005:CLA:C1C	2.59	0.79
18:4:120:ILE:HG22	18:4:121:ILE:N	1.96	0.79
1:A:22:VAL:O	1:A:22:VAL:CG2	2.28	0.79
1:A:388:ASP:CG	1:A:391:THR:OG1	2.21	0.79
2:B:257:ILE:C	2:B:497:TRP:HZ3	1.86	0.79
2:B:469:LYS:NZ	2:B:471:THR:H	1.80	0.79
2:B:527:LEU:O	2:B:527:LEU:HD12	1.82	0.79
5:E:79:LYS:HE3	5:E:84:TYR:OH	1.81	0.79
5:E:127:GLU:O	5:E:128:VAL:CG2	2.29	0.79
8:H:119:ASP:CG	8:H:121:LEU:HG	2.03	0.79
9:I:7:LEU:CD1	21:I:6021:BCR:H333	2.08	0.79
22:L:7029:LMU:H5B	22:L:7029:LMU:C4'	2.09	0.79
22:L:7029:LMU:O2B	22:L:7029:LMU:H6E	1.82	0.79
13:N:138:ALA:HB3	13:N:140:GLN:HG3	1.65	0.79
18:4:94:ALA:O	18:4:98:ASN:OD1	2.01	0.79
1:A:684:PHE:C	1:A:684:PHE:CD2	2.56	0.79
21:A:6011:BCR:H313	19:A:9013:CLA:C14	2.11	0.79
2:B:93:ASP:OD1	2:B:96:PHE:CD1	2.35	0.79
2:B:334:LEU:HG	2:B:334:LEU:O	1.81	0.79
2:B:475:ASP:O	2:B:476:ILE:CG2	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:ARG:NH2	7:G:117:ASN:O	2.14	0.79
7:G:90:GLN:CB	7:G:91:VAL:C	2.51	0.79
7:G:131:GLY:CA	7:G:136:VAL:HG23	2.13	0.79
22:G:7026:LMU:H2B	22:G:7026:LMU:O3'	1.83	0.79
19:J:1308:CLA:H2A	19:J:1308:CLA:O2A	1.80	0.79
12:L:91:THR:HA	12:L:98:ARG:HH12	1.47	0.79
15:1:77:GLU:HG3	15:1:80:LYS:CD	2.13	0.79
15:1:170:PRO:CD	15:1:173:TYR:CE2	2.66	0.79
15:1:182:GLU:OE1	19:1:1001:CLA:C1D	2.31	0.79
16:2:224:ASN:OD1	16:2:227:LEU:HD22	1.82	0.79
17:3:201:ALA:CB	17:3:202:TYR:HD2	1.94	0.79
1:A:77:LYS:O	1:A:80:SER:OG	2.00	0.79
1:A:484:LEU:HD22	1:A:484:LEU:N	1.96	0.79
1:A:567:ARG:NH1	4:D:89:GLY:CA	2.45	0.79
2:B:363:GLN:H	2:B:365:PHE:HB3	1.46	0.79
19:B:1223:CLA:CED	19:B:1231:CLA:HBB2	2.11	0.79
20:B:5002:PQN:H2M1	20:B:5002:PQN:H142	1.64	0.79
3:C:1:MET:H1	3:C:4:SER:N	1.79	0.79
4:D:167:HIS:N	4:D:168:PRO:CD	2.45	0.79
15:1:78:ARG:NH2	15:1:179:LYS:CD	2.37	0.79
15:1:162:LYS:O	15:1:164:PRO:HD3	1.83	0.79
15:1:172:GLY:HA2	15:1:173:TYR:CG	2.17	0.79
19:1:1014:CLA:H41	19:1:1014:CLA:C7	2.04	0.79
16:2:229:MET:SD	16:2:230:LEU:N	2.55	0.79
17:3:148:TYR:N	17:3:149:ASN:ND2	2.30	0.79
22:3:7003:LMU:C3B	22:3:7005:LMU:O5B	2.30	0.79
1:A:255:LEU:HD13	1:A:280:PHE:CZ	2.12	0.79
1:A:452:PHE:CE1	19:A:1136:CLA:CBB	2.66	0.79
2:B:25:ILE:O	2:B:25:ILE:CG1	2.27	0.79
2:B:53:GLN:HG3	19:B:1202:CLA:HHB	1.65	0.79
2:B:310:PRO:CG	2:B:311:PRO:CD	2.61	0.79
2:B:454:LEU:HD12	2:B:454:LEU:O	1.82	0.79
4:D:156:ARG:NE	4:D:164:GLN:HB2	1.98	0.79
7:G:69:GLY:HA2	7:G:72:LEU:HG	1.65	0.79
7:G:134:GLY:O	7:G:135:HIS:CG	2.36	0.79
13:N:148:ASP:N	13:N:149:ASP:CB	2.45	0.79
15:1:92:LEU:HA	15:1:95:PRO:CG	2.12	0.79
15:1:97:ILE:CD1	15:1:98:LEU:HB2	2.12	0.79
1:A:68:THR:HG23	1:A:70:ASP:H	1.47	0.79
1:A:316:MET:HB3	1:A:317:TYR:CG	2.18	0.79
2:B:557:PHE:N	2:B:558:PRO:CD	2.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:7101:LMG:O3	3:C:70:TRP:NE1	2.16	0.79
4:D:99:PHE:CB	4:D:157:VAL:HG12	2.13	0.79
8:H:61:THR:HA	8:H:62:THR:HG22	1.64	0.79
13:N:130:ASN:O	13:N:132:THR:HG22	1.78	0.79
16:2:115:LEU:O	16:2:118:ALA:HB3	1.82	0.79
16:2:269:LYS:HA	16:2:269:LYS:CE	2.12	0.79
18:4:123:VAL:N	18:4:124:PRO:HD3	1.98	0.79
18:4:232:LEU:CB	18:4:236:ILE:HD12	2.12	0.79
1:A:158:ILE:CG1	1:A:159:THR:N	2.28	0.78
1:A:207:LEU:CB	19:A:1119:CLA:HBB2	2.13	0.78
19:A:1124:CLA:H72	19:A:1125:CLA:HED1	1.54	0.78
2:B:87:ILE:CA	2:B:115:ASN:HA	2.12	0.78
11:K:115:ILE:HA	11:K:118:VAL:HG21	1.63	0.78
15:1:97:ILE:CD1	15:1:98:LEU:CD2	2.61	0.78
17:3:96:ARG:NH1	17:3:96:ARG:HG3	1.98	0.78
17:3:254:GLN:HG3	17:3:255:ASN:N	1.98	0.78
22:A:7016:LMU:H22	22:A:7016:LMU:C6	2.02	0.78
2:B:232:LEU:HD11	2:B:235:GLN:CG	2.14	0.78
19:B:1218:CLA:HHD	19:B:1218:CLA:CBC	2.13	0.78
15:1:190:ASN:HD21	19:1:1002:CLA:C4D	1.97	0.78
19:3:3016:CLA:HMC1	19:3:3016:CLA:CBC	2.13	0.78
1:A:545:HIS:O	1:A:549:ILE:HG13	1.82	0.78
1:A:628:ILE:HD12	1:A:632:GLY:HA2	1.64	0.78
19:A:1124:CLA:H2	19:A:1124:CLA:O1A	1.80	0.78
2:B:317:ARG:NH1	2:B:410:ARG:HG2	1.98	0.78
2:B:462:TRP:CZ3	19:B:1231:CLA:HBC2	2.19	0.78
15:1:190:ASN:ND2	19:1:1002:CLA:CHA	2.46	0.78
22:1:7013:LMU:O6B	22:1:7013:LMU:H1B	1.82	0.78
16:2:148:ASP:O	16:2:149:THR:OG1	2.00	0.78
17:3:187:PHE:C	17:3:187:PHE:HD1	1.86	0.78
18:4:173:LYS:O	18:4:194:PHE:CD2	2.36	0.78
1:A:148:GLY:O	1:A:152:ILE:HD12	1.84	0.78
1:A:492:ILE:CD1	19:A:1133:CLA:HMC3	2.06	0.78
1:A:578:ARG:CZ	1:A:578:ARG:CB	2.61	0.78
19:A:1112:CLA:CHC	21:A:6002:BCR:C19	2.61	0.78
19:A:1123:CLA:HMD2	19:A:1123:CLA:H142	1.65	0.78
3:C:62:PHE:CE1	5:E:80:GLU:HB3	2.17	0.78
4:D:99:PHE:HB2	4:D:157:VAL:HG12	1.64	0.78
5:E:89:SER:OG	5:E:106:ARG:CG	2.30	0.78
19:H:1241:CLA:HAC1	21:I:6021:BCR:C3	2.13	0.78
12:L:79:ILE:HG23	12:L:80:ALA:HA	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:95:PRO:O	12:L:98:ARG:N	2.16	0.78
12:L:168:GLY:C	12:L:170:LYS:H	1.87	0.78
22:4:7034:LMU:H101	22:4:7052:LMU:O3'	1.83	0.78
1:A:555:ILE:CD1	19:A:9023:CLA:OBD	2.31	0.78
19:A:1121:CLA:HAA1	11:K:78:ARG:CZ	2.12	0.78
2:B:645:VAL:HG11	19:B:1205:CLA:HAC1	1.65	0.78
3:C:44:ARG:HB3	4:D:182:GLN:HE22	1.47	0.78
19:K:1142:CLA:CED	19:K:1143:CLA:CMB	2.62	0.78
17:3:111:LEU:HG	17:3:112:GLY:H	0.63	0.78
18:4:110:LEU:O	18:4:113:GLU:CG	2.30	0.78
1:A:201:SER:O	1:A:204:ASN:HB2	1.84	0.78
1:A:203:LEU:HD22	19:A:1123:CLA:HED1	1.63	0.78
19:A:1124:CLA:O1A	19:A:1125:CLA:HED3	1.84	0.78
6:F:220:GLU:OE1	6:F:225:GLU:HB2	1.83	0.78
19:2:2014:CLA:H72	19:2:2014:CLA:C4	2.12	0.78
19:3:3008:CLA:HBD	19:3:3008:CLA:CBA	2.06	0.78
18:4:173:LYS:O	18:4:194:PHE:CE2	2.36	0.78
19:A:1149:CLA:O1D	19:A:1149:CLA:CAA	2.31	0.78
3:C:52:LYS:NZ	3:C:64:SER:CB	2.47	0.78
5:E:111:ASN:HD21	5:E:113:ALA:N	1.80	0.78
6:F:190:LYS:HG3	6:F:192:THR:HG23	1.66	0.78
15:1:128:PRO:HG2	15:1:131:TRP:CZ3	2.18	0.78
16:2:171:ILE:HG13	16:2:172:LEU:CB	2.14	0.78
16:2:261:THR:CG2	16:2:262:ILE:H	1.96	0.78
17:3:103:VAL:O	17:3:107:ARG:CD	2.31	0.78
1:A:27:ILE:O	1:A:27:ILE:HG22	1.83	0.78
1:A:421:ASP:OD1	1:A:422:TYR:CE1	2.36	0.78
1:A:492:ILE:HD11	19:A:1133:CLA:C2C	2.12	0.78
2:B:216:LEU:HG	2:B:218:TYR:H	1.48	0.78
7:G:90:GLN:HB2	7:G:92:PRO:CD	2.13	0.78
9:I:7:LEU:HD12	21:I:6021:BCR:C33	2.09	0.78
12:L:210:PRO:C	12:L:211:TYR:CD2	2.57	0.78
22:L:7029:LMU:H4'	22:L:7029:LMU:C5B	2.11	0.78
13:N:148:ASP:H	13:N:149:ASP:C	1.87	0.78
15:1:176:ASP:HB3	15:1:180:LEU:HD12	0.79	0.78
16:2:172:LEU:CA	16:2:173:ASN:HD22	1.96	0.78
19:2:2007:CLA:HMD2	19:3:2009:CLA:HMD3	1.65	0.78
1:A:603:PHE:HZ	1:A:693:LEU:HD21	1.49	0.78
22:H:7011:LMU:H122	22:H:7011:LMU:H82	1.66	0.78
17:3:125:VAL:HG21	19:3:3010:CLA:C2C	2.13	0.78
17:3:151:TRP:CD1	17:3:151:TRP:N	2.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:THR:O	1:A:427:ARG:CD	2.31	0.78
1:A:502:THR:HB	1:A:504:ALA:CB	2.13	0.78
2:B:36:ASP:O	2:B:41:ARG:NE	2.17	0.78
13:N:165:ASN:OD1	13:N:167:PHE:HA	1.84	0.78
15:1:150:HIS:CG	15:1:151:GLN:HE22	2.00	0.78
16:2:254:LEU:HD22	16:2:255:ALA:H	1.49	0.78
19:2:2002:CLA:H93	19:2:2002:CLA:H51	1.65	0.78
18:4:87:ASN:CB	18:4:90:TRP:CD2	2.67	0.78
18:4:205:ILE:HG12	18:4:206:ALA:H	1.47	0.78
1:A:190:ALA:CB	1:A:191:PRO:HD3	2.11	0.77
1:A:328:LYS:HZ3	1:A:345:GLY:CA	1.94	0.77
1:A:484:LEU:CD2	1:A:484:LEU:N	2.47	0.77
2:B:242:HIS:ND1	2:B:244:PHE:HA	1.99	0.77
2:B:303:TYR:HA	2:B:306:GLU:CB	2.13	0.77
2:B:648:TRP:CZ3	21:B:6017:BCR:H392	2.19	0.77
20:B:5002:PQN:C16	21:B:6017:BCR:H331	2.10	0.77
4:D:167:HIS:N	4:D:168:PRO:HD2	2.00	0.77
7:G:123:ASN:CA	7:G:126:ASP:OD2	2.33	0.77
22:R:7021:LMU:H31	22:R:7021:LMU:C1'	2.13	0.77
15:1:78:ARG:CG	15:1:81:GLU:OE1	2.32	0.77
15:1:206:SER:O	15:1:209:PRO:CD	2.32	0.77
15:1:207:ALA:C	15:1:209:PRO:HD3	2.05	0.77
18:4:90:TRP:C	18:4:91:PHE:HD1	1.87	0.77
1:A:40:PHE:H	1:A:44:ILE:CG2	1.97	0.77
1:A:291:THR:O	1:A:291:THR:HG22	1.83	0.77
19:B:1222:CLA:HED1	19:B:1223:CLA:HMD1	1.65	0.77
16:2:112:TRP:CZ3	16:2:164:GLU:HG3	2.19	0.77
18:4:211:MET:SD	19:4:4002:CLA:CBB	2.73	0.77
2:B:255:LEU:CA	2:B:271:THR:HB	2.06	0.77
2:B:664:LEU:C	2:B:667:TRP:HZ3	1.87	0.77
19:B:1226:CLA:H72	24:B:7101:LMG:H311	1.66	0.77
5:E:83:TRP:CE3	5:E:83:TRP:N	2.51	0.77
8:H:77:ASN:ND2	8:H:78:PRO:HG2	1.98	0.77
13:N:132:THR:OG1	13:N:138:ALA:C	2.22	0.77
14:R:27:UNK:O	14:R:29:UNK:O	2.03	0.77
15:1:87:CYS:SG	15:1:88:ARG:N	2.58	0.77
15:1:177:PRO:HG2	15:1:179:LYS:C	2.04	0.77
16:2:184:PRO:HD3	16:2:187:LYS:HG2	1.66	0.77
16:2:222:ILE:O	16:2:226:ARG:HB2	1.83	0.77
18:4:226:LYS:CD	18:4:226:LYS:N	2.47	0.77
1:A:360:ILE:HD13	21:A:6007:BCR:H371	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:VAL:O	1:A:636:HIS:CD2	2.37	0.77
19:A:1122:CLA:CHD	21:A:6007:BCR:C19	2.58	0.77
2:B:123:TRP:O	2:B:126:THR:HG22	1.84	0.77
2:B:154:TRP:O	2:B:157:LEU:HB3	1.84	0.77
2:B:455:ILE:HG23	6:F:148:LEU:HD11	1.67	0.77
19:B:1239:CLA:H102	9:I:21:MET:SD	2.25	0.77
6:F:83:THR:HB	6:F:84:PRO:HD2	1.67	0.77
7:G:84:ARG:HG3	7:G:85:GLU:HB3	1.63	0.77
19:H:1241:CLA:C3C	21:I:6021:BCR:C2	2.62	0.77
11:K:118:VAL:HG23	11:K:121:VAL:CG2	2.11	0.77
13:N:150:LEU:HB2	13:N:152:LEU:HD23	1.67	0.77
15:1:73:PRO:O	15:1:77:GLU:HB2	1.84	0.77
15:1:177:PRO:HD2	15:1:180:LEU:CA	2.15	0.77
15:1:183:LEU:O	15:1:184:LYS:HG2	1.85	0.77
16:2:125:PHE:O	16:2:127:THR:HG23	1.83	0.77
16:2:243:GLY:C	16:2:244:THR:HG23	2.05	0.77
1:A:85:GLN:C	1:A:87:SER:O	2.22	0.77
1:A:726:SER:O	1:A:728:VAL:N	2.18	0.77
22:A:7010:LMU:H3'	22:A:7010:LMU:O2B	1.85	0.77
19:A:9022:CLA:C11	21:B:6017:BCR:H19C	2.14	0.77
2:B:103:ALA:HB1	2:B:106:ARG:CD	2.14	0.77
2:B:247:THR:HG22	2:B:248:GLN:H	1.49	0.77
2:B:374:HIS:CG	2:B:374:HIS:O	2.38	0.77
19:B:1228:CLA:HHD	19:B:1228:CLA:HBC3	1.66	0.77
4:D:93:LYS:CG	4:D:96:VAL:HG13	2.14	0.77
7:G:72:LEU:HD23	7:G:124:ILE:HG13	1.67	0.77
7:G:99:HIS:O	7:G:101:GLU:HB2	1.83	0.77
10:J:5:LYS:CD	16:2:178:ASN:OD1	2.32	0.77
12:L:153:PHE:CD1	12:L:155:GLU:OE1	2.38	0.77
14:R:3:UNK:O	14:R:4:UNK:CB	2.33	0.77
17:3:111:LEU:O	17:3:115:GLY:N	2.17	0.77
19:3:3011:CLA:HMA2	19:3:3011:CLA:C1	2.12	0.77
22:3:7003:LMU:C3B	22:3:7005:LMU:C6B	2.62	0.77
18:4:123:VAL:O	18:4:123:VAL:HG13	1.82	0.77
1:A:51:THR:CB	19:A:1139:CLA:CBB	2.63	0.77
1:A:202:MET:HG3	19:A:1111:CLA:HBC2	1.65	0.77
1:A:508:THR:O	1:A:509:ALA:CB	2.30	0.77
2:B:732:LYS:CB	2:B:733:PHE:CA	2.62	0.77
6:F:103:GLN:CD	6:F:104:ALA:H	1.87	0.77
7:G:99:HIS:C	7:G:101:GLU:N	2.37	0.77
8:H:58:LEU:CB	8:H:61:THR:CG2	2.51	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:9:SER:O	10:J:10:VAL:HB	1.85	0.77
19:J:1311:CLA:HBC3	19:J:1311:CLA:HHD	1.65	0.77
17:3:243:ILE:HG12	19:3:3005:CLA:C3C	2.14	0.77
18:4:177:LEU:CG	18:4:178:PRO:CD	2.59	0.77
1:A:581:CYS:CB	1:A:590:CYS:HA	2.14	0.77
1:A:669:GLY:H	2:B:445:ALA:CA	1.95	0.77
19:A:1103:CLA:H151	21:A:6002:BCR:H393	1.66	0.77
2:B:174:ARG:CB	19:B:1210:CLA:HBC2	2.11	0.77
2:B:615:TYR:HD1	2:B:615:TYR:H	1.32	0.77
19:K:3009:CLA:HBA1	19:K:3009:CLA:O2D	1.84	0.77
12:L:168:GLY:C	12:L:170:LYS:N	2.35	0.77
15:1:170:PRO:O	15:1:173:TYR:CE2	2.38	0.77
17:3:98:LEU:O	17:3:101:GLY:CA	2.33	0.77
18:4:87:ASN:CB	18:4:90:TRP:CZ3	2.66	0.77
19:4:4002:CLA:HBA1	19:4:4002:CLA:CMA	1.94	0.77
19:4:4014:CLA:HHD	19:4:4014:CLA:CBC	2.14	0.77
1:A:472:ARG:HE	1:A:474:GLN:HG3	1.49	0.77
3:C:42:ALA:HB1	3:C:43:PRO:HD2	1.65	0.77
6:F:119:ILE:CG1	6:F:120:LYS:H	1.94	0.77
13:N:122:PHE:HD2	13:N:122:PHE:H	1.32	0.77
13:N:156:GLY:HA2	13:N:157:LYS:HD2	1.64	0.77
15:1:114:TRP:CZ3	15:1:121:GLN:HA	2.19	0.77
17:3:135:ALA:HB1	17:3:139:THR:CG2	2.14	0.77
19:A:1108:CLA:HBB2	19:A:1111:CLA:HMA3	1.65	0.77
19:A:1119:CLA:C3C	19:A:1125:CLA:H172	2.15	0.77
2:B:586:THR:C	2:B:588:GLY:H	1.87	0.77
19:B:1209:CLA:HAC2	19:B:1210:CLA:HBB2	0.81	0.77
5:E:83:TRP:HE3	5:E:83:TRP:H	1.29	0.77
16:2:224:ASN:O	16:2:227:LEU:HB3	1.85	0.77
2:B:130:ARG:HG3	2:B:130:ARG:NH1	1.99	0.77
2:B:160:LYS:HD3	2:B:161:TRP:CZ2	2.20	0.77
2:B:261:PHE:HE2	2:B:499:ASN:C	1.87	0.77
2:B:374:HIS:HB2	19:B:1224:CLA:NB	2.00	0.77
19:B:1222:CLA:HED1	19:B:1223:CLA:CMD	2.15	0.77
3:C:8:TYR:O	3:C:60:THR:HA	1.85	0.77
3:C:33:GLY:HA2	3:C:37:LYS:HE2	1.67	0.77
11:K:89:ARG:CG	11:K:89:ARG:HH11	1.98	0.77
19:K:1142:CLA:CMD	19:K:1143:CLA:NA	2.47	0.77
17:3:134:LEU:HD12	17:3:134:LEU:N	2.00	0.77
17:3:207:PHE:HD1	17:3:207:PHE:C	1.84	0.77
18:4:103:MET:HE3	18:4:208:GLY:HA3	1.63	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1124:CLA:CED	19:A:1125:CLA:C3D	2.58	0.76
19:A:9022:CLA:H101	21:B:6017:BCR:H17C	1.68	0.76
19:A:9023:CLA:CBC	19:A:9023:CLA:HMC1	2.16	0.76
2:B:267:SER:HB2	2:B:356:PRO:O	1.84	0.76
2:B:314:ARG:HH12	15:1:67:LEU:CG	1.98	0.76
2:B:732:LYS:CB	2:B:733:PHE:HA	2.14	0.76
4:D:156:ARG:NH2	4:D:163:VAL:O	2.18	0.76
4:D:158:PHE:HB3	4:D:159:PRO:CD	2.08	0.76
5:E:79:LYS:CA	5:E:84:TYR:HE1	1.99	0.76
7:G:120:VAL:O	7:G:120:VAL:HG12	1.84	0.76
11:K:47:ASP:CA	11:K:51:SER:HB2	2.15	0.76
19:1:1303:CLA:HMC1	19:4:1304:CLA:HMB3	1.66	0.76
19:4:1306:CLA:HBC3	19:4:1306:CLA:CMC	2.12	0.76
1:A:284:ARG:HA	1:A:284:ARG:CZ	2.14	0.76
1:A:295:TRP:O	1:A:298:ASP:OD2	2.03	0.76
1:A:714:LEU:HD13	21:F:6016:BCR:C39	2.15	0.76
19:A:1125:CLA:HMC1	19:A:1125:CLA:CBC	2.15	0.76
2:B:87:ILE:HA	2:B:115:ASN:HB2	1.66	0.76
2:B:247:THR:HG23	2:B:248:GLN:N	1.94	0.76
2:B:293:THR:O	2:B:295:PHE:CD2	2.38	0.76
4:D:103:THR:CG2	4:D:128:LEU:HG	2.15	0.76
21:J:6012:BCR:H393	21:J:6012:BCR:C23	2.14	0.76
13:N:143:VAL:CB	13:N:144:PRO:CD	2.62	0.76
16:2:107:LEU:HD12	16:2:108:VAL:N	1.99	0.76
16:2:182:ILE:C	16:2:187:LYS:HG3	2.05	0.76
16:2:195:TYR:CE2	16:2:198:GLY:HA3	2.20	0.76
19:3:3016:CLA:H142	19:3:3016:CLA:H101	1.64	0.76
1:A:56:ASN:O	1:A:57:LEU:CB	2.24	0.76
1:A:426:THR:CA	1:A:428:TYR:CZ	2.69	0.76
1:A:525:ASN:HD22	1:A:526:LYS:HE3	1.50	0.76
1:A:534:LEU:CD1	1:A:535:GLY:H	1.90	0.76
19:A:1117:CLA:HBB2	19:A:1117:CLA:H8	1.65	0.76
19:A:1134:CLA:O1A	19:A:1141:CLA:HBB1	1.84	0.76
22:A:7023:LMU:H2B	22:A:7023:LMU:H6'2	1.68	0.76
2:B:174:ARG:O	2:B:175:LEU:HB3	1.85	0.76
6:F:200:VAL:HG11	10:J:7:TYR:CB	2.11	0.76
7:G:64:ILE:O	7:G:64:ILE:HG13	1.83	0.76
7:G:124:ILE:CG1	7:G:128:LEU:CD1	2.62	0.76
11:K:50:GLY:C	11:K:52:PRO:HD2	2.06	0.76
12:L:115:VAL:HG11	12:L:130:GLY:N	1.95	0.76
19:L:1148:CLA:CBC	19:L:1148:CLA:CHD	2.62	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:172:LEU:CB	16:2:173:ASN:ND2	2.48	0.76
1:A:127:VAL:CG2	19:A:1107:CLA:CBB	2.63	0.76
1:A:150:PHE:N	1:A:153:TRP:HB2	2.01	0.76
1:A:343:HIS:O	1:A:346:LEU:CB	2.33	0.76
1:A:368:LEU:CD1	19:A:1125:CLA:H61	2.15	0.76
1:A:411:ALA:HB2	21:A:6008:BCR:C39	2.16	0.76
1:A:746:THR:HA	1:A:749:PHE:HB3	1.66	0.76
4:D:100:TYR:CD1	4:D:134:LYS:CG	2.66	0.76
12:L:54:TYR:CE1	12:L:57:ILE:HG23	2.19	0.76
15:1:177:PRO:CD	15:1:180:LEU:HD23	2.15	0.76
17:3:161:GLU:OE1	17:3:162:MET:HA	1.84	0.76
1:A:23:ASP:CG	1:A:33:GLN:CG	2.54	0.76
1:A:351:THR:C	19:A:1123:CLA:H191	2.05	0.76
21:A:6002:BCR:H341	21:A:6002:BCR:C12	2.15	0.76
2:B:655:LEU:CD2	19:B:1239:CLA:HBB1	2.15	0.76
4:D:101:VAL:HG12	4:D:130:LYS:CB	2.16	0.76
6:F:139:LEU:CD1	6:F:149:ILE:HD13	2.15	0.76
10:J:23:ALA:O	10:J:26:LEU:HB3	1.85	0.76
22:K:7001:LMU:H42	22:K:7001:LMU:H81	1.67	0.76
12:L:153:PHE:CA	12:L:179:ALA:HB2	2.10	0.76
13:N:110:THR:CG2	13:N:111:GLY:N	2.47	0.76
14:R:34:UNK:H	14:R:36:UNK:CB	1.99	0.76
16:2:261:THR:HG22	16:2:262:ILE:N	1.98	0.76
17:3:109:ALA:O	17:3:111:LEU:HB3	1.86	0.76
19:3:3011:CLA:CBC	19:3:3012:CLA:CHA	2.63	0.76
1:A:193:LEU:HA	1:A:196:PHE:CE2	2.18	0.76
1:A:279:ASP:C	1:A:281:LEU:HG	2.06	0.76
2:B:292:ARG:NH2	2:B:297:ILE:N	2.33	0.76
2:B:353:TYR:O	2:B:354:SER:HB2	1.84	0.76
2:B:517:PHE:O	2:B:517:PHE:HD2	1.66	0.76
2:B:732:LYS:HG2	2:B:733:PHE:CA	2.15	0.76
4:D:140:LEU:HD13	4:D:144:LEU:CB	2.11	0.76
7:G:88:ALA:HB3	7:G:90:GLN:O	1.86	0.76
14:R:37:UNK:O	14:R:42:UNK:C	2.34	0.76
15:1:73:PRO:CG	15:1:74:ALA:N	2.49	0.76
19:1:1010:CLA:HMA2	19:1:1010:CLA:HBA2	1.65	0.76
17:3:125:VAL:HG11	19:3:3010:CLA:CHC	2.16	0.76
17:3:177:ALA:O	17:3:178:LYS:HB2	1.84	0.76
18:4:246:GLN:O	18:4:246:GLN:HG2	1.84	0.76
1:A:270:PHE:CE1	19:A:1141:CLA:H2	2.21	0.76
1:A:389:TYR:HE1	1:A:625:TRP:CD1	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ARG:NH2	2:B:566:GLY:O	2.17	0.76
2:B:69:ALA:HB1	2:B:135:LEU:HD12	1.65	0.76
2:B:203:ARG:HH22	2:B:254:ILE:HG22	1.50	0.76
5:E:89:SER:O	5:E:105:VAL:HB	1.86	0.76
7:G:63:VAL:CG2	7:G:64:ILE:N	2.45	0.76
11:K:76:ALA:N	11:K:78:ARG:HH12	1.81	0.76
12:L:129:ALA:O	12:L:201:TYR:CB	2.25	0.76
19:1:1010:CLA:CHD	19:1:1010:CLA:CBC	2.63	0.76
16:2:128:LYS:CB	16:2:131:ILE:HG12	2.16	0.76
1:A:23:ASP:HB3	1:A:33:GLN:OE1	1.84	0.76
1:A:431:LEU:O	1:A:435:VAL:HG12	1.85	0.76
1:A:457:SER:O	1:A:544:ILE:HD13	1.85	0.76
19:A:1237:CLA:HMC2	19:B:1238:CLA:H11	1.68	0.76
2:B:160:LYS:NZ	2:B:161:TRP:CD2	2.54	0.76
2:B:233:TYR:CD1	2:B:254:ILE:HG13	2.20	0.76
2:B:387:PHE:O	2:B:391:PRO:HD3	1.86	0.76
2:B:493:TRP:HE1	19:B:1213:CLA:CAC	1.99	0.76
4:D:147:LYS:C	4:D:148:TYR:CG	2.57	0.76
4:D:156:ARG:HB2	4:D:166:LEU:CD1	2.15	0.76
5:E:90:VAL:O	5:E:91:VAL:CG2	2.34	0.76
6:F:200:VAL:HG12	10:J:7:TYR:CA	2.15	0.76
8:H:109:LEU:HD23	19:H:1207:CLA:C7	2.14	0.76
15:1:157:ASP:OD1	15:1:175:LYS:HE3	1.86	0.76
16:2:184:PRO:CG	16:2:187:LYS:N	2.49	0.76
1:A:92:TRP:CD1	19:A:1105:CLA:HBB2	2.20	0.76
1:A:98:PHE:O	1:A:99:HIS:C	2.24	0.76
19:A:1105:CLA:CMB	21:J:6012:BCR:HC7	2.15	0.76
2:B:69:ALA:CB	2:B:135:LEU:HD12	2.15	0.76
2:B:229:GLN:O	7:G:63:VAL:CG2	2.34	0.76
4:D:128:LEU:O	4:D:128:LEU:HD23	1.85	0.76
5:E:89:SER:OG	5:E:106:ARG:NE	2.15	0.76
5:E:111:ASN:ND2	5:E:113:ALA:N	2.31	0.76
9:I:11:LEU:HD12	21:I:6021:BCR:C10	2.15	0.76
15:1:78:ARG:CD	19:1:1011:CLA:CMC	2.64	0.76
19:1:1303:CLA:HMC1	19:1:1303:CLA:CBC	2.14	0.76
18:4:173:LYS:CB	18:4:194:PHE:HD2	1.97	0.76
1:A:170:GLY:O	1:A:173:VAL:HG22	1.86	0.76
1:A:217:SER:OG	21:A:6002:BCR:C17	2.34	0.76
1:A:281:LEU:HD22	19:A:1115:CLA:CMA	2.11	0.76
1:A:603:PHE:CZ	1:A:735:VAL:HG22	2.21	0.76
1:A:661:ALA:HA	1:A:664:VAL:HG13	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:LYS:HB3	2:B:470:THR:OG1	1.86	0.76
2:B:500:ALA:O	2:B:501:ILE:CG1	2.31	0.76
2:B:510:LEU:HD11	2:B:597:LYS:NZ	2.00	0.76
21:B:6006:BCR:H331	21:B:6006:BCR:HC8	1.66	0.76
4:D:99:PHE:HB3	4:D:157:VAL:HB	1.67	0.76
5:E:89:SER:CB	5:E:106:ARG:CD	2.61	0.76
6:F:207:LEU:HD21	6:F:208:PHE:HD1	1.48	0.76
10:J:5:LYS:HD2	16:2:178:ASN:CA	2.15	0.76
13:N:122:PHE:N	13:N:122:PHE:CD2	2.36	0.76
15:1:69:LEU:CA	15:1:73:PRO:HD3	2.16	0.76
22:1:7004:LMU:O2'	22:1:7004:LMU:H11	1.84	0.76
16:2:160:ILE:CB	19:2:2012:CLA:CBB	2.64	0.76
1:A:163:GLN:CG	1:A:164:LEU:N	2.37	0.75
1:A:187:HIS:HE1	19:A:1109:CLA:C4D	1.86	0.75
1:A:475:ASP:OD2	12:L:120:LEU:HA	1.85	0.75
2:B:200:PRO:O	2:B:204:GLY:CA	2.33	0.75
2:B:545:LYS:CG	2:B:546:LEU:N	2.48	0.75
4:D:138:LEU:C	4:D:140:LEU:O	2.25	0.75
6:F:129:ARG:HB3	6:F:133:TYR:CZ	2.21	0.75
6:F:225:GLU:N	6:F:227:VAL:HG12	2.01	0.75
11:K:127:ILE:O	11:K:130:LEU:HD23	1.86	0.75
15:1:84:LEU:O	15:1:87:CYS:SG	2.44	0.75
1:A:127:VAL:HG21	19:A:1107:CLA:HBB2	1.69	0.75
19:A:1105:CLA:HBA2	19:A:1107:CLA:H12	1.68	0.75
19:A:1106:CLA:HMB1	19:A:1107:CLA:H11	1.68	0.75
19:A:9022:CLA:H93	19:A:9023:CLA:C9	2.11	0.75
2:B:459:PHE:CB	19:B:1235:CLA:CAD	2.64	0.75
6:F:160:PHE:O	6:F:164:GLY:HA3	1.86	0.75
6:F:173:TRP:CE3	6:F:211:PHE:N	2.54	0.75
12:L:175:GLN:O	12:L:176:LEU:HB2	1.86	0.75
19:2:2014:CLA:H102	19:2:2014:CLA:C15	2.15	0.75
19:3:3008:CLA:HMC1	19:3:3008:CLA:CBC	2.13	0.75
1:A:422:TYR:HD1	1:A:422:TYR:H	0.82	0.75
1:A:425:THR:C	1:A:428:TYR:CE1	2.60	0.75
1:A:523:VAL:HG13	1:A:524:GLY:H	1.49	0.75
1:A:624:VAL:O	1:A:636:HIS:HD2	1.69	0.75
1:A:701:GLN:OE1	5:E:112:TYR:OH	2.01	0.75
19:A:1136:CLA:H171	19:L:1504:CLA:HBB2	1.67	0.75
2:B:257:ILE:C	2:B:497:TRP:CZ3	2.57	0.75
2:B:709:GLY:O	2:B:710:LEU:HB2	1.84	0.75
8:H:98:LEU:HD22	12:L:146:THR:HG21	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:1311:CLA:O1A	19:J:1311:CLA:H143	1.86	0.75
11:K:115:ILE:HG12	11:K:121:VAL:C	2.06	0.75
12:L:55:GLN:C	12:L:57:ILE:H	1.90	0.75
13:N:146:LEU:HD21	17:3:142:ILE:O	1.84	0.75
13:N:157:LYS:CB	13:N:159:LYS:H	1.98	0.75
16:2:184:PRO:CD	16:2:187:LYS:CD	2.63	0.75
19:2:2007:CLA:HBC2	19:3:2009:CLA:CED	1.89	0.75
2:B:679:ALA:O	2:B:683:GLU:CD	2.25	0.75
5:E:74:VAL:HG22	5:E:90:VAL:HG22	1.67	0.75
6:F:207:LEU:CD2	6:F:208:PHE:CD1	2.69	0.75
7:G:84:ARG:HA	19:G:1242:CLA:CMA	2.16	0.75
7:G:102:ALA:HA	7:G:104:ASP:OD2	1.85	0.75
8:H:97:LEU:CD1	8:H:100:PHE:HB3	2.13	0.75
11:K:63:LEU:H	11:K:63:LEU:CD2	1.90	0.75
11:K:84:LEU:HG	11:K:85:LYS:CG	2.10	0.75
19:3:3008:CLA:CGD	19:3:3008:CLA:CBA	2.64	0.75
18:4:177:LEU:CD2	18:4:178:PRO:CD	2.64	0.75
19:4:4015:CLA:HBC3	19:4:4015:CLA:HHD	1.68	0.75
22:4:7034:LMU:C8	22:4:7052:LMU:C1'	2.58	0.75
1:A:128:GLY:HA3	2:B:446:PHE:CD2	2.21	0.75
1:A:154:ARG:CZ	1:A:384:TYR:CE1	2.68	0.75
1:A:196:PHE:H	1:A:196:PHE:HD2	1.33	0.75
1:A:349:ILE:HG22	1:A:350:LEU:CA	2.16	0.75
19:A:1124:CLA:HBA2	19:A:1137:CLA:CED	2.16	0.75
19:A:1124:CLA:C6	19:A:1125:CLA:HED1	2.15	0.75
2:B:88:ALA:H	2:B:115:ASN:HA	1.50	0.75
2:B:323:TYR:O	2:B:327:ASN:HB2	1.86	0.75
2:B:628:SER:O	2:B:629:SER:C	2.24	0.75
2:B:694:ARG:HD3	9:I:28:VAL:HG13	1.67	0.75
20:B:5002:PQN:H162	21:B:6017:BCR:H331	1.62	0.75
4:D:103:THR:HG21	4:D:128:LEU:CD1	2.16	0.75
5:E:91:VAL:HG12	5:E:92:ALA:H	1.51	0.75
11:K:127:ILE:HB	11:K:129:ALA:CB	2.16	0.75
12:L:153:PHE:HD1	12:L:155:GLU:OE1	1.70	0.75
15:1:134:LEU:N	15:1:135:PRO:HD3	2.00	0.75
19:4:4003:CLA:HMC1	19:4:4003:CLA:CBC	2.14	0.75
1:A:163:GLN:O	1:A:166:CYS:N	2.07	0.75
1:A:485:GLN:CD	1:A:485:GLN:N	2.40	0.75
2:B:53:GLN:C	2:B:55:ALA:H	1.90	0.75
2:B:694:ARG:HD3	9:I:28:VAL:CG1	2.17	0.75
9:I:8:PHE:CB	19:I:1204:CLA:OBD	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:H	1:A:243:PRO:HD2	1.48	0.75
1:A:308:ILE:O	1:A:312:ILE:N	2.16	0.75
1:A:349:ILE:HG22	1:A:350:LEU:HA	1.67	0.75
1:A:470:LEU:HD11	2:B:95:HIS:HB3	1.68	0.75
19:A:1124:CLA:H43	19:A:1136:CLA:HBA1	1.67	0.75
19:A:9012:CLA:HED2	19:A:9012:CLA:CAD	2.16	0.75
3:C:25:VAL:HA	3:C:43:PRO:CG	2.17	0.75
11:K:115:ILE:CA	11:K:118:VAL:CG2	2.59	0.75
13:N:104:LYS:N	13:N:107:LEU:HD13	2.02	0.75
13:N:156:GLY:N	13:N:157:LYS:HE2	2.02	0.75
15:1:77:GLU:HA	15:1:80:LYS:HD2	1.69	0.75
16:2:182:ILE:C	16:2:187:LYS:HG2	2.07	0.75
18:4:172:PHE:CD1	18:4:173:LYS:O	2.40	0.75
1:A:555:ILE:HD13	19:A:9023:CLA:CMD	2.17	0.75
1:A:700:TRP:O	1:A:704:ILE:HB	1.87	0.75
2:B:625:TRP:HE3	2:B:626:LEU:N	1.85	0.75
19:B:1222:CLA:HBC2	19:B:1222:CLA:CHD	2.12	0.75
19:B:1222:CLA:H52	19:B:1236:CLA:CAD	2.17	0.75
4:D:93:LYS:HG2	4:D:96:VAL:HG13	1.67	0.75
22:G:7026:LMU:H41	22:G:7026:LMU:H82	1.69	0.75
12:L:211:TYR:CD2	12:L:211:TYR:N	2.49	0.75
16:2:184:PRO:CD	16:2:187:LYS:HG2	2.16	0.75
16:2:229:MET:SD	16:2:230:LEU:CD1	2.75	0.75
19:2:2013:CLA:HMC1	19:2:2013:CLA:CBC	2.17	0.75
1:A:93:LEU:HA	1:A:96:MET:HB2	1.69	0.75
19:A:1117:CLA:HBB2	19:A:1117:CLA:H121	1.68	0.75
19:B:1205:CLA:HBA1	19:B:1224:CLA:OBD	1.87	0.75
6:F:88:SER:OG	6:F:91:PHE:CB	2.35	0.75
7:G:63:VAL:HG23	7:G:64:ILE:N	2.01	0.75
1:A:168:ALA:O	1:A:171:ALA:HB3	1.86	0.74
1:A:284:ARG:HB3	1:A:295:TRP:CD1	2.22	0.74
1:A:336:GLY:HA3	19:A:1151:CLA:HMC2	1.69	0.74
1:A:514:THR:O	1:A:531:PRO:O	2.05	0.74
1:A:711:HIS:HB3	1:A:717:ALA:HB2	1.66	0.74
19:A:1126:CLA:C20	21:J:6012:BCR:H17C	2.17	0.74
21:A:6011:BCR:C31	19:A:9013:CLA:H142	2.17	0.74
2:B:87:ILE:HA	2:B:115:ASN:CB	2.15	0.74
2:B:308:HIS:ND1	2:B:309:ILE:N	2.32	0.74
2:B:461:GLN:O	2:B:464:GLN:HG2	1.86	0.74
3:C:73:THR:OG1	3:C:76:SER:N	2.20	0.74
12:L:67:GLY:O	12:L:68:SER:HB3	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:128:GLN:CA	12:L:130:GLY:HA3	2.14	0.74
13:N:132:THR:HA	13:N:136:ASP:OD1	1.86	0.74
19:R:1150:CLA:HBA2	19:R:1150:CLA:CBD	2.16	0.74
17:3:156:THR:C	17:3:158:PHE:O	2.25	0.74
18:4:87:ASN:CG	18:4:90:TRP:CD2	2.59	0.74
1:A:209:GLY:HA2	1:A:213:LEU:HD13	1.68	0.74
19:A:1124:CLA:HED3	19:A:1125:CLA:HMD1	1.68	0.74
19:A:1124:CLA:C4B	21:A:6008:BCR:H373	2.17	0.74
19:B:1203:CLA:HBB2	19:B:1225:CLA:HHC	1.68	0.74
22:B:7040:LMU:O3'	22:B:7040:LMU:H1B	1.87	0.74
3:C:52:LYS:HE3	3:C:64:SER:HB3	1.69	0.74
22:3:7003:LMU:C3B	22:3:7005:LMU:H6'1	2.09	0.74
1:A:63:ASP:HB2	19:A:1128:CLA:HED3	1.69	0.74
1:A:129:GLN:O	1:A:130:GLU:CB	2.35	0.74
4:D:159:PRO:O	4:D:159:PRO:CD	2.34	0.74
6:F:180:SER:C	6:F:182:LEU:H	1.91	0.74
6:F:207:LEU:CD2	6:F:208:PHE:N	2.50	0.74
7:G:145:THR:HG23	7:G:146:SER:H	1.50	0.74
12:L:172:GLU:O	12:L:173:PRO:C	2.24	0.74
14:R:44:UNK:O	14:R:45:UNK:C	2.35	0.74
19:R:1144:CLA:CHA	19:R:1144:CLA:CED	2.65	0.74
16:2:117:ALA:HB1	16:2:230:LEU:CD1	2.17	0.74
17:3:191:GLU:O	17:3:191:GLU:HG2	1.85	0.74
1:A:25:ASP:OD1	1:A:26:PRO:HG3	1.87	0.74
1:A:284:ARG:CZ	1:A:284:ARG:C	2.56	0.74
21:A:6008:BCR:HC8	21:A:6008:BCR:C33	2.15	0.74
3:C:62:PHE:CD1	4:D:191:ILE:HG22	2.21	0.74
4:D:156:ARG:NH1	4:D:158:PHE:CD1	2.37	0.74
13:N:155:GLU:HB3	13:N:157:LYS:HE2	1.67	0.74
14:R:24:UNK:O	14:R:27:UNK:CB	2.35	0.74
15:1:97:ILE:HD12	15:1:98:LEU:CB	2.17	0.74
15:1:178:LYS:HD2	15:1:178:LYS:C	2.08	0.74
16:2:153:PHE:CE2	16:2:157:LEU:CD2	2.70	0.74
17:3:150:TYR:CD1	17:3:151:TRP:N	2.54	0.74
18:4:159:ASP:OD2	18:4:163:PRO:HA	1.86	0.74
1:A:479:ASP:HA	1:A:536:THR:CG2	2.15	0.74
1:A:513:LEU:HD12	1:A:513:LEU:O	1.86	0.74
21:A:6011:BCR:H393	21:A:6011:BCR:C23	2.15	0.74
2:B:314:ARG:HH22	15:1:67:LEU:HG	1.51	0.74
2:B:500:ALA:HB1	2:B:503:GLU:OE2	1.87	0.74
3:C:24:ASP:CB	23:C:8002:SF4:S2	2.73	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:K:7042:LMU:C6'	22:K:7042:LMU:H32	2.18	0.74
13:N:147:SER:HB2	13:N:151:ASP:OD1	1.88	0.74
1:A:423:ASP:CB	1:A:424:PRO:CD	2.63	0.74
1:A:452:PHE:HE1	19:A:1136:CLA:CBB	1.99	0.74
1:A:523:VAL:CG1	1:A:524:GLY:N	2.51	0.74
19:A:1102:CLA:C1	19:A:1109:CLA:H61	2.12	0.74
19:A:1133:CLA:HMC1	19:A:1133:CLA:CBC	2.17	0.74
2:B:295:PHE:N	2:B:295:PHE:HD2	1.85	0.74
2:B:310:PRO:O	19:B:1301:CLA:HHD	1.86	0.74
2:B:390:GLY:O	21:B:6010:BCR:HC42	1.86	0.74
6:F:89:LYS:HG2	6:F:90:GLN:H	1.51	0.74
6:F:103:GLN:HG3	6:F:104:ALA:N	1.99	0.74
7:G:89:LYS:N	7:G:89:LYS:HZ2	1.84	0.74
14:R:7:UNK:O	14:R:11:UNK:N	2.20	0.74
15:1:123:THR:HG22	15:1:124:TYR:O	1.86	0.74
15:1:147:PHE:CD1	15:1:147:PHE:C	2.60	0.74
16:2:218:ARG:HB2	16:2:219:THR:HG23	1.68	0.74
17:3:96:ARG:NH1	17:3:100:TYR:CZ	2.47	0.74
18:4:201:LYS:O	18:4:201:LYS:HG2	1.86	0.74
1:A:163:GLN:HA	1:A:166:CYS:HG	1.52	0.74
1:A:283:PHE:O	1:A:284:ARG:NH1	2.19	0.74
1:A:328:LYS:HZ2	1:A:345:GLY:CA	1.99	0.74
1:A:693:LEU:HD21	1:A:735:VAL:H	1.51	0.74
2:B:160:LYS:CE	2:B:161:TRP:CE3	2.71	0.74
2:B:216:LEU:CD2	2:B:218:TYR:O	2.31	0.74
2:B:230:TRP:CH2	7:G:67:SER:HB2	2.21	0.74
2:B:295:PHE:HE2	7:G:94:GLN:HE22	1.35	0.74
2:B:317:ARG:NE	2:B:317:ARG:HA	2.02	0.74
5:E:74:VAL:HG22	5:E:90:VAL:CG2	2.17	0.74
8:H:77:ASN:CG	8:H:78:PRO:CD	2.55	0.74
8:H:112:LEU:N	8:H:112:LEU:CD2	2.51	0.74
11:K:115:ILE:C	11:K:118:VAL:HG22	2.08	0.74
22:2:7006:LMU:H22	22:2:7006:LMU:C2'	2.18	0.74
1:A:41:SER:O	1:A:44:ILE:HA	1.88	0.74
1:A:208:ALA:HB2	1:A:314:GLY:HA3	1.68	0.74
1:A:336:GLY:CA	19:A:1151:CLA:HMC2	2.18	0.74
1:A:336:GLY:HA2	19:A:1151:CLA:CMC	2.18	0.74
1:A:349:ILE:O	1:A:352:THR:N	2.21	0.74
1:A:470:LEU:HD13	2:B:95:HIS:HB3	1.68	0.74
1:A:542:HIS:HA	1:A:545:HIS:HD2	1.53	0.74
1:A:733:VAL:HG21	19:A:1140:CLA:CMD	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:GLN:O	2:B:14:GLN:NE2	2.20	0.74
2:B:25:ILE:CG2	21:L:6019:BCR:H282	2.18	0.74
22:F:7036:LMU:H4'	22:F:7036:LMU:O2B	1.87	0.74
8:H:67:SER:O	8:H:68:TYR:CG	2.41	0.74
8:H:77:ASN:HD21	8:H:78:PRO:HG2	1.51	0.74
12:L:164:LEU:CB	12:L:165:THR:HG23	2.16	0.74
15:1:83:GLU:OE2	15:1:83:GLU:HA	1.87	0.74
16:2:246:PRO:HB2	16:2:247:ILE:HG12	1.70	0.74
1:A:281:LEU:CD1	19:A:1115:CLA:HED2	1.94	0.74
1:A:296:LEU:HD12	1:A:296:LEU:C	2.08	0.74
19:A:1101:CLA:H42	19:A:1140:CLA:C6	2.07	0.74
2:B:53:GLN:HE21	19:B:1201:CLA:HBB1	1.50	0.74
2:B:70:TRP:CD1	2:B:71:GLN:OE1	2.40	0.74
2:B:330:ILE:HD11	19:B:1202:CLA:C19	2.18	0.74
2:B:429:LEU:C	2:B:525:LEU:CD1	2.53	0.74
2:B:469:LYS:HZ3	2:B:471:THR:H	1.34	0.74
2:B:504:ASN:O	2:B:504:ASN:CG	2.25	0.74
2:B:527:LEU:CD2	19:B:1222:CLA:ND	2.50	0.74
4:D:167:HIS:NE2	4:D:172:VAL:CG2	2.50	0.74
22:H:7030:LMU:H52	22:H:7030:LMU:C9	2.16	0.74
12:L:141:LEU:CD1	21:L:6019:BCR:C31	2.65	0.74
12:L:190:PHE:CZ	12:L:194:ILE:HD12	2.21	0.74
15:1:73:PRO:HG2	15:1:74:ALA:N	2.03	0.74
16:2:184:PRO:CD	16:2:185:ASN:C	2.53	0.74
16:2:220:LYS:NZ	19:2:2004:CLA:OBD	2.15	0.74
17:3:101:GLY:HA2	17:3:104:ILE:CD1	2.18	0.74
19:3:3016:CLA:C10	19:3:3016:CLA:C14	2.57	0.74
18:4:141:LEU:CD2	18:4:141:LEU:N	2.48	0.74
1:A:316:MET:HG2	1:A:317:TYR:CE1	2.21	0.74
1:A:692:PHE:CE2	19:A:1140:CLA:HBC3	2.23	0.74
19:A:1140:CLA:C14	21:A:6011:BCR:C2	2.62	0.74
2:B:32:GLU:HG2	2:B:42:LEU:CD2	2.18	0.74
19:B:1220:CLA:H102	19:B:1220:CLA:C15	2.12	0.74
6:F:173:TRP:HE3	6:F:211:PHE:N	1.86	0.74
13:N:165:ASN:C	13:N:167:PHE:N	2.39	0.74
15:1:225:TRP:HD1	15:1:226:HIS:CE1	2.06	0.74
17:3:197:SER:OG	17:3:206:PRO:CD	2.35	0.74
18:4:123:VAL:N	18:4:124:PRO:CD	2.51	0.74
2:B:90:ALA:HA	2:B:113:VAL:CG1	2.02	0.73
3:C:26:LEU:H	3:C:43:PRO:HG3	1.53	0.73
3:C:73:THR:HG23	3:C:76:SER:OG	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100:TYR:HE1	4:D:134:LYS:CG	2.01	0.73
22:E:7037:LMU:H12	22:E:7037:LMU:H51	1.69	0.73
7:G:128:LEU:HD23	7:G:128:LEU:O	1.88	0.73
13:N:139:LYS:CE	13:N:142:LYS:CE	2.51	0.73
15:1:78:ARG:HG2	19:1:1011:CLA:HMC1	1.69	0.73
16:2:254:LEU:C	16:2:254:LEU:HD23	2.05	0.73
1:A:591:GLN:HA	1:A:591:GLN:HE21	1.53	0.73
19:A:1136:CLA:H192	19:L:1130:CLA:CBB	2.18	0.73
21:A:6002:BCR:H12C	21:A:6002:BCR:C34	2.17	0.73
2:B:349:ALA:HB2	2:B:375:HIS:HB3	1.69	0.73
2:B:516:ASP:O	2:B:520:HIS:HB2	1.88	0.73
2:B:711:VAL:O	2:B:711:VAL:HG12	1.85	0.73
4:D:148:TYR:O	4:D:149:LYS:HG2	1.89	0.73
7:G:98:THR:OG1	7:G:101:GLU:CB	2.35	0.73
8:H:70:SER:O	8:H:73:PRO:CD	2.37	0.73
12:L:155:GLU:HA	12:L:178:THR:HG21	1.68	0.73
14:R:35:UNK:O	14:R:36:UNK:C	2.35	0.73
17:3:111:LEU:C	17:3:114:VAL:H	1.91	0.73
1:A:218:TRP:O	1:A:222:GLN:HB2	1.87	0.73
19:A:1124:CLA:HHD	19:A:1124:CLA:CBC	2.15	0.73
2:B:550:LYS:O	2:B:550:LYS:HG2	1.87	0.73
3:C:42:ALA:O	4:D:183:GLY:HA3	1.88	0.73
3:C:44:ARG:CB	4:D:182:GLN:OE1	2.37	0.73
3:C:67:VAL:HG13	3:C:68:TYR:HA	1.70	0.73
4:D:167:HIS:NE2	4:D:172:VAL:HG21	2.02	0.73
5:E:78:ARG:HH12	5:E:125:ILE:HG21	1.51	0.73
22:G:7026:LMU:C5	22:G:7026:LMU:H12	2.17	0.73
19:L:1130:CLA:HAC2	19:L:1504:CLA:HMC3	1.70	0.73
13:N:157:LYS:HB3	13:N:158:ASP:CA	2.18	0.73
16:2:139:THR:CG2	16:2:140:ALA:N	2.51	0.73
16:2:212:GLN:HG2	16:2:213:LYS:HG2	1.71	0.73
17:3:96:ARG:HA	17:3:99:ALA:H	1.41	0.73
19:3:3013:CLA:H2A	19:3:3013:CLA:O1D	1.88	0.73
18:4:100:ARG:O	18:4:104:LEU:HD12	1.89	0.73
18:4:232:LEU:HD12	18:4:234:GLN:HA	1.69	0.73
1:A:150:PHE:N	1:A:153:TRP:HE3	1.86	0.73
1:A:284:ARG:CZ	1:A:284:ARG:O	2.35	0.73
19:A:1107:CLA:CBB	19:B:1230:CLA:HMD2	2.18	0.73
2:B:75:GLU:HB2	2:B:132:ASN:CB	2.19	0.73
4:D:167:HIS:CE1	4:D:172:VAL:CG1	2.58	0.73
14:R:38:UNK:O	14:R:41:UNK:CB	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:170:PRO:HD2	15:1:173:TYR:HE2	1.49	0.73
17:3:201:ALA:CA	17:3:202:TYR:HD2	2.02	0.73
17:3:210:PRO:CD	17:3:211:LEU:H	2.02	0.73
18:4:211:MET:CG	19:4:4002:CLA:CBB	2.65	0.73
1:A:29:THR:HG23	1:A:29:THR:O	1.89	0.73
1:A:73:GLU:OE1	1:A:186:TYR:OH	2.07	0.73
1:A:89:ILE:O	1:A:93:LEU:HD22	1.89	0.73
1:A:217:SER:HA	21:A:6002:BCR:H351	1.68	0.73
1:A:258:LEU:O	1:A:259:TYR:HB2	1.87	0.73
19:A:9023:CLA:H3A	19:A:9023:CLA:O2A	1.87	0.73
4:D:174:PRO:C	4:D:175:GLU:HG2	2.08	0.73
7:G:137:VAL:O	7:G:137:VAL:HG23	1.87	0.73
19:J:1308:CLA:H91	19:2:2014:CLA:O1D	1.87	0.73
19:1:1002:CLA:HMC1	19:1:1002:CLA:HBC3	1.71	0.73
18:4:173:LYS:HB2	18:4:194:PHE:CD2	2.22	0.73
18:4:201:LYS:HD3	18:4:201:LYS:N	2.03	0.73
1:A:293:GLY:O	1:A:294:LEU:CB	2.37	0.73
1:A:328:LYS:NZ	1:A:345:GLY:HA3	2.01	0.73
1:A:521:VAL:O	1:A:521:VAL:HG12	1.86	0.73
19:A:1119:CLA:CBA	19:A:1123:CLA:HBB2	2.18	0.73
19:A:1125:CLA:HBB2	19:A:1133:CLA:C3A	2.14	0.73
21:A:6002:BCR:H373	19:3:1147:CLA:HBC1	1.68	0.73
19:A:9012:CLA:C3B	2:B:589:TRP:HH2	2.02	0.73
2:B:11:GLY:CA	3:C:71:HIS:CD2	2.61	0.73
2:B:486:LEU:CD1	2:B:489:GLY:N	2.49	0.73
2:B:545:LYS:HG2	2:B:546:LEU:N	2.01	0.73
19:B:1205:CLA:H102	19:B:1205:CLA:H142	1.71	0.73
3:C:52:LYS:O	3:C:52:LYS:CG	2.37	0.73
3:C:73:THR:HG21	3:C:76:SER:HB3	1.70	0.73
7:G:99:HIS:O	7:G:101:GLU:CB	2.36	0.73
8:H:80:GLN:HA	8:H:83:LEU:HD23	1.70	0.73
12:L:110:LEU:HA	12:L:113:PRO:HG2	1.71	0.73
12:L:210:PRO:O	12:L:211:TYR:CG	2.42	0.73
16:2:269:LYS:NZ	16:2:269:LYS:CA	2.47	0.73
17:3:202:TYR:HB3	17:3:203:PRO:HD2	1.69	0.73
19:A:1237:CLA:C20	12:L:110:LEU:HD21	2.18	0.73
19:A:9022:CLA:H13	19:B:1206:CLA:HBB2	1.70	0.73
2:B:515:GLY:CA	2:B:613:SER:HB2	2.18	0.73
7:G:75:GLY:C	7:G:77:PHE:N	2.35	0.73
7:G:88:ALA:C	7:G:90:GLN:O	2.27	0.73
7:G:89:LYS:CA	7:G:89:LYS:HZ2	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:92:PHE:N	17:3:92:PHE:CD1	2.57	0.73
1:A:635:THR:O	1:A:635:THR:HG22	1.88	0.73
19:A:1122:CLA:C1D	21:A:6007:BCR:C19	2.67	0.73
2:B:256:THR:O	2:B:272:ASP:CG	2.27	0.73
6:F:228:ASP:OD2	6:F:231:PHE:CD1	2.41	0.73
8:H:119:ASP:C	8:H:120:ILE:HG22	2.07	0.73
19:H:1145:CLA:CED	19:H:1145:CLA:HAA1	2.19	0.73
19:K:1146:CLA:O1A	19:K:1146:CLA:CMA	2.37	0.73
15:1:155:GLU:O	15:1:156:LYS:HB2	1.88	0.73
21:1:6023:BCR:HC8	21:1:6023:BCR:HC21	1.70	0.73
16:2:192:ASP:OD2	16:2:194:GLY:HA2	1.87	0.73
17:3:238:ILE:HG23	17:3:241:TYR:OH	1.88	0.73
1:A:328:LYS:HG3	1:A:332:GLU:CB	2.19	0.73
1:A:575:LEU:HD11	1:A:579:PHE:HB3	1.71	0.73
19:A:1124:CLA:HED1	19:A:1125:CLA:CAD	2.12	0.73
2:B:261:PHE:CE2	2:B:500:ALA:N	2.57	0.73
2:B:493:TRP:O	2:B:495:PRO:HD3	1.88	0.73
2:B:531:THR:O	2:B:535:VAL:HG12	1.89	0.73
19:B:1228:CLA:CBC	19:B:1228:CLA:CHD	2.66	0.73
3:C:1:MET:N	3:C:3:HIS:C	2.42	0.73
3:C:65:VAL:CG2	3:C:66:ARG:H	1.97	0.73
4:D:141:GLY:N	4:D:144:LEU:H	1.84	0.73
5:E:96:ASP:CB	5:E:98:ASN:H	1.94	0.73
12:L:54:TYR:CD1	12:L:54:TYR:N	2.53	0.73
15:1:162:LYS:C	15:1:164:PRO:CD	2.56	0.73
16:2:153:PHE:CE2	16:2:157:LEU:HD21	2.24	0.73
19:3:3008:CLA:CGD	19:3:3008:CLA:CGA	2.66	0.73
1:A:309:LEU:HD21	19:A:1119:CLA:CMC	2.19	0.73
1:A:349:ILE:HG22	1:A:350:LEU:N	2.01	0.73
2:B:310:PRO:CG	19:B:1220:CLA:HMA1	2.17	0.73
2:B:622:ASP:HB3	2:B:626:LEU:CD1	2.18	0.73
4:D:100:TYR:HE1	4:D:134:LYS:CE	2.00	0.73
5:E:89:SER:HG	5:E:106:ARG:HD3	1.49	0.73
6:F:222:LEU:HD23	6:F:222:LEU:N	2.03	0.73
19:H:1145:CLA:O2D	19:H:1145:CLA:HAA2	1.89	0.73
19:J:1311:CLA:H2	19:J:1311:CLA:C16	2.18	0.73
12:L:128:GLN:HG2	12:L:132:LEU:HD22	1.69	0.73
16:2:167:ARG:NE	16:2:167:ARG:CA	2.51	0.73
16:2:177:VAL:CG1	16:2:178:ASN:CG	2.56	0.73
1:A:93:LEU:HA	1:A:96:MET:H	1.53	0.72
1:A:150:PHE:O	1:A:151:GLN:CG	2.34	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ASN:HD22	1:A:464:ASN:N	1.85	0.72
2:B:53:GLN:HG2	19:B:1202:CLA:HMB2	1.69	0.72
2:B:87:ILE:HD12	2:B:87:ILE:N	2.03	0.72
2:B:190:TRP:HA	19:B:1211:CLA:HBB2	1.69	0.72
4:D:147:LYS:HA	4:D:148:TYR:CD1	2.23	0.72
5:E:129:GLU:CA	5:E:129:GLU:OE1	2.35	0.72
10:J:5:LYS:CG	16:2:178:ASN:OD1	2.36	0.72
15:1:170:PRO:CD	15:1:173:TYR:CD2	2.71	0.72
19:4:1304:CLA:C20	19:4:1304:CLA:C15	2.63	0.72
1:A:379:MET:CE	19:A:1125:CLA:HMC2	2.18	0.72
2:B:124:TRP:CD1	2:B:129:LEU:HB3	2.24	0.72
2:B:125:TYR:CE1	2:B:130:ARG:NH1	2.56	0.72
2:B:294:ASN:HB2	7:G:94:GLN:NE2	2.03	0.72
2:B:486:LEU:CD1	2:B:489:GLY:H	2.02	0.72
2:B:542:ARG:HH11	2:B:542:ARG:HB3	1.52	0.72
2:B:553:PHE:O	2:B:555:TYR:N	2.22	0.72
19:B:1205:CLA:H141	19:B:1224:CLA:H91	1.71	0.72
24:B:7101:LMG:HC61	3:C:70:TRP:CH2	2.25	0.72
8:H:109:LEU:CD2	19:H:1207:CLA:C5	2.67	0.72
17:3:150:TYR:C	17:3:151:TRP:HD1	1.90	0.72
17:3:173:PHE:CD1	17:3:174:GLN:N	2.51	0.72
1:A:210:LEU:HD13	19:A:1111:CLA:HMB2	1.70	0.72
1:A:267:THR:HG22	1:A:269:PHE:CD2	2.23	0.72
1:A:478:SER:HB3	1:A:644:GLN:NE2	1.94	0.72
1:A:588:GLY:N	2:B:668:ARG:HD3	2.03	0.72
2:B:131:THR:HB	2:B:134:ASP:HB2	1.71	0.72
2:B:216:LEU:HD21	2:B:221:GLY:HA2	1.71	0.72
2:B:457:PRO:HB3	2:B:517:PHE:CB	2.19	0.72
3:C:5:VAL:HG23	3:C:65:VAL:CG2	2.19	0.72
7:G:63:VAL:HG22	7:G:64:ILE:H	1.51	0.72
7:G:129:ALA:O	7:G:131:GLY:N	2.23	0.72
8:H:111:TYR:CD1	8:H:112:LEU:CD2	2.72	0.72
19:J:1308:CLA:C9	19:2:2014:CLA:CGD	2.67	0.72
11:K:127:ILE:O	11:K:130:LEU:HG	1.90	0.72
12:L:51:LYS:N	12:L:52:PRO:HD3	2.04	0.72
13:N:157:LYS:N	13:N:157:LYS:CE	2.52	0.72
16:2:188:LEU:HD22	16:2:188:LEU:H	1.53	0.72
17:3:94:GLU:C	17:3:94:GLU:CD	2.47	0.72
19:3:3016:CLA:H2A	19:3:3016:CLA:O2D	1.88	0.72
18:4:98:ASN:CB	18:4:212:LEU:HD21	2.20	0.72
1:A:558:LYS:HZ2	2:B:674:LEU:HB2	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1112:CLA:HBA2	19:3:1147:CLA:HMC3	1.71	0.72
21:A:6011:BCR:C32	21:J:6012:BCR:H391	2.19	0.72
2:B:256:THR:OG1	2:B:258:LEU:N	2.23	0.72
2:B:430:GLY:CA	2:B:525:LEU:HD11	2.17	0.72
3:C:12:ILE:O	3:C:38:GLN:HG3	1.89	0.72
5:E:79:LYS:CG	5:E:84:TYR:CE1	2.73	0.72
6:F:100:LYS:O	6:F:103:GLN:CB	2.31	0.72
6:F:207:LEU:HD22	6:F:208:PHE:HA	1.70	0.72
22:F:7036:LMU:O2B	22:F:7036:LMU:H6D	1.89	0.72
7:G:96:GLY:O	7:G:97:LEU:CG	2.37	0.72
8:H:113:SER:OG	19:H:1207:CLA:C5	2.37	0.72
15:1:224:PRO:HA	15:1:225:TRP:HB2	1.69	0.72
1:A:188:LYS:HE2	1:A:190:ALA:HA	1.72	0.72
1:A:475:ASP:HB3	19:A:1132:CLA:HED3	1.69	0.72
1:A:579:PHE:N	1:A:579:PHE:CD1	2.53	0.72
19:A:1105:CLA:C3B	21:J:6012:BCR:H333	2.19	0.72
2:B:160:LYS:CD	2:B:161:TRP:CD2	2.72	0.72
2:B:521:HIS:CE1	19:B:1235:CLA:NA	2.56	0.72
3:C:1:MET:H1	3:C:3:HIS:C	1.93	0.72
4:D:176:LYS:HG3	4:D:177:VAL:N	2.02	0.72
22:G:7026:LMU:H41	22:G:7026:LMU:C8	2.19	0.72
15:1:64:PHE:CE1	15:1:66:PRO:HD3	2.24	0.72
17:3:156:THR:CA	17:3:158:PHE:O	2.36	0.72
19:4:1304:CLA:O1D	19:4:1304:CLA:H2A	1.90	0.72
1:A:34:TRP:O	1:A:35:ALA:HB3	1.89	0.72
1:A:345:GLY:C	1:A:347:TYR:N	2.35	0.72
1:A:351:THR:O	19:A:1123:CLA:H201	1.89	0.72
19:A:1141:CLA:HBC3	19:A:1141:CLA:HHD	1.70	0.72
2:B:293:THR:HG23	7:G:94:GLN:HG2	1.69	0.72
2:B:362:ALA:O	2:B:363:GLN:HB3	1.88	0.72
2:B:459:PHE:H	19:B:1235:CLA:CAD	2.02	0.72
2:B:576:PHE:HE2	19:B:1226:CLA:HAC1	1.53	0.72
3:C:52:LYS:NZ	3:C:64:SER:HB2	2.03	0.72
4:D:162:GLU:C	4:D:163:VAL:HG23	2.10	0.72
4:D:201:LYS:O	4:D:202:PHE:HB3	1.87	0.72
11:K:97:ASP:CA	11:K:101:PHE:CE2	2.73	0.72
13:N:139:LYS:HD2	13:N:142:LYS:NZ	2.01	0.72
15:1:134:LEU:N	15:1:135:PRO:CD	2.52	0.72
19:1:1005:CLA:HMC1	19:1:1005:CLA:CBC	2.20	0.72
16:2:249:ASN:ND2	16:2:254:LEU:HG	2.04	0.72
1:A:93:LEU:HA	1:A:96:MET:CB	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PRO:O	1:A:290:LEU:CB	2.37	0.72
1:A:355:HIS:CE1	1:A:416:ILE:HG21	2.24	0.72
2:B:77:TRP:O	2:B:81:PRO:HG3	1.89	0.72
2:B:135:LEU:HD12	2:B:135:LEU:O	1.90	0.72
2:B:469:LYS:HZ2	2:B:471:THR:C	1.93	0.72
2:B:639:VAL:HG22	2:B:640:CYS:H	1.55	0.72
19:B:1214:CLA:HBD	19:B:1223:CLA:HBB2	1.70	0.72
19:B:1222:CLA:HBB1	19:B:1236:CLA:CHB	2.19	0.72
7:G:89:LYS:HZ2	7:G:89:LYS:H	1.38	0.72
8:H:94:ARG:O	8:H:95:GLY:C	2.28	0.72
15:1:70:GLY:C	15:1:73:PRO:HD2	2.08	0.72
15:1:161:LYS:HE2	15:1:162:LYS:CB	2.17	0.72
16:2:165:GLY:C	16:2:167:ARG:CG	2.58	0.72
17:3:103:VAL:HG13	17:3:107:ARG:CZ	2.19	0.72
18:4:103:MET:HE2	18:4:207:ASN:C	1.90	0.72
18:4:169:ASP:HB3	19:4:4001:CLA:HMB3	1.70	0.72
19:4:1306:CLA:O2A	19:4:1306:CLA:H2A	1.89	0.72
1:A:284:ARG:CG	1:A:295:TRP:CG	2.73	0.72
1:A:346:LEU:C	1:A:346:LEU:CD2	2.58	0.72
1:A:355:HIS:ND1	1:A:416:ILE:CG2	2.52	0.72
1:A:422:TYR:N	1:A:422:TYR:CD1	2.31	0.72
1:A:499:ALA:CB	19:A:1133:CLA:CED	2.64	0.72
19:A:1140:CLA:C4	19:A:1140:CLA:NC	2.53	0.72
21:A:6002:BCR:H402	21:A:6002:BCR:C23	2.20	0.72
2:B:75:GLU:HB2	2:B:132:ASN:CG	2.09	0.72
2:B:293:THR:CG2	19:B:1209:CLA:HMA2	2.19	0.72
2:B:430:GLY:HA2	2:B:525:LEU:CD1	2.19	0.72
19:B:1211:CLA:HMB2	21:B:6006:BCR:C8	2.19	0.72
3:C:73:THR:CG2	3:C:76:SER:OG	2.38	0.72
5:E:93:VAL:HG23	5:E:103:VAL:CB	2.19	0.72
6:F:138:LEU:HD23	6:F:146:PRO:HB3	1.71	0.72
15:1:170:PRO:O	15:1:173:TYR:OH	2.08	0.72
16:2:206:TRP:O	16:2:208:SER:HB2	1.90	0.72
22:4:7009:LMU:H3'	22:4:7009:LMU:O5B	1.89	0.72
1:A:27:ILE:O	1:A:28:LYS:CG	2.38	0.72
1:A:126:ILE:HD11	19:A:1107:CLA:HMA3	1.70	0.72
19:A:9023:CLA:HMC1	19:A:9023:CLA:HBC3	1.71	0.72
2:B:120:VAL:HA	2:B:123:TRP:NE1	2.05	0.72
2:B:230:TRP:N	7:G:63:VAL:CG2	2.49	0.72
19:B:1203:CLA:H91	19:B:1203:CLA:H193	1.71	0.72
3:C:27:GLU:OE1	3:C:39:ILE:C	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:PHE:CE2	5:E:80:GLU:OE2	2.42	0.72
19:H:1145:CLA:CED	19:H:1145:CLA:CAA	2.68	0.72
12:L:112:GLY:HA3	19:L:1503:CLA:HHC	1.69	0.72
19:L:1130:CLA:H52	19:L:1504:CLA:CHB	2.19	0.72
15:1:179:LYS:HG2	15:1:180:LEU:O	1.89	0.72
18:4:232:LEU:HB2	18:4:236:ILE:CD1	2.18	0.72
1:A:316:MET:CG	1:A:317:TYR:HD1	1.97	0.72
2:B:639:VAL:HG22	2:B:640:CYS:N	2.05	0.72
19:B:1216:CLA:OBD	19:B:1219:CLA:HBC3	1.90	0.72
3:C:5:VAL:HG23	3:C:65:VAL:HG23	1.71	0.72
3:C:72:GLU:CG	3:C:77:MET:CE	2.66	0.72
3:C:80:ALA:O	3:C:81:TYR:CB	2.35	0.72
5:E:78:ARG:HH12	5:E:125:ILE:CG2	2.00	0.72
22:E:7037:LMU:H12	22:E:7037:LMU:C5	2.20	0.72
22:E:7048:LMU:H22	22:E:7048:LMU:O5'	1.90	0.72
7:G:64:ILE:O	7:G:68:THR:HG21	1.88	0.72
7:G:144:THR:HG23	7:G:147:ASN:O	1.90	0.72
22:N:7049:LMU:O1'	22:N:7049:LMU:H41	1.88	0.72
15:1:92:LEU:CA	15:1:95:PRO:HD2	2.19	0.72
16:2:167:ARG:HE	16:2:168:TRP:H	1.37	0.72
1:A:57:LEU:C	1:A:57:LEU:CD2	2.57	0.71
1:A:293:GLY:O	1:A:294:LEU:HB3	1.89	0.71
2:B:74:PHE:O	2:B:76:ALA:N	2.23	0.71
2:B:231:ASN:HD21	7:G:61:ALA:HB3	1.53	0.71
2:B:317:ARG:NH2	2:B:410:ARG:HG3	2.05	0.71
2:B:729:THR:O	2:B:729:THR:HG22	1.90	0.71
6:F:96:LYS:O	6:F:100:LYS:CB	2.37	0.71
19:J:1308:CLA:HMA3	19:2:2014:CLA:CED	2.20	0.71
11:K:63:LEU:H	11:K:63:LEU:CD1	1.99	0.71
11:K:118:VAL:CG2	11:K:121:VAL:CG2	2.68	0.71
12:L:51:LYS:N	12:L:52:PRO:CD	2.52	0.71
17:3:252:PRO:HB3	17:3:254:GLN:NE2	2.04	0.71
18:4:226:LYS:H	18:4:226:LYS:NZ	1.87	0.71
1:A:246:HIS:CA	1:A:248:PHE:CE2	2.60	0.71
1:A:472:ARG:HH22	12:L:120:LEU:HD11	1.54	0.71
19:A:1141:CLA:C12	19:A:1141:CLA:H72	2.18	0.71
2:B:493:TRP:CZ3	19:B:1232:CLA:HMA2	2.25	0.71
2:B:510:LEU:HD11	2:B:597:LYS:HZ3	1.54	0.71
3:C:26:LEU:N	3:C:43:PRO:HG3	2.05	0.71
4:D:188:PHE:N	4:D:188:PHE:CD1	2.52	0.71
11:K:56:ILE:HG23	11:K:59:THR:CG2	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:116:ILE:HG23	11:K:117:GLY:N	2.05	0.71
11:K:127:ILE:CB	11:K:130:LEU:HG	2.20	0.71
12:L:110:LEU:HB3	12:L:114:PHE:CE1	2.22	0.71
15:1:101:GLU:O	15:1:101:GLU:HG2	1.89	0.71
15:1:150:HIS:CE1	15:1:151:GLN:HE22	2.07	0.71
16:2:184:PRO:HD3	16:2:187:LYS:N	2.05	0.71
17:3:104:ILE:HG21	19:3:3004:CLA:C4D	2.20	0.71
18:4:225:GLY:HA2	18:4:226:LYS:HZ2	1.55	0.71
1:A:92:TRP:O	1:A:93:LEU:CB	2.38	0.71
1:A:387:THR:CG2	1:A:523:VAL:HG11	2.20	0.71
1:A:472:ARG:NH1	12:L:120:LEU:CD2	2.50	0.71
19:A:1117:CLA:H202	19:A:1125:CLA:H3A	1.71	0.71
22:A:7016:LMU:H61	22:A:7016:LMU:C2	2.16	0.71
2:B:315:LEU:HD11	2:B:317:ARG:HD2	1.73	0.71
2:B:395:ILE:HD12	2:B:396:ARG:HG2	1.73	0.71
2:B:693:TRP:CD1	19:B:1238:CLA:C1D	2.74	0.71
19:B:1235:CLA:H121	21:F:6016:BCR:H312	1.70	0.71
22:B:7038:LMU:H4'	22:B:7038:LMU:O2B	1.88	0.71
3:C:72:GLU:HG2	3:C:77:MET:CE	2.19	0.71
5:E:83:TRP:CZ3	5:E:111:ASN:HB2	2.25	0.71
11:K:89:ARG:HG3	11:K:89:ARG:HH11	1.55	0.71
19:K:1142:CLA:HED2	19:K:1143:CLA:HMB2	1.70	0.71
12:L:67:GLY:O	12:L:68:SER:CB	2.38	0.71
21:L:6019:BCR:H403	21:L:6019:BCR:C27	2.19	0.71
16:2:124:GLU:O	16:2:127:THR:CG2	2.37	0.71
16:2:227:LEU:HD21	19:2:2004:CLA:NC	2.05	0.71
17:3:98:LEU:HD21	19:3:3012:CLA:C3D	2.20	0.71
19:A:1102:CLA:HMC3	19:A:1104:CLA:O2D	1.90	0.71
19:A:1124:CLA:H172	21:A:6007:BCR:H332	1.71	0.71
6:F:224:GLY:C	6:F:227:VAL:CG1	2.54	0.71
11:K:59:THR:O	11:K:63:LEU:CD2	2.38	0.71
11:K:98:PRO:CD	11:K:99:ALA:H	2.01	0.71
13:N:139:LYS:CD	13:N:142:LYS:CE	2.68	0.71
15:1:67:LEU:HD12	15:1:68:GLY:H	1.51	0.71
16:2:96:PRO:HD3	17:3:85:ASP:OD2	1.87	0.71
16:2:121:PHE:H	16:2:121:PHE:HD2	1.36	0.71
16:2:226:ARG:HH11	16:2:226:ARG:HB2	1.56	0.71
1:A:555:ILE:CD1	19:A:9023:CLA:HMD1	2.19	0.71
19:A:1102:CLA:H12	19:A:1109:CLA:H92	1.72	0.71
2:B:331:HIS:CE1	2:B:392:ILE:HG21	2.25	0.71
19:B:1223:CLA:C8	21:B:6010:BCR:H14C	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:170:ILE:CG2	21:F:6014:BCR:H372	2.21	0.71
12:L:94:SER:O	12:L:96:LEU:CD2	2.38	0.71
13:N:99:LYS:CB	13:N:102:ASN:HD21	2.03	0.71
15:1:189:LYS:CB	19:1:1007:CLA:HMC1	2.15	0.71
16:2:154:ILE:HG12	16:2:155:VAL:N	2.04	0.71
16:2:223:LYS:O	16:2:226:ARG:HB3	1.90	0.71
17:3:150:TYR:CD2	17:3:151:TRP:CD2	2.78	0.71
1:A:187:HIS:CE1	19:A:1109:CLA:C4D	2.67	0.71
1:A:258:LEU:HG	1:A:280:PHE:CE1	2.26	0.71
1:A:370:ILE:HG23	1:A:403:GLY:CA	2.16	0.71
1:A:478:SER:HB2	1:A:644:GLN:CD	2.10	0.71
1:A:479:ASP:OD1	1:A:536:THR:HG22	1.91	0.71
21:B:6004:BCR:H343	7:G:77:PHE:CD1	2.25	0.71
3:C:63:LEU:HD21	3:C:65:VAL:H	1.53	0.71
4:D:106:SER:OG	4:D:124:GLU:HG2	1.91	0.71
4:D:133:ARG:H	4:D:136:GLN:HE22	1.36	0.71
8:H:77:ASN:OD1	8:H:78:PRO:HD2	1.91	0.71
19:K:1146:CLA:HBC2	19:K:1146:CLA:HMC1	1.73	0.71
22:L:7029:LMU:H31	22:L:7029:LMU:C1'	2.16	0.71
17:3:204:GLY:H	17:3:207:PHE:HA	1.56	0.71
18:4:226:LYS:N	18:4:226:LYS:HD3	2.04	0.71
1:A:615:HIS:CE1	19:A:1135:CLA:HBC3	2.26	0.71
19:A:1102:CLA:O2D	19:A:1102:CLA:H2A	1.90	0.71
2:B:600:THR:O	2:B:604:GLY:HA2	1.89	0.71
19:B:1225:CLA:OBD	19:B:1225:CLA:O1D	1.97	0.71
3:C:44:ARG:HA	4:D:182:GLN:OE1	1.90	0.71
5:E:89:SER:HB3	5:E:106:ARG:NE	2.06	0.71
8:H:98:LEU:HD21	12:L:143:LEU:HD22	1.73	0.71
11:K:70:PHE:HD1	11:K:70:PHE:O	1.74	0.71
15:1:83:GLU:CA	15:1:86:HIS:CD2	2.74	0.71
17:3:150:TYR:CA	17:3:152:ALA:HB2	2.21	0.71
22:3:7003:LMU:O2B	22:3:7005:LMU:O5B	2.09	0.71
18:4:96:LEU:HD12	18:4:96:LEU:O	1.91	0.71
18:4:167:ASN:ND2	19:4:4014:CLA:C2	2.53	0.71
1:A:252:ARG:NH1	1:A:261:SER:OG	2.23	0.71
1:A:328:LYS:CG	1:A:332:GLU:CB	2.68	0.71
1:A:723:ARG:HH11	1:A:723:ARG:HG2	1.56	0.71
2:B:88:ALA:N	2:B:115:ASN:HA	2.05	0.71
2:B:322:LEU:O	2:B:326:ILE:HG22	1.90	0.71
2:B:622:ASP:HB3	2:B:626:LEU:HG	1.72	0.71
3:C:62:PHE:CG	4:D:191:ILE:HG21	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:VAL:HG12	5:E:91:VAL:H	1.56	0.71
6:F:207:LEU:CG	6:F:208:PHE:N	2.54	0.71
19:H:1241:CLA:HAC1	21:I:6021:BCR:HC31	1.69	0.71
12:L:143:LEU:H	12:L:145:LEU:H	1.35	0.71
18:4:173:LYS:HZ2	18:4:201:LYS:CG	2.01	0.71
18:4:242:ASN:O	18:4:243:THR:CG2	2.35	0.71
2:B:125:TYR:CD1	2:B:130:ARG:NH1	2.58	0.71
3:C:52:LYS:NZ	3:C:65:VAL:O	2.24	0.71
5:E:94:ASP:HB2	5:E:102:PRO:HB3	1.72	0.71
10:J:2:ARG:NH1	10:J:8:LEU:HD13	2.01	0.71
12:L:209:LEU:CG	12:L:210:PRO:HD2	2.21	0.71
19:1:1303:CLA:CMA	19:1:1303:CLA:HBA2	2.19	0.71
18:4:122:ASN:CB	18:4:124:PRO:HD3	2.19	0.71
1:A:62:HIS:ND1	1:A:62:HIS:N	2.39	0.71
19:A:1112:CLA:HMC2	21:A:6002:BCR:C17	2.20	0.71
2:B:293:THR:CG2	7:G:94:GLN:CD	2.54	0.71
19:B:1231:CLA:HMD2	19:B:1232:CLA:C2C	2.21	0.71
5:E:81:SER:OG	5:E:120:TYR:CZ	2.37	0.71
19:K:1143:CLA:HBC1	22:K:7001:LMU:C3B	2.21	0.71
16:2:171:ILE:HG13	16:2:172:LEU:CA	2.19	0.71
17:3:150:TYR:CA	17:3:151:TRP:HD1	2.04	0.71
18:4:174:GLN:O	18:4:194:PHE:CD1	2.44	0.71
1:A:66:SER:O	1:A:67:HIS:HB2	1.89	0.70
1:A:362:LEU:HB3	1:A:410:ALA:HB2	1.73	0.70
1:A:545:HIS:HB3	19:A:1135:CLA:HBB2	1.71	0.70
1:A:680:LEU:HB3	19:A:9012:CLA:O2A	1.91	0.70
19:A:1140:CLA:H161	21:A:6011:BCR:HC22	1.72	0.70
19:A:9022:CLA:C9	19:A:9023:CLA:C9	2.69	0.70
2:B:70:TRP:HB3	2:B:136:TYR:HH	1.55	0.70
3:C:44:ARG:HB3	4:D:182:GLN:OE1	1.89	0.70
3:C:49:VAL:HG22	3:C:50:GLY:H	1.55	0.70
5:E:82:TYR:HB3	5:E:83:TRP:HE3	1.54	0.70
7:G:84:ARG:NE	7:G:89:LYS:CE	2.51	0.70
12:L:82:TYR:O	12:L:83:LEU:HB3	1.91	0.70
15:1:151:GLN:HE21	15:1:151:GLN:CA	2.02	0.70
16:2:120:ILE:CG1	16:2:121:PHE:N	2.51	0.70
16:2:134:THR:OG1	16:2:135:PRO:HD3	1.89	0.70
16:2:160:ILE:CG2	19:2:2012:CLA:CAB	2.68	0.70
18:4:169:ASP:OD1	18:4:174:GLN:HB2	1.90	0.70
18:4:172:PHE:CA	18:4:194:PHE:HE2	1.94	0.70
18:4:211:MET:HG3	19:4:4002:CLA:HBB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD11	1:A:674:ALA:CB	2.20	0.70
1:A:188:LYS:HD2	1:A:189:ALA:N	2.06	0.70
1:A:379:MET:HE1	19:A:1125:CLA:HHC	1.73	0.70
1:A:389:TYR:HE2	1:A:526:LYS:HD3	1.56	0.70
2:B:400:PRO:HD2	4:D:197:PRO:HD3	1.72	0.70
2:B:663:PHE:O	2:B:664:LEU:CB	2.39	0.70
3:C:65:VAL:CG2	3:C:66:ARG:N	2.55	0.70
6:F:139:LEU:HD13	6:F:149:ILE:HD12	1.72	0.70
6:F:213:TRP:CB	6:F:216:ALA:HB2	2.17	0.70
6:F:225:GLU:O	6:F:227:VAL:HG13	1.92	0.70
19:F:1302:CLA:CMA	21:F:6016:BCR:HC32	2.21	0.70
10:J:11:ALA:HB1	10:J:12:PRO:CD	2.12	0.70
16:2:131:ILE:O	16:2:132:LEU:CB	2.39	0.70
16:2:173:ASN:ND2	16:2:173:ASN:N	2.36	0.70
17:3:156:THR:HA	17:3:158:PHE:O	1.89	0.70
17:3:225:LEU:HD13	17:3:228:VAL:HG21	1.72	0.70
1:A:532:ILE:HG23	1:A:532:ILE:O	1.90	0.70
19:A:1237:CLA:C14	12:L:141:LEU:HD23	2.17	0.70
21:A:6007:BCR:H382	21:A:6007:BCR:C23	2.21	0.70
2:B:110:LEU:CD1	2:B:111:GLY:N	2.53	0.70
2:B:127:ILE:O	2:B:127:ILE:CG1	2.38	0.70
2:B:680:TRP:O	2:B:681:ALA:O	2.08	0.70
3:C:31:TRP:CD1	3:C:32:GLY:N	2.58	0.70
4:D:123:ARG:O	4:D:124:GLU:HB2	1.91	0.70
6:F:159:GLU:HG2	10:J:38:ILE:HG12	1.72	0.70
21:I:6021:BCR:H322	21:I:6021:BCR:HC42	1.72	0.70
11:K:115:ILE:O	11:K:118:VAL:HG22	1.91	0.70
19:K:3009:CLA:H91	19:3:3007:CLA:HAC2	1.74	0.70
14:R:37:UNK:O	14:R:43:UNK:N	2.24	0.70
16:2:176:CYS:O	16:2:177:VAL:CG2	2.36	0.70
19:2:2014:CLA:OBD	19:2:2014:CLA:CED	2.38	0.70
17:3:103:VAL:CG1	17:3:107:ARG:NE	2.42	0.70
22:3:7003:LMU:C2B	22:3:7005:LMU:O5B	2.39	0.70
1:A:284:ARG:CG	1:A:295:TRP:CD1	2.73	0.70
2:B:25:ILE:CG2	21:L:6019:BCR:H292	2.15	0.70
2:B:160:LYS:HZ2	2:B:161:TRP:CB	2.02	0.70
19:B:1223:CLA:HED1	19:B:1231:CLA:CBB	2.19	0.70
3:C:43:PRO:HA	4:D:182:GLN:CB	2.20	0.70
5:E:129:GLU:C	5:E:129:GLU:OE1	2.30	0.70
6:F:190:LYS:CG	6:F:192:THR:HG23	2.22	0.70
6:F:204:SER:O	6:F:207:LEU:CD1	2.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:ARG:HH12	10:J:8:LEU:CD1	2.00	0.70
13:N:99:LYS:CB	13:N:102:ASN:ND2	2.55	0.70
13:N:165:ASN:O	13:N:167:PHE:N	2.24	0.70
17:3:150:TYR:O	17:3:152:ALA:CA	2.38	0.70
17:3:156:THR:O	17:3:156:THR:HG23	1.90	0.70
18:4:111:LEU:HD12	18:4:112:PRO:HG3	1.74	0.70
1:A:27:ILE:O	1:A:28:LYS:HG3	1.92	0.70
1:A:86:LEU:CD1	1:A:178:MET:CE	2.69	0.70
2:B:244:PHE:HD2	2:B:244:PHE:O	1.75	0.70
2:B:615:TYR:HD1	2:B:615:TYR:N	1.89	0.70
19:B:1209:CLA:H61	19:B:1209:CLA:H11	1.73	0.70
19:B:1209:CLA:HMC1	21:B:6005:BCR:H373	1.72	0.70
4:D:100:TYR:HE1	4:D:134:LYS:CD	2.04	0.70
7:G:124:ILE:O	7:G:128:LEU:CB	2.39	0.70
13:N:131:PHE:C	13:N:132:THR:HG22	2.11	0.70
13:N:152:LEU:C	13:N:153:GLU:CG	2.57	0.70
16:2:183:PHE:N	16:2:187:LYS:CG	2.53	0.70
22:4:7053:LMU:H6E	22:4:7053:LMU:C1B	2.20	0.70
1:A:246:HIS:O	1:A:248:PHE:CD2	2.43	0.70
2:B:58:PHE:HB3	2:B:146:SER:HB3	1.73	0.70
2:B:334:LEU:HB2	19:B:1202:CLA:HMD3	1.71	0.70
2:B:469:LYS:CE	2:B:470:THR:HG23	2.21	0.70
19:B:1235:CLA:H121	21:F:6016:BCR:C31	2.21	0.70
4:D:113:GLU:O	4:D:114:MET:HB3	1.91	0.70
22:R:7021:LMU:H1'	22:R:7021:LMU:C3	2.20	0.70
16:2:154:ILE:CG1	16:2:155:VAL:N	2.53	0.70
1:A:346:LEU:C	1:A:346:LEU:HD23	2.11	0.70
19:A:1124:CLA:H2	19:A:1125:CLA:HED3	1.73	0.70
21:A:6008:BCR:H331	21:A:6008:BCR:C8	2.21	0.70
2:B:131:THR:C	2:B:135:LEU:HD23	2.12	0.70
2:B:188:LEU:CD1	19:B:1212:CLA:HBB2	2.20	0.70
2:B:232:LEU:HD11	2:B:235:GLN:HB2	1.72	0.70
2:B:256:THR:O	2:B:257:ILE:HD13	1.92	0.70
2:B:314:ARG:HH12	15:1:67:LEU:CD1	2.05	0.70
2:B:329:SER:OG	2:B:332:PHE:HB2	1.91	0.70
2:B:457:PRO:CB	2:B:517:PHE:HD1	2.04	0.70
5:E:79:LYS:HG3	5:E:84:TYR:OH	1.90	0.70
7:G:124:ILE:CG2	7:G:125:VAL:N	2.54	0.70
19:K:1142:CLA:HED2	19:K:1143:CLA:CMB	2.21	0.70
12:L:73:VAL:HG21	19:L:1130:CLA:OBD	1.90	0.70
12:L:91:THR:CA	12:L:98:ARG:HH12	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:120:VAL:O	13:N:120:VAL:CG1	2.40	0.70
13:N:139:LYS:HG3	13:N:142:LYS:CE	2.22	0.70
15:1:150:HIS:CG	15:1:151:GLN:NE2	2.60	0.70
17:3:148:TYR:N	17:3:149:ASN:CG	2.45	0.70
18:4:211:MET:CG	19:4:4002:CLA:HBB1	2.21	0.70
1:A:207:LEU:HB3	19:A:1119:CLA:CBB	2.22	0.70
1:A:236:GLY:C	1:A:237:VAL:HG22	2.12	0.70
1:A:430:ASP:H	1:A:433:ASP:CG	1.95	0.70
1:A:581:CYS:HB2	1:A:590:CYS:CA	2.18	0.70
2:B:5:ILE:HG22	2:B:6:PRO:N	2.05	0.70
19:B:1222:CLA:HHD	19:B:1222:CLA:CBC	2.16	0.70
21:B:6020:BCR:C33	19:L:1502:CLA:NB	2.48	0.70
4:D:95:GLN:HG3	4:D:96:VAL:N	2.06	0.70
5:E:83:TRP:CH2	5:E:116:SER:HB2	2.27	0.70
7:G:82:PHE:HB2	7:G:83:GLN:CG	2.21	0.70
10:J:4:LEU:O	10:J:5:LYS:HB2	1.89	0.70
11:K:78:ARG:HA	11:K:78:ARG:HE	1.52	0.70
19:R:1144:CLA:H2A	19:R:1144:CLA:O1A	1.92	0.70
16:2:229:MET:SD	16:2:229:MET:C	2.70	0.70
18:4:200:ALA:O	18:4:202:GLU:N	2.25	0.70
19:4:1004:CLA:HBC2	19:4:1004:CLA:CHD	2.16	0.70
1:A:244:LEU:HD13	1:A:247:GLU:OE2	1.92	0.70
1:A:564:ARG:NH2	1:A:564:ARG:CB	2.54	0.70
19:A:1112:CLA:HHC	21:A:6002:BCR:C17	2.22	0.70
19:A:1132:CLA:HBC3	19:A:1132:CLA:HMC1	1.73	0.70
19:B:1239:CLA:H192	9:I:21:MET:HB3	1.73	0.70
3:C:44:ARG:NH2	4:D:181:ARG:HG2	2.06	0.70
5:E:126:VAL:O	5:E:127:GLU:HB2	1.92	0.70
12:L:172:GLU:N	12:L:173:PRO:CD	2.40	0.70
13:N:157:LYS:HB3	13:N:158:ASP:HA	1.73	0.70
15:1:81:GLU:C	15:1:83:GLU:N	2.40	0.70
15:1:103:LEU:HD23	15:1:103:LEU:N	2.02	0.70
16:2:148:ASP:HB3	16:2:152:LEU:HG	1.71	0.70
19:3:2009:CLA:CHA	19:3:2009:CLA:CBA	2.70	0.70
18:4:173:LYS:HZ2	18:4:201:LYS:HG2	1.57	0.70
1:A:50:THR:HG22	1:A:52:THR:H	1.57	0.70
2:B:212:PHE:CZ	19:B:1211:CLA:HHD	2.26	0.70
2:B:551:LYS:O	2:B:552:ASP:CG	2.30	0.70
5:E:78:ARG:NH1	5:E:125:ILE:HB	2.07	0.70
6:F:138:LEU:CD2	6:F:146:PRO:HB3	2.22	0.70
11:K:115:ILE:HD13	11:K:122:LEU:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:182:ILE:HB	16:2:187:LYS:HG3	1.64	0.70
18:4:109:MET:O	18:4:111:LEU:N	2.25	0.70
18:4:153:GLU:OE2	19:4:4012:CLA:C4B	2.39	0.70
1:A:83:PHE:CE1	19:A:1111:CLA:CED	2.75	0.69
1:A:531:PRO:O	1:A:532:ILE:CG2	2.39	0.69
19:A:1115:CLA:H193	11:K:64:MET:HE3	1.71	0.69
19:A:1237:CLA:C6	19:A:1237:CLA:H112	2.20	0.69
19:B:1206:CLA:H41	21:I:6018:BCR:C23	2.21	0.69
4:D:145:ARG:HH12	4:D:173:TYR:HE1	1.38	0.69
5:E:82:TYR:CE1	5:E:111:ASN:HA	2.27	0.69
22:H:7011:LMU:O6'	22:H:7011:LMU:H4B	1.92	0.69
11:K:115:ILE:CG1	11:K:121:VAL:C	2.47	0.69
12:L:51:LYS:HB3	12:L:51:LYS:NZ	2.06	0.69
12:L:143:LEU:CD2	12:L:146:THR:HG22	2.15	0.69
19:L:1148:CLA:H2	19:L:1148:CLA:HED3	1.70	0.69
13:N:155:GLU:CB	13:N:157:LYS:N	2.17	0.69
15:1:112:GLN:HG2	15:1:113:GLU:N	2.03	0.69
17:3:187:PHE:CD1	17:3:188:LEU:N	2.60	0.69
18:4:142:PHE:CD1	19:4:4010:CLA:C3C	2.75	0.69
22:4:7034:LMU:C8	22:4:7052:LMU:H1'	2.14	0.69
1:A:105:ASN:HB2	1:A:119:SER:O	1.93	0.69
1:A:370:ILE:HG22	1:A:400:MET:CA	2.21	0.69
19:A:1101:CLA:C4	19:A:1140:CLA:H61	2.07	0.69
2:B:229:GLN:OE1	2:B:229:GLN:HA	1.92	0.69
3:C:67:VAL:HG22	3:C:67:VAL:O	1.90	0.69
10:J:5:LYS:HD2	16:2:178:ASN:CG	2.12	0.69
19:K:3009:CLA:C9	19:3:3007:CLA:HAC2	2.23	0.69
15:1:98:LEU:O	15:1:98:LEU:HD13	1.92	0.69
19:1:1014:CLA:HHD	19:1:1014:CLA:CBC	2.12	0.69
16:2:113:ALA:CB	16:2:114:MET:HE3	2.21	0.69
17:3:150:TYR:HB3	17:3:151:TRP:HE1	1.56	0.69
19:3:3008:CLA:CB	19:3:3008:CLA:CBA	2.65	0.69
18:4:120:ILE:HG22	18:4:121:ILE:HG23	1.74	0.69
18:4:188:ILE:HG22	18:4:189:PHE:N	2.05	0.69
19:A:1105:CLA:HAA2	19:A:1107:CLA:CED	2.22	0.69
19:A:1106:CLA:HBB2	19:A:1107:CLA:C4D	2.23	0.69
19:A:1119:CLA:HBA1	19:A:1123:CLA:HBB2	1.74	0.69
19:A:1122:CLA:CAB	21:A:6007:BCR:H351	2.22	0.69
2:B:187:SER:O	2:B:189:ALA:N	2.25	0.69
4:D:80:SER:HG	4:D:126:PRO:CD	1.94	0.69
6:F:207:LEU:HD22	6:F:208:PHE:CB	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:64:ILE:HG13	7:G:68:THR:CG2	2.22	0.69
12:L:131:SER:N	12:L:201:TYR:CD2	2.59	0.69
13:N:124:SER:O	13:N:125:CYS:HB2	1.91	0.69
13:N:156:GLY:CA	13:N:157:LYS:HD2	2.22	0.69
15:1:201:PHE:CD1	15:1:204:GLN:NE2	2.59	0.69
19:1:1014:CLA:C10	19:1:1014:CLA:C5	2.58	0.69
19:1:1303:CLA:HBA2	19:1:1303:CLA:HMA3	1.74	0.69
16:2:243:GLY:CA	16:2:244:THR:HG23	2.22	0.69
1:A:472:ARG:HH22	12:L:120:LEU:CD1	2.04	0.69
19:A:1237:CLA:HMB2	19:L:1502:CLA:HBC1	1.73	0.69
2:B:118:SER:HB2	19:B:1205:CLA:OBD	1.92	0.69
2:B:373:THR:HA	2:B:376:GLN:HB2	1.73	0.69
2:B:438:VAL:HG22	19:B:1230:CLA:CMC	2.21	0.69
6:F:193:GLN:HA	6:F:195:GLU:OE1	1.92	0.69
7:G:116:SER:CA	7:G:119:PRO:HG2	2.21	0.69
12:L:137:LEU:HD23	12:L:137:LEU:O	1.91	0.69
13:N:89:GLU:OE1	13:N:89:GLU:O	2.11	0.69
15:1:67:LEU:HD12	15:1:67:LEU:C	2.12	0.69
15:1:157:ASP:CB	15:1:178:LYS:CA	2.50	0.69
17:3:93:ILE:O	17:3:93:ILE:HG23	1.92	0.69
17:3:98:LEU:HD21	19:3:3012:CLA:C2D	2.22	0.69
17:3:233:LEU:HA	17:3:236:LEU:HB3	1.73	0.69
22:3:7005:LMU:H3'	22:3:7005:LMU:O2B	1.91	0.69
1:A:74:ILE:O	1:A:77:LYS:N	2.22	0.69
1:A:351:THR:O	19:A:1123:CLA:C20	2.41	0.69
1:A:690:LEU:HD23	1:A:693:LEU:HD12	1.74	0.69
2:B:44:GLN:OE1	2:B:163:PRO:HB2	1.91	0.69
2:B:224:PRO:O	2:B:226:LEU:N	2.25	0.69
2:B:508:LEU:HB3	2:B:509:PHE:CD2	2.28	0.69
2:B:527:LEU:CD1	19:B:1236:CLA:HMA3	2.22	0.69
3:C:14:CYS:C	3:C:17:CYS:SG	2.69	0.69
7:G:76:ARG:NH2	7:G:117:ASN:HA	2.07	0.69
7:G:77:PHE:O	7:G:79:PHE:HB3	1.92	0.69
11:K:114:HIS:O	11:K:115:ILE:C	2.31	0.69
12:L:168:GLY:O	12:L:170:LYS:N	2.25	0.69
12:L:172:GLU:O	12:L:174:ASP:O	2.10	0.69
12:L:205:TYR:CE1	12:L:207:LEU:CD1	2.75	0.69
14:R:51:UNK:O	14:R:52:UNK:CB	2.41	0.69
15:1:65:ASP:OD2	15:1:66:PRO:CA	2.40	0.69
15:1:97:ILE:HD12	15:1:98:LEU:HB2	1.73	0.69
15:1:147:PHE:O	15:1:150:HIS:HB3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:192:LYS:HA	17:3:192:LYS:NZ	2.06	0.69
1:A:73:GLU:CG	1:A:74:ILE:N	2.55	0.69
1:A:281:LEU:HD13	19:A:1115:CLA:O2D	1.89	0.69
19:A:1134:CLA:CMA	19:A:1141:CLA:HBB2	2.22	0.69
19:A:9012:CLA:H12	2:B:616:LEU:HD13	1.73	0.69
6:F:170:ILE:O	6:F:173:TRP:CD1	2.44	0.69
7:G:90:GLN:CB	7:G:91:VAL:O	2.38	0.69
8:H:114:ALA:O	8:H:115:THR:CG2	2.40	0.69
10:J:42:PHE:HD1	18:4:244:ILE:HG21	1.58	0.69
19:J:1308:CLA:HBA2	19:J:1308:CLA:CBD	2.14	0.69
11:K:125:LYS:HB2	11:K:128:GLY:H	1.57	0.69
12:L:54:TYR:HE1	12:L:57:ILE:HG23	1.58	0.69
12:L:155:GLU:HA	12:L:178:THR:HG22	1.74	0.69
15:1:170:PRO:CD	15:1:173:TYR:HE2	2.05	0.69
16:2:94:SER:O	16:2:95:ASP:HB2	1.90	0.69
1:A:173:VAL:HG23	1:A:174:PHE:HD1	1.57	0.69
1:A:217:SER:OG	21:A:6002:BCR:H17C	1.92	0.69
19:A:1112:CLA:HED2	19:A:1112:CLA:H2A	1.74	0.69
19:A:1123:CLA:OBD	19:A:1123:CLA:H112	1.93	0.69
19:A:9023:CLA:H3A	19:A:9023:CLA:CGA	2.22	0.69
2:B:21:ILE:HD11	19:B:1238:CLA:HMA1	1.74	0.69
2:B:87:ILE:N	2:B:87:ILE:CD1	2.55	0.69
2:B:308:HIS:CG	2:B:309:ILE:N	2.61	0.69
19:B:1211:CLA:HMB3	21:B:6006:BCR:H311	1.73	0.69
6:F:103:GLN:O	6:F:104:ALA:C	2.30	0.69
6:F:138:LEU:O	6:F:140:CYS:SG	2.48	0.69
22:G:7039:LMU:H6'2	22:G:7039:LMU:H3'	1.74	0.69
12:L:204:LEU:HD13	12:L:205:TYR:N	2.08	0.69
13:N:99:LYS:CA	13:N:102:ASN:OD1	2.33	0.69
19:1:1013:CLA:CAD	19:1:1013:CLA:HED2	2.22	0.69
17:3:91:GLY:O	17:3:93:ILE:N	2.25	0.69
17:3:243:ILE:HD11	19:3:3005:CLA:C1C	2.20	0.69
18:4:145:GLU:CG	18:4:146:PHE:CD1	2.58	0.69
18:4:207:ASN:HD21	19:4:4002:CLA:C1A	2.06	0.69
1:A:49:ASP:HB2	1:A:720:THR:HA	1.75	0.69
1:A:491:TRP:NE1	19:A:1135:CLA:C1	2.50	0.69
1:A:684:PHE:C	1:A:684:PHE:HD2	1.95	0.69
21:A:6011:BCR:C31	21:A:6011:BCR:C8	2.70	0.69
2:B:53:GLN:HE22	19:B:1201:CLA:HBB1	1.53	0.69
2:B:141:PHE:HA	2:B:144:PHE:CD1	2.28	0.69
2:B:315:LEU:CD1	2:B:315:LEU:C	2.54	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:625:TRP:CE3	2:B:626:LEU:N	2.60	0.69
4:D:82:ILE:CG2	4:D:121:ILE:O	2.40	0.69
4:D:140:LEU:CD1	4:D:140:LEU:C	2.32	0.69
19:F:1302:CLA:HBC2	19:F:1302:CLA:HHD	1.75	0.69
7:G:87:VAL:O	7:G:88:ALA:HB3	1.92	0.69
7:G:136:VAL:O	7:G:137:VAL:C	2.28	0.69
8:H:115:THR:O	8:H:116:ALA:HB3	1.90	0.69
22:H:7011:LMU:H2B	22:H:7011:LMU:C6'	2.22	0.69
15:1:206:SER:O	15:1:209:PRO:HD3	1.92	0.69
15:1:217:LEU:HD23	15:1:218:ALA:HA	1.74	0.69
16:2:95:ASP:HB3	17:3:85:ASP:OD2	1.82	0.69
16:2:158:VAL:CG2	16:2:159:PHE:N	2.54	0.69
17:3:159:VAL:CG1	17:3:160:LEU:H	2.05	0.69
17:3:191:GLU:O	17:3:192:LYS:HE2	1.91	0.69
1:A:575:LEU:CD1	1:A:576:GLY:CA	2.57	0.69
19:A:9022:CLA:H151	21:B:6017:BCR:C19	2.22	0.69
2:B:127:ILE:O	2:B:127:ILE:HG13	1.93	0.69
19:B:1223:CLA:H41	19:B:1223:CLA:H72	1.74	0.69
3:C:10:THR:CG2	5:E:101:TYR:CD2	2.71	0.69
4:D:80:SER:CB	4:D:127:ASN:H	2.06	0.69
7:G:89:LYS:NZ	7:G:89:LYS:N	2.41	0.69
14:R:34:UNK:C	14:R:38:UNK:CB	2.71	0.69
15:1:170:PRO:O	15:1:173:TYR:HE2	1.73	0.69
19:1:1013:CLA:HAA2	19:1:1013:CLA:CGD	2.22	0.69
16:2:172:LEU:C	16:2:173:ASN:HD22	1.95	0.69
16:2:215:LYS:O	16:2:215:LYS:HG2	1.92	0.69
22:3:7005:LMU:H32	22:3:7005:LMU:H1'	1.73	0.69
1:A:209:GLY:CA	1:A:213:LEU:HD13	2.23	0.69
1:A:336:GLY:CA	19:A:1151:CLA:CMC	2.71	0.69
1:A:443:ILE:HG21	1:A:558:LYS:HB2	1.75	0.69
1:A:453:LEU:HD13	1:A:547:PHE:HA	1.73	0.69
1:A:740:LEU:HD21	19:A:1140:CLA:HMA3	1.73	0.69
19:A:1115:CLA:H2A	19:A:1115:CLA:HED3	0.74	0.69
3:C:44:ARG:HE	4:D:182:GLN:NE2	1.90	0.69
10:J:31:ARG:HA	10:J:34:PRO:HA	1.75	0.69
12:L:82:TYR:O	12:L:82:TYR:CG	2.46	0.69
15:1:84:LEU:O	15:1:88:ARG:CG	2.38	0.69
15:1:84:LEU:C	15:1:88:ARG:HG3	2.14	0.69
15:1:178:LYS:CG	15:1:179:LYS:N	2.55	0.69
16:2:131:ILE:O	16:2:131:ILE:CG2	2.41	0.69
19:2:2014:CLA:H152	19:2:2014:CLA:H91	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:3011:CLA:HBC1	19:3:3012:CLA:CHA	2.22	0.69
18:4:153:GLU:OE2	19:4:4012:CLA:CHC	2.41	0.69
20:A:5001:PQN:H241	20:A:5001:PQN:H272	1.76	0.68
2:B:262:HIS:ND1	2:B:265:THR:OG1	2.26	0.68
2:B:530:THR:HG21	19:B:1222:CLA:HAC1	1.74	0.68
2:B:535:VAL:O	2:B:539:LEU:CD2	2.41	0.68
2:B:545:LYS:CD	2:B:546:LEU:N	2.50	0.68
2:B:654:HIS:CE1	19:B:9010:CLA:NB	2.60	0.68
3:C:55:GLU:C	3:C:57:ALA:H	1.96	0.68
8:H:119:ASP:CB	8:H:121:LEU:HG	2.22	0.68
12:L:164:LEU:C	12:L:165:THR:CG2	2.61	0.68
15:1:66:PRO:CD	15:1:67:LEU:N	2.56	0.68
17:3:93:ILE:CD1	17:3:95:PRO:O	2.41	0.68
17:3:104:ILE:HG21	19:3:3004:CLA:ND	2.08	0.68
1:A:103:PHE:CE1	19:A:1105:CLA:O1D	2.43	0.68
1:A:120:ALA:N	1:A:145:ILE:HD12	1.97	0.68
1:A:220:ARG:O	1:A:221:HIS:HB2	1.92	0.68
1:A:453:LEU:CD2	19:A:1136:CLA:CBB	2.71	0.68
2:B:90:ALA:N	2:B:113:VAL:CG1	2.55	0.68
6:F:105:SER:O	6:F:106:LEU:C	2.31	0.68
11:K:127:ILE:HA	11:K:130:LEU:CD1	2.23	0.68
12:L:112:GLY:N	12:L:113:PRO:HD2	2.08	0.68
12:L:198:ILE:O	12:L:202:PHE:N	2.21	0.68
13:N:157:LYS:CG	13:N:159:LYS:H	2.07	0.68
15:1:95:PRO:C	15:1:98:LEU:CB	2.60	0.68
15:1:158:PRO:HA	15:1:175:LYS:CG	2.21	0.68
15:1:162:LYS:HG2	15:1:163:TYR:H	1.59	0.68
16:2:182:ILE:O	16:2:183:PHE:CD1	2.46	0.68
22:4:7033:LMU:H3'	22:4:7033:LMU:C6B	2.23	0.68
1:A:258:LEU:O	1:A:259:TYR:CB	2.42	0.68
1:A:508:THR:O	1:A:509:ALA:HB2	1.90	0.68
2:B:620:LEU:HD12	2:B:624:LEU:HD21	1.74	0.68
6:F:160:PHE:O	6:F:164:GLY:CA	2.40	0.68
8:H:98:LEU:HD21	12:L:143:LEU:CD2	2.24	0.68
12:L:190:PHE:CZ	12:L:194:ILE:CD1	2.77	0.68
15:1:135:PRO:HD2	15:1:136:THR:H	1.59	0.68
15:1:171:LEU:HA	15:1:173:TYR:CD2	2.26	0.68
16:2:226:ARG:HD3	16:2:230:LEU:CD2	2.23	0.68
17:3:109:ALA:CA	17:3:111:LEU:HD22	2.23	0.68
22:3:7005:LMU:H32	22:3:7005:LMU:C1'	2.22	0.68
18:4:121:ILE:HG13	18:4:122:ASN:N	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:146:PHE:CE1	19:4:4013:CLA:C1C	2.77	0.68
1:A:217:SER:OG	21:A:6002:BCR:C16	2.40	0.68
1:A:249:ILE:N	17:3:137:PHE:HZ	1.91	0.68
1:A:668:TYR:CB	2:B:445:ALA:HB2	2.23	0.68
19:A:1133:CLA:C3D	19:A:1134:CLA:HAC1	2.22	0.68
21:A:6011:BCR:H313	19:A:9013:CLA:H143	1.74	0.68
2:B:314:ARG:HH12	15:1:67:LEU:HD11	1.59	0.68
2:B:469:LYS:NZ	2:B:471:THR:O	2.27	0.68
5:E:103:VAL:CG1	5:E:120:TYR:O	2.42	0.68
7:G:64:ILE:HG13	7:G:68:THR:HG23	1.74	0.68
11:K:55:LEU:O	11:K:58:VAL:HG12	1.94	0.68
13:N:139:LYS:CA	13:N:142:LYS:NZ	2.51	0.68
13:N:147:SER:CA	13:N:149:ASP:HB2	2.23	0.68
17:3:206:PRO:HG2	17:3:208:PHE:CZ	2.28	0.68
1:A:57:LEU:HD23	1:A:58:HIS:N	2.08	0.68
2:B:475:ASP:CA	2:B:480:SER:HA	2.23	0.68
19:B:1209:CLA:CMC	21:B:6005:BCR:H373	2.24	0.68
19:B:1215:CLA:CGA	19:B:1215:CLA:H3A	2.23	0.68
4:D:124:GLU:OE1	4:D:125:GLY:CA	2.41	0.68
8:H:114:ALA:O	8:H:115:THR:HG23	1.93	0.68
9:I:11:LEU:HG	21:I:6021:BCR:C7	2.23	0.68
11:K:47:ASP:OD2	11:K:48:PHE:N	2.27	0.68
12:L:161:ALA:N	12:L:162:PRO:HD2	2.07	0.68
13:N:139:LYS:CG	13:N:142:LYS:CE	2.71	0.68
15:1:170:PRO:C	15:1:171:LEU:HD23	2.14	0.68
16:2:131:ILE:O	16:2:132:LEU:CD1	2.41	0.68
16:2:171:ILE:HD11	16:2:173:ASN:HD21	1.59	0.68
16:2:184:PRO:HD2	16:2:185:ASN:O	1.93	0.68
16:2:240:ILE:HG22	16:2:263:PHE:HB3	1.72	0.68
18:4:154:ILE:O	18:4:158:GLN:HG2	1.93	0.68
1:A:193:LEU:CA	1:A:196:PHE:HE2	2.03	0.68
2:B:22:TRP:NE1	19:B:1238:CLA:CBB	2.47	0.68
2:B:247:THR:C	2:B:250:ALA:H	1.96	0.68
2:B:454:LEU:HD12	2:B:454:LEU:C	2.13	0.68
2:B:633:ASN:OD1	2:B:633:ASN:O	2.11	0.68
3:C:17:CYS:CB	3:C:58:CYS:SG	2.74	0.68
3:C:66:ARG:CG	3:C:66:ARG:NH2	2.49	0.68
16:2:167:ARG:HE	16:2:168:TRP:N	1.90	0.68
16:2:182:ILE:O	16:2:183:PHE:CG	2.47	0.68
17:3:154:ASN:O	17:3:155:TYR:CG	2.46	0.68
19:3:3017:CLA:HBC3	19:3:3017:CLA:HMC1	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:145:GLU:CG	18:4:146:PHE:HD1	2.03	0.68
1:A:110:LEU:O	1:A:113:PRO:HD3	1.94	0.68
22:A:7016:LMU:O6'	22:A:7016:LMU:H51	1.94	0.68
2:B:266:GLN:O	2:B:267:SER:CB	2.41	0.68
2:B:666:SER:HB3	2:B:671:TRP:NE1	2.05	0.68
19:B:1226:CLA:H62	24:B:7101:LMG:H182	1.75	0.68
3:C:52:LYS:NZ	3:C:64:SER:HB3	2.08	0.68
6:F:200:VAL:CG1	10:J:7:TYR:CA	2.71	0.68
22:H:7011:LMU:O6'	22:H:7011:LMU:H1B	1.93	0.68
11:K:79:LYS:O	11:K:80:ALA:HB3	1.91	0.68
18:4:202:GLU:O	18:4:205:ILE:CG1	2.40	0.68
1:A:281:LEU:CD1	1:A:282:THR:H	2.07	0.68
1:A:464:ASN:HD22	1:A:464:ASN:H	1.41	0.68
19:A:1125:CLA:H143	19:A:1125:CLA:H101	1.74	0.68
22:A:7023:LMU:H91	22:A:7023:LMU:C2	2.24	0.68
2:B:82:PHE:O	2:B:84:VAL:N	2.22	0.68
2:B:98:GLN:O	2:B:100:ALA:CA	2.42	0.68
2:B:444:LEU:CD2	2:B:452:GLN:NE2	2.56	0.68
3:C:12:ILE:HG22	3:C:38:GLN:O	1.93	0.68
3:C:44:ARG:NH2	4:D:181:ARG:CB	2.56	0.68
6:F:92:ALA:O	6:F:95:GLU:HB2	1.94	0.68
7:G:86:ASN:O	7:G:89:LYS:NZ	2.26	0.68
8:H:89:ALA:O	8:H:92:THR:N	2.27	0.68
12:L:68:SER:O	12:L:69:LEU:C	2.30	0.68
12:L:69:LEU:O	12:L:71:THR:HG23	1.94	0.68
18:4:194:PHE:O	18:4:195:ALA:HB3	1.91	0.68
1:A:63:ASP:HA	19:A:1128:CLA:HED2	1.76	0.68
1:A:490:GLN:HG3	1:A:490:GLN:O	1.93	0.68
1:A:728:VAL:HG22	1:A:731:ARG:NH1	2.09	0.68
19:A:1129:CLA:HMB2	19:L:1130:CLA:C1D	2.23	0.68
2:B:57:ILE:HD13	21:B:6005:BCR:H321	1.76	0.68
2:B:190:TRP:HE3	19:B:1211:CLA:CBB	2.06	0.68
3:C:43:PRO:HD2	3:C:43:PRO:O	1.94	0.68
5:E:111:ASN:ND2	5:E:111:ASN:C	2.46	0.68
12:L:150:ILE:HD12	12:L:151:SER:N	2.08	0.68
15:1:142:PHE:HA	15:1:145:ILE:HD12	1.74	0.68
15:1:177:PRO:HG2	15:1:180:LEU:N	2.09	0.68
16:2:183:PHE:C	16:2:185:ASN:HA	2.14	0.68
16:2:184:PRO:N	16:2:187:LYS:HG2	2.09	0.68
16:2:263:PHE:CG	16:2:263:PHE:O	2.47	0.68
19:2:2014:CLA:H152	19:2:2014:CLA:C9	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:215:LYS:HB2	17:3:216:ASP:HA	1.75	0.68
1:A:545:HIS:CG	19:A:1135:CLA:CBB	2.69	0.68
1:A:628:ILE:HD12	1:A:629:ASN:N	2.09	0.68
19:A:1126:CLA:H102	21:A:6011:BCR:H372	1.76	0.68
2:B:476:ILE:HG23	2:B:476:ILE:O	1.93	0.68
5:E:78:ARG:HH12	5:E:125:ILE:CB	2.07	0.68
7:G:76:ARG:NH1	7:G:120:VAL:HB	2.08	0.68
15:1:73:PRO:CD	15:1:74:ALA:H	2.07	0.68
15:1:140:ILE:HD13	15:1:140:ILE:N	2.09	0.68
18:4:141:LEU:HD22	18:4:141:LEU:N	2.01	0.68
1:A:75:SER:HB3	1:A:354:TRP:CZ2	2.29	0.67
1:A:445:HIS:O	1:A:446:LEU:CB	2.42	0.67
1:A:553:VAL:H	1:A:556:LEU:HD12	1.59	0.67
1:A:555:ILE:CD1	19:A:9023:CLA:CMD	2.71	0.67
2:B:104:PHE:O	2:B:105:THR:OG1	2.09	0.67
19:B:1203:CLA:H71	24:B:7101:LMG:H381	1.76	0.67
22:D:7050:LMU:O2B	22:D:7050:LMU:H5B	1.92	0.67
15:1:137:ILE:CG2	19:1:1013:CLA:HBB2	2.22	0.67
16:2:122:ILE:O	16:2:126:LEU:CG	2.40	0.67
16:2:166:ARG:CA	16:2:167:ARG:CB	2.70	0.67
16:2:167:ARG:HA	16:2:167:ARG:HE	1.55	0.67
16:2:174:PRO:HD2	16:2:189:THR:OG1	1.94	0.67
16:2:184:PRO:HD3	16:2:187:LYS:HD2	1.75	0.67
18:4:100:ARG:O	18:4:104:LEU:CD1	2.42	0.67
18:4:172:PHE:O	18:4:173:LYS:HB2	1.94	0.67
18:4:198:LEU:HG	18:4:199:GLU:H	1.58	0.67
18:4:214:PHE:O	18:4:215:LEU:C	2.29	0.67
1:A:21:LEU:N	1:A:22:VAL:CB	2.57	0.67
1:A:249:ILE:CG1	1:A:250:LEU:N	2.52	0.67
1:A:304:LEU:HG	19:A:1115:CLA:CAB	2.24	0.67
1:A:684:PHE:HD2	1:A:685:VAL:N	1.93	0.67
2:B:69:ALA:CB	2:B:135:LEU:CD1	2.71	0.67
2:B:310:PRO:HG2	2:B:311:PRO:HD3	1.75	0.67
19:B:1202:CLA:H151	19:B:1202:CLA:OBD	1.94	0.67
5:E:101:TYR:HA	5:E:121:ALA:HB2	1.76	0.67
13:N:99:LYS:HB3	13:N:102:ASN:ND2	2.09	0.67
14:R:26:UNK:O	14:R:27:UNK:C	2.42	0.67
15:1:145:ILE:HA	15:1:148:VAL:HG12	1.76	0.67
16:2:164:GLU:OE2	19:2:2012:CLA:NB	2.26	0.67
18:4:124:PRO:HB2	18:4:126:TRP:N	2.07	0.67
18:4:173:LYS:CA	18:4:194:PHE:HD2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:THR:O	1:A:720:THR:HG22	1.95	0.67
19:A:1126:CLA:H111	21:J:6012:BCR:H353	1.74	0.67
2:B:176:ASN:ND2	2:B:291:TYR:O	2.27	0.67
2:B:294:ASN:HD21	7:G:94:GLN:HA	1.57	0.67
2:B:424:TRP:CZ2	19:B:1228:CLA:HAC1	2.29	0.67
2:B:501:ILE:HG13	2:B:502:ASN:N	2.09	0.67
21:B:6020:BCR:H23C	21:B:6020:BCR:H383	1.75	0.67
4:D:114:MET:HG3	4:D:115:PRO:CA	2.23	0.67
5:E:122:LEU:O	5:E:125:ILE:N	2.28	0.67
22:H:7011:LMU:C7	22:H:7011:LMU:H111	2.23	0.67
9:I:12:VAL:O	9:I:17:PRO:CD	2.41	0.67
19:J:1308:CLA:H92	19:2:2014:CLA:O2D	1.93	0.67
11:K:127:ILE:O	11:K:129:ALA:HA	1.94	0.67
12:L:92:ALA:H	12:L:98:ARG:HH12	1.22	0.67
13:N:139:LYS:CE	13:N:142:LYS:NZ	2.57	0.67
22:N:7049:LMU:C1	22:N:7049:LMU:C6	2.71	0.67
15:1:129:VAL:CB	15:1:130:PRO:HD3	2.24	0.67
15:1:225:TRP:HB3	15:1:226:HIS:HA	1.73	0.67
17:3:238:ILE:HA	17:3:241:TYR:CE1	2.30	0.67
1:A:408:VAL:HG21	1:A:602:LEU:HG	1.76	0.67
1:A:536:THR:HA	1:A:539:PHE:HB2	1.76	0.67
19:A:1115:CLA:H193	11:K:64:MET:HE1	1.76	0.67
2:B:85:ARG:HH11	2:B:85:ARG:CG	2.05	0.67
2:B:233:TYR:O	2:B:253:ALA:HB1	1.94	0.67
2:B:459:PHE:CZ	19:B:1235:CLA:HMD2	2.29	0.67
4:D:95:GLN:CD	4:D:95:GLN:C	2.52	0.67
4:D:102:ILE:O	4:D:102:ILE:HG23	1.93	0.67
5:E:107:PHE:CD2	5:E:109:LYS:HE3	2.28	0.67
15:1:68:GLY:O	15:1:72:VAL:CB	2.40	0.67
15:1:151:GLN:NE2	15:1:151:GLN:CA	2.57	0.67
15:1:201:PHE:O	15:1:204:GLN:HB2	1.95	0.67
16:2:100:ARG:O	16:2:102:ASN:N	2.26	0.67
16:2:226:ARG:HH11	16:2:226:ARG:CG	2.08	0.67
18:4:121:ILE:CG1	18:4:122:ASN:N	2.57	0.67
22:4:7053:LMU:H1B	22:4:7053:LMU:C6'	2.17	0.67
1:A:207:LEU:HA	1:A:211:LEU:CG	2.25	0.67
1:A:251:ASN:OD1	17:3:137:PHE:HD1	1.55	0.67
1:A:304:LEU:CG	19:A:1115:CLA:CBB	2.72	0.67
1:A:373:ALA:O	1:A:396:PHE:CD1	2.48	0.67
2:B:411:MET:CE	19:B:1220:CLA:CMC	2.72	0.67
6:F:103:GLN:CD	6:F:104:ALA:N	2.47	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:GLN:OE1	6:F:103:GLN:CA	2.42	0.67
6:F:170:ILE:HG22	21:F:6014:BCR:H372	1.76	0.67
7:G:62:LEU:O	7:G:65:SER:HB3	1.94	0.67
11:K:56:ILE:HA	11:K:59:THR:HG23	1.76	0.67
14:R:26:UNK:O	14:R:28:UNK:N	2.27	0.67
15:1:73:PRO:CG	15:1:74:ALA:H	2.07	0.67
15:1:93:ALA:CB	19:1:1006:CLA:HHC	2.09	0.67
21:1:6023:BCR:C8	21:1:6023:BCR:HC21	2.23	0.67
16:2:211:PRO:O	16:2:212:GLN:CB	2.41	0.67
22:2:7027:LMU:O2'	22:2:7027:LMU:H12	1.95	0.67
19:3:2009:CLA:HBD	19:3:2009:CLA:CBA	2.22	0.67
2:B:292:ARG:NH2	2:B:297:ILE:HG13	2.10	0.67
2:B:324:ASP:O	2:B:328:ASN:HB2	1.94	0.67
2:B:414:HIS:CD2	19:B:1227:CLA:HMA3	2.30	0.67
2:B:542:ARG:HH21	4:D:197:PRO:HG3	1.59	0.67
19:B:1223:CLA:H71	21:B:6010:BCR:H14C	1.76	0.67
7:G:114:LEU:HD12	7:G:115:LYS:N	2.09	0.67
8:H:113:SER:OG	19:H:1207:CLA:H52	1.92	0.67
15:1:85:ILE:CG1	15:1:88:ARG:CZ	2.69	0.67
16:2:103:VAL:HG12	16:2:104:GLN:OE1	1.94	0.67
19:2:2001:CLA:HMC1	19:2:2001:CLA:HBC2	1.74	0.67
18:4:175:TYR:HB2	18:4:195:ALA:N	2.09	0.67
19:4:4015:CLA:HBA1	19:4:4015:CLA:CBD	2.25	0.67
1:A:87:SER:O	1:A:88:ILE:HB	1.94	0.67
1:A:193:LEU:O	1:A:196:PHE:CD2	2.48	0.67
1:A:207:LEU:HB3	19:A:1119:CLA:HBB2	1.76	0.67
22:A:7016:LMU:C2	22:A:7016:LMU:C6	2.72	0.67
2:B:29:HIS:CD2	19:B:1202:CLA:CBB	2.77	0.67
2:B:73:ASN:H	2:B:73:ASN:ND2	1.90	0.67
2:B:299:HIS:HE1	19:B:1219:CLA:HMD1	1.58	0.67
2:B:594:TRP:CD1	2:B:594:TRP:C	2.68	0.67
4:D:103:THR:CG2	4:D:128:LEU:HD12	2.23	0.67
5:E:83:TRP:HH2	5:E:116:SER:CB	2.07	0.67
7:G:68:THR:HB	7:G:128:LEU:HG	1.77	0.67
15:1:199:VAL:CG1	15:1:200:GLY:N	2.56	0.67
17:3:96:ARG:N	17:3:99:ALA:H	1.93	0.67
18:4:83:GLU:HB3	18:4:84:ASP:OD1	1.94	0.67
18:4:205:ILE:HD12	19:4:4004:CLA:CHA	2.25	0.67
1:A:102:ARG:C	1:A:103:PHE:CD2	2.62	0.67
1:A:224:HIS:O	1:A:225:VAL:HG22	1.95	0.67
1:A:246:HIS:C	1:A:248:PHE:CD2	2.68	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:PHE:C	1:A:284:ARG:HH11	1.98	0.67
1:A:334:HIS:ND1	1:A:334:HIS:N	2.41	0.67
1:A:503:THR:HB	19:A:1134:CLA:HBA1	1.75	0.67
2:B:292:ARG:NH1	2:B:296:GLY:N	2.41	0.67
2:B:318:GLY:O	2:B:407:VAL:HG13	1.95	0.67
2:B:438:VAL:CG2	19:B:1230:CLA:HMC1	2.24	0.67
2:B:606:VAL:O	2:B:607:SER:C	2.33	0.67
11:K:49:ILE:C	11:K:52:PRO:HD3	2.15	0.67
19:1:1008:CLA:CGD	19:1:1008:CLA:HAA2	2.25	0.67
18:4:159:ASP:CG	18:4:171:ILE:CD1	2.55	0.67
1:A:40:PHE:N	1:A:44:ILE:HG23	2.10	0.67
1:A:127:VAL:CG2	1:A:128:GLY:H	2.03	0.67
2:B:273:VAL:O	2:B:277:HIS:HD2	1.78	0.67
19:B:1231:CLA:HMD2	19:B:1232:CLA:C1C	2.24	0.67
19:B:1235:CLA:CBC	6:F:160:PHE:CZ	2.77	0.67
5:E:125:ILE:O	5:E:125:ILE:CG1	2.30	0.67
5:E:127:GLU:C	5:E:128:VAL:HG23	2.15	0.67
12:L:110:LEU:HA	12:L:113:PRO:CG	2.25	0.67
13:N:139:LYS:CD	13:N:142:LYS:NZ	2.55	0.67
15:1:182:GLU:O	15:1:183:LEU:HB2	1.93	0.67
19:1:1007:CLA:H122	19:1:1007:CLA:H61	1.77	0.67
16:2:126:LEU:O	16:2:128:LYS:N	2.27	0.67
17:3:191:GLU:O	17:3:192:LYS:HD2	1.95	0.67
18:4:167:ASN:HD21	19:4:4014:CLA:C2	2.08	0.67
1:A:79:PHE:CE1	19:A:1111:CLA:CED	2.78	0.67
2:B:92:TRP:O	2:B:92:TRP:CD1	2.48	0.67
2:B:270:LEU:HD12	2:B:270:LEU:C	2.15	0.67
2:B:353:TYR:HB2	2:B:594:TRP:HH2	1.60	0.67
19:B:1222:CLA:CBB	19:B:1236:CLA:CMB	2.73	0.67
19:B:1226:CLA:HMC1	19:B:1226:CLA:HBC3	1.74	0.67
3:C:52:LYS:CE	3:C:64:SER:HB3	2.24	0.67
4:D:102:ILE:O	4:D:102:ILE:CG2	2.43	0.67
4:D:146:SER:C	4:D:147:LYS:HG3	2.12	0.67
7:G:139:TYR:CG	7:G:139:TYR:O	2.45	0.67
8:H:108:THR:O	8:H:109:LEU:C	2.29	0.67
19:H:1145:CLA:C2	19:H:1145:CLA:CMA	2.71	0.67
19:H:1207:CLA:CHD	21:I:6018:BCR:H342	2.25	0.67
13:N:139:LYS:O	13:N:142:LYS:CD	2.43	0.67
13:N:143:VAL:HG12	13:N:144:PRO:HD3	1.77	0.67
16:2:107:LEU:HD12	16:2:107:LEU:C	2.15	0.67
16:2:212:GLN:HG2	16:2:213:LYS:N	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:226:ARG:CD	16:2:230:LEU:HD22	2.25	0.67
17:3:154:ASN:HA	17:3:155:TYR:CE2	2.29	0.67
18:4:122:ASN:C	18:4:124:PRO:HD3	2.15	0.67
18:4:220:GLN:CD	19:4:1306:CLA:HAC2	2.14	0.67
1:A:64:PHE:CD2	1:A:74:ILE:HD13	2.30	0.66
1:A:214:GLY:O	1:A:215:SER:HB3	1.94	0.66
1:A:458:PHE:CD2	19:A:9022:CLA:HMB2	2.29	0.66
1:A:577:PHE:O	1:A:593:SER:OG	2.13	0.66
1:A:711:HIS:NE2	19:A:1139:CLA:HAC1	2.10	0.66
2:B:75:GLU:HB2	2:B:132:ASN:HB3	1.76	0.66
2:B:638:LEU:O	2:B:639:VAL:CG1	2.40	0.66
8:H:58:LEU:CB	8:H:61:THR:HG21	2.08	0.66
8:H:61:THR:CA	8:H:62:THR:CG2	2.24	0.66
11:K:112:VAL:O	11:K:113:GLY:C	2.34	0.66
15:1:128:PRO:CG	15:1:131:TRP:CH2	2.75	0.66
15:1:170:PRO:HG2	15:1:171:LEU:N	2.09	0.66
16:2:148:ASP:CB	16:2:152:LEU:CB	2.51	0.66
16:2:182:ILE:CG2	16:2:187:LYS:CG	2.65	0.66
17:3:108:PHE:CB	19:3:3013:CLA:H42	2.24	0.66
17:3:197:SER:HB3	17:3:206:PRO:CD	2.21	0.66
18:4:98:ASN:HB3	18:4:212:LEU:HD21	1.77	0.66
18:4:109:MET:C	18:4:111:LEU:H	1.97	0.66
18:4:232:LEU:CB	18:4:236:ILE:CD1	2.72	0.66
1:A:149:PHE:HB3	1:A:153:TRP:CE3	2.31	0.66
1:A:451:ILE:HD11	19:A:1131:CLA:HED1	1.78	0.66
1:A:755:ILE:O	1:A:756:ALA:HB3	1.95	0.66
19:A:1102:CLA:H2A	19:A:1102:CLA:CED	2.25	0.66
21:A:6003:BCR:C40	21:A:6003:BCR:C23	2.73	0.66
2:B:310:PRO:HB2	2:B:311:PRO:CD	2.12	0.66
2:B:315:LEU:HD11	2:B:317:ARG:HG2	1.72	0.66
2:B:576:PHE:CE2	19:B:1226:CLA:HAC1	2.29	0.66
19:B:1239:CLA:HED1	24:B:7101:LMG:C21	2.25	0.66
3:C:61:ASP:OD2	5:E:118:ASN:ND2	2.26	0.66
5:E:122:LEU:O	5:E:122:LEU:HD12	1.95	0.66
6:F:188:GLU:OE2	16:2:180:ASP:OD1	2.13	0.66
7:G:84:ARG:CG	7:G:85:GLU:HB3	2.26	0.66
8:H:109:LEU:HD23	19:H:1207:CLA:H72	1.77	0.66
11:K:56:ILE:O	11:K:59:THR:HG23	1.95	0.66
11:K:99:ALA:O	11:K:103:LEU:HD12	1.95	0.66
15:1:58:ALA:HB3	15:1:59:PRO:CD	2.25	0.66
16:2:182:ILE:CA	16:2:187:LYS:HG3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:237:PHE:O	16:2:237:PHE:HD1	1.77	0.66
19:2:2014:CLA:H41	19:2:2014:CLA:H93	1.75	0.66
1:A:295:TRP:C	1:A:297:THR:H	1.96	0.66
2:B:455:ILE:HD13	6:F:148:LEU:HD21	1.77	0.66
2:B:691:ILE:O	2:B:691:ILE:CG2	2.43	0.66
4:D:86:SER:HA	12:L:69:LEU:HD21	1.78	0.66
8:H:121:LEU:CB	8:H:122:PRO:HD2	2.05	0.66
11:K:47:ASP:HA	11:K:51:SER:CB	2.25	0.66
13:N:168:TRP:HE3	13:N:168:TRP:O	1.78	0.66
15:1:219:THR:O	15:1:220:HIS:HB3	1.95	0.66
19:1:1008:CLA:HMC1	19:1:1008:CLA:HBC3	1.77	0.66
19:3:1147:CLA:CMC	19:3:1147:CLA:HBC2	2.20	0.66
18:4:158:GLN:CA	19:4:1004:CLA:CMA	2.67	0.66
19:4:4006:CLA:C10	19:4:4006:CLA:H41	2.25	0.66
1:A:308:ILE:HG23	19:A:1115:CLA:H111	1.77	0.66
19:A:1138:CLA:H191	6:F:181:TYR:CB	2.19	0.66
19:A:1140:CLA:NC	19:A:1140:CLA:H43	2.11	0.66
2:B:80:ASP:OD1	2:B:80:ASP:O	2.14	0.66
2:B:231:ASN:O	2:B:233:TYR:N	2.28	0.66
2:B:459:PHE:HB2	19:B:1235:CLA:CBD	2.26	0.66
2:B:479:SER:O	2:B:480:SER:HB3	1.96	0.66
3:C:73:THR:CG2	3:C:76:SER:CB	2.74	0.66
4:D:167:HIS:NE2	4:D:172:VAL:CB	2.57	0.66
5:E:82:TYR:CZ	5:E:111:ASN:HA	2.30	0.66
5:E:82:TYR:CB	5:E:83:TRP:CE3	2.74	0.66
5:E:90:VAL:O	5:E:91:VAL:HG23	1.94	0.66
6:F:130:PHE:HB3	6:F:132:ASN:ND2	2.09	0.66
8:H:78:PRO:HG3	19:L:1501:CLA:HMD1	1.76	0.66
11:K:52:PRO:CD	11:K:53:THR:N	2.51	0.66
11:K:87:GLU:O	11:K:87:GLU:CD	2.34	0.66
12:L:70:GLU:CG	12:L:74:THR:HG21	2.24	0.66
13:N:120:VAL:O	13:N:121:GLU:C	2.34	0.66
16:2:97:GLU:HG2	16:2:97:GLU:O	1.96	0.66
16:2:166:ARG:NH2	19:2:4009:CLA:O1D	2.29	0.66
17:3:96:ARG:NH1	17:3:100:TYR:CE2	2.63	0.66
17:3:130:GLN:CA	17:3:132:THR:H	2.08	0.66
22:A:7010:LMU:C6'	22:K:7047:LMU:H111	2.25	0.66
2:B:67:HIS:O	2:B:88:ALA:O	2.14	0.66
2:B:120:VAL:O	2:B:123:TRP:N	2.28	0.66
2:B:317:ARG:NE	2:B:317:ARG:CA	2.55	0.66
2:B:411:MET:CE	19:B:1220:CLA:HMC2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:LYS:CB	2:B:470:THR:OG1	2.43	0.66
19:B:1217:CLA:H2	19:B:1217:CLA:NB	2.09	0.66
11:K:47:ASP:CA	11:K:51:SER:CB	2.73	0.66
13:N:151:ASP:O	13:N:152:LEU:HG	1.96	0.66
16:2:148:ASP:CG	16:2:152:LEU:CB	2.63	0.66
1:A:207:LEU:HD11	1:A:314:GLY:HA2	1.78	0.66
19:A:1115:CLA:HBC3	19:A:1115:CLA:CMC	2.14	0.66
19:A:1124:CLA:C5	19:A:1125:CLA:HED1	2.25	0.66
19:A:1138:CLA:CBC	21:F:6014:BCR:H332	2.25	0.66
2:B:123:TRP:CA	2:B:126:THR:HG21	2.18	0.66
2:B:175:LEU:O	2:B:179:LEU:HG	1.96	0.66
5:E:79:LYS:CE	5:E:84:TYR:OH	2.43	0.66
5:E:111:ASN:C	5:E:111:ASN:HD22	1.99	0.66
6:F:202:LEU:O	6:F:203:ALA:HB3	1.94	0.66
7:G:145:THR:CG2	7:G:146:SER:N	2.57	0.66
8:H:66:ASP:O	8:H:67:SER:C	2.34	0.66
19:J:1311:CLA:CHA	19:J:1311:CLA:CED	2.74	0.66
11:K:63:LEU:HB3	11:K:102:THR:OG1	1.95	0.66
12:L:73:VAL:CG1	19:L:1504:CLA:HMA3	2.23	0.66
12:L:174:ASP:CG	12:L:175:GLN:N	2.48	0.66
17:3:100:TYR:CB	17:3:229:LYS:HE2	2.24	0.66
17:3:110:MET:O	17:3:114:VAL:N	2.29	0.66
18:4:169:ASP:OD1	18:4:174:GLN:CB	2.43	0.66
1:A:109:TRP:HA	1:A:116:ILE:HG13	1.77	0.66
1:A:377:TYR:CD1	1:A:616:PHE:HE1	2.14	0.66
19:A:1124:CLA:HBB2	19:A:1137:CLA:HMA1	1.76	0.66
2:B:117:TYR:HE2	2:B:366:THR:HG21	1.60	0.66
2:B:131:THR:HG22	2:B:134:ASP:CA	2.26	0.66
2:B:211:ASN:HB2	2:B:214:ASP:HB3	1.75	0.66
2:B:310:PRO:O	19:B:1301:CLA:C1D	2.44	0.66
2:B:508:LEU:CB	2:B:509:PHE:HD2	2.08	0.66
4:D:140:LEU:HD22	4:D:144:LEU:CD1	2.26	0.66
11:K:111:VAL:HA	11:K:114:HIS:CG	2.30	0.66
12:L:142:SER:O	12:L:143:LEU:CD2	2.43	0.66
15:1:77:GLU:CA	15:1:80:LYS:HD2	2.25	0.66
17:3:207:PHE:O	17:3:207:PHE:CD1	2.39	0.66
18:4:126:TRP:CG	18:4:127:TYR:N	2.63	0.66
18:4:143:VAL:HG12	18:4:144:ILE:N	2.11	0.66
18:4:209:ARG:HB2	19:4:4004:CLA:C3A	2.26	0.66
1:A:150:PHE:N	1:A:153:TRP:CE3	2.62	0.66
1:A:203:LEU:HD21	19:A:1123:CLA:C3D	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:PHE:CD2	1:A:533:PRO:HB2	2.31	0.66
1:A:710:ALA:CB	19:A:1138:CLA:HED2	2.26	0.66
4:D:148:TYR:O	4:D:149:LYS:CG	2.44	0.66
6:F:110:ALA:HA	6:F:113:SER:HB2	1.78	0.66
7:G:102:ALA:CA	7:G:104:ASP:CG	2.60	0.66
7:G:131:GLY:O	7:G:136:VAL:CB	2.42	0.66
9:I:9:VAL:HG12	9:I:10:PRO:HD3	1.78	0.66
12:L:153:PHE:CB	12:L:155:GLU:OE1	2.38	0.66
13:N:91:TYR:O	13:N:93:GLU:N	2.27	0.66
15:1:162:LYS:CA	15:1:164:PRO:HG3	2.26	0.66
16:2:269:LYS:CE	16:2:269:LYS:CA	2.73	0.66
18:4:103:MET:HE2	18:4:207:ASN:O	1.96	0.66
18:4:175:TYR:HB3	18:4:194:PHE:HD1	1.54	0.66
18:4:223:VAL:O	18:4:223:VAL:CG1	2.38	0.66
1:A:358:LEU:HD11	1:A:413:HIS:CB	2.26	0.66
1:A:396:PHE:CE2	1:A:616:PHE:CG	2.84	0.66
1:A:483:GLN:CB	1:A:485:GLN:NE2	2.56	0.66
1:A:606:TYR:O	1:A:610:SER:CB	2.44	0.66
1:A:678:PHE:O	1:A:680:LEU:N	2.28	0.66
1:A:715:LYS:CE	6:F:230:ASN:OD1	2.44	0.66
19:A:1105:CLA:HMB3	19:A:1106:CLA:HHB	1.78	0.66
19:A:1125:CLA:CBB	19:A:1133:CLA:C3A	2.70	0.66
19:A:1139:CLA:CGA	19:A:1139:CLA:H42	2.25	0.66
19:A:1140:CLA:C14	21:A:6011:BCR:HC21	2.25	0.66
22:A:7023:LMU:H2B	22:A:7023:LMU:C6B	2.24	0.66
2:B:123:TRP:HA	2:B:126:THR:HB	1.58	0.66
3:C:31:TRP:O	3:C:33:GLY:N	2.29	0.66
4:D:185:GLY:O	4:D:186:GLN:CB	2.43	0.66
5:E:128:VAL:O	5:E:129:GLU:C	2.30	0.66
6:F:149:ILE:O	6:F:150:VAL:HG12	1.96	0.66
11:K:69:ARG:HG3	11:K:73:ALA:HB2	1.77	0.66
11:K:127:ILE:O	11:K:130:LEU:CG	2.44	0.66
1:A:112:ASP:O	1:A:115:HIS:CD2	2.49	0.66
1:A:733:VAL:O	1:A:733:VAL:CG1	2.44	0.66
2:B:305:LEU:CD2	19:B:1220:CLA:O1D	2.45	0.66
2:B:527:LEU:HD12	19:B:1236:CLA:HMA3	1.78	0.66
3:C:12:ILE:HG21	3:C:27:GLU:OE1	1.96	0.66
7:G:102:ALA:CA	7:G:104:ASP:OD1	2.39	0.66
22:H:7017:LMU:O3'	22:H:7017:LMU:H1B	1.96	0.66
12:L:92:ALA:N	12:L:98:ARG:NH2	2.41	0.66
16:2:237:PHE:CE1	16:2:241:TYR:CE1	2.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:4009:CLA:H151	19:2:4009:CLA:H8	1.75	0.66
1:A:328:LYS:HZ2	1:A:345:GLY:HA3	1.60	0.65
1:A:402:ILE:CG1	19:A:1127:CLA:HBB2	2.26	0.65
1:A:578:ARG:O	1:A:579:PHE:C	2.33	0.65
19:A:1106:CLA:HBB2	19:A:1107:CLA:C3D	2.26	0.65
2:B:79:GLN:O	2:B:80:ASP:CB	2.43	0.65
19:B:1205:CLA:CBB	19:B:1205:CLA:C9	2.73	0.65
4:D:140:LEU:CD1	4:D:141:GLY:H	1.82	0.65
6:F:181:TYR:HB2	6:F:203:ALA:HB2	1.78	0.65
22:F:7036:LMU:C6'	22:F:7036:LMU:O2B	2.45	0.65
7:G:125:VAL:O	7:G:129:ALA:N	2.29	0.65
12:L:205:TYR:H	12:L:205:TYR:HD2	1.40	0.65
13:N:148:ASP:H	13:N:149:ASP:CB	2.08	0.65
15:1:66:PRO:O	15:1:69:LEU:O	2.14	0.65
19:1:1006:CLA:CAC	19:1:1010:CLA:CMB	2.73	0.65
19:4:1304:CLA:H151	19:4:1304:CLA:H202	1.77	0.65
19:A:1131:CLA:O1A	19:A:1237:CLA:H11	1.96	0.65
19:A:9011:CLA:HMC3	2:B:624:LEU:HG	1.77	0.65
19:A:9022:CLA:H13	19:B:1206:CLA:CBB	2.26	0.65
2:B:58:PHE:HB2	2:B:146:SER:HB2	1.78	0.65
2:B:120:VAL:O	2:B:123:TRP:HD1	1.79	0.65
2:B:476:ILE:HG23	2:B:479:SER:OG	1.94	0.65
3:C:73:THR:CB	3:C:76:SER:OG	2.43	0.65
4:D:99:PHE:HB3	4:D:157:VAL:CB	2.25	0.65
8:H:64:GLN:CB	8:H:67:SER:H	2.09	0.65
8:H:85:GLU:CG	8:H:86:THR:H	1.98	0.65
15:1:86:HIS:CD2	15:1:86:HIS:H	2.01	0.65
15:1:201:PHE:CD1	15:1:204:GLN:CD	2.70	0.65
16:2:115:LEU:HD21	19:2:2011:CLA:NB	2.12	0.65
18:4:103:MET:HE1	18:4:207:ASN:HB3	1.79	0.65
19:A:1115:CLA:H191	11:K:64:MET:HE3	1.79	0.65
2:B:596:TRP:CH2	2:B:612:SER:C	2.67	0.65
6:F:172:GLY:O	6:F:176:TRP:HB2	1.96	0.65
8:H:58:LEU:CD1	8:H:61:THR:HA	2.26	0.65
11:K:89:ARG:NH1	11:K:89:ARG:CG	2.58	0.65
12:L:141:LEU:HD12	12:L:145:LEU:CD1	2.24	0.65
15:1:79:TYR:CB	19:1:1012:CLA:OBD	2.44	0.65
18:4:211:MET:SD	19:4:4002:CLA:HBB1	2.36	0.65
22:4:7034:LMU:C11	22:4:7052:LMU:C2'	2.72	0.65
1:A:385:LEU:O	1:A:386:ALA:CB	2.43	0.65
1:A:711:HIS:CE1	19:A:1139:CLA:HAC1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1126:CLA:H43	19:A:1126:CLA:CBA	2.25	0.65
19:A:9012:CLA:C1	2:B:616:LEU:HD12	2.14	0.65
2:B:292:ARG:NH2	2:B:297:ILE:CG1	2.60	0.65
2:B:320:LYS:O	2:B:406:ASN:ND2	2.18	0.65
7:G:89:LYS:O	7:G:90:GLN:HG2	1.95	0.65
8:H:119:ASP:HB3	8:H:121:LEU:HG	1.78	0.65
18:4:245:VAL:HG22	18:4:246:GLN:N	2.10	0.65
1:A:90:PHE:CD1	19:A:1103:CLA:H91	2.31	0.65
1:A:250:LEU:HD12	17:3:136:TRP:HZ2	1.61	0.65
1:A:660:GLN:O	1:A:661:ALA:CB	2.43	0.65
19:A:1112:CLA:HMC2	21:A:6002:BCR:C15	2.26	0.65
2:B:69:ALA:HB2	2:B:135:LEU:CD1	2.27	0.65
2:B:615:TYR:N	2:B:615:TYR:CD1	2.62	0.65
2:B:645:VAL:HG22	19:B:1206:CLA:HHD	1.77	0.65
19:B:1219:CLA:H72	19:B:1219:CLA:CBB	2.24	0.65
19:B:1224:CLA:HMC1	19:B:1224:CLA:HBC3	1.79	0.65
3:C:55:GLU:O	3:C:57:ALA:N	2.20	0.65
4:D:95:GLN:NE2	4:D:96:VAL:CA	2.52	0.65
8:H:67:SER:C	8:H:68:TYR:CG	2.69	0.65
13:N:110:THR:CG2	13:N:111:GLY:H	2.10	0.65
15:1:91:MET:O	15:1:91:MET:SD	2.55	0.65
17:3:254:GLN:CG	17:3:255:ASN:H	2.06	0.65
1:A:40:PHE:N	1:A:44:ILE:CG2	2.59	0.65
1:A:101:ALA:HB2	1:A:164:LEU:HB2	1.77	0.65
1:A:525:ASN:ND2	1:A:526:LYS:HE3	2.12	0.65
1:A:747:TRP:CE3	21:A:6011:BCR:H401	2.31	0.65
19:A:1119:CLA:HMD1	19:A:1120:CLA:HHD	1.79	0.65
2:B:5:ILE:CG2	2:B:6:PRO:CD	2.62	0.65
2:B:98:GLN:N	2:B:99:PRO:HD2	2.11	0.65
2:B:444:LEU:HD21	2:B:452:GLN:HE22	1.61	0.65
3:C:73:THR:CG2	3:C:76:SER:HB3	2.26	0.65
11:K:87:GLU:O	11:K:87:GLU:OE1	2.15	0.65
13:N:152:LEU:CB	13:N:153:GLU:HG3	2.27	0.65
13:N:169:LYS:CB	13:N:170:TRP:CD1	2.74	0.65
15:1:150:HIS:CE1	15:1:151:GLN:NE2	2.65	0.65
17:3:91:GLY:C	17:3:92:PHE:CD1	2.69	0.65
18:4:158:GLN:CG	19:4:1004:CLA:HMA3	2.23	0.65
18:4:169:ASP:O	18:4:173:LYS:CA	2.45	0.65
1:A:356:ALA:HB2	1:A:417:PHE:HD2	1.61	0.65
1:A:425:THR:OG1	1:A:428:TYR:CE1	2.49	0.65
1:A:586:ARG:CG	3:C:49:VAL:HG21	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:GLY:H	2:B:668:ARG:NH1	1.95	0.65
1:A:740:LEU:CD2	19:A:1140:CLA:CMA	2.75	0.65
2:B:65:LEU:HD22	2:B:124:TRP:CE3	2.31	0.65
2:B:171:ALA:O	2:B:172:GLU:HB2	1.97	0.65
3:C:26:LEU:H	3:C:43:PRO:CG	2.08	0.65
4:D:140:LEU:CD1	4:D:144:LEU:H	2.10	0.65
6:F:205:SER:C	6:F:207:LEU:HD12	2.17	0.65
7:G:69:GLY:CA	7:G:72:LEU:HG	2.26	0.65
7:G:89:LYS:NZ	7:G:89:LYS:H	1.95	0.65
11:K:75:SER:O	11:K:76:ALA:HB3	1.97	0.65
14:R:36:UNK:O	14:R:38:UNK:N	2.30	0.65
15:1:208:TYR:N	15:1:209:PRO:CD	2.59	0.65
16:2:156:GLU:O	16:2:160:ILE:HD13	1.96	0.65
17:3:96:ARG:CA	17:3:99:ALA:N	2.51	0.65
18:4:158:GLN:HA	19:4:1004:CLA:H2A	1.78	0.65
1:A:105:ASN:OD1	1:A:119:SER:N	2.28	0.65
1:A:692:PHE:CZ	19:A:1140:CLA:HBC3	2.32	0.65
19:A:1115:CLA:H191	11:K:64:MET:CE	2.26	0.65
21:A:6011:BCR:H313	19:A:9013:CLA:H142	1.79	0.65
2:B:127:ILE:O	2:B:127:ILE:HD12	1.97	0.65
2:B:280:ILE:HD13	19:B:1215:CLA:HBB2	1.79	0.65
2:B:394:PHE:O	2:B:542:ARG:CD	2.45	0.65
19:B:1220:CLA:C4	19:B:1220:CLA:C1A	2.65	0.65
6:F:101:LYS:C	6:F:103:GLN:N	2.46	0.65
6:F:139:LEU:CD1	6:F:149:ILE:CD1	2.71	0.65
22:F:7036:LMU:H72	22:F:7036:LMU:C11	2.27	0.65
8:H:98:LEU:CD2	12:L:146:THR:CG2	2.71	0.65
19:L:1502:CLA:HAC1	21:L:6019:BCR:H322	1.78	0.65
15:1:176:ASP:HB3	15:1:180:LEU:CG	2.24	0.65
17:3:112:GLY:HA2	17:3:115:GLY:O	1.97	0.65
17:3:136:TRP:O	17:3:139:THR:N	2.29	0.65
22:3:7005:LMU:H51	22:3:7005:LMU:O1'	1.97	0.65
18:4:149:SER:HB2	18:4:153:GLU:OE1	1.95	0.65
1:A:246:HIS:O	1:A:248:PHE:N	2.25	0.65
1:A:331:LEU:HD21	1:A:343:HIS:C	2.16	0.65
19:A:1131:CLA:C16	21:L:6019:BCR:C36	2.75	0.65
19:A:1139:CLA:H43	6:F:198:ILE:HD13	1.78	0.65
2:B:196:HIS:CE1	19:B:1212:CLA:HED2	2.32	0.65
2:B:312:GLY:CA	2:B:315:LEU:HB2	2.24	0.65
21:B:6020:BCR:H333	19:L:1502:CLA:C1C	2.26	0.65
3:C:17:CYS:C	3:C:58:CYS:HB2	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:111:ASN:ND2	5:E:112:TYR:N	2.45	0.65
11:K:128:GLY:N	11:K:129:ALA:CA	2.55	0.65
22:N:7049:LMU:H12	22:N:7049:LMU:C6	2.12	0.65
15:1:65:ASP:OD2	15:1:66:PRO:N	2.29	0.65
16:2:152:LEU:CD1	16:2:153:PHE:N	2.55	0.65
16:2:258:GLY:O	16:2:259:HIS:ND1	2.29	0.65
17:3:210:PRO:HD2	17:3:211:LEU:H	1.62	0.65
19:3:3011:CLA:HBC2	19:3:3012:CLA:CHA	2.26	0.65
22:4:7009:LMU:H3'	22:4:7009:LMU:C5B	2.27	0.65
2:B:123:TRP:HB2	2:B:126:THR:CG2	2.26	0.65
2:B:361:ILE:CG2	2:B:368:GLN:OE1	2.44	0.65
2:B:456:GLU:HA	2:B:514:PRO:CD	2.27	0.65
19:B:1222:CLA:HBB1	19:B:1236:CLA:HMB3	1.78	0.65
19:B:1235:CLA:H152	21:F:6016:BCR:H313	1.76	0.65
5:E:121:ALA:O	5:E:125:ILE:HG21	1.97	0.65
6:F:97:GLN:O	6:F:98:ALA:C	2.32	0.65
7:G:62:LEU:O	7:G:65:SER:CB	2.44	0.65
12:L:72:PRO:C	12:L:73:VAL:HG22	2.15	0.65
19:L:1502:CLA:HBC3	19:L:1502:CLA:HMC1	1.78	0.65
13:N:146:LEU:HD11	17:3:142:ILE:C	2.03	0.65
16:2:152:LEU:HD22	16:2:153:PHE:N	2.12	0.65
17:3:177:ALA:O	17:3:178:LYS:CB	2.45	0.65
18:4:112:PRO:HA	18:4:117:SER:OG	1.96	0.65
18:4:193:ASN:C	18:4:194:PHE:CD1	2.69	0.65
1:A:328:LYS:HD2	1:A:332:GLU:CB	2.19	0.64
1:A:467:MET:HA	1:A:470:LEU:HB2	1.79	0.64
1:A:740:LEU:HD21	19:A:1140:CLA:HMA1	1.77	0.64
19:A:1102:CLA:HBA2	19:A:1109:CLA:H62	1.79	0.64
19:A:1120:CLA:H2A	19:A:1120:CLA:O1D	1.97	0.64
19:A:1124:CLA:HMA1	21:A:6008:BCR:H16C	1.79	0.64
19:A:1133:CLA:O1A	19:A:1134:CLA:HBC3	1.97	0.64
2:B:292:ARG:NH2	2:B:297:ILE:O	2.30	0.64
2:B:292:ARG:HH21	2:B:297:ILE:C	1.99	0.64
2:B:444:LEU:O	2:B:445:ALA:HB3	1.97	0.64
10:J:18:TRP:CH2	10:J:22:LEU:HD22	2.32	0.64
12:L:71:THR:HB	12:L:72:PRO:HD2	1.78	0.64
12:L:174:ASP:OD2	12:L:175:GLN:N	2.29	0.64
15:1:58:ALA:HB1	19:1:1015:CLA:C3B	2.27	0.64
15:1:170:PRO:HG2	15:1:173:TYR:CE2	2.32	0.64
19:1:1014:CLA:CHD	19:1:1014:CLA:CBC	2.72	0.64
16:2:133:ASN:HD22	16:2:134:THR:HB	0.92	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:THR:HG22	1:A:46:LYS:NZ	2.11	0.64
1:A:207:LEU:CD1	1:A:314:GLY:CA	2.75	0.64
1:A:223:VAL:HG23	1:A:227:LEU:HD12	0.79	0.64
1:A:274:TRP:CG	1:A:277:TYR:O	2.49	0.64
1:A:370:ILE:CD1	19:A:1124:CLA:CAD	2.74	0.64
1:A:388:ASP:CG	1:A:391:THR:HG1	1.97	0.64
19:A:1133:CLA:CAD	19:A:1134:CLA:HAC1	2.27	0.64
21:A:6011:BCR:H323	21:J:6012:BCR:H391	1.77	0.64
2:B:188:LEU:O	2:B:191:ALA:N	2.30	0.64
2:B:558:PRO:CG	2:B:703:VAL:CG2	2.62	0.64
2:B:607:SER:O	2:B:610:ASN:HB2	1.96	0.64
19:B:1227:CLA:HAA1	19:B:1227:CLA:HED2	1.80	0.64
3:C:73:THR:CB	3:C:76:SER:HG	2.05	0.64
4:D:102:ILE:HG13	4:D:153:GLN:O	1.97	0.64
6:F:117:LEU:HA	6:F:119:ILE:HG12	1.78	0.64
12:L:154:ASN:C	12:L:178:THR:CG2	2.62	0.64
19:R:1150:CLA:H92	22:R:7007:LMU:O4'	1.97	0.64
15:1:78:ARG:HH21	15:1:179:LYS:HD3	1.55	0.64
16:2:125:PHE:O	16:2:126:LEU:C	2.36	0.64
19:2:2014:CLA:H41	19:2:2014:CLA:C8	2.26	0.64
1:A:204:ASN:O	1:A:205:HIS:CB	2.45	0.64
1:A:281:LEU:HD12	1:A:282:THR:H	1.62	0.64
1:A:374:GLN:O	1:A:377:TYR:HD2	1.81	0.64
1:A:382:TYR:CE2	19:A:1127:CLA:HED3	2.33	0.64
1:A:555:ILE:CG1	19:A:9023:CLA:OBD	2.45	0.64
1:A:618:TRP:O	1:A:622:SER:HB3	1.98	0.64
1:A:705:GLU:HA	1:A:708:VAL:HB	1.80	0.64
19:A:1132:CLA:C4	12:L:110:LEU:HD23	2.27	0.64
2:B:152:ALA:O	2:B:153:GLY:C	2.35	0.64
2:B:362:ALA:O	2:B:363:GLN:CB	2.46	0.64
2:B:561:GLY:HA3	3:C:52:LYS:CG	2.25	0.64
19:B:1235:CLA:CBC	6:F:160:PHE:HZ	2.10	0.64
8:H:58:LEU:CD1	8:H:61:THR:CB	2.52	0.64
11:K:115:ILE:HG12	11:K:122:LEU:CD1	2.27	0.64
13:N:114:PHE:CE2	13:N:116:ARG:HD2	2.33	0.64
14:R:38:UNK:C	14:R:39:UNK:O	2.45	0.64
16:2:184:PRO:HD3	16:2:187:LYS:HB2	1.71	0.64
19:3:3017:CLA:HBC3	19:3:3017:CLA:CMC	2.24	0.64
22:3:7003:LMU:H3B	22:3:7005:LMU:C6B	2.19	0.64
1:A:52:THR:OG1	1:A:53:TRP:CE3	2.50	0.64
1:A:113:PRO:O	1:A:114:THR:CG2	2.35	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:CD1	1:A:297:THR:HG22	2.22	0.64
1:A:392:GLN:HA	1:A:395:LEU:HD23	1.78	0.64
1:A:393:LEU:HG	1:A:394:SER:H	1.62	0.64
2:B:174:ARG:NH1	19:B:1221:CLA:HMD1	2.13	0.64
3:C:63:LEU:CD2	3:C:65:VAL:N	2.59	0.64
6:F:97:GLN:NE2	6:F:98:ALA:N	2.45	0.64
7:G:61:ALA:O	7:G:63:VAL:HG13	1.97	0.64
12:L:104:LEU:HD21	12:L:199:TRP:CZ2	2.29	0.64
13:N:139:LYS:CD	13:N:142:LYS:HE2	2.28	0.64
13:N:150:LEU:H	13:N:150:LEU:HD22	1.63	0.64
19:2:2001:CLA:CGA	19:2:2001:CLA:C4	2.74	0.64
17:3:150:TYR:CB	17:3:151:TRP:NE1	2.48	0.64
1:A:40:PHE:H	1:A:44:ILE:HG23	1.62	0.64
1:A:174:PHE:CE2	19:A:1103:CLA:H152	2.31	0.64
1:A:302:HIS:HB2	19:A:1116:CLA:CHB	2.27	0.64
2:B:622:ASP:HB3	2:B:626:LEU:CG	2.27	0.64
19:B:1212:CLA:O2D	19:B:1212:CLA:OBD	2.11	0.64
4:D:77:ASN:HB3	4:D:79:PRO:CD	2.27	0.64
12:L:209:LEU:CD1	12:L:210:PRO:CD	2.59	0.64
13:N:135:GLN:HA	13:N:136:ASP:C	2.12	0.64
15:1:93:ALA:HA	19:1:1006:CLA:C4B	2.28	0.64
15:1:223:ASP:OD1	18:4:140:THR:CG2	2.46	0.64
16:2:177:VAL:HG13	16:2:178:ASN:CG	2.17	0.64
17:3:111:LEU:O	17:3:114:VAL:CB	2.45	0.64
18:4:111:LEU:CD1	18:4:112:PRO:HG3	2.26	0.64
1:A:44:ILE:O	1:A:45:ALA:C	2.36	0.64
1:A:554:LEU:CD2	19:A:9023:CLA:O2D	2.46	0.64
2:B:310:PRO:HG2	2:B:311:PRO:CD	2.27	0.64
21:B:6020:BCR:H23C	21:B:6020:BCR:C38	2.28	0.64
3:C:26:LEU:CD2	4:D:181:ARG:NH1	2.61	0.64
3:C:67:VAL:HG13	3:C:68:TYR:N	2.09	0.64
19:F:1302:CLA:HHB	21:F:6016:BCR:H333	1.79	0.64
11:K:62:SER:OG	11:K:63:LEU:CD1	2.42	0.64
11:K:63:LEU:N	11:K:63:LEU:CD1	2.45	0.64
13:N:110:THR:HG22	13:N:111:GLY:N	2.12	0.64
16:2:126:LEU:C	16:2:128:LYS:H	1.97	0.64
19:2:2007:CLA:HMC1	19:2:2007:CLA:HBC3	1.79	0.64
1:A:76:ARG:HH12	1:A:193:LEU:HD22	1.62	0.64
1:A:645:SER:OG	1:A:655:ASP:OD1	2.15	0.64
2:B:469:LYS:NZ	2:B:471:THR:N	2.46	0.64
3:C:63:LEU:HD23	3:C:65:VAL:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:93:LYS:NZ	4:D:97:GLU:OE2	2.30	0.64
4:D:98:GLU:CB	4:D:100:TYR:HE2	2.11	0.64
6:F:214:PRO:O	6:F:215:VAL:CB	2.45	0.64
11:K:59:THR:O	11:K:63:LEU:CD1	2.46	0.64
12:L:83:LEU:O	12:L:83:LEU:CD1	2.46	0.64
12:L:210:PRO:HB2	12:L:211:TYR:CD2	2.33	0.64
16:2:184:PRO:HG2	16:2:185:ASN:N	2.12	0.64
16:2:211:PRO:HD2	16:2:212:GLN:N	2.12	0.64
16:2:256:ASP:N	16:2:256:ASP:OD1	2.29	0.64
17:3:135:ALA:HB3	17:3:139:THR:HB	1.77	0.64
18:4:158:GLN:NE2	19:4:1004:CLA:CHA	2.44	0.64
18:4:169:ASP:C	18:4:173:LYS:CA	2.57	0.64
1:A:57:LEU:HD23	1:A:57:LEU:O	1.98	0.64
1:A:62:HIS:ND1	19:A:1128:CLA:HBA1	2.12	0.64
1:A:92:TRP:O	1:A:93:LEU:HB3	1.97	0.64
1:A:336:GLY:C	1:A:339:THR:HG1	2.01	0.64
1:A:338:PHE:CD1	19:A:1151:CLA:HBB2	2.33	0.64
1:A:378:SER:O	1:A:379:MET:HG3	1.97	0.64
1:A:497:ALA:CB	1:A:510:SER:OG	2.45	0.64
22:A:7045:LMU:O5B	22:A:7045:LMU:H5'	1.97	0.64
19:A:9013:CLA:H93	2:B:431:PHE:CD1	2.33	0.64
19:A:9023:CLA:HHB	19:A:9023:CLA:C4	2.27	0.64
2:B:3:LEU:CD1	9:I:29:GLU:OE1	2.44	0.64
2:B:73:ASN:O	2:B:121:TYR:HE1	1.79	0.64
2:B:202:SER:O	2:B:245:GLY:HA2	1.98	0.64
2:B:280:ILE:HA	2:B:283:LEU:HD12	1.79	0.64
2:B:293:THR:CG2	7:G:94:GLN:CG	2.72	0.64
2:B:295:PHE:CD2	2:B:295:PHE:N	2.59	0.64
2:B:683:GLU:OE2	2:B:693:TRP:HH2	1.80	0.64
2:B:692:ARG:HH22	2:B:694:ARG:HH22	1.44	0.64
4:D:103:THR:CG2	4:D:128:LEU:CG	2.75	0.64
5:E:127:GLU:HB3	5:E:128:VAL:C	2.18	0.64
13:N:157:LYS:HB3	13:N:158:ASP:C	2.17	0.64
15:1:143:LEU:N	15:1:143:LEU:HD12	2.13	0.64
18:4:202:GLU:O	18:4:205:ILE:CD1	2.45	0.64
1:A:130:GLU:OE1	1:A:130:GLU:CA	2.45	0.64
1:A:261:SER:O	1:A:262:PHE:CG	2.51	0.64
1:A:345:GLY:O	1:A:347:TYR:N	2.23	0.64
1:A:401:TRP:CD1	19:A:1126:CLA:CHC	2.80	0.64
22:A:7016:LMU:C7	22:A:7016:LMU:H112	2.28	0.64
2:B:232:LEU:HD11	2:B:235:GLN:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:418:ILE:O	2:B:422:LEU:HD12	1.97	0.64
2:B:510:LEU:HD22	2:B:597:LYS:HD2	1.79	0.64
4:D:186:GLN:C	4:D:187:ASN:ND2	2.50	0.64
7:G:114:LEU:HD12	7:G:114:LEU:C	2.18	0.64
8:H:97:LEU:HD13	8:H:100:PHE:CB	2.28	0.64
14:R:27:UNK:O	14:R:29:UNK:N	2.31	0.64
15:1:224:PRO:HA	15:1:225:TRP:CB	2.26	0.64
19:2:2007:CLA:CAC	19:3:2009:CLA:HED1	2.09	0.64
17:3:176:TRP:O	17:3:178:LYS:CG	2.45	0.64
18:4:112:PRO:HB3	18:4:116:THR:O	1.98	0.64
19:4:1304:CLA:CGD	19:4:1304:CLA:C2A	2.75	0.64
1:A:59:ALA:O	1:A:60:ASP:C	2.36	0.64
1:A:430:ASP:OD1	1:A:433:ASP:OD2	2.15	0.64
1:A:455:PHE:HD1	19:A:1131:CLA:HMA2	1.63	0.64
19:A:1117:CLA:H203	19:A:1125:CLA:HAA1	1.80	0.64
2:B:453:ILE:O	2:B:453:ILE:CG2	2.41	0.64
2:B:476:ILE:HG22	2:B:479:SER:OG	1.98	0.64
8:H:120:ILE:O	8:H:120:ILE:CG1	2.40	0.64
12:L:71:THR:HB	12:L:72:PRO:CD	2.27	0.64
12:L:146:THR:O	12:L:148:TYR:N	2.30	0.64
13:N:139:LYS:CA	13:N:142:LYS:HD3	2.27	0.64
16:2:206:TRP:O	16:2:208:SER:N	2.31	0.64
18:4:87:ASN:O	18:4:90:TRP:HB2	1.98	0.64
19:4:1304:CLA:H203	19:4:1304:CLA:C15	2.23	0.64
1:A:58:HIS:HE1	19:A:1101:CLA:ND	1.97	0.63
1:A:188:LYS:CE	1:A:190:ALA:HA	2.27	0.63
1:A:245:PRO:O	1:A:248:PHE:CE2	2.51	0.63
1:A:451:ILE:HD11	19:A:1131:CLA:CED	2.29	0.63
1:A:555:ILE:HD13	19:A:9023:CLA:HMD2	1.78	0.63
19:A:1111:CLA:HMA2	19:A:1111:CLA:C2	2.28	0.63
2:B:212:PHE:CZ	19:B:1211:CLA:HAC1	2.33	0.63
2:B:622:ASP:CB	2:B:626:LEU:HD11	2.28	0.63
2:B:711:VAL:HG22	24:B:7101:LMG:H391	1.80	0.63
4:D:100:TYR:CZ	4:D:134:LYS:HE3	2.32	0.63
4:D:103:THR:CG2	4:D:128:LEU:CD1	2.76	0.63
4:D:129:LEU:HD13	12:L:65:PHE:CE1	2.33	0.63
4:D:163:VAL:C	4:D:164:GLN:HG3	2.18	0.63
21:F:6016:BCR:HC8	21:F:6016:BCR:H311	1.79	0.63
8:H:78:PRO:CG	19:L:1501:CLA:CMD	2.69	0.63
13:N:142:LYS:HE3	13:N:142:LYS:CA	2.11	0.63
15:1:95:PRO:C	15:1:98:LEU:HB2	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:131:ILE:O	16:2:132:LEU:HD12	1.98	0.63
16:2:145:TYR:O	16:2:146:PHE:CG	2.51	0.63
16:2:211:PRO:CD	16:2:212:GLN:H	2.09	0.63
17:3:141:VAL:CG2	17:3:142:ILE:HG12	2.16	0.63
18:4:207:ASN:O	18:4:211:MET:HE2	1.97	0.63
1:A:218:TRP:N	19:A:1112:CLA:HBB2	2.13	0.63
2:B:120:VAL:C	2:B:123:TRP:HD1	2.00	0.63
2:B:256:THR:HG1	2:B:258:LEU:H	1.44	0.63
2:B:292:ARG:NH2	2:B:297:ILE:H	1.95	0.63
2:B:454:LEU:HB2	2:B:514:PRO:HB3	1.79	0.63
3:C:73:THR:O	3:C:77:MET:HG2	1.97	0.63
19:F:1305:CLA:C4	19:4:1306:CLA:HAA1	2.23	0.63
13:N:169:LYS:HB3	13:N:170:TRP:HD1	1.48	0.63
15:1:158:PRO:CG	15:1:159:GLU:N	2.61	0.63
15:1:176:ASP:HB2	15:1:180:LEU:HD12	1.72	0.63
18:4:158:GLN:NE2	19:4:1004:CLA:C2A	2.61	0.63
18:4:158:GLN:HE22	19:4:1004:CLA:C4D	2.12	0.63
22:4:7053:LMU:H6E	22:4:7053:LMU:H2B	1.79	0.63
19:A:1129:CLA:HMB2	19:L:1130:CLA:C2D	2.27	0.63
2:B:117:TYR:CE2	2:B:366:THR:HG21	2.33	0.63
3:C:73:THR:OG1	3:C:76:SER:CB	2.46	0.63
4:D:83:PHE:CZ	4:D:114:MET:HE2	2.33	0.63
4:D:140:LEU:HD13	4:D:144:LEU:N	2.13	0.63
5:E:74:VAL:CG2	5:E:90:VAL:HG22	2.27	0.63
22:H:7032:LMU:H31	22:H:7032:LMU:C2B	2.28	0.63
11:K:115:ILE:HG12	11:K:122:LEU:HD13	1.78	0.63
22:K:7042:LMU:H32	22:K:7042:LMU:H6D	1.80	0.63
12:L:153:PHE:N	12:L:153:PHE:HD2	1.92	0.63
22:R:7020:LMU:C5B	22:R:7020:LMU:C6'	2.64	0.63
15:1:133:THR:C	15:1:135:PRO:CD	2.66	0.63
16:2:163:ALA:O	16:2:167:ARG:HD2	1.98	0.63
16:2:182:ILE:HD13	16:2:187:LYS:O	1.98	0.63
16:2:189:THR:HG23	16:2:193:VAL:O	1.97	0.63
22:3:7005:LMU:O3'	22:3:7005:LMU:H1B	1.99	0.63
1:A:432:LEU:HA	1:A:435:VAL:HG13	1.81	0.63
1:A:434:ARG:O	1:A:437:ARG:HB2	1.98	0.63
1:A:536:THR:O	1:A:537:ALA:HB3	1.98	0.63
1:A:569:ILE:HB	1:A:572:LYS:HB2	1.80	0.63
1:A:585:GLY:O	1:A:589:THR:OG1	2.17	0.63
1:A:699:TYR:OH	2:B:533:ILE:CG2	2.43	0.63
19:A:1237:CLA:H92	21:L:6019:BCR:H321	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:LEU:O	2:B:619:TRP:HB2	1.98	0.63
4:D:83:PHE:CZ	4:D:114:MET:CE	2.81	0.63
5:E:91:VAL:O	5:E:93:VAL:N	2.31	0.63
7:G:72:LEU:HD22	7:G:124:ILE:CD1	2.02	0.63
7:G:82:PHE:HB2	7:G:83:GLN:HG3	1.79	0.63
11:K:81:THR:OG1	11:K:82:ALA:N	2.32	0.63
22:K:7042:LMU:O3'	22:K:7042:LMU:H1B	1.96	0.63
15:1:77:GLU:OE1	15:1:77:GLU:N	2.31	0.63
16:2:165:GLY:C	16:2:167:ARG:HG2	2.19	0.63
16:2:252:ALA:HB1	16:2:254:LEU:HB2	1.80	0.63
17:3:243:ILE:HD13	19:3:3005:CLA:C1C	2.29	0.63
18:4:87:ASN:ND2	18:4:90:TRP:CE2	2.67	0.63
1:A:42:ARG:NH1	1:A:42:ARG:O	2.32	0.63
1:A:54:ILE:O	1:A:58:HIS:HD2	1.80	0.63
1:A:711:HIS:NE2	19:A:1139:CLA:CAC	2.62	0.63
21:A:6003:BCR:H403	21:A:6003:BCR:H23C	1.80	0.63
2:B:551:LYS:HZ1	4:D:194:ASN:C	2.01	0.63
4:D:112:PHE:O	4:D:119:ALA:HB1	1.98	0.63
6:F:139:LEU:HD12	6:F:147:HIS:O	1.99	0.63
21:F:6016:BCR:H271	21:F:6016:BCR:H403	1.80	0.63
14:R:7:UNK:O	14:R:10:UNK:CB	2.47	0.63
15:1:201:PHE:HA	15:1:204:GLN:HB2	1.80	0.63
16:2:160:ILE:O	16:2:161:GLY:C	2.34	0.63
1:A:58:HIS:HB3	19:A:1102:CLA:HBC1	1.81	0.63
1:A:71:LEU:HD12	1:A:71:LEU:C	2.18	0.63
1:A:197:GLN:NE2	1:A:351:THR:O	2.32	0.63
1:A:281:LEU:HD12	1:A:282:THR:N	2.14	0.63
1:A:368:LEU:HD22	19:A:1117:CLA:H92	1.77	0.63
1:A:582:ASP:HB3	1:A:589:THR:HG22	1.80	0.63
2:B:568:CYS:O	2:B:570:ILE:N	2.31	0.63
6:F:191:PRO:HG2	6:F:191:PRO:O	1.99	0.63
7:G:84:ARG:HE	7:G:85:GLU:HB3	1.60	0.63
8:H:86:THR:O	8:H:88:ALA:C	2.37	0.63
8:H:94:ARG:O	8:H:95:GLY:O	2.16	0.63
9:I:10:PRO:HA	9:I:14:LEU:HB2	1.80	0.63
11:K:59:THR:O	11:K:63:LEU:HD11	1.98	0.63
19:2:2002:CLA:HBC2	19:2:2002:CLA:CHD	2.23	0.63
17:3:96:ARG:CB	17:3:99:ALA:HB3	2.27	0.63
18:4:175:TYR:HB2	18:4:195:ALA:H	1.63	0.63
1:A:401:TRP:O	1:A:405:PHE:HB2	1.98	0.63
1:A:568:LEU:HG	2:B:676:GLU:OE2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:MET:HB2	19:A:9013:CLA:C1C	2.28	0.63
19:A:1110:CLA:C3D	19:A:1111:CLA:HMC3	2.29	0.63
19:A:1140:CLA:H62	19:A:9013:CLA:H193	1.79	0.63
2:B:225:LEU:C	2:B:227:THR:O	2.37	0.63
2:B:544:SER:O	2:B:547:MET:N	2.32	0.63
6:F:204:SER:C	6:F:207:LEU:HD12	2.19	0.63
6:F:206:LEU:O	6:F:209:ARG:HB2	1.99	0.63
19:R:1144:CLA:HED3	19:R:1144:CLA:C4D	2.28	0.63
17:3:131:GLU:O	17:3:134:LEU:N	2.17	0.63
18:4:86:GLU:CD	18:4:86:GLU:H	1.98	0.63
18:4:145:GLU:CG	18:4:146:PHE:CE1	2.78	0.63
1:A:98:PHE:HD1	1:A:99:HIS:H	1.43	0.63
1:A:448:TRP:CD1	19:A:1131:CLA:HED2	2.32	0.63
2:B:21:ILE:O	2:B:24:GLY:N	2.31	0.63
2:B:292:ARG:NE	2:B:297:ILE:O	2.31	0.63
2:B:348:VAL:HA	19:B:1215:CLA:H42	1.79	0.63
2:B:353:TYR:C	2:B:355:LEU:H	2.02	0.63
3:C:12:ILE:HD13	3:C:39:ILE:HG13	1.81	0.63
4:D:100:TYR:CD2	4:D:100:TYR:N	2.65	0.63
11:K:98:PRO:HD2	11:K:99:ALA:N	2.06	0.63
22:K:7041:LMU:H6'2	22:K:7042:LMU:H21	1.79	0.63
12:L:210:PRO:O	12:L:211:TYR:CB	2.46	0.63
15:1:225:TRP:CD1	15:1:226:HIS:CE1	2.86	0.63
16:2:233:MET:HA	16:2:236:TRP:HB2	1.80	0.63
1:A:210:LEU:HD12	19:A:1111:CLA:HMB2	1.81	0.63
1:A:370:ILE:HD11	19:A:1124:CLA:C3D	2.29	0.63
19:A:1113:CLA:CED	19:A:1113:CLA:HAA1	2.29	0.63
19:A:1119:CLA:H92	21:A:6007:BCR:H373	0.74	0.63
19:A:1124:CLA:HED2	19:A:1124:CLA:CAA	2.29	0.63
2:B:103:ALA:CA	2:B:105:THR:N	2.61	0.63
2:B:174:ARG:HH11	19:B:1221:CLA:HMD1	1.64	0.63
2:B:422:LEU:CD1	2:B:535:VAL:HG11	2.26	0.63
3:C:44:ARG:CB	4:D:182:GLN:NE2	2.51	0.63
4:D:112:PHE:O	4:D:119:ALA:CB	2.47	0.63
5:E:78:ARG:CD	5:E:78:ARG:H	2.11	0.63
7:G:93:GLU:OE2	7:G:98:THR:N	2.31	0.63
8:H:58:LEU:HD11	8:H:62:THR:CG2	1.92	0.63
11:K:70:PHE:CD1	11:K:70:PHE:O	2.51	0.63
12:L:131:SER:N	12:L:201:TYR:CZ	2.58	0.63
21:L:6019:BCR:H403	21:L:6019:BCR:H271	1.79	0.63
14:R:31:UNK:C	14:R:32:UNK:O	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:202:TYR:HB3	17:3:203:PRO:HD3	1.79	0.63
18:4:133:GLU:O	18:4:134:TYR:CD1	2.51	0.63
18:4:157:TRP:HB2	19:4:4012:CLA:CMA	2.29	0.63
18:4:172:PHE:CA	18:4:194:PHE:CE2	2.77	0.63
1:A:336:GLY:C	1:A:339:THR:OG1	2.36	0.62
1:A:364:MET:O	1:A:368:LEU:HB2	1.99	0.62
19:A:1111:CLA:HBA1	19:A:1123:CLA:C4	2.27	0.62
19:A:1134:CLA:H3A	19:A:1141:CLA:CBB	2.19	0.62
2:B:356:PRO:O	2:B:356:PRO:HD2	1.99	0.62
2:B:470:THR:H	2:B:502:ASN:H	1.45	0.62
2:B:598:HIS:HB3	2:B:602:TRP:CZ3	2.34	0.62
2:B:663:PHE:O	2:B:664:LEU:HG	1.99	0.62
19:B:1222:CLA:HBB1	19:B:1236:CLA:CMB	2.29	0.62
19:B:1227:CLA:HMB2	19:B:1228:CLA:CHB	2.28	0.62
19:B:1235:CLA:HHB	19:B:1236:CLA:OBD	1.98	0.62
3:C:7:ILE:O	3:C:8:TYR:C	2.36	0.62
4:D:158:PHE:CB	4:D:159:PRO:HD2	2.17	0.62
7:G:72:LEU:HD12	7:G:73:PHE:CZ	2.33	0.62
7:G:111:VAL:HG23	7:G:111:VAL:O	1.97	0.62
19:G:1242:CLA:H11	22:G:7026:LMU:H61	1.81	0.62
8:H:94:ARG:HH11	8:H:94:ARG:HB2	1.64	0.62
19:J:1311:CLA:H152	19:2:2014:CLA:HMB1	1.79	0.62
15:1:75:ASN:O	15:1:76:LEU:C	2.34	0.62
19:1:1008:CLA:HMA3	19:1:1008:CLA:HBA2	1.80	0.62
19:1:1010:CLA:HHD	19:1:1010:CLA:CBC	2.09	0.62
16:2:128:LYS:CB	16:2:131:ILE:HG23	2.29	0.62
16:2:171:ILE:CG1	16:2:173:ASN:HD21	2.12	0.62
16:2:247:ILE:O	16:2:248:ASP:HB2	1.98	0.62
18:4:90:TRP:O	18:4:91:PHE:CD1	2.52	0.62
1:A:105:ASN:OD1	1:A:118:PRO:CA	2.44	0.62
1:A:381:PRO:CB	19:A:1117:CLA:HAA2	2.29	0.62
1:A:681:GLY:HA2	1:A:684:PHE:HB3	1.79	0.62
1:A:723:ARG:HG2	1:A:723:ARG:NH1	2.13	0.62
22:A:7016:LMU:H31	22:A:7016:LMU:C1'	2.29	0.62
2:B:32:GLU:HG2	2:B:42:LEU:HD21	1.81	0.62
2:B:230:TRP:HH2	7:G:67:SER:HB2	1.64	0.62
2:B:459:PHE:HB2	19:B:1235:CLA:HBD	1.80	0.62
2:B:552:ASP:OD1	2:B:553:PHE:CE2	2.52	0.62
2:B:625:TRP:C	2:B:625:TRP:CD2	2.71	0.62
19:B:1220:CLA:O2D	19:B:1220:CLA:C2A	2.47	0.62
3:C:25:VAL:HA	3:C:43:PRO:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:85:LYS:O	5:E:86:GLY:C	2.37	0.62
6:F:89:LYS:O	6:F:92:ALA:N	2.32	0.62
6:F:173:TRP:HE3	6:F:210:GLY:C	2.01	0.62
22:H:7011:LMU:C6'	22:H:7011:LMU:H1B	2.28	0.62
11:K:56:ILE:CA	11:K:59:THR:HG23	2.29	0.62
11:K:127:ILE:O	11:K:130:LEU:CD2	2.47	0.62
12:L:86:LEU:HD12	12:L:86:LEU:H	1.64	0.62
15:1:78:ARG:O	15:1:81:GLU:HG2	1.98	0.62
15:1:138:LEU:HA	15:1:141:GLU:CG	2.29	0.62
16:2:201:PHE:CE1	16:2:202:ASP:HB3	2.34	0.62
19:4:4002:CLA:HMA2	19:4:4002:CLA:CGA	2.29	0.62
1:A:364:MET:O	1:A:368:LEU:N	2.32	0.62
1:A:389:TYR:CD1	1:A:625:TRP:CG	2.87	0.62
1:A:426:THR:CG2	1:A:428:TYR:HE2	2.04	0.62
19:A:1124:CLA:C6	19:A:1125:CLA:CED	2.77	0.62
2:B:269:TRP:HA	2:B:269:TRP:CE3	2.34	0.62
2:B:353:TYR:HB2	2:B:594:TRP:CH2	2.33	0.62
2:B:538:ALA:O	2:B:539:LEU:C	2.38	0.62
2:B:664:LEU:O	2:B:667:TRP:CZ3	2.52	0.62
2:B:691:ILE:O	2:B:691:ILE:HG22	1.98	0.62
3:C:11:CYS:SG	3:C:12:ILE:N	2.72	0.62
5:E:79:LYS:CB	5:E:84:TYR:CE1	2.82	0.62
5:E:103:VAL:CG2	5:E:104:VAL:O	2.47	0.62
6:F:101:LYS:O	6:F:103:GLN:N	2.32	0.62
22:H:7011:LMU:H111	22:H:7011:LMU:H72	1.81	0.62
19:J:1311:CLA:HBC3	19:J:1311:CLA:CHD	2.28	0.62
11:K:47:ASP:O	11:K:48:PHE:HB2	1.99	0.62
13:N:142:LYS:O	13:N:145:PHE:O	2.16	0.62
17:3:135:ALA:C	17:3:139:THR:OG1	2.38	0.62
18:4:146:PHE:HD1	18:4:146:PHE:N	1.97	0.62
18:4:223:VAL:O	18:4:224:THR:HG23	1.99	0.62
1:A:443:ILE:HG22	2:B:674:LEU:HD11	1.80	0.62
2:B:488:ALA:HB1	19:B:1233:CLA:C1C	2.29	0.62
6:F:200:VAL:HG11	10:J:7:TYR:CG	2.34	0.62
7:G:84:ARG:CD	7:G:85:GLU:HB3	2.30	0.62
7:G:139:TYR:O	7:G:139:TYR:CD1	2.52	0.62
9:I:9:VAL:CG1	9:I:10:PRO:HD3	2.29	0.62
13:N:142:LYS:CA	13:N:145:PHE:O	2.47	0.62
15:1:85:ILE:CG1	15:1:88:ARG:NH2	2.62	0.62
16:2:118:ALA:CB	16:2:121:PHE:HE2	2.11	0.62
16:2:137:TRP:O	16:2:139:THR:CG2	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:174:PRO:HB2	16:2:194:GLY:CA	2.22	0.62
17:3:113:ALA:HB2	17:3:239:LEU:HD12	1.70	0.62
17:3:148:TYR:CG	17:3:148:TYR:O	2.51	0.62
19:4:1304:CLA:CED	19:4:1304:CLA:CAA	2.66	0.62
1:A:284:ARG:HB2	1:A:295:TRP:HB2	1.80	0.62
1:A:747:TRP:CD2	21:A:6011:BCR:H401	2.34	0.62
2:B:144:PHE:CD2	2:B:144:PHE:O	2.52	0.62
2:B:207:VAL:HG13	2:B:207:VAL:O	1.99	0.62
2:B:550:LYS:O	2:B:550:LYS:CG	2.46	0.62
19:B:1222:CLA:CBB	19:B:1236:CLA:HHB	2.24	0.62
19:B:1222:CLA:HED2	19:B:1223:CLA:HMD1	1.81	0.62
5:E:107:PHE:CE2	5:E:109:LYS:CD	2.82	0.62
6:F:94:ARG:HA	6:F:94:ARG:HE	1.62	0.62
7:G:89:LYS:O	7:G:90:GLN:CB	2.48	0.62
8:H:86:THR:HG22	8:H:87:PHE:C	2.19	0.62
10:J:26:LEU:C	10:J:26:LEU:HD23	2.20	0.62
15:1:112:GLN:CG	15:1:113:GLU:N	2.62	0.62
16:2:98:SER:O	16:2:100:ARG:CB	2.47	0.62
1:A:57:LEU:O	1:A:61:ALA:HB2	1.99	0.62
19:A:1125:CLA:HBA2	21:A:6008:BCR:H12C	1.81	0.62
19:A:1151:CLA:O2D	19:A:1151:CLA:HBA2	2.00	0.62
21:A:6011:BCR:HC31	21:F:6014:BCR:H17C	1.81	0.62
2:B:98:GLN:HA	2:B:98:GLN:NE2	2.14	0.62
2:B:247:THR:N	2:B:250:ALA:HB2	2.15	0.62
2:B:255:LEU:H	2:B:271:THR:CG2	2.13	0.62
2:B:337:ALA:HA	19:B:1221:CLA:HAA1	1.82	0.62
2:B:379:ALA:O	2:B:383:MET:HG2	1.98	0.62
5:E:107:PHE:CD2	5:E:109:LYS:HD2	2.34	0.62
7:G:84:ARG:HG3	7:G:85:GLU:HB2	1.76	0.62
7:G:100:PHE:CD2	7:G:100:PHE:O	2.53	0.62
8:H:113:SER:CB	19:H:1207:CLA:H2	2.29	0.62
15:1:225:TRP:CB	15:1:226:HIS:HA	2.29	0.62
17:3:130:GLN:CA	17:3:132:THR:N	2.63	0.62
18:4:120:ILE:CG1	18:4:226:LYS:HG3	2.17	0.62
1:A:63:ASP:HB2	19:A:1128:CLA:CED	2.28	0.62
1:A:104:SER:C	1:A:106:TYR:H	2.02	0.62
1:A:123:VAL:O	1:A:124:TRP:HB2	1.99	0.62
1:A:150:PHE:C	1:A:151:GLN:HG3	2.19	0.62
1:A:159:THR:HG22	1:A:160:SER:H	1.64	0.62
1:A:733:VAL:CG2	19:A:1140:CLA:C3D	2.78	0.62
2:B:295:PHE:HE2	7:G:94:GLN:NE2	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:LYS:C	3:C:54:CYS:H	2.03	0.62
3:C:74:THR:HG23	3:C:75:ARG:N	2.13	0.62
4:D:140:LEU:CD2	4:D:144:LEU:HD11	2.30	0.62
6:F:103:GLN:OE1	6:F:103:GLN:HA	2.00	0.62
8:H:98:LEU:HG	8:H:98:LEU:O	1.99	0.62
10:J:5:LYS:HD2	16:2:178:ASN:CB	2.30	0.62
11:K:115:ILE:CD1	11:K:122:LEU:HD12	2.29	0.62
16:2:186:ASN:O	16:2:187:LYS:HB2	1.99	0.62
17:3:155:TYR:O	17:3:157:LEU:N	2.32	0.62
1:A:21:LEU:HD12	1:A:21:LEU:C	2.20	0.62
1:A:207:LEU:CD1	1:A:314:GLY:N	2.62	0.62
1:A:250:LEU:CG	17:3:136:TRP:CZ2	2.83	0.62
1:A:360:ILE:O	1:A:361:ASN:CB	2.47	0.62
1:A:452:PHE:CE1	19:A:1136:CLA:HBB2	2.34	0.62
1:A:485:GLN:N	1:A:485:GLN:OE1	2.32	0.62
1:A:532:ILE:O	1:A:533:PRO:C	2.34	0.62
19:A:1101:CLA:HBB2	19:A:1102:CLA:NC	2.15	0.62
2:B:686:PRO:HG2	19:L:1130:CLA:H12	1.82	0.62
3:C:14:CYS:SG	3:C:14:CYS:O	2.58	0.62
3:C:20:ALA:O	3:C:21:CYS:CB	2.47	0.62
3:C:58:CYS:HB3	23:C:8003:SF4:S2	2.40	0.62
4:D:167:HIS:NE2	4:D:172:VAL:HG13	2.02	0.62
4:D:172:VAL:O	4:D:173:TYR:CB	2.48	0.62
13:N:91:TYR:C	13:N:93:GLU:N	2.50	0.62
15:1:65:ASP:HA	15:1:69:LEU:HD13	1.80	0.62
19:1:1001:CLA:HMA2	19:1:1001:CLA:HBA1	1.82	0.62
19:2:2004:CLA:O1A	19:3:2009:CLA:CBC	2.48	0.62
17:3:204:GLY:CA	17:3:206:PRO:O	2.48	0.62
1:A:211:LEU:O	1:A:214:GLY:O	2.18	0.62
1:A:224:HIS:CE1	19:A:1113:CLA:C4C	2.83	0.62
1:A:229:ILE:CG2	1:A:229:ILE:O	2.46	0.62
1:A:298:ASP:OD2	1:A:298:ASP:N	2.32	0.62
1:A:351:THR:O	19:A:1123:CLA:H18	1.98	0.62
1:A:497:ALA:HB1	1:A:510:SER:OG	1.99	0.62
1:A:603:PHE:HZ	1:A:693:LEU:CD2	2.13	0.62
1:A:682:ALA:H	1:A:685:VAL:HG23	1.65	0.62
2:B:141:PHE:O	2:B:143:LEU:N	2.33	0.62
2:B:233:TYR:N	2:B:233:TYR:CD2	2.68	0.62
2:B:400:PRO:HD2	4:D:197:PRO:CD	2.29	0.62
2:B:438:VAL:HG23	19:B:1230:CLA:HAC1	1.82	0.62
19:B:1203:CLA:H191	19:B:1224:CLA:H141	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1221:CLA:HMA2	19:B:1221:CLA:H61	1.82	0.62
3:C:1:MET:CG	3:C:4:SER:OG	2.42	0.62
3:C:25:VAL:HA	3:C:43:PRO:HG2	1.79	0.62
3:C:39:ILE:HG12	3:C:40:ALA:H	1.65	0.62
9:I:24:LEU:C	9:I:26:LEU:N	2.51	0.62
13:N:110:THR:H	13:N:113:ASN:ND2	1.98	0.62
15:1:190:ASN:ND2	19:1:1002:CLA:ND	2.48	0.62
16:2:128:LYS:O	16:2:129:LEU:C	2.37	0.62
16:2:144:GLU:HA	16:2:144:GLU:OE2	1.97	0.62
16:2:156:GLU:HG3	16:2:157:LEU:HD13	1.74	0.62
16:2:266:PHE:CZ	16:2:267:THR:O	2.53	0.62
17:3:110:MET:O	17:3:113:ALA:CB	2.41	0.62
18:4:90:TRP:CD1	18:4:91:PHE:N	2.67	0.62
18:4:201:LYS:H	18:4:201:LYS:CD	2.12	0.62
1:A:93:LEU:N	1:A:96:MET:H	1.98	0.62
1:A:98:PHE:O	1:A:101:ALA:N	2.33	0.62
1:A:373:ALA:HB1	1:A:396:PHE:CD1	2.35	0.62
1:A:399:HIS:O	1:A:400:MET:HB2	2.00	0.62
19:A:1104:CLA:H51	19:A:1128:CLA:C4C	2.30	0.62
19:A:1115:CLA:CED	19:A:1115:CLA:C2A	2.44	0.62
19:A:1117:CLA:C20	19:A:1125:CLA:H3A	2.30	0.62
19:A:9023:CLA:H92	19:B:1239:CLA:HBB2	1.82	0.62
2:B:178:HIS:HE1	19:B:1210:CLA:NC	1.97	0.62
2:B:262:HIS:O	2:B:265:THR:O	2.18	0.62
4:D:93:LYS:CG	4:D:96:VAL:CG1	2.74	0.62
22:H:7043:LMU:H62	22:H:7043:LMU:C10	2.28	0.62
19:L:1503:CLA:CBC	19:L:1503:CLA:CHD	2.65	0.62
16:2:95:ASP:OD2	17:3:85:ASP:O	2.13	0.62
17:3:134:LEU:HD12	17:3:134:LEU:H	1.64	0.62
17:3:201:ALA:O	17:3:202:TYR:HB2	2.00	0.62
1:A:54:ILE:O	1:A:58:HIS:CD2	2.53	0.61
1:A:96:MET:CE	19:A:1106:CLA:HED2	2.29	0.61
1:A:126:ILE:O	1:A:127:VAL:CG2	2.41	0.61
1:A:227:LEU:HD22	1:A:296:LEU:O	1.99	0.61
1:A:578:ARG:CB	1:A:578:ARG:NH1	2.63	0.61
2:B:139:ALA:O	2:B:140:ILE:C	2.36	0.61
2:B:449:PRO:O	2:B:452:GLN:HB2	2.00	0.61
2:B:557:PHE:CD1	2:B:571:SER:HB3	2.34	0.61
2:B:663:PHE:O	2:B:664:LEU:HB2	1.99	0.61
2:B:685:THR:OG1	19:L:1130:CLA:C3A	2.47	0.61
19:B:1235:CLA:H202	21:F:6016:BCR:HC41	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:ARG:NE	4:D:182:GLN:HE21	1.97	0.61
4:D:142:THR:O	4:D:143:ARG:C	2.38	0.61
6:F:203:ALA:HB1	6:F:206:LEU:HD12	1.80	0.61
12:L:150:ILE:C	12:L:150:ILE:CD1	2.63	0.61
19:L:1503:CLA:HAA1	19:L:1503:CLA:O1D	2.00	0.61
13:N:148:ASP:N	13:N:149:ASP:C	2.53	0.61
15:1:170:PRO:HD2	15:1:173:TYR:HD2	1.56	0.61
17:3:151:TRP:HD1	17:3:151:TRP:N	1.93	0.61
22:4:7033:LMU:H3'	22:4:7033:LMU:H6'2	1.82	0.61
1:A:188:LYS:O	1:A:190:ALA:CB	2.43	0.61
1:A:193:LEU:O	1:A:196:PHE:CE2	2.52	0.61
1:A:389:TYR:CE1	1:A:625:TRP:CG	2.87	0.61
1:A:459:GLY:O	1:A:462:ILE:HG22	2.00	0.61
1:A:701:GLN:O	1:A:704:ILE:N	2.33	0.61
19:A:1117:CLA:OBD	19:A:1127:CLA:H43	2.01	0.61
19:A:1131:CLA:C16	21:L:6019:BCR:H361	2.29	0.61
2:B:278:LEU:HG	19:B:1213:CLA:HMA2	1.82	0.61
4:D:141:GLY:H	4:D:144:LEU:N	1.86	0.61
5:E:107:PHE:HD2	5:E:109:LYS:HD2	1.65	0.61
6:F:171:ALA:HA	6:F:174:ILE:HG12	1.80	0.61
11:K:110:GLY:O	11:K:114:HIS:CD2	2.53	0.61
13:N:147:SER:O	13:N:148:ASP:CB	2.48	0.61
15:1:93:ALA:CB	19:1:1006:CLA:C4B	2.78	0.61
16:2:104:GLN:H	16:2:104:GLN:CD	2.02	0.61
16:2:168:TRP:HA	16:2:171:ILE:CG2	2.19	0.61
17:3:192:LYS:HZ3	17:3:192:LYS:CA	2.12	0.61
17:3:202:TYR:CD2	17:3:202:TYR:N	2.67	0.61
17:3:243:ILE:CG1	19:3:3005:CLA:C3C	2.78	0.61
18:4:96:LEU:HD13	18:4:100:ARG:CZ	2.30	0.61
22:4:7052:LMU:H61	22:4:7052:LMU:C1	2.29	0.61
1:A:236:GLY:O	1:A:237:VAL:CG1	2.48	0.61
1:A:263:ALA:O	1:A:264:GLU:CG	2.47	0.61
1:A:302:HIS:HB2	19:A:1116:CLA:C1B	2.30	0.61
1:A:309:LEU:O	1:A:310:PHE:HB2	2.00	0.61
1:A:575:LEU:CD1	1:A:579:PHE:HB3	2.30	0.61
19:A:1119:CLA:HMC1	19:A:1119:CLA:CBC	2.29	0.61
19:A:1124:CLA:CHC	21:A:6008:BCR:H373	2.30	0.61
2:B:175:LEU:HD21	19:B:1216:CLA:CMA	2.30	0.61
2:B:298:GLY:HA2	19:B:1218:CLA:CMD	2.28	0.61
2:B:438:VAL:HG22	19:B:1230:CLA:HMC3	1.81	0.61
2:B:493:TRP:O	2:B:495:PRO:CD	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:525:LEU:HD23	2:B:525:LEU:O	1.99	0.61
3:C:42:ALA:HB1	3:C:43:PRO:CD	2.30	0.61
3:C:74:THR:OG1	3:C:80:ALA:HB2	2.00	0.61
3:C:74:THR:OG1	3:C:80:ALA:CB	2.48	0.61
6:F:157:TRP:HE3	19:F:1305:CLA:HMC2	1.65	0.61
22:H:7032:LMU:H3'	22:H:7032:LMU:C5B	2.29	0.61
12:L:204:LEU:HD13	12:L:205:TYR:C	2.19	0.61
15:1:112:GLN:O	15:1:113:GLU:HB2	2.00	0.61
15:1:184:LYS:HE3	19:1:1001:CLA:OBD	2.00	0.61
16:2:104:GLN:OE1	16:2:104:GLN:N	2.33	0.61
16:2:160:ILE:O	16:2:163:ALA:N	2.34	0.61
16:2:172:LEU:CA	16:2:173:ASN:ND2	2.62	0.61
19:2:2007:CLA:H2A	19:2:2007:CLA:O1D	2.01	0.61
19:2:4009:CLA:H18	19:2:4009:CLA:ND	2.14	0.61
18:4:87:ASN:ND2	18:4:90:TRP:CZ2	2.68	0.61
1:A:93:LEU:HA	1:A:96:MET:N	2.15	0.61
1:A:483:GLN:HB3	1:A:485:GLN:HE22	1.61	0.61
19:A:1112:CLA:C3B	21:A:6002:BCR:C19	2.72	0.61
19:A:1124:CLA:H52	19:A:1125:CLA:HED1	1.81	0.61
19:A:1237:CLA:H152	21:B:6020:BCR:H352	1.80	0.61
2:B:120:VAL:HG13	2:B:123:TRP:CD1	2.35	0.61
2:B:202:SER:C	2:B:204:GLY:H	2.03	0.61
2:B:266:GLN:O	2:B:267:SER:HB3	1.98	0.61
2:B:544:SER:N	2:B:547:MET:O	2.34	0.61
2:B:714:SER:O	2:B:718:ILE:HG22	2.01	0.61
19:B:1215:CLA:CGA	19:B:1215:CLA:C3A	2.77	0.61
19:B:1227:CLA:HED2	19:B:1227:CLA:CAA	2.30	0.61
3:C:72:GLU:OE2	3:C:77:MET:HE1	2.00	0.61
4:D:80:SER:N	4:D:81:PRO:HD3	2.16	0.61
4:D:83:PHE:CE1	4:D:114:MET:HE2	2.35	0.61
21:F:6016:BCR:H403	21:F:6016:BCR:C27	2.30	0.61
9:I:14:LEU:C	9:I:17:PRO:HD2	2.20	0.61
11:K:60:SER:CA	11:K:63:LEU:HD21	2.28	0.61
12:L:201:TYR:O	12:L:202:PHE:C	2.37	0.61
13:N:112:ALA:N	13:N:118:TYR:CD1	2.69	0.61
13:N:147:SER:C	13:N:149:ASP:HB2	2.21	0.61
15:1:184:LYS:CE	19:1:1001:CLA:OBD	2.47	0.61
17:3:204:GLY:HA3	17:3:207:PHE:C	2.20	0.61
17:3:238:ILE:CG1	19:3:3003:CLA:HMC2	2.31	0.61
18:4:243:THR:HG23	18:4:244:ILE:C	2.20	0.61
22:4:7034:LMU:C10	22:4:7052:LMU:O3'	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:O	1:A:259:TYR:CD2	2.54	0.61
1:A:304:LEU:HG	19:A:1115:CLA:HBB2	1.82	0.61
1:A:379:MET:HE2	19:A:1125:CLA:HMC2	1.80	0.61
1:A:438:HIS:CE1	1:A:442:ILE:HD11	2.35	0.61
1:A:554:LEU:HD21	19:A:9023:CLA:O2D	1.99	0.61
1:A:604:TRP:HE1	19:A:9023:CLA:C1D	2.14	0.61
19:A:1116:CLA:HMC1	19:A:1116:CLA:HBC3	1.81	0.61
2:B:293:THR:O	2:B:295:PHE:HD2	1.82	0.61
2:B:421:HIS:NE2	19:B:1228:CLA:C4D	2.63	0.61
6:F:101:LYS:O	6:F:102:LEU:C	2.38	0.61
6:F:228:ASP:O	6:F:231:PHE:CB	2.49	0.61
7:G:76:ARG:NH2	7:G:117:ASN:C	2.54	0.61
19:1:1005:CLA:HMC3	19:1:1012:CLA:CAC	2.29	0.61
21:3:6022:BCR:C8	21:3:6022:BCR:H311	2.29	0.61
18:4:177:LEU:N	18:4:178:PRO:HD2	2.16	0.61
18:4:201:LYS:N	18:4:201:LYS:CD	2.63	0.61
1:A:296:LEU:HD12	1:A:297:THR:N	2.16	0.61
1:A:296:LEU:C	1:A:296:LEU:CD1	2.69	0.61
1:A:618:TRP:CZ2	1:A:655:ASP:HB2	2.35	0.61
1:A:700:TRP:CZ3	19:A:9013:CLA:O1D	2.53	0.61
19:A:1103:CLA:H42	21:A:6003:BCR:H313	1.82	0.61
19:A:1131:CLA:HAA1	21:B:6020:BCR:C13	2.30	0.61
22:A:7010:LMU:O6'	22:K:7047:LMU:H111	2.00	0.61
2:B:552:ASP:OD1	2:B:553:PHE:HD2	1.82	0.61
3:C:62:PHE:CG	4:D:191:ILE:CG2	2.84	0.61
4:D:173:TYR:O	4:D:173:TYR:CD2	2.52	0.61
6:F:204:SER:O	6:F:206:LEU:N	2.33	0.61
8:H:67:SER:C	8:H:68:TYR:CD2	2.74	0.61
16:2:133:ASN:HD21	16:2:134:THR:CB	2.10	0.61
16:2:154:ILE:O	16:2:158:VAL:HG12	2.01	0.61
16:2:160:ILE:CG2	19:2:2012:CLA:HBB2	2.11	0.61
17:3:130:GLN:C	17:3:132:THR:N	2.49	0.61
18:4:115:PHE:O	18:4:116:THR:C	2.38	0.61
18:4:142:PHE:HA	18:4:145:GLU:CD	2.20	0.61
1:A:375:HIS:CE1	19:A:1125:CLA:NC	2.69	0.61
1:A:648:THR:CG2	1:A:651:GLY:H	2.09	0.61
1:A:707:ILE:O	1:A:711:HIS:CD2	2.53	0.61
19:A:1106:CLA:H142	21:J:6012:BCR:C14	2.31	0.61
19:A:1119:CLA:CMD	19:A:1121:CLA:CBB	2.64	0.61
2:B:8:PHE:O	2:B:35:ASP:OD2	2.18	0.61
2:B:98:GLN:O	2:B:100:ALA:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:LEU:HD12	2:B:317:ARG:N	2.15	0.61
2:B:378:ILE:HA	2:B:381:PHE:HB2	1.82	0.61
2:B:480:SER:O	2:B:481:THR:CG2	2.45	0.61
2:B:607:SER:O	2:B:610:ASN:CB	2.49	0.61
2:B:623:TYR:H	2:B:626:LEU:HB2	1.66	0.61
2:B:638:LEU:C	2:B:639:VAL:HG12	2.21	0.61
19:B:1220:CLA:HAA2	19:B:1220:CLA:HBD	1.81	0.61
19:F:1302:CLA:C3B	19:F:1305:CLA:CAC	2.68	0.61
19:K:1142:CLA:HMD1	19:K:1143:CLA:C1A	2.30	0.61
12:L:51:LYS:CA	12:L:51:LYS:CE	2.75	0.61
15:1:158:PRO:CA	15:1:175:LYS:HG3	2.26	0.61
17:3:98:LEU:O	17:3:99:ALA:C	2.39	0.61
1:A:690:LEU:HD21	1:A:738:TYR:HE1	1.66	0.61
2:B:123:TRP:CB	2:B:126:THR:HG22	2.26	0.61
2:B:390:GLY:N	2:B:391:PRO:CD	2.64	0.61
2:B:558:PRO:HG2	2:B:703:VAL:CG1	2.31	0.61
2:B:633:ASN:CG	2:B:636:THR:HB	2.19	0.61
2:B:692:ARG:HH22	2:B:694:ARG:NH2	1.98	0.61
2:B:696:LYS:HG2	3:C:80:ALA:CA	2.24	0.61
3:C:51:CYS:N	23:C:8002:SF4:S4	2.63	0.61
3:C:78:GLY:O	3:C:81:TYR:HE1	1.84	0.61
4:D:82:ILE:O	4:D:82:ILE:CG1	2.46	0.61
4:D:156:ARG:HB2	4:D:166:LEU:HD12	1.81	0.61
13:N:130:ASN:HB2	13:N:139:LYS:HD3	1.80	0.61
22:R:7020:LMU:H5B	22:R:7020:LMU:O6'	1.99	0.61
15:1:177:PRO:CG	15:1:180:LEU:HD23	2.31	0.61
17:3:156:THR:O	17:3:158:PHE:O	2.18	0.61
1:A:284:ARG:CB	1:A:295:TRP:CD1	2.84	0.61
1:A:393:LEU:CD1	1:A:750:PHE:CE1	2.83	0.61
19:A:1120:CLA:CAD	19:A:1121:CLA:HMA1	2.31	0.61
19:A:1122:CLA:HBC1	21:A:6007:BCR:H393	1.83	0.61
19:A:1134:CLA:O1A	19:A:1141:CLA:CBB	2.49	0.61
2:B:426:SER:O	2:B:430:GLY:N	2.33	0.61
2:B:668:ARG:HG3	2:B:699:ALA:O	2.01	0.61
19:K:1146:CLA:O1A	19:K:1146:CLA:C2A	2.48	0.61
12:L:106:HIS:HD2	19:L:1502:CLA:HED1	1.64	0.61
12:L:209:LEU:O	12:L:210:PRO:C	2.38	0.61
15:1:67:LEU:CD1	15:1:68:GLY:H	2.10	0.61
1:A:342:GLY:O	1:A:343:HIS:C	2.39	0.61
1:A:716:VAL:O	19:A:1139:CLA:HMD3	2.01	0.61
2:B:75:GLU:HB3	2:B:132:ASN:HD22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:GLN:O	2:B:126:THR:CA	2.49	0.61
2:B:178:HIS:O	2:B:180:SER:N	2.34	0.61
2:B:463:ILE:O	2:B:464:GLN:CB	2.49	0.61
2:B:469:LYS:CD	2:B:470:THR:HG23	2.30	0.61
11:K:76:ALA:HA	11:K:78:ARG:HH11	1.65	0.61
12:L:82:TYR:CE1	19:L:1130:CLA:H93	2.35	0.61
13:N:143:VAL:HG12	13:N:144:PRO:CD	2.31	0.61
22:R:7007:LMU:H1'	22:R:7007:LMU:O6'	2.00	0.61
15:1:77:GLU:O	15:1:80:LYS:CG	2.41	0.61
19:1:1014:CLA:C5	19:1:1014:CLA:H101	2.29	0.61
16:2:101:TRP:N	16:2:103:VAL:N	2.49	0.61
19:4:4002:CLA:HAA2	19:4:4002:CLA:O1D	2.01	0.61
1:A:76:ARG:O	1:A:186:TYR:HD2	1.84	0.60
1:A:101:ALA:HB1	1:A:161:GLU:O	2.01	0.60
1:A:545:HIS:HB3	19:A:1135:CLA:CBB	2.30	0.60
2:B:681:ALA:O	2:B:684:ARG:N	2.33	0.60
19:B:1222:CLA:HMB2	19:B:1236:CLA:O1A	1.99	0.60
3:C:12:ILE:CG2	3:C:38:GLN:O	2.49	0.60
3:C:24:ASP:O	3:C:43:PRO:HG2	2.01	0.60
6:F:152:GLY:O	19:F:1302:CLA:HAC2	2.00	0.60
10:J:5:LYS:CD	16:2:178:ASN:HA	2.28	0.60
19:J:1308:CLA:CHD	19:J:1308:CLA:HBC3	2.25	0.60
14:R:41:UNK:CA	14:R:42:UNK:CB	2.77	0.60
16:2:155:VAL:O	16:2:158:VAL:HG13	2.01	0.60
16:2:172:LEU:CB	16:2:173:ASN:HD22	2.13	0.60
18:4:158:GLN:CD	19:4:1004:CLA:O1D	2.37	0.60
18:4:174:GLN:C	18:4:176:SER:N	2.49	0.60
1:A:107:GLU:CD	1:A:161:GLU:HG3	2.21	0.60
1:A:207:LEU:O	1:A:310:PHE:CB	2.49	0.60
1:A:346:LEU:O	1:A:346:LEU:HD22	2.01	0.60
1:A:425:THR:O	1:A:427:ARG:NE	2.33	0.60
1:A:534:LEU:HD12	1:A:535:GLY:CA	2.26	0.60
1:A:723:ARG:HH11	1:A:723:ARG:HG3	1.65	0.60
2:B:27:THR:O	2:B:28:ALA:C	2.39	0.60
2:B:230:TRP:O	2:B:231:ASN:C	2.39	0.60
2:B:440:ASN:OD1	2:B:614:THR:HG23	1.96	0.60
2:B:553:PHE:CD1	2:B:557:PHE:HB3	2.36	0.60
2:B:664:LEU:O	2:B:667:TRP:HZ3	1.84	0.60
3:C:9:ASP:OD1	3:C:61:ASP:OD2	2.19	0.60
4:D:208:TYR:CG	4:D:208:TYR:O	2.53	0.60
7:G:100:PHE:H	7:G:101:GLU:HB2	1.62	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:81:SER:O	8:H:82:LYS:C	2.37	0.60
14:R:35:UNK:C	14:R:38:UNK:CB	2.79	0.60
15:1:169:ASP:OD2	15:1:170:PRO:HD2	2.00	0.60
15:1:189:LYS:HE2	15:1:189:LYS:N	2.16	0.60
16:2:167:ARG:CA	16:2:167:ARG:HE	2.13	0.60
17:3:131:GLU:O	17:3:134:LEU:HD12	2.02	0.60
18:4:89:ARG:NH1	18:4:90:TRP:HA	2.16	0.60
1:A:68:THR:HG22	1:A:70:ASP:N	2.14	0.60
1:A:174:PHE:O	1:A:175:ALA:HB2	2.01	0.60
1:A:246:HIS:ND1	1:A:246:HIS:N	2.50	0.60
1:A:362:LEU:HD11	19:A:1128:CLA:HBB2	1.84	0.60
1:A:679:PHE:HE1	1:A:749:PHE:HB2	1.66	0.60
19:A:1132:CLA:H41	12:L:110:LEU:HD23	1.82	0.60
19:A:1141:CLA:HBC3	19:A:1141:CLA:CHD	2.32	0.60
19:A:9012:CLA:HMB3	19:B:9010:CLA:C18	2.30	0.60
2:B:25:ILE:CG2	21:L:6019:BCR:C29	2.77	0.60
2:B:302:LYS:O	2:B:303:TYR:CB	2.37	0.60
2:B:553:PHE:O	2:B:554:GLY:O	2.19	0.60
2:B:704:GLN:O	2:B:708:VAL:HG23	2.02	0.60
2:B:715:VAL:HG13	2:B:719:PHE:HD2	1.64	0.60
19:B:1216:CLA:HBB2	19:B:1221:CLA:H41	1.83	0.60
7:G:76:ARG:NH2	7:G:117:ASN:CA	2.64	0.60
7:G:128:LEU:C	7:G:128:LEU:CD2	2.70	0.60
11:K:56:ILE:CG2	11:K:59:THR:HG23	2.28	0.60
12:L:142:SER:O	12:L:143:LEU:HD23	2.01	0.60
13:N:145:PHE:CA	13:N:146:LEU:O	2.49	0.60
16:2:101:TRP:HA	16:2:103:VAL:H	1.64	0.60
22:4:7034:LMU:C10	22:4:7052:LMU:C2'	2.78	0.60
1:A:23:ASP:CB	1:A:33:GLN:OE1	2.50	0.60
1:A:50:THR:CG2	1:A:51:THR:H	2.15	0.60
1:A:250:LEU:CG	17:3:136:TRP:HZ2	2.15	0.60
1:A:442:ILE:CG2	19:A:1129:CLA:HMC3	2.31	0.60
19:A:1115:CLA:H141	19:A:1115:CLA:C17	2.13	0.60
21:A:6008:BCR:C33	21:A:6008:BCR:C8	2.75	0.60
19:A:9012:CLA:H11	2:B:616:LEU:CB	2.30	0.60
2:B:469:LYS:NZ	2:B:471:THR:C	2.55	0.60
2:B:478:LEU:O	2:B:478:LEU:CD2	2.44	0.60
19:B:1212:CLA:H2A	19:B:1212:CLA:O1D	2.02	0.60
4:D:156:ARG:CZ	4:D:164:GLN:HB2	2.32	0.60
5:E:78:ARG:CZ	5:E:125:ILE:HG22	2.32	0.60
5:E:82:TYR:CB	5:E:83:TRP:CZ3	2.72	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:207:LEU:N	6:F:207:LEU:CD1	2.64	0.60
7:G:144:THR:OG1	7:G:148:GLY:N	2.34	0.60
11:K:47:ASP:N	11:K:51:SER:HB2	2.17	0.60
15:1:85:ILE:HA	15:1:88:ARG:NE	2.14	0.60
15:1:150:HIS:NE2	15:1:151:GLN:NE2	2.47	0.60
16:2:122:ILE:N	16:2:123:PRO:CD	2.64	0.60
16:2:152:LEU:HD22	16:2:152:LEU:C	2.21	0.60
18:4:149:SER:CB	18:4:153:GLU:OE1	2.50	0.60
18:4:174:GLN:C	18:4:176:SER:H	2.03	0.60
1:A:34:TRP:O	1:A:35:ALA:CB	2.49	0.60
1:A:206:HIS:O	1:A:211:LEU:HD23	2.00	0.60
1:A:287:LEU:HD22	1:A:292:GLY:O	2.00	0.60
1:A:327:ILE:O	1:A:328:LYS:C	2.37	0.60
1:A:331:LEU:CD2	1:A:331:LEU:C	2.69	0.60
1:A:704:ILE:HA	1:A:707:ILE:HG13	1.83	0.60
1:A:725:LEU:HD21	19:A:1140:CLA:HMD3	1.83	0.60
1:A:735:VAL:O	1:A:739:LEU:HG	2.00	0.60
2:B:294:ASN:CG	7:G:94:GLN:CG	2.57	0.60
2:B:652:PHE:O	2:B:656:VAL:HG23	2.00	0.60
19:B:1212:CLA:HMA1	21:B:6006:BCR:H372	1.83	0.60
21:B:6010:BCR:H23C	21:B:6010:BCR:C38	2.27	0.60
4:D:112:PHE:C	4:D:112:PHE:CD2	2.75	0.60
5:E:107:PHE:CD2	5:E:109:LYS:CE	2.84	0.60
7:G:83:GLN:O	7:G:84:ARG:HB3	2.01	0.60
19:H:1145:CLA:H143	19:H:1145:CLA:C19	2.29	0.60
9:I:8:PHE:CE1	19:I:1204:CLA:H43	2.36	0.60
15:1:143:LEU:N	15:1:143:LEU:CD1	2.63	0.60
15:1:170:PRO:HG2	15:1:171:LEU:C	2.22	0.60
16:2:130:GLY:CA	16:2:131:ILE:HG12	1.99	0.60
16:2:184:PRO:CB	16:2:187:LYS:CD	2.68	0.60
16:2:184:PRO:N	16:2:185:ASN:HA	2.16	0.60
16:2:266:PHE:CG	16:2:267:THR:N	2.70	0.60
22:2:7031:LMU:H4'	22:2:7031:LMU:O2B	2.01	0.60
17:3:150:TYR:C	17:3:152:ALA:H	2.01	0.60
18:4:127:TYR:CD1	18:4:127:TYR:O	2.54	0.60
18:4:205:ILE:HG13	18:4:206:ALA:N	2.14	0.60
1:A:109:TRP:O	1:A:113:PRO:N	2.35	0.60
1:A:242:ILE:HG13	1:A:243:PRO:HD3	0.74	0.60
2:B:131:THR:CG2	2:B:134:ASP:CB	2.74	0.60
2:B:131:THR:O	2:B:134:ASP:N	2.34	0.60
2:B:159:PRO:O	2:B:160:LYS:C	2.38	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:TRP:HH2	19:B:1232:CLA:HMA2	1.61	0.60
19:B:1239:CLA:H151	12:L:144:CYS:SG	2.42	0.60
4:D:148:TYR:C	4:D:149:LYS:HG2	2.22	0.60
5:E:107:PHE:HD2	5:E:109:LYS:CD	2.12	0.60
5:E:127:GLU:CD	5:E:129:GLU:O	2.40	0.60
7:G:144:THR:HG23	7:G:144:THR:O	2.01	0.60
13:N:127:PHE:CD2	13:N:127:PHE:N	2.68	0.60
15:1:97:ILE:HD11	15:1:98:LEU:CD2	2.27	0.60
16:2:154:ILE:O	16:2:158:VAL:CG1	2.49	0.60
22:2:7006:LMU:H22	22:2:7006:LMU:O2'	2.01	0.60
17:3:104:ILE:HG21	19:3:3004:CLA:C2D	2.30	0.60
17:3:150:TYR:CG	17:3:151:TRP:NE1	2.47	0.60
17:3:245:GLY:C	17:3:246:LEU:HD22	2.22	0.60
19:4:4006:CLA:CMA	22:4:7034:LMU:H62	2.23	0.60
1:A:479:ASP:CG	1:A:536:THR:CG2	2.70	0.60
19:A:1141:CLA:H121	19:A:1141:CLA:H72	1.79	0.60
19:A:9012:CLA:H122	19:A:9012:CLA:H92	1.83	0.60
2:B:31:PHE:HB2	2:B:42:LEU:CD1	2.32	0.60
2:B:141:PHE:HD2	2:B:144:PHE:CE1	2.20	0.60
2:B:315:LEU:HD11	2:B:317:ARG:CD	2.30	0.60
2:B:493:TRP:CZ2	19:B:1214:CLA:H122	2.36	0.60
2:B:686:PRO:HD2	19:L:1130:CLA:O1A	2.01	0.60
4:D:87:THR:H	12:L:69:LEU:HD11	1.67	0.60
5:E:110:VAL:O	5:E:111:ASN:HB3	2.00	0.60
7:G:94:GLN:O	7:G:97:LEU:CD2	2.46	0.60
7:G:131:GLY:CA	7:G:136:VAL:CG2	2.75	0.60
7:G:145:THR:CG2	7:G:146:SER:H	2.13	0.60
14:R:35:UNK:N	14:R:38:UNK:CB	2.65	0.60
15:1:64:PHE:C	15:1:69:LEU:CD1	2.70	0.60
19:3:3008:CLA:O1A	19:3:3008:CLA:HED3	2.01	0.60
1:A:92:TRP:CD1	19:A:1105:CLA:CBB	2.83	0.60
1:A:281:LEU:CG	19:A:1115:CLA:HED2	2.23	0.60
1:A:281:LEU:O	1:A:282:THR:C	2.38	0.60
1:A:707:ILE:C	1:A:711:HIS:HD2	2.05	0.60
2:B:349:ALA:CB	2:B:375:HIS:HB3	2.31	0.60
2:B:443:MET:O	2:B:446:PHE:CB	2.48	0.60
19:B:1206:CLA:H143	19:B:1224:CLA:H18	1.83	0.60
4:D:95:GLN:CG	4:D:96:VAL:N	2.63	0.60
5:E:129:GLU:OE1	5:E:129:GLU:HA	2.00	0.60
6:F:129:ARG:HB3	6:F:133:TYR:CE1	2.37	0.60
12:L:153:PHE:O	12:L:178:THR:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:7029:LMU:O2B	22:L:7029:LMU:C6'	2.50	0.60
15:1:150:HIS:C	15:1:150:HIS:ND1	2.53	0.60
15:1:179:LYS:CG	15:1:180:LEU:O	2.49	0.60
1:A:29:THR:OG1	1:A:31:PHE:HB2	2.02	0.60
1:A:343:HIS:HA	1:A:431:LEU:HD22	1.83	0.60
21:A:6008:BCR:HC8	21:A:6008:BCR:H331	1.82	0.60
19:A:9022:CLA:C13	19:B:1206:CLA:HBB2	2.32	0.60
2:B:4:ARG:C	2:B:4:ARG:NE	2.55	0.60
2:B:275:HIS:HD1	19:B:1214:CLA:HMB1	1.65	0.60
3:C:43:PRO:CA	4:D:182:GLN:HG3	2.32	0.60
4:D:114:MET:HG3	4:D:115:PRO:N	2.17	0.60
5:E:72:ALA:O	5:E:73:LYS:HB3	2.02	0.60
19:F:1305:CLA:H42	19:4:1306:CLA:CAA	2.25	0.60
11:K:62:SER:HG	11:K:63:LEU:HD13	1.62	0.60
12:L:169:ARG:HG2	12:L:172:GLU:HA	1.84	0.60
13:N:132:THR:CG2	13:N:139:LYS:CD	2.46	0.60
13:N:165:ASN:OD1	13:N:167:PHE:CA	2.49	0.60
22:R:7014:LMU:H11	22:R:7014:LMU:C6	2.22	0.60
16:2:112:TRP:HZ3	16:2:164:GLU:HG3	1.66	0.60
17:3:191:GLU:O	17:3:191:GLU:CG	2.49	0.60
2:B:508:LEU:CB	2:B:509:PHE:CD2	2.85	0.60
2:B:732:LYS:CG	2:B:733:PHE:CA	2.78	0.60
3:C:62:PHE:HZ	5:E:80:GLU:OE2	1.74	0.60
4:D:96:VAL:O	4:D:96:VAL:HG22	2.00	0.60
6:F:207:LEU:CD2	6:F:208:PHE:CB	2.80	0.60
6:F:228:ASP:HA	6:F:231:PHE:HB3	1.84	0.60
7:G:105:THR:OG1	7:G:106:ARG:N	2.34	0.60
8:H:60:ASN:O	8:H:62:THR:HA	2.01	0.60
8:H:62:THR:H	8:H:63:GLY:HA2	1.67	0.60
8:H:89:ALA:O	8:H:93:LYS:N	2.32	0.60
12:L:155:GLU:CA	12:L:178:THR:CG2	2.75	0.60
14:R:4:UNK:O	14:R:5:UNK:CB	2.50	0.60
15:1:114:TRP:HH2	15:1:121:GLN:HA	1.65	0.60
16:2:223:LYS:O	16:2:226:ARG:CB	2.50	0.60
18:4:161:LYS:HD2	18:4:161:LYS:C	2.22	0.60
1:A:84:GLY:O	1:A:87:SER:O	2.19	0.59
1:A:107:GLU:HA	1:A:110:LEU:HD21	1.83	0.59
1:A:158:ILE:HG13	1:A:163:GLN:HE22	1.65	0.59
1:A:165:TYR:CD2	1:A:165:TYR:O	2.55	0.59
1:A:253:ASP:HB3	1:A:254:LEU:HD22	1.83	0.59
1:A:266:ALA:O	1:A:267:THR:C	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ASP:CA	1:A:536:THR:HG21	2.21	0.59
2:B:246:THR:O	2:B:246:THR:HG23	2.00	0.59
2:B:438:VAL:O	2:B:441:ASP:N	2.35	0.59
2:B:607:SER:O	2:B:610:ASN:N	2.35	0.59
22:B:7038:LMU:C6	22:B:7038:LMU:H101	2.31	0.59
22:B:7040:LMU:O3'	22:B:7040:LMU:C1B	2.50	0.59
3:C:55:GLU:C	3:C:57:ALA:N	2.50	0.59
6:F:159:GLU:CG	10:J:38:ILE:HG12	2.31	0.59
6:F:167:PHE:HA	21:F:6014:BCR:H392	1.84	0.59
19:L:1148:CLA:C2	19:L:1148:CLA:O1A	2.50	0.59
15:1:95:PRO:HA	15:1:98:LEU:CB	2.31	0.59
15:1:157:ASP:CB	15:1:178:LYS:HB2	2.23	0.59
15:1:170:PRO:O	15:1:171:LEU:HD23	2.02	0.59
16:2:183:PHE:CA	16:2:187:LYS:HG2	2.31	0.59
18:4:103:MET:CE	18:4:207:ASN:O	2.48	0.59
18:4:221:HIS:O	18:4:224:THR:N	2.33	0.59
1:A:195:TRP:CH2	19:A:1108:CLA:HMA1	2.38	0.59
1:A:361:ASN:O	1:A:365:LEU:N	2.34	0.59
1:A:580:PRO:HB3	1:A:727:ILE:HG21	1.84	0.59
21:A:6002:BCR:H402	21:A:6002:BCR:H23C	1.83	0.59
2:B:222:LEU:HD13	2:B:225:LEU:HD23	1.84	0.59
3:C:52:LYS:C	3:C:54:CYS:N	2.54	0.59
22:D:7050:LMU:O2B	22:D:7050:LMU:C4'	2.46	0.59
5:E:78:ARG:HD2	5:E:78:ARG:H	1.66	0.59
5:E:121:ALA:O	5:E:125:ILE:CG2	2.50	0.59
19:F:1302:CLA:H2A	19:F:1302:CLA:O1D	2.02	0.59
7:G:88:ALA:O	7:G:90:GLN:O	2.20	0.59
8:H:94:ARG:NH2	8:H:97:LEU:O	2.35	0.59
19:2:2001:CLA:C4	19:2:2001:CLA:O2A	2.50	0.59
18:4:90:TRP:O	18:4:91:PHE:HD1	1.84	0.59
18:4:165:SER:O	18:4:168:GLN:N	2.34	0.59
1:A:90:PHE:CE1	19:A:1103:CLA:C9	2.82	0.59
1:A:447:ASN:ND2	2:B:678:LEU:HD21	2.17	0.59
19:A:1126:CLA:H171	21:J:6012:BCR:H15C	1.83	0.59
20:A:5001:PQN:H142	21:F:6014:BCR:HC22	1.83	0.59
2:B:126:THR:OG1	2:B:358:TYR:CD1	2.49	0.59
2:B:180:SER:OG	2:B:181:GLY:N	2.35	0.59
2:B:189:ALA:HB2	19:B:1225:CLA:C20	2.26	0.59
2:B:378:ILE:HG22	2:B:379:ALA:H	1.66	0.59
21:B:6020:BCR:C33	21:B:6020:BCR:C8	2.77	0.59
5:E:78:ARG:HB2	5:E:80:GLU:OE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:105:SER:HB2	6:F:108:LEU:HD13	1.83	0.59
7:G:82:PHE:HB2	7:G:83:GLN:HG2	1.84	0.59
12:L:74:THR:HG22	12:L:75:SER:CB	2.31	0.59
13:N:169:LYS:HA	13:N:170:TRP:CD1	2.37	0.59
16:2:164:GLU:HG2	19:2:2012:CLA:HMA3	1.84	0.59
16:2:240:ILE:HG23	16:2:263:PHE:CB	2.27	0.59
19:2:2002:CLA:H2A	19:2:2002:CLA:O1D	2.02	0.59
1:A:112:ASP:HB3	1:A:116:ILE:HD11	1.84	0.59
1:A:130:GLU:OE1	1:A:130:GLU:HA	2.02	0.59
1:A:308:ILE:CD1	19:A:1115:CLA:CBB	2.77	0.59
1:A:472:ARG:HH12	12:L:120:LEU:CD2	2.10	0.59
1:A:679:PHE:O	1:A:683:HIS:HB2	2.03	0.59
19:A:1106:CLA:HBB1	19:A:1126:CLA:H151	1.84	0.59
19:A:1237:CLA:HAA2	19:L:1130:CLA:HMB1	1.84	0.59
2:B:32:GLU:HG2	2:B:42:LEU:HD22	1.85	0.59
2:B:46:ILE:HD11	19:B:1202:CLA:H192	1.83	0.59
2:B:89:HIS:CA	2:B:113:VAL:HG11	2.22	0.59
2:B:463:ILE:O	2:B:464:GLN:HG2	2.01	0.59
2:B:618:GLY:HA2	2:B:621:ARG:H	1.67	0.59
6:F:180:SER:C	6:F:182:LEU:N	2.56	0.59
6:F:225:GLU:N	6:F:227:VAL:CG1	2.64	0.59
8:H:79:LEU:O	8:H:80:GLN:C	2.40	0.59
11:K:118:VAL:O	11:K:121:VAL:HG22	1.99	0.59
15:1:81:GLU:C	15:1:83:GLU:H	2.05	0.59
15:1:189:LYS:HB3	19:1:1007:CLA:HMC2	1.77	0.59
15:1:193:LEU:C	15:1:193:LEU:CD2	2.68	0.59
17:3:154:ASN:C	17:3:155:TYR:CG	2.75	0.59
18:4:87:ASN:OD1	18:4:88:LEU:N	2.35	0.59
22:4:7052:LMU:O1'	22:4:7052:LMU:C6	2.45	0.59
1:A:23:ASP:OD1	1:A:33:GLN:CG	2.51	0.59
1:A:60:ASP:CG	1:A:60:ASP:O	2.40	0.59
1:A:73:GLU:HB2	1:A:186:TYR:HE2	1.67	0.59
1:A:368:LEU:HD21	19:A:1117:CLA:H91	1.75	0.59
1:A:451:ILE:HD12	19:A:1131:CLA:CED	2.03	0.59
1:A:472:ARG:O	1:A:474:GLN:N	2.36	0.59
19:A:1151:CLA:HBA2	19:A:1151:CLA:CED	2.32	0.59
2:B:549:ASP:CG	3:C:63:LEU:HB2	2.22	0.59
20:B:5002:PQN:H291	24:B:7101:LMG:H201	1.83	0.59
4:D:162:GLU:O	4:D:163:VAL:CG2	2.30	0.59
4:D:201:LYS:CD	4:D:201:LYS:N	2.47	0.59
22:D:7050:LMU:C6'	22:D:7050:LMU:O2B	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:136:VAL:HG22	7:G:137:VAL:HG13	1.83	0.59
7:G:144:THR:OG1	7:G:148:GLY:CA	2.50	0.59
11:K:58:VAL:O	11:K:62:SER:HB3	2.02	0.59
15:1:76:LEU:CB	15:1:77:GLU:OE1	2.48	0.59
15:1:189:LYS:HB3	19:1:1007:CLA:CMC	2.27	0.59
16:2:240:ILE:HG21	16:2:263:PHE:HB3	1.79	0.59
17:3:98:LEU:CD2	19:3:3012:CLA:C3D	2.81	0.59
1:A:274:TRP:CD2	1:A:277:TYR:O	2.55	0.59
1:A:349:ILE:O	1:A:350:LEU:C	2.39	0.59
1:A:454:GLY:H	1:A:457:SER:CB	2.05	0.59
1:A:575:LEU:CD1	1:A:576:GLY:N	2.48	0.59
1:A:747:TRP:CD2	21:A:6011:BCR:C40	2.85	0.59
2:B:195:VAL:HA	2:B:199:ILE:HG13	1.84	0.59
2:B:293:THR:HG22	7:G:94:GLN:NE2	2.18	0.59
2:B:388:ALA:C	2:B:391:PRO:CD	2.69	0.59
2:B:455:ILE:HG23	6:F:148:LEU:CD1	2.32	0.59
19:B:1201:CLA:C4C	21:I:6021:BCR:H401	2.33	0.59
4:D:96:VAL:O	4:D:96:VAL:CG2	2.49	0.59
4:D:141:GLY:O	4:D:142:THR:C	2.39	0.59
4:D:173:TYR:O	4:D:175:GLU:CG	2.51	0.59
6:F:185:ILE:C	6:F:186:ARG:CG	2.71	0.59
7:G:125:VAL:O	7:G:129:ALA:HB3	2.03	0.59
13:N:126:LYS:NZ	13:N:126:LYS:CB	2.65	0.59
14:R:26:UNK:C	14:R:28:UNK:N	2.66	0.59
15:1:102:ALA:CA	15:1:103:LEU:HD23	2.33	0.59
15:1:145:ILE:O	15:1:148:VAL:CG1	2.51	0.59
16:2:263:PHE:O	16:2:263:PHE:CD2	2.56	0.59
18:4:142:PHE:CG	19:4:4010:CLA:C3C	2.85	0.59
18:4:155:ARG:O	18:4:158:GLN:HB2	2.02	0.59
18:4:158:GLN:NE2	19:4:1004:CLA:C4A	2.65	0.59
22:4:7034:LMU:H81	22:4:7052:LMU:O2'	1.97	0.59
1:A:330:ILE:O	1:A:334:HIS:HE1	1.86	0.59
1:A:393:LEU:HG	1:A:394:SER:N	2.17	0.59
1:A:426:THR:HA	1:A:428:TYR:CE1	2.36	0.59
1:A:455:PHE:HD1	19:A:1131:CLA:CMA	2.15	0.59
1:A:636:HIS:O	1:A:637:ILE:C	2.41	0.59
19:A:1139:CLA:H42	19:A:1139:CLA:O1A	2.02	0.59
2:B:90:ALA:N	2:B:113:VAL:HG13	2.18	0.59
19:B:1213:CLA:HBA2	19:B:1213:CLA:HED2	1.85	0.59
3:C:44:ARG:NH2	4:D:181:ARG:HB3	2.16	0.59
9:I:22:ALA:O	9:I:23:SER:C	2.40	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:78:ARG:CA	11:K:78:ARG:CZ	2.80	0.59
13:N:147:SER:HA	13:N:149:ASP:CB	2.32	0.59
14:R:39:UNK:CB	14:R:40:UNK:HA	2.33	0.59
15:1:171:LEU:CD2	15:1:173:TYR:OH	2.51	0.59
16:2:217:LEU:HD12	16:2:218:ARG:HG3	1.85	0.59
17:3:184:LYS:O	17:3:185:GLN:HB3	2.02	0.59
1:A:46:LYS:HB2	1:A:48:PRO:O	2.03	0.59
1:A:71:LEU:HD12	1:A:72:GLU:O	2.03	0.59
1:A:129:GLN:HE21	19:A:1107:CLA:MG	1.09	0.59
1:A:426:THR:HG23	1:A:428:TYR:CZ	2.38	0.59
1:A:492:ILE:HA	1:A:495:THR:HG22	1.83	0.59
2:B:90:ALA:CA	2:B:113:VAL:CG1	2.63	0.59
2:B:255:LEU:CA	2:B:271:THR:CB	2.70	0.59
2:B:289:LEU:HD21	19:B:1217:CLA:NA	2.17	0.59
2:B:290:MET:HA	19:B:1218:CLA:CAC	2.32	0.59
2:B:489:GLY:HA3	19:B:1232:CLA:OBD	2.01	0.59
19:B:1223:CLA:C7	21:B:6010:BCR:H14C	2.33	0.59
4:D:181:ARG:HB3	4:D:182:GLN:HG2	1.83	0.59
7:G:69:GLY:C	7:G:72:LEU:HG	2.23	0.59
7:G:99:HIS:CB	7:G:100:PHE:HB3	2.33	0.59
19:H:1145:CLA:CED	19:H:1145:CLA:HAA2	2.33	0.59
11:K:55:LEU:O	11:K:58:VAL:CG1	2.51	0.59
12:L:158:PRO:O	12:L:159:SER:CB	2.51	0.59
12:L:164:LEU:CD1	12:L:165:THR:N	2.61	0.59
19:L:1148:CLA:CED	19:L:1148:CLA:CGA	2.80	0.59
13:N:133:GLY:HA3	13:N:134:CYS:C	2.21	0.59
13:N:147:SER:HA	13:N:149:ASP:HB2	1.83	0.59
19:1:1007:CLA:O1D	22:4:7008:LMU:O2'	2.19	0.59
16:2:184:PRO:HG2	16:2:186:ASN:N	2.17	0.59
16:2:226:ARG:CD	16:2:230:LEU:HD23	2.30	0.59
16:2:246:PRO:HB2	16:2:247:ILE:CG1	2.32	0.59
18:4:133:GLU:O	18:4:134:TYR:HB2	2.01	0.59
18:4:225:GLY:CA	18:4:226:LYS:NZ	2.66	0.59
1:A:40:PHE:C	1:A:41:SER:O	2.41	0.59
1:A:43:THR:HG22	1:A:46:LYS:HZ3	1.67	0.59
1:A:136:VAL:CG2	1:A:140:PHE:O	2.51	0.59
1:A:267:THR:CG2	1:A:267:THR:O	2.50	0.59
1:A:360:ILE:O	1:A:361:ASN:HB2	2.02	0.59
1:A:461:TYR:CE1	1:A:540:LEU:CD1	2.85	0.59
1:A:555:ILE:HD13	19:A:9023:CLA:HMD1	1.83	0.59
19:A:9011:CLA:HAA1	19:B:9010:CLA:HBB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:GLU:OE1	2:B:640:CYS:O	2.20	0.59
2:B:178:HIS:C	2:B:180:SER:H	2.04	0.59
2:B:207:VAL:O	2:B:207:VAL:CG1	2.50	0.59
3:C:39:ILE:O	3:C:40:ALA:HB3	2.03	0.59
5:E:76:ILE:HG23	5:E:78:ARG:HD3	1.85	0.59
6:F:129:ARG:C	6:F:133:TYR:CE1	2.76	0.59
7:G:76:ARG:HH12	7:G:120:VAL:CA	2.16	0.59
7:G:88:ALA:CB	7:G:90:GLN:O	2.49	0.59
11:K:115:ILE:HD12	11:K:118:VAL:HG23	1.85	0.59
16:2:129:LEU:O	16:2:130:GLY:O	2.20	0.59
18:4:146:PHE:CD1	18:4:146:PHE:N	2.70	0.59
18:4:177:LEU:HD22	18:4:177:LEU:C	2.22	0.59
18:4:232:LEU:HD12	18:4:234:GLN:CA	2.32	0.59
1:A:63:ASP:OD2	1:A:65:ASP:N	2.30	0.59
1:A:628:ILE:CD1	1:A:629:ASN:H	2.13	0.59
1:A:700:TRP:CZ2	20:A:5001:PQN:H2M3	2.38	0.59
19:A:9012:CLA:CAD	19:A:9012:CLA:CED	2.81	0.59
2:B:224:PRO:C	2:B:227:THR:HB	2.23	0.59
2:B:315:LEU:HD11	2:B:317:ARG:CG	2.30	0.59
2:B:623:TYR:O	2:B:624:LEU:HB3	2.03	0.59
19:B:1222:CLA:CED	19:B:1223:CLA:OBD	2.50	0.59
19:B:1226:CLA:HMD2	24:B:7101:LMG:H341	1.85	0.59
19:J:1308:CLA:O1D	19:J:1308:CLA:CGA	2.51	0.59
12:L:73:VAL:CA	19:L:1504:CLA:HMA3	2.31	0.59
12:L:76:SER:O	12:L:77:PRO:C	2.41	0.59
13:N:104:LYS:O	13:N:107:LEU:CB	2.49	0.59
15:1:64:PHE:CE1	15:1:65:ASP:HB3	2.38	0.59
19:1:1013:CLA:CAD	19:1:1013:CLA:CED	2.79	0.59
16:2:103:VAL:C	16:2:105:ALA:N	2.53	0.59
16:2:145:TYR:O	16:2:146:PHE:CB	2.51	0.59
16:2:217:LEU:O	16:2:218:ARG:C	2.42	0.59
17:3:96:ARG:HA	17:3:99:ALA:HB2	1.78	0.59
1:A:105:ASN:CB	1:A:119:SER:O	2.51	0.58
1:A:154:ARG:CD	1:A:384:TYR:HE1	2.11	0.58
1:A:197:GLN:NE2	1:A:351:THR:C	2.57	0.58
1:A:253:ASP:O	1:A:256:ALA:HB3	2.02	0.58
1:A:604:TRP:O	1:A:607:ASN:N	2.31	0.58
1:A:699:TYR:HD1	1:A:700:TRP:CD1	2.21	0.58
2:B:8:PHE:HE2	2:B:27:THR:HG1	1.50	0.58
2:B:127:ILE:O	2:B:127:ILE:CD1	2.51	0.58
2:B:277:HIS:HE1	19:B:1215:CLA:NC	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:THR:O	2:B:436:LEU:O	2.20	0.58
2:B:503:GLU:CG	2:B:503:GLU:O	2.49	0.58
2:B:535:VAL:HG13	2:B:536:LYS:N	2.17	0.58
2:B:551:LYS:O	2:B:553:PHE:CE2	2.56	0.58
19:B:1222:CLA:H72	19:B:1236:CLA:C2D	2.33	0.58
3:C:73:THR:OG1	3:C:76:SER:CA	2.51	0.58
5:E:79:LYS:N	5:E:84:TYR:HE1	2.00	0.58
12:L:102:VAL:HG13	19:L:1502:CLA:CED	2.33	0.58
15:1:179:LYS:HE3	15:1:181:GLU:HA	1.85	0.58
16:2:130:GLY:HA3	16:2:131:ILE:CG1	1.92	0.58
16:2:160:ILE:HB	19:2:2012:CLA:CBB	2.33	0.58
17:3:238:ILE:HG13	19:3:3003:CLA:CMC	2.33	0.58
1:A:93:LEU:O	1:A:97:TYR:HD2	1.85	0.58
19:A:1101:CLA:HBB2	19:A:1102:CLA:C1C	2.32	0.58
19:A:1115:CLA:C19	11:K:64:MET:HE1	2.32	0.58
19:A:1117:CLA:H121	19:A:1117:CLA:CBB	2.34	0.58
2:B:455:ILE:O	2:B:514:PRO:HG3	2.02	0.58
19:B:1214:CLA:HBD	19:B:1223:CLA:CBB	2.31	0.58
19:B:1239:CLA:C19	9:I:21:MET:HB3	2.32	0.58
20:B:5002:PQN:C19	21:B:6017:BCR:C10	2.80	0.58
3:C:34:CYS:H	3:C:37:LYS:CB	2.09	0.58
6:F:128:LYS:O	6:F:129:ARG:HD3	2.03	0.58
12:L:146:THR:C	12:L:148:TYR:H	2.05	0.58
22:R:7022:LMU:C2'	22:R:7022:LMU:C2	2.76	0.58
16:2:167:ARG:HD3	19:2:2012:CLA:HMA3	1.85	0.58
16:2:183:PHE:CD1	16:2:183:PHE:C	2.77	0.58
16:2:203:PRO:O	16:2:204:LEU:HB2	2.03	0.58
18:4:87:ASN:OD1	18:4:90:TRP:CG	2.55	0.58
22:4:7034:LMU:H81	22:4:7052:LMU:C3'	2.23	0.58
1:A:278:ALA:O	1:A:281:LEU:HD11	2.03	0.58
1:A:581:CYS:CB	1:A:590:CYS:O	2.50	0.58
19:A:1136:CLA:C19	19:L:1130:CLA:HBB1	2.29	0.58
2:B:175:LEU:HD12	19:B:1221:CLA:HED1	1.84	0.58
2:B:298:GLY:N	19:B:1218:CLA:HMD3	2.17	0.58
2:B:555:TYR:O	2:B:571:SER:HB2	2.03	0.58
2:B:631:LEU:HD23	2:B:631:LEU:H	1.68	0.58
19:B:1223:CLA:H122	21:B:6010:BCR:C13	2.32	0.58
19:B:1229:CLA:H51	21:F:6016:BCR:C40	2.33	0.58
5:E:84:TYR:CD2	5:E:85:LYS:HG3	2.38	0.58
5:E:90:VAL:O	5:E:91:VAL:HG22	2.03	0.58
6:F:173:TRP:CZ3	6:F:211:PHE:CB	2.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:99:HIS:O	7:G:101:GLU:N	2.37	0.58
8:H:109:LEU:HD22	19:H:1207:CLA:H52	1.85	0.58
11:K:112:VAL:C	11:K:114:HIS:H	2.06	0.58
13:N:132:THR:CB	13:N:139:LYS:HD3	2.29	0.58
22:R:7020:LMU:O6'	22:R:7020:LMU:H3B	2.03	0.58
19:1:1014:CLA:H71	19:1:1014:CLA:C4	2.19	0.58
16:2:148:ASP:C	16:2:149:THR:HG1	2.00	0.58
16:2:266:PHE:CE1	16:2:267:THR:O	2.55	0.58
17:3:162:MET:CE	19:3:3010:CLA:C3D	2.81	0.58
18:4:88:LEU:O	18:4:90:TRP:CD1	2.55	0.58
18:4:228:PRO:CB	18:4:229:PHE:CD1	2.72	0.58
18:4:232:LEU:CD1	18:4:234:GLN:HA	2.33	0.58
1:A:50:THR:HG23	1:A:51:THR:H	1.69	0.58
1:A:90:PHE:HA	1:A:93:LEU:CD2	2.34	0.58
1:A:255:LEU:CD1	1:A:280:PHE:CZ	2.82	0.58
1:A:746:THR:HG1	19:A:9011:CLA:CGD	2.13	0.58
2:B:378:ILE:CA	2:B:381:PHE:HB2	2.34	0.58
2:B:409:ALA:O	2:B:410:ARG:CB	2.34	0.58
2:B:654:HIS:HE1	19:B:9010:CLA:NB	2.01	0.58
19:B:1222:CLA:CHD	19:B:1222:CLA:CBC	2.79	0.58
24:B:7101:LMG:HO3	3:C:70:TRP:HE1	1.46	0.58
5:E:78:ARG:HH12	5:E:125:ILE:HB	1.65	0.58
9:I:23:SER:O	9:I:26:LEU:HG	2.04	0.58
19:K:1142:CLA:CMD	19:K:1143:CLA:C1A	2.82	0.58
19:L:1501:CLA:HED2	19:L:1501:CLA:HAA2	1.85	0.58
13:N:130:ASN:O	13:N:130:ASN:OD1	2.20	0.58
14:R:35:UNK:C	14:R:36:UNK:O	2.51	0.58
15:1:223:ASP:OD1	18:4:140:THR:HG21	2.03	0.58
19:1:1005:CLA:HMC1	19:1:1005:CLA:HBC3	1.85	0.58
16:2:226:ARG:HH11	16:2:226:ARG:CA	2.16	0.58
18:4:161:LYS:C	18:4:161:LYS:CD	2.72	0.58
18:4:220:GLN:NE2	19:4:1306:CLA:HAC2	2.18	0.58
1:A:216:LEU:HD12	21:A:6002:BCR:H353	1.85	0.58
1:A:230:ASN:HA	1:A:233:LEU:HB2	1.85	0.58
1:A:332:GLU:HA	1:A:344:LYS:HG2	1.85	0.58
1:A:338:PHE:CZ	19:A:1151:CLA:CBB	2.81	0.58
1:A:368:LEU:CD2	19:A:1117:CLA:H93	2.24	0.58
2:B:29:HIS:CG	19:B:1202:CLA:HBB2	2.38	0.58
2:B:194:LEU:O	2:B:199:ILE:HG13	2.04	0.58
2:B:213:LEU:CD1	2:B:214:ASP:N	2.60	0.58
2:B:460:ALA:O	2:B:461:GLN:C	2.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1213:CLA:CBC	19:B:1213:CLA:CHD	2.81	0.58
19:B:1223:CLA:H8	21:B:6010:BCR:H14C	1.84	0.58
3:C:34:CYS:O	3:C:35:LYS:HB2	2.04	0.58
4:D:150:ILE:O	4:D:151:LYS:CG	2.47	0.58
4:D:156:ARG:HE	4:D:164:GLN:HB2	1.64	0.58
5:E:96:ASP:OD2	5:E:98:ASN:ND2	2.36	0.58
5:E:103:VAL:HG22	5:E:104:VAL:O	2.03	0.58
6:F:99:LEU:HB3	6:F:127:LYS:HE2	1.85	0.58
8:H:77:ASN:ND2	8:H:78:PRO:CG	2.66	0.58
22:K:7042:LMU:H2B	22:K:7042:LMU:H3'	1.85	0.58
12:L:143:LEU:N	12:L:145:LEU:H	2.01	0.58
13:N:127:PHE:O	13:N:128:PRO:C	2.42	0.58
13:N:139:LYS:CA	13:N:142:LYS:CD	2.81	0.58
15:1:116:ALA:O	15:1:117:LEU:HD22	2.02	0.58
16:2:195:TYR:CE2	16:2:198:GLY:CA	2.87	0.58
19:A:1107:CLA:HMC1	19:A:1107:CLA:HBC3	1.85	0.58
19:A:1237:CLA:HBB2	19:B:1238:CLA:HMD1	1.85	0.58
2:B:70:TRP:CD1	2:B:70:TRP:N	2.71	0.58
2:B:182:LEU:HA	19:B:1210:CLA:HMB2	1.86	0.58
2:B:290:MET:HA	19:B:1218:CLA:HAC2	1.85	0.58
2:B:469:LYS:CG	2:B:470:THR:HA	2.31	0.58
2:B:558:PRO:HB3	2:B:706:ARG:HH21	1.68	0.58
2:B:732:LYS:C	2:B:733:PHE:O	2.41	0.58
3:C:66:ARG:HB3	3:C:66:ARG:NH2	2.18	0.58
6:F:129:ARG:C	6:F:133:TYR:HE1	2.07	0.58
6:F:227:VAL:O	6:F:230:ASN:N	2.37	0.58
12:L:70:GLU:HG2	12:L:74:THR:CG2	2.31	0.58
14:R:52:UNK:CB	14:R:53:UNK:CB	2.82	0.58
19:1:1013:CLA:HED2	19:1:1013:CLA:OBD	2.03	0.58
16:2:122:ILE:HG13	16:2:126:LEU:HD21	1.84	0.58
17:3:161:GLU:CD	17:3:161:GLU:C	2.61	0.58
17:3:192:LYS:CE	17:3:192:LYS:CA	2.59	0.58
18:4:121:ILE:C	18:4:123:VAL:H	2.07	0.58
1:A:210:LEU:HD13	19:A:1111:CLA:HHB	1.85	0.58
1:A:453:LEU:HD23	19:A:1136:CLA:HBB1	1.86	0.58
1:A:603:PHE:CZ	1:A:735:VAL:CG2	2.86	0.58
19:A:1117:CLA:O1A	19:A:1127:CLA:H71	2.04	0.58
19:A:1124:CLA:O2A	19:A:1137:CLA:O2D	2.21	0.58
19:A:9022:CLA:C14	19:B:1206:CLA:HBB2	2.34	0.58
2:B:145:LEU:HA	2:B:148:ILE:HD12	1.85	0.58
2:B:190:TRP:CA	19:B:1211:CLA:HBB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ASN:HB2	7:G:94:GLN:OE1	1.89	0.58
2:B:341:LEU:O	2:B:345:THR:OG1	2.14	0.58
2:B:394:PHE:O	2:B:542:ARG:HD3	2.04	0.58
2:B:438:VAL:CG2	19:B:1230:CLA:CMC	2.80	0.58
2:B:560:ASP:OD1	3:C:52:LYS:NZ	2.35	0.58
2:B:696:LYS:CG	3:C:80:ALA:HA	2.24	0.58
2:B:697:PRO:O	3:C:79:LEU:CD1	2.49	0.58
19:B:1205:CLA:HMC2	21:B:6017:BCR:C28	2.31	0.58
19:B:1218:CLA:HMD2	21:B:6004:BCR:C32	2.34	0.58
4:D:77:ASN:HB3	4:D:79:PRO:HD2	1.85	0.58
5:E:90:VAL:CG1	5:E:91:VAL:N	2.65	0.58
12:L:91:THR:O	12:L:92:ALA:C	2.41	0.58
15:1:133:THR:C	15:1:135:PRO:HD2	2.24	0.58
15:1:162:LYS:CB	15:1:164:PRO:HG3	2.34	0.58
19:1:1007:CLA:CBC	19:1:1007:CLA:CHD	2.82	0.58
18:4:172:PHE:O	18:4:173:LYS:CB	2.51	0.58
1:A:29:THR:OG1	1:A:31:PHE:CB	2.51	0.58
1:A:159:THR:C	1:A:163:GLN:NE2	2.57	0.58
1:A:281:LEU:HB2	19:A:1115:CLA:HED2	1.85	0.58
1:A:284:ARG:HG2	1:A:295:TRP:CG	2.37	0.58
1:A:396:PHE:HE2	1:A:616:PHE:CB	2.17	0.58
1:A:397:THR:HG21	1:A:613:ILE:HG13	1.82	0.58
1:A:443:ILE:CG1	1:A:557:LEU:HD22	2.32	0.58
19:A:9013:CLA:H2	19:A:9013:CLA:HMA1	1.85	0.58
2:B:115:ASN:C	2:B:115:ASN:OD1	2.41	0.58
2:B:154:TRP:O	2:B:157:LEU:N	2.36	0.58
2:B:388:ALA:O	2:B:391:PRO:HD2	2.02	0.58
2:B:475:ASP:O	2:B:480:SER:N	2.26	0.58
2:B:692:ARG:NH2	2:B:694:ARG:NH2	2.52	0.58
3:C:34:CYS:N	3:C:37:LYS:HB3	2.10	0.58
10:J:5:LYS:HD2	16:2:178:ASN:OD1	2.02	0.58
14:R:37:UNK:C	14:R:42:UNK:O	2.52	0.58
17:3:171:ARG:CG	17:3:175:ASP:OD1	2.50	0.58
22:3:7005:LMU:C1'	22:3:7005:LMU:C3	2.80	0.58
18:4:173:LYS:NZ	18:4:201:LYS:HG2	2.14	0.58
18:4:210:LEU:HD23	19:4:4002:CLA:CBB	2.34	0.58
1:A:104:SER:O	1:A:106:TYR:N	2.28	0.58
1:A:711:HIS:HB3	1:A:717:ALA:CB	2.34	0.58
19:A:9013:CLA:H11	2:B:431:PHE:CE1	2.39	0.58
2:B:25:ILE:O	2:B:26:ALA:CB	2.51	0.58
2:B:29:HIS:CD2	19:B:1202:CLA:HBB1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:HIS:O	2:B:36:ASP:N	2.37	0.58
2:B:212:PHE:CE1	19:B:1211:CLA:HHD	2.38	0.58
2:B:375:HIS:HE1	19:B:1225:CLA:NC	2.01	0.58
10:J:11:ALA:CB	10:J:12:PRO:HD2	2.10	0.58
11:K:60:SER:HA	11:K:63:LEU:CD2	2.28	0.58
19:K:1142:CLA:HMD3	19:K:1143:CLA:ND	2.19	0.58
12:L:73:VAL:CA	19:L:1504:CLA:CMA	2.78	0.58
12:L:108:TYR:HB2	12:L:200:ALA:HB2	1.85	0.58
13:N:120:VAL:O	13:N:122:PHE:CD2	2.57	0.58
13:N:156:GLY:C	13:N:157:LYS:HD2	2.24	0.58
15:1:65:ASP:O	15:1:68:GLY:N	2.37	0.58
15:1:157:ASP:OD2	15:1:175:LYS:HD2	2.04	0.58
16:2:201:PHE:HD1	16:2:202:ASP:CA	2.16	0.58
17:3:103:VAL:HG11	17:3:229:LYS:HG2	1.84	0.58
19:4:4006:CLA:H43	22:4:7034:LMU:H91	1.86	0.58
1:A:253:ASP:O	1:A:256:ALA:CB	2.52	0.58
1:A:284:ARG:NH1	1:A:284:ARG:C	2.57	0.58
1:A:329:ASP:O	1:A:332:GLU:O	2.22	0.58
2:B:187:SER:O	2:B:188:LEU:C	2.40	0.58
19:B:1220:CLA:H93	19:B:1227:CLA:HBC1	1.86	0.58
19:B:1229:CLA:CBB	21:F:6014:BCR:H23C	2.34	0.58
5:E:107:PHE:HD2	5:E:109:LYS:CG	2.17	0.58
8:H:77:ASN:ND2	8:H:78:PRO:CD	2.67	0.58
8:H:97:LEU:HD12	8:H:100:PHE:HB2	1.83	0.58
12:L:128:GLN:HG2	12:L:132:LEU:CD2	2.02	0.58
15:1:155:GLU:OE2	15:1:155:GLU:N	2.30	0.58
15:1:171:LEU:HB3	15:1:173:TYR:CZ	2.39	0.58
16:2:171:ILE:HG13	16:2:172:LEU:HB2	1.84	0.58
16:2:249:ASN:C	16:2:249:ASN:OD1	2.42	0.58
1:A:111:ASN:O	1:A:113:PRO:HD2	2.03	0.57
1:A:217:SER:CA	21:A:6002:BCR:H351	2.34	0.57
1:A:270:PHE:CZ	19:A:1141:CLA:H2	2.39	0.57
2:B:37:ILE:HD12	2:B:37:ILE:O	2.04	0.57
2:B:74:PHE:O	2:B:77:TRP:N	2.36	0.57
19:B:1214:CLA:H52	19:B:1223:CLA:CMB	2.30	0.57
11:K:79:LYS:O	11:K:79:LYS:HG3	2.04	0.57
13:N:131:PHE:N	13:N:132:THR:HG22	2.19	0.57
13:N:143:VAL:CG1	13:N:144:PRO:CD	2.82	0.57
19:1:1006:CLA:CAB	19:1:1013:CLA:CHD	2.82	0.57
16:2:113:ALA:HB1	16:2:114:MET:HE3	1.84	0.57
16:2:121:PHE:CD2	16:2:121:PHE:N	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:2014:CLA:H41	19:2:2014:CLA:C9	2.33	0.57
1:A:40:PHE:H	1:A:44:ILE:HG22	1.68	0.57
1:A:51:THR:HG22	1:A:723:ARG:HB2	1.84	0.57
1:A:187:HIS:HE1	19:A:1109:CLA:CHA	2.17	0.57
1:A:346:LEU:O	1:A:347:TYR:HB2	2.04	0.57
1:A:423:ASP:N	1:A:424:PRO:CD	2.65	0.57
1:A:705:GLU:HB3	2:B:545:LYS:NZ	2.19	0.57
21:A:6002:BCR:C31	21:A:6002:BCR:C8	2.69	0.57
2:B:317:ARG:HA	2:B:317:ARG:HE	1.68	0.57
2:B:560:ASP:CB	3:C:66:ARG:NE	2.65	0.57
3:C:12:ILE:O	3:C:12:ILE:HG22	2.03	0.57
3:C:12:ILE:HB	3:C:39:ILE:HA	1.86	0.57
5:E:91:VAL:HG12	5:E:92:ALA:N	2.18	0.57
6:F:152:GLY:O	6:F:157:TRP:CH2	2.57	0.57
7:G:103:GLY:N	7:G:104:ASP:HA	2.19	0.57
19:J:1308:CLA:H2A	19:J:1308:CLA:H2	1.86	0.57
12:L:79:ILE:HD12	19:L:1504:CLA:CMA	2.34	0.57
13:N:127:PHE:H	13:N:127:PHE:HD2	1.50	0.57
14:R:38:UNK:C	14:R:42:UNK:O	2.52	0.57
15:1:73:PRO:HG2	15:1:74:ALA:H	1.65	0.57
15:1:170:PRO:HG2	15:1:171:LEU:HA	1.85	0.57
16:2:251:PHE:O	16:2:251:PHE:CG	2.57	0.57
22:2:7006:LMU:H22	22:2:7006:LMU:H2'	1.86	0.57
18:4:172:PHE:C	18:4:194:PHE:CE2	2.77	0.57
1:A:707:ILE:C	1:A:711:HIS:CD2	2.77	0.57
19:A:9023:CLA:HMC1	2:B:661:PHE:CB	2.34	0.57
2:B:154:TRP:O	2:B:157:LEU:CB	2.52	0.57
2:B:282:PHE:O	2:B:286:ILE:HG13	2.03	0.57
2:B:393:PHE:CD2	2:B:397:ASP:OD1	2.49	0.57
2:B:414:HIS:O	2:B:414:HIS:CG	2.57	0.57
19:B:1203:CLA:C4	24:B:7101:LMG:H321	2.34	0.57
19:B:1235:CLA:CGA	19:B:1235:CLA:C1A	2.82	0.57
3:C:33:GLY:HA2	3:C:37:LYS:CE	2.33	0.57
13:N:114:PHE:HE2	13:N:116:ARG:HD2	1.69	0.57
15:1:134:LEU:CA	15:1:137:ILE:CD1	2.71	0.57
17:3:226:LYS:HG3	17:3:229:LYS:HE3	1.86	0.57
18:4:93:GLN:OE1	18:4:170:PRO:HB2	2.04	0.57
1:A:111:ASN:OD1	1:A:238:ASP:HA	2.04	0.57
1:A:282:THR:O	1:A:283:PHE:O	2.22	0.57
1:A:558:LYS:HZ1	2:B:674:LEU:HB2	1.67	0.57
19:A:1102:CLA:HBB2	19:A:1104:CLA:C4D	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1109:CLA:HMC1	19:A:1109:CLA:HBC3	1.86	0.57
19:A:9023:CLA:CMC	2:B:661:PHE:CB	2.81	0.57
2:B:51:PHE:CD1	19:B:1210:CLA:HED1	2.40	0.57
2:B:155:LEU:O	2:B:161:TRP:NE1	2.38	0.57
2:B:486:LEU:HD13	2:B:489:GLY:N	2.19	0.57
2:B:710:LEU:C	2:B:712:HIS:N	2.56	0.57
2:B:711:VAL:O	2:B:711:VAL:CG1	2.52	0.57
4:D:98:GLU:HB2	4:D:100:TYR:HE2	1.68	0.57
11:K:116:ILE:CG2	11:K:117:GLY:N	2.68	0.57
19:K:1142:CLA:HED1	19:K:1143:CLA:CMB	2.30	0.57
12:L:55:GLN:O	12:L:57:ILE:N	2.38	0.57
12:L:55:GLN:C	12:L:57:ILE:N	2.57	0.57
12:L:82:TYR:O	12:L:82:TYR:CD1	2.57	0.57
13:N:147:SER:CB	13:N:151:ASP:OD1	2.52	0.57
15:1:129:VAL:HB	15:1:130:PRO:HD3	1.85	0.57
16:2:154:ILE:HG12	16:2:155:VAL:H	1.70	0.57
16:2:182:ILE:CB	16:2:187:LYS:CB	2.61	0.57
18:4:120:ILE:O	18:4:121:ILE:C	2.43	0.57
18:4:209:ARG:O	18:4:212:LEU:C	2.42	0.57
18:4:222:ASN:O	18:4:223:VAL:CB	2.39	0.57
19:4:1004:CLA:CBC	19:4:1004:CLA:CHD	2.75	0.57
1:A:174:PHE:O	1:A:175:ALA:CB	2.51	0.57
1:A:225:VAL:O	1:A:229:ILE:HB	2.04	0.57
1:A:246:HIS:C	1:A:248:PHE:HD2	2.05	0.57
1:A:338:PHE:CD1	1:A:338:PHE:N	2.72	0.57
1:A:344:LYS:C	1:A:346:LEU:H	2.08	0.57
1:A:412:ALA:HA	1:A:598:VAL:HG21	1.86	0.57
19:A:1133:CLA:H2A	19:A:1133:CLA:O1D	2.04	0.57
21:A:6011:BCR:H19C	19:A:9012:CLA:H172	1.86	0.57
2:B:155:LEU:O	2:B:161:TRP:CD1	2.57	0.57
2:B:486:LEU:HD12	2:B:489:GLY:H	1.68	0.57
20:B:5002:PQN:H161	21:B:6017:BCR:H331	1.87	0.57
21:B:6020:BCR:H331	19:L:1502:CLA:C4B	2.06	0.57
3:C:31:TRP:CD1	3:C:31:TRP:C	2.78	0.57
8:H:91:PHE:HB3	12:L:187:GLY:HA3	1.86	0.57
9:I:2:ILE:HG12	9:I:3:ASN:ND2	2.20	0.57
11:K:118:VAL:O	11:K:120:VAL:HA	2.03	0.57
13:N:146:LEU:HD13	17:3:142:ILE:O	1.75	0.57
15:1:78:ARG:HH22	15:1:179:LYS:CB	2.16	0.57
15:1:115:ALA:O	15:1:116:ALA:HB3	2.05	0.57
15:1:171:LEU:HD22	15:1:173:TYR:OH	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:115:LEU:O	16:2:118:ALA:CB	2.52	0.57
17:3:103:VAL:O	17:3:107:ARG:CB	2.49	0.57
19:3:3013:CLA:O1D	19:3:3013:CLA:C2A	2.52	0.57
18:4:194:PHE:O	18:4:195:ALA:CB	2.51	0.57
18:4:225:GLY:CA	18:4:226:LYS:HZ2	2.17	0.57
1:A:278:ALA:O	1:A:279:ASP:O	2.22	0.57
1:A:340:GLY:O	1:A:343:HIS:CB	2.45	0.57
1:A:665:ILE:O	2:B:621:ARG:HD3	2.04	0.57
1:A:723:ARG:N	19:A:1139:CLA:HBB1	2.16	0.57
19:A:1122:CLA:NC	21:A:6007:BCR:H19C	2.20	0.57
2:B:70:TRP:HD1	2:B:70:TRP:H	1.50	0.57
2:B:93:ASP:OD1	2:B:96:PHE:HD1	1.87	0.57
2:B:347:LEU:HD13	2:B:351:HIS:HD1	1.70	0.57
20:B:5002:PQN:H191	21:B:6017:BCR:C10	2.34	0.57
3:C:1:MET:N	3:C:4:SER:CB	2.67	0.57
5:E:83:TRP:CH2	5:E:116:SER:CB	2.86	0.57
11:K:125:LYS:HE3	11:K:125:LYS:O	2.04	0.57
12:L:95:PRO:O	12:L:97:LEU:N	2.38	0.57
12:L:100:ILE:CG2	12:L:191:PHE:O	2.50	0.57
15:1:77:GLU:C	15:1:80:LYS:HG3	2.23	0.57
15:1:182:GLU:O	15:1:183:LEU:CB	2.53	0.57
19:1:1001:CLA:CMC	19:1:1001:CLA:CBC	2.80	0.57
16:2:171:ILE:CD1	16:2:173:ASN:HD21	2.17	0.57
17:3:155:TYR:CD2	17:3:155:TYR:N	2.72	0.57
17:3:210:PRO:CD	17:3:211:LEU:N	2.67	0.57
18:4:133:GLU:O	18:4:134:TYR:CB	2.51	0.57
1:A:51:THR:CG2	19:A:1139:CLA:CBB	2.61	0.57
1:A:240:LYS:CA	1:A:243:PRO:HD2	2.33	0.57
19:A:1119:CLA:C2C	19:A:1125:CLA:C17	2.82	0.57
19:A:1134:CLA:O2A	19:A:1141:CLA:HBB1	2.04	0.57
19:A:9013:CLA:H93	2:B:431:PHE:HD1	1.69	0.57
2:B:120:VAL:O	2:B:121:TYR:C	2.41	0.57
2:B:438:VAL:HG21	19:B:1230:CLA:HMC1	1.86	0.57
2:B:457:PRO:HG3	2:B:517:PHE:HB2	1.87	0.57
4:D:100:TYR:N	4:D:100:TYR:HD2	2.01	0.57
22:D:7050:LMU:H42	22:D:7050:LMU:H82	1.85	0.57
11:K:76:ALA:HA	11:K:78:ARG:NH1	2.18	0.57
11:K:114:HIS:O	11:K:116:ILE:N	2.38	0.57
13:N:146:LEU:O	13:N:147:SER:HB2	2.04	0.57
15:1:69:LEU:O	15:1:70:GLY:C	2.39	0.57
15:1:93:ALA:HB1	19:1:1006:CLA:C4B	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:97:ILE:HG12	15:1:98:LEU:N	2.18	0.57
17:3:104:ILE:CG2	19:3:3004:CLA:C1D	2.83	0.57
18:4:90:TRP:C	18:4:91:PHE:CD1	2.74	0.57
18:4:159:ASP:O	18:4:163:PRO:HA	2.04	0.57
1:A:86:LEU:HD13	1:A:178:MET:HE2	1.85	0.57
1:A:213:LEU:O	1:A:217:SER:HB2	2.04	0.57
1:A:259:TYR:CE2	1:A:280:PHE:HA	2.40	0.57
1:A:331:LEU:HD23	1:A:331:LEU:C	2.17	0.57
2:B:91:ILE:HG12	2:B:112:PRO:O	2.04	0.57
2:B:254:ILE:HB	2:B:255:LEU:CD2	2.32	0.57
2:B:649:MET:O	2:B:653:GLY:N	2.37	0.57
19:B:1222:CLA:HMB3	21:B:6010:BCR:C35	2.35	0.57
3:C:1:MET:H2	3:C:3:HIS:N	2.02	0.57
4:D:181:ARG:CB	4:D:182:GLN:HG2	2.35	0.57
6:F:200:VAL:HG13	10:J:7:TYR:N	2.02	0.57
7:G:144:THR:OG1	7:G:148:GLY:HA3	2.05	0.57
13:N:139:LYS:HA	13:N:142:LYS:CE	2.34	0.57
13:N:144:PRO:HG2	13:N:158:ASP:O	2.05	0.57
15:1:92:LEU:CA	15:1:95:PRO:HD3	2.35	0.57
17:3:204:GLY:N	17:3:207:PHE:HA	2.18	0.57
19:3:3016:CLA:O1A	19:3:3016:CLA:HMA2	2.04	0.57
1:A:110:LEU:HD11	1:A:239:PRO:HG2	1.86	0.57
1:A:250:LEU:CB	17:3:136:TRP:HH2	2.02	0.57
1:A:308:ILE:CG2	19:A:1115:CLA:H111	2.35	0.57
1:A:389:TYR:CD1	1:A:625:TRP:CD1	2.92	0.57
1:A:603:PHE:CE2	1:A:735:VAL:HG22	2.40	0.57
19:A:1106:CLA:HMC3	19:A:1107:CLA:HHD	1.86	0.57
2:B:53:GLN:C	2:B:55:ALA:N	2.58	0.57
2:B:276:HIS:HB2	19:B:1214:CLA:C1B	2.35	0.57
2:B:302:LYS:NZ	7:G:103:GLY:HA3	2.19	0.57
2:B:303:TYR:N	2:B:306:GLU:HB2	2.19	0.57
2:B:454:LEU:HD13	2:B:514:PRO:HG2	1.86	0.57
2:B:469:LYS:HG3	2:B:470:THR:CB	2.35	0.57
2:B:471:THR:CG2	2:B:502:ASN:HD22	2.18	0.57
2:B:486:LEU:HD13	2:B:489:GLY:H	1.70	0.57
19:B:1205:CLA:C4C	19:B:1205:CLA:H42	2.35	0.57
3:C:2:SER:O	3:C:69:LEU:HB3	2.05	0.57
4:D:172:VAL:O	4:D:173:TYR:HB3	2.05	0.57
5:E:89:SER:OG	5:E:106:ARG:HG3	2.05	0.57
22:E:7048:LMU:H3'	22:E:7048:LMU:C5B	2.34	0.57
6:F:150:VAL:HG21	6:F:160:PHE:CB	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:157:TRP:HB3	19:F:1305:CLA:HHC	1.85	0.57
7:G:63:VAL:HG23	7:G:64:ILE:H	1.59	0.57
7:G:69:GLY:O	7:G:72:LEU:CB	2.53	0.57
12:L:54:TYR:O	12:L:55:GLN:HB3	2.05	0.57
15:1:71:GLU:HG2	15:1:72:VAL:HG23	1.85	0.57
15:1:77:GLU:CD	15:1:80:LYS:HZ1	2.08	0.57
15:1:78:ARG:HH21	15:1:179:LYS:CB	2.07	0.57
15:1:97:ILE:HD11	15:1:98:LEU:HD23	1.85	0.57
16:2:128:LYS:CG	16:2:131:ILE:HG23	2.35	0.57
16:2:168:TRP:O	16:2:169:ALA:C	2.43	0.57
17:3:130:GLN:CB	17:3:132:THR:N	2.37	0.57
19:4:4014:CLA:CBC	19:4:4014:CLA:CHD	2.83	0.57
1:A:284:ARG:CA	1:A:298:ASP:OD1	2.53	0.57
1:A:484:LEU:H	1:A:484:LEU:HD23	1.66	0.57
1:A:502:THR:C	1:A:504:ALA:N	2.51	0.57
1:A:567:ARG:HH11	4:D:89:GLY:CA	2.16	0.57
1:A:697:ARG:HD3	2:B:566:GLY:O	2.05	0.57
19:A:1132:CLA:O1D	12:L:119:PRO:HA	2.05	0.57
19:A:1136:CLA:CGA	19:A:1136:CLA:C1A	2.83	0.57
2:B:232:LEU:CD1	2:B:235:GLN:HB2	2.35	0.57
2:B:233:TYR:HB3	2:B:254:ILE:O	2.04	0.57
2:B:643:LEU:HD22	2:B:646:TRP:CD1	2.40	0.57
2:B:668:ARG:NE	2:B:699:ALA:O	2.38	0.57
5:E:111:ASN:CG	5:E:116:SER:HB3	2.25	0.57
6:F:195:GLU:H	6:F:195:GLU:CD	2.07	0.57
8:H:78:PRO:O	8:H:79:LEU:C	2.39	0.57
13:N:139:LYS:C	13:N:142:LYS:HZ2	2.09	0.57
13:N:146:LEU:CG	13:N:148:ASP:O	2.52	0.57
16:2:195:TYR:CD1	16:2:196:PRO:CD	2.60	0.57
16:2:201:PHE:HD1	16:2:202:ASP:N	2.00	0.57
19:2:2002:CLA:HHD	19:2:2002:CLA:CBC	2.28	0.57
18:4:87:ASN:OD1	18:4:90:TRP:CD1	2.58	0.57
1:A:73:GLU:O	1:A:74:ILE:C	2.43	0.56
1:A:206:HIS:C	1:A:211:LEU:HD23	2.26	0.56
1:A:390:ALA:HB1	1:A:754:ILE:HD13	1.86	0.56
1:A:638:THR:O	1:A:639:ALA:C	2.44	0.56
1:A:705:GLU:HB3	2:B:545:LYS:HZ1	1.68	0.56
19:A:1131:CLA:H101	19:A:1131:CLA:C14	2.35	0.56
19:A:1135:CLA:HBD	19:A:1135:CLA:HBA2	1.85	0.56
2:B:88:ALA:H	2:B:115:ASN:CA	2.17	0.56
2:B:457:PRO:CG	2:B:517:PHE:HB2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:570:ILE:O	2:B:570:ILE:HG13	2.04	0.56
2:B:725:LEU:HD12	2:B:726:ILE:N	2.20	0.56
21:B:6020:BCR:C38	21:B:6020:BCR:C23	2.82	0.56
4:D:100:TYR:HE1	4:D:134:LYS:HG3	1.58	0.56
4:D:102:ILE:CG1	4:D:154:PHE:HB3	2.35	0.56
4:D:177:VAL:HG22	4:D:178:ASN:HA	1.87	0.56
4:D:177:VAL:O	4:D:177:VAL:HG13	2.05	0.56
6:F:102:LEU:C	6:F:103:GLN:O	2.42	0.56
6:F:114:ALA:N	6:F:115:PRO:HD3	2.20	0.56
7:G:96:GLY:O	7:G:97:LEU:CD2	2.53	0.56
7:G:99:HIS:HA	7:G:100:PHE:HB2	1.85	0.56
19:H:1145:CLA:H101	19:H:1145:CLA:C14	2.22	0.56
11:K:58:VAL:HG12	11:K:59:THR:N	2.19	0.56
11:K:76:ALA:N	11:K:78:ARG:NH1	2.46	0.56
11:K:115:ILE:HD12	11:K:118:VAL:CG2	2.34	0.56
12:L:164:LEU:HD12	12:L:165:THR:CA	2.34	0.56
12:L:164:LEU:C	12:L:165:THR:HG23	2.24	0.56
13:N:132:THR:OG1	13:N:137:LEU:C	2.43	0.56
13:N:148:ASP:CA	13:N:149:ASP:O	2.53	0.56
15:1:95:PRO:CA	15:1:98:LEU:CB	2.83	0.56
16:2:195:TYR:CE1	16:2:196:PRO:HD2	2.37	0.56
19:2:2004:CLA:O1A	19:3:2009:CLA:HBC2	2.05	0.56
17:3:159:VAL:O	17:3:161:GLU:CA	2.53	0.56
18:4:146:PHE:HE2	19:4:4013:CLA:C3C	2.17	0.56
1:A:97:TYR:O	1:A:98:PHE:O	2.23	0.56
1:A:146:THR:O	19:A:1126:CLA:HMA2	2.04	0.56
1:A:236:GLY:O	1:A:237:VAL:CG2	2.53	0.56
1:A:370:ILE:CD1	19:A:1124:CLA:O1D	2.53	0.56
1:A:438:HIS:HB2	1:A:441:ALA:HB3	1.85	0.56
1:A:497:ALA:HB1	1:A:510:SER:HG	1.71	0.56
1:A:558:LYS:NZ	2:B:674:LEU:HD22	2.20	0.56
19:A:1105:CLA:HHB	19:A:1106:CLA:HMB3	1.86	0.56
19:A:1124:CLA:CHD	19:A:1124:CLA:CBC	2.77	0.56
19:A:1124:CLA:O1A	19:A:1124:CLA:C2	2.51	0.56
2:B:143:LEU:C	2:B:145:LEU:H	2.08	0.56
2:B:371:LEU:HD21	19:B:1225:CLA:HED3	1.87	0.56
19:B:1213:CLA:HED2	19:B:1213:CLA:CBA	2.36	0.56
3:C:26:LEU:HD21	4:D:181:ARG:NH1	2.20	0.56
4:D:138:LEU:O	4:D:138:LEU:HD23	2.05	0.56
4:D:167:HIS:CD2	4:D:167:HIS:O	2.59	0.56
4:D:187:ASN:N	4:D:187:ASN:ND2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:106:ARG:C	5:E:106:ARG:HE	2.09	0.56
6:F:82:LEU:CG	6:F:83:THR:N	2.58	0.56
6:F:207:LEU:CD2	6:F:208:PHE:CG	2.88	0.56
7:G:133:ILE:HG23	7:G:133:ILE:O	2.03	0.56
22:H:7002:LMU:H1B	22:H:7002:LMU:O6B	2.05	0.56
15:1:78:ARG:CD	19:1:1011:CLA:HMC2	2.16	0.56
16:2:117:ALA:HB3	16:2:230:LEU:CG	2.20	0.56
16:2:195:TYR:HB3	16:2:201:PHE:CE2	2.39	0.56
17:3:214:GLY:HA3	17:3:215:LYS:HE2	1.85	0.56
19:4:4015:CLA:HBC3	19:4:4015:CLA:CHD	2.34	0.56
1:A:111:ASN:HB3	1:A:112:ASP:OD1	2.04	0.56
1:A:203:LEU:CD2	19:A:1123:CLA:CED	2.83	0.56
1:A:224:HIS:HE1	19:A:1113:CLA:C4C	2.18	0.56
1:A:263:ALA:O	1:A:264:GLU:HG2	2.06	0.56
1:A:462:ILE:HD11	19:A:9022:CLA:C5	2.32	0.56
1:A:631:GLN:O	1:A:632:GLY:C	2.41	0.56
1:A:733:VAL:HG22	19:A:1140:CLA:C3D	2.35	0.56
19:A:1112:CLA:CAB	21:A:6002:BCR:H19C	2.36	0.56
19:A:1119:CLA:C4C	19:A:1125:CLA:H172	2.35	0.56
19:A:9022:CLA:CBB	19:A:9023:CLA:CHB	2.79	0.56
19:A:9023:CLA:H142	21:I:6018:BCR:C4	2.36	0.56
2:B:293:THR:H	19:B:1217:CLA:CED	2.18	0.56
2:B:457:PRO:O	2:B:458:ILE:C	2.44	0.56
2:B:495:PRO:O	2:B:499:ASN:ND2	2.39	0.56
19:B:1206:CLA:H203	21:I:6018:BCR:H372	1.85	0.56
19:B:1206:CLA:H122	21:I:6018:BCR:H373	1.87	0.56
21:B:6010:BCR:H321	21:B:6010:BCR:HC8	1.88	0.56
4:D:104:TRP:N	4:D:104:TRP:CD1	2.73	0.56
6:F:215:VAL:O	6:F:218:TYR:N	2.38	0.56
7:G:90:GLN:N	7:G:90:GLN:OE1	2.39	0.56
19:H:1145:CLA:CBC	19:H:1145:CLA:CMC	2.77	0.56
10:J:10:VAL:CG1	10:J:11:ALA:N	2.68	0.56
11:K:57:MET:O	11:K:61:THR:OG1	2.22	0.56
11:K:70:PHE:CB	11:K:98:PRO:HB3	2.32	0.56
12:L:141:LEU:CD1	21:L:6019:BCR:H312	2.17	0.56
15:1:64:PHE:CD1	15:1:65:ASP:HB3	2.40	0.56
15:1:91:MET:SD	15:1:94:VAL:HB	2.45	0.56
16:2:150:THR:O	16:2:152:LEU:HD13	2.05	0.56
16:2:172:LEU:O	16:2:174:PRO:CD	2.46	0.56
19:2:2001:CLA:O1A	19:2:2001:CLA:C1A	2.53	0.56
17:3:184:LYS:O	17:3:185:GLN:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:111:LEU:HD12	18:4:112:PRO:HD3	1.78	0.56
18:4:154:ILE:CD1	19:4:1009:CLA:HMD1	2.35	0.56
18:4:156:ARG:HD2	19:4:4011:CLA:C2D	2.35	0.56
18:4:177:LEU:N	18:4:178:PRO:CD	2.68	0.56
18:4:226:LYS:N	18:4:226:LYS:HZ3	2.04	0.56
18:4:246:GLN:O	18:4:246:GLN:CG	2.52	0.56
19:4:1306:CLA:H2	19:4:1306:CLA:CED	2.31	0.56
1:A:68:THR:HG23	1:A:69:SER:N	2.20	0.56
1:A:187:HIS:CE1	19:A:1109:CLA:C1A	2.74	0.56
1:A:430:ASP:C	1:A:432:LEU:H	2.08	0.56
19:A:1138:CLA:CBB	19:A:1138:CLA:H101	2.35	0.56
2:B:25:ILE:CG2	21:L:6019:BCR:C28	2.83	0.56
2:B:175:LEU:CD1	19:B:1221:CLA:HED1	2.35	0.56
2:B:312:GLY:C	2:B:314:ARG:N	2.59	0.56
2:B:315:LEU:O	2:B:315:LEU:HD22	2.06	0.56
2:B:558:PRO:HG3	2:B:574:ASP:OD1	2.06	0.56
19:B:1220:CLA:H43	19:B:1220:CLA:CAA	2.31	0.56
3:C:7:ILE:HD13	3:C:54:CYS:SG	2.45	0.56
3:C:23:THR:HG21	3:C:47:ASP:OD2	2.06	0.56
11:K:50:GLY:N	11:K:52:PRO:CD	2.68	0.56
15:1:170:PRO:O	15:1:173:TYR:CZ	2.58	0.56
15:1:189:LYS:CA	15:1:189:LYS:CE	2.74	0.56
16:2:112:TRP:CG	19:2:2012:CLA:O1D	2.58	0.56
16:2:165:GLY:HA2	16:2:167:ARG:HG2	1.86	0.56
16:2:192:ASP:OD1	16:2:194:GLY:C	2.43	0.56
17:3:162:MET:HE1	19:3:3010:CLA:C3D	2.36	0.56
18:4:95:GLU:HA	18:4:98:ASN:OD1	2.05	0.56
18:4:121:ILE:CG1	18:4:122:ASN:H	2.18	0.56
1:A:242:ILE:CB	1:A:243:PRO:HD3	2.34	0.56
1:A:267:THR:CG2	1:A:269:PHE:CE2	2.59	0.56
1:A:281:LEU:HD22	19:A:1115:CLA:HED2	1.83	0.56
1:A:438:HIS:HA	4:D:87:THR:OG1	2.05	0.56
1:A:564:ARG:CB	1:A:564:ARG:CZ	2.83	0.56
1:A:570:PRO:C	1:A:572:LYS:H	2.07	0.56
1:A:578:ARG:HB2	1:A:578:ARG:NH1	2.19	0.56
19:A:1102:CLA:CBA	19:A:1109:CLA:H62	2.35	0.56
19:A:9023:CLA:HBA2	19:A:9023:CLA:HED3	1.87	0.56
2:B:131:THR:HG22	2:B:131:THR:O	2.04	0.56
2:B:230:TRP:H	7:G:63:VAL:HG21	1.63	0.56
2:B:560:ASP:CG	3:C:66:ARG:NH1	2.59	0.56
20:B:5002:PQN:H302	21:L:6019:BCR:H24C	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:MET:H3	3:C:4:SER:CB	2.16	0.56
3:C:67:VAL:CG1	3:C:68:TYR:N	2.68	0.56
4:D:147:LYS:O	4:D:148:TYR:CG	2.58	0.56
5:E:78:ARG:NH1	5:E:125:ILE:CB	2.65	0.56
6:F:221:LEU:CD2	6:F:222:LEU:HD21	2.31	0.56
11:K:127:ILE:HG12	11:K:130:LEU:CD1	2.28	0.56
11:K:127:ILE:HG23	11:K:130:LEU:HG	1.64	0.56
13:N:133:GLY:O	13:N:134:CYS:SG	2.60	0.56
13:N:146:LEU:HG	13:N:148:ASP:O	2.06	0.56
15:1:85:ILE:C	15:1:88:ARG:HB2	2.26	0.56
15:1:123:THR:O	15:1:124:TYR:CB	2.53	0.56
15:1:221:LEU:CD1	19:1:1003:CLA:HAC1	2.29	0.56
17:3:124:LYS:HZ1	17:3:148:TYR:N	2.04	0.56
17:3:164:LEU:CD1	17:3:165:MET:SD	2.93	0.56
17:3:204:GLY:O	17:3:205:GLY:C	2.42	0.56
18:4:145:GLU:OE2	18:4:146:PHE:HE1	1.88	0.56
18:4:207:ASN:OD1	19:4:4002:CLA:NB	2.39	0.56
1:A:331:LEU:CD2	1:A:331:LEU:O	2.52	0.56
1:A:685:VAL:HG22	19:A:1140:CLA:HBB2	1.86	0.56
1:A:700:TRP:HZ3	19:A:9013:CLA:O1D	1.89	0.56
2:B:117:TYR:H	19:B:1205:CLA:HMD1	1.71	0.56
2:B:193:HIS:HB2	19:B:1211:CLA:CHC	2.36	0.56
2:B:351:HIS:O	2:B:355:LEU:HB2	2.05	0.56
2:B:355:LEU:HD21	2:B:508:LEU:HD21	1.87	0.56
19:B:1205:CLA:H142	19:B:1205:CLA:C10	2.34	0.56
4:D:140:LEU:CD1	4:D:144:LEU:N	2.69	0.56
5:E:90:VAL:CG1	5:E:91:VAL:H	2.19	0.56
6:F:199:ASP:HA	10:J:9:SER:HA	1.87	0.56
8:H:82:LYS:HG2	8:H:85:GLU:CB	2.36	0.56
8:H:82:LYS:HG2	8:H:85:GLU:HB3	1.87	0.56
13:N:113:ASN:OD1	13:N:113:ASN:O	2.24	0.56
22:R:7021:LMU:H41	22:R:7021:LMU:H6D	1.87	0.56
15:1:151:GLN:NE2	15:1:151:GLN:HA	2.19	0.56
15:1:170:PRO:CG	15:1:173:TYR:CE2	2.88	0.56
16:2:157:LEU:HD13	16:2:157:LEU:N	2.19	0.56
18:4:158:GLN:CD	19:4:1004:CLA:C1A	2.70	0.56
18:4:212:LEU:O	18:4:213:ALA:HB3	2.04	0.56
1:A:57:LEU:CD2	1:A:58:HIS:N	2.68	0.56
1:A:349:ILE:CG2	1:A:350:LEU:N	2.66	0.56
1:A:426:THR:CG2	1:A:428:TYR:CZ	2.88	0.56
1:A:451:ILE:HD13	19:A:1131:CLA:HED1	1.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ILE:CG2	19:A:1132:CLA:HMC3	2.35	0.56
19:A:1112:CLA:CHC	21:A:6002:BCR:C17	2.82	0.56
19:A:1127:CLA:H51	21:A:6003:BCR:H331	1.87	0.56
2:B:436:LEU:O	2:B:437:TYR:HB2	2.06	0.56
2:B:614:THR:CG2	2:B:614:THR:O	2.50	0.56
2:B:730:SER:C	2:B:731:GLY:O	2.42	0.56
5:E:75:LYS:HA	5:E:87:THR:CG2	2.31	0.56
6:F:88:SER:O	6:F:91:PHE:N	2.39	0.56
6:F:148:LEU:O	6:F:148:LEU:CD1	2.48	0.56
7:G:151:PRO:O	7:G:151:PRO:HD2	2.05	0.56
8:H:121:LEU:C	8:H:122:PRO:O	2.44	0.56
10:J:31:ARG:NH2	19:J:1311:CLA:C3B	2.69	0.56
22:R:7021:LMU:H22	22:R:7021:LMU:C6	2.33	0.56
15:1:81:GLU:CG	15:1:82:SER:N	2.68	0.56
15:1:117:LEU:N	15:1:117:LEU:CD1	2.67	0.56
15:1:170:PRO:CG	15:1:171:LEU:N	2.58	0.56
16:2:185:ASN:C	16:2:185:ASN:OD1	2.43	0.56
17:3:125:VAL:HG21	19:3:3010:CLA:C1C	2.35	0.56
1:A:58:HIS:CE1	19:A:1101:CLA:ND	2.74	0.56
1:A:190:ALA:HB1	1:A:191:PRO:HD2	1.85	0.56
1:A:544:ILE:HD11	19:A:9011:CLA:H193	1.88	0.56
1:A:567:ARG:HH11	4:D:88:GLY:C	2.09	0.56
19:A:1116:CLA:H52	19:A:1133:CLA:HBA1	1.87	0.56
19:A:1119:CLA:H18	21:A:6007:BCR:H383	1.87	0.56
19:A:1127:CLA:CHD	21:A:6003:BCR:H333	2.36	0.56
2:B:317:ARG:CZ	2:B:410:ARG:CG	2.68	0.56
24:B:7101:LMG:O3	3:C:70:TRP:HZ2	1.84	0.56
3:C:43:PRO:O	3:C:43:PRO:CD	2.54	0.56
3:C:66:ARG:HG2	3:C:66:ARG:NH2	1.95	0.56
5:E:73:LYS:O	5:E:73:LYS:HG3	2.06	0.56
6:F:215:VAL:O	6:F:218:TYR:HB2	2.06	0.56
10:J:2:ARG:HB3	10:J:7:TYR:CZ	2.41	0.56
12:L:67:GLY:C	12:L:68:SER:OG	2.45	0.56
12:L:93:VAL:O	12:L:94:SER:C	2.41	0.56
15:1:78:ARG:HH21	15:1:179:LYS:CG	2.15	0.56
15:1:147:PHE:CD1	15:1:147:PHE:O	2.59	0.56
15:1:161:LYS:O	15:1:161:LYS:HD2	2.06	0.56
19:1:1001:CLA:HMC1	19:1:1001:CLA:CBC	2.17	0.56
16:2:146:PHE:N	16:2:146:PHE:CD1	2.73	0.56
16:2:226:ARG:HA	16:2:229:MET:HB3	1.87	0.56
16:2:269:LYS:HE3	16:2:269:LYS:C	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:210:PRO:CG	17:3:211:LEU:N	2.69	0.56
22:3:7003:LMU:C2B	22:3:7005:LMU:HG1	2.36	0.56
18:4:103:MET:HE1	18:4:207:ASN:CA	2.35	0.56
1:A:177:LEU:C	1:A:179:LEU:H	2.09	0.56
1:A:252:ARG:NH2	1:A:261:SER:OG	2.39	0.56
1:A:426:THR:CA	1:A:428:TYR:CE2	2.84	0.56
1:A:484:LEU:C	1:A:485:GLN:NE2	2.59	0.56
1:A:580:PRO:HA	1:A:728:VAL:CG2	2.36	0.56
1:A:586:ARG:HG3	3:C:49:VAL:CG2	2.31	0.56
1:A:639:ALA:O	1:A:641:ASN:N	2.39	0.56
19:A:1124:CLA:CHB	21:A:6008:BCR:H363	2.35	0.56
19:A:9023:CLA:H142	21:I:6018:BCR:HC42	1.87	0.56
2:B:12:ILE:HG22	2:B:13:ALA:N	2.20	0.56
2:B:154:TRP:CD1	2:B:154:TRP:C	2.78	0.56
2:B:197:VAL:O	2:B:198:ALA:HB2	2.06	0.56
2:B:419:ILE:HG12	2:B:536:LYS:HB2	1.88	0.56
2:B:457:PRO:HB3	2:B:517:PHE:CG	2.40	0.56
2:B:505:SER:OG	2:B:506:ASN:OD1	2.23	0.56
5:E:79:LYS:N	5:E:84:TYR:CE1	2.74	0.56
6:F:228:ASP:C	6:F:231:PHE:HB3	2.25	0.56
7:G:89:LYS:HA	7:G:89:LYS:HZ1	1.63	0.56
7:G:102:ALA:C	7:G:104:ASP:OD1	2.44	0.56
8:H:109:LEU:HD23	19:H:1207:CLA:H52	1.86	0.56
11:K:97:ASP:O	11:K:98:PRO:C	2.44	0.56
13:N:131:PHE:CA	13:N:132:THR:HG22	2.35	0.56
14:R:36:UNK:C	14:R:38:UNK:N	2.66	0.56
19:3:3013:CLA:H91	19:3:3013:CLA:H121	1.87	0.56
18:4:172:PHE:C	18:4:194:PHE:CD2	2.79	0.56
19:4:4002:CLA:CBA	19:4:4002:CLA:CMA	2.67	0.56
1:A:159:THR:HG22	1:A:160:SER:N	2.20	0.56
1:A:193:LEU:O	1:A:194:ALA:C	2.44	0.56
1:A:358:LEU:HD21	1:A:413:HIS:ND1	2.21	0.56
1:A:545:HIS:CE1	1:A:612:VAL:HG22	2.41	0.56
2:B:86:PRO:C	2:B:87:ILE:HD12	2.26	0.56
2:B:471:THR:HG22	2:B:502:ASN:HD22	1.71	0.56
2:B:493:TRP:O	2:B:495:PRO:HG3	2.06	0.56
2:B:655:LEU:CD2	19:B:1239:CLA:CBB	2.84	0.56
2:B:707:LEU:O	2:B:710:LEU:HB3	2.06	0.56
2:B:732:LYS:HG2	2:B:733:PHE:HA	1.88	0.56
19:B:1203:CLA:C19	19:B:1224:CLA:H141	2.36	0.56
4:D:184:VAL:HG12	4:D:185:GLY:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:103:VAL:HG13	5:E:120:TYR:C	2.26	0.56
6:F:168:LEU:O	6:F:171:ALA:O	2.23	0.56
9:I:10:PRO:O	9:I:15:LEU:N	2.32	0.56
10:J:32:PHE:HE2	10:J:33:PHE:CZ	2.23	0.56
11:K:56:ILE:O	11:K:56:ILE:HG22	2.05	0.56
19:K:1146:CLA:O1A	19:K:1146:CLA:H2A	2.05	0.56
12:L:51:LYS:N	12:L:51:LYS:CD	2.66	0.56
12:L:164:LEU:O	12:L:165:THR:HG22	2.05	0.56
15:1:170:PRO:HG2	15:1:173:TYR:CD2	2.41	0.56
16:2:122:ILE:N	16:2:123:PRO:HD3	2.20	0.56
16:2:122:ILE:HD12	19:2:2002:CLA:HMB1	1.87	0.56
17:3:204:GLY:C	17:3:206:PRO:C	2.65	0.56
1:A:42:ARG:C	1:A:44:ILE:N	2.60	0.55
1:A:630:ASP:O	1:A:631:GLN:C	2.45	0.55
19:A:9012:CLA:C3B	2:B:589:TRP:CH2	2.85	0.55
2:B:382:ILE:CG2	2:B:383:MET:N	2.48	0.55
2:B:438:VAL:CG2	19:B:1230:CLA:HAC1	2.35	0.55
2:B:440:ASN:CG	2:B:614:THR:CG2	2.71	0.55
2:B:596:TRP:O	2:B:597:LYS:HB3	2.06	0.55
19:B:1220:CLA:H93	19:B:1227:CLA:CBC	2.37	0.55
6:F:149:ILE:HG22	6:F:151:SER:N	2.21	0.55
6:F:200:VAL:CG2	6:F:204:SER:N	2.70	0.55
9:I:14:LEU:O	9:I:17:PRO:HD2	2.06	0.55
11:K:50:GLY:C	11:K:52:PRO:CD	2.71	0.55
11:K:124:LEU:O	11:K:126:ASN:CB	2.54	0.55
19:K:1146:CLA:HMD2	22:K:7001:LMU:H32	1.87	0.55
12:L:82:TYR:O	12:L:83:LEU:CB	2.54	0.55
12:L:104:LEU:HD11	12:L:199:TRP:CZ2	2.41	0.55
19:L:1148:CLA:CED	19:L:1148:CLA:C1	2.77	0.55
15:1:125:LEU:O	15:1:125:LEU:HD23	2.06	0.55
16:2:150:THR:O	16:2:153:PHE:N	2.39	0.55
16:2:254:LEU:HD22	16:2:256:ASP:H	1.69	0.55
1:A:362:LEU:CB	1:A:410:ALA:HB2	2.36	0.55
19:A:1124:CLA:HED2	19:A:1124:CLA:HAA1	1.87	0.55
19:A:1131:CLA:H52	21:B:6017:BCR:C34	2.34	0.55
19:A:1141:CLA:H71	19:A:1141:CLA:C12	2.09	0.55
2:B:290:MET:O	2:B:290:MET:HG2	2.06	0.55
2:B:347:LEU:HD22	2:B:351:HIS:CE1	2.42	0.55
2:B:356:PRO:O	2:B:356:PRO:CD	2.55	0.55
2:B:463:ILE:HD11	19:B:1231:CLA:HMC3	1.88	0.55
4:D:123:ARG:NH2	22:D:7050:LMU:H6'1	1.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:90:GLN:HG2	6:F:143:ASP:H	1.70	0.55
8:H:111:TYR:CD1	8:H:112:LEU:HD21	2.41	0.55
9:I:28:VAL:O	9:I:29:GLU:CD	2.45	0.55
12:L:169:ARG:HG2	12:L:172:GLU:CA	2.37	0.55
12:L:172:GLU:C	12:L:173:PRO:O	2.41	0.55
13:N:155:GLU:CB	13:N:157:LYS:CA	2.79	0.55
22:N:7049:LMU:O1'	22:N:7049:LMU:C6	2.55	0.55
16:2:183:PHE:C	16:2:183:PHE:HD1	2.09	0.55
1:A:245:PRO:C	1:A:248:PHE:HE2	2.09	0.55
1:A:316:MET:CA	1:A:317:TYR:HB2	2.31	0.55
1:A:393:LEU:HD11	1:A:750:PHE:CE1	2.41	0.55
19:A:1124:CLA:H2	19:A:1125:CLA:CED	2.35	0.55
19:A:1126:CLA:C20	21:J:6012:BCR:C17	2.79	0.55
2:B:98:GLN:O	2:B:100:ALA:CB	2.55	0.55
2:B:292:ARG:HH21	2:B:297:ILE:HG13	1.70	0.55
2:B:293:THR:HG21	19:B:1209:CLA:HMA3	1.88	0.55
2:B:459:PHE:CD2	19:B:1235:CLA:C1D	2.66	0.55
2:B:556:SER:C	2:B:558:PRO:CD	2.71	0.55
3:C:11:CYS:C	3:C:13:GLY:H	2.10	0.55
7:G:106:ARG:HB2	7:G:107:ALA:HA	1.88	0.55
8:H:61:THR:HA	8:H:62:THR:HG23	0.63	0.55
11:K:78:ARG:CZ	11:K:78:ARG:H	2.20	0.55
11:K:81:THR:HG23	11:K:82:ALA:N	2.22	0.55
11:K:97:ASP:HA	11:K:101:PHE:CE2	2.41	0.55
12:L:141:LEU:O	12:L:145:LEU:HD12	2.07	0.55
13:N:99:LYS:HA	13:N:102:ASN:CG	2.23	0.55
13:N:139:LYS:HG3	13:N:142:LYS:CG	2.37	0.55
15:1:112:GLN:C	15:1:113:GLU:OE2	2.44	0.55
18:4:191:PRO:O	18:4:192:LEU:HB2	2.06	0.55
22:4:7053:LMU:H6E	22:4:7053:LMU:C2B	2.36	0.55
1:A:29:THR:O	1:A:29:THR:CG2	2.54	0.55
1:A:74:ILE:O	1:A:75:SER:C	2.44	0.55
1:A:541:VAL:HG12	1:A:545:HIS:NE2	2.22	0.55
1:A:629:ASN:O	1:A:632:GLY:N	2.39	0.55
19:A:9011:CLA:HMB3	19:A:9012:CLA:CAD	2.37	0.55
19:A:9023:CLA:HBC1	2:B:665:ILE:HD12	1.89	0.55
2:B:352:MET:HE2	19:B:1225:CLA:OBD	2.04	0.55
2:B:459:PHE:CG	19:B:1235:CLA:CAD	2.89	0.55
2:B:617:MET:HG3	2:B:618:GLY:N	2.21	0.55
2:B:622:ASP:CB	2:B:626:LEU:CG	2.85	0.55
3:C:12:ILE:HB	3:C:38:GLN:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:96:ASP:CB	5:E:98:ASN:OD1	2.54	0.55
5:E:102:PRO:O	5:E:120:TYR:O	2.24	0.55
6:F:94:ARG:HA	6:F:94:ARG:NE	2.21	0.55
7:G:68:THR:OG1	7:G:69:GLY:N	2.39	0.55
12:L:92:ALA:CB	12:L:98:ARG:CZ	2.84	0.55
19:L:1148:CLA:HAA1	19:L:1148:CLA:O1D	2.03	0.55
15:1:60:GLY:O	15:1:61:ASP:C	2.45	0.55
15:1:141:GLU:O	15:1:145:ILE:CG1	2.53	0.55
17:3:94:GLU:HB3	17:3:95:PRO:HD3	1.88	0.55
22:3:7003:LMU:O2B	22:3:7005:LMU:C6B	2.55	0.55
18:4:95:GLU:CG	18:4:96:LEU:N	2.69	0.55
1:A:107:GLU:OE2	1:A:161:GLU:CG	2.45	0.55
1:A:158:ILE:HD13	19:A:1112:CLA:CED	2.36	0.55
1:A:201:SER:O	1:A:204:ASN:N	2.40	0.55
1:A:338:PHE:HB3	19:A:1129:CLA:HBD	1.89	0.55
1:A:430:ASP:C	1:A:432:LEU:N	2.60	0.55
2:B:542:ARG:NH1	2:B:542:ARG:HB3	2.18	0.55
2:B:670:TYR:C	2:B:670:TYR:CD1	2.80	0.55
4:D:80:SER:H	4:D:81:PRO:HD3	1.70	0.55
6:F:100:LYS:O	6:F:100:LYS:CD	2.53	0.55
12:L:102:VAL:CA	19:L:1502:CLA:HED2	2.33	0.55
15:1:68:GLY:C	15:1:72:VAL:HB	2.25	0.55
15:1:137:ILE:C	15:1:141:GLU:OE2	2.45	0.55
17:3:161:GLU:HA	17:3:164:LEU:CG	2.32	0.55
22:3:7003:LMU:H3B	22:3:7005:LMU:C3B	2.31	0.55
19:4:4002:CLA:CGD	19:4:4002:CLA:CAA	2.75	0.55
1:A:64:PHE:N	1:A:64:PHE:CD1	2.73	0.55
1:A:470:LEU:HG	19:B:1206:CLA:HMC3	1.89	0.55
1:A:507:ALA:O	1:A:508:THR:C	2.44	0.55
19:A:1106:CLA:H111	21:J:6012:BCR:C11	2.36	0.55
2:B:49:SER:O	2:B:52:GLY:N	2.40	0.55
2:B:175:LEU:HA	2:B:178:HIS:HB2	1.88	0.55
2:B:275:HIS:ND1	19:B:1214:CLA:HMB1	2.22	0.55
19:B:1229:CLA:HMB3	19:B:1230:CLA:HBB2	1.87	0.55
21:B:6010:BCR:H382	21:B:6010:BCR:C23	2.34	0.55
21:B:6017:BCR:H23C	21:B:6017:BCR:C38	2.26	0.55
4:D:173:TYR:O	4:D:175:GLU:HG3	2.07	0.55
5:E:82:TYR:CB	5:E:83:TRP:HZ3	2.14	0.55
6:F:123:MET:O	6:F:126:THR:N	2.39	0.55
7:G:74:LEU:C	7:G:77:PHE:H	2.10	0.55
8:H:89:ALA:N	8:H:90:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:112:VAL:C	11:K:114:HIS:N	2.53	0.55
13:N:104:LYS:O	13:N:107:LEU:CA	2.55	0.55
13:N:139:LYS:HG3	13:N:142:LYS:HE2	1.87	0.55
15:1:137:ILE:HB	15:1:141:GLU:OE2	2.07	0.55
16:2:165:GLY:O	16:2:167:ARG:CG	2.54	0.55
18:4:173:LYS:CA	18:4:194:PHE:CD2	2.89	0.55
18:4:174:GLN:CA	18:4:176:SER:H	2.19	0.55
1:A:230:ASN:OD1	1:A:296:LEU:HD22	2.07	0.55
1:A:373:ALA:O	1:A:396:PHE:HD1	1.88	0.55
1:A:420:ARG:HB3	1:A:420:ARG:CZ	2.32	0.55
1:A:710:ALA:HB1	19:A:1138:CLA:HED2	1.88	0.55
19:A:9012:CLA:CED	19:B:9010:CLA:H2	2.36	0.55
2:B:18:THR:O	2:B:21:ILE:N	2.40	0.55
2:B:312:GLY:C	2:B:314:ARG:H	2.07	0.55
2:B:707:LEU:CD1	2:B:711:VAL:HG21	2.37	0.55
2:B:732:LYS:CG	2:B:733:PHE:HA	2.37	0.55
19:B:1205:CLA:CGA	19:B:1205:CLA:C1A	2.85	0.55
19:B:1225:CLA:H101	21:B:6006:BCR:H343	1.89	0.55
4:D:129:LEU:HD12	4:D:130:LYS:H	1.71	0.55
5:E:69:LYS:HE3	5:E:69:LYS:H	1.71	0.55
5:E:106:ARG:NE	5:E:106:ARG:C	2.60	0.55
19:G:1242:CLA:O1A	22:G:7026:LMU:H101	2.07	0.55
13:N:105:LYS:O	13:N:106:ARG:C	2.44	0.55
13:N:146:LEU:HD13	17:3:142:ILE:HB	1.89	0.55
13:N:155:GLU:CB	13:N:157:LYS:CE	2.78	0.55
13:N:169:LYS:CA	13:N:170:TRP:HD1	2.20	0.55
15:1:122:ALA:HB3	15:1:124:TYR:H	1.72	0.55
17:3:110:MET:CE	17:3:238:ILE:H	2.20	0.55
17:3:154:ASN:HA	17:3:155:TYR:CD2	2.41	0.55
22:3:7005:LMU:C2B	22:3:7005:LMU:C3'	2.85	0.55
1:A:109:TRP:CH2	1:A:154:ARG:HD3	2.42	0.55
19:A:1113:CLA:HBA2	19:A:1113:CLA:H42	1.88	0.55
19:A:1131:CLA:HAA1	21:B:6020:BCR:C14	2.37	0.55
19:A:1237:CLA:H112	19:A:1237:CLA:H61	1.87	0.55
21:A:6011:BCR:C19	19:A:9012:CLA:H172	2.37	0.55
22:A:7010:LMU:H22	22:K:7047:LMU:H101	1.89	0.55
2:B:160:LYS:CE	2:B:161:TRP:CD2	2.90	0.55
2:B:334:LEU:O	2:B:334:LEU:CG	2.51	0.55
2:B:376:GLN:OE1	2:B:376:GLN:HA	2.06	0.55
2:B:473:GLY:O	2:B:474:PHE:HB2	2.06	0.55
2:B:502:ASN:ND2	2:B:511:THR:HG21	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:SER:O	2:B:508:LEU:HB2	2.05	0.55
2:B:607:SER:OG	2:B:608:GLN:N	2.39	0.55
4:D:98:GLU:HB2	4:D:100:TYR:CE2	2.42	0.55
4:D:146:SER:O	4:D:147:LYS:CG	2.51	0.55
5:E:93:VAL:O	5:E:93:VAL:CG1	2.54	0.55
6:F:194:LYS:O	6:F:197:ILE:O	2.25	0.55
19:F:1305:CLA:HED2	19:F:1305:CLA:CAD	2.36	0.55
7:G:134:GLY:O	7:G:135:HIS:ND1	2.40	0.55
22:H:7032:LMU:H31	22:H:7032:LMU:O5B	2.07	0.55
16:2:101:TRP:CA	16:2:103:VAL:N	2.62	0.55
17:3:96:ARG:CA	17:3:99:ALA:HB2	2.34	0.55
18:4:124:PRO:O	18:4:125:LYS:CB	2.55	0.55
18:4:158:GLN:HE21	19:4:1004:CLA:C4A	2.18	0.55
18:4:169:ASP:O	18:4:173:LYS:CB	2.54	0.55
19:4:4002:CLA:O1A	19:4:4002:CLA:C2	2.52	0.55
22:4:7033:LMU:H3'	22:4:7033:LMU:O5B	2.05	0.55
1:A:229:ILE:HG22	1:A:229:ILE:O	2.06	0.55
1:A:281:LEU:HD22	19:A:1115:CLA:H2A	1.87	0.55
1:A:466:THR:HG22	2:B:648:TRP:NE1	2.21	0.55
1:A:472:ARG:N	1:A:473:PRO:CD	2.68	0.55
2:B:224:PRO:HB2	2:B:227:THR:CG2	2.36	0.55
2:B:348:VAL:HG12	2:B:349:ALA:N	2.22	0.55
19:B:1210:CLA:H41	19:B:1215:CLA:CBC	2.36	0.55
3:C:62:PHE:CE1	5:E:80:GLU:CB	2.87	0.55
4:D:167:HIS:HD2	4:D:167:HIS:O	1.90	0.55
22:E:7048:LMU:C7	22:E:7048:LMU:C11	2.83	0.55
7:G:134:GLY:O	7:G:135:HIS:CD2	2.60	0.55
19:G:1242:CLA:H3A	19:G:1242:CLA:O2A	2.06	0.55
8:H:107:SER:O	8:H:111:TYR:HB2	2.07	0.55
19:H:1145:CLA:O2D	19:H:1145:CLA:CAA	2.55	0.55
12:L:205:TYR:CD1	12:L:207:LEU:HD13	2.33	0.55
13:N:145:PHE:C	13:N:146:LEU:O	2.45	0.55
15:1:170:PRO:HB2	15:1:171:LEU:O	2.06	0.55
15:1:171:LEU:HD23	15:1:171:LEU:N	2.22	0.55
22:1:7004:LMU:H3'	22:1:7004:LMU:C1	2.25	0.55
19:2:2014:CLA:C4A	19:2:2014:CLA:HBA2	2.35	0.55
17:3:206:PRO:HD2	17:3:206:PRO:O	2.07	0.55
18:4:172:PHE:HB2	18:4:173:LYS:O	2.06	0.55
1:A:70:ASP:O	1:A:71:LEU:C	2.44	0.55
1:A:86:LEU:CD1	1:A:178:MET:HE2	2.35	0.55
1:A:250:LEU:CD1	17:3:136:TRP:HZ2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:TYR:CE1	1:A:540:LEU:HD11	2.42	0.55
1:A:607:ASN:HD21	19:A:9022:CLA:C2C	2.19	0.55
19:A:1140:CLA:H192	10:J:19:PHE:CD2	2.42	0.55
19:A:9013:CLA:H3A	19:A:9013:CLA:CGA	2.37	0.55
2:B:104:PHE:O	2:B:105:THR:CB	2.54	0.55
2:B:256:THR:C	2:B:257:ILE:HD13	2.27	0.55
2:B:560:ASP:OD1	3:C:65:VAL:O	2.25	0.55
19:B:1213:CLA:HBC2	19:B:1213:CLA:CHD	2.29	0.55
19:B:1235:CLA:C15	21:F:6016:BCR:H313	2.25	0.55
3:C:26:LEU:HD22	4:D:181:ARG:HH11	1.71	0.55
4:D:101:VAL:HA	4:D:130:LYS:HA	1.87	0.55
4:D:203:THR:HG22	4:D:205:LYS:N	2.16	0.55
6:F:158:GLY:O	10:J:38:ILE:HG23	2.06	0.55
6:F:225:GLU:O	6:F:227:VAL:CG1	2.54	0.55
19:G:1242:CLA:HAA2	19:G:1242:CLA:HBD	1.88	0.55
22:K:7042:LMU:H32	22:K:7042:LMU:O5'	2.06	0.55
12:L:125:ILE:HG12	12:L:127:GLY:H	1.72	0.55
13:N:118:TYR:O	13:N:119:THR:CG2	2.53	0.55
13:N:169:LYS:HA	13:N:170:TRP:HD1	1.71	0.55
15:1:170:PRO:CD	15:1:173:TYR:HD2	2.16	0.55
15:1:193:LEU:HD23	15:1:193:LEU:O	2.07	0.55
16:2:149:THR:O	16:2:152:LEU:HD11	2.07	0.55
16:2:184:PRO:N	16:2:187:LYS:CD	2.70	0.55
17:3:98:LEU:HD21	17:3:102:GLU:HG3	1.88	0.55
17:3:185:GLN:CG	17:3:186:TYR:N	2.33	0.55
18:4:202:GLU:HA	18:4:205:ILE:HG23	1.89	0.55
22:4:7053:LMU:H72	22:4:7053:LMU:C11	2.37	0.55
1:A:75:SER:HB3	1:A:354:TRP:HZ2	1.71	0.54
1:A:448:TRP:CD1	19:A:1131:CLA:CED	2.90	0.54
1:A:622:SER:OG	1:A:642:PHE:HB2	2.07	0.54
1:A:728:VAL:HG22	1:A:731:ARG:HH12	1.72	0.54
22:A:7023:LMU:C6B	22:A:7023:LMU:C2B	2.82	0.54
2:B:167:TRP:CZ2	19:B:1208:CLA:HMA1	2.42	0.54
2:B:261:PHE:HE2	2:B:500:ALA:N	1.98	0.54
2:B:314:ARG:NH1	15:1:67:LEU:HD11	2.23	0.54
2:B:330:ILE:HD11	19:B:1202:CLA:H193	1.87	0.54
2:B:594:TRP:C	2:B:594:TRP:HD1	2.10	0.54
19:B:1201:CLA:HBC3	19:B:1226:CLA:H51	1.88	0.54
8:H:111:TYR:C	8:H:112:LEU:CD2	2.70	0.54
21:I:6021:BCR:C39	21:L:6019:BCR:C40	2.81	0.54
10:J:10:VAL:HG13	10:J:11:ALA:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:1311:CLA:H141	19:2:2014:CLA:HMB3	1.88	0.54
11:K:56:ILE:O	11:K:56:ILE:CG2	2.55	0.54
15:1:130:PRO:O	15:1:131:TRP:CE3	2.42	0.54
15:1:145:ILE:O	15:1:148:VAL:HG12	2.07	0.54
16:2:269:LYS:HA	16:2:269:LYS:HZ1	1.65	0.54
19:3:3011:CLA:H3A	19:3:3011:CLA:CGA	2.37	0.54
1:A:51:THR:OG1	19:A:1139:CLA:CAB	2.54	0.54
1:A:146:THR:H	19:A:1106:CLA:HMD1	1.72	0.54
1:A:286:GLY:O	1:A:295:TRP:CD1	2.59	0.54
1:A:295:TRP:CD1	1:A:295:TRP:N	2.75	0.54
1:A:396:PHE:HE2	1:A:616:PHE:CG	2.26	0.54
1:A:426:THR:HA	1:A:428:TYR:CD2	2.43	0.54
19:A:1101:CLA:O1D	19:A:1101:CLA:HBA2	2.07	0.54
19:A:1120:CLA:HBC3	19:A:1122:CLA:HED1	1.90	0.54
21:A:6007:BCR:H23C	21:A:6007:BCR:C38	2.21	0.54
2:B:20:ARG:CG	2:B:20:ARG:NH1	2.49	0.54
2:B:124:TRP:NE1	2:B:129:LEU:O	2.36	0.54
2:B:229:GLN:OE1	2:B:229:GLN:CA	2.53	0.54
2:B:462:TRP:CZ3	19:B:1231:CLA:HBC1	2.42	0.54
19:B:1221:CLA:C8	19:B:1223:CLA:H43	2.38	0.54
3:C:79:LEU:CD2	3:C:81:TYR:C	2.76	0.54
4:D:112:PHE:C	4:D:112:PHE:HD2	2.09	0.54
4:D:125:GLY:HA2	4:D:127:ASN:N	2.22	0.54
11:K:69:ARG:O	11:K:70:PHE:C	2.42	0.54
12:L:76:SER:OG	12:L:78:LEU:CD1	2.55	0.54
17:3:174:GLN:O	17:3:175:ASP:C	2.46	0.54
1:A:203:LEU:HD21	19:A:1123:CLA:C4D	2.37	0.54
1:A:285:GLY:O	1:A:294:LEU:CD1	2.56	0.54
19:A:1126:CLA:C10	21:A:6011:BCR:H372	2.38	0.54
19:A:1135:CLA:HBD	19:A:1135:CLA:CBA	2.37	0.54
2:B:70:TRP:NE1	2:B:71:GLN:OE1	2.40	0.54
2:B:160:LYS:NZ	2:B:161:TRP:CB	2.69	0.54
2:B:174:ARG:NH1	19:B:1221:CLA:CMD	2.70	0.54
2:B:303:TYR:HA	2:B:306:GLU:CG	2.36	0.54
2:B:326:ILE:O	2:B:326:ILE:HG12	2.07	0.54
4:D:115:PRO:C	4:D:116:THR:HG1	1.96	0.54
7:G:84:ARG:HG2	7:G:85:GLU:H	1.72	0.54
7:G:88:ALA:O	7:G:89:LYS:C	2.41	0.54
16:2:133:ASN:ND2	16:2:134:THR:CA	2.52	0.54
16:2:150:THR:C	16:2:152:LEU:CD1	2.76	0.54
19:2:2006:CLA:H102	19:2:2006:CLA:H161	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:239:LEU:HA	17:3:242:PHE:HB2	1.89	0.54
18:4:127:TYR:O	18:4:128:ALA:CB	2.55	0.54
1:A:73:GLU:HB2	1:A:186:TYR:CE2	2.42	0.54
1:A:76:ARG:HD3	1:A:191:PRO:O	2.07	0.54
1:A:261:SER:C	1:A:262:PHE:CD1	2.79	0.54
1:A:302:HIS:HD2	19:A:1116:CLA:NB	2.03	0.54
1:A:471:GLY:O	1:A:472:ARG:HG2	2.07	0.54
1:A:672:LEU:HD23	1:A:672:LEU:H	1.72	0.54
1:A:693:LEU:HD11	1:A:738:TYR:CD1	2.43	0.54
19:A:1105:CLA:HAA2	19:A:1107:CLA:HED1	1.90	0.54
2:B:22:TRP:CE2	19:B:1238:CLA:HMB1	2.41	0.54
2:B:124:TRP:CD1	2:B:124:TRP:C	2.80	0.54
2:B:233:TYR:H	2:B:233:TYR:HD2	1.55	0.54
2:B:292:ARG:HH22	2:B:297:ILE:HG12	1.73	0.54
2:B:297:ILE:HG21	7:G:77:PHE:CZ	2.43	0.54
2:B:450:GLU:O	2:B:451:LYS:CB	2.52	0.54
2:B:454:LEU:HD11	6:F:147:HIS:CA	2.29	0.54
3:C:44:ARG:NE	4:D:182:GLN:NE2	2.55	0.54
4:D:100:TYR:HE1	4:D:134:LYS:HE3	1.61	0.54
10:J:22:LEU:O	10:J:25:LEU:N	2.41	0.54
22:K:7041:LMU:H1B	22:K:7041:LMU:O6'	2.08	0.54
12:L:91:THR:C	12:L:98:ARG:HH12	2.11	0.54
13:N:104:LYS:H	13:N:107:LEU:HD13	1.73	0.54
16:2:184:PRO:CG	16:2:186:ASN:N	2.71	0.54
16:2:249:ASN:HD22	16:2:254:LEU:HG	1.71	0.54
17:3:107:ARG:NH1	17:3:233:LEU:H	2.06	0.54
17:3:156:THR:C	17:3:158:PHE:C	2.65	0.54
22:3:7005:LMU:O2B	22:3:7005:LMU:C3'	2.55	0.54
1:A:73:GLU:O	1:A:76:ARG:CA	2.55	0.54
1:A:129:GLN:HE22	19:A:1107:CLA:C1A	2.13	0.54
1:A:261:SER:C	1:A:263:ALA:H	2.08	0.54
1:A:370:ILE:HD12	19:A:1124:CLA:O1D	2.07	0.54
1:A:656:PHE:HD2	1:A:657:LEU:HD12	1.72	0.54
19:A:1237:CLA:C14	12:L:141:LEU:HD22	2.36	0.54
2:B:33:SER:H	2:B:37:ILE:HD13	1.73	0.54
2:B:160:LYS:HE3	2:B:161:TRP:CE3	2.41	0.54
2:B:241:ASN:CG	2:B:241:ASN:O	2.45	0.54
2:B:646:TRP:CH2	2:B:726:ILE:HG21	2.43	0.54
2:B:668:ARG:NH2	2:B:672:GLN:OE1	2.41	0.54
2:B:720:THR:O	2:B:724:PHE:N	2.41	0.54
4:D:83:PHE:CE1	4:D:114:MET:CE	2.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:163:VAL:O	4:D:164:GLN:CB	2.56	0.54
7:G:84:ARG:CG	7:G:85:GLU:CB	2.71	0.54
13:N:139:LYS:O	13:N:142:LYS:NZ	2.40	0.54
13:N:169:LYS:CA	13:N:170:TRP:CD1	2.91	0.54
15:1:70:GLY:O	15:1:71:GLU:C	2.42	0.54
15:1:201:PHE:CE1	15:1:204:GLN:NE2	2.75	0.54
16:2:243:GLY:C	16:2:244:THR:CG2	2.76	0.54
17:3:139:THR:CG2	17:3:140:GLY:N	2.38	0.54
18:4:168:GLN:O	18:4:173:LYS:C	2.46	0.54
18:4:178:PRO:O	18:4:194:PHE:HZ	1.89	0.54
18:4:201:LYS:CG	18:4:201:LYS:O	2.52	0.54
1:A:436:LEU:O	1:A:439:ARG:HB3	2.07	0.54
1:A:491:TRP:CE2	19:A:1135:CLA:H12	2.42	0.54
1:A:706:SER:HB3	2:B:419:ILE:O	2.07	0.54
19:A:1133:CLA:C1B	21:A:6008:BCR:H333	2.37	0.54
19:A:1138:CLA:C6	21:F:6014:BCR:H12C	2.33	0.54
19:A:9022:CLA:H152	21:B:6017:BCR:H20C	1.85	0.54
19:A:9023:CLA:HBC3	2:B:661:PHE:HB3	1.89	0.54
2:B:228:GLY:O	2:B:229:GLN:OE1	2.26	0.54
2:B:361:ILE:O	2:B:362:ALA:HB3	2.08	0.54
2:B:557:PHE:N	2:B:558:PRO:HD2	2.16	0.54
2:B:631:LEU:HB3	2:B:727:ALA:HB1	1.90	0.54
2:B:663:PHE:O	2:B:664:LEU:CG	2.55	0.54
19:B:1218:CLA:CHD	19:B:1218:CLA:CBC	2.76	0.54
19:B:1220:CLA:HAA2	19:B:1220:CLA:CBD	2.37	0.54
19:B:1232:CLA:HBB2	21:B:6010:BCR:H281	1.89	0.54
4:D:170:ASP:HB2	4:D:181:ARG:HH21	1.71	0.54
5:E:90:VAL:C	5:E:91:VAL:HG23	2.28	0.54
6:F:92:ALA:O	6:F:96:LYS:HG3	2.06	0.54
7:G:98:THR:OG1	7:G:101:GLU:CG	2.54	0.54
22:G:7051:LMU:H5'	22:G:7051:LMU:O2'	2.04	0.54
19:H:1241:CLA:O1D	19:H:1241:CLA:H2A	2.07	0.54
10:J:5:LYS:CD	16:2:178:ASN:CG	2.76	0.54
11:K:47:ASP:O	11:K:48:PHE:CB	2.55	0.54
12:L:60:ILE:HG12	12:L:68:SER:OG	2.08	0.54
13:N:110:THR:HG23	13:N:111:GLY:N	2.22	0.54
13:N:123:GLY:CA	13:N:131:PHE:CD1	2.90	0.54
15:1:69:LEU:O	15:1:73:PRO:HD3	2.07	0.54
16:2:128:LYS:HB3	16:2:131:ILE:CG2	2.33	0.54
17:3:96:ARG:O	17:3:100:TYR:CD2	2.61	0.54
17:3:103:VAL:CG1	17:3:107:ARG:CZ	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:176:TRP:CZ2	17:3:199:ASN:OD1	2.61	0.54
1:A:207:LEU:HA	1:A:211:LEU:HB2	1.89	0.54
1:A:284:ARG:CB	1:A:295:TRP:HB2	2.37	0.54
1:A:432:LEU:C	1:A:434:ARG:N	2.60	0.54
19:A:1140:CLA:C19	10:J:19:PHE:CD2	2.90	0.54
2:B:137:THR:OG1	2:B:140:ILE:HG12	2.08	0.54
2:B:233:TYR:N	2:B:233:TYR:HD2	2.04	0.54
2:B:236:ASN:N	2:B:237:PRO:HD3	2.23	0.54
2:B:544:SER:O	2:B:545:LYS:C	2.45	0.54
19:B:1222:CLA:HED2	19:B:1223:CLA:OBD	2.07	0.54
6:F:204:SER:O	6:F:207:LEU:CB	2.55	0.54
7:G:72:LEU:HD21	7:G:124:ILE:HD11	1.84	0.54
8:H:81:SER:O	8:H:83:LEU:N	2.41	0.54
8:H:109:LEU:HD23	19:H:1207:CLA:C5	2.36	0.54
22:H:7011:LMU:C6'	22:H:7011:LMU:C1B	2.86	0.54
19:J:1308:CLA:O1D	19:J:1308:CLA:C1	2.56	0.54
11:K:76:ALA:CA	11:K:78:ARG:NH1	2.71	0.54
13:N:156:GLY:CA	13:N:157:LYS:HE2	2.36	0.54
15:1:170:PRO:CG	15:1:173:TYR:CD2	2.91	0.54
15:1:225:TRP:HB3	15:1:226:HIS:ND1	2.22	0.54
16:2:211:PRO:CD	16:2:212:GLN:N	2.70	0.54
16:2:249:ASN:O	16:2:250:LEU:HB3	2.06	0.54
17:3:150:TYR:CE2	17:3:151:TRP:CD2	2.96	0.54
19:4:4006:CLA:HBA2	19:4:4006:CLA:HBD	1.89	0.54
1:A:25:ASP:OD1	1:A:26:PRO:CG	2.56	0.54
1:A:425:THR:OG1	1:A:428:TYR:HE1	1.82	0.54
1:A:618:TRP:CZ2	1:A:655:ASP:CB	2.91	0.54
2:B:225:LEU:O	2:B:230:TRP:NE1	2.40	0.54
2:B:334:LEU:CA	19:B:1202:CLA:HMD3	2.38	0.54
2:B:393:PHE:CZ	2:B:398:TYR:HD2	2.24	0.54
2:B:486:LEU:HD12	2:B:489:GLY:N	2.21	0.54
2:B:625:TRP:CE3	2:B:625:TRP:O	2.59	0.54
22:G:7026:LMU:H12	22:G:7026:LMU:H51	1.89	0.54
8:H:108:THR:OG1	8:H:109:LEU:N	2.38	0.54
19:K:1142:CLA:OBD	19:K:1143:CLA:CHB	2.56	0.54
19:K:1146:CLA:O1A	19:K:1146:CLA:C3A	2.56	0.54
12:L:81:TRP:O	12:L:83:LEU:N	2.37	0.54
12:L:172:GLU:O	12:L:173:PRO:O	2.25	0.54
13:N:144:PRO:CG	13:N:158:ASP:O	2.56	0.54
15:1:67:LEU:O	15:1:69:LEU:O	2.26	0.54
15:1:68:GLY:O	15:1:73:PRO:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:104:GLY:O	15:1:105:TYR:HB2	2.08	0.54
15:1:177:PRO:O	15:1:179:LYS:N	2.41	0.54
15:1:183:LEU:O	15:1:184:LYS:CG	2.55	0.54
18:4:103:MET:HE1	18:4:207:ASN:CB	2.38	0.54
18:4:148:LEU:O	18:4:149:SER:C	2.45	0.54
1:A:394:SER:HB2	19:A:1126:CLA:CMA	2.30	0.54
1:A:398:HIS:CD2	19:A:1126:CLA:ND	2.76	0.54
1:A:402:ILE:HG13	19:A:1127:CLA:CBB	2.33	0.54
1:A:453:LEU:HD21	19:A:1136:CLA:CBB	2.38	0.54
19:A:1125:CLA:HBA1	19:A:1125:CLA:CGD	2.37	0.54
2:B:324:ASP:O	2:B:328:ASN:CB	2.54	0.54
2:B:440:ASN:O	2:B:444:LEU:HD23	2.07	0.54
3:C:79:LEU:CD2	3:C:81:TYR:O	2.56	0.54
4:D:99:PHE:CB	4:D:157:VAL:CG1	2.84	0.54
4:D:99:PHE:HB3	4:D:157:VAL:CG1	2.38	0.54
4:D:100:TYR:HD1	4:D:134:LYS:CG	2.18	0.54
4:D:157:VAL:HG13	4:D:158:PHE:O	2.06	0.54
5:E:118:ASN:OD1	5:E:119:ASN:N	2.41	0.54
6:F:149:ILE:HG22	6:F:150:VAL:N	2.21	0.54
6:F:228:ASP:CA	6:F:231:PHE:HB3	2.38	0.54
7:G:80:PHE:O	7:G:81:ASN:C	2.44	0.54
7:G:89:LYS:HE3	7:G:89:LYS:CA	2.22	0.54
8:H:97:LEU:HD11	8:H:100:PHE:HB2	1.66	0.54
13:N:150:LEU:O	13:N:151:ASP:HB2	2.07	0.54
15:1:71:GLU:CG	15:1:72:VAL:N	2.71	0.54
15:1:171:LEU:N	15:1:173:TYR:CE2	2.76	0.54
18:4:193:ASN:O	18:4:194:PHE:CB	2.52	0.54
1:A:29:THR:OG1	1:A:31:PHE:N	2.40	0.54
1:A:79:PHE:CE1	19:A:1111:CLA:HED3	2.39	0.54
1:A:119:SER:HA	1:A:145:ILE:HD12	1.90	0.54
1:A:155:ALA:O	1:A:156:SER:C	2.40	0.54
1:A:158:ILE:HG12	1:A:159:THR:H	1.68	0.54
1:A:479:ASP:OD1	1:A:536:THR:CG2	2.55	0.54
1:A:628:ILE:CG1	1:A:629:ASN:N	2.70	0.54
19:A:1104:CLA:H51	19:A:1128:CLA:NC	2.23	0.54
2:B:55:ALA:HB1	2:B:150:LEU:CD1	2.38	0.54
2:B:255:LEU:H	2:B:271:THR:HG21	1.73	0.54
2:B:269:TRP:HE3	2:B:270:LEU:H	1.55	0.54
2:B:343:VAL:CG1	19:B:1223:CLA:H2	2.38	0.54
2:B:442:VAL:HG21	19:B:1230:CLA:CAC	2.33	0.54
2:B:545:LYS:O	2:B:548:PRO:HD3	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1205:CLA:CMC	21:B:6017:BCR:H281	2.37	0.54
5:E:89:SER:C	5:E:106:ARG:H	2.07	0.54
6:F:215:VAL:O	6:F:216:ALA:C	2.45	0.54
13:N:93:GLU:HG2	13:N:94:LYS:N	2.23	0.54
22:R:7007:LMU:H71	22:R:7007:LMU:H11	1.90	0.54
15:1:114:TRP:CH2	15:1:121:GLN:CA	2.89	0.54
15:1:188:ILE:O	15:1:189:LYS:C	2.44	0.54
16:2:244:THR:O	16:2:246:PRO:C	2.46	0.54
16:2:254:LEU:HD22	16:2:256:ASP:N	2.23	0.54
18:4:98:ASN:HB2	18:4:212:LEU:HD21	1.90	0.54
18:4:197:THR:OG1	19:4:4001:CLA:HBA2	2.07	0.54
1:A:249:ILE:CG2	17:3:137:PHE:CE2	2.92	0.53
1:A:252:ARG:CD	1:A:252:ARG:N	2.52	0.53
1:A:274:TRP:HB3	1:A:277:TYR:H	1.73	0.53
2:B:135:LEU:O	2:B:135:LEU:HG	2.07	0.53
2:B:212:PHE:HZ	19:B:1211:CLA:HHD	1.73	0.53
2:B:462:TRP:CH2	19:B:1231:CLA:HBC1	2.43	0.53
2:B:509:PHE:CD2	2:B:509:PHE:N	2.76	0.53
19:B:1216:CLA:C3	19:B:1221:CLA:H92	2.38	0.53
5:E:79:LYS:CB	5:E:84:TYR:HE1	2.19	0.53
8:H:64:GLN:C	8:H:66:ASP:HA	2.29	0.53
12:L:51:LYS:N	12:L:51:LYS:HD2	2.23	0.53
13:N:132:THR:CA	13:N:137:LEU:O	2.56	0.53
13:N:150:LEU:CB	13:N:152:LEU:HD23	2.38	0.53
15:1:123:THR:O	15:1:124:TYR:HB2	2.08	0.53
16:2:172:LEU:C	16:2:174:PRO:HD3	2.26	0.53
16:2:215:LYS:HA	16:2:217:LEU:HD23	1.89	0.53
16:2:218:ARG:CB	16:2:219:THR:HG22	2.28	0.53
16:2:254:LEU:CD2	16:2:256:ASP:H	2.20	0.53
17:3:232:ARG:HA	17:3:235:MET:HB2	1.90	0.53
18:4:124:PRO:O	18:4:125:LYS:HG3	2.08	0.53
18:4:217:PHE:CD1	18:4:221:HIS:ND1	2.76	0.53
18:4:226:LYS:H	18:4:226:LYS:HD3	1.57	0.53
1:A:23:ASP:OD2	1:A:24:ARG:CZ	2.56	0.53
1:A:62:HIS:CE1	19:A:1128:CLA:CGA	2.92	0.53
1:A:64:PHE:HE2	1:A:74:ILE:CG2	2.12	0.53
1:A:453:LEU:HD23	19:A:1136:CLA:CBB	2.37	0.53
19:A:1137:CLA:HBC3	19:A:1137:CLA:CMC	2.34	0.53
2:B:247:THR:HG22	2:B:248:GLN:N	2.15	0.53
2:B:278:LEU:HG	19:B:1213:CLA:CMA	2.38	0.53
2:B:304:ILE:O	2:B:308:HIS:CB	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:PRO:HB3	2:B:538:ALA:CA	2.30	0.53
2:B:469:LYS:HE3	2:B:470:THR:CG2	2.34	0.53
4:D:87:THR:N	12:L:69:LEU:HD11	2.22	0.53
4:D:158:PHE:CB	4:D:159:PRO:O	2.46	0.53
5:E:84:TYR:HD2	5:E:85:LYS:HG3	1.72	0.53
8:H:98:LEU:O	8:H:102:ILE:HG13	2.08	0.53
15:1:66:PRO:O	15:1:69:LEU:C	2.46	0.53
15:1:77:GLU:CD	15:1:80:LYS:HE3	2.28	0.53
16:2:164:GLU:HA	16:2:167:ARG:NH1	2.22	0.53
19:3:2009:CLA:CBD	19:3:2009:CLA:CBA	2.85	0.53
18:4:131:LYS:O	18:4:131:LYS:HG2	2.08	0.53
18:4:198:LEU:O	18:4:199:GLU:C	2.46	0.53
18:4:209:ARG:O	18:4:212:LEU:N	2.41	0.53
18:4:209:ARG:HG2	18:4:210:LEU:N	2.15	0.53
1:A:462:ILE:CD1	19:A:9022:CLA:H72	2.38	0.53
1:A:534:LEU:HD12	1:A:534:LEU:C	2.17	0.53
2:B:196:HIS:CE1	19:B:1212:CLA:ND	2.75	0.53
2:B:223:GLY:O	2:B:224:PRO:C	2.45	0.53
2:B:353:TYR:C	2:B:355:LEU:N	2.61	0.53
2:B:551:LYS:NZ	4:D:194:ASN:O	2.34	0.53
2:B:625:TRP:CD2	2:B:625:TRP:O	2.61	0.53
19:B:1220:CLA:HMD2	19:B:1221:CLA:HBB1	1.88	0.53
3:C:62:PHE:CD1	5:E:80:GLU:HB3	2.43	0.53
6:F:227:VAL:HG23	6:F:228:ASP:N	2.23	0.53
11:K:113:GLY:O	11:K:116:ILE:CG2	2.34	0.53
13:N:90:GLU:OE1	13:N:91:TYR:CZ	2.61	0.53
19:1:1303:CLA:HBC2	19:4:1304:CLA:HMB3	1.88	0.53
16:2:266:PHE:CE2	16:2:267:THR:O	2.62	0.53
22:3:7005:LMU:O2B	22:3:7005:LMU:H5'	2.09	0.53
18:4:142:PHE:HA	18:4:145:GLU:CG	2.38	0.53
18:4:165:SER:O	18:4:166:VAL:C	2.45	0.53
1:A:328:LYS:O	1:A:329:ASP:C	2.46	0.53
1:A:431:LEU:H	1:A:434:ARG:NE	2.06	0.53
1:A:534:LEU:HB2	1:A:538:ASP:CB	2.39	0.53
1:A:696:GLY:HA3	2:B:569:ASP:HB2	1.89	0.53
19:A:1107:CLA:HBB2	19:B:1230:CLA:HMD1	1.86	0.53
2:B:65:LEU:HD22	2:B:124:TRP:HE3	1.72	0.53
2:B:66:PHE:O	2:B:66:PHE:CG	2.60	0.53
2:B:367:THR:O	2:B:367:THR:CG2	2.56	0.53
2:B:482:ASN:O	2:B:484:PRO:HD2	2.08	0.53
3:C:65:VAL:H	3:C:66:ARG:HH22	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:VAL:N	3:C:66:ARG:HH22	2.06	0.53
4:D:80:SER:HB2	4:D:127:ASN:HA	1.90	0.53
4:D:156:ARG:HB2	4:D:166:LEU:HD11	1.89	0.53
11:K:108:ALA:O	11:K:109:CYS:C	2.45	0.53
13:N:99:LYS:HB2	13:N:102:ASN:ND2	2.24	0.53
22:R:7021:LMU:H41	22:R:7021:LMU:C6'	2.38	0.53
15:1:81:GLU:HG2	15:1:82:SER:N	2.22	0.53
15:1:183:LEU:C	15:1:184:LYS:CG	2.69	0.53
16:2:125:PHE:O	16:2:127:THR:CG2	2.56	0.53
16:2:228:ALA:O	16:2:229:MET:C	2.44	0.53
22:2:7006:LMU:O6B	22:2:7006:LMU:H3'	2.08	0.53
17:3:156:THR:O	17:3:157:LEU:C	2.46	0.53
18:4:215:LEU:O	18:4:217:PHE:N	2.41	0.53
1:A:79:PHE:CE2	1:A:185:HIS:NE2	2.76	0.53
1:A:466:THR:O	1:A:470:LEU:HG	2.08	0.53
1:A:482:ILE:CG2	1:A:482:ILE:O	2.55	0.53
1:A:624:VAL:HG12	1:A:625:TRP:N	2.22	0.53
1:A:628:ILE:CD1	1:A:629:ASN:N	2.71	0.53
1:A:703:LEU:O	1:A:707:ILE:HG12	2.08	0.53
2:B:316:GLY:O	2:B:317:ARG:NE	2.41	0.53
2:B:459:PHE:N	19:B:1235:CLA:CAD	2.71	0.53
2:B:508:LEU:HB3	2:B:509:PHE:CE2	2.42	0.53
2:B:509:PHE:HD2	2:B:509:PHE:N	2.06	0.53
3:C:2:SER:O	3:C:3:HIS:ND1	2.42	0.53
6:F:176:TRP:CZ3	6:F:217:ALA:HB2	2.43	0.53
6:F:203:ALA:O	6:F:205:SER:N	2.42	0.53
8:H:58:LEU:CB	8:H:61:THR:CB	2.60	0.53
12:L:190:PHE:CE2	12:L:194:ILE:HD12	2.44	0.53
13:N:126:LYS:HD2	13:N:127:PHE:HD2	1.74	0.53
13:N:143:VAL:O	13:N:151:ASP:OD1	2.26	0.53
13:N:148:ASP:CA	13:N:149:ASP:C	2.77	0.53
15:1:199:VAL:HG13	15:1:200:GLY:N	2.23	0.53
16:2:168:TRP:CD1	16:2:171:ILE:HD13	2.43	0.53
17:3:132:THR:HG23	17:3:133:ALA:N	2.23	0.53
17:3:156:THR:O	17:3:156:THR:HG22	2.06	0.53
1:A:281:LEU:HD12	1:A:282:THR:HG23	1.91	0.53
1:A:362:LEU:HB3	1:A:406:LEU:O	2.08	0.53
1:A:466:THR:HG22	2:B:648:TRP:HE1	1.72	0.53
1:A:707:ILE:HG22	1:A:711:HIS:CD2	2.41	0.53
19:A:1106:CLA:CMB	19:A:1107:CLA:H11	2.36	0.53
19:A:1119:CLA:C2C	19:A:1125:CLA:H172	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1126:CLA:C17	21:J:6012:BCR:H17C	2.36	0.53
19:A:9012:CLA:NB	19:A:9013:CLA:HBB2	2.24	0.53
2:B:464:GLN:HG3	2:B:464:GLN:O	2.01	0.53
2:B:574:ASP:O	2:B:578:LEU:HG	2.08	0.53
19:B:1216:CLA:HBD	19:B:1216:CLA:HBA1	1.90	0.53
19:B:1222:CLA:CMB	21:B:6010:BCR:H352	2.39	0.53
6:F:192:THR:O	6:F:193:GLN:CG	2.56	0.53
6:F:228:ASP:O	6:F:231:PHE:HD1	1.90	0.53
7:G:123:ASN:O	7:G:126:ASP:OD2	2.27	0.53
8:H:77:ASN:ND2	8:H:78:PRO:O	2.42	0.53
8:H:119:ASP:OD2	8:H:121:LEU:CG	2.50	0.53
22:H:7028:LMU:O6'	22:H:7028:LMU:H1'	2.09	0.53
12:L:109:LEU:O	12:L:110:LEU:C	2.47	0.53
12:L:141:LEU:HD11	12:L:145:LEU:HD11	1.90	0.53
12:L:205:TYR:CD2	12:L:205:TYR:O	2.62	0.53
15:1:176:ASP:C	15:1:180:LEU:HG	2.29	0.53
15:1:199:VAL:O	15:1:201:PHE:N	2.41	0.53
15:1:199:VAL:O	15:1:200:GLY:C	2.47	0.53
17:3:88:GLY:O	17:3:89:THR:C	2.47	0.53
18:4:217:PHE:CE1	18:4:221:HIS:ND1	2.77	0.53
1:A:307:ALA:O	1:A:308:ILE:C	2.48	0.53
1:A:449:VAL:HG22	19:A:1137:CLA:HMC3	1.90	0.53
1:A:472:ARG:N	1:A:473:PRO:HD2	2.22	0.53
19:A:1106:CLA:H93	21:J:6012:BCR:H311	1.89	0.53
19:A:1131:CLA:H152	21:L:6019:BCR:C36	2.39	0.53
21:A:6002:BCR:C23	21:A:6002:BCR:C40	2.87	0.53
2:B:278:LEU:O	2:B:281:ALA:N	2.42	0.53
2:B:292:ARG:NH2	2:B:297:ILE:CA	2.71	0.53
2:B:411:MET:HE2	19:B:1220:CLA:CMC	2.39	0.53
19:B:1235:CLA:H61	21:F:6016:BCR:H323	1.91	0.53
19:B:1239:CLA:H51	20:B:5002:PQN:H251	1.90	0.53
22:B:7038:LMU:H101	22:B:7038:LMU:H61	1.91	0.53
3:C:12:ILE:CB	3:C:38:GLN:O	2.56	0.53
4:D:100:TYR:CD1	4:D:134:LYS:HG2	2.42	0.53
12:L:63:ASP:OD1	12:L:63:ASP:O	2.26	0.53
14:R:26:UNK:O	14:R:28:UNK:CA	2.57	0.53
15:1:177:PRO:HD3	15:1:180:LEU:HD21	1.85	0.53
16:2:118:ALA:C	16:2:121:PHE:CD2	2.75	0.53
16:2:156:GLU:HG3	16:2:157:LEU:CD1	2.36	0.53
17:3:150:TYR:N	17:3:152:ALA:CB	2.32	0.53
1:A:209:GLY:HA2	1:A:213:LEU:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:HIS:CE1	19:A:1113:CLA:NC	2.77	0.53
1:A:492:ILE:CD1	19:A:1133:CLA:C2C	2.85	0.53
1:A:750:PHE:O	1:A:752:ALA:N	2.41	0.53
19:A:1122:CLA:CBB	21:A:6007:BCR:H353	2.36	0.53
19:A:1125:CLA:HMA2	21:A:6008:BCR:H10C	1.90	0.53
2:B:364:ASP:OD2	2:B:367:THR:HB	2.08	0.53
2:B:367:THR:O	2:B:367:THR:HG22	2.08	0.53
19:B:1220:CLA:C9	19:B:1227:CLA:HBC2	2.39	0.53
4:D:140:LEU:HD12	4:D:144:LEU:H	1.74	0.53
5:E:100:ARG:O	5:E:121:ALA:CB	2.57	0.53
6:F:160:PHE:O	6:F:164:GLY:N	2.42	0.53
7:G:98:THR:HB	7:G:101:GLU:OE2	1.81	0.53
12:L:98:ARG:O	12:L:102:VAL:HG23	2.07	0.53
13:N:130:ASN:HB2	13:N:132:THR:HG21	1.91	0.53
15:1:101:GLU:O	15:1:101:GLU:CG	2.54	0.53
15:1:176:ASP:CB	15:1:180:LEU:CD1	2.39	0.53
19:1:1014:CLA:H52	19:1:1014:CLA:H101	1.79	0.53
16:2:126:LEU:O	16:2:129:LEU:N	2.41	0.53
16:2:137:TRP:O	16:2:137:TRP:CD1	2.62	0.53
16:2:240:ILE:CG2	16:2:263:PHE:CB	2.65	0.53
17:3:155:TYR:C	17:3:157:LEU:H	2.12	0.53
22:4:7053:LMU:H5B	22:4:7053:LMU:O2B	2.08	0.53
1:A:32:GLU:OE1	1:A:33:GLN:N	2.38	0.53
1:A:284:ARG:O	1:A:284:ARG:NE	2.42	0.53
1:A:612:VAL:O	1:A:615:HIS:HB3	2.09	0.53
19:A:1126:CLA:C17	21:J:6012:BCR:H15C	2.39	0.53
19:A:1131:CLA:H11	19:A:1237:CLA:H43	1.90	0.53
2:B:232:LEU:CD1	2:B:235:GLN:CB	2.86	0.53
2:B:282:PHE:HE2	19:B:1213:CLA:H3A	1.74	0.53
2:B:298:GLY:H	19:B:1218:CLA:HMD3	1.73	0.53
2:B:311:PRO:HG3	19:B:1301:CLA:NC	2.24	0.53
2:B:312:GLY:HA3	2:B:315:LEU:HB3	1.87	0.53
2:B:440:ASN:CG	2:B:614:THR:HG23	2.29	0.53
2:B:469:LYS:C	2:B:470:THR:OG1	2.47	0.53
2:B:595:HIS:CE1	2:B:599:ILE:HD11	2.43	0.53
2:B:622:ASP:HB3	2:B:626:LEU:HD11	1.91	0.53
5:E:78:ARG:HB2	5:E:80:GLU:CD	2.29	0.53
6:F:181:TYR:O	6:F:181:TYR:CD2	2.61	0.53
19:L:1148:CLA:O2D	19:L:1148:CLA:CAA	2.52	0.53
15:1:81:GLU:O	15:1:82:SER:C	2.46	0.53
16:2:128:LYS:O	16:2:131:ILE:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:237:PHE:CD1	16:2:237:PHE:O	2.57	0.53
16:2:246:PRO:HB2	16:2:247:ILE:CD1	2.36	0.53
19:2:2007:CLA:C1B	19:2:2007:CLA:H2	2.38	0.53
17:3:104:ILE:HG21	19:3:3004:CLA:C3D	2.39	0.53
18:4:150:HIS:CE1	18:4:154:ILE:HD11	2.43	0.53
19:4:1004:CLA:O1D	19:4:1004:CLA:H2A	2.08	0.53
1:A:157:GLY:C	1:A:229:ILE:HG21	2.28	0.53
1:A:302:HIS:HE1	19:A:1117:CLA:CHB	2.22	0.53
1:A:346:LEU:CD2	1:A:346:LEU:O	2.56	0.53
1:A:415:ALA:HB2	1:A:560:VAL:HG12	1.91	0.53
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.44	0.53
1:A:443:ILE:HG22	2:B:674:LEU:CD1	2.39	0.53
1:A:464:ASN:H	1:A:464:ASN:ND2	2.07	0.53
19:A:9023:CLA:H111	21:B:6017:BCR:C35	2.39	0.53
2:B:66:PHE:O	2:B:66:PHE:CD2	2.61	0.53
2:B:120:VAL:CB	2:B:123:TRP:HE1	2.21	0.53
2:B:310:PRO:CD	2:B:311:PRO:CD	2.87	0.53
2:B:325:THR:HG21	2:B:403:ASN:HD21	1.74	0.53
2:B:330:ILE:CD1	19:B:1202:CLA:C19	2.86	0.53
2:B:486:LEU:HD13	19:B:1232:CLA:HMD1	1.89	0.53
2:B:577:TYR:CE2	2:B:578:LEU:HD23	2.45	0.53
2:B:580:VAL:CG1	2:B:710:LEU:HD21	2.39	0.53
2:B:609:PHE:O	2:B:613:SER:N	2.36	0.53
4:D:129:LEU:CD1	12:L:65:PHE:CD1	2.92	0.53
5:E:75:LYS:CA	5:E:87:THR:HG22	2.31	0.53
5:E:89:SER:O	5:E:105:VAL:CB	2.56	0.53
22:E:7048:LMU:O5'	22:E:7048:LMU:C2	2.57	0.53
6:F:228:ASP:O	6:F:231:PHE:CD1	2.62	0.53
9:I:20:ALA:O	9:I:24:LEU:HB3	2.08	0.53
15:1:77:GLU:C	15:1:80:LYS:CG	2.77	0.53
15:1:134:LEU:O	15:1:137:ILE:HG12	2.09	0.53
16:2:184:PRO:HD2	16:2:186:ASN:N	2.22	0.53
17:3:150:TYR:CG	17:3:151:TRP:N	2.77	0.53
18:4:220:GLN:NE2	19:4:1306:CLA:CAC	2.72	0.53
1:A:106:TYR:O	1:A:107:GLU:C	2.43	0.52
1:A:479:ASP:CG	1:A:536:THR:HG22	2.29	0.52
1:A:582:ASP:HB3	1:A:589:THR:CG2	2.38	0.52
19:A:1124:CLA:HED3	19:A:1125:CLA:CMD	2.30	0.52
2:B:127:ILE:HD13	2:B:193:HIS:HE1	1.74	0.52
2:B:244:PHE:CD2	2:B:245:GLY:N	2.77	0.52
2:B:294:ASN:ND2	7:G:94:GLN:CB	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:LEU:CD2	2:B:351:HIS:CE1	2.92	0.52
2:B:353:TYR:O	2:B:355:LEU:N	2.41	0.52
2:B:687:LEU:HD12	21:B:6020:BCR:HC31	1.91	0.52
2:B:708:VAL:O	2:B:710:LEU:O	2.27	0.52
19:B:1203:CLA:H91	19:B:1203:CLA:H161	1.91	0.52
19:B:1216:CLA:OBD	19:B:1219:CLA:CBC	2.57	0.52
4:D:133:ARG:H	4:D:136:GLN:HE21	1.53	0.52
4:D:167:HIS:H	4:D:168:PRO:CD	2.21	0.52
4:D:205:LYS:N	4:D:205:LYS:HE2	2.24	0.52
6:F:228:ASP:OD2	6:F:231:PHE:CG	2.63	0.52
12:L:143:LEU:H	12:L:145:LEU:N	2.05	0.52
14:R:32:UNK:CB	14:R:33:UNK:CA	2.76	0.52
22:1:7004:LMU:O6B	22:1:7004:LMU:C1B	2.55	0.52
22:1:7004:LMU:O2'	22:1:7004:LMU:C1	2.50	0.52
16:2:101:TRP:H	16:2:103:VAL:CG1	2.21	0.52
18:4:193:ASN:C	18:4:201:LYS:NZ	2.62	0.52
1:A:746:THR:O	1:A:750:PHE:N	2.36	0.52
19:A:9012:CLA:HED1	19:B:9010:CLA:H61	1.90	0.52
2:B:414:HIS:HD2	19:B:1227:CLA:HMA3	1.71	0.52
2:B:429:LEU:HD11	19:B:1235:CLA:CMB	2.39	0.52
2:B:486:LEU:HB2	19:B:1232:CLA:CMD	2.28	0.52
2:B:569:ASP:OD1	2:B:706:ARG:NE	2.42	0.52
2:B:608:GLN:O	2:B:612:SER:HB2	2.08	0.52
19:B:1231:CLA:ND	19:B:1232:CLA:HBB1	2.24	0.52
4:D:129:LEU:HD13	12:L:65:PHE:CZ	2.44	0.52
6:F:214:PRO:C	6:F:215:VAL:HG23	2.30	0.52
7:G:84:ARG:CG	7:G:85:GLU:H	2.13	0.52
7:G:136:VAL:O	7:G:137:VAL:HG22	2.09	0.52
19:J:1308:CLA:H2A	19:J:1308:CLA:C2	2.39	0.52
11:K:62:SER:HG	11:K:63:LEU:CD1	2.21	0.52
11:K:62:SER:O	11:K:63:LEU:C	2.46	0.52
12:L:55:GLN:O	12:L:57:ILE:HG13	2.08	0.52
12:L:73:VAL:HA	19:L:1504:CLA:HMA1	1.85	0.52
12:L:205:TYR:HD1	12:L:207:LEU:CD1	1.90	0.52
13:N:133:GLY:CA	13:N:134:CYS:O	2.54	0.52
13:N:143:VAL:CG1	13:N:144:PRO:HD2	2.39	0.52
13:N:150:LEU:HD13	13:N:150:LEU:N	2.25	0.52
13:N:152:LEU:CA	13:N:153:GLU:HG3	2.39	0.52
15:1:65:ASP:OD2	15:1:66:PRO:HA	2.08	0.52
16:2:176:CYS:H	16:2:188:LEU:HB2	1.73	0.52
17:3:225:LEU:HD13	17:3:228:VAL:CG2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:7005:LMU:O3'	22:3:7005:LMU:C1B	2.57	0.52
18:4:93:GLN:CD	18:4:170:PRO:HB2	2.30	0.52
18:4:174:GLN:HB3	18:4:195:ALA:HA	1.92	0.52
18:4:195:ALA:CB	18:4:197:THR:O	2.55	0.52
1:A:309:LEU:O	1:A:310:PHE:CB	2.56	0.52
1:A:690:LEU:CD2	2:B:661:PHE:HE1	2.21	0.52
19:A:1105:CLA:C4B	21:J:6012:BCR:C33	2.86	0.52
19:A:1117:CLA:H93	19:A:1117:CLA:H193	1.91	0.52
19:A:1126:CLA:H43	19:A:1126:CLA:CGA	2.39	0.52
19:A:9023:CLA:HMB3	19:B:1239:CLA:HMC3	1.92	0.52
2:B:297:ILE:HG21	7:G:77:PHE:HZ	1.73	0.52
2:B:376:GLN:HB3	2:B:587:ILE:HD12	1.92	0.52
19:B:1226:CLA:HBC2	19:B:1226:CLA:CMC	2.36	0.52
19:B:1227:CLA:HMB2	19:B:1228:CLA:C4A	2.39	0.52
3:C:26:LEU:HD22	4:D:181:ARG:NH1	2.23	0.52
4:D:148:TYR:O	4:D:149:LYS:CB	2.56	0.52
6:F:132:ASN:C	6:F:133:TYR:CD1	2.74	0.52
7:G:60:SER:OG	7:G:61:ALA:N	2.42	0.52
7:G:72:LEU:CD1	7:G:73:PHE:CZ	2.93	0.52
7:G:125:VAL:HG13	7:G:129:ALA:HB2	1.88	0.52
10:J:37:LEU:C	10:J:38:ILE:HG13	2.25	0.52
19:J:1308:CLA:CBA	19:J:1308:CLA:CBD	2.83	0.52
19:K:1143:CLA:CGA	19:K:1143:CLA:C3A	2.85	0.52
12:L:102:VAL:HA	19:L:1502:CLA:HED1	1.89	0.52
13:N:114:PHE:O	13:N:118:TYR:N	2.42	0.52
13:N:136:ASP:OD1	13:N:137:LEU:O	2.28	0.52
15:I:69:LEU:C	15:I:73:PRO:CD	2.72	0.52
16:2:113:ALA:HB1	16:2:114:MET:CE	2.38	0.52
16:2:133:ASN:HD21	16:2:134:THR:HB	1.57	0.52
17:3:233:LEU:O	17:3:236:LEU:N	2.43	0.52
19:4:1304:CLA:CAA	19:4:1304:CLA:CGD	2.87	0.52
1:A:205:HIS:CE1	19:A:1111:CLA:HMC2	2.44	0.52
1:A:252:ARG:NH2	1:A:252:ARG:O	2.42	0.52
1:A:458:PHE:CD2	19:A:9022:CLA:CMB	2.92	0.52
1:A:592:VAL:HG23	1:A:593:SER:N	2.25	0.52
19:A:1135:CLA:HBA2	19:A:1135:CLA:O1D	2.09	0.52
2:B:42:LEU:O	2:B:43:TYR:C	2.47	0.52
2:B:221:GLY:O	2:B:222:LEU:C	2.46	0.52
2:B:444:LEU:C	2:B:446:PHE:H	2.11	0.52
2:B:574:ASP:OD2	2:B:706:ARG:NE	2.43	0.52
2:B:624:LEU:CD2	19:B:9010:CLA:H93	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:668:ARG:HH12	2:B:672:GLN:HG2	1.73	0.52
2:B:673:GLU:O	2:B:676:GLU:HB2	2.09	0.52
2:B:715:VAL:O	2:B:716:GLY:C	2.48	0.52
19:B:1222:CLA:HBB2	19:B:1236:CLA:HMB3	1.91	0.52
6:F:190:LYS:CG	6:F:192:THR:CG2	2.88	0.52
7:G:85:GLU:HG3	7:G:86:ASN:N	2.24	0.52
8:H:116:ALA:CB	8:H:117:SER:CA	2.85	0.52
19:H:1505:CLA:HAA1	19:H:1505:CLA:H42	1.92	0.52
16:2:114:MET:HE3	16:2:114:MET:N	2.25	0.52
17:3:213:PHE:HB2	17:3:215:LYS:N	2.24	0.52
1:A:240:LYS:O	1:A:240:LYS:HD2	2.10	0.52
1:A:245:PRO:C	1:A:248:PHE:CE2	2.82	0.52
1:A:365:LEU:HD22	19:A:1103:CLA:HED3	1.87	0.52
1:A:599:PHE:CE2	1:A:735:VAL:HG21	2.45	0.52
1:A:607:ASN:ND2	19:A:9022:CLA:C2C	2.73	0.52
19:A:1149:CLA:HBC2	19:A:1149:CLA:CMC	2.33	0.52
19:A:9012:CLA:HBB2	19:A:9013:CLA:C1B	2.39	0.52
2:B:135:LEU:O	2:B:135:LEU:CD1	2.57	0.52
2:B:183:PHE:HB3	2:B:284:PHE:HD2	1.74	0.52
2:B:350:GLN:O	2:B:353:TYR:CD1	2.62	0.52
2:B:353:TYR:O	2:B:354:SER:CB	2.47	0.52
2:B:465:SER:O	2:B:466:ALA:C	2.44	0.52
2:B:662:MET:HE2	20:B:5002:PQN:H2M3	1.92	0.52
3:C:36:ALA:O	3:C:37:LYS:HG2	2.09	0.52
4:D:100:TYR:HD1	4:D:134:LYS:HG3	1.64	0.52
5:E:91:VAL:HB	5:E:104:VAL:CG1	2.40	0.52
7:G:69:GLY:HA2	7:G:72:LEU:CG	2.38	0.52
8:H:67:SER:O	8:H:68:TYR:CD1	2.62	0.52
19:I:1204:CLA:C14	21:I:6018:BCR:H392	2.37	0.52
12:L:51:LYS:HB3	12:L:51:LYS:HZ3	1.73	0.52
12:L:194:ILE:O	12:L:195:SER:CB	2.58	0.52
12:L:205:TYR:CG	12:L:207:LEU:HD12	2.36	0.52
19:L:1148:CLA:O2D	19:L:1148:CLA:CGA	2.57	0.52
13:N:123:GLY:CA	13:N:131:PHE:HD1	2.22	0.52
13:N:147:SER:O	13:N:148:ASP:HB2	2.10	0.52
15:1:163:TYR:N	15:1:164:PRO:HD3	2.23	0.52
19:1:1303:CLA:HBC2	19:1:1303:CLA:CMC	2.18	0.52
16:2:103:VAL:C	16:2:105:ALA:H	2.13	0.52
16:2:113:ALA:CB	16:2:114:MET:CE	2.87	0.52
19:3:3008:CLA:H2A	19:3:3008:CLA:O2A	2.09	0.52
18:4:174:GLN:HA	18:4:176:SER:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:177:LEU:HD22	18:4:178:PRO:CA	2.40	0.52
18:4:241:HIS:CE1	18:4:242:ASN:OD1	2.62	0.52
1:A:39:HIS:ND1	1:A:39:HIS:O	2.43	0.52
1:A:49:ASP:OD2	1:A:49:ASP:N	2.41	0.52
1:A:553:VAL:HG23	19:A:1124:CLA:HMC2	1.91	0.52
1:A:629:ASN:OD1	1:A:630:ASP:N	2.43	0.52
19:A:9012:CLA:H12	2:B:616:LEU:CD1	2.32	0.52
2:B:272:ASP:C	2:B:274:ALA:H	2.13	0.52
2:B:443:MET:HG2	2:B:451:LYS:O	2.10	0.52
2:B:510:LEU:C	2:B:510:LEU:HD12	2.29	0.52
2:B:694:ARG:CD	9:I:28:VAL:CG1	2.87	0.52
3:C:12:ILE:CB	3:C:39:ILE:HA	2.39	0.52
5:E:127:GLU:CG	5:E:129:GLU:O	2.57	0.52
22:F:7036:LMU:O2B	22:F:7036:LMU:C4'	2.58	0.52
19:H:1241:CLA:HAC1	21:I:6021:BCR:HC32	1.90	0.52
12:L:76:SER:O	12:L:79:ILE:N	2.42	0.52
16:2:155:VAL:HA	16:2:158:VAL:CG1	2.40	0.52
19:2:2004:CLA:O1A	19:3:2009:CLA:HBC3	2.10	0.52
17:3:103:VAL:HG11	17:3:229:LYS:CG	2.39	0.52
17:3:109:ALA:HA	17:3:111:LEU:CD1	2.39	0.52
19:3:2009:CLA:C5	19:3:2009:CLA:C9	2.26	0.52
19:3:3008:CLA:HBC2	19:3:3008:CLA:CMC	2.19	0.52
18:4:174:GLN:O	18:4:175:TYR:CB	2.58	0.52
1:A:63:ASP:CG	1:A:65:ASP:H	2.13	0.52
1:A:396:PHE:CG	1:A:396:PHE:O	2.62	0.52
1:A:587:GLY:HA3	2:B:668:ARG:CZ	2.40	0.52
19:A:9022:CLA:H151	21:B:6017:BCR:H19C	1.92	0.52
2:B:224:PRO:HG3	7:G:153:PHE:CB	2.40	0.52
2:B:323:TYR:CE1	19:B:1221:CLA:HBC1	2.45	0.52
10:J:26:LEU:H	10:J:28:GLU:H	1.56	0.52
12:L:93:VAL:HG12	12:L:94:SER:O	2.10	0.52
13:N:157:LYS:HG2	13:N:159:LYS:HG3	1.92	0.52
14:R:39:UNK:CA	14:R:41:UNK:CB	2.88	0.52
15:1:149:GLU:HG2	15:1:152:ARG:HH11	1.61	0.52
15:1:171:LEU:CB	15:1:173:TYR:CZ	2.93	0.52
17:3:155:TYR:C	17:3:157:LEU:N	2.62	0.52
19:3:3008:CLA:O1A	19:3:3008:CLA:CED	2.58	0.52
18:4:112:PRO:CB	18:4:116:THR:O	2.57	0.52
18:4:131:LYS:O	18:4:131:LYS:CG	2.57	0.52
1:A:73:GLU:HG3	1:A:74:ILE:CA	2.40	0.52
1:A:100:GLY:HA3	1:A:153:TRP:HH2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TRP:CZ3	19:A:1112:CLA:HMB3	2.45	0.52
1:A:435:VAL:HA	1:A:438:HIS:HE1	1.75	0.52
1:A:692:PHE:CD2	1:A:733:VAL:HG12	2.45	0.52
1:A:711:HIS:CD2	19:A:1139:CLA:CBC	2.84	0.52
19:A:9011:CLA:H192	19:A:9022:CLA:C2B	2.39	0.52
19:A:9012:CLA:H11	2:B:616:LEU:HB2	1.92	0.52
2:B:25:ILE:O	2:B:26:ALA:HB3	2.08	0.52
2:B:135:LEU:O	2:B:135:LEU:CG	2.58	0.52
2:B:186:SER:C	2:B:187:SER:O	2.48	0.52
2:B:278:LEU:HD21	19:B:1213:CLA:CGA	2.40	0.52
2:B:334:LEU:CB	19:B:1202:CLA:HMD3	2.38	0.52
2:B:393:PHE:CE2	2:B:398:TYR:HD2	2.27	0.52
2:B:463:ILE:O	2:B:464:GLN:HB3	2.08	0.52
2:B:609:PHE:O	2:B:613:SER:OG	2.27	0.52
19:B:1221:CLA:H61	19:B:1221:CLA:CMA	2.40	0.52
3:C:5:VAL:HG23	3:C:65:VAL:HG21	1.91	0.52
3:C:43:PRO:HA	4:D:182:GLN:HG3	1.92	0.52
3:C:44:ARG:NH2	4:D:181:ARG:NE	2.49	0.52
6:F:193:GLN:CA	6:F:195:GLU:OE1	2.57	0.52
10:J:9:SER:O	10:J:10:VAL:CB	2.57	0.52
12:L:104:LEU:HD12	12:L:196:GLY:CA	2.38	0.52
13:N:165:ASN:OD1	13:N:167:PHE:N	2.42	0.52
16:2:182:ILE:CA	16:2:187:LYS:CG	2.87	0.52
17:3:148:TYR:CD2	17:3:148:TYR:C	2.78	0.52
1:A:176:GLY:O	1:A:180:PHE:HB2	2.10	0.52
1:A:181:ALA:HB2	19:A:1108:CLA:HBC2	1.92	0.52
1:A:246:HIS:C	1:A:248:PHE:CE2	2.83	0.52
1:A:373:ALA:HB1	1:A:396:PHE:HD1	1.75	0.52
1:A:379:MET:HE1	19:A:1125:CLA:HMC2	1.90	0.52
1:A:553:VAL:HG22	21:A:6008:BCR:H401	1.91	0.52
1:A:574:ASN:OD1	1:A:574:ASN:N	2.42	0.52
1:A:595:TRP:HE3	1:A:596:ASP:OD2	1.92	0.52
19:A:1137:CLA:HBA2	19:A:1137:CLA:CHA	2.39	0.52
19:A:1237:CLA:H152	21:B:6020:BCR:C35	2.40	0.52
2:B:44:GLN:OE1	2:B:163:PRO:CB	2.57	0.52
2:B:110:LEU:HD12	2:B:111:GLY:HA2	1.88	0.52
2:B:123:TRP:HB2	2:B:126:THR:HG21	1.82	0.52
2:B:211:ASN:CB	2:B:214:ASP:HB3	2.39	0.52
2:B:363:GLN:HG3	2:B:363:GLN:O	2.09	0.52
2:B:387:PHE:HE2	19:B:1222:CLA:HHC	1.75	0.52
2:B:636:THR:O	2:B:636:THR:HG23	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:ARG:NH2	2:B:694:ARG:CG	2.47	0.52
19:F:1305:CLA:HED2	19:F:1305:CLA:OBD	2.09	0.52
11:K:122:LEU:HD22	11:K:122:LEU:C	2.30	0.52
22:K:7042:LMU:H71	22:K:7042:LMU:H22	1.92	0.52
12:L:161:ALA:H	12:L:162:PRO:HD2	1.72	0.52
13:N:136:ASP:OD1	13:N:136:ASP:N	2.43	0.52
19:R:1144:CLA:C1A	19:R:1144:CLA:CED	2.83	0.52
15:1:78:ARG:CG	19:1:1011:CLA:HMC1	2.40	0.52
19:1:1008:CLA:HAA2	19:1:1008:CLA:CBD	2.40	0.52
22:3:7003:LMU:O4'	22:3:7005:LMU:C4B	2.56	0.52
18:4:93:GLN:HE22	18:4:171:ILE:HG12	1.75	0.52
18:4:139:SER:O	18:4:141:LEU:HD22	2.09	0.52
1:A:44:ILE:O	1:A:45:ALA:O	2.28	0.52
1:A:51:THR:HG23	1:A:52:THR:N	2.25	0.52
1:A:130:GLU:O	1:A:130:GLU:CD	2.48	0.52
1:A:157:GLY:CA	1:A:229:ILE:HG22	2.25	0.52
1:A:478:SER:HB2	1:A:644:GLN:OE1	2.08	0.52
1:A:483:GLN:CB	1:A:485:GLN:HE22	2.21	0.52
1:A:664:VAL:CG2	1:A:665:ILE:HG23	2.40	0.52
1:A:733:VAL:HG21	19:A:1140:CLA:C3D	2.40	0.52
19:A:1149:CLA:O1D	19:A:1149:CLA:CBA	2.58	0.52
19:A:9022:CLA:O2A	2:B:651:LEU:HB3	2.10	0.52
2:B:200:PRO:O	2:B:204:GLY:HA2	2.10	0.52
2:B:455:ILE:HA	6:F:148:LEU:HG	1.91	0.52
2:B:628:SER:O	2:B:630:GLN:N	2.43	0.52
2:B:693:TRP:CD1	19:B:1238:CLA:HMD3	2.45	0.52
4:D:155:TYR:CE1	4:D:168:PRO:HG3	2.45	0.52
4:D:173:TYR:O	4:D:175:GLU:HG2	2.10	0.52
5:E:78:ARG:NH2	5:E:125:ILE:HG22	2.19	0.52
6:F:207:LEU:CD1	6:F:208:PHE:N	2.51	0.52
8:H:104:GLY:O	8:H:105:GLY:C	2.47	0.52
11:K:60:SER:O	11:K:61:THR:C	2.44	0.52
12:L:169:ARG:NE	12:L:169:ARG:O	2.43	0.52
13:N:132:THR:CA	13:N:136:ASP:OD1	2.54	0.52
15:1:77:GLU:CD	15:1:80:LYS:CE	2.78	0.52
16:2:103:VAL:O	16:2:104:GLN:C	2.48	0.52
16:2:118:ALA:HA	16:2:121:PHE:CD2	2.34	0.52
16:2:152:LEU:CD1	16:2:152:LEU:N	2.73	0.52
16:2:247:ILE:O	16:2:248:ASP:CB	2.58	0.52
1:A:154:ARG:HG3	1:A:383:PRO:HB2	1.92	0.51
1:A:291:THR:O	1:A:293:GLY:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:C	1:A:404:GLY:H	2.13	0.51
1:A:545:HIS:ND1	19:A:1135:CLA:HBB2	2.22	0.51
1:A:555:ILE:HG23	2:B:670:TYR:HE2	1.75	0.51
1:A:691:MET:HE2	20:A:5001:PQN:H2M2	1.92	0.51
19:A:1132:CLA:HBC2	19:H:1207:CLA:HBC1	1.92	0.51
19:A:9022:CLA:H122	19:A:9022:CLA:H71	1.92	0.51
19:A:9023:CLA:CAD	2:B:670:TYR:OH	2.58	0.51
2:B:527:LEU:CD2	19:B:1222:CLA:C1D	2.87	0.51
2:B:597:LYS:O	2:B:598:HIS:HB2	2.10	0.51
2:B:693:TRP:NE1	19:B:1238:CLA:HMD3	2.24	0.51
19:B:1238:CLA:HBC2	19:B:1238:CLA:HMC1	1.92	0.51
3:C:28:MET:HG3	4:D:175:GLU:HA	1.92	0.51
4:D:129:LEU:HD11	12:L:65:PHE:CD1	2.44	0.51
21:I:6021:BCR:H392	21:L:6019:BCR:C40	2.39	0.51
11:K:56:ILE:HG12	11:K:59:THR:HG21	1.92	0.51
12:L:178:THR:HG22	12:L:179:ALA:H	1.74	0.51
13:N:90:GLU:OE1	13:N:91:TYR:CE1	2.62	0.51
13:N:109:THR:O	13:N:111:GLY:N	2.42	0.51
15:1:90:ALA:O	15:1:91:MET:C	2.45	0.51
15:1:157:ASP:O	15:1:158:PRO:C	2.48	0.51
18:4:121:ILE:O	18:4:123:VAL:N	2.41	0.51
18:4:144:ILE:O	18:4:145:GLU:C	2.46	0.51
1:A:374:GLN:O	1:A:377:TYR:CD2	2.63	0.51
1:A:421:ASP:OD1	1:A:421:ASP:N	2.43	0.51
1:A:603:PHE:CZ	1:A:693:LEU:CD2	2.93	0.51
1:A:694:PHE:HZ	2:B:661:PHE:CD1	2.28	0.51
19:A:1103:CLA:H201	21:A:6003:BCR:C18	2.40	0.51
19:A:1112:CLA:CMB	21:A:6002:BCR:H382	2.36	0.51
19:A:9011:CLA:HMB3	19:A:9012:CLA:HMD1	1.92	0.51
19:A:9022:CLA:H62	2:B:648:TRP:CZ2	2.45	0.51
19:A:9023:CLA:HED3	19:A:9023:CLA:CBA	2.40	0.51
19:B:1203:CLA:CBB	19:B:1225:CLA:HHC	2.39	0.51
19:B:1239:CLA:C19	9:I:21:MET:CB	2.88	0.51
22:B:7038:LMU:C6	22:B:7038:LMU:C10	2.88	0.51
3:C:67:VAL:O	3:C:67:VAL:CG2	2.57	0.51
4:D:171:GLY:O	4:D:172:VAL:CG2	2.53	0.51
7:G:89:LYS:O	7:G:90:GLN:CG	2.57	0.51
8:H:121:LEU:O	8:H:122:PRO:C	2.47	0.51
12:L:110:LEU:CA	12:L:113:PRO:HG2	2.40	0.51
14:R:39:UNK:CA	14:R:42:UNK:CB	2.85	0.51
15:1:150:HIS:ND1	15:1:150:HIS:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:157:ASP:OD2	15:1:178:LYS:HA	2.08	0.51
19:1:1005:CLA:HMC1	19:1:1005:CLA:HBC2	1.93	0.51
17:3:159:VAL:HG12	17:3:160:LEU:H	1.75	0.51
17:3:176:TRP:O	17:3:178:LYS:CA	2.57	0.51
17:3:210:PRO:CG	17:3:211:LEU:H	2.23	0.51
18:4:173:LYS:HD2	18:4:201:LYS:CE	2.33	0.51
1:A:23:ASP:CB	1:A:33:GLN:CD	2.74	0.51
1:A:411:ALA:CB	21:A:6008:BCR:H392	2.34	0.51
1:A:461:TYR:CZ	1:A:540:LEU:CD1	2.93	0.51
19:A:1126:CLA:CGA	19:A:1126:CLA:C1A	2.89	0.51
2:B:102:GLU:OE2	2:B:641:ASN:HA	2.09	0.51
2:B:620:LEU:CD1	19:B:9010:CLA:H93	2.39	0.51
22:B:7038:LMU:H1B	22:B:7038:LMU:O6'	2.10	0.51
6:F:83:THR:HB	6:F:84:PRO:CD	2.36	0.51
6:F:150:VAL:O	6:F:150:VAL:CG1	2.49	0.51
6:F:184:ALA:C	6:F:185:ILE:HG23	2.29	0.51
8:H:80:GLN:CA	8:H:83:LEU:HD23	2.40	0.51
22:H:7011:LMU:H6E	22:H:7011:LMU:C2B	2.32	0.51
12:L:205:TYR:CE1	12:L:207:LEU:HD13	2.45	0.51
12:L:211:TYR:N	12:L:211:TYR:HD2	2.07	0.51
13:N:120:VAL:HG12	13:N:122:PHE:CE2	2.45	0.51
14:R:38:UNK:O	14:R:42:UNK:C	2.59	0.51
15:1:77:GLU:HG3	15:1:80:LYS:NZ	2.25	0.51
15:1:93:ALA:HA	19:1:1006:CLA:C3B	2.41	0.51
16:2:177:VAL:CG1	16:2:178:ASN:N	2.73	0.51
16:2:249:ASN:OD1	16:2:249:ASN:O	2.28	0.51
17:3:192:LYS:NZ	17:3:192:LYS:CA	2.71	0.51
1:A:207:LEU:CD2	19:A:1119:CLA:CBB	2.83	0.51
1:A:368:LEU:CD1	19:A:1125:CLA:C6	2.88	0.51
19:A:1126:CLA:H18	19:A:9012:CLA:H18	1.92	0.51
19:A:1132:CLA:H111	21:B:6020:BCR:H10C	1.91	0.51
19:A:1135:CLA:HBA2	19:A:1135:CLA:CGD	2.39	0.51
2:B:98:GLN:NE2	2:B:98:GLN:CA	2.71	0.51
2:B:315:LEU:CD1	2:B:317:ARG:HD2	2.40	0.51
2:B:317:ARG:CZ	2:B:317:ARG:HB3	2.39	0.51
2:B:494:LEU:O	2:B:494:LEU:HD12	2.11	0.51
2:B:561:GLY:HA3	3:C:52:LYS:CB	2.41	0.51
2:B:561:GLY:CA	3:C:52:LYS:HG2	2.36	0.51
2:B:662:MET:HG2	20:B:5002:PQN:O1	2.11	0.51
4:D:95:GLN:NE2	4:D:95:GLN:C	2.64	0.51
5:E:73:LYS:HG3	5:E:128:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:202:LEU:O	6:F:203:ALA:CB	2.59	0.51
6:F:221:LEU:C	6:F:222:LEU:HD23	2.31	0.51
19:J:1308:CLA:O1D	19:J:1308:CLA:C2	2.58	0.51
11:K:64:MET:O	11:K:67:ALA:HB3	2.11	0.51
19:K:1142:CLA:HMD1	19:K:1143:CLA:C4A	2.39	0.51
13:N:157:LYS:N	13:N:157:LYS:CD	2.74	0.51
15:1:182:GLU:OE1	19:1:1001:CLA:C2D	2.58	0.51
16:2:122:ILE:HD11	19:2:2002:CLA:CBB	2.26	0.51
17:3:113:ALA:CB	17:3:239:LEU:HD12	2.28	0.51
17:3:134:LEU:CD1	17:3:134:LEU:N	2.65	0.51
18:4:95:GLU:O	18:4:98:ASN:N	2.43	0.51
18:4:96:LEU:CD1	18:4:96:LEU:O	2.57	0.51
1:A:295:TRP:HB3	1:A:297:THR:HG23	1.92	0.51
1:A:374:GLN:O	1:A:376:MET:N	2.43	0.51
1:A:571:ASP:HB3	3:C:53:ARG:HH12	1.74	0.51
1:A:628:ILE:HG13	1:A:629:ASN:N	2.25	0.51
1:A:665:ILE:C	1:A:665:ILE:HD12	2.30	0.51
1:A:678:PHE:O	1:A:681:GLY:O	2.29	0.51
19:A:1125:CLA:HBA2	21:A:6008:BCR:C12	2.41	0.51
2:B:340:SER:O	2:B:344:ILE:HG13	2.11	0.51
2:B:404:ALA:O	2:B:405:ASP:CG	2.48	0.51
2:B:558:PRO:HG2	2:B:703:VAL:HG13	1.92	0.51
2:B:639:VAL:CG2	2:B:640:CYS:N	2.74	0.51
19:F:1302:CLA:HBC2	19:F:1302:CLA:CHD	2.38	0.51
15:1:67:LEU:CG	15:1:68:GLY:N	2.73	0.51
15:1:84:LEU:N	15:1:86:HIS:HD2	2.07	0.51
15:1:168:PHE:O	15:1:169:ASP:CB	2.39	0.51
16:2:184:PRO:CA	16:2:187:LYS:HD2	2.40	0.51
16:2:200:TRP:N	16:2:200:TRP:CD1	2.79	0.51
19:2:4009:CLA:H152	19:2:4009:CLA:C19	2.33	0.51
1:A:214:GLY:O	1:A:215:SER:CB	2.58	0.51
1:A:274:TRP:NE1	1:A:277:TYR:CD2	2.78	0.51
1:A:483:GLN:CA	1:A:485:GLN:HE22	2.23	0.51
1:A:488:PHE:HB3	1:A:535:GLY:H	1.76	0.51
1:A:575:LEU:HD11	1:A:579:PHE:CG	2.45	0.51
19:A:1101:CLA:HBB1	19:A:1109:CLA:H151	1.91	0.51
19:A:1105:CLA:HBA2	19:A:1107:CLA:C1	2.40	0.51
19:A:1107:CLA:HBA2	19:A:1107:CLA:CHA	2.40	0.51
19:A:1124:CLA:CHC	21:A:6008:BCR:C37	2.89	0.51
19:A:1124:CLA:HAA2	19:A:1125:CLA:CAD	2.41	0.51
19:A:9012:CLA:C4B	19:A:9013:CLA:HBB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:GLN:HE21	2:B:101:VAL:HG23	1.76	0.51
2:B:225:LEU:N	2:B:227:THR:O	2.44	0.51
2:B:257:ILE:HD13	2:B:257:ILE:N	2.25	0.51
2:B:324:ASP:O	2:B:328:ASN:CG	2.48	0.51
2:B:365:PHE:HD1	2:B:602:TRP:CE2	2.29	0.51
2:B:555:TYR:CD2	2:B:573:TRP:HB2	2.44	0.51
2:B:558:PRO:CB	2:B:703:VAL:CG2	2.64	0.51
2:B:564:ARG:NH2	3:C:66:ARG:HH12	2.09	0.51
19:B:1220:CLA:HAA1	19:B:1220:CLA:H12	1.93	0.51
4:D:74:LEU:HD11	12:L:58:GLN:OE1	2.10	0.51
6:F:161:ILE:O	6:F:164:GLY:N	2.36	0.51
11:K:60:SER:O	11:K:63:LEU:HD22	2.11	0.51
13:N:152:LEU:O	13:N:153:GLU:HG3	2.08	0.51
13:N:168:TRP:O	13:N:168:TRP:CE3	2.63	0.51
14:R:37:UNK:O	14:R:42:UNK:O	2.29	0.51
16:2:201:PHE:CD1	16:2:202:ASP:CA	2.93	0.51
18:4:201:LYS:HD3	18:4:201:LYS:H	1.71	0.51
1:A:79:PHE:CD1	19:A:1111:CLA:CED	2.90	0.51
1:A:468:SER:HB2	1:A:476:MET:SD	2.51	0.51
1:A:660:GLN:HE21	1:A:660:GLN:H	1.58	0.51
19:A:1115:CLA:HED3	19:A:1115:CLA:C1A	2.36	0.51
19:A:1126:CLA:H71	21:A:6011:BCR:H372	1.93	0.51
19:A:1131:CLA:C16	21:L:6019:BCR:H362	2.40	0.51
2:B:230:TRP:O	2:B:232:LEU:N	2.43	0.51
2:B:292:ARG:HH22	2:B:297:ILE:CG1	2.24	0.51
2:B:378:ILE:H	2:B:381:PHE:HD1	1.59	0.51
2:B:493:TRP:CB	19:B:1232:CLA:HED2	2.41	0.51
2:B:621:ARG:O	2:B:625:TRP:CB	2.52	0.51
19:B:1205:CLA:H102	19:B:1205:CLA:C14	2.40	0.51
19:B:1228:CLA:HBC2	19:B:1228:CLA:CHD	2.35	0.51
3:C:1:MET:N	3:C:3:HIS:N	2.59	0.51
3:C:5:VAL:HG23	3:C:5:VAL:O	2.11	0.51
4:D:172:VAL:HG12	4:D:173:TYR:N	2.26	0.51
5:E:96:ASP:CG	5:E:98:ASN:OD1	2.49	0.51
6:F:131:ASP:OD2	6:F:131:ASP:N	2.43	0.51
19:J:1311:CLA:C1A	19:J:1311:CLA:CED	2.83	0.51
15:1:178:LYS:C	15:1:178:LYS:CD	2.71	0.51
17:3:96:ARG:CG	17:3:96:ARG:NH1	2.39	0.51
18:4:94:ALA:HA	19:4:4012:CLA:OBD	2.11	0.51
1:A:240:LYS:O	1:A:240:LYS:CG	2.58	0.51
1:A:332:GLU:HA	1:A:344:LYS:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:O	1:A:438:HIS:ND1	2.43	0.51
1:A:755:ILE:O	1:A:756:ALA:CB	2.59	0.51
2:B:160:LYS:NZ	2:B:161:TRP:CG	2.65	0.51
2:B:288:GLY:O	2:B:289:LEU:HB2	2.10	0.51
2:B:596:TRP:O	2:B:597:LYS:CB	2.58	0.51
19:B:1222:CLA:CHB	19:B:1236:CLA:HAA2	2.41	0.51
4:D:123:ARG:HG2	4:D:124:GLU:N	2.24	0.51
5:E:103:VAL:HG23	5:E:104:VAL:O	2.11	0.51
8:H:58:LEU:N	8:H:61:THR:HG21	2.23	0.51
8:H:94:ARG:HB2	8:H:94:ARG:NH1	2.25	0.51
12:L:107:GLY:O	12:L:109:LEU:N	2.44	0.51
13:N:146:LEU:C	13:N:147:SER:O	2.48	0.51
14:R:27:UNK:C	14:R:29:UNK:N	2.74	0.51
14:R:30:UNK:O	14:R:32:UNK:N	2.43	0.51
15:1:162:LYS:N	15:1:164:PRO:CG	2.49	0.51
19:2:2004:CLA:H43	19:3:2009:CLA:HBC3	1.93	0.51
22:2:7006:LMU:H122	22:3:7005:LMU:O3'	2.10	0.51
17:3:96:ARG:H	17:3:99:ALA:H	1.58	0.51
17:3:125:VAL:CB	17:3:126:GLY:HA2	2.31	0.51
17:3:159:VAL:C	17:3:161:GLU:N	2.56	0.51
18:4:108:GLY:C	18:4:109:MET:O	2.49	0.51
19:4:1304:CLA:H2A	19:4:1304:CLA:CGD	2.41	0.51
1:A:431:LEU:CA	1:A:434:ARG:HB2	2.41	0.51
19:A:1106:CLA:H112	19:A:1126:CLA:H91	1.93	0.51
19:A:1117:CLA:ND	19:A:1127:CLA:H72	2.26	0.51
19:A:1126:CLA:C7	21:A:6011:BCR:C37	2.88	0.51
2:B:89:HIS:C	2:B:113:VAL:HG13	1.98	0.51
2:B:189:ALA:HB1	19:B:1225:CLA:H203	1.91	0.51
2:B:194:LEU:O	2:B:198:ALA:HB3	2.11	0.51
2:B:256:THR:O	2:B:272:ASP:OD2	2.29	0.51
2:B:290:MET:SD	2:B:291:TYR:CE1	3.04	0.51
2:B:297:ILE:HD11	19:B:1217:CLA:O2D	2.10	0.51
2:B:304:ILE:HD13	19:B:1216:CLA:CED	2.38	0.51
2:B:458:ILE:O	2:B:461:GLN:N	2.43	0.51
3:C:63:LEU:HD21	3:C:65:VAL:N	2.24	0.51
6:F:82:LEU:O	6:F:140:CYS:O	2.29	0.51
10:J:42:PHE:CD1	18:4:244:ILE:HG21	2.43	0.51
19:K:1143:CLA:HMC1	19:K:1143:CLA:HBC2	1.93	0.51
13:N:123:GLY:HA3	13:N:131:PHE:CD1	2.45	0.51
16:2:157:LEU:CD1	16:2:157:LEU:N	2.73	0.51
16:2:183:PHE:O	16:2:185:ASN:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:162:MET:O	17:3:163:ALA:C	2.46	0.51
17:3:191:GLU:O	17:3:192:LYS:CE	2.57	0.51
17:3:201:ALA:O	17:3:202:TYR:CB	2.58	0.51
18:4:133:GLU:O	18:4:134:TYR:HD1	1.93	0.51
18:4:226:LYS:N	18:4:226:LYS:NZ	2.56	0.51
1:A:270:PHE:CD2	1:A:270:PHE:N	2.79	0.51
1:A:583:GLY:O	1:A:585:GLY:N	2.44	0.51
19:A:1113:CLA:HAA1	19:A:1113:CLA:HED2	1.91	0.51
19:A:1122:CLA:CAB	21:A:6007:BCR:C35	2.86	0.51
2:B:544:SER:O	2:B:547:MET:C	2.49	0.51
2:B:560:ASP:OD2	3:C:66:ARG:NH1	2.44	0.51
3:C:42:ALA:CB	3:C:43:PRO:CD	2.88	0.51
11:K:115:ILE:CG1	11:K:122:LEU:CD1	2.89	0.51
15:1:69:LEU:HA	15:1:73:PRO:HD3	1.91	0.51
15:1:177:PRO:HG3	15:1:180:LEU:HD23	1.93	0.51
19:1:1010:CLA:O1D	19:1:1010:CLA:C4D	2.50	0.51
16:2:153:PHE:CD2	16:2:157:LEU:HD22	2.45	0.51
16:2:201:PHE:CD1	16:2:202:ASP:HB3	2.46	0.51
17:3:226:LYS:O	17:3:229:LYS:HB3	2.11	0.51
17:3:233:LEU:C	17:3:235:MET:N	2.65	0.51
1:A:39:HIS:HA	1:A:44:ILE:HG21	1.92	0.50
1:A:233:LEU:C	1:A:235:ALA:H	2.14	0.50
1:A:333:ALA:HB3	1:A:334:HIS:ND1	2.27	0.50
1:A:484:LEU:C	1:A:485:GLN:CD	2.70	0.50
19:A:1106:CLA:H43	21:A:6011:BCR:H383	1.92	0.50
2:B:122:GLN:HG2	2:B:361:ILE:HG13	1.94	0.50
2:B:229:GLN:O	7:G:63:VAL:HG11	2.12	0.50
2:B:710:LEU:C	2:B:712:HIS:H	2.13	0.50
4:D:91:LEU:C	4:D:91:LEU:HD12	2.32	0.50
6:F:88:SER:O	6:F:89:LYS:C	2.48	0.50
7:G:75:GLY:O	7:G:78:VAL:N	2.45	0.50
8:H:60:ASN:C	8:H:60:ASN:OD1	2.47	0.50
9:I:29:GLU:HA	9:I:29:GLU:OE2	2.11	0.50
12:L:96:LEU:HG	12:L:97:LEU:CD2	2.41	0.50
12:L:106:HIS:HD2	19:L:1502:CLA:CED	2.23	0.50
13:N:123:GLY:HA3	13:N:131:PHE:HD1	1.76	0.50
13:N:142:LYS:O	13:N:145:PHE:CD1	2.64	0.50
14:R:38:UNK:C	14:R:42:UNK:C	2.89	0.50
16:2:161:GLY:N	19:2:2012:CLA:HBB2	2.26	0.50
17:3:100:TYR:HB3	17:3:229:LYS:HE2	1.92	0.50
18:4:127:TYR:O	18:4:128:ALA:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASP:OD2	1:A:141:ARG:N	2.44	0.50
1:A:285:GLY:O	1:A:294:LEU:HD11	2.11	0.50
1:A:340:GLY:O	1:A:343:HIS:N	2.33	0.50
1:A:377:TYR:HD1	1:A:616:PHE:HE1	1.56	0.50
1:A:492:ILE:O	1:A:493:GLN:C	2.47	0.50
19:A:9012:CLA:HED2	19:A:9012:CLA:C3D	2.41	0.50
19:A:9012:CLA:H91	19:A:9012:CLA:H152	1.92	0.50
2:B:120:VAL:HG13	2:B:123:TRP:NE1	2.27	0.50
2:B:303:TYR:H	2:B:306:GLU:HB2	1.76	0.50
2:B:556:SER:O	24:B:7101:LMG:HC2	2.11	0.50
2:B:583:MET:HA	19:B:1222:CLA:HBC1	1.93	0.50
2:B:598:HIS:HB3	2:B:602:TRP:CH2	2.46	0.50
19:B:1220:CLA:CBC	19:B:1220:CLA:CMC	2.74	0.50
19:B:1238:CLA:H91	21:I:6018:BCR:H333	1.93	0.50
3:C:44:ARG:CA	4:D:182:GLN:CD	2.69	0.50
4:D:126:PRO:HB2	4:D:128:LEU:HB2	1.93	0.50
5:E:128:VAL:O	5:E:129:GLU:O	2.28	0.50
7:G:99:HIS:C	7:G:101:GLU:CB	2.68	0.50
10:J:14:VAL:O	10:J:14:VAL:HG13	2.11	0.50
13:N:144:PRO:HA	13:N:151:ASP:CG	2.31	0.50
14:R:35:UNK:O	14:R:42:UNK:O	2.30	0.50
16:2:120:ILE:C	16:2:123:PRO:HD2	2.31	0.50
16:2:126:LEU:HB3	19:2:2006:CLA:C19	2.29	0.50
16:2:126:LEU:HD13	19:2:2006:CLA:H172	1.93	0.50
16:2:236:TRP:CZ2	19:2:2003:CLA:CHB	2.94	0.50
17:3:95:PRO:O	17:3:96:ARG:CD	2.58	0.50
17:3:97:TRP:O	17:3:98:LEU:C	2.48	0.50
17:3:233:LEU:C	17:3:235:MET:H	2.14	0.50
18:4:147:ILE:O	18:4:150:HIS:HB3	2.10	0.50
1:A:472:ARG:O	1:A:474:GLN:HG3	2.12	0.50
1:A:626:GLY:O	1:A:627:THR:HG22	2.11	0.50
19:A:1102:CLA:HBC3	19:A:1102:CLA:HHD	1.92	0.50
19:A:1103:CLA:C4	21:A:6003:BCR:H313	2.41	0.50
19:A:1128:CLA:C10	19:A:1128:CLA:H152	2.41	0.50
19:A:1135:CLA:HBA2	19:A:1135:CLA:CBD	2.41	0.50
2:B:429:LEU:HD21	19:B:1235:CLA:C3B	2.42	0.50
2:B:573:TRP:O	2:B:577:TYR:N	2.37	0.50
4:D:180:GLY:O	4:D:182:GLN:N	2.44	0.50
6:F:209:ARG:O	6:F:212:SER:C	2.50	0.50
11:K:115:ILE:O	11:K:118:VAL:N	2.44	0.50
13:N:142:LYS:CE	13:N:142:LYS:CA	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:148:ASP:H	13:N:150:LEU:N	2.09	0.50
14:R:44:UNK:O	14:R:45:UNK:O	2.30	0.50
16:2:114:MET:HG3	16:2:230:LEU:HB2	1.92	0.50
16:2:241:TYR:HD2	16:2:242:THR:N	2.10	0.50
17:3:154:ASN:O	17:3:155:TYR:CD2	2.62	0.50
17:3:176:TRP:O	17:3:177:ALA:C	2.49	0.50
18:4:161:LYS:NZ	18:4:162:ASN:ND2	2.60	0.50
1:A:109:TRP:O	1:A:112:ASP:N	2.44	0.50
1:A:284:ARG:HG3	1:A:295:TRP:NE1	2.26	0.50
1:A:502:THR:O	1:A:504:ALA:O	2.30	0.50
1:A:536:THR:O	1:A:536:THR:HG23	2.11	0.50
1:A:550:HIS:O	1:A:552:THR:O	2.29	0.50
1:A:734:GLY:O	1:A:736:THR:N	2.44	0.50
2:B:351:HIS:NE2	19:B:1223:CLA:NC	2.59	0.50
2:B:594:TRP:HD1	2:B:595:HIS:HB2	1.76	0.50
2:B:622:ASP:HB2	2:B:626:LEU:HD11	1.84	0.50
2:B:682:HIS:O	2:B:683:GLU:C	2.50	0.50
19:B:1203:CLA:H43	24:B:7101:LMG:H321	1.92	0.50
19:B:1218:CLA:HMA3	19:B:1219:CLA:C4D	2.41	0.50
3:C:10:THR:HG23	5:E:101:TYR:CG	2.41	0.50
6:F:88:SER:HG	6:F:91:PHE:HB3	1.73	0.50
19:K:1143:CLA:CAC	22:K:7001:LMU:C3B	2.86	0.50
19:L:1130:CLA:H92	19:L:1504:CLA:H2	1.92	0.50
13:N:104:LYS:O	13:N:107:LEU:N	2.44	0.50
13:N:120:VAL:CG1	13:N:122:PHE:CE2	2.94	0.50
22:R:7025:LMU:H21	22:R:7025:LMU:O2'	2.11	0.50
15:1:225:TRP:HB3	15:1:226:HIS:CA	2.41	0.50
16:2:187:LYS:HE3	16:2:187:LYS:C	2.31	0.50
16:2:227:LEU:CD2	19:2:2004:CLA:NC	2.72	0.50
16:2:261:THR:CG2	16:2:262:ILE:N	2.59	0.50
17:3:201:ALA:CB	17:3:202:TYR:CE2	2.74	0.50
18:4:232:LEU:HD12	18:4:233:LEU:C	2.31	0.50
1:A:245:PRO:O	1:A:248:PHE:CZ	2.64	0.50
1:A:455:PHE:CD1	19:A:1131:CLA:HMA2	2.45	0.50
1:A:747:TRP:CE3	21:A:6011:BCR:C40	2.94	0.50
19:A:9022:CLA:C10	21:B:6017:BCR:H19C	2.40	0.50
2:B:6:PRO:O	2:B:6:PRO:HG2	2.12	0.50
2:B:8:PHE:O	2:B:35:ASP:CG	2.50	0.50
2:B:196:HIS:NE2	19:B:1212:CLA:ND	2.59	0.50
2:B:247:THR:CA	2:B:250:ALA:HB3	2.20	0.50
2:B:330:ILE:HG13	2:B:330:ILE:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:ILE:C	2:B:420:SER:OG	2.50	0.50
2:B:451:LYS:HD3	19:B:1230:CLA:O2D	2.10	0.50
2:B:593:TYR:O	2:B:596:TRP:O	2.29	0.50
19:B:1224:CLA:CGA	19:B:1224:CLA:H3A	2.34	0.50
5:E:127:GLU:OE1	5:E:129:GLU:O	2.28	0.50
6:F:173:TRP:CZ3	6:F:211:PHE:N	2.80	0.50
6:F:226:LEU:HA	6:F:230:ASN:HD22	1.77	0.50
7:G:81:ASN:OD1	7:G:82:PHE:N	2.43	0.50
7:G:87:VAL:O	7:G:88:ALA:CB	2.57	0.50
8:H:78:PRO:HG3	19:L:1501:CLA:CMD	2.40	0.50
12:L:166:LEU:O	12:L:167:THR:C	2.45	0.50
12:L:208:ASP:OD2	12:L:209:LEU:O	2.29	0.50
14:R:38:UNK:O	14:R:39:UNK:O	2.30	0.50
19:1:1008:CLA:HBA2	19:1:1008:CLA:CMA	2.42	0.50
16:2:145:TYR:C	16:2:146:PHE:CG	2.85	0.50
22:4:7033:LMU:H6'2	22:4:7033:LMU:O2'	2.12	0.50
1:A:23:ASP:OD1	1:A:33:GLN:HG3	2.12	0.50
1:A:203:LEU:CD2	19:A:1123:CLA:O2D	2.59	0.50
1:A:656:PHE:O	1:A:659:ALA:N	2.45	0.50
19:A:1104:CLA:HBA2	19:A:1104:CLA:HED2	1.93	0.50
19:A:1112:CLA:CHC	21:A:6002:BCR:H17C	2.31	0.50
19:A:9012:CLA:HED1	19:B:9010:CLA:H2	1.94	0.50
19:A:9023:CLA:HMC1	2:B:661:PHE:HB2	1.89	0.50
2:B:31:PHE:O	2:B:32:GLU:C	2.50	0.50
2:B:92:TRP:CZ2	9:I:6:SER:HB2	2.47	0.50
2:B:175:LEU:HD12	2:B:179:LEU:HD23	1.93	0.50
2:B:292:ARG:HH21	2:B:297:ILE:CA	2.25	0.50
2:B:354:SER:O	2:B:508:LEU:HD23	2.12	0.50
2:B:456:GLU:CB	6:F:147:HIS:ND1	2.75	0.50
2:B:667:TRP:O	2:B:669:GLY:N	2.44	0.50
2:B:686:PRO:C	2:B:688:ALA:H	2.14	0.50
19:B:1208:CLA:HBD	19:B:1208:CLA:O2A	2.11	0.50
19:B:1209:CLA:H61	19:B:1209:CLA:C1	2.42	0.50
19:B:1222:CLA:O1A	19:B:1236:CLA:HAA1	2.12	0.50
3:C:29:ILE:HG22	3:C:30:PRO:O	2.12	0.50
22:H:7032:LMU:H22	22:H:7032:LMU:H6'2	1.93	0.50
11:K:115:ILE:O	11:K:116:ILE:C	2.47	0.50
13:N:155:GLU:O	13:N:157:LYS:CE	2.08	0.50
22:R:7020:LMU:H6E	22:R:7020:LMU:O6B	2.11	0.50
16:2:219:THR:O	16:2:223:LYS:HB2	2.12	0.50
1:A:148:GLY:O	1:A:152:ILE:CD1	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HD13	19:A:1124:CLA:CAD	2.40	0.50
1:A:425:THR:HG1	1:A:428:TYR:HH	1.59	0.50
1:A:578:ARG:O	1:A:579:PHE:O	2.30	0.50
1:A:655:ASP:O	1:A:660:GLN:NE2	2.45	0.50
1:A:662:SER:O	1:A:666:GLN:HB2	2.12	0.50
1:A:705:GLU:CB	2:B:545:LYS:NZ	2.75	0.50
19:A:1141:CLA:H72	19:A:1141:CLA:H122	1.90	0.50
2:B:163:PRO:C	2:B:164:SER:OG	2.48	0.50
2:B:224:PRO:HG3	7:G:153:PHE:HB3	1.94	0.50
2:B:330:ILE:HD12	2:B:333:GLN:HE21	1.77	0.50
2:B:519:VAL:HG11	2:B:593:TYR:HB2	1.94	0.50
2:B:626:LEU:O	2:B:627:ASN:CB	2.47	0.50
2:B:685:THR:HG1	19:L:1130:CLA:H3A	1.73	0.50
19:B:1221:CLA:HMB2	19:B:1223:CLA:H92	1.93	0.50
4:D:140:LEU:HD22	4:D:144:LEU:HD11	1.92	0.50
4:D:147:LYS:CA	4:D:148:TYR:CD1	2.93	0.50
4:D:184:VAL:HG12	4:D:185:GLY:H	1.76	0.50
6:F:88:SER:HG	6:F:91:PHE:CB	2.25	0.50
8:H:55:LEU:O	8:H:56:GLU:C	2.50	0.50
11:K:51:SER:H	11:K:52:PRO:HD3	1.75	0.50
15:1:168:PHE:O	15:1:168:PHE:HD1	1.95	0.50
19:1:1005:CLA:CHA	19:1:1005:CLA:HBA1	2.42	0.50
17:3:109:ALA:O	17:3:111:LEU:CD2	2.60	0.50
17:3:246:LEU:HB3	17:3:248:THR:HG23	1.92	0.50
18:4:188:ILE:HG22	18:4:189:PHE:HD2	1.77	0.50
1:A:431:LEU:N	1:A:434:ARG:HE	2.10	0.50
2:B:348:VAL:HG21	19:B:1225:CLA:HHD	1.94	0.50
2:B:420:SER:O	2:B:424:TRP:N	2.36	0.50
2:B:431:PHE:HE2	19:B:1229:CLA:CED	2.25	0.50
2:B:508:LEU:HB2	2:B:509:PHE:HD2	1.76	0.50
2:B:693:TRP:CD1	19:B:1238:CLA:CMD	2.94	0.50
4:D:103:THR:OG1	4:D:153:GLN:HB2	2.11	0.50
6:F:105:SER:O	6:F:107:LYS:N	2.45	0.50
7:G:89:LYS:C	7:G:90:GLN:CG	2.78	0.50
22:H:7002:LMU:O6B	22:H:7002:LMU:C1B	2.58	0.50
12:L:70:GLU:OE2	12:L:75:SER:OG	2.19	0.50
13:N:90:GLU:OE1	13:N:91:TYR:CD1	2.65	0.50
13:N:139:LYS:C	13:N:142:LYS:NZ	2.64	0.50
13:N:168:TRP:CZ3	13:N:170:TRP:HB3	2.47	0.50
14:R:8:UNK:CB	19:R:1144:CLA:CED	2.90	0.50
14:R:34:UNK:O	14:R:36:UNK:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:150:HIS:O	15:1:153:SER:HB3	2.12	0.50
16:2:224:ASN:C	16:2:227:LEU:H	2.15	0.50
16:2:249:ASN:OD1	16:2:250:LEU:O	2.30	0.50
17:3:104:ILE:CG2	19:3:3004:CLA:C2D	2.90	0.50
17:3:111:LEU:C	17:3:113:ALA:N	2.62	0.50
18:4:120:ILE:HD11	18:4:226:LYS:HG3	0.51	0.50
18:4:122:ASN:HB3	18:4:124:PRO:CD	2.36	0.50
22:4:7034:LMU:C10	22:4:7052:LMU:C3'	2.90	0.50
1:A:167:THR:HG22	19:A:1112:CLA:CAA	2.23	0.50
1:A:240:LYS:O	1:A:240:LYS:HG3	2.12	0.50
1:A:255:LEU:O	1:A:256:ALA:C	2.49	0.50
1:A:302:HIS:CD2	19:A:1116:CLA:NB	2.78	0.50
1:A:344:LYS:C	1:A:346:LEU:N	2.60	0.50
1:A:348:GLU:O	1:A:351:THR:HG22	2.12	0.50
1:A:348:GLU:O	1:A:351:THR:CG2	2.60	0.50
2:B:23:PHE:O	2:B:24:GLY:C	2.49	0.50
2:B:317:ARG:NH1	2:B:405:ASP:C	2.58	0.50
2:B:338:LEU:O	2:B:339:ALA:HB3	2.11	0.50
2:B:472:TYR:O	2:B:472:TYR:HD1	1.95	0.50
2:B:620:LEU:CA	2:B:624:LEU:HD23	2.32	0.50
2:B:707:LEU:HD11	2:B:711:VAL:HG21	1.93	0.50
2:B:732:LYS:CG	2:B:734:GLY:CA	2.88	0.50
19:B:1202:CLA:H162	19:B:1210:CLA:OBD	2.12	0.50
19:B:1239:CLA:HMC1	19:B:1239:CLA:CBC	2.35	0.50
6:F:129:ARG:NH1	6:F:132:ASN:OD1	2.45	0.50
6:F:169:TYR:C	6:F:169:TYR:CD2	2.85	0.50
19:J:1308:CLA:HBD	19:J:1308:CLA:CGA	2.42	0.50
11:K:53:THR:HA	11:K:56:ILE:HB	1.94	0.50
11:K:116:ILE:HG23	11:K:117:GLY:H	1.74	0.50
12:L:112:GLY:N	12:L:113:PRO:CD	2.75	0.50
12:L:138:VAL:HG21	12:L:194:ILE:HG13	1.94	0.50
13:N:132:THR:HG21	13:N:139:LYS:HD3	0.66	0.50
14:R:35:UNK:O	14:R:36:UNK:O	2.30	0.50
15:1:133:THR:C	15:1:137:ILE:HD13	2.31	0.50
15:1:137:ILE:O	15:1:141:GLU:CG	2.49	0.50
16:2:161:GLY:O	16:2:162:TRP:C	2.50	0.50
17:3:108:PHE:HD2	19:3:3013:CLA:H43	1.77	0.50
17:3:109:ALA:HA	17:3:111:LEU:HB3	1.60	0.50
18:4:161:LYS:HZ1	18:4:162:ASN:HD21	1.58	0.50
18:4:167:ASN:O	18:4:168:GLN:HB2	2.12	0.50
1:A:378:SER:OG	19:A:1125:CLA:HBC2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ALA:HB3	1:A:500:PRO:CD	2.42	0.49
1:A:701:GLN:HA	1:A:701:GLN:NE2	2.26	0.49
1:A:744:ALA:HB2	21:A:6011:BCR:H391	0.69	0.49
19:A:1126:CLA:H72	21:A:6011:BCR:H371	1.94	0.49
2:B:46:ILE:HG21	19:B:1202:CLA:HBC3	1.94	0.49
2:B:69:ALA:HB1	2:B:135:LEU:CD1	2.37	0.49
2:B:275:HIS:O	2:B:278:LEU:HB3	2.11	0.49
2:B:306:GLU:CG	2:B:307:ALA:H	2.00	0.49
2:B:434:LEU:O	2:B:438:VAL:HG13	2.12	0.49
2:B:592:PHE:HA	2:B:721:TYR:OH	2.12	0.49
19:B:1225:CLA:H142	21:B:6006:BCR:C10	2.42	0.49
4:D:132:ALA:CB	4:D:136:GLN:HE22	2.21	0.49
5:E:76:ILE:O	5:E:84:TYR:O	2.30	0.49
7:G:102:ALA:CA	7:G:104:ASP:OD2	2.59	0.49
7:G:144:THR:CG2	7:G:147:ASN:O	2.58	0.49
22:H:7032:LMU:H31	22:H:7032:LMU:H2B	1.93	0.49
14:R:38:UNK:O	14:R:42:UNK:O	2.30	0.49
22:R:7007:LMU:O6B	22:R:7007:LMU:H1B	2.12	0.49
15:1:77:GLU:HG3	15:1:80:LYS:CE	2.42	0.49
16:2:171:ILE:CG1	16:2:172:LEU:H	2.23	0.49
17:3:161:GLU:CA	17:3:164:LEU:HG	2.39	0.49
17:3:192:LYS:HZ3	17:3:192:LYS:C	2.15	0.49
18:4:170:PRO:HG2	18:4:171:ILE:HG13	1.94	0.49
19:4:1004:CLA:OBD	19:4:1004:CLA:O2D	2.29	0.49
1:A:150:PHE:H	1:A:153:TRP:CB	2.19	0.49
1:A:217:SER:HG	21:A:6002:BCR:H17C	1.76	0.49
1:A:233:LEU:O	1:A:235:ALA:N	2.30	0.49
1:A:262:PHE:O	1:A:265:GLY:N	2.44	0.49
1:A:382:TYR:HE2	19:A:1127:CLA:HED3	1.75	0.49
1:A:686:TRP:O	1:A:689:SER:OG	2.19	0.49
1:A:692:PHE:CE2	1:A:733:VAL:HG11	2.46	0.49
19:A:1132:CLA:HBC3	19:A:1132:CLA:CMC	2.41	0.49
19:A:1141:CLA:O2D	19:A:1141:CLA:O1A	2.29	0.49
21:A:6011:BCR:H353	19:A:9012:CLA:H41	1.94	0.49
2:B:91:ILE:HG21	19:B:1206:CLA:HMD1	1.95	0.49
2:B:244:PHE:CD2	2:B:244:PHE:O	2.58	0.49
2:B:393:PHE:CZ	2:B:398:TYR:CD2	3.01	0.49
2:B:396:ARG:NH1	19:B:1226:CLA:HED2	2.27	0.49
19:B:1205:CLA:H42	19:B:1205:CLA:CHD	2.42	0.49
19:B:1222:CLA:H72	19:B:1236:CLA:C3D	2.41	0.49
19:B:1225:CLA:H62	21:B:6006:BCR:HC7	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1235:CLA:C12	21:F:6016:BCR:C31	2.90	0.49
3:C:5:VAL:CG2	3:C:65:VAL:HG21	2.35	0.49
3:C:7:ILE:C	3:C:8:TYR:O	2.50	0.49
4:D:105:ASP:HB2	4:D:151:LYS:HB2	1.94	0.49
5:E:127:GLU:C	5:E:128:VAL:CG2	2.77	0.49
19:H:1207:CLA:HBB2	9:I:13:GLY:O	2.11	0.49
11:K:127:ILE:CA	11:K:129:ALA:HA	2.40	0.49
22:K:7042:LMU:H5'	22:K:7042:LMU:C2B	2.41	0.49
12:L:124:GLU:O	12:L:124:GLU:HG3	2.13	0.49
13:N:90:GLU:OE1	13:N:91:TYR:CE2	2.65	0.49
13:N:147:SER:O	13:N:148:ASP:CG	2.50	0.49
22:R:7020:LMU:O2'	22:R:7020:LMU:H5'	2.12	0.49
15:1:207:ALA:C	15:1:209:PRO:CD	2.79	0.49
19:2:2002:CLA:C4C	19:2:2002:CLA:H42	2.42	0.49
17:3:197:SER:OG	17:3:205:GLY:C	2.50	0.49
1:A:130:GLU:OE1	1:A:130:GLU:O	2.29	0.49
1:A:267:THR:HG21	1:A:269:PHE:HE2	1.67	0.49
1:A:284:ARG:CZ	1:A:284:ARG:CA	2.88	0.49
1:A:539:PHE:HD2	1:A:539:PHE:O	1.95	0.49
19:A:1141:CLA:HMA2	19:A:1141:CLA:O2A	2.11	0.49
2:B:10:GLN:O	2:B:11:GLY:C	2.49	0.49
2:B:222:LEU:HB3	19:B:1212:CLA:CAD	2.43	0.49
3:C:17:CYS:SG	3:C:18:VAL:N	2.86	0.49
4:D:95:GLN:NE2	4:D:96:VAL:N	2.60	0.49
22:E:7048:LMU:O4'	22:F:7036:LMU:C6'	2.60	0.49
7:G:116:SER:OG	7:G:119:PRO:HG2	2.12	0.49
12:L:137:LEU:C	12:L:137:LEU:CD2	2.64	0.49
15:1:125:LEU:HD22	15:1:125:LEU:N	2.13	0.49
15:1:158:PRO:CD	15:1:159:GLU:H	2.24	0.49
17:3:99:ALA:C	17:3:101:GLY:N	2.64	0.49
17:3:164:LEU:HD12	17:3:164:LEU:C	2.33	0.49
18:4:174:GLN:C	18:4:195:ALA:H	2.15	0.49
1:A:159:THR:C	1:A:160:SER:OG	2.50	0.49
1:A:251:ASN:OD1	17:3:137:PHE:CD1	2.45	0.49
1:A:312:ILE:O	1:A:313:ALA:HB2	2.11	0.49
1:A:369:THR:HG21	1:A:402:ILE:CG2	2.42	0.49
1:A:372:VAL:HG22	19:A:1117:CLA:C4	2.42	0.49
1:A:432:LEU:O	1:A:435:VAL:N	2.45	0.49
1:A:462:ILE:HG21	19:A:1132:CLA:HMC3	1.95	0.49
1:A:673:SER:OG	2:B:445:ALA:O	2.16	0.49
19:A:1115:CLA:CB	19:A:1115:CLA:CMC	2.82	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1119:CLA:C9	21:A:6007:BCR:C37	2.53	0.49
2:B:123:TRP:CA	2:B:126:THR:HB	2.37	0.49
2:B:312:GLY:O	2:B:314:ARG:N	2.36	0.49
2:B:330:ILE:CD1	19:B:1202:CLA:H193	2.43	0.49
2:B:462:TRP:HZ3	19:B:1231:CLA:CBC	2.10	0.49
2:B:500:ALA:HB3	2:B:507:SER:O	2.13	0.49
19:B:1217:CLA:HBB2	7:G:74:LEU:HD22	1.94	0.49
19:B:1223:CLA:H41	19:B:1223:CLA:C7	2.32	0.49
4:D:105:ASP:HB2	4:D:151:LYS:CB	2.42	0.49
6:F:89:LYS:O	6:F:90:GLN:C	2.47	0.49
7:G:89:LYS:O	7:G:90:GLN:HB2	2.11	0.49
10:J:10:VAL:HG13	10:J:11:ALA:H	1.76	0.49
12:L:76:SER:O	12:L:78:LEU:N	2.45	0.49
13:N:150:LEU:O	13:N:151:ASP:CB	2.60	0.49
19:1:1008:CLA:H43	19:1:1008:CLA:CGA	2.42	0.49
16:2:211:PRO:O	16:2:212:GLN:HB3	2.11	0.49
17:3:204:GLY:C	17:3:206:PRO:HD2	2.33	0.49
22:4:7052:LMU:H12	22:4:7052:LMU:H52	1.93	0.49
1:A:401:TRP:HB3	19:A:1126:CLA:HMC3	1.94	0.49
1:A:598:VAL:O	1:A:598:VAL:HG12	2.13	0.49
19:A:1102:CLA:HBA2	19:A:1109:CLA:C6	2.41	0.49
2:B:172:GLU:C	2:B:176:ASN:HB2	2.29	0.49
2:B:396:ARG:HH11	19:B:1226:CLA:HED2	1.78	0.49
2:B:646:TRP:CZ2	2:B:726:ILE:HG21	2.48	0.49
19:B:1205:CLA:H71	19:B:1205:CLA:H2	1.95	0.49
19:B:1214:CLA:H12	19:B:1214:CLA:C1A	2.42	0.49
19:B:1229:CLA:HBB2	21:F:6014:BCR:H23C	1.94	0.49
4:D:206:GLN:O	4:D:208:TYR:N	2.45	0.49
7:G:62:LEU:HB3	7:G:65:SER:CB	2.16	0.49
7:G:89:LYS:CA	7:G:89:LYS:HZ1	2.19	0.49
8:H:99:LYS:O	8:H:102:ILE:N	2.42	0.49
22:H:7011:LMU:C6'	22:H:7011:LMU:C2B	2.90	0.49
12:L:164:LEU:HD13	12:L:165:THR:OG1	2.12	0.49
13:N:89:GLU:O	13:N:89:GLU:CD	2.51	0.49
13:N:133:GLY:CA	13:N:134:CYS:CB	2.89	0.49
15:1:157:ASP:OD1	15:1:157:ASP:O	2.29	0.49
16:2:182:ILE:HD13	16:2:190:GLY:CA	2.34	0.49
16:2:200:TRP:HB3	16:2:202:ASP:OD1	2.12	0.49
18:4:232:LEU:HB3	18:4:236:ILE:CD1	2.42	0.49
18:4:239:PRO:HD2	18:4:240:TRP:H	1.78	0.49
1:A:104:SER:C	1:A:106:TYR:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:O	1:A:126:ILE:HG13	2.11	0.49
1:A:385:LEU:O	1:A:386:ALA:HB3	2.12	0.49
1:A:503:THR:HB	19:A:1134:CLA:CBA	2.43	0.49
1:A:571:ASP:O	1:A:574:ASN:ND2	2.46	0.49
1:A:623:ASP:O	1:A:624:VAL:HB	2.12	0.49
21:A:6002:BCR:C12	21:A:6002:BCR:C34	2.84	0.49
2:B:131:THR:CG2	2:B:134:ASP:N	2.55	0.49
2:B:160:LYS:HG3	2:B:161:TRP:H	1.75	0.49
2:B:224:PRO:C	2:B:227:THR:CB	2.81	0.49
2:B:639:VAL:CG2	2:B:640:CYS:H	2.23	0.49
3:C:62:PHE:CE1	5:E:80:GLU:CG	2.93	0.49
7:G:76:ARG:HH11	7:G:120:VAL:HB	1.78	0.49
11:K:111:VAL:C	11:K:114:HIS:HB2	2.27	0.49
15:1:186:LYS:O	15:1:189:LYS:HG2	2.12	0.49
16:2:200:TRP:H	16:2:200:TRP:HD1	1.61	0.49
17:3:107:ARG:CZ	17:3:233:LEU:N	2.75	0.49
18:4:203:LYS:NZ	19:4:4002:CLA:CAD	2.71	0.49
1:A:88:ILE:O	1:A:92:TRP:HB2	2.13	0.49
1:A:216:LEU:HD12	21:A:6002:BCR:C35	2.43	0.49
1:A:218:TRP:HZ3	19:A:1112:CLA:HMB3	1.77	0.49
1:A:377:TYR:CD1	1:A:616:PHE:CE1	2.99	0.49
1:A:397:THR:HG21	1:A:613:ILE:CG1	2.41	0.49
1:A:446:LEU:CD2	1:A:554:LEU:HA	2.38	0.49
1:A:462:ILE:HD13	19:A:9022:CLA:H93	1.95	0.49
1:A:618:TRP:O	1:A:618:TRP:CD1	2.66	0.49
1:A:618:TRP:CH2	1:A:655:ASP:HB2	2.48	0.49
1:A:656:PHE:O	1:A:658:TRP:N	2.46	0.49
2:B:197:VAL:O	2:B:198:ALA:CB	2.60	0.49
2:B:270:LEU:HD12	2:B:271:THR:CA	2.43	0.49
2:B:311:PRO:HG3	19:B:1301:CLA:C4C	2.42	0.49
2:B:321:GLY:O	2:B:322:LEU:C	2.49	0.49
2:B:399:ASN:O	2:B:402:GLN:N	2.45	0.49
2:B:471:THR:O	2:B:472:TYR:C	2.48	0.49
2:B:618:GLY:CA	2:B:621:ARG:H	2.26	0.49
19:B:1205:CLA:CMC	21:B:6017:BCR:C28	2.91	0.49
3:C:29:ILE:HD11	4:D:180:GLY:O	2.12	0.49
3:C:39:ILE:O	3:C:40:ALA:CB	2.61	0.49
3:C:66:ARG:NH2	3:C:66:ARG:CB	2.75	0.49
22:E:7037:LMU:H5B	22:E:7037:LMU:O2B	2.12	0.49
6:F:204:SER:O	6:F:205:SER:C	2.51	0.49
6:F:224:GLY:O	6:F:226:LEU:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:11:LEU:CD1	21:I:6021:BCR:C10	2.81	0.49
12:L:52:PRO:O	12:L:53:THR:C	2.50	0.49
13:N:156:GLY:HA2	13:N:157:LYS:CD	2.38	0.49
13:N:156:GLY:CA	13:N:157:LYS:CE	2.91	0.49
15:1:97:ILE:HD12	15:1:98:LEU:CD2	2.32	0.49
16:2:218:ARG:HH12	19:2:2001:CLA:HBB2	1.78	0.49
17:3:206:PRO:HG2	17:3:208:PHE:CD2	2.47	0.49
19:3:2009:CLA:H92	19:3:2009:CLA:H52	0.60	0.49
1:A:23:ASP:OD1	1:A:24:ARG:CD	2.56	0.49
1:A:75:SER:CB	1:A:354:TRP:HZ2	2.24	0.49
1:A:89:ILE:O	1:A:93:LEU:CD2	2.61	0.49
1:A:110:LEU:C	1:A:113:PRO:HD3	2.32	0.49
1:A:184:PHE:CE2	19:A:1108:CLA:C2D	2.96	0.49
19:A:1126:CLA:H2A	19:A:1126:CLA:O1D	2.12	0.49
19:A:1138:CLA:HBC3	21:F:6014:BCR:H332	1.93	0.49
2:B:87:ILE:O	2:B:121:TYR:HE2	1.96	0.49
2:B:103:ALA:HB2	2:B:105:THR:O	2.13	0.49
2:B:129:LEU:CD1	19:B:1211:CLA:HMA2	2.43	0.49
2:B:216:LEU:HD21	2:B:221:GLY:CA	2.42	0.49
2:B:257:ILE:HG22	2:B:495:PRO:HG2	1.95	0.49
2:B:394:PHE:CE2	2:B:412:LEU:HD21	2.48	0.49
2:B:476:ILE:CG2	2:B:476:ILE:O	2.58	0.49
2:B:492:ILE:O	2:B:493:TRP:HB2	2.13	0.49
2:B:506:ASN:CG	2:B:506:ASN:O	2.51	0.49
2:B:527:LEU:HD23	19:B:1222:CLA:C1D	2.43	0.49
2:B:614:THR:HG23	2:B:614:THR:O	2.12	0.49
2:B:707:LEU:HD11	19:B:1226:CLA:C9	2.42	0.49
2:B:718:ILE:HD13	19:B:1224:CLA:HMC2	1.95	0.49
19:B:1222:CLA:HMB3	21:B:6010:BCR:H352	1.93	0.49
3:C:28:MET:HB3	4:D:176:LYS:O	2.13	0.49
3:C:73:THR:OG1	3:C:76:SER:OG	1.76	0.49
19:H:1145:CLA:H193	19:H:1145:CLA:C14	2.37	0.49
10:J:20:GLY:O	10:J:21:ALA:HB3	2.11	0.49
11:K:78:ARG:HB3	11:K:79:LYS:H	1.49	0.49
12:L:111:VAL:C	12:L:113:PRO:HD2	2.32	0.49
12:L:137:LEU:HD23	12:L:138:VAL:N	2.28	0.49
13:N:126:LYS:HZ3	13:N:126:LYS:HB3	1.77	0.49
15:1:73:PRO:CD	15:1:74:ALA:N	2.72	0.49
15:1:85:ILE:N	15:1:88:ARG:HG3	2.27	0.49
15:1:158:PRO:HA	15:1:175:LYS:CB	2.42	0.49
15:1:177:PRO:CD	15:1:180:LEU:CA	2.89	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:95:ASP:CB	17:3:85:ASP:OD2	2.50	0.49
16:2:149:THR:O	16:2:152:LEU:CD1	2.61	0.49
17:3:150:TYR:C	17:3:151:TRP:CD1	2.77	0.49
1:A:223:VAL:O	1:A:228:PRO:HD3	2.13	0.49
1:A:244:LEU:CD1	1:A:247:GLU:OE2	2.56	0.49
1:A:312:ILE:O	1:A:313:ALA:CB	2.60	0.49
1:A:355:HIS:O	1:A:358:LEU:HG	2.12	0.49
1:A:370:ILE:CD1	19:A:1124:CLA:C3D	2.90	0.49
1:A:487:VAL:CG1	1:A:489:ALA:N	2.55	0.49
1:A:705:GLU:CB	2:B:545:LYS:HZ2	2.26	0.49
1:A:740:LEU:CD2	19:A:1140:CLA:HMA1	2.41	0.49
19:A:1107:CLA:HBA2	19:A:1107:CLA:HBD	1.93	0.49
2:B:175:LEU:HD21	19:B:1216:CLA:HMA1	1.95	0.49
2:B:223:GLY:O	2:B:225:LEU:HB3	2.13	0.49
2:B:232:LEU:HD12	2:B:235:GLN:HG3	1.78	0.49
2:B:326:ILE:O	2:B:326:ILE:CG1	2.60	0.49
2:B:469:LYS:HG3	2:B:470:THR:OG1	2.12	0.49
2:B:622:ASP:CB	2:B:626:LEU:HG	2.40	0.49
6:F:149:ILE:HG22	6:F:151:SER:H	1.78	0.49
7:G:61:ALA:O	7:G:63:VAL:CG1	2.61	0.49
7:G:119:PRO:HB2	7:G:120:VAL:HG23	1.95	0.49
12:L:101:GLU:HG3	19:L:1501:CLA:C1A	2.43	0.49
13:N:127:PHE:HD1	13:N:128:PRO:HA	1.78	0.49
19:R:1144:CLA:HBA2	19:R:1144:CLA:HBD	1.95	0.49
15:1:84:LEU:N	15:1:84:LEU:HD12	2.28	0.49
15:1:204:GLN:HE21	19:1:1003:CLA:CBB	2.26	0.49
15:1:223:ASP:CB	15:1:224:PRO:HD2	2.43	0.49
16:2:149:THR:OG1	16:2:150:THR:N	2.46	0.49
16:2:182:ILE:HG21	16:2:187:LYS:HE2	1.95	0.49
19:2:2002:CLA:CHD	19:2:2002:CLA:CBC	2.90	0.49
17:3:171:ARG:O	17:3:172:ARG:C	2.49	0.49
17:3:206:PRO:CD	17:3:206:PRO:O	2.61	0.49
18:4:87:ASN:OD1	18:4:90:TRP:CD2	2.66	0.49
18:4:170:PRO:O	18:4:171:ILE:C	2.50	0.49
18:4:177:LEU:HD22	18:4:178:PRO:CB	2.43	0.49
18:4:177:LEU:CD2	18:4:178:PRO:N	2.68	0.49
18:4:202:GLU:HA	18:4:205:ILE:CG2	2.42	0.49
1:A:224:HIS:HE1	19:A:1113:CLA:CHD	2.26	0.49
1:A:226:SER:O	1:A:230:ASN:ND2	2.46	0.49
1:A:302:HIS:HE1	19:A:1117:CLA:C1B	2.25	0.49
1:A:532:ILE:O	1:A:532:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LEU:HD11	1:A:579:PHE:CB	2.40	0.49
1:A:628:ILE:CD1	1:A:629:ASN:O	2.61	0.49
1:A:723:ARG:H	19:A:1139:CLA:CBB	2.17	0.49
19:A:1138:CLA:H52	19:A:1138:CLA:NC	2.27	0.49
19:A:1138:CLA:CMD	21:F:6014:BCR:HC41	2.36	0.49
19:A:9022:CLA:H71	19:A:9022:CLA:C12	2.41	0.49
19:A:9022:CLA:H142	19:B:1206:CLA:HBB2	1.94	0.49
2:B:120:VAL:O	2:B:123:TRP:CD1	2.64	0.49
2:B:549:ASP:HB2	3:C:63:LEU:HD12	1.95	0.49
2:B:590:VAL:O	2:B:593:TYR:HB3	2.13	0.49
2:B:649:MET:SD	2:B:723:ALA:HB2	2.53	0.49
19:B:1221:CLA:CMB	19:B:1223:CLA:H92	2.43	0.49
6:F:199:ASP:CA	10:J:9:SER:HA	2.42	0.49
7:G:83:GLN:OE1	19:G:1242:CLA:C2D	2.60	0.49
8:H:98:LEU:O	8:H:99:LYS:O	2.30	0.49
11:K:63:LEU:O	11:K:64:MET:C	2.50	0.49
12:L:54:TYR:CD1	12:L:57:ILE:HG23	2.47	0.49
12:L:81:TRP:C	12:L:83:LEU:H	2.17	0.49
13:N:148:ASP:H	13:N:149:ASP:CA	2.26	0.49
13:N:164:SER:CA	13:N:165:ASN:C	2.77	0.49
15:1:158:PRO:CD	15:1:159:GLU:N	2.76	0.49
16:2:125:PHE:CA	16:2:127:THR:CG2	2.60	0.49
17:3:157:LEU:O	17:3:160:LEU:HB3	2.12	0.49
17:3:167:PHE:O	17:3:168:ALA:C	2.50	0.49
18:4:112:PRO:CA	18:4:117:SER:OG	2.61	0.49
1:A:39:HIS:HA	1:A:44:ILE:CG2	2.43	0.48
1:A:246:HIS:NE2	19:3:1147:CLA:O1D	2.46	0.48
1:A:366:GLY:O	1:A:403:GLY:HA2	2.13	0.48
1:A:378:SER:OG	1:A:512:SER:OG	2.29	0.48
1:A:412:ALA:O	1:A:415:ALA:HB3	2.13	0.48
1:A:423:ASP:H	1:A:424:PRO:HD3	1.76	0.48
1:A:488:PHE:CD1	1:A:535:GLY:N	2.81	0.48
19:A:1131:CLA:H101	19:A:1131:CLA:H143	1.94	0.48
19:A:1132:CLA:O1D	12:L:119:PRO:O	2.31	0.48
2:B:85:ARG:HG2	2:B:85:ARG:NH1	2.04	0.48
2:B:143:LEU:C	2:B:145:LEU:N	2.66	0.48
2:B:421:HIS:O	19:B:1236:CLA:HMC3	2.13	0.48
2:B:427:LEU:HB3	19:B:1229:CLA:HED1	1.95	0.48
2:B:438:VAL:O	2:B:442:VAL:N	2.44	0.48
2:B:454:LEU:HD13	2:B:514:PRO:CG	2.43	0.48
2:B:507:SER:O	2:B:508:LEU:CB	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:657:TRP:O	2:B:660:GLY:N	2.34	0.48
19:B:1225:CLA:H62	21:B:6006:BCR:C32	2.42	0.48
19:F:1302:CLA:C3B	19:F:1305:CLA:HAC2	2.41	0.48
7:G:99:HIS:O	7:G:101:GLU:CA	2.61	0.48
7:G:116:SER:OG	7:G:119:PRO:HB2	2.13	0.48
22:G:7026:LMU:H3'	22:G:7026:LMU:H11	1.94	0.48
19:J:1311:CLA:O1A	19:J:1311:CLA:C14	2.59	0.48
13:N:146:LEU:HD21	13:N:148:ASP:O	2.12	0.48
15:1:85:ILE:CA	15:1:88:ARG:CG	2.72	0.48
21:1:6023:BCR:HC8	21:1:6023:BCR:C2	2.42	0.48
16:2:153:PHE:CD2	16:2:157:LEU:CD2	2.96	0.48
16:2:226:ARG:CG	16:2:226:ARG:NH1	2.67	0.48
17:3:100:TYR:HA	17:3:229:LYS:HE2	1.94	0.48
17:3:182:MET:HG2	17:3:183:GLY:N	2.28	0.48
17:3:238:ILE:HD12	19:3:3003:CLA:HMC2	1.87	0.48
18:4:107:ALA:O	18:4:110:LEU:HB3	2.13	0.48
1:A:258:LEU:HG	1:A:280:PHE:CD1	2.47	0.48
1:A:439:ARG:HG2	1:A:562:PHE:CE2	2.47	0.48
1:A:464:ASN:O	1:A:468:SER:N	2.42	0.48
1:A:552:THR:O	1:A:553:VAL:HB	2.13	0.48
1:A:618:TRP:HB2	1:A:656:PHE:CE1	2.48	0.48
1:A:679:PHE:O	1:A:683:HIS:CB	2.61	0.48
19:A:1123:CLA:HMD2	19:A:1123:CLA:C14	2.41	0.48
19:A:1151:CLA:CED	19:A:1151:CLA:CBA	2.91	0.48
19:A:1237:CLA:HMD2	21:B:6017:BCR:H313	1.95	0.48
19:A:9022:CLA:CAD	19:B:9010:CLA:HMB3	2.42	0.48
2:B:4:ARG:CZ	2:B:4:ARG:O	2.60	0.48
2:B:317:ARG:HH12	2:B:410:ARG:HG2	1.75	0.48
5:E:83:TRP:CH2	5:E:116:SER:OG	2.63	0.48
7:G:100:PHE:O	7:G:100:PHE:HD2	1.96	0.48
7:G:120:VAL:O	7:G:120:VAL:CG1	2.57	0.48
10:J:14:VAL:O	10:J:14:VAL:CG1	2.59	0.48
16:2:150:THR:C	16:2:152:LEU:HD13	2.33	0.48
16:2:189:THR:O	16:2:190:GLY:C	2.50	0.48
17:3:108:PHE:CD2	19:3:3013:CLA:H43	2.48	0.48
18:4:123:VAL:O	18:4:123:VAL:HG22	2.13	0.48
18:4:239:PRO:HD2	18:4:240:TRP:N	2.28	0.48
1:A:39:HIS:O	1:A:40:PHE:HB3	2.12	0.48
1:A:309:LEU:HA	1:A:312:ILE:O	2.13	0.48
1:A:350:LEU:HA	1:A:350:LEU:HD23	1.37	0.48
1:A:382:TYR:HB2	1:A:385:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ALA:HA	1:A:444:SER:HB3	1.95	0.48
1:A:482:ILE:O	1:A:482:ILE:HG23	2.13	0.48
1:A:665:ILE:HD13	2:B:621:ARG:HG3	1.95	0.48
19:A:1139:CLA:O1A	19:A:1139:CLA:C3	2.62	0.48
21:A:6007:BCR:C23	21:A:6007:BCR:C38	2.85	0.48
2:B:70:TRP:CB	2:B:136:TYR:HH	2.25	0.48
2:B:165:VAL:O	2:B:166:SER:C	2.50	0.48
2:B:361:ILE:O	2:B:362:ALA:O	2.31	0.48
2:B:373:THR:O	2:B:377:TYR:N	2.36	0.48
2:B:404:ALA:O	2:B:405:ASP:OD1	2.30	0.48
19:B:1218:CLA:HMA3	19:B:1219:CLA:C3D	2.43	0.48
19:B:1222:CLA:HED1	19:B:1223:CLA:HMD2	1.95	0.48
3:C:43:PRO:HA	4:D:182:GLN:CG	2.43	0.48
4:D:140:LEU:CB	4:D:143:ARG:HB2	2.40	0.48
6:F:78:ASP:OD1	6:F:154:GLN:NE2	2.39	0.48
6:F:220:GLU:HG3	6:F:220:GLU:O	2.13	0.48
10:J:21:ALA:O	10:J:23:ALA:N	2.46	0.48
11:K:115:ILE:CG1	11:K:122:LEU:HD12	2.43	0.48
12:L:205:TYR:O	12:L:205:TYR:CG	2.65	0.48
15:1:199:VAL:HG12	15:1:200:GLY:N	2.28	0.48
16:2:122:ILE:CD1	19:2:2002:CLA:HMB1	2.42	0.48
17:3:205:GLY:H	17:3:206:PRO:HD2	1.76	0.48
18:4:179:ALA:O	18:4:180:GLY:C	2.49	0.48
1:A:249:ILE:HG23	17:3:137:PHE:CE2	2.49	0.48
1:A:250:LEU:H	17:3:136:TRP:HH2	1.60	0.48
1:A:370:ILE:HD11	19:A:1124:CLA:CAD	2.41	0.48
1:A:420:ARG:CZ	1:A:420:ARG:CB	2.91	0.48
1:A:619:LYS:O	1:A:621:GLN:N	2.46	0.48
19:A:1103:CLA:H141	19:A:1103:CLA:H161	1.68	0.48
19:A:1122:CLA:ND	21:A:6007:BCR:H19C	2.27	0.48
19:A:1128:CLA:H192	21:A:6011:BCR:H20C	1.95	0.48
2:B:98:GLN:HB2	2:B:99:PRO:HD2	1.96	0.48
2:B:314:ARG:CZ	15:1:67:LEU:CD2	2.77	0.48
2:B:560:ASP:CG	3:C:66:ARG:CZ	2.81	0.48
2:B:666:SER:CB	2:B:671:TRP:HE1	2.13	0.48
2:B:707:LEU:HD13	24:B:7101:LMG:H301	1.96	0.48
19:B:1202:CLA:HAC1	19:B:1226:CLA:HMA1	1.94	0.48
19:B:1231:CLA:HMC3	19:B:1234:CLA:H2	1.94	0.48
19:B:1234:CLA:HBC3	19:B:1234:CLA:CMC	2.35	0.48
4:D:173:TYR:O	4:D:173:TYR:CG	2.62	0.48
9:I:19:VAL:O	9:I:23:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:21:ALA:O	10:J:22:LEU:C	2.51	0.48
11:K:125:LYS:CG	11:K:128:GLY:HA2	2.43	0.48
13:N:110:THR:O	13:N:112:ALA:O	2.31	0.48
13:N:147:SER:O	13:N:151:ASP:CG	2.52	0.48
15:1:223:ASP:O	15:1:225:TRP:HB2	2.13	0.48
16:2:160:ILE:CB	19:2:2012:CLA:HBB1	2.37	0.48
16:2:169:ALA:O	16:2:170:ASP:HB3	2.13	0.48
16:2:184:PRO:N	16:2:187:LYS:HD2	2.28	0.48
18:4:206:ALA:C	18:4:208:GLY:N	2.66	0.48
1:A:130:GLU:OE1	1:A:133:ASN:HB3	2.13	0.48
1:A:502:THR:CB	1:A:504:ALA:H	2.25	0.48
1:A:681:GLY:C	1:A:683:HIS:H	2.16	0.48
1:A:733:VAL:HG21	19:A:1140:CLA:HMD3	1.94	0.48
19:A:1119:CLA:H162	21:A:6008:BCR:H271	1.96	0.48
19:A:1128:CLA:HBD	19:A:1128:CLA:HAA1	1.96	0.48
19:A:1138:CLA:HBC3	19:A:1138:CLA:HHD	1.96	0.48
2:B:230:TRP:CE3	19:B:1213:CLA:HAA2	2.49	0.48
2:B:374:HIS:HB2	19:B:1224:CLA:C4B	2.42	0.48
2:B:560:ASP:CG	2:B:561:GLY:N	2.66	0.48
2:B:697:PRO:CG	19:B:1238:CLA:HBC3	2.44	0.48
3:C:7:ILE:HG21	3:C:54:CYS:SG	2.54	0.48
6:F:83:THR:CB	6:F:84:PRO:CD	2.91	0.48
6:F:230:ASN:C	6:F:231:PHE:O	2.51	0.48
7:G:84:ARG:NH1	7:G:89:LYS:H	2.11	0.48
8:H:113:SER:OG	19:H:1207:CLA:H2	2.12	0.48
22:K:7042:LMU:H71	22:K:7042:LMU:C2	2.43	0.48
13:N:139:LYS:O	13:N:140:GLN:C	2.51	0.48
13:N:143:VAL:HG11	13:N:155:GLU:OE1	2.14	0.48
15:1:68:GLY:HA2	15:1:72:VAL:HB	1.93	0.48
15:1:83:GLU:OE2	15:1:83:GLU:CA	2.55	0.48
15:1:163:TYR:N	15:1:164:PRO:CD	2.76	0.48
16:2:145:TYR:C	16:2:146:PHE:CD1	2.87	0.48
18:4:169:ASP:HA	18:4:173:LYS:C	2.33	0.48
18:4:207:ASN:ND2	19:4:4002:CLA:C1A	2.72	0.48
1:A:73:GLU:O	1:A:76:ARG:HB2	2.14	0.48
1:A:182:GLY:C	19:A:1109:CLA:HAC1	2.33	0.48
1:A:282:THR:O	1:A:283:PHE:C	2.52	0.48
1:A:390:ALA:HA	1:A:393:LEU:CD2	2.44	0.48
1:A:680:LEU:HD21	2:B:617:MET:CE	2.43	0.48
1:A:691:MET:CE	20:A:5001:PQN:H2M2	2.44	0.48
19:A:1119:CLA:HAA2	19:A:1123:CLA:HBB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1140:CLA:H102	19:A:9013:CLA:H152	1.95	0.48
2:B:22:TRP:HE1	19:B:1238:CLA:CAB	2.17	0.48
2:B:138:GLY:O	2:B:139:ALA:C	2.50	0.48
2:B:620:LEU:O	2:B:621:ARG:C	2.50	0.48
2:B:709:GLY:O	2:B:710:LEU:CB	2.59	0.48
19:B:1214:CLA:H112	19:B:1232:CLA:H3A	1.96	0.48
3:C:61:ASP:CG	5:E:118:ASN:HD21	2.14	0.48
3:C:73:THR:HG23	3:C:76:SER:CB	2.42	0.48
4:D:123:ARG:NH2	22:D:7050:LMU:H4B	1.98	0.48
4:D:148:TYR:C	4:D:148:TYR:CD2	2.86	0.48
7:G:73:PHE:O	7:G:76:ARG:CB	2.56	0.48
7:G:89:LYS:C	7:G:90:GLN:HG2	2.34	0.48
7:G:98:THR:OG1	7:G:100:PHE:N	2.47	0.48
8:H:111:TYR:CD1	8:H:112:LEU:HD23	2.48	0.48
12:L:148:TYR:C	12:L:150:ILE:H	2.16	0.48
13:N:118:TYR:C	13:N:119:THR:OG1	2.52	0.48
13:N:144:PRO:C	13:N:151:ASP:OD1	2.52	0.48
22:R:7020:LMU:H6E	22:R:7020:LMU:C6B	2.42	0.48
15:1:58:ALA:CB	19:1:1015:CLA:C2B	2.91	0.48
19:1:1007:CLA:HAA1	22:4:7008:LMU:O3'	2.13	0.48
22:1:7013:LMU:O6B	22:1:7013:LMU:C1B	2.58	0.48
1:A:87:SER:HB3	1:A:178:MET:O	2.14	0.48
1:A:98:PHE:O	1:A:100:GLY:CA	2.62	0.48
1:A:402:ILE:HD11	19:A:1127:CLA:CBB	2.44	0.48
1:A:462:ILE:HG21	19:A:1132:CLA:CMC	2.43	0.48
19:A:1105:CLA:CGA	19:A:1107:CLA:H12	2.43	0.48
19:A:1133:CLA:C2B	21:A:6008:BCR:H333	2.44	0.48
19:A:9011:CLA:CBB	19:A:9012:CLA:HED1	2.43	0.48
2:B:98:GLN:CB	2:B:99:PRO:HD2	2.44	0.48
2:B:103:ALA:HA	2:B:105:THR:CA	2.43	0.48
2:B:103:ALA:CB	2:B:105:THR:O	2.61	0.48
2:B:131:THR:C	2:B:135:LEU:CD2	2.80	0.48
2:B:183:PHE:HE1	19:B:1210:CLA:H71	1.79	0.48
2:B:305:LEU:HD23	19:B:1220:CLA:O1D	2.14	0.48
2:B:326:ILE:HG13	2:B:332:PHE:HB3	1.96	0.48
2:B:389:HIS:HE1	19:B:1226:CLA:NC	2.11	0.48
2:B:436:LEU:O	2:B:437:TYR:CB	2.61	0.48
2:B:559:CYS:SG	2:B:560:ASP:N	2.86	0.48
2:B:649:MET:CE	21:B:6017:BCR:H272	2.44	0.48
19:B:1202:CLA:H43	21:B:6005:BCR:C31	2.38	0.48
19:B:1224:CLA:O1D	19:B:1225:CLA:CMA	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:SER:CA	12:L:69:LEU:HD21	2.43	0.48
8:H:86:THR:HG23	8:H:89:ALA:HB2	1.94	0.48
11:K:116:ILE:CG2	11:K:117:GLY:H	2.26	0.48
19:L:1502:CLA:HBC3	19:L:1502:CLA:CMC	2.44	0.48
13:N:139:LYS:CG	13:N:142:LYS:HE2	2.41	0.48
13:N:155:GLU:OE2	13:N:157:LYS:O	2.32	0.48
15:1:74:ALA:HB3	15:1:75:ASN:CG	2.34	0.48
16:2:157:LEU:HD12	16:2:157:LEU:HA	1.59	0.48
16:2:233:MET:SD	16:2:236:TRP:CD1	3.07	0.48
17:3:191:GLU:O	17:3:192:LYS:CD	2.62	0.48
18:4:168:GLN:O	18:4:172:PHE:CD1	2.66	0.48
18:4:209:ARG:O	18:4:212:LEU:CA	2.61	0.48
1:A:93:LEU:H	1:A:96:MET:H	1.60	0.48
1:A:188:LYS:O	1:A:188:LYS:HD2	2.14	0.48
1:A:281:LEU:CB	19:A:1115:CLA:HED2	2.44	0.48
1:A:316:MET:CA	1:A:317:TYR:HD1	2.27	0.48
1:A:316:MET:HA	1:A:317:TYR:HD1	1.79	0.48
1:A:547:PHE:HE2	19:A:9023:CLA:O1A	1.97	0.48
1:A:690:LEU:HD21	2:B:661:PHE:HE1	1.78	0.48
19:A:1110:CLA:C4D	19:A:1111:CLA:HMC3	2.43	0.48
19:A:9023:CLA:HMC1	19:A:9023:CLA:HBC2	1.96	0.48
2:B:7:ARG:NH1	2:B:7:ARG:CB	2.69	0.48
2:B:382:ILE:HD11	19:B:1203:CLA:H142	1.95	0.48
2:B:493:TRP:HB2	19:B:1232:CLA:HED2	1.96	0.48
3:C:1:MET:SD	3:C:4:SER:CB	3.02	0.48
3:C:66:ARG:HB3	3:C:66:ARG:CZ	2.44	0.48
6:F:82:LEU:HG	6:F:83:THR:OG1	2.14	0.48
6:F:142:SER:C	6:F:144:GLY:H	2.17	0.48
11:K:48:PHE:HB2	11:K:50:GLY:H	1.79	0.48
19:K:1142:CLA:HBD	19:K:1142:CLA:HAA2	1.94	0.48
13:N:133:GLY:CA	13:N:134:CYS:HB2	2.44	0.48
13:N:148:ASP:N	13:N:149:ASP:CA	2.76	0.48
13:N:157:LYS:CB	13:N:159:LYS:N	2.57	0.48
22:N:7049:LMU:O1'	22:N:7049:LMU:C4	2.61	0.48
15:1:189:LYS:N	15:1:189:LYS:CE	2.77	0.48
16:2:229:MET:CE	16:2:230:LEU:HD13	2.43	0.48
18:4:243:THR:CG2	18:4:244:ILE:O	2.53	0.48
1:A:249:ILE:HG22	17:3:137:PHE:CE2	2.49	0.48
1:A:390:ALA:CB	1:A:754:ILE:HD13	2.43	0.48
19:A:1119:CLA:H43	19:A:1122:CLA:H2	1.96	0.48
19:A:1136:CLA:H71	19:A:1136:CLA:H112	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1140:CLA:H62	19:A:9013:CLA:H171	1.96	0.48
19:A:9011:CLA:C1A	19:B:9010:CLA:HBB2	2.44	0.48
2:B:62:SER:OG	2:B:63:GLY:N	2.47	0.48
2:B:405:ASP:C	2:B:405:ASP:OD1	2.52	0.48
2:B:500:ALA:CB	2:B:503:GLU:OE2	2.60	0.48
2:B:594:TRP:CD2	2:B:598:HIS:CE1	3.02	0.48
2:B:685:THR:O	2:B:685:THR:HG22	2.14	0.48
22:B:7038:LMU:O6'	22:B:7038:LMU:C1B	2.62	0.48
3:C:36:ALA:C	3:C:37:LYS:HG2	2.34	0.48
4:D:165:TYR:CD2	4:D:168:PRO:HG2	2.49	0.48
6:F:194:LYS:N	6:F:195:GLU:OE2	2.47	0.48
6:F:204:SER:O	6:F:207:LEU:HB3	2.14	0.48
11:K:125:LYS:CD	11:K:128:GLY:HA2	2.44	0.48
19:L:1148:CLA:HED3	19:L:1148:CLA:H72	1.96	0.48
13:N:132:THR:CB	13:N:137:LEU:O	2.62	0.48
14:R:38:UNK:O	14:R:39:UNK:C	2.62	0.48
15:1:77:GLU:CG	15:1:80:LYS:CD	2.78	0.48
15:1:92:LEU:N	15:1:95:PRO:HD3	2.26	0.48
15:1:162:LYS:CG	15:1:163:TYR:H	2.24	0.48
16:2:128:LYS:HB3	16:2:131:ILE:CG1	2.35	0.48
16:2:184:PRO:CG	16:2:185:ASN:N	2.77	0.48
18:4:131:LYS:CD	18:4:131:LYS:N	2.69	0.48
18:4:177:LEU:CD1	18:4:178:PRO:CD	2.59	0.48
22:4:7019:LMU:H32	22:4:7019:LMU:O2'	2.13	0.48
1:A:316:MET:CA	1:A:317:TYR:CB	2.91	0.48
1:A:348:GLU:O	1:A:349:ILE:C	2.52	0.48
1:A:358:LEU:O	1:A:361:ASN:HB3	2.14	0.48
1:A:426:THR:HG23	1:A:428:TYR:CE2	2.45	0.48
1:A:493:GLN:HG2	1:A:516:GLY:H	1.79	0.48
1:A:588:GLY:N	2:B:668:ARG:NH1	2.60	0.48
1:A:664:VAL:HG23	1:A:665:ILE:HG23	1.95	0.48
1:A:701:GLN:NE2	1:A:724:ALA:H	2.12	0.48
1:A:733:VAL:HG22	19:A:1140:CLA:CAD	2.43	0.48
19:A:1112:CLA:CBA	19:3:1147:CLA:HMC3	2.42	0.48
2:B:172:GLU:OE1	2:B:301:ILE:HG13	2.14	0.48
2:B:416:GLU:CD	2:B:416:GLU:H	2.16	0.48
2:B:469:LYS:C	2:B:501:ILE:CA	2.68	0.48
2:B:618:GLY:HA2	2:B:621:ARG:CB	2.40	0.48
19:B:1231:CLA:HMB3	19:B:1234:CLA:HED3	1.96	0.48
6:F:207:LEU:HD13	6:F:207:LEU:N	2.28	0.48
7:G:80:PHE:CE1	7:G:83:GLN:O	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:85:ASN:O	12:L:92:ALA:CB	2.55	0.48
13:N:96:LYS:HG3	13:N:97:THR:HG1	1.75	0.48
13:N:133:GLY:HA2	13:N:134:CYS:HB2	1.96	0.48
15:1:94:VAL:O	15:1:98:LEU:HB2	2.14	0.48
19:2:2001:CLA:HBA2	19:2:2001:CLA:H3A	1.67	0.48
17:3:96:ARG:NH1	17:3:100:TYR:OH	2.43	0.48
1:A:63:ASP:CA	19:A:1128:CLA:HED2	2.43	0.47
1:A:70:ASP:C	1:A:72:GLU:HG2	2.34	0.47
1:A:93:LEU:CA	1:A:96:MET:N	2.69	0.47
1:A:211:LEU:HB3	1:A:310:PHE:CD2	2.49	0.47
1:A:545:HIS:ND1	19:A:1135:CLA:CBB	2.76	0.47
19:A:1124:CLA:H43	19:A:1136:CLA:CBA	2.39	0.47
19:A:1126:CLA:C7	21:A:6011:BCR:H371	2.44	0.47
19:A:1128:CLA:H152	19:A:1128:CLA:H101	1.96	0.47
19:A:9022:CLA:OBD	19:B:9010:CLA:HMB3	2.14	0.47
2:B:377:TYR:O	2:B:378:ILE:HB	2.14	0.47
2:B:542:ARG:CG	2:B:542:ARG:NH1	2.41	0.47
2:B:586:THR:C	2:B:588:GLY:N	2.56	0.47
2:B:658:ALA:O	2:B:661:PHE:HD2	1.96	0.47
4:D:97:GLU:HB2	4:D:98:GLU:HG2	1.96	0.47
4:D:149:LYS:HE3	4:D:149:LYS:HB3	1.28	0.47
6:F:121:ALA:HB1	6:F:125:LYS:HB3	1.95	0.47
6:F:208:PHE:O	6:F:209:ARG:C	2.48	0.47
8:H:81:SER:O	8:H:83:LEU:HD22	2.14	0.47
19:H:1145:CLA:HAA1	19:H:1145:CLA:HED2	1.93	0.47
19:K:1143:CLA:HAC2	22:K:7001:LMU:H3O1	1.66	0.47
12:L:112:GLY:C	19:L:1503:CLA:HMC3	2.34	0.47
13:N:132:THR:CB	13:N:139:LYS:CD	2.90	0.47
15:1:93:ALA:CA	19:1:1006:CLA:C4B	2.91	0.47
15:1:114:TRP:HH2	15:1:121:GLN:CA	2.27	0.47
19:1:1303:CLA:HMC1	19:4:1304:CLA:CMB	2.40	0.47
16:2:128:LYS:HD2	16:2:128:LYS:HA	1.61	0.47
18:4:142:PHE:O	18:4:143:VAL:C	2.51	0.47
18:4:169:ASP:OD1	18:4:174:GLN:CA	2.62	0.47
18:4:177:LEU:HD13	18:4:178:PRO:HD2	1.95	0.47
18:4:209:ARG:HA	18:4:212:LEU:HD12	1.95	0.47
22:4:7034:LMU:C11	22:4:7052:LMU:O3'	2.61	0.47
1:A:122:VAL:O	19:A:1105:CLA:HED2	2.14	0.47
1:A:252:ARG:O	1:A:252:ARG:CZ	2.62	0.47
1:A:258:LEU:O	1:A:259:TYR:HD2	1.96	0.47
1:A:261:SER:C	1:A:263:ALA:N	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:TRP:CZ3	1:A:728:VAL:HG13	2.50	0.47
19:A:1106:CLA:ND	19:A:1126:CLA:H42	2.29	0.47
19:A:1117:CLA:HBC1	21:A:6003:BCR:H12C	1.96	0.47
2:B:167:TRP:CZ2	19:B:1210:CLA:CAC	2.97	0.47
2:B:203:ARG:O	2:B:245:GLY:C	2.53	0.47
2:B:495:PRO:HD2	2:B:497:TRP:HB2	1.95	0.47
2:B:607:SER:HA	2:B:610:ASN:ND2	2.29	0.47
2:B:668:ARG:CG	2:B:699:ALA:O	2.62	0.47
19:B:1214:CLA:H8	19:B:1232:CLA:HMA1	1.96	0.47
19:B:1227:CLA:H3A	19:B:1227:CLA:HBA2	1.50	0.47
3:C:11:CYS:SG	23:C:8003:SF4:S3	3.12	0.47
12:L:52:PRO:HB2	12:L:55:GLN:C	2.32	0.47
12:L:79:ILE:HD12	19:L:1504:CLA:HMA2	1.95	0.47
12:L:161:ALA:N	12:L:162:PRO:CD	2.77	0.47
15:1:58:ALA:HB3	15:1:59:PRO:HD3	1.96	0.47
15:1:145:ILE:O	15:1:148:VAL:HG13	2.14	0.47
16:2:184:PRO:CD	16:2:185:ASN:HA	2.44	0.47
18:4:138:SER:O	18:4:139:SER:CB	2.61	0.47
18:4:225:GLY:HA2	18:4:226:LYS:NZ	2.24	0.47
1:A:50:THR:HG22	1:A:52:THR:N	2.27	0.47
1:A:64:PHE:CG	1:A:74:ILE:HD13	2.49	0.47
1:A:91:LEU:O	19:A:1105:CLA:HMC3	2.13	0.47
1:A:220:ARG:O	1:A:221:HIS:CB	2.62	0.47
1:A:350:LEU:O	1:A:350:LEU:HD22	2.14	0.47
1:A:362:LEU:HG	1:A:406:LEU:HG	1.96	0.47
1:A:438:HIS:HB2	1:A:441:ALA:CB	2.44	0.47
1:A:651:GLY:O	1:A:655:ASP:N	2.41	0.47
1:A:653:LEU:HD13	19:B:9010:CLA:HBC2	1.96	0.47
1:A:697:ARG:C	1:A:699:TYR:H	2.17	0.47
2:B:19:ARG:O	2:B:23:PHE:HB2	2.15	0.47
2:B:55:ALA:HB1	2:B:150:LEU:HD12	1.97	0.47
2:B:183:PHE:HB3	2:B:284:PHE:CD2	2.48	0.47
2:B:198:ALA:H	2:B:200:PRO:HG2	1.80	0.47
2:B:292:ARG:HH12	2:B:295:PHE:N	2.13	0.47
2:B:469:LYS:C	2:B:501:ILE:HA	2.34	0.47
2:B:587:ILE:HA	2:B:587:ILE:HD13	1.72	0.47
19:B:1206:CLA:HAA1	19:B:1206:CLA:H12	1.97	0.47
21:B:6006:BCR:HC8	21:B:6006:BCR:C33	2.39	0.47
6:F:85:CYS:O	6:F:86:LYS:C	2.52	0.47
6:F:99:LEU:O	6:F:102:LEU:CG	2.30	0.47
6:F:127:LYS:O	6:F:129:ARG:CA	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:ASP:N	11:K:51:SER:CB	2.77	0.47
11:K:75:SER:O	11:K:76:ALA:CB	2.61	0.47
12:L:83:LEU:HD13	12:L:88:ALA:CB	2.44	0.47
12:L:209:LEU:CG	12:L:210:PRO:CD	2.92	0.47
13:N:120:VAL:HG12	13:N:122:PHE:CD2	2.49	0.47
16:2:168:TRP:NE1	16:2:171:ILE:HG21	2.21	0.47
16:2:212:GLN:CG	16:2:213:LYS:N	2.74	0.47
18:4:214:PHE:O	18:4:215:LEU:O	2.32	0.47
1:A:27:ILE:O	1:A:28:LYS:CD	2.62	0.47
1:A:44:ILE:HG22	1:A:45:ALA:H	1.79	0.47
1:A:126:ILE:CD1	19:A:1107:CLA:CMA	2.86	0.47
1:A:349:ILE:O	1:A:351:THR:N	2.47	0.47
1:A:405:PHE:O	19:A:1128:CLA:HMC1	2.15	0.47
1:A:483:GLN:CB	1:A:485:GLN:CD	2.79	0.47
1:A:619:LYS:HG2	1:A:642:PHE:CE1	2.50	0.47
1:A:629:ASN:CG	1:A:630:ASP:N	2.68	0.47
19:A:1126:CLA:HBD	19:A:1126:CLA:HAA1	1.95	0.47
2:B:98:GLN:CB	2:B:99:PRO:CD	2.92	0.47
2:B:130:ARG:NH1	2:B:130:ARG:CG	2.71	0.47
2:B:375:HIS:CE1	19:B:1225:CLA:NC	2.82	0.47
2:B:693:TRP:HD1	19:B:1238:CLA:C3D	2.27	0.47
4:D:132:ALA:HB3	4:D:136:GLN:NE2	2.21	0.47
6:F:192:THR:O	6:F:193:GLN:HG3	2.14	0.47
19:H:1145:CLA:HAA1	19:H:1145:CLA:HED1	1.96	0.47
19:J:1311:CLA:C15	19:2:2014:CLA:HMB1	2.43	0.47
12:L:91:THR:HA	12:L:98:ARG:NH1	2.22	0.47
12:L:143:LEU:N	12:L:145:LEU:N	2.60	0.47
12:L:181:GLY:O	12:L:184:LYS:HG2	2.14	0.47
13:N:157:LYS:HG2	13:N:159:LYS:CG	2.44	0.47
16:2:261:THR:C	16:2:262:ILE:HG23	2.35	0.47
17:3:124:LYS:CG	17:3:124:LYS:O	2.62	0.47
17:3:159:VAL:O	17:3:161:GLU:C	2.53	0.47
18:4:176:SER:OG	18:4:177:LEU:HD13	2.14	0.47
1:A:73:GLU:O	1:A:76:ARG:CB	2.62	0.47
1:A:130:GLU:O	1:A:131:ILE:C	2.51	0.47
1:A:143:ILE:HG23	1:A:143:ILE:HD12	1.64	0.47
1:A:304:LEU:CD1	19:A:1115:CLA:CBB	2.93	0.47
1:A:330:ILE:O	1:A:330:ILE:HG22	2.13	0.47
1:A:454:GLY:N	1:A:457:SER:HB3	2.07	0.47
19:A:1102:CLA:H12	19:A:1109:CLA:C6	2.20	0.47
19:A:1106:CLA:ND	19:A:1126:CLA:C4	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1138:CLA:HBB1	19:A:1138:CLA:H122	1.97	0.47
19:A:1237:CLA:HMB2	19:L:1502:CLA:CBC	2.42	0.47
19:A:9012:CLA:H152	19:A:9012:CLA:H101	1.94	0.47
2:B:73:ASN:ND2	2:B:73:ASN:N	2.61	0.47
2:B:157:LEU:HB3	2:B:158:GLN:HG2	1.96	0.47
2:B:224:PRO:CB	2:B:227:THR:OG1	2.62	0.47
2:B:365:PHE:HD1	2:B:602:TRP:NE1	2.12	0.47
2:B:544:SER:O	2:B:546:LEU:N	2.48	0.47
6:F:97:GLN:O	6:F:99:LEU:N	2.47	0.47
6:F:185:ILE:O	6:F:186:ARG:CG	2.37	0.47
8:H:120:ILE:O	8:H:121:LEU:O	2.31	0.47
9:I:4:LEU:HG	9:I:4:LEU:O	2.15	0.47
12:L:59:PRO:O	12:L:60:ILE:HB	2.14	0.47
22:R:7014:LMU:H1B	22:R:7014:LMU:H3'	1.27	0.47
16:2:123:PRO:O	16:2:124:GLU:C	2.50	0.47
18:4:159:ASP:OD2	18:4:163:PRO:CA	2.60	0.47
18:4:161:LYS:NZ	18:4:162:ASN:HD21	2.12	0.47
18:4:214:PHE:O	18:4:218:ILE:HG13	2.15	0.47
1:A:159:THR:CA	1:A:163:GLN:HE22	2.27	0.47
1:A:246:HIS:C	1:A:248:PHE:H	2.15	0.47
1:A:279:ASP:O	1:A:281:LEU:HD11	2.12	0.47
1:A:308:ILE:O	1:A:311:LEU:HB2	2.14	0.47
1:A:310:PHE:H	1:A:313:ALA:HB3	1.79	0.47
1:A:452:PHE:O	1:A:456:HIS:ND1	2.35	0.47
1:A:709:TRP:CH2	2:B:417:ALA:HB2	2.50	0.47
19:A:1133:CLA:H3A	19:A:1133:CLA:HBA2	1.58	0.47
19:A:1237:CLA:HMC3	19:B:1238:CLA:C1D	2.45	0.47
2:B:124:TRP:O	2:B:124:TRP:HD1	1.98	0.47
2:B:260:GLY:O	2:B:262:HIS:NE2	2.47	0.47
2:B:411:MET:HE3	19:B:1220:CLA:HMC2	1.96	0.47
2:B:493:TRP:O	2:B:495:PRO:CG	2.62	0.47
2:B:527:LEU:CD2	19:B:1222:CLA:C4D	2.92	0.47
19:B:1201:CLA:HBC2	19:B:1201:CLA:HMC1	1.97	0.47
19:B:1214:CLA:HMC2	19:B:1214:CLA:H141	1.97	0.47
3:C:28:MET:SD	4:D:176:LYS:C	2.93	0.47
6:F:207:LEU:HD22	6:F:208:PHE:CG	2.49	0.47
7:G:130:TRP:O	7:G:134:GLY:CA	2.55	0.47
10:J:31:ARG:NH2	19:J:1311:CLA:CHC	2.77	0.47
12:L:114:PHE:HD1	12:L:114:PHE:H	1.61	0.47
14:R:46:UNK:CB	14:R:47:UNK:CA	2.92	0.47
15:1:65:ASP:OD1	15:1:66:PRO:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:129:VAL:HG12	15:1:130:PRO:CG	2.45	0.47
15:1:155:GLU:OE1	15:1:156:LYS:N	2.45	0.47
16:2:168:TRP:CD1	16:2:171:ILE:HG23	2.19	0.47
1:A:25:ASP:OD1	1:A:26:PRO:CD	2.62	0.47
1:A:51:THR:HG21	1:A:723:ARG:H	1.80	0.47
1:A:89:ILE:O	1:A:92:TRP:CB	2.55	0.47
1:A:167:THR:CG2	19:A:1112:CLA:CAA	2.87	0.47
1:A:201:SER:O	1:A:204:ASN:CB	2.58	0.47
1:A:223:VAL:CG1	1:A:224:HIS:N	2.77	0.47
1:A:270:PHE:CZ	19:A:1141:CLA:C2	2.97	0.47
1:A:281:LEU:CD2	19:A:1115:CLA:HED2	2.37	0.47
1:A:296:LEU:HD12	1:A:297:THR:CG2	2.31	0.47
1:A:309:LEU:HD23	1:A:309:LEU:C	2.35	0.47
1:A:346:LEU:CD2	1:A:347:TYR:HB2	2.45	0.47
1:A:346:LEU:HD11	19:A:1122:CLA:HBC3	1.97	0.47
1:A:390:ALA:HA	1:A:393:LEU:HD23	1.96	0.47
1:A:466:THR:CG2	2:B:648:TRP:HE1	2.28	0.47
1:A:581:CYS:HB3	1:A:590:CYS:O	2.14	0.47
1:A:584:PRO:HB2	3:C:67:VAL:HA	1.96	0.47
1:A:599:PHE:CD2	1:A:735:VAL:HG21	2.49	0.47
1:A:661:ALA:O	1:A:665:ILE:HG13	2.15	0.47
19:A:1102:CLA:O1A	19:A:1109:CLA:HBA2	2.15	0.47
19:A:1104:CLA:HBA2	19:A:1104:CLA:CED	2.45	0.47
19:A:1106:CLA:H111	21:J:6012:BCR:C10	2.45	0.47
19:A:1120:CLA:O2D	19:A:1120:CLA:OBD	2.33	0.47
19:A:1121:CLA:HAA1	11:K:78:ARG:NH1	2.29	0.47
19:A:1122:CLA:C1B	21:A:6007:BCR:C15	2.93	0.47
19:A:1129:CLA:HMB2	19:L:1130:CLA:C3D	2.45	0.47
19:A:1138:CLA:H52	19:A:1138:CLA:C4C	2.45	0.47
2:B:34:HIS:O	2:B:37:ILE:HG23	2.15	0.47
2:B:154:TRP:O	2:B:158:GLN:HG2	2.14	0.47
2:B:197:VAL:O	2:B:197:VAL:HG12	2.15	0.47
2:B:224:PRO:O	2:B:227:THR:N	2.43	0.47
2:B:497:TRP:C	2:B:499:ASN:N	2.62	0.47
2:B:503:GLU:O	2:B:503:GLU:HG2	2.13	0.47
2:B:564:ARG:NH2	3:C:66:ARG:NH1	2.63	0.47
2:B:655:LEU:HD21	19:B:1239:CLA:CBB	2.37	0.47
2:B:710:LEU:HA	2:B:713:PHE:HB3	1.97	0.47
2:B:732:LYS:HG2	2:B:734:GLY:H	1.58	0.47
19:B:1201:CLA:HBB2	19:B:1203:CLA:C4D	2.45	0.47
19:B:1206:CLA:H43	21:I:6018:BCR:H21C	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:PHE:CE1	5:E:80:GLU:OE1	2.68	0.47
4:D:100:TYR:CE2	4:D:156:ARG:HG3	2.50	0.47
4:D:100:TYR:OH	4:D:134:LYS:HE3	2.14	0.47
4:D:114:MET:CG	4:D:115:PRO:N	2.78	0.47
6:F:123:MET:O	6:F:125:LYS:N	2.48	0.47
6:F:168:LEU:HD13	6:F:168:LEU:HA	1.75	0.47
7:G:100:PHE:CD2	7:G:100:PHE:C	2.87	0.47
19:H:1207:CLA:HHD	21:I:6018:BCR:H342	1.96	0.47
10:J:19:PHE:O	10:J:23:ALA:HB3	2.14	0.47
10:J:25:LEU:HA	10:J:28:GLU:HB2	1.97	0.47
21:J:6012:BCR:C23	21:J:6012:BCR:C39	2.83	0.47
11:K:101:PHE:O	11:K:104:ALA:HB3	2.15	0.47
12:L:104:LEU:HD12	12:L:196:GLY:HA2	1.97	0.47
12:L:105:ALA:HB2	19:L:1501:CLA:HMA1	1.97	0.47
13:N:146:LEU:O	13:N:147:SER:O	2.33	0.47
15:1:133:THR:O	15:1:135:PRO:HD2	2.15	0.47
15:1:186:LYS:O	15:1:187:GLU:C	2.49	0.47
15:1:216:ASN:O	15:1:217:LEU:HB2	2.12	0.47
22:1:7013:LMU:H41	22:1:7013:LMU:H1'	1.97	0.47
16:2:150:THR:CG2	16:2:151:THR:N	2.76	0.47
16:2:269:LYS:HE3	16:2:269:LYS:O	2.15	0.47
17:3:101:GLY:O	17:3:102:GLU:C	2.53	0.47
19:3:3017:CLA:H3A	19:3:3017:CLA:HBA1	1.29	0.47
18:4:81:LEU:O	18:4:83:GLU:OE2	2.33	0.47
18:4:99:GLY:O	18:4:103:MET:HG3	2.14	0.47
18:4:172:PHE:CD1	18:4:176:SER:O	2.68	0.47
18:4:211:MET:CE	19:4:4002:CLA:CBB	2.92	0.47
18:4:217:PHE:HE1	18:4:221:HIS:CG	2.31	0.47
22:4:7052:LMU:H111	22:4:7052:LMU:H82	1.67	0.47
1:A:207:LEU:HA	1:A:211:LEU:CB	2.44	0.47
1:A:252:ARG:O	1:A:252:ARG:NE	2.48	0.47
1:A:369:THR:HG21	1:A:402:ILE:HG22	1.96	0.47
1:A:644:GLN:HG3	1:A:644:GLN:O	2.15	0.47
19:A:1105:CLA:HBA2	19:A:1105:CLA:H3A	1.49	0.47
19:A:1136:CLA:ND	19:A:1136:CLA:H11	2.29	0.47
19:A:9011:CLA:CMC	2:B:624:LEU:HG	2.44	0.47
19:A:9013:CLA:H2	19:A:9013:CLA:CMA	2.44	0.47
19:A:9023:CLA:CMB	19:A:9023:CLA:H41	2.45	0.47
2:B:30:ASP:CG	2:B:30:ASP:O	2.53	0.47
2:B:172:GLU:CD	2:B:301:ILE:HG13	2.35	0.47
2:B:312:GLY:O	19:B:1301:CLA:CAD	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:GLU:OE1	6:F:143:ASP:OD2	2.33	0.47
2:B:666:SER:O	2:B:667:TRP:HB2	2.14	0.47
19:B:1219:CLA:H3A	19:B:1219:CLA:HBA2	1.51	0.47
3:C:10:THR:CG2	5:E:101:TYR:CG	2.98	0.47
3:C:69:LEU:HD12	3:C:70:TRP:H	1.78	0.47
4:D:99:PHE:C	4:D:100:TYR:HD2	2.18	0.47
4:D:135:GLU:O	4:D:139:ALA:HB2	2.13	0.47
4:D:162:GLU:C	4:D:163:VAL:CG2	2.81	0.47
6:F:100:LYS:HA	6:F:100:LYS:HD3	1.30	0.47
6:F:172:GLY:O	6:F:176:TRP:CB	2.61	0.47
10:J:5:LYS:CE	16:2:178:ASN:OD1	2.63	0.47
11:K:81:THR:CG2	11:K:83:GLY:N	2.49	0.47
11:K:86:LEU:O	11:K:87:GLU:CB	2.62	0.47
13:N:157:LYS:CB	13:N:158:ASP:HA	2.42	0.47
22:1:7013:LMU:H42	22:1:7013:LMU:H11	1.81	0.47
16:2:100:ARG:N	16:2:101:TRP:HB2	2.29	0.47
16:2:122:ILE:O	16:2:126:LEU:CD2	2.62	0.47
16:2:142:GLU:O	16:2:143:GLN:HG2	2.15	0.47
16:2:172:LEU:O	16:2:172:LEU:HD12	2.15	0.47
19:2:2002:CLA:O2D	19:2:2002:CLA:OBD	2.33	0.47
19:2:2014:CLA:OBD	19:2:2014:CLA:O2D	2.32	0.47
22:4:7008:LMU:C6'	22:4:7008:LMU:H1B	2.45	0.47
1:A:281:LEU:HD21	19:A:1115:CLA:HED1	1.94	0.47
1:A:370:ILE:CG2	1:A:403:GLY:HA3	2.26	0.47
1:A:532:ILE:HD13	19:A:1135:CLA:CMD	2.45	0.47
1:A:594:ALA:O	1:A:598:VAL:HG23	2.14	0.47
1:A:736:THR:HG21	19:A:1128:CLA:H91	1.96	0.47
19:A:1119:CLA:H61	21:A:6008:BCR:H19C	1.96	0.47
19:A:1124:CLA:HAA1	19:A:1124:CLA:HBD	1.97	0.47
19:A:1126:CLA:H193	19:A:1126:CLA:H162	1.77	0.47
19:A:1140:CLA:HBA2	19:A:1140:CLA:H3A	1.47	0.47
21:A:6011:BCR:H333	19:B:1230:CLA:HBB2	1.95	0.47
2:B:4:ARG:HE	2:B:4:ARG:HB2	1.46	0.47
2:B:124:TRP:C	2:B:124:TRP:HD1	2.17	0.47
2:B:225:LEU:HD11	2:B:233:TYR:OH	2.06	0.47
2:B:459:PHE:CD2	19:B:1235:CLA:HMD1	2.45	0.47
2:B:560:ASP:OD1	3:C:66:ARG:HB3	2.15	0.47
2:B:679:ALA:HB1	2:B:683:GLU:OE2	2.15	0.47
7:G:136:VAL:O	7:G:137:VAL:CG2	2.63	0.47
10:J:15:SER:HA	10:J:18:TRP:HB3	1.96	0.47
12:L:206:VAL:O	12:L:207:LEU:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:142:LYS:HB3	13:N:143:VAL:H	1.61	0.47
14:R:34:UNK:CB	14:R:35:UNK:CA	2.80	0.47
16:2:155:VAL:HA	16:2:158:VAL:HG13	1.97	0.47
16:2:215:LYS:O	16:2:215:LYS:CG	2.60	0.47
17:3:94:GLU:CB	17:3:95:PRO:HD3	2.45	0.47
18:4:140:THR:O	18:4:144:ILE:HD12	2.15	0.47
1:A:360:ILE:HD11	19:A:1123:CLA:HMB2	1.97	0.47
1:A:603:PHE:CE2	2:B:665:ILE:HG21	2.50	0.47
19:A:1115:CLA:C14	19:A:1115:CLA:C17	2.75	0.47
19:A:1119:CLA:HMC1	19:A:1119:CLA:HBC2	1.96	0.47
19:A:1133:CLA:C3D	19:A:1134:CLA:CAC	2.92	0.47
21:A:6003:BCR:C8	21:A:6003:BCR:H311	2.44	0.47
2:B:154:TRP:O	2:B:155:LEU:C	2.52	0.47
2:B:224:PRO:CB	2:B:227:THR:HG21	2.45	0.47
2:B:235:GLN:O	2:B:236:ASN:C	2.53	0.47
2:B:290:MET:HG3	19:B:1218:CLA:C2C	2.45	0.47
2:B:343:VAL:HG11	19:B:1223:CLA:H2	1.96	0.47
2:B:555:TYR:CE2	2:B:573:TRP:HA	2.50	0.47
2:B:605:ASN:C	2:B:605:ASN:OD1	2.53	0.47
19:B:1205:CLA:HBB2	19:B:1205:CLA:C9	2.29	0.47
19:B:1210:CLA:H192	19:B:1215:CLA:OBD	2.15	0.47
21:B:6017:BCR:C33	21:B:6017:BCR:HC8	2.45	0.47
3:C:11:CYS:O	3:C:13:GLY:N	2.48	0.47
3:C:12:ILE:O	3:C:38:GLN:CG	2.62	0.47
4:D:99:PHE:HB3	4:D:157:VAL:HG12	1.95	0.47
4:D:177:VAL:HG23	4:D:178:ASN:C	2.35	0.47
5:E:110:VAL:O	5:E:111:ASN:CB	2.61	0.47
6:F:207:LEU:HD21	6:F:208:PHE:CG	2.48	0.47
7:G:124:ILE:CG2	7:G:125:VAL:H	2.26	0.47
8:H:108:THR:O	8:H:109:LEU:O	2.33	0.47
22:H:7032:LMU:O2'	22:H:7032:LMU:H12	2.15	0.47
10:J:2:ARG:NH1	10:J:8:LEU:HB2	2.30	0.47
11:K:55:LEU:O	11:K:58:VAL:HB	2.15	0.47
11:K:78:ARG:CZ	11:K:78:ARG:N	2.78	0.47
12:L:79:ILE:HD12	19:L:1504:CLA:HMA1	1.97	0.47
22:R:7021:LMU:O3'	22:R:7021:LMU:H1B	2.13	0.47
16:2:145:TYR:O	16:2:146:PHE:HB2	2.15	0.47
16:2:264:ALA:O	16:2:265:ALA:CB	2.63	0.47
17:3:107:ARG:NH1	17:3:229:LYS:O	2.47	0.47
17:3:109:ALA:O	17:3:111:LEU:HD23	2.14	0.47
17:3:161:GLU:O	17:3:162:MET:C	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:83:GLU:O	18:4:84:ASP:CG	2.53	0.47
18:4:144:ILE:HA	18:4:147:ILE:HD13	1.97	0.47
18:4:209:ARG:O	18:4:212:LEU:HB2	2.15	0.47
1:A:84:GLY:O	1:A:88:ILE:HD12	2.15	0.46
1:A:126:ILE:CD1	19:A:1107:CLA:HMA3	2.42	0.46
1:A:263:ALA:O	1:A:264:GLU:HG3	2.13	0.46
1:A:358:LEU:C	1:A:358:LEU:HD12	2.35	0.46
1:A:581:CYS:HB2	1:A:590:CYS:O	2.14	0.46
1:A:592:VAL:HG23	1:A:593:SER:H	1.80	0.46
1:A:739:LEU:O	1:A:743:ILE:HG13	2.15	0.46
19:A:1119:CLA:CAA	19:A:1123:CLA:HBB2	2.45	0.46
19:A:1124:CLA:H162	19:A:1124:CLA:H111	1.96	0.46
19:A:1138:CLA:HBD	19:A:1138:CLA:HAA1	1.95	0.46
19:A:1237:CLA:HMC3	19:B:1238:CLA:ND	2.30	0.46
2:B:15:ASP:O	2:B:20:ARG:HG3	2.15	0.46
2:B:290:MET:HG3	19:B:1218:CLA:HMC3	1.97	0.46
2:B:487:ASN:C	2:B:487:ASN:OD1	2.53	0.46
2:B:649:MET:HE2	21:B:6017:BCR:H272	1.96	0.46
3:C:62:PHE:CD1	4:D:191:ILE:CG2	2.92	0.46
4:D:123:ARG:HH21	22:D:7050:LMU:C6B	2.17	0.46
6:F:121:ALA:C	6:F:123:MET:N	2.69	0.46
6:F:192:THR:O	6:F:193:GLN:CB	2.63	0.46
8:H:98:LEU:O	8:H:98:LEU:CG	2.63	0.46
19:H:1505:CLA:HAA2	19:H:1505:CLA:HBD	1.96	0.46
22:H:7030:LMU:H61	22:H:7030:LMU:H32	1.62	0.46
11:K:56:ILE:CA	11:K:59:THR:CG2	2.81	0.46
11:K:115:ILE:O	11:K:118:VAL:CG2	2.60	0.46
12:L:82:TYR:OH	19:L:1502:CLA:HBA2	2.15	0.46
12:L:131:SER:O	12:L:132:LEU:HB3	2.15	0.46
12:L:178:THR:HG22	12:L:179:ALA:N	2.30	0.46
13:N:160:TYR:O	13:N:164:SER:O	2.33	0.46
15:1:77:GLU:CD	15:1:80:LYS:NZ	2.69	0.46
15:1:133:THR:O	15:1:136:THR:CG2	2.53	0.46
16:2:174:PRO:CD	16:2:189:THR:OG1	2.61	0.46
16:2:229:MET:CE	16:2:230:LEU:CD1	2.94	0.46
18:4:173:LYS:CE	18:4:201:LYS:HG3	2.43	0.46
18:4:178:PRO:O	18:4:194:PHE:CZ	2.67	0.46
18:4:238:ASP:OD2	18:4:238:ASP:N	2.47	0.46
1:A:124:TRP:HA	1:A:124:TRP:CE3	2.50	0.46
1:A:129:GLN:NE2	19:A:1107:CLA:NB	2.64	0.46
1:A:185:HIS:O	1:A:186:TYR:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:HIS:HE1	19:A:1109:CLA:C1A	2.06	0.46
1:A:245:PRO:O	1:A:248:PHE:HE2	1.93	0.46
1:A:308:ILE:CG2	19:A:1115:CLA:C11	2.94	0.46
1:A:473:PRO:O	1:A:475:ASP:N	2.48	0.46
1:A:536:THR:O	1:A:537:ALA:CB	2.63	0.46
1:A:564:ARG:HA	1:A:573:ALA:HB2	1.97	0.46
19:A:1101:CLA:H42	19:A:1140:CLA:H8	1.97	0.46
19:A:1105:CLA:C4B	21:J:6012:BCR:H333	2.45	0.46
2:B:80:ASP:HA	2:B:81:PRO:HD3	1.75	0.46
2:B:320:LYS:HG3	2:B:321:GLY:H	1.80	0.46
2:B:353:TYR:CB	2:B:594:TRP:CZ3	2.98	0.46
2:B:471:THR:O	2:B:472:TYR:HD1	1.92	0.46
2:B:488:ALA:HB2	19:B:1233:CLA:C3C	2.45	0.46
2:B:564:ARG:CZ	3:C:64:SER:H	2.28	0.46
2:B:645:VAL:HG21	19:B:1206:CLA:HMD2	1.96	0.46
2:B:668:ARG:NH1	2:B:672:GLN:HG2	2.30	0.46
19:B:1222:CLA:H11	19:B:1236:CLA:CBD	2.46	0.46
19:B:1233:CLA:HBA2	19:B:1233:CLA:H3A	1.71	0.46
3:C:79:LEU:HD22	3:C:81:TYR:O	2.15	0.46
4:D:172:VAL:CG1	4:D:173:TYR:N	2.78	0.46
6:F:169:TYR:OH	6:F:211:PHE:HA	2.15	0.46
22:H:7032:LMU:H1B	22:H:7032:LMU:O1'	2.15	0.46
10:J:26:LEU:HA	10:J:29:ILE:HG22	1.97	0.46
11:K:48:PHE:C	11:K:52:PRO:HD3	2.34	0.46
14:R:6:UNK:CB	14:R:10:UNK:CB	2.92	0.46
22:R:7021:LMU:H41	22:R:7021:LMU:O6'	2.16	0.46
15:1:179:LYS:HG2	15:1:180:LEU:C	2.35	0.46
19:1:1001:CLA:HBA1	19:1:1001:CLA:CMA	2.44	0.46
19:1:1001:CLA:H3A	19:1:1001:CLA:HBA2	1.30	0.46
16:2:128:LYS:HB2	16:2:131:ILE:HG12	1.96	0.46
17:3:187:PHE:CE1	17:3:188:LEU:HB2	2.51	0.46
1:A:393:LEU:HD11	1:A:750:PHE:CD1	2.51	0.46
19:A:1149:CLA:O1D	19:A:1149:CLA:HBA2	2.14	0.46
2:B:38:THR:HG23	2:B:41:ARG:NH1	2.30	0.46
2:B:469:LYS:HZ3	2:B:471:THR:N	2.07	0.46
2:B:595:HIS:HD2	2:B:623:TYR:OH	1.99	0.46
2:B:596:TRP:CD1	2:B:623:TYR:HB2	2.50	0.46
2:B:693:TRP:HD1	19:B:1238:CLA:C1D	2.18	0.46
3:C:18:VAL:HB	3:C:58:CYS:HB2	1.97	0.46
4:D:140:LEU:HD22	4:D:144:LEU:HG	1.96	0.46
4:D:147:LYS:C	4:D:148:TYR:CD1	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:73:LYS:HG3	5:E:128:VAL:CG1	2.46	0.46
7:G:123:ASN:O	7:G:124:ILE:C	2.52	0.46
9:I:8:PHE:CE1	21:I:6021:BCR:HC7	2.50	0.46
10:J:2:ARG:HB3	10:J:7:TYR:CE1	2.50	0.46
22:K:7047:LMU:O2B	22:K:7047:LMU:H6E	2.16	0.46
12:L:92:ALA:N	12:L:98:ARG:HH22	2.12	0.46
13:N:115:ALA:O	13:N:116:ARG:C	2.49	0.46
22:N:7049:LMU:H4'	22:N:7049:LMU:O6B	2.15	0.46
15:1:66:PRO:CD	15:1:67:LEU:H	2.06	0.46
15:1:103:LEU:N	15:1:103:LEU:CD2	2.71	0.46
19:1:1010:CLA:O1D	19:1:1010:CLA:C3D	2.54	0.46
16:2:184:PRO:CD	16:2:185:ASN:CA	2.93	0.46
16:2:218:ARG:NH1	19:2:2001:CLA:HBB2	2.30	0.46
16:2:267:THR:O	16:2:267:THR:HG23	2.14	0.46
21:3:6022:BCR:C39	21:3:6022:BCR:C23	2.63	0.46
1:A:244:LEU:CB	1:A:247:GLU:CD	2.81	0.46
1:A:389:TYR:HD1	1:A:625:TRP:CG	2.32	0.46
19:A:1102:CLA:HBB2	19:A:1104:CLA:C3D	2.46	0.46
19:A:1138:CLA:H191	6:F:181:TYR:CG	2.51	0.46
19:A:1140:CLA:H43	19:A:1140:CLA:ND	2.30	0.46
19:A:9023:CLA:HMC1	2:B:661:PHE:HB3	1.98	0.46
2:B:247:THR:O	2:B:250:ALA:N	2.49	0.46
2:B:294:ASN:ND2	7:G:93:GLU:C	2.66	0.46
2:B:310:PRO:HD2	2:B:311:PRO:HD2	1.97	0.46
2:B:655:LEU:HD22	19:B:1239:CLA:CBB	2.45	0.46
19:B:1220:CLA:C9	19:B:1227:CLA:CBC	2.94	0.46
19:B:1225:CLA:H62	21:B:6006:BCR:H321	1.97	0.46
4:D:114:MET:SD	4:D:115:PRO:HD2	2.55	0.46
4:D:147:LYS:O	4:D:148:TYR:CD2	2.68	0.46
5:E:111:ASN:CG	5:E:112:TYR:N	2.68	0.46
6:F:133:TYR:CD1	6:F:133:TYR:N	2.83	0.46
19:J:1311:CLA:O1A	19:J:1311:CLA:C15	2.64	0.46
11:K:97:ASP:O	11:K:97:ASP:OD1	2.32	0.46
12:L:172:GLU:CG	12:L:173:PRO:N	2.73	0.46
13:N:159:LYS:O	13:N:160:TYR:C	2.54	0.46
15:1:75:ASN:O	15:1:76:LEU:O	2.34	0.46
15:1:157:ASP:OD1	15:1:157:ASP:C	2.53	0.46
17:3:182:MET:CG	17:3:183:GLY:N	2.78	0.46
18:4:112:PRO:O	18:4:115:PHE:O	2.34	0.46
19:4:4014:CLA:HBC2	19:4:4014:CLA:CHD	2.34	0.46
1:A:42:ARG:O	1:A:44:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:C	1:A:132:LEU:N	2.65	0.46
1:A:163:GLN:HG2	1:A:164:LEU:H	1.74	0.46
1:A:313:ALA:C	1:A:315:HIS:H	2.19	0.46
1:A:392:GLN:CG	1:A:392:GLN:O	2.64	0.46
1:A:539:PHE:HE2	1:A:543:HIS:CE1	2.34	0.46
1:A:586:ARG:HA	3:C:77:MET:O	2.15	0.46
1:A:626:GLY:O	1:A:627:THR:CG2	2.64	0.46
1:A:692:PHE:CD2	1:A:733:VAL:CG1	2.97	0.46
1:A:725:LEU:HD21	19:A:1140:CLA:CMD	2.46	0.46
19:A:1124:CLA:HMB3	21:A:6008:BCR:C18	2.45	0.46
19:A:1237:CLA:H201	12:L:110:LEU:CD2	2.34	0.46
20:A:5001:PQN:H243	20:A:5001:PQN:H212	1.76	0.46
2:B:15:ASP:O	2:B:20:ARG:CG	2.63	0.46
2:B:377:TYR:CD1	2:B:718:ILE:HD12	2.51	0.46
2:B:594:TRP:CD1	2:B:595:HIS:N	2.84	0.46
19:B:1217:CLA:HMA1	7:G:77:PHE:CG	2.51	0.46
22:E:7048:LMU:H3'	22:E:7048:LMU:O5B	2.15	0.46
9:I:9:VAL:H	9:I:10:PRO:CD	2.28	0.46
9:I:12:VAL:HG12	9:I:13:GLY:N	2.31	0.46
10:J:2:ARG:HH22	10:J:8:LEU:HD22	1.80	0.46
19:J:1308:CLA:H93	19:J:1308:CLA:H61	1.70	0.46
12:L:96:LEU:HG	12:L:97:LEU:HD23	1.97	0.46
12:L:109:LEU:HG	12:L:110:LEU:H	1.81	0.46
12:L:113:PRO:O	12:L:117:ALA:HB3	2.16	0.46
16:2:189:THR:CG2	16:2:193:VAL:O	2.61	0.46
17:3:94:GLU:CD	17:3:94:GLU:O	2.54	0.46
17:3:94:GLU:CA	17:3:94:GLU:OE2	2.63	0.46
18:4:93:GLN:O	18:4:97:VAL:HG23	2.15	0.46
18:4:107:ALA:O	18:4:109:MET:O	2.33	0.46
18:4:176:SER:C	18:4:178:PRO:HD2	2.35	0.46
18:4:237:SER:O	18:4:238:ASP:C	2.50	0.46
1:A:426:THR:N	1:A:428:TYR:CZ	2.84	0.46
1:A:430:ASP:HA	1:A:434:ARG:HH21	1.80	0.46
1:A:497:ALA:HB2	1:A:510:SER:OG	2.14	0.46
19:A:1104:CLA:HED2	19:A:1104:CLA:H12	1.97	0.46
19:A:9013:CLA:HBC2	19:A:9013:CLA:HMC1	1.98	0.46
2:B:139:ALA:O	2:B:141:PHE:N	2.49	0.46
2:B:321:GLY:O	2:B:325:THR:HG22	2.15	0.46
2:B:450:GLU:C	2:B:452:GLN:H	2.18	0.46
19:B:1220:CLA:H42	19:B:1220:CLA:CHB	2.43	0.46
21:B:6004:BCR:H343	7:G:77:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:CYS:SG	3:C:53:ARG:N	2.89	0.46
6:F:95:GLU:OE1	6:F:129:ARG:O	2.33	0.46
6:F:152:GLY:HA2	6:F:157:TRP:CE3	2.51	0.46
12:L:175:GLN:O	12:L:176:LEU:CB	2.55	0.46
13:N:132:THR:CB	13:N:139:LYS:NZ	2.57	0.46
14:R:1:UNK:O	14:R:2:UNK:O	2.34	0.46
15:1:84:LEU:HA	15:1:87:CYS:HB3	1.97	0.46
15:1:138:LEU:O	15:1:139:ALA:C	2.53	0.46
16:2:172:LEU:HB3	16:2:173:ASN:HD21	1.73	0.46
16:2:177:VAL:HG13	16:2:178:ASN:OD1	2.14	0.46
16:2:184:PRO:HG2	16:2:185:ASN:CA	2.45	0.46
19:2:2001:CLA:O1A	19:2:2001:CLA:NA	2.49	0.46
17:3:150:TYR:CE2	17:3:151:TRP:CE2	2.99	0.46
19:3:3013:CLA:O2D	19:3:3013:CLA:OBD	2.33	0.46
1:A:284:ARG:HH12	1:A:507:ALA:HB2	1.10	0.46
1:A:309:LEU:HD21	19:A:1119:CLA:HMC3	1.97	0.46
1:A:409:GLY:C	1:A:411:ALA:H	2.19	0.46
1:A:467:MET:HE3	1:A:467:MET:HB3	1.69	0.46
1:A:584:PRO:HB2	3:C:67:VAL:CA	2.45	0.46
1:A:697:ARG:NH1	1:A:724:ALA:HB3	2.30	0.46
19:A:1117:CLA:HBC1	21:A:6003:BCR:C12	2.46	0.46
19:A:1135:CLA:H2	19:A:1135:CLA:O1A	2.16	0.46
21:A:6003:BCR:C23	21:A:6003:BCR:H402	2.44	0.46
2:B:21:ILE:O	2:B:22:TRP:C	2.54	0.46
2:B:435:GLY:HA3	19:B:1230:CLA:HBB1	1.97	0.46
2:B:536:LYS:O	2:B:537:GLY:C	2.54	0.46
2:B:587:ILE:O	2:B:587:ILE:CG2	2.62	0.46
2:B:605:ASN:OD1	2:B:605:ASN:O	2.34	0.46
2:B:623:TYR:O	2:B:624:LEU:CB	2.64	0.46
19:B:1235:CLA:CBB	19:B:1235:CLA:C9	2.66	0.46
3:C:69:LEU:H	3:C:69:LEU:HG	1.20	0.46
5:E:124:GLU:HB2	5:E:126:VAL:HG13	1.97	0.46
6:F:132:ASN:O	6:F:132:ASN:CG	2.54	0.46
6:F:167:PHE:CD1	21:F:6014:BCR:H23C	2.51	0.46
6:F:180:SER:O	6:F:182:LEU:N	2.38	0.46
6:F:190:LYS:HA	6:F:191:PRO:HD3	1.54	0.46
7:G:131:GLY:C	7:G:136:VAL:HB	2.35	0.46
7:G:134:GLY:O	7:G:135:HIS:CE1	2.69	0.46
8:H:76:TYR:HH	12:L:90:ARG:NE	1.83	0.46
8:H:86:THR:HA	8:H:92:THR:HG21	1.98	0.46
19:L:1130:CLA:H72	19:L:1504:CLA:HBA1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:8:UNK:CB	19:R:1144:CLA:HED1	2.46	0.46
16:2:114:MET:O	16:2:117:ALA:HB3	2.16	0.46
16:2:122:ILE:HG13	16:2:126:LEU:CD2	2.46	0.46
19:3:3016:CLA:H102	19:3:3016:CLA:H143	1.90	0.46
22:3:7005:LMU:H3'	22:3:7005:LMU:C2B	2.46	0.46
18:4:154:ILE:HD12	19:4:1009:CLA:HMD1	1.98	0.46
1:A:199:VAL:O	1:A:199:VAL:CG1	2.58	0.46
1:A:284:ARG:CB	1:A:295:TRP:CG	2.99	0.46
1:A:341:GLN:HE21	1:A:341:GLN:HB2	1.56	0.46
1:A:402:ILE:CD1	19:A:1127:CLA:CBB	2.94	0.46
1:A:655:ASP:O	1:A:659:ALA:HB3	2.16	0.46
1:A:708:VAL:HA	1:A:711:HIS:HD2	1.80	0.46
19:A:1109:CLA:C4A	19:A:1109:CLA:CBA	2.92	0.46
2:B:53:GLN:O	2:B:55:ALA:N	2.41	0.46
2:B:196:HIS:CE1	19:B:1212:CLA:C4D	2.98	0.46
2:B:217:PRO:HD2	19:B:1212:CLA:HED1	1.98	0.46
19:B:1235:CLA:C6	21:F:6016:BCR:H323	2.46	0.46
3:C:7:ILE:O	3:C:60:THR:HA	2.16	0.46
4:D:90:LEU:O	12:L:66:ILE:HG23	2.16	0.46
4:D:141:GLY:O	4:D:142:THR:O	2.34	0.46
6:F:96:LYS:C	6:F:97:GLN:O	2.53	0.46
11:K:95:THR:O	11:K:95:THR:HG22	2.16	0.46
11:K:124:LEU:HD12	11:K:124:LEU:C	2.36	0.46
12:L:131:SER:HA	12:L:197:VAL:CG1	2.45	0.46
12:L:155:GLU:H	12:L:155:GLU:HG2	1.15	0.46
19:L:1504:CLA:H62	19:L:1504:CLA:H41	1.62	0.46
22:L:7029:LMU:H1'	22:L:7029:LMU:C3	2.23	0.46
15:1:83:GLU:HA	15:1:86:HIS:CD2	2.51	0.46
15:1:97:ILE:HD11	15:1:98:LEU:HD22	1.97	0.46
15:1:201:PHE:CE1	15:1:204:GLN:OE1	2.69	0.46
19:2:4009:CLA:H71	19:2:4009:CLA:H111	1.68	0.46
17:3:184:LYS:HD3	19:3:2009:CLA:H61	1.60	0.46
19:3:2009:CLA:O1A	19:3:2009:CLA:CBD	2.44	0.46
18:4:98:ASN:HB3	18:4:212:LEU:CD2	2.45	0.46
18:4:206:ALA:O	18:4:207:ASN:C	2.54	0.46
1:A:71:LEU:HD12	1:A:72:GLU:C	2.36	0.46
1:A:112:ASP:N	1:A:113:PRO:CD	2.78	0.46
1:A:196:PHE:CD2	1:A:196:PHE:N	2.76	0.46
1:A:431:LEU:H	1:A:434:ARG:HE	1.62	0.46
1:A:473:PRO:O	1:A:474:GLN:C	2.54	0.46
1:A:555:ILE:HD11	19:A:9023:CLA:CAD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:LYS:CD	6:F:230:ASN:ND2	2.48	0.46
19:A:1117:CLA:H71	19:A:1117:CLA:CAB	2.46	0.46
19:A:1126:CLA:H71	21:A:6011:BCR:C37	2.45	0.46
19:A:1237:CLA:CGA	19:A:1237:CLA:C1A	2.94	0.46
2:B:21:ILE:CD1	19:B:1238:CLA:HMA1	2.43	0.46
2:B:29:HIS:NE2	19:B:1202:CLA:HBB1	2.31	0.46
2:B:100:ALA:O	2:B:102:GLU:O	2.33	0.46
2:B:255:LEU:N	2:B:271:THR:HG21	2.31	0.46
2:B:330:ILE:HD12	2:B:333:GLN:NE2	2.30	0.46
19:B:1222:CLA:H52	19:B:1236:CLA:CBD	2.45	0.46
5:E:73:LYS:O	5:E:73:LYS:CG	2.64	0.46
5:E:73:LYS:CG	5:E:128:VAL:HG11	2.44	0.46
5:E:93:VAL:O	5:E:93:VAL:HG12	2.15	0.46
6:F:153:ASP:N	6:F:153:ASP:OD1	2.47	0.46
6:F:177:VAL:CA	6:F:180:SER:OG	2.57	0.46
7:G:82:PHE:CB	7:G:83:GLN:HG2	2.46	0.46
7:G:98:THR:OG1	7:G:99:HIS:C	2.55	0.46
9:I:12:VAL:HG13	21:I:6018:BCR:H271	1.97	0.46
19:L:1130:CLA:H142	19:L:1504:CLA:H43	1.97	0.46
15:1:224:PRO:HA	15:1:225:TRP:C	2.36	0.46
16:2:157:LEU:O	16:2:161:GLY:N	2.39	0.46
16:2:206:TRP:O	16:2:208:SER:CB	2.62	0.46
18:4:103:MET:HG2	18:4:211:MET:HB2	1.96	0.46
18:4:154:ILE:O	18:4:155:ARG:C	2.54	0.46
1:A:105:ASN:HA	1:A:140:PHE:HE2	1.81	0.46
1:A:308:ILE:HD11	19:A:1115:CLA:C4B	2.46	0.46
1:A:308:ILE:HG21	19:A:1115:CLA:C11	2.46	0.46
1:A:520:LEU:HB3	22:A:7044:LMU:H2'	1.62	0.46
1:A:654:ARG:HG3	1:A:655:ASP:N	2.30	0.46
1:A:701:GLN:OE1	5:E:112:TYR:CE1	2.69	0.46
19:A:9022:CLA:H91	19:A:9023:CLA:C9	2.43	0.46
2:B:25:ILE:HG21	21:L:6019:BCR:C28	2.45	0.46
2:B:317:ARG:HH22	2:B:410:ARG:CB	2.28	0.46
2:B:646:TRP:CH2	2:B:726:ILE:HD13	2.50	0.46
19:B:1208:CLA:HAA2	19:B:1208:CLA:H12	1.98	0.46
19:B:1234:CLA:O2D	19:B:1234:CLA:OBD	2.34	0.46
4:D:80:SER:HB2	4:D:127:ASN:H	1.80	0.46
4:D:95:GLN:HE21	4:D:96:VAL:CB	2.29	0.46
5:E:108:ASN:OD1	5:E:109:LYS:N	2.49	0.46
22:E:7037:LMU:C5	22:E:7037:LMU:C1	2.92	0.46
6:F:139:LEU:O	6:F:140:CYS:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:184:ALA:C	6:F:185:ILE:CG2	2.84	0.46
8:H:91:PHE:HB3	12:L:187:GLY:CA	2.46	0.46
22:H:7011:LMU:H111	22:H:7011:LMU:C6	2.46	0.46
11:K:94:GLN:CD	11:K:94:GLN:N	2.69	0.46
13:N:156:GLY:CA	13:N:157:LYS:CD	2.94	0.46
15:1:91:MET:O	15:1:94:VAL:HB	2.16	0.46
15:1:201:PHE:CD1	15:1:204:GLN:OE1	2.69	0.46
18:4:83:GLU:C	18:4:84:ASP:CG	2.74	0.46
1:A:70:ASP:CB	1:A:72:GLU:HG2	2.46	0.45
1:A:90:PHE:O	1:A:91:LEU:C	2.52	0.45
1:A:120:ALA:HB3	19:A:1106:CLA:HED3	1.98	0.45
1:A:183:TRP:O	1:A:185:HIS:N	2.49	0.45
1:A:240:LYS:H	1:A:243:PRO:CD	2.24	0.45
1:A:451:ILE:HD13	19:A:1131:CLA:CED	2.35	0.45
1:A:502:THR:HG22	1:A:503:THR:N	2.32	0.45
1:A:592:VAL:O	1:A:597:HIS:CD2	2.69	0.45
1:A:660:GLN:O	1:A:661:ALA:HB3	2.16	0.45
2:B:5:ILE:CG2	2:B:6:PRO:N	2.75	0.45
2:B:65:LEU:HD11	21:B:6006:BCR:HC42	1.97	0.45
2:B:95:HIS:CE1	19:B:1206:CLA:HMB3	2.52	0.45
2:B:199:ILE:CG2	2:B:270:LEU:HD11	2.43	0.45
2:B:229:GLN:NE2	7:G:154:PHE:CE1	2.79	0.45
2:B:377:TYR:OH	2:B:717:TYR:HE1	1.99	0.45
2:B:394:PHE:C	2:B:542:ARG:HD3	2.36	0.45
2:B:407:VAL:C	2:B:409:ALA:O	2.55	0.45
2:B:447:GLY:C	2:B:449:PRO:HD3	2.37	0.45
2:B:551:LYS:HE3	2:B:551:LYS:HB3	1.55	0.45
19:B:1229:CLA:HBB2	21:F:6014:BCR:C26	2.46	0.45
4:D:103:THR:C	4:D:104:TRP:HD1	2.19	0.45
21:F:6016:BCR:H24C	21:F:6016:BCR:H371	1.75	0.45
11:K:98:PRO:CD	11:K:99:ALA:N	2.64	0.45
22:R:7020:LMU:H92	22:R:7020:LMU:H62	1.54	0.45
15:1:156:LYS:HB3	15:1:158:PRO:CD	2.46	0.45
17:3:109:ALA:HA	17:3:111:LEU:HD13	1.97	0.45
17:3:209:ASN:HD22	17:3:209:ASN:HA	1.55	0.45
17:3:238:ILE:HA	17:3:241:TYR:CZ	2.50	0.45
18:4:89:ARG:CD	18:4:89:ARG:N	2.79	0.45
18:4:121:ILE:HG12	18:4:122:ASN:H	1.81	0.45
18:4:223:VAL:C	18:4:224:THR:HG23	2.36	0.45
1:A:23:ASP:HA	1:A:24:ARG:HE	1.81	0.45
1:A:252:ARG:CZ	1:A:261:SER:OG	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1101:CLA:C1	19:A:1140:CLA:H2	2.47	0.45
19:A:1122:CLA:HBC1	21:A:6007:BCR:C39	2.46	0.45
19:A:1237:CLA:CMD	21:B:6017:BCR:H313	2.46	0.45
19:A:1237:CLA:CMD	21:B:6017:BCR:HC31	2.39	0.45
2:B:50:HIS:HB2	2:B:53:GLN:HB2	1.98	0.45
2:B:240:SER:O	2:B:242:HIS:N	2.49	0.45
2:B:463:ILE:O	2:B:464:GLN:CG	2.64	0.45
2:B:636:THR:O	2:B:636:THR:CG2	2.64	0.45
2:B:683:GLU:OE1	4:D:91:LEU:HD13	2.16	0.45
4:D:78:THR:N	4:D:79:PRO:CD	2.79	0.45
22:E:7037:LMU:H4B	22:E:7037:LMU:H1B	1.54	0.45
22:G:7039:LMU:H4B	22:G:7039:LMU:H1B	1.64	0.45
8:H:86:THR:O	8:H:88:ALA:N	2.49	0.45
8:H:94:ARG:CZ	8:H:97:LEU:O	2.65	0.45
11:K:50:GLY:CA	11:K:52:PRO:HD2	2.45	0.45
13:N:90:GLU:OE2	13:N:91:TYR:CG	2.69	0.45
13:N:127:PHE:CD1	13:N:128:PRO:HA	2.51	0.45
15:1:155:GLU:O	15:1:156:LYS:CB	2.61	0.45
15:1:181:GLU:O	15:1:182:GLU:HB3	2.16	0.45
16:2:266:PHE:CD1	16:2:267:THR:O	2.68	0.45
22:2:7006:LMU:O5B	22:2:7006:LMU:C5'	2.50	0.45
17:3:192:LYS:O	17:3:193:GLY:C	2.54	0.45
22:4:7053:LMU:O2B	22:4:7053:LMU:C5B	2.60	0.45
1:A:23:ASP:OD1	1:A:24:ARG:N	2.50	0.45
1:A:164:LEU:HA	1:A:167:THR:OG1	2.17	0.45
1:A:462:ILE:CG2	19:A:1132:CLA:CMC	2.94	0.45
1:A:596:ASP:HA	1:A:599:PHE:CB	2.38	0.45
19:A:1132:CLA:H172	19:A:1136:CLA:C20	2.46	0.45
19:A:9011:CLA:HBB2	19:A:9012:CLA:HED1	1.98	0.45
19:A:9012:CLA:HBB2	19:A:9013:CLA:C2B	2.47	0.45
19:A:9023:CLA:H141	19:A:9023:CLA:H161	1.72	0.45
2:B:224:PRO:CA	2:B:227:THR:OG1	2.64	0.45
2:B:451:LYS:CD	19:B:1230:CLA:O2D	2.65	0.45
19:B:1223:CLA:C7	19:B:1223:CLA:C4	2.94	0.45
3:C:28:MET:HA	3:C:29:ILE:O	2.17	0.45
3:C:69:LEU:HD12	3:C:70:TRP:O	2.11	0.45
4:D:121:ILE:O	4:D:121:ILE:HG13	2.17	0.45
22:D:7050:LMU:H82	22:D:7050:LMU:C4	2.46	0.45
5:E:85:LYS:O	5:E:87:THR:CG2	2.64	0.45
6:F:99:LEU:CA	6:F:102:LEU:CD2	2.89	0.45
7:G:70:LEU:O	7:G:70:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:ARG:NH1	7:G:120:VAL:CA	2.80	0.45
11:K:66:PHE:HE2	11:K:102:THR:HG22	1.82	0.45
11:K:126:ASN:OD1	11:K:126:ASN:O	2.34	0.45
15:1:64:PHE:CD1	15:1:65:ASP:CB	2.99	0.45
16:2:127:THR:OG1	16:2:129:LEU:N	2.49	0.45
18:4:135:PHE:H	18:4:136:ALA:HB2	1.81	0.45
1:A:43:THR:HG22	1:A:43:THR:O	2.17	0.45
1:A:70:ASP:O	1:A:72:GLU:HB2	2.16	0.45
1:A:95:GLY:O	1:A:96:MET:C	2.52	0.45
1:A:107:GLU:HA	1:A:110:LEU:CD2	2.46	0.45
1:A:149:PHE:O	1:A:150:PHE:CB	2.36	0.45
1:A:165:TYR:O	1:A:165:TYR:HD2	1.97	0.45
1:A:421:ASP:OD1	1:A:422:TYR:HE1	1.92	0.45
1:A:492:ILE:O	1:A:495:THR:HG22	2.17	0.45
1:A:553:VAL:O	1:A:557:LEU:HB2	2.16	0.45
2:B:97:GLY:O	2:B:100:ALA:HB2	2.17	0.45
2:B:261:PHE:CE2	2:B:499:ASN:C	2.76	0.45
2:B:339:ALA:O	2:B:340:SER:CB	2.64	0.45
2:B:564:ARG:CZ	3:C:64:SER:N	2.80	0.45
2:B:564:ARG:HH21	3:C:66:ARG:NH1	2.14	0.45
19:B:1223:CLA:H72	19:B:1223:CLA:C4	2.45	0.45
4:D:116:THR:O	4:D:117:GLY:O	2.34	0.45
4:D:123:ARG:O	4:D:124:GLU:CB	2.63	0.45
5:E:99:THR:CG2	5:E:100:ARG:N	2.42	0.45
6:F:224:GLY:CA	6:F:227:VAL:CG1	2.94	0.45
19:L:1502:CLA:HBA1	19:L:1502:CLA:CHA	2.47	0.45
15:1:145:ILE:HG13	15:1:145:ILE:H	1.52	0.45
19:1:1007:CLA:HHD	19:1:1007:CLA:HBC3	1.96	0.45
17:3:101:GLY:C	17:3:103:VAL:N	2.65	0.45
17:3:186:TYR:HD2	17:3:188:LEU:O	1.99	0.45
17:3:233:LEU:HA	17:3:236:LEU:CB	2.44	0.45
18:4:124:PRO:O	18:4:125:LYS:HB2	2.17	0.45
18:4:124:PRO:O	18:4:125:LYS:CG	2.63	0.45
18:4:217:PHE:CE1	18:4:221:HIS:CG	3.04	0.45
22:4:7033:LMU:H5'	22:4:7033:LMU:H1B	1.73	0.45
1:A:379:MET:HE1	19:A:1125:CLA:CHC	2.43	0.45
1:A:532:ILE:HG12	1:A:619:LYS:HZ1	1.82	0.45
21:A:6003:BCR:C8	21:A:6003:BCR:C31	2.95	0.45
2:B:73:ASN:H	2:B:73:ASN:HD22	1.59	0.45
2:B:336:LEU:HD13	19:B:1221:CLA:CBB	2.46	0.45
2:B:395:ILE:HD13	2:B:555:TYR:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:LEU:O	2:B:498:LEU:HD23	2.16	0.45
2:B:505:SER:OG	2:B:506:ASN:N	2.49	0.45
2:B:533:ILE:CD1	2:B:579:ALA:HA	2.46	0.45
2:B:646:TRP:O	2:B:649:MET:HB3	2.17	0.45
19:B:1230:CLA:HED2	19:B:1230:CLA:H2A	1.98	0.45
19:B:1231:CLA:HBA2	19:B:1231:CLA:H3A	1.53	0.45
19:B:9010:CLA:H161	19:B:9010:CLA:H193	1.74	0.45
3:C:63:LEU:HD23	3:C:63:LEU:C	2.37	0.45
5:E:123:ASP:HA	5:E:124:GLU:HA	1.57	0.45
6:F:103:GLN:OE1	6:F:104:ALA:N	2.50	0.45
6:F:157:TRP:CE3	19:F:1305:CLA:HMC2	2.49	0.45
12:L:158:PRO:O	12:L:159:SER:HB3	2.16	0.45
12:L:167:THR:OG1	12:L:168:GLY:N	2.47	0.45
13:N:90:GLU:OE1	13:N:91:TYR:CD2	2.69	0.45
22:R:7007:LMU:H6D	22:R:7007:LMU:O5B	2.17	0.45
22:R:7014:LMU:H62	22:R:7014:LMU:C1	2.25	0.45
16:2:158:VAL:O	16:2:159:PHE:C	2.52	0.45
17:3:176:TRP:O	17:3:178:LYS:HG3	2.16	0.45
18:4:170:PRO:C	18:4:173:LYS:N	2.70	0.45
19:4:1304:CLA:HAA2	19:4:1304:CLA:O2D	2.13	0.45
1:A:109:TRP:O	1:A:112:ASP:CA	2.65	0.45
1:A:136:VAL:HG23	1:A:140:PHE:O	2.15	0.45
1:A:210:LEU:N	1:A:213:LEU:H	2.15	0.45
1:A:252:ARG:HE	1:A:252:ARG:HB2	1.34	0.45
1:A:362:LEU:HD11	19:A:1128:CLA:CBB	2.45	0.45
1:A:401:TRP:HD1	19:A:1126:CLA:CHC	2.30	0.45
1:A:496:HIS:O	1:A:499:ALA:HB2	2.17	0.45
1:A:569:ILE:HG22	1:A:571:ASP:N	2.32	0.45
1:A:708:VAL:O	1:A:711:HIS:HB2	2.17	0.45
19:A:1101:CLA:HMB1	19:A:1109:CLA:H18	1.99	0.45
2:B:7:ARG:HD2	2:B:7:ARG:N	2.31	0.45
2:B:57:ILE:HG12	19:B:1203:CLA:HMC2	1.97	0.45
2:B:141:PHE:O	2:B:144:PHE:N	2.50	0.45
2:B:305:LEU:O	2:B:308:HIS:CB	2.65	0.45
2:B:469:LYS:CG	2:B:470:THR:OG1	2.65	0.45
2:B:515:GLY:HA3	2:B:613:SER:CB	2.39	0.45
19:B:1203:CLA:H193	19:B:1203:CLA:H161	1.78	0.45
19:B:1230:CLA:H3A	19:B:1230:CLA:HBA1	1.70	0.45
4:D:104:TRP:NE1	4:D:127:ASN:OD1	2.48	0.45
5:E:89:SER:CB	5:E:106:ARG:NH1	2.57	0.45
6:F:124:GLU:N	6:F:127:LYS:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:128:LYS:O	6:F:129:ARG:CD	2.64	0.45
6:F:200:VAL:HG12	10:J:7:TYR:C	2.36	0.45
8:H:113:SER:HG	19:H:1207:CLA:H61	1.76	0.45
8:H:115:THR:O	8:H:116:ALA:CB	2.58	0.45
11:K:125:LYS:CB	11:K:128:GLY:H	2.26	0.45
22:K:7042:LMU:H6D	22:K:7042:LMU:C3	2.44	0.45
12:L:143:LEU:HA	12:L:146:THR:N	2.18	0.45
12:L:206:VAL:O	12:L:206:VAL:HG22	2.17	0.45
13:N:136:ASP:O	13:N:137:LEU:CD2	2.51	0.45
15:1:114:TRP:CZ3	15:1:121:GLN:CA	2.96	0.45
16:2:215:LYS:HB2	16:2:217:LEU:HG	1.98	0.45
16:2:241:TYR:CD2	16:2:242:THR:N	2.84	0.45
22:2:7031:LMU:H21	22:2:7031:LMU:H52	1.56	0.45
17:3:98:LEU:O	17:3:101:GLY:HA3	2.16	0.45
17:3:108:PHE:CD2	19:3:3013:CLA:C4	2.99	0.45
17:3:176:TRP:C	17:3:178:LYS:N	2.67	0.45
19:3:3006:CLA:C3B	19:3:3013:CLA:H11	2.46	0.45
18:4:172:PHE:CD2	18:4:172:PHE:N	2.82	0.45
18:4:215:LEU:O	18:4:218:ILE:N	2.49	0.45
19:4:4001:CLA:HAA2	19:4:4001:CLA:HBD	1.99	0.45
1:A:105:ASN:HA	1:A:105:ASN:HD22	1.55	0.45
1:A:185:HIS:O	1:A:188:LYS:N	2.49	0.45
1:A:421:ASP:OD1	1:A:422:TYR:CD1	2.70	0.45
1:A:443:ILE:CG2	2:B:674:LEU:CD1	2.95	0.45
1:A:525:ASN:HD22	1:A:526:LYS:CE	2.24	0.45
1:A:555:ILE:HG23	2:B:670:TYR:CE2	2.51	0.45
1:A:685:VAL:O	1:A:688:PHE:HB3	2.17	0.45
1:A:691:MET:O	20:A:5001:PQN:O1	2.35	0.45
19:A:1110:CLA:HBD	19:A:1110:CLA:HAA1	1.98	0.45
19:A:1115:CLA:H93	19:A:1115:CLA:H61	1.81	0.45
19:A:1116:CLA:C4C	19:A:1116:CLA:H62	2.47	0.45
19:A:1138:CLA:HBC2	19:A:1139:CLA:NC	2.32	0.45
19:A:9012:CLA:H41	19:A:9012:CLA:H62	1.80	0.45
2:B:302:LYS:HZ3	7:G:103:GLY:HA3	1.78	0.45
2:B:315:LEU:CD1	2:B:316:GLY:C	2.85	0.45
2:B:444:LEU:C	2:B:446:PHE:N	2.68	0.45
2:B:606:VAL:O	2:B:608:GLN:N	2.49	0.45
2:B:608:GLN:O	2:B:608:GLN:HG3	2.16	0.45
3:C:12:ILE:CG2	3:C:39:ILE:HA	2.47	0.45
4:D:74:LEU:CD1	12:L:58:GLN:OE1	2.64	0.45
4:D:101:VAL:O	4:D:101:VAL:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:111:ASN:CG	5:E:116:SER:CB	2.85	0.45
19:H:1145:CLA:H3A	19:H:1145:CLA:HBA1	1.35	0.45
10:J:22:LEU:O	10:J:23:ALA:C	2.55	0.45
22:N:7049:LMU:H41	22:N:7049:LMU:H5'	1.98	0.45
15:1:205:GLN:HE21	15:1:205:GLN:HB2	1.62	0.45
16:2:167:ARG:NE	16:2:168:TRP:H	2.10	0.45
17:3:154:ASN:O	17:3:158:PHE:CZ	2.70	0.45
19:3:3006:CLA:HHC	19:3:3013:CLA:H11	1.98	0.45
19:4:1304:CLA:C2	19:4:1304:CLA:O1A	2.64	0.45
1:A:75:SER:HB3	1:A:354:TRP:CE2	2.52	0.45
1:A:170:GLY:C	1:A:173:VAL:HG22	2.37	0.45
1:A:213:LEU:HD12	1:A:311:LEU:HD21	1.97	0.45
1:A:254:LEU:HA	1:A:254:LEU:HD13	1.41	0.45
1:A:413:HIS:ND1	1:A:416:ILE:HD12	2.32	0.45
1:A:569:ILE:CG1	1:A:586:ARG:NH1	2.80	0.45
1:A:639:ALA:O	1:A:640:GLY:C	2.53	0.45
1:A:668:TYR:HA	2:B:445:ALA:HB1	1.98	0.45
1:A:708:VAL:HA	1:A:711:HIS:CD2	2.52	0.45
19:A:1104:CLA:O1A	19:A:1128:CLA:HMB2	2.16	0.45
19:A:1106:CLA:HBA2	19:A:1106:CLA:H3A	1.35	0.45
2:B:29:HIS:CG	19:B:1202:CLA:CBB	2.99	0.45
2:B:175:LEU:HD13	19:B:1221:CLA:O2D	2.16	0.45
2:B:182:LEU:O	2:B:186:SER:HB2	2.17	0.45
2:B:726:ILE:C	2:B:728:SER:H	2.19	0.45
19:B:1203:CLA:H41	24:B:7101:LMG:H321	1.98	0.45
3:C:44:ARG:CD	4:D:182:GLN:NE2	2.80	0.45
3:C:72:GLU:CB	3:C:77:MET:HE2	2.45	0.45
5:E:111:ASN:HB3	5:E:116:SER:HG	1.78	0.45
6:F:129:ARG:HD2	6:F:129:ARG:HA	1.61	0.45
7:G:109:GLU:HG3	7:G:109:GLU:O	2.17	0.45
19:G:1242:CLA:HBC3	19:G:1242:CLA:HHD	1.97	0.45
19:H:1207:CLA:HMA2	19:H:1207:CLA:C1	2.46	0.45
10:J:5:LYS:CE	16:2:178:ASN:CG	2.85	0.45
12:L:54:TYR:HE1	12:L:57:ILE:CG2	2.28	0.45
21:L:6019:BCR:C8	21:L:6019:BCR:H331	2.46	0.45
15:1:68:GLY:O	15:1:73:PRO:CD	2.65	0.45
15:1:151:GLN:NE2	15:1:151:GLN:N	2.56	0.45
15:1:183:LEU:O	15:1:184:LYS:C	2.54	0.45
16:2:160:ILE:HG22	16:2:161:GLY:N	2.32	0.45
16:2:249:ASN:O	16:2:250:LEU:C	2.47	0.45
19:2:2007:CLA:CGA	19:2:2007:CLA:C1A	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:3008:CLA:CGA	19:3:3008:CLA:O1D	2.64	0.45
19:4:1304:CLA:H161	19:4:1304:CLA:H122	1.38	0.45
1:A:42:ARG:O	1:A:44:ILE:N	2.49	0.45
1:A:74:ILE:O	1:A:76:ARG:N	2.50	0.45
1:A:119:SER:CA	1:A:145:ILE:HD12	2.47	0.45
1:A:249:ILE:HG22	17:3:137:PHE:HE2	1.82	0.45
1:A:284:ARG:N	1:A:298:ASP:OD1	2.49	0.45
1:A:418:MET:O	1:A:564:ARG:HD2	2.16	0.45
1:A:421:ASP:H	1:A:422:TYR:HD1	1.64	0.45
1:A:536:THR:HA	1:A:539:PHE:CB	2.46	0.45
19:A:1117:CLA:HAC2	21:A:6003:BCR:H352	1.98	0.45
19:A:1126:CLA:H171	21:J:6012:BCR:H351	1.98	0.45
22:A:7010:LMU:O5'	22:K:7047:LMU:H122	2.17	0.45
2:B:156:HIS:O	2:B:163:PRO:HB3	2.17	0.45
2:B:167:TRP:CZ2	19:B:1210:CLA:HAC2	2.52	0.45
2:B:255:LEU:HA	2:B:271:THR:OG1	2.16	0.45
2:B:284:PHE:CE1	19:B:1216:CLA:HHC	2.52	0.45
2:B:370:ALA:HB2	2:B:725:LEU:HD11	1.99	0.45
2:B:503:GLU:O	2:B:504:ASN:C	2.55	0.45
2:B:637:PRO:O	2:B:639:VAL:N	2.44	0.45
19:B:1223:CLA:H202	19:B:1223:CLA:H162	1.80	0.45
3:C:36:ALA:O	3:C:37:LYS:CG	2.65	0.45
3:C:44:ARG:HG3	3:C:44:ARG:O	2.17	0.45
4:D:113:GLU:O	4:D:114:MET:CB	2.59	0.45
6:F:123:MET:C	6:F:127:LYS:HB2	2.37	0.45
6:F:181:TYR:CD2	6:F:181:TYR:C	2.90	0.45
19:F:1302:CLA:HMA1	21:F:6016:BCR:C5	2.47	0.45
7:G:101:GLU:HA	7:G:105:THR:HG21	1.12	0.45
7:G:137:VAL:O	7:G:137:VAL:CG2	2.60	0.45
7:G:149:TYR:CG	7:G:150:ASP:OD1	2.70	0.45
19:J:1311:CLA:O1A	19:J:1311:CLA:H152	2.16	0.45
11:K:58:VAL:CG1	11:K:59:THR:N	2.76	0.45
12:L:54:TYR:O	12:L:55:GLN:CB	2.65	0.45
12:L:148:TYR:O	12:L:151:SER:HB3	2.17	0.45
12:L:156:GLY:N	12:L:178:THR:HG21	2.32	0.45
12:L:207:LEU:HD23	12:L:208:ASP:C	2.37	0.45
13:N:90:GLU:OE1	13:N:91:TYR:CG	2.70	0.45
13:N:114:PHE:HE2	13:N:116:ARG:CD	2.29	0.45
13:N:155:GLU:CA	13:N:157:LYS:H	2.19	0.45
16:2:120:ILE:CG1	16:2:121:PHE:H	2.24	0.45
16:2:152:LEU:HD13	16:2:152:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:164:GLU:HG2	16:2:167:ARG:HD3	1.98	0.45
16:2:244:THR:O	16:2:245:GLY:C	2.55	0.45
18:4:201:LYS:O	18:4:205:ILE:HG23	2.17	0.45
1:A:98:PHE:HZ	19:A:1105:CLA:HMD3	1.79	0.45
1:A:159:THR:O	1:A:163:GLN:OE1	2.35	0.45
1:A:196:PHE:HD2	1:A:196:PHE:N	2.07	0.45
1:A:217:SER:CB	21:A:6002:BCR:H351	2.46	0.45
1:A:531:PRO:O	1:A:532:ILE:CB	2.65	0.45
19:A:1106:CLA:C4	21:A:6011:BCR:H383	2.46	0.45
19:A:1119:CLA:HMB2	19:A:1125:CLA:H92	1.99	0.45
19:A:1138:CLA:HBC1	21:F:6014:BCR:C33	2.47	0.45
2:B:129:LEU:HA	19:B:1211:CLA:HED3	1.99	0.45
2:B:172:GLU:HG3	2:B:301:ILE:CG1	2.47	0.45
2:B:193:HIS:HD2	19:B:1211:CLA:NC	2.15	0.45
2:B:289:LEU:O	19:B:1218:CLA:HAC1	2.16	0.45
2:B:355:LEU:HD11	19:B:1223:CLA:HMC2	1.99	0.45
19:B:1202:CLA:H2	19:B:1202:CLA:H62	1.37	0.45
6:F:80:ALA:O	6:F:81:GLY:C	2.55	0.45
6:F:199:ASP:HB2	10:J:7:TYR:O	2.17	0.45
7:G:99:HIS:CA	7:G:100:PHE:CB	2.62	0.45
11:K:55:LEU:O	11:K:58:VAL:CB	2.65	0.45
22:K:7041:LMU:H1B	22:K:7041:LMU:H4B	1.67	0.45
12:L:92:ALA:H	12:L:98:ARG:HH22	1.59	0.45
12:L:131:SER:CB	12:L:201:TYR:HE2	2.05	0.45
12:L:168:GLY:O	12:L:170:LYS:O	2.34	0.45
12:L:169:ARG:CZ	12:L:169:ARG:HA	2.47	0.45
19:L:1148:CLA:CED	19:L:1148:CLA:HAA1	2.46	0.45
15:1:161:LYS:CD	15:1:161:LYS:C	2.85	0.45
15:1:178:LYS:HD2	15:1:178:LYS:O	2.17	0.45
16:2:211:PRO:O	16:2:212:GLN:HB2	2.17	0.45
16:2:227:LEU:HD21	19:2:2004:CLA:C4B	2.46	0.45
16:2:250:LEU:HD23	16:2:251:PHE:CD1	2.52	0.45
18:4:89:ARG:CD	18:4:90:TRP:N	2.45	0.45
19:4:4006:CLA:HMA1	22:4:7034:LMU:C6	2.28	0.45
1:A:239:PRO:O	1:A:240:LYS:HB3	2.17	0.44
1:A:629:ASN:CG	1:A:630:ASP:H	2.21	0.44
19:A:1116:CLA:H12	19:A:1116:CLA:C4A	2.47	0.44
19:A:1132:CLA:H172	19:A:1136:CLA:H202	1.99	0.44
19:A:1132:CLA:H3A	19:A:1132:CLA:HBA1	1.78	0.44
21:A:6011:BCR:H322	21:J:6012:BCR:H391	1.97	0.44
2:B:38:THR:OG1	2:B:41:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:LEU:HD13	2:B:275:HIS:HB2	1.99	0.44
2:B:292:ARG:NH1	2:B:295:PHE:N	2.65	0.44
2:B:382:ILE:O	2:B:385:GLY:N	2.48	0.44
2:B:420:SER:H	2:B:422:LEU:H	1.65	0.44
2:B:535:VAL:CG1	2:B:536:LYS:N	2.79	0.44
2:B:580:VAL:HG11	2:B:710:LEU:HD11	1.98	0.44
2:B:593:TYR:CZ	19:B:1234:CLA:HBC2	2.52	0.44
2:B:697:PRO:CB	19:B:1238:CLA:HBC3	2.48	0.44
4:D:77:ASN:C	4:D:79:PRO:CD	2.86	0.44
4:D:95:GLN:HE21	4:D:96:VAL:N	2.16	0.44
4:D:131:LEU:HD13	4:D:136:GLN:HB3	1.99	0.44
4:D:140:LEU:CD2	4:D:144:LEU:CG	2.96	0.44
5:E:82:TYR:CB	5:E:83:TRP:HE3	2.20	0.44
5:E:89:SER:O	5:E:105:VAL:CA	2.65	0.44
7:G:151:PRO:O	7:G:151:PRO:CD	2.65	0.44
8:H:61:THR:C	8:H:62:THR:HG23	2.25	0.44
22:H:7028:LMU:O6'	22:H:7028:LMU:C1'	2.65	0.44
12:L:69:LEU:HD23	12:L:69:LEU:HA	1.80	0.44
12:L:112:GLY:HA2	12:L:115:VAL:HG22	1.99	0.44
15:1:58:ALA:HB3	15:1:59:PRO:HD2	1.99	0.44
15:1:70:GLY:N	15:1:73:PRO:CD	2.80	0.44
15:1:138:LEU:HA	15:1:141:GLU:HG3	1.99	0.44
22:3:7005:LMU:C2	22:3:7005:LMU:O5'	2.64	0.44
18:4:168:GLN:O	18:4:172:PHE:HD1	2.00	0.44
22:4:7033:LMU:H61	22:4:7033:LMU:H31	1.83	0.44
1:A:59:ALA:O	1:A:61:ALA:N	2.50	0.44
1:A:163:GLN:CA	1:A:166:CYS:HG	2.27	0.44
1:A:209:GLY:C	1:A:213:LEU:HB2	2.37	0.44
1:A:331:LEU:HD22	1:A:343:HIS:O	2.15	0.44
1:A:431:LEU:N	1:A:434:ARG:HB2	2.32	0.44
1:A:499:ALA:HB1	19:A:1133:CLA:O2D	2.14	0.44
1:A:555:ILE:HD11	19:A:9023:CLA:CMD	2.48	0.44
1:A:567:ARG:HH11	4:D:89:GLY:N	2.15	0.44
19:A:1120:CLA:C2D	19:A:1121:CLA:HMB3	2.47	0.44
2:B:120:VAL:CA	2:B:123:TRP:NE1	2.71	0.44
2:B:131:THR:O	2:B:135:LEU:N	2.49	0.44
2:B:256:THR:OG1	2:B:257:ILE:N	2.50	0.44
2:B:261:PHE:HE2	2:B:499:ASN:O	2.00	0.44
2:B:279:ALA:HA	19:B:1213:CLA:HMA1	1.99	0.44
2:B:378:ILE:HG22	2:B:379:ALA:N	2.32	0.44
2:B:458:ILE:N	19:B:1235:CLA:HMD1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:TRP:HB3	2:B:494:LEU:H	1.54	0.44
2:B:584:LEU:HD11	2:B:714:SER:OG	2.18	0.44
2:B:597:LYS:HG2	19:B:1234:CLA:HBC1	1.99	0.44
2:B:644:SER:O	2:B:645:VAL:C	2.54	0.44
2:B:718:ILE:HD11	19:B:1224:CLA:HHC	1.97	0.44
19:B:1226:CLA:C20	19:B:1239:CLA:HBA1	2.47	0.44
4:D:145:ARG:NH1	4:D:173:TYR:HE1	2.12	0.44
5:E:85:LYS:HE3	5:E:85:LYS:HB3	1.67	0.44
5:E:127:GLU:HA	5:E:128:VAL:O	2.13	0.44
6:F:154:GLN:C	6:F:154:GLN:OE1	2.55	0.44
6:F:190:LYS:HZ2	6:F:192:THR:HG21	0.48	0.44
7:G:64:ILE:CG1	7:G:68:THR:HG23	2.45	0.44
7:G:76:ARG:HH12	7:G:120:VAL:N	2.16	0.44
7:G:119:PRO:HB3	19:G:1242:CLA:CBC	2.47	0.44
7:G:144:THR:OG1	7:G:147:ASN:C	2.56	0.44
11:K:86:LEU:O	11:K:87:GLU:HB2	2.16	0.44
11:K:111:VAL:HA	11:K:114:HIS:ND1	2.30	0.44
12:L:182:TRP:O	12:L:186:THR:HG23	2.17	0.44
19:L:1501:CLA:H3A	19:L:1501:CLA:HBA2	1.57	0.44
13:N:132:THR:HA	13:N:137:LEU:O	2.18	0.44
15:1:68:GLY:CA	15:1:72:VAL:HB	2.47	0.44
15:1:73:PRO:O	15:1:74:ALA:C	2.54	0.44
15:1:177:PRO:O	15:1:178:LYS:HG3	2.17	0.44
15:1:202:CYS:O	15:1:202:CYS:SG	2.71	0.44
16:2:131:ILE:C	16:2:133:ASN:H	2.20	0.44
17:3:124:LYS:NZ	17:3:148:TYR:N	2.65	0.44
18:4:173:LYS:CD	18:4:201:LYS:HG3	2.46	0.44
22:4:7053:LMU:H51	22:4:7053:LMU:H21	1.57	0.44
1:A:85:GLN:O	1:A:89:ILE:HG13	2.18	0.44
1:A:106:TYR:O	1:A:110:LEU:CD2	2.50	0.44
1:A:359:SER:OG	1:A:414:ALA:HB2	2.16	0.44
1:A:488:PHE:CD1	1:A:488:PHE:N	2.83	0.44
1:A:493:GLN:HE21	1:A:515:TRP:HA	1.82	0.44
1:A:499:ALA:HB3	1:A:500:PRO:HD2	1.99	0.44
1:A:502:THR:CG2	1:A:503:THR:N	2.81	0.44
19:A:1103:CLA:H161	19:A:1103:CLA:H202	1.62	0.44
19:A:1103:CLA:HMB3	19:A:1104:CLA:HAA1	1.99	0.44
19:A:1112:CLA:C4B	21:A:6002:BCR:C20	2.94	0.44
19:A:1140:CLA:H43	19:A:1140:CLA:C4C	2.46	0.44
2:B:244:PHE:HD2	2:B:245:GLY:N	2.15	0.44
2:B:292:ARG:CZ	2:B:297:ILE:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1220:CLA:H141	19:B:1220:CLA:H161	1.67	0.44
3:C:44:ARG:O	3:C:44:ARG:CG	2.65	0.44
4:D:80:SER:HB2	4:D:127:ASN:CA	2.47	0.44
6:F:200:VAL:CG2	6:F:203:ALA:C	2.85	0.44
7:G:75:GLY:C	7:G:77:PHE:H	2.20	0.44
7:G:84:ARG:NE	7:G:89:LYS:CD	2.80	0.44
10:J:26:LEU:HD23	10:J:26:LEU:O	2.17	0.44
14:R:5:UNK:O	14:R:6:UNK:CB	2.65	0.44
15:1:116:ALA:HA	15:1:117:LEU:HD22	1.99	0.44
15:1:177:PRO:HG2	15:1:180:LEU:CA	2.47	0.44
16:2:171:ILE:HG12	16:2:172:LEU:N	2.26	0.44
19:2:2006:CLA:H112	19:2:2006:CLA:H71	1.72	0.44
17:3:151:TRP:CG	17:3:152:ALA:N	2.84	0.44
17:3:200:PRO:O	17:3:201:ALA:C	2.54	0.44
17:3:224:LYS:O	17:3:226:LYS:N	2.50	0.44
19:4:1304:CLA:CAA	19:4:1304:CLA:O2D	2.65	0.44
22:4:7052:LMU:H12	22:4:7052:LMU:C5	2.47	0.44
1:A:308:ILE:CG1	19:A:1115:CLA:CBB	2.96	0.44
1:A:432:LEU:HB3	1:A:433:ASP:H	1.71	0.44
1:A:539:PHE:HE2	1:A:543:HIS:HE1	1.65	0.44
1:A:549:ILE:O	1:A:552:THR:O	2.34	0.44
1:A:615:HIS:ND1	19:A:1135:CLA:HBC3	2.32	0.44
1:A:669:GLY:CA	2:B:445:ALA:HA	2.44	0.44
2:B:120:VAL:CB	2:B:123:TRP:NE1	2.80	0.44
2:B:316:GLY:O	2:B:317:ARG:CD	2.64	0.44
2:B:495:PRO:HB2	2:B:496:GLY:H	1.40	0.44
19:B:1217:CLA:NA	19:B:1217:CLA:O2A	2.51	0.44
19:B:1229:CLA:H143	19:B:1229:CLA:H162	1.84	0.44
3:C:11:CYS:C	3:C:13:GLY:N	2.71	0.44
4:D:173:TYR:CZ	4:D:175:GLU:OE2	2.70	0.44
4:D:199:GLU:O	4:D:200:VAL:C	2.56	0.44
6:F:149:ILE:O	6:F:150:VAL:CG1	2.64	0.44
12:L:205:TYR:N	12:L:205:TYR:CD2	2.84	0.44
13:N:104:LYS:HB3	13:N:105:LYS:H	1.53	0.44
15:1:68:GLY:O	15:1:72:VAL:CA	2.64	0.44
16:2:113:ALA:CA	16:2:114:MET:HE3	2.45	0.44
16:2:183:PHE:O	16:2:184:PRO:C	2.55	0.44
17:3:93:ILE:HA	17:3:95:PRO:HD2	1.99	0.44
17:3:164:LEU:HD12	17:3:165:MET:SD	2.58	0.44
17:3:190:LEU:HD23	17:3:190:LEU:HA	1.78	0.44
19:3:3011:CLA:CAC	19:3:3012:CLA:C2A	2.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASP:CG	1:A:24:ARG:HD2	2.37	0.44
1:A:98:PHE:CD1	1:A:99:HIS:N	2.77	0.44
1:A:107:GLU:CD	1:A:161:GLU:CG	2.85	0.44
1:A:122:VAL:HG13	1:A:133:ASN:HD21	1.83	0.44
1:A:190:ALA:HA	1:A:191:PRO:HD3	1.77	0.44
1:A:218:TRP:CA	19:A:1112:CLA:HBB2	2.48	0.44
1:A:227:LEU:O	1:A:231:GLN:HB2	2.18	0.44
1:A:389:TYR:HD1	1:A:625:TRP:CD2	2.36	0.44
1:A:680:LEU:HB3	19:A:9012:CLA:C2	2.48	0.44
1:A:684:PHE:CD2	1:A:685:VAL:N	2.78	0.44
19:A:1107:CLA:HBA2	19:A:1107:CLA:CB D	2.47	0.44
19:A:1125:CLA:CBA	21:A:6008:BCR:H12C	2.45	0.44
19:A:1140:CLA:H71	19:A:9013:CLA:H171	1.98	0.44
2:B:33:SER:H	2:B:37:ILE:CD1	2.30	0.44
2:B:75:GLU:O	2:B:79:GLN:HG2	2.17	0.44
2:B:167:TRP:CZ2	19:B:1210:CLA:HAC1	2.53	0.44
2:B:469:LYS:CD	2:B:470:THR:CA	2.60	0.44
2:B:664:LEU:C	2:B:667:TRP:CZ3	2.76	0.44
2:B:697:PRO:HB3	19:B:1238:CLA:HBC3	1.99	0.44
19:B:1229:CLA:CBB	21:F:6014:BCR:C23	2.96	0.44
3:C:10:THR:HG23	5:E:101:TYR:HD2	1.67	0.44
4:D:99:PHE:CD1	4:D:99:PHE:O	2.71	0.44
4:D:141:GLY:N	4:D:143:ARG:N	2.66	0.44
7:G:116:SER:O	7:G:119:PRO:N	2.50	0.44
8:H:97:LEU:HG	8:H:98:LEU:N	2.32	0.44
11:K:49:ILE:CA	11:K:52:PRO:HG2	2.23	0.44
12:L:56:VAL:HG23	12:L:56:VAL:O	2.17	0.44
12:L:108:TYR:C	12:L:109:LEU:O	2.52	0.44
12:L:114:PHE:N	12:L:114:PHE:CD1	2.85	0.44
12:L:138:VAL:CG2	12:L:194:ILE:HG13	2.47	0.44
12:L:146:THR:C	12:L:148:TYR:N	2.69	0.44
13:N:113:ASN:OD1	13:N:113:ASN:C	2.56	0.44
16:2:97:GLU:OE1	16:2:97:GLU:N	2.51	0.44
16:2:156:GLU:OE2	19:2:2013:CLA:HHD	2.11	0.44
16:2:184:PRO:N	16:2:187:LYS:CG	2.74	0.44
16:2:195:TYR:HD1	16:2:196:PRO:N	2.14	0.44
16:2:226:ARG:NH1	16:2:226:ARG:HG2	2.33	0.44
17:3:151:TRP:HD1	17:3:152:ALA:N	1.97	0.44
17:3:226:LYS:O	17:3:226:LYS:HG2	2.18	0.44
1:A:51:THR:CG2	1:A:723:ARG:HB2	2.47	0.44
1:A:148:GLY:C	1:A:149:PHE:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:CYS:O	1:A:453:LEU:O	2.35	0.44
1:A:527:VAL:CB	1:A:626:GLY:HA3	2.41	0.44
1:A:723:ARG:CG	1:A:723:ARG:NH1	2.57	0.44
1:A:729:GLN:HE21	19:A:1140:CLA:HMD1	1.83	0.44
19:A:1119:CLA:HBA1	19:A:1123:CLA:CBB	2.46	0.44
19:A:1139:CLA:C4	6:F:198:ILE:HD13	2.45	0.44
19:A:1140:CLA:C6	19:A:9013:CLA:H193	2.45	0.44
22:A:7023:LMU:H41	22:A:7023:LMU:H92	1.99	0.44
2:B:55:ALA:HB1	2:B:150:LEU:HD11	2.00	0.44
2:B:182:LEU:HD13	19:B:1210:CLA:HHB	1.99	0.44
2:B:387:PHE:HB2	2:B:534:LEU:HD13	1.98	0.44
3:C:9:ASP:OD1	3:C:61:ASP:HB2	2.17	0.44
3:C:62:PHE:CD1	5:E:80:GLU:CB	3.00	0.44
4:D:148:TYR:O	4:D:149:LYS:NZ	2.44	0.44
4:D:151:LYS:HB3	4:D:151:LYS:HE2	1.72	0.44
5:E:122:LEU:O	5:E:124:GLU:C	2.56	0.44
5:E:128:VAL:C	5:E:129:GLU:O	2.56	0.44
7:G:79:PHE:CE2	7:G:80:PHE:HB2	2.53	0.44
8:H:89:ALA:HB3	8:H:90:PRO:HD3	1.99	0.44
8:H:112:LEU:HD22	8:H:112:LEU:HA	1.74	0.44
9:I:12:VAL:CG1	21:I:6018:BCR:H271	2.48	0.44
22:K:7042:LMU:O2B	22:K:7042:LMU:C5'	2.59	0.44
12:L:83:LEU:HD13	12:L:88:ALA:HB3	1.98	0.44
12:L:208:ASP:OD2	12:L:208:ASP:C	2.55	0.44
13:N:90:GLU:OE2	13:N:91:TYR:N	2.51	0.44
22:R:7022:LMU:H81	22:R:7022:LMU:H111	1.72	0.44
15:1:73:PRO:HD2	15:1:74:ALA:H	1.82	0.44
16:2:128:LYS:HG3	16:2:131:ILE:HG23	1.98	0.44
16:2:164:GLU:HB3	19:2:2012:CLA:CHB	2.47	0.44
17:3:96:ARG:NH2	17:3:100:TYR:OH	2.51	0.44
17:3:164:LEU:O	17:3:167:PHE:HB2	2.18	0.44
22:3:7005:LMU:O1'	22:3:7005:LMU:C5	2.63	0.44
18:4:158:GLN:HB3	19:4:1004:CLA:HMA3	0.45	0.44
18:4:232:LEU:HB3	18:4:236:ILE:HD13	1.99	0.44
1:A:49:ASP:HA	6:F:193:GLN:OE1	2.18	0.44
1:A:93:LEU:HA	1:A:96:MET:CG	2.48	0.44
1:A:132:LEU:O	1:A:671:SER:C	2.52	0.44
1:A:357:GLN:OE1	1:A:357:GLN:O	2.36	0.44
1:A:358:LEU:HD11	1:A:413:HIS:CD2	2.48	0.44
1:A:370:ILE:HD11	19:A:1124:CLA:O1D	2.17	0.44
1:A:538:ASP:O	1:A:542:HIS:CD2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:GLY:HA3	2:B:668:ARG:HB3	1.99	0.44
1:A:648:THR:C	1:A:650:ASN:H	2.21	0.44
2:B:10:GLN:HE21	2:B:10:GLN:HB2	1.53	0.44
2:B:160:LYS:NZ	2:B:161:TRP:HB3	2.32	0.44
2:B:294:ASN:CB	7:G:94:GLN:CG	2.96	0.44
2:B:488:ALA:HB2	19:B:1233:CLA:C2C	2.48	0.44
2:B:510:LEU:CD2	2:B:597:LYS:HD2	2.47	0.44
2:B:707:LEU:HD13	24:B:7101:LMG:H331	1.98	0.44
19:B:1229:CLA:HBD	19:B:1229:CLA:HBA1	1.98	0.44
4:D:83:PHE:CZ	4:D:114:MET:HE3	2.51	0.44
4:D:110:GLN:O	4:D:122:MET:HG3	2.18	0.44
5:E:81:SER:OG	5:E:120:TYR:CE1	2.68	0.44
6:F:207:LEU:C	6:F:209:ARG:H	2.21	0.44
7:G:144:THR:O	7:G:144:THR:CG2	2.66	0.44
11:K:110:GLY:O	11:K:114:HIS:CG	2.70	0.44
12:L:76:SER:H	12:L:79:ILE:HG22	1.83	0.44
12:L:153:PHE:CG	12:L:155:GLU:OE1	2.71	0.44
12:L:155:GLU:CA	12:L:178:THR:HG21	2.43	0.44
13:N:126:LYS:NZ	13:N:126:LYS:HB3	2.32	0.44
15:1:138:LEU:HA	15:1:141:GLU:CD	2.38	0.44
16:2:137:TRP:CD1	16:2:139:THR:HG22	2.53	0.44
19:3:3008:CLA:CBC	19:3:3008:CLA:CMC	2.86	0.44
18:4:170:PRO:C	18:4:173:LYS:H	2.21	0.44
18:4:242:ASN:O	18:4:243:THR:CB	2.66	0.44
1:A:89:ILE:O	1:A:92:TRP:C	2.54	0.44
1:A:159:THR:O	1:A:163:GLN:CD	2.56	0.44
1:A:406:LEU:HD11	19:A:1104:CLA:HMB3	1.99	0.44
1:A:620:MET:HG3	1:A:625:TRP:CE2	2.52	0.44
19:A:1119:CLA:HMB2	19:A:1123:CLA:HMA3	1.98	0.44
19:A:1126:CLA:H171	19:A:1126:CLA:H122	2.00	0.44
19:A:1131:CLA:HBB2	19:A:1132:CLA:H2	2.00	0.44
19:A:1141:CLA:H41	19:A:1141:CLA:H62	1.48	0.44
2:B:37:ILE:HG13	4:D:202:PHE:HD2	1.83	0.44
2:B:163:PRO:O	2:B:164:SER:CB	2.66	0.44
2:B:444:LEU:O	2:B:445:ALA:CB	2.62	0.44
2:B:535:VAL:HG13	2:B:536:LYS:H	1.83	0.44
19:B:1206:CLA:C4	21:I:6018:BCR:H21C	2.48	0.44
19:B:1218:CLA:HBA2	19:B:1219:CLA:O1A	2.18	0.44
19:B:1220:CLA:C4	19:B:1220:CLA:HAA1	2.33	0.44
22:B:7012:LMU:H1B	22:B:7012:LMU:H3'	1.36	0.44
3:C:59:PRO:HB3	3:C:61:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:84:PRO:HA	6:F:138:LEU:O	2.18	0.44
6:F:128:LYS:C	6:F:129:ARG:HD3	2.37	0.44
19:H:1505:CLA:H41	19:H:1505:CLA:C10	2.47	0.44
19:K:1143:CLA:H43	19:K:1143:CLA:O2A	2.18	0.44
12:L:68:SER:O	12:L:70:GLU:N	2.50	0.44
12:L:100:ILE:HG22	12:L:188:GLY:O	2.18	0.44
13:N:131:PHE:HA	13:N:133:GLY:H	1.83	0.44
14:R:34:UNK:C	14:R:36:UNK:O	2.66	0.44
15:1:161:LYS:HG3	15:1:162:LYS:N	2.33	0.44
15:1:189:LYS:CG	19:1:1007:CLA:CMC	2.53	0.44
15:1:223:ASP:HB3	15:1:224:PRO:HD2	1.99	0.44
16:2:122:ILE:CD1	19:2:2002:CLA:C2B	2.89	0.44
16:2:241:TYR:O	16:2:242:THR:C	2.52	0.44
17:3:155:TYR:HB2	17:3:157:LEU:HG	1.99	0.44
17:3:204:GLY:HA3	17:3:207:PHE:O	2.17	0.44
19:3:3016:CLA:CBC	19:3:3016:CLA:CMC	2.87	0.44
18:4:83:GLU:C	18:4:84:ASP:OD1	2.56	0.44
1:A:109:TRP:O	1:A:112:ASP:C	2.56	0.44
1:A:119:SER:OG	1:A:136:VAL:HG11	2.18	0.44
1:A:701:GLN:OE1	5:E:112:TYR:CZ	2.71	0.44
19:A:1124:CLA:HAA2	19:A:1125:CLA:OBD	2.18	0.44
2:B:214:ASP:OD1	2:B:214:ASP:O	2.36	0.44
2:B:586:THR:O	2:B:590:VAL:HG12	2.17	0.44
3:C:61:ASP:O	3:C:62:PHE:CD2	2.71	0.44
6:F:83:THR:CB	6:F:84:PRO:HD2	2.41	0.44
6:F:102:LEU:HD12	6:F:103:GLN:N	2.33	0.44
7:G:138:ALA:O	7:G:140:TYR:N	2.50	0.44
19:H:1145:CLA:CAA	19:H:1145:CLA:HED1	2.44	0.44
11:K:84:LEU:HG	11:K:85:LYS:N	2.33	0.44
11:K:127:ILE:HA	11:K:130:LEU:CD2	2.42	0.44
12:L:164:LEU:C	12:L:165:THR:HG22	2.37	0.44
12:L:173:PRO:CD	12:L:173:PRO:O	2.65	0.44
15:1:114:TRP:CH2	15:1:121:GLN:CG	2.95	0.44
15:1:114:TRP:HZ3	15:1:121:GLN:HA	1.76	0.44
16:2:112:TRP:CZ3	16:2:164:GLU:CG	2.97	0.44
19:3:3011:CLA:H92	19:3:3011:CLA:H142	1.99	0.44
18:4:172:PHE:O	18:4:194:PHE:CD2	2.71	0.44
1:A:133:ASN:HA	1:A:142:GLY:O	2.18	0.43
1:A:181:ALA:HA	1:A:184:PHE:HB3	1.99	0.43
1:A:398:HIS:HD2	19:A:1126:CLA:ND	2.15	0.43
1:A:473:PRO:C	1:A:475:ASP:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:HIS:O	1:A:716:VAL:HG22	2.18	0.43
19:A:1115:CLA:H61	19:A:1115:CLA:H41	1.68	0.43
19:A:1138:CLA:OBD	2:B:427:LEU:HD22	2.18	0.43
19:A:1139:CLA:OBD	6:F:182:LEU:HD11	2.18	0.43
2:B:14:GLN:O	2:B:15:ASP:C	2.56	0.43
2:B:31:PHE:CD1	19:B:1202:CLA:HMC2	2.53	0.43
2:B:170:ASN:O	2:B:171:ALA:HB3	2.18	0.43
2:B:304:ILE:O	2:B:308:HIS:CD2	2.71	0.43
2:B:309:ILE:HG22	2:B:319:HIS:HD2	1.82	0.43
2:B:310:PRO:HD2	2:B:311:PRO:CD	2.48	0.43
2:B:337:ALA:O	2:B:339:ALA:O	2.35	0.43
2:B:388:ALA:HA	2:B:391:PRO:CG	2.48	0.43
2:B:454:LEU:HD11	6:F:146:PRO:O	2.18	0.43
2:B:513:GLY:O	2:B:516:ASP:OD1	2.36	0.43
2:B:529:THR:O	2:B:532:LEU:HG	2.17	0.43
2:B:549:ASP:HB2	3:C:63:LEU:HB2	2.00	0.43
19:B:1206:CLA:H93	19:B:1206:CLA:H61	1.83	0.43
19:B:1223:CLA:C10	21:B:6010:BCR:H14C	2.48	0.43
3:C:12:ILE:HG21	3:C:39:ILE:CA	2.47	0.43
8:H:65:TRP:N	8:H:66:ASP:CA	2.74	0.43
8:H:109:LEU:HD23	19:H:1207:CLA:C6	2.47	0.43
19:H:1145:CLA:CGA	19:H:1145:CLA:C3A	2.95	0.43
11:K:125:LYS:HD2	11:K:128:GLY:CA	2.48	0.43
12:L:76:SER:OG	12:L:78:LEU:HD11	2.17	0.43
12:L:125:ILE:HG23	12:L:128:GLN:H	1.82	0.43
14:R:27:UNK:O	14:R:29:UNK:C	2.65	0.43
14:R:50:UNK:HA	14:R:51:UNK:HA	1.70	0.43
19:1:1303:CLA:CMC	19:4:1304:CLA:HMB3	2.43	0.43
16:2:101:TRP:N	16:2:103:VAL:CB	2.66	0.43
16:2:182:ILE:HG22	16:2:187:LYS:CD	2.48	0.43
16:2:182:ILE:CD1	16:2:187:LYS:O	2.64	0.43
17:3:204:GLY:CA	17:3:207:PHE:HA	2.48	0.43
18:4:158:GLN:O	19:4:1004:CLA:HMA2	2.13	0.43
18:4:204:GLU:O	18:4:205:ILE:C	2.54	0.43
18:4:220:GLN:CD	19:4:1306:CLA:CAC	2.85	0.43
22:4:7034:LMU:H92	22:4:7052:LMU:C1	2.47	0.43
1:A:23:ASP:CG	1:A:24:ARG:CD	2.87	0.43
1:A:36:LYS:HA	1:A:37:PRO:HD3	1.60	0.43
1:A:188:LYS:C	1:A:188:LYS:CD	2.65	0.43
1:A:336:GLY:HA3	19:A:1151:CLA:CMC	2.37	0.43
1:A:662:SER:HA	1:A:665:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1131:CLA:CB	19:A:1136:CLA:HBC2	2.48	0.43
2:B:98:GLN:H	2:B:99:PRO:HD2	1.82	0.43
2:B:175:LEU:HD21	19:B:1216:CLA:HMA3	1.99	0.43
2:B:216:LEU:HD11	2:B:221:GLY:HA2	2.00	0.43
2:B:224:PRO:HB3	2:B:227:THR:HG21	2.00	0.43
2:B:317:ARG:CZ	2:B:317:ARG:CB	2.94	0.43
2:B:618:GLY:HA2	2:B:621:ARG:N	2.31	0.43
19:B:1205:CLA:C14	19:B:1224:CLA:H91	2.44	0.43
19:B:1205:CLA:H193	19:B:1224:CLA:H192	1.99	0.43
19:B:1208:CLA:HBD	19:B:1208:CLA:C1	2.48	0.43
21:B:6010:BCR:C8	21:B:6010:BCR:H311	2.47	0.43
4:D:129:LEU:HD13	12:L:65:PHE:CD1	2.53	0.43
4:D:133:ARG:N	4:D:136:GLN:HE22	2.09	0.43
11:K:84:LEU:HD11	11:K:85:LYS:HE3	2.01	0.43
11:K:113:GLY:O	11:K:114:HIS:O	2.36	0.43
13:N:90:GLU:HA	13:N:91:TYR:CD2	2.53	0.43
13:N:146:LEU:HD22	17:3:142:ILE:O	2.11	0.43
16:2:100:ARG:O	16:2:101:TRP:C	2.55	0.43
16:2:147:THR:HG22	16:2:148:ASP:CG	2.35	0.43
16:2:226:ARG:HD3	16:2:226:ARG:HA	1.60	0.43
22:2:7006:LMU:H3'	22:2:7006:LMU:C5B	2.48	0.43
1:A:207:LEU:CG	19:A:1119:CLA:HBB2	2.49	0.43
1:A:244:LEU:HB3	1:A:247:GLU:HG2	1.92	0.43
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.39	0.43
1:A:262:PHE:CD2	1:A:262:PHE:C	2.91	0.43
1:A:270:PHE:HE1	19:A:1141:CLA:H2	1.78	0.43
19:A:1124:CLA:H61	19:A:1125:CLA:CED	2.49	0.43
19:A:1136:CLA:H18	19:A:1136:CLA:H151	1.84	0.43
22:A:7016:LMU:H112	22:A:7016:LMU:H71	1.97	0.43
2:B:293:THR:O	2:B:295:PHE:CE2	2.72	0.43
2:B:420:SER:HA	2:B:423:SER:OG	2.19	0.43
2:B:532:LEU:HA	2:B:535:VAL:HG12	2.00	0.43
19:B:1201:CLA:CHD	21:I:6021:BCR:H401	2.48	0.43
19:B:1201:CLA:HBA2	19:B:1201:CLA:H3A	1.57	0.43
19:B:1215:CLA:CGA	19:B:1215:CLA:C4A	2.96	0.43
19:B:1235:CLA:H41	21:F:6016:BCR:H323	2.00	0.43
6:F:136:TYR:HD1	6:F:138:LEU:CD1	2.30	0.43
11:K:124:LEU:O	11:K:126:ASN:HB3	2.17	0.43
12:L:79:ILE:O	12:L:80:ALA:C	2.56	0.43
12:L:110:LEU:HA	12:L:113:PRO:HG3	2.00	0.43
12:L:170:LYS:HE2	12:L:170:LYS:HB2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:7029:LMU:C4'	22:L:7029:LMU:C5B	2.82	0.43
13:N:138:ALA:O	13:N:139:LYS:HD2	2.17	0.43
15:1:176:ASP:HB3	15:1:180:LEU:HD11	1.74	0.43
16:2:182:ILE:CG2	16:2:187:LYS:HE2	2.48	0.43
19:2:2014:CLA:H91	19:2:2014:CLA:H151	1.96	0.43
18:4:177:LEU:CD2	18:4:177:LEU:C	2.84	0.43
18:4:198:LEU:HG	18:4:199:GLU:CA	2.48	0.43
18:4:220:GLN:HG3	19:4:1306:CLA:CAC	2.42	0.43
18:4:228:PRO:CG	18:4:228:PRO:O	2.66	0.43
1:A:22:VAL:H	1:A:25:ASP:HB2	1.83	0.43
1:A:27:ILE:O	1:A:28:LYS:CB	2.65	0.43
1:A:400:MET:HG3	1:A:609:ILE:HG23	2.00	0.43
1:A:401:TRP:CZ3	1:A:609:ILE:HB	2.52	0.43
1:A:411:ALA:O	1:A:412:ALA:C	2.57	0.43
1:A:478:SER:OG	1:A:481:ALA:N	2.45	0.43
1:A:599:PHE:CE2	1:A:735:VAL:CG2	3.00	0.43
1:A:707:ILE:HG12	1:A:707:ILE:H	1.49	0.43
19:A:1125:CLA:H101	19:A:1125:CLA:C14	2.44	0.43
19:A:1136:CLA:O1D	19:A:1136:CLA:H2A	2.18	0.43
2:B:285:LEU:HD11	19:B:1217:CLA:HBC2	2.00	0.43
2:B:304:ILE:O	2:B:308:HIS:CG	2.72	0.43
2:B:469:LYS:CG	2:B:470:THR:CB	2.97	0.43
2:B:493:TRP:CZ2	19:B:1214:CLA:C12	3.01	0.43
2:B:497:TRP:C	2:B:499:ASN:H	2.21	0.43
2:B:599:ILE:O	2:B:734:GLY:C	2.57	0.43
2:B:620:LEU:O	2:B:625:TRP:HB3	2.18	0.43
19:B:1216:CLA:C2	19:B:1221:CLA:H92	2.49	0.43
4:D:100:TYR:CE1	4:D:134:LYS:CD	2.88	0.43
4:D:100:TYR:CE1	4:D:134:LYS:HE2	2.50	0.43
6:F:90:GLN:CG	6:F:143:ASP:HA	2.48	0.43
19:H:1241:CLA:H92	19:H:1241:CLA:H62	1.88	0.43
22:K:7042:LMU:H32	22:K:7042:LMU:C5'	2.49	0.43
12:L:97:LEU:O	12:L:98:ARG:C	2.55	0.43
12:L:165:THR:O	12:L:166:LEU:C	2.57	0.43
16:2:128:LYS:C	16:2:130:GLY:N	2.66	0.43
16:2:243:GLY:N	16:2:244:THR:HG23	2.33	0.43
22:2:7027:LMU:O2'	22:2:7027:LMU:C1	2.66	0.43
17:3:103:VAL:C	17:3:107:ARG:HD2	2.38	0.43
18:4:190:ASN:HA	18:4:191:PRO:HD3	1.74	0.43
1:A:71:LEU:O	1:A:72:GLU:C	2.53	0.43
1:A:207:LEU:CB	19:A:1119:CLA:CBB	2.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:TYR:CD2	19:A:1127:CLA:HED3	2.53	0.43
1:A:457:SER:OG	1:A:544:ILE:HA	2.19	0.43
1:A:479:ASP:CA	1:A:536:THR:CG2	2.90	0.43
19:A:1102:CLA:HBB2	19:A:1104:CLA:CHA	2.49	0.43
19:A:1129:CLA:HMB2	19:L:1130:CLA:C4D	2.49	0.43
19:A:1131:CLA:H93	19:A:1131:CLA:H61	1.86	0.43
19:A:9023:CLA:H202	19:A:9023:CLA:H162	1.85	0.43
2:B:110:LEU:HD12	2:B:110:LEU:C	2.34	0.43
2:B:303:TYR:CA	2:B:306:GLU:CB	2.85	0.43
2:B:471:THR:HG23	2:B:502:ASN:HB2	1.99	0.43
2:B:514:PRO:HG2	6:F:147:HIS:CE1	2.54	0.43
19:B:1222:CLA:C2B	21:B:6010:BCR:C35	2.97	0.43
3:C:1:MET:N	3:C:4:SER:N	2.57	0.43
4:D:87:THR:HG23	12:L:69:LEU:CG	2.45	0.43
4:D:95:GLN:O	4:D:159:PRO:HG3	2.17	0.43
21:F:6016:BCR:C31	21:F:6016:BCR:HC8	2.40	0.43
7:G:69:GLY:O	7:G:72:LEU:CD1	2.67	0.43
8:H:114:ALA:O	8:H:115:THR:HG22	2.15	0.43
8:H:119:ASP:HB3	8:H:121:LEU:CG	2.47	0.43
10:J:41:PHE:CD1	10:J:41:PHE:N	2.87	0.43
22:K:7042:LMU:H81	22:K:7042:LMU:H52	1.52	0.43
13:N:136:ASP:CG	13:N:137:LEU:N	2.71	0.43
15:1:98:LEU:HA	15:1:98:LEU:HD22	1.45	0.43
16:2:269:LYS:CE	16:2:269:LYS:C	2.87	0.43
17:3:149:ASN:HA	17:3:150:TYR:HA	1.40	0.43
17:3:211:LEU:HD12	17:3:211:LEU:H	1.84	0.43
18:4:100:ARG:O	18:4:104:LEU:HD13	2.19	0.43
18:4:111:LEU:CD1	18:4:112:PRO:HD3	2.48	0.43
18:4:120:ILE:HD11	18:4:226:LYS:CA	2.48	0.43
1:A:334:HIS:HB3	19:A:1120:CLA:CMA	2.49	0.43
1:A:372:VAL:O	1:A:374:GLN:N	2.51	0.43
1:A:409:GLY:C	1:A:411:ALA:N	2.72	0.43
1:A:607:ASN:O	1:A:608:SER:C	2.57	0.43
2:B:172:GLU:HG3	2:B:301:ILE:HG12	2.00	0.43
2:B:212:PHE:HZ	19:B:1211:CLA:HAC1	1.77	0.43
2:B:500:ALA:CB	2:B:507:SER:O	2.66	0.43
2:B:568:CYS:HB3	2:B:569:ASP:H	1.65	0.43
19:B:1201:CLA:HBC3	19:B:1226:CLA:H41	2.00	0.43
19:B:1220:CLA:O1D	19:B:1220:CLA:OBD	2.35	0.43
19:B:1222:CLA:H11	19:B:1236:CLA:HBD	2.00	0.43
19:B:1225:CLA:H141	19:B:1225:CLA:H162	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ASP:OD1	4:D:134:LYS:NZ	2.51	0.43
6:F:167:PHE:HA	21:F:6014:BCR:C39	2.47	0.43
7:G:89:LYS:CE	7:G:89:LYS:CA	2.47	0.43
8:H:76:TYR:HH	12:L:90:ARG:HD3	1.72	0.43
22:H:7043:LMU:H71	22:H:7043:LMU:H112	2.00	0.43
11:K:56:ILE:C	11:K:59:THR:HG23	2.39	0.43
13:N:132:THR:O	13:N:133:GLY:C	2.55	0.43
15:1:71:GLU:OE1	15:1:76:LEU:HD11	2.17	0.43
15:1:97:ILE:HD13	15:1:98:LEU:HB2	1.78	0.43
15:1:117:LEU:HD13	15:1:117:LEU:H	1.78	0.43
15:1:155:GLU:HB2	15:1:160:LYS:HD2	1.99	0.43
15:1:177:PRO:CD	15:1:180:LEU:N	2.82	0.43
19:2:2004:CLA:HBC2	19:2:2004:CLA:HMC1	2.01	0.43
17:3:210:PRO:CD	17:3:211:LEU:HD12	2.48	0.43
19:3:3016:CLA:O1A	19:3:3016:CLA:CMA	2.67	0.43
1:A:23:ASP:OD2	1:A:33:GLN:HG2	2.16	0.43
1:A:40:PHE:O	1:A:44:ILE:HA	2.18	0.43
1:A:63:ASP:OD2	1:A:64:PHE:N	2.52	0.43
1:A:113:PRO:C	1:A:114:THR:HG22	2.29	0.43
1:A:183:TRP:CZ3	1:A:188:LYS:HB3	2.54	0.43
1:A:295:TRP:HB3	1:A:297:THR:CG2	2.48	0.43
1:A:338:PHE:CZ	19:A:1151:CLA:HBB1	2.38	0.43
1:A:561:LEU:HA	1:A:561:LEU:HD23	1.77	0.43
1:A:575:LEU:HD12	1:A:575:LEU:C	2.32	0.43
19:A:1105:CLA:HMB2	21:J:6012:BCR:HC7	1.98	0.43
19:A:9011:CLA:H111	19:A:9011:CLA:H71	1.87	0.43
2:B:188:LEU:HG	2:B:189:ALA:N	2.34	0.43
2:B:689:ASN:OD1	2:B:689:ASN:N	2.52	0.43
19:B:1209:CLA:C3C	19:B:1210:CLA:HBB2	2.40	0.43
20:B:5002:PQN:H192	21:B:6017:BCR:C8	2.48	0.43
22:B:7038:LMU:H1B	22:B:7038:LMU:C6'	2.48	0.43
4:D:140:LEU:HD13	4:D:144:LEU:CA	2.49	0.43
4:D:167:HIS:HD2	4:D:172:VAL:CG2	2.03	0.43
5:E:81:SER:O	5:E:82:TYR:C	2.53	0.43
6:F:117:LEU:CA	6:F:119:ILE:HG12	2.46	0.43
6:F:121:ALA:O	6:F:123:MET:N	2.50	0.43
6:F:205:SER:C	6:F:207:LEU:CD1	2.86	0.43
7:G:75:GLY:N	7:G:77:PHE:H	2.17	0.43
8:H:98:LEU:C	8:H:99:LYS:O	2.56	0.43
12:L:135:GLY:O	12:L:138:VAL:HG22	2.19	0.43
12:L:171:LYS:O	12:L:173:PRO:CD	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:204:LEU:CD1	12:L:205:TYR:C	2.85	0.43
13:N:139:LYS:HA	13:N:139:LYS:HD2	1.14	0.43
13:N:145:PHE:N	13:N:145:PHE:CD1	2.80	0.43
15:1:58:ALA:HB1	19:1:1015:CLA:C2B	2.48	0.43
15:1:77:GLU:CG	15:1:80:LYS:CE	2.96	0.43
15:1:114:TRP:HH2	15:1:121:GLN:HG3	1.75	0.43
15:1:136:THR:O	15:1:137:ILE:C	2.56	0.43
16:2:119:GLY:O	16:2:123:PRO:HD3	2.14	0.43
17:3:150:TYR:C	17:3:152:ALA:CB	2.83	0.43
17:3:238:ILE:HD13	17:3:238:ILE:N	2.34	0.43
18:4:193:ASN:O	18:4:201:LYS:NZ	2.52	0.43
19:4:1304:CLA:H3A	19:4:1304:CLA:HBA2	1.19	0.43
22:4:7053:LMU:C11	22:4:7053:LMU:C7	2.97	0.43
19:A:1120:CLA:HBA2	19:A:1120:CLA:H3A	1.84	0.43
19:A:1138:CLA:HBB2	19:B:1229:CLA:H43	2.00	0.43
2:B:29:HIS:CB	19:B:1226:CLA:HBA1	2.49	0.43
2:B:50:HIS:CA	2:B:53:GLN:HB2	2.49	0.43
2:B:161:TRP:O	2:B:162:LYS:C	2.57	0.43
2:B:224:PRO:CB	2:B:227:THR:CG2	2.96	0.43
2:B:323:TYR:HD2	7:G:104:ASP:H	1.65	0.43
2:B:431:PHE:CE2	19:B:1229:CLA:CED	3.02	0.43
2:B:517:PHE:O	2:B:517:PHE:CG	2.64	0.43
2:B:557:PHE:N	2:B:558:PRO:HD3	2.30	0.43
2:B:596:TRP:NE1	2:B:623:TYR:HB2	2.34	0.43
3:C:61:ASP:CG	5:E:118:ASN:ND2	2.72	0.43
4:D:103:THR:HG22	4:D:128:LEU:CB	2.48	0.43
6:F:96:LYS:O	6:F:97:GLN:O	2.36	0.43
8:H:94:ARG:HD2	12:L:183:ALA:HB1	2.00	0.43
9:I:24:LEU:HD23	21:L:6019:BCR:H23C	2.01	0.43
12:L:102:VAL:HG22	19:L:1502:CLA:HED2	2.01	0.43
12:L:111:VAL:O	12:L:115:VAL:N	2.52	0.43
12:L:174:ASP:O	12:L:175:GLN:O	2.36	0.43
16:2:148:ASP:O	16:2:151:THR:N	2.52	0.43
17:3:187:PHE:HD1	17:3:188:LEU:N	2.08	0.43
18:4:198:LEU:CG	18:4:199:GLU:N	2.59	0.43
18:4:245:VAL:HG22	18:4:246:GLN:H	1.82	0.43
1:A:369:THR:O	1:A:372:VAL:HB	2.19	0.43
1:A:408:VAL:HG11	1:A:602:LEU:HD23	2.00	0.43
1:A:711:HIS:CB	1:A:717:ALA:HB2	2.43	0.43
2:B:242:HIS:O	2:B:243:LEU:HB2	2.19	0.43
2:B:290:MET:O	2:B:299:HIS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:HIS:CE1	19:B:1229:CLA:NB	2.72	0.43
2:B:662:MET:O	2:B:663:PHE:C	2.57	0.43
19:B:1203:CLA:H3A	19:B:1203:CLA:HBA1	1.74	0.43
19:B:1209:CLA:HMC2	21:B:6005:BCR:H373	2.01	0.43
19:B:1214:CLA:HBA2	19:B:1214:CLA:H3A	1.33	0.43
19:B:1220:CLA:C2A	19:B:1220:CLA:CGD	2.96	0.43
4:D:122:MET:O	4:D:123:ARG:HB3	2.19	0.43
5:E:86:GLY:HA3	5:E:109:LYS:NZ	2.33	0.43
6:F:205:SER:O	6:F:207:LEU:CD1	2.67	0.43
6:F:207:LEU:C	6:F:209:ARG:N	2.69	0.43
9:I:8:PHE:CZ	21:I:6021:BCR:C7	3.02	0.43
11:K:60:SER:O	11:K:63:LEU:CD2	2.67	0.43
11:K:127:ILE:HG23	11:K:130:LEU:CD1	2.46	0.43
12:L:207:LEU:HD23	12:L:208:ASP:N	2.33	0.43
16:2:148:ASP:CA	16:2:152:LEU:HB3	2.41	0.43
16:2:186:ASN:O	16:2:187:LYS:CB	2.65	0.43
22:2:7046:LMU:H41	22:2:7046:LMU:H6D	2.01	0.43
17:3:197:SER:CB	17:3:206:PRO:CG	2.97	0.43
19:3:3016:CLA:H41	19:3:3016:CLA:H61	1.58	0.43
21:3:6022:BCR:H14C	21:3:6022:BCR:H11C	1.56	0.43
18:4:85:PRO:HB3	18:4:188:ILE:HA	2.00	0.43
19:4:1306:CLA:H92	19:4:1306:CLA:H61	1.87	0.43
1:A:615:HIS:CE1	19:A:1135:CLA:CBC	3.00	0.43
1:A:732:ALA:HB1	19:A:1140:CLA:HED2	2.01	0.43
19:A:1134:CLA:HBD	19:A:1134:CLA:HAA1	2.01	0.43
19:A:9013:CLA:HHH	19:A:9013:CLA:HAC1	1.88	0.43
2:B:98:GLN:CA	2:B:98:GLN:HE21	2.30	0.43
2:B:119:GLY:O	2:B:122:GLN:OE1	2.37	0.43
2:B:222:LEU:HA	19:B:1212:CLA:CMD	2.40	0.43
2:B:444:LEU:HD23	2:B:452:GLN:HE22	1.80	0.43
2:B:456:GLU:HA	2:B:514:PRO:HG3	2.01	0.43
2:B:496:GLY:O	2:B:499:ASN:HB2	2.19	0.43
7:G:90:GLN:HB2	7:G:91:VAL:C	2.36	0.43
22:H:7011:LMU:C7	22:H:7011:LMU:C11	2.94	0.43
10:J:5:LYS:HE3	16:2:178:ASN:CG	2.38	0.43
19:K:1143:CLA:O2A	19:K:1143:CLA:C4	2.67	0.43
22:R:7022:LMU:O2'	22:R:7022:LMU:H1B	2.19	0.43
15:1:171:LEU:N	15:1:171:LEU:CD2	2.81	0.43
16:2:156:GLU:OE2	19:2:2013:CLA:C1D	2.67	0.43
16:2:157:LEU:HD11	19:2:2012:CLA:HMC3	2.00	0.43
18:4:110:LEU:HA	18:4:113:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:7053:LMU:C1B	22:4:7053:LMU:C6'	2.89	0.43
1:A:119:SER:OG	1:A:143:ILE:C	2.57	0.42
1:A:255:LEU:O	1:A:259:TYR:O	2.37	0.42
1:A:498:LEU:HD23	1:A:498:LEU:HA	1.83	0.42
1:A:538:ASP:O	1:A:542:HIS:HD2	2.02	0.42
1:A:600:LEU:HD13	19:A:9023:CLA:HMD3	2.00	0.42
1:A:682:ALA:HA	1:A:685:VAL:HB	2.01	0.42
1:A:744:ALA:HA	1:A:747:TRP:HB3	2.00	0.42
2:B:229:GLN:O	7:G:63:VAL:CG1	2.67	0.42
2:B:315:LEU:CD1	2:B:315:LEU:O	2.54	0.42
2:B:390:GLY:HA3	21:B:6010:BCR:HC22	2.01	0.42
2:B:395:ILE:HG21	2:B:554:GLY:HA3	2.00	0.42
2:B:498:LEU:O	2:B:499:ASN:OD1	2.36	0.42
2:B:721:TYR:HA	2:B:724:PHE:HB3	2.00	0.42
19:B:1222:CLA:HMB3	21:B:6010:BCR:H351	1.99	0.42
20:B:5002:PQN:H192	21:B:6017:BCR:C10	2.49	0.42
3:C:74:THR:CG2	3:C:75:ARG:N	2.81	0.42
4:D:124:GLU:OE1	4:D:125:GLY:N	2.52	0.42
7:G:76:ARG:NH1	7:G:120:VAL:CB	2.78	0.42
7:G:96:GLY:O	7:G:97:LEU:HD23	2.18	0.42
8:H:70:SER:O	8:H:73:PRO:HD2	2.19	0.42
8:H:110:ALA:HA	8:H:113:SER:HB2	2.01	0.42
10:J:5:LYS:HE3	16:2:178:ASN:ND2	2.34	0.42
13:N:132:THR:CG2	13:N:139:LYS:CE	2.97	0.42
21:1:6023:BCR:C33	21:1:6023:BCR:H322	2.31	0.42
22:2:7027:LMU:H62	22:2:7027:LMU:H31	1.51	0.42
1:A:96:MET:O	1:A:99:HIS:HB2	2.18	0.42
1:A:154:ARG:HA	1:A:154:ARG:HD2	1.48	0.42
1:A:205:HIS:CG	19:A:1111:CLA:HMC2	2.54	0.42
1:A:396:PHE:CE2	1:A:616:PHE:CB	2.99	0.42
19:A:1237:CLA:H61	19:A:1237:CLA:C11	2.49	0.42
2:B:75:GLU:HB3	2:B:132:ASN:ND2	2.17	0.42
2:B:78:VAL:O	2:B:79:GLN:C	2.56	0.42
2:B:177:HIS:CE1	19:B:1209:CLA:NC	2.86	0.42
2:B:377:TYR:O	2:B:378:ILE:CB	2.66	0.42
2:B:414:HIS:CD2	2:B:414:HIS:O	2.72	0.42
2:B:476:ILE:HG21	2:B:479:SER:OG	2.12	0.42
2:B:575:ASP:O	2:B:579:ALA:N	2.49	0.42
2:B:710:LEU:H	2:B:713:PHE:H	1.66	0.42
3:C:9:ASP:OD1	3:C:61:ASP:CG	2.57	0.42
4:D:80:SER:HB2	4:D:127:ASN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:GLY:HA3	5:E:107:PHE:HB2	2.01	0.42
6:F:103:GLN:OE1	6:F:103:GLN:C	2.57	0.42
6:F:207:LEU:CD1	6:F:207:LEU:H	2.32	0.42
8:H:64:GLN:HB2	8:H:67:SER:N	2.23	0.42
12:L:209:LEU:HG	12:L:210:PRO:CD	2.49	0.42
14:R:8:UNK:CB	19:R:1144:CLA:O2D	2.67	0.42
16:2:150:THR:CA	16:2:152:LEU:CD1	2.97	0.42
16:2:189:THR:OG1	16:2:193:VAL:O	2.36	0.42
19:2:2002:CLA:HBA2	19:2:2002:CLA:H3A	1.76	0.42
19:2:2004:CLA:O1D	19:3:2009:CLA:HBB2	2.19	0.42
17:3:133:ALA:HB3	17:3:134:LEU:CG	2.49	0.42
17:3:210:PRO:HG2	17:3:211:LEU:N	2.33	0.42
17:3:233:LEU:C	17:3:236:LEU:H	2.22	0.42
1:A:27:ILE:O	1:A:27:ILE:CG2	2.54	0.42
1:A:159:THR:O	1:A:160:SER:OG	2.34	0.42
1:A:249:ILE:HG23	17:3:137:PHE:CZ	2.54	0.42
1:A:337:PRO:HB2	19:A:1151:CLA:HBB2	2.00	0.42
1:A:427:ARG:HG2	1:A:428:TYR:HA	2.02	0.42
1:A:452:PHE:CD1	19:A:1136:CLA:HBB2	2.54	0.42
1:A:476:MET:O	1:A:477:PHE:HB2	2.19	0.42
1:A:551:VAL:HG21	1:A:604:TRP:CZ2	2.53	0.42
1:A:569:ILE:HG22	1:A:572:LYS:N	2.34	0.42
1:A:628:ILE:HD11	1:A:629:ASN:O	2.20	0.42
19:A:1119:CLA:C1C	19:A:1125:CLA:H171	2.49	0.42
19:A:1126:CLA:C7	21:A:6011:BCR:H372	2.49	0.42
19:A:1135:CLA:H11	19:A:1136:CLA:O1A	2.19	0.42
19:A:1139:CLA:O1A	19:A:1139:CLA:C4	2.67	0.42
19:A:1141:CLA:O1A	19:A:1141:CLA:H2A	2.08	0.42
2:B:120:VAL:CG1	2:B:123:TRP:CD1	3.01	0.42
2:B:267:SER:OG	2:B:268:LEU:N	2.49	0.42
2:B:289:LEU:HA	19:B:1217:CLA:O1D	2.19	0.42
2:B:366:THR:HA	2:B:729:THR:HG21	2.00	0.42
2:B:449:PRO:O	2:B:452:GLN:CB	2.67	0.42
2:B:463:ILE:CG2	2:B:467:HIS:HE1	2.32	0.42
2:B:490:ARG:NH1	2:B:490:ARG:CG	2.47	0.42
2:B:493:TRP:CZ3	19:B:1232:CLA:CMA	3.01	0.42
2:B:633:ASN:HB2	2:B:636:THR:H	1.84	0.42
2:B:684:ARG:HD3	2:B:684:ARG:HA	1.76	0.42
19:B:1206:CLA:HED1	19:I:1204:CLA:HMA2	2.00	0.42
19:B:1238:CLA:H172	19:B:1239:CLA:H13	2.02	0.42
4:D:101:VAL:HG12	4:D:130:LYS:HB3	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:77:PHE:CE2	7:G:79:PHE:CD2	3.07	0.42
7:G:150:ASP:N	7:G:151:PRO:HD3	2.33	0.42
19:K:1142:CLA:OBD	19:K:1143:CLA:C1B	2.68	0.42
12:L:111:VAL:H	12:L:113:PRO:HD2	1.84	0.42
15:1:116:ALA:CA	15:1:117:LEU:HD22	2.49	0.42
16:2:204:LEU:CD1	16:2:210:SER:O	2.62	0.42
16:2:224:ASN:HD21	16:2:227:LEU:HD23	1.84	0.42
18:4:122:ASN:OD1	18:4:124:PRO:HA	2.19	0.42
18:4:144:ILE:HA	18:4:147:ILE:CD1	2.49	0.42
18:4:231:ASN:O	18:4:235:HIS:HB3	2.18	0.42
22:4:7034:LMU:C10	22:4:7052:LMU:H2'	2.45	0.42
1:A:350:LEU:O	1:A:350:LEU:CD2	2.67	0.42
1:A:427:ARG:HE	1:A:428:TYR:HD1	1.66	0.42
1:A:645:SER:O	1:A:651:GLY:HA3	2.19	0.42
1:A:733:VAL:HG13	1:A:737:HIS:CE1	2.54	0.42
19:A:1131:CLA:O1A	19:A:1237:CLA:C1	2.65	0.42
19:A:1132:CLA:H41	19:A:1132:CLA:H61	1.60	0.42
2:B:50:HIS:HA	2:B:53:GLN:H	1.85	0.42
2:B:230:TRP:H	7:G:63:VAL:CG2	2.23	0.42
2:B:299:HIS:CE1	19:B:1219:CLA:OBD	2.73	0.42
2:B:310:PRO:HG3	19:B:1220:CLA:CMA	2.33	0.42
2:B:316:GLY:O	2:B:317:ARG:HD2	2.19	0.42
2:B:424:TRP:CH2	19:B:1228:CLA:HAC1	2.55	0.42
2:B:486:LEU:O	2:B:487:ASN:HB3	2.20	0.42
2:B:674:LEU:O	2:B:678:LEU:HB2	2.19	0.42
4:D:123:ARG:HH21	22:D:7050:LMU:C5B	2.13	0.42
4:D:137:CYS:O	4:D:138:LEU:C	2.55	0.42
6:F:88:SER:O	6:F:91:PHE:HB3	2.19	0.42
21:I:6018:BCR:H272	21:I:6021:BCR:H352	2.01	0.42
10:J:36:ALA:O	10:J:37:LEU:HB2	2.18	0.42
19:J:1308:CLA:CBD	19:J:1308:CLA:CGA	2.97	0.42
13:N:104:LYS:O	13:N:105:LYS:C	2.58	0.42
13:N:147:SER:C	13:N:151:ASP:N	2.71	0.42
15:1:72:VAL:O	15:1:73:PRO:C	2.54	0.42
17:3:132:THR:CG2	17:3:133:ALA:N	2.82	0.42
17:3:236:LEU:C	17:3:238:ILE:H	2.17	0.42
19:3:3016:CLA:O1A	19:3:3016:CLA:C3A	2.68	0.42
22:3:7005:LMU:O2B	22:3:7005:LMU:C5'	2.67	0.42
1:A:94:SER:OG	1:A:95:GLY:N	2.53	0.42
1:A:249:ILE:CG2	17:3:137:PHE:CZ	3.03	0.42
1:A:331:LEU:CD2	1:A:343:HIS:C	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLN:C	1:A:376:MET:N	2.71	0.42
1:A:613:ILE:HG23	1:A:750:PHE:HE2	1.83	0.42
19:A:1131:CLA:C15	21:L:6019:BCR:C36	2.97	0.42
19:A:1138:CLA:HMC1	20:A:5001:PQN:H251	2.01	0.42
2:B:252:THR:HG22	2:B:252:THR:O	2.19	0.42
2:B:256:THR:N	2:B:271:THR:OG1	2.52	0.42
2:B:292:ARG:NE	2:B:292:ARG:HA	2.34	0.42
2:B:408:LEU:O	2:B:411:MET:HB2	2.20	0.42
2:B:596:TRP:CH2	2:B:612:SER:HB3	2.55	0.42
2:B:615:TYR:O	2:B:619:TRP:HD1	2.03	0.42
19:B:1234:CLA:HMC1	19:B:1234:CLA:CBC	2.35	0.42
4:D:77:ASN:HB3	4:D:79:PRO:HD3	2.01	0.42
4:D:139:ALA:O	4:D:142:THR:CG2	2.59	0.42
6:F:130:PHE:O	6:F:131:ASP:C	2.56	0.42
6:F:138:LEU:HD22	6:F:146:PRO:HB3	2.01	0.42
6:F:181:TYR:C	6:F:181:TYR:HD2	2.22	0.42
8:H:66:ASP:C	8:H:68:TYR:N	2.71	0.42
12:L:78:LEU:HD12	12:L:79:ILE:H	1.79	0.42
12:L:95:PRO:O	12:L:98:ARG:HG3	2.19	0.42
13:N:108:ALA:C	13:N:109:THR:HG1	2.23	0.42
13:N:112:ALA:O	13:N:113:ASN:C	2.58	0.42
13:N:134:CYS:O	13:N:136:ASP:O	2.37	0.42
13:N:155:GLU:CB	13:N:157:LYS:HA	2.50	0.42
16:2:167:ARG:HE	16:2:167:ARG:C	2.22	0.42
17:3:99:ALA:O	17:3:100:TYR:C	2.58	0.42
18:4:96:LEU:CD1	18:4:100:ARG:NE	2.83	0.42
18:4:217:PHE:CE1	18:4:221:HIS:CE1	3.08	0.42
18:4:233:LEU:H	18:4:233:LEU:HG	1.79	0.42
1:A:68:THR:HG22	1:A:70:ASP:O	2.20	0.42
1:A:149:PHE:HB3	1:A:153:TRP:CZ3	2.53	0.42
1:A:652:TRP:O	1:A:656:PHE:HB3	2.19	0.42
1:A:741:GLY:O	1:A:743:ILE:N	2.53	0.42
19:A:1101:CLA:C4	19:A:1140:CLA:H8	2.50	0.42
2:B:319:HIS:CE1	2:B:322:LEU:HD11	2.50	0.42
2:B:346:SER:O	2:B:350:GLN:N	2.50	0.42
2:B:429:LEU:HD11	19:B:1235:CLA:HMB3	2.00	0.42
2:B:450:GLU:O	2:B:451:LYS:HB2	2.19	0.42
2:B:488:ALA:CB	19:B:1233:CLA:C1C	2.96	0.42
19:B:1202:CLA:CAB	19:B:1203:CLA:HBA2	2.49	0.42
3:C:38:GLN:HE21	3:C:38:GLN:HB3	1.65	0.42
4:D:204:GLY:C	4:D:205:LYS:HE2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:VAL:CG1	5:E:92:ALA:H	2.26	0.42
6:F:97:GLN:HE21	6:F:97:GLN:HB3	1.52	0.42
12:L:104:LEU:HA	12:L:192:GLY:O	2.19	0.42
22:L:7029:LMU:O2'	22:L:7029:LMU:H11	2.20	0.42
14:R:38:UNK:C	14:R:42:UNK:CA	2.97	0.42
15:1:177:PRO:O	15:1:178:LYS:CB	2.68	0.42
16:2:104:GLN:CD	16:2:104:GLN:N	2.72	0.42
16:2:107:LEU:CD1	16:2:108:VAL:HG23	2.49	0.42
16:2:195:TYR:CD2	16:2:198:GLY:CA	2.93	0.42
17:3:95:PRO:C	17:3:96:ARG:CG	2.85	0.42
17:3:174:GLN:HE21	17:3:174:GLN:HB2	1.47	0.42
18:4:89:ARG:HD3	18:4:89:ARG:N	2.33	0.42
18:4:120:ILE:CG2	18:4:121:ILE:N	2.65	0.42
18:4:189:PHE:N	18:4:189:PHE:CD2	2.88	0.42
1:A:119:SER:HA	1:A:145:ILE:CD1	2.50	0.42
1:A:261:SER:C	1:A:262:PHE:CG	2.93	0.42
1:A:299:ILE:HA	1:A:299:ILE:HD12	1.78	0.42
19:A:1103:CLA:HBA1	19:A:1103:CLA:H3A	1.71	0.42
19:A:1136:CLA:H203	19:L:1130:CLA:HBB2	2.02	0.42
2:B:160:LYS:HB2	2:B:160:LYS:HE2	1.43	0.42
2:B:225:LEU:CA	2:B:227:THR:O	2.67	0.42
2:B:262:HIS:HB2	2:B:265:THR:O	2.20	0.42
2:B:278:LEU:O	2:B:279:ALA:C	2.58	0.42
2:B:556:SER:CA	2:B:558:PRO:HD2	2.50	0.42
2:B:628:SER:O	2:B:629:SER:O	2.38	0.42
7:G:83:GLN:O	7:G:84:ARG:CB	2.67	0.42
11:K:115:ILE:HG12	11:K:122:LEU:HD12	1.99	0.42
12:L:82:TYR:HE1	19:L:1130:CLA:H93	1.80	0.42
12:L:150:ILE:HD12	12:L:150:ILE:O	2.18	0.42
15:1:142:PHE:C	15:1:143:LEU:HD12	2.40	0.42
15:1:148:VAL:O	15:1:148:VAL:HG22	2.19	0.42
15:1:168:PHE:O	15:1:168:PHE:CD1	2.72	0.42
15:1:198:PHE:C	15:1:199:VAL:O	2.57	0.42
16:2:114:MET:HG2	16:2:227:LEU:CA	2.36	0.42
16:2:167:ARG:HB3	16:2:169:ALA:H	1.84	0.42
16:2:238:GLN:O	16:2:239:HIS:C	2.57	0.42
17:3:238:ILE:HG13	19:3:3003:CLA:HMC2	1.93	0.42
18:4:121:ILE:O	18:4:122:ASN:HB3	2.20	0.42
1:A:53:TRP:O	1:A:56:ASN:O	2.38	0.42
1:A:60:ASP:O	1:A:60:ASP:OD1	2.38	0.42
1:A:93:LEU:O	1:A:97:TYR:CD2	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:THR:O	1:A:271:THR:HG22	2.20	0.42
1:A:335:LYS:HG2	1:A:336:GLY:N	2.35	0.42
1:A:534:LEU:HB2	1:A:538:ASP:HB3	2.02	0.42
1:A:660:GLN:O	1:A:661:ALA:HB2	2.17	0.42
1:A:733:VAL:CG2	19:A:1140:CLA:C2D	2.87	0.42
19:A:1119:CLA:HMC1	19:A:1119:CLA:HBC3	1.99	0.42
2:B:126:THR:HG21	2:B:358:TYR:CE1	2.54	0.42
2:B:202:SER:C	2:B:204:GLY:N	2.58	0.42
2:B:350:GLN:HG3	2:B:372:TYR:HE1	1.85	0.42
2:B:431:PHE:CE2	19:B:1229:CLA:HED3	2.55	0.42
2:B:445:ALA:N	2:B:447:GLY:H	2.17	0.42
2:B:631:LEU:HG	2:B:632:ILE:N	2.34	0.42
2:B:715:VAL:O	2:B:719:PHE:N	2.42	0.42
3:C:8:TYR:HB2	3:C:41:SER:OG	2.18	0.42
4:D:130:LYS:O	4:D:130:LYS:HG3	2.19	0.42
5:E:111:ASN:CB	5:E:116:SER:OG	2.54	0.42
6:F:205:SER:CA	6:F:207:LEU:HD12	2.49	0.42
7:G:76:ARG:HH12	7:G:120:VAL:H	1.66	0.42
22:H:7002:LMU:O2'	22:H:7002:LMU:H5'	2.19	0.42
10:J:9:SER:HB2	10:J:10:VAL:H	1.67	0.42
19:J:1311:CLA:H152	19:2:2014:CLA:CMB	2.48	0.42
12:L:78:LEU:HD22	19:L:1504:CLA:CED	2.42	0.42
12:L:145:LEU:O	12:L:182:TRP:HZ3	2.02	0.42
12:L:209:LEU:HG	12:L:210:PRO:N	2.33	0.42
13:N:112:ALA:O	13:N:113:ASN:O	2.37	0.42
15:1:92:LEU:HA	15:1:95:PRO:HD2	1.92	0.42
15:1:148:VAL:O	15:1:148:VAL:CG2	2.65	0.42
16:2:118:ALA:CB	16:2:121:PHE:CE2	2.96	0.42
16:2:238:GLN:HA	16:2:241:TYR:CE2	2.54	0.42
17:3:107:ARG:HG2	17:3:232:ARG:HB2	2.01	0.42
18:4:162:ASN:HA	18:4:163:PRO:HD3	1.68	0.42
18:4:171:ILE:N	18:4:173:LYS:H	2.17	0.42
19:4:4006:CLA:HED2	19:4:4006:CLA:H2A	2.01	0.42
1:A:68:THR:CG2	1:A:69:SER:N	2.79	0.42
1:A:250:LEU:HD12	17:3:136:TRP:CZ2	2.49	0.42
1:A:389:TYR:CE2	1:A:526:LYS:HD3	2.45	0.42
1:A:457:SER:O	1:A:544:ILE:CD1	2.64	0.42
1:A:488:PHE:HD1	1:A:535:GLY:CA	2.33	0.42
1:A:554:LEU:HD11	2:B:674:LEU:HD21	2.01	0.42
1:A:555:ILE:HD11	19:A:9023:CLA:C3D	2.49	0.42
19:A:1138:CLA:H2A	19:A:1138:CLA:CED	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:7045:LMU:H21	22:A:7045:LMU:H1'	1.69	0.42
2:B:74:PHE:C	2:B:76:ALA:N	2.73	0.42
2:B:123:TRP:HB3	2:B:126:THR:HG21	1.99	0.42
2:B:144:PHE:O	2:B:144:PHE:HD2	2.02	0.42
2:B:182:LEU:HG	2:B:183:PHE:N	2.34	0.42
2:B:310:PRO:HG2	2:B:311:PRO:HD2	1.99	0.42
2:B:331:HIS:CE1	2:B:392:ILE:CG2	2.97	0.42
2:B:387:PHE:CB	2:B:534:LEU:HD13	2.50	0.42
2:B:399:ASN:OD1	2:B:402:GLN:HB2	2.20	0.42
2:B:430:GLY:CA	2:B:525:LEU:CD1	2.88	0.42
2:B:648:TRP:HZ3	21:B:6017:BCR:H383	1.84	0.42
2:B:655:LEU:HD22	19:B:1239:CLA:CAB	2.50	0.42
2:B:692:ARG:NH2	2:B:694:ARG:HH22	2.10	0.42
2:B:694:ARG:HE	12:L:151:SER:HA	1.85	0.42
19:B:1201:CLA:H2A	19:B:1201:CLA:O1D	2.19	0.42
19:B:1208:CLA:H8	19:B:1208:CLA:H51	1.75	0.42
19:B:1220:CLA:H203	19:B:1220:CLA:H11	2.02	0.42
20:B:5002:PQN:H2M1	20:B:5002:PQN:H111	1.78	0.42
4:D:101:VAL:O	4:D:101:VAL:CG2	2.67	0.42
6:F:100:LYS:NZ	6:F:103:GLN:HB2	2.35	0.42
7:G:102:ALA:N	7:G:104:ASP:OD2	2.53	0.42
7:G:123:ASN:C	7:G:126:ASP:OD2	2.58	0.42
7:G:125:VAL:O	7:G:129:ALA:CB	2.67	0.42
9:I:20:ALA:O	9:I:24:LEU:N	2.52	0.42
10:J:18:TRP:CZ2	10:J:22:LEU:HD22	2.55	0.42
19:J:1308:CLA:O2A	19:J:1308:CLA:C2A	2.53	0.42
11:K:48:PHE:O	11:K:52:PRO:CD	2.57	0.42
11:K:125:LYS:HD2	11:K:128:GLY:HA3	2.01	0.42
13:N:92:LEU:HD12	13:N:92:LEU:HA	1.68	0.42
13:N:133:GLY:CA	13:N:134:CYS:C	2.86	0.42
13:N:146:LEU:HD12	13:N:146:LEU:HA	1.72	0.42
16:2:133:ASN:ND2	16:2:134:THR:OG1	2.50	0.42
16:2:184:PRO:CD	16:2:186:ASN:C	2.87	0.42
16:2:226:ARG:HD3	16:2:229:MET:HB3	2.01	0.42
17:3:94:GLU:N	17:3:95:PRO:CD	2.83	0.42
17:3:98:LEU:CD2	19:3:3012:CLA:C2D	2.94	0.42
18:4:142:PHE:CA	18:4:145:GLU:OE1	2.63	0.42
18:4:192:LEU:CD1	18:4:193:ASN:H	2.33	0.42
1:A:92:TRP:O	1:A:93:LEU:CG	2.68	0.42
1:A:132:LEU:O	1:A:143:ILE:HD11	2.20	0.42
1:A:288:ASP:HB2	1:A:291:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:SER:O	1:A:512:SER:OG	2.29	0.42
1:A:580:PRO:HA	1:A:728:VAL:HG23	2.01	0.42
1:A:584:PRO:HG3	2:B:559:CYS:SG	2.59	0.42
1:A:651:GLY:O	1:A:655:ASP:HB2	2.20	0.42
19:A:1115:CLA:H51	19:A:1115:CLA:H11	1.74	0.42
19:A:1122:CLA:ND	21:A:6007:BCR:C19	2.83	0.42
19:A:1129:CLA:HHB	19:L:1130:CLA:CAD	2.50	0.42
19:A:1139:CLA:H3A	19:A:1139:CLA:HBA1	1.69	0.42
2:B:202:SER:CB	2:B:270:LEU:HD22	2.46	0.42
2:B:273:VAL:O	2:B:277:HIS:CD2	2.65	0.42
2:B:292:ARG:HH12	2:B:295:PHE:H	1.66	0.42
2:B:343:VAL:HG12	19:B:1223:CLA:H2	2.02	0.42
2:B:398:TYR:CD1	2:B:400:PRO:HD3	2.55	0.42
2:B:623:TYR:HH	2:B:721:TYR:HH	1.68	0.42
19:B:1229:CLA:H51	21:F:6016:BCR:H403	2.01	0.42
3:C:1:MET:H2	3:C:3:HIS:H	1.66	0.42
5:E:79:LYS:CA	5:E:84:TYR:CD1	2.90	0.42
6:F:117:LEU:CD1	6:F:120:LYS:HB2	2.49	0.42
8:H:98:LEU:HD23	12:L:146:THR:CG2	2.41	0.42
19:H:1207:CLA:H102	19:H:1207:CLA:H152	2.02	0.42
12:L:79:ILE:HG22	12:L:80:ALA:N	2.30	0.42
13:N:146:LEU:HD11	13:N:148:ASP:O	2.20	0.42
15:1:155:GLU:CD	15:1:156:LYS:N	2.73	0.42
15:1:173:TYR:O	15:1:174:SER:OG	2.29	0.42
16:2:149:THR:HG1	16:2:150:THR:N	2.18	0.42
16:2:226:ARG:CA	16:2:226:ARG:NH1	2.83	0.42
17:3:136:TRP:N	17:3:139:THR:HG1	2.17	0.42
17:3:158:PHE:HA	17:3:159:VAL:C	2.40	0.42
18:4:157:TRP:HE3	19:4:4012:CLA:HMA2	1.84	0.42
18:4:193:ASN:C	18:4:194:PHE:CG	2.87	0.42
19:4:1304:CLA:C15	19:4:1304:CLA:H202	2.40	0.42
1:A:64:PHE:CZ	1:A:74:ILE:HG23	2.52	0.41
1:A:75:SER:CB	1:A:354:TRP:CZ2	2.98	0.41
1:A:93:LEU:HA	1:A:96:MET:HG2	2.02	0.41
1:A:252:ARG:NE	1:A:252:ARG:CA	2.77	0.41
1:A:363:ALA:N	1:A:410:ALA:CB	2.83	0.41
1:A:448:TRP:HD1	19:A:1131:CLA:CED	2.32	0.41
1:A:485:GLN:OE1	1:A:485:GLN:CA	2.67	0.41
1:A:525:ASN:CB	1:A:526:LYS:CG	2.90	0.41
1:A:701:GLN:HE21	1:A:724:ALA:HB2	1.85	0.41
19:A:1101:CLA:H12	19:A:1140:CLA:C6	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:LEU:O	2:B:45:ASN:N	2.53	0.41
2:B:120:VAL:CG2	2:B:123:TRP:NE1	2.57	0.41
2:B:344:ILE:HD13	19:B:1215:CLA:H71	2.02	0.41
2:B:645:VAL:HG13	21:B:6017:BCR:H282	2.02	0.41
2:B:661:PHE:HA	2:B:664:LEU:HB2	2.02	0.41
19:B:1211:CLA:C2B	21:B:6006:BCR:H11C	2.50	0.41
4:D:196:SER:HA	4:D:197:PRO:HD3	1.33	0.41
4:D:203:THR:CG2	4:D:205:LYS:HG2	2.50	0.41
5:E:122:LEU:HD12	5:E:122:LEU:HA	1.57	0.41
6:F:140:CYS:H	6:F:146:PRO:HA	1.85	0.41
6:F:184:ALA:O	6:F:185:ILE:CG2	2.68	0.41
7:G:124:ILE:CD1	7:G:128:LEU:CD1	2.98	0.41
8:H:58:LEU:HG	8:H:61:THR:HB	1.93	0.41
12:L:92:ALA:HB3	12:L:98:ARG:CZ	2.50	0.41
15:1:130:PRO:HB2	15:1:131:TRP:H	1.63	0.41
15:1:177:PRO:CG	15:1:180:LEU:N	2.79	0.41
15:1:201:PHE:CA	15:1:204:GLN:HB2	2.48	0.41
19:2:2004:CLA:H2	19:2:2007:CLA:HMD3	2.02	0.41
17:3:204:GLY:HA3	17:3:207:PHE:CA	2.49	0.41
19:3:3013:CLA:H51	19:3:3013:CLA:H12	1.83	0.41
18:4:122:ASN:O	18:4:123:VAL:CG1	2.59	0.41
18:4:173:LYS:CB	18:4:194:PHE:CD2	2.87	0.41
22:4:7033:LMU:H3'	22:4:7033:LMU:H1B	1.73	0.41
1:A:240:LYS:HA	1:A:243:PRO:HD2	2.01	0.41
1:A:293:GLY:O	1:A:380:PRO:O	2.37	0.41
1:A:349:ILE:CG2	1:A:350:LEU:HA	2.45	0.41
1:A:400:MET:HE3	1:A:612:VAL:HG11	2.01	0.41
1:A:488:PHE:CD1	1:A:535:GLY:CA	3.03	0.41
1:A:564:ARG:CZ	1:A:564:ARG:HB2	2.49	0.41
19:A:1131:CLA:H191	20:B:5002:PQN:H303	2.02	0.41
2:B:4:ARG:HH21	2:B:5:ILE:N	2.19	0.41
2:B:37:ILE:HD12	2:B:37:ILE:C	2.41	0.41
2:B:110:LEU:CG	2:B:111:GLY:N	2.83	0.41
2:B:141:PHE:O	2:B:142:LEU:C	2.58	0.41
2:B:314:ARG:HH22	15:1:67:LEU:CG	2.28	0.41
2:B:365:PHE:CD1	2:B:602:TRP:CD1	3.08	0.41
2:B:431:PHE:HE2	19:B:1229:CLA:HED3	1.85	0.41
2:B:621:ARG:C	2:B:625:TRP:HB3	2.35	0.41
19:B:1229:CLA:C5	21:F:6016:BCR:H403	2.49	0.41
4:D:187:ASN:HB2	4:D:188:PHE:H	1.60	0.41
5:E:66:ILE:HG13	5:E:67:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:82:TYR:CD2	5:E:83:TRP:CE3	3.08	0.41
6:F:173:TRP:CZ3	6:F:211:PHE:CA	3.03	0.41
6:F:224:GLY:O	6:F:227:VAL:HG12	2.14	0.41
19:F:1305:CLA:HAA2	19:F:1305:CLA:HBD	2.02	0.41
7:G:90:GLN:CB	7:G:92:PRO:N	2.83	0.41
22:K:7041:LMU:O2'	22:K:7041:LMU:H5'	2.20	0.41
12:L:73:VAL:CB	19:L:1504:CLA:HMA3	2.50	0.41
12:L:114:PHE:HD1	12:L:114:PHE:N	2.17	0.41
13:N:114:PHE:CD2	13:N:116:ARG:HD2	2.55	0.41
15:1:158:PRO:HD2	15:1:159:GLU:O	2.20	0.41
16:2:103:VAL:HG13	16:2:104:GLN:N	2.35	0.41
17:3:241:TYR:OH	19:3:3003:CLA:CHC	2.68	0.41
17:3:243:ILE:CG1	19:3:3005:CLA:C4C	2.79	0.41
22:3:7003:LMU:C2B	22:3:7005:LMU:C6B	2.96	0.41
18:4:120:ILE:HD11	18:4:226:LYS:CD	2.29	0.41
18:4:202:GLU:O	18:4:205:ILE:HD13	2.19	0.41
1:A:105:ASN:HB2	1:A:140:PHE:HZ	1.86	0.41
1:A:121:GLN:NE2	19:A:1107:CLA:HMD1	2.35	0.41
1:A:158:ILE:O	1:A:159:THR:CB	2.68	0.41
1:A:210:LEU:HD12	19:A:1111:CLA:CMB	2.48	0.41
1:A:443:ILE:HD12	1:A:443:ILE:N	2.35	0.41
1:A:553:VAL:CG2	21:A:6008:BCR:H401	2.50	0.41
19:A:1103:CLA:HMC3	19:A:1128:CLA:HMA1	2.01	0.41
19:A:1117:CLA:HBA2	19:A:1117:CLA:H3A	1.62	0.41
19:A:1119:CLA:C2C	19:A:1125:CLA:H171	2.50	0.41
19:A:1131:CLA:HED1	19:A:1237:CLA:O1A	2.20	0.41
19:A:9011:CLA:H162	19:A:9011:CLA:H122	1.68	0.41
19:A:9023:CLA:C9	19:B:1239:CLA:HBB2	2.48	0.41
2:B:75:GLU:HB2	2:B:132:ASN:HD22	1.63	0.41
2:B:212:PHE:HE1	19:B:1211:CLA:CMD	2.33	0.41
2:B:323:TYR:CD1	19:B:1221:CLA:HBC1	2.54	0.41
2:B:583:MET:O	2:B:587:ILE:HB	2.20	0.41
2:B:661:PHE:O	2:B:665:ILE:N	2.52	0.41
21:B:6017:BCR:C38	21:B:6017:BCR:C23	2.97	0.41
6:F:170:ILE:CG2	21:F:6014:BCR:H371	2.32	0.41
8:H:97:LEU:HD11	8:H:101:LEU:H	1.85	0.41
11:K:115:ILE:CD1	11:K:122:LEU:H	2.32	0.41
12:L:164:LEU:H	12:L:164:LEU:HG	1.53	0.41
12:L:171:LYS:CA	12:L:173:PRO:HD3	2.48	0.41
19:L:1501:CLA:H11	19:L:1501:CLA:C4D	2.50	0.41
16:2:125:PHE:C	16:2:127:THR:N	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:192:ASP:OD2	16:2:194:GLY:CA	2.65	0.41
19:2:2001:CLA:O2A	19:2:2001:CLA:H43	2.20	0.41
19:2:2004:CLA:HED2	19:3:2009:CLA:CAB	2.50	0.41
17:3:208:PHE:HD1	17:3:208:PHE:HA	1.76	0.41
1:A:123:VAL:HG23	1:A:124:TRP:O	2.19	0.41
1:A:218:TRP:NE1	1:A:222:GLN:OE1	2.54	0.41
1:A:365:LEU:O	1:A:369:THR:HG23	2.21	0.41
1:A:443:ILE:CG2	2:B:674:LEU:HD11	2.47	0.41
1:A:578:ARG:NH1	1:A:578:ARG:HB3	2.32	0.41
2:B:77:TRP:O	2:B:81:PRO:HB3	2.20	0.41
2:B:87:ILE:C	2:B:115:ASN:HA	2.40	0.41
2:B:497:TRP:O	2:B:498:LEU:HB3	2.21	0.41
2:B:718:ILE:CD1	19:B:1224:CLA:HMC2	2.50	0.41
19:B:1229:CLA:CBB	21:F:6014:BCR:C26	2.99	0.41
19:F:1305:CLA:CAD	19:F:1305:CLA:CED	2.97	0.41
22:H:7032:LMU:H1B	22:H:7032:LMU:H5'	1.84	0.41
11:K:112:VAL:O	11:K:114:HIS:N	2.53	0.41
16:2:123:PRO:HA	16:2:126:LEU:HG	2.00	0.41
17:3:135:ALA:HB1	17:3:139:THR:HG21	1.98	0.41
17:3:137:PHE:CD2	17:3:137:PHE:N	2.88	0.41
17:3:204:GLY:O	17:3:206:PRO:C	2.59	0.41
22:4:7034:LMU:H81	22:4:7052:LMU:H2'	0.42	0.41
1:A:158:ILE:CD1	19:A:1112:CLA:HED3	2.40	0.41
1:A:214:GLY:HA3	21:A:6003:BCR:C15	2.51	0.41
1:A:258:LEU:HG	1:A:280:PHE:HE1	1.82	0.41
1:A:336:GLY:HA2	19:A:1151:CLA:HMC3	2.00	0.41
1:A:656:PHE:O	1:A:657:LEU:C	2.58	0.41
19:A:1138:CLA:HBC3	19:A:1138:CLA:CHD	2.50	0.41
19:A:1139:CLA:H42	19:A:1139:CLA:O2A	2.19	0.41
2:B:104:PHE:HZ	2:B:645:VAL:HG23	1.84	0.41
2:B:193:HIS:CD2	19:B:1211:CLA:NB	2.88	0.41
2:B:268:LEU:O	2:B:269:TRP:C	2.58	0.41
2:B:430:GLY:N	2:B:525:LEU:CD1	2.83	0.41
2:B:502:ASN:OD1	2:B:502:ASN:C	2.59	0.41
2:B:580:VAL:HG11	2:B:710:LEU:HD21	2.02	0.41
2:B:594:TRP:HD1	2:B:595:HIS:N	2.17	0.41
2:B:645:VAL:HA	19:B:1206:CLA:HAC1	2.03	0.41
2:B:715:VAL:O	2:B:719:PHE:HB2	2.20	0.41
2:B:724:PHE:CE1	19:B:9010:CLA:HMD1	2.55	0.41
19:B:1211:CLA:H111	19:B:1211:CLA:H71	1.47	0.41
19:B:1225:CLA:H3A	19:B:1225:CLA:HBA2	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1228:CLA:HBC3	19:B:1228:CLA:CHD	2.41	0.41
4:D:140:LEU:CD1	4:D:141:GLY:CA	2.80	0.41
6:F:118:ALA:O	6:F:121:ALA:O	2.38	0.41
6:F:157:TRP:HZ3	19:F:1302:CLA:CMC	2.34	0.41
6:F:188:GLU:HB3	6:F:189:LYS:H	1.23	0.41
7:G:127:VAL:O	7:G:128:LEU:C	2.57	0.41
19:1:1006:CLA:HHC	19:1:1013:CLA:HBC1	2.02	0.41
16:2:117:ALA:HB1	16:2:230:LEU:HD12	2.01	0.41
16:2:264:ALA:O	16:2:265:ALA:HB3	2.20	0.41
19:2:2004:CLA:C3	19:3:2009:CLA:HBC3	2.50	0.41
1:A:79:PHE:CE1	19:A:1111:CLA:HED1	2.55	0.41
1:A:109:TRP:HH2	1:A:154:ARG:HD3	1.83	0.41
1:A:119:SER:C	1:A:145:ILE:HD12	2.41	0.41
1:A:123:VAL:HB	1:A:124:TRP:O	2.21	0.41
1:A:328:LYS:HZ2	1:A:345:GLY:N	2.17	0.41
1:A:355:HIS:ND1	1:A:416:ILE:HG22	2.31	0.41
1:A:425:THR:O	1:A:428:TYR:CE1	2.73	0.41
1:A:431:LEU:O	1:A:435:VAL:CG1	2.61	0.41
1:A:685:VAL:HG22	19:A:1140:CLA:CBB	2.48	0.41
19:A:1106:CLA:O2D	19:A:1106:CLA:H2A	2.21	0.41
19:A:1107:CLA:CHA	19:A:1107:CLA:CBA	2.98	0.41
19:A:1116:CLA:HHD	19:A:1116:CLA:HAC2	1.96	0.41
2:B:67:HIS:CD2	2:B:89:HIS:HB2	2.55	0.41
2:B:93:ASP:HA	2:B:94:PRO:HD2	1.48	0.41
2:B:152:ALA:HB2	19:B:1208:CLA:C2C	2.50	0.41
2:B:192:GLY:HA2	19:B:1212:CLA:CHC	2.51	0.41
2:B:217:PRO:HB2	2:B:218:TYR:HD1	1.85	0.41
2:B:397:ASP:O	2:B:398:TYR:HB3	2.20	0.41
2:B:443:MET:CG	2:B:451:LYS:O	2.68	0.41
2:B:680:TRP:O	2:B:684:ARG:HB2	2.20	0.41
19:B:1203:CLA:O1D	19:B:1203:CLA:C2A	2.60	0.41
19:B:1210:CLA:C15	19:B:1225:CLA:HMD2	2.35	0.41
3:C:12:ILE:HG21	3:C:39:ILE:C	2.40	0.41
7:G:97:LEU:O	7:G:98:THR:O	2.39	0.41
7:G:116:SER:O	7:G:119:PRO:CD	2.68	0.41
8:H:109:LEU:HD21	19:H:1207:CLA:C5	2.50	0.41
12:L:63:ASP:OD1	12:L:63:ASP:C	2.59	0.41
12:L:210:PRO:O	12:L:211:TYR:HB3	2.18	0.41
13:N:146:LEU:HD22	17:3:142:ILE:CA	2.50	0.41
14:R:27:UNK:C	14:R:29:UNK:C	2.98	0.41
15:1:77:GLU:OE1	15:1:80:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:115:ALA:O	15:1:116:ALA:CB	2.69	0.41
19:1:1002:CLA:HMA2	19:1:1002:CLA:CGA	2.51	0.41
19:1:1014:CLA:H102	19:1:1014:CLA:C5	2.18	0.41
17:3:107:ARG:NH1	17:3:233:LEU:N	2.69	0.41
17:3:197:SER:OG	17:3:198:GLY:N	2.53	0.41
19:3:3013:CLA:H3A	19:3:3013:CLA:HBA2	1.87	0.41
18:4:110:LEU:HA	18:4:113:GLU:CD	2.40	0.41
1:A:110:LEU:O	1:A:111:ASN:C	2.57	0.41
1:A:249:ILE:HG12	17:3:136:TRP:HH2	1.85	0.41
1:A:389:TYR:HE2	1:A:526:LYS:CD	2.29	0.41
1:A:417:PHE:CD1	1:A:417:PHE:C	2.94	0.41
1:A:537:ALA:O	1:A:642:PHE:HE2	2.04	0.41
1:A:691:MET:CE	20:A:5001:PQN:C2M	2.98	0.41
1:A:708:VAL:N	1:A:711:HIS:HD2	2.19	0.41
19:A:1122:CLA:CBC	21:A:6007:BCR:H393	2.51	0.41
19:A:1126:CLA:C11	21:J:6012:BCR:H353	2.48	0.41
2:B:91:ILE:HG21	2:B:91:ILE:HD13	1.78	0.41
2:B:98:GLN:N	2:B:99:PRO:CD	2.81	0.41
2:B:98:GLN:NE2	2:B:101:VAL:HG23	2.36	0.41
2:B:160:LYS:NZ	2:B:161:TRP:N	2.69	0.41
2:B:289:LEU:HD22	21:B:6004:BCR:H352	2.02	0.41
2:B:294:ASN:HB2	7:G:94:GLN:CG	2.45	0.41
2:B:458:ILE:HD11	6:F:149:ILE:HG13	2.02	0.41
2:B:549:ASP:CB	3:C:63:LEU:HB2	2.51	0.41
2:B:573:TRP:CZ3	2:B:703:VAL:HG13	2.55	0.41
19:B:1239:CLA:H2	20:B:5002:PQN:H251	2.02	0.41
3:C:58:CYS:HA	3:C:59:PRO:HD2	1.57	0.41
5:E:76:ILE:CB	5:E:84:TYR:O	2.53	0.41
5:E:77:LEU:C	5:E:78:ARG:HD2	2.40	0.41
22:E:7048:LMU:O4'	22:F:7036:LMU:H6E	2.15	0.41
19:F:1305:CLA:H12	19:4:1306:CLA:HAA1	2.02	0.41
10:J:19:PHE:CD2	10:J:19:PHE:C	2.94	0.41
22:K:7041:LMU:H82	22:K:7041:LMU:H111	1.95	0.41
12:L:83:LEU:HA	12:L:86:LEU:HD13	2.02	0.41
15:1:138:LEU:O	15:1:141:GLU:HG3	2.21	0.41
19:1:1008:CLA:HBC3	19:1:1008:CLA:CMC	2.48	0.41
19:1:1014:CLA:C12	19:1:1014:CLA:H91	2.50	0.41
16:2:155:VAL:CA	16:2:158:VAL:HG13	2.50	0.41
16:2:202:ASP:OD2	16:2:202:ASP:C	2.58	0.41
19:2:2006:CLA:H72	19:2:2006:CLA:H41	2.02	0.41
19:2:2014:CLA:C15	19:2:2014:CLA:C9	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:158:GLN:CD	19:4:1004:CLA:C2A	2.89	0.41
18:4:210:LEU:HD23	19:4:4002:CLA:CAB	2.51	0.41
1:A:57:LEU:HD22	1:A:58:HIS:CD2	2.54	0.41
1:A:109:TRP:HD1	1:A:116:ILE:HB	1.84	0.41
1:A:349:ILE:CG2	1:A:350:LEU:CA	2.95	0.41
1:A:479:ASP:CB	1:A:536:THR:CG2	2.99	0.41
1:A:514:THR:HA	1:A:530:LEU:O	2.21	0.41
1:A:547:PHE:CE2	19:A:9023:CLA:O1A	2.73	0.41
1:A:709:TRP:CZ3	2:B:417:ALA:HA	2.55	0.41
22:A:7016:LMU:H1'	22:A:7016:LMU:H6D	1.76	0.41
2:B:52:GLY:O	2:B:56:ILE:HG12	2.21	0.41
2:B:208:ARG:HA	2:B:208:ARG:HD2	1.98	0.41
2:B:353:TYR:CB	2:B:594:TRP:CH2	3.01	0.41
2:B:410:ARG:HA	2:B:410:ARG:HD2	1.49	0.41
2:B:622:ASP:CA	2:B:626:LEU:HD12	2.48	0.41
3:C:33:GLY:HA2	3:C:37:LYS:HB3	2.02	0.41
4:D:114:MET:HG2	4:D:115:PRO:O	1.98	0.41
9:I:8:PHE:CD1	19:I:1204:CLA:H12	2.56	0.41
19:J:1308:CLA:H93	19:2:2014:CLA:O1D	2.13	0.41
19:J:1311:CLA:HBA2	19:J:1311:CLA:H3A	1.27	0.41
11:K:47:ASP:C	11:K:51:SER:H	2.24	0.41
11:K:127:ILE:O	11:K:130:LEU:CA	2.69	0.41
22:K:7001:LMU:H42	22:K:7001:LMU:H102	2.01	0.41
12:L:91:THR:O	12:L:91:THR:OG1	2.34	0.41
12:L:210:PRO:HB2	12:L:211:TYR:CE2	2.55	0.41
13:N:127:PHE:CG	13:N:128:PRO:HD3	2.55	0.41
13:N:164:SER:HA	13:N:165:ASN:O	2.18	0.41
15:1:85:ILE:HG12	15:1:88:ARG:NE	2.26	0.41
15:1:200:GLY:HA3	19:1:1003:CLA:HBB2	2.02	0.41
15:1:201:PHE:HA	15:1:204:GLN:CB	2.49	0.41
16:2:110:SER:HB3	16:2:227:LEU:HD13	2.02	0.41
19:2:2014:CLA:H91	19:2:2014:CLA:C16	2.51	0.41
19:3:3011:CLA:H11	19:3:3011:CLA:HBA2	1.88	0.41
18:4:154:ILE:HD13	19:4:1009:CLA:HMD1	2.03	0.41
18:4:169:ASP:OD1	18:4:174:GLN:N	2.54	0.41
18:4:175:TYR:CB	18:4:194:PHE:CD1	2.90	0.41
1:A:173:VAL:O	1:A:175:ALA:O	2.39	0.41
1:A:212:GLY:C	1:A:214:GLY:H	2.23	0.41
1:A:288:ASP:O	1:A:292:GLY:HA2	2.20	0.41
1:A:288:ASP:OD1	1:A:295:TRP:CD2	2.74	0.41
1:A:378:SER:O	1:A:378:SER:OG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:THR:HG22	2:B:648:TRP:CE2	2.56	0.41
1:A:580:PRO:HB3	1:A:727:ILE:CG2	2.51	0.41
1:A:604:TRP:O	1:A:605:MET:C	2.59	0.41
1:A:663:GLN:HB3	1:A:752:ALA:O	2.21	0.41
19:A:1102:CLA:HBC3	19:A:1102:CLA:CHD	2.50	0.41
19:A:1126:CLA:C17	19:A:1126:CLA:H122	2.50	0.41
2:B:4:ARG:C	2:B:5:ILE:HG12	2.41	0.41
2:B:4:ARG:NH2	2:B:5:ILE:N	2.69	0.41
2:B:7:ARG:CD	2:B:7:ARG:H	2.32	0.41
2:B:73:ASN:C	2:B:121:TYR:OH	2.48	0.41
2:B:88:ALA:HB1	19:B:1205:CLA:O2D	2.20	0.41
2:B:142:LEU:O	2:B:145:LEU:HB3	2.21	0.41
2:B:175:LEU:HD13	19:B:1221:CLA:CED	2.51	0.41
2:B:305:LEU:HD22	19:B:1220:CLA:O1D	2.18	0.41
2:B:355:LEU:HD21	2:B:508:LEU:CD2	2.51	0.41
2:B:395:ILE:H	2:B:395:ILE:HG13	1.75	0.41
2:B:439:HIS:HB2	19:B:1230:CLA:C1C	2.50	0.41
2:B:478:LEU:O	2:B:478:LEU:CG	2.68	0.41
2:B:724:PHE:CD1	19:B:9010:CLA:HMD1	2.56	0.41
2:B:729:THR:O	2:B:729:THR:CG2	2.61	0.41
19:B:1214:CLA:H12	19:B:1214:CLA:NA	2.36	0.41
19:B:1229:CLA:HMD2	19:B:1229:CLA:H13	2.03	0.41
3:C:39:ILE:CG1	3:C:40:ALA:H	2.32	0.41
4:D:110:GLN:O	4:D:122:MET:CG	2.69	0.41
5:E:106:ARG:CZ	5:E:106:ARG:O	2.67	0.41
5:E:127:GLU:HB3	5:E:129:GLU:C	2.32	0.41
22:E:7048:LMU:H4'	22:E:7048:LMU:H1'	1.79	0.41
6:F:101:LYS:O	6:F:104:ALA:HB3	2.21	0.41
6:F:116:ALA:O	6:F:119:ILE:HD13	2.21	0.41
6:F:214:PRO:C	6:F:215:VAL:CG2	2.86	0.41
8:H:107:SER:O	8:H:111:TYR:CB	2.68	0.41
8:H:111:TYR:CB	8:H:112:LEU:HD23	2.51	0.41
8:H:111:TYR:CG	8:H:112:LEU:HD23	2.56	0.41
8:H:113:SER:HG	19:H:1207:CLA:C6	2.31	0.41
22:H:7017:LMU:H1B	22:H:7017:LMU:H6'2	1.72	0.41
9:I:11:LEU:O	9:I:16:PHE:N	2.51	0.41
11:K:50:GLY:N	11:K:52:PRO:HD2	2.33	0.41
22:K:7042:LMU:H121	22:K:7042:LMU:H91	1.75	0.41
12:L:103:GLY:HA3	12:L:192:GLY:HA3	2.02	0.41
12:L:111:VAL:HG23	12:L:112:GLY:H	1.86	0.41
15:1:65:ASP:CG	15:1:66:PRO:CA	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:135:PRO:HD2	15:1:136:THR:N	2.32	0.41
19:1:1303:CLA:CBC	19:1:1303:CLA:CMC	2.86	0.41
16:2:94:SER:O	16:2:95:ASP:CB	2.62	0.41
16:2:106:GLU:HG2	19:2:2004:CLA:HBC2	2.02	0.41
16:2:266:PHE:CD2	16:2:267:THR:O	2.74	0.41
17:3:111:LEU:CD2	17:3:112:GLY:H	2.21	0.41
17:3:178:LYS:HB3	17:3:179:PRO:HD3	2.03	0.41
17:3:178:LYS:HB3	17:3:179:PRO:CD	2.49	0.41
22:3:7005:LMU:H71	22:3:7005:LMU:H42	1.79	0.41
18:4:95:GLU:HG3	18:4:96:LEU:N	2.35	0.41
18:4:121:ILE:C	18:4:123:VAL:N	2.71	0.41
19:4:1004:CLA:H11	19:4:1004:CLA:H52	1.83	0.41
1:A:236:GLY:O	1:A:237:VAL:CB	2.69	0.41
1:A:281:LEU:CD2	19:A:1115:CLA:HED3	2.22	0.41
1:A:484:LEU:CA	1:A:485:GLN:NE2	2.84	0.41
1:A:684:PHE:HB2	19:A:9012:CLA:HAA1	2.02	0.41
1:A:720:THR:O	1:A:720:THR:CG2	2.65	0.41
19:A:1104:CLA:H11	19:A:1128:CLA:O2A	2.21	0.41
19:A:1106:CLA:H142	21:J:6012:BCR:C13	2.50	0.41
19:A:1106:CLA:CBB	19:A:1107:CLA:C3D	2.95	0.41
19:A:1119:CLA:H112	19:A:1119:CLA:H91	1.83	0.41
22:A:7010:LMU:H3'	22:A:7010:LMU:H2O1	1.83	0.41
2:B:131:THR:O	2:B:135:LEU:CD2	2.62	0.41
2:B:334:LEU:HD22	19:B:1202:CLA:CHD	2.51	0.41
2:B:366:THR:HG22	2:B:366:THR:O	2.21	0.41
4:D:93:LYS:HG3	4:D:96:VAL:HG11	1.99	0.41
4:D:185:GLY:O	4:D:186:GLN:HB2	2.19	0.41
22:E:7037:LMU:O2B	22:E:7037:LMU:C5B	2.66	0.41
22:E:7048:LMU:H6'2	22:E:7048:LMU:O2'	2.21	0.41
6:F:201:PRO:O	6:F:202:LEU:HB2	2.21	0.41
7:G:87:VAL:O	7:G:90:GLN:O	2.38	0.41
22:G:7039:LMU:H82	22:G:7039:LMU:H112	1.61	0.41
11:K:92:GLY:O	11:K:93:LEU:CB	2.66	0.41
22:K:7041:LMU:H2B	22:K:7041:LMU:H4'	1.79	0.41
15:1:68:GLY:O	15:1:73:PRO:N	2.55	0.41
19:1:1014:CLA:H121	19:1:1014:CLA:C9	2.51	0.41
16:2:107:LEU:HD11	16:2:108:VAL:HG23	2.03	0.41
16:2:184:PRO:CD	16:2:186:ASN:N	2.83	0.41
19:2:2004:CLA:C4	19:3:2009:CLA:HBC3	2.51	0.41
17:3:156:THR:C	17:3:158:PHE:N	2.69	0.41
17:3:157:LEU:O	17:3:160:LEU:CA	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:1306:CLA:CBC	19:4:1306:CLA:CMC	2.79	0.41
1:A:23:ASP:OD1	1:A:23:ASP:C	2.59	0.40
1:A:127:VAL:CG2	19:A:1107:CLA:HBB2	2.39	0.40
1:A:201:SER:O	1:A:204:ASN:CA	2.69	0.40
1:A:208:ALA:HA	1:A:310:PHE:C	2.37	0.40
1:A:375:HIS:ND1	1:A:375:HIS:N	2.69	0.40
1:A:539:PHE:C	1:A:539:PHE:CD2	2.94	0.40
1:A:648:THR:O	1:A:649:ILE:HG22	2.21	0.40
2:B:15:ASP:HA	2:B:16:PRO:HD3	1.89	0.40
2:B:29:HIS:HB3	19:B:1226:CLA:HBA1	2.03	0.40
2:B:169:LYS:O	2:B:170:ASN:O	2.39	0.40
2:B:289:LEU:O	19:B:1218:CLA:HMC1	2.22	0.40
2:B:373:THR:C	2:B:375:HIS:H	2.24	0.40
2:B:535:VAL:CG1	2:B:536:LYS:H	2.34	0.40
19:B:1235:CLA:HBC1	6:F:160:PHE:CE1	2.48	0.40
20:B:5002:PQN:H161	20:B:5002:PQN:H141	1.60	0.40
3:C:70:TRP:O	3:C:71:HIS:C	2.59	0.40
4:D:125:GLY:HA2	4:D:127:ASN:H	1.85	0.40
4:D:134:LYS:HE2	4:D:166:LEU:HD11	2.03	0.40
6:F:102:LEU:O	6:F:103:GLN:O	2.39	0.40
22:F:7036:LMU:H1'	22:F:7036:LMU:O6'	2.21	0.40
7:G:136:VAL:C	7:G:137:VAL:HG22	2.41	0.40
11:K:50:GLY:N	11:K:52:PRO:HD3	2.36	0.40
12:L:145:LEU:CG	21:L:6019:BCR:HC7	2.41	0.40
13:N:118:TYR:O	13:N:119:THR:OG1	2.39	0.40
13:N:155:GLU:CB	13:N:157:LYS:NZ	2.82	0.40
15:I:68:GLY:C	15:I:69:LEU:O	2.56	0.40
17:3:85:ASP:HA	17:3:86:PRO:HD3	1.40	0.40
17:3:201:ALA:O	17:3:202:TYR:CD2	2.74	0.40
19:3:3013:CLA:HHD	19:3:3013:CLA:HBC2	2.02	0.40
18:4:180:GLY:O	18:4:183:GLY:N	2.54	0.40
19:4:4006:CLA:HBA2	19:4:4006:CLA:CBF	2.51	0.40
1:A:177:LEU:C	1:A:179:LEU:N	2.75	0.40
1:A:284:ARG:O	1:A:285:GLY:C	2.56	0.40
1:A:363:ALA:N	1:A:410:ALA:HB2	2.36	0.40
1:A:434:ARG:HA	1:A:437:ARG:HD2	2.03	0.40
1:A:586:ARG:HB2	1:A:589:THR:OG1	2.22	0.40
21:A:6011:BCR:H323	21:J:6012:BCR:C39	2.49	0.40
19:A:9023:CLA:O2A	19:A:9023:CLA:C3A	2.65	0.40
2:B:285:LEU:HD12	21:B:6004:BCR:C17	2.50	0.40
2:B:310:PRO:CG	2:B:311:PRO:HD2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:LYS:HG3	2:B:321:GLY:N	2.37	0.40
2:B:475:ASP:CG	2:B:480:SER:HA	2.35	0.40
2:B:593:TYR:CD1	19:B:1234:CLA:HMC2	2.57	0.40
2:B:631:LEU:O	2:B:634:GLY:N	2.53	0.40
19:B:1232:CLA:CBB	21:B:6010:BCR:C28	2.99	0.40
4:D:155:TYR:CD1	4:D:168:PRO:HG3	2.57	0.40
4:D:169:LYS:HB2	4:D:169:LYS:NZ	2.36	0.40
4:D:169:LYS:HB2	4:D:169:LYS:HZ3	1.85	0.40
5:E:108:ASN:O	5:E:109:LYS:C	2.57	0.40
6:F:113:SER:C	6:F:115:PRO:HD3	2.42	0.40
6:F:116:ALA:O	6:F:119:ILE:HG12	2.20	0.40
7:G:90:GLN:HB2	7:G:92:PRO:N	2.37	0.40
7:G:131:GLY:HA2	7:G:136:VAL:CB	2.50	0.40
22:G:7039:LMU:H3'	22:G:7039:LMU:C6B	2.49	0.40
11:K:56:ILE:HG12	11:K:59:THR:CG2	2.50	0.40
22:K:7042:LMU:H22	22:K:7042:LMU:C7	2.50	0.40
12:L:182:TRP:CZ3	12:L:186:THR:HG21	2.56	0.40
12:L:194:ILE:O	12:L:195:SER:HB3	2.21	0.40
15:1:140:ILE:N	15:1:140:ILE:CD1	2.72	0.40
19:1:1003:CLA:HED1	19:1:1008:CLA:HMB1	2.04	0.40
16:2:95:ASP:HA	16:2:96:PRO:HD3	1.93	0.40
17:3:108:PHE:HD2	19:3:3013:CLA:C4	2.34	0.40
18:4:88:LEU:O	18:4:90:TRP:CB	2.59	0.40
18:4:108:GLY:O	18:4:109:MET:O	2.39	0.40
18:4:126:TRP:HA	19:4:4006:CLA:HMD3	2.02	0.40
18:4:149:SER:OG	18:4:150:HIS:N	2.54	0.40
18:4:153:GLU:OE2	19:4:4012:CLA:HHC	2.17	0.40
18:4:232:LEU:HD12	18:4:234:GLN:N	2.36	0.40
18:4:243:THR:HG23	18:4:244:ILE:N	2.36	0.40
1:A:39:HIS:ND1	1:A:39:HIS:C	2.75	0.40
1:A:94:SER:O	1:A:95:GLY:C	2.58	0.40
1:A:98:PHE:C	1:A:100:GLY:N	2.68	0.40
1:A:170:GLY:O	1:A:173:VAL:CG2	2.64	0.40
1:A:352:THR:HG22	19:A:1123:CLA:H201	2.03	0.40
1:A:409:GLY:O	1:A:411:ALA:N	2.55	0.40
1:A:472:ARG:HH22	12:L:120:LEU:HD13	1.85	0.40
1:A:492:ILE:HD13	19:A:1133:CLA:CHC	2.50	0.40
1:A:569:ILE:HG12	1:A:586:ARG:NH1	2.36	0.40
1:A:631:GLN:O	1:A:631:GLN:HG2	2.21	0.40
1:A:755:ILE:H	1:A:755:ILE:HG13	1.62	0.40
19:A:1119:CLA:CGA	19:A:1123:CLA:HBB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1120:CLA:CGA	19:A:1120:CLA:C1A	2.99	0.40
19:A:9013:CLA:H91	19:A:9013:CLA:H112	1.78	0.40
2:B:262:HIS:HB2	2:B:265:THR:OG1	2.21	0.40
2:B:653:GLY:HA3	2:B:720:THR:OG1	2.20	0.40
2:B:700:LEU:HD23	2:B:700:LEU:N	2.36	0.40
19:B:1205:CLA:H162	19:B:1224:CLA:H192	2.03	0.40
20:B:5002:PQN:H141	21:B:6017:BCR:H331	2.04	0.40
21:B:6004:BCR:H15C	21:B:6004:BCR:H351	1.88	0.40
22:B:7040:LMU:C1B	22:B:7040:LMU:H3O2	2.34	0.40
4:D:140:LEU:HD22	4:D:144:LEU:CG	2.49	0.40
21:F:6014:BCR:C33	21:F:6014:BCR:HC8	2.52	0.40
7:G:66:LEU:HD23	7:G:69:GLY:HA3	2.03	0.40
8:H:103:LEU:O	8:H:107:SER:HB3	2.22	0.40
10:J:5:LYS:CG	16:2:178:ASN:HA	2.52	0.40
19:K:1143:CLA:CBC	22:K:7001:LMU:C3B	2.91	0.40
13:N:123:GLY:O	13:N:124:SER:O	2.39	0.40
15:1:177:PRO:HG2	15:1:180:LEU:HA	2.03	0.40
16:2:160:ILE:HG21	19:2:2012:CLA:CAB	2.41	0.40
16:2:172:LEU:HD12	16:2:172:LEU:HA	1.75	0.40
17:3:197:SER:HB3	17:3:206:PRO:CG	2.51	0.40
19:3:3011:CLA:H41	19:3:3011:CLA:H62	1.80	0.40
18:4:217:PHE:O	18:4:220:GLN:HB2	2.21	0.40
22:4:7009:LMU:C3'	22:4:7009:LMU:H5B	2.52	0.40
1:A:261:SER:O	1:A:262:PHE:CE1	2.73	0.40
1:A:295:TRP:CB	1:A:297:THR:HG23	2.51	0.40
1:A:334:HIS:HB3	19:A:1120:CLA:HMA1	2.04	0.40
1:A:368:LEU:HD12	19:A:1125:CLA:C6	2.52	0.40
1:A:397:THR:OG1	19:A:1126:CLA:CMB	2.70	0.40
19:A:1107:CLA:HBC3	19:A:1107:CLA:CMC	2.52	0.40
19:A:1119:CLA:H101	19:A:1122:CLA:H93	2.02	0.40
19:A:1119:CLA:H8	21:A:6008:BCR:H19C	2.03	0.40
19:A:1124:CLA:H172	21:A:6007:BCR:C33	2.46	0.40
19:A:1138:CLA:H202	19:A:1139:CLA:H41	2.03	0.40
19:A:1138:CLA:HMC3	19:A:1139:CLA:ND	2.36	0.40
2:B:178:HIS:C	2:B:180:SER:N	2.72	0.40
2:B:440:ASN:OD1	2:B:452:GLN:CD	2.60	0.40
2:B:569:ASP:HB3	2:B:574:ASP:HB3	2.04	0.40
2:B:586:THR:O	2:B:589:TRP:N	2.54	0.40
2:B:596:TRP:CZ2	2:B:612:SER:HB3	2.56	0.40
2:B:635:ILE:O	2:B:636:THR:O	2.38	0.40
19:B:1235:CLA:H121	21:F:6016:BCR:H311	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1235:CLA:C12	21:F:6016:BCR:H311	2.51	0.40
4:D:148:TYR:O	4:D:149:LYS:HB3	2.21	0.40
22:E:7037:LMU:C7	22:E:7037:LMU:H32	2.51	0.40
6:F:130:PHE:O	6:F:132:ASN:O	2.39	0.40
6:F:154:GLN:OE1	6:F:155:ARG:N	2.55	0.40
6:F:230:ASN:O	6:F:231:PHE:O	2.40	0.40
7:G:140:TYR:CG	7:G:141:ILE:N	2.86	0.40
9:I:15:LEU:HD12	9:I:18:ALA:HB3	2.03	0.40
11:K:123:GLY:HA3	11:K:124:LEU:HA	1.82	0.40
11:K:127:ILE:CB	11:K:129:ALA:HB1	2.33	0.40
12:L:195:SER:C	12:L:197:VAL:H	2.25	0.40
12:L:210:PRO:CB	12:L:211:TYR:CD2	3.03	0.40
13:N:114:PHE:C	13:N:117:ALA:HB3	2.39	0.40
19:1:1006:CLA:CAB	19:1:1013:CLA:HHD	2.51	0.40
19:1:1007:CLA:H11	19:1:1007:CLA:H51	1.92	0.40
16:2:222:ILE:O	16:2:226:ARG:N	2.51	0.40
19:2:2004:CLA:HED2	19:3:2009:CLA:CBB	2.51	0.40
19:2:2006:CLA:HED2	19:2:2006:CLA:OBD	2.22	0.40
17:3:111:LEU:CD2	17:3:112:GLY:N	2.83	0.40
17:3:124:LYS:CG	17:3:149:ASN:HB3	2.49	0.40
19:3:1147:CLA:HBA2	19:3:1147:CLA:H3A	1.72	0.40
18:4:169:ASP:HB3	19:4:4001:CLA:CMB	2.43	0.40
18:4:212:LEU:O	18:4:213:ALA:CB	2.70	0.40
1:A:146:THR:HA	1:A:391:THR:HG22	2.03	0.40
1:A:195:TRP:CZ2	19:A:1108:CLA:HMA2	2.52	0.40
1:A:222:GLN:O	1:A:227:LEU:HG	2.21	0.40
1:A:286:GLY:O	1:A:295:TRP:NE1	2.55	0.40
1:A:447:ASN:ND2	2:B:678:LEU:CD2	2.82	0.40
1:A:672:LEU:C	1:A:674:ALA:H	2.16	0.40
1:A:697:ARG:C	1:A:699:TYR:N	2.74	0.40
1:A:705:GLU:HG2	2:B:545:LYS:HZ2	1.86	0.40
19:A:1101:CLA:H12	19:A:1140:CLA:H61	2.02	0.40
19:A:1104:CLA:HBA2	19:A:1104:CLA:H12	1.79	0.40
19:A:9022:CLA:C14	19:H:1207:CLA:HBC3	2.52	0.40
2:B:120:VAL:CB	2:B:123:TRP:CD1	3.03	0.40
2:B:185:VAL:HA	2:B:188:LEU:HB3	2.04	0.40
2:B:421:HIS:CE1	19:B:1228:CLA:C4D	3.04	0.40
2:B:463:ILE:HD12	19:B:1234:CLA:CGA	2.51	0.40
2:B:488:ALA:CB	19:B:1233:CLA:C2C	3.00	0.40
2:B:557:PHE:O	2:B:557:PHE:CD2	2.74	0.40
2:B:649:MET:HE1	19:B:1205:CLA:HBC3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:668:ARG:HG3	2:B:699:ALA:C	2.42	0.40
19:B:1202:CLA:HMC3	19:B:1226:CLA:H3A	2.02	0.40
19:B:1218:CLA:CBA	19:B:1219:CLA:O1A	2.70	0.40
21:B:6005:BCR:H321	21:B:6005:BCR:HC7	1.87	0.40
6:F:103:GLN:O	6:F:105:SER:N	2.54	0.40
6:F:121:ALA:HA	6:F:124:GLU:HB3	2.04	0.40
6:F:123:MET:O	6:F:127:LYS:N	2.54	0.40
22:G:7026:LMU:C8	22:G:7026:LMU:C4	2.96	0.40
8:H:91:PHE:CZ	8:H:98:LEU:HD13	2.56	0.40
19:K:1143:CLA:HBC2	19:K:1143:CLA:CMC	2.52	0.40
12:L:52:PRO:O	12:L:54:TYR:N	2.55	0.40
13:N:91:TYR:HD2	13:N:91:TYR:HA	1.68	0.40
15:1:65:ASP:HA	15:1:69:LEU:CD1	2.49	0.40
15:1:94:VAL:C	15:1:96:GLY:N	2.73	0.40
15:1:155:GLU:CD	15:1:155:GLU:H	2.19	0.40
15:1:173:TYR:HD2	15:1:173:TYR:HA	1.49	0.40
15:1:192:ARG:CG	15:1:193:LEU:N	2.82	0.40
16:2:170:ASP:C	16:2:172:LEU:N	2.67	0.40
19:2:2002:CLA:H72	19:2:2002:CLA:H41	2.04	0.40
19:2:2014:CLA:HED3	19:2:2014:CLA:CAD	2.50	0.40
17:3:197:SER:CB	17:3:206:PRO:HG3	2.52	0.40
22:4:7034:LMU:H71	22:4:7052:LMU:C1	2.38	0.40

All (130) 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)
15:1:173:TYR:OH	16:2:132:LEU:C[2_646]	0.71	1.49
6:F:130:PHE:CG	12:L:170:LYS:NZ[2_556]	0.72	1.48
2:B:205:GLU:OE2	11:K:69:ARG:NH1[1_554]	0.79	1.41
12:L:123:THR:O	18:4:180:GLY:CA[1_455]	0.88	1.32
15:1:171:LEU:N	16:2:132:LEU:N[2_646]	0.98	1.22
15:1:173:TYR:OH	16:2:132:LEU:CA[2_646]	1.01	1.19
12:L:203:LEU:C	18:4:184:TYR:OH[1_455]	1.02	1.18
12:L:205:TYR:OH	18:4:181:GLU:O[1_455]	1.02	1.18
12:L:124:GLU:OE1	18:4:172:PHE:CE2[1_455]	1.06	1.14
15:1:171:LEU:CD2	16:2:131:ILE:C[2_646]	1.07	1.13
15:1:171:LEU:CD2	16:2:131:ILE:O[2_646]	1.08	1.12
12:L:124:GLU:OE1	18:4:172:PHE:CZ[1_455]	1.09	1.11
2:B:248:GLN:NE2	19:K:3009:CLA:C2C[1_554]	1.11	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:124:GLU:CD	18:4:172:PHE:CE2[1_455]	1.11	1.09
15:1:173:TYR:CE1	16:2:132:LEU:O[2_646]	1.13	1.07
12:L:124:GLU:CD	18:4:172:PHE:CZ[1_455]	1.15	1.05
15:1:118:PRO:O	17:3:89:THR:CG2[1_554]	1.17	1.03
6:F:130:PHE:CD2	12:L:170:LYS:NZ[2_556]	1.18	1.02
6:F:130:PHE:CE1	12:L:170:LYS:CE[2_556]	1.18	1.02
2:B:205:GLU:OE2	11:K:69:ARG:CZ[1_554]	1.19	1.01
15:1:170:PRO:O	16:2:132:LEU:CB[2_646]	1.20	1.00
12:L:203:LEU:O	18:4:184:TYR:CE2[1_455]	1.27	0.93
15:1:170:PRO:O	16:2:132:LEU:CA[2_646]	1.30	0.90
6:F:130:PHE:CD1	12:L:170:LYS:NZ[2_556]	1.32	0.88
6:F:131:ASP:OD2	12:L:170:LYS:CD[2_556]	1.32	0.88
1:A:348:GLU:OE2	7:G:147:ASN:OD1[1_556]	1.33	0.87
15:1:173:TYR:CZ	16:2:132:LEU:O[2_646]	1.37	0.83
6:F:131:ASP:OD1	12:L:170:LYS:CG[2_556]	1.38	0.82
2:B:205:GLU:CD	11:K:69:ARG:NH1[1_554]	1.39	0.81
4:D:160:ASN:CG	6:F:101:LYS:NZ[2_546]	1.39	0.81
2:B:248:GLN:NE2	19:K:3009:CLA:CMC[1_554]	1.40	0.80
12:L:203:LEU:O	18:4:184:TYR:CZ[1_455]	1.40	0.80
12:L:122:ASN:ND2	18:4:181:GLU:OE1[1_455]	1.46	0.74
15:1:173:TYR:CZ	16:2:132:LEU:C[2_646]	1.47	0.73
2:B:248:GLN:NE2	19:K:3009:CLA:C1C[1_554]	1.49	0.71
6:F:131:ASP:CG	12:L:170:LYS:CD[2_556]	1.49	0.71
12:L:123:THR:O	18:4:180:GLY:N[1_455]	1.50	0.70
12:L:124:GLU:OE2	18:4:172:PHE:CZ[1_455]	1.50	0.70
8:H:81:SER:OG	18:4:240:TRP:CZ3[2_546]	1.51	0.69
12:L:124:GLU:OE2	18:4:172:PHE:CE1[1_455]	1.52	0.68
6:F:130:PHE:CZ	12:L:170:LYS:CE[2_556]	1.53	0.67
12:L:124:GLU:N	18:4:177:LEU:O[1_455]	1.54	0.66
12:L:205:TYR:OH	18:4:181:GLU:C[1_455]	1.55	0.65
15:1:171:LEU:CG	16:2:131:ILE:CA[2_646]	1.55	0.65
6:F:130:PHE:CD1	12:L:170:LYS:CE[2_556]	1.56	0.64
12:L:203:LEU:O	18:4:184:TYR:OH[1_455]	1.58	0.62
15:1:170:PRO:C	16:2:132:LEU:N[2_646]	1.58	0.62
15:1:173:TYR:CZ	16:2:132:LEU:CA[2_646]	1.59	0.61
12:L:122:ASN:CG	18:4:181:GLU:OE1[1_455]	1.60	0.60
12:L:202:PHE:O	18:4:184:TYR:OH[1_455]	1.61	0.59
6:F:131:ASP:OD1	12:L:170:LYS:CD[2_556]	1.62	0.58
15:1:171:LEU:CG	16:2:131:ILE:C[2_646]	1.62	0.58
12:L:122:ASN:OD1	18:4:181:GLU:OE1[1_455]	1.64	0.56
12:L:124:GLU:OE2	18:4:176:SER:O[1_455]	1.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:173:TYR:OH	16:2:132:LEU:O[2_646]	1.66	0.54
15:1:118:PRO:C	17:3:89:THR:CG2[1_554]	1.67	0.53
12:L:203:LEU:CA	18:4:184:TYR:OH[1_455]	1.68	0.52
15:1:171:LEU:CG	16:2:131:ILE:N[2_646]	1.68	0.52
2:B:205:GLU:OE2	11:K:69:ARG:NH2[1_554]	1.70	0.50
19:K:1142:CLA:O2A	19:1:1008:CLA:O2D[1_456]	1.70	0.50
15:1:173:TYR:OH	16:2:133:ASN:N[2_646]	1.71	0.49
4:D:160:ASN:ND2	6:F:101:LYS:NZ[2_546]	1.72	0.48
15:1:171:LEU:CD1	16:2:131:ILE:CB[2_646]	1.72	0.48
15:1:173:TYR:OH	16:2:132:LEU:CB[2_646]	1.72	0.48
6:F:120:LYS:NZ	12:L:155:GLU:CG[2_556]	1.73	0.47
15:1:171:LEU:CA	16:2:132:LEU:N[2_646]	1.73	0.47
12:L:124:GLU:OE2	18:4:172:PHE:CE2[1_455]	1.74	0.46
12:L:204:LEU:N	18:4:184:TYR:OH[1_455]	1.75	0.45
12:L:124:GLU:OE2	18:4:172:PHE:CD1[1_455]	1.76	0.44
12:L:203:LEU:C	18:4:184:TYR:CZ[1_455]	1.76	0.44
15:1:170:PRO:C	16:2:132:LEU:CA[2_646]	1.81	0.39
12:L:205:TYR:CZ	18:4:181:GLU:O[1_455]	1.83	0.37
15:1:170:PRO:O	16:2:132:LEU:CG[2_646]	1.83	0.37
1:A:348:GLU:OE2	7:G:147:ASN:CG[1_556]	1.84	0.36
6:F:120:LYS:NZ	12:L:155:GLU:CD[2_556]	1.85	0.35
6:F:130:PHE:CE2	12:L:170:LYS:NZ[2_556]	1.85	0.35
1:A:200:GLU:OE1	2:B:220:GLN:NE2[1_556]	1.86	0.34
8:H:81:SER:OG	18:4:240:TRP:CH2[2_546]	1.86	0.34
6:F:130:PHE:CE1	12:L:170:LYS:CD[2_556]	1.88	0.32
15:1:171:LEU:CD2	16:2:132:LEU:N[2_646]	1.88	0.32
6:F:130:PHE:CD1	12:L:170:LYS:CD[2_556]	1.89	0.31
12:L:122:ASN:OD1	18:4:181:GLU:CD[1_455]	1.91	0.29
2:B:248:GLN:NE2	19:K:3009:CLA:CHC[1_554]	1.92	0.28
6:F:120:LYS:CE	12:L:155:GLU:CG[2_556]	1.92	0.28
12:L:204:LEU:CD2	18:4:185:PRO:O[1_455]	1.92	0.28
15:1:171:LEU:CG	16:2:132:LEU:N[2_646]	1.93	0.27
12:L:124:GLU:OE2	18:4:172:PHE:CD2[1_455]	1.95	0.25
7:G:85:GLU:OE2	22:K:7047:LMU:C7[2_546]	1.96	0.24
15:1:171:LEU:CD2	16:2:133:ASN:N[2_646]	1.96	0.24
2:B:205:GLU:OE1	11:K:69:ARG:NH1[1_554]	1.97	0.23
12:L:124:GLU:OE2	18:4:172:PHE:CG[1_455]	1.97	0.23
15:1:171:LEU:CB	16:2:132:LEU:N[2_646]	1.97	0.23
15:1:173:TYR:CE2	16:2:132:LEU:CA[2_646]	1.97	0.23
6:F:130:PHE:CE1	12:L:170:LYS:NZ[2_556]	1.98	0.22
2:B:248:GLN:CD	19:K:3009:CLA:CMC[1_554]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:GLN:CD	19:K:3009:CLA:C2C[1_554]	1.99	0.21
2:B:5:ILE:CD1	6:F:111:ASP:OD1[2_546]	2.00	0.20
6:F:131:ASP:CG	12:L:170:LYS:CG[2_556]	2.01	0.19
15:1:170:PRO:O	16:2:132:LEU:N[2_646]	2.01	0.19
12:L:122:ASN:O	18:4:179:ALA:N[1_455]	2.02	0.18
12:L:203:LEU:N	18:4:184:TYR:OH[1_455]	2.02	0.18
4:D:160:ASN:OD1	6:F:101:LYS:NZ[2_546]	2.03	0.17
12:L:202:PHE:C	18:4:184:TYR:OH[1_455]	2.03	0.17
15:1:171:LEU:N	16:2:132:LEU:CA[2_646]	2.03	0.17
1:A:348:GLU:OE2	7:G:147:ASN:ND2[1_556]	2.04	0.16
2:B:239:SER:OG	19:K:3009:CLA:CAA[1_554]	2.04	0.16
4:D:160:ASN:CB	6:F:101:LYS:NZ[2_546]	2.04	0.16
6:F:120:LYS:NZ	12:L:155:GLU:OE2[2_556]	2.05	0.15
15:1:171:LEU:N	16:2:131:ILE:C[2_646]	2.06	0.14
7:G:85:GLU:OE2	22:K:7047:LMU:C9[2_546]	2.07	0.13
1:A:348:GLU:CD	7:G:147:ASN:OD1[1_556]	2.10	0.10
15:1:171:LEU:CD2	16:2:131:ILE:CA[2_646]	2.10	0.10
6:F:130:PHE:CE2	12:L:170:LYS:CE[2_556]	2.11	0.09
12:L:123:THR:C	18:4:180:GLY:CA[1_455]	2.11	0.09
1:A:474:GLN:O	18:4:175:TYR:OH[1_455]	2.12	0.08
12:L:124:GLU:CD	18:4:172:PHE:CD2[1_455]	2.12	0.08
12:L:209:LEU:CD2	18:4:189:PHE:CE1[1_455]	2.13	0.07
15:1:173:TYR:CE1	16:2:132:LEU:C[2_646]	2.13	0.07
6:F:130:PHE:CG	12:L:170:LYS:CE[2_556]	2.14	0.06
12:L:204:LEU:CD2	18:4:185:PRO:C[1_455]	2.14	0.06
15:1:171:LEU:CD1	16:2:131:ILE:N[2_646]	2.14	0.06
6:F:130:PHE:CZ	12:L:170:LYS:NZ[2_556]	2.15	0.05
12:L:204:LEU:N	18:4:184:TYR:CZ[1_455]	2.15	0.05
15:1:171:LEU:CG	16:2:131:ILE:CB[2_646]	2.15	0.05
12:L:203:LEU:C	18:4:184:TYR:CE2[1_455]	2.16	0.04
12:L:123:THR:C	18:4:180:GLY:N[1_455]	2.17	0.03
6:F:112:ASP:OD2	9:I:30:LYS:NZ[2_556]	2.18	0.02
12:L:124:GLU:CD	18:4:172:PHE:CE1[1_455]	2.18	0.02
12:L:202:PHE:O	18:4:184:TYR:CZ[1_455]	2.19	0.01
15:1:171:LEU:CD1	16:2:131:ILE:CA[2_646]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/738 (98%)	483 (66%)	139 (19%)	104 (14%)	0	1
2	B	731/733 (100%)	527 (72%)	111 (15%)	93 (13%)	0	1
3	C	79/81 (98%)	42 (53%)	18 (23%)	19 (24%)	0	0
4	D	136/138 (99%)	94 (69%)	24 (18%)	18 (13%)	0	1
5	E	62/64 (97%)	44 (71%)	11 (18%)	7 (11%)	0	2
6	F	152/154 (99%)	105 (69%)	27 (18%)	20 (13%)	0	1
7	G	93/95 (98%)	60 (64%)	22 (24%)	11 (12%)	0	2
8	H	67/69 (97%)	49 (73%)	9 (13%)	9 (13%)	0	1
9	I	28/30 (93%)	11 (39%)	9 (32%)	8 (29%)	0	0
10	J	40/42 (95%)	19 (48%)	11 (28%)	10 (25%)	0	0
11	K	82/84 (98%)	66 (80%)	9 (11%)	7 (8%)	1	5
12	L	159/161 (99%)	110 (69%)	23 (14%)	26 (16%)	0	1
13	N	83/85 (98%)	50 (60%)	19 (23%)	14 (17%)	0	1
15	1	161/170 (95%)	119 (74%)	28 (17%)	14 (9%)	1	5
16	2	174/176 (99%)	129 (74%)	26 (15%)	19 (11%)	0	2
17	3	148/172 (86%)	111 (75%)	20 (14%)	17 (12%)	0	2
18	4	164/166 (99%)	129 (79%)	21 (13%)	14 (8%)	1	5
All	All	3085/3158 (98%)	2148 (70%)	527 (17%)	410 (13%)	0	1

All (410) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	41	SER
1	A	98	PHE
1	A	99	HIS
1	A	158	ILE

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Mol	Chain	Res	Type
1	A	164	LEU
1	A	175	ALA
1	A	205	HIS
1	A	221	HIS
1	A	237	VAL
1	A	268	PRO
1	A	279	ASP
1	A	283	PHE
1	A	307	ALA
1	A	310	PHE
1	A	317	TYR
1	A	329	ASP
1	A	333	ALA
1	A	346	LEU
1	A	361	ASN
1	A	386	ALA
1	A	389	TYR
1	A	424	PRO
1	A	431	LEU
1	A	433	ASP
1	A	473	PRO
1	A	474	GLN
1	A	477	PHE
1	A	509	ALA
1	A	523	VAL
1	A	532	ILE
1	A	553	VAL
1	A	594	ALA
1	A	643	ALA
1	A	657	LEU
1	A	673	SER
1	A	679	PHE
1	A	727	ILE
1	A	735	VAL
1	A	750	PHE
1	A	751	LEU
1	A	752	ALA
1	A	757	VAL
2	B	35	ASP
2	B	80	ASP
2	B	83	HIS
2	B	99	PRO

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Mol	Chain	Res	Type
2	B	105	THR
2	B	142	LEU
2	B	160	LYS
2	B	170	ASN
2	B	182	LEU
2	B	187	SER
2	B	198	ALA
2	B	208	ARG
2	B	231	ASN
2	B	267	SER
2	B	308	HIS
2	B	321	GLY
2	B	378	ILE
2	B	382	ILE
2	B	383	MET
2	B	420	SER
2	B	490	ARG
2	B	495	PRO
2	B	506	ASN
2	B	512	ILE
2	B	545	LYS
2	B	554	GLY
2	B	555	TYR
2	B	569	ASP
2	B	587	ILE
2	B	599	ILE
2	B	629	SER
2	B	639	VAL
2	B	661	PHE
2	B	662	MET
2	B	668	ARG
2	B	681	ALA
2	B	710	LEU
2	B	733	PHE
3	C	8	TYR
3	C	21	CYS
3	C	32	GLY
3	C	49	VAL
3	C	56	SER
3	C	59	PRO
3	C	62	PHE
3	C	65	VAL

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Mol	Chain	Res	Type
4	D	107	PRO
4	D	124	GLU
4	D	132	ALA
4	D	151	LYS
4	D	173	TYR
4	D	186	GLN
4	D	193	LYS
4	D	207	PRO
5	E	73	LYS
5	E	92	ALA
5	E	102	PRO
5	E	103	VAL
5	E	128	VAL
6	F	84	PRO
6	F	119	ILE
6	F	124	GLU
6	F	191	PRO
6	F	193	GLN
7	G	84	ARG
7	G	92	PRO
7	G	98	THR
7	G	130	TRP
7	G	142	LEU
7	G	150	ASP
8	H	62	THR
8	H	99	LYS
9	I	22	ALA
9	I	23	SER
10	J	5	LYS
10	J	6	THR
10	J	10	VAL
10	J	22	LEU
10	J	26	LEU
10	J	38	ILE
11	K	87	GLU
11	K	93	LEU
12	L	60	ILE
12	L	73	VAL
12	L	83	LEU
12	L	121	ARG
12	L	122	ASN
12	L	143	LEU

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Mol	Chain	Res	Type
12	L	169	ARG
12	L	195	SER
13	N	97	THR
13	N	125	CYS
13	N	134	CYS
13	N	146	LEU
13	N	148	ASP
13	N	149	ASP
15	1	65	ASP
15	1	97	ILE
15	1	130	PRO
15	1	156	LYS
15	1	169	ASP
15	1	170	PRO
15	1	177	PRO
15	1	217	LEU
15	1	225	TRP
16	2	139	THR
16	2	174	PRO
16	2	183	PHE
16	2	207	GLY
16	2	212	GLN
16	2	246	PRO
16	2	257	PRO
16	2	265	ALA
17	3	92	PHE
17	3	129	PRO
17	3	151	TRP
17	3	160	LEU
17	3	178	LYS
17	3	254	GLN
18	4	85	PRO
18	4	109	MET
18	4	120	ILE
18	4	134	TYR
1	A	22	VAL
1	A	35	ALA
1	A	57	LEU
1	A	160	SER
1	A	163	GLN
1	A	210	LEU
1	A	215	SER

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Mol	Chain	Res	Type
1	A	247	GLU
1	A	249	ILE
1	A	250	LEU
1	A	294	LEU
1	A	308	ILE
1	A	313	ALA
1	A	347	TYR
1	A	373	ALA
1	A	400	MET
1	A	439	ARG
1	A	446	LEU
1	A	476	MET
1	A	592	VAL
1	A	624	VAL
1	A	640	GLY
1	A	649	ILE
1	A	661	ALA
1	A	671	SER
1	A	717	ALA
2	B	26	ALA
2	B	153	GLY
2	B	178	HIS
2	B	179	LEU
2	B	188	LEU
2	B	330	ILE
2	B	371	LEU
2	B	375	HIS
2	B	379	ALA
2	B	437	TYR
2	B	501	ILE
2	B	505	SER
2	B	528	HIS
2	B	657	TRP
2	B	664	LEU
2	B	707	LEU
2	B	731	GLY
2	B	732	LYS
3	C	10	THR
3	C	12	ILE
3	C	28	MET
3	C	40	ALA
3	C	66	ARG

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Mol	Chain	Res	Type
4	D	76	PRO
4	D	81	PRO
4	D	119	ALA
4	D	149	LYS
4	D	164	GLN
5	E	110	VAL
5	E	111	ASN
6	F	128	LYS
6	F	135	LYS
6	F	138	LEU
6	F	140	CYS
6	F	205	SER
7	G	62	LEU
7	G	141	ILE
8	H	64	GLN
8	H	100	PHE
8	H	116	ALA
9	I	25	PHE
10	J	37	LEU
11	K	86	LEU
11	K	114	HIS
11	K	126	ASN
12	L	68	SER
12	L	200	ALA
13	N	109	THR
13	N	119	THR
13	N	147	SER
15	1	59	PRO
16	2	104	GLN
16	2	133	ASN
16	2	146	PHE
16	2	248	ASP
17	3	152	ALA
17	3	250	VAL
17	3	252	PRO
18	4	192	LEU
1	A	127	VAL
1	A	184	PHE
1	A	213	LEU
1	A	243	PRO
1	A	421	ASP
1	A	498	LEU

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Mol	Chain	Res	Type
1	A	742	GLY
2	B	42	LEU
2	B	81	PRO
2	B	141	PHE
2	B	189	ALA
2	B	273	VAL
2	B	335	GLY
2	B	362	ALA
2	B	470	THR
2	B	558	PRO
2	B	592	PHE
3	C	23	THR
3	C	52	LYS
4	D	88	GLY
4	D	175	GLU
4	D	184	VAL
6	F	102	LEU
6	F	103	GLN
6	F	121	ALA
6	F	186	ARG
8	H	98	LEU
10	J	9	SER
10	J	23	ALA
10	J	39	PHE
12	L	193	GLY
13	N	110	THR
13	N	132	THR
13	N	142	LYS
13	N	159	LYS
15	1	224	PRO
16	2	168	TRP
17	3	112	GLY
18	4	173	LYS
18	4	201	LYS
18	4	228	PRO
18	4	230	ASP
1	A	67	HIS
1	A	186	TYR
1	A	234	ASN
1	A	259	TYR
1	A	306	ILE
1	A	404	GLY

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Mol	Chain	Res	Type
1	A	574	ASN
1	A	701	GLN
2	B	41	ARG
2	B	43	TYR
2	B	69	ALA
2	B	164	SER
2	B	281	ALA
2	B	309	ILE
2	B	474	PHE
2	B	476	ILE
2	B	593	TYR
2	B	595	HIS
6	F	97	GLN
6	F	115	PRO
6	F	123	MET
6	F	160	PHE
8	H	69	GLY
8	H	117	SER
9	I	2	ILE
9	I	5	PRO
9	I	9	VAL
12	L	56	VAL
12	L	57	ILE
12	L	59	PRO
12	L	131	SER
12	L	159	SER
12	L	181	GLY
15	1	220	HIS
16	2	203	PRO
17	3	140	GLY
17	3	156	THR
17	3	248	THR
1	A	151	GLN
1	A	179	LEU
1	A	230	ASN
1	A	472	ARG
1	A	580	PRO
1	A	718	PRO
2	B	172	GLU
2	B	265	THR
2	B	278	LEU
2	B	311	PRO

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Mol	Chain	Res	Type
2	B	391	PRO
2	B	398	TYR
2	B	457	PRO
2	B	514	PRO
2	B	596	TRP
2	B	623	TYR
2	B	730	SER
3	C	55	GLU
3	C	58	CYS
4	D	202	PHE
7	G	90	GLN
7	G	149	TYR
8	H	120	ILE
11	K	48	PHE
11	K	80	ALA
12	L	55	GLN
12	L	175	GLN
15	1	119	GLY
16	2	95	ASP
16	2	206	TRP
17	3	202	TYR
17	3	230	ASN
17	3	234	ALA
18	4	179	ALA
18	4	223	VAL
18	4	243	THR
1	A	36	LYS
1	A	130	GLU
1	A	225	VAL
1	A	289	PRO
1	A	542	HIS
1	A	721	GLN
2	B	598	HIS
3	C	71	HIS
6	F	214	PRO
16	2	135	PRO
18	4	195	ALA
1	A	223	VAL
1	A	584	PRO
2	B	557	PHE
2	B	711	VAL
2	B	716	GLY

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Mol	Chain	Res	Type
3	C	22	PRO
4	D	89	GLY
15	1	223	ASP
1	A	112	ASP
1	A	125	PRO
1	A	229	ILE
1	A	754	ILE
2	B	708	VAL
12	L	192	GLY
16	2	196	PRO
17	3	245	GLY
2	B	219	PRO
12	L	107	GLY
12	L	118	GLY
12	L	158	PRO
1	A	124	TRP
1	A	190	ALA
6	F	215	VAL
7	G	78	VAL
9	I	12	VAL
12	L	99	GLY
13	N	166	VAL
16	2	130	GLY
18	4	163	PRO
9	I	10	PRO
12	L	62	GLY
12	L	115	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	590/599 (98%)	475 (80%)	115 (20%)	1	5
2	B	597/599 (100%)	468 (78%)	129 (22%)	1	4
3	C	70/70 (100%)	60 (86%)	10 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	117/117 (100%)	83 (71%)	34 (29%)	0	1
5	E	56/56 (100%)	42 (75%)	14 (25%)	0	2
6	F	127/127 (100%)	91 (72%)	36 (28%)	0	1
7	G	78/79 (99%)	60 (77%)	18 (23%)	1	3
8	H	55/55 (100%)	42 (76%)	13 (24%)	1	3
9	I	26/26 (100%)	23 (88%)	3 (12%)	5	22
10	J	35/36 (97%)	26 (74%)	9 (26%)	0	2
11	K	62/62 (100%)	45 (73%)	17 (27%)	0	1
12	L	127/127 (100%)	105 (83%)	22 (17%)	2	8
13	N	74/74 (100%)	49 (66%)	25 (34%)	0	1
15	1	126/134 (94%)	76 (60%)	50 (40%)	0	0
16	2	139/142 (98%)	91 (66%)	48 (34%)	0	1
17	3	113/129 (88%)	74 (66%)	39 (34%)	0	1
18	4	136/140 (97%)	107 (79%)	29 (21%)	1	4
All	All	2528/2572 (98%)	1917 (76%)	611 (24%)	0	2

All (611) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	24	ARG
1	A	25	ASP
1	A	31	PHE
1	A	34	TRP
1	A	39	HIS
1	A	55	TRP
1	A	57	LEU
1	A	60	ASP
1	A	62	HIS
1	A	63	ASP
1	A	68	THR
1	A	78	VAL
1	A	93	LEU
1	A	103	PHE
1	A	104	SER
1	A	105	ASN
1	A	110	LEU

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Mol	Chain	Res	Type
1	A	124	TRP
1	A	129	GLN
1	A	132	LEU
1	A	153	TRP
1	A	159	THR
1	A	160	SER
1	A	172	LEU
1	A	180	PHE
1	A	187	HIS
1	A	188	LYS
1	A	195	TRP
1	A	196	PHE
1	A	224	HIS
1	A	232	PHE
1	A	233	LEU
1	A	246	HIS
1	A	248	PHE
1	A	250	LEU
1	A	252	ARG
1	A	254	LEU
1	A	255	LEU
1	A	270	PHE
1	A	277	TYR
1	A	284	ARG
1	A	296	LEU
1	A	297	THR
1	A	298	ASP
1	A	317	TYR
1	A	328	LYS
1	A	331	LEU
1	A	334	HIS
1	A	338	PHE
1	A	341	GLN
1	A	350	LEU
1	A	351	THR
1	A	353	SER
1	A	357	GLN
1	A	368	LEU
1	A	369	THR
1	A	375	HIS
1	A	377	TYR
1	A	384	TYR

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Mol	Chain	Res	Type
1	A	392	GLN
1	A	393	LEU
1	A	400	MET
1	A	402	ILE
1	A	405	PHE
1	A	408	VAL
1	A	420	ARG
1	A	421	ASP
1	A	422	TYR
1	A	426	THR
1	A	427	ARG
1	A	433	ASP
1	A	434	ARG
1	A	435	VAL
1	A	438	HIS
1	A	439	ARG
1	A	444	SER
1	A	462	ILE
1	A	464	ASN
1	A	477	PHE
1	A	484	LEU
1	A	485	GLN
1	A	488	PHE
1	A	490	GLN
1	A	498	LEU
1	A	519	ASP
1	A	523	VAL
1	A	538	ASP
1	A	539	PHE
1	A	553	VAL
1	A	558	LYS
1	A	561	LEU
1	A	564	ARG
1	A	577	PHE
1	A	578	ARG
1	A	579	PHE
1	A	590	CYS
1	A	591	GLN
1	A	605	MET
1	A	637	ILE
1	A	642	PHE
1	A	646	SER

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Mol	Chain	Res	Type
1	A	654	ARG
1	A	660	GLN
1	A	662	SER
1	A	684	PHE
1	A	689	SER
1	A	691	MET
1	A	697	ARG
1	A	707	ILE
1	A	715	LYS
1	A	723	ARG
1	A	726	SER
1	A	727	ILE
1	A	754	ILE
2	B	4	ARG
2	B	6	PRO
2	B	7	ARG
2	B	8	PHE
2	B	10	GLN
2	B	12	ILE
2	B	19	ARG
2	B	20	ARG
2	B	46	ILE
2	B	50	HIS
2	B	51	PHE
2	B	67	HIS
2	B	70	TRP
2	B	73	ASN
2	B	78	VAL
2	B	83	HIS
2	B	85	ARG
2	B	87	ILE
2	B	96	PHE
2	B	98	GLN
2	B	106	ARG
2	B	113	VAL
2	B	115	ASN
2	B	121	TYR
2	B	123	TRP
2	B	124	TRP
2	B	129	LEU
2	B	130	ARG
2	B	131	THR

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Mol	Chain	Res	Type
2	B	135	LEU
2	B	144	PHE
2	B	154	TRP
2	B	158	GLN
2	B	160	LYS
2	B	161	TRP
2	B	165	VAL
2	B	177	HIS
2	B	178	HIS
2	B	188	LEU
2	B	195	VAL
2	B	206	TYR
2	B	212	PHE
2	B	229	GLN
2	B	233	TYR
2	B	241	ASN
2	B	244	PHE
2	B	247	THR
2	B	248	GLN
2	B	262	HIS
2	B	267	SER
2	B	269	TRP
2	B	285	LEU
2	B	291	TYR
2	B	292	ARG
2	B	295	PHE
2	B	299	HIS
2	B	317	ARG
2	B	319	HIS
2	B	320	LYS
2	B	332	PHE
2	B	347	LEU
2	B	348	VAL
2	B	350	GLN
2	B	353	TYR
2	B	361	ILE
2	B	365	PHE
2	B	367	THR
2	B	374	HIS
2	B	382	ILE
2	B	393	PHE
2	B	395	ILE

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Mol	Chain	Res	Type
2	B	396	ARG
2	B	410	ARG
2	B	420	SER
2	B	422	LEU
2	B	428	PHE
2	B	437	TYR
2	B	438	VAL
2	B	440	ASN
2	B	443	MET
2	B	448	THR
2	B	451	LYS
2	B	455	ILE
2	B	464	GLN
2	B	469	LYS
2	B	472	TYR
2	B	474	PHE
2	B	490	ARG
2	B	492	ILE
2	B	497	TRP
2	B	509	PHE
2	B	516	ASP
2	B	521	HIS
2	B	528	HIS
2	B	542	ARG
2	B	545	LYS
2	B	555	TYR
2	B	564	ARG
2	B	577	TYR
2	B	580	VAL
2	B	583	MET
2	B	587	ILE
2	B	592	PHE
2	B	594	TRP
2	B	596	TRP
2	B	608	GLN
2	B	613	SER
2	B	614	THR
2	B	615	TYR
2	B	617	MET
2	B	620	LEU
2	B	622	ASP
2	B	629	SER

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Mol	Chain	Res	Type
2	B	630	GLN
2	B	662	MET
2	B	670	TYR
2	B	677	THR
2	B	682	HIS
2	B	685	THR
2	B	690	LEU
2	B	692	ARG
2	B	694	ARG
2	B	696	LYS
2	B	701	SER
2	B	710	LEU
2	B	712	HIS
2	B	719	PHE
2	B	732	LYS
2	B	733	PHE
3	C	18	VAL
3	C	24	ASP
3	C	28	MET
3	C	38	GLN
3	C	45	THR
3	C	48	CYS
3	C	52	LYS
3	C	58	CYS
3	C	66	ARG
3	C	70	TRP
4	D	75	ASP
4	D	78	THR
4	D	80	SER
4	D	82	ILE
4	D	83	PHE
4	D	92	ARG
4	D	95	GLN
4	D	97	GLU
4	D	99	PHE
4	D	100	TYR
4	D	101	VAL
4	D	104	TRP
4	D	105	ASP
4	D	112	PHE
4	D	122	MET
4	D	124	GLU

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Mol	Chain	Res	Type
4	D	130	LYS
4	D	133	ARG
4	D	135	GLU
4	D	140	LEU
4	D	147	LYS
4	D	149	LYS
4	D	152	TYR
4	D	162	GLU
4	D	165	TYR
4	D	169	LYS
4	D	176	LYS
4	D	177	VAL
4	D	187	ASN
4	D	188	PHE
4	D	198	ILE
4	D	200	VAL
4	D	201	LYS
4	D	205	LYS
5	E	66	ILE
5	E	69	LYS
5	E	70	ARG
5	E	77	LEU
5	E	78	ARG
5	E	79	LYS
5	E	83	TRP
5	E	93	VAL
5	E	106	ARG
5	E	111	ASN
5	E	114	ASN
5	E	126	VAL
5	E	128	VAL
5	E	129	GLU
6	F	79	ILE
6	F	86	LYS
6	F	89	LYS
6	F	91	PHE
6	F	94	ARG
6	F	97	GLN
6	F	100	LYS
6	F	103	GLN
6	F	106	LEU
6	F	107	LYS

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Mol	Chain	Res	Type
6	F	125	LYS
6	F	128	LYS
6	F	129	ARG
6	F	131	ASP
6	F	136	TYR
6	F	138	LEU
6	F	151	SER
6	F	154	GLN
6	F	156	HIS
6	F	160	PHE
6	F	165	ILE
6	F	168	LEU
6	F	170	ILE
6	F	173	TRP
6	F	177	VAL
6	F	181	TYR
6	F	183	ILE
6	F	188	GLU
6	F	200	VAL
6	F	207	LEU
6	F	208	PHE
6	F	213	TRP
6	F	218	TYR
6	F	219	ARG
6	F	221	LEU
6	F	231	PHE
7	G	66	LEU
7	G	73	PHE
7	G	76	ARG
7	G	80	PHE
7	G	87	VAL
7	G	89	LYS
7	G	90	GLN
7	G	94	GLN
7	G	95	ASN
7	G	97	LEU
7	G	98	THR
7	G	101	GLU
7	G	104	ASP
7	G	116	SER
7	G	125	VAL
7	G	144	THR

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Mol	Chain	Res	Type
7	G	147	ASN
7	G	149	TYR
8	H	66	ASP
8	H	76	TYR
8	H	79	LEU
8	H	80	GLN
8	H	93	LYS
8	H	94	ARG
8	H	99	LYS
8	H	100	PHE
8	H	109	LEU
8	H	111	TYR
8	H	112	LEU
8	H	113	SER
8	H	119	ASP
9	I	3	ASN
9	I	7	LEU
9	I	11	LEU
10	J	2	ARG
10	J	3	ASP
10	J	5	LYS
10	J	9	SER
10	J	16	THR
10	J	19	PHE
10	J	35	ASP
10	J	37	LEU
10	J	41	PHE
11	K	51	SER
11	K	53	THR
11	K	58	VAL
11	K	59	THR
11	K	63	LEU
11	K	65	LEU
11	K	66	PHE
11	K	70	PHE
11	K	77	ASN
11	K	78	ARG
11	K	89	ARG
11	K	102	THR
11	K	103	LEU
11	K	114	HIS
11	K	122	LEU

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Mol	Chain	Res	Type
11	K	125	LYS
11	K	130	LEU
12	L	51	LYS
12	L	54	TYR
12	L	86	LEU
12	L	96	LEU
12	L	114	PHE
12	L	116	LYS
12	L	122	ASN
12	L	128	GLN
12	L	141	LEU
12	L	142	SER
12	L	145	LEU
12	L	151	SER
12	L	153	PHE
12	L	155	GLU
12	L	171	LYS
12	L	172	GLU
12	L	182	TRP
12	L	186	THR
12	L	191	PHE
12	L	201	TYR
12	L	205	TYR
12	L	211	TYR
13	N	90	GLU
13	N	91	TYR
13	N	94	LYS
13	N	96	LYS
13	N	104	LYS
13	N	105	LYS
13	N	106	ARG
13	N	110	THR
13	N	114	PHE
13	N	118	TYR
13	N	122	PHE
13	N	126	LYS
13	N	127	PHE
13	N	135	GLN
13	N	139	LYS
13	N	142	LYS
13	N	145	PHE
13	N	150	LEU

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Mol	Chain	Res	Type
13	N	157	LYS
13	N	160	TYR
13	N	161	LYS
13	N	162	CYS
13	N	167	PHE
13	N	168	TRP
13	N	170	TRP
15	1	62	PHE
15	1	71	GLU
15	1	76	LEU
15	1	77	GLU
15	1	81	GLU
15	1	86	HIS
15	1	87	CYS
15	1	91	MET
15	1	92	LEU
15	1	94	VAL
15	1	97	ILE
15	1	98	LEU
15	1	101	GLU
15	1	103	LEU
15	1	117	LEU
15	1	124	TYR
15	1	125	LEU
15	1	131	TRP
15	1	133	THR
15	1	136	THR
15	1	137	ILE
15	1	138	LEU
15	1	141	GLU
15	1	145	ILE
15	1	147	PHE
15	1	149	GLU
15	1	150	HIS
15	1	151	GLN
15	1	155	GLU
15	1	161	LYS
15	1	163	TYR
15	1	168	PHE
15	1	169	ASP
15	1	170	PRO
15	1	171	LEU

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Mol	Chain	Res	Type
15	1	173	TYR
15	1	175	LYS
15	1	178	LYS
15	1	181	GLU
15	1	189	LYS
15	1	193	LEU
15	1	198	PHE
15	1	199	VAL
15	1	203	VAL
15	1	205	GLN
15	1	206	SER
15	1	211	THR
15	1	214	LEU
15	1	225	TRP
15	1	226	HIS
16	2	99	LEU
16	2	101	TRP
16	2	104	GLN
16	2	114	MET
16	2	121	PHE
16	2	128	LYS
16	2	133	ASN
16	2	138	TYR
16	2	139	THR
16	2	144	GLU
16	2	145	TYR
16	2	150	THR
16	2	152	LEU
16	2	154	ILE
16	2	156	GLU
16	2	157	LEU
16	2	159	PHE
16	2	167	ARG
16	2	168	TRP
16	2	173	ASN
16	2	183	PHE
16	2	185	ASN
16	2	187	LYS
16	2	188	LEU
16	2	189	THR
16	2	192	ASP
16	2	195	TYR

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Mol	Chain	Res	Type
16	2	200	TRP
16	2	201	PHE
16	2	202	ASP
16	2	215	LYS
16	2	217	LEU
16	2	219	THR
16	2	220	LYS
16	2	222	ILE
16	2	226	ARG
16	2	229	MET
16	2	230	LEU
16	2	232	VAL
16	2	237	PHE
16	2	241	TYR
16	2	242	THR
16	2	244	THR
16	2	251	PHE
16	2	254	LEU
16	2	256	ASP
16	2	259	HIS
16	2	269	LYS
17	3	87	GLU
17	3	92	PHE
17	3	93	ILE
17	3	94	GLU
17	3	96	ARG
17	3	97	TRP
17	3	107	ARG
17	3	108	PHE
17	3	111	LEU
17	3	124	LYS
17	3	134	LEU
17	3	136	TRP
17	3	137	PHE
17	3	138	GLN
17	3	151	TRP
17	3	153	ASP
17	3	155	TYR
17	3	156	THR
17	3	158	PHE
17	3	161	GLU
17	3	165	MET

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Mol	Chain	Res	Type
17	3	167	PHE
17	3	173	PHE
17	3	174	GLN
17	3	175	ASP
17	3	181	SER
17	3	185	GLN
17	3	187	PHE
17	3	192	LYS
17	3	202	TYR
17	3	207	PHE
17	3	208	PHE
17	3	209	ASN
17	3	215	LYS
17	3	229	LYS
17	3	232	ARG
17	3	235	MET
17	3	242	PHE
17	3	253	TYR
18	4	86	GLU
18	4	89	ARG
18	4	90	TRP
18	4	95	GLU
18	4	96	LEU
18	4	101	TRP
18	4	115	PHE
18	4	118	ILE
18	4	131	LYS
18	4	139	SER
18	4	141	LEU
18	4	143	VAL
18	4	146	PHE
18	4	151	TYR
18	4	157	TRP
18	4	161	LYS
18	4	165	SER
18	4	172	PHE
18	4	175	TYR
18	4	177	LEU
18	4	192	LEU
18	4	201	LYS
18	4	214	PHE
18	4	226	LYS

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Mol	Chain	Res	Type
18	4	234	GLN
18	4	238	ASP
18	4	240	TRP
18	4	241	HIS
18	4	245	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	82	HIS
1	A	115	HIS
1	A	129	GLN
1	A	163	GLN
1	A	224	HIS
1	A	303	HIS
1	A	341	GLN
1	A	398	HIS
1	A	464	ASN
1	A	485	GLN
1	A	493	GLN
1	A	525	ASN
1	A	542	HIS
1	A	545	HIS
1	A	591	GLN
1	A	607	ASN
1	A	636	HIS
1	A	644	GLN
1	A	660	GLN
1	A	683	HIS
1	A	711	HIS
1	A	729	GLN
2	B	10	GLN
2	B	50	HIS
2	B	53	GLN
2	B	67	HIS
2	B	73	ASN
2	B	98	GLN
2	B	158	GLN
2	B	178	HIS
2	B	193	HIS
2	B	231	ASN

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Mol	Chain	Res	Type
2	B	277	HIS
2	B	294	ASN
2	B	319	HIS
2	B	331	HIS
2	B	333	GLN
2	B	375	HIS
2	B	403	ASN
2	B	432	HIS
2	B	452	GLN
2	B	464	GLN
2	B	502	ASN
2	B	521	HIS
2	B	528	HIS
2	B	595	HIS
2	B	610	ASN
2	B	633	ASN
2	B	712	HIS
3	C	71	HIS
4	D	95	GLN
4	D	110	GLN
4	D	136	GLN
4	D	182	GLN
4	D	187	ASN
4	D	206	GLN
5	E	111	ASN
6	F	97	GLN
6	F	193	GLN
8	H	77	ASN
8	H	80	GLN
11	K	77	ASN
11	K	114	HIS
12	L	85	ASN
12	L	122	ASN
13	N	113	ASN
13	N	130	ASN
15	1	86	HIS
15	1	112	GLN
15	1	151	GLN
15	1	190	ASN
15	1	204	GLN
15	1	205	GLN
15	1	226	HIS

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Mol	Chain	Res	Type
16	2	133	ASN
16	2	173	ASN
16	2	238	GLN
17	3	149	ASN
17	3	174	GLN
17	3	209	ASN
17	3	254	GLN
18	4	158	GLN
18	4	190	ASN
18	4	246	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

252 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	LMU	H	7002	-	36,36,36	0.61	0	47,47,47	1.50	7 (14%)
22	LMU	E	7048	-	36,36,36	0.83	1 (2%)	47,47,47	2.04	10 (21%)
19	CLA	B	1201	-	33,53,73	2.29	9 (27%)	27,89,113	4.10	10 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1230	-	41,58,73	2.15	11 (26%)	37,95,113	4.12	14 (37%)
22	LMU	H	7030	-	36,36,36	0.75	2 (5%)	47,47,47	1.19	4 (8%)
19	CLA	A	1110	-	45,62,73	2.02	9 (20%)	41,99,113	3.26	12 (29%)
19	CLA	2	2004	-	41,58,73	2.08	9 (21%)	37,95,113	3.93	14 (37%)
19	CLA	A	1125	-	56,73,73	1.80	9 (16%)	55,113,113	3.07	11 (20%)
19	CLA	4	4010	-	18,32,73	1.77	6 (33%)	22,54,113	3.98	13 (59%)
21	BCR	A	6007	-	41,41,41	1.55	4 (9%)	56,56,56	3.81	31 (55%)
19	CLA	A	1120	-	42,59,73	2.14	10 (23%)	38,96,113	3.76	15 (39%)
21	BCR	I	6018	-	41,41,41	1.47	4 (9%)	56,56,56	4.70	32 (57%)
22	LMU	B	7038	-	36,36,36	0.74	0	47,47,47	1.68	10 (21%)
19	CLA	B	1235	-	56,73,73	1.73	10 (17%)	55,113,113	2.69	11 (20%)
22	LMU	E	7037	-	36,36,36	0.72	1 (2%)	47,47,47	1.75	11 (23%)
19	CLA	3	3006	-	18,32,73	1.75	4 (22%)	22,54,113	4.07	14 (63%)
22	LMU	R	7024	-	36,36,36	0.76	1 (2%)	47,47,47	1.46	8 (17%)
19	CLA	A	1136	-	56,73,73	1.80	10 (17%)	55,113,113	3.23	14 (25%)
23	SF4	C	8002	3	0,12,12	0.00	-	-	-	-
19	CLA	A	1128	-	56,73,73	1.83	10 (17%)	55,113,113	3.61	17 (30%)
19	CLA	3	3012	-	18,32,73	1.76	5 (27%)	22,54,113	4.20	13 (59%)
19	CLA	A	1103	-	56,73,73	1.91	11 (19%)	55,113,113	2.98	15 (27%)
19	CLA	B	1202	-	56,73,73	1.88	11 (19%)	55,113,113	3.65	16 (29%)
19	CLA	2	2005	-	18,32,73	1.60	4 (22%)	22,54,113	3.99	11 (50%)
19	CLA	3	3004	-	18,32,73	2.01	6 (33%)	22,54,113	4.10	11 (50%)
21	BCR	B	6017	-	41,41,41	1.53	5 (12%)	56,56,56	3.97	25 (44%)
19	CLA	B	1215	-	51,68,73	1.82	10 (19%)	49,107,113	3.59	15 (30%)
19	CLA	A	1101	-	41,58,73	2.09	8 (19%)	37,95,113	3.83	15 (40%)
19	CLA	A	1137	-	38,55,73	2.18	11 (28%)	33,91,113	3.85	12 (36%)
19	CLA	L	1502	-	38,55,73	2.24	7 (18%)	33,91,113	4.16	15 (45%)
19	CLA	3	3011	-	56,73,73	1.83	10 (17%)	55,113,113	2.61	15 (27%)
22	LMU	B	7012	-	26,26,36	0.78	1 (3%)	37,37,47	1.41	7 (18%)
22	LMU	G	7039	-	36,36,36	0.68	0	47,47,47	1.35	4 (8%)
22	LMU	K	7047	-	36,36,36	0.79	1 (2%)	47,47,47	1.04	3 (6%)
19	CLA	A	1106	-	56,73,73	1.76	10 (17%)	55,113,113	3.13	18 (32%)
19	CLA	A	1123	-	56,73,73	1.77	9 (16%)	55,113,113	2.56	13 (23%)
19	CLA	B	1219	-	46,63,73	2.20	11 (23%)	43,101,113	3.63	10 (23%)
19	CLA	L	1501	12	41,58,73	2.13	9 (21%)	37,95,113	3.83	13 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1209	-	46,63,73	1.94	9 (19%)	43,101,113	3.68	13 (30%)
19	CLA	L	1504	-	46,63,73	2.10	10 (21%)	43,101,113	3.00	16 (37%)
19	CLA	A	1108	-	33,53,73	2.20	8 (24%)	27,89,113	4.77	12 (44%)
19	CLA	B	1222	-	49,66,73	1.95	11 (22%)	46,104,113	3.39	14 (30%)
19	CLA	3	3015	-	18,32,73	1.66	5 (27%)	22,54,113	3.74	11 (50%)
19	CLA	H	1241	-	46,63,73	2.19	8 (17%)	43,101,113	3.80	18 (41%)
19	CLA	B	1217	-	41,58,73	2.08	10 (24%)	37,95,113	3.82	13 (35%)
22	LMU	4	7018	-	36,36,36	0.74	1 (2%)	47,47,47	1.07	3 (6%)
21	BCR	B	6004	-	41,41,41	1.29	3 (7%)	56,56,56	4.27	29 (51%)
19	CLA	H	1505	-	46,63,73	2.13	9 (19%)	43,101,113	3.70	13 (30%)
19	CLA	3	3003	-	27,44,73	2.43	8 (29%)	27,78,113	4.14	12 (44%)
19	CLA	A	1112	-	33,53,73	2.35	8 (24%)	27,89,113	4.37	11 (40%)
19	CLA	3	3016	-	56,73,73	1.85	11 (19%)	55,113,113	3.19	15 (27%)
19	CLA	A	1138	-	56,73,73	1.85	10 (17%)	55,113,113	3.15	14 (25%)
19	CLA	A	1134	1	33,53,73	2.16	8 (24%)	27,89,113	4.44	11 (40%)
22	LMU	H	7017	-	36,36,36	0.73	1 (2%)	47,47,47	1.90	11 (23%)
19	CLA	3	1118	-	27,44,73	2.42	9 (33%)	27,78,113	4.69	10 (37%)
19	CLA	A	1127	-	46,63,73	2.06	10 (21%)	43,101,113	3.61	14 (32%)
19	CLA	A	1139	-	42,59,73	2.14	10 (23%)	38,96,113	3.81	15 (39%)
19	CLA	B	1218	-	37,54,73	2.19	9 (24%)	32,90,113	4.29	12 (37%)
21	BCR	A	6003	-	41,41,41	1.48	3 (7%)	56,56,56	4.08	27 (48%)
22	LMU	4	7034	-	36,36,36	0.62	0	47,47,47	0.70	0
23	SF4	A	8001	1,2	0,12,12	0.00	-	-	-	-
22	LMU	4	7019	-	36,36,36	0.81	1 (2%)	47,47,47	1.35	9 (19%)
21	BCR	F	6016	-	41,41,41	1.67	11 (26%)	56,56,56	3.64	27 (48%)
19	CLA	L	1148	-	46,63,73	2.23	14 (30%)	43,101,113	4.25	21 (48%)
19	CLA	1	1011	-	27,44,73	2.80	10 (37%)	27,78,113	5.22	10 (37%)
19	CLA	J	1308	-	46,63,73	2.07	11 (23%)	43,101,113	3.53	17 (39%)
22	LMU	A	7016	-	36,36,36	0.68	0	47,47,47	1.43	6 (12%)
19	CLA	A	1109	19	56,73,73	1.85	10 (17%)	55,113,113	2.92	16 (29%)
19	CLA	1	1002	-	38,55,73	2.31	9 (23%)	33,91,113	3.68	16 (48%)
21	BCR	1	6023	-	41,41,41	1.73	3 (7%)	56,56,56	6.25	30 (53%)
19	CLA	B	1220	-	56,73,73	1.99	11 (19%)	55,113,113	3.38	16 (29%)
19	CLA	A	9011	-	56,73,73	1.81	10 (17%)	55,113,113	3.55	15 (27%)
19	CLA	1	1010	-	37,54,73	2.36	11 (29%)	32,90,113	4.84	19 (59%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	4	4002	18	43,60,73	2.17	13 (30%)	39,97,113	4.64	25 (64%)
22	LMU	R	7007	-	36,36,36	0.58	1 (2%)	47,47,47	0.80	2 (4%)
19	CLA	A	1119	-	56,73,73	1.85	9 (16%)	55,113,113	3.41	17 (30%)
22	LMU	4	7008	-	36,36,36	0.58	0	47,47,47	0.87	1 (2%)
22	LMU	1	7013	-	36,36,36	0.71	1 (2%)	47,47,47	1.04	1 (2%)
19	CLA	L	1503	-	41,58,73	2.37	13 (31%)	37,95,113	4.47	14 (37%)
19	CLA	4	4007	-	43,60,73	2.12	9 (20%)	39,97,113	3.68	15 (38%)
19	CLA	B	1301	-	27,44,73	2.58	9 (33%)	27,78,113	4.58	12 (44%)
19	CLA	3	3010	-	18,32,73	1.69	6 (33%)	22,54,113	3.89	12 (54%)
19	CLA	2	2011	-	18,32,73	1.71	4 (22%)	22,54,113	4.01	14 (63%)
19	CLA	3	3014	-	18,32,73	1.85	5 (27%)	22,54,113	4.25	14 (63%)
22	LMU	R	7022	-	36,36,36	0.71	1 (2%)	47,47,47	1.31	6 (12%)
19	CLA	B	1231	19	33,53,73	2.31	7 (21%)	27,89,113	4.37	12 (44%)
19	CLA	4	1304	-	56,73,73	1.98	13 (23%)	55,113,113	3.54	20 (36%)
19	CLA	1	1007	-	52,69,73	2.01	10 (19%)	50,108,113	2.98	15 (30%)
19	CLA	4	4001	-	41,58,73	2.23	10 (24%)	37,95,113	4.14	14 (37%)
23	SF4	C	8003	3	0,12,12	0.00	-	-	-	-
22	LMU	A	7045	-	36,36,36	0.75	1 (2%)	47,47,47	1.48	8 (17%)
19	CLA	2	2001	-	42,59,73	2.09	10 (23%)	38,96,113	3.57	14 (36%)
19	CLA	3	3007	-	33,50,73	2.18	8 (24%)	27,85,113	4.67	10 (37%)
19	CLA	A	9013	-	56,73,73	1.97	10 (17%)	55,113,113	3.29	16 (29%)
19	CLA	4	1306	-	46,63,73	2.05	10 (21%)	43,101,113	3.38	13 (30%)
19	CLA	A	1113	-	41,58,73	2.22	8 (19%)	37,95,113	3.77	17 (45%)
19	CLA	A	1102	19	46,63,73	2.09	9 (19%)	43,101,113	2.80	15 (34%)
19	CLA	A	1309	-	18,32,73	1.66	5 (27%)	22,54,113	3.81	11 (50%)
22	LMU	A	7023	-	36,36,36	0.60	0	47,47,47	1.18	4 (8%)
19	CLA	J	1311	-	52,69,73	1.89	10 (19%)	50,108,113	3.41	14 (28%)
19	CLA	B	1223	-	56,73,73	1.82	11 (19%)	55,113,113	3.16	16 (29%)
19	CLA	B	1212	-	51,68,73	1.88	9 (17%)	49,107,113	2.88	13 (26%)
19	CLA	A	1140	-	56,73,73	1.77	10 (17%)	55,113,113	3.15	14 (25%)
19	CLA	A	1115	-	56,73,73	1.87	11 (19%)	55,113,113	3.19	15 (27%)
22	LMU	K	7001	-	36,36,36	0.82	2 (5%)	47,47,47	1.37	7 (14%)
19	CLA	B	1203	-	56,73,73	1.89	12 (21%)	55,113,113	3.18	19 (34%)
19	CLA	4	1004	-	46,63,73	2.17	13 (28%)	43,101,113	3.71	14 (32%)
19	CLA	B	1210	-	56,73,73	1.86	10 (17%)	55,113,113	3.20	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	3	1147	-	37,54,73	2.77	12 (32%)	32,90,113	3.85	19 (59%)
19	CLA	B	9010	-	56,73,73	1.75	10 (17%)	55,113,113	3.34	18 (32%)
19	CLA	1	1005	-	37,54,73	2.74	10 (27%)	32,90,113	2.70	11 (34%)
19	CLA	4	4014	-	38,55,73	2.07	9 (23%)	33,91,113	4.70	13 (39%)
22	LMU	R	7025	-	36,36,36	0.76	1 (2%)	47,47,47	1.20	5 (10%)
22	LMU	R	7021	-	36,36,36	0.74	1 (2%)	47,47,47	1.34	5 (10%)
19	CLA	A	1149	-	37,54,73	2.57	11 (29%)	36,90,113	5.93	22 (61%)
19	CLA	A	1104	-	48,65,73	1.94	8 (16%)	45,103,113	3.57	16 (35%)
22	LMU	4	7009	-	35,35,36	1.34	2 (5%)	46,46,47	1.24	4 (8%)
19	CLA	4	4003	-	46,63,73	2.07	10 (21%)	43,101,113	3.21	13 (30%)
19	CLA	B	1236	-	38,55,73	2.13	10 (26%)	33,91,113	3.81	13 (39%)
19	CLA	L	1130	-	56,73,73	1.97	9 (16%)	55,113,113	2.63	15 (27%)
22	LMU	R	7020	-	36,36,36	0.67	0	47,47,47	1.39	6 (12%)
19	CLA	B	1211	-	56,73,73	1.94	10 (17%)	55,113,113	2.64	12 (21%)
22	LMU	C	7015	-	36,36,36	0.69	1 (2%)	47,47,47	1.27	6 (12%)
22	LMU	4	7052	-	36,36,36	1.22	4 (11%)	47,47,47	1.78	8 (17%)
19	CLA	3	3005	-	18,32,73	1.71	5 (27%)	22,54,113	4.02	13 (59%)
22	LMU	K	7041	-	36,36,36	0.57	0	47,47,47	1.06	3 (6%)
22	LMU	B	7040	-	36,36,36	0.74	1 (2%)	47,47,47	1.61	10 (21%)
19	CLA	2	2003	-	18,32,73	1.80	5 (27%)	22,54,113	3.98	12 (54%)
22	LMU	D	7050	-	36,36,36	0.62	1 (2%)	47,47,47	0.82	1 (2%)
19	CLA	B	1239	-	56,73,73	1.79	11 (19%)	55,113,113	2.83	15 (27%)
19	CLA	A	9023	-	56,73,73	1.83	8 (14%)	55,113,113	2.93	18 (32%)
19	CLA	A	9022	-	56,73,73	1.91	10 (17%)	55,113,113	3.20	14 (25%)
19	CLA	3	3017	-	41,58,73	2.18	10 (24%)	37,95,113	4.47	18 (48%)
19	CLA	1	1015	-	18,32,73	1.72	5 (27%)	22,54,113	3.94	13 (59%)
19	CLA	1	1008	-	42,59,73	2.24	11 (26%)	38,96,113	4.25	16 (42%)
22	LMU	A	7010	-	36,36,36	1.29	2 (5%)	47,47,47	1.20	5 (10%)
19	CLA	A	1133	-	41,58,73	2.14	11 (26%)	37,95,113	3.76	14 (37%)
20	PQN	A	5001	-	34,34,34	1.70	2 (5%)	42,45,45	1.43	5 (11%)
22	LMU	N	7049	-	36,36,36	0.58	1 (2%)	47,47,47	1.34	4 (8%)
19	CLA	B	1221	-	45,62,73	2.19	11 (24%)	41,99,113	2.82	14 (34%)
22	LMU	4	7053	-	35,35,36	0.70	1 (2%)	46,46,47	1.25	6 (13%)
19	CLA	1	1303	-	42,59,73	2.39	12 (28%)	38,96,113	4.91	16 (42%)
21	BCR	B	6020	-	41,41,41	2.21	11 (26%)	56,56,56	4.46	27 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	K	1146	-	41,58,73	2.22	10 (24%)	37,95,113	4.08	17 (45%)
19	CLA	A	1126	-	56,73,73	1.86	9 (16%)	55,113,113	3.70	20 (36%)
19	CLA	F	1302	-	32,49,73	2.40	10 (31%)	26,84,113	4.37	11 (42%)
22	LMU	A	7044	-	36,36,36	0.87	1 (2%)	47,47,47	1.57	9 (19%)
19	CLA	B	1229	-	56,73,73	1.91	9 (16%)	55,113,113	3.24	16 (29%)
19	CLA	B	1208	-	45,62,73	2.27	9 (20%)	46,100,113	3.53	18 (39%)
19	CLA	1	1012	-	27,44,73	2.39	6 (22%)	27,78,113	4.18	9 (33%)
19	CLA	1	1014	-	52,69,73	1.97	9 (17%)	50,108,113	3.30	12 (24%)
19	CLA	2	2007	-	56,73,73	1.86	8 (14%)	55,113,113	3.11	17 (30%)
19	CLA	3	2009	-	47,64,73	2.09	13 (27%)	44,102,113	3.83	15 (34%)
19	CLA	B	1224	-	56,73,73	1.90	10 (17%)	55,113,113	3.63	15 (27%)
19	CLA	B	1213	-	37,54,73	2.23	9 (24%)	32,90,113	3.91	12 (37%)
19	CLA	B	1214	-	50,67,73	2.00	10 (20%)	47,105,113	2.84	14 (29%)
19	CLA	B	1227	-	41,58,73	2.15	8 (19%)	37,95,113	3.71	13 (35%)
19	CLA	1	1310	-	18,32,73	1.92	4 (22%)	22,54,113	4.29	13 (59%)
19	CLA	2	2014	-	52,69,73	1.89	10 (19%)	50,108,113	3.42	17 (34%)
19	CLA	A	1122	-	46,63,73	2.11	10 (21%)	43,101,113	3.56	13 (30%)
19	CLA	2	4009	-	56,73,73	1.84	9 (16%)	55,113,113	3.84	16 (29%)
22	LMU	2	7031	-	36,36,36	1.23	3 (8%)	47,47,47	1.32	5 (10%)
19	CLA	B	1234	-	51,68,73	1.92	9 (17%)	49,107,113	3.51	11 (22%)
19	CLA	3	3013	-	56,73,73	1.86	10 (17%)	55,113,113	3.79	15 (27%)
19	CLA	G	1242	-	42,59,73	2.17	10 (23%)	38,96,113	3.73	17 (44%)
22	LMU	G	7051	-	36,36,36	0.86	1 (2%)	47,47,47	2.07	12 (25%)
22	LMU	R	7014	-	36,36,36	0.92	2 (5%)	47,47,47	2.02	8 (17%)
19	CLA	2	2010	-	18,32,73	1.77	6 (33%)	22,54,113	3.69	9 (40%)
19	CLA	A	1121	1	33,50,73	2.32	7 (21%)	27,85,113	4.65	11 (40%)
19	CLA	B	1228	-	41,58,73	2.10	9 (21%)	37,95,113	3.67	15 (40%)
19	CLA	4	4005	-	18,32,73	1.83	5 (27%)	22,54,113	4.00	11 (50%)
19	CLA	K	1142	-	33,53,73	2.12	9 (27%)	27,89,113	4.42	11 (40%)
22	LMU	L	7029	-	36,36,36	0.68	1 (2%)	47,47,47	0.73	0
19	CLA	K	3009	-	56,73,73	1.89	8 (14%)	55,113,113	2.95	15 (27%)
19	CLA	A	1107	-	46,63,73	2.00	10 (21%)	43,101,113	3.29	16 (37%)
19	CLA	B	1216	-	52,69,73	1.81	9 (17%)	50,108,113	3.53	14 (28%)
19	CLA	A	1151	-	41,58,73	2.25	9 (21%)	37,95,113	3.89	12 (32%)
19	CLA	B	1238	-	56,73,73	1.84	10 (17%)	55,113,113	2.94	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LMU	F	7036	-	35,35,36	0.76	1 (2%)	46,46,47	1.41	6 (13%)
19	CLA	4	4004	-	18,32,73	1.78	5 (27%)	22,54,113	4.06	14 (63%)
19	CLA	A	1237	-	56,73,73	1.85	10 (17%)	55,113,113	3.66	15 (27%)
21	BCR	B	6006	-	41,41,41	1.52	9 (21%)	56,56,56	4.50	26 (46%)
19	CLA	I	1204	-	51,68,73	1.86	9 (17%)	49,107,113	3.69	12 (24%)
19	CLA	4	4015	-	37,54,73	2.22	11 (29%)	32,90,113	3.45	12 (37%)
21	BCR	A	6008	-	41,41,41	1.38	4 (9%)	56,56,56	4.07	29 (51%)
19	CLA	R	1144	-	48,65,73	2.02	9 (18%)	45,103,113	3.93	16 (35%)
19	CLA	4	1009	-	27,44,73	2.67	9 (33%)	27,78,113	4.76	12 (44%)
19	CLA	4	4006	-	46,63,73	2.04	8 (17%)	43,101,113	3.09	14 (32%)
19	CLA	A	1111	-	45,62,73	1.95	10 (22%)	41,99,113	3.46	15 (36%)
19	CLA	F	1240	-	27,44,73	2.32	7 (25%)	27,78,113	3.72	15 (55%)
22	LMU	2	7046	-	36,36,36	0.71	1 (2%)	47,47,47	0.86	2 (4%)
22	LMU	K	7042	-	36,36,36	0.62	0	47,47,47	1.16	5 (10%)
19	CLA	2	2008	-	18,32,73	1.69	4 (22%)	22,54,113	3.98	11 (50%)
19	CLA	1	1001	-	37,54,73	2.53	13 (35%)	32,90,113	4.57	14 (43%)
21	BCR	B	6010	-	41,41,41	1.39	3 (7%)	56,56,56	4.27	28 (50%)
19	CLA	B	1233	-	42,59,73	2.24	9 (21%)	38,96,113	4.21	13 (34%)
21	BCR	B	6005	-	41,41,41	1.37	4 (9%)	56,56,56	4.72	32 (57%)
22	LMU	H	7011	-	36,36,36	0.77	2 (5%)	47,47,47	1.93	10 (21%)
22	LMU	3	7005	-	36,36,36	0.71	0	47,47,47	2.09	14 (29%)
19	CLA	2	1307	-	18,32,73	1.80	6 (33%)	22,54,113	3.96	11 (50%)
19	CLA	A	1117	-	56,73,73	1.82	10 (17%)	55,113,113	2.93	16 (29%)
19	CLA	3	3008	-	41,58,73	2.12	10 (24%)	37,95,113	4.12	15 (40%)
19	CLA	1	1013	-	42,59,73	2.50	15 (35%)	38,96,113	4.55	17 (44%)
20	PQN	B	5002	-	34,34,34	1.60	2 (5%)	42,45,45	1.53	6 (14%)
19	CLA	3	3001	-	18,32,73	1.82	6 (33%)	22,54,113	4.03	13 (59%)
19	CLA	H	1207	-	56,73,73	1.86	9 (16%)	55,113,113	3.31	13 (23%)
21	BCR	F	6014	-	41,41,41	1.34	6 (14%)	56,56,56	4.82	27 (48%)
19	CLA	A	1129	-	41,58,73	2.12	11 (26%)	37,95,113	4.11	14 (37%)
19	CLA	A	1132	-	56,73,73	1.86	9 (16%)	55,113,113	3.17	16 (29%)
19	CLA	A	1135	-	42,59,73	2.11	10 (23%)	38,96,113	3.82	14 (36%)
19	CLA	2	2013	-	41,58,73	2.19	9 (21%)	37,95,113	4.35	14 (37%)
19	CLA	2	2006	-	56,73,73	1.93	9 (16%)	55,113,113	3.37	11 (20%)
19	CLA	4	4011	-	18,32,73	1.71	5 (27%)	22,54,113	4.03	13 (59%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LMU	A	7035	-	36,36,36	0.61	0	47,47,47	1.54	8 (17%)
22	LMU	4	7033	-	36,36,36	0.75	0	47,47,47	1.59	9 (19%)
22	LMU	H	7032	-	36,36,36	0.72	1 (2%)	47,47,47	1.44	6 (12%)
19	CLA	B	1226	-	56,73,73	1.72	9 (16%)	55,113,113	2.98	14 (25%)
19	CLA	2	2012	16	41,58,73	2.18	9 (21%)	37,95,113	3.79	12 (32%)
19	CLA	4	4012	-	27,44,73	2.46	8 (29%)	27,78,113	4.78	10 (37%)
19	CLA	H	1145	-	56,73,73	1.82	11 (19%)	55,113,113	3.71	16 (29%)
19	CLA	1	1006	-	27,44,73	2.64	9 (33%)	27,78,113	4.48	10 (37%)
19	CLA	A	1131	-	56,73,73	1.84	11 (19%)	55,113,113	3.16	14 (25%)
19	CLA	B	1206	2	56,73,73	1.78	9 (16%)	55,113,113	3.32	14 (25%)
21	BCR	L	6019	-	41,41,41	1.75	12 (29%)	56,56,56	4.27	25 (44%)
21	BCR	J	6012	-	41,41,41	1.47	5 (12%)	56,56,56	5.42	26 (46%)
21	BCR	A	6011	-	41,41,41	1.36	5 (12%)	56,56,56	4.17	32 (57%)
19	CLA	A	9012	-	56,73,73	1.91	11 (19%)	55,113,113	3.04	16 (29%)
24	LMG	B	7101	-	49,49,55	1.04	3 (6%)	57,57,63	1.02	3 (5%)
19	CLA	2	2002	-	47,64,73	2.05	9 (19%)	44,102,113	3.29	18 (40%)
19	CLA	B	1232	19	33,53,73	2.27	8 (24%)	27,89,113	4.29	10 (37%)
19	CLA	3	3002	-	18,32,73	1.77	5 (27%)	22,54,113	3.80	11 (50%)
19	CLA	B	1205	-	56,73,73	1.90	9 (16%)	55,113,113	3.16	15 (27%)
19	CLA	B	1225	-	56,73,73	1.81	9 (16%)	55,113,113	3.13	15 (27%)
19	CLA	R	1150	-	56,73,73	2.07	10 (17%)	55,113,113	3.09	17 (30%)
21	BCR	A	6002	-	41,41,41	1.87	6 (14%)	56,56,56	4.62	34 (60%)
22	LMU	1	7004	-	36,36,36	0.66	1 (2%)	47,47,47	0.79	1 (2%)
21	BCR	3	6022	-	41,41,41	1.35	4 (9%)	56,56,56	4.91	25 (44%)
19	CLA	4	4013	18	18,32,73	1.59	5 (27%)	22,54,113	3.60	12 (54%)
19	CLA	A	1141	-	56,73,73	1.84	10 (17%)	55,113,113	3.10	13 (23%)
22	LMU	2	7006	-	36,36,36	0.63	1 (2%)	47,47,47	0.73	0
22	LMU	3	7003	-	36,36,36	0.80	0	47,47,47	1.48	7 (14%)
19	CLA	A	1124	-	56,73,73	1.81	10 (17%)	55,113,113	3.12	13 (23%)
21	BCR	I	6021	-	41,41,41	2.04	8 (19%)	56,56,56	4.79	32 (57%)
19	CLA	F	1305	-	44,61,73	2.32	14 (31%)	40,98,113	3.78	16 (40%)
19	CLA	1	1003	-	38,55,73	2.23	9 (23%)	33,91,113	4.48	13 (39%)
22	LMU	H	7028	-	36,36,36	0.59	0	47,47,47	0.97	2 (4%)
19	CLA	A	1105	-	37,54,73	2.18	8 (21%)	32,90,113	4.71	12 (37%)
22	LMU	G	7026	-	36,36,36	0.88	2 (5%)	47,47,47	1.49	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LMU	2	7027	-	36,36,36	0.81	1 (2%)	47,47,47	1.67	10 (21%)
22	LMU	H	7043	-	36,36,36	0.83	1 (2%)	47,47,47	1.64	10 (21%)
19	CLA	A	1116	-	43,60,73	2.18	9 (20%)	39,97,113	3.95	15 (38%)
19	CLA	K	1143	-	41,58,73	2.10	10 (24%)	37,95,113	3.72	16 (43%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMU	H	7002	-	-	14/21/61/61	0/2/2/2
22	LMU	E	7048	-	-	12/21/61/61	0/2/2/2
19	CLA	B	1201	-	1/1/11/20	6/11/91/115	-
19	CLA	B	1230	-	1/1/12/20	6/19/97/115	-
22	LMU	H	7030	-	-	14/21/61/61	0/2/2/2
19	CLA	A	1110	-	1/1/12/20	12/24/102/115	-
19	CLA	2	2004	-	1/1/12/20	8/19/97/115	-
19	CLA	A	1125	-	2/2/15/20	23/37/115/115	-
19	CLA	4	4010	-	1/1/4/20	-	-
21	BCR	A	6007	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1120	-	1/1/12/20	9/21/99/115	-
21	BCR	I	6018	-	-	14/29/63/63	0/2/2/2
22	LMU	B	7038	-	-	13/21/61/61	0/2/2/2
19	CLA	B	1235	-	2/2/15/20	13/37/115/115	-
22	LMU	E	7037	-	-	16/21/61/61	0/2/2/2
19	CLA	3	3006	-	1/1/4/20	-	-
22	LMU	R	7024	-	-	14/21/61/61	0/2/2/2
19	CLA	A	1136	-	2/2/15/20	12/37/115/115	-
23	SF4	C	8002	3	-	-	0/6/5/5
19	CLA	A	1128	-	2/2/15/20	18/37/115/115	-
19	CLA	3	3012	-	1/1/4/20	-	-
19	CLA	A	1103	-	2/2/15/20	24/37/115/115	-
19	CLA	B	1202	-	2/2/15/20	21/37/115/115	-
19	CLA	2	2005	-	1/1/4/20	-	-
19	CLA	3	3004	-	1/1/4/20	-	-
21	BCR	B	6017	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1215	-	2/2/14/20	13/31/109/115	-
19	CLA	A	1101	-	1/1/12/20	5/19/97/115	-
19	CLA	A	1137	-	1/1/11/20	9/16/94/115	-
19	CLA	L	1502	-	1/1/11/20	8/16/94/115	-
19	CLA	3	3011	-	2/2/15/20	19/37/115/115	-
22	LMU	B	7012	-	-	5/11/51/61	0/2/2/2
22	LMU	G	7039	-	-	17/21/61/61	0/2/2/2
22	LMU	K	7047	-	-	9/21/61/61	0/2/2/2
19	CLA	A	1106	-	2/2/15/20	22/37/115/115	-
19	CLA	A	1123	-	2/2/15/20	20/37/115/115	-
19	CLA	B	1219	-	2/2/13/20	9/25/103/115	-
19	CLA	L	1501	12	1/1/12/20	7/19/97/115	-
19	CLA	B	1209	-	2/2/13/20	10/25/103/115	-
19	CLA	L	1504	-	2/2/13/20	7/25/103/115	-
19	CLA	A	1108	-	1/1/11/20	2/11/91/115	-
19	CLA	B	1222	-	2/2/13/20	16/29/107/115	-
19	CLA	3	3015	-	1/1/4/20	-	-
19	CLA	H	1241	-	2/2/13/20	7/25/103/115	-
19	CLA	B	1217	-	1/1/12/20	6/19/97/115	-
22	LMU	4	7018	-	-	13/21/61/61	0/2/2/2
21	BCR	B	6004	-	-	16/29/63/63	0/2/2/2
19	CLA	H	1505	-	2/2/13/20	13/25/103/115	-
19	CLA	3	3003	-	1/1/9/20	-	-
19	CLA	A	1112	-	1/1/11/20	7/11/91/115	-
19	CLA	3	3016	-	2/2/15/20	22/37/115/115	-
19	CLA	A	1138	-	2/2/15/20	21/37/115/115	-
19	CLA	A	1134	1	1/1/11/20	5/11/91/115	-
22	LMU	H	7017	-	-	13/21/61/61	0/2/2/2
19	CLA	3	1118	-	1/1/9/20	-	-
19	CLA	A	1127	-	2/2/13/20	11/25/103/115	-
19	CLA	A	1139	-	1/1/12/20	11/21/99/115	-
19	CLA	B	1218	-	1/1/11/20	12/15/93/115	-
21	BCR	A	6003	-	-	14/29/63/63	0/2/2/2
22	LMU	4	7034	-	-	12/21/61/61	0/2/2/2
23	SF4	A	8001	1,2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMU	4	7019	-	-	15/21/61/61	0/2/2/2
21	BCR	F	6016	-	-	13/29/63/63	0/2/2/2
19	CLA	L	1148	-	3/3/13/20	12/25/103/115	-
19	CLA	1	1011	-	1/1/9/20	-	-
19	CLA	J	1308	-	2/2/13/20	16/25/103/115	-
22	LMU	A	7016	-	-	11/21/61/61	0/2/2/2
19	CLA	A	1109	19	2/2/15/20	25/37/115/115	-
19	CLA	1	1002	-	1/1/11/20	9/16/94/115	-
21	BCR	1	6023	-	-	15/29/63/63	0/2/2/2
19	CLA	B	1220	-	1/1/15/20	21/37/115/115	-
19	CLA	A	9011	-	2/2/15/20	23/37/115/115	-
19	CLA	1	1010	-	1/1/11/20	7/15/93/115	-
19	CLA	4	4002	18	2/2/12/20	6/22/100/115	-
22	LMU	R	7007	-	-	16/21/61/61	0/2/2/2
19	CLA	A	1119	-	2/2/15/20	17/37/115/115	-
22	LMU	4	7008	-	-	12/21/61/61	0/2/2/2
22	LMU	1	7013	-	-	10/21/61/61	0/2/2/2
19	CLA	L	1503	-	2/2/12/20	10/19/97/115	-
19	CLA	4	4007	-	1/1/12/20	9/22/100/115	-
19	CLA	B	1301	-	1/1/9/20	-	-
19	CLA	3	3010	-	1/1/4/20	-	-
19	CLA	2	2011	-	1/1/4/20	-	-
19	CLA	3	3014	-	1/1/4/20	-	-
22	LMU	R	7022	-	-	14/21/61/61	0/2/2/2
19	CLA	B	1231	19	1/1/11/20	9/11/91/115	-
19	CLA	4	1304	-	3/3/15/20	20/37/115/115	-
19	CLA	1	1007	-	2/2/14/20	20/33/111/115	-
19	CLA	4	4001	-	1/1/12/20	6/19/97/115	-
23	SF4	C	8003	3	-	-	0/6/5/5
22	LMU	A	7045	-	-	14/21/61/61	0/2/2/2
19	CLA	2	2001	-	1/1/12/20	9/21/99/115	-
19	CLA	3	3007	-	1/1/10/20	5/10/88/115	-
19	CLA	A	9013	-	2/2/15/20	25/37/115/115	-
19	CLA	4	1306	-	2/2/13/20	12/25/103/115	-
19	CLA	A	1113	-	1/1/12/20	10/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1102	19	2/2/13/20	12/25/103/115	-
19	CLA	A	1309	-	1/1/4/20	-	-
22	LMU	A	7023	-	-	17/21/61/61	0/2/2/2
19	CLA	J	1311	-	2/2/14/20	24/33/111/115	-
19	CLA	B	1223	-	2/2/15/20	18/37/115/115	-
19	CLA	B	1212	-	2/2/14/20	14/31/109/115	-
19	CLA	A	1140	-	2/2/15/20	17/37/115/115	-
19	CLA	A	1115	-	2/2/15/20	17/37/115/115	-
22	LMU	K	7001	-	-	13/21/61/61	0/2/2/2
19	CLA	B	1203	-	2/2/15/20	16/37/115/115	-
19	CLA	4	1004	-	2/2/13/20	9/25/103/115	-
19	CLA	B	1210	-	2/2/15/20	23/37/115/115	-
19	CLA	3	1147	-	1/1/11/20	8/15/93/115	-
19	CLA	B	9010	-	2/2/15/20	20/37/115/115	-
19	CLA	1	1005	-	1/1/11/20	6/15/93/115	-
19	CLA	4	4014	-	1/1/11/20	13/16/94/115	-
22	LMU	R	7025	-	-	13/21/61/61	0/2/2/2
22	LMU	R	7021	-	-	14/21/61/61	0/2/2/2
19	CLA	A	1149	-	3/3/11/20	12/16/92/115	-
19	CLA	A	1104	-	2/2/13/20	7/28/106/115	-
22	LMU	4	7009	-	-	13/20/60/61	0/2/2/2
19	CLA	4	4003	-	2/2/13/20	15/25/103/115	-
19	CLA	B	1236	-	1/1/11/20	8/16/94/115	-
19	CLA	L	1130	-	2/2/15/20	18/37/115/115	-
22	LMU	R	7020	-	-	10/21/61/61	0/2/2/2
19	CLA	B	1211	-	2/2/15/20	23/37/115/115	-
22	LMU	C	7015	-	-	14/21/61/61	0/2/2/2
22	LMU	4	7052	-	-	19/21/61/61	0/2/2/2
19	CLA	3	3005	-	1/1/4/20	-	-
22	LMU	K	7041	-	-	12/21/61/61	0/2/2/2
22	LMU	B	7040	-	-	13/21/61/61	0/2/2/2
19	CLA	2	2003	-	1/1/4/20	-	-
22	LMU	D	7050	-	-	11/21/61/61	0/2/2/2
19	CLA	B	1239	-	2/2/15/20	18/37/115/115	-
19	CLA	A	9023	-	2/2/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	9022	-	2/2/15/20	16/37/115/115	-
19	CLA	3	3017	-	1/1/12/20	7/19/97/115	-
19	CLA	1	1015	-	1/1/4/20	-	-
19	CLA	1	1008	-	2/2/12/20	9/21/99/115	-
22	LMU	A	7010	-	-	18/21/61/61	0/2/2/2
19	CLA	A	1133	-	1/1/12/20	11/19/97/115	-
20	PQN	A	5001	-	1/1/8/9	11/23/43/43	0/2/2/2
22	LMU	N	7049	-	-	16/21/61/61	0/2/2/2
19	CLA	B	1221	-	1/1/12/20	9/24/102/115	-
22	LMU	4	7053	-	-	13/20/60/61	0/2/2/2
19	CLA	1	1303	-	3/3/12/20	11/21/99/115	-
21	BCR	B	6020	-	-	14/29/63/63	0/2/2/2
19	CLA	K	1146	-	1/1/12/20	8/19/97/115	-
19	CLA	A	1126	-	2/2/15/20	14/37/115/115	-
19	CLA	F	1302	-	1/1/10/20	5/8/86/115	-
22	LMU	A	7044	-	-	15/21/61/61	0/2/2/2
19	CLA	B	1229	-	2/2/15/20	18/37/115/115	-
19	CLA	B	1208	-	2/2/13/20	9/25/101/115	-
19	CLA	1	1012	-	1/1/9/20	-	-
19	CLA	1	1014	-	2/2/14/20	15/33/111/115	-
19	CLA	2	2007	-	2/2/15/20	16/37/115/115	-
19	CLA	3	2009	-	2/2/13/20	13/27/105/115	-
19	CLA	B	1224	-	2/2/15/20	16/37/115/115	-
19	CLA	B	1213	-	1/1/11/20	11/15/93/115	-
19	CLA	B	1214	-	2/2/13/20	11/30/108/115	-
19	CLA	B	1227	-	1/1/12/20	9/19/97/115	-
19	CLA	1	1310	-	1/1/4/20	-	-
19	CLA	2	2014	-	2/2/14/20	20/33/111/115	-
19	CLA	A	1122	-	2/2/13/20	8/25/103/115	-
19	CLA	2	4009	-	2/2/15/20	16/37/115/115	-
22	LMU	2	7031	-	-	11/21/61/61	0/2/2/2
19	CLA	B	1234	-	2/2/14/20	13/31/109/115	-
19	CLA	3	3013	-	2/2/15/20	17/37/115/115	-
19	CLA	G	1242	-	1/1/12/20	10/21/99/115	-
22	LMU	G	7051	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMU	R	7014	-	-	12/21/61/61	0/2/2/2
19	CLA	2	2010	-	1/1/4/20	-	-
19	CLA	A	1121	1	1/1/10/20	2/10/88/115	-
19	CLA	B	1228	-	1/1/12/20	12/19/97/115	-
19	CLA	4	4005	-	1/1/4/20	-	-
19	CLA	K	1142	-	1/1/11/20	3/11/91/115	-
22	LMU	L	7029	-	-	16/21/61/61	0/2/2/2
19	CLA	K	3009	-	2/2/15/20	21/37/115/115	-
19	CLA	A	1107	-	2/2/13/20	11/25/103/115	-
19	CLA	B	1216	-	2/2/14/20	16/33/111/115	-
19	CLA	A	1151	-	1/1/12/20	10/19/97/115	-
19	CLA	B	1238	-	2/2/15/20	19/37/115/115	-
22	LMU	F	7036	-	-	11/20/60/61	0/2/2/2
19	CLA	4	4004	-	1/1/4/20	-	-
19	CLA	A	1237	-	2/2/15/20	19/37/115/115	-
21	BCR	B	6006	-	-	12/29/63/63	0/2/2/2
19	CLA	I	1204	-	2/2/14/20	13/31/109/115	-
19	CLA	4	4015	-	1/1/11/20	11/15/93/115	-
21	BCR	A	6008	-	-	15/29/63/63	0/2/2/2
19	CLA	R	1144	-	2/2/13/20	13/28/106/115	-
19	CLA	4	1009	-	1/1/9/20	-	-
19	CLA	4	4006	-	2/2/13/20	12/25/103/115	-
19	CLA	A	1111	-	1/1/12/20	13/24/102/115	-
19	CLA	F	1240	-	1/1/9/20	-	-
22	LMU	2	7046	-	-	16/21/61/61	0/2/2/2
22	LMU	K	7042	-	-	18/21/61/61	0/2/2/2
19	CLA	2	2008	-	1/1/4/20	-	-
19	CLA	1	1001	-	1/1/11/20	10/15/93/115	-
21	BCR	B	6010	-	-	13/29/63/63	0/2/2/2
19	CLA	B	1233	-	1/1/12/20	10/21/99/115	-
21	BCR	B	6005	-	-	9/29/63/63	0/2/2/2
22	LMU	H	7011	-	-	17/21/61/61	0/2/2/2
22	LMU	3	7005	-	-	15/21/61/61	0/2/2/2
19	CLA	2	1307	-	1/1/4/20	-	-
19	CLA	A	1117	-	2/2/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	3	3008	-	1/1/12/20	6/19/97/115	-
19	CLA	1	1013	-	2/2/12/20	8/21/99/115	-
20	PQN	B	5002	-	1/1/8/9	9/23/43/43	0/2/2/2
19	CLA	3	3001	-	1/1/4/20	-	-
19	CLA	H	1207	-	2/2/15/20	19/37/115/115	-
21	BCR	F	6014	-	-	17/29/63/63	0/2/2/2
19	CLA	A	1129	-	1/1/12/20	3/19/97/115	-
19	CLA	A	1132	-	2/2/15/20	24/37/115/115	-
19	CLA	A	1135	-	1/1/12/20	9/21/99/115	-
19	CLA	2	2013	-	1/1/12/20	11/19/97/115	-
19	CLA	2	2006	-	2/2/15/20	17/37/115/115	-
19	CLA	4	4011	-	1/1/4/20	-	-
22	LMU	A	7035	-	-	13/21/61/61	0/2/2/2
22	LMU	4	7033	-	-	12/21/61/61	0/2/2/2
22	LMU	H	7032	-	-	17/21/61/61	0/2/2/2
19	CLA	B	1226	-	2/2/15/20	26/37/115/115	-
19	CLA	2	2012	16	1/1/12/20	6/19/97/115	-
19	CLA	4	4012	-	1/1/9/20	-	-
19	CLA	H	1145	-	3/3/15/20	20/37/115/115	-
19	CLA	1	1006	-	1/1/9/20	-	-
19	CLA	A	1131	-	2/2/15/20	19/37/115/115	-
19	CLA	B	1206	2	2/2/15/20	17/37/115/115	-
21	BCR	L	6019	-	-	13/29/63/63	0/2/2/2
21	BCR	J	6012	-	-	13/29/63/63	0/2/2/2
21	BCR	A	6011	-	-	11/29/63/63	0/2/2/2
19	CLA	A	9012	-	2/2/15/20	20/37/115/115	-
24	LMG	B	7101	-	-	24/44/64/70	0/1/1/1
19	CLA	2	2002	-	2/2/13/20	9/27/105/115	-
19	CLA	B	1232	19	1/1/11/20	6/11/91/115	-
19	CLA	3	3002	-	1/1/4/20	-	-
19	CLA	B	1205	-	2/2/15/20	11/37/115/115	-
19	CLA	B	1225	-	2/2/15/20	15/37/115/115	-
19	CLA	R	1150	-	2/2/15/20	19/37/115/115	-
21	BCR	A	6002	-	-	16/29/63/63	0/2/2/2
22	LMU	1	7004	-	-	16/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	3	6022	-	-	19/29/63/63	0/2/2/2
19	CLA	4	4013	18	1/1/4/20	-	-
19	CLA	A	1141	-	2/2/15/20	19/37/115/115	-
22	LMU	2	7006	-	-	14/21/61/61	0/2/2/2
22	LMU	3	7003	-	-	14/21/61/61	0/2/2/2
19	CLA	A	1124	-	2/2/15/20	19/37/115/115	-
21	BCR	I	6021	-	-	13/29/63/63	0/2/2/2
19	CLA	F	1305	-	4/4/12/20	10/23/101/115	-
19	CLA	1	1003	-	1/1/11/20	8/16/94/115	-
22	LMU	H	7028	-	-	13/21/61/61	0/2/2/2
19	CLA	A	1105	-	1/1/11/20	7/15/93/115	-
22	LMU	G	7026	-	-	15/21/61/61	0/2/2/2
22	LMU	2	7027	-	-	11/21/61/61	0/2/2/2
22	LMU	H	7043	-	-	11/21/61/61	0/2/2/2
19	CLA	A	1116	-	1/1/12/20	13/22/100/115	-
19	CLA	K	1143	-	1/1/12/20	4/19/97/115	-

All (1756) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1005	CLA	OBD-CAD	10.52	1.37	1.22
19	1	1011	CLA	CAB-C3B	-8.86	1.33	1.51
19	1	1006	CLA	CAB-C3B	-8.85	1.33	1.51
19	4	1009	CLA	CAB-C3B	-8.52	1.33	1.51
19	B	1208	CLA	CAB-C3B	-8.25	1.34	1.51
19	4	4012	CLA	CAB-C3B	-8.24	1.34	1.51
19	B	1301	CLA	CAB-C3B	-8.17	1.34	1.51
19	3	1147	CLA	C3B-CAB	-8.15	1.31	1.47
19	1	1012	CLA	CAB-C3B	-8.04	1.34	1.51
19	A	1149	CLA	CAB-C3B	-7.96	1.35	1.51
19	1	1013	CLA	C3B-CAB	-7.88	1.31	1.47
19	B	1220	CLA	C3B-CAB	-7.86	1.31	1.47
19	B	1203	CLA	C3B-CAB	-7.83	1.32	1.47
19	A	9013	CLA	C3B-CAB	-7.82	1.32	1.47
19	3	1118	CLA	CAB-C3B	-7.77	1.35	1.51
20	A	5001	PQN	C3-C2	7.66	1.49	1.35
19	3	1147	CLA	C1B-NB	-7.55	1.28	1.35
19	B	1205	CLA	C3B-CAB	-7.53	1.32	1.47
20	B	5002	PQN	C3-C2	7.52	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1210	CLA	C3B-CAB	-7.50	1.32	1.47
19	2	2012	CLA	C3B-CAB	-7.47	1.32	1.47
19	A	1139	CLA	C3B-CAB	-7.44	1.32	1.47
19	3	3003	CLA	CAB-C3B	-7.44	1.36	1.51
19	A	9023	CLA	C3B-CAB	-7.37	1.32	1.47
19	A	1138	CLA	C3B-CAB	-7.28	1.33	1.47
19	A	1126	CLA	C3B-CAB	-7.27	1.33	1.47
19	A	1135	CLA	C3B-CAB	-7.26	1.33	1.47
19	B	1221	CLA	C3B-CAB	-7.25	1.33	1.47
19	4	1304	CLA	C3B-CAB	-7.21	1.33	1.47
19	B	1219	CLA	C3B-CAB	-7.19	1.33	1.47
19	A	1137	CLA	C3B-CAB	-7.18	1.33	1.47
19	A	1136	CLA	C3B-CAB	-7.17	1.33	1.47
19	J	1308	CLA	C3B-CAB	-7.16	1.33	1.47
19	B	1229	CLA	C3B-CAB	-7.16	1.33	1.47
19	3	3013	CLA	C3B-CAB	-7.14	1.33	1.47
19	B	1235	CLA	C3B-CAB	-7.11	1.33	1.47
19	A	1127	CLA	C3B-CAB	-7.09	1.33	1.47
19	A	1103	CLA	C3B-CAB	-7.09	1.33	1.47
19	A	9022	CLA	C3B-CAB	-7.06	1.33	1.47
19	A	1124	CLA	C3B-CAB	-7.06	1.33	1.47
19	B	1234	CLA	C3B-CAB	-7.05	1.33	1.47
21	A	6002	BCR	C11-C10	7.04	1.65	1.43
19	A	1125	CLA	C3B-CAB	-7.02	1.33	1.47
21	B	6020	BCR	C21-C22	-7.00	1.26	1.35
19	A	9012	CLA	C3B-CAB	-6.99	1.33	1.47
19	4	4015	CLA	C3B-CAB	-6.97	1.33	1.47
19	R	1150	CLA	C3B-CAB	-6.96	1.33	1.47
19	F	1240	CLA	CAB-C3B	-6.94	1.37	1.51
19	R	1150	CLA	OBD-CAD	6.94	1.32	1.22
19	B	1222	CLA	C3B-CAB	-6.91	1.33	1.47
19	B	1211	CLA	C3B-CAB	-6.91	1.33	1.47
19	B	1231	CLA	C3B-CAB	-6.91	1.33	1.47
21	1	6023	BCR	C11-C10	-6.91	1.22	1.43
19	1	1014	CLA	C3B-CAB	-6.90	1.33	1.47
19	A	1141	CLA	C3B-CAB	-6.90	1.33	1.47
19	3	3016	CLA	C3B-CAB	-6.86	1.34	1.47
19	3	2009	CLA	C3B-CAB	-6.85	1.34	1.47
19	K	1146	CLA	C3B-CAB	-6.85	1.34	1.47
19	L	1130	CLA	C3B-CAB	-6.85	1.34	1.47
19	B	1223	CLA	C3B-CAB	-6.82	1.34	1.47
19	B	1232	CLA	C3B-CAB	-6.82	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	1305	CLA	C3B-CAB	-6.81	1.34	1.47
19	A	1237	CLA	C3B-CAB	-6.81	1.34	1.47
19	4	4003	CLA	C3B-CAB	-6.79	1.34	1.47
19	F	1302	CLA	C3B-CAB	-6.78	1.34	1.47
19	4	1004	CLA	C3B-CAB	-6.77	1.34	1.47
19	A	1115	CLA	C3B-CAB	-6.75	1.34	1.47
19	B	1227	CLA	C3B-CAB	-6.75	1.34	1.47
19	4	1306	CLA	C3B-CAB	-6.74	1.34	1.47
19	1	1007	CLA	C3B-CAB	-6.72	1.34	1.47
19	B	1225	CLA	C3B-CAB	-6.72	1.34	1.47
19	B	1202	CLA	C3B-CAB	-6.71	1.34	1.47
19	B	1224	CLA	C3B-CAB	-6.71	1.34	1.47
19	3	3008	CLA	C3B-CAB	-6.71	1.34	1.47
19	L	1504	CLA	OBD-CAD	6.70	1.31	1.22
19	2	2014	CLA	C3B-CAB	-6.70	1.34	1.47
19	A	1140	CLA	C3B-CAB	-6.69	1.34	1.47
19	A	1132	CLA	C3B-CAB	-6.69	1.34	1.47
19	B	1233	CLA	C3B-CAB	-6.68	1.34	1.47
19	L	1503	CLA	C3B-CAB	-6.68	1.34	1.47
19	I	1204	CLA	C3B-CAB	-6.66	1.34	1.47
19	L	1502	CLA	C3B-CAB	-6.66	1.34	1.47
19	A	1131	CLA	C3B-CAB	-6.66	1.34	1.47
19	A	9011	CLA	C3B-CAB	-6.60	1.34	1.47
19	A	1113	CLA	C3B-CAB	-6.60	1.34	1.47
19	H	1145	CLA	C3B-CAB	-6.58	1.34	1.47
19	B	1239	CLA	C3B-CAB	-6.58	1.34	1.47
19	A	1101	CLA	C3B-CAB	-6.56	1.34	1.47
19	A	1107	CLA	C3B-CAB	-6.56	1.34	1.47
19	J	1311	CLA	C3B-CAB	-6.55	1.34	1.47
19	2	2001	CLA	C3B-CAB	-6.55	1.34	1.47
19	2	2006	CLA	C3B-CAB	-6.55	1.34	1.47
19	A	1116	CLA	C3B-CAB	-6.54	1.34	1.47
19	1	1005	CLA	C3B-CAB	-6.53	1.34	1.47
19	A	1134	CLA	C3B-CAB	-6.53	1.34	1.47
19	B	1206	CLA	C3B-CAB	-6.52	1.34	1.47
19	A	1121	CLA	C3B-CAB	-6.52	1.34	1.47
19	B	1216	CLA	C3B-CAB	-6.51	1.34	1.47
21	I	6021	BCR	C30-C25	-6.51	1.44	1.53
19	H	1505	CLA	O2D-CGD	6.49	1.49	1.33
19	A	1109	CLA	C3B-CAB	-6.48	1.34	1.47
19	1	1014	CLA	O2D-CGD	6.47	1.49	1.33
19	A	1117	CLA	C3B-CAB	-6.46	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1303	CLA	C3B-CAB	-6.46	1.34	1.47
19	4	4007	CLA	C3B-CAB	-6.45	1.34	1.47
19	K	1143	CLA	C3B-CAB	-6.44	1.34	1.47
19	H	1241	CLA	C3B-CAB	-6.41	1.34	1.47
19	1	1010	CLA	C3B-CAB	-6.35	1.35	1.47
19	A	1149	CLA	O2D-CGD	6.34	1.48	1.33
19	B	1215	CLA	C3B-CAB	-6.34	1.35	1.47
19	K	3009	CLA	C3B-CAB	-6.33	1.35	1.47
19	B	1217	CLA	C3B-CAB	-6.32	1.35	1.47
19	3	3011	CLA	C3B-CAB	-6.32	1.35	1.47
19	3	3017	CLA	C3B-CAB	-6.32	1.35	1.47
19	B	1231	CLA	OBD-CAD	6.29	1.31	1.22
19	A	1123	CLA	C3B-CAB	-6.29	1.35	1.47
19	H	1505	CLA	C3B-CAB	-6.28	1.35	1.47
19	L	1501	CLA	C3B-CAB	-6.28	1.35	1.47
19	1	1303	CLA	OBD-CAD	6.26	1.31	1.22
19	1	1002	CLA	O2D-CGD	6.26	1.48	1.33
19	2	2013	CLA	C3B-CAB	-6.25	1.35	1.47
19	1	1001	CLA	O2D-CGD	6.24	1.48	1.33
19	1	1008	CLA	C3B-CAB	-6.24	1.35	1.47
19	A	1122	CLA	C3B-CAB	-6.23	1.35	1.47
19	1	1001	CLA	OBD-CAD	6.22	1.31	1.22
19	A	1112	CLA	C3B-CAB	-6.22	1.35	1.47
19	1	1003	CLA	C3B-CAB	-6.21	1.35	1.47
19	B	1214	CLA	C3B-CAB	-6.21	1.35	1.47
19	3	3013	CLA	O2D-CGD	6.21	1.48	1.33
19	H	1207	CLA	C3B-CAB	-6.21	1.35	1.47
19	H	1241	CLA	O2D-CGD	6.21	1.48	1.33
19	A	1133	CLA	C3B-CAB	-6.19	1.35	1.47
19	B	1201	CLA	C3B-CAB	-6.18	1.35	1.47
19	2	4009	CLA	C3B-CAB	-6.18	1.35	1.47
19	A	1112	CLA	OBD-CAD	6.18	1.30	1.22
19	A	1151	CLA	C3B-CAB	-6.18	1.35	1.47
19	L	1504	CLA	C3B-CAB	-6.17	1.35	1.47
19	G	1242	CLA	O2D-CGD	6.16	1.48	1.33
19	K	1142	CLA	C3B-CAB	-6.15	1.35	1.47
19	B	1238	CLA	C3B-CAB	-6.15	1.35	1.47
19	B	1219	CLA	O2D-CGD	6.15	1.48	1.33
19	A	1116	CLA	O2D-CGD	6.14	1.48	1.33
19	L	1503	CLA	O2D-CGD	6.14	1.48	1.33
19	1	1002	CLA	C3B-CAB	-6.14	1.35	1.47
19	4	1009	CLA	OBD-CAD	6.14	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1228	CLA	C3B-CAB	-6.12	1.35	1.47
19	1	1007	CLA	O2D-CGD	6.10	1.48	1.33
19	2	2006	CLA	OBD-CAD	6.09	1.30	1.22
19	B	9010	CLA	C3B-CAB	-6.07	1.35	1.47
19	B	1218	CLA	O2D-CGD	6.07	1.48	1.33
19	2	2006	CLA	O2D-CGD	6.07	1.48	1.33
19	4	4006	CLA	C3B-CAB	-6.07	1.35	1.47
19	A	1121	CLA	OBD-CAD	6.06	1.30	1.22
19	R	1150	CLA	O2D-CGD	6.06	1.48	1.33
19	L	1501	CLA	O2D-CGD	6.05	1.48	1.33
19	4	4001	CLA	C3B-CAB	-6.04	1.35	1.47
19	H	1241	CLA	OBD-CAD	6.04	1.30	1.22
19	3	3007	CLA	C3B-CAB	-6.03	1.35	1.47
19	G	1242	CLA	C3B-CAB	-6.03	1.35	1.47
19	A	1120	CLA	C3B-CAB	-6.02	1.35	1.47
19	A	1104	CLA	C3B-CAB	-6.02	1.35	1.47
19	A	1105	CLA	C3B-CAB	-6.01	1.35	1.47
19	B	1213	CLA	OBD-CAD	6.00	1.30	1.22
19	1	1001	CLA	C3B-CAB	-6.00	1.35	1.47
19	4	4006	CLA	O2D-CGD	5.99	1.47	1.33
19	4	4007	CLA	O2D-CGD	5.98	1.47	1.33
19	A	1119	CLA	C3B-CAB	-5.98	1.35	1.47
19	A	1113	CLA	O2D-CGD	5.97	1.47	1.33
21	A	6003	BCR	C24-C23	5.97	1.51	1.33
19	4	4001	CLA	O2D-CGD	5.96	1.47	1.33
19	A	1151	CLA	OBD-CAD	5.96	1.30	1.22
19	2	2007	CLA	C3B-CAB	-5.95	1.35	1.47
19	B	1233	CLA	O2D-CGD	5.93	1.47	1.33
19	F	1305	CLA	OBD-CAD	5.93	1.30	1.22
19	1	1006	CLA	OBD-CAD	5.93	1.30	1.22
19	B	1233	CLA	OBD-CAD	5.92	1.30	1.22
19	B	1212	CLA	C3B-CAB	-5.92	1.35	1.47
19	B	1221	CLA	OBD-CAD	5.92	1.30	1.22
19	3	1118	CLA	OBD-CAD	5.91	1.30	1.22
19	A	1106	CLA	C3B-CAB	-5.91	1.35	1.47
19	A	9013	CLA	OBD-CAD	5.91	1.30	1.22
19	B	1228	CLA	O2D-CGD	5.91	1.47	1.33
21	A	6002	BCR	C11-C12	5.91	1.49	1.34
19	4	4006	CLA	OBD-CAD	5.90	1.30	1.22
19	A	1121	CLA	O2D-CGD	5.90	1.47	1.33
19	2	2007	CLA	OBD-CAD	5.90	1.30	1.22
19	A	1108	CLA	O2D-CGD	5.89	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1111	CLA	C3B-CAB	-5.89	1.35	1.47
19	2	2013	CLA	O2D-CGD	5.88	1.47	1.33
19	A	1133	CLA	O2D-CGD	5.87	1.47	1.33
19	B	1236	CLA	C3B-CAB	-5.86	1.36	1.47
19	B	1209	CLA	C3B-CAB	-5.86	1.36	1.47
19	L	1148	CLA	C3B-CAB	-5.86	1.36	1.47
19	R	1144	CLA	O2D-CGD	5.85	1.47	1.33
19	A	1120	CLA	O2D-CGD	5.85	1.47	1.33
19	3	3008	CLA	O2D-CGD	5.85	1.47	1.33
19	B	1213	CLA	O2D-CGD	5.84	1.47	1.33
19	3	3007	CLA	O2D-CGD	5.84	1.47	1.33
19	B	1214	CLA	O2D-CGD	5.84	1.47	1.33
19	K	1146	CLA	O2D-CGD	5.83	1.47	1.33
19	1	1005	CLA	O2D-CGD	5.83	1.47	1.33
19	B	1201	CLA	OBD-CAD	5.83	1.30	1.22
19	J	1311	CLA	O2D-CGD	5.83	1.47	1.33
19	2	2002	CLA	O2D-CGD	5.82	1.47	1.33
19	B	1213	CLA	C3B-CAB	-5.82	1.36	1.47
19	A	1110	CLA	O2D-CGD	5.82	1.47	1.33
19	B	1301	CLA	OBD-CAD	5.82	1.30	1.22
19	1	1013	CLA	O2D-CGD	5.81	1.47	1.33
21	1	6023	BCR	C10-C9	-5.81	1.28	1.35
19	A	1103	CLA	O2D-CGD	5.81	1.47	1.33
19	A	1149	CLA	O2A-CGA	5.80	1.50	1.33
19	3	1147	CLA	C4B-NB	-5.80	1.30	1.35
19	2	2004	CLA	C3B-CAB	-5.78	1.36	1.47
19	1	1007	CLA	OBD-CAD	5.77	1.30	1.22
19	B	1230	CLA	C3B-CAB	-5.77	1.36	1.47
19	4	4001	CLA	OBD-CAD	5.77	1.30	1.22
21	B	6020	BCR	C17-C18	-5.76	1.28	1.35
19	A	1122	CLA	O2D-CGD	5.76	1.47	1.33
19	L	1502	CLA	O2D-CGD	5.75	1.47	1.33
19	2	2007	CLA	O2D-CGD	5.75	1.47	1.33
19	A	1119	CLA	O2D-CGD	5.74	1.47	1.33
19	H	1207	CLA	O2D-CGD	5.74	1.47	1.33
19	A	1104	CLA	O2D-CGD	5.74	1.47	1.33
19	A	1102	CLA	C3B-CAB	-5.73	1.36	1.47
19	A	1112	CLA	O2D-CGD	5.73	1.47	1.33
19	K	3009	CLA	OBD-CAD	5.73	1.30	1.22
19	A	1129	CLA	C3B-CAB	-5.72	1.36	1.47
19	B	1231	CLA	O2D-CGD	5.72	1.47	1.33
19	2	4009	CLA	O2D-CGD	5.72	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1230	CLA	O2D-CGD	5.72	1.47	1.33
19	4	4014	CLA	O2D-CGD	5.70	1.47	1.33
19	B	1205	CLA	O2D-CGD	5.69	1.47	1.33
19	R	1144	CLA	C3B-CAB	-5.68	1.36	1.47
19	B	1219	CLA	OBD-CAD	5.68	1.30	1.22
19	A	1102	CLA	OBD-CAD	5.67	1.30	1.22
19	B	1227	CLA	O2D-CGD	5.66	1.47	1.33
19	B	1232	CLA	O2D-CGD	5.64	1.47	1.33
19	L	1504	CLA	O2D-CGD	5.63	1.46	1.33
19	B	1212	CLA	O2D-CGD	5.61	1.46	1.33
19	B	1211	CLA	OBD-CAD	5.61	1.30	1.22
19	A	1151	CLA	O2D-CGD	5.60	1.46	1.33
19	B	1211	CLA	O2D-CGD	5.60	1.46	1.33
19	1	1008	CLA	O2D-CGD	5.60	1.46	1.33
19	1	1003	CLA	OBD-CAD	5.59	1.30	1.22
19	A	1128	CLA	C3B-CAB	-5.59	1.36	1.47
19	A	9011	CLA	O2D-CGD	5.58	1.46	1.33
19	A	1237	CLA	O2D-CGD	5.57	1.46	1.33
19	L	1130	CLA	O2D-CGD	5.57	1.46	1.33
19	A	1105	CLA	O2D-CGD	5.57	1.46	1.33
19	B	1208	CLA	O2A-CGA	5.57	1.49	1.33
21	L	6019	BCR	C21-C22	-5.57	1.28	1.35
19	A	1132	CLA	O2D-CGD	5.56	1.46	1.33
19	3	3003	CLA	OBD-CAD	5.55	1.30	1.22
19	4	4014	CLA	O2A-CGA	5.55	1.49	1.33
19	B	1223	CLA	O2D-CGD	5.54	1.46	1.33
19	A	1104	CLA	OBD-CAD	5.54	1.30	1.22
19	L	1503	CLA	OBD-CAD	5.53	1.30	1.22
19	B	1236	CLA	O2D-CGD	5.53	1.46	1.33
19	F	1302	CLA	O2D-CGD	5.52	1.46	1.33
19	4	4003	CLA	O2D-CGD	5.51	1.46	1.33
19	A	1110	CLA	C3B-CAB	-5.51	1.36	1.47
19	2	2002	CLA	C3B-CAB	-5.50	1.36	1.47
19	4	4002	CLA	O2D-CGD	5.50	1.46	1.33
19	G	1242	CLA	OBD-CAD	5.50	1.30	1.22
19	A	1128	CLA	O2D-CGD	5.50	1.46	1.33
19	3	2009	CLA	O2D-CGD	5.49	1.46	1.33
19	A	1141	CLA	O2D-CGD	5.49	1.46	1.33
19	4	1004	CLA	O2D-CGD	5.48	1.46	1.33
19	4	1306	CLA	OBD-CAD	5.48	1.30	1.22
19	B	1218	CLA	C3B-CAB	-5.48	1.36	1.47
19	2	2004	CLA	O2D-CGD	5.48	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3011	CLA	O2D-CGD	5.48	1.46	1.33
19	B	1215	CLA	O2D-CGD	5.47	1.46	1.33
19	A	1122	CLA	O2A-CGA	5.47	1.49	1.33
19	B	1209	CLA	O2D-CGD	5.45	1.46	1.33
19	1	1303	CLA	O2D-CGD	5.45	1.46	1.33
19	4	1306	CLA	O2D-CGD	5.45	1.46	1.33
19	3	3007	CLA	OBD-CAD	5.45	1.29	1.22
19	K	1143	CLA	O2D-CGD	5.44	1.46	1.33
19	A	9012	CLA	O2D-CGD	5.43	1.46	1.33
19	4	4002	CLA	C1B-NB	-5.42	1.30	1.35
19	B	1221	CLA	O2D-CGD	5.41	1.46	1.33
19	A	9023	CLA	O2D-CGD	5.41	1.46	1.33
19	A	1103	CLA	O2A-CGA	5.41	1.49	1.33
19	3	3016	CLA	O2D-CGD	5.40	1.46	1.33
19	H	1207	CLA	OBD-CAD	5.40	1.29	1.22
19	1	1008	CLA	OBD-CAD	5.38	1.29	1.22
19	4	4007	CLA	OBD-CAD	5.38	1.29	1.22
19	2	2002	CLA	O2A-CGA	5.37	1.49	1.33
21	I	6018	BCR	C10-C9	-5.37	1.28	1.35
19	A	1108	CLA	OBD-CAD	5.37	1.29	1.22
19	B	1214	CLA	OBD-CAD	5.36	1.29	1.22
19	A	1127	CLA	O2D-CGD	5.36	1.46	1.33
19	B	1224	CLA	O2D-CGD	5.36	1.46	1.33
19	1	1002	CLA	O2A-CGA	5.35	1.49	1.33
19	A	1129	CLA	O2A-CGA	5.35	1.49	1.33
19	J	1308	CLA	O2D-CGD	5.35	1.46	1.33
19	A	1109	CLA	O2D-CGD	5.34	1.46	1.33
19	2	2013	CLA	O2A-CGA	5.34	1.49	1.33
19	2	2001	CLA	O2D-CGD	5.34	1.46	1.33
19	A	1140	CLA	O2D-CGD	5.33	1.46	1.33
19	A	1139	CLA	O2D-CGD	5.33	1.46	1.33
19	A	1102	CLA	O2A-CGA	5.33	1.48	1.33
19	B	1238	CLA	O2D-CGD	5.32	1.46	1.33
19	4	4012	CLA	OBD-CAD	5.32	1.29	1.22
19	A	9022	CLA	O2D-CGD	5.32	1.46	1.33
19	B	1217	CLA	O2D-CGD	5.31	1.46	1.33
19	4	4003	CLA	OBD-CAD	5.31	1.29	1.22
19	2	4009	CLA	OBD-CAD	5.30	1.29	1.22
19	A	1138	CLA	O2D-CGD	5.30	1.46	1.33
21	I	6021	BCR	C24-C23	5.30	1.49	1.33
19	2	2014	CLA	O2D-CGD	5.29	1.46	1.33
19	1	1003	CLA	O2D-CGD	5.29	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1218	CLA	OBD-CAD	5.29	1.29	1.22
19	L	1130	CLA	OBD-CAD	5.28	1.29	1.22
19	A	1122	CLA	OBD-CAD	5.28	1.29	1.22
19	B	1202	CLA	O2D-CGD	5.27	1.46	1.33
19	K	3009	CLA	O2D-CGD	5.27	1.46	1.33
19	A	9022	CLA	OBD-CAD	5.26	1.29	1.22
19	4	4002	CLA	C3B-CAB	-5.25	1.37	1.47
21	I	6021	BCR	C10-C9	-5.25	1.28	1.35
19	2	2013	CLA	OBD-CAD	5.24	1.29	1.22
19	A	1105	CLA	OBD-CAD	5.24	1.29	1.22
19	R	1144	CLA	O2A-CGA	5.23	1.48	1.33
19	A	1113	CLA	OBD-CAD	5.23	1.29	1.22
19	B	1239	CLA	O2D-CGD	5.23	1.46	1.33
19	4	1304	CLA	O2D-CGD	5.23	1.46	1.33
21	F	6016	BCR	C30-C25	-5.22	1.46	1.53
19	B	1220	CLA	C1B-NB	-5.22	1.30	1.35
19	B	1214	CLA	O2A-CGA	5.21	1.48	1.33
19	B	1211	CLA	O2A-CGA	5.21	1.48	1.33
19	A	1134	CLA	O2D-CGD	5.20	1.45	1.33
19	B	1202	CLA	O2A-CGA	5.19	1.48	1.33
19	A	9013	CLA	O2D-CGD	5.19	1.45	1.33
19	K	1142	CLA	O2D-CGD	5.18	1.45	1.33
19	1	1002	CLA	OBD-CAD	5.18	1.29	1.22
19	B	1225	CLA	OBD-CAD	5.17	1.29	1.22
19	A	1120	CLA	OBD-CAD	5.16	1.29	1.22
19	B	1208	CLA	OBD-CAD	5.16	1.29	1.22
19	A	1117	CLA	O2A-CGA	5.16	1.48	1.33
19	A	1101	CLA	O2D-CGD	5.14	1.45	1.33
19	B	1203	CLA	O2D-CGD	5.14	1.45	1.33
19	A	1131	CLA	OBD-CAD	5.14	1.29	1.22
19	B	1227	CLA	O2A-CGA	5.14	1.48	1.33
19	B	9010	CLA	OBD-CAD	5.14	1.29	1.22
19	I	1204	CLA	O2A-CGA	5.14	1.48	1.33
19	A	1101	CLA	OBD-CAD	5.13	1.29	1.22
19	A	1110	CLA	O2A-CGA	5.13	1.48	1.33
19	A	1110	CLA	OBD-CAD	5.13	1.29	1.22
19	B	1210	CLA	O2D-CGD	5.12	1.45	1.33
21	B	6017	BCR	C10-C9	-5.12	1.29	1.35
19	A	1135	CLA	O2D-CGD	5.12	1.45	1.33
19	1	1010	CLA	O2D-CGD	5.11	1.45	1.33
19	A	1111	CLA	O2D-CGD	5.11	1.45	1.33
19	B	1230	CLA	OBD-CAD	5.11	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1141	CLA	OBD-CAD	5.11	1.29	1.22
20	A	5001	PQN	C10-C5	5.10	1.49	1.40
19	A	1127	CLA	O2A-CGA	5.10	1.48	1.33
19	H	1505	CLA	OBD-CAD	5.09	1.29	1.22
19	B	1216	CLA	O2D-CGD	5.09	1.45	1.33
19	3	3011	CLA	OBD-CAD	5.09	1.29	1.22
19	B	1201	CLA	O2D-CGD	5.09	1.45	1.33
19	3	1147	CLA	OBD-CAD	5.09	1.29	1.22
19	I	1204	CLA	O2D-CGD	5.09	1.45	1.33
19	B	1226	CLA	O2D-CGD	5.09	1.45	1.33
19	A	1116	CLA	O2A-CGA	5.09	1.48	1.33
19	H	1145	CLA	O2D-CGD	5.07	1.45	1.33
19	B	1229	CLA	O2A-CGA	5.07	1.48	1.33
19	A	1125	CLA	O2D-CGD	5.07	1.45	1.33
19	2	2001	CLA	OBD-CAD	5.07	1.29	1.22
19	A	1128	CLA	OBD-CAD	5.07	1.29	1.22
19	A	1129	CLA	O2D-CGD	5.06	1.45	1.33
19	B	1226	CLA	C3B-CAB	-5.06	1.37	1.47
19	A	1102	CLA	O2D-CGD	5.05	1.45	1.33
19	3	3017	CLA	O2D-CGD	5.05	1.45	1.33
19	F	1240	CLA	OBD-CAD	5.05	1.29	1.22
19	K	1143	CLA	OBD-CAD	5.05	1.29	1.22
19	B	1208	CLA	O2D-CGD	5.04	1.45	1.33
19	A	1117	CLA	O2D-CGD	5.04	1.45	1.33
19	2	2002	CLA	OBD-CAD	5.04	1.29	1.22
19	L	1501	CLA	O2A-CGA	5.03	1.48	1.33
19	A	1237	CLA	OBD-CAD	5.03	1.29	1.22
19	B	1222	CLA	O2D-CGD	5.03	1.45	1.33
19	A	9022	CLA	O2A-CGA	5.02	1.48	1.33
19	R	1150	CLA	O2A-CGA	5.02	1.48	1.33
19	B	1232	CLA	OBD-CAD	5.02	1.29	1.22
19	F	1302	CLA	OBD-CAD	5.00	1.29	1.22
19	B	1206	CLA	O2D-CGD	5.00	1.45	1.33
19	A	1136	CLA	O2D-CGD	4.99	1.45	1.33
19	K	3009	CLA	O2A-CGA	4.98	1.47	1.33
19	4	1304	CLA	OBD-CAD	4.98	1.29	1.22
19	4	1306	CLA	O2A-CGA	4.97	1.47	1.33
19	3	3016	CLA	OBD-CAD	4.96	1.29	1.22
19	F	1305	CLA	O2D-CGD	4.95	1.45	1.33
19	A	1137	CLA	O2D-CGD	4.95	1.45	1.33
19	1	1014	CLA	OBD-CAD	4.94	1.29	1.22
19	L	1502	CLA	OBD-CAD	4.93	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	1504	CLA	O2A-CGA	4.93	1.47	1.33
19	A	9012	CLA	OBD-CAD	4.93	1.29	1.22
19	3	3017	CLA	OBD-CAD	4.92	1.29	1.22
19	B	1238	CLA	O2A-CGA	4.92	1.47	1.33
19	B	1233	CLA	O2A-CGA	4.92	1.47	1.33
19	B	1218	CLA	O2A-CGA	4.92	1.48	1.33
19	A	1126	CLA	OBD-CAD	4.91	1.29	1.22
19	2	2012	CLA	O2D-CGD	4.91	1.45	1.33
19	1	1013	CLA	OBD-CAD	4.91	1.29	1.22
19	A	9012	CLA	O2A-CGA	4.90	1.47	1.33
19	A	1115	CLA	O2D-CGD	4.90	1.45	1.33
19	B	1236	CLA	O2A-CGA	4.89	1.47	1.33
19	B	9010	CLA	O2D-CGD	4.88	1.45	1.33
19	A	1106	CLA	O2D-CGD	4.88	1.45	1.33
19	B	1216	CLA	O2A-CGA	4.88	1.47	1.33
19	A	1138	CLA	OBD-CAD	4.88	1.29	1.22
19	B	1234	CLA	O2D-CGD	4.88	1.45	1.33
19	B	1229	CLA	OBD-CAD	4.88	1.29	1.22
19	B	1234	CLA	O2A-CGA	4.88	1.47	1.33
19	A	1107	CLA	OBD-CAD	4.87	1.29	1.22
19	A	1113	CLA	O2A-CGA	4.87	1.47	1.33
24	B	7101	LMG	O7-C10	4.87	1.48	1.34
19	2	4009	CLA	O2A-CGA	4.86	1.47	1.33
19	A	1127	CLA	OBD-CAD	4.86	1.29	1.22
19	A	1108	CLA	C3B-CAB	-4.85	1.38	1.47
19	A	1111	CLA	O2A-CGA	4.85	1.47	1.33
19	4	4003	CLA	O2A-CGA	4.85	1.47	1.33
19	B	1239	CLA	O2A-CGA	4.85	1.47	1.33
19	B	1228	CLA	O2A-CGA	4.84	1.47	1.33
19	A	1132	CLA	O2A-CGA	4.84	1.47	1.33
19	J	1311	CLA	OBD-CAD	4.84	1.29	1.22
19	A	1123	CLA	O2D-CGD	4.84	1.45	1.33
19	1	1008	CLA	O2A-CGA	4.84	1.47	1.33
19	2	2014	CLA	OBD-CAD	4.84	1.29	1.22
19	A	1124	CLA	O2D-CGD	4.83	1.45	1.33
19	A	1135	CLA	OBD-CAD	4.82	1.29	1.22
19	H	1207	CLA	O2A-CGA	4.82	1.47	1.33
19	L	1502	CLA	O2A-CGA	4.82	1.47	1.33
19	A	1119	CLA	OBD-CAD	4.82	1.29	1.22
19	3	2009	CLA	O2A-CGA	4.81	1.47	1.33
19	4	4014	CLA	OBD-CAD	4.80	1.29	1.22
19	1	1014	CLA	O2A-CGA	4.80	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	1130	CLA	O2A-CGA	4.80	1.47	1.33
19	1	1001	CLA	O2D-CED	4.78	1.56	1.45
19	B	1209	CLA	OBD-CAD	4.77	1.29	1.22
19	B	1217	CLA	O2A-CGA	4.76	1.47	1.33
19	A	1109	CLA	O2A-CGA	4.76	1.47	1.33
19	A	9023	CLA	O2A-CGA	4.76	1.47	1.33
19	B	1225	CLA	O2D-CGD	4.75	1.44	1.33
19	1	1013	CLA	O2A-CGA	4.74	1.47	1.33
19	L	1503	CLA	O2A-CGA	4.74	1.47	1.33
19	A	1116	CLA	OBD-CAD	4.74	1.28	1.22
19	B	1221	CLA	O2A-CGA	4.74	1.47	1.33
19	4	1004	CLA	OBD-CAD	4.74	1.28	1.22
19	A	1125	CLA	O2A-CGA	4.73	1.47	1.33
19	H	1241	CLA	O2A-CGA	4.73	1.47	1.33
21	A	6007	BCR	C30-C25	-4.73	1.47	1.53
21	A	6007	BCR	C20-C21	4.73	1.58	1.43
19	3	3011	CLA	O2A-CGA	4.72	1.47	1.33
19	B	1210	CLA	O2A-CGA	4.72	1.47	1.33
19	A	1134	CLA	OBD-CAD	4.72	1.28	1.22
19	2	2007	CLA	O2A-CGA	4.71	1.47	1.33
19	B	1224	CLA	OBD-CAD	4.71	1.28	1.22
19	A	1133	CLA	O2A-CGA	4.71	1.47	1.33
19	H	1505	CLA	O2A-CGA	4.71	1.47	1.33
19	A	1119	CLA	O2A-CGA	4.70	1.47	1.33
19	L	1148	CLA	O2A-CGA	4.70	1.47	1.33
19	A	1107	CLA	O2A-CGA	4.70	1.47	1.33
19	4	4007	CLA	O2A-CGA	4.69	1.47	1.33
19	1	1013	CLA	C3D-CAD	-4.69	1.34	1.46
19	K	1142	CLA	OBD-CAD	4.69	1.28	1.22
19	A	1131	CLA	O2D-CGD	4.68	1.44	1.33
19	B	1229	CLA	O2D-CGD	4.68	1.44	1.33
19	B	1212	CLA	O2A-CGA	4.68	1.47	1.33
19	A	1139	CLA	OBD-CAD	4.67	1.28	1.22
19	B	1226	CLA	OBD-CAD	4.67	1.28	1.22
19	A	1149	CLA	OBD-CAD	4.67	1.28	1.22
19	1	1005	CLA	O2A-CGA	4.67	1.47	1.33
19	3	3016	CLA	O2A-CGA	4.65	1.46	1.33
19	J	1311	CLA	O2A-CGA	4.65	1.46	1.33
19	A	1120	CLA	O2A-CGA	4.64	1.46	1.33
19	1	1007	CLA	O2A-CGA	4.64	1.46	1.33
20	B	5002	PQN	C10-C5	4.64	1.48	1.40
19	B	1205	CLA	OBD-CAD	4.64	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	1145	CLA	OBD-CAD	4.63	1.28	1.22
19	L	1501	CLA	OBD-CAD	4.62	1.28	1.22
19	R	1144	CLA	OBD-CAD	4.61	1.28	1.22
19	A	1101	CLA	O2A-CGA	4.61	1.46	1.33
19	2	2004	CLA	O2A-CGA	4.61	1.46	1.33
19	B	1212	CLA	OBD-CAD	4.60	1.28	1.22
19	A	1133	CLA	OBD-CAD	4.60	1.28	1.22
19	2	2012	CLA	O2A-CGA	4.59	1.46	1.33
19	B	1235	CLA	O2D-CGD	4.59	1.44	1.33
19	1	1011	CLA	C3A-C2A	-4.59	1.50	1.54
19	4	4001	CLA	O2A-CGA	4.57	1.46	1.33
19	1	1011	CLA	OBD-CAD	4.57	1.28	1.22
19	A	1136	CLA	OBD-CAD	4.57	1.28	1.22
19	A	1124	CLA	OBD-CAD	4.57	1.28	1.22
19	K	1146	CLA	OBD-CAD	4.57	1.28	1.22
19	G	1242	CLA	O2A-CGA	4.56	1.46	1.33
19	2	2004	CLA	OBD-CAD	4.56	1.28	1.22
19	A	1107	CLA	O2D-CGD	4.56	1.44	1.33
19	A	1137	CLA	OBD-CAD	4.56	1.28	1.22
19	B	1222	CLA	O2A-CGA	4.55	1.46	1.33
19	A	1109	CLA	OBD-CAD	4.55	1.28	1.22
19	B	1238	CLA	OBD-CAD	4.55	1.28	1.22
19	1	1003	CLA	O2A-CGA	4.55	1.46	1.33
19	1	1012	CLA	OBD-CAD	4.55	1.28	1.22
19	4	4015	CLA	O2A-CGA	4.54	1.47	1.33
19	J	1308	CLA	OBD-CAD	4.54	1.28	1.22
19	A	1151	CLA	O2A-CGA	4.54	1.46	1.33
19	A	1126	CLA	O2D-CGD	4.54	1.44	1.33
19	B	1206	CLA	OBD-CAD	4.53	1.28	1.22
19	A	1108	CLA	C4C-CHD	4.53	1.53	1.41
19	A	1113	CLA	C4C-CHD	4.53	1.53	1.41
19	A	1131	CLA	O2A-CGA	4.52	1.46	1.33
19	A	1140	CLA	OBD-CAD	4.52	1.28	1.22
19	B	1227	CLA	OBD-CAD	4.52	1.28	1.22
19	B	1202	CLA	OBD-CAD	4.50	1.28	1.22
19	B	1219	CLA	O2A-CGA	4.49	1.46	1.33
21	B	6010	BCR	C21-C22	-4.48	1.29	1.35
19	2	2007	CLA	C4C-CHD	4.48	1.53	1.41
19	A	1151	CLA	C4C-CHD	4.48	1.53	1.41
19	B	1222	CLA	OBD-CAD	4.48	1.28	1.22
19	A	1126	CLA	C4C-CHD	4.47	1.53	1.41
19	2	2012	CLA	C4C-CHD	4.46	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	9013	CLA	C4C-CHD	4.46	1.53	1.41
19	A	1141	CLA	O2A-CGA	4.46	1.46	1.33
19	2	2012	CLA	OBD-CAD	4.46	1.28	1.22
19	L	1148	CLA	OBD-CAD	4.46	1.28	1.22
19	1	1303	CLA	C3A-C2A	-4.45	1.42	1.54
19	B	1209	CLA	O2A-CGA	4.44	1.46	1.33
19	B	1234	CLA	OBD-CAD	4.44	1.28	1.22
19	1	1303	CLA	O2A-CGA	4.43	1.46	1.33
19	A	1106	CLA	O2A-CGA	4.43	1.46	1.33
19	L	1130	CLA	C4C-CHD	4.43	1.53	1.41
19	B	1224	CLA	C4C-CHD	4.43	1.53	1.41
19	A	1128	CLA	O2A-CGA	4.42	1.46	1.33
19	B	1202	CLA	C4C-CHD	4.42	1.53	1.41
19	3	1147	CLA	C3B-C2B	-4.42	1.34	1.40
19	4	4015	CLA	O2D-CGD	4.42	1.44	1.33
21	B	6020	BCR	C30-C25	-4.41	1.47	1.53
19	B	1223	CLA	O2A-CGA	4.41	1.46	1.33
19	H	1241	CLA	C4C-CHD	4.41	1.53	1.41
19	A	1123	CLA	O2A-CGA	4.40	1.46	1.33
19	B	1235	CLA	O2A-CGA	4.39	1.46	1.33
19	B	1223	CLA	OBD-CAD	4.39	1.28	1.22
19	B	1230	CLA	O2A-CGA	4.39	1.46	1.33
19	B	1228	CLA	OBD-CAD	4.39	1.28	1.22
19	A	1151	CLA	C4C-NC	4.38	1.39	1.35
19	4	4006	CLA	O2A-CGA	4.37	1.46	1.33
19	B	1219	CLA	C4C-CHD	4.37	1.53	1.41
19	3	1147	CLA	O2D-CGD	4.37	1.43	1.33
19	B	1205	CLA	O2A-CGA	4.37	1.46	1.33
19	H	1241	CLA	C4C-NC	4.37	1.39	1.35
19	A	1140	CLA	O2A-CGA	4.36	1.46	1.33
19	3	3017	CLA	C4C-CHD	4.36	1.53	1.41
19	A	1117	CLA	OBD-CAD	4.36	1.28	1.22
19	A	1135	CLA	O2A-CGA	4.36	1.46	1.33
19	A	1132	CLA	OBD-CAD	4.36	1.28	1.22
19	A	1111	CLA	OBD-CAD	4.35	1.28	1.22
19	B	1227	CLA	C4C-CHD	4.35	1.53	1.41
19	A	9011	CLA	OBD-CAD	4.34	1.28	1.22
19	A	1139	CLA	O2A-CGA	4.34	1.46	1.33
19	A	1121	CLA	C4C-CHD	4.34	1.53	1.41
19	2	2001	CLA	O2A-CGA	4.34	1.46	1.33
19	A	1106	CLA	OBD-CAD	4.34	1.28	1.22
21	A	6008	BCR	C10-C9	-4.33	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	1148	CLA	O2D-CGD	4.33	1.43	1.33
19	B	1208	CLA	C4C-CHD	4.32	1.53	1.41
19	F	1305	CLA	C3A-C2A	-4.31	1.42	1.54
19	A	1138	CLA	O2A-CGA	4.31	1.45	1.33
19	1	1011	CLA	C1B-NB	-4.31	1.31	1.35
19	4	1004	CLA	O2A-CGA	4.31	1.45	1.33
19	2	2006	CLA	O2A-CGA	4.31	1.45	1.33
19	B	1235	CLA	C4C-CHD	4.30	1.53	1.41
19	A	1120	CLA	C4C-CHD	4.30	1.52	1.41
19	A	1104	CLA	O2A-CGA	4.29	1.45	1.33
19	A	1107	CLA	C4C-CHD	4.29	1.52	1.41
19	3	3004	CLA	C1B-NB	-4.29	1.31	1.35
21	A	6007	BCR	C10-C9	-4.29	1.30	1.35
19	A	9023	CLA	OBD-CAD	4.28	1.28	1.22
19	A	1115	CLA	OBD-CAD	4.28	1.28	1.22
19	A	1149	CLA	C4C-CHD	4.28	1.52	1.41
19	B	1205	CLA	C4C-CHD	4.28	1.52	1.41
19	B	1211	CLA	C4C-CHD	4.28	1.52	1.41
19	A	1132	CLA	C4C-CHD	4.27	1.52	1.41
19	L	1502	CLA	C4C-CHD	4.27	1.52	1.41
19	2	2002	CLA	C4C-CHD	4.27	1.52	1.41
19	F	1302	CLA	C3A-C2A	-4.26	1.50	1.54
21	B	6005	BCR	C10-C9	-4.26	1.30	1.35
21	A	6008	BCR	C21-C22	-4.25	1.30	1.35
19	F	1240	CLA	C4C-CHD	4.25	1.52	1.41
19	B	1201	CLA	C4C-CHD	4.25	1.52	1.41
19	A	1110	CLA	C4C-CHD	4.24	1.52	1.41
19	A	1103	CLA	C4C-CHD	4.24	1.52	1.41
19	B	1234	CLA	C4C-CHD	4.23	1.52	1.41
19	4	1304	CLA	C4C-CHD	4.23	1.52	1.41
19	1	1010	CLA	O2A-CGA	4.22	1.46	1.33
19	3	3008	CLA	O2A-CGA	4.22	1.45	1.33
19	3	2009	CLA	OBD-CAD	4.22	1.28	1.22
19	3	3008	CLA	OBD-CAD	4.21	1.28	1.22
19	K	1143	CLA	O2A-CGA	4.21	1.45	1.33
19	A	1112	CLA	C4C-CHD	4.20	1.52	1.41
19	B	1215	CLA	O2A-CGA	4.19	1.45	1.33
19	A	1137	CLA	O2A-CGA	4.19	1.45	1.33
19	A	1123	CLA	OBD-CAD	4.19	1.28	1.22
19	B	1238	CLA	C4C-CHD	4.19	1.52	1.41
19	A	1102	CLA	C4C-CHD	4.18	1.52	1.41
19	A	1105	CLA	O2A-CGA	4.18	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1237	CLA	O2A-CGA	4.18	1.45	1.33
19	A	9011	CLA	O2A-CGA	4.18	1.45	1.33
19	4	4005	CLA	C4C-CHD	4.18	1.52	1.43
19	A	1123	CLA	C4C-CHD	4.18	1.52	1.41
19	B	1217	CLA	OBD-CAD	4.17	1.28	1.22
19	1	1010	CLA	OBD-CAD	4.17	1.28	1.22
19	A	1129	CLA	OBD-CAD	4.17	1.28	1.22
19	K	1146	CLA	O2A-CGA	4.17	1.45	1.33
19	B	1214	CLA	C4C-CHD	4.17	1.52	1.41
19	4	4002	CLA	O2A-CGA	4.15	1.45	1.33
19	A	1105	CLA	C4C-CHD	4.15	1.52	1.41
19	G	1242	CLA	C4C-CHD	4.15	1.52	1.41
19	A	1101	CLA	C4C-CHD	4.15	1.52	1.41
19	B	1226	CLA	O2A-CGA	4.15	1.45	1.33
19	3	3013	CLA	O2A-CGA	4.14	1.45	1.33
19	A	1129	CLA	C4C-CHD	4.14	1.52	1.41
19	J	1308	CLA	O2A-CGA	4.14	1.45	1.33
19	3	3017	CLA	O2A-CGA	4.14	1.45	1.33
21	F	6016	BCR	C21-C22	-4.13	1.30	1.35
19	B	1203	CLA	O2A-CGA	4.13	1.45	1.33
19	4	1306	CLA	C4C-CHD	4.13	1.52	1.41
19	B	1224	CLA	O2A-CGA	4.13	1.45	1.33
19	3	3003	CLA	C4C-CHD	4.13	1.52	1.41
19	A	1133	CLA	C4C-CHD	4.13	1.52	1.41
19	A	1104	CLA	C4C-CHD	4.12	1.52	1.41
19	A	1119	CLA	C4C-CHD	4.11	1.52	1.41
19	A	1136	CLA	O2A-CGA	4.11	1.45	1.33
19	4	4003	CLA	C4C-CHD	4.10	1.52	1.41
19	A	1115	CLA	O2A-CGA	4.10	1.45	1.33
19	A	9022	CLA	C4C-CHD	4.10	1.52	1.41
19	H	1145	CLA	O2A-CGA	4.09	1.45	1.33
19	R	1144	CLA	C4C-CHD	4.09	1.52	1.41
19	A	1116	CLA	C4C-CHD	4.09	1.52	1.41
19	B	1221	CLA	C4C-CHD	4.08	1.52	1.41
19	A	1124	CLA	O2A-CGA	4.08	1.45	1.33
19	3	3001	CLA	C4C-CHD	4.08	1.52	1.43
19	A	1109	CLA	C4C-CHD	4.08	1.52	1.41
19	A	1122	CLA	C4C-CHD	4.08	1.52	1.41
19	B	1220	CLA	O2A-CGA	4.08	1.45	1.33
19	B	1232	CLA	C4C-CHD	4.08	1.52	1.41
19	B	1239	CLA	OBD-CAD	4.07	1.28	1.22
19	A	1128	CLA	C4C-CHD	4.07	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1003	CLA	C4C-CHD	4.07	1.52	1.41
19	1	1006	CLA	C4C-CHD	4.07	1.52	1.41
19	1	1012	CLA	C4C-CHD	4.07	1.52	1.41
21	J	6012	BCR	C21-C22	-4.07	1.30	1.35
19	1	1001	CLA	O2A-CGA	4.06	1.45	1.33
19	A	1111	CLA	C4C-CHD	4.06	1.52	1.41
19	K	1143	CLA	C4C-CHD	4.05	1.52	1.41
19	1	1010	CLA	C1B-NB	-4.05	1.31	1.35
19	2	2004	CLA	C4C-CHD	4.05	1.52	1.41
21	3	6022	BCR	C30-C25	-4.05	1.48	1.53
19	3	3011	CLA	C4C-CHD	4.04	1.52	1.41
19	A	1131	CLA	C4C-CHD	4.04	1.52	1.41
19	H	1505	CLA	C4C-CHD	4.04	1.52	1.41
19	A	1106	CLA	C4C-CHD	4.04	1.52	1.41
19	1	1310	CLA	C4C-CHD	4.03	1.52	1.43
19	3	1118	CLA	C4C-CHD	4.03	1.52	1.41
19	A	1138	CLA	C4C-CHD	4.03	1.52	1.41
19	B	1203	CLA	C4C-CHD	4.02	1.52	1.41
19	B	1206	CLA	C4C-CHD	4.01	1.52	1.41
19	L	1148	CLA	C4C-NC	4.01	1.38	1.35
19	3	3012	CLA	C4C-CHD	4.01	1.51	1.43
19	B	1218	CLA	C4C-CHD	4.01	1.52	1.41
24	B	7101	LMG	O8-C28	4.01	1.45	1.33
19	A	1126	CLA	O2A-CGA	3.99	1.45	1.33
19	2	2003	CLA	C4C-CHD	3.99	1.51	1.43
19	1	1005	CLA	C4C-CHD	3.99	1.52	1.41
19	B	1225	CLA	O2A-CGA	3.99	1.45	1.33
19	2	2014	CLA	O2A-CGA	3.99	1.45	1.33
19	4	1004	CLA	O2D-CED	3.98	1.54	1.45
19	L	1503	CLA	C4C-CHD	3.98	1.52	1.41
19	A	9013	CLA	O2A-CGA	3.98	1.45	1.33
19	B	9010	CLA	O2A-CGA	3.98	1.45	1.33
19	2	2001	CLA	C4C-CHD	3.97	1.52	1.41
19	3	3013	CLA	OBD-CAD	3.97	1.27	1.22
19	B	1213	CLA	O2A-CGA	3.97	1.45	1.33
19	3	3007	CLA	C4C-CHD	3.97	1.52	1.41
19	4	1009	CLA	C3A-C2A	-3.96	1.50	1.54
19	1	1310	CLA	MG-NA	-3.96	1.96	2.06
19	1	1303	CLA	C1B-NB	-3.96	1.31	1.35
19	A	1141	CLA	C4C-CHD	3.96	1.52	1.41
19	H	1207	CLA	C4C-CHD	3.95	1.52	1.41
19	L	1504	CLA	C4C-CHD	3.95	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1117	CLA	C4C-CHD	3.95	1.52	1.41
19	B	1216	CLA	OBD-CAD	3.94	1.27	1.22
19	B	1220	CLA	O2D-CGD	3.94	1.42	1.33
19	4	4001	CLA	C4C-CHD	3.94	1.51	1.41
19	4	4007	CLA	C4C-CHD	3.94	1.51	1.41
19	2	2010	CLA	C4C-CHD	3.94	1.51	1.43
19	B	9010	CLA	C4C-CHD	3.93	1.51	1.41
19	A	1135	CLA	C4C-CHD	3.93	1.51	1.41
19	A	1140	CLA	C4C-CHD	3.93	1.51	1.41
19	1	1015	CLA	C4C-CHD	3.93	1.51	1.43
19	B	1229	CLA	C4B-CHC	3.93	1.51	1.41
19	B	1228	CLA	C4C-CHD	3.92	1.51	1.41
19	B	1210	CLA	OBD-CAD	3.91	1.27	1.22
19	3	3004	CLA	MG-NA	-3.91	1.97	2.06
19	3	3008	CLA	C4C-CHD	3.91	1.51	1.41
19	B	1236	CLA	OBD-CAD	3.91	1.27	1.22
19	B	1233	CLA	C4C-CHD	3.91	1.51	1.41
19	1	1303	CLA	C4C-CHD	3.91	1.51	1.41
19	4	4006	CLA	C4C-CHD	3.91	1.51	1.41
19	B	1210	CLA	C4B-CHC	3.91	1.51	1.41
19	B	1213	CLA	C4C-CHD	3.91	1.51	1.41
19	A	1134	CLA	C4C-CHD	3.90	1.51	1.41
19	B	1223	CLA	C4C-CHD	3.90	1.51	1.41
19	A	1127	CLA	C4C-CHD	3.90	1.51	1.41
19	4	4015	CLA	OBD-CAD	3.90	1.27	1.22
19	4	1304	CLA	O2A-CGA	3.90	1.44	1.33
19	A	1136	CLA	C4C-CHD	3.90	1.51	1.41
19	3	3016	CLA	C4C-CHD	3.90	1.51	1.41
19	R	1150	CLA	C4C-CHD	3.89	1.51	1.41
19	4	4004	CLA	C4C-CHD	3.89	1.51	1.43
19	A	1237	CLA	C4C-CHD	3.89	1.51	1.41
19	F	1302	CLA	C4C-CHD	3.88	1.51	1.41
19	1	1002	CLA	C4C-CHD	3.88	1.51	1.41
19	L	1130	CLA	C4C-NC	3.88	1.38	1.35
19	A	1124	CLA	C4C-CHD	3.88	1.51	1.41
19	K	3009	CLA	C4C-CHD	3.88	1.51	1.41
19	A	9011	CLA	C4B-CHC	3.87	1.51	1.41
21	B	6010	BCR	C30-C25	-3.87	1.48	1.53
19	B	1217	CLA	C4C-CHD	3.87	1.51	1.41
19	1	1003	CLA	C4B-CHC	3.86	1.51	1.41
19	4	4010	CLA	C4C-CHD	3.86	1.51	1.43
19	F	1305	CLA	O2A-CGA	3.86	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1230	CLA	C4C-CHD	3.85	1.51	1.41
19	G	1242	CLA	C4B-CHC	3.85	1.51	1.41
19	A	1137	CLA	C4C-CHD	3.85	1.51	1.41
19	A	1139	CLA	C4C-CHD	3.85	1.51	1.41
19	K	1146	CLA	C1B-NB	-3.85	1.31	1.35
19	A	1120	CLA	C4B-CHC	3.85	1.51	1.41
19	1	1008	CLA	C4C-CHD	3.85	1.51	1.41
19	K	3009	CLA	C4B-CHC	3.85	1.51	1.41
19	A	1125	CLA	OBD-CAD	3.85	1.27	1.22
19	B	1206	CLA	O2A-CGA	3.84	1.44	1.33
19	2	4009	CLA	C4C-CHD	3.84	1.51	1.41
19	K	1142	CLA	C4C-CHD	3.84	1.51	1.41
19	B	1210	CLA	C4C-CHD	3.84	1.51	1.41
21	B	6006	BCR	C24-C23	3.83	1.44	1.33
19	3	3005	CLA	C4C-CHD	3.83	1.51	1.43
19	B	1233	CLA	C4B-CHC	3.83	1.51	1.41
19	B	1215	CLA	OBD-CAD	3.83	1.27	1.22
19	1	1012	CLA	C4B-CHC	3.83	1.51	1.41
19	B	1212	CLA	C4B-CHC	3.83	1.51	1.41
19	B	1231	CLA	C4C-CHD	3.82	1.51	1.41
19	R	1150	CLA	C4B-CHC	3.81	1.51	1.41
19	A	9012	CLA	C4C-CHD	3.81	1.51	1.41
19	4	1004	CLA	C4C-CHD	3.81	1.51	1.41
19	H	1505	CLA	C4C-NC	3.80	1.38	1.35
19	3	3002	CLA	C4C-CHD	3.80	1.51	1.43
19	B	1301	CLA	C3A-C2A	-3.80	1.51	1.54
19	B	1201	CLA	C4C-NC	3.80	1.38	1.35
19	F	1302	CLA	C4B-CHC	3.79	1.51	1.41
19	J	1311	CLA	C4C-CHD	3.79	1.51	1.41
19	I	1204	CLA	C4B-CHC	3.79	1.51	1.41
19	1	1007	CLA	C4C-CHD	3.79	1.51	1.41
19	B	1222	CLA	C4C-CHD	3.79	1.51	1.41
19	L	1148	CLA	C4B-NB	-3.78	1.31	1.35
19	K	1146	CLA	C4C-CHD	3.78	1.51	1.41
21	B	6004	BCR	C10-C9	-3.78	1.30	1.35
22	4	7052	LMU	O6'-C6'	3.78	1.58	1.42
19	A	9011	CLA	C4C-CHD	3.77	1.51	1.41
19	A	9023	CLA	C4C-CHD	3.77	1.51	1.41
19	L	1148	CLA	C4C-CHD	3.77	1.51	1.41
19	2	2011	CLA	C4B-CHC	3.77	1.51	1.43
19	B	1217	CLA	C4B-CHC	3.77	1.51	1.41
19	2	2006	CLA	C4C-CHD	3.76	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	6012	BCR	C10-C9	-3.76	1.30	1.35
19	B	1216	CLA	C4C-CHD	3.76	1.51	1.41
19	2	2002	CLA	C4B-CHC	3.76	1.51	1.41
19	B	1209	CLA	C4C-CHD	3.75	1.51	1.41
19	3	3002	CLA	C4B-CHC	3.75	1.51	1.43
19	I	1204	CLA	C4C-CHD	3.75	1.51	1.41
19	4	1009	CLA	C4C-CHD	3.75	1.51	1.41
19	B	1212	CLA	C4C-CHD	3.74	1.51	1.41
21	A	6011	BCR	C21-C22	-3.74	1.30	1.35
19	4	4012	CLA	C4C-CHD	3.73	1.51	1.41
19	1	1002	CLA	C1B-NB	-3.73	1.31	1.35
19	B	1229	CLA	C4C-CHD	3.72	1.51	1.41
19	A	1126	CLA	C4C-NC	3.72	1.38	1.35
19	A	1110	CLA	C4B-CHC	3.72	1.51	1.41
19	4	4002	CLA	OBD-CAD	3.71	1.27	1.22
19	3	3014	CLA	C4C-CHD	3.71	1.51	1.43
19	B	1301	CLA	C4C-CHD	3.71	1.51	1.41
19	3	3004	CLA	C4C-CHD	3.71	1.51	1.43
19	B	1203	CLA	OBD-CAD	3.71	1.27	1.22
19	L	1148	CLA	C4B-CHC	3.70	1.51	1.41
19	3	3006	CLA	C4C-CHD	3.70	1.51	1.43
21	I	6018	BCR	C20-C21	-3.70	1.32	1.43
19	4	4014	CLA	C4C-CHD	3.70	1.51	1.41
19	A	1119	CLA	C4B-CHC	3.69	1.51	1.41
19	A	1102	CLA	C4B-CHC	3.69	1.51	1.41
19	A	1115	CLA	C4C-CHD	3.69	1.51	1.41
19	3	2009	CLA	C4C-CHD	3.69	1.51	1.41
21	3	6022	BCR	C21-C22	-3.69	1.30	1.35
19	H	1505	CLA	C4B-CHC	3.68	1.51	1.41
21	B	6005	BCR	C30-C25	-3.68	1.48	1.53
19	B	1224	CLA	C4B-CHC	3.68	1.51	1.41
21	B	6004	BCR	C21-C22	-3.68	1.30	1.35
21	J	6012	BCR	C20-C21	-3.67	1.32	1.43
19	B	1215	CLA	C4C-CHD	3.67	1.51	1.41
21	B	6005	BCR	C21-C22	-3.67	1.30	1.35
19	A	1102	CLA	C4C-NC	3.67	1.38	1.35
19	B	1208	CLA	C4B-CHC	3.67	1.51	1.41
21	B	6020	BCR	C31-C1	-3.67	1.46	1.53
19	2	2012	CLA	C4C-NC	3.66	1.38	1.35
19	1	1013	CLA	C3B-C2B	-3.66	1.35	1.40
19	B	1225	CLA	C4C-CHD	3.66	1.51	1.41
19	L	1502	CLA	C4B-CHC	3.65	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	1145	CLA	C4C-CHD	3.65	1.51	1.41
19	F	1305	CLA	C3B-C2B	-3.65	1.35	1.40
19	A	1103	CLA	OBD-CAD	3.64	1.27	1.22
21	L	6019	BCR	C10-C9	-3.64	1.31	1.35
19	L	1503	CLA	C4B-CHC	3.64	1.51	1.41
21	B	6020	BCR	C20-C21	-3.64	1.32	1.43
19	3	3015	CLA	C4C-CHD	3.64	1.51	1.43
19	1	1010	CLA	MG-NA	-3.63	1.97	2.06
19	2	2004	CLA	C4B-CHC	3.63	1.51	1.41
19	A	1116	CLA	C4B-CHC	3.63	1.51	1.41
19	4	4012	CLA	C4B-CHC	3.63	1.51	1.41
19	A	1108	CLA	C4B-CHC	3.63	1.51	1.41
19	3	3001	CLA	C4B-CHC	3.62	1.51	1.43
19	A	1125	CLA	C4C-CHD	3.62	1.51	1.41
19	B	1236	CLA	C4B-CHC	3.62	1.51	1.41
21	A	6002	BCR	C20-C21	-3.62	1.32	1.43
19	4	4012	CLA	C3A-C2A	-3.62	1.51	1.54
19	F	1240	CLA	C3A-C2A	-3.62	1.51	1.54
19	B	1301	CLA	C4B-CHC	3.62	1.51	1.41
19	2	2013	CLA	C4C-CHD	3.62	1.51	1.41
19	3	3014	CLA	MG-NA	-3.61	1.97	2.06
19	B	1236	CLA	C4C-CHD	3.61	1.51	1.41
19	L	1501	CLA	C4B-CHC	3.61	1.51	1.41
19	B	1213	CLA	C4B-CHC	3.59	1.51	1.41
19	B	1239	CLA	C4C-CHD	3.59	1.51	1.41
19	4	4002	CLA	C4C-CHD	3.59	1.51	1.41
19	4	4006	CLA	C4B-CHC	3.59	1.51	1.41
19	F	1305	CLA	C4C-CHD	3.58	1.51	1.41
19	L	1501	CLA	C4C-CHD	3.58	1.50	1.41
19	A	1123	CLA	C4C-NC	3.58	1.38	1.35
21	B	6017	BCR	C21-C22	-3.57	1.31	1.35
19	4	4001	CLA	C4B-CHC	3.57	1.50	1.41
19	A	1112	CLA	C4B-CHC	3.57	1.50	1.41
19	A	1309	CLA	C4C-CHD	3.57	1.51	1.43
19	1	1010	CLA	C4C-CHD	3.57	1.50	1.41
19	B	1235	CLA	OBD-CAD	3.56	1.27	1.22
19	1	1011	CLA	C4C-CHD	3.56	1.50	1.41
19	B	1232	CLA	C4B-CHC	3.56	1.50	1.41
19	3	3003	CLA	C4B-CHC	3.55	1.50	1.41
19	4	4005	CLA	C4B-CHC	3.55	1.51	1.43
19	B	1238	CLA	C4B-CHC	3.55	1.50	1.41
19	1	1008	CLA	C4B-CHC	3.54	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	4011	CLA	C4B-CHC	3.54	1.51	1.43
21	B	6006	BCR	C20-C21	-3.53	1.32	1.43
19	1	1012	CLA	C4C-NC	3.52	1.38	1.35
19	B	1214	CLA	C4B-CHC	3.52	1.50	1.41
19	B	1231	CLA	C4B-CHC	3.52	1.50	1.41
19	B	1226	CLA	C4C-CHD	3.52	1.50	1.41
19	1	1001	CLA	C4C-CHD	3.52	1.50	1.41
19	G	1242	CLA	C4C-NC	3.52	1.38	1.35
19	A	1113	CLA	C4B-CHC	3.51	1.50	1.41
19	A	1122	CLA	C4B-CHC	3.51	1.50	1.41
19	1	1011	CLA	MG-NA	-3.51	1.97	2.06
19	A	1126	CLA	C4B-CHC	3.51	1.50	1.41
19	4	4011	CLA	C4C-CHD	3.50	1.50	1.43
19	3	3014	CLA	C4B-CHC	3.50	1.50	1.43
19	A	9022	CLA	C4B-CHC	3.50	1.50	1.41
19	A	1140	CLA	C4B-CHC	3.49	1.50	1.41
19	2	2003	CLA	MG-NA	-3.49	1.98	2.06
19	2	2008	CLA	MG-NA	-3.48	1.98	2.06
19	A	1135	CLA	C4B-CHC	3.48	1.50	1.41
19	A	1124	CLA	C4B-CHC	3.48	1.50	1.41
19	1	1014	CLA	C4C-CHD	3.48	1.50	1.41
19	A	1107	CLA	C4C-NC	3.48	1.38	1.35
19	B	1227	CLA	C4B-CHC	3.48	1.50	1.41
19	1	1006	CLA	C4C-NC	3.48	1.38	1.35
19	1	1007	CLA	C4B-CHC	3.47	1.50	1.41
21	B	6020	BCR	C20-C19	-3.47	1.25	1.34
21	3	6022	BCR	C20-C21	-3.47	1.32	1.43
19	A	9013	CLA	C4B-CHC	3.47	1.50	1.41
21	B	6010	BCR	C10-C9	-3.47	1.31	1.35
19	2	2014	CLA	C4C-CHD	3.47	1.50	1.41
19	R	1144	CLA	C4B-CHC	3.46	1.50	1.41
19	H	1241	CLA	C4B-CHC	3.46	1.50	1.41
19	2	2006	CLA	C4B-CHC	3.46	1.50	1.41
19	J	1308	CLA	C4C-CHD	3.45	1.50	1.41
21	B	6017	BCR	C32-C1	3.45	1.60	1.53
19	4	4001	CLA	C4C-NC	3.45	1.38	1.35
19	K	1142	CLA	C4B-CHC	3.45	1.50	1.41
21	F	6016	BCR	C32-C1	-3.45	1.47	1.53
19	B	1206	CLA	C4B-CHC	3.45	1.50	1.41
19	B	1223	CLA	C4B-CHC	3.44	1.50	1.41
19	3	3003	CLA	C4C-NC	3.44	1.38	1.35
19	L	1503	CLA	C4C-NC	3.43	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	1307	CLA	C4C-CHD	3.43	1.50	1.43
19	A	1115	CLA	C4B-CHC	3.43	1.50	1.41
22	2	7031	LMU	O1'-C1'	3.43	1.46	1.40
19	2	2001	CLA	C4B-CHC	3.42	1.50	1.41
19	3	3016	CLA	C4B-CHC	3.42	1.50	1.41
19	A	9012	CLA	C4B-CHC	3.42	1.50	1.41
19	A	1106	CLA	C4B-CHC	3.42	1.50	1.41
19	1	1006	CLA	C4B-CHC	3.41	1.50	1.41
19	B	1220	CLA	C4B-CHC	3.41	1.50	1.41
19	4	4002	CLA	MG-NA	-3.41	1.98	2.06
19	4	4013	CLA	C4B-CHC	3.41	1.50	1.43
19	3	3015	CLA	C4B-CHC	3.41	1.50	1.43
21	B	6017	BCR	C30-C25	-3.40	1.49	1.53
19	A	1141	CLA	C4B-CHC	3.40	1.50	1.41
21	F	6014	BCR	C30-C25	-3.40	1.49	1.53
19	B	1218	CLA	C4B-CHC	3.39	1.50	1.41
19	L	1504	CLA	C4B-CHC	3.39	1.50	1.41
19	A	1103	CLA	C4C-NC	3.39	1.38	1.35
19	3	1118	CLA	C4B-CHC	3.39	1.50	1.41
19	3	2009	CLA	C4B-CHC	3.39	1.50	1.41
19	1	1001	CLA	C1B-NB	-3.38	1.32	1.35
19	4	1009	CLA	C4B-CHC	3.38	1.50	1.41
19	1	1005	CLA	C4B-CHC	3.38	1.50	1.41
19	4	4014	CLA	C4B-CHC	3.38	1.50	1.41
19	3	3013	CLA	C4C-CHD	3.38	1.50	1.41
19	3	3010	CLA	C4C-CHD	3.38	1.50	1.43
19	4	4013	CLA	C4C-CHD	3.37	1.50	1.43
19	2	2011	CLA	C4C-CHD	3.37	1.50	1.43
19	A	1137	CLA	C4B-CHC	3.37	1.50	1.41
19	J	1311	CLA	C4B-CHC	3.37	1.50	1.41
19	B	1208	CLA	C4C-NC	3.37	1.38	1.35
19	F	1240	CLA	C4B-CHC	3.36	1.50	1.41
19	3	3006	CLA	C4B-CHC	3.36	1.50	1.43
19	2	2008	CLA	C4C-CHD	3.36	1.50	1.43
19	B	1222	CLA	C4B-CHC	3.36	1.50	1.41
19	B	9010	CLA	C4B-CHC	3.36	1.50	1.41
19	1	1014	CLA	C4B-CHC	3.35	1.50	1.41
19	F	1305	CLA	C4B-CHC	3.35	1.50	1.41
21	J	6012	BCR	C30-C25	-3.35	1.49	1.53
19	B	1220	CLA	C4C-CHD	3.34	1.50	1.41
19	L	1130	CLA	C4B-CHC	3.34	1.50	1.41
19	1	1007	CLA	C4C-NC	3.34	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	4015	CLA	C4C-CHD	3.34	1.50	1.41
19	1	1003	CLA	C4C-NC	3.34	1.38	1.35
19	A	1125	CLA	C4B-CHC	3.33	1.50	1.41
19	B	1225	CLA	C4B-CHC	3.32	1.50	1.41
19	A	1112	CLA	C4C-NC	3.32	1.38	1.35
19	3	3008	CLA	C4B-CHC	3.32	1.50	1.41
19	4	4007	CLA	C4B-CHC	3.32	1.50	1.41
19	H	1207	CLA	C4B-CHC	3.32	1.50	1.41
19	A	1109	CLA	C4B-CHC	3.32	1.50	1.41
19	A	1138	CLA	C4B-CHC	3.31	1.50	1.41
19	2	2012	CLA	C4B-CHC	3.31	1.50	1.41
19	A	1112	CLA	C3B-C2B	-3.31	1.35	1.40
19	1	1013	CLA	C4C-CHD	3.31	1.50	1.41
19	K	1146	CLA	C4B-CHC	3.31	1.50	1.41
19	B	1219	CLA	C4B-CHC	3.31	1.50	1.41
19	A	1136	CLA	C4B-CHC	3.31	1.50	1.41
19	2	2013	CLA	C4B-CHC	3.31	1.50	1.41
19	2	2006	CLA	C4C-NC	3.31	1.38	1.35
19	A	1134	CLA	C4B-CHC	3.30	1.50	1.41
19	4	4010	CLA	C4B-CHC	3.30	1.50	1.43
21	A	6011	BCR	C30-C25	-3.30	1.49	1.53
19	2	2014	CLA	C4B-CHC	3.30	1.50	1.41
19	A	1151	CLA	C4B-CHC	3.30	1.50	1.41
19	L	1148	CLA	C3A-C2A	-3.29	1.45	1.54
19	A	1128	CLA	C4B-CHC	3.29	1.50	1.41
19	A	1105	CLA	C4B-CHC	3.29	1.50	1.41
19	2	4009	CLA	C4B-CHC	3.29	1.50	1.41
19	4	1004	CLA	C4B-CHC	3.29	1.50	1.41
19	B	1211	CLA	C4B-CHC	3.28	1.50	1.41
19	A	1123	CLA	C4B-CHC	3.28	1.50	1.41
21	A	6011	BCR	C10-C9	-3.28	1.31	1.35
19	A	1139	CLA	C4B-CHC	3.28	1.50	1.41
21	A	6003	BCR	C10-C9	-3.28	1.31	1.35
19	B	1228	CLA	C4B-CHC	3.27	1.50	1.41
19	B	1201	CLA	C4B-CHC	3.27	1.50	1.41
19	A	1127	CLA	C4B-CHC	3.26	1.50	1.41
19	A	1133	CLA	C4B-CHC	3.26	1.50	1.41
19	K	3009	CLA	C4C-NC	3.26	1.38	1.35
19	4	1304	CLA	C3B-C2B	-3.25	1.35	1.40
19	A	1104	CLA	C4B-CHC	3.25	1.50	1.41
19	A	1129	CLA	C4B-CHC	3.25	1.50	1.41
19	3	3017	CLA	C1B-NB	-3.24	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	4003	CLA	C4B-CHC	3.24	1.50	1.41
19	B	1230	CLA	C4B-CHC	3.24	1.50	1.41
19	B	1209	CLA	C4B-CHC	3.24	1.50	1.41
19	K	1143	CLA	C4B-CHC	3.24	1.50	1.41
19	L	1148	CLA	C3D-CAD	-3.24	1.37	1.46
21	I	6021	BCR	C26-C25	-3.24	1.28	1.34
19	B	1205	CLA	C4B-CHC	3.23	1.50	1.41
19	B	1216	CLA	C4B-CHC	3.23	1.50	1.41
19	A	1111	CLA	C4B-CHC	3.23	1.50	1.41
19	A	1237	CLA	C4B-CHC	3.23	1.50	1.41
19	B	1215	CLA	C4B-CHC	3.23	1.50	1.41
19	B	1220	CLA	MG-NA	-3.22	1.98	2.06
19	2	2010	CLA	C4B-CHC	3.22	1.50	1.43
22	4	7019	LMU	O1'-C1'	3.22	1.45	1.40
19	3	3011	CLA	C4B-CHC	3.21	1.49	1.41
19	A	9022	CLA	C4C-NC	3.21	1.38	1.35
19	3	3005	CLA	C4B-CHC	3.21	1.50	1.43
19	2	1307	CLA	MG-NA	-3.21	1.98	2.06
19	B	1220	CLA	C3B-C2B	-3.21	1.35	1.40
19	L	1148	CLA	CMA-C3A	3.20	1.60	1.53
19	I	1204	CLA	OBD-CAD	3.20	1.26	1.22
19	A	1105	CLA	C4C-NC	3.20	1.38	1.35
19	B	1226	CLA	C3D-CAD	-3.20	1.38	1.46
19	2	2005	CLA	C4B-CHC	3.20	1.50	1.43
19	A	1129	CLA	C4C-NC	3.20	1.38	1.35
19	B	1224	CLA	C4C-NC	3.20	1.38	1.35
19	3	3007	CLA	C4B-CHC	3.19	1.49	1.41
22	A	7010	LMU	O1'-C1'	3.19	1.45	1.40
19	4	4011	CLA	MG-NA	-3.19	1.98	2.06
19	B	1221	CLA	C4B-CHC	3.19	1.49	1.41
19	4	1304	CLA	C4C-NC	3.19	1.38	1.35
19	4	4015	CLA	C4B-CHC	3.19	1.49	1.41
19	A	1120	CLA	C4C-NC	3.18	1.38	1.35
19	B	1202	CLA	C4C-NC	3.18	1.38	1.35
19	J	1308	CLA	C3D-CAD	-3.17	1.38	1.46
19	2	2010	CLA	MG-NA	-3.17	1.98	2.06
19	1	1010	CLA	C3B-C2B	-3.17	1.36	1.40
19	B	1233	CLA	C4C-NC	3.17	1.38	1.35
19	A	1131	CLA	C4B-CHC	3.16	1.49	1.41
19	4	4004	CLA	C4B-CHC	3.16	1.50	1.43
19	K	1146	CLA	MG-NA	-3.16	1.98	2.06
19	A	1117	CLA	C4B-CHC	3.16	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1015	CLA	C4B-CHC	3.16	1.50	1.43
19	1	1001	CLA	C3D-CAD	-3.16	1.38	1.46
19	3	3013	CLA	C3D-CAD	-3.15	1.38	1.46
19	A	1113	CLA	C4C-NC	3.15	1.38	1.35
19	J	1308	CLA	C4B-CHC	3.15	1.49	1.41
19	1	1010	CLA	C3D-CAD	-3.15	1.38	1.46
19	A	9023	CLA	C4B-CHC	3.15	1.49	1.41
21	A	6011	BCR	C8-C7	3.15	1.42	1.33
19	2	2003	CLA	C4B-CHC	3.14	1.50	1.43
19	4	1304	CLA	C1B-NB	-3.13	1.32	1.35
19	B	1239	CLA	C4B-CHC	3.13	1.49	1.41
19	1	1008	CLA	C2A-C1A	-3.13	1.45	1.52
19	4	4004	CLA	MG-NA	-3.13	1.98	2.06
21	A	6008	BCR	C30-C25	-3.12	1.49	1.53
19	A	9011	CLA	C3B-C2B	-3.11	1.36	1.40
19	A	1101	CLA	C4B-CHC	3.11	1.49	1.41
19	H	1145	CLA	C4B-CHC	3.11	1.49	1.41
19	A	1149	CLA	C4B-CHC	3.10	1.49	1.41
19	B	1220	CLA	C3D-CAD	-3.10	1.38	1.46
19	2	2007	CLA	C4B-CHC	3.10	1.49	1.41
19	A	1122	CLA	C4C-NC	3.10	1.38	1.35
19	3	3012	CLA	MG-NA	-3.10	1.98	2.06
21	L	6019	BCR	C17-C18	-3.10	1.31	1.35
19	A	1309	CLA	C4B-CHC	3.10	1.50	1.43
22	4	7009	LMU	O1'-C1'	3.09	1.45	1.40
21	1	6023	BCR	C11-C12	-3.09	1.26	1.34
21	F	6014	BCR	C40-C30	3.09	1.59	1.53
19	4	4005	CLA	C4C-NC	3.09	1.38	1.35
19	B	1203	CLA	MG-NA	-3.09	1.98	2.06
19	A	1309	CLA	MG-NA	-3.09	1.98	2.06
21	A	6002	BCR	C21-C22	-3.08	1.31	1.35
19	2	2005	CLA	C4C-CHD	3.08	1.50	1.43
19	H	1145	CLA	MG-NA	-3.07	1.99	2.06
19	2	2002	CLA	C4C-NC	3.07	1.37	1.35
19	A	1121	CLA	C4B-CHC	3.07	1.49	1.41
19	2	2008	CLA	CHA-C1A	3.07	1.50	1.41
19	4	1009	CLA	C4C-NC	3.07	1.37	1.35
19	J	1308	CLA	MG-NA	-3.06	1.99	2.06
19	1	1013	CLA	C1B-NB	-3.06	1.32	1.35
19	3	3008	CLA	C3D-CAD	-3.06	1.38	1.46
19	3	3006	CLA	CHA-C1A	3.06	1.50	1.41
19	1	1310	CLA	C4B-CHC	3.06	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1116	CLA	C4C-NC	3.05	1.37	1.35
19	B	1202	CLA	C4B-CHC	3.05	1.49	1.41
19	2	2005	CLA	MG-NA	-3.05	1.99	2.06
19	3	3010	CLA	MG-NA	-3.05	1.99	2.06
19	2	2008	CLA	C4B-CHC	3.05	1.50	1.43
19	R	1150	CLA	C4C-NC	3.04	1.37	1.35
21	A	6003	BCR	C30-C25	-3.04	1.49	1.53
21	I	6018	BCR	C30-C25	-3.03	1.49	1.53
19	B	1234	CLA	C3D-CAD	-3.03	1.38	1.46
21	B	6020	BCR	C11-C12	-3.03	1.26	1.34
19	4	4006	CLA	C4C-NC	3.02	1.37	1.35
19	4	4010	CLA	MG-NA	-3.02	1.99	2.06
22	G	7051	LMU	O1'-C1'	3.02	1.45	1.40
19	A	1109	CLA	C4C-NC	3.02	1.37	1.35
19	B	1214	CLA	C4C-NC	3.01	1.37	1.35
19	3	3014	CLA	CHB-C4A	-3.01	1.32	1.34
19	1	1011	CLA	C4B-CHC	3.01	1.49	1.41
19	A	1132	CLA	C4C-NC	3.01	1.37	1.35
21	B	6020	BCR	C2-C1	-3.00	1.47	1.54
19	A	1132	CLA	C4B-CHC	3.00	1.49	1.41
19	1	1013	CLA	C3D-C2D	-3.00	1.34	1.39
19	4	4005	CLA	MG-NA	-2.99	1.99	2.06
21	L	6019	BCR	C31-C1	-2.99	1.47	1.53
19	A	1119	CLA	C4C-NC	2.98	1.37	1.35
19	1	1002	CLA	C4B-CHC	2.98	1.49	1.41
19	3	3010	CLA	C4B-CHC	2.98	1.49	1.43
19	2	2011	CLA	MG-NA	-2.97	1.99	2.06
19	3	3001	CLA	CHA-C1A	2.97	1.49	1.41
19	3	3001	CLA	MG-NA	-2.97	1.99	2.06
19	3	2009	CLA	C3D-CAD	-2.97	1.38	1.46
19	2	2004	CLA	C4C-NC	2.96	1.37	1.35
19	B	1226	CLA	C4B-CHC	2.96	1.49	1.41
19	2	2013	CLA	C3D-CAD	-2.96	1.38	1.46
19	3	3012	CLA	CHA-C1A	2.96	1.49	1.41
19	F	1305	CLA	CAA-C2A	-2.96	1.48	1.54
19	3	3011	CLA	C4C-NC	2.95	1.37	1.35
19	3	3005	CLA	CHA-C1A	2.95	1.49	1.41
19	1	1011	CLA	C3D-CAD	-2.95	1.38	1.46
19	4	1306	CLA	C4B-CHC	2.95	1.49	1.41
19	3	3006	CLA	MG-NA	-2.94	1.99	2.06
21	L	6019	BCR	C24-C23	2.94	1.42	1.33
19	3	1147	CLA	MG-NA	-2.94	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	4015	CLA	C3B-C2B	-2.94	1.36	1.40
19	4	4015	CLA	C3D-CAD	-2.94	1.38	1.46
19	1	1310	CLA	C1B-NB	-2.94	1.32	1.35
21	B	6004	BCR	C30-C25	-2.93	1.49	1.53
19	A	1103	CLA	C4B-CHC	2.93	1.49	1.41
19	R	1144	CLA	C4C-NC	2.93	1.37	1.35
21	B	6006	BCR	C10-C9	-2.93	1.31	1.35
19	A	1117	CLA	C3B-C2B	-2.93	1.36	1.40
19	A	1121	CLA	C4C-NC	2.91	1.37	1.35
21	I	6021	BCR	C32-C1	-2.91	1.48	1.53
19	R	1150	CLA	C1B-CHB	2.91	1.49	1.41
19	I	1204	CLA	C4C-NC	2.90	1.37	1.35
19	B	1225	CLA	C1B-CHB	2.90	1.49	1.41
19	3	3013	CLA	C4B-CHC	2.89	1.49	1.41
19	A	1149	CLA	C4C-NC	2.89	1.37	1.35
19	1	1002	CLA	C4C-NC	2.89	1.37	1.35
19	H	1145	CLA	C3D-CAD	-2.89	1.38	1.46
19	B	1234	CLA	C4B-CHC	2.87	1.49	1.41
19	F	1305	CLA	C1B-NB	-2.87	1.32	1.35
19	1	1003	CLA	C3D-CAD	-2.86	1.38	1.46
19	B	1230	CLA	C3D-CAD	-2.86	1.38	1.46
19	4	4014	CLA	C3D-CAD	-2.86	1.38	1.46
19	3	3017	CLA	C3D-CAD	-2.86	1.38	1.46
19	L	1503	CLA	CMA-C3A	2.85	1.59	1.53
19	L	1504	CLA	C1B-CHB	2.85	1.48	1.41
19	L	1148	CLA	MG-NA	-2.84	1.99	2.06
19	B	1229	CLA	C4C-NC	2.84	1.37	1.35
21	B	6020	BCR	C11-C10	2.84	1.52	1.43
22	4	7052	LMU	O1'-C1'	2.84	1.45	1.40
19	B	1218	CLA	C3D-CAD	-2.84	1.38	1.46
19	1	1013	CLA	C4B-CHC	2.83	1.48	1.41
22	A	7044	LMU	O1'-C1'	2.83	1.45	1.40
19	B	1229	CLA	C3D-CAD	-2.83	1.38	1.46
19	H	1207	CLA	C3D-CAD	-2.83	1.38	1.46
19	L	1501	CLA	C1B-CHB	2.83	1.48	1.41
19	B	1238	CLA	C4C-NC	2.83	1.37	1.35
19	L	1148	CLA	C3B-C2B	-2.83	1.36	1.40
21	3	6022	BCR	C10-C9	-2.83	1.32	1.35
19	4	4002	CLA	C1C-C2C	-2.83	1.36	1.42
21	F	6014	BCR	C10-C9	-2.82	1.32	1.35
19	B	1235	CLA	C4B-CHC	2.81	1.48	1.41
19	A	1121	CLA	C1B-CHB	2.81	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1006	CLA	C3A-C2A	-2.81	1.51	1.54
19	B	1203	CLA	C3B-C2B	-2.81	1.36	1.40
19	2	1307	CLA	C4B-CHC	2.81	1.49	1.43
19	A	1115	CLA	C3B-C2B	-2.80	1.36	1.40
19	I	1204	CLA	C3D-CAD	-2.80	1.39	1.46
19	A	1127	CLA	C4C-NC	2.80	1.37	1.35
19	4	4013	CLA	CHA-C1A	2.80	1.49	1.41
19	B	1236	CLA	C4C-NC	2.80	1.37	1.35
19	1	1013	CLA	C1B-CHB	2.80	1.48	1.41
19	B	1226	CLA	MG-NA	-2.79	1.99	2.06
19	1	1015	CLA	MG-NA	-2.78	1.99	2.06
19	4	1304	CLA	C4B-CHC	2.78	1.48	1.41
21	F	6016	BCR	C10-C9	-2.78	1.32	1.35
19	4	4001	CLA	C1B-CHB	2.78	1.48	1.41
19	B	1203	CLA	C4B-CHC	2.78	1.48	1.41
19	B	1206	CLA	C4C-NC	2.77	1.37	1.35
19	1	1011	CLA	C1C-C2C	-2.77	1.36	1.42
19	1	1014	CLA	C3D-CAD	-2.77	1.39	1.46
19	B	1212	CLA	C4C-NC	2.77	1.37	1.35
19	4	4014	CLA	MG-NA	-2.77	1.99	2.06
19	2	2014	CLA	C1B-NB	-2.77	1.32	1.35
19	K	1146	CLA	C1C-C2C	-2.76	1.36	1.42
19	4	4002	CLA	C3D-CAD	-2.76	1.39	1.46
19	1	1001	CLA	MG-NA	-2.76	1.99	2.06
19	B	1216	CLA	C1B-CHB	2.76	1.48	1.41
19	R	1144	CLA	C3D-CAD	-2.75	1.39	1.46
19	B	1222	CLA	C3D-CAD	-2.75	1.39	1.46
21	B	6005	BCR	C20-C21	-2.74	1.34	1.43
19	3	3012	CLA	C4B-CHC	2.74	1.49	1.43
19	A	1237	CLA	C1B-CHB	2.74	1.48	1.41
19	1	1015	CLA	CHA-C1A	2.74	1.49	1.41
19	3	3007	CLA	C1B-CHB	2.74	1.48	1.41
19	B	1228	CLA	C4C-NC	2.73	1.37	1.35
22	H	7032	LMU	O1'-C1'	2.73	1.44	1.40
19	3	3004	CLA	CHB-C4A	-2.73	1.32	1.34
19	B	1234	CLA	C1B-CHB	2.73	1.48	1.41
19	2	2007	CLA	C4C-NC	2.73	1.37	1.35
19	4	1004	CLA	C5-C3	2.72	1.56	1.51
19	A	1108	CLA	C4C-NC	2.72	1.37	1.35
19	3	3010	CLA	CHA-C1A	2.72	1.49	1.41
19	3	3015	CLA	CHA-C1A	2.71	1.49	1.41
19	2	2011	CLA	CHA-C1A	2.71	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1115	CLA	C3D-CAD	-2.71	1.39	1.46
19	F	1305	CLA	C2A-C1A	-2.71	1.46	1.52
19	4	4004	CLA	CHA-C1A	2.71	1.49	1.41
19	B	1224	CLA	C3D-CAD	-2.71	1.39	1.46
21	F	6014	BCR	C20-C21	-2.71	1.35	1.43
19	3	3015	CLA	MG-NA	-2.71	1.99	2.06
22	R	7025	LMU	O1'-C1'	2.70	1.44	1.40
19	3	3005	CLA	MG-NA	-2.70	1.99	2.06
19	1	1007	CLA	C1B-CHB	2.70	1.48	1.41
19	3	1147	CLA	O2A-CGA	2.70	1.41	1.33
19	4	4002	CLA	C4B-CHC	2.70	1.48	1.41
19	4	4007	CLA	C1B-CHB	2.70	1.48	1.41
19	3	3002	CLA	MG-NA	-2.69	1.99	2.06
19	3	3017	CLA	C4B-CHC	2.69	1.48	1.41
21	B	6006	BCR	C23-C22	2.69	1.51	1.45
19	4	1304	CLA	MG-NA	-2.69	1.99	2.06
19	1	1010	CLA	C4B-CHC	2.68	1.48	1.41
19	F	1240	CLA	C4C-NC	2.68	1.37	1.35
19	A	1128	CLA	C3D-CAD	-2.68	1.39	1.46
21	F	6016	BCR	C39-C30	2.68	1.59	1.53
19	B	1232	CLA	C4C-NC	2.68	1.37	1.35
19	4	4006	CLA	C1B-CHB	2.67	1.48	1.41
19	1	1303	CLA	C4B-CHC	2.67	1.48	1.41
19	A	1237	CLA	C3D-CAD	-2.66	1.39	1.46
19	1	1303	CLA	C1C-C2C	-2.66	1.36	1.42
19	2	1307	CLA	CHA-C1A	2.66	1.48	1.41
22	2	7046	LMU	O1'-C1'	2.65	1.44	1.40
19	B	1206	CLA	C3D-CAD	-2.65	1.39	1.46
19	3	3002	CLA	CHA-C1A	2.65	1.48	1.41
19	A	1149	CLA	C1B-CHB	2.65	1.48	1.41
19	A	9012	CLA	C4C-NC	2.65	1.37	1.35
19	A	1115	CLA	MG-NA	-2.64	2.00	2.06
19	2	1307	CLA	C1B-NB	-2.64	1.32	1.35
19	A	1117	CLA	C4C-NC	2.64	1.37	1.35
19	L	1503	CLA	C3D-CAD	-2.64	1.39	1.46
19	B	1234	CLA	C4C-NC	2.64	1.37	1.35
19	1	1005	CLA	C3D-CAD	-2.63	1.39	1.46
19	4	4015	CLA	MG-NA	-2.63	2.00	2.06
19	2	4009	CLA	C3D-CAD	-2.63	1.39	1.46
19	A	1107	CLA	C4B-CHC	2.62	1.48	1.41
19	B	1211	CLA	C4C-NC	2.62	1.37	1.35
19	1	1008	CLA	C3D-CAD	-2.62	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	7029	LMU	O1'-C1'	2.61	1.44	1.40
19	A	1123	CLA	C3D-CAD	-2.61	1.39	1.46
19	A	9023	CLA	MG-NA	-2.60	2.00	2.06
19	A	1101	CLA	C1B-CHB	2.60	1.48	1.41
19	A	1127	CLA	C3B-C2B	-2.60	1.36	1.40
19	4	1304	CLA	C1C-C2C	-2.60	1.36	1.42
19	K	1142	CLA	C4C-NC	2.60	1.37	1.35
19	3	3003	CLA	C3A-C2A	-2.60	1.52	1.54
19	K	3009	CLA	C1B-CHB	2.60	1.48	1.41
19	B	1202	CLA	MG-NA	-2.60	2.00	2.06
19	3	3014	CLA	CHA-C1A	2.59	1.48	1.41
19	3	1118	CLA	C1B-CHB	2.59	1.48	1.41
19	3	3013	CLA	C1B-CHB	2.59	1.48	1.41
19	A	1128	CLA	C3B-C2B	-2.59	1.36	1.40
19	A	1149	CLA	C3D-CAD	-2.58	1.39	1.46
19	4	4015	CLA	C1B-CHB	2.58	1.48	1.41
21	B	6020	BCR	C14-C13	-2.58	1.32	1.35
19	B	1233	CLA	C1B-CHB	2.58	1.48	1.41
19	B	1219	CLA	C4C-NC	2.58	1.37	1.35
21	I	6021	BCR	C21-C22	-2.58	1.32	1.35
19	H	1505	CLA	C1B-CHB	2.57	1.48	1.41
19	B	1221	CLA	C3D-CAD	-2.57	1.39	1.46
19	1	1006	CLA	C1B-CHB	2.57	1.48	1.41
19	A	1125	CLA	C3D-CAD	-2.57	1.39	1.46
19	A	1105	CLA	C1B-CHB	2.57	1.48	1.41
19	1	1005	CLA	MG-NA	-2.56	2.00	2.06
22	H	7043	LMU	O1'-C1'	2.56	1.44	1.40
22	K	7047	LMU	O1'-C1'	2.56	1.44	1.40
19	A	1124	CLA	C4C-NC	2.56	1.37	1.35
19	A	1133	CLA	C4C-NC	2.56	1.37	1.35
22	4	7052	LMU	O1'-C1	2.56	1.50	1.43
19	4	4010	CLA	CHA-C1A	2.56	1.48	1.41
19	4	1004	CLA	C3D-CAD	-2.56	1.39	1.46
19	A	1139	CLA	MG-NA	-2.56	2.00	2.06
19	A	1103	CLA	C3B-C2B	-2.55	1.36	1.40
19	A	1106	CLA	C3B-C2B	-2.55	1.36	1.40
19	2	2012	CLA	C1B-CHB	2.55	1.48	1.41
19	1	1010	CLA	C3D-C2D	-2.55	1.34	1.39
19	2	2013	CLA	C1B-NB	-2.54	1.32	1.35
19	A	1107	CLA	C1B-CHB	2.54	1.48	1.41
19	B	1215	CLA	C3D-CAD	-2.54	1.39	1.46
19	F	1302	CLA	C3D-CAD	-2.54	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	7009	LMU	O6'-C6'	2.54	1.53	1.42
19	A	1129	CLA	C3D-CAD	-2.54	1.39	1.46
19	B	1219	CLA	C1B-NB	-2.54	1.32	1.35
19	2	4009	CLA	C1B-CHB	2.53	1.48	1.41
19	K	1142	CLA	MG-NA	-2.53	2.00	2.06
19	B	1238	CLA	MG-NA	-2.53	2.00	2.06
19	1	1014	CLA	MG-NA	-2.53	2.00	2.06
19	A	1134	CLA	C3D-CAD	-2.53	1.39	1.46
21	A	6007	BCR	C21-C22	-2.53	1.32	1.35
19	B	1215	CLA	C1B-CHB	2.52	1.48	1.41
19	A	1107	CLA	C1C-C2C	-2.52	1.36	1.42
19	B	1221	CLA	C3B-C2B	-2.52	1.36	1.40
19	B	1216	CLA	C3D-CAD	-2.52	1.39	1.46
19	A	1141	CLA	MG-NA	-2.52	2.00	2.06
22	4	7018	LMU	O1'-C1'	2.52	1.44	1.40
19	2	2010	CLA	CHA-C1A	2.51	1.48	1.41
19	2	2006	CLA	C3D-CAD	-2.51	1.39	1.46
19	A	1125	CLA	MG-NA	-2.51	2.00	2.06
19	B	1301	CLA	C1B-CHB	2.51	1.48	1.41
21	F	6016	BCR	C17-C18	-2.51	1.32	1.35
19	A	1309	CLA	CHA-C1A	2.51	1.48	1.41
19	A	9013	CLA	MG-NA	-2.51	2.00	2.06
19	2	2006	CLA	C1B-CHB	2.51	1.48	1.41
19	A	1237	CLA	C4C-NC	2.51	1.37	1.35
19	A	1109	CLA	C3B-C2B	-2.50	1.36	1.40
19	B	1225	CLA	C3D-CAD	-2.50	1.39	1.46
19	B	1239	CLA	C3D-CAD	-2.50	1.39	1.46
19	B	1217	CLA	C4C-NC	2.50	1.37	1.35
19	R	1144	CLA	C1B-CHB	2.50	1.47	1.41
19	A	1116	CLA	C1B-CHB	2.50	1.47	1.41
21	I	6021	BCR	C31-C1	-2.50	1.48	1.53
19	B	1206	CLA	C1B-NB	-2.50	1.33	1.35
22	G	7026	LMU	O1'-C1'	2.49	1.44	1.40
19	3	3017	CLA	MG-NA	-2.49	2.00	2.06
19	A	1115	CLA	C1B-NB	-2.49	1.33	1.35
19	4	4002	CLA	C3A-C2A	-2.49	1.47	1.54
22	G	7026	LMU	O3B-C3B	2.49	1.48	1.43
19	3	1147	CLA	C4C-CHD	2.49	1.47	1.41
19	B	1232	CLA	C3D-CAD	-2.49	1.39	1.46
19	A	1132	CLA	C3D-CAD	-2.49	1.39	1.46
19	1	1005	CLA	C4C-NC	2.49	1.37	1.35
19	B	1213	CLA	C4C-NC	2.49	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1222	CLA	C1B-CHB	2.49	1.47	1.41
19	K	1146	CLA	C3D-CAD	-2.48	1.39	1.46
19	A	1131	CLA	C3D-CAD	-2.48	1.39	1.46
19	A	1116	CLA	C3D-CAD	-2.48	1.39	1.46
19	B	1235	CLA	C1B-CHB	2.48	1.47	1.41
19	B	1213	CLA	C1B-CHB	2.47	1.47	1.41
19	B	1210	CLA	C4C-NC	2.47	1.37	1.35
19	3	3015	CLA	C1B-CHB	2.47	1.48	1.43
19	L	1504	CLA	C4C-NC	2.47	1.37	1.35
19	B	1228	CLA	C3D-CAD	-2.47	1.39	1.46
22	R	7014	LMU	O2B-C2B	2.47	1.48	1.43
19	A	1106	CLA	C3D-CAD	-2.47	1.39	1.46
19	2	2014	CLA	C3D-CAD	-2.47	1.39	1.46
19	1	1012	CLA	C1B-CHB	2.47	1.47	1.41
19	4	4014	CLA	C3B-CAB	-2.46	1.42	1.47
19	A	9012	CLA	C3D-CAD	-2.46	1.39	1.46
19	B	1239	CLA	C1B-CHB	2.46	1.47	1.41
19	B	1209	CLA	C3D-CAD	-2.46	1.39	1.46
19	B	1201	CLA	C3B-C2B	-2.46	1.37	1.40
19	2	1307	CLA	CHB-C4A	-2.46	1.32	1.34
19	2	2001	CLA	C4C-NC	2.46	1.37	1.35
19	4	4003	CLA	C4C-NC	2.46	1.37	1.35
19	2	2005	CLA	CHA-C1A	2.46	1.48	1.41
19	A	1124	CLA	C3D-CAD	-2.45	1.39	1.46
19	L	1501	CLA	C4C-NC	2.45	1.37	1.35
22	A	7045	LMU	O1'-C1'	2.45	1.44	1.40
21	F	6016	BCR	C20-C19	-2.45	1.28	1.34
19	1	1008	CLA	C1B-CHB	2.45	1.47	1.41
19	B	1236	CLA	C1B-CHB	2.45	1.47	1.41
19	K	1143	CLA	C4C-NC	2.45	1.37	1.35
22	H	7030	LMU	O6B-C6B	2.45	1.52	1.42
19	2	2003	CLA	CHA-C1A	2.45	1.48	1.41
19	4	1009	CLA	C3D-CAD	-2.45	1.39	1.46
19	A	1136	CLA	C3D-CAD	-2.44	1.39	1.46
19	A	1134	CLA	MG-NA	-2.44	2.00	2.06
19	A	9012	CLA	C1B-NB	-2.44	1.33	1.35
19	3	3017	CLA	C1C-C2C	-2.44	1.37	1.42
19	B	1221	CLA	C4C-NC	2.43	1.37	1.35
19	4	4011	CLA	C4C-NC	2.43	1.37	1.35
21	A	6002	BCR	C30-C25	-2.43	1.50	1.53
21	L	6019	BCR	C2-C1	-2.43	1.48	1.54
19	B	1205	CLA	C4C-NC	2.43	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	7012	LMU	O1'-C1'	2.43	1.44	1.40
19	3	3008	CLA	MG-NA	-2.43	2.00	2.06
19	3	1118	CLA	C4C-NC	2.42	1.37	1.35
19	A	1103	CLA	C1B-CHB	2.42	1.47	1.41
19	B	1238	CLA	C4B-NB	2.42	1.37	1.35
19	3	3010	CLA	C1B-NB	-2.42	1.33	1.35
21	I	6021	BCR	C11-C10	2.42	1.50	1.43
21	L	6019	BCR	C20-C19	-2.42	1.28	1.34
19	A	1124	CLA	MG-NA	-2.42	2.00	2.06
19	A	1122	CLA	C3D-CAD	-2.42	1.39	1.46
19	1	1013	CLA	CBD-CGD	-2.42	1.44	1.52
19	B	1226	CLA	C1B-CHB	2.41	1.47	1.41
19	B	1223	CLA	C3D-CAD	-2.41	1.39	1.46
21	B	6006	BCR	C30-C25	-2.41	1.50	1.53
19	A	1131	CLA	MG-NA	-2.41	2.00	2.06
19	3	3003	CLA	C1B-CHB	2.41	1.47	1.41
19	A	1125	CLA	C1B-CHB	2.41	1.47	1.41
19	B	1217	CLA	C1B-CHB	2.41	1.47	1.41
19	J	1311	CLA	C4C-NC	2.41	1.37	1.35
21	L	6019	BCR	C20-C21	-2.40	1.36	1.43
19	J	1311	CLA	C3D-CAD	-2.40	1.40	1.46
21	F	6014	BCR	C21-C22	-2.40	1.32	1.35
19	H	1505	CLA	C3D-CAD	-2.40	1.40	1.46
19	B	1201	CLA	MG-NA	-2.40	2.00	2.06
19	B	1217	CLA	C3D-CAD	-2.40	1.40	1.46
19	A	1113	CLA	C1B-CHB	2.39	1.47	1.41
19	1	1003	CLA	C1B-CHB	2.39	1.47	1.41
19	A	1131	CLA	C4C-NC	2.39	1.37	1.35
19	B	1232	CLA	C1B-CHB	2.39	1.47	1.41
19	1	1303	CLA	MG-NA	-2.39	2.00	2.06
19	4	1009	CLA	CBD-CHA	-2.39	1.48	1.51
19	2	2007	CLA	C1B-CHB	2.39	1.47	1.41
19	A	1137	CLA	C3D-CAD	-2.38	1.40	1.46
19	A	1133	CLA	C3D-CAD	-2.38	1.40	1.46
19	1	1001	CLA	O1D-CGD	2.38	1.27	1.21
19	A	1129	CLA	C1B-CHB	2.38	1.47	1.41
19	A	1138	CLA	C4C-NC	2.37	1.37	1.35
19	A	1138	CLA	C1B-CHB	2.37	1.47	1.41
19	B	1301	CLA	C3D-CAD	-2.37	1.40	1.46
19	2	2002	CLA	C3D-CAD	-2.37	1.40	1.46
19	A	1136	CLA	MG-NA	-2.37	2.00	2.06
19	A	1120	CLA	C3D-CAD	-2.37	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1230	CLA	C1B-CHB	2.37	1.47	1.41
19	B	1210	CLA	MG-NA	-2.37	2.00	2.06
21	L	6019	BCR	C30-C25	-2.36	1.50	1.53
21	F	6016	BCR	C1-C6	-2.36	1.50	1.53
19	A	1137	CLA	MG-NA	-2.36	2.00	2.06
19	A	1135	CLA	C4C-NC	2.36	1.37	1.35
19	F	1305	CLA	C3D-CAD	-2.36	1.40	1.46
19	B	1236	CLA	C3D-CAD	-2.36	1.40	1.46
19	A	1103	CLA	C3D-CAD	-2.35	1.40	1.46
19	3	2009	CLA	MG-NA	-2.35	2.00	2.06
19	B	1203	CLA	C4C-NC	2.35	1.37	1.35
19	A	1119	CLA	C3D-CAD	-2.35	1.40	1.46
19	B	1208	CLA	C1B-CHB	2.35	1.47	1.41
19	4	1004	CLA	MG-NA	-2.35	2.00	2.06
19	1	1014	CLA	C1B-CHB	2.35	1.47	1.41
19	B	1230	CLA	C1C-C2C	-2.35	1.37	1.42
19	4	1306	CLA	C4C-NC	2.35	1.37	1.35
19	3	3016	CLA	C4C-NC	2.35	1.37	1.35
19	4	1004	CLA	C4C-NC	2.35	1.37	1.35
19	A	1135	CLA	MG-NA	-2.35	2.00	2.06
19	B	9010	CLA	C3B-C2B	-2.35	1.37	1.40
19	B	1212	CLA	C1B-CHB	2.34	1.47	1.41
19	1	1006	CLA	C3D-CAD	-2.34	1.40	1.46
19	A	1133	CLA	C1B-NB	-2.34	1.33	1.35
19	A	9022	CLA	C3B-C2B	-2.34	1.37	1.40
19	J	1308	CLA	C1B-NB	-2.34	1.33	1.35
19	3	3016	CLA	MG-NA	-2.33	2.00	2.06
19	3	3004	CLA	CHA-C1A	2.33	1.47	1.41
19	A	1109	CLA	C3D-CAD	-2.33	1.40	1.46
19	2	2004	CLA	C1B-CHB	2.33	1.47	1.41
19	B	1231	CLA	C3D-CAD	-2.33	1.40	1.46
19	4	1304	CLA	C3D-CAD	-2.33	1.40	1.46
19	K	1143	CLA	C3D-CAD	-2.33	1.40	1.46
19	B	1223	CLA	MG-NA	-2.33	2.00	2.06
19	3	3016	CLA	C3D-CAD	-2.33	1.40	1.46
19	2	2010	CLA	C4C-NC	2.33	1.37	1.35
19	A	1110	CLA	C4C-NC	2.32	1.37	1.35
19	A	1139	CLA	C3D-CAD	-2.32	1.40	1.46
22	R	7024	LMU	O1'-C1'	2.32	1.44	1.40
19	A	9012	CLA	MG-NA	-2.32	2.00	2.06
19	A	1128	CLA	C1B-CHB	2.32	1.47	1.41
21	L	6019	BCR	C11-C10	2.32	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	7010	LMU	C4-C3	2.32	1.64	1.51
19	A	9013	CLA	C1B-NB	-2.32	1.33	1.35
19	A	1111	CLA	C4C-NC	2.32	1.37	1.35
19	4	1304	CLA	CBD-CHA	-2.32	1.41	1.52
19	4	1306	CLA	C1B-CHB	2.31	1.47	1.41
19	2	2012	CLA	C3D-CAD	-2.31	1.40	1.46
19	B	1222	CLA	C4C-NC	2.31	1.37	1.35
19	4	4005	CLA	CHA-C1A	2.31	1.47	1.41
19	A	1135	CLA	C1B-CHB	2.31	1.47	1.41
19	B	1201	CLA	C3D-CAD	-2.31	1.40	1.46
19	B	1230	CLA	C1B-NB	-2.31	1.33	1.35
19	A	1104	CLA	MG-NA	-2.31	2.00	2.06
19	B	1238	CLA	C3D-CAD	-2.30	1.40	1.46
19	2	2003	CLA	C4C-NC	2.30	1.37	1.35
19	3	3013	CLA	MG-NA	-2.30	2.00	2.06
19	G	1242	CLA	C3D-CAD	-2.30	1.40	1.46
19	H	1241	CLA	C1B-CHB	2.30	1.47	1.41
19	B	1210	CLA	C1B-NB	-2.30	1.33	1.35
22	2	7027	LMU	O1'-C1'	2.30	1.44	1.40
19	A	1138	CLA	MG-NA	-2.30	2.00	2.06
19	3	3007	CLA	C4C-NC	2.30	1.37	1.35
19	H	1145	CLA	C1B-NB	-2.30	1.33	1.35
19	1	1005	CLA	C1B-CHB	2.29	1.47	1.41
19	2	2014	CLA	MG-NA	-2.29	2.00	2.06
19	A	9022	CLA	MG-NA	-2.29	2.00	2.06
19	4	4003	CLA	C3D-CAD	-2.29	1.40	1.46
19	2	2002	CLA	MG-NA	-2.29	2.00	2.06
19	J	1311	CLA	MG-NA	-2.28	2.00	2.06
19	4	4013	CLA	C1B-CHB	2.28	1.48	1.43
19	1	1002	CLA	C3D-CAD	-2.28	1.40	1.46
19	4	4014	CLA	C1B-CHB	2.28	1.47	1.41
19	A	1137	CLA	C1B-CHB	2.28	1.47	1.41
19	B	1228	CLA	C1B-CHB	2.28	1.47	1.41
19	A	1149	CLA	CMA-C3A	2.28	1.58	1.53
19	1	1008	CLA	C4C-NC	2.27	1.37	1.35
21	F	6014	BCR	C20-C19	-2.27	1.28	1.34
19	3	1118	CLA	C3A-C2A	-2.27	1.52	1.54
19	A	1141	CLA	C3D-CAD	-2.27	1.40	1.46
19	A	1133	CLA	MG-NA	-2.27	2.00	2.06
19	3	3007	CLA	C3D-CAD	-2.27	1.40	1.46
19	B	1211	CLA	C3B-C2B	-2.27	1.37	1.40
19	L	1148	CLA	C1B-NB	-2.27	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1132	CLA	C1B-CHB	2.26	1.47	1.41
19	A	1126	CLA	C3D-CAD	-2.26	1.40	1.46
19	B	1235	CLA	C3D-CAD	-2.26	1.40	1.46
19	B	1223	CLA	C1B-CHB	2.26	1.47	1.41
19	3	3010	CLA	CHB-C4A	-2.26	1.33	1.34
22	K	7001	LMU	O3B-C3B	2.26	1.48	1.43
19	L	1503	CLA	CBD-CGD	-2.26	1.45	1.52
19	A	9013	CLA	C4C-NC	2.26	1.37	1.35
19	2	2001	CLA	MG-NA	-2.26	2.00	2.06
19	B	1203	CLA	C1C-C2C	-2.26	1.37	1.42
19	B	1211	CLA	C3D-CAD	-2.26	1.40	1.46
19	B	1215	CLA	C4C-NC	2.26	1.37	1.35
19	B	1219	CLA	C3D-CAD	-2.26	1.40	1.46
19	B	1231	CLA	C1B-CHB	2.25	1.47	1.41
19	1	1008	CLA	C3A-C2A	-2.25	1.48	1.54
19	3	3012	CLA	C1B-NB	-2.25	1.33	1.35
21	J	6012	BCR	C32-C1	2.25	1.58	1.53
19	B	1224	CLA	MG-NA	-2.25	2.00	2.06
19	B	1208	CLA	C3D-CAD	-2.25	1.40	1.46
19	B	1210	CLA	C3D-CAD	-2.25	1.40	1.46
22	F	7036	LMU	O1'-C1'	2.24	1.44	1.40
19	B	1218	CLA	C4C-NC	2.24	1.37	1.35
19	K	1142	CLA	C3D-CAD	-2.24	1.40	1.46
19	J	1308	CLA	C3B-C2B	-2.24	1.37	1.40
19	B	1230	CLA	MG-NA	-2.24	2.00	2.06
19	B	1225	CLA	C3B-C2B	-2.24	1.37	1.40
19	A	1140	CLA	C1B-CHB	2.24	1.47	1.41
19	B	1203	CLA	C4B-NB	-2.24	1.33	1.35
19	L	1502	CLA	C3D-CAD	-2.24	1.40	1.46
19	4	4004	CLA	CHB-C4A	-2.23	1.33	1.34
19	4	4012	CLA	MG-NA	-2.23	2.01	2.06
19	B	1213	CLA	C3D-CAD	-2.23	1.40	1.46
19	B	1214	CLA	C3D-CAD	-2.23	1.40	1.46
19	K	1143	CLA	C1B-CHB	2.23	1.47	1.41
19	A	1127	CLA	C1B-CHB	2.23	1.47	1.41
19	3	3004	CLA	C4B-CHC	2.23	1.48	1.43
19	4	4002	CLA	CAA-C2A	-2.22	1.50	1.54
19	B	1235	CLA	C4C-NC	2.22	1.37	1.35
19	R	1150	CLA	C3B-C2B	-2.22	1.37	1.40
19	B	1233	CLA	C3D-CAD	-2.22	1.40	1.46
19	A	1106	CLA	MG-NA	-2.22	2.01	2.06
19	J	1311	CLA	C1B-CHB	2.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	1145	CLA	C4C-NC	2.22	1.37	1.35
19	B	1221	CLA	C1B-NB	-2.21	1.33	1.35
19	3	3011	CLA	C3D-CAD	-2.21	1.40	1.46
19	A	1124	CLA	C1B-CHB	2.21	1.47	1.41
19	3	1147	CLA	C3D-CAD	-2.21	1.40	1.46
19	2	2010	CLA	C1B-CHB	2.21	1.48	1.43
21	A	6008	BCR	C40-C30	-2.21	1.49	1.53
19	A	1140	CLA	MG-NA	-2.21	2.01	2.06
19	A	1112	CLA	C1B-CHB	2.21	1.47	1.41
19	A	9011	CLA	C1B-CHB	2.21	1.47	1.41
19	I	1204	CLA	C1B-CHB	2.20	1.47	1.41
19	1	1013	CLA	MG-NA	-2.20	2.01	2.06
19	A	1141	CLA	C4C-NC	2.20	1.37	1.35
19	A	1101	CLA	C3B-C2B	-2.20	1.37	1.40
19	3	2009	CLA	C4-C3	2.20	1.56	1.50
22	B	7040	LMU	O1'-C1'	2.20	1.43	1.40
19	G	1242	CLA	C1B-CHB	2.20	1.47	1.41
19	B	9010	CLA	C1B-CHB	2.20	1.47	1.41
19	B	9010	CLA	MG-NA	-2.20	2.01	2.06
19	B	1209	CLA	C1B-CHB	2.20	1.47	1.41
19	A	1102	CLA	C3B-C2B	-2.20	1.37	1.40
19	3	2009	CLA	C4C-NC	2.19	1.37	1.35
19	A	1107	CLA	C3D-CAD	-2.19	1.40	1.46
19	B	1203	CLA	C3D-CAD	-2.19	1.40	1.46
21	B	6017	BCR	C39-C30	-2.19	1.49	1.53
21	A	6011	BCR	C31-C1	-2.19	1.49	1.53
19	A	1108	CLA	C1B-CHB	2.19	1.47	1.41
21	B	6006	BCR	C37-C22	2.19	1.55	1.50
19	A	9022	CLA	C3D-CAD	-2.19	1.40	1.46
19	B	1223	CLA	C4C-NC	2.19	1.37	1.35
19	F	1305	CLA	C1B-CHB	2.19	1.47	1.41
19	A	1135	CLA	C3D-CAD	-2.19	1.40	1.46
19	4	4011	CLA	CHA-C1A	2.18	1.47	1.41
19	3	3001	CLA	C4C-NC	2.18	1.37	1.35
19	B	1227	CLA	C3D-CAD	-2.18	1.40	1.46
19	1	1007	CLA	C3D-CAD	-2.18	1.40	1.46
19	A	1117	CLA	C1B-CHB	2.18	1.47	1.41
19	4	4003	CLA	C1B-CHB	2.18	1.47	1.41
19	1	1303	CLA	C3B-C2B	-2.18	1.37	1.40
19	L	1130	CLA	C1B-CHB	2.18	1.47	1.41
19	A	1140	CLA	C3D-CAD	-2.18	1.40	1.46
19	B	1212	CLA	C3D-CAD	-2.18	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1224	CLA	C1B-CHB	2.18	1.47	1.41
19	A	1139	CLA	C1B-CHB	2.18	1.47	1.41
19	A	9012	CLA	C3B-C2B	-2.18	1.37	1.40
19	1	1001	CLA	C4B-CHC	2.18	1.47	1.41
21	B	6020	BCR	C39-C30	-2.18	1.49	1.53
19	3	3005	CLA	C4C-NC	2.18	1.37	1.35
19	1	1013	CLA	C1C-C2C	-2.18	1.37	1.42
19	A	1109	CLA	C1B-CHB	2.17	1.47	1.41
21	F	6016	BCR	C11-C10	2.17	1.50	1.43
19	A	1111	CLA	C1B-CHB	2.17	1.47	1.41
21	L	6019	BCR	C39-C30	-2.17	1.49	1.53
19	F	1302	CLA	MG-NA	-2.17	2.01	2.06
19	2	2001	CLA	C3D-CAD	-2.17	1.40	1.46
19	A	1119	CLA	C1B-CHB	2.17	1.47	1.41
19	A	1136	CLA	C1B-CHB	2.17	1.47	1.41
19	A	1111	CLA	C3D-CAD	-2.17	1.40	1.46
19	B	1219	CLA	MG-NA	-2.17	2.01	2.06
19	B	1214	CLA	C1B-CHB	2.17	1.47	1.41
19	1	1011	CLA	C3C-C2C	-2.17	1.34	1.41
19	A	1117	CLA	MG-NA	-2.16	2.01	2.06
19	4	1009	CLA	C1B-CHB	2.16	1.47	1.41
19	B	1239	CLA	C3B-C2B	-2.16	1.37	1.40
21	B	6006	BCR	C31-C1	-2.16	1.49	1.53
19	A	9011	CLA	C3D-CAD	-2.16	1.40	1.46
22	4	7052	LMU	C2-C1	2.16	1.60	1.51
19	4	4007	CLA	C3D-CAD	-2.16	1.40	1.46
19	3	3013	CLA	C1C-C2C	-2.15	1.37	1.42
19	4	4012	CLA	C3D-CAD	-2.15	1.40	1.46
22	E	7037	LMU	O1'-C1'	2.15	1.43	1.40
19	A	1138	CLA	C3D-CAD	-2.15	1.40	1.46
19	B	1205	CLA	C1B-CHB	2.15	1.47	1.41
19	3	3011	CLA	MG-NA	-2.15	2.01	2.06
22	H	7030	LMU	O1'-C1'	2.15	1.43	1.40
19	3	3008	CLA	C1B-CHB	2.15	1.47	1.41
19	2	2013	CLA	C4C-NC	2.14	1.37	1.35
19	3	2009	CLA	C1B-NB	-2.14	1.33	1.35
19	4	1004	CLA	C2-C3	2.14	1.38	1.33
22	1	7004	LMU	O1'-C1'	2.14	1.43	1.40
19	K	1143	CLA	MG-NA	-2.14	2.01	2.06
19	A	1134	CLA	C1B-CHB	2.14	1.46	1.41
19	B	1219	CLA	C1B-CHB	2.14	1.46	1.41
19	F	1302	CLA	C1B-CHB	2.14	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1104	CLA	C1B-CHB	2.13	1.46	1.41
19	K	1142	CLA	C1B-CHB	2.13	1.46	1.41
22	H	7011	LMU	O1'-C1'	2.13	1.43	1.40
22	N	7049	LMU	O1'-C1'	2.13	1.43	1.40
19	A	1120	CLA	MG-NA	-2.13	2.01	2.06
19	B	1214	CLA	C1B-NB	-2.13	1.33	1.35
19	B	1239	CLA	C4C-NC	2.13	1.37	1.35
21	F	6016	BCR	C31-C1	-2.13	1.49	1.53
19	F	1302	CLA	C4C-NC	2.12	1.37	1.35
19	4	1004	CLA	C1B-CHB	2.12	1.46	1.41
19	3	3016	CLA	C1B-NB	-2.12	1.33	1.35
19	L	1503	CLA	C1B-CHB	2.12	1.46	1.41
21	L	6019	BCR	C32-C1	-2.12	1.49	1.53
22	H	7017	LMU	O1'-C1'	2.12	1.43	1.40
19	1	1001	CLA	C1C-C2C	-2.12	1.37	1.42
19	R	1150	CLA	C3D-CAD	-2.12	1.40	1.46
19	2	4009	CLA	C1B-NB	-2.12	1.33	1.35
19	A	1137	CLA	C3B-C2B	-2.12	1.37	1.40
19	1	1007	CLA	MG-NA	-2.12	2.01	2.06
19	B	1301	CLA	MG-NA	-2.12	2.01	2.06
19	A	1131	CLA	C1B-CHB	2.12	1.46	1.41
19	A	1110	CLA	MG-NA	-2.11	2.01	2.06
19	B	1227	CLA	C4C-NC	2.11	1.37	1.35
19	4	4010	CLA	C4C-NC	2.11	1.37	1.35
22	C	7015	LMU	O1'-C1'	2.11	1.43	1.40
19	B	1217	CLA	MG-NA	-2.11	2.01	2.06
19	H	1207	CLA	MG-NA	-2.11	2.01	2.06
22	E	7048	LMU	O1'-C1'	2.11	1.43	1.40
19	1	1013	CLA	C2-C3	2.11	1.38	1.33
19	B	1211	CLA	C1B-CHB	2.10	1.46	1.41
19	B	1229	CLA	C1B-CHB	2.10	1.46	1.41
19	A	1108	CLA	MG-NA	-2.10	2.01	2.06
19	B	1235	CLA	C1B-NB	-2.10	1.33	1.35
19	4	4007	CLA	C4C-NC	2.10	1.37	1.35
22	4	7053	LMU	O1'-C1'	2.10	1.43	1.40
19	B	1216	CLA	MG-NA	-2.10	2.01	2.06
19	2	2014	CLA	C3A-C2A	-2.10	1.48	1.54
19	B	1301	CLA	C4C-NC	2.10	1.37	1.35
19	3	2009	CLA	C1B-CHB	2.10	1.46	1.41
19	L	1501	CLA	C3D-CAD	-2.10	1.40	1.46
19	B	1205	CLA	C3B-C2B	-2.10	1.37	1.40
21	F	6016	BCR	C11-C12	-2.10	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1120	CLA	C1B-CHB	2.10	1.46	1.41
19	B	1209	CLA	MG-NA	-2.10	2.01	2.06
19	B	1239	CLA	MG-NA	-2.10	2.01	2.06
24	B	7101	LMG	O1-C1	2.10	1.43	1.40
19	A	1237	CLA	MG-NA	-2.09	2.01	2.06
19	1	1015	CLA	C1B-CHB	2.09	1.48	1.43
19	2	2001	CLA	C1B-CHB	2.09	1.46	1.41
19	A	1309	CLA	C1B-CHB	2.09	1.48	1.43
22	R	7014	LMU	O1'-C1'	2.09	1.43	1.40
19	B	1220	CLA	C1C-C2C	-2.09	1.37	1.42
19	L	1504	CLA	MG-NA	-2.09	2.01	2.06
19	A	1133	CLA	C1B-CHB	2.09	1.46	1.41
19	4	4013	CLA	MG-NA	-2.09	2.01	2.06
19	A	1106	CLA	C4C-NC	2.09	1.37	1.35
19	L	1503	CLA	C1B-NB	-2.09	1.33	1.35
22	K	7001	LMU	O1'-C1'	2.08	1.43	1.40
19	A	1122	CLA	C1B-NB	-2.08	1.33	1.35
19	B	1202	CLA	C3D-CAD	-2.08	1.40	1.46
22	1	7013	LMU	O1'-C1'	2.08	1.43	1.40
19	A	1151	CLA	C3D-CAD	-2.08	1.40	1.46
21	A	6002	BCR	C39-C30	-2.08	1.49	1.53
19	H	1207	CLA	C4C-NC	2.08	1.37	1.35
19	2	2004	CLA	MG-NA	-2.08	2.01	2.06
19	1	1006	CLA	MG-NA	-2.08	2.01	2.06
22	R	7021	LMU	O1'-C1'	2.07	1.43	1.40
21	I	6018	BCR	C21-C22	-2.07	1.33	1.35
19	A	9023	CLA	C1B-CHB	2.07	1.46	1.41
19	A	1122	CLA	C1B-CHB	2.07	1.46	1.41
19	4	4012	CLA	C1B-CHB	2.07	1.46	1.41
19	4	1306	CLA	MG-NA	-2.07	2.01	2.06
19	B	9010	CLA	C3D-CAD	-2.07	1.40	1.46
22	2	7006	LMU	O1'-C1'	2.07	1.43	1.40
19	4	4010	CLA	CHB-C4A	-2.07	1.33	1.34
19	3	1147	CLA	O2D-CED	-2.07	1.40	1.45
19	J	1308	CLA	C1C-C2C	-2.07	1.37	1.42
22	R	7022	LMU	O1'-C1'	2.07	1.43	1.40
19	B	1223	CLA	C1B-NB	-2.07	1.33	1.35
19	L	1503	CLA	C3B-C2B	-2.07	1.37	1.40
19	A	1139	CLA	C1B-NB	-2.07	1.33	1.35
19	F	1305	CLA	MG-NA	-2.07	2.01	2.06
19	4	1306	CLA	C3D-CAD	-2.07	1.40	1.46
19	A	1126	CLA	C1B-CHB	2.07	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1123	CLA	C1B-CHB	2.07	1.46	1.41
22	2	7031	LMU	C6'-C5'	2.06	1.58	1.51
19	3	3011	CLA	C1B-NB	-2.06	1.33	1.35
19	L	1130	CLA	C3D-CAD	-2.06	1.40	1.46
19	B	1222	CLA	MG-NA	-2.06	2.01	2.06
19	B	1236	CLA	MG-NA	-2.06	2.01	2.06
19	3	1118	CLA	C3D-CAD	-2.06	1.40	1.46
19	B	1202	CLA	C1C-C2C	-2.06	1.37	1.42
19	A	1136	CLA	C4C-NC	2.05	1.37	1.35
19	A	1149	CLA	C2A-C1A	-2.05	1.47	1.52
19	1	1303	CLA	C4B-NB	-2.05	1.33	1.35
19	A	1128	CLA	C4C-NC	2.05	1.37	1.35
22	H	7011	LMU	O5B-C1B	2.05	1.47	1.41
19	1	1001	CLA	C3D-C2D	-2.05	1.35	1.39
19	B	1202	CLA	C1B-CHB	2.04	1.46	1.41
19	A	9011	CLA	MG-NA	-2.04	2.01	2.06
19	3	3016	CLA	C1B-CHB	2.04	1.46	1.41
19	3	1147	CLA	C3A-C2A	-2.04	1.48	1.54
19	A	1140	CLA	C4C-NC	2.04	1.37	1.35
19	A	1103	CLA	MG-NA	-2.04	2.01	2.06
19	A	1141	CLA	C1B-CHB	2.03	1.46	1.41
19	3	1118	CLA	MG-NA	-2.03	2.01	2.06
19	A	1131	CLA	C1B-NB	-2.03	1.33	1.35
19	3	3003	CLA	C3D-CAD	-2.03	1.40	1.46
19	3	3002	CLA	C4C-NC	2.03	1.37	1.35
19	L	1504	CLA	C3D-CAD	-2.03	1.40	1.46
19	4	4002	CLA	C2A-C1A	-2.03	1.47	1.52
19	B	1218	CLA	MG-NA	-2.03	2.01	2.06
19	F	1240	CLA	C3D-CAD	-2.02	1.40	1.46
19	B	1220	CLA	C1B-CHB	2.02	1.46	1.41
19	A	1127	CLA	MG-NA	-2.02	2.01	2.06
21	B	6006	BCR	C32-C1	-2.02	1.49	1.53
21	B	6006	BCR	C19-C18	2.02	1.50	1.45
19	4	4003	CLA	MG-NA	-2.02	2.01	2.06
19	A	1129	CLA	C2-C3	2.02	1.38	1.32
19	H	1145	CLA	C3A-C2A	-2.02	1.48	1.54
19	3	3001	CLA	C1B-CHB	2.02	1.47	1.43
19	A	1111	CLA	MG-NA	-2.01	2.01	2.06
19	A	1110	CLA	C1B-CHB	2.01	1.46	1.41
19	4	4001	CLA	C5-C3	2.01	1.55	1.50
22	D	7050	LMU	O1'-C1'	2.01	1.43	1.40
19	3	2009	CLA	C3B-C2B	-2.01	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1222	CLA	CBC-CAC	2.01	1.63	1.50
19	A	1151	CLA	MG-NA	-2.01	2.01	2.06
19	B	1215	CLA	MG-NA	-2.01	2.01	2.06
19	B	1221	CLA	C2-C3	2.01	1.37	1.33
22	2	7031	LMU	O5'-C1'	2.01	1.47	1.41
19	A	9013	CLA	C3B-C2B	-2.01	1.37	1.40
19	A	1129	CLA	MG-NA	-2.01	2.01	2.06
19	A	1115	CLA	C4C-NC	2.00	1.37	1.35
19	A	1137	CLA	C4C-NC	2.00	1.37	1.35
19	A	1102	CLA	C1B-CHB	2.00	1.46	1.41
19	G	1242	CLA	MG-NA	-2.00	2.01	2.06
22	R	7007	LMU	O1'-C1'	2.00	1.43	1.40
19	3	3008	CLA	C4C-NC	2.00	1.37	1.35
19	4	4015	CLA	CBD-CGD	-2.00	1.46	1.52
19	4	4001	CLA	C3D-CAD	-2.00	1.41	1.46

All (3333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	6012	BCR	C20-C21-C22	30.06	170.21	127.31
21	A	6002	BCR	C20-C21-C22	24.71	162.58	127.31
21	3	6022	BCR	C20-C21-C22	24.52	162.30	127.31
21	F	6014	BCR	C20-C21-C22	22.67	159.67	127.31
21	B	6005	BCR	C20-C21-C22	22.24	159.05	127.31
19	1	1303	CLA	OBD-CAD-CBD	-21.66	94.95	125.89
21	L	6019	BCR	C20-C21-C22	21.15	157.50	127.31
21	B	6006	BCR	C20-C21-C22	20.73	156.90	127.31
21	1	6023	BCR	C11-C10-C9	20.61	156.72	127.31
21	1	6023	BCR	C2-C1-C6	-20.53	78.87	110.48
21	B	6010	BCR	C20-C21-C22	20.16	156.09	127.31
21	B	6020	BCR	C20-C21-C22	19.95	155.79	127.31
21	B	6004	BCR	C20-C21-C22	18.64	153.91	127.31
19	A	1105	CLA	OBD-CAD-CBD	-18.62	99.29	125.89
19	2	4009	CLA	OBD-CAD-C3D	-17.64	98.70	127.98
21	I	6018	BCR	C11-C10-C9	17.57	152.38	127.31
19	1	1013	CLA	OBD-CAD-C3D	-17.17	99.48	127.98
19	A	1149	CLA	C4D-C3D-CAD	17.00	117.95	108.47
21	A	6008	BCR	C20-C21-C22	16.85	151.36	127.31
19	3	3013	CLA	OBD-CAD-C3D	-16.81	100.06	127.98
21	B	6017	BCR	C20-C21-C22	16.68	151.11	127.31
19	A	1126	CLA	OBD-CAD-CBD	-16.52	102.29	125.89
19	B	1215	CLA	OBD-CAD-CBD	-16.16	102.81	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	4002	CLA	OBD-CAD-CBD	-16.15	102.82	125.89
19	4	4014	CLA	OBD-CAD-CBD	-16.04	102.97	125.89
19	A	1151	CLA	OBD-CAD-CBD	-15.99	103.05	125.89
19	A	1237	CLA	OBD-CAD-CBD	-15.95	103.10	125.89
21	B	6006	BCR	C11-C10-C9	15.82	149.89	127.31
21	J	6012	BCR	C11-C10-C9	15.60	149.57	127.31
19	I	1204	CLA	OBD-CAD-CBD	-15.57	103.64	125.89
19	4	4014	CLA	OBD-CAD-C3D	-15.50	102.24	127.98
19	2	4009	CLA	OBD-CAD-CBD	-15.47	103.80	125.89
21	I	6021	BCR	C24-C23-C22	-15.46	102.88	126.23
19	2	2006	CLA	OBD-CAD-C3D	-15.42	102.38	127.98
19	A	9011	CLA	OBD-CAD-CBD	-15.23	104.14	125.89
19	2	2004	CLA	OBD-CAD-CBD	-15.21	104.16	125.89
19	2	2013	CLA	OBD-CAD-CBD	-15.20	104.18	125.89
19	1	1010	CLA	OBD-CAD-CBD	-15.18	104.21	125.89
21	I	6018	BCR	C20-C21-C22	15.12	148.89	127.31
19	1	1011	CLA	CAB-C3B-C4B	-15.08	105.28	128.46
19	L	1503	CLA	OBD-CAD-C3D	-15.06	102.97	127.98
19	H	1241	CLA	OBD-CAD-CBD	-14.96	104.53	125.89
19	1	1303	CLA	OBD-CAD-C3D	-14.93	103.20	127.98
19	3	3013	CLA	OBD-CAD-CBD	-14.90	104.60	125.89
21	A	6007	BCR	C11-C10-C9	14.86	148.52	127.31
19	B	1210	CLA	OBD-CAD-CBD	-14.82	104.72	125.89
19	A	1108	CLA	OBD-CAD-CBD	-14.78	104.78	125.89
19	3	2009	CLA	OBD-CAD-CBD	-14.77	104.79	125.89
19	A	1129	CLA	OBD-CAD-C3D	-14.77	103.45	127.98
19	4	4001	CLA	OBD-CAD-CBD	-14.76	104.81	125.89
19	H	1207	CLA	OBD-CAD-C3D	-14.71	103.56	127.98
19	B	1233	CLA	OBD-CAD-C3D	-14.70	103.57	127.98
21	1	6023	BCR	C29-C30-C25	-14.70	87.86	110.48
19	B	1234	CLA	OBD-CAD-C3D	-14.68	103.61	127.98
21	A	6011	BCR	C20-C21-C22	14.67	148.24	127.31
19	B	1224	CLA	OBD-CAD-C3D	-14.66	103.64	127.98
21	I	6021	BCR	C20-C21-C22	14.63	148.18	127.31
21	A	6011	BCR	C11-C10-C9	14.62	148.17	127.31
21	F	6014	BCR	C21-C20-C19	14.61	168.81	123.22
19	3	3007	CLA	OBD-CAD-CBD	-14.61	105.02	125.89
19	R	1144	CLA	OBD-CAD-CBD	-14.61	105.03	125.89
19	3	3017	CLA	OBD-CAD-C3D	-14.57	103.80	127.98
19	A	1149	CLA	OBD-CAD-C3D	-14.56	103.81	127.98
19	I	1204	CLA	OBD-CAD-C3D	-14.54	103.84	127.98
19	B	1202	CLA	OBD-CAD-CBD	-14.51	105.17	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1237	CLA	OBD-CAD-C3D	-14.47	103.95	127.98
19	A	1128	CLA	OBD-CAD-CBD	-14.39	105.34	125.89
19	B	1218	CLA	OBD-CAD-C3D	-14.39	104.09	127.98
19	A	1128	CLA	OBD-CAD-C3D	-14.38	104.10	127.98
19	B	1224	CLA	OBD-CAD-CBD	-14.33	105.42	125.89
19	A	1135	CLA	OBD-CAD-CBD	-14.30	105.46	125.89
19	A	1119	CLA	OBD-CAD-C3D	-14.25	104.32	127.98
19	A	1112	CLA	OBD-CAD-CBD	-14.22	105.58	125.89
21	F	6016	BCR	C20-C21-C22	14.21	147.59	127.31
19	B	1233	CLA	OBD-CAD-CBD	-14.14	105.70	125.89
19	B	1219	CLA	OBD-CAD-CBD	-14.12	105.72	125.89
19	H	1145	CLA	OBD-CAD-C3D	-14.11	104.56	127.98
21	A	6002	BCR	C21-C20-C19	14.08	167.16	123.22
19	1	1001	CLA	OBD-CAD-C3D	-14.03	104.69	127.98
19	1	1006	CLA	OBD-CAD-C3D	-13.95	104.81	127.98
19	2	2013	CLA	OBD-CAD-C3D	-13.85	104.98	127.98
19	H	1145	CLA	C4D-C3D-CAD	13.85	116.19	108.47
19	L	1148	CLA	OBD-CAD-C3D	-13.79	105.08	127.98
19	B	1206	CLA	OBD-CAD-C3D	-13.77	105.12	127.98
21	3	6022	BCR	C21-C20-C19	13.75	166.13	123.22
19	A	1126	CLA	OBD-CAD-C3D	-13.74	105.17	127.98
19	4	1004	CLA	OBD-CAD-C3D	-13.73	105.18	127.98
19	B	1216	CLA	OBD-CAD-CBD	-13.72	106.29	125.89
19	B	1220	CLA	OBD-CAD-C3D	-13.69	105.25	127.98
19	4	1009	CLA	CAB-C3B-C4B	-13.68	107.43	128.46
19	A	1106	CLA	OBD-CAD-C3D	-13.63	105.34	127.98
21	B	6005	BCR	C11-C10-C9	13.63	146.76	127.31
19	B	1230	CLA	OBD-CAD-C3D	-13.62	105.37	127.98
19	B	1301	CLA	CAB-C3B-C4B	-13.58	107.59	128.46
21	1	6023	BCR	C32-C1-C6	-13.56	88.31	110.30
19	A	1140	CLA	OBD-CAD-CBD	-13.56	106.53	125.89
19	A	9011	CLA	C4D-C3D-CAD	13.55	116.03	108.47
19	1	1013	CLA	C4D-C3D-CAD	13.51	116.00	108.47
19	3	1118	CLA	OBD-CAD-C3D	-13.38	105.76	127.98
19	4	4012	CLA	CAB-C3B-C4B	-13.38	107.89	128.46
19	4	4002	CLA	OBD-CAD-C3D	-13.33	105.85	127.98
19	A	1134	CLA	OBD-CAD-C3D	-13.31	105.87	127.98
19	B	1232	CLA	OBD-CAD-C3D	-13.31	105.89	127.98
19	B	1220	CLA	OBD-CAD-CBD	-13.30	106.89	125.89
19	A	1138	CLA	OBD-CAD-CBD	-13.28	106.92	125.89
19	A	1122	CLA	OBD-CAD-C3D	-13.22	106.03	127.98
21	A	6003	BCR	C20-C21-C22	13.21	146.16	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1223	CLA	OBD-CAD-CBD	-13.17	107.08	125.89
19	L	1501	CLA	OBD-CAD-CBD	-13.13	107.13	125.89
19	1	1003	CLA	C4D-C3D-CAD	13.13	115.79	108.47
19	4	4001	CLA	OBD-CAD-C3D	-13.12	106.19	127.98
19	1	1001	CLA	C4D-C3D-CAD	13.10	115.78	108.47
19	B	1209	CLA	OBD-CAD-C3D	-12.99	106.41	127.98
19	A	9013	CLA	OBD-CAD-C3D	-12.98	106.43	127.98
19	3	3016	CLA	OBD-CAD-C3D	-12.96	106.45	127.98
19	L	1503	CLA	OBD-CAD-CBD	-12.94	107.41	125.89
19	B	1231	CLA	OBD-CAD-C3D	-12.93	106.52	127.98
19	3	1147	CLA	C4D-C3D-CAD	12.90	115.66	108.47
19	A	1120	CLA	OBD-CAD-C3D	-12.90	106.56	127.98
19	F	1305	CLA	OBD-CAD-C3D	-12.90	106.57	127.98
19	B	1226	CLA	C4D-C3D-CAD	12.89	115.66	108.47
19	H	1505	CLA	OBD-CAD-CBD	-12.89	107.48	125.89
19	A	1136	CLA	OBD-CAD-CBD	-12.88	107.50	125.89
21	B	6017	BCR	C11-C10-C9	12.87	145.68	127.31
19	1	1003	CLA	OBD-CAD-CBD	-12.86	107.52	125.89
19	A	1149	CLA	CAB-C3B-C4B	-12.86	108.70	128.46
19	2	2014	CLA	OBD-CAD-C3D	-12.84	106.67	127.98
19	A	1108	CLA	OBD-CAD-C3D	-12.83	106.68	127.98
19	A	9022	CLA	OBD-CAD-CBD	-12.82	107.58	125.89
19	B	1206	CLA	OBD-CAD-CBD	-12.78	107.64	125.89
19	3	3008	CLA	OBD-CAD-C3D	-12.78	106.77	127.98
21	J	6012	BCR	C21-C20-C19	12.76	163.04	123.22
19	A	1127	CLA	OBD-CAD-CBD	-12.75	107.68	125.89
19	1	1014	CLA	OBD-CAD-C3D	-12.74	106.83	127.98
19	4	1304	CLA	OBD-CAD-C3D	-12.73	106.84	127.98
19	1	1012	CLA	CAB-C3B-C4B	-12.72	108.92	128.46
19	A	1103	CLA	OBD-CAD-C3D	-12.69	106.90	127.98
19	A	1116	CLA	OBD-CAD-C3D	-12.68	106.92	127.98
19	A	1119	CLA	OBD-CAD-CBD	-12.68	107.78	125.89
19	3	1118	CLA	CAB-C3B-C4B	-12.66	109.01	128.46
19	A	1131	CLA	OBD-CAD-C3D	-12.63	107.02	127.98
19	3	3008	CLA	C4D-C3D-CAD	12.63	115.51	108.47
19	1	1008	CLA	C4D-C3D-CAD	12.62	115.51	108.47
19	4	1009	CLA	OBD-CAD-C3D	-12.62	107.03	127.98
19	K	1142	CLA	OBD-CAD-CBD	-12.62	107.87	125.89
19	4	4012	CLA	OBD-CAD-C3D	-12.61	107.04	127.98
19	A	1104	CLA	OBD-CAD-C3D	-12.60	107.06	127.98
19	A	1104	CLA	OBD-CAD-CBD	-12.59	107.90	125.89
19	R	1144	CLA	C4D-C3D-CAD	12.56	115.47	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1139	CLA	OBD-CAD-C3D	-12.56	107.13	127.98
19	3	3017	CLA	C4D-C3D-CAD	12.53	115.46	108.47
19	A	1115	CLA	OBD-CAD-C3D	-12.53	107.18	127.98
19	R	1144	CLA	OBD-CAD-C3D	-12.53	107.18	127.98
19	A	1124	CLA	OBD-CAD-C3D	-12.52	107.20	127.98
21	I	6021	BCR	C11-C10-C9	12.51	145.17	127.31
19	A	1129	CLA	OBD-CAD-CBD	-12.51	108.02	125.89
19	A	1125	CLA	OBD-CAD-C3D	-12.50	107.22	127.98
19	2	2006	CLA	OBD-CAD-CBD	-12.50	108.04	125.89
21	B	6005	BCR	C21-C20-C19	12.48	162.16	123.22
21	A	6008	BCR	C11-C10-C9	12.47	145.11	127.31
21	F	6014	BCR	C11-C10-C9	12.42	145.04	127.31
19	1	1010	CLA	OBD-CAD-C3D	-12.42	107.36	127.98
21	1	6023	BCR	C10-C11-C12	12.41	161.95	123.22
19	A	1116	CLA	OBD-CAD-CBD	-12.41	108.17	125.89
19	3	2009	CLA	OBD-CAD-C3D	-12.40	107.39	127.98
19	1	1011	CLA	OBD-CAD-C3D	-12.39	107.40	127.98
19	1	1003	CLA	OBD-CAD-C3D	-12.39	107.42	127.98
19	G	1242	CLA	OBD-CAD-CBD	-12.38	108.20	125.89
19	K	1146	CLA	OBD-CAD-CBD	-12.38	108.20	125.89
19	A	1121	CLA	C4D-C3D-CAD	12.38	115.37	108.47
19	F	1302	CLA	OBD-CAD-C3D	-12.35	107.48	127.98
19	B	9010	CLA	OBD-CAD-CBD	-12.24	108.41	125.89
19	J	1311	CLA	OBD-CAD-CBD	-12.24	108.41	125.89
19	1	1011	CLA	C4D-C3D-CAD	12.23	115.29	108.47
19	3	3016	CLA	OBD-CAD-CBD	-12.19	108.48	125.89
19	B	1228	CLA	OBD-CAD-C3D	-12.18	107.75	127.98
19	B	1231	CLA	C4D-C3D-CAD	12.18	115.26	108.47
19	B	1218	CLA	C4D-C3D-CAD	12.17	115.26	108.47
19	B	1236	CLA	OBD-CAD-CBD	-12.17	108.51	125.89
19	3	3008	CLA	OBD-CAD-CBD	-12.16	108.52	125.89
19	A	1141	CLA	OBD-CAD-C3D	-12.16	107.79	127.98
19	J	1311	CLA	OBD-CAD-C3D	-12.14	107.82	127.98
19	A	1139	CLA	OBD-CAD-CBD	-12.13	108.57	125.89
19	B	9010	CLA	OBD-CAD-C3D	-12.11	107.87	127.98
19	A	1113	CLA	OBD-CAD-CBD	-12.10	108.60	125.89
19	F	1305	CLA	OBD-CAD-CBD	-12.10	108.61	125.89
19	H	1207	CLA	OBD-CAD-CBD	-12.07	108.65	125.89
19	B	1217	CLA	C4D-C3D-CAD	12.07	115.20	108.47
19	H	1145	CLA	OBD-CAD-CBD	-12.07	108.65	125.89
19	B	1216	CLA	OBD-CAD-C3D	-12.06	107.95	127.98
19	K	1142	CLA	OBD-CAD-C3D	-12.06	107.97	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3007	CLA	OBD-CAD-C3D	-12.05	107.98	127.98
19	A	1121	CLA	OBD-CAD-CBD	-12.04	108.69	125.89
19	K	1146	CLA	OBD-CAD-C3D	-12.04	108.00	127.98
19	4	1004	CLA	OBD-CAD-CBD	-12.03	108.71	125.89
19	B	1202	CLA	OBD-CAD-C3D	-12.01	108.04	127.98
19	A	9022	CLA	OBD-CAD-C3D	-12.00	108.06	127.98
21	B	6020	BCR	C15-C16-C17	-11.99	98.91	123.47
19	K	1143	CLA	OBD-CAD-C3D	-11.99	108.08	127.98
19	3	2009	CLA	C4D-C3D-CAD	11.98	115.15	108.47
19	B	1222	CLA	OBD-CAD-C3D	-11.96	108.12	127.98
19	A	1133	CLA	OBD-CAD-CBD	-11.95	108.83	125.89
19	A	1101	CLA	OBD-CAD-C3D	-11.91	108.20	127.98
19	A	1122	CLA	C4D-C3D-CAD	11.89	115.10	108.47
19	A	1113	CLA	OBD-CAD-C3D	-11.88	108.25	127.98
19	A	9012	CLA	OBD-CAD-C3D	-11.87	108.27	127.98
19	B	1234	CLA	C4D-C3D-CAD	11.86	115.08	108.47
19	K	1143	CLA	OBD-CAD-CBD	-11.85	108.96	125.89
19	R	1150	CLA	OBD-CAD-CBD	-11.84	108.97	125.89
19	3	3003	CLA	OBD-CAD-C3D	-11.84	108.32	127.98
19	2	2012	CLA	OBD-CAD-C3D	-11.83	108.34	127.98
19	B	1222	CLA	OBD-CAD-CBD	-11.82	109.00	125.89
19	B	1209	CLA	OBD-CAD-CBD	-11.81	109.02	125.89
19	B	1227	CLA	OBD-CAD-CBD	-11.77	109.07	125.89
19	A	1125	CLA	OBD-CAD-CBD	-11.74	109.13	125.89
19	A	1136	CLA	OBD-CAD-C3D	-11.73	108.50	127.98
19	3	3017	CLA	OBD-CAD-CBD	-11.72	109.15	125.89
19	B	1230	CLA	C4D-C3D-CAD	11.72	115.00	108.47
19	4	1306	CLA	C4D-C3D-CAD	11.71	115.00	108.47
19	A	1149	CLA	OBD-CAD-CBD	-11.66	109.23	125.89
19	2	2012	CLA	C4D-C3D-CAD	11.66	114.97	108.47
19	A	1137	CLA	OBD-CAD-C3D	-11.65	108.64	127.98
19	4	4012	CLA	C4D-C3D-CAD	11.65	114.97	108.47
19	L	1148	CLA	OBD-CAD-CBD	-11.64	109.27	125.89
19	H	1241	CLA	OBD-CAD-C3D	-11.62	108.69	127.98
19	B	1229	CLA	OBD-CAD-C3D	-11.62	108.69	127.98
19	A	1116	CLA	C4D-C3D-CAD	11.62	114.95	108.47
21	1	6023	BCR	C31-C1-C6	-11.54	91.58	110.30
19	4	4007	CLA	OBD-CAD-CBD	-11.51	109.45	125.89
19	A	1105	CLA	OBD-CAD-C3D	-11.50	108.89	127.98
19	4	1009	CLA	C4D-C3D-CAD	11.48	114.87	108.47
19	B	1239	CLA	C4D-C3D-CAD	11.48	114.87	108.47
19	A	1115	CLA	OBD-CAD-CBD	-11.48	109.50	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1111	CLA	OBD-CAD-CBD	-11.46	109.52	125.89
19	4	4006	CLA	C4D-C3D-CAD	11.45	114.85	108.47
19	B	1227	CLA	OBD-CAD-C3D	-11.45	108.97	127.98
19	B	1209	CLA	C4D-C3D-CAD	11.45	114.85	108.47
21	B	6004	BCR	C11-C10-C9	11.45	143.65	127.31
19	1	1006	CLA	C4D-C3D-CAD	11.44	114.85	108.47
19	B	1230	CLA	OBD-CAD-CBD	-11.43	109.56	125.89
19	A	1134	CLA	OBD-CAD-CBD	-11.42	109.58	125.89
19	K	1146	CLA	C4D-C3D-CAD	11.41	114.83	108.47
19	B	1217	CLA	OBD-CAD-C3D	-11.40	109.05	127.98
19	F	1302	CLA	C4D-C3D-CAD	11.39	114.82	108.47
19	H	1505	CLA	OBD-CAD-C3D	-11.38	109.09	127.98
19	A	1124	CLA	OBD-CAD-CBD	-11.37	109.64	125.89
19	A	1137	CLA	OBD-CAD-CBD	-11.37	109.65	125.89
19	1	1007	CLA	C4D-C3D-CAD	11.34	114.79	108.47
19	B	1228	CLA	OBD-CAD-CBD	-11.33	109.70	125.89
19	1	1010	CLA	C4D-C3D-CAD	11.32	114.78	108.47
19	A	9013	CLA	OBD-CAD-CBD	-11.31	109.73	125.89
19	B	1203	CLA	OBD-CAD-C3D	-11.31	109.21	127.98
19	B	1215	CLA	OBD-CAD-C3D	-11.30	109.22	127.98
19	B	1219	CLA	C4D-C3D-CAD	11.29	114.77	108.47
19	A	1133	CLA	OBD-CAD-C3D	-11.29	109.24	127.98
19	B	1201	CLA	C4D-C3D-CAD	11.29	114.76	108.47
19	A	1117	CLA	OBD-CAD-CBD	-11.28	109.78	125.89
19	H	1505	CLA	C4D-C3D-CAD	11.26	114.75	108.47
19	B	1211	CLA	C4D-C3D-CAD	11.25	114.74	108.47
19	A	1131	CLA	C4D-C3D-CAD	11.25	114.74	108.47
19	B	9010	CLA	C4D-C3D-CAD	11.23	114.73	108.47
19	2	2001	CLA	OBD-CAD-C3D	-11.21	109.36	127.98
19	A	1131	CLA	OBD-CAD-CBD	-11.21	109.88	125.89
19	J	1308	CLA	OBD-CAD-C3D	-11.21	109.38	127.98
19	L	1502	CLA	OBD-CAD-CBD	-11.20	109.90	125.89
19	A	1140	CLA	OBD-CAD-C3D	-11.18	109.42	127.98
19	B	1223	CLA	OBD-CAD-C3D	-11.18	109.42	127.98
19	L	1502	CLA	OBD-CAD-C3D	-11.13	109.50	127.98
19	A	1135	CLA	OBD-CAD-C3D	-11.12	109.52	127.98
19	A	9012	CLA	OBD-CAD-CBD	-11.12	110.01	125.89
19	4	4003	CLA	OBD-CAD-C3D	-11.09	109.57	127.98
19	A	1141	CLA	C4D-C3D-CAD	11.09	114.65	108.47
19	A	1127	CLA	OBD-CAD-C3D	-11.08	109.58	127.98
19	B	1202	CLA	C4D-C3D-CAD	11.08	114.65	108.47
21	I	6018	BCR	C24-C23-C22	-11.07	109.51	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1150	CLA	C4D-C3D-CAD	11.06	114.64	108.47
19	B	1219	CLA	OBD-CAD-C3D	-11.06	109.61	127.98
19	K	3009	CLA	OBD-CAD-CBD	-11.06	110.10	125.89
19	B	1212	CLA	OBD-CAD-C3D	-11.05	109.63	127.98
19	1	1002	CLA	C4D-C3D-CAD	11.05	114.63	108.47
19	B	1208	CLA	CAB-C3B-C4B	-11.03	111.51	128.46
19	B	1225	CLA	C4D-C3D-CAD	11.02	114.62	108.47
19	4	1004	CLA	C4D-C3D-CAD	11.01	114.61	108.47
19	3	3003	CLA	CAB-C3B-C4B	-11.01	111.54	128.46
19	B	1232	CLA	C4D-C3D-CAD	11.01	114.61	108.47
19	4	4007	CLA	OBD-CAD-C3D	-11.00	109.72	127.98
19	A	1136	CLA	C4D-C3D-CAD	10.98	114.59	108.47
19	A	1109	CLA	C4D-C3D-CAD	10.98	114.59	108.47
19	4	4007	CLA	C4D-C3D-CAD	10.97	114.59	108.47
19	2	2002	CLA	C4D-C3D-CAD	10.96	114.58	108.47
19	B	1205	CLA	C4D-C3D-CAD	10.96	114.58	108.47
19	1	1014	CLA	OBD-CAD-CBD	-10.93	110.28	125.89
19	2	2007	CLA	OBD-CAD-CBD	-10.93	110.28	125.89
19	2	2014	CLA	C4D-C3D-CAD	10.92	114.56	108.47
19	3	3007	CLA	C4D-C3D-CAD	10.91	114.56	108.47
19	J	1311	CLA	C4D-C3D-CAD	10.90	114.55	108.47
19	A	1132	CLA	OBD-CAD-CBD	-10.89	110.34	125.89
19	A	1138	CLA	OBD-CAD-C3D	-10.88	109.91	127.98
19	B	1206	CLA	C4D-C3D-CAD	10.88	114.54	108.47
19	2	2004	CLA	C4D-C3D-CAD	10.88	114.54	108.47
19	4	1304	CLA	OBD-CAD-CBD	-10.87	110.37	125.89
19	2	2007	CLA	OBD-CAD-C3D	-10.87	109.94	127.98
19	A	1139	CLA	C4D-C3D-CAD	10.87	114.53	108.47
19	B	1217	CLA	OBD-CAD-CBD	-10.85	110.39	125.89
19	B	1213	CLA	OBD-CAD-C3D	-10.83	110.00	127.98
19	A	1110	CLA	OBD-CAD-CBD	-10.82	110.43	125.89
19	B	1238	CLA	C4D-C3D-CAD	10.82	114.50	108.47
19	A	1120	CLA	C4D-C3D-CAD	10.80	114.50	108.47
19	K	1142	CLA	C4D-C3D-CAD	10.80	114.49	108.47
19	B	1236	CLA	OBD-CAD-C3D	-10.79	110.07	127.98
19	A	1237	CLA	C4D-C3D-CAD	10.79	114.48	108.47
19	B	1233	CLA	C4D-C3D-CAD	10.78	114.48	108.47
19	L	1501	CLA	OBD-CAD-C3D	-10.77	110.09	127.98
19	A	9013	CLA	C4D-C3D-CAD	10.76	114.47	108.47
19	2	2001	CLA	OBD-CAD-CBD	-10.74	110.55	125.89
19	3	3006	CLA	C1D-CHD-C4C	-10.74	113.06	129.64
19	B	1216	CLA	C4D-C3D-CAD	10.73	114.45	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1134	CLA	C4D-C3D-CAD	10.72	114.45	108.47
19	B	1223	CLA	C4D-C3D-CAD	10.70	114.44	108.47
19	4	1306	CLA	OBD-CAD-C3D	-10.70	110.22	127.98
19	A	1128	CLA	C4D-C3D-CAD	10.66	114.42	108.47
19	A	1132	CLA	C4D-C3D-CAD	10.66	114.42	108.47
19	3	1118	CLA	C4D-C3D-CAD	10.66	114.41	108.47
19	4	4001	CLA	C4D-C3D-CAD	10.65	114.41	108.47
19	B	1222	CLA	C4D-C3D-CAD	10.65	114.41	108.47
21	B	6010	BCR	C11-C10-C9	10.63	142.48	127.31
19	B	1213	CLA	C4D-C3D-CAD	10.63	114.40	108.47
19	K	3009	CLA	C4D-C3D-CAD	10.62	114.39	108.47
19	B	1201	CLA	OBD-CAD-C3D	-10.61	110.37	127.98
19	A	1132	CLA	OBD-CAD-C3D	-10.59	110.39	127.98
19	A	9023	CLA	C4D-C3D-CAD	10.59	114.38	108.47
19	1	1011	CLA	CAB-C3B-C2B	-10.59	103.95	124.69
19	4	4010	CLA	C1D-CHD-C4C	-10.59	113.30	129.64
19	A	1119	CLA	C4D-C3D-CAD	10.58	114.37	108.47
19	L	1148	CLA	C4D-C3D-CAD	10.58	114.37	108.47
19	4	4003	CLA	C4D-C3D-CAD	10.57	114.37	108.47
19	2	2001	CLA	C4D-C3D-CAD	10.56	114.36	108.47
19	2	2006	CLA	C4D-C3D-CAD	10.54	114.35	108.47
19	F	1240	CLA	C4D-C3D-CAD	10.51	114.33	108.47
19	A	1106	CLA	C4D-C3D-CAD	10.49	114.32	108.47
19	L	1502	CLA	C4D-C3D-CAD	10.49	114.32	108.47
19	A	1133	CLA	C4D-C3D-CAD	10.49	114.32	108.47
19	F	1302	CLA	OBD-CAD-CBD	-10.48	110.92	125.89
19	G	1242	CLA	OBD-CAD-C3D	-10.47	110.60	127.98
19	B	1229	CLA	C4D-C3D-CAD	10.46	114.31	108.47
19	A	1117	CLA	C4D-C3D-CAD	10.46	114.30	108.47
21	B	6020	BCR	C7-C8-C9	-10.46	110.43	126.23
19	A	1122	CLA	OBD-CAD-CBD	-10.45	110.96	125.89
19	B	1213	CLA	OBD-CAD-CBD	-10.43	111.00	125.89
19	A	1141	CLA	OBD-CAD-CBD	-10.43	111.00	125.89
19	2	2002	CLA	OBD-CAD-C3D	-10.42	110.67	127.98
19	A	1111	CLA	C4D-C3D-CAD	10.42	114.28	108.47
19	L	1501	CLA	C4D-C3D-CAD	10.42	114.28	108.47
19	B	1205	CLA	OBD-CAD-CBD	-10.41	111.02	125.89
19	4	1304	CLA	C4D-C3D-CAD	10.40	114.27	108.47
21	A	6003	BCR	C11-C10-C9	10.40	142.15	127.31
19	A	1126	CLA	C4D-C3D-CAD	10.37	114.25	108.47
19	3	3005	CLA	C1D-CHD-C4C	-10.36	113.65	129.64
19	2	2004	CLA	OBD-CAD-C3D	-10.36	110.79	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1208	CLA	C4D-C3D-CAD	10.35	114.24	108.47
19	B	1301	CLA	C4D-C3D-CAD	10.35	114.24	108.47
19	A	1140	CLA	C4D-C3D-CAD	10.35	114.24	108.47
21	L	6019	BCR	C11-C10-C9	10.35	142.08	127.31
19	A	1149	CLA	C3D-CAD-CBD	-10.34	93.99	107.61
19	A	1137	CLA	C4D-C3D-CAD	10.33	114.23	108.47
19	2	2014	CLA	OBD-CAD-CBD	-10.32	111.15	125.89
19	4	4005	CLA	C1D-CHD-C4C	-10.32	113.71	129.64
19	L	1503	CLA	C4D-C3D-CAD	10.32	114.22	108.47
19	J	1308	CLA	OBD-CAD-CBD	-10.31	111.17	125.89
19	2	4009	CLA	C4D-C3D-CAD	10.28	114.20	108.47
19	H	1207	CLA	C4D-C3D-CAD	10.27	114.20	108.47
21	I	6018	BCR	C7-C8-C9	-10.27	110.72	126.23
19	B	1226	CLA	OBD-CAD-C3D	-10.26	110.94	127.98
19	A	1125	CLA	C4D-C3D-CAD	10.26	114.19	108.47
19	B	1218	CLA	OBD-CAD-CBD	-10.23	111.28	125.89
19	3	3004	CLA	C1C-CHC-C4B	-10.22	113.86	129.64
19	A	1138	CLA	C4D-C3D-CAD	10.22	114.17	108.47
19	A	1121	CLA	OBD-CAD-C3D	-10.21	111.03	127.98
19	1	1014	CLA	C4D-C3D-CAD	10.21	114.16	108.47
19	A	1120	CLA	OBD-CAD-CBD	-10.20	111.32	125.89
19	A	1107	CLA	OBD-CAD-CBD	-10.20	111.33	125.89
19	A	1104	CLA	C4D-C3D-CAD	10.19	114.16	108.47
19	B	1227	CLA	C4D-C3D-CAD	10.18	114.14	108.47
21	3	6022	BCR	C11-C10-C9	10.16	141.81	127.31
19	4	4004	CLA	C1D-CHD-C4C	-10.15	113.96	129.64
21	B	6006	BCR	C21-C20-C19	10.14	154.87	123.22
19	A	1105	CLA	C4D-C3D-CAD	10.13	114.12	108.47
19	3	3012	CLA	C1C-CHC-C4B	-10.13	114.00	129.64
19	1	1012	CLA	C4D-C3D-CAD	10.12	114.11	108.47
19	B	1224	CLA	C4D-C3D-CAD	10.12	114.11	108.47
19	A	1110	CLA	OBD-CAD-C3D	-10.11	111.19	127.98
19	B	1301	CLA	OBD-CAD-C3D	-10.10	111.21	127.98
19	2	2010	CLA	C1D-CHD-C4C	-10.09	114.06	129.64
19	A	1124	CLA	C4D-C3D-CAD	10.09	114.10	108.47
19	B	1210	CLA	C4D-C3D-CAD	10.08	114.09	108.47
19	2	2005	CLA	C1C-CHC-C4B	-10.08	114.07	129.64
19	A	1101	CLA	C4D-C3D-CAD	10.08	114.09	108.47
19	A	1110	CLA	C4D-C3D-CAD	10.07	114.09	108.47
19	3	3002	CLA	C1D-CHD-C4C	-10.07	114.10	129.64
19	2	2008	CLA	C1D-CHD-C4C	-10.06	114.10	129.64
19	1	1008	CLA	OBD-CAD-C3D	-10.04	111.31	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3016	CLA	C4D-C3D-CAD	10.04	114.07	108.47
19	J	1308	CLA	C4D-C3D-CAD	10.03	114.06	108.47
19	A	1112	CLA	OBD-CAD-C3D	-10.03	111.33	127.98
19	A	1151	CLA	OBD-CAD-C3D	-10.02	111.35	127.98
19	3	3001	CLA	C1D-CHD-C4C	-10.00	114.19	129.64
19	B	1203	CLA	OBD-CAD-CBD	-10.00	111.61	125.89
19	A	1113	CLA	C4D-C3D-CAD	9.98	114.04	108.47
19	A	1135	CLA	C4D-C3D-CAD	9.97	114.03	108.47
19	2	2011	CLA	C1D-CHD-C4C	-9.97	114.24	129.64
19	2	2003	CLA	C1D-CHD-C4C	-9.93	114.31	129.64
21	A	6011	BCR	C21-C20-C19	9.92	154.16	123.22
19	4	4011	CLA	C1D-CHD-C4C	-9.92	114.33	129.64
19	B	1215	CLA	C4D-C3D-CAD	9.91	114.00	108.47
19	K	1143	CLA	C4D-C3D-CAD	9.91	113.99	108.47
19	L	1504	CLA	C4D-C3D-CAD	9.89	113.99	108.47
19	2	2013	CLA	C4D-C3D-CAD	9.86	113.97	108.47
19	A	1112	CLA	C4D-C3D-CAD	9.85	113.97	108.47
19	A	1103	CLA	C4D-C3D-CAD	9.85	113.96	108.47
19	H	1241	CLA	C4D-C3D-CAD	9.84	113.96	108.47
19	3	3011	CLA	OBD-CAD-C3D	-9.82	111.68	127.98
19	A	1123	CLA	C4D-C3D-CAD	9.81	113.94	108.47
19	A	1107	CLA	OBD-CAD-C3D	-9.81	111.69	127.98
19	4	4002	CLA	C4D-C3D-CAD	9.77	113.92	108.47
21	A	6003	BCR	C21-C20-C19	9.76	153.69	123.22
19	3	3010	CLA	C1D-CHD-C4C	-9.76	114.58	129.64
19	1	1008	CLA	OBD-CAD-CBD	-9.74	111.99	125.89
19	3	3015	CLA	C1D-CHD-C4C	-9.73	114.62	129.64
19	B	1232	CLA	OBD-CAD-CBD	-9.73	112.00	125.89
19	B	1238	CLA	OBD-CAD-C3D	-9.72	111.85	127.98
21	B	6004	BCR	C21-C20-C19	9.72	153.54	123.22
19	B	1210	CLA	OBD-CAD-C3D	-9.69	111.89	127.98
19	2	2007	CLA	C4D-C3D-CAD	9.69	113.87	108.47
19	4	4014	CLA	C4D-C3D-CAD	9.68	113.87	108.47
19	1	1310	CLA	C1D-CHD-C4C	-9.68	114.69	129.64
19	1	1007	CLA	OBD-CAD-C3D	-9.68	111.91	127.98
19	A	1107	CLA	C4D-C3D-CAD	9.67	113.86	108.47
19	B	1203	CLA	C4D-C3D-CAD	9.67	113.86	108.47
19	B	1225	CLA	OBD-CAD-C3D	-9.66	111.95	127.98
19	A	1103	CLA	OBD-CAD-CBD	-9.64	112.13	125.89
19	1	1015	CLA	C1D-CHD-C4C	-9.63	114.76	129.64
19	A	9023	CLA	OBD-CAD-C3D	-9.63	111.99	127.98
19	G	1242	CLA	C4D-C3D-CAD	9.62	113.83	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	9011	CLA	OBD-CAD-C3D	-9.55	112.12	127.98
21	B	6010	BCR	C21-C20-C19	9.55	153.00	123.22
19	A	1115	CLA	C4D-C3D-CAD	9.54	113.79	108.47
21	1	6023	BCR	C24-C23-C22	-9.52	111.85	126.23
19	A	1309	CLA	C1C-CHC-C4B	-9.50	114.97	129.64
19	B	1239	CLA	OBD-CAD-C3D	-9.50	112.21	127.98
19	4	4013	CLA	C1D-CHD-C4C	-9.48	115.00	129.64
21	L	6019	BCR	C21-C20-C19	9.45	152.70	123.22
19	K	3009	CLA	OBD-CAD-C3D	-9.44	112.31	127.98
19	A	1151	CLA	C4D-C3D-CAD	9.44	113.73	108.47
19	A	1111	CLA	OBD-CAD-C3D	-9.42	112.33	127.98
19	A	1309	CLA	C1D-CHD-C4C	-9.40	115.12	129.64
19	A	9023	CLA	OBD-CAD-CBD	-9.38	112.50	125.89
19	B	1214	CLA	C4D-C3D-CAD	9.37	113.70	108.47
19	I	1204	CLA	C4D-C3D-CAD	9.34	113.68	108.47
19	3	3014	CLA	C1C-CHC-C4B	-9.34	115.22	129.64
19	4	4006	CLA	OBD-CAD-C3D	-9.34	112.48	127.98
19	B	1236	CLA	C4D-C3D-CAD	9.31	113.66	108.47
19	A	1127	CLA	C4D-C3D-CAD	9.31	113.66	108.47
19	3	3013	CLA	C4D-C3D-CAD	9.31	113.66	108.47
21	B	6020	BCR	C21-C20-C19	9.28	152.19	123.22
19	1	1006	CLA	CAB-C3B-C4B	-9.28	114.20	128.46
19	A	1108	CLA	C4D-C3D-CAD	9.27	113.64	108.47
19	A	1123	CLA	OBD-CAD-C3D	-9.27	112.58	127.98
19	A	1101	CLA	OBD-CAD-CBD	-9.26	112.67	125.89
19	B	1231	CLA	OBD-CAD-CBD	-9.24	112.69	125.89
19	A	9012	CLA	C4D-C3D-CAD	9.21	113.61	108.47
19	4	4010	CLA	C1C-CHC-C4B	-9.21	115.42	129.64
19	2	1307	CLA	C1D-CHD-C4C	-9.18	115.46	129.64
19	3	3015	CLA	C1C-CHC-C4B	-9.17	115.49	129.64
19	L	1503	CLA	O2D-CGD-CBD	9.15	127.53	111.27
19	B	1212	CLA	OBD-CAD-CBD	-9.15	112.82	125.89
19	1	1310	CLA	C1C-CHC-C4B	-9.12	115.55	129.64
19	3	3004	CLA	C1D-CHD-C4C	-9.12	115.56	129.64
19	3	3006	CLA	C1C-CHC-C4B	-9.12	115.56	129.64
19	B	1235	CLA	OBD-CAD-C3D	-9.12	112.84	127.98
19	B	1221	CLA	C4D-C3D-CAD	9.11	113.55	108.47
19	2	2003	CLA	C1C-CHC-C4B	-9.10	115.59	129.64
19	B	1238	CLA	OBD-CAD-CBD	-9.09	112.90	125.89
19	2	2005	CLA	C1D-CHD-C4C	-9.09	115.61	129.64
19	3	1147	CLA	OBD-CAD-CBD	-9.09	112.91	125.89
19	3	3005	CLA	C1C-CHC-C4B	-9.07	115.64	129.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	2012	CLA	OBD-CAD-CBD	-9.07	112.94	125.89
19	3	3014	CLA	C1D-CHD-C4C	-9.06	115.64	129.64
21	F	6016	BCR	C21-C20-C19	9.06	151.49	123.22
19	1	1012	CLA	CAB-C3B-C2B	-9.05	106.96	124.69
21	3	6022	BCR	C10-C11-C12	9.05	151.45	123.22
19	4	4013	CLA	C1C-CHC-C4B	-9.03	115.69	129.64
19	B	1214	CLA	OBD-CAD-C3D	-9.03	112.98	127.98
19	4	4005	CLA	C1C-CHC-C4B	-9.01	115.73	129.64
19	3	3010	CLA	C1C-CHC-C4B	-8.99	115.75	129.64
21	A	6003	BCR	C10-C11-C12	8.97	151.22	123.22
19	2	2008	CLA	C1C-CHC-C4B	-8.97	115.79	129.64
19	2	2011	CLA	C1C-CHC-C4B	-8.96	115.81	129.64
19	A	1109	CLA	OBD-CAD-CBD	-8.94	113.13	125.89
19	4	4015	CLA	C4D-C3D-CAD	8.92	113.44	108.47
19	4	4015	CLA	OBD-CAD-C3D	-8.91	113.18	127.98
19	B	1229	CLA	CAA-C2A-C3A	-8.91	88.39	112.78
19	L	1504	CLA	OBD-CAD-C3D	-8.90	113.20	127.98
19	3	3003	CLA	C4D-C3D-CAD	8.90	113.43	108.47
19	B	1235	CLA	C4D-C3D-CAD	8.90	113.43	108.47
19	2	2010	CLA	C1C-CHC-C4B	-8.89	115.91	129.64
21	A	6008	BCR	C21-C20-C19	8.88	150.92	123.22
19	4	1304	CLA	C3D-CAD-CBD	-8.87	95.93	107.61
21	B	6020	BCR	C15-C14-C13	-8.86	114.67	127.31
19	A	1102	CLA	OBD-CAD-CBD	-8.84	113.27	125.89
19	A	1117	CLA	OBD-CAD-C3D	-8.82	113.33	127.98
19	1	1015	CLA	C1C-CHC-C4B	-8.80	116.06	129.64
19	B	1229	CLA	OBD-CAD-CBD	-8.79	113.33	125.89
19	A	1149	CLA	CAB-C3B-C2B	-8.78	107.50	124.69
21	I	6021	BCR	C16-C15-C14	-8.77	105.50	123.47
21	A	6003	BCR	C24-C23-C22	-8.77	112.99	126.23
19	1	1002	CLA	OBD-CAD-CBD	-8.77	113.37	125.89
19	1	1001	CLA	C4A-NA-C1A	8.75	110.64	106.71
19	L	1130	CLA	OBD-CAD-C3D	-8.75	113.46	127.98
19	3	3002	CLA	C1C-CHC-C4B	-8.73	116.17	129.64
19	B	1301	CLA	CAB-C3B-C2B	-8.71	107.63	124.69
19	A	1129	CLA	C4D-C3D-CAD	8.67	113.31	108.47
21	A	6011	BCR	C10-C11-C12	8.66	150.25	123.22
19	4	4003	CLA	OBD-CAD-CBD	-8.66	113.52	125.89
19	4	4011	CLA	C1C-CHC-C4B	-8.65	116.28	129.64
19	A	1109	CLA	OBD-CAD-C3D	-8.65	113.62	127.98
19	3	3011	CLA	C4D-C3D-CAD	8.61	113.27	108.47
19	B	1234	CLA	OBD-CAD-CBD	-8.60	113.60	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1101	CLA	O2D-CGD-CBD	8.60	126.55	111.27
19	B	1220	CLA	C4D-C3D-CAD	8.60	113.26	108.47
21	B	6017	BCR	C21-C20-C19	8.59	150.03	123.22
19	B	1225	CLA	OBD-CAD-CBD	-8.56	113.66	125.89
21	I	6018	BCR	C21-C20-C19	8.53	149.84	123.22
19	B	1201	CLA	OBD-CAD-CBD	-8.41	113.87	125.89
19	A	1106	CLA	OBD-CAD-CBD	-8.35	113.97	125.89
19	B	1212	CLA	C4D-C3D-CAD	8.34	113.12	108.47
19	1	1007	CLA	OBD-CAD-CBD	-8.32	114.00	125.89
21	F	6014	BCR	C10-C11-C12	8.31	149.16	123.22
19	A	9022	CLA	C4D-C3D-CAD	8.29	113.09	108.47
19	1	1002	CLA	OBD-CAD-C3D	-8.29	114.22	127.98
22	H	7011	LMU	C1B-O1B-C4'	-8.29	97.46	117.96
21	I	6021	BCR	C30-C25-C26	-8.26	110.98	122.61
19	3	3001	CLA	C1C-CHC-C4B	-8.25	116.90	129.64
19	B	1214	CLA	OBD-CAD-CBD	-8.22	114.14	125.89
19	4	4015	CLA	OBD-CAD-CBD	-8.22	114.15	125.89
19	B	1228	CLA	C4D-C3D-CAD	8.18	113.03	108.47
19	B	1211	CLA	OBD-CAD-C3D	-8.18	114.40	127.98
19	4	4004	CLA	C1C-CHC-C4B	-8.18	117.02	129.64
19	3	3012	CLA	C1D-CHD-C4C	-8.13	117.09	129.64
19	1	1008	CLA	C3A-C2A-C1A	8.10	113.48	101.34
19	2	1307	CLA	C1C-CHC-C4B	-8.10	117.13	129.64
19	B	1235	CLA	OBD-CAD-CBD	-8.09	114.33	125.89
19	A	1102	CLA	C4D-C3D-CAD	8.08	112.97	108.47
19	L	1130	CLA	C4D-C3D-CAD	8.07	112.97	108.47
19	A	9011	CLA	C3D-CAD-CBD	-8.01	97.05	107.61
19	1	1012	CLA	OBD-CAD-C3D	-8.01	114.68	127.98
19	A	1127	CLA	O2D-CGD-CBD	8.00	125.48	111.27
19	R	1150	CLA	OBD-CAD-C3D	-7.97	114.75	127.98
19	B	1208	CLA	OBD-CAD-C3D	-7.92	114.83	127.98
19	1	1001	CLA	OBD-CAD-CBD	-7.92	114.58	125.89
19	B	1239	CLA	OBD-CAD-CBD	-7.90	114.61	125.89
19	F	1240	CLA	OBD-CAD-C3D	-7.85	114.95	127.98
19	B	1205	CLA	O2D-CGD-CBD	7.84	125.20	111.27
21	L	6019	BCR	C10-C11-C12	7.81	147.60	123.22
19	3	1118	CLA	CAB-C3B-C2B	-7.80	109.41	124.69
19	B	1225	CLA	O2D-CGD-CBD	7.79	125.12	111.27
19	L	1130	CLA	OBD-CAD-CBD	-7.78	114.77	125.89
21	A	6007	BCR	C24-C23-C22	-7.77	114.49	126.23
21	J	6012	BCR	C10-C11-C12	7.77	147.45	123.22
21	B	6005	BCR	C10-C11-C12	7.76	147.44	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	1145	CLA	C3D-CAD-CBD	-7.67	97.50	107.61
21	3	6022	BCR	C16-C17-C18	-7.67	116.37	127.31
19	B	1205	CLA	OBD-CAD-C3D	-7.65	115.27	127.98
19	4	1306	CLA	OBD-CAD-CBD	-7.65	114.96	125.89
21	A	6007	BCR	C10-C11-C12	7.63	147.02	123.22
21	1	6023	BCR	C30-C25-C26	-7.60	111.91	122.61
21	B	6020	BCR	C3-C4-C5	-7.54	100.61	114.08
21	B	6006	BCR	C24-C23-C22	-7.51	114.89	126.23
21	F	6016	BCR	C11-C10-C9	7.46	137.96	127.31
21	I	6021	BCR	C21-C20-C19	7.46	146.49	123.22
19	1	1013	CLA	OBD-CAD-CBD	-7.43	115.28	125.89
19	4	1304	CLA	CGD-CBD-CAD	7.37	134.60	110.73
19	B	1211	CLA	OBD-CAD-CBD	-7.30	115.47	125.89
19	3	3011	CLA	OBD-CAD-CBD	-7.28	115.49	125.89
19	B	1208	CLA	CAB-C3B-C2B	-7.28	110.43	124.69
19	1	1005	CLA	O2D-CGD-CBD	7.28	124.20	111.27
21	B	6006	BCR	C10-C11-C12	7.27	145.91	123.22
19	2	2002	CLA	OBD-CAD-CBD	-7.27	115.51	125.89
19	L	1503	CLA	C3D-CAD-CBD	-7.26	98.05	107.61
19	3	3017	CLA	O2D-CGD-CBD	7.23	124.12	111.27
19	B	1226	CLA	O2D-CGD-CBD	7.22	124.10	111.27
21	A	6008	BCR	C10-C11-C12	7.20	145.68	123.22
19	4	4006	CLA	OBD-CAD-CBD	-7.18	115.63	125.89
19	F	1305	CLA	C4D-C3D-CAD	7.14	112.45	108.47
21	B	6010	BCR	C10-C11-C12	7.12	145.43	123.22
19	2	2007	CLA	O2D-CGD-CBD	7.09	123.86	111.27
19	3	3013	CLA	O2D-CGD-CBD	7.02	123.74	111.27
19	L	1148	CLA	O2D-CGD-CBD	6.98	123.67	111.27
21	I	6018	BCR	C3-C4-C5	-6.97	101.63	114.08
19	B	1208	CLA	OBD-CAD-CBD	-6.93	116.00	125.89
19	F	1240	CLA	C1B-C2B-C3B	-6.93	100.48	106.92
21	1	6023	BCR	C21-C20-C19	6.91	144.78	123.22
19	1	1310	CLA	C2B-C1B-NB	6.90	116.16	110.11
19	B	1234	CLA	O2D-CGD-CBD	6.89	123.51	111.27
19	B	1201	CLA	O2D-CGD-CBD	6.88	123.50	111.27
19	A	1129	CLA	O2D-CGD-CBD	6.88	123.49	111.27
19	4	4012	CLA	CAB-C3B-C2B	-6.88	111.21	124.69
21	F	6016	BCR	C15-C14-C13	-6.85	117.53	127.31
22	G	7051	LMU	O1B-C4'-C3'	6.85	125.51	107.28
21	A	6007	BCR	C20-C21-C22	6.85	137.09	127.31
19	L	1501	CLA	O2D-CGD-CBD	6.83	123.40	111.27
21	I	6018	BCR	C40-C30-C25	6.81	121.35	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1306	CLA	O2D-CGD-CBD	6.81	123.37	111.27
19	3	3003	CLA	CAB-C3B-C2B	-6.79	111.38	124.69
22	E	7048	LMU	C1B-C2B-C3B	-6.79	95.86	110.00
19	1	1013	CLA	C3D-CAD-CBD	-6.74	98.72	107.61
19	A	1128	CLA	O2D-CGD-CBD	6.74	123.25	111.27
19	3	3012	CLA	C2B-C1B-NB	6.71	115.98	110.11
19	B	1235	CLA	O2D-CGD-CBD	6.70	123.18	111.27
19	4	1009	CLA	CAB-C3B-C2B	-6.70	111.56	124.69
19	B	1216	CLA	O2D-CGD-CBD	6.69	123.16	111.27
19	4	4015	CLA	O2D-CGD-CBD	6.69	123.15	111.27
22	3	7005	LMU	C2'-C3'-C4'	-6.66	94.48	109.68
19	A	1132	CLA	O2D-CGD-CBD	6.66	123.10	111.27
19	A	1149	CLA	O2D-CGD-CBD	6.65	123.09	111.27
19	B	1202	CLA	CAA-C2A-C3A	-6.65	94.58	112.78
21	B	6004	BCR	C10-C11-C12	6.64	143.95	123.22
19	L	1148	CLA	C1-C2-C3	-6.64	114.56	126.04
19	A	1121	CLA	O2D-CGD-CBD	6.63	123.04	111.27
21	I	6021	BCR	C34-C9-C10	-6.61	113.66	122.92
22	E	7048	LMU	C3B-C4B-C5B	6.61	122.03	110.24
19	L	1504	CLA	O2D-CGD-CBD	6.54	122.88	111.27
22	R	7014	LMU	C4B-C3B-C2B	-6.53	99.42	110.82
21	B	6017	BCR	C10-C11-C12	6.50	143.50	123.22
21	I	6021	BCR	C16-C17-C18	-6.50	118.04	127.31
19	B	1225	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	3	3014	CLA	C2B-C1B-NB	6.47	115.78	110.11
19	B	1224	CLA	O2D-CGD-CBD	6.46	122.75	111.27
19	1	1303	CLA	O2D-CGD-CBD	6.45	122.73	111.27
21	A	6011	BCR	C15-C14-C13	-6.44	118.12	127.31
19	H	1241	CLA	O2D-CGD-CBD	6.40	122.64	111.27
19	A	1108	CLA	O2D-CGD-CBD	6.39	122.62	111.27
21	A	6003	BCR	C32-C1-C6	-6.34	100.01	110.30
19	J	1311	CLA	O2D-CGD-CBD	6.34	122.53	111.27
19	A	1102	CLA	OBD-CAD-C3D	-6.31	117.50	127.98
19	2	2011	CLA	C2B-C1B-NB	6.30	115.63	110.11
19	L	1502	CLA	CAA-C2A-C3A	-6.29	95.54	112.78
21	B	6006	BCR	C16-C17-C18	-6.29	118.33	127.31
21	I	6021	BCR	C2-C1-C6	-6.28	100.81	110.48
19	B	1221	CLA	O2D-CGD-CBD	6.28	122.43	111.27
19	B	1203	CLA	O2D-CGD-CBD	6.28	122.42	111.27
19	4	4004	CLA	C2B-C1B-NB	6.28	115.61	110.11
21	A	6007	BCR	C16-C17-C18	-6.27	118.36	127.31
19	3	3004	CLA	C4A-NA-C1A	6.26	109.52	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	7002	LMU	O1B-C4'-C3'	6.25	123.90	107.28
19	1	1003	CLA	O2D-CGD-CBD	6.22	122.32	111.27
19	B	1230	CLA	O2D-CGD-CBD	6.22	122.31	111.27
19	B	1236	CLA	O2D-CGD-CBD	6.21	122.31	111.27
19	B	1229	CLA	O2D-CGD-CBD	6.19	122.26	111.27
19	A	1149	CLA	CAA-C2A-C3A	6.18	129.71	112.78
19	B	1202	CLA	O2D-CGD-CBD	6.17	122.24	111.27
19	B	1228	CLA	O2D-CGD-CBD	6.16	122.21	111.27
19	1	1303	CLA	CAA-C2A-C1A	6.15	132.14	111.97
19	A	1123	CLA	OBD-CAD-CBD	-6.15	117.11	125.89
19	3	3004	CLA	C2B-C1B-NB	6.12	115.47	110.11
19	3	1147	CLA	OBD-CAD-C3D	-6.08	117.89	127.98
21	1	6023	BCR	C28-C27-C26	-6.06	103.26	114.08
19	2	2003	CLA	C2B-C1B-NB	6.06	115.42	110.11
19	2	4009	CLA	O2D-CGD-CBD	6.05	122.01	111.27
19	3	3001	CLA	C2B-C1B-NB	6.04	115.40	110.11
19	B	1208	CLA	O2D-CGD-CBD	6.04	122.00	111.27
19	2	1307	CLA	C2B-C1B-NB	6.04	115.40	110.11
19	A	1105	CLA	O2D-CGD-CBD	6.02	121.97	111.27
19	A	9022	CLA	O2D-CGD-CBD	6.01	121.95	111.27
19	L	1502	CLA	O2D-CGD-CBD	6.01	121.95	111.27
19	A	1121	CLA	C3D-CAD-CBD	-6.00	99.71	107.61
22	H	7017	LMU	C1B-O1B-C4'	-5.99	103.13	117.96
21	B	6010	BCR	C24-C23-C22	-5.99	117.18	126.23
19	A	1112	CLA	O2D-CGD-CBD	5.96	121.86	111.27
19	4	4011	CLA	C2B-C1B-NB	5.94	115.31	110.11
19	2	2002	CLA	O2D-CGD-CBD	5.94	121.82	111.27
20	B	5002	PQN	C11-C12-C13	-5.94	116.91	126.79
19	1	1013	CLA	C4A-NA-C1A	5.92	109.37	106.71
21	B	6005	BCR	C31-C1-C6	-5.92	100.70	110.30
19	1	1014	CLA	O2D-CGD-CBD	5.91	121.77	111.27
19	1	1010	CLA	CGD-CBD-CAD	-5.90	91.61	110.73
19	K	3009	CLA	O2D-CGD-CBD	5.88	121.72	111.27
19	L	1130	CLA	O2D-CGD-CBD	5.87	121.70	111.27
19	3	3010	CLA	C2B-C1B-NB	5.86	115.25	110.11
21	A	6008	BCR	C16-C17-C18	-5.85	118.96	127.31
19	A	1107	CLA	O2D-CGD-CBD	5.83	121.63	111.27
19	4	4002	CLA	CAA-C2A-C1A	5.83	131.09	111.97
19	1	1005	CLA	C4D-C3D-CAD	5.83	111.72	108.47
19	4	4010	CLA	C2B-C1B-NB	5.83	115.22	110.11
22	A	7035	LMU	O1B-C4'-C3'	5.83	122.79	107.28
19	1	1006	CLA	CAB-C3B-C2B	-5.81	113.30	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	9013	CLA	O2D-CGD-CBD	5.79	121.56	111.27
19	1	1008	CLA	O2D-CGD-CBD	5.79	121.56	111.27
21	1	6023	BCR	C40-C30-C29	-5.79	85.76	108.91
19	B	1213	CLA	O2D-CGD-CBD	5.78	121.54	111.27
19	G	1242	CLA	C4-C3-C5	5.77	122.58	115.98
19	2	2012	CLA	C4A-NA-C1A	5.76	109.30	106.71
19	4	4004	CLA	C3A-C4A-CHB	-5.73	116.90	123.91
19	1	1010	CLA	C3D-CAD-CBD	-5.72	100.08	107.61
21	F	6014	BCR	C37-C22-C21	-5.72	114.92	122.92
21	A	6007	BCR	C31-C1-C6	-5.70	101.05	110.30
19	3	3014	CLA	C3A-C4A-CHB	-5.69	116.94	123.91
19	2	2013	CLA	C4A-NA-C1A	5.68	109.26	106.71
21	F	6014	BCR	C32-C1-C6	-5.68	101.09	110.30
22	3	7005	LMU	C1B-O5B-C5B	-5.67	102.55	113.69
21	B	6010	BCR	C7-C8-C9	-5.66	117.68	126.23
19	4	4005	CLA	C2B-C1B-NB	5.65	115.05	110.11
19	A	1120	CLA	O2D-CGD-CBD	5.63	121.27	111.27
22	G	7051	LMU	C3'-C4'-C5'	-5.62	98.05	110.93
19	1	1005	CLA	OBD-CAD-C3D	-5.61	118.66	127.98
19	J	1308	CLA	O2D-CGD-CBD	5.61	121.23	111.27
21	B	6004	BCR	C32-C1-C6	-5.61	101.20	110.30
19	F	1240	CLA	CAB-C3B-C4B	-5.60	119.85	128.46
19	2	2012	CLA	O2D-CGD-CBD	5.60	121.23	111.27
19	3	3002	CLA	C2B-C1B-NB	5.60	115.02	110.11
19	B	1221	CLA	OBD-CAD-C3D	-5.60	118.69	127.98
19	2	2008	CLA	C2B-C1B-NB	5.58	115.00	110.11
19	2	2010	CLA	C2B-C1B-NB	5.58	114.99	110.11
21	A	6003	BCR	C23-C24-C25	-5.57	111.55	127.20
21	J	6012	BCR	C24-C23-C22	-5.57	117.82	126.23
21	A	6008	BCR	C31-C1-C6	-5.57	101.27	110.30
21	A	6011	BCR	C7-C8-C9	-5.55	117.85	126.23
21	I	6021	BCR	C8-C9-C10	5.55	127.46	118.94
19	B	1234	CLA	O2D-CGD-O1D	-5.54	113.00	123.84
19	4	4003	CLA	O2D-CGD-CBD	5.54	121.12	111.27
19	B	1221	CLA	OBD-CAD-CBD	-5.54	117.98	125.89
22	3	7003	LMU	C4B-C3B-C2B	5.52	120.47	110.82
21	I	6021	BCR	C1-C6-C5	-5.52	114.83	122.61
19	2	2013	CLA	O2D-CGD-CBD	5.52	121.07	111.27
19	3	3006	CLA	C3A-C4A-CHB	-5.51	117.16	123.91
21	I	6021	BCR	C38-C26-C27	5.50	124.19	113.62
19	B	1205	CLA	O1D-CGD-CBD	-5.49	113.24	124.48
21	A	6003	BCR	C16-C17-C18	-5.49	119.47	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1238	CLA	O2D-CGD-CBD	5.48	121.01	111.27
19	1	1008	CLA	CBA-CAA-C2A	-5.48	97.69	113.86
21	1	6023	BCR	C20-C19-C18	5.47	141.79	126.42
19	F	1305	CLA	CMA-C3A-C4A	5.47	126.47	111.77
19	3	3006	CLA	C2B-C1B-NB	5.46	114.89	110.11
21	B	6004	BCR	C16-C17-C18	-5.45	119.53	127.31
19	1	1015	CLA	C2B-C1B-NB	5.45	114.89	110.11
19	3	3005	CLA	C2B-C1B-NB	5.44	114.88	110.11
19	B	1217	CLA	C3D-CAD-CBD	-5.44	100.44	107.61
19	A	1309	CLA	C2B-C1B-NB	5.44	114.87	110.11
21	F	6016	BCR	C3-C4-C5	-5.43	104.38	114.08
22	N	7049	LMU	C1B-O1B-C4'	-5.42	104.54	117.96
19	3	2009	CLA	C3D-CAD-CBD	-5.42	100.47	107.61
19	A	1135	CLA	O2D-CGD-CBD	5.40	120.86	111.27
19	2	2014	CLA	O2D-CGD-CBD	5.40	120.86	111.27
19	F	1305	CLA	O2D-CGD-CBD	5.39	120.84	111.27
19	A	1124	CLA	O2D-CGD-CBD	5.38	120.83	111.27
19	1	1008	CLA	C3D-CAD-CBD	-5.38	100.52	107.61
21	I	6021	BCR	C38-C26-C25	-5.38	118.49	124.53
19	3	3015	CLA	C2B-C1B-NB	5.37	114.81	110.11
21	1	6023	BCR	C39-C30-C25	5.35	118.98	110.30
21	F	6016	BCR	C24-C23-C22	-5.34	118.16	126.23
19	G	1242	CLA	O2D-CGD-CBD	5.34	120.76	111.27
19	2	2014	CLA	CAA-C2A-C3A	-5.33	98.17	112.78
19	B	1205	CLA	C4A-NA-C1A	5.32	109.10	106.71
19	A	1106	CLA	O2D-CGD-CBD	5.32	120.73	111.27
19	B	1218	CLA	C3D-CAD-CBD	-5.32	100.60	107.61
21	B	6004	BCR	C15-C14-C13	-5.32	119.72	127.31
21	1	6023	BCR	C39-C30-C29	-5.31	87.65	108.91
19	A	1237	CLA	O2D-CGD-CBD	5.31	120.71	111.27
19	A	9022	CLA	C4-C3-C5	5.31	124.20	115.27
22	4	7052	LMU	O1'-C1'-C2'	5.30	116.58	108.30
19	I	1204	CLA	O2D-CGD-CBD	5.30	120.68	111.27
19	A	1137	CLA	O2D-CGD-CBD	5.29	120.67	111.27
19	B	1206	CLA	C3D-CAD-CBD	-5.28	100.65	107.61
21	3	6022	BCR	C7-C8-C9	-5.28	118.26	126.23
19	2	2001	CLA	O2D-CGD-CBD	5.28	120.65	111.27
19	3	1147	CLA	C3D-CAD-CBD	-5.27	100.66	107.61
19	3	3001	CLA	C3A-C4A-CHB	-5.27	117.46	123.91
21	3	6022	BCR	C16-C15-C14	-5.27	112.69	123.47
19	1	1310	CLA	C3A-C4A-CHB	-5.26	117.46	123.91
19	1	1010	CLA	CAA-C2A-C1A	5.26	129.22	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	6017	BCR	C31-C1-C6	-5.26	101.77	110.30
19	A	1115	CLA	O2D-CGD-CBD	5.26	120.61	111.27
19	A	9023	CLA	C3D-CAD-CBD	-5.26	100.69	107.61
19	J	1308	CLA	C4A-NA-C1A	5.24	109.06	106.71
19	R	1144	CLA	C3D-CAD-CBD	-5.24	100.71	107.61
21	1	6023	BCR	C38-C26-C25	-5.23	118.65	124.53
19	L	1504	CLA	OBD-CAD-CBD	-5.22	118.43	125.89
21	F	6016	BCR	C32-C1-C6	-5.22	101.83	110.30
21	L	6019	BCR	C31-C1-C6	-5.22	101.83	110.30
19	4	4002	CLA	C3A-C2A-C1A	5.22	109.16	101.34
19	B	1232	CLA	O2D-CGD-CBD	5.22	120.54	111.27
21	A	6007	BCR	C21-C20-C19	5.21	139.49	123.22
19	B	1217	CLA	O2D-CGD-CBD	5.21	120.53	111.27
19	B	1230	CLA	C3D-CAD-CBD	-5.21	100.74	107.61
19	1	1015	CLA	C3A-C4A-CHB	-5.21	117.53	123.91
19	A	1122	CLA	C3D-CAD-CBD	-5.21	100.75	107.61
19	3	3017	CLA	CBC-CAC-C3C	-5.21	99.00	112.27
19	3	3005	CLA	C3A-C4A-CHB	-5.21	117.53	123.91
19	B	1214	CLA	O2D-CGD-CBD	5.20	120.50	111.27
19	1	1001	CLA	O2D-CGD-CBD	5.19	120.50	111.27
19	3	3007	CLA	O2D-CGD-CBD	5.19	120.50	111.27
21	1	6023	BCR	C15-C14-C13	-5.19	119.90	127.31
19	1	1003	CLA	C3D-CAD-CBD	-5.19	100.77	107.61
19	1	1310	CLA	C3B-C2B-C1B	-5.19	101.84	106.29
21	F	6016	BCR	C10-C11-C12	5.19	139.42	123.22
19	2	2005	CLA	C2B-C1B-NB	5.19	114.65	110.11
19	2	2008	CLA	C4A-NA-C1A	5.18	109.04	106.71
19	4	1304	CLA	CAA-C2A-C3A	-5.18	98.59	112.78
19	1	1008	CLA	CGD-CBD-CAD	-5.17	94.00	110.73
19	1	1010	CLA	O2D-CGD-CBD	5.17	120.45	111.27
21	A	6008	BCR	C20-C19-C18	-5.16	111.91	126.42
19	1	1002	CLA	C4A-NA-C1A	5.16	109.03	106.71
19	B	9010	CLA	C3D-CAD-CBD	-5.16	100.82	107.61
19	3	3016	CLA	O2D-CGD-CBD	5.15	120.43	111.27
19	L	1148	CLA	CMA-C3A-C4A	5.15	125.62	111.77
22	G	7026	LMU	C1'-O5'-C5'	5.15	123.79	113.69
21	B	6017	BCR	C15-C14-C13	-5.14	119.97	127.31
19	K	1146	CLA	O2D-CGD-CBD	5.14	120.40	111.27
19	1	1310	CLA	C2A-C1A-CHA	-5.14	113.87	122.63
19	1	1303	CLA	C4-C3-C5	5.13	121.85	115.98
21	A	6008	BCR	C32-C1-C6	-5.13	101.98	110.30
19	2	2011	CLA	C3A-C4A-CHB	-5.13	117.63	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1007	CLA	O2D-CGD-CBD	5.12	120.38	111.27
19	B	1239	CLA	C3D-CAD-CBD	-5.11	100.87	107.61
21	1	6023	BCR	C40-C30-C25	5.11	118.58	110.30
21	A	6008	BCR	C15-C14-C13	-5.08	120.06	127.31
19	B	1231	CLA	C3D-CAD-CBD	-5.07	100.92	107.61
19	B	1213	CLA	C3D-CAD-CBD	-5.07	100.93	107.61
19	1	1007	CLA	C3D-CAD-CBD	-5.07	100.93	107.61
22	A	7044	LMU	O1'-C1'-C2'	5.07	116.22	108.30
21	F	6014	BCR	C7-C8-C9	-5.07	118.58	126.23
19	4	4014	CLA	O2D-CGD-CBD	5.07	120.27	111.27
22	E	7037	LMU	C1B-O5B-C5B	-5.06	103.75	113.69
19	B	1205	CLA	C3D-CAD-CBD	-5.06	100.94	107.61
21	B	6004	BCR	C24-C23-C22	-5.05	118.60	126.23
19	B	1203	CLA	C4A-NA-C1A	5.05	108.98	106.71
19	B	1223	CLA	O2D-CGD-CBD	5.05	120.24	111.27
22	4	7033	LMU	C3B-C4B-C5B	5.04	119.23	110.24
19	3	3012	CLA	C3B-C2B-C1B	-5.04	101.98	106.29
19	1	1310	CLA	C4A-NA-C1A	5.04	108.97	106.71
19	4	4010	CLA	C3A-C4A-CHB	-5.03	117.75	123.91
19	K	1142	CLA	O2D-CGD-CBD	5.02	120.19	111.27
19	A	1116	CLA	O2D-CGD-CBD	5.02	120.19	111.27
19	A	1134	CLA	O2D-CGD-CBD	5.02	120.19	111.27
19	L	1148	CLA	O2D-CGD-O1D	-5.01	114.05	123.84
21	I	6021	BCR	C29-C30-C25	-5.01	102.78	110.48
19	A	1119	CLA	O2D-CGD-CBD	5.00	120.16	111.27
19	B	1232	CLA	C3D-CAD-CBD	-5.00	101.02	107.61
21	A	6007	BCR	C15-C14-C13	-5.00	120.17	127.31
21	L	6019	BCR	C24-C23-C22	-5.00	118.68	126.23
19	A	1141	CLA	O2D-CGD-CBD	5.00	120.15	111.27
19	A	1149	CLA	CMD-C2D-C3D	-5.00	115.33	124.68
19	A	1138	CLA	O2D-CGD-CBD	5.00	120.15	111.27
19	A	1111	CLA	O2D-CGD-CBD	4.99	120.13	111.27
19	3	3017	CLA	C3D-CAD-CBD	-4.99	101.04	107.61
19	4	4006	CLA	C3D-CAD-CBD	-4.98	101.04	107.61
19	A	1136	CLA	O2D-CGD-CBD	4.98	120.11	111.27
19	3	3012	CLA	C2D-C3D-C4D	-4.98	102.01	106.30
19	3	1147	CLA	C4A-NA-C1A	4.98	108.94	106.71
19	B	1233	CLA	C4-C3-C5	4.97	121.67	115.98
21	A	6002	BCR	C15-C14-C13	-4.97	120.22	127.31
19	A	1131	CLA	C3D-CAD-CBD	-4.96	101.07	107.61
19	A	1149	CLA	C4A-NA-C1A	4.96	108.94	106.71
19	B	1239	CLA	C4A-NA-C1A	4.96	108.94	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1008	CLA	C2A-C3A-C4A	-4.96	93.86	101.87
19	3	3004	CLA	C2A-C1A-CHA	-4.94	114.20	122.63
19	4	4004	CLA	C3B-C2B-C1B	-4.94	102.06	106.29
19	4	4005	CLA	C2A-C1A-CHA	-4.94	114.21	122.63
21	A	6011	BCR	C32-C1-C6	-4.94	102.29	110.30
19	A	1116	CLA	C3D-CAD-CBD	-4.93	101.12	107.61
19	4	4002	CLA	C3D-CAD-CBD	-4.92	101.13	107.61
19	2	2005	CLA	C2A-C1A-CHA	-4.92	114.25	122.63
21	A	6008	BCR	C7-C8-C9	-4.91	118.82	126.23
19	L	1148	CLA	C4-C3-C5	4.89	123.50	115.27
19	A	1133	CLA	O2D-CGD-CBD	4.89	119.96	111.27
19	1	1008	CLA	C4A-NA-C1A	4.88	108.90	106.71
19	A	1104	CLA	O2D-CGD-CBD	4.88	119.94	111.27
19	2	2011	CLA	C3B-C2B-C1B	-4.87	102.12	106.29
21	1	6023	BCR	C36-C18-C19	4.86	125.74	118.08
19	R	1150	CLA	C3D-CAD-CBD	-4.86	101.21	107.61
19	3	1147	CLA	O2D-CGD-CBD	4.86	119.90	111.27
21	I	6018	BCR	C16-C15-C14	-4.86	113.53	123.47
19	4	4011	CLA	C3B-C2B-C1B	-4.85	102.14	106.29
21	A	6002	BCR	C32-C1-C6	-4.85	102.44	110.30
21	L	6019	BCR	C7-C8-C9	-4.85	118.91	126.23
19	3	3014	CLA	C2D-C3D-C4D	-4.85	102.13	106.30
19	1	1002	CLA	C3D-CAD-CBD	-4.84	101.23	107.61
19	B	1233	CLA	O2D-CGD-CBD	4.84	119.88	111.27
21	B	6010	BCR	C31-C1-C6	-4.84	102.45	110.30
19	2	2008	CLA	C3A-C4A-CHB	-4.84	117.99	123.91
19	1	1013	CLA	O2A-CGA-O1A	-4.83	111.39	123.59
19	A	1139	CLA	O2D-CGD-CBD	4.83	119.85	111.27
19	A	1102	CLA	C1-O2A-CGA	4.83	129.12	116.44
19	2	2005	CLA	C2D-C3D-C4D	-4.82	102.15	106.30
21	A	6007	BCR	C7-C8-C9	-4.82	118.95	126.23
19	3	3014	CLA	C3B-C2B-C1B	-4.82	102.17	106.29
21	B	6010	BCR	C29-C30-C25	-4.82	103.07	110.48
21	F	6014	BCR	C15-C14-C13	-4.80	120.45	127.31
21	A	6003	BCR	C7-C8-C9	-4.79	119.00	126.23
22	R	7014	LMU	O2B-C2B-C3B	4.78	121.41	110.35
19	K	1143	CLA	O2D-CGD-CBD	4.78	119.77	111.27
21	A	6003	BCR	C3-C4-C5	-4.78	105.55	114.08
19	B	1234	CLA	C3D-CAD-CBD	-4.77	101.32	107.61
19	A	1151	CLA	C3D-CAD-CBD	-4.77	101.32	107.61
19	4	4001	CLA	O2D-CGD-CBD	4.77	119.75	111.27
19	B	1213	CLA	C4A-NA-C1A	4.77	108.85	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3008	CLA	C3D-CAD-CBD	-4.77	101.33	107.61
19	3	3011	CLA	O2D-CGD-CBD	4.77	119.74	111.27
21	B	6017	BCR	C7-C8-C9	-4.75	119.05	126.23
19	3	3010	CLA	C3A-C4A-CHB	-4.75	118.09	123.91
19	A	1111	CLA	C3D-CAD-CBD	-4.75	101.35	107.61
19	4	1306	CLA	C3D-CAD-CBD	-4.75	101.35	107.61
22	E	7037	LMU	C4B-C3B-C2B	-4.74	102.55	110.82
21	F	6016	BCR	C16-C17-C18	-4.74	120.55	127.31
19	B	1229	CLA	C3D-CAD-CBD	-4.74	101.37	107.61
19	B	1211	CLA	C3D-CAD-CBD	-4.73	101.38	107.61
22	4	7052	LMU	C1'-O5'-C5'	-4.73	104.41	113.69
22	F	7036	LMU	O1'-C1'-C2'	4.72	115.68	108.30
21	B	6005	BCR	C16-C17-C18	-4.72	120.58	127.31
19	B	1211	CLA	CMD-C2D-C3D	-4.72	115.85	124.68
21	1	6023	BCR	C16-C15-C14	-4.72	113.81	123.47
19	H	1505	CLA	C3D-CAD-CBD	-4.72	101.39	107.61
19	1	1008	CLA	CAA-C2A-C3A	4.72	125.69	112.78
21	F	6016	BCR	C31-C1-C6	-4.72	102.65	110.30
19	2	2002	CLA	C3D-CAD-CBD	-4.72	101.39	107.61
19	4	4007	CLA	C3D-CAD-CBD	-4.71	101.40	107.61
19	H	1207	CLA	O2D-CGD-CBD	4.70	119.62	111.27
19	3	3008	CLA	O2D-CGD-CBD	4.70	119.62	111.27
19	2	2003	CLA	C3A-C4A-CHB	-4.69	118.16	123.91
19	B	1208	CLA	C3D-CAD-CBD	-4.69	101.42	107.61
19	1	1013	CLA	CMD-C2D-C3D	-4.69	115.90	124.68
19	4	1009	CLA	C1B-C2B-C3B	-4.69	102.56	106.92
21	B	6005	BCR	C32-C1-C6	-4.69	102.69	110.30
21	1	6023	BCR	C19-C18-C17	-4.69	111.75	118.94
19	F	1302	CLA	C3D-CAD-CBD	-4.69	101.43	107.61
22	4	7033	LMU	C1B-O1B-C4'	-4.69	106.37	117.96
19	2	1307	CLA	C3A-C4A-CHB	-4.68	118.18	123.91
19	A	1127	CLA	C3D-CAD-CBD	-4.68	101.44	107.61
21	3	6022	BCR	C2-C1-C6	-4.67	103.29	110.48
22	R	7014	LMU	O1B-C1B-C2B	4.67	120.19	108.10
19	2	1307	CLA	C2D-C3D-C4D	-4.66	102.29	106.30
19	3	3012	CLA	C3D-C4D-ND	4.66	114.19	110.14
19	3	3007	CLA	C3D-CAD-CBD	-4.66	101.47	107.61
22	R	7021	LMU	O1B-C4'-C3'	4.66	119.67	107.28
19	2	2012	CLA	C3D-CAD-CBD	-4.66	101.47	107.61
19	1	1001	CLA	C3D-CAD-CBD	-4.65	101.48	107.61
19	1	1001	CLA	CHB-C4A-NA	4.64	130.94	124.51
19	4	4007	CLA	O2D-CGD-CBD	4.64	119.51	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3002	CLA	C2A-C1A-CHA	-4.64	114.72	122.63
21	B	6004	BCR	C20-C19-C18	-4.63	113.41	126.42
21	B	6004	BCR	C7-C8-C9	-4.63	119.24	126.23
19	B	1210	CLA	C3D-CAD-CBD	-4.62	101.52	107.61
19	A	1128	CLA	C4A-NA-C1A	4.62	108.78	106.71
19	4	1306	CLA	C4A-NA-C1A	4.62	108.78	106.71
21	A	6007	BCR	C32-C1-C6	-4.61	102.81	110.30
21	J	6012	BCR	C15-C14-C13	-4.61	120.73	127.31
22	H	7032	LMU	C1B-O5B-C5B	4.61	122.73	113.69
19	4	4001	CLA	C3D-CAD-CBD	-4.60	101.54	107.61
19	3	3014	CLA	C2A-C1A-CHA	-4.60	114.79	122.63
19	2	1307	CLA	C2A-C1A-CHA	-4.59	114.80	122.63
19	A	1101	CLA	C3D-CAD-CBD	-4.59	101.56	107.61
19	3	3008	CLA	CMD-C2D-C3D	-4.59	116.09	124.68
19	3	3012	CLA	C3A-C4A-CHB	-4.59	118.29	123.91
19	F	1305	CLA	C1-C2-C3	-4.59	118.11	126.04
19	B	1225	CLA	O2D-CGD-O1D	-4.58	114.88	123.84
19	A	1121	CLA	O1D-CGD-CBD	-4.58	115.12	124.48
19	1	1013	CLA	O2A-CGA-CBA	4.58	126.27	111.91
19	B	1209	CLA	C3D-CAD-CBD	-4.58	101.58	107.61
19	B	1231	CLA	C4A-NA-C1A	4.58	108.76	106.71
19	4	4011	CLA	C2A-C1A-CHA	-4.57	114.83	122.63
19	3	3013	CLA	O1D-CGD-CBD	-4.57	115.13	124.48
19	2	2001	CLA	C3D-CAD-CBD	-4.57	101.59	107.61
19	A	1140	CLA	O2D-CGD-CBD	4.57	119.39	111.27
19	3	3012	CLA	C3D-C2D-C1D	4.57	110.24	106.30
19	R	1144	CLA	O2D-CGD-CBD	4.56	119.38	111.27
19	A	1109	CLA	C3D-CAD-CBD	-4.56	101.60	107.61
19	1	1014	CLA	C3D-CAD-CBD	-4.56	101.60	107.61
21	A	6007	BCR	C2-C1-C6	-4.56	103.47	110.48
19	J	1308	CLA	C3D-CAD-CBD	-4.55	101.62	107.61
21	A	6002	BCR	C11-C10-C9	-4.54	120.82	127.31
19	2	2010	CLA	C3A-C4A-CHB	-4.54	118.35	123.91
19	4	4002	CLA	C4A-NA-C1A	4.54	108.75	106.71
19	B	1209	CLA	O2D-CGD-CBD	4.54	119.33	111.27
19	A	1125	CLA	O2D-CGD-CBD	4.54	119.33	111.27
19	B	1226	CLA	C4A-NA-C1A	4.54	108.75	106.71
21	B	6004	BCR	C31-C1-C6	-4.54	102.94	110.30
21	3	6022	BCR	C37-C22-C21	-4.53	116.57	122.92
19	A	1119	CLA	C3D-CAD-CBD	-4.53	101.64	107.61
19	4	4011	CLA	C3A-C4A-CHB	-4.53	118.36	123.91
19	A	1126	CLA	C3D-CAD-CBD	-4.53	101.64	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1139	CLA	C3D-CAD-CBD	-4.53	101.64	107.61
21	1	6023	BCR	C3-C4-C5	-4.52	106.00	114.08
21	L	6019	BCR	C29-C30-C25	-4.52	103.52	110.48
19	B	1226	CLA	C3D-CAD-CBD	-4.52	101.66	107.61
19	A	1121	CLA	C4A-NA-C1A	4.51	108.73	106.71
19	B	1222	CLA	C3D-CAD-CBD	-4.51	101.66	107.61
19	R	1150	CLA	O2A-C1-C2	4.51	120.48	108.64
19	A	1136	CLA	C3D-CAD-CBD	-4.51	101.67	107.61
19	B	1229	CLA	O2D-CGD-O1D	-4.51	115.03	123.84
19	A	1309	CLA	C2A-C1A-CHA	-4.51	114.95	122.63
19	1	1005	CLA	O2D-CGD-O1D	-4.50	115.03	123.84
19	B	1220	CLA	C6-C5-C3	-4.50	101.65	113.45
19	A	1115	CLA	C1-C2-C3	-4.50	118.26	126.04
21	3	6022	BCR	C31-C1-C6	-4.50	103.00	110.30
19	A	1141	CLA	C3D-CAD-CBD	-4.50	101.68	107.61
19	3	3001	CLA	C3B-C2B-C1B	-4.49	102.44	106.29
19	A	1112	CLA	C3D-CAD-CBD	-4.49	101.69	107.61
19	B	1225	CLA	C3D-CAD-CBD	-4.49	101.70	107.61
21	I	6021	BCR	C31-C1-C6	-4.49	103.02	110.30
19	L	1148	CLA	CMD-C2D-C3D	-4.47	116.31	124.68
19	2	2003	CLA	C2A-C1A-CHA	-4.47	115.01	122.63
19	A	1117	CLA	C3D-CAD-CBD	-4.46	101.73	107.61
19	2	1307	CLA	C3D-C4D-ND	4.46	114.02	110.14
19	B	1201	CLA	O2D-CGD-O1D	-4.46	115.11	123.84
19	4	4013	CLA	C2B-C1B-NB	4.46	114.02	110.11
19	L	1502	CLA	C3D-CAD-CBD	-4.46	101.73	107.61
19	A	1102	CLA	O2A-CGA-CBA	4.46	125.90	111.91
19	4	4002	CLA	CMB-C2B-C3B	4.45	133.01	124.68
19	4	4007	CLA	C4A-NA-C1A	4.45	108.71	106.71
19	L	1148	CLA	C3D-CAD-CBD	-4.45	101.75	107.61
19	2	2014	CLA	C3D-CAD-CBD	-4.45	101.75	107.61
19	F	1302	CLA	O2D-CGD-CBD	4.45	119.17	111.27
19	L	1130	CLA	C4-C3-C5	4.44	122.74	115.27
19	J	1311	CLA	C3D-CAD-CBD	-4.44	101.76	107.61
19	A	9013	CLA	C3D-CAD-CBD	-4.44	101.76	107.61
19	2	2007	CLA	O2D-CGD-O1D	-4.44	115.16	123.84
19	3	3001	CLA	C2A-C1A-CHA	-4.43	115.07	122.63
19	A	1134	CLA	C3D-CAD-CBD	-4.43	101.77	107.61
19	B	1219	CLA	C3D-CAD-CBD	-4.43	101.78	107.61
19	3	3005	CLA	C4A-NA-C1A	4.42	108.69	106.71
19	2	2008	CLA	C2A-C1A-CHA	-4.42	115.09	122.63
22	E	7048	LMU	C1B-O1B-C4'	-4.42	107.03	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3015	CLA	C2A-C1A-CHA	-4.42	115.10	122.63
19	4	1004	CLA	C3D-CAD-CBD	-4.42	101.79	107.61
19	K	1142	CLA	C3D-CAD-CBD	-4.41	101.80	107.61
21	I	6018	BCR	C28-C27-C26	-4.41	106.20	114.08
19	4	4012	CLA	C1B-C2B-C3B	-4.41	102.82	106.92
19	B	1218	CLA	O2D-CGD-CBD	4.41	119.10	111.27
21	F	6014	BCR	C24-C23-C22	-4.41	119.57	126.23
19	B	1227	CLA	O2D-CGD-CBD	4.41	119.10	111.27
19	B	1220	CLA	O2D-CGD-CBD	4.41	119.10	111.27
21	A	6008	BCR	C3-C4-C5	-4.40	106.21	114.08
19	3	3014	CLA	C3D-C2D-C1D	4.40	110.10	106.30
19	L	1503	CLA	O1D-CGD-CBD	-4.40	115.47	124.48
19	B	1201	CLA	C3D-CAD-CBD	-4.40	101.81	107.61
19	3	3010	CLA	C2A-C1A-CHA	-4.40	115.14	122.63
19	A	1149	CLA	O2A-CGA-CBA	4.39	125.70	111.91
19	3	3004	CLA	C3A-C4A-CHB	-4.39	118.53	123.91
19	K	3009	CLA	C3D-CAD-CBD	-4.39	101.82	107.61
19	B	1222	CLA	O2D-CGD-CBD	4.39	119.06	111.27
19	B	1212	CLA	O2D-CGD-CBD	4.38	119.06	111.27
19	L	1504	CLA	O2D-CGD-O1D	-4.38	115.27	123.84
19	B	1223	CLA	C3D-CAD-CBD	-4.38	101.84	107.61
21	L	6019	BCR	C39-C30-C25	4.38	117.40	110.30
19	A	1124	CLA	C3D-CAD-CBD	-4.37	101.85	107.61
21	A	6003	BCR	C31-C1-C6	-4.37	103.21	110.30
19	4	4003	CLA	C3D-CAD-CBD	-4.37	101.85	107.61
19	A	1109	CLA	C4A-NA-C1A	4.37	108.67	106.71
19	A	1149	CLA	C3A-C2A-C1A	4.37	107.88	101.34
19	3	3015	CLA	C3A-C4A-CHB	-4.37	118.56	123.91
19	H	1145	CLA	CHB-C4A-NA	4.37	130.55	124.51
19	1	1011	CLA	CMD-C2D-C3D	-4.37	116.51	124.68
19	B	1226	CLA	OBD-CAD-CBD	-4.36	119.66	125.89
19	1	1003	CLA	CMD-C2D-C3D	-4.36	116.52	124.68
19	A	1149	CLA	O2D-CGD-O1D	-4.36	115.32	123.84
19	A	1110	CLA	O2D-CGD-CBD	4.35	119.01	111.27
19	B	1226	CLA	CMD-C2D-C3D	-4.35	116.54	124.68
21	1	6023	BCR	C38-C26-C27	4.35	121.97	113.62
21	B	6020	BCR	C4-C5-C6	-4.34	116.42	122.73
22	3	7005	LMU	O1B-C1B-O5B	-4.34	98.54	110.67
19	1	1310	CLA	C2D-C3D-C4D	-4.34	102.56	106.30
21	A	6011	BCR	C31-C1-C6	-4.34	103.26	110.30
19	B	1227	CLA	C3D-CAD-CBD	-4.34	101.90	107.61
19	B	1238	CLA	CMD-C2D-C3D	-4.33	116.57	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	1307	CLA	C3B-C2B-C1B	-4.33	102.58	106.29
19	A	1131	CLA	O2D-CGD-CBD	4.33	118.97	111.27
19	1	1013	CLA	CGD-CBD-CAD	-4.33	96.71	110.73
19	B	1220	CLA	C3D-CAD-CBD	-4.33	101.91	107.61
19	A	1133	CLA	C3D-CAD-CBD	-4.32	101.91	107.61
19	4	4005	CLA	C3A-C4A-CHB	-4.32	118.61	123.91
19	A	1138	CLA	C3D-CAD-CBD	-4.32	101.91	107.61
19	B	1216	CLA	C3D-CAD-CBD	-4.32	101.92	107.61
19	4	4010	CLA	C3B-C2B-C1B	-4.31	102.60	106.29
19	1	1003	CLA	O2D-CGD-O1D	-4.31	115.41	123.84
19	2	2005	CLA	C3D-C4D-ND	4.31	113.89	110.14
19	A	1132	CLA	C4-C3-C5	4.31	122.52	115.27
19	A	1137	CLA	C3D-CAD-CBD	-4.31	101.93	107.61
19	F	1305	CLA	O2D-CGD-O1D	-4.30	115.43	123.84
21	A	6003	BCR	C15-C14-C13	-4.30	121.17	127.31
19	3	3006	CLA	C4A-NA-C1A	4.30	108.64	106.71
19	1	1310	CLA	C3D-C4D-ND	4.30	113.87	110.14
19	K	1143	CLA	C3D-CAD-CBD	-4.30	101.95	107.61
21	B	6017	BCR	C15-C16-C17	-4.29	114.68	123.47
19	A	1309	CLA	C3A-C4A-CHB	-4.29	118.65	123.91
19	A	1120	CLA	C3D-CAD-CBD	-4.29	101.95	107.61
22	4	7019	LMU	C2'-C3'-C4'	4.29	119.48	109.68
19	4	4002	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
19	3	1147	CLA	CAA-C2A-C1A	4.28	126.00	111.97
21	I	6018	BCR	C10-C11-C12	4.28	136.57	123.22
19	A	1109	CLA	CMD-C2D-C3D	-4.28	116.67	124.68
21	1	6023	BCR	C40-C30-C39	4.28	121.66	108.53
21	A	6007	BCR	C20-C19-C18	-4.28	114.40	126.42
19	A	1132	CLA	CMD-C2D-C3D	-4.28	116.68	124.68
19	H	1505	CLA	C4-C3-C5	4.27	122.46	115.27
21	L	6019	BCR	C3-C4-C5	-4.27	106.45	114.08
19	3	3002	CLA	C3A-C4A-CHB	-4.27	118.68	123.91
19	A	1126	CLA	C1-C2-C3	-4.27	118.67	126.04
19	A	1107	CLA	C3D-CAD-CBD	-4.26	101.99	107.61
19	3	3006	CLA	C3B-C2B-C1B	-4.26	102.64	106.29
19	A	9023	CLA	CHB-C4A-NA	4.26	130.40	124.51
19	3	3012	CLA	C2A-C1A-CHA	-4.26	115.37	122.63
22	B	7040	LMU	O5B-C5B-C4B	-4.25	101.97	109.69
19	1	1001	CLA	CMD-C2D-C3D	-4.25	116.73	124.68
19	4	4014	CLA	C4A-NA-C1A	4.25	108.62	106.71
19	A	1101	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
22	2	7031	LMU	O1B-C1B-C2B	4.24	119.10	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	6017	BCR	C32-C1-C6	-4.24	103.42	110.30
19	1	1003	CLA	CGD-CBD-CAD	-4.24	97.00	110.73
19	3	3002	CLA	C4A-NA-C1A	4.24	108.61	106.71
21	I	6018	BCR	C29-C30-C25	-4.24	103.96	110.48
21	A	6007	BCR	C33-C5-C6	-4.24	119.77	124.53
19	A	1140	CLA	C3D-CAD-CBD	-4.23	102.03	107.61
19	B	1238	CLA	C3D-CAD-CBD	-4.23	102.03	107.61
19	A	9012	CLA	O2D-CGD-CBD	4.23	118.79	111.27
19	3	3010	CLA	C4A-NA-C1A	4.23	108.61	106.71
22	R	7014	LMU	C1'-C2'-C3'	-4.23	101.19	110.00
19	A	1111	CLA	C4A-NA-C1A	4.22	108.61	106.71
19	A	9012	CLA	C3D-CAD-CBD	-4.22	102.04	107.61
19	A	1105	CLA	C3D-CAD-CBD	-4.22	102.05	107.61
19	A	1237	CLA	C4A-NA-C1A	4.22	108.60	106.71
19	3	3001	CLA	C4A-NA-C1A	4.22	108.60	106.71
19	4	4012	CLA	C4A-NA-C1A	4.21	108.60	106.71
21	A	6003	BCR	C2-C1-C6	-4.21	104.00	110.48
19	B	1215	CLA	O2D-CGD-CBD	4.21	118.75	111.27
19	2	2012	CLA	O2D-CGD-O1D	-4.21	115.62	123.84
21	3	6022	BCR	C33-C5-C6	-4.21	119.81	124.53
21	L	6019	BCR	C23-C24-C25	-4.20	115.40	127.20
19	B	1301	CLA	C4A-NA-C1A	4.20	108.59	106.71
19	3	3012	CLA	C4A-NA-C1A	4.20	108.59	106.71
22	H	7017	LMU	C1'-O5'-C5'	4.20	121.93	113.69
19	3	3016	CLA	C3D-CAD-CBD	-4.20	102.08	107.61
22	4	7052	LMU	C1'-C2'-C3'	4.20	118.73	110.00
19	A	1126	CLA	O2D-CGD-CBD	4.19	118.72	111.27
19	1	1002	CLA	CAA-C2A-C1A	4.19	125.72	111.97
19	A	1113	CLA	C3D-CAD-CBD	-4.19	102.09	107.61
19	B	1210	CLA	O2D-CGD-CBD	4.18	118.70	111.27
19	4	4010	CLA	C2A-C1A-CHA	-4.18	115.50	122.63
19	A	1115	CLA	C4-C3-C5	4.18	122.30	115.27
19	1	1006	CLA	C4A-NA-C1A	4.18	108.58	106.71
19	1	1015	CLA	C2A-C1A-CHA	-4.18	115.51	122.63
19	3	3014	CLA	C3D-C4D-ND	4.17	113.77	110.14
19	1	1015	CLA	C3B-C2B-C1B	-4.17	102.72	106.29
19	4	4015	CLA	C3D-CAD-CBD	-4.17	102.11	107.61
19	R	1150	CLA	O2A-CGA-CBA	4.16	124.98	111.91
19	2	2005	CLA	C3A-C4A-CHB	-4.16	118.81	123.91
19	L	1504	CLA	C4A-NA-C1A	4.16	108.58	106.71
19	4	4015	CLA	O1D-CGD-CBD	-4.16	115.97	124.48
19	2	1307	CLA	C4A-NA-C1A	4.16	108.58	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3014	CLA	C4A-NA-C1A	4.16	108.58	106.71
19	4	4013	CLA	C3A-C4A-CHB	-4.16	118.82	123.91
21	I	6018	BCR	C23-C22-C21	4.15	125.31	118.94
19	3	3013	CLA	CED-O2D-CGD	4.15	125.33	115.94
21	A	6002	BCR	C31-C1-C6	-4.15	103.57	110.30
19	B	9010	CLA	C4A-NA-C1A	4.15	108.57	106.71
19	L	1504	CLA	C3D-CAD-CBD	-4.14	102.15	107.61
19	A	1125	CLA	C3D-CAD-CBD	-4.14	102.15	107.61
19	B	1202	CLA	C3D-CAD-CBD	-4.14	102.16	107.61
19	A	1103	CLA	C3D-CAD-CBD	-4.14	102.16	107.61
24	B	7101	LMG	O7-C10-C11	4.14	120.42	111.50
19	1	1008	CLA	CMD-C2D-C3D	-4.14	116.94	124.68
19	1	1015	CLA	C4A-NA-C1A	4.13	108.56	106.71
19	2	2010	CLA	C2A-C1A-CHA	-4.13	115.58	122.63
21	A	6011	BCR	C2-C1-C6	-4.13	104.12	110.48
22	G	7039	LMU	C1B-O5B-C5B	-4.13	105.58	113.69
20	A	5001	PQN	C14-C13-C15	4.13	122.22	115.27
19	F	1305	CLA	C3D-CAD-CBD	-4.13	102.17	107.61
21	F	6014	BCR	C29-C30-C25	-4.11	104.15	110.48
19	B	1203	CLA	C3D-CAD-CBD	-4.11	102.19	107.61
22	R	7014	LMU	O1'-C1'-C2'	4.11	114.72	108.30
19	3	3001	CLA	C3D-C2D-C1D	4.11	109.84	106.30
19	B	1202	CLA	C4A-NA-C1A	4.10	108.55	106.71
22	B	7040	LMU	C1B-O1B-C4'	-4.10	107.82	117.96
21	F	6016	BCR	C8-C7-C6	-4.09	115.70	127.20
19	B	1234	CLA	CMD-C2D-C3D	-4.09	117.02	124.68
19	A	1129	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
19	1	1010	CLA	C4A-NA-C1A	4.08	108.54	106.71
19	2	2003	CLA	C4A-NA-C1A	4.08	108.54	106.71
19	K	1146	CLA	CMB-C2B-C3B	4.08	132.32	124.68
19	4	4004	CLA	C4A-NA-C1A	4.08	108.54	106.71
19	A	1135	CLA	C3D-CAD-CBD	-4.08	102.23	107.61
19	B	1235	CLA	O2D-CGD-O1D	-4.08	115.86	123.84
21	B	6005	BCR	C38-C26-C25	-4.08	119.94	124.53
22	1	7013	LMU	O1B-C4'-C3'	4.08	118.14	107.28
19	A	1237	CLA	C3D-CAD-CBD	-4.08	102.24	107.61
19	B	1203	CLA	CHB-C4A-NA	4.07	130.15	124.51
21	A	6002	BCR	C7-C8-C9	-4.07	120.08	126.23
21	I	6021	BCR	C15-C16-C17	4.07	131.82	123.47
22	H	7043	LMU	O5B-C5B-C4B	4.07	117.09	109.69
22	H	7043	LMU	C1B-O5B-C5B	4.07	121.68	113.69
19	B	1235	CLA	C4-C3-C5	4.07	122.12	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1144	CLA	CMD-C2D-C3D	-4.07	117.06	124.68
19	2	2004	CLA	O2D-CGD-CBD	4.07	118.50	111.27
19	B	1215	CLA	C3D-CAD-CBD	-4.07	102.25	107.61
19	R	1150	CLA	CMD-C2D-C3D	-4.07	117.07	124.68
19	G	1242	CLA	C3D-CAD-CBD	-4.07	102.25	107.61
19	A	9022	CLA	C4A-NA-C1A	4.06	108.53	106.71
21	A	6011	BCR	C33-C5-C6	-4.06	119.97	124.53
19	3	3010	CLA	C3B-C2B-C1B	-4.05	102.82	106.29
19	B	1221	CLA	C4A-NA-C1A	4.05	108.53	106.71
19	2	2006	CLA	C4A-NA-C1A	4.05	108.53	106.71
22	K	7001	LMU	C1B-C2B-C3B	4.05	118.43	110.00
19	2	2003	CLA	C3B-C2B-C1B	-4.04	102.83	106.29
19	A	1113	CLA	O2D-CGD-CBD	4.04	118.45	111.27
19	A	1103	CLA	O2D-CGD-CBD	4.04	118.45	111.27
19	L	1502	CLA	CHB-C4A-NA	4.04	130.10	124.51
21	A	6002	BCR	C11-C12-C13	-4.04	115.06	126.42
19	B	1202	CLA	CMD-C2D-C3D	-4.04	117.12	124.68
19	F	1240	CLA	C4B-C3B-C2B	4.03	110.67	106.92
19	A	1104	CLA	C3D-CAD-CBD	-4.03	102.30	107.61
19	H	1241	CLA	C3D-CAD-CBD	-4.02	102.31	107.61
21	B	6004	BCR	C23-C24-C25	-4.02	115.90	127.20
19	L	1148	CLA	C1B-CHB-C4A	-4.02	122.15	130.12
19	B	1208	CLA	C1B-C2B-C3B	-4.02	103.18	106.92
19	1	1006	CLA	C1B-C2B-C3B	-4.02	103.18	106.92
19	B	1233	CLA	C3D-CAD-CBD	-4.02	102.32	107.61
19	4	4013	CLA	C2A-C1A-CHA	-4.02	115.78	122.63
19	L	1501	CLA	C3D-CAD-CBD	-4.01	102.32	107.61
19	H	1505	CLA	CMD-C2D-C3D	-4.01	117.17	124.68
21	B	6020	BCR	C33-C5-C4	4.01	121.33	113.62
21	B	6020	BCR	C36-C18-C19	4.01	124.40	118.08
19	4	4012	CLA	CBD-CHA-C1A	4.01	133.85	127.43
21	A	6002	BCR	C2-C1-C6	-4.01	104.31	110.48
21	A	6008	BCR	C23-C24-C25	-4.01	115.95	127.20
19	A	1115	CLA	C3D-CAD-CBD	-4.00	102.33	107.61
19	4	4011	CLA	C4A-NA-C1A	4.00	108.51	106.71
21	A	6011	BCR	C23-C24-C25	-4.00	115.96	127.20
21	I	6021	BCR	C8-C7-C6	-4.00	115.96	127.20
19	4	4005	CLA	C3B-C2B-C1B	-4.00	102.86	106.29
19	B	1224	CLA	O2A-CGA-CBA	4.00	124.46	111.91
22	G	7051	LMU	O1'-C1'-C2'	4.00	114.55	108.30
19	3	3005	CLA	C3B-C2B-C1B	-4.00	102.87	106.29
19	H	1145	CLA	CMA-C3A-C4A	-4.00	101.03	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1211	CLA	O2D-CGD-CBD	4.00	118.37	111.27
21	B	6010	BCR	C38-C26-C27	3.99	121.29	113.62
19	A	1111	CLA	C1-C2-C3	-3.99	119.14	126.04
21	B	6005	BCR	C34-C9-C10	-3.99	117.34	122.92
19	A	9022	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
19	B	1208	CLA	CMD-C2D-C3D	-3.98	117.23	124.68
21	B	6020	BCR	C8-C9-C10	3.98	125.05	118.94
19	3	3017	CLA	CMD-C2D-C3D	-3.98	117.23	124.68
19	B	1212	CLA	C3D-CAD-CBD	-3.97	102.37	107.61
19	B	1220	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
22	B	7038	LMU	C3'-C4'-C5'	-3.97	101.82	110.93
19	A	1116	CLA	O2A-CGA-CBA	3.97	124.37	111.91
19	A	1110	CLA	C3D-CAD-CBD	-3.97	102.38	107.61
19	B	1217	CLA	C4A-NA-C1A	3.97	108.49	106.71
19	3	3005	CLA	C2A-C1A-CHA	-3.97	115.87	122.63
19	2	1307	CLA	C3D-C2D-C1D	3.97	109.72	106.30
19	4	4005	CLA	C4A-NA-C1A	3.97	108.49	106.71
19	B	1221	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
19	B	1219	CLA	C4-C3-C5	3.96	121.94	115.27
19	A	1103	CLA	C4A-NA-C1A	3.96	108.49	106.71
21	1	6023	BCR	C32-C1-C2	3.96	124.75	108.91
21	B	6005	BCR	C15-C14-C13	-3.96	121.66	127.31
21	B	6006	BCR	C40-C30-C25	3.96	116.72	110.30
19	H	1505	CLA	O2D-CGD-CBD	3.96	118.30	111.27
19	K	3009	CLA	O2D-CGD-O1D	-3.96	116.10	123.84
22	H	7017	LMU	O5B-C5B-C4B	-3.95	102.51	109.69
19	B	1215	CLA	C4A-NA-C1A	3.95	108.48	106.71
22	E	7048	LMU	O5B-C5B-C6B	3.95	116.25	106.44
19	4	1004	CLA	O2D-CGD-CBD	3.95	118.28	111.27
19	B	1301	CLA	CAA-C2A-C3A	-3.95	106.89	116.10
19	3	3001	CLA	C2D-C3D-C4D	-3.95	102.90	106.30
19	4	4011	CLA	C3D-C2D-C1D	3.94	109.70	106.30
19	2	2006	CLA	C3D-CAD-CBD	-3.94	102.42	107.61
19	2	2007	CLA	C3D-CAD-CBD	-3.94	102.42	107.61
19	3	3017	CLA	C4A-NA-C1A	3.94	108.48	106.71
19	B	1221	CLA	C3D-CAD-CBD	-3.94	102.42	107.61
19	B	1239	CLA	O2A-CGA-CBA	3.94	124.26	111.91
19	B	1231	CLA	O2D-CGD-CBD	3.94	118.26	111.27
19	2	2005	CLA	C3D-C2D-C1D	3.93	109.69	106.30
19	4	4002	CLA	O2A-CGA-CBA	3.93	124.23	111.91
19	2	2004	CLA	C3D-CAD-CBD	-3.93	102.44	107.61
21	F	6016	BCR	C39-C30-C25	3.93	116.67	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	4015	CLA	C4A-NA-C1A	3.92	108.47	106.71
19	A	9013	CLA	C1-C2-C3	3.92	132.82	126.04
19	1	1002	CLA	CED-O2D-CGD	3.92	124.80	115.94
19	2	2013	CLA	C3D-CAD-CBD	-3.91	102.45	107.61
19	A	1151	CLA	CMD-C2D-C3D	-3.91	117.36	124.68
21	I	6018	BCR	C12-C13-C14	-3.91	112.94	118.94
19	4	4004	CLA	C2A-C1A-CHA	-3.91	115.97	122.63
19	2	2002	CLA	CMD-C2D-C3D	-3.91	117.36	124.68
19	B	1201	CLA	CMD-C2D-C3D	-3.90	117.37	124.68
19	3	1147	CLA	CBA-CAA-C2A	-3.90	102.34	113.86
22	2	7027	LMU	C1B-O1B-C4'	-3.90	108.31	117.96
22	R	7024	LMU	O5B-C1B-C2B	3.90	118.61	110.35
19	A	1123	CLA	C3D-CAD-CBD	-3.90	102.47	107.61
21	F	6016	BCR	C20-C19-C18	-3.90	115.47	126.42
21	I	6018	BCR	C4-C5-C6	-3.89	117.08	122.73
19	B	1220	CLA	C2A-C1A-CHA	-3.89	117.06	123.86
19	H	1207	CLA	C3D-CAD-CBD	-3.89	102.48	107.61
22	A	7016	LMU	C4B-C3B-C2B	3.89	117.61	110.82
19	A	1120	CLA	C4-C3-C5	3.89	120.43	115.98
22	3	7003	LMU	C1B-O1B-C4'	-3.89	108.34	117.96
19	B	1224	CLA	O1D-CGD-CBD	-3.88	116.54	124.48
19	A	1109	CLA	C1-C2-C3	-3.88	119.34	126.04
19	F	1305	CLA	CBA-CAA-C2A	-3.88	102.42	113.86
19	A	1132	CLA	C3D-CAD-CBD	-3.87	102.51	107.61
19	F	1240	CLA	CMB-C2B-C3B	3.87	132.26	124.69
19	1	1011	CLA	C1B-C2B-C3B	-3.87	103.32	106.92
21	A	6003	BCR	C15-C16-C17	-3.87	115.56	123.47
22	H	7017	LMU	C4B-C3B-C2B	3.87	117.57	110.82
19	1	1015	CLA	C2D-C3D-C4D	-3.86	102.97	106.30
19	4	4002	CLA	CBC-CAC-C3C	-3.86	102.43	112.27
22	B	7038	LMU	C1'-O5'-C5'	3.86	121.27	113.69
19	4	4011	CLA	C2D-C3D-C4D	-3.86	102.98	106.30
19	F	1240	CLA	C4A-NA-C1A	3.86	108.44	106.71
21	A	6002	BCR	C10-C11-C12	-3.86	111.18	123.22
19	4	4005	CLA	C3D-C2D-C1D	3.85	109.62	106.30
19	B	1228	CLA	C4A-NA-C1A	3.85	108.44	106.71
21	B	6005	BCR	C24-C23-C22	-3.85	120.41	126.23
22	A	7023	LMU	C2'-C3'-C4'	3.85	118.47	109.68
21	A	6003	BCR	C38-C26-C25	-3.85	120.21	124.53
19	2	2011	CLA	C2A-C1A-CHA	-3.85	116.07	122.63
19	K	1146	CLA	C3D-CAD-CBD	-3.85	102.54	107.61
22	B	7038	LMU	C1B-O5B-C5B	3.84	121.23	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1130	CLA	CMB-C2B-C3B	3.84	131.87	124.68
19	A	1119	CLA	CMD-C2D-C3D	-3.84	117.49	124.68
19	1	1006	CLA	CBD-CHA-C1A	3.84	133.58	127.43
19	4	4006	CLA	O2D-CGD-CBD	3.84	118.09	111.27
19	4	1304	CLA	CMD-C2D-C3D	-3.84	117.50	124.68
19	B	1203	CLA	C6-C5-C3	-3.83	103.40	113.45
21	A	6002	BCR	C39-C30-C25	3.83	116.52	110.30
19	1	1010	CLA	C3A-C2A-C1A	3.83	107.07	101.34
19	B	1209	CLA	C4A-NA-C1A	3.82	108.42	106.71
21	B	6010	BCR	C15-C14-C13	-3.82	121.86	127.31
19	A	1309	CLA	C3B-C2B-C1B	-3.82	103.02	106.29
21	B	6005	BCR	C33-C5-C4	3.82	120.96	113.62
21	A	6002	BCR	C28-C27-C26	-3.82	107.26	114.08
19	A	9023	CLA	CGD-CBD-CAD	3.82	123.11	110.73
19	3	3006	CLA	C2A-C1A-CHA	-3.82	116.12	122.63
21	B	6010	BCR	C2-C1-C6	-3.82	104.60	110.48
21	I	6021	BCR	C15-C14-C13	3.82	132.76	127.31
19	A	1132	CLA	O1D-CGD-CBD	-3.82	116.68	124.48
19	B	1230	CLA	O1D-CGD-CBD	-3.82	116.68	124.48
19	B	1205	CLA	C1-C2-C3	-3.81	119.45	126.04
19	A	1106	CLA	C3D-CAD-CBD	-3.81	102.59	107.61
19	A	1128	CLA	C3D-CAD-CBD	-3.81	102.59	107.61
21	I	6021	BCR	C27-C26-C25	-3.80	117.21	122.73
22	2	7027	LMU	O1'-C1'-C2'	3.80	114.24	108.30
22	R	7021	LMU	C1B-O5B-C5B	3.80	121.15	113.69
19	4	4002	CLA	C2A-C3A-C4A	-3.80	95.73	101.87
19	4	4013	CLA	C4A-NA-C1A	3.80	108.41	106.71
19	B	1236	CLA	C3D-CAD-CBD	-3.80	102.61	107.61
22	G	7051	LMU	C1'-O5'-C5'	-3.79	106.24	113.69
19	B	1227	CLA	C1-O2A-CGA	3.79	126.39	116.44
22	2	7031	LMU	O1'-C1'-C2'	3.79	114.22	108.30
21	B	6017	BCR	C16-C17-C18	-3.79	121.90	127.31
21	I	6021	BCR	C7-C8-C9	3.79	131.96	126.23
21	A	6003	BCR	C20-C19-C18	-3.79	115.78	126.42
21	B	6020	BCR	C7-C6-C5	-3.79	112.29	121.46
19	3	3015	CLA	C3B-C2B-C1B	-3.79	103.05	106.29
22	R	7020	LMU	C1B-O5B-C5B	3.79	121.12	113.69
19	B	1224	CLA	C3D-CAD-CBD	-3.78	102.63	107.61
21	J	6012	BCR	C15-C16-C17	-3.78	115.73	123.47
19	A	1123	CLA	O2D-CGD-CBD	3.78	117.98	111.27
19	F	1240	CLA	CMD-C2D-C3D	-3.78	117.61	124.68
19	B	1202	CLA	CHB-C4A-NA	3.78	129.74	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1203	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
19	A	1151	CLA	O2D-CGD-CBD	3.78	117.98	111.27
19	3	3011	CLA	C3D-CAD-CBD	-3.77	102.64	107.61
19	B	1224	CLA	CMD-C2D-C3D	-3.77	117.62	124.68
19	3	3017	CLA	CHB-C4A-NA	3.77	129.72	124.51
21	F	6014	BCR	C31-C1-C6	-3.77	104.19	110.30
19	3	3004	CLA	C3B-C2B-C1B	-3.77	103.06	106.29
19	2	2008	CLA	C3D-C4D-ND	3.77	113.41	110.14
19	A	1120	CLA	CMD-C2D-C3D	-3.76	117.64	124.68
19	R	1150	CLA	C1-C2-C3	3.76	132.54	126.04
19	K	1146	CLA	O2A-CGA-CBA	3.76	123.69	111.91
19	3	1118	CLA	C1B-C2B-C3B	-3.75	103.43	106.92
19	B	1214	CLA	C3D-CAD-CBD	-3.75	102.66	107.61
19	3	3003	CLA	C1B-C2B-C3B	-3.75	103.43	106.92
19	A	1106	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
21	B	6004	BCR	C2-C1-C6	-3.75	104.71	110.48
21	F	6014	BCR	C2-C1-C6	-3.74	104.72	110.48
19	A	1108	CLA	CMD-C2D-C3D	-3.74	117.67	124.68
19	A	1107	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
19	L	1501	CLA	CED-O2D-CGD	3.74	124.39	115.94
19	A	1237	CLA	C6-C5-C3	-3.73	103.67	113.45
19	B	1301	CLA	CBD-CHA-C1A	3.73	133.41	127.43
19	A	9012	CLA	CAA-C2A-C1A	3.73	124.20	111.97
19	B	9010	CLA	O2D-CGD-CBD	3.73	117.89	111.27
21	F	6014	BCR	C20-C19-C18	-3.73	115.94	126.42
21	B	6006	BCR	C16-C15-C14	-3.73	115.84	123.47
19	2	4009	CLA	C3D-CAD-CBD	-3.73	102.70	107.61
19	A	1133	CLA	CMD-C2D-C3D	-3.73	117.71	124.68
19	A	9022	CLA	CHB-C4A-NA	3.72	129.66	124.51
21	B	6017	BCR	C24-C23-C22	-3.72	120.61	126.23
21	L	6019	BCR	C15-C16-C17	-3.72	115.85	123.47
19	H	1145	CLA	CAA-C2A-C3A	-3.72	102.59	112.78
19	A	1110	CLA	C4A-NA-C1A	3.72	108.38	106.71
21	B	6006	BCR	C20-C19-C18	-3.72	115.97	126.42
19	4	4004	CLA	C2D-C3D-C4D	-3.71	103.10	106.30
19	A	9013	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
21	3	6022	BCR	C38-C26-C25	-3.71	120.36	124.53
21	L	6019	BCR	C27-C26-C25	-3.71	117.34	122.73
21	A	6002	BCR	C38-C26-C25	-3.71	120.36	124.53
21	F	6014	BCR	C33-C5-C6	-3.71	120.36	124.53
21	A	6011	BCR	C29-C30-C25	-3.71	104.77	110.48
21	B	6017	BCR	C39-C30-C25	3.71	116.32	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	6008	BCR	C24-C23-C22	-3.71	120.63	126.23
19	L	1502	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
19	A	1102	CLA	CMD-C2D-C3D	-3.71	117.74	124.68
19	B	1220	CLA	CAA-C2A-C1A	-3.71	99.83	111.97
19	B	1218	CLA	CHB-C4A-NA	3.71	129.64	124.51
21	A	6003	BCR	C16-C15-C14	-3.71	115.88	123.47
21	A	6007	BCR	C3-C4-C5	-3.70	107.46	114.08
19	H	1505	CLA	C4A-NA-C1A	3.70	108.37	106.71
19	A	1136	CLA	C1-C2-C3	-3.70	119.64	126.04
22	E	7037	LMU	C1B-O1B-C4'	-3.70	108.81	117.96
19	1	1005	CLA	CED-O2D-CGD	3.69	124.29	115.94
19	2	2007	CLA	C6-C5-C3	-3.69	103.78	113.45
21	J	6012	BCR	C2-C1-C6	-3.69	104.80	110.48
19	L	1502	CLA	C4A-NA-C1A	3.69	108.36	106.71
22	4	7052	LMU	O5'-C5'-C4'	-3.69	101.98	109.75
19	A	1127	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
21	B	6010	BCR	C16-C17-C18	-3.68	122.06	127.31
19	B	1235	CLA	C3D-CAD-CBD	-3.67	102.77	107.61
21	B	6020	BCR	C37-C22-C23	3.67	123.86	118.08
21	A	6007	BCR	C33-C5-C4	3.67	120.67	113.62
19	L	1503	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
19	A	1109	CLA	CAA-C2A-C3A	-3.67	102.73	112.78
20	B	5002	PQN	C2M-C2-C3	-3.67	118.42	124.40
19	A	1129	CLA	C3D-CAD-CBD	-3.67	102.78	107.61
21	B	6004	BCR	C28-C27-C26	-3.67	107.53	114.08
19	K	1146	CLA	CMD-C2D-C3D	-3.66	117.82	124.68
21	F	6014	BCR	C38-C26-C25	-3.66	120.41	124.53
19	L	1504	CLA	C4-C3-C5	3.66	121.43	115.27
19	3	3007	CLA	C4A-NA-C1A	3.66	108.35	106.71
19	2	2008	CLA	C2D-C3D-C4D	-3.66	103.15	106.30
21	A	6007	BCR	C34-C9-C10	-3.66	117.80	122.92
21	A	6003	BCR	C33-C5-C6	-3.66	120.42	124.53
19	B	1228	CLA	C1-C2-C3	-3.66	120.84	126.75
19	A	1107	CLA	CMD-C2D-C3D	-3.65	117.85	124.68
21	A	6008	BCR	C38-C26-C25	-3.65	120.43	124.53
21	B	6005	BCR	C29-C30-C25	-3.65	104.87	110.48
19	A	1129	CLA	O2A-CGA-CBA	3.65	123.35	111.91
19	B	1218	CLA	CMD-C2D-C3D	-3.64	117.86	124.68
19	3	3005	CLA	C2D-C3D-C4D	-3.64	103.17	106.30
21	F	6016	BCR	C34-C9-C8	3.64	123.81	118.08
19	3	3007	CLA	CMD-C2D-C3D	-3.64	117.87	124.68
21	A	6007	BCR	C23-C24-C25	-3.64	116.98	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1011	CLA	C4A-NA-C1A	3.64	108.34	106.71
21	A	6007	BCR	C29-C30-C25	-3.64	104.88	110.48
21	B	6017	BCR	C29-C30-C25	-3.64	104.88	110.48
19	3	3008	CLA	O2A-CGA-CBA	3.63	123.30	111.91
19	1	1002	CLA	O2A-CGA-CBA	3.63	123.29	111.91
19	4	4006	CLA	C4-C3-C5	3.63	121.37	115.27
19	2	2003	CLA	C3D-C4D-ND	3.62	113.29	110.14
21	B	6004	BCR	C34-C9-C10	-3.62	117.85	122.92
19	A	1309	CLA	C4A-NA-C1A	3.62	108.33	106.71
19	4	4006	CLA	C4A-NA-C1A	3.62	108.33	106.71
19	2	2006	CLA	CED-O2D-CGD	3.62	124.12	115.94
21	F	6014	BCR	C23-C22-C21	3.62	124.49	118.94
19	A	1121	CLA	CAA-C2A-C1A	3.62	120.14	112.14
22	A	7044	LMU	O2'-C2'-C1'	3.61	118.83	110.05
21	B	6010	BCR	C38-C26-C25	-3.61	120.47	124.53
22	F	7036	LMU	O1B-C1B-C2B	3.61	117.46	108.10
21	B	6017	BCR	C37-C22-C21	-3.61	117.86	122.92
19	A	1116	CLA	CMD-C2D-C3D	-3.61	117.92	124.68
22	G	7039	LMU	O1B-C1B-C2B	3.61	117.45	108.10
19	1	1012	CLA	CMD-C2D-C3D	-3.61	117.92	124.68
19	B	1202	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
19	4	4005	CLA	C2D-C3D-C4D	-3.61	103.19	106.30
22	4	7009	LMU	O1'-C1'-C2'	3.61	113.94	108.30
19	L	1148	CLA	O2A-CGA-CBA	3.61	123.23	111.91
19	A	1138	CLA	CMD-C2D-C3D	-3.61	117.93	124.68
21	I	6018	BCR	C30-C25-C24	3.60	125.97	115.78
19	A	1102	CLA	O2D-CGD-CBD	3.60	117.67	111.27
19	4	4015	CLA	CGD-CBD-CAD	-3.60	99.07	110.73
22	C	7015	LMU	C1B-C2B-C3B	3.60	117.49	110.00
19	2	2002	CLA	C1-O2A-CGA	3.60	125.89	116.44
19	3	3011	CLA	CHB-C4A-NA	3.60	129.49	124.51
21	B	6020	BCR	C20-C19-C18	-3.60	116.31	126.42
21	B	6004	BCR	C3-C4-C5	-3.60	107.66	114.08
19	B	1219	CLA	CMD-C2D-C3D	-3.60	117.95	124.68
19	F	1302	CLA	CMD-C2D-C3D	-3.59	117.96	124.68
19	A	1108	CLA	C2A-C1A-CHA	-3.59	117.58	123.86
19	3	3017	CLA	CAA-C2A-C3A	-3.59	102.95	112.78
19	L	1130	CLA	C3D-CAD-CBD	-3.59	102.88	107.61
21	F	6016	BCR	C29-C30-C25	-3.59	104.96	110.48
19	B	1226	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
19	2	2011	CLA	C2D-C3D-C4D	-3.58	103.22	106.30
19	3	3005	CLA	C3D-C2D-C1D	3.58	109.39	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	7051	LMU	C1B-O1B-C4'	3.58	126.83	117.96
19	A	1113	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
19	A	1104	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
21	L	6019	BCR	C33-C5-C6	-3.58	120.51	124.53
19	3	3002	CLA	C3B-C2B-C1B	-3.57	103.23	106.29
19	B	1228	CLA	C3D-CAD-CBD	-3.57	102.90	107.61
19	2	2002	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
21	J	6012	BCR	C7-C8-C9	-3.57	120.84	126.23
21	B	6004	BCR	C33-C5-C6	-3.57	120.52	124.53
19	H	1145	CLA	CAA-C2A-C1A	3.56	123.66	111.97
22	R	7020	LMU	O1'-C1'-C2'	3.56	113.87	108.30
21	F	6016	BCR	C30-C25-C26	-3.56	117.60	122.61
19	A	9011	CLA	CED-O2D-CGD	3.56	123.99	115.94
21	B	6005	BCR	C33-C5-C6	-3.56	120.53	124.53
22	E	7048	LMU	C1B-O5B-C5B	-3.56	106.71	113.69
19	A	1126	CLA	CMD-C2D-C3D	-3.55	118.03	124.68
19	4	1306	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
22	A	7045	LMU	O5B-C1B-C2B	3.55	117.86	110.35
22	G	7051	LMU	O5'-C5'-C6'	3.55	115.26	106.44
19	L	1148	CLA	C4-C3-C2	-3.55	114.58	123.68
22	H	7032	LMU	C1B-C2B-C3B	-3.55	102.61	110.00
19	A	1139	CLA	CMD-C2D-C3D	-3.55	118.05	124.68
19	J	1308	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
21	L	6019	BCR	C36-C18-C19	3.54	123.66	118.08
19	R	1144	CLA	O2A-CGA-CBA	3.54	123.02	111.91
19	R	1150	CLA	O2D-CGD-CBD	3.54	117.56	111.27
19	A	1127	CLA	C1-O2A-CGA	3.54	125.72	116.44
21	B	6004	BCR	C33-C5-C4	3.53	120.41	113.62
21	A	6007	BCR	C38-C26-C25	-3.53	120.56	124.53
22	R	7025	LMU	C1'-O5'-C5'	3.53	120.62	113.69
21	B	6006	BCR	C27-C26-C25	-3.53	117.61	122.73
19	B	1238	CLA	O2A-CGA-CBA	3.53	122.98	111.91
22	A	7035	LMU	C3'-C4'-C5'	-3.53	102.84	110.93
19	2	2013	CLA	CGD-CBD-CAD	-3.53	99.31	110.73
21	A	6011	BCR	C15-C16-C17	-3.52	116.26	123.47
19	B	9010	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
19	A	1123	CLA	C4-C3-C5	3.52	121.19	115.27
21	B	6006	BCR	C29-C30-C25	-3.52	105.06	110.48
19	A	1102	CLA	C3D-CAD-CBD	-3.52	102.97	107.61
19	4	4001	CLA	O2A-CGA-CBA	3.52	122.95	111.91
19	4	1004	CLA	CMD-C2D-C3D	-3.52	118.10	124.68
19	A	1123	CLA	CMD-C2D-C3D	-3.52	118.10	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1225	CLA	CHB-C4A-NA	3.52	129.37	124.51
21	I	6018	BCR	C38-C26-C27	3.51	120.37	113.62
19	A	1133	CLA	C1-C2-C3	-3.51	121.07	126.75
19	2	2001	CLA	CMD-C2D-C3D	-3.51	118.12	124.68
19	A	1107	CLA	C4A-NA-C1A	3.51	108.28	106.71
19	1	1015	CLA	C3D-C4D-ND	3.50	113.19	110.14
19	3	2009	CLA	CMD-C2D-C3D	-3.50	118.12	124.68
22	B	7038	LMU	O5B-C5B-C4B	3.50	116.06	109.69
19	3	3013	CLA	C4A-NA-C1A	3.50	108.28	106.71
19	A	9023	CLA	O2D-CGD-CBD	3.50	117.49	111.27
19	4	1004	CLA	C1-C2-C3	-3.50	119.99	126.04
19	4	4014	CLA	C3D-CAD-CBD	-3.50	103.00	107.61
21	B	6020	BCR	C1-C6-C7	3.50	125.67	115.78
22	4	7052	LMU	C6'-C5'-C4'	3.50	123.50	113.33
19	K	1146	CLA	CHB-C4A-NA	3.49	129.34	124.51
19	J	1308	CLA	CHB-C4A-NA	3.49	129.34	124.51
19	A	1141	CLA	CMD-C2D-C3D	-3.49	118.15	124.68
19	1	1011	CLA	CBD-CHA-C1A	3.49	133.02	127.43
19	A	9012	CLA	O2A-CGA-CBA	3.49	122.85	111.91
21	J	6012	BCR	C28-C27-C26	-3.49	107.85	114.08
19	2	2005	CLA	C3B-C2B-C1B	-3.49	103.30	106.29
19	B	1225	CLA	O2A-CGA-CBA	3.49	122.85	111.91
19	A	1134	CLA	CMD-C2D-C3D	-3.49	118.16	124.68
21	B	6005	BCR	C38-C26-C27	3.48	120.31	113.62
21	A	6007	BCR	C28-C27-C26	-3.48	107.86	114.08
19	4	4006	CLA	C4-C3-C2	-3.47	114.77	123.68
19	2	2003	CLA	C2D-C3D-C4D	-3.47	103.31	106.30
21	3	6022	BCR	C11-C12-C13	-3.47	116.68	126.42
21	J	6012	BCR	C23-C24-C25	-3.46	117.47	127.20
19	4	1306	CLA	CMD-C2D-C3D	-3.46	118.20	124.68
19	A	1108	CLA	C3D-CAD-CBD	-3.46	103.05	107.61
19	B	1230	CLA	CED-O2D-CGD	3.46	123.76	115.94
21	B	6004	BCR	C29-C30-C25	-3.46	105.16	110.48
19	1	1002	CLA	CMB-C2B-C3B	3.46	131.15	124.68
19	A	1128	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
21	B	6017	BCR	C2-C1-C6	-3.45	105.16	110.48
21	J	6012	BCR	C8-C7-C6	-3.45	117.50	127.20
19	2	2001	CLA	C4-C3-C5	3.45	119.93	115.98
19	B	1209	CLA	CMD-C2D-C3D	-3.45	118.22	124.68
22	A	7045	LMU	C3B-C4B-C5B	-3.45	104.09	110.24
19	1	1013	CLA	CBA-CAA-C2A	3.44	124.03	113.86
22	B	7040	LMU	O3'-C3'-C2'	-3.44	102.39	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	7024	LMU	C3B-C4B-C5B	-3.44	104.10	110.24
19	4	4004	CLA	C3D-C4D-ND	3.44	113.13	110.14
22	H	7011	LMU	C3'-C4'-C5'	3.44	118.81	110.93
19	I	1204	CLA	C3D-CAD-CBD	-3.44	103.08	107.61
19	H	1145	CLA	CMD-C2D-C3D	-3.44	118.24	124.68
19	A	1128	CLA	C4-C3-C5	3.44	121.05	115.27
19	A	1237	CLA	C1-C2-C3	-3.43	120.10	126.04
21	A	6011	BCR	C28-C27-C26	-3.43	107.95	114.08
21	B	6010	BCR	C34-C9-C10	-3.43	118.11	122.92
19	2	2013	CLA	CAA-C2A-C1A	3.43	123.22	111.97
19	2	2010	CLA	C3B-C2B-C1B	-3.43	103.35	106.29
21	B	6010	BCR	C37-C22-C21	-3.43	118.12	122.92
19	B	1222	CLA	CMD-C2D-C3D	-3.43	118.27	124.68
22	H	7030	LMU	C3B-C4B-C5B	-3.43	104.13	110.24
19	2	2011	CLA	C4A-NA-C1A	3.42	108.25	106.71
21	B	6005	BCR	C3-C4-C5	-3.42	107.97	114.08
21	F	6016	BCR	C15-C16-C17	-3.42	116.47	123.47
22	A	7016	LMU	C2'-C3'-C4'	3.42	117.49	109.68
19	4	4011	CLA	C3D-C4D-ND	3.42	113.11	110.14
19	3	1118	CLA	CMD-C2D-C3D	-3.42	118.28	124.68
19	A	1121	CLA	CMD-C2D-C3D	-3.42	118.28	124.68
19	B	1205	CLA	CHB-C4A-NA	3.42	129.24	124.51
19	K	1143	CLA	CMD-C2D-C3D	-3.42	118.29	124.68
21	A	6002	BCR	C3-C4-C5	-3.42	107.98	114.08
19	3	3008	CLA	C4A-NA-C1A	3.41	108.24	106.71
19	4	4002	CLA	O2A-CGA-O1A	-3.41	114.98	123.59
19	4	1304	CLA	O2A-CGA-O1A	-3.41	114.98	123.59
21	A	6011	BCR	C38-C26-C27	3.41	120.17	113.62
19	A	1109	CLA	C11-C12-C13	-3.41	104.89	115.92
19	2	2005	CLA	C4A-NA-C1A	3.41	108.24	106.71
19	3	3015	CLA	C4A-NA-C1A	3.41	108.24	106.71
19	B	9010	CLA	CBA-CAA-C2A	-3.41	103.80	113.86
22	R	7014	LMU	C1B-O1B-C4'	-3.41	109.53	117.96
19	3	2009	CLA	O2D-CGD-CBD	3.41	117.32	111.27
19	B	1233	CLA	CMD-C2D-C3D	-3.40	118.31	124.68
21	3	6022	BCR	C20-C19-C18	-3.40	116.86	126.42
22	G	7051	LMU	O3'-C3'-C2'	-3.40	102.48	110.35
21	B	6004	BCR	C40-C30-C25	3.40	115.81	110.30
21	J	6012	BCR	C29-C30-C25	-3.40	105.25	110.48
22	B	7040	LMU	O1B-C1B-C2B	3.40	116.91	108.10
21	A	6002	BCR	C23-C24-C25	-3.40	117.65	127.20
19	A	9023	CLA	C4A-NA-C1A	3.40	108.23	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1012	CLA	C4A-NA-C1A	3.40	108.23	106.71
19	H	1207	CLA	CMB-C2B-C3B	3.40	131.03	124.68
19	H	1241	CLA	CHB-C4A-NA	3.40	129.21	124.51
19	A	1111	CLA	CHB-C4A-NA	3.39	129.21	124.51
19	4	4014	CLA	CHB-C4A-NA	3.39	129.21	124.51
19	A	1136	CLA	CMD-C2D-C3D	-3.39	118.33	124.68
22	G	7039	LMU	C1B-C2B-C3B	-3.39	102.93	110.00
21	A	6002	BCR	C24-C23-C22	-3.39	121.11	126.23
19	2	2012	CLA	CMD-C2D-C3D	-3.39	118.34	124.68
21	B	6004	BCR	C38-C26-C25	-3.39	120.73	124.53
22	H	7017	LMU	O4'-C4B-C5B	-3.39	100.89	109.30
19	B	1215	CLA	O2A-CGA-CBA	3.39	122.53	111.91
22	R	7024	LMU	C1B-O5B-C5B	3.38	120.33	113.69
21	L	6019	BCR	C38-C26-C27	3.38	120.12	113.62
22	A	7045	LMU	C1B-O5B-C5B	3.38	120.33	113.69
22	H	7043	LMU	O5B-C1B-C2B	3.38	117.51	110.35
19	3	1118	CLA	C4A-NA-C1A	3.38	108.23	106.71
19	A	1135	CLA	CMD-C2D-C3D	-3.38	118.36	124.68
19	2	2010	CLA	C4A-NA-C1A	3.38	108.22	106.71
22	F	7036	LMU	C2'-C3'-C4'	-3.38	101.97	109.68
22	H	7032	LMU	C2'-C3'-C4'	3.38	117.39	109.68
19	B	1205	CLA	O2A-CGA-CBA	3.38	122.50	111.91
19	A	1115	CLA	CHB-C4A-NA	3.37	129.18	124.51
19	1	1010	CLA	C2A-C3A-C4A	-3.37	96.42	101.87
19	3	3013	CLA	C4-C3-C5	3.37	120.94	115.27
19	A	1124	CLA	CMD-C2D-C3D	-3.37	118.38	124.68
19	A	1137	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
19	A	1149	CLA	CED-O2D-CGD	3.37	123.55	115.94
21	J	6012	BCR	C31-C1-C6	-3.37	104.84	110.30
19	3	3013	CLA	C3D-CAD-CBD	-3.36	103.18	107.61
19	B	1221	CLA	O2A-CGA-CBA	3.36	122.46	111.91
19	1	1008	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
19	1	1303	CLA	C4D-C3D-CAD	3.36	110.34	108.47
22	G	7026	LMU	C1B-O1B-C4'	-3.36	109.65	117.96
21	B	6010	BCR	C33-C5-C6	-3.36	120.76	124.53
19	B	1220	CLA	CBC-CAC-C3C	-3.35	103.74	112.27
21	B	6010	BCR	C36-C18-C19	3.35	123.35	118.08
19	1	1013	CLA	C1-C2-C3	-3.35	120.25	126.04
19	H	1505	CLA	CED-O2D-CGD	3.35	123.51	115.94
19	1	1015	CLA	C3D-C2D-C1D	3.34	109.18	106.30
19	B	1217	CLA	CMD-C2D-C3D	-3.34	118.42	124.68
19	2	2014	CLA	CHB-C4A-NA	3.34	129.13	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	9012	CLA	CHB-C4A-NA	3.34	129.13	124.51
19	A	1107	CLA	O2A-CGA-CBA	3.34	122.39	111.91
19	1	1010	CLA	CMD-C2D-C3D	-3.34	118.43	124.68
22	H	7043	LMU	C1B-C2B-C3B	3.34	116.95	110.00
19	4	1009	CLA	CMD-C2D-C3D	-3.34	118.44	124.68
21	L	6019	BCR	C28-C27-C26	-3.34	108.12	114.08
19	4	4003	CLA	CMD-C2D-C3D	-3.33	118.44	124.68
19	B	1227	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
22	A	7044	LMU	C3'-C4'-C5'	3.33	118.56	110.93
22	A	7045	LMU	O1'-C1'-C2'	3.33	113.50	108.30
19	A	1134	CLA	C4A-NA-C1A	3.32	108.20	106.71
19	B	1301	CLA	C1B-C2B-C3B	-3.32	103.83	106.92
19	K	1146	CLA	C1-C2-C3	-3.32	121.38	126.75
19	3	3001	CLA	C3D-C4D-ND	3.32	113.03	110.14
19	A	1117	CLA	O2D-CGD-CBD	3.32	117.17	111.27
19	A	9012	CLA	O2A-C1-C2	3.32	117.35	108.64
19	R	1150	CLA	C4A-NA-C1A	3.31	108.20	106.71
21	B	6010	BCR	C3-C4-C5	-3.31	108.16	114.08
19	A	9022	CLA	C3D-CAD-CBD	-3.31	103.25	107.61
21	A	6002	BCR	C33-C5-C6	-3.31	120.81	124.53
19	F	1240	CLA	CHB-C4A-NA	3.31	129.09	124.51
19	A	1122	CLA	O2D-CGD-CBD	3.31	117.15	111.27
19	B	1203	CLA	O2A-CGA-CBA	3.31	122.29	111.91
19	A	1126	CLA	O2A-CGA-CBA	3.31	122.29	111.91
19	2	2008	CLA	C3B-C2B-C1B	-3.31	103.46	106.29
19	L	1501	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
22	B	7038	LMU	C2'-C3'-C4'	-3.30	102.14	109.68
19	K	1146	CLA	CMA-C3A-C4A	-3.30	102.89	111.77
19	J	1311	CLA	CMD-C2D-C3D	-3.30	118.50	124.68
19	B	1212	CLA	C4-C3-C5	3.30	120.83	115.27
19	A	9023	CLA	C1-O2A-CGA	3.30	125.11	116.44
19	B	1238	CLA	CMB-C2B-C3B	3.30	130.86	124.68
19	3	1118	CLA	CBD-CHA-C1A	3.30	132.72	127.43
19	4	4002	CLA	CBA-CAA-C2A	-3.30	104.12	113.86
19	1	1014	CLA	C1-C2-C3	-3.30	120.33	126.04
19	H	1145	CLA	C4A-NA-C1A	3.30	108.19	106.71
19	1	1007	CLA	C4A-NA-C1A	3.30	108.19	106.71
19	A	9022	CLA	C5-C3-C2	-3.30	114.44	121.12
21	A	6007	BCR	C40-C30-C25	3.30	115.65	110.30
19	L	1148	CLA	CBA-CAA-C2A	3.30	123.60	113.86
22	H	7011	LMU	O1B-C1B-O5B	3.30	119.89	110.67
22	R	7022	LMU	C1-O1'-C1'	3.30	119.31	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	7053	LMU	O1B-C1B-C2B	3.30	116.64	108.10
19	B	1221	CLA	CHB-C4A-NA	3.30	129.07	124.51
19	1	1002	CLA	CMD-C2D-C3D	-3.29	118.51	124.68
19	A	1113	CLA	O2A-CGA-CBA	3.29	122.25	111.91
21	F	6014	BCR	C16-C17-C18	-3.29	122.61	127.31
19	2	2013	CLA	CHB-C4A-NA	3.29	129.07	124.51
21	J	6012	BCR	C34-C9-C10	-3.29	118.31	122.92
19	J	1308	CLA	CED-O2D-CGD	3.29	123.38	115.94
21	I	6018	BCR	C15-C14-C13	3.29	132.01	127.31
19	B	1202	CLA	O2A-CGA-CBA	3.29	122.23	111.91
19	B	1213	CLA	O1D-CGD-CBD	-3.29	117.75	124.48
21	F	6014	BCR	C3-C4-C5	-3.29	108.20	114.08
22	C	7015	LMU	O1'-C1'-C2'	3.29	113.44	108.30
19	1	1014	CLA	O1D-CGD-CBD	-3.29	117.76	124.48
19	B	1221	CLA	CGD-CBD-CAD	-3.29	100.09	110.73
22	H	7043	LMU	O1B-C4'-C3'	3.28	116.02	107.28
19	1	1008	CLA	CAA-CBA-CGA	3.28	122.84	113.25
22	A	7010	LMU	O5'-C5'-C6'	3.28	114.59	106.44
19	B	1218	CLA	O1D-CGD-CBD	-3.28	117.77	124.48
19	4	4012	CLA	CHB-C4A-NA	3.28	129.05	124.51
20	A	5001	PQN	C2M-C2-C3	-3.28	119.05	124.40
19	1	1303	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
19	3	3010	CLA	C2D-C3D-C4D	-3.28	103.48	106.30
21	B	6005	BCR	C7-C8-C9	-3.27	121.30	126.23
19	A	1108	CLA	CMA-C3A-C2A	-3.27	100.64	113.83
19	A	1127	CLA	C4A-NA-C1A	3.27	108.17	106.71
19	B	1230	CLA	C4A-NA-C1A	3.27	108.17	106.71
19	A	1117	CLA	C1-C2-C3	-3.27	120.39	126.04
19	3	3011	CLA	C1-C2-C3	-3.27	120.39	126.04
21	1	6023	BCR	C7-C8-C9	-3.27	121.30	126.23
19	I	1204	CLA	O2A-CGA-CBA	3.26	122.15	111.91
19	A	9011	CLA	C4A-NA-C1A	3.26	108.17	106.71
19	A	1107	CLA	C4-C3-C5	3.26	120.76	115.27
19	2	2006	CLA	C4-C3-C5	3.26	120.76	115.27
19	2	2004	CLA	CMD-C2D-C3D	-3.26	118.58	124.68
19	2	2002	CLA	O2A-CGA-CBA	3.26	122.13	111.91
19	2	2014	CLA	C4-C3-C5	3.26	120.75	115.27
21	3	6022	BCR	C34-C9-C10	-3.25	118.36	122.92
19	A	1141	CLA	C4A-NA-C1A	3.25	108.17	106.71
21	A	6008	BCR	C33-C5-C6	-3.25	120.87	124.53
22	3	7005	LMU	C1'-O5'-C5'	3.25	120.07	113.69
21	B	6005	BCR	C28-C27-C26	-3.25	108.27	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	1305	CLA	C4-C3-C5	3.25	120.74	115.27
22	2	7027	LMU	C1'-O5'-C5'	3.25	120.07	113.69
19	B	1215	CLA	C1-C2-C3	-3.25	120.42	126.04
22	B	7012	LMU	C3B-C4B-C5B	3.25	116.03	110.24
21	A	6011	BCR	C34-C9-C10	-3.25	118.38	122.92
19	R	1144	CLA	C4-C3-C5	3.25	120.73	115.27
22	4	7009	LMU	C2'-C3'-C4'	3.24	117.09	109.68
19	L	1502	CLA	CMD-C2D-C3D	-3.24	118.61	124.68
19	B	1231	CLA	CMD-C2D-C3D	-3.24	118.61	124.68
19	1	1310	CLA	C3D-C2D-C1D	3.24	109.10	106.30
19	B	1235	CLA	CBC-CAC-C3C	-3.24	104.01	112.27
21	A	6002	BCR	C37-C22-C21	-3.24	118.38	122.92
19	A	1127	CLA	O1D-CGD-CBD	-3.24	117.86	124.48
19	4	4010	CLA	C4A-NA-C1A	3.24	108.16	106.71
19	4	1306	CLA	CHB-C4A-NA	3.24	128.99	124.51
21	B	6017	BCR	C34-C9-C10	-3.24	118.39	122.92
19	K	1142	CLA	CMD-C2D-C3D	-3.24	118.62	124.68
19	B	1214	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
19	4	4002	CLA	O2D-CGD-CBD	3.24	117.02	111.27
21	A	6003	BCR	C39-C30-C25	3.23	115.54	110.30
22	K	7001	LMU	O5B-C5B-C6B	3.23	114.47	106.44
19	H	1241	CLA	C4-C3-C5	3.23	120.71	115.27
19	B	1235	CLA	CMD-C2D-C3D	-3.23	118.63	124.68
19	3	3016	CLA	C4-C3-C5	3.23	120.70	115.27
19	4	1304	CLA	O2A-CGA-CBA	3.23	122.04	111.91
21	A	6007	BCR	C38-C26-C27	3.23	119.81	113.62
19	2	2007	CLA	C4A-NA-C1A	3.23	108.16	106.71
19	4	1304	CLA	O2D-CGD-CBD	3.23	117.00	111.27
19	4	4012	CLA	CAA-C2A-C3A	-3.22	108.57	116.10
19	B	1227	CLA	CED-O2D-CGD	3.22	123.23	115.94
19	A	1117	CLA	C4-C3-C5	3.22	120.69	115.27
19	1	1013	CLA	CAA-C2A-C1A	-3.22	101.41	111.97
19	A	1106	CLA	CHB-C4A-NA	3.22	128.97	124.51
19	1	1011	CLA	CAA-C2A-C3A	-3.22	108.58	116.10
19	J	1308	CLA	C1-C2-C3	-3.22	120.47	126.04
19	A	1140	CLA	C1-C2-C3	-3.22	120.48	126.04
19	3	3010	CLA	C3D-C2D-C1D	3.22	109.07	106.30
21	3	6022	BCR	C15-C14-C13	-3.21	122.72	127.31
21	A	6011	BCR	C36-C18-C19	3.21	123.14	118.08
19	1	1005	CLA	CMD-C2D-C3D	-3.21	118.67	124.68
19	G	1242	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
19	A	1101	CLA	O1D-CGD-CBD	-3.21	117.92	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	6018	BCR	C38-C26-C25	-3.21	120.92	124.53
22	4	7053	LMU	C4B-C3B-C2B	-3.21	105.22	110.82
19	B	1231	CLA	CHB-C4A-NA	3.21	128.95	124.51
22	H	7002	LMU	O5'-C5'-C6'	3.21	114.41	106.44
19	1	1003	CLA	C4A-NA-C1A	3.21	108.15	106.71
19	2	2012	CLA	CHB-C4A-NA	3.20	128.94	124.51
19	2	2006	CLA	O2D-CGD-CBD	3.20	116.96	111.27
22	H	7028	LMU	O1'-C1'-C2'	3.20	113.30	108.30
22	4	7033	LMU	C4B-C3B-C2B	3.20	116.41	110.82
22	H	7017	LMU	O5B-C5B-C6B	3.20	114.39	106.44
19	2	2014	CLA	CMB-C2B-C3B	3.20	130.66	124.68
21	I	6021	BCR	C20-C19-C18	-3.20	117.44	126.42
19	4	1004	CLA	C4A-NA-C1A	3.19	108.14	106.71
22	2	7027	LMU	C2'-C3'-C4'	3.19	116.96	109.68
21	A	6011	BCR	C24-C23-C22	-3.19	121.42	126.23
21	A	6011	BCR	C38-C26-C25	-3.19	120.95	124.53
19	3	2009	CLA	C4-C3-C5	3.18	120.62	115.27
19	J	1308	CLA	CMD-C2D-C3D	-3.18	118.73	124.68
19	4	4004	CLA	C3D-C2D-C1D	3.18	109.04	106.30
21	I	6018	BCR	C39-C30-C25	3.18	115.45	110.30
22	A	7016	LMU	O1'-C1'-C2'	3.18	113.26	108.30
22	4	7018	LMU	C1B-O5B-C5B	3.18	119.92	113.69
19	B	1212	CLA	CED-O2D-CGD	3.18	123.12	115.94
19	H	1241	CLA	CED-O2D-CGD	3.18	123.12	115.94
21	B	6020	BCR	C16-C17-C18	-3.17	122.78	127.31
19	2	4009	CLA	CMD-C2D-C3D	-3.17	118.75	124.68
19	A	1137	CLA	CMD-C2D-C3D	-3.17	118.75	124.68
19	L	1148	CLA	CAA-CBA-CGA	-3.17	104.00	113.25
19	4	4002	CLA	C6-C5-C3	-3.17	109.44	114.62
22	B	7038	LMU	O1B-C4'-C3'	3.17	115.71	107.28
21	A	6011	BCR	C16-C17-C18	-3.17	122.79	127.31
19	K	1142	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
19	B	1216	CLA	C1-C2-C3	-3.16	120.57	126.04
19	3	3017	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
19	B	1210	CLA	CMD-C2D-C3D	-3.16	118.76	124.68
22	4	7052	LMU	C3'-C4'-C5'	-3.16	103.68	110.93
22	G	7051	LMU	O5B-C1B-C2B	-3.16	103.66	110.35
19	4	4014	CLA	CMD-C2D-C3D	-3.16	118.77	124.68
22	E	7037	LMU	O5B-C5B-C6B	3.16	114.29	106.44
19	A	1131	CLA	C4A-NA-C1A	3.15	108.12	106.71
19	B	1208	CLA	O2A-CGA-CBA	3.15	121.80	111.91
19	A	1109	CLA	CAA-C2A-C1A	-3.15	101.65	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1112	CLA	O1D-CGD-CBD	-3.15	118.04	124.48
19	A	1113	CLA	CMD-C2D-C3D	-3.15	118.79	124.68
19	A	1136	CLA	C4A-NA-C1A	3.15	108.12	106.71
19	1	1303	CLA	CGD-CBD-CAD	-3.15	100.54	110.73
21	A	6003	BCR	C33-C5-C4	3.15	119.66	113.62
19	A	1149	CLA	CBA-CAA-C2A	3.15	123.15	113.86
19	4	4014	CLA	O2A-CGA-CBA	3.15	121.78	111.91
19	L	1130	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
19	A	1309	CLA	C2D-C3D-C4D	-3.15	103.59	106.30
22	R	7024	LMU	C2'-C3'-C4'	3.14	116.86	109.68
19	3	3006	CLA	C2D-C3D-C4D	-3.14	103.59	106.30
21	B	6006	BCR	C31-C1-C6	-3.14	105.20	110.30
19	A	1131	CLA	CMD-C2D-C3D	-3.14	118.80	124.68
19	B	9010	CLA	CHB-C4A-NA	3.14	128.86	124.51
19	1	1014	CLA	C4A-NA-C1A	3.14	108.12	106.71
21	I	6021	BCR	C10-C11-C12	3.14	133.01	123.22
21	A	6002	BCR	C16-C17-C18	-3.14	122.83	127.31
19	A	1104	CLA	C4A-NA-C1A	3.14	108.12	106.71
19	B	1214	CLA	CMD-C2D-C3D	-3.14	118.81	124.68
22	4	7033	LMU	O5'-C1'-C2'	3.13	116.98	110.35
19	A	1126	CLA	CHB-C4A-NA	3.13	128.85	124.51
19	A	1125	CLA	C4A-NA-C1A	3.13	108.11	106.71
19	B	1228	CLA	O2A-C1-C2	3.13	116.86	108.64
19	2	2002	CLA	C4-C3-C2	-3.13	115.65	123.68
19	B	1236	CLA	C4A-NA-C1A	3.13	108.11	106.71
19	1	1303	CLA	O2A-CGA-CBA	3.13	121.72	111.91
19	H	1145	CLA	O2A-CGA-CBA	3.13	121.72	111.91
19	A	9013	CLA	CHB-C4A-NA	3.13	128.84	124.51
19	A	1117	CLA	O2A-CGA-CBA	3.12	121.71	111.91
19	K	3009	CLA	C4A-NA-C1A	3.12	108.11	106.71
22	A	7045	LMU	C2'-C3'-C4'	3.12	116.81	109.68
19	A	9011	CLA	CHB-C4A-NA	3.12	128.82	124.51
19	4	4013	CLA	C3B-C2B-C1B	-3.12	103.62	106.29
19	3	3008	CLA	C1-C2-C3	-3.11	121.71	126.75
19	F	1305	CLA	CBC-CAC-C3C	-3.11	104.34	112.27
19	A	9012	CLA	O2A-CGA-O1A	-3.11	115.74	123.59
21	B	6020	BCR	C24-C23-C22	-3.11	121.54	126.23
19	B	1301	CLA	CMA-C3A-C2A	-3.11	108.84	116.10
19	A	1106	CLA	CMD-C2D-C3D	-3.11	118.86	124.68
19	B	1223	CLA	CMD-C2D-C3D	-3.11	118.86	124.68
19	3	3016	CLA	CMD-C2D-C3D	-3.11	118.86	124.68
22	3	7003	LMU	O4'-C4B-C3B	3.10	117.53	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1209	CLA	C4-C3-C2	-3.10	115.72	123.68
19	A	1117	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
19	1	1005	CLA	C4A-NA-C1A	3.10	108.10	106.71
19	A	9013	CLA	CMD-C2D-C3D	-3.10	118.88	124.68
19	4	4006	CLA	CMD-C2D-C3D	-3.10	118.88	124.68
19	1	1006	CLA	CMD-C2D-C3D	-3.10	118.88	124.68
22	A	7044	LMU	O5'-C5'-C4'	3.09	116.27	109.75
21	B	6010	BCR	C27-C26-C25	-3.09	118.24	122.73
19	B	1220	CLA	CBA-CAA-C2A	3.09	122.98	113.86
19	3	3004	CLA	C2D-C3D-C4D	-3.09	103.64	106.30
21	B	6006	BCR	C38-C26-C27	3.09	119.55	113.62
19	R	1144	CLA	CED-O2D-CGD	3.09	122.92	115.94
19	B	1230	CLA	CMD-C2D-C3D	-3.09	118.90	124.68
19	B	1212	CLA	CMB-C2B-C3B	3.09	130.45	124.68
19	A	1110	CLA	CMD-C2D-C3D	-3.09	118.90	124.68
21	1	6023	BCR	C8-C7-C6	-3.09	118.53	127.20
19	A	1309	CLA	C3D-C2D-C1D	3.08	108.96	106.30
22	A	7010	LMU	C2'-C3'-C4'	3.08	116.72	109.68
22	B	7012	LMU	O5B-C5B-C4B	3.08	115.29	109.69
19	A	1123	CLA	O2A-CGA-CBA	3.08	121.58	111.91
19	A	1106	CLA	C6-C5-C3	-3.08	105.37	113.45
19	B	1221	CLA	CMD-C2D-C3D	-3.08	118.92	124.68
19	A	1131	CLA	O2A-CGA-CBA	3.08	121.56	111.91
19	2	2011	CLA	C3D-C4D-ND	3.08	112.81	110.14
19	B	1219	CLA	CED-O2D-CGD	3.08	122.89	115.94
19	A	1108	CLA	CMB-C2B-C3B	3.07	130.43	124.68
19	A	1104	CLA	CMB-C2B-C3B	3.07	130.43	124.68
19	B	1236	CLA	O1D-CGD-CBD	-3.07	118.19	124.48
19	L	1148	CLA	CMB-C2B-C3B	3.07	130.42	124.68
21	A	6011	BCR	C40-C30-C39	3.07	117.95	108.53
19	2	2013	CLA	O2A-CGA-CBA	3.07	121.54	111.91
19	L	1504	CLA	CMD-C2D-C3D	-3.07	118.94	124.68
19	H	1505	CLA	O2A-CGA-CBA	3.07	121.53	111.91
19	A	1101	CLA	C1-C2-C3	-3.06	121.79	126.75
19	B	1221	CLA	CAA-CBA-CGA	-3.06	104.30	113.25
19	B	1226	CLA	C2A-C1A-CHA	-3.06	118.50	123.86
19	3	3017	CLA	O1D-CGD-CBD	-3.06	118.22	124.48
19	A	1110	CLA	CHB-C4A-NA	3.06	128.74	124.51
19	B	1231	CLA	CED-O2D-CGD	3.06	122.86	115.94
19	B	1223	CLA	C4-C3-C5	3.06	120.42	115.27
19	B	1212	CLA	O2A-CGA-CBA	3.06	121.50	111.91
19	B	1208	CLA	O2D-CGD-O1D	-3.05	117.87	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	6022	BCR	C23-C24-C25	-3.05	118.63	127.20
19	B	9010	CLA	O2A-CGA-CBA	3.05	121.49	111.91
22	A	7044	LMU	C3B-C4B-C5B	3.05	115.68	110.24
19	B	1216	CLA	C4-C3-C5	3.05	120.40	115.27
19	B	1222	CLA	C4A-NA-C1A	3.05	108.08	106.71
22	3	7005	LMU	O1B-C4'-C3'	3.05	115.38	107.28
19	A	1139	CLA	C4-C3-C5	3.04	119.46	115.98
22	2	7027	LMU	C1'-C2'-C3'	3.04	116.33	110.00
19	A	1115	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	H	7032	LMU	C4B-C3B-C2B	-3.04	105.52	110.82
19	4	4005	CLA	C3D-C4D-ND	3.04	112.78	110.14
22	E	7037	LMU	O4'-C4B-C5B	3.04	116.84	109.30
19	A	1149	CLA	CGD-CBD-CAD	3.04	120.57	110.73
22	R	7014	LMU	O5B-C5B-C6B	3.04	113.99	106.44
22	K	7001	LMU	C3B-C4B-C5B	-3.04	104.82	110.24
19	B	1205	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
19	A	1112	CLA	CMD-C2D-C3D	-3.04	119.00	124.68
19	4	1009	CLA	CMB-C2B-C3B	3.04	130.63	124.69
22	H	7017	LMU	C1B-O5B-C5B	-3.04	107.73	113.69
22	H	7028	LMU	C1B-O1B-C4'	-3.04	110.45	117.96
22	H	7011	LMU	O1B-C4'-C3'	3.03	115.35	107.28
19	2	2002	CLA	C4-C3-C5	3.03	120.37	115.27
19	A	1103	CLA	CMD-C2D-C3D	-3.03	119.01	124.68
19	B	1206	CLA	CMB-C2B-C3B	3.03	130.35	124.68
19	B	1201	CLA	C4A-NA-C1A	3.03	108.07	106.71
21	I	6021	BCR	C30-C25-C24	3.03	124.35	115.78
19	L	1148	CLA	CHB-C4A-NA	3.03	128.70	124.51
19	1	1007	CLA	C4-C3-C5	3.03	120.36	115.27
21	B	6020	BCR	C19-C18-C17	-3.03	114.30	118.94
19	A	1109	CLA	CMB-C2B-C1B	3.02	133.11	128.46
19	1	1001	CLA	CBC-CAC-C3C	-3.02	104.57	112.27
22	A	7016	LMU	C1B-C2B-C3B	3.02	116.29	110.00
21	B	6017	BCR	C36-C18-C19	3.02	122.84	118.08
19	A	1104	CLA	C1-C2-C3	-3.02	120.82	126.04
19	B	1215	CLA	CGD-CBD-CAD	-3.02	100.95	110.73
19	A	9013	CLA	O2A-C1-C2	3.02	116.57	108.64
19	J	1311	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
22	B	7012	LMU	O1'-C1'-C2'	3.02	113.02	108.30
19	A	9022	CLA	C1-O2A-CGA	3.02	124.36	116.44
22	H	7017	LMU	C3B-C4B-C5B	3.01	115.62	110.24
19	4	4015	CLA	CHB-C4A-NA	3.01	128.68	124.51
22	H	7011	LMU	O3'-C3'-C4'	-3.01	101.96	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	6010	BCR	C28-C27-C26	-3.01	108.70	114.08
19	B	1210	CLA	C4A-NA-C1A	3.01	108.06	106.71
19	K	1146	CLA	O2A-CGA-O1A	-3.00	116.01	123.59
22	K	7041	LMU	C4B-C3B-C2B	-3.00	105.59	110.82
19	1	1303	CLA	CMA-C3A-C4A	3.00	119.83	111.77
19	A	1122	CLA	CMD-C2D-C3D	-3.00	119.07	124.68
21	I	6018	BCR	C24-C25-C26	-3.00	114.20	121.46
19	A	1140	CLA	CMD-C2D-C3D	-3.00	119.07	124.68
21	A	6002	BCR	C33-C5-C4	3.00	119.37	113.62
19	B	1224	CLA	O2A-CGA-O1A	-3.00	116.03	123.59
19	K	1146	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
19	A	1111	CLA	CMD-C2D-C3D	-3.00	119.07	124.68
19	A	1115	CLA	C4A-NA-C1A	2.99	108.05	106.71
21	1	6023	BCR	C30-C25-C24	2.99	124.25	115.78
19	A	1135	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	B	1216	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
21	B	6017	BCR	C16-C15-C14	-2.99	117.34	123.47
19	A	1141	CLA	C4-C3-C5	2.99	120.30	115.27
19	B	1205	CLA	O2A-CGA-O1A	-2.99	116.04	123.59
19	J	1308	CLA	C4-C3-C5	2.99	120.30	115.27
19	A	1149	CLA	CAA-C2A-C1A	2.99	121.77	111.97
19	B	1214	CLA	C4A-NA-C1A	2.99	108.05	106.71
19	B	1213	CLA	CMD-C2D-C3D	-2.99	119.09	124.68
19	2	2002	CLA	C4A-NA-C1A	2.99	108.05	106.71
19	B	1226	CLA	CMA-C3A-C2A	-2.99	101.78	113.83
21	3	6022	BCR	C32-C1-C6	-2.99	105.45	110.30
19	A	1102	CLA	CMB-C2B-C3B	2.99	130.27	124.68
19	A	1138	CLA	C4-C3-C5	2.99	120.30	115.27
21	B	6005	BCR	C39-C30-C25	2.98	115.13	110.30
19	B	1201	CLA	CHB-C4A-NA	2.98	128.63	124.51
19	3	3006	CLA	C3D-C2D-C1D	2.98	108.87	106.30
21	B	6005	BCR	C2-C1-C6	-2.98	105.90	110.48
19	4	4001	CLA	CMD-C2D-C3D	-2.97	119.11	124.68
21	A	6002	BCR	C32-C1-C31	2.97	117.66	108.53
19	2	2013	CLA	C1-O2A-CGA	2.97	124.24	116.44
19	4	1009	CLA	CAA-C2A-C3A	-2.97	109.17	116.10
19	B	1224	CLA	CAA-C2A-C3A	-2.97	104.64	112.78
19	4	1306	CLA	C4-C3-C5	2.97	120.27	115.27
19	L	1148	CLA	CMA-C3A-C2A	2.97	125.81	113.83
21	F	6016	BCR	C34-C9-C10	-2.97	118.76	122.92
19	L	1502	CLA	CGD-CBD-CAD	-2.97	101.12	110.73
21	B	6017	BCR	C28-C27-C26	-2.97	108.78	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1007	CLA	O2A-CGA-CBA	2.97	121.22	111.91
19	B	1203	CLA	CMD-C2D-C3D	-2.96	119.13	124.68
19	A	1116	CLA	C1-O2A-CGA	2.96	124.22	116.44
22	B	7038	LMU	O5'-C1'-C2'	2.96	116.62	110.35
21	F	6016	BCR	C27-C26-C25	-2.96	118.43	122.73
19	L	1130	CLA	O2A-CGA-CBA	2.96	121.19	111.91
21	A	6003	BCR	C28-C27-C26	-2.96	108.80	114.08
19	1	1012	CLA	C1B-C2B-C3B	-2.96	104.17	106.92
19	A	9023	CLA	CMA-C3A-C4A	-2.96	103.83	111.77
19	A	1109	CLA	O2D-CGD-CBD	2.96	116.52	111.27
19	2	4009	CLA	O2A-CGA-CBA	2.95	121.17	111.91
19	A	1131	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
19	B	1229	CLA	C4-C3-C5	2.95	120.23	115.27
19	3	1147	CLA	O1D-CGD-CBD	-2.95	118.45	124.48
19	B	1206	CLA	C4A-NA-C1A	2.95	108.03	106.71
19	A	1101	CLA	CMB-C2B-C3B	2.95	130.19	124.68
22	A	7044	LMU	O2'-C2'-C3'	-2.95	103.54	110.35
19	2	2014	CLA	O2A-CGA-CBA	2.95	121.15	111.91
19	H	1145	CLA	C4-C3-C5	2.94	120.22	115.27
22	4	7053	LMU	O1B-C4'-C5'	2.94	117.52	109.45
19	A	1141	CLA	CHB-C4A-NA	2.94	128.58	124.51
19	B	1218	CLA	C4A-NA-C1A	2.94	108.03	106.71
21	B	6006	BCR	C34-C9-C10	-2.94	118.80	122.92
19	R	1144	CLA	C1-O2A-CGA	2.94	124.16	116.44
19	B	1229	CLA	CHB-C4A-NA	2.94	128.57	124.51
19	B	1214	CLA	O2A-CGA-CBA	2.94	121.13	111.91
19	H	1241	CLA	O2A-CGA-CBA	2.94	121.13	111.91
19	A	1104	CLA	CMD-C2D-C3D	-2.94	119.18	124.68
20	B	5002	PQN	C2M-C2-C1	2.94	121.14	116.27
19	A	1133	CLA	O2A-CGA-CBA	2.94	121.12	111.91
22	E	7048	LMU	O4'-C4B-C5B	-2.93	102.01	109.30
19	3	3011	CLA	CMD-C2D-C3D	-2.93	119.19	124.68
19	B	1219	CLA	O2D-CGD-CBD	2.93	116.48	111.27
21	J	6012	BCR	C38-C26-C25	-2.93	121.23	124.53
19	B	1239	CLA	CHB-C4A-NA	2.93	128.57	124.51
22	R	7024	LMU	C1'-C2'-C3'	2.93	116.10	110.00
19	B	1208	CLA	CAA-C2A-C3A	-2.93	104.75	112.78
19	3	3011	CLA	C4A-NA-C1A	2.93	108.02	106.71
19	R	1150	CLA	CED-O2D-CGD	2.93	122.57	115.94
19	B	1227	CLA	CMD-C2D-C3D	-2.93	119.19	124.68
19	2	2008	CLA	C3D-C2D-C1D	2.93	108.83	106.30
19	A	1122	CLA	C4-C3-C5	2.93	120.20	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	1242	CLA	C4A-NA-C1A	2.93	108.02	106.71
22	K	7041	LMU	O1B-C1B-C2B	2.93	115.68	108.10
21	A	6011	BCR	C3-C4-C5	-2.93	108.85	114.08
19	B	1238	CLA	C4A-NA-C1A	2.92	108.02	106.71
22	K	7001	LMU	O1'-C1'-C2'	2.92	112.87	108.30
19	4	4013	CLA	C2D-C3D-C4D	-2.92	103.78	106.30
21	B	6005	BCR	C4-C5-C6	-2.92	118.49	122.73
19	2	2011	CLA	C3D-C2D-C1D	2.92	108.82	106.30
19	A	1149	CLA	C1B-C2B-C3B	-2.92	104.20	106.92
21	I	6021	BCR	C32-C1-C31	2.92	117.50	108.53
19	3	3005	CLA	C3D-C4D-ND	2.92	112.68	110.14
19	A	1104	CLA	O2A-CGA-CBA	2.92	121.07	111.91
19	B	1222	CLA	C4-C3-C5	2.92	120.18	115.27
21	B	6004	BCR	C38-C26-C27	2.92	119.22	113.62
19	I	1204	CLA	C4A-NA-C1A	2.92	108.02	106.71
19	L	1503	CLA	C1-C2-C3	-2.92	122.03	126.75
22	E	7048	LMU	O1B-C1B-C2B	2.92	115.66	108.10
19	A	1132	CLA	CMA-C3A-C2A	-2.92	102.06	113.83
22	K	7047	LMU	O1B-C4'-C5'	2.92	117.44	109.45
19	1	1002	CLA	CHB-C4A-NA	2.92	128.54	124.51
19	B	1211	CLA	CHB-C4A-NA	2.92	128.54	124.51
19	A	1104	CLA	CED-O2D-CGD	2.91	122.53	115.94
19	B	1225	CLA	C16-C15-C13	-2.91	106.50	115.92
22	R	7022	LMU	O1B-C4'-C3'	2.91	115.02	107.28
19	1	1310	CLA	CHB-C4A-NA	2.91	128.79	124.34
19	J	1311	CLA	CED-O2D-CGD	2.91	122.51	115.94
19	B	1235	CLA	O2A-CGA-CBA	2.90	121.02	111.91
19	4	4004	CLA	C2A-C3A-C4A	-2.90	99.62	104.18
19	A	1126	CLA	C4A-NA-C1A	2.90	108.01	106.71
19	A	1137	CLA	C4A-NA-C1A	2.90	108.01	106.71
19	A	1104	CLA	C2A-C1A-CHA	-2.90	118.80	123.86
19	A	1124	CLA	C4A-NA-C1A	2.90	108.01	106.71
19	G	1242	CLA	CHB-C4A-NA	2.89	128.51	124.51
21	A	6003	BCR	C29-C30-C25	-2.89	106.03	110.48
19	3	3005	CLA	CHB-C4A-NA	2.89	128.77	124.34
19	J	1311	CLA	O2A-CGA-CBA	2.89	120.98	111.91
19	4	4007	CLA	CMB-C2B-C3B	2.89	130.08	124.68
19	A	1133	CLA	CHB-C4A-NA	2.89	128.51	124.51
19	4	1009	CLA	C4A-NA-C1A	2.89	108.00	106.71
19	4	1004	CLA	CHB-C4A-NA	2.89	128.50	124.51
19	1	1001	CLA	CED-O2D-CGD	2.89	122.46	115.94
19	1	1001	CLA	O1D-CGD-CBD	-2.88	118.58	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1224	CLA	CHB-C4A-NA	2.88	128.50	124.51
19	1	1006	CLA	CHB-C4A-NA	2.88	128.50	124.51
19	A	1101	CLA	CMD-C2D-C3D	-2.88	119.29	124.68
21	F	6014	BCR	C39-C30-C25	2.88	114.97	110.30
22	3	7005	LMU	O2'-C2'-C1'	2.88	117.03	110.05
21	B	6010	BCR	C40-C30-C39	2.88	117.36	108.53
19	4	4001	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
21	A	6003	BCR	C34-C9-C10	-2.87	118.90	122.92
19	4	4002	CLA	CGD-CBD-CAD	2.87	120.04	110.73
19	2	2011	CLA	C2A-C3A-C4A	-2.87	99.67	104.18
19	A	1115	CLA	CMD-C2D-C3D	-2.87	119.31	124.68
19	L	1130	CLA	CMD-C2D-C3D	-2.87	119.31	124.68
19	4	1304	CLA	C11-C10-C8	-2.87	106.64	115.92
19	3	3008	CLA	CED-O2D-CGD	2.87	122.43	115.94
22	4	7052	LMU	O5'-C1'-O1'	-2.87	103.18	109.97
19	A	1113	CLA	C1-O2A-CGA	2.87	123.97	116.44
21	I	6021	BCR	C23-C24-C25	-2.87	119.15	127.20
21	A	6002	BCR	C29-C30-C25	-2.87	106.07	110.48
19	A	9013	CLA	C4A-NA-C1A	2.87	108.00	106.71
19	R	1144	CLA	C4A-NA-C1A	2.86	107.99	106.71
19	B	1206	CLA	O2A-CGA-O1A	-2.86	116.36	123.59
21	B	6020	BCR	C39-C30-C25	2.86	114.94	110.30
19	L	1504	CLA	C2A-C1A-CHA	-2.86	118.85	123.86
19	1	1002	CLA	O2D-CGD-CBD	2.86	116.36	111.27
22	R	7020	LMU	C3B-C4B-C5B	-2.86	105.13	110.24
19	B	1219	CLA	C5-C3-C2	-2.86	115.33	121.12
19	K	3009	CLA	O2A-CGA-CBA	2.86	120.89	111.91
19	A	1106	CLA	CMB-C2B-C3B	2.86	130.03	124.68
19	B	1232	CLA	O1D-CGD-CBD	-2.86	118.63	124.48
22	H	7043	LMU	C1'-O5'-C5'	2.86	119.30	113.69
19	B	1216	CLA	CAA-C2A-C1A	2.86	121.35	111.97
19	A	1106	CLA	C4A-NA-C1A	2.86	107.99	106.71
21	A	6002	BCR	C38-C26-C27	2.86	119.10	113.62
22	A	7010	LMU	C4B-C3B-C2B	2.86	115.81	110.82
19	A	1124	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
19	H	1145	CLA	CGD-CBD-CAD	2.85	119.98	110.73
21	B	6004	BCR	C39-C30-C25	2.85	114.93	110.30
19	B	1239	CLA	C4-C3-C5	2.85	120.07	115.27
19	A	1103	CLA	O2A-CGA-CBA	2.85	120.85	111.91
19	B	1227	CLA	CGD-CBD-CAD	2.85	119.96	110.73
22	K	7042	LMU	C1B-O1B-C4'	-2.85	110.92	117.96
19	A	9011	CLA	CMD-C2D-C3D	-2.85	119.35	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	1143	CLA	C4A-NA-C1A	2.85	107.99	106.71
19	A	1140	CLA	O2A-CGA-CBA	2.85	120.84	111.91
19	B	1228	CLA	CED-O2D-CGD	2.85	122.37	115.94
19	1	1012	CLA	CBD-CHA-C1A	2.84	131.99	127.43
19	4	4007	CLA	CMD-C2D-C3D	-2.84	119.36	124.68
21	I	6018	BCR	C33-C5-C4	2.84	119.08	113.62
21	B	6005	BCR	C1-C6-C5	-2.84	118.61	122.61
22	3	7005	LMU	O5B-C5B-C6B	2.84	113.50	106.44
22	2	7027	LMU	C6B-C5B-C4B	2.84	119.66	113.00
19	A	1127	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	3	7005	LMU	O5B-C5B-C4B	-2.84	104.54	109.69
19	R	1144	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	3	3004	CLA	C3D-C2D-C1D	2.84	108.75	106.30
19	3	3004	CLA	C3D-C4D-ND	2.84	112.61	110.14
19	A	1122	CLA	CHB-C4A-NA	2.84	128.44	124.51
19	3	3013	CLA	C2A-C1A-CHA	-2.84	118.90	123.86
19	A	1102	CLA	O2A-CGA-O1A	-2.84	116.43	123.59
19	H	1241	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
21	A	6008	BCR	C37-C22-C23	2.84	122.54	118.08
19	A	9023	CLA	O2A-CGA-CBA	2.83	120.80	111.91
19	1	1303	CLA	O2A-CGA-O1A	-2.83	116.44	123.59
22	E	7037	LMU	O5'-C5'-C6'	2.83	113.48	106.44
21	B	6010	BCR	C32-C1-C6	-2.83	105.70	110.30
21	3	6022	BCR	C38-C26-C27	2.83	119.06	113.62
19	A	1109	CLA	CHB-C4A-NA	2.83	128.43	124.51
19	4	4002	CLA	CED-O2D-CGD	2.83	122.34	115.94
22	3	7005	LMU	O1B-C1B-C2B	2.83	115.43	108.10
19	B	1236	CLA	CMD-C2D-C3D	-2.83	119.39	124.68
19	A	1103	CLA	CED-O2D-CGD	2.83	122.33	115.94
22	K	7001	LMU	O5B-C5B-C4B	-2.83	104.56	109.69
19	2	2003	CLA	C3D-C2D-C1D	2.83	108.74	106.30
19	B	1209	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
19	L	1148	CLA	C1-O2A-CGA	2.82	123.85	116.44
21	J	6012	BCR	C16-C17-C18	-2.82	123.28	127.31
19	R	1144	CLA	O2A-CGA-O1A	-2.82	116.47	123.59
19	K	1142	CLA	CAA-CBA-CGA	-2.82	107.52	113.59
19	4	4010	CLA	C2D-C3D-C4D	-2.82	103.87	106.30
19	A	1132	CLA	CED-O2D-CGD	2.82	122.31	115.94
19	B	1205	CLA	CMD-C2D-C3D	-2.82	119.41	124.68
19	3	3002	CLA	C3D-C4D-ND	2.82	112.59	110.14
19	3	1147	CLA	O2A-CGA-O1A	-2.82	114.32	123.14
19	J	1308	CLA	CGD-CBD-CAD	-2.82	101.61	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1311	CLA	C4-C3-C5	2.81	120.00	115.27
19	A	1106	CLA	CAA-C2A-C1A	-2.81	102.76	111.97
19	K	1143	CLA	O2A-CGA-CBA	2.81	120.73	111.91
22	B	7040	LMU	O2'-C2'-C3'	-2.81	103.85	110.35
19	4	4003	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
19	A	1107	CLA	O2A-C1-C2	2.81	116.02	108.64
22	E	7037	LMU	O1B-C1B-O5B	2.81	118.52	110.67
19	A	1120	CLA	O2A-CGA-CBA	2.81	120.71	111.91
19	L	1504	CLA	O2A-CGA-CBA	2.80	120.70	111.91
19	H	1207	CLA	CMD-C2D-C3D	-2.80	119.43	124.68
21	A	6008	BCR	C33-C5-C4	2.80	119.00	113.62
19	L	1130	CLA	C4A-NA-C1A	2.80	107.96	106.71
19	1	1013	CLA	CHB-C4A-NA	2.80	128.38	124.51
19	2	2013	CLA	O1D-CGD-CBD	-2.80	118.76	124.48
21	B	6006	BCR	C40-C30-C39	2.80	117.11	108.53
19	3	3006	CLA	C3D-C4D-ND	2.80	112.57	110.14
19	A	9023	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
19	2	2006	CLA	CMD-C2D-C3D	-2.79	119.45	124.68
22	R	7025	LMU	O5'-C5'-C4'	2.79	115.64	109.75
19	F	1302	CLA	CMA-C3A-C2A	-2.79	109.58	116.10
21	B	6010	BCR	C16-C15-C14	-2.79	117.75	123.47
22	C	7015	LMU	C4B-C3B-C2B	2.79	115.70	110.82
19	B	1229	CLA	CMD-C2D-C3D	-2.79	119.46	124.68
19	1	1008	CLA	CMB-C2B-C3B	2.79	129.90	124.68
22	B	7040	LMU	C1'-C2'-C3'	2.79	115.81	110.00
19	4	1004	CLA	O2A-CGA-CBA	2.79	120.66	111.91
19	B	1206	CLA	C4-C3-C5	2.79	119.96	115.27
19	K	1146	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
19	B	1213	CLA	CHB-C4A-NA	2.79	128.37	124.51
19	A	1108	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
19	3	3001	CLA	CHB-C4A-NA	2.79	128.61	124.34
19	A	1133	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
22	4	7019	LMU	C1'-C2'-C3'	2.78	115.80	110.00
19	K	1146	CLA	CED-O2D-CGD	2.78	122.24	115.94
21	A	6002	BCR	C20-C19-C18	-2.78	118.59	126.42
21	B	6006	BCR	C28-C27-C26	-2.78	109.11	114.08
19	A	1132	CLA	CHB-C4A-NA	2.78	128.36	124.51
19	4	1304	CLA	CED-O2D-CGD	2.78	122.23	115.94
19	B	1215	CLA	CHB-C4A-NA	2.78	128.36	124.51
21	B	6020	BCR	C8-C7-C6	-2.78	119.39	127.20
19	B	1233	CLA	CED-O2D-CGD	2.78	122.23	115.94
19	B	1239	CLA	O2A-CGA-O1A	-2.78	116.57	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	1305	CLA	O2A-CGA-CBA	2.78	120.64	111.91
19	A	9023	CLA	CMD-C2D-C3D	-2.78	119.47	124.68
19	L	1502	CLA	CED-O2D-CGD	2.78	122.22	115.94
21	A	6007	BCR	C15-C16-C17	-2.78	117.78	123.47
21	J	6012	BCR	C38-C26-C27	2.78	118.95	113.62
19	A	1309	CLA	C3D-C4D-ND	2.78	112.55	110.14
22	A	7044	LMU	C1B-O5B-C5B	2.77	119.13	113.69
22	H	7017	LMU	O5'-C1'-C2'	2.77	116.22	110.35
22	A	7010	LMU	O1'-C1'-C2'	2.77	112.63	108.30
19	4	4004	CLA	CHB-C4A-NA	2.77	128.58	124.34
21	I	6018	BCR	C27-C26-C25	-2.77	118.71	122.73
19	G	1242	CLA	CMD-C2D-C3D	-2.77	119.49	124.68
22	4	7018	LMU	O1'-C1'-C2'	2.77	112.63	108.30
19	3	3003	CLA	CBD-CHA-C1A	2.77	131.87	127.43
19	2	2008	CLA	CHB-C4A-NA	2.77	128.58	124.34
19	3	3016	CLA	O2A-CGA-CBA	2.77	120.60	111.91
22	3	7005	LMU	O3'-C3'-C4'	2.77	117.28	109.94
19	4	1304	CLA	CBC-CAC-C3C	-2.77	105.22	112.27
19	H	1505	CLA	C1-O2A-CGA	2.76	123.70	116.44
19	F	1305	CLA	CED-O2D-CGD	2.76	122.19	115.94
19	A	1103	CLA	C1-O2A-CGA	2.76	123.70	116.44
19	B	1232	CLA	CMD-C2D-C3D	-2.76	119.51	124.68
19	3	3003	CLA	C4A-NA-C1A	2.76	107.95	106.71
19	3	3013	CLA	O2A-CGA-CBA	2.76	120.57	111.91
19	4	1306	CLA	O2A-CGA-CBA	2.76	120.57	111.91
19	B	1222	CLA	O2A-CGA-CBA	2.76	120.57	111.91
22	4	7052	LMU	O6'-C6'-C5'	-2.76	101.83	111.29
19	3	3011	CLA	CED-O2D-CGD	2.76	122.18	115.94
19	B	1215	CLA	O2A-C1-C2	2.76	115.88	108.64
22	H	7030	LMU	O1'-C1'-C2'	2.75	112.60	108.30
22	B	7038	LMU	O1B-C1B-C2B	2.75	115.23	108.10
19	B	1216	CLA	O1D-CGD-CBD	-2.75	118.85	124.48
19	B	1301	CLA	CMD-C2D-C3D	-2.75	119.53	124.68
19	3	3011	CLA	CMB-C2B-C3B	2.75	129.82	124.68
19	4	4006	CLA	CED-O2D-CGD	2.75	122.16	115.94
19	2	2007	CLA	CMD-C2D-C3D	-2.75	119.53	124.68
19	1	1001	CLA	CAA-C2A-C3A	-2.75	105.25	112.78
19	B	1227	CLA	C1-C2-C3	-2.75	122.30	126.75
19	A	1120	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
19	A	9011	CLA	O2A-CGA-CBA	2.75	120.53	111.91
20	A	5001	PQN	C21-C20-C18	-2.75	107.05	115.92
19	A	1124	CLA	O2A-CGA-CBA	2.74	120.52	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1206	CLA	CGD-CBD-CAD	2.74	119.62	110.73
19	K	1142	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
19	3	1147	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
21	A	6008	BCR	C38-C26-C27	2.74	118.88	113.62
19	A	1101	CLA	O2A-CGA-CBA	2.74	120.51	111.91
19	A	1101	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
21	I	6018	BCR	C31-C1-C6	-2.74	105.86	110.30
19	4	4002	CLA	CMA-C3A-C4A	-2.74	104.41	111.77
19	2	4009	CLA	CMB-C2B-C3B	2.74	129.80	124.68
19	F	1240	CLA	CAA-C2A-C3A	-2.74	109.71	116.10
19	1	1013	CLA	O2D-CGD-CBD	2.74	116.13	111.27
19	B	1202	CLA	C4-C3-C5	2.73	119.87	115.27
19	3	3014	CLA	CHB-C4A-NA	2.73	128.53	124.34
21	B	6010	BCR	C32-C1-C31	2.73	116.92	108.53
19	A	9012	CLA	O1D-CGD-CBD	-2.73	118.89	124.48
19	1	1005	CLA	CAA-C2A-C3A	-2.73	105.29	112.78
19	2	2014	CLA	C3A-C2A-C1A	2.73	105.43	101.34
21	F	6014	BCR	C34-C9-C10	-2.73	119.10	122.92
19	B	1202	CLA	C1-C2-C3	2.73	130.77	126.04
19	A	9023	CLA	CED-O2D-CGD	2.73	122.11	115.94
22	E	7048	LMU	C1'-C2'-C3'	-2.73	104.31	110.00
19	A	1149	CLA	O2A-CGA-O1A	-2.73	116.70	123.59
19	H	1207	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
21	A	6003	BCR	C11-C12-C13	-2.73	118.75	126.42
19	B	1224	CLA	CMB-C2B-C3B	2.73	129.78	124.68
21	I	6018	BCR	C34-C9-C10	-2.73	119.10	122.92
19	3	3015	CLA	C3D-C4D-ND	2.73	112.51	110.14
19	I	1204	CLA	CMD-C2D-C3D	-2.73	119.58	124.68
19	B	1228	CLA	O2A-CGA-CBA	2.73	120.46	111.91
19	3	3004	CLA	CHB-C4A-NA	2.72	128.51	124.34
19	B	1214	CLA	CMB-C2B-C3B	2.72	129.77	124.68
21	B	6017	BCR	C3-C4-C5	-2.72	109.22	114.08
22	H	7043	LMU	C1'-C2'-C3'	2.72	115.66	110.00
19	3	3016	CLA	C1-C2-C3	-2.72	121.34	126.04
19	A	1110	CLA	O2A-CGA-CBA	2.72	120.44	111.91
19	1	1003	CLA	O2A-CGA-CBA	2.72	120.44	111.91
19	B	1228	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
19	3	3008	CLA	O2A-CGA-O1A	-2.71	116.74	123.59
21	I	6018	BCR	C8-C9-C10	2.71	123.11	118.94
19	2	2007	CLA	O2A-CGA-CBA	2.71	120.42	111.91
19	A	1122	CLA	C4A-NA-C1A	2.71	107.92	106.71
19	B	1216	CLA	C4A-NA-C1A	2.71	107.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	2014	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
19	B	1234	CLA	C1-O2A-CGA	2.71	123.55	116.44
19	3	3006	CLA	CHB-C4A-NA	2.71	128.49	124.34
19	A	1132	CLA	O2A-CGA-CBA	2.71	120.41	111.91
19	R	1150	CLA	CGD-CBD-CAD	-2.71	101.96	110.73
19	3	3014	CLA	C2A-C3A-C4A	-2.71	99.93	104.18
19	3	3011	CLA	C4-C3-C5	2.71	119.83	115.27
21	B	6005	BCR	C20-C19-C18	-2.71	118.81	126.42
21	B	6020	BCR	C34-C9-C10	-2.71	119.13	122.92
22	3	7005	LMU	C1'-C2'-C3'	-2.71	104.36	110.00
19	H	1207	CLA	O2A-CGA-CBA	2.71	120.40	111.91
19	1	1015	CLA	C2A-C3A-C4A	-2.71	99.93	104.18
19	F	1240	CLA	CAB-C3B-C2B	-2.71	119.39	124.69
21	B	6017	BCR	C27-C26-C25	-2.71	118.80	122.73
22	R	7024	LMU	O5'-C5'-C6'	2.71	113.16	106.44
19	A	1103	CLA	C4-C3-C5	2.70	119.82	115.27
19	A	1105	CLA	CMD-C2D-C3D	-2.70	119.62	124.68
21	B	6017	BCR	C38-C26-C27	2.70	118.81	113.62
21	B	6005	BCR	C16-C15-C14	-2.70	117.94	123.47
19	A	1117	CLA	CMB-C2B-C3B	2.70	129.73	124.68
19	A	1134	CLA	CHB-C4A-NA	2.70	128.25	124.51
19	A	1128	CLA	CED-O2D-CGD	2.70	122.04	115.94
19	B	1217	CLA	O2A-CGA-CBA	2.70	120.38	111.91
19	B	1225	CLA	CMA-C3A-C2A	-2.70	102.94	113.83
19	4	1304	CLA	C7-C6-C5	-2.70	106.03	113.36
19	A	1125	CLA	CMD-C2D-C3D	-2.70	119.63	124.68
19	4	4007	CLA	CHB-C4A-NA	2.70	128.24	124.51
19	1	1002	CLA	C3A-C2A-C1A	2.70	105.38	101.34
19	K	3009	CLA	CMD-C2D-C3D	-2.70	119.64	124.68
19	A	1105	CLA	CAA-C2A-C1A	-2.69	103.14	111.97
22	R	7020	LMU	O5B-C1B-C2B	2.69	116.05	110.35
22	R	7022	LMU	O1B-C1B-C2B	2.69	115.08	108.10
19	B	1211	CLA	C4A-NA-C1A	2.69	107.92	106.71
19	A	9013	CLA	O2A-CGA-CBA	2.69	120.36	111.91
22	R	7020	LMU	C1B-C2B-C3B	2.69	115.60	110.00
19	A	1129	CLA	CMD-C2D-C3D	-2.69	119.64	124.68
19	A	1131	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	3	7003	LMU	O2B-C2B-C3B	2.69	116.57	110.35
19	L	1502	CLA	O2A-CGA-CBA	2.69	120.35	111.91
19	A	1124	CLA	C1-C2-C3	-2.69	121.39	126.04
19	A	1108	CLA	O1D-CGD-CBD	-2.69	118.98	124.48
19	4	4007	CLA	C1-C2-C3	-2.69	121.39	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	1240	CLA	CBD-CHA-C1A	2.69	131.74	127.43
22	4	7053	LMU	C1'-C2'-C3'	2.69	115.59	110.00
19	B	1230	CLA	CMB-C2B-C3B	2.69	129.71	124.68
19	B	1209	CLA	CHB-C4A-NA	2.69	128.23	124.51
21	A	6007	BCR	C8-C7-C6	-2.69	119.66	127.20
19	A	1105	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
19	B	1229	CLA	C4A-NA-C1A	2.68	107.91	106.71
21	J	6012	BCR	C40-C30-C25	2.68	114.65	110.30
19	1	1008	CLA	O2A-CGA-CBA	2.68	120.33	111.91
19	4	4002	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	A	1126	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
19	2	4009	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
21	A	6003	BCR	C38-C26-C27	2.68	118.76	113.62
19	3	3006	CLA	C2A-C3A-C4A	-2.68	99.98	104.18
19	4	4005	CLA	CHB-C4A-NA	2.68	128.44	124.34
19	A	1120	CLA	CHB-C4A-NA	2.68	128.21	124.51
21	3	6022	BCR	C32-C1-C31	2.68	116.74	108.53
19	G	1242	CLA	C1-C2-C3	-2.67	121.42	126.04
19	A	1134	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
22	R	7024	LMU	O1'-C1'-C2'	2.67	112.48	108.30
19	A	1115	CLA	O2A-CGA-CBA	2.67	120.29	111.91
19	B	1203	CLA	CBC-CAC-C3C	-2.67	105.46	112.27
19	A	1111	CLA	CAA-C2A-C1A	-2.67	103.22	111.97
21	B	6020	BCR	C37-C22-C21	-2.67	119.18	122.92
19	A	1123	CLA	CHB-C4A-NA	2.67	128.20	124.51
19	A	1137	CLA	O2A-CGA-CBA	2.67	120.28	111.91
19	1	1303	CLA	C4A-NA-C1A	-2.67	105.51	106.71
19	B	1230	CLA	O2A-CGA-CBA	2.67	120.28	111.91
19	3	3003	CLA	CMD-C2D-C3D	-2.67	119.69	124.68
22	R	7020	LMU	C3'-C4'-C5'	-2.67	104.81	110.93
22	R	7014	LMU	O5'-C1'-O1'	2.66	116.28	109.97
19	L	1502	CLA	CMA-C3A-C4A	-2.66	104.62	111.77
19	F	1302	CLA	CAA-C2A-C3A	-2.66	109.89	116.10
21	F	6014	BCR	C33-C5-C4	2.66	118.73	113.62
19	B	1212	CLA	C4-C3-C2	-2.66	116.86	123.68
19	A	1237	CLA	C6-C7-C8	-2.66	107.33	115.92
21	3	6022	BCR	C24-C23-C22	-2.66	122.22	126.23
21	B	6006	BCR	C23-C24-C25	-2.66	119.74	127.20
21	A	6011	BCR	C27-C26-C25	-2.66	118.88	122.73
21	A	6003	BCR	C40-C30-C25	2.65	114.61	110.30
21	A	6011	BCR	C8-C7-C6	-2.65	119.75	127.20
19	B	1226	CLA	O1D-CGD-CBD	-2.65	119.06	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	6011	BCR	C33-C5-C4	2.65	118.71	113.62
19	A	1131	CLA	CMB-C2B-C3B	2.65	129.63	124.68
19	A	1123	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
22	H	7002	LMU	O1'-C1'-C2'	2.65	112.44	108.30
19	H	1241	CLA	O1D-CGD-CBD	-2.65	119.07	124.48
19	B	1233	CLA	C4A-NA-C1A	2.65	107.90	106.71
21	1	6023	BCR	C31-C1-C2	2.65	119.49	108.91
19	A	1119	CLA	C1-O2A-CGA	2.65	123.38	116.44
22	2	7046	LMU	O1B-C4'-C3'	2.65	114.32	107.28
19	4	1009	CLA	CHB-C4A-NA	2.64	128.17	124.51
22	A	7035	LMU	O5'-C5'-C4'	-2.64	104.18	109.75
19	A	1105	CLA	O1D-CGD-CBD	-2.64	119.08	124.48
21	B	6006	BCR	C15-C14-C13	-2.64	123.54	127.31
22	H	7032	LMU	C3'-C4'-C5'	2.64	116.98	110.93
19	A	1119	CLA	CED-O2D-CGD	2.64	121.90	115.94
19	A	1103	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	A	9012	CLA	C1-C2-C3	-2.64	121.48	126.04
19	A	1124	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	B	6020	BCR	C30-C25-C26	2.64	126.33	122.61
19	B	1221	CLA	C1-O2A-CGA	2.64	123.36	116.44
22	4	7019	LMU	C1B-C2B-C3B	2.64	115.48	110.00
22	F	7036	LMU	O2'-C2'-C1'	2.64	116.45	110.05
21	L	6019	BCR	C40-C30-C39	2.63	116.61	108.53
19	1	1010	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	3	3002	CLA	C2D-C3D-C4D	-2.63	104.03	106.30
21	B	6005	BCR	C23-C24-C25	-2.63	119.81	127.20
19	A	1106	CLA	O2A-CGA-O1A	-2.63	116.95	123.59
19	2	2010	CLA	C2A-C3A-C4A	-2.63	100.05	104.18
19	A	1116	CLA	O1D-CGD-CBD	-2.63	119.10	124.48
20	A	5001	PQN	C2M-C2-C1	2.63	120.62	116.27
19	B	1209	CLA	C5-C3-C2	2.63	126.43	121.12
19	1	1007	CLA	CMD-C2D-C3D	-2.63	119.77	124.68
19	B	1212	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
19	2	2011	CLA	C2B-C3B-C4B	2.62	108.53	106.29
19	3	3016	CLA	CHB-C4A-NA	2.62	128.14	124.51
19	4	4003	CLA	CED-O2D-CGD	2.62	121.87	115.94
19	A	1113	CLA	CGD-CBD-CAD	2.62	119.22	110.73
19	A	1101	CLA	C4A-NA-C1A	2.62	107.88	106.71
19	H	1505	CLA	CGD-CBD-CAD	-2.62	102.25	110.73
19	B	1202	CLA	CAA-C2A-C1A	-2.62	103.39	111.97
21	L	6019	BCR	C32-C1-C6	-2.62	106.05	110.30
19	A	1138	CLA	O2A-CGA-CBA	2.62	120.13	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1503	CLA	O2A-CGA-CBA	2.62	120.13	111.91
19	A	1104	CLA	CHB-C4A-NA	2.62	128.13	124.51
19	A	1104	CLA	CAA-C2A-C1A	-2.62	103.39	111.97
19	A	1109	CLA	C3A-C2A-C1A	2.62	105.26	101.34
20	B	5002	PQN	C16-C15-C13	-2.62	106.59	113.45
21	I	6018	BCR	C35-C13-C12	2.62	122.20	118.08
19	3	3002	CLA	C3D-C2D-C1D	2.62	108.56	106.30
19	A	1108	CLA	CED-O2D-CGD	2.61	121.85	115.94
19	A	1116	CLA	CED-O2D-CGD	2.61	121.85	115.94
21	A	6002	BCR	C8-C9-C10	2.61	122.95	118.94
19	A	1119	CLA	C4-C3-C5	2.61	119.67	115.27
19	H	1207	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	A	1110	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	1	1010	CLA	CMB-C2B-C3B	2.61	129.56	124.68
19	H	1241	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
19	B	1301	CLA	CGD-CBD-CAD	-2.61	103.60	114.30
19	A	1128	CLA	CAA-C2A-C1A	-2.61	103.42	111.97
19	A	1237	CLA	O1D-CGD-CBD	-2.61	119.15	124.48
19	L	1501	CLA	C1-O2A-CGA	2.61	123.29	116.44
22	H	7030	LMU	C4B-C3B-C2B	-2.61	106.27	110.82
19	3	1147	CLA	C3B-C4B-NB	2.61	112.58	109.21
21	F	6016	BCR	C35-C13-C14	-2.61	119.27	122.92
19	A	1132	CLA	C4A-NA-C1A	2.61	107.88	106.71
19	B	1235	CLA	C4A-NA-C1A	2.61	107.88	106.71
19	A	1151	CLA	O1D-CGD-CBD	-2.61	119.15	124.48
21	B	6005	BCR	C40-C30-C39	2.61	116.53	108.53
19	4	4014	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
19	B	1206	CLA	O2A-CGA-CBA	2.61	120.08	111.91
19	4	1304	CLA	C16-C15-C13	-2.61	107.50	115.92
19	A	1129	CLA	CAA-C2A-C3A	-2.60	105.65	112.78
22	H	7002	LMU	O5B-C1B-C2B	-2.60	104.84	110.35
19	4	4010	CLA	C3D-C2D-C1D	2.60	108.55	106.30
21	3	6022	BCR	C40-C30-C39	2.60	116.52	108.53
19	A	1136	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
21	B	6004	BCR	C16-C15-C14	-2.60	118.14	123.47
19	B	1232	CLA	C4A-NA-C1A	2.60	107.88	106.71
19	R	1150	CLA	C4-C3-C2	-2.60	117.00	123.68
19	A	1113	CLA	C1-C2-C3	-2.60	122.54	126.75
19	B	1238	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
19	B	1214	CLA	CHB-C4A-NA	2.60	128.11	124.51
21	B	6010	BCR	C15-C16-C17	-2.60	118.15	123.47
21	A	6008	BCR	C29-C30-C25	-2.60	106.48	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1222	CLA	C1-C2-C3	-2.60	121.55	126.04
19	A	1138	CLA	CED-O2D-CGD	2.60	121.81	115.94
19	B	1301	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	K	1143	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	A	1115	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
19	2	1307	CLA	CHB-C4A-NA	2.59	128.31	124.34
19	R	1150	CLA	CMA-C3A-C4A	2.59	118.74	111.77
19	A	1102	CLA	CBA-CAA-C2A	2.59	121.51	113.86
19	1	1014	CLA	CMD-C2D-C3D	-2.59	119.83	124.68
22	N	7049	LMU	C1B-C2B-C3B	-2.59	104.60	110.00
19	A	1136	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	A	1138	CLA	C4A-NA-C1A	2.59	107.87	106.71
19	A	1141	CLA	O2A-CGA-CBA	2.59	120.02	111.91
19	3	3002	CLA	CHB-C4A-NA	2.59	128.30	124.34
19	3	3015	CLA	C2D-C3D-C4D	-2.58	104.08	106.30
22	H	7030	LMU	O5B-C5B-C6B	2.58	112.86	106.44
22	2	7027	LMU	C3B-C4B-C5B	2.58	114.85	110.24
19	A	1140	CLA	C4A-NA-C1A	2.58	107.87	106.71
19	L	1501	CLA	C4A-NA-C1A	2.58	107.87	106.71
19	A	9011	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
22	B	7012	LMU	C2'-C3'-C4'	2.58	115.57	109.68
19	4	4014	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
19	L	1501	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
22	4	7033	LMU	O5B-C5B-C6B	2.58	112.84	106.44
19	L	1503	CLA	CAA-C2A-C1A	2.58	120.42	111.97
19	B	1214	CLA	CED-O2D-CGD	2.58	121.76	115.94
22	H	7043	LMU	C6'-C5'-C4'	-2.58	105.83	113.33
19	J	1311	CLA	CHB-C4A-NA	2.58	128.07	124.51
19	B	1230	CLA	CAA-CBA-CGA	-2.57	105.73	113.25
19	G	1242	CLA	CED-O2D-CGD	2.57	121.76	115.94
19	A	1117	CLA	CMD-C2D-C3D	-2.57	119.86	124.68
19	2	2004	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	3	3006	CLA	C2B-C3B-C4B	2.57	108.49	106.29
21	F	6016	BCR	C31-C1-C2	2.57	119.19	108.91
19	3	1118	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	B	1201	CLA	CMB-C2B-C3B	2.57	129.49	124.68
19	L	1504	CLA	C4-C3-C2	-2.57	117.09	123.68
19	3	3010	CLA	C3D-C4D-ND	2.57	112.37	110.14
19	3	3013	CLA	C4-C3-C2	-2.57	117.09	123.68
19	A	1128	CLA	C1-C2-C3	-2.57	121.60	126.04
19	B	1203	CLA	C16-C15-C13	-2.57	107.62	115.92
19	1	1310	CLA	C2A-C3A-C4A	-2.57	100.15	104.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1211	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
21	A	6007	BCR	C32-C1-C31	2.57	116.41	108.53
22	R	7025	LMU	C1B-O1B-C4'	-2.57	111.61	117.96
19	B	1228	CLA	O1D-CGD-CBD	-2.56	119.24	124.48
19	B	1203	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
19	B	9010	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
19	2	2007	CLA	CGD-CBD-CAD	2.56	119.03	110.73
19	1	1003	CLA	CHB-C4A-NA	2.56	128.05	124.51
19	2	2004	CLA	CED-O2D-CGD	2.56	121.72	115.94
19	3	3016	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
19	2	2001	CLA	O2A-CGA-CBA	2.56	119.93	111.91
19	4	1004	CLA	C4-C3-C5	2.56	119.57	115.27
19	A	1136	CLA	O2A-CGA-CBA	2.55	119.92	111.91
22	3	7005	LMU	O5'-C5'-C6'	2.55	112.78	106.44
22	K	7047	LMU	C1'-O5'-C5'	2.55	118.69	113.69
19	2	2007	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	B	1223	CLA	O2A-CGA-CBA	2.54	119.89	111.91
21	F	6016	BCR	C38-C26-C27	2.54	118.50	113.62
21	J	6012	BCR	C39-C30-C25	2.54	114.42	110.30
19	2	2001	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	B	1229	CLA	C1-O2A-CGA	2.54	123.11	116.44
21	A	6002	BCR	C1-C6-C7	2.54	122.96	115.78
21	A	6002	BCR	C34-C9-C10	-2.54	119.36	122.92
22	A	7035	LMU	O5'-C1'-C2'	2.54	115.72	110.35
19	1	1010	CLA	O2A-CGA-CBA	2.54	122.27	112.23
22	H	7011	LMU	O5B-C5B-C6B	2.54	112.75	106.44
19	B	1210	CLA	CMB-C2B-C3B	2.54	129.43	124.68
19	A	1133	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
19	3	3011	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
19	4	4010	CLA	C2A-C3A-C4A	-2.54	100.20	104.18
19	4	4002	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
19	A	1126	CLA	C1-O2A-CGA	2.54	123.10	116.44
19	A	9011	CLA	C6-C7-C8	-2.53	107.73	115.92
22	B	7040	LMU	C2'-C3'-C4'	2.53	115.47	109.68
21	1	6023	BCR	C23-C24-C25	2.53	134.31	127.20
19	B	1205	CLA	O2A-C1-C2	2.53	115.29	108.64
19	A	1132	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
19	A	1237	CLA	CMD-C2D-C3D	-2.53	119.94	124.68
19	A	1119	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	B	1238	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
21	B	6017	BCR	C34-C9-C8	2.52	122.05	118.08
21	B	6005	BCR	C37-C22-C23	2.52	122.05	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1005	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
19	A	1129	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
19	A	9012	CLA	CED-O2D-CGD	2.52	121.64	115.94
19	4	4011	CLA	C2B-C3B-C4B	2.52	108.45	106.29
21	B	6004	BCR	C4-C5-C6	-2.52	119.07	122.73
19	A	1116	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	A	9013	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
19	4	4003	CLA	O2A-CGA-CBA	2.52	119.81	111.91
21	I	6018	BCR	C31-C1-C2	2.52	118.98	108.91
21	A	6002	BCR	C15-C16-C17	-2.52	118.31	123.47
19	G	1242	CLA	CAA-CBA-CGA	-2.52	105.89	113.25
19	A	1133	CLA	C4A-NA-C1A	2.52	107.84	106.71
19	B	1218	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
19	A	1151	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	K	7042	LMU	O5'-C5'-C6'	2.52	112.69	106.44
22	H	7032	LMU	O5'-C1'-C2'	-2.52	105.02	110.35
19	3	1118	CLA	CAA-C2A-C3A	-2.52	110.23	116.10
19	A	1105	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
22	A	7045	LMU	C1'-C2'-C3'	2.51	115.23	110.00
19	A	9011	CLA	CMB-C2B-C3B	2.51	129.38	124.68
21	A	6008	BCR	C16-C15-C14	-2.51	118.33	123.47
21	B	6010	BCR	C33-C5-C4	2.51	118.44	113.62
19	A	1137	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	A	7023	LMU	O1'-C1'-C2'	2.51	112.22	108.30
21	B	6006	BCR	C8-C7-C6	-2.51	120.15	127.20
22	4	7009	LMU	O1B-C1B-C2B	2.51	114.61	108.10
19	2	4009	CLA	C4A-NA-C1A	2.51	107.83	106.71
19	B	1223	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
19	B	1203	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
19	B	1210	CLA	C4-C3-C5	2.51	119.49	115.27
22	4	7019	LMU	O5B-C5B-C6B	2.51	112.68	106.44
19	A	1119	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
19	A	1107	CLA	C5-C3-C2	-2.51	116.04	121.12
21	I	6018	BCR	C39-C30-C29	-2.51	98.88	108.91
19	B	1210	CLA	C11-C10-C8	-2.51	107.82	115.92
19	B	1233	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	A	9012	CLA	C4-C3-C5	2.51	119.48	115.27
21	F	6014	BCR	C23-C24-C25	-2.50	120.17	127.20
19	F	1240	CLA	CAA-C2A-C1A	-2.50	105.62	111.81
19	1	1015	CLA	CHB-C4A-NA	2.50	128.17	124.34
19	A	1116	CLA	C4A-NA-C1A	2.50	107.83	106.71
19	B	1236	CLA	CAA-C2A-C3A	-2.50	105.93	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	2009	CLA	C6-C7-C8	-2.50	107.85	115.92
19	A	1140	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	2	2014	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
19	2	2004	CLA	C4A-NA-C1A	2.50	107.83	106.71
19	B	1222	CLA	CHB-C4A-NA	2.50	127.96	124.51
19	A	1138	CLA	C1-C2-C3	-2.50	121.73	126.04
19	4	1304	CLA	C1-C2-C3	-2.50	121.73	126.04
21	B	6005	BCR	C32-C1-C2	2.50	118.89	108.91
22	K	7041	LMU	C1'-O5'-C5'	2.49	118.58	113.69
19	H	1241	CLA	C4-C3-C2	-2.49	117.28	123.68
19	B	1236	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	A	1113	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
19	B	1239	CLA	CAA-CBA-CGA	2.49	120.54	113.25
19	A	1125	CLA	O2A-CGA-CBA	2.49	119.73	111.91
19	K	1143	CLA	CBC-CAC-C3C	-2.49	105.92	112.27
19	A	1129	CLA	CGD-CBD-CAD	2.49	118.81	110.73
19	B	1228	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	3	3003	CLA	CAC-C3C-C4C	-2.49	124.64	128.46
19	A	1125	CLA	CHB-C4A-NA	2.49	127.96	124.51
24	B	7101	LMG	O8-C28-C29	2.49	119.72	111.91
19	2	4009	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
22	H	7002	LMU	O3'-C3'-C2'	-2.49	104.59	110.35
19	A	1120	CLA	CED-O2D-CGD	2.49	121.56	115.94
19	2	2004	CLA	CAA-C2A-C3A	-2.49	105.97	112.78
19	B	1227	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	A	1101	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	B	7038	LMU	C6B-C5B-C4B	-2.48	107.19	113.00
21	I	6021	BCR	C39-C30-C25	2.48	114.33	110.30
19	1	1011	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	K	7001	LMU	O1B-C4'-C5'	2.48	116.25	109.45
19	A	9013	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
19	4	4003	CLA	C4-C3-C5	2.48	119.45	115.27
19	3	3003	CLA	CMB-C2B-C3B	2.48	129.55	124.69
19	A	1122	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
19	K	3009	CLA	C1-O2A-CGA	2.48	122.95	116.44
22	2	7031	LMU	O5B-C5B-C4B	2.48	114.19	109.69
19	B	1208	CLA	O2A-C1-C2	2.48	115.15	108.64
22	A	7035	LMU	C2'-C3'-C4'	-2.48	104.02	109.68
19	A	1120	CLA	C1-C2-C3	-2.48	121.76	126.04
22	R	7021	LMU	O1'-C1'-C2'	2.48	112.17	108.30
19	B	1211	CLA	CED-O2D-CGD	2.48	121.54	115.94
19	A	9022	CLA	O2A-CGA-CBA	2.48	119.68	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	2003	CLA	CHB-C4A-NA	2.48	128.13	124.34
19	B	1233	CLA	O2A-CGA-CBA	2.47	119.67	111.91
19	B	1238	CLA	C4-C3-C5	2.47	119.43	115.27
19	A	1115	CLA	CMB-C2B-C3B	2.47	129.31	124.68
19	B	1206	CLA	CHB-C4A-NA	2.47	127.93	124.51
21	J	6012	BCR	C33-C5-C6	-2.47	121.75	124.53
19	2	2007	CLA	C1-O2A-CGA	2.47	122.93	116.44
19	A	1128	CLA	CMD-C2D-C3D	-2.47	120.05	124.68
19	B	1238	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	B	1206	CLA	O2D-CGD-CBD	2.47	115.66	111.27
19	B	1229	CLA	C1-C2-C3	-2.47	121.77	126.04
19	A	1106	CLA	C1-C2-C3	-2.47	121.77	126.04
22	1	7004	LMU	O1'-C1'-C2'	2.47	112.16	108.30
19	4	1304	CLA	CMA-C3A-C4A	2.47	118.41	111.77
19	H	1145	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
21	F	6014	BCR	C38-C26-C27	2.47	118.35	113.62
21	3	6022	BCR	C28-C27-C26	-2.47	109.67	114.08
19	3	3007	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
22	2	7027	LMU	O5'-C5'-C6'	2.46	112.56	106.44
22	A	7016	LMU	C1'-O5'-C5'	-2.46	108.85	113.69
19	K	3009	CLA	C4-C3-C5	2.46	119.41	115.27
19	4	4013	CLA	C3D-C2D-C1D	2.46	108.42	106.30
22	H	7011	LMU	O3B-C3B-C4B	-2.46	104.66	110.35
19	L	1130	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	2	2001	CLA	C4A-NA-C1A	2.46	107.81	106.71
19	A	1122	CLA	C1-C2-C3	-2.46	121.80	126.04
19	A	1123	CLA	CMB-C2B-C3B	2.46	129.27	124.68
19	B	1215	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
19	A	1105	CLA	C4A-NA-C1A	2.45	107.81	106.71
19	L	1130	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
19	B	1224	CLA	C4-C3-C5	2.45	119.39	115.27
19	B	1223	CLA	C1-C2-C3	-2.45	121.81	126.04
21	A	6007	BCR	C23-C22-C21	-2.45	115.18	118.94
19	A	1120	CLA	CMB-C2B-C3B	2.45	129.26	124.68
19	A	1151	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
19	3	3010	CLA	C2A-C3A-C4A	-2.45	100.34	104.18
19	4	4010	CLA	C3D-C4D-ND	2.45	112.27	110.14
19	A	1126	CLA	CMB-C2B-C3B	2.45	129.25	124.68
19	B	1226	CLA	C7-C6-C5	-2.45	106.72	113.36
19	3	3016	CLA	C4A-NA-C1A	2.44	107.81	106.71
19	A	1107	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
19	B	1229	CLA	C3A-C2A-C1A	2.44	105.00	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1238	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
22	4	7018	LMU	O5'-C5'-C6'	2.44	112.51	106.44
21	1	6023	BCR	C27-C26-C25	-2.44	119.19	122.73
19	B	1210	CLA	O2A-CGA-CBA	2.44	119.57	111.91
19	4	4013	CLA	C3D-C4D-ND	2.44	112.26	110.14
19	B	1229	CLA	CAA-CBA-CGA	-2.44	106.12	113.25
19	A	1135	CLA	O2A-CGA-CBA	2.44	119.56	111.91
21	A	6011	BCR	C37-C22-C23	2.44	121.92	118.08
22	A	7035	LMU	O3'-C3'-C4'	2.44	116.41	109.94
22	G	7051	LMU	O3B-C3B-C4B	-2.44	104.71	110.35
19	I	1204	CLA	CHB-C4A-NA	2.44	127.88	124.51
19	F	1240	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
19	B	1225	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
19	A	1139	CLA	C4A-NA-C1A	2.44	107.80	106.71
19	A	1111	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
19	3	3007	CLA	CHB-C4A-NA	2.43	127.88	124.51
19	J	1311	CLA	C4A-NA-C1A	2.43	107.80	106.71
19	A	1125	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
21	B	6006	BCR	C30-C25-C26	-2.43	119.19	122.61
19	B	1216	CLA	O2A-CGA-CBA	2.43	119.53	111.91
19	B	1214	CLA	C1-O2A-CGA	2.43	122.81	116.44
21	F	6014	BCR	C16-C15-C14	-2.43	118.50	123.47
19	A	9012	CLA	CMB-C2B-C3B	2.43	129.22	124.68
19	F	1305	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
19	A	1138	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
19	1	1303	CLA	CBA-CAA-C2A	-2.43	106.70	113.86
21	A	6011	BCR	C39-C30-C25	2.43	114.23	110.30
19	A	1136	CLA	C4-C3-C5	2.42	119.35	115.27
19	2	2002	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	3	3012	CLA	C2B-C3B-C4B	2.42	108.36	106.29
19	B	1210	CLA	CBA-CAA-C2A	-2.42	106.71	113.86
19	J	1311	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
19	3	3008	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
19	A	1123	CLA	C4A-NA-C1A	2.42	107.79	106.71
19	B	9010	CLA	CMB-C2B-C3B	2.42	129.20	124.68
19	B	1230	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
21	F	6016	BCR	C33-C5-C4	2.42	118.26	113.62
19	3	2009	CLA	C4-C3-C2	-2.42	117.47	123.68
22	E	7037	LMU	C3B-C4B-C5B	-2.42	105.93	110.24
22	2	7031	LMU	C1-O1'-C1'	2.42	117.84	113.84
19	B	1233	CLA	C1-C2-C3	-2.41	121.87	126.04
19	A	1138	CLA	C2A-C1A-CHA	-2.41	119.64	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1308	CLA	O2A-CGA-CBA	2.41	119.48	111.91
22	G	7051	LMU	O5'-C5'-C4'	-2.41	104.67	109.75
19	B	1212	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	B	1228	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
19	B	1234	CLA	O2A-CGA-CBA	2.41	119.48	111.91
19	1	1001	CLA	CBA-CAA-C2A	-2.41	106.74	113.86
19	3	3014	CLA	C2B-C3B-C4B	2.41	108.35	106.29
19	A	1109	CLA	C4-C3-C5	2.41	119.33	115.27
19	B	1215	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
19	B	1239	CLA	O2D-CGD-CBD	2.41	115.55	111.27
19	I	1204	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
19	4	4012	CLA	CMD-C2D-C3D	-2.41	120.17	124.68
19	A	1126	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
19	A	1135	CLA	C2A-C1A-CHA	-2.40	119.65	123.86
19	H	1241	CLA	CMD-C2D-C3D	-2.40	120.18	124.68
19	F	1302	CLA	CHB-C4A-NA	2.40	127.84	124.51
21	B	6004	BCR	C35-C13-C12	2.40	121.86	118.08
21	3	6022	BCR	C36-C18-C17	-2.40	119.56	122.92
19	L	1148	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
19	3	1147	CLA	O2A-CGA-CBA	2.40	121.72	112.23
19	A	1112	CLA	CED-O2D-CGD	2.40	121.37	115.94
19	A	1139	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	3	3013	CLA	CMD-C2D-C3D	-2.40	120.19	124.68
19	A	1128	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
22	N	7049	LMU	O1'-C1'-C2'	2.40	112.05	108.30
19	A	1135	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	L	1502	CLA	CMB-C2B-C3B	2.40	129.16	124.68
19	L	1503	CLA	CMD-C2D-C3D	-2.40	120.19	124.68
19	4	4007	CLA	CAA-C2A-C1A	-2.40	104.12	111.97
21	B	6017	BCR	C33-C5-C6	-2.39	121.84	124.53
19	4	4001	CLA	CED-O2D-CGD	2.39	121.35	115.94
19	2	4009	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
19	A	1141	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
19	A	1115	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
21	I	6018	BCR	C37-C22-C21	-2.39	119.58	122.92
19	B	1217	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	R	1144	CLA	C4-C3-C2	-2.39	117.55	123.68
19	B	1218	CLA	CMB-C2B-C3B	2.39	129.15	124.68
21	I	6018	BCR	C2-C1-C6	-2.39	106.80	110.48
22	G	7026	LMU	O4'-C4B-C5B	2.39	115.23	109.30
22	2	7027	LMU	O1B-C1B-C2B	2.39	114.29	108.10
19	1	1005	CLA	CHB-C4A-NA	2.39	127.81	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	6006	BCR	C3-C4-C5	-2.39	109.81	114.08
19	A	1107	CLA	CMC-C2C-C3C	2.39	129.44	124.94
19	A	1106	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
22	A	7023	LMU	O5B-C5B-C6B	2.38	112.36	106.44
19	A	1126	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
19	B	1239	CLA	CMA-C3A-C2A	-2.38	104.22	113.83
19	A	1105	CLA	CGD-CBD-CAD	-2.38	103.02	110.73
19	A	1119	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
21	A	6008	BCR	C32-C1-C2	2.38	118.42	108.91
19	L	1130	CLA	C1-O2A-CGA	2.38	122.69	116.44
19	2	2004	CLA	O2A-CGA-CBA	2.38	119.37	111.91
19	2	2007	CLA	C6-C7-C8	-2.38	108.23	115.92
19	4	4007	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
19	A	1125	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
19	A	1149	CLA	CAA-CBA-CGA	-2.38	106.31	113.25
19	F	1305	CLA	CHB-C4A-NA	2.37	127.80	124.51
22	4	7019	LMU	O5'-C5'-C4'	2.37	114.76	109.75
22	H	7002	LMU	C3'-C4'-C5'	-2.37	105.49	110.93
22	H	7017	LMU	O1B-C1B-C2B	2.37	114.25	108.10
19	A	1129	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	3	3017	CLA	CMB-C2B-C3B	2.37	129.12	124.68
19	G	1242	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
19	B	1208	CLA	C4A-NA-C1A	2.37	107.77	106.71
19	4	4003	CLA	C4A-NA-C1A	2.37	107.77	106.71
21	A	6008	BCR	C8-C7-C6	-2.37	120.55	127.20
19	3	3017	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
19	A	9011	CLA	C3B-C4B-NB	-2.37	106.15	109.21
19	2	2006	CLA	CHB-C4A-NA	2.37	127.78	124.51
19	4	4011	CLA	CHB-C4A-NA	2.37	127.96	124.34
19	B	1224	CLA	CAA-C2A-C1A	-2.36	104.23	111.97
19	2	4009	CLA	CED-O2D-CGD	2.36	121.28	115.94
22	G	7026	LMU	O5'-C5'-C4'	2.36	114.73	109.75
19	R	1150	CLA	CAA-CBA-CGA	2.36	120.15	113.25
19	3	3007	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
19	3	3011	CLA	O2A-C1-C2	2.36	114.84	108.64
19	A	1119	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
19	1	1005	CLA	CGD-CBD-CAD	2.36	118.37	110.73
19	B	1214	CLA	C1-C2-C3	-2.36	121.97	126.04
19	3	3010	CLA	CHB-C4A-NA	2.36	127.95	124.34
19	1	1014	CLA	C4-C3-C5	2.36	119.23	115.27
20	A	5001	PQN	C30-C28-C29	2.36	121.37	110.51
19	B	1223	CLA	C4A-NA-C1A	2.35	107.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1128	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
21	B	6020	BCR	C10-C11-C12	2.35	130.56	123.22
19	3	3008	CLA	CHB-C4A-NA	2.35	127.77	124.51
19	A	1136	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
19	A	1112	CLA	C4A-NA-C1A	2.35	107.76	106.71
19	2	4009	CLA	C4-C3-C2	-2.35	117.65	123.68
19	A	1109	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
19	A	1106	CLA	O2A-C1-C2	2.35	114.81	108.64
19	1	1014	CLA	O2A-CGA-CBA	2.35	119.28	111.91
19	A	1113	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	3	2009	CLA	C4A-NA-C1A	2.35	107.76	106.71
19	2	2014	CLA	CMD-C2D-C3D	-2.35	120.29	124.68
19	A	1107	CLA	C1-C2-C3	2.35	130.10	126.04
19	4	4015	CLA	CBA-CAA-C2A	-2.35	106.94	113.86
19	A	1120	CLA	C4A-NA-C1A	2.34	107.76	106.71
19	A	1126	CLA	CMA-C3A-C4A	-2.34	105.47	111.77
21	A	6007	BCR	C34-C9-C8	2.34	121.77	118.08
19	3	3008	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
19	A	1138	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	A	1122	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
19	A	1151	CLA	C5-C3-C4	2.34	119.77	114.60
22	A	7016	LMU	C3'-C4'-C5'	2.34	116.28	110.93
19	1	1012	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	H	1207	CLA	C1-C2-C3	2.34	130.08	126.04
19	4	4006	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
22	A	7023	LMU	C3'-C4'-C5'	2.33	116.28	110.93
19	B	1225	CLA	C11-C12-C13	-2.33	108.38	115.92
19	G	1242	CLA	O2A-CGA-CBA	2.33	119.23	111.91
22	2	7031	LMU	O5'-C1'-O1'	2.33	115.50	109.97
22	E	7037	LMU	O1B-C1B-C2B	2.33	114.14	108.10
19	B	1208	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	B	1239	CLA	CMD-C2D-C3D	-2.33	120.32	124.68
19	A	1106	CLA	O2A-CGA-CBA	2.33	119.22	111.91
22	B	7038	LMU	O5'-C5'-C6'	2.33	112.22	106.44
19	4	4007	CLA	CED-O2D-CGD	2.33	121.20	115.94
21	A	6008	BCR	C40-C30-C25	2.32	114.07	110.30
19	4	4001	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
19	K	3009	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
19	1	1010	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
19	4	1306	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
19	B	1230	CLA	C1-O2A-CGA	2.32	122.54	116.44
19	4	4003	CLA	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1127	CLA	O2A-CGA-CBA	2.32	119.19	111.91
19	B	1232	CLA	CED-O2D-CGD	2.32	121.18	115.94
22	K	7042	LMU	O5B-C1B-C2B	2.32	115.26	110.35
19	4	4002	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
19	A	9022	CLA	CAA-C2A-C1A	2.32	119.57	111.97
19	3	3016	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
19	A	9013	CLA	CGD-CBD-CAD	2.32	118.23	110.73
19	B	1222	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
19	B	1236	CLA	CED-O2D-CGD	2.31	121.17	115.94
21	A	6002	BCR	C8-C7-C6	-2.31	120.71	127.20
22	4	7053	LMU	O2B-C2B-C3B	-2.31	105.00	110.35
19	B	1210	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
19	2	2004	CLA	CMB-C2B-C3B	2.31	129.00	124.68
19	B	1221	CLA	CBC-CAC-C3C	-2.31	106.39	112.27
19	G	1242	CLA	CMB-C2B-C3B	2.31	129.00	124.68
21	B	6005	BCR	C34-C9-C8	2.31	121.71	118.08
19	1	1007	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
19	A	1102	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
19	B	1238	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
19	H	1145	CLA	CMB-C2B-C3B	2.30	128.99	124.68
19	4	4002	CLA	C4-C3-C2	-2.30	117.77	123.68
19	4	4006	CLA	O2A-CGA-CBA	2.30	119.13	111.91
19	4	4004	CLA	C2B-C3B-C4B	2.30	108.26	106.29
21	L	6019	BCR	C33-C5-C4	2.30	118.03	113.62
19	A	1139	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
19	3	3015	CLA	CHB-C4A-NA	2.30	127.86	124.34
22	A	7035	LMU	O5'-C5'-C6'	2.30	112.14	106.44
19	A	1113	CLA	CMB-C2B-C3B	2.30	128.97	124.68
19	B	1208	CLA	C1-O2A-CGA	2.30	122.47	116.44
19	K	3009	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	B	1213	CLA	CED-O2D-CGD	2.29	121.12	115.94
19	3	3001	CLA	C2A-C3A-C4A	-2.29	100.58	104.18
19	F	1305	CLA	C4-C3-C2	-2.29	117.80	123.68
19	A	1112	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	K	1146	CLA	C5-C3-C4	2.29	119.66	114.60
19	1	1013	CLA	CMB-C2B-C1B	2.29	131.98	128.46
19	2	2001	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
19	3	3011	CLA	C5-C3-C2	-2.29	116.49	121.12
19	1	1007	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
19	J	1308	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	A	1111	CLA	CMB-C2B-C3B	2.29	128.96	124.68
19	L	1504	CLA	C1-O2A-CGA	2.29	122.44	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	4009	CLA	C4-C3-C5	2.28	119.11	115.27
19	A	9011	CLA	CMA-C3A-C2A	-2.28	104.61	113.83
22	B	7040	LMU	O3B-C3B-C2B	-2.28	105.07	110.35
22	4	7033	LMU	C1'-C2'-C3'	2.28	114.75	110.00
19	A	1113	CLA	CED-O2D-CGD	2.28	121.10	115.94
19	1	1303	CLA	CMB-C2B-C3B	2.28	128.95	124.68
22	A	7035	LMU	O1B-C4'-C5'	2.28	115.70	109.45
21	B	6020	BCR	C31-C1-C6	-2.28	106.60	110.30
19	B	1203	CLA	CMA-C3A-C2A	-2.28	104.63	113.83
21	F	6014	BCR	C40-C30-C39	2.28	115.53	108.53
19	4	1004	CLA	CED-O2D-CGD	2.28	121.09	115.94
19	A	1139	CLA	O2A-CGA-CBA	2.28	119.06	111.91
19	B	9010	CLA	C16-C17-C18	-2.28	105.24	115.98
19	4	4010	CLA	CHB-C4A-NA	2.28	127.83	124.34
19	A	1102	CLA	C4-C3-C5	2.28	119.10	115.27
19	B	1212	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
19	1	1303	CLA	O1D-CGD-CBD	-2.28	119.83	124.48
22	B	7040	LMU	O1'-C1'-C2'	2.28	111.86	108.30
19	B	1236	CLA	O2A-CGA-CBA	2.28	119.05	111.91
19	B	1216	CLA	CMD-C2D-C3D	-2.27	120.42	124.68
22	H	7043	LMU	O5'-C5'-C6'	2.27	112.09	106.44
19	2	2006	CLA	O2A-CGA-CBA	2.27	119.04	111.91
19	2	2013	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
19	B	1203	CLA	C11-C12-C13	-2.27	108.58	115.92
19	R	1150	CLA	CAA-C2A-C1A	2.27	119.41	111.97
19	3	2009	CLA	CGD-CBD-CAD	-2.27	103.39	110.73
19	B	1232	CLA	CHB-C4A-NA	2.27	127.65	124.51
19	B	9010	CLA	CBC-CAC-C3C	-2.27	106.49	112.27
19	1	1310	CLA	C2B-C3B-C4B	2.27	108.23	106.29
22	A	7044	LMU	C2'-C3'-C4'	2.27	114.86	109.68
19	A	1102	CLA	CHB-C4A-NA	2.27	127.64	124.51
19	3	3013	CLA	C1-O2A-CGA	2.27	122.39	116.44
19	1	1001	CLA	CGD-CBD-CAD	-2.27	103.40	110.73
19	4	4015	CLA	CMB-C2B-C3B	2.26	128.91	124.68
21	F	6016	BCR	C33-C5-C6	-2.26	121.99	124.53
22	H	7017	LMU	C1'-C2'-C3'	2.26	114.71	110.00
19	A	1128	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
19	B	1202	CLA	C11-C12-C13	-2.26	108.61	115.92
19	H	1145	CLA	C1-C2-C3	-2.26	122.13	126.04
19	2	2002	CLA	C3A-C2A-C1A	2.26	104.72	101.34
21	B	6010	BCR	C40-C30-C25	-2.26	106.64	110.30
19	A	1101	CLA	C5-C3-C4	2.26	119.59	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	6019	BCR	C8-C7-C6	-2.26	120.86	127.20
19	I	1204	CLA	C1-O2A-CGA	2.26	122.37	116.44
19	2	2004	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
19	A	1117	CLA	CHB-C4A-NA	2.26	127.63	124.51
21	A	6002	BCR	C7-C6-C5	-2.26	116.00	121.46
19	B	1217	CLA	C5-C3-C4	2.26	119.59	114.60
19	K	1146	CLA	C4A-NA-C1A	2.26	107.72	106.71
22	H	7043	LMU	O5'-C1'-C2'	2.26	115.12	110.35
19	J	1308	CLA	CAA-C2A-C3A	-2.25	106.60	112.78
19	2	2005	CLA	CHB-C4A-NA	2.25	127.79	124.34
21	F	6014	BCR	C15-C16-C17	-2.25	118.86	123.47
19	A	1117	CLA	CAA-CBA-CGA	-2.25	106.67	113.25
19	4	1306	CLA	C1-O2A-CGA	2.25	122.36	116.44
19	2	2012	CLA	O2A-CGA-CBA	2.25	118.98	111.91
19	B	1233	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
19	3	2009	CLA	O2A-CGA-CBA	2.25	118.97	111.91
19	2	2007	CLA	CMC-C2C-C3C	2.25	129.19	124.94
19	B	1215	CLA	CED-O2D-CGD	2.25	121.03	115.94
21	A	6011	BCR	C19-C18-C17	-2.25	115.49	118.94
19	A	9022	CLA	CMD-C2D-C3D	-2.25	120.47	124.68
19	4	4011	CLA	C2A-C3A-C4A	-2.25	100.65	104.18
21	A	6008	BCR	C28-C27-C26	-2.25	110.06	114.08
19	B	1223	CLA	CHB-C4A-NA	2.25	127.62	124.51
19	B	1217	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
19	B	1236	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
19	A	1140	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
19	2	4009	CLA	C1-O2A-CGA	2.24	122.33	116.44
19	A	1103	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
19	2	2011	CLA	CHB-C4A-NA	2.24	127.78	124.34
22	4	7033	LMU	C2'-C3'-C4'	2.24	114.81	109.68
19	3	3012	CLA	CHB-C4A-NA	2.24	127.77	124.34
22	G	7026	LMU	O1B-C1B-C2B	2.24	113.91	108.10
19	R	1150	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
19	3	3017	CLA	O2A-CGA-CBA	2.24	118.94	111.91
21	F	6016	BCR	C37-C22-C21	-2.24	119.79	122.92
22	N	7049	LMU	O5B-C5B-C4B	-2.24	105.63	109.69
19	A	1151	CLA	O2A-CGA-CBA	2.24	118.93	111.91
19	B	1229	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
22	R	7007	LMU	O1'-C1'-C2'	2.23	111.79	108.30
22	4	7019	LMU	O2'-C2'-C3'	-2.23	105.19	110.35
19	K	1143	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
19	B	1225	CLA	O1D-CGD-CBD	-2.23	119.92	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	1143	CLA	C1-C2-C3	-2.23	123.14	126.75
21	3	6022	BCR	C37-C22-C23	2.23	121.59	118.08
19	A	1151	CLA	CMB-C2B-C3B	2.23	128.85	124.68
19	A	1117	CLA	C4A-NA-C1A	2.23	107.71	106.71
22	E	7037	LMU	O2'-C2'-C1'	-2.23	104.63	110.05
19	K	1142	CLA	CMB-C2B-C3B	2.23	128.85	124.68
19	2	2011	CLA	C3A-C4A-NA	2.23	114.59	109.92
19	B	1226	CLA	O2A-CGA-CBA	2.22	118.89	111.91
19	B	1211	CLA	O2A-CGA-CBA	2.22	118.88	111.91
21	L	6019	BCR	C37-C22-C21	-2.22	119.81	122.92
19	B	1210	CLA	C16-C15-C13	-2.22	108.74	115.92
22	C	7015	LMU	O2'-C2'-C3'	2.22	115.48	110.35
19	A	1126	CLA	C4-C3-C2	-2.22	117.98	123.68
19	B	1203	CLA	C1-C2-C3	-2.22	122.20	126.04
19	1	1007	CLA	CBC-CAC-C3C	2.22	117.92	112.27
19	A	1116	CLA	O2A-C1-C2	2.22	114.47	108.64
19	4	4006	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
21	A	6002	BCR	C16-C15-C14	-2.22	118.93	123.47
19	A	1127	CLA	CMD-C2D-C3D	-2.22	120.53	124.68
19	3	1147	CLA	CMD-C2D-C3D	-2.22	120.53	124.68
19	A	1129	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
19	4	1304	CLA	CHA-C1A-NA	-2.22	121.32	126.40
19	A	1119	CLA	O2A-CGA-CBA	2.22	118.86	111.91
21	I	6021	BCR	C28-C27-C26	-2.21	110.12	114.08
19	L	1130	CLA	CBA-CAA-C2A	2.21	120.40	113.86
22	K	7042	LMU	C4B-C3B-C2B	-2.21	106.96	110.82
21	A	6007	BCR	C40-C30-C39	2.21	115.32	108.53
19	2	2002	CLA	CAA-C2A-C1A	-2.21	104.73	111.97
19	A	1134	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
19	4	4014	CLA	CED-O2D-CGD	2.21	120.94	115.94
19	A	1112	CLA	CMB-C2B-C1B	2.21	131.86	128.46
19	A	1121	CLA	CHB-C4A-NA	2.21	127.57	124.51
19	3	2009	CLA	CHB-C4A-NA	2.21	127.57	124.51
19	L	1504	CLA	CED-O2D-CGD	2.21	120.93	115.94
22	G	7026	LMU	O3'-C3'-C4'	2.21	115.79	109.94
19	2	2014	CLA	C1-C2-C3	-2.21	122.23	126.04
19	3	3005	CLA	C2B-C3B-C4B	2.21	108.18	106.29
19	L	1503	CLA	CHB-C4A-NA	2.21	127.56	124.51
19	A	1149	CLA	C2A-C3A-C4A	-2.21	98.31	101.87
22	2	7027	LMU	C3'-C4'-C5'	2.20	115.98	110.93
19	A	1104	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
19	B	9010	CLA	C7-C6-C5	-2.20	107.38	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	2012	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
21	A	6002	BCR	C40-C30-C39	2.20	115.29	108.53
19	3	3003	CLA	CHB-C4A-NA	2.20	127.56	124.51
19	A	1110	CLA	CED-O2D-CGD	2.20	120.92	115.94
19	A	1141	CLA	C6-C5-C3	-2.20	107.69	113.45
21	A	6007	BCR	C16-C15-C14	-2.20	118.97	123.47
19	B	1225	CLA	C1-C2-C3	-2.20	122.24	126.04
21	B	6005	BCR	C15-C16-C17	-2.20	118.97	123.47
19	B	1219	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
19	3	3014	CLA	C3A-C4A-NA	2.20	114.53	109.92
19	2	2001	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
19	4	1304	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
19	B	1209	CLA	C2A-C1A-CHA	-2.19	120.02	123.86
19	4	4006	CLA	CHB-C4A-NA	2.19	127.55	124.51
19	A	1119	CLA	CMB-C2B-C3B	2.19	128.78	124.68
19	4	4004	CLA	C3A-C4A-NA	2.19	114.52	109.92
19	B	1217	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
19	L	1504	CLA	CHB-C4A-NA	2.19	127.54	124.51
19	4	1004	CLA	C4-C3-C2	-2.19	118.06	123.68
19	H	1241	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
19	A	1139	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
19	B	9010	CLA	C1-O2A-CGA	2.19	122.19	116.44
20	B	5002	PQN	C14-C13-C12	-2.19	118.07	123.68
19	B	1223	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
21	A	6007	BCR	C4-C5-C6	-2.18	119.56	122.73
22	R	7021	LMU	C6B-C5B-C4B	-2.18	107.89	113.00
22	4	7053	LMU	O1'-C1'-C2'	2.18	111.71	108.30
19	3	1147	CLA	CAA-CBA-CGA	2.18	119.63	113.25
22	C	7015	LMU	O5B-C5B-C4B	-2.18	105.73	109.69
21	L	6019	BCR	C19-C18-C17	-2.18	115.59	118.94
19	A	1133	CLA	CMA-C3A-C4A	-2.18	105.91	111.77
22	4	7033	LMU	O1B-C1B-C2B	2.18	113.75	108.10
19	H	1207	CLA	CED-O2D-CGD	2.18	120.87	115.94
22	E	7037	LMU	C1'-C2'-C3'	2.18	114.53	110.00
19	4	4013	CLA	C2A-C3A-C4A	-2.18	100.76	104.18
19	A	1149	CLA	CHB-C4A-NA	2.18	127.52	124.51
19	A	1237	CLA	CHB-C4A-NA	2.18	127.52	124.51
19	1	1007	CLA	CMB-C2B-C3B	2.18	128.75	124.68
19	A	1135	CLA	C4-C3-C5	2.18	118.47	115.98
19	3	3012	CLA	C2A-C3A-C4A	-2.18	100.76	104.18
19	4	4001	CLA	C4A-NA-C1A	2.18	107.69	106.71
19	2	2001	CLA	O2A-CGA-O1A	-2.18	118.10	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	9013	CLA	C16-C15-C13	-2.18	108.89	115.92
19	A	1135	CLA	C1-C2-C3	-2.18	122.28	126.04
19	A	1137	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
19	A	1126	CLA	C11-C10-C8	-2.17	108.90	115.92
19	B	1220	CLA	C6-C7-C8	-2.17	108.90	115.92
19	A	1139	CLA	CMB-C2B-C3B	2.17	128.74	124.68
19	3	3005	CLA	C2A-C3A-C4A	-2.17	100.77	104.18
19	B	1239	CLA	CMB-C2B-C1B	2.17	131.80	128.46
19	A	1309	CLA	CHB-C4A-NA	2.17	127.66	124.34
19	A	1131	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	B	7101	LMG	O7-C10-O9	-2.17	118.46	123.70
22	H	7002	LMU	C1B-O1B-C4'	2.17	123.33	117.96
19	L	1504	CLA	CMA-C3A-C4A	2.17	117.60	111.77
19	3	1147	CLA	CBC-CAC-C3C	-2.17	106.75	112.27
19	2	2003	CLA	C2A-C3A-C4A	-2.17	100.78	104.18
19	A	1126	CLA	C6-C7-C8	-2.17	108.92	115.92
19	A	1122	CLA	CMB-C2B-C3B	2.17	128.73	124.68
21	B	6005	BCR	C36-C18-C19	2.17	121.49	118.08
19	A	1111	CLA	CBC-CAC-C3C	-2.17	106.75	112.27
19	4	4003	CLA	C1-O2A-CGA	2.16	122.12	116.44
19	A	1116	CLA	C4-C3-C5	2.16	118.91	115.27
19	A	1128	CLA	CHB-C4A-NA	2.16	127.50	124.51
19	A	1135	CLA	CMB-C2B-C3B	2.16	128.73	124.68
19	A	1110	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
19	1	1002	CLA	C1-O2A-CGA	2.16	123.01	116.73
19	L	1503	CLA	CMB-C2B-C3B	2.16	128.72	124.68
19	1	1010	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
19	J	1311	CLA	C1-O2A-CGA	2.16	122.11	116.44
22	4	7033	LMU	O5'-C5'-C6'	2.16	111.80	106.44
19	B	9010	CLA	C11-C10-C8	-2.16	108.94	115.92
19	2	2004	CLA	C1-O2A-CGA	2.16	122.10	116.44
21	B	6020	BCR	C39-C30-C29	-2.16	100.28	108.91
19	B	1227	CLA	CMB-C2B-C3B	2.16	128.71	124.68
19	3	3003	CLA	CAC-C3C-C2C	2.16	128.91	124.69
19	B	1226	CLA	CHB-C4A-NA	2.16	127.49	124.51
19	2	2012	CLA	C5-C3-C4	2.16	119.36	114.60
19	K	1142	CLA	CHB-C4A-NA	2.15	127.49	124.51
19	2	2014	CLA	CBC-CAC-C3C	-2.15	106.78	112.27
22	K	7001	LMU	C4B-C3B-C2B	2.15	114.58	110.82
19	A	1119	CLA	CMC-C2C-C3C	2.15	129.00	124.94
19	4	1009	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
19	G	1242	CLA	C4-C3-C2	-2.15	118.16	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1124	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
19	4	1304	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
19	K	3009	CLA	CAA-CBA-CGA	-2.15	106.97	113.25
19	H	1207	CLA	C1-O2A-CGA	2.15	122.08	116.44
19	K	3009	CLA	C6-C7-C8	-2.15	108.98	115.92
19	3	2009	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
19	A	1237	CLA	O2A-CGA-CBA	2.14	118.64	111.91
19	4	4010	CLA	C3A-C4A-NA	2.14	114.42	109.92
19	2	2010	CLA	CHB-C4A-NA	2.14	127.62	124.34
19	B	1234	CLA	C4A-NA-C1A	2.14	107.67	106.71
22	3	7003	LMU	O1'-C1'-C2'	2.14	111.65	108.30
19	A	1102	CLA	C3B-C4B-NB	-2.14	106.44	109.21
21	A	6007	BCR	C27-C26-C25	-2.14	119.63	122.73
19	A	9012	CLA	C4A-NA-C1A	2.14	107.67	106.71
21	A	6008	BCR	C34-C9-C10	-2.14	119.93	122.92
19	1	1003	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
21	A	6011	BCR	C11-C12-C13	-2.13	120.42	126.42
19	B	1213	CLA	CAA-C2A-C1A	2.13	118.97	111.97
19	A	1140	CLA	C4-C3-C5	2.13	118.86	115.27
19	A	1123	CLA	CED-O2D-CGD	2.13	120.76	115.94
19	2	2014	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
19	F	1302	CLA	C2A-C1A-CHA	-2.13	120.13	123.85
22	K	7047	LMU	C1B-O5B-C5B	2.13	117.87	113.69
19	1	1013	CLA	O2A-C1-C2	2.13	114.23	108.64
19	L	1501	CLA	CMB-C2B-C3B	2.13	128.66	124.68
19	A	1136	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
19	A	9023	CLA	CMA-C3A-C2A	-2.13	105.24	113.83
19	A	1140	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
19	B	1208	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
21	B	6017	BCR	C32-C1-C2	2.13	117.41	108.91
22	4	7019	LMU	C3'-C4'-C5'	2.13	115.80	110.93
19	4	4014	CLA	C1-O2A-CGA	2.13	122.91	116.73
22	R	7022	LMU	O5'-C5'-C4'	2.13	114.23	109.75
19	A	1134	CLA	CED-O2D-CGD	2.12	120.74	115.94
19	F	1240	CLA	CGD-CBD-CAD	-2.12	105.59	114.30
22	K	7042	LMU	C1'-O5'-C5'	-2.12	109.52	113.69
21	B	6004	BCR	C8-C7-C6	-2.12	121.24	127.20
19	3	3001	CLA	C2B-C3B-C4B	2.12	108.10	106.29
22	H	7011	LMU	O1'-C1'-C2'	2.12	111.62	108.30
19	J	1308	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
19	4	1004	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
19	A	1107	CLA	C2A-C1A-CHA	-2.12	120.15	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	6014	BCR	C32-C1-C31	2.12	115.04	108.53
19	A	1132	CLA	CMC-C2C-C3C	2.12	128.94	124.94
22	F	7036	LMU	O5'-C5'-C6'	2.12	111.71	106.44
19	A	1137	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
19	4	4013	CLA	CHB-C4A-NA	2.12	127.58	124.34
22	B	7012	LMU	O5'-C5'-C4'	2.12	114.22	109.75
19	A	1132	CLA	C5-C3-C2	-2.12	116.83	121.12
19	1	1002	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
19	B	1211	CLA	O2A-C1-C2	2.12	114.20	108.64
19	1	1003	CLA	CAA-CBA-CGA	-2.12	107.07	113.25
21	B	6004	BCR	C40-C30-C29	-2.12	100.44	108.91
19	3	3015	CLA	C3D-C2D-C1D	2.11	108.12	106.30
22	H	7011	LMU	O5B-C1B-C2B	2.11	114.82	110.35
19	4	1009	CLA	CBD-CHA-C1A	2.11	130.81	127.43
19	A	1111	CLA	C4-C3-C5	2.11	118.83	115.27
19	B	1217	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
19	3	3006	CLA	C3A-C4A-NA	2.11	114.35	109.92
21	A	6011	BCR	C35-C13-C14	-2.11	119.97	122.92
22	R	7022	LMU	O5B-C5B-C4B	2.11	113.53	109.69
19	A	1141	CLA	CED-O2D-CGD	2.11	120.71	115.94
19	3	1147	CLA	CMB-C2B-C3B	2.11	128.63	124.68
21	A	6008	BCR	C15-C16-C17	-2.11	119.15	123.47
19	3	3016	CLA	CED-O2D-CGD	2.11	120.71	115.94
19	3	3016	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
19	B	1206	CLA	CED-O2D-CGD	2.11	120.70	115.94
19	H	1505	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
19	1	1014	CLA	CHB-C4A-NA	2.11	127.42	124.51
19	3	3017	CLA	C1-C2-C3	-2.11	123.34	126.75
19	4	4001	CLA	C5-C3-C4	2.10	119.25	114.60
22	3	7003	LMU	C6B-C5B-C4B	-2.10	108.08	113.00
22	3	7005	LMU	O5'-C1'-C2'	2.10	114.80	110.35
22	R	7025	LMU	O1B-C1B-C2B	2.10	113.54	108.10
19	B	1231	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
19	2	2013	CLA	CMD-C2D-C3D	-2.10	120.75	124.68
19	3	1147	CLA	CGD-CBD-CAD	-2.10	103.94	110.73
19	3	1147	CLA	CHB-C4A-NA	2.10	127.41	124.51
21	J	6012	BCR	C34-C9-C8	2.10	121.38	118.08
19	1	1007	CLA	C1-O2A-CGA	2.10	121.94	116.44
19	I	1204	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
19	A	1127	CLA	CGD-CBD-CAD	2.10	117.52	110.73
19	L	1501	CLA	O2A-CGA-CBA	2.09	118.48	111.91
19	4	4007	CLA	O2A-CGA-CBA	2.09	118.48	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	9023	CLA	CMC-C2C-C3C	2.09	128.89	124.94
19	B	1223	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
19	K	1143	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
19	B	1208	CLA	C4-C3-C5	2.09	118.79	115.27
19	A	1103	CLA	C6-C7-C8	-2.09	109.16	115.92
21	I	6018	BCR	C40-C30-C29	-2.09	100.55	108.91
21	L	6019	BCR	C40-C30-C29	-2.09	100.55	108.91
21	I	6021	BCR	C31-C1-C2	2.09	117.26	108.91
19	B	1209	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
21	B	6006	BCR	C1-C6-C7	2.09	121.68	115.78
19	A	1133	CLA	C1-O2A-CGA	2.09	121.92	116.44
19	A	1117	CLA	C3A-C2A-C1A	2.09	104.46	101.34
19	3	2009	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
19	1	1015	CLA	C3A-C4A-NA	2.09	114.30	109.92
21	A	6008	BCR	C35-C13-C12	2.08	121.36	118.08
21	J	6012	BCR	C40-C30-C39	2.08	114.93	108.53
19	B	1213	CLA	O2A-CGA-CBA	2.08	120.47	112.23
19	A	1126	CLA	C7-C6-C5	-2.08	107.70	113.36
21	B	6006	BCR	C36-C18-C17	-2.08	120.00	122.92
22	A	7010	LMU	C3B-C4B-C5B	2.08	113.96	110.24
19	B	1205	CLA	C3A-C2A-C1A	2.08	104.46	101.34
22	B	7012	LMU	C3'-C4'-C5'	2.08	115.70	110.93
19	B	1202	CLA	CBC-CAC-C3C	-2.08	106.96	112.27
19	A	1113	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
19	B	1224	CLA	O2A-C1-C2	2.08	114.10	108.64
19	2	2001	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
19	B	1238	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
19	A	1237	CLA	CED-O2D-CGD	2.08	120.64	115.94
22	A	7045	LMU	O1'-C1-C2	2.08	116.85	109.56
21	J	6012	BCR	C16-C15-C14	-2.08	119.22	123.47
21	B	6006	BCR	C35-C13-C12	2.08	121.35	118.08
19	K	1143	CLA	CED-O2D-CGD	2.08	120.64	115.94
19	4	4007	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
21	A	6008	BCR	C2-C1-C6	-2.08	107.28	110.48
22	A	7044	LMU	O5B-C5B-C4B	2.08	113.46	109.69
19	A	1139	CLA	CAA-CBA-CGA	-2.08	107.19	113.25
19	1	1013	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
19	1	1007	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
19	A	1116	CLA	CMC-C2C-C3C	2.07	128.85	124.94
19	B	1222	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
19	F	1302	CLA	C4A-NA-C1A	2.07	107.64	106.71
19	1	1010	CLA	O2A-CGA-O1A	-2.07	116.64	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3008	CLA	CMB-C2B-C3B	2.07	128.55	124.68
19	A	1124	CLA	C4-C3-C5	2.07	118.75	115.27
19	B	1220	CLA	CMA-C3A-C4A	-2.07	106.21	111.77
19	4	4002	CLA	CAA-C2A-C3A	2.07	118.44	112.78
19	A	1117	CLA	C6-C5-C3	-2.07	108.03	113.45
19	1	1010	CLA	CAA-C2A-C3A	2.07	118.44	112.78
22	A	7045	LMU	C4B-C3B-C2B	-2.07	107.21	110.82
21	B	6006	BCR	C35-C13-C14	-2.07	120.03	122.92
19	A	1120	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
19	1	1010	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
19	B	1218	CLA	O2A-CGA-CBA	2.07	120.39	112.23
19	L	1148	CLA	CAA-C2A-C1A	2.06	118.74	111.97
19	B	9010	CLA	CMD-C2D-C3D	-2.06	120.82	124.68
19	2	2007	CLA	CED-O2D-CGD	2.06	120.61	115.94
21	A	6011	BCR	C1-C6-C7	2.06	121.61	115.78
19	B	1220	CLA	O2A-CGA-CBA	2.06	118.38	111.91
19	A	1127	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
19	3	3017	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
19	1	1006	CLA	CMA-C3A-C2A	-2.06	111.29	116.10
19	L	1501	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
19	A	1128	CLA	C5-C3-C2	-2.06	116.95	121.12
19	A	1135	CLA	C4A-NA-C1A	2.06	107.63	106.71
22	R	7022	LMU	O1'-C1'-C2'	2.06	111.52	108.30
21	J	6012	BCR	C36-C18-C19	2.06	121.32	118.08
22	R	7007	LMU	C1B-O5B-C5B	2.06	117.73	113.69
19	2	2002	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
19	4	4002	CLA	CMD-C2D-C3D	-2.06	120.83	124.68
22	4	7019	LMU	O5'-C5'-C6'	2.06	111.55	106.44
21	B	6005	BCR	C27-C26-C25	-2.06	119.75	122.73
19	4	4001	CLA	CGD-CBD-CAD	-2.05	104.08	110.73
22	G	7039	LMU	C1B-O1B-C4'	-2.05	112.88	117.96
22	G	7051	LMU	O2B-C2B-C3B	-2.05	105.60	110.35
19	A	1139	CLA	C1-O2A-CGA	2.05	121.83	116.44
19	A	1131	CLA	C4-C3-C5	2.05	118.72	115.27
19	A	9023	CLA	C6-C7-C8	-2.05	109.29	115.92
19	H	1241	CLA	CMB-C2B-C3B	2.05	128.52	124.68
21	F	6016	BCR	C4-C5-C6	-2.05	119.75	122.73
21	I	6021	BCR	C32-C1-C6	-2.05	106.97	110.30
19	2	2007	CLA	CMB-C2B-C3B	2.05	128.51	124.68
22	4	7019	LMU	O1'-C1'-C2'	2.05	111.50	108.30
19	4	4001	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
19	A	1121	CLA	CED-O2D-CGD	2.05	120.57	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	7011	LMU	O5'-C1'-C2'	-2.05	106.02	110.35
19	A	1119	CLA	CGD-CBD-CAD	2.05	117.36	110.73
22	3	7005	LMU	C6B-C5B-C4B	2.05	117.80	113.00
19	A	1113	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
22	D	7050	LMU	C1'-O5'-C5'	-2.05	109.67	113.69
19	A	1111	CLA	C1-O2A-CGA	2.04	121.81	116.44
19	1	1303	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
21	B	6004	BCR	C15-C16-C17	-2.04	119.29	123.47
22	3	7003	LMU	O1B-C4'-C3'	2.04	112.72	107.28
19	B	1239	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
19	1	1002	CLA	CAA-CBA-CGA	2.04	119.22	113.25
19	B	1216	CLA	CMB-C2B-C3B	2.04	128.50	124.68
19	B	1231	CLA	CMB-C2B-C3B	2.04	128.50	124.68
22	B	7012	LMU	C1'-C2'-C3'	2.04	114.25	110.00
21	A	6003	BCR	C37-C22-C23	2.04	121.29	118.08
21	I	6021	BCR	C35-C13-C12	2.04	121.29	118.08
19	3	3017	CLA	CBA-CAA-C2A	-2.04	107.84	113.86
19	A	1140	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
19	B	1222	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	A	9011	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
19	B	1215	CLA	CMB-C2B-C3B	2.04	128.49	124.68
21	B	6010	BCR	C1-C6-C7	2.04	121.54	115.78
19	A	9023	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
22	4	7008	LMU	O2'-C2'-C3'	-2.04	105.64	110.35
21	B	6020	BCR	C23-C24-C25	-2.04	121.48	127.20
21	F	6016	BCR	C28-C27-C26	-2.04	110.44	114.08
19	B	1220	CLA	O2A-C1-C2	2.03	113.98	108.64
20	B	5002	PQN	C14-C13-C15	2.03	118.69	115.27
19	K	1143	CLA	C5-C3-C4	2.03	119.10	114.60
19	A	1131	CLA	C1-O2A-CGA	2.03	121.78	116.44
21	I	6018	BCR	C30-C25-C26	-2.03	119.75	122.61
22	R	7025	LMU	O3B-C3B-C4B	2.03	115.05	110.35
19	4	4015	CLA	O2A-CGA-CBA	2.03	120.26	112.23
19	B	1220	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
21	B	6006	BCR	C40-C30-C29	-2.03	100.78	108.91
22	E	7048	LMU	O5'-C5'-C6'	2.03	111.49	106.44
19	3	3013	CLA	CMB-C2B-C3B	2.03	128.48	124.68
21	B	6020	BCR	C33-C5-C6	-2.03	122.25	124.53
19	H	1241	CLA	C4A-NA-C1A	2.03	107.62	106.71
22	C	7015	LMU	C6B-C5B-C4B	2.03	117.76	113.00
19	B	1206	CLA	CMD-C2D-C3D	-2.03	120.88	124.68
22	R	7024	LMU	O5B-C5B-C6B	2.03	111.48	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1210	CLA	CHB-C4A-NA	2.03	127.32	124.51
21	I	6021	BCR	C7-C6-C5	2.03	126.38	121.46
22	R	7021	LMU	O5B-C5B-C4B	2.03	113.38	109.69
19	B	1223	CLA	CMB-C2B-C3B	2.03	128.47	124.68
19	A	1103	CLA	O1A-CGA-CBA	-2.03	115.82	123.73
22	E	7048	LMU	O1B-C1B-O5B	2.02	116.33	110.67
19	L	1503	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
19	B	1231	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
22	2	7046	LMU	O5'-C5'-C6'	2.02	111.47	106.44
19	B	1228	CLA	CMD-C2D-C3D	-2.02	120.89	124.68
19	2	2002	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
22	G	7051	LMU	C1'-C2'-C3'	2.02	114.21	110.00
19	R	1144	CLA	CGD-CBD-CAD	-2.02	104.19	110.73
21	A	6011	BCR	C23-C22-C21	-2.02	115.84	118.94
21	I	6021	BCR	C33-C5-C6	-2.02	122.26	124.53
21	A	6002	BCR	C40-C30-C29	-2.02	100.83	108.91
21	L	6019	BCR	C8-C9-C10	2.02	122.04	118.94
19	A	1106	CLA	C1-O2A-CGA	2.02	121.74	116.44
19	B	1234	CLA	C4-C3-C5	2.02	118.66	115.27
19	A	1129	CLA	C1-O2A-CGA	2.02	121.73	116.44
22	4	7009	LMU	C4B-C3B-C2B	2.02	114.34	110.82
19	2	2002	CLA	CED-O2D-CGD	2.02	120.50	115.94
19	R	1144	CLA	CAA-C2A-C1A	2.01	118.57	111.97
19	K	1143	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
21	A	6008	BCR	C39-C30-C25	2.01	113.56	110.30
21	A	6002	BCR	C4-C5-C6	-2.01	119.81	122.73
21	J	6012	BCR	C27-C26-C25	-2.01	119.81	122.73
22	B	7040	LMU	O5B-C1B-C2B	2.01	114.60	110.35
22	F	7036	LMU	O5B-C5B-C6B	2.01	111.42	106.44
19	A	1237	CLA	C2A-C1A-CHA	-2.01	120.35	123.86
22	G	7026	LMU	C4B-C3B-C2B	-2.00	107.32	110.82
19	B	1223	CLA	C1-O2A-CGA	2.00	121.70	116.44
19	B	1203	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
19	H	1241	CLA	C1B-CHB-C4A	-2.00	126.15	130.12

All (271) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1101	CLA	ND
19	A	1102	CLA	ND
19	A	1102	CLA	C8
19	A	1103	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1103	CLA	C8
19	A	1104	CLA	ND
19	A	1104	CLA	C8
19	A	1105	CLA	ND
19	A	1106	CLA	ND
19	A	1106	CLA	C8
19	A	1107	CLA	ND
19	A	1107	CLA	C8
19	A	1108	CLA	ND
19	A	1109	CLA	ND
19	A	1109	CLA	C8
19	A	1110	CLA	ND
19	A	1111	CLA	ND
19	A	1112	CLA	ND
19	A	1113	CLA	ND
19	A	1115	CLA	ND
19	A	1115	CLA	C8
19	A	1116	CLA	ND
19	A	1117	CLA	ND
19	A	1117	CLA	C8
19	A	1119	CLA	ND
19	A	1119	CLA	C8
19	A	1120	CLA	ND
19	A	1121	CLA	ND
19	A	1122	CLA	ND
19	A	1122	CLA	C8
19	A	1123	CLA	ND
19	A	1123	CLA	C8
19	A	1124	CLA	ND
19	A	1124	CLA	C8
19	A	1125	CLA	ND
19	A	1125	CLA	C8
19	A	1126	CLA	ND
19	A	1126	CLA	C8
19	A	1127	CLA	ND
19	A	1127	CLA	C8
19	A	1128	CLA	ND
19	A	1128	CLA	C8
19	A	1129	CLA	ND
19	A	1131	CLA	ND
19	A	1131	CLA	C8
19	A	1132	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1132	CLA	C8
19	A	1133	CLA	ND
19	A	1134	CLA	ND
19	A	1135	CLA	ND
19	A	1136	CLA	ND
19	A	1136	CLA	C8
19	A	1137	CLA	ND
19	A	1138	CLA	ND
19	A	1138	CLA	C8
19	A	1139	CLA	ND
19	A	1140	CLA	ND
19	A	1140	CLA	C8
19	A	1141	CLA	ND
19	A	1141	CLA	C8
19	A	1149	CLA	ND
19	A	1149	CLA	CBD
19	A	1149	CLA	C2A
19	A	1151	CLA	ND
19	A	1237	CLA	ND
19	A	1237	CLA	C8
19	A	1309	CLA	ND
19	A	9011	CLA	ND
19	A	9011	CLA	C8
19	A	9012	CLA	ND
19	A	9012	CLA	C8
19	A	9013	CLA	ND
19	A	9013	CLA	C8
19	A	9022	CLA	ND
19	A	9022	CLA	C8
19	A	9023	CLA	ND
19	A	9023	CLA	C8
19	B	1201	CLA	ND
19	B	1202	CLA	ND
19	B	1202	CLA	C8
19	B	1203	CLA	ND
19	B	1203	CLA	C8
19	B	1205	CLA	ND
19	B	1205	CLA	C8
19	B	1206	CLA	ND
19	B	1206	CLA	C8
19	B	1208	CLA	ND
19	B	1208	CLA	C8

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Mol	Chain	Res	Type	Atom
19	B	1209	CLA	ND
19	B	1209	CLA	C8
19	B	1210	CLA	ND
19	B	1210	CLA	C8
19	B	1211	CLA	ND
19	B	1211	CLA	C8
19	B	1212	CLA	ND
19	B	1212	CLA	C8
19	B	1213	CLA	ND
19	B	1214	CLA	ND
19	B	1214	CLA	C8
19	B	1215	CLA	ND
19	B	1215	CLA	C8
19	B	1216	CLA	ND
19	B	1216	CLA	C8
19	B	1217	CLA	ND
19	B	1218	CLA	ND
19	B	1219	CLA	ND
19	B	1219	CLA	C8
19	B	1220	CLA	ND
19	B	1221	CLA	ND
19	B	1222	CLA	ND
19	B	1222	CLA	C8
19	B	1223	CLA	ND
19	B	1223	CLA	C8
19	B	1224	CLA	ND
19	B	1224	CLA	C8
19	B	1225	CLA	ND
19	B	1225	CLA	C8
19	B	1226	CLA	ND
19	B	1226	CLA	C8
19	B	1227	CLA	ND
19	B	1228	CLA	ND
19	B	1229	CLA	ND
19	B	1229	CLA	C8
19	B	1230	CLA	ND
19	B	1231	CLA	ND
19	B	1232	CLA	ND
19	B	1233	CLA	ND
19	B	1234	CLA	ND
19	B	1234	CLA	C8
19	B	1235	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	1235	CLA	C8
19	B	1236	CLA	ND
19	B	1238	CLA	ND
19	B	1238	CLA	C8
19	B	1239	CLA	ND
19	B	1239	CLA	C8
19	B	1301	CLA	ND
19	B	9010	CLA	ND
19	B	9010	CLA	C8
19	F	1240	CLA	ND
19	F	1302	CLA	ND
19	F	1305	CLA	ND
19	F	1305	CLA	CBD
19	F	1305	CLA	C2A
19	F	1305	CLA	C3A
19	G	1242	CLA	ND
19	H	1145	CLA	ND
19	H	1145	CLA	C8
19	H	1145	CLA	CBD
19	H	1207	CLA	ND
19	H	1207	CLA	C8
19	H	1241	CLA	ND
19	H	1241	CLA	C8
19	H	1505	CLA	ND
19	H	1505	CLA	C8
19	I	1204	CLA	ND
19	I	1204	CLA	C8
19	J	1308	CLA	ND
19	J	1308	CLA	C8
19	J	1311	CLA	ND
19	J	1311	CLA	C8
19	K	1142	CLA	ND
19	K	1143	CLA	ND
19	K	1146	CLA	ND
19	K	3009	CLA	ND
19	K	3009	CLA	C8
19	L	1130	CLA	ND
19	L	1130	CLA	C8
19	L	1148	CLA	ND
19	L	1148	CLA	C2A
19	L	1148	CLA	C3A
19	L	1501	CLA	ND

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Mol	Chain	Res	Type	Atom
19	L	1502	CLA	ND
19	L	1503	CLA	ND
19	L	1503	CLA	CBD
19	L	1504	CLA	ND
19	L	1504	CLA	C8
19	R	1144	CLA	ND
19	R	1144	CLA	C8
19	R	1150	CLA	ND
19	R	1150	CLA	C8
19	1	1001	CLA	ND
19	1	1002	CLA	ND
19	1	1003	CLA	ND
19	1	1005	CLA	ND
19	1	1006	CLA	ND
19	1	1007	CLA	ND
19	1	1007	CLA	C8
19	1	1008	CLA	ND
19	1	1008	CLA	C2A
19	1	1010	CLA	ND
19	1	1011	CLA	ND
19	1	1012	CLA	ND
19	1	1013	CLA	ND
19	1	1013	CLA	CBD
19	1	1014	CLA	ND
19	1	1014	CLA	C8
19	1	1015	CLA	ND
19	1	1303	CLA	ND
19	1	1303	CLA	C2A
19	1	1303	CLA	C3A
19	1	1310	CLA	ND
19	2	1307	CLA	ND
19	2	2001	CLA	ND
19	2	2002	CLA	ND
19	2	2002	CLA	C8
19	2	2003	CLA	ND
19	2	2004	CLA	ND
19	2	2005	CLA	ND
19	2	2006	CLA	ND
19	2	2006	CLA	C8
19	2	2007	CLA	ND
19	2	2007	CLA	C8
19	2	2008	CLA	ND

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Mol	Chain	Res	Type	Atom
19	2	2010	CLA	ND
19	2	2011	CLA	ND
19	2	2012	CLA	ND
19	2	2013	CLA	ND
19	2	2014	CLA	ND
19	2	2014	CLA	C8
19	2	4009	CLA	ND
19	2	4009	CLA	C8
19	3	1118	CLA	ND
19	3	1147	CLA	ND
19	3	2009	CLA	ND
19	3	2009	CLA	C8
19	3	3001	CLA	ND
19	3	3002	CLA	ND
19	3	3003	CLA	ND
19	3	3004	CLA	ND
19	3	3005	CLA	ND
19	3	3006	CLA	ND
19	3	3007	CLA	ND
19	3	3008	CLA	ND
19	3	3010	CLA	ND
19	3	3011	CLA	ND
19	3	3011	CLA	C8
19	3	3012	CLA	ND
19	3	3013	CLA	ND
19	3	3013	CLA	C8
19	3	3014	CLA	ND
19	3	3015	CLA	ND
19	3	3016	CLA	ND
19	3	3016	CLA	C8
19	3	3017	CLA	ND
19	4	1004	CLA	ND
19	4	1004	CLA	C8
19	4	1009	CLA	ND
19	4	1304	CLA	ND
19	4	1304	CLA	C8
19	4	1304	CLA	CBD
19	4	1306	CLA	ND
19	4	1306	CLA	C8
19	4	4001	CLA	ND
19	4	4002	CLA	ND
19	4	4002	CLA	C2A

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Mol	Chain	Res	Type	Atom
19	4	4003	CLA	ND
19	4	4003	CLA	C8
19	4	4004	CLA	ND
19	4	4005	CLA	ND
19	4	4006	CLA	ND
19	4	4006	CLA	C8
19	4	4007	CLA	ND
19	4	4010	CLA	ND
19	4	4011	CLA	ND
19	4	4012	CLA	ND
19	4	4013	CLA	ND
19	4	4014	CLA	ND
19	4	4015	CLA	ND
20	A	5001	PQN	C23
20	B	5002	PQN	C23

All (2879) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	1101	CLA	C3A-C2A-CAA-CBA
19	A	1102	CLA	C3A-C2A-CAA-CBA
19	A	1102	CLA	CBA-CGA-O2A-C1
19	A	1102	CLA	O1A-CGA-O2A-C1
19	A	1102	CLA	CBD-CGD-O2D-CED
19	A	1103	CLA	C1A-C2A-CAA-CBA
19	A	1103	CLA	C3A-C2A-CAA-CBA
19	A	1103	CLA	C2-C3-C5-C6
19	A	1103	CLA	C4-C3-C5-C6
19	A	1104	CLA	CBA-CGA-O2A-C1
19	A	1104	CLA	O1A-CGA-O2A-C1
19	A	1104	CLA	CBD-CGD-O2D-CED
19	A	1105	CLA	C1A-C2A-CAA-CBA
19	A	1105	CLA	C3A-C2A-CAA-CBA
19	A	1105	CLA	CBA-CGA-O2A-C1
19	A	1106	CLA	C1A-C2A-CAA-CBA
19	A	1106	CLA	C3A-C2A-CAA-CBA
19	A	1107	CLA	C1A-C2A-CAA-CBA
19	A	1107	CLA	C2C-C3C-CAC-CBC
19	A	1107	CLA	O2A-C1-C2-C3
19	A	1108	CLA	CBD-CGD-O2D-CED
19	A	1109	CLA	C2C-C3C-CAC-CBC
19	A	1109	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	1111	CLA	CBD-CGD-O2D-CED
19	A	1112	CLA	C1A-C2A-CAA-CBA
19	A	1112	CLA	C2A-CAA-CBA-CGA
19	A	1112	CLA	C2C-C3C-CAC-CBC
19	A	1113	CLA	C1A-C2A-CAA-CBA
19	A	1113	CLA	CBA-CGA-O2A-C1
19	A	1113	CLA	O1A-CGA-O2A-C1
19	A	1113	CLA	C2C-C3C-CAC-CBC
19	A	1113	CLA	C4C-C3C-CAC-CBC
19	A	1113	CLA	CHA-CBD-CGD-O1D
19	A	1113	CLA	CHA-CBD-CGD-O2D
19	A	1113	CLA	CBD-CGD-O2D-CED
19	A	1115	CLA	CBA-CGA-O2A-C1
19	A	1115	CLA	O1A-CGA-O2A-C1
19	A	1115	CLA	C2C-C3C-CAC-CBC
19	A	1115	CLA	C4C-C3C-CAC-CBC
19	A	1115	CLA	C2-C3-C5-C6
19	A	1115	CLA	C4-C3-C5-C6
19	A	1116	CLA	C1A-C2A-CAA-CBA
19	A	1116	CLA	C3A-C2A-CAA-CBA
19	A	1116	CLA	C2C-C3C-CAC-CBC
19	A	1116	CLA	CHA-CBD-CGD-O1D
19	A	1116	CLA	CHA-CBD-CGD-O2D
19	A	1116	CLA	CBD-CGD-O2D-CED
19	A	1117	CLA	C1A-C2A-CAA-CBA
19	A	1117	CLA	C3A-C2A-CAA-CBA
19	A	1117	CLA	CBA-CGA-O2A-C1
19	A	1117	CLA	O1A-CGA-O2A-C1
19	A	1117	CLA	CAD-CBD-CGD-O1D
19	A	1117	CLA	CAD-CBD-CGD-O2D
19	A	1117	CLA	CBD-CGD-O2D-CED
19	A	1119	CLA	C2C-C3C-CAC-CBC
19	A	1119	CLA	C4C-C3C-CAC-CBC
19	A	1120	CLA	CAD-CBD-CGD-O1D
19	A	1120	CLA	CAD-CBD-CGD-O2D
19	A	1121	CLA	C1A-C2A-CAA-CBA
19	A	1121	CLA	C3A-C2A-CAA-CBA
19	A	1122	CLA	C1A-C2A-CAA-CBA
19	A	1124	CLA	C2C-C3C-CAC-CBC
19	A	1124	CLA	C4C-C3C-CAC-CBC
19	A	1124	CLA	CBD-CGD-O2D-CED
19	A	1125	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	A	1125	CLA	C4C-C3C-CAC-CBC
19	A	1125	CLA	O2A-C1-C2-C3
19	A	1125	CLA	C11-C10-C8-C9
19	A	1128	CLA	C1A-C2A-CAA-CBA
19	A	1128	CLA	C3A-C2A-CAA-CBA
19	A	1128	CLA	CHA-CBD-CGD-O1D
19	A	1128	CLA	CHA-CBD-CGD-O2D
19	A	1128	CLA	CBD-CGD-O2D-CED
19	A	1131	CLA	CBD-CGD-O2D-CED
19	A	1132	CLA	C1A-C2A-CAA-CBA
19	A	1132	CLA	C2C-C3C-CAC-CBC
19	A	1133	CLA	C1A-C2A-CAA-CBA
19	A	1133	CLA	C3A-C2A-CAA-CBA
19	A	1133	CLA	C2C-C3C-CAC-CBC
19	A	1133	CLA	C4C-C3C-CAC-CBC
19	A	1134	CLA	C2A-CAA-CBA-CGA
19	A	1135	CLA	C1A-C2A-CAA-CBA
19	A	1135	CLA	CBD-CGD-O2D-CED
19	A	1136	CLA	CAD-CBD-CGD-O1D
19	A	1136	CLA	CAD-CBD-CGD-O2D
19	A	1137	CLA	C1A-C2A-CAA-CBA
19	A	1137	CLA	C2C-C3C-CAC-CBC
19	A	1139	CLA	C1A-C2A-CAA-CBA
19	A	1139	CLA	CBD-CGD-O2D-CED
19	A	1139	CLA	O2A-C1-C2-C3
19	A	1140	CLA	C1A-C2A-CAA-CBA
19	A	1140	CLA	C3A-C2A-CAA-CBA
19	A	1141	CLA	C2-C3-C5-C6
19	A	1141	CLA	C4-C3-C5-C6
19	A	1149	CLA	C1A-C2A-CAA-CBA
19	A	1149	CLA	C2C-C3C-CAC-CBC
19	A	1149	CLA	CAD-CBD-CGD-O1D
19	A	1149	CLA	CAD-CBD-CGD-O2D
19	A	1149	CLA	CBD-CGD-O2D-CED
19	A	1151	CLA	C3A-C2A-CAA-CBA
19	A	1151	CLA	CHA-CBD-CGD-O1D
19	A	1151	CLA	CHA-CBD-CGD-O2D
19	A	1151	CLA	CBD-CGD-O2D-CED
19	A	1237	CLA	C11-C10-C8-C7
19	A	9011	CLA	C3A-C2A-CAA-CBA
19	A	9012	CLA	CBD-CGD-O2D-CED
19	A	9012	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	9012	CLA	C6-C7-C8-C9
19	A	9013	CLA	C2C-C3C-CAC-CBC
19	A	9013	CLA	CHA-CBD-CGD-O1D
19	A	9013	CLA	CHA-CBD-CGD-O2D
19	A	9013	CLA	O2A-C1-C2-C3
19	A	9022	CLA	C2-C3-C5-C6
19	A	9022	CLA	C4-C3-C5-C6
19	A	9023	CLA	C2C-C3C-CAC-CBC
19	A	9023	CLA	C4C-C3C-CAC-CBC
19	B	1201	CLA	C1A-C2A-CAA-CBA
19	B	1201	CLA	C3A-C2A-CAA-CBA
19	B	1201	CLA	C2C-C3C-CAC-CBC
19	B	1202	CLA	C1A-C2A-CAA-CBA
19	B	1202	CLA	C2-C1-O2A-CGA
19	B	1202	CLA	CAD-CBD-CGD-O1D
19	B	1202	CLA	CAD-CBD-CGD-O2D
19	B	1203	CLA	CBD-CGD-O2D-CED
19	B	1205	CLA	C11-C10-C8-C9
19	B	1205	CLA	C12-C13-C15-C16
19	B	1206	CLA	C1A-C2A-CAA-CBA
19	B	1206	CLA	O2A-C1-C2-C3
19	B	1208	CLA	C1A-C2A-CAA-CBA
19	B	1208	CLA	C3A-C2A-CAA-CBA
19	B	1208	CLA	CBA-CGA-O2A-C1
19	B	1208	CLA	O1A-CGA-O2A-C1
19	B	1210	CLA	C1A-C2A-CAA-CBA
19	B	1210	CLA	CHA-CBD-CGD-O1D
19	B	1210	CLA	CHA-CBD-CGD-O2D
19	B	1210	CLA	CAD-CBD-CGD-O1D
19	B	1210	CLA	CAD-CBD-CGD-O2D
19	B	1211	CLA	C1A-C2A-CAA-CBA
19	B	1211	CLA	C3A-C2A-CAA-CBA
19	B	1211	CLA	C2A-CAA-CBA-CGA
19	B	1212	CLA	CAD-CBD-CGD-O1D
19	B	1212	CLA	CAD-CBD-CGD-O2D
19	B	1213	CLA	C2C-C3C-CAC-CBC
19	B	1213	CLA	C4C-C3C-CAC-CBC
19	B	1213	CLA	CBD-CGD-O2D-CED
19	B	1214	CLA	C1A-C2A-CAA-CBA
19	B	1214	CLA	C3A-C2A-CAA-CBA
19	B	1214	CLA	C2A-CAA-CBA-CGA
19	B	1214	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B	1215	CLA	C1A-C2A-CAA-CBA
19	B	1215	CLA	C3A-C2A-CAA-CBA
19	B	1216	CLA	C1A-C2A-CAA-CBA
19	B	1216	CLA	C3A-C2A-CAA-CBA
19	B	1216	CLA	CBD-CGD-O2D-CED
19	B	1217	CLA	CBD-CGD-O2D-CED
19	B	1218	CLA	C2C-C3C-CAC-CBC
19	B	1218	CLA	C4C-C3C-CAC-CBC
19	B	1218	CLA	CBD-CGD-O2D-CED
19	B	1219	CLA	C1A-C2A-CAA-CBA
19	B	1219	CLA	C3A-C2A-CAA-CBA
19	B	1220	CLA	CBA-CGA-O2A-C1
19	B	1220	CLA	O1A-CGA-O2A-C1
19	B	1220	CLA	C2C-C3C-CAC-CBC
19	B	1220	CLA	C4C-C3C-CAC-CBC
19	B	1220	CLA	CHA-CBD-CGD-O1D
19	B	1222	CLA	C2C-C3C-CAC-CBC
19	B	1222	CLA	C4C-C3C-CAC-CBC
19	B	1222	CLA	CBD-CGD-O2D-CED
19	B	1222	CLA	C2-C3-C5-C6
19	B	1222	CLA	C4-C3-C5-C6
19	B	1223	CLA	C1A-C2A-CAA-CBA
19	B	1223	CLA	C3A-C2A-CAA-CBA
19	B	1223	CLA	C11-C12-C13-C14
19	B	1224	CLA	C3A-C2A-CAA-CBA
19	B	1224	CLA	C2C-C3C-CAC-CBC
19	B	1224	CLA	C4C-C3C-CAC-CBC
19	B	1224	CLA	CBD-CGD-O2D-CED
19	B	1225	CLA	C1A-C2A-CAA-CBA
19	B	1225	CLA	C3A-C2A-CAA-CBA
19	B	1226	CLA	C2C-C3C-CAC-CBC
19	B	1226	CLA	C4C-C3C-CAC-CBC
19	B	1226	CLA	CHA-CBD-CGD-O1D
19	B	1226	CLA	CHA-CBD-CGD-O2D
19	B	1226	CLA	CAD-CBD-CGD-O1D
19	B	1227	CLA	C1A-C2A-CAA-CBA
19	B	1227	CLA	C3A-C2A-CAA-CBA
19	B	1227	CLA	CHA-CBD-CGD-O1D
19	B	1227	CLA	CHA-CBD-CGD-O2D
19	B	1227	CLA	CBD-CGD-O2D-CED
19	B	1228	CLA	C1A-C2A-CAA-CBA
19	B	1228	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B	1228	CLA	C2C-C3C-CAC-CBC
19	B	1228	CLA	C4C-C3C-CAC-CBC
19	B	1228	CLA	CHA-CBD-CGD-O1D
19	B	1228	CLA	CHA-CBD-CGD-O2D
19	B	1229	CLA	C1A-C2A-CAA-CBA
19	B	1230	CLA	C1A-C2A-CAA-CBA
19	B	1230	CLA	C3A-C2A-CAA-CBA
19	B	1230	CLA	CBD-CGD-O2D-CED
19	B	1231	CLA	C1A-C2A-CAA-CBA
19	B	1231	CLA	C3A-C2A-CAA-CBA
19	B	1231	CLA	CHA-CBD-CGD-O1D
19	B	1231	CLA	CHA-CBD-CGD-O2D
19	B	1231	CLA	CAD-CBD-CGD-O1D
19	B	1231	CLA	CAD-CBD-CGD-O2D
19	B	1231	CLA	CBD-CGD-O2D-CED
19	B	1232	CLA	CBD-CGD-O2D-CED
19	B	1233	CLA	C3A-C2A-CAA-CBA
19	B	1233	CLA	O1A-CGA-O2A-C1
19	B	1233	CLA	C2-C3-C5-C6
19	B	1234	CLA	C2C-C3C-CAC-CBC
19	B	1238	CLA	C2C-C3C-CAC-CBC
19	B	1239	CLA	C3A-C2A-CAA-CBA
19	B	1239	CLA	C2C-C3C-CAC-CBC
19	B	1239	CLA	C4C-C3C-CAC-CBC
19	B	9010	CLA	CBD-CGD-O2D-CED
19	F	1302	CLA	CBD-CGD-O2D-CED
19	F	1302	CLA	O1D-CGD-O2D-CED
19	F	1305	CLA	C1A-C2A-CAA-CBA
19	F	1305	CLA	CBD-CGD-O2D-CED
19	F	1305	CLA	O1D-CGD-O2D-CED
19	G	1242	CLA	CAD-CBD-CGD-O1D
19	G	1242	CLA	CAD-CBD-CGD-O2D
19	G	1242	CLA	CBD-CGD-O2D-CED
19	G	1242	CLA	C2-C3-C5-C6
19	G	1242	CLA	C4-C3-C5-C6
19	H	1145	CLA	C1A-C2A-CAA-CBA
19	H	1145	CLA	C3A-C2A-CAA-CBA
19	H	1145	CLA	C2C-C3C-CAC-CBC
19	H	1145	CLA	C4C-C3C-CAC-CBC
19	H	1145	CLA	CBD-CGD-O2D-CED
19	H	1145	CLA	O1D-CGD-O2D-CED
19	H	1207	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
19	H	1241	CLA	CAD-CBD-CGD-O1D
19	H	1241	CLA	CAD-CBD-CGD-O2D
19	H	1241	CLA	CBD-CGD-O2D-CED
19	H	1505	CLA	C2A-CAA-CBA-CGA
19	H	1505	CLA	C2-C3-C5-C6
19	H	1505	CLA	C4-C3-C5-C6
19	I	1204	CLA	CHA-CBD-CGD-O1D
19	I	1204	CLA	CHA-CBD-CGD-O2D
19	J	1308	CLA	C1A-C2A-CAA-CBA
19	J	1308	CLA	C2C-C3C-CAC-CBC
19	J	1308	CLA	C4C-C3C-CAC-CBC
19	J	1308	CLA	CAD-CBD-CGD-O1D
19	J	1308	CLA	CAD-CBD-CGD-O2D
19	J	1308	CLA	CBD-CGD-O2D-CED
19	J	1311	CLA	C3A-C2A-CAA-CBA
19	J	1311	CLA	C2A-CAA-CBA-CGA
19	J	1311	CLA	CHA-CBD-CGD-O1D
19	J	1311	CLA	CHA-CBD-CGD-O2D
19	J	1311	CLA	CBD-CGD-O2D-CED
19	K	1143	CLA	C2C-C3C-CAC-CBC
19	K	1143	CLA	O2A-C1-C2-C3
19	K	1146	CLA	C2C-C3C-CAC-CBC
19	K	3009	CLA	C3A-C2A-CAA-CBA
19	K	3009	CLA	C2-C1-O2A-CGA
19	K	3009	CLA	CHA-CBD-CGD-O1D
19	K	3009	CLA	CHA-CBD-CGD-O2D
19	L	1130	CLA	C1A-C2A-CAA-CBA
19	L	1130	CLA	CHA-CBD-CGD-O1D
19	L	1130	CLA	CHA-CBD-CGD-O2D
19	L	1130	CLA	CBD-CGD-O2D-CED
19	L	1130	CLA	O1D-CGD-O2D-CED
19	L	1130	CLA	C2-C3-C5-C6
19	L	1130	CLA	C4-C3-C5-C6
19	L	1148	CLA	C1A-C2A-CAA-CBA
19	L	1148	CLA	C2-C1-O2A-CGA
19	L	1148	CLA	C2C-C3C-CAC-CBC
19	L	1148	CLA	C4C-C3C-CAC-CBC
19	L	1501	CLA	C1A-C2A-CAA-CBA
19	L	1501	CLA	C3A-C2A-CAA-CBA
19	L	1501	CLA	CBD-CGD-O2D-CED
19	L	1502	CLA	C1A-C2A-CAA-CBA
19	L	1502	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	L	1502	CLA	CBD-CGD-O2D-CED
19	L	1503	CLA	C1A-C2A-CAA-CBA
19	L	1503	CLA	C2C-C3C-CAC-CBC
19	L	1503	CLA	C4C-C3C-CAC-CBC
19	L	1504	CLA	CBD-CGD-O2D-CED
19	L	1504	CLA	C2-C3-C5-C6
19	L	1504	CLA	C4-C3-C5-C6
19	R	1144	CLA	C1A-C2A-CAA-CBA
19	R	1144	CLA	O1A-CGA-O2A-C1
19	R	1144	CLA	CHA-CBD-CGD-O1D
19	R	1144	CLA	CHA-CBD-CGD-O2D
19	R	1144	CLA	CBD-CGD-O2D-CED
19	R	1144	CLA	C2-C3-C5-C6
19	R	1144	CLA	C4-C3-C5-C6
19	R	1150	CLA	C1A-C2A-CAA-CBA
19	R	1150	CLA	CAD-CBD-CGD-O1D
19	R	1150	CLA	O2A-C1-C2-C3
19	1	1001	CLA	C1A-C2A-CAA-CBA
19	1	1001	CLA	C3A-C2A-CAA-CBA
19	1	1001	CLA	CBA-CGA-O2A-C1
19	1	1001	CLA	C2C-C3C-CAC-CBC
19	1	1002	CLA	C2C-C3C-CAC-CBC
19	1	1002	CLA	C4C-C3C-CAC-CBC
19	1	1002	CLA	CBD-CGD-O2D-CED
19	1	1005	CLA	C1A-C2A-CAA-CBA
19	1	1005	CLA	C2C-C3C-CAC-CBC
19	1	1005	CLA	C4C-C3C-CAC-CBC
19	1	1005	CLA	CBD-CGD-O2D-CED
19	1	1005	CLA	O1D-CGD-O2D-CED
19	1	1007	CLA	C1A-C2A-CAA-CBA
19	1	1007	CLA	C2C-C3C-CAC-CBC
19	1	1007	CLA	C4C-C3C-CAC-CBC
19	1	1007	CLA	CHA-CBD-CGD-O1D
19	1	1007	CLA	CHA-CBD-CGD-O2D
19	1	1008	CLA	C2C-C3C-CAC-CBC
19	1	1008	CLA	C2-C3-C5-C6
19	1	1008	CLA	C4-C3-C5-C6
19	1	1010	CLA	C1A-C2A-CAA-CBA
19	1	1010	CLA	CBA-CGA-O2A-C1
19	1	1010	CLA	CBD-CGD-O2D-CED
19	1	1013	CLA	CBD-CGD-O2D-CED
19	1	1014	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	1	1014	CLA	C4C-C3C-CAC-CBC
19	1	1014	CLA	CBD-CGD-O2D-CED
19	1	1303	CLA	C3A-C2A-CAA-CBA
19	1	1303	CLA	C2C-C3C-CAC-CBC
19	1	1303	CLA	C4C-C3C-CAC-CBC
19	1	1303	CLA	C2-C3-C5-C6
19	2	2001	CLA	C1A-C2A-CAA-CBA
19	2	2001	CLA	C3A-C2A-CAA-CBA
19	2	2001	CLA	C2C-C3C-CAC-CBC
19	2	2001	CLA	C4C-C3C-CAC-CBC
19	2	2001	CLA	O2A-C1-C2-C3
19	2	2002	CLA	C1A-C2A-CAA-CBA
19	2	2002	CLA	C3A-C2A-CAA-CBA
19	2	2002	CLA	C2C-C3C-CAC-CBC
19	2	2002	CLA	C4C-C3C-CAC-CBC
19	2	2002	CLA	CAD-CBD-CGD-O1D
19	2	2002	CLA	C2-C3-C5-C6
19	2	2002	CLA	C4-C3-C5-C6
19	2	2004	CLA	C2-C1-O2A-CGA
19	2	2004	CLA	C2C-C3C-CAC-CBC
19	2	2006	CLA	C1A-C2A-CAA-CBA
19	2	2006	CLA	CBD-CGD-O2D-CED
19	2	2007	CLA	CBA-CGA-O2A-C1
19	2	2007	CLA	O1A-CGA-O2A-C1
19	2	2007	CLA	C2C-C3C-CAC-CBC
19	2	2012	CLA	CHA-CBD-CGD-O1D
19	2	2012	CLA	CHA-CBD-CGD-O2D
19	2	2013	CLA	CBA-CGA-O2A-C1
19	2	2013	CLA	O1A-CGA-O2A-C1
19	2	2013	CLA	C2C-C3C-CAC-CBC
19	2	2013	CLA	C4C-C3C-CAC-CBC
19	2	2014	CLA	C1A-C2A-CAA-CBA
19	2	2014	CLA	C3A-C2A-CAA-CBA
19	2	2014	CLA	CHA-CBD-CGD-O1D
19	2	2014	CLA	CAD-CBD-CGD-O1D
19	2	2014	CLA	CAD-CBD-CGD-O2D
19	2	2014	CLA	CBD-CGD-O2D-CED
19	2	4009	CLA	C2-C1-O2A-CGA
19	2	4009	CLA	C14-C13-C15-C16
19	3	1147	CLA	C2C-C3C-CAC-CBC
19	3	1147	CLA	C4C-C3C-CAC-CBC
19	3	1147	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	3	2009	CLA	C1A-C2A-CAA-CBA
19	3	2009	CLA	C2-C3-C5-C6
19	3	2009	CLA	C4-C3-C5-C6
19	3	3007	CLA	C1A-C2A-CAA-CBA
19	3	3008	CLA	C1A-C2A-CAA-CBA
19	3	3008	CLA	C2C-C3C-CAC-CBC
19	3	3008	CLA	C4C-C3C-CAC-CBC
19	3	3013	CLA	C1A-C2A-CAA-CBA
19	3	3013	CLA	C3A-C2A-CAA-CBA
19	3	3013	CLA	CAD-CBD-CGD-O1D
19	3	3013	CLA	CAD-CBD-CGD-O2D
19	3	3016	CLA	O1A-CGA-O2A-C1
19	3	3016	CLA	C2C-C3C-CAC-CBC
19	3	3016	CLA	C4C-C3C-CAC-CBC
19	3	3017	CLA	C2C-C3C-CAC-CBC
19	4	1004	CLA	C2C-C3C-CAC-CBC
19	4	1004	CLA	C4C-C3C-CAC-CBC
19	4	1304	CLA	C3A-C2A-CAA-CBA
19	4	1304	CLA	CHA-CBD-CGD-O1D
19	4	1304	CLA	CHA-CBD-CGD-O2D
19	4	1304	CLA	C6-C7-C8-C9
19	4	1306	CLA	C2C-C3C-CAC-CBC
19	4	1306	CLA	C4C-C3C-CAC-CBC
19	4	4002	CLA	C2-C1-O2A-CGA
19	4	4003	CLA	C1A-C2A-CAA-CBA
19	4	4003	CLA	C3A-C2A-CAA-CBA
19	4	4003	CLA	C2C-C3C-CAC-CBC
19	4	4003	CLA	C4C-C3C-CAC-CBC
19	4	4003	CLA	CBD-CGD-O2D-CED
19	4	4003	CLA	O1D-CGD-O2D-CED
19	4	4006	CLA	CBD-CGD-O2D-CED
19	4	4014	CLA	C3A-C2A-CAA-CBA
19	4	4014	CLA	C2C-C3C-CAC-CBC
19	4	4014	CLA	C4C-C3C-CAC-CBC
19	4	4014	CLA	CBD-CGD-O2D-CED
19	4	4015	CLA	C1A-C2A-CAA-CBA
20	A	5001	PQN	C14-C13-C15-C16
20	B	5002	PQN	C14-C13-C15-C16
21	A	6002	BCR	C11-C10-C9-C8
21	A	6002	BCR	C11-C10-C9-C34
21	A	6002	BCR	C10-C11-C12-C13
21	A	6002	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
21	A	6002	BCR	C19-C20-C21-C22
21	A	6002	BCR	C20-C21-C22-C23
21	A	6002	BCR	C20-C21-C22-C37
21	A	6002	BCR	C21-C22-C23-C24
21	A	6002	BCR	C37-C22-C23-C24
21	A	6003	BCR	C5-C6-C7-C8
21	A	6003	BCR	C7-C8-C9-C10
21	A	6003	BCR	C7-C8-C9-C34
21	A	6003	BCR	C21-C22-C23-C24
21	A	6003	BCR	C23-C24-C25-C26
21	A	6003	BCR	C23-C24-C25-C30
21	A	6007	BCR	C21-C22-C23-C24
21	A	6007	BCR	C37-C22-C23-C24
21	A	6007	BCR	C23-C24-C25-C26
21	A	6007	BCR	C23-C24-C25-C30
21	A	6008	BCR	C5-C6-C7-C8
21	A	6008	BCR	C7-C8-C9-C10
21	A	6008	BCR	C7-C8-C9-C34
21	A	6008	BCR	C11-C12-C13-C14
21	A	6008	BCR	C11-C12-C13-C35
21	A	6008	BCR	C17-C18-C19-C20
21	A	6008	BCR	C36-C18-C19-C20
21	A	6011	BCR	C7-C8-C9-C10
21	A	6011	BCR	C7-C8-C9-C34
21	B	6004	BCR	C7-C8-C9-C10
21	B	6004	BCR	C7-C8-C9-C34
21	B	6004	BCR	C10-C11-C12-C13
21	B	6004	BCR	C11-C12-C13-C35
21	B	6004	BCR	C17-C18-C19-C20
21	B	6004	BCR	C36-C18-C19-C20
21	B	6004	BCR	C23-C24-C25-C26
21	B	6004	BCR	C23-C24-C25-C30
21	B	6005	BCR	C5-C6-C7-C8
21	B	6005	BCR	C18-C19-C20-C21
21	B	6006	BCR	C11-C10-C9-C8
21	B	6006	BCR	C11-C10-C9-C34
21	B	6006	BCR	C11-C12-C13-C14
21	B	6006	BCR	C11-C12-C13-C35
21	B	6010	BCR	C9-C10-C11-C12
21	B	6017	BCR	C5-C6-C7-C8
21	B	6017	BCR	C21-C22-C23-C24
21	B	6017	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	B	6020	BCR	C11-C10-C9-C8
21	B	6020	BCR	C11-C10-C9-C34
21	B	6020	BCR	C11-C12-C13-C14
21	B	6020	BCR	C11-C12-C13-C35
21	B	6020	BCR	C13-C14-C15-C16
21	B	6020	BCR	C37-C22-C23-C24
21	F	6014	BCR	C9-C10-C11-C12
21	F	6014	BCR	C18-C19-C20-C21
21	F	6014	BCR	C19-C20-C21-C22
21	F	6016	BCR	C11-C10-C9-C8
21	F	6016	BCR	C11-C10-C9-C34
21	F	6016	BCR	C11-C12-C13-C14
21	F	6016	BCR	C11-C12-C13-C35
21	I	6018	BCR	C11-C12-C13-C35
21	I	6018	BCR	C21-C22-C23-C24
21	I	6018	BCR	C37-C22-C23-C24
21	I	6021	BCR	C10-C11-C12-C13
21	I	6021	BCR	C17-C18-C19-C20
21	I	6021	BCR	C36-C18-C19-C20
21	I	6021	BCR	C21-C22-C23-C24
21	I	6021	BCR	C37-C22-C23-C24
21	J	6012	BCR	C7-C8-C9-C10
21	J	6012	BCR	C7-C8-C9-C34
21	J	6012	BCR	C17-C18-C19-C20
21	J	6012	BCR	C36-C18-C19-C20
21	J	6012	BCR	C18-C19-C20-C21
21	J	6012	BCR	C20-C21-C22-C23
21	J	6012	BCR	C20-C21-C22-C37
21	J	6012	BCR	C37-C22-C23-C24
21	L	6019	BCR	C1-C6-C7-C8
21	L	6019	BCR	C11-C10-C9-C8
21	L	6019	BCR	C11-C10-C9-C34
21	L	6019	BCR	C10-C11-C12-C13
21	L	6019	BCR	C20-C21-C22-C37
21	1	6023	BCR	C1-C6-C7-C8
21	1	6023	BCR	C5-C6-C7-C8
21	1	6023	BCR	C11-C10-C9-C8
21	1	6023	BCR	C11-C10-C9-C34
21	1	6023	BCR	C10-C11-C12-C13
21	1	6023	BCR	C21-C22-C23-C24
21	1	6023	BCR	C37-C22-C23-C24
21	1	6023	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
21	3	6022	BCR	C1-C6-C7-C8
21	3	6022	BCR	C5-C6-C7-C8
21	3	6022	BCR	C15-C16-C17-C18
21	3	6022	BCR	C17-C18-C19-C20
21	3	6022	BCR	C36-C18-C19-C20
21	3	6022	BCR	C18-C19-C20-C21
21	3	6022	BCR	C19-C20-C21-C22
21	3	6022	BCR	C20-C21-C22-C23
21	3	6022	BCR	C20-C21-C22-C37
21	3	6022	BCR	C37-C22-C23-C24
22	A	7010	LMU	C2'-C1'-O1'-C1
22	A	7010	LMU	O5'-C1'-O1'-C1
22	A	7010	LMU	C2-C1-O1'-C1'
22	A	7023	LMU	C2'-C1'-O1'-C1
22	A	7023	LMU	O5'-C1'-O1'-C1
22	A	7045	LMU	C2-C1-O1'-C1'
22	B	7040	LMU	C2'-C1'-O1'-C1
22	B	7040	LMU	O5'-C1'-O1'-C1
22	C	7015	LMU	C2'-C1'-O1'-C1
22	C	7015	LMU	O5'-C1'-O1'-C1
22	D	7050	LMU	C2B-C1B-O1B-C4'
22	D	7050	LMU	C2'-C1'-O1'-C1
22	D	7050	LMU	O5'-C1'-O1'-C1
22	E	7037	LMU	C2'-C1'-O1'-C1
22	E	7037	LMU	O5'-C1'-O1'-C1
22	E	7037	LMU	C2-C1-O1'-C1'
22	F	7036	LMU	C2B-C1B-O1B-C4'
22	F	7036	LMU	O5'-C1'-O1'-C1
22	F	7036	LMU	C2-C1-O1'-C1'
22	G	7026	LMU	C2'-C1'-O1'-C1
22	G	7026	LMU	O5'-C1'-O1'-C1
22	G	7026	LMU	C2-C1-O1'-C1'
22	G	7051	LMU	C2'-C1'-O1'-C1
22	G	7051	LMU	O5'-C1'-O1'-C1
22	H	7002	LMU	C2'-C1'-O1'-C1
22	H	7002	LMU	C2-C1-O1'-C1'
22	H	7011	LMU	O5'-C1'-O1'-C1
22	H	7028	LMU	C2-C1-O1'-C1'
22	H	7030	LMU	C2-C1-O1'-C1'
22	H	7032	LMU	O5'-C1'-O1'-C1
22	H	7043	LMU	O5'-C1'-O1'-C1
22	K	7041	LMU	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
22	K	7041	LMU	C2'-C1'-O1'-C1
22	K	7041	LMU	O5'-C1'-O1'-C1
22	K	7042	LMU	O5'-C1'-O1'-C1
22	K	7047	LMU	C2-C1-O1'-C1'
22	L	7029	LMU	O5'-C1'-O1'-C1
22	R	7007	LMU	C2'-C1'-O1'-C1
22	R	7007	LMU	O5'-C1'-O1'-C1
22	R	7007	LMU	C2-C1-O1'-C1'
22	R	7014	LMU	C2'-C1'-O1'-C1
22	R	7014	LMU	O5'-C1'-O1'-C1
22	R	7020	LMU	C2-C1-O1'-C1'
22	R	7022	LMU	O5'-C1'-O1'-C1
22	R	7022	LMU	C2-C1-O1'-C1'
22	R	7024	LMU	C2'-C1'-O1'-C1
22	R	7024	LMU	O5'-C1'-O1'-C1
22	R	7025	LMU	C2'-C1'-O1'-C1
22	1	7004	LMU	C2'-C1'-O1'-C1
22	1	7004	LMU	O5'-C1'-O1'-C1
22	1	7013	LMU	C2-C1-O1'-C1'
22	2	7006	LMU	O5'-C1'-O1'-C1
22	2	7027	LMU	O5'-C1'-O1'-C1
22	2	7031	LMU	C2B-C1B-O1B-C4'
22	2	7046	LMU	O5'-C1'-O1'-C1
22	3	7003	LMU	C2'-C1'-O1'-C1
22	3	7003	LMU	O5'-C1'-O1'-C1
22	3	7005	LMU	O5'-C1'-O1'-C1
22	4	7008	LMU	O5'-C1'-O1'-C1
22	4	7009	LMU	C2'-C1'-O1'-C1
22	4	7009	LMU	O5'-C1'-O1'-C1
22	4	7018	LMU	C2'-C1'-O1'-C1
22	4	7018	LMU	O5'-C1'-O1'-C1
22	4	7019	LMU	C2'-C1'-O1'-C1
22	4	7019	LMU	O5'-C1'-O1'-C1
22	4	7034	LMU	C2'-C1'-O1'-C1
22	4	7034	LMU	O5'-C1'-O1'-C1
22	4	7052	LMU	C2'-C1'-O1'-C1
22	4	7052	LMU	O5'-C1'-O1'-C1
22	4	7053	LMU	C2'-C1'-O1'-C1
22	4	7053	LMU	O5'-C1'-O1'-C1
24	B	7101	LMG	C2-C1-O1-C7
24	B	7101	LMG	O6-C1-O1-C7
24	B	7101	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
22	G	7051	LMU	C3'-C4'-O1B-C1B
22	H	7002	LMU	C3'-C4'-O1B-C1B
22	K	7042	LMU	C3'-C4'-O1B-C1B
22	4	7008	LMU	C5'-C4'-O1B-C1B
19	A	1104	CLA	O1D-CGD-O2D-CED
19	A	1115	CLA	O1D-CGD-O2D-CED
19	A	1116	CLA	O1D-CGD-O2D-CED
19	A	1123	CLA	O1D-CGD-O2D-CED
19	A	1151	CLA	O1D-CGD-O2D-CED
19	B	1213	CLA	O1D-CGD-O2D-CED
19	B	1217	CLA	O1D-CGD-O2D-CED
19	B	1222	CLA	O1D-CGD-O2D-CED
19	H	1505	CLA	O1D-CGD-O2D-CED
19	L	1501	CLA	O1D-CGD-O2D-CED
19	R	1144	CLA	O1D-CGD-O2D-CED
19	1	1001	CLA	O1D-CGD-O2D-CED
19	1	1303	CLA	O1D-CGD-O2D-CED
19	3	3007	CLA	O1D-CGD-O2D-CED
19	4	4007	CLA	O1D-CGD-O2D-CED
22	H	7011	LMU	O5B-C1B-O1B-C4'
22	R	7007	LMU	O5B-C1B-O1B-C4'
22	3	7005	LMU	O5B-C1B-O1B-C4'
22	H	7011	LMU	C2B-C1B-O1B-C4'
22	H	7043	LMU	C3'-C4'-O1B-C1B
22	1	7013	LMU	C3'-C4'-O1B-C1B
22	2	7006	LMU	C5'-C4'-O1B-C1B
22	4	7034	LMU	C5'-C4'-O1B-C1B
22	4	7053	LMU	C5'-C4'-O1B-C1B
19	A	1105	CLA	O1D-CGD-O2D-CED
19	A	1109	CLA	O1D-CGD-O2D-CED
19	A	1113	CLA	O1D-CGD-O2D-CED
19	A	1117	CLA	O1D-CGD-O2D-CED
19	A	1131	CLA	O1D-CGD-O2D-CED
19	A	1139	CLA	O1D-CGD-O2D-CED
19	A	1149	CLA	O1D-CGD-O2D-CED
19	B	1208	CLA	O1D-CGD-O2D-CED
19	B	1214	CLA	O1D-CGD-O2D-CED
19	B	1218	CLA	O1D-CGD-O2D-CED
19	B	1224	CLA	O1D-CGD-O2D-CED
19	B	1230	CLA	O1D-CGD-O2D-CED
19	G	1242	CLA	O1D-CGD-O2D-CED
19	L	1502	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	1	1002	CLA	O1D-CGD-O2D-CED
19	1	1007	CLA	O1D-CGD-O2D-CED
19	1	1008	CLA	O1D-CGD-O2D-CED
19	1	1010	CLA	O1D-CGD-O2D-CED
19	2	2006	CLA	O1D-CGD-O2D-CED
19	2	2014	CLA	O1D-CGD-O2D-CED
19	3	1147	CLA	O1D-CGD-O2D-CED
19	4	4014	CLA	O1D-CGD-O2D-CED
19	A	1105	CLA	CBD-CGD-O2D-CED
19	A	1107	CLA	CBD-CGD-O2D-CED
19	A	1112	CLA	CBD-CGD-O2D-CED
19	A	1115	CLA	CBD-CGD-O2D-CED
19	A	1122	CLA	CBD-CGD-O2D-CED
19	A	1123	CLA	CBD-CGD-O2D-CED
19	A	1125	CLA	CBD-CGD-O2D-CED
19	A	1126	CLA	CBD-CGD-O2D-CED
19	A	1132	CLA	CBD-CGD-O2D-CED
19	A	1138	CLA	CBD-CGD-O2D-CED
19	B	1202	CLA	CBD-CGD-O2D-CED
19	B	1208	CLA	CBD-CGD-O2D-CED
19	B	1212	CLA	CBD-CGD-O2D-CED
19	B	1220	CLA	CBD-CGD-O2D-CED
19	B	1226	CLA	CBD-CGD-O2D-CED
19	B	1229	CLA	CBD-CGD-O2D-CED
19	B	1234	CLA	CBD-CGD-O2D-CED
19	H	1505	CLA	CBD-CGD-O2D-CED
19	I	1204	CLA	CBD-CGD-O2D-CED
19	K	3009	CLA	CBD-CGD-O2D-CED
19	L	1503	CLA	CBD-CGD-O2D-CED
19	1	1001	CLA	CBD-CGD-O2D-CED
19	1	1003	CLA	CBD-CGD-O2D-CED
19	1	1007	CLA	CBD-CGD-O2D-CED
19	1	1008	CLA	CBD-CGD-O2D-CED
19	1	1303	CLA	CBD-CGD-O2D-CED
19	2	2013	CLA	CBD-CGD-O2D-CED
19	2	4009	CLA	CBD-CGD-O2D-CED
19	3	3007	CLA	CBD-CGD-O2D-CED
19	4	1306	CLA	CBD-CGD-O2D-CED
19	4	4001	CLA	CBD-CGD-O2D-CED
19	4	4007	CLA	CBD-CGD-O2D-CED
19	4	4015	CLA	CBD-CGD-O2D-CED
19	A	1133	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	9011	CLA	O1A-CGA-O2A-C1
19	B	1206	CLA	O1A-CGA-O2A-C1
19	B	1214	CLA	O1A-CGA-O2A-C1
19	B	1236	CLA	O1A-CGA-O2A-C1
19	H	1505	CLA	O1A-CGA-O2A-C1
19	R	1150	CLA	O1A-CGA-O2A-C1
19	3	3011	CLA	O1A-CGA-O2A-C1
22	4	7052	LMU	O5B-C1B-O1B-C4'
22	3	7005	LMU	C2B-C1B-O1B-C4'
19	1	1003	CLA	C2-C1-O2A-CGA
22	B	7012	LMU	C3'-C4'-O1B-C1B
22	R	7014	LMU	C3'-C4'-O1B-C1B
22	R	7021	LMU	C3'-C4'-O1B-C1B
22	R	7022	LMU	C3'-C4'-O1B-C1B
22	3	7005	LMU	C3'-C4'-O1B-C1B
19	A	1112	CLA	O1D-CGD-O2D-CED
19	A	1124	CLA	O1D-CGD-O2D-CED
19	A	1138	CLA	O1D-CGD-O2D-CED
19	B	1203	CLA	O1D-CGD-O2D-CED
19	B	1212	CLA	O1D-CGD-O2D-CED
19	B	1220	CLA	O1D-CGD-O2D-CED
19	B	1227	CLA	O1D-CGD-O2D-CED
19	J	1308	CLA	O1D-CGD-O2D-CED
19	1	1003	CLA	O1D-CGD-O2D-CED
19	1	1013	CLA	O1D-CGD-O2D-CED
19	4	4001	CLA	O1D-CGD-O2D-CED
24	B	7101	LMG	C8-C9-O8-C28
22	A	7045	LMU	O5B-C1B-O1B-C4'
22	B	7038	LMU	O5B-C1B-O1B-C4'
22	E	7037	LMU	O5B-C1B-O1B-C4'
22	K	7042	LMU	O5B-C1B-O1B-C4'
22	R	7020	LMU	O5B-C1B-O1B-C4'
22	R	7024	LMU	O5B-C1B-O1B-C4'
22	1	7004	LMU	O5B-C1B-O1B-C4'
22	B	7038	LMU	C2B-C1B-O1B-C4'
22	E	7037	LMU	C2B-C1B-O1B-C4'
19	A	1107	CLA	O1D-CGD-O2D-CED
19	A	1126	CLA	O1D-CGD-O2D-CED
19	A	1128	CLA	O1D-CGD-O2D-CED
19	B	1202	CLA	O1D-CGD-O2D-CED
19	B	1232	CLA	O1D-CGD-O2D-CED
19	J	1311	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	K	3009	CLA	O1D-CGD-O2D-CED
19	L	1504	CLA	O1D-CGD-O2D-CED
19	4	4006	CLA	O1D-CGD-O2D-CED
19	4	4015	CLA	O1D-CGD-O2D-CED
19	A	1133	CLA	CBA-CGA-O2A-C1
19	A	9011	CLA	CBA-CGA-O2A-C1
19	B	1214	CLA	CBA-CGA-O2A-C1
19	B	1221	CLA	CBA-CGA-O2A-C1
19	B	1233	CLA	CBA-CGA-O2A-C1
19	B	1236	CLA	CBA-CGA-O2A-C1
19	H	1505	CLA	CBA-CGA-O2A-C1
19	3	3011	CLA	CBA-CGA-O2A-C1
22	E	7048	LMU	C4'-C5'-C6'-O6'
22	2	7027	LMU	C4B-C5B-C6B-O6B
19	A	1110	CLA	CBD-CGD-O2D-CED
19	A	1120	CLA	CBD-CGD-O2D-CED
19	A	1133	CLA	CBD-CGD-O2D-CED
19	A	1136	CLA	CBD-CGD-O2D-CED
19	A	1140	CLA	CBD-CGD-O2D-CED
19	A	9022	CLA	CBD-CGD-O2D-CED
19	A	9023	CLA	CBD-CGD-O2D-CED
19	B	1211	CLA	CBD-CGD-O2D-CED
19	H	1207	CLA	CBD-CGD-O2D-CED
19	3	2009	CLA	CBD-CGD-O2D-CED
19	3	3011	CLA	CBD-CGD-O2D-CED
19	A	1116	CLA	O1A-CGA-O2A-C1
19	A	1126	CLA	O1A-CGA-O2A-C1
19	A	1151	CLA	O1A-CGA-O2A-C1
19	A	1237	CLA	O1A-CGA-O2A-C1
19	A	9013	CLA	O1A-CGA-O2A-C1
19	B	1217	CLA	O1A-CGA-O2A-C1
19	B	1221	CLA	O1A-CGA-O2A-C1
19	B	1228	CLA	O1A-CGA-O2A-C1
19	B	9010	CLA	O1A-CGA-O2A-C1
19	J	1311	CLA	O1A-CGA-O2A-C1
19	K	1143	CLA	O1A-CGA-O2A-C1
19	1	1007	CLA	O1A-CGA-O2A-C1
19	1	1008	CLA	O1A-CGA-O2A-C1
19	2	4009	CLA	O1A-CGA-O2A-C1
19	3	3017	CLA	O1A-CGA-O2A-C1
19	4	4007	CLA	O1A-CGA-O2A-C1
19	A	1105	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	1	1001	CLA	O1A-CGA-O2A-C1
19	A	1102	CLA	O1D-CGD-O2D-CED
19	A	1108	CLA	O1D-CGD-O2D-CED
19	A	1135	CLA	O1D-CGD-O2D-CED
19	B	1216	CLA	O1D-CGD-O2D-CED
19	B	1231	CLA	O1D-CGD-O2D-CED
22	2	7046	LMU	O5B-C1B-O1B-C4'
22	A	7035	LMU	C3'-C4'-O1B-C1B
22	K	7001	LMU	C5'-C4'-O1B-C1B
22	K	7047	LMU	C5'-C4'-O1B-C1B
19	A	1111	CLA	O1D-CGD-O2D-CED
19	H	1241	CLA	O1D-CGD-O2D-CED
22	G	7039	LMU	O5B-C1B-O1B-C4'
22	K	7041	LMU	O5B-C1B-O1B-C4'
22	K	7042	LMU	C2B-C1B-O1B-C4'
22	L	7029	LMU	C2B-C1B-O1B-C4'
19	2	2004	CLA	CBD-CGD-O2D-CED
19	3	2009	CLA	C5-C6-C7-C8
19	B	1226	CLA	O1D-CGD-O2D-CED
19	1	1014	CLA	O1D-CGD-O2D-CED
24	B	7101	LMG	O9-C10-O7-C8
22	R	7021	LMU	C4B-C5B-C6B-O6B
19	B	1213	CLA	CBA-CGA-O2A-C1
19	4	4015	CLA	CBA-CGA-O2A-C1
22	A	7045	LMU	C5'-C4'-O1B-C1B
19	B	1213	CLA	O1A-CGA-O2A-C1
19	A	1103	CLA	C3-C5-C6-C7
19	A	1117	CLA	C3-C5-C6-C7
19	A	1126	CLA	C3-C5-C6-C7
19	A	1128	CLA	C3-C5-C6-C7
19	A	1131	CLA	C3-C5-C6-C7
19	A	9022	CLA	C3-C5-C6-C7
19	B	1202	CLA	C3-C5-C6-C7
19	B	1238	CLA	C3-C5-C6-C7
19	H	1505	CLA	C3-C5-C6-C7
19	J	1308	CLA	C3-C5-C6-C7
19	L	1504	CLA	C3-C5-C6-C7
19	4	1306	CLA	C3-C5-C6-C7
19	A	1126	CLA	CBA-CGA-O2A-C1
19	A	1137	CLA	CBA-CGA-O2A-C1
19	A	1237	CLA	CBA-CGA-O2A-C1
19	B	1206	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	1209	CLA	CBA-CGA-O2A-C1
19	B	9010	CLA	CBA-CGA-O2A-C1
19	F	1305	CLA	CBA-CGA-O2A-C1
19	K	1143	CLA	CBA-CGA-O2A-C1
19	L	1503	CLA	CBA-CGA-O2A-C1
19	R	1144	CLA	CBA-CGA-O2A-C1
19	R	1150	CLA	CBA-CGA-O2A-C1
19	1	1007	CLA	CBA-CGA-O2A-C1
19	1	1008	CLA	CBA-CGA-O2A-C1
19	3	3016	CLA	CBA-CGA-O2A-C1
19	3	3017	CLA	CBA-CGA-O2A-C1
22	4	7018	LMU	O5'-C5'-C6'-O6'
22	A	7044	LMU	C4B-C5B-C6B-O6B
22	4	7019	LMU	O5B-C1B-O1B-C4'
19	A	1122	CLA	O1D-CGD-O2D-CED
19	B	9010	CLA	O1D-CGD-O2D-CED
19	3	3016	CLA	CBD-CGD-O2D-CED
19	4	4014	CLA	C2-C1-O2A-CGA
22	R	7024	LMU	O5B-C5B-C6B-O6B
22	4	7009	LMU	O5B-C5B-C6B-O6B
19	4	4015	CLA	O1A-CGA-O2A-C1
22	B	7040	LMU	C3'-C4'-O1B-C1B
22	4	7019	LMU	C2B-C1B-O1B-C4'
19	4	4007	CLA	C3-C5-C6-C7
22	E	7048	LMU	O5'-C5'-C6'-O6'
22	4	7052	LMU	O5B-C5B-C6B-O6B
19	1	1014	CLA	C4-C3-C5-C6
19	3	3011	CLA	C4-C3-C5-C6
19	1	1014	CLA	C2-C3-C5-C6
20	A	5001	PQN	C12-C13-C15-C16
20	B	5002	PQN	C12-C13-C15-C16
19	A	1119	CLA	CBD-CGD-O2D-CED
19	B	1209	CLA	CBD-CGD-O2D-CED
19	B	1215	CLA	CBD-CGD-O2D-CED
19	R	1150	CLA	CBD-CGD-O2D-CED
19	A	1103	CLA	C2A-CAA-CBA-CGA
19	A	1105	CLA	C2A-CAA-CBA-CGA
19	A	1115	CLA	C2A-CAA-CBA-CGA
19	A	1116	CLA	C2A-CAA-CBA-CGA
19	A	1131	CLA	C2A-CAA-CBA-CGA
19	A	1133	CLA	C2A-CAA-CBA-CGA
19	A	1138	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	1139	CLA	C2A-CAA-CBA-CGA
19	A	1141	CLA	C2A-CAA-CBA-CGA
19	A	9011	CLA	C2A-CAA-CBA-CGA
19	B	1210	CLA	C2A-CAA-CBA-CGA
19	B	1218	CLA	C2A-CAA-CBA-CGA
19	B	1219	CLA	C2A-CAA-CBA-CGA
19	B	1227	CLA	C2A-CAA-CBA-CGA
19	B	1238	CLA	C2A-CAA-CBA-CGA
19	H	1207	CLA	C2A-CAA-CBA-CGA
19	L	1130	CLA	C2A-CAA-CBA-CGA
19	2	2006	CLA	C2A-CAA-CBA-CGA
19	A	1127	CLA	C3-C5-C6-C7
19	A	1140	CLA	C3-C5-C6-C7
19	B	1219	CLA	C3-C5-C6-C7
19	B	1234	CLA	C3-C5-C6-C7
19	B	1239	CLA	C3-C5-C6-C7
19	A	1116	CLA	CBA-CGA-O2A-C1
19	A	1138	CLA	CBA-CGA-O2A-C1
19	A	1149	CLA	CBA-CGA-O2A-C1
19	A	1151	CLA	CBA-CGA-O2A-C1
19	A	9013	CLA	CBA-CGA-O2A-C1
19	B	1216	CLA	CBA-CGA-O2A-C1
19	B	1217	CLA	CBA-CGA-O2A-C1
19	B	1228	CLA	CBA-CGA-O2A-C1
19	H	1241	CLA	CBA-CGA-O2A-C1
19	J	1311	CLA	CBA-CGA-O2A-C1
19	2	4009	CLA	CBA-CGA-O2A-C1
19	3	2009	CLA	CBA-CGA-O2A-C1
19	4	4007	CLA	CBA-CGA-O2A-C1
22	G	7051	LMU	O5'-C5'-C6'-O6'
22	H	7002	LMU	O5B-C5B-C6B-O6B
22	R	7022	LMU	O5'-C5'-C6'-O6'
22	4	7053	LMU	O5B-C5B-C6B-O6B
22	K	7041	LMU	C4'-C5'-C6'-O6'
22	R	7014	LMU	C4'-C5'-C6'-O6'
22	4	7033	LMU	C3'-C4'-O1B-C1B
19	A	1134	CLA	CBD-CGD-O2D-CED
19	B	1228	CLA	CBD-CGD-O2D-CED
19	B	1239	CLA	CBD-CGD-O2D-CED
19	A	1125	CLA	O1D-CGD-O2D-CED
19	B	1229	CLA	O1D-CGD-O2D-CED
19	2	2013	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	2	4009	CLA	O1D-CGD-O2D-CED
22	R	7014	LMU	O5'-C5'-C6'-O6'
22	B	7038	LMU	C4B-C5B-C6B-O6B
22	K	7042	LMU	C4B-C5B-C6B-O6B
22	L	7029	LMU	C4B-C5B-C6B-O6B
19	A	1107	CLA	O1A-CGA-O2A-C1
19	B	1216	CLA	O1A-CGA-O2A-C1
19	H	1241	CLA	O1A-CGA-O2A-C1
19	3	2009	CLA	O1A-CGA-O2A-C1
19	K	1142	CLA	C2A-CAA-CBA-CGA
19	1	1010	CLA	O1A-CGA-O2A-C1
21	B	6020	BCR	C15-C16-C17-C18
21	I	6018	BCR	C19-C20-C21-C22
21	I	6021	BCR	C9-C10-C11-C12
21	J	6012	BCR	C19-C20-C21-C22
21	1	6023	BCR	C9-C10-C11-C12
21	3	6022	BCR	C9-C10-C11-C12
19	2	2006	CLA	C15-C16-C17-C18
22	E	7037	LMU	O5'-C5'-C6'-O6'
22	H	7028	LMU	O5'-C5'-C6'-O6'
22	R	7025	LMU	O5B-C5B-C6B-O6B
22	4	7033	LMU	O5'-C5'-C6'-O6'
22	A	7010	LMU	C4'-C5'-C6'-O6'
22	4	7008	LMU	C4'-C5'-C6'-O6'
19	A	9013	CLA	CBD-CGD-O2D-CED
19	B	1236	CLA	CBD-CGD-O2D-CED
19	I	1204	CLA	O1D-CGD-O2D-CED
19	A	1119	CLA	C3-C5-C6-C7
19	A	1122	CLA	C3-C5-C6-C7
19	B	1208	CLA	C3-C5-C6-C7
19	B	1215	CLA	C3-C5-C6-C7
19	K	3009	CLA	C3-C5-C6-C7
19	2	2007	CLA	C3-C5-C6-C7
19	3	3016	CLA	C3-C5-C6-C7
20	A	5001	PQN	C13-C15-C16-C17
19	H	1207	CLA	CBA-CGA-O2A-C1
22	3	7005	LMU	C2-C3-C4-C5
19	A	1137	CLA	O1A-CGA-O2A-C1
19	F	1305	CLA	O1A-CGA-O2A-C1
19	L	1503	CLA	O1A-CGA-O2A-C1
22	D	7050	LMU	O5B-C5B-C6B-O6B
22	G	7051	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
22	N	7049	LMU	O5B-C5B-C6B-O6B
22	R	7022	LMU	O5B-C5B-C6B-O6B
22	B	7012	LMU	C4'-C5'-C6'-O6'
22	2	7006	LMU	C4'-C5'-C6'-O6'
22	4	7018	LMU	C4'-C5'-C6'-O6'
19	A	1132	CLA	O1D-CGD-O2D-CED
19	B	1218	CLA	CBA-CGA-O2A-C1
19	4	4002	CLA	CBD-CGD-O2D-CED
22	N	7049	LMU	O5'-C5'-C6'-O6'
22	4	7019	LMU	O5'-C5'-C6'-O6'
22	H	7002	LMU	C4B-C5B-C6B-O6B
22	H	7030	LMU	C3-C4-C5-C6
22	K	7001	LMU	C5-C6-C7-C8
22	2	7006	LMU	O5B-C1B-O1B-C4'
22	E	7048	LMU	C11-C10-C9-C8
22	H	7011	LMU	C6-C7-C8-C9
22	3	7005	LMU	C4-C5-C6-C7
22	A	7035	LMU	O5'-C5'-C6'-O6'
22	H	7032	LMU	O5'-C5'-C6'-O6'
22	2	7006	LMU	O5'-C5'-C6'-O6'
22	2	7046	LMU	O5'-C5'-C6'-O6'
22	G	7051	LMU	C4'-C5'-C6'-O6'
22	N	7049	LMU	C4B-C5B-C6B-O6B
22	R	7024	LMU	C4B-C5B-C6B-O6B
22	A	7016	LMU	C2-C3-C4-C5
22	A	7044	LMU	C3'-C4'-O1B-C1B
22	B	7038	LMU	C6-C7-C8-C9
22	E	7048	LMU	C5-C6-C7-C8
22	2	7027	LMU	C3-C4-C5-C6
22	2	7046	LMU	C5'-C4'-O1B-C1B
19	2	4009	CLA	C3-C5-C6-C7
19	A	1107	CLA	CBA-CGA-O2A-C1
19	A	1128	CLA	CBA-CGA-O2A-C1
19	4	4006	CLA	CBA-CGA-O2A-C1
19	B	1234	CLA	O1D-CGD-O2D-CED
22	H	7017	LMU	O5B-C5B-C6B-O6B
22	A	7023	LMU	C4B-C5B-C6B-O6B
22	A	7044	LMU	C4'-C5'-C6'-O6'
22	H	7028	LMU	C4'-C5'-C6'-O6'
22	4	7053	LMU	C4B-C5B-C6B-O6B
22	H	7011	LMU	C11-C10-C9-C8
22	K	7042	LMU	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
22	R	7007	LMU	C7-C8-C9-C10
22	R	7022	LMU	C11-C10-C9-C8
19	A	1149	CLA	O1A-CGA-O2A-C1
19	B	1209	CLA	O1A-CGA-O2A-C1
22	R	7020	LMU	C6-C7-C8-C9
22	A	7010	LMU	O5'-C5'-C6'-O6'
22	A	7044	LMU	O5B-C5B-C6B-O6B
22	B	7038	LMU	O5B-C5B-C6B-O6B
22	G	7039	LMU	O5'-C5'-C6'-O6'
22	H	7011	LMU	O5'-C5'-C6'-O6'
22	H	7028	LMU	O5B-C5B-C6B-O6B
22	H	7030	LMU	O5B-C5B-C6B-O6B
22	K	7041	LMU	O5'-C5'-C6'-O6'
22	R	7021	LMU	O5B-C5B-C6B-O6B
22	2	7027	LMU	O5B-C5B-C6B-O6B
22	4	7008	LMU	O5'-C5'-C6'-O6'
19	A	1132	CLA	C4-C3-C5-C6
19	A	9012	CLA	C4-C3-C5-C6
19	B	1216	CLA	C4-C3-C5-C6
19	B	1223	CLA	C4-C3-C5-C6
19	3	3016	CLA	C4-C3-C5-C6
22	R	7025	LMU	C4B-C5B-C6B-O6B
22	4	7009	LMU	C4B-C5B-C6B-O6B
22	4	7033	LMU	C4'-C5'-C6'-O6'
19	A	1132	CLA	C2-C3-C5-C6
19	A	9012	CLA	C2-C3-C5-C6
19	B	1216	CLA	C2-C3-C5-C6
19	B	1223	CLA	C2-C3-C5-C6
19	3	3016	CLA	C2-C3-C5-C6
19	R	1144	CLA	C2A-CAA-CBA-CGA
19	3	2009	CLA	C2A-CAA-CBA-CGA
22	E	7037	LMU	C3-C4-C5-C6
22	H	7030	LMU	O5'-C5'-C6'-O6'
22	K	7042	LMU	O5B-C5B-C6B-O6B
22	R	7024	LMU	O5'-C5'-C6'-O6'
22	3	7003	LMU	O5'-C5'-C6'-O6'
22	4	7019	LMU	O5B-C5B-C6B-O6B
19	A	1138	CLA	O1A-CGA-O2A-C1
19	H	1207	CLA	O1A-CGA-O2A-C1
24	B	7101	LMG	O10-C28-O8-C9
22	L	7029	LMU	C4'-C5'-C6'-O6'
22	R	7022	LMU	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
22	A	7016	LMU	O5'-C1'-O1'-C1
22	E	7048	LMU	O5'-C1'-O1'-C1
22	H	7002	LMU	O5'-C1'-O1'-C1
22	H	7032	LMU	C5-C6-C7-C8
22	E	7037	LMU	C1-C2-C3-C4
19	2	2004	CLA	CBA-CGA-O2A-C1
19	2	2012	CLA	CBA-CGA-O2A-C1
19	4	4014	CLA	CBA-CGA-O2A-C1
24	B	7101	LMG	C29-C28-O8-C9
22	G	7039	LMU	C11-C10-C9-C8
22	H	7043	LMU	C7-C8-C9-C10
19	4	1306	CLA	O1D-CGD-O2D-CED
22	A	7010	LMU	C4B-C5B-C6B-O6B
22	A	7010	LMU	C3'-C4'-O1B-C1B
19	A	1133	CLA	O1D-CGD-O2D-CED
19	L	1503	CLA	O1D-CGD-O2D-CED
19	A	1128	CLA	O1A-CGA-O2A-C1
22	E	7037	LMU	C4'-C5'-C6'-O6'
22	4	7052	LMU	C4B-C5B-C6B-O6B
22	A	7044	LMU	C2-C3-C4-C5
22	4	7019	LMU	C7-C8-C9-C10
19	A	1136	CLA	O1D-CGD-O2D-CED
19	H	1207	CLA	O1D-CGD-O2D-CED
19	3	2009	CLA	O1D-CGD-O2D-CED
19	A	1141	CLA	CBD-CGD-O2D-CED
22	2	7031	LMU	C2-C3-C4-C5
22	A	7035	LMU	C4'-C5'-C6'-O6'
22	G	7051	LMU	C4B-C5B-C6B-O6B
19	2	2004	CLA	O1A-CGA-O2A-C1
19	2	2012	CLA	O1A-CGA-O2A-C1
19	4	4006	CLA	O1A-CGA-O2A-C1
19	4	4014	CLA	O1A-CGA-O2A-C1
19	B	1211	CLA	O1D-CGD-O2D-CED
19	A	1110	CLA	CBA-CGA-O2A-C1
19	A	1139	CLA	CBA-CGA-O2A-C1
19	A	1140	CLA	CBA-CGA-O2A-C1
19	K	1146	CLA	CBA-CGA-O2A-C1
19	L	1501	CLA	CBA-CGA-O2A-C1
19	1	1013	CLA	CBA-CGA-O2A-C1
19	2	2001	CLA	CBA-CGA-O2A-C1
19	4	1306	CLA	CBA-CGA-O2A-C1
19	A	1106	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	1	7013	LMU	C1-C2-C3-C4
19	A	1127	CLA	CBD-CGD-O2D-CED
22	H	7030	LMU	C4B-C5B-C6B-O6B
22	4	7019	LMU	C4B-C5B-C6B-O6B
19	B	1231	CLA	C2A-CAA-CBA-CGA
21	B	6020	BCR	C9-C10-C11-C12
21	F	6016	BCR	C15-C16-C17-C18
21	1	6023	BCR	C13-C14-C15-C16
19	B	1214	CLA	C10-C11-C12-C13
22	A	7044	LMU	C5'-C4'-O1B-C1B
19	A	9013	CLA	C8-C10-C11-C12
19	L	1130	CLA	C5-C6-C7-C8
22	4	7018	LMU	O5B-C5B-C6B-O6B
22	H	7017	LMU	C4B-C5B-C6B-O6B
22	H	7030	LMU	C4'-C5'-C6'-O6'
22	R	7024	LMU	C4'-C5'-C6'-O6'
22	2	7046	LMU	C4'-C5'-C6'-O6'
22	E	7048	LMU	C3'-C4'-O1B-C1B
22	3	7005	LMU	O1'-C1-C2-C3
22	3	7003	LMU	C4'-C5'-C6'-O6'
19	A	1138	CLA	C13-C15-C16-C17
19	B	1223	CLA	C15-C16-C17-C18
19	A	1116	CLA	C3-C5-C6-C7
22	H	7028	LMU	C2'-C1'-O1'-C1
22	H	7030	LMU	C2'-C1'-O1'-C1
22	H	7032	LMU	C2'-C1'-O1'-C1
22	H	7043	LMU	C2'-C1'-O1'-C1
22	2	7006	LMU	C2'-C1'-O1'-C1
22	2	7031	LMU	C2'-C1'-O1'-C1
22	4	7008	LMU	C2'-C1'-O1'-C1
19	2	2006	CLA	CBA-CGA-O2A-C1
19	A	1140	CLA	O1A-CGA-O2A-C1
22	A	7023	LMU	O5B-C5B-C6B-O6B
22	B	7012	LMU	O5'-C5'-C6'-O6'
22	L	7029	LMU	O5B-C5B-C6B-O6B
22	L	7029	LMU	O5'-C5'-C6'-O6'
22	H	7028	LMU	C4B-C5B-C6B-O6B
19	A	1115	CLA	C14-C13-C15-C16
19	A	1117	CLA	C6-C7-C8-C9
19	A	1123	CLA	C11-C10-C8-C9
19	A	1123	CLA	C14-C13-C15-C16
19	A	1132	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A	1138	CLA	C11-C10-C8-C9
19	A	1138	CLA	C14-C13-C15-C16
19	A	9013	CLA	C11-C10-C8-C9
19	A	9023	CLA	C14-C13-C15-C16
19	B	1206	CLA	C11-C10-C8-C9
19	B	1211	CLA	C14-C13-C15-C16
19	B	1220	CLA	C14-C13-C15-C16
19	B	1222	CLA	C11-C10-C8-C9
19	B	1224	CLA	C6-C7-C8-C9
19	B	1226	CLA	C11-C10-C8-C9
19	B	1229	CLA	C11-C10-C8-C9
19	B	1229	CLA	C14-C13-C15-C16
19	B	9010	CLA	C11-C12-C13-C14
19	J	1311	CLA	C11-C12-C13-C14
19	R	1150	CLA	C11-C10-C8-C9
19	R	1150	CLA	C11-C12-C13-C14
19	1	1014	CLA	C11-C12-C13-C14
19	3	2009	CLA	C6-C7-C8-C9
20	A	5001	PQN	C21-C22-C23-C24
19	A	1110	CLA	O1D-CGD-O2D-CED
19	A	9023	CLA	O1D-CGD-O2D-CED
19	2	2004	CLA	O1D-CGD-O2D-CED
19	3	3011	CLA	O1D-CGD-O2D-CED
19	G	1242	CLA	C2A-CAA-CBA-CGA
21	A	6003	BCR	C11-C12-C13-C35
21	A	6003	BCR	C37-C22-C23-C24
21	A	6007	BCR	C7-C8-C9-C34
21	A	6007	BCR	C11-C12-C13-C35
21	A	6008	BCR	C37-C22-C23-C24
21	B	6004	BCR	C37-C22-C23-C24
21	B	6006	BCR	C37-C22-C23-C24
21	B	6010	BCR	C36-C18-C19-C20
21	B	6017	BCR	C7-C8-C9-C34
21	F	6014	BCR	C37-C22-C23-C24
21	L	6019	BCR	C7-C8-C9-C34
21	3	6022	BCR	C11-C12-C13-C35
21	A	6003	BCR	C11-C12-C13-C14
21	A	6007	BCR	C7-C8-C9-C10
21	B	6004	BCR	C21-C22-C23-C24
21	B	6006	BCR	C21-C22-C23-C24
21	B	6017	BCR	C7-C8-C9-C10
21	B	6020	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	F	6014	BCR	C21-C22-C23-C24
21	J	6012	BCR	C21-C22-C23-C24
21	L	6019	BCR	C7-C8-C9-C10
21	L	6019	BCR	C21-C22-C23-C24
21	3	6022	BCR	C11-C12-C13-C14
21	3	6022	BCR	C21-C22-C23-C24
22	A	7023	LMU	O5'-C5'-C6'-O6'
22	H	7032	LMU	C4'-C5'-C6'-O6'
22	H	7043	LMU	C4B-C5B-C6B-O6B
19	A	1109	CLA	C5-C6-C7-C8
19	B	1224	CLA	C8-C10-C11-C12
19	J	1311	CLA	C8-C10-C11-C12
19	L	1130	CLA	C10-C11-C12-C13
20	B	5002	PQN	C15-C16-C17-C18
19	A	1140	CLA	O1D-CGD-O2D-CED
22	K	7042	LMU	C5-C6-C7-C8
22	C	7015	LMU	O5'-C5'-C6'-O6'
22	H	7017	LMU	O5'-C5'-C6'-O6'
22	R	7007	LMU	O5B-C5B-C6B-O6B
22	G	7039	LMU	C4'-C5'-C6'-O6'
22	H	7011	LMU	C4'-C5'-C6'-O6'
22	K	7042	LMU	C4'-C5'-C6'-O6'
22	R	7022	LMU	C4B-C5B-C6B-O6B
19	A	1107	CLA	C5-C6-C7-C8
19	A	1119	CLA	C10-C11-C12-C13
19	A	1140	CLA	C10-C11-C12-C13
19	A	9011	CLA	C10-C11-C12-C13
19	B	1206	CLA	C5-C6-C7-C8
19	B	1216	CLA	C10-C11-C12-C13
19	L	1130	CLA	C13-C15-C16-C17
19	1	1007	CLA	C8-C10-C11-C12
19	3	3016	CLA	C13-C15-C16-C17
19	4	4006	CLA	C5-C6-C7-C8
20	B	5002	PQN	C18-C20-C21-C22
20	B	5002	PQN	C20-C21-C22-C23
22	2	7027	LMU	C1-C2-C3-C4
19	A	9022	CLA	O1D-CGD-O2D-CED
22	4	7052	LMU	C5'-C4'-O1B-C1B
19	A	1126	CLA	C15-C16-C17-C18
19	A	1127	CLA	C5-C6-C7-C8
19	A	1138	CLA	C15-C16-C17-C18
19	A	1140	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	A	1237	CLA	C8-C10-C11-C12
19	A	9011	CLA	C5-C6-C7-C8
19	A	9023	CLA	C10-C11-C12-C13
19	B	1206	CLA	C10-C11-C12-C13
19	B	1206	CLA	C15-C16-C17-C18
19	B	1211	CLA	C5-C6-C7-C8
19	B	1214	CLA	C8-C10-C11-C12
19	B	1220	CLA	C13-C15-C16-C17
19	B	1229	CLA	C13-C15-C16-C17
19	B	1234	CLA	C5-C6-C7-C8
19	B	1235	CLA	C13-C15-C16-C17
19	B	1238	CLA	C10-C11-C12-C13
19	B	1239	CLA	C15-C16-C17-C18
19	H	1207	CLA	C8-C10-C11-C12
19	R	1150	CLA	C8-C10-C11-C12
22	N	7049	LMU	C4'-C5'-C6'-O6'
22	R	7007	LMU	C4B-C5B-C6B-O6B
19	A	1120	CLA	O1D-CGD-O2D-CED
19	A	1139	CLA	O1A-CGA-O2A-C1
19	4	1306	CLA	O1A-CGA-O2A-C1
22	R	7021	LMU	O5'-C5'-C6'-O6'
22	H	7028	LMU	O1'-C1-C2-C3
22	R	7025	LMU	O1'-C1-C2-C3
19	A	1117	CLA	C10-C11-C12-C13
19	A	1140	CLA	C5-C6-C7-C8
19	A	9023	CLA	C13-C15-C16-C17
19	B	1209	CLA	C5-C6-C7-C8
19	B	1229	CLA	C10-C11-C12-C13
19	B	1235	CLA	C8-C10-C11-C12
19	I	1204	CLA	C5-C6-C7-C8
19	I	1204	CLA	C8-C10-C11-C12
20	A	5001	PQN	C20-C21-C22-C23
19	B	1220	CLA	C3-C5-C6-C7
19	B	1226	CLA	C3-C5-C6-C7
22	3	7005	LMU	O5'-C5'-C6'-O6'
19	A	1103	CLA	C2-C1-O2A-CGA
19	A	1123	CLA	C2-C1-O2A-CGA
19	A	1124	CLA	C2-C1-O2A-CGA
19	A	1139	CLA	C2-C1-O2A-CGA
19	1	1007	CLA	C2-C1-O2A-CGA
19	B	1215	CLA	C10-C11-C12-C13
22	G	7026	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
19	B	1201	CLA	C2A-CAA-CBA-CGA
19	B	1218	CLA	O1A-CGA-O2A-C1
19	A	1104	CLA	C5-C6-C7-C8
19	A	1123	CLA	C10-C11-C12-C13
19	B	1226	CLA	C5-C6-C7-C8
22	H	7030	LMU	C2B-C1B-O1B-C4'
19	A	1106	CLA	C12-C13-C15-C16
19	A	1237	CLA	C11-C12-C13-C15
19	A	9011	CLA	C12-C13-C15-C16
19	A	9023	CLA	C6-C7-C8-C10
19	B	1211	CLA	C11-C10-C8-C7
19	B	1220	CLA	C11-C12-C13-C15
19	B	1224	CLA	C6-C7-C8-C10
19	B	1226	CLA	C11-C10-C8-C7
19	L	1130	CLA	C12-C13-C15-C16
19	2	2014	CLA	C11-C12-C13-C15
19	3	3011	CLA	C11-C10-C8-C7
19	4	1304	CLA	C12-C13-C15-C16
22	G	7026	LMU	C1-C2-C3-C4
19	A	9011	CLA	C3-C5-C6-C7
19	A	1110	CLA	O1A-CGA-O2A-C1
19	K	1146	CLA	O1A-CGA-O2A-C1
19	L	1501	CLA	O1A-CGA-O2A-C1
19	2	2001	CLA	O1A-CGA-O2A-C1
21	F	6016	BCR	C9-C10-C11-C12
21	L	6019	BCR	C15-C16-C17-C18
19	A	1122	CLA	C2A-CAA-CBA-CGA
19	A	1124	CLA	C2A-CAA-CBA-CGA
19	B	1226	CLA	C2A-CAA-CBA-CGA
19	B	1215	CLA	O1D-CGD-O2D-CED
19	A	9023	CLA	C15-C16-C17-C18
19	B	1205	CLA	C8-C10-C11-C12
19	B	1210	CLA	C15-C16-C17-C18
19	B	1222	CLA	C5-C6-C7-C8
19	3	3011	CLA	C8-C10-C11-C12
22	1	7013	LMU	O1'-C1-C2-C3
22	A	7016	LMU	C4-C5-C6-C7
22	A	7023	LMU	O1'-C1-C2-C3
22	H	7032	LMU	O1'-C1-C2-C3
19	B	1221	CLA	CBD-CGD-O2D-CED
22	H	7030	LMU	O5'-C1'-O1'-C1
22	R	7025	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
19	A	1141	CLA	C5-C6-C7-C8
19	B	1219	CLA	C5-C6-C7-C8
22	2	7046	LMU	O1'-C1-C2-C3
21	A	6008	BCR	C10-C11-C12-C13
21	B	6006	BCR	C10-C11-C12-C13
21	B	6010	BCR	C10-C11-C12-C13
21	B	6020	BCR	C10-C11-C12-C13
21	I	6018	BCR	C10-C11-C12-C13
22	R	7025	LMU	C6-C7-C8-C9
19	A	1132	CLA	C3-C5-C6-C7
19	A	9013	CLA	C15-C16-C17-C18
19	B	1202	CLA	C15-C16-C17-C18
19	B	1225	CLA	C10-C11-C12-C13
19	R	1150	CLA	C10-C11-C12-C13
19	2	4009	CLA	C10-C11-C12-C13
19	3	3016	CLA	C5-C6-C7-C8
19	4	1304	CLA	C8-C10-C11-C12
19	1	1013	CLA	O1A-CGA-O2A-C1
19	2	2006	CLA	O1A-CGA-O2A-C1
19	3	1147	CLA	CBA-CGA-O2A-C1
22	K	7042	LMU	O1'-C1-C2-C3
22	R	7007	LMU	C3'-C4'-O1B-C1B
19	A	1109	CLA	C10-C11-C12-C13
19	A	1117	CLA	C5-C6-C7-C8
19	A	1117	CLA	C15-C16-C17-C18
19	A	1132	CLA	C8-C10-C11-C12
19	B	1226	CLA	C15-C16-C17-C18
19	1	1014	CLA	C10-C11-C12-C13
22	H	7043	LMU	C6-C7-C8-C9
19	B	1228	CLA	O1D-CGD-O2D-CED
22	A	7010	LMU	C5'-C4'-O1B-C1B
19	A	1131	CLA	C15-C16-C17-C18
19	A	1136	CLA	C5-C6-C7-C8
19	A	1237	CLA	C15-C16-C17-C18
19	A	9022	CLA	C13-C15-C16-C17
19	B	1205	CLA	C15-C16-C17-C18
19	B	1206	CLA	C8-C10-C11-C12
19	B	1210	CLA	C10-C11-C12-C13
19	B	1211	CLA	C10-C11-C12-C13
19	2	4009	CLA	C8-C10-C11-C12
19	A	1109	CLA	C3-C5-C6-C7
22	1	7004	LMU	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
22	2	7006	LMU	O1'-C1-C2-C3
22	4	7033	LMU	O1'-C1-C2-C3
22	N	7049	LMU	C1-C2-C3-C4
19	A	1125	CLA	CBA-CGA-O2A-C1
19	B	1215	CLA	CBA-CGA-O2A-C1
19	G	1242	CLA	CBA-CGA-O2A-C1
19	A	1119	CLA	C5-C6-C7-C8
19	A	1123	CLA	C15-C16-C17-C18
19	A	9013	CLA	C10-C11-C12-C13
19	2	4009	CLA	C5-C6-C7-C8
19	R	1150	CLA	O1D-CGD-O2D-CED
19	4	4002	CLA	O1D-CGD-O2D-CED
19	R	1144	CLA	C8-C10-C11-C12
19	B	1239	CLA	O1D-CGD-O2D-CED
19	3	3011	CLA	C2-C3-C5-C6
22	A	7016	LMU	C11-C10-C9-C8
22	4	7009	LMU	C5'-C4'-O1B-C1B
19	A	1110	CLA	C2A-CAA-CBA-CGA
19	B	1222	CLA	C2A-CAA-CBA-CGA
19	B	1223	CLA	C2A-CAA-CBA-CGA
19	A	1109	CLA	C16-C17-C18-C19
19	A	1136	CLA	C16-C17-C18-C19
20	B	5002	PQN	C26-C27-C28-C30
19	B	1221	CLA	C3-C5-C6-C7
19	4	4006	CLA	C3-C5-C6-C7
19	3	3016	CLA	O1D-CGD-O2D-CED
19	2	2014	CLA	CBA-CGA-O2A-C1
20	A	5001	PQN	C25-C26-C27-C28
22	K	7001	LMU	O5'-C5'-C6'-O6'
22	4	7052	LMU	O1'-C1-C2-C3
19	B	1211	CLA	C13-C15-C16-C17
22	R	7024	LMU	O1'-C1-C2-C3
21	A	6011	BCR	C19-C20-C21-C22
21	F	6016	BCR	C13-C14-C15-C16
21	I	6018	BCR	C9-C10-C11-C12
21	1	6023	BCR	C19-C20-C21-C22
22	3	7005	LMU	C7-C8-C9-C10
24	B	7101	LMG	C33-C34-C35-C36
19	A	9012	CLA	C13-C15-C16-C17
19	4	1304	CLA	C5-C6-C7-C8
21	A	6003	BCR	C11-C10-C9-C34
21	B	6004	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
21	B	6005	BCR	C20-C21-C22-C37
21	B	6006	BCR	C20-C21-C22-C37
21	B	6010	BCR	C11-C10-C9-C34
21	B	6020	BCR	C20-C21-C22-C37
21	F	6016	BCR	C20-C21-C22-C37
21	I	6021	BCR	C20-C21-C22-C37
21	3	6022	BCR	C11-C10-C9-C34
22	F	7036	LMU	O5'-C5'-C6'-O6'
22	A	7035	LMU	C6-C7-C8-C9
22	C	7015	LMU	C7-C8-C9-C10
22	C	7015	LMU	C11-C10-C9-C8
22	E	7048	LMU	C2-C3-C4-C5
22	2	7046	LMU	C6-C7-C8-C9
22	3	7003	LMU	C4-C5-C6-C7
22	4	7008	LMU	C3-C4-C5-C6
22	D	7050	LMU	C4'-C5'-C6'-O6'
19	B	1209	CLA	O1D-CGD-O2D-CED
19	A	1237	CLA	C16-C17-C18-C20
19	H	1145	CLA	C16-C17-C18-C19
19	I	1204	CLA	C11-C12-C13-C14
19	3	3011	CLA	C16-C17-C18-C19
20	A	5001	PQN	C26-C27-C28-C30
19	1	1003	CLA	CBA-CGA-O2A-C1
22	H	7032	LMU	C4-C5-C6-C7
22	K	7041	LMU	C4-C5-C6-C7
22	R	7024	LMU	C2-C3-C4-C5
22	1	7013	LMU	C5-C6-C7-C8
22	2	7031	LMU	C3-C4-C5-C6
22	4	7034	LMU	C3-C4-C5-C6
22	4	7052	LMU	C3-C4-C5-C6
19	B	1236	CLA	O1D-CGD-O2D-CED
19	A	1131	CLA	C13-C15-C16-C17
19	3	3013	CLA	C5-C6-C7-C8
19	A	1111	CLA	C5-C6-C7-C8
22	K	7042	LMU	C6-C7-C8-C9
22	N	7049	LMU	C11-C10-C9-C8
22	R	7014	LMU	C2-C3-C4-C5
22	4	7019	LMU	C3-C4-C5-C6
19	A	1119	CLA	O1D-CGD-O2D-CED
19	B	1215	CLA	O1A-CGA-O2A-C1
22	A	7044	LMU	O5'-C5'-C6'-O6'
22	C	7015	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	D	7050	LMU	C6-C7-C8-C9
22	H	7030	LMU	C4-C5-C6-C7
22	3	7005	LMU	C5-C6-C7-C8
19	H	1145	CLA	C8-C10-C11-C12
22	A	7044	LMU	C5-C6-C7-C8
22	B	7038	LMU	O1'-C1-C2-C3
22	H	7011	LMU	O1'-C1-C2-C3
22	N	7049	LMU	C7-C8-C9-C10
22	1	7013	LMU	C3-C4-C5-C6
19	A	1124	CLA	C3-C5-C6-C7
19	4	1004	CLA	C3-C5-C6-C7
19	2	2007	CLA	CBD-CGD-O2D-CED
19	2	2012	CLA	CBD-CGD-O2D-CED
21	A	6003	BCR	C11-C10-C9-C8
21	B	6004	BCR	C11-C10-C9-C8
21	B	6006	BCR	C20-C21-C22-C23
21	B	6010	BCR	C11-C10-C9-C8
21	B	6020	BCR	C20-C21-C22-C23
21	I	6021	BCR	C20-C21-C22-C23
21	L	6019	BCR	C20-C21-C22-C23
21	3	6022	BCR	C11-C10-C9-C8
22	A	7035	LMU	C2'-C1'-O1'-C1
22	N	7049	LMU	C2'-C1'-O1'-C1
22	3	7005	LMU	C2'-C1'-O1'-C1
19	A	1135	CLA	CBA-CGA-O2A-C1
22	A	7045	LMU	C6-C7-C8-C9
22	G	7026	LMU	C3-C4-C5-C6
22	2	7027	LMU	C2-C3-C4-C5
24	B	7101	LMG	C32-C33-C34-C35
19	B	1203	CLA	C13-C15-C16-C17
19	B	1210	CLA	C5-C6-C7-C8
19	H	1505	CLA	C5-C6-C7-C8
19	A	1127	CLA	C6-C7-C8-C9
19	B	1234	CLA	C11-C12-C13-C14
19	B	1235	CLA	C16-C17-C18-C19
19	B	1238	CLA	C16-C17-C18-C19
19	H	1207	CLA	C16-C17-C18-C20
19	2	2007	CLA	C16-C17-C18-C20
19	3	3016	CLA	C16-C17-C18-C20
19	4	4006	CLA	C6-C7-C8-C9
22	A	7010	LMU	O5B-C5B-C6B-O6B
22	H	7002	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
19	A	1131	CLA	C4-C3-C5-C6
19	B	1205	CLA	C4-C3-C5-C6
22	A	7010	LMU	C5-C6-C7-C8
22	K	7042	LMU	C4-C5-C6-C7
22	1	7004	LMU	C5-C6-C7-C8
22	1	7013	LMU	C6-C7-C8-C9
22	2	7006	LMU	C7-C8-C9-C10
24	B	7101	LMG	C35-C36-C37-C38
19	A	1106	CLA	C11-C12-C13-C14
19	A	1109	CLA	C6-C7-C8-C9
19	A	1119	CLA	C14-C13-C15-C16
19	A	1124	CLA	C11-C12-C13-C14
19	A	1125	CLA	C14-C13-C15-C16
19	A	1141	CLA	C14-C13-C15-C16
19	A	9012	CLA	C11-C12-C13-C14
19	B	1205	CLA	C14-C13-C15-C16
19	B	1210	CLA	C6-C7-C8-C9
19	B	1235	CLA	C11-C12-C13-C14
19	A	1134	CLA	O1D-CGD-O2D-CED
19	B	1221	CLA	C5-C6-C7-C8
22	A	7045	LMU	C11-C10-C9-C8
22	4	7018	LMU	C7-C8-C9-C10
19	A	1103	CLA	C13-C15-C16-C17
19	R	1150	CLA	C5-C6-C7-C8
19	A	1123	CLA	C2A-CAA-CBA-CGA
19	A	1129	CLA	C2A-CAA-CBA-CGA
19	B	1228	CLA	C2A-CAA-CBA-CGA
19	J	1308	CLA	C2A-CAA-CBA-CGA
19	K	1146	CLA	C2A-CAA-CBA-CGA
19	1	1013	CLA	C2A-CAA-CBA-CGA
19	3	3013	CLA	C2A-CAA-CBA-CGA
19	A	1125	CLA	O1A-CGA-O2A-C1
21	A	6007	BCR	C36-C18-C19-C20
21	B	6010	BCR	C37-C22-C23-C24
21	L	6019	BCR	C37-C22-C23-C24
22	L	7029	LMU	C11-C10-C9-C8
22	R	7007	LMU	C2-C3-C4-C5
21	A	6007	BCR	C17-C18-C19-C20
21	A	6008	BCR	C21-C22-C23-C24
19	A	1111	CLA	C3-C5-C6-C7
22	F	7036	LMU	O5B-C5B-C6B-O6B
19	A	1119	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	A	1128	CLA	C13-C15-C16-C17
19	A	9011	CLA	C8-C10-C11-C12
22	K	7047	LMU	C6-C7-C8-C9
22	4	7034	LMU	C2-C3-C4-C5
24	B	7101	LMG	C37-C38-C39-C40
22	L	7029	LMU	O5B-C1B-O1B-C4'
19	A	1110	CLA	C5-C6-C7-C8
22	A	7023	LMU	C3-C4-C5-C6
22	A	7035	LMU	C11-C10-C9-C8
22	E	7037	LMU	C7-C8-C9-C10
22	E	7037	LMU	C11-C10-C9-C8
22	H	7017	LMU	C11-C10-C9-C8
22	H	7028	LMU	C2-C3-C4-C5
22	H	7032	LMU	C7-C8-C9-C10
22	K	7001	LMU	C6-C7-C8-C9
22	K	7001	LMU	C7-C8-C9-C10
22	4	7009	LMU	C6-C7-C8-C9
22	4	7018	LMU	C4-C5-C6-C7
22	4	7034	LMU	C4-C5-C6-C7
19	A	1106	CLA	C16-C17-C18-C19
19	A	1124	CLA	C16-C17-C18-C19
19	A	1128	CLA	C16-C17-C18-C19
19	A	1237	CLA	C16-C17-C18-C19
19	A	9012	CLA	C16-C17-C18-C19
19	A	9012	CLA	C16-C17-C18-C20
19	B	1211	CLA	C16-C17-C18-C19
19	B	1229	CLA	C16-C17-C18-C20
19	I	1204	CLA	C11-C12-C13-C15
19	3	3011	CLA	C16-C17-C18-C20
22	N	7049	LMU	O5'-C1'-O1'-C1
19	B	1223	CLA	C8-C10-C11-C12
22	G	7051	LMU	C6-C7-C8-C9
22	H	7017	LMU	C6-C7-C8-C9
22	H	7032	LMU	C5'-C4'-O1B-C1B
22	R	7007	LMU	C11-C10-C9-C8
22	4	7019	LMU	C6-C7-C8-C9
22	4	7052	LMU	C5-C6-C7-C8
22	R	7020	LMU	C1-C2-C3-C4
22	R	7024	LMU	C1-C2-C3-C4
19	A	9013	CLA	O1D-CGD-O2D-CED
22	A	7010	LMU	C4-C5-C6-C7
22	A	7035	LMU	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	A	7035	LMU	C7-C8-C9-C10
22	H	7028	LMU	C6-C7-C8-C9
22	K	7001	LMU	C11-C10-C9-C8
22	2	7027	LMU	C4-C5-C6-C7
22	3	7003	LMU	C11-C10-C9-C8
22	4	7018	LMU	C2-C3-C4-C5
24	B	7101	LMG	C11-C12-C13-C14
22	4	7052	LMU	C2B-C1B-O1B-C4'
19	B	9010	CLA	C10-C11-C12-C13
20	B	5002	PQN	C23-C25-C26-C27
22	G	7026	LMU	C6-C7-C8-C9
22	4	7033	LMU	C6-C7-C8-C9
24	B	7101	LMG	C40-C41-C42-C43
19	A	1110	CLA	C3-C5-C6-C7
22	B	7040	LMU	O5B-C5B-C6B-O6B
19	A	1123	CLA	CBA-CGA-O2A-C1
19	A	1104	CLA	C3A-C2A-CAA-CBA
19	A	1107	CLA	C3A-C2A-CAA-CBA
19	A	1111	CLA	C3A-C2A-CAA-CBA
19	A	1112	CLA	C3A-C2A-CAA-CBA
19	A	1113	CLA	C3A-C2A-CAA-CBA
19	A	1125	CLA	C3A-C2A-CAA-CBA
19	A	1132	CLA	C3A-C2A-CAA-CBA
19	A	1139	CLA	C3A-C2A-CAA-CBA
19	B	1206	CLA	C3A-C2A-CAA-CBA
19	B	1210	CLA	C3A-C2A-CAA-CBA
19	B	1212	CLA	C3A-C2A-CAA-CBA
19	B	1213	CLA	C3A-C2A-CAA-CBA
19	F	1305	CLA	C3A-C2A-CAA-CBA
19	L	1130	CLA	C3A-C2A-CAA-CBA
19	L	1148	CLA	C3A-C2A-CAA-CBA
19	L	1502	CLA	C3A-C2A-CAA-CBA
19	R	1144	CLA	C3A-C2A-CAA-CBA
19	1	1003	CLA	C3A-C2A-CAA-CBA
19	1	1007	CLA	C3A-C2A-CAA-CBA
19	2	2006	CLA	C3A-C2A-CAA-CBA
19	2	4009	CLA	C3A-C2A-CAA-CBA
19	3	2009	CLA	C3A-C2A-CAA-CBA
19	4	4006	CLA	C3A-C2A-CAA-CBA
19	B	1203	CLA	C10-C11-C12-C13
21	A	6003	BCR	C9-C10-C11-C12
22	H	7002	LMU	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
22	H	7011	LMU	C1-C2-C3-C4
22	R	7021	LMU	C1-C2-C3-C4
22	A	7044	LMU	C2-C1-O1'-C1'
22	2	7031	LMU	C2-C1-O1'-C1'
22	3	7003	LMU	C2-C1-O1'-C1'
22	A	7016	LMU	C5-C6-C7-C8
22	L	7029	LMU	C7-C8-C9-C10
22	N	7049	LMU	C5-C6-C7-C8
24	B	7101	LMG	C17-C18-C19-C20
19	A	1109	CLA	C16-C17-C18-C20
19	A	1128	CLA	C16-C17-C18-C20
19	H	1145	CLA	C16-C17-C18-C20
19	L	1148	CLA	C6-C7-C8-C9
19	4	4006	CLA	C6-C7-C8-C10
22	A	7045	LMU	C2-C3-C4-C5
22	G	7039	LMU	C5-C6-C7-C8
22	4	7052	LMU	O5'-C5'-C6'-O6'
22	G	7051	LMU	C1-C2-C3-C4
22	R	7014	LMU	C11-C10-C9-C8
22	2	7046	LMU	C2-C3-C4-C5
22	4	7008	LMU	C4-C5-C6-C7
19	A	1237	CLA	O2A-C1-C2-C3
22	N	7049	LMU	C6-C7-C8-C9
22	1	7004	LMU	C11-C10-C9-C8
22	2	7046	LMU	C4-C5-C6-C7
19	B	1216	CLA	C5-C6-C7-C8
19	B	1225	CLA	C5-C6-C7-C8
19	F	1305	CLA	C4-C3-C5-C6
19	L	1148	CLA	C4-C3-C5-C6
19	B	1205	CLA	C2-C3-C5-C6
19	F	1305	CLA	C2-C3-C5-C6
22	A	7016	LMU	C6-C7-C8-C9
22	F	7036	LMU	C11-C10-C9-C8
22	F	7036	LMU	C4'-C5'-C6'-O6'
22	A	7045	LMU	C5-C6-C7-C8
22	H	7017	LMU	C7-C8-C9-C10
22	H	7032	LMU	C3'-C4'-O1B-C1B
22	R	7007	LMU	C5'-C4'-O1B-C1B
22	4	7008	LMU	C5-C6-C7-C8
19	G	1242	CLA	O1A-CGA-O2A-C1
22	K	7042	LMU	O5'-C5'-C6'-O6'
22	A	7010	LMU	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	R	7021	LMU	O1'-C1-C2-C3
22	B	7040	LMU	C1-C2-C3-C4
22	D	7050	LMU	C4B-C5B-C6B-O6B
19	B	1202	CLA	C10-C11-C12-C13
22	A	7023	LMU	C4-C5-C6-C7
22	A	7045	LMU	O1'-C1-C2-C3
22	H	7030	LMU	O5B-C1B-O1B-C4'
22	E	7037	LMU	O5B-C5B-C6B-O6B
22	1	7013	LMU	O5'-C5'-C6'-O6'
22	A	7010	LMU	C1-C2-C3-C4
19	L	1148	CLA	CBA-CGA-O2A-C1
22	A	7044	LMU	C11-C10-C9-C8
22	B	7038	LMU	C11-C10-C9-C8
22	F	7036	LMU	C2-C3-C4-C5
22	H	7028	LMU	C7-C8-C9-C10
22	K	7047	LMU	C2-C3-C4-C5
19	2	2014	CLA	O1A-CGA-O2A-C1
19	A	1119	CLA	C8-C10-C11-C12
19	B	9010	CLA	C5-C6-C7-C8
22	4	7009	LMU	C1-C2-C3-C4
19	A	9022	CLA	C2-C1-O2A-CGA
19	B	1229	CLA	C2-C1-O2A-CGA
19	3	3013	CLA	C2-C1-O2A-CGA
22	R	7014	LMU	C4B-C5B-C6B-O6B
22	G	7039	LMU	C2-C3-C4-C5
22	K	7041	LMU	C3-C4-C5-C6
22	K	7042	LMU	C11-C10-C9-C8
22	N	7049	LMU	C2-C3-C4-C5
22	4	7033	LMU	C11-C10-C9-C8
24	B	7101	LMG	C15-C16-C17-C18
19	A	1132	CLA	C13-C15-C16-C17
19	B	1203	CLA	C8-C10-C11-C12
19	J	1308	CLA	C5-C6-C7-C8
19	A	1135	CLA	O1A-CGA-O2A-C1
19	1	1003	CLA	O1A-CGA-O2A-C1
22	2	7046	LMU	C1-C2-C3-C4
22	4	7008	LMU	C1-C2-C3-C4
22	B	7040	LMU	C11-C10-C9-C8
22	2	7031	LMU	C5-C6-C7-C8
22	4	7052	LMU	C3'-C4'-O1B-C1B
19	A	1127	CLA	C6-C7-C8-C10
19	B	1234	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	B	1211	CLA	C3-C5-C6-C7
19	H	1145	CLA	C3-C5-C6-C7
19	2	2006	CLA	C3-C5-C6-C7
21	A	6002	BCR	C23-C24-C25-C26
21	A	6002	BCR	C23-C24-C25-C30
21	A	6003	BCR	C1-C6-C7-C8
21	A	6007	BCR	C1-C6-C7-C8
21	A	6007	BCR	C5-C6-C7-C8
21	A	6008	BCR	C1-C6-C7-C8
21	A	6008	BCR	C23-C24-C25-C26
21	A	6008	BCR	C23-C24-C25-C30
21	A	6011	BCR	C1-C6-C7-C8
21	A	6011	BCR	C5-C6-C7-C8
21	A	6011	BCR	C23-C24-C25-C26
21	A	6011	BCR	C23-C24-C25-C30
21	B	6005	BCR	C1-C6-C7-C8
21	B	6010	BCR	C1-C6-C7-C8
21	B	6010	BCR	C5-C6-C7-C8
21	B	6017	BCR	C1-C6-C7-C8
21	B	6017	BCR	C23-C24-C25-C26
21	F	6014	BCR	C1-C6-C7-C8
21	F	6014	BCR	C5-C6-C7-C8
21	F	6014	BCR	C23-C24-C25-C26
21	F	6014	BCR	C23-C24-C25-C30
21	I	6018	BCR	C1-C6-C7-C8
21	I	6018	BCR	C5-C6-C7-C8
21	J	6012	BCR	C1-C6-C7-C8
21	J	6012	BCR	C5-C6-C7-C8
21	L	6019	BCR	C5-C6-C7-C8
21	1	6023	BCR	C23-C24-C25-C26
22	A	7016	LMU	O1'-C1-C2-C3
22	1	7004	LMU	C7-C8-C9-C10
19	B	1223	CLA	CBA-CGA-O2A-C1
19	B	1238	CLA	C8-C10-C11-C12
19	K	3009	CLA	C13-C15-C16-C17
19	4	1306	CLA	C5-C6-C7-C8
22	A	7010	LMU	C6-C7-C8-C9
22	A	7044	LMU	C3-C4-C5-C6
22	H	7017	LMU	C4-C5-C6-C7
22	H	7028	LMU	C5-C6-C7-C8
22	R	7021	LMU	C7-C8-C9-C10
19	J	1311	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	2	7027	LMU	C7-C8-C9-C10
22	4	7018	LMU	C11-C10-C9-C8
22	4	7053	LMU	C11-C10-C9-C8
19	A	1106	CLA	C6-C7-C8-C10
19	A	1106	CLA	C11-C12-C13-C15
19	A	1109	CLA	C6-C7-C8-C10
19	A	1109	CLA	C12-C13-C15-C16
19	A	1119	CLA	C12-C13-C15-C16
19	A	1123	CLA	C11-C10-C8-C7
19	A	1123	CLA	C12-C13-C15-C16
19	A	1124	CLA	C11-C12-C13-C15
19	A	1125	CLA	C2-C3-C5-C6
19	A	1131	CLA	C2-C3-C5-C6
19	A	1141	CLA	C12-C13-C15-C16
19	A	9012	CLA	C11-C12-C13-C15
19	B	1203	CLA	C11-C10-C8-C7
19	B	1203	CLA	C11-C12-C13-C15
19	B	1210	CLA	C6-C7-C8-C10
19	B	1210	CLA	C12-C13-C15-C16
19	B	1211	CLA	C12-C13-C15-C16
19	B	1224	CLA	C11-C10-C8-C7
19	B	1229	CLA	C11-C12-C13-C15
19	B	1229	CLA	C12-C13-C15-C16
19	B	9010	CLA	C6-C7-C8-C10
19	J	1311	CLA	C6-C7-C8-C10
19	L	1148	CLA	C2-C3-C5-C6
19	R	1150	CLA	C6-C7-C8-C10
19	R	1150	CLA	C11-C12-C13-C15
19	1	1014	CLA	C6-C7-C8-C10
19	3	2009	CLA	C6-C7-C8-C10
20	B	5002	PQN	C21-C22-C23-C25
19	A	1123	CLA	O1A-CGA-O2A-C1
22	A	7023	LMU	C7-C8-C9-C10
22	H	7011	LMU	C5'-C4'-O1B-C1B
22	L	7029	LMU	C6-C7-C8-C9
22	N	7049	LMU	C3'-C4'-O1B-C1B
22	1	7004	LMU	C2-C3-C4-C5
19	A	1115	CLA	C5-C6-C7-C8
19	A	1128	CLA	C8-C10-C11-C12
19	B	1203	CLA	C15-C16-C17-C18
21	B	6005	BCR	C19-C20-C21-C22
21	B	6017	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
19	H	1207	CLA	C16-C17-C18-C19
19	A	1109	CLA	CBA-CGA-O2A-C1
19	B	1202	CLA	CBA-CGA-O2A-C1
19	B	1210	CLA	CBA-CGA-O2A-C1
19	B	1226	CLA	CBA-CGA-O2A-C1
19	L	1504	CLA	CBA-CGA-O2A-C1
22	R	7007	LMU	C9-C10-C11-C12
22	R	7022	LMU	O1'-C1-C2-C3
22	2	7006	LMU	C5-C6-C7-C8
22	R	7007	LMU	C1-C2-C3-C4
19	A	1135	CLA	C2A-CAA-CBA-CGA
19	A	1140	CLA	C2A-CAA-CBA-CGA
19	4	1004	CLA	C2A-CAA-CBA-CGA
19	B	1226	CLA	C8-C10-C11-C12
22	K	7042	LMU	C9-C10-C11-C12
19	2	2014	CLA	C12-C13-C15-C16
19	A	1103	CLA	C15-C16-C17-C18
19	A	9012	CLA	C15-C16-C17-C18
19	3	3016	CLA	C8-C10-C11-C12
22	2	7006	LMU	C2-C3-C4-C5
22	4	7034	LMU	C11-C10-C9-C8
22	E	7048	LMU	C5'-C4'-O1B-C1B
22	D	7050	LMU	O5'-C5'-C6'-O6'
19	2	2007	CLA	C16-C17-C18-C19
22	H	7017	LMU	C4'-C5'-C6'-O6'
19	A	9013	CLA	C13-C15-C16-C17
19	H	1145	CLA	C15-C16-C17-C18
22	K	7001	LMU	C1-C2-C3-C4
22	4	7009	LMU	C5-C6-C7-C8
21	B	6017	BCR	C18-C19-C20-C21
21	3	6022	BCR	C10-C11-C12-C13
22	R	7025	LMU	C3-C4-C5-C6
19	A	1123	CLA	C5-C6-C7-C8
19	B	1216	CLA	C8-C10-C11-C12
19	B	1224	CLA	C10-C11-C12-C13
19	A	1137	CLA	CBD-CGD-O2D-CED
22	4	7009	LMU	C3'-C4'-O1B-C1B
22	C	7015	LMU	C5-C6-C7-C8
22	R	7025	LMU	C4-C5-C6-C7
22	L	7029	LMU	C2'-C1'-O1'-C1
22	2	7027	LMU	C2'-C1'-O1'-C1
22	A	7044	LMU	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	R	7024	LMU	C7-C8-C9-C10
22	2	7046	LMU	C11-C10-C9-C8
22	3	7005	LMU	C6-C7-C8-C9
19	B	1223	CLA	O1A-CGA-O2A-C1
19	B	1238	CLA	C16-C17-C18-C20
19	3	3016	CLA	C16-C17-C18-C19
19	4	1306	CLA	C6-C7-C8-C10
22	A	7045	LMU	C7-C8-C9-C10
22	L	7029	LMU	C2-C3-C4-C5
22	2	7046	LMU	C7-C8-C9-C10
22	4	7033	LMU	C5'-C4'-O1B-C1B
22	B	7040	LMU	O5'-C5'-C6'-O6'
19	A	1125	CLA	C8-C10-C11-C12
19	A	1125	CLA	C4-C3-C5-C6
19	1	1007	CLA	C4-C3-C5-C6
19	B	1211	CLA	C2-C3-C5-C6
22	G	7026	LMU	C2-C3-C4-C5
22	G	7051	LMU	C7-C8-C9-C10
19	A	1103	CLA	C11-C10-C8-C9
19	A	1109	CLA	C11-C12-C13-C14
19	A	1109	CLA	C14-C13-C15-C16
19	A	1123	CLA	C11-C12-C13-C14
19	A	1125	CLA	C6-C7-C8-C9
19	A	1237	CLA	C11-C10-C8-C9
19	A	1237	CLA	C11-C12-C13-C14
19	A	9023	CLA	C6-C7-C8-C9
19	B	1203	CLA	C11-C10-C8-C9
19	B	1203	CLA	C11-C12-C13-C14
19	B	1210	CLA	C14-C13-C15-C16
19	B	1220	CLA	C11-C12-C13-C14
19	B	1224	CLA	C11-C10-C8-C9
19	B	1229	CLA	C11-C12-C13-C14
19	B	9010	CLA	C11-C10-C8-C9
19	K	3009	CLA	C14-C13-C15-C16
19	L	1130	CLA	C14-C13-C15-C16
19	2	2007	CLA	C14-C13-C15-C16
19	3	3016	CLA	C11-C10-C8-C9
19	4	1304	CLA	C14-C13-C15-C16
20	B	5002	PQN	C21-C22-C23-C24
19	A	1141	CLA	O1D-CGD-O2D-CED
22	4	7052	LMU	C6-C7-C8-C9
19	A	1106	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	L	1502	CLA	C2A-CAA-CBA-CGA
22	L	7029	LMU	C1-C2-C3-C4
22	B	7038	LMU	C3-C4-C5-C6
22	H	7002	LMU	C6-C7-C8-C9
22	1	7004	LMU	C3-C4-C5-C6
22	B	7038	LMU	O5'-C5'-C6'-O6'
22	R	7020	LMU	O5'-C5'-C6'-O6'
19	B	1208	CLA	C5-C6-C7-C8
19	B	1235	CLA	C15-C16-C17-C18
22	A	7045	LMU	C3-C4-C5-C6
22	4	7009	LMU	C2-C3-C4-C5
24	B	7101	LMG	C13-C14-C15-C16
21	B	6004	BCR	C11-C12-C13-C14
19	B	1226	CLA	O1A-CGA-O2A-C1
19	A	1101	CLA	C1A-C2A-CAA-CBA
19	A	1102	CLA	C1A-C2A-CAA-CBA
19	A	1111	CLA	C1A-C2A-CAA-CBA
19	A	1125	CLA	C1A-C2A-CAA-CBA
19	A	1134	CLA	C1A-C2A-CAA-CBA
19	A	1151	CLA	C1A-C2A-CAA-CBA
19	A	9011	CLA	C1A-C2A-CAA-CBA
19	A	9022	CLA	C1A-C2A-CAA-CBA
19	B	1212	CLA	C1A-C2A-CAA-CBA
19	B	1213	CLA	C1A-C2A-CAA-CBA
19	B	1224	CLA	C1A-C2A-CAA-CBA
19	B	1233	CLA	C1A-C2A-CAA-CBA
19	B	1236	CLA	C1A-C2A-CAA-CBA
19	B	1239	CLA	C1A-C2A-CAA-CBA
19	J	1311	CLA	C1A-C2A-CAA-CBA
19	K	3009	CLA	C1A-C2A-CAA-CBA
19	1	1003	CLA	C1A-C2A-CAA-CBA
19	1	1303	CLA	C1A-C2A-CAA-CBA
19	2	4009	CLA	C1A-C2A-CAA-CBA
19	4	1304	CLA	C1A-C2A-CAA-CBA
19	4	4006	CLA	C1A-C2A-CAA-CBA
19	4	4014	CLA	C1A-C2A-CAA-CBA
19	A	1117	CLA	C16-C17-C18-C19
19	B	1211	CLA	C16-C17-C18-C20
19	B	1229	CLA	C16-C17-C18-C19
22	A	7016	LMU	C7-C8-C9-C10
21	A	6007	BCR	C19-C20-C21-C22
19	3	3013	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	A	7016	LMU	C1-C2-C3-C4
22	B	7038	LMU	C5-C6-C7-C8
22	R	7025	LMU	C9-C10-C11-C12
22	2	7031	LMU	O5'-C5'-C6'-O6'
19	A	1106	CLA	C3-C5-C6-C7
19	B	1210	CLA	O1A-CGA-O2A-C1
19	A	1109	CLA	C8-C10-C11-C12
19	B	1238	CLA	CBA-CGA-O2A-C1
22	B	7040	LMU	C4-C5-C6-C7
22	G	7039	LMU	C1-C2-C3-C4
22	4	7053	LMU	C1-C2-C3-C4
22	R	7025	LMU	O5'-C5'-C6'-O6'
22	3	7005	LMU	O5B-C5B-C6B-O6B
19	A	1136	CLA	C16-C17-C18-C20
19	3	3013	CLA	C16-C17-C18-C20
22	A	7023	LMU	C2-C3-C4-C5
22	H	7032	LMU	C11-C10-C9-C8
22	4	7034	LMU	C1-C2-C3-C4
22	K	7041	LMU	C6-C7-C8-C9
22	K	7047	LMU	C7-C8-C9-C10
22	A	7023	LMU	C4'-C5'-C6'-O6'
19	A	1132	CLA	CBA-CGA-O2A-C1
22	K	7047	LMU	O5B-C5B-C6B-O6B
19	B	1211	CLA	C4-C3-C5-C6
19	3	3007	CLA	C3A-C2A-CAA-CBA
22	B	7040	LMU	C5'-C4'-O1B-C1B
19	B	1211	CLA	C8-C10-C11-C12
19	B	1239	CLA	C10-C11-C12-C13
22	H	7002	LMU	C11-C10-C9-C8
22	R	7020	LMU	C11-C10-C9-C8
19	L	1148	CLA	O1A-CGA-O2A-C1
19	L	1504	CLA	O1A-CGA-O2A-C1
19	B	1225	CLA	C2A-CAA-CBA-CGA
19	L	1503	CLA	C2A-CAA-CBA-CGA
19	B	1209	CLA	C6-C7-C8-C10
24	B	7101	LMG	O1-C7-C8-C9
19	A	1129	CLA	CBA-CGA-O2A-C1
22	K	7001	LMU	O5B-C5B-C6B-O6B
22	4	7009	LMU	O5'-C5'-C6'-O6'
19	L	1148	CLA	C5-C6-C7-C8
22	H	7017	LMU	C1-C2-C3-C4
22	E	7048	LMU	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	R	7007	LMU	C5-C6-C7-C8
22	2	7006	LMU	C9-C10-C11-C12
22	A	7010	LMU	C2B-C1B-O1B-C4'
22	G	7026	LMU	C9-C10-C11-C12
22	2	7031	LMU	C4-C5-C6-C7
22	4	7033	LMU	C2-C3-C4-C5
22	G	7051	LMU	C9-C10-C11-C12
19	A	9022	CLA	C16-C17-C18-C19
19	A	1111	CLA	C6-C7-C8-C9
22	A	7044	LMU	C9-C10-C11-C12
22	E	7037	LMU	O1'-C1-C2-C3
22	H	7011	LMU	O5B-C5B-C6B-O6B
21	A	6002	BCR	C9-C10-C11-C12
22	R	7024	LMU	C5'-C4'-O1B-C1B
22	2	7027	LMU	C5-C6-C7-C8
19	3	3011	CLA	C5-C6-C7-C8
19	B	1202	CLA	O1A-CGA-O2A-C1
22	G	7039	LMU	C9-C10-C11-C12
22	R	7024	LMU	C5-C6-C7-C8
22	4	7018	LMU	C1-C2-C3-C4
19	B	1221	CLA	C6-C7-C8-C9
22	4	7053	LMU	C2-C3-C4-C5
24	B	7101	LMG	C39-C40-C41-C42
19	3	3013	CLA	C10-C11-C12-C13
21	F	6014	BCR	C11-C10-C9-C34
19	A	1110	CLA	C4-C3-C5-C6
19	B	1209	CLA	C4-C3-C5-C6
19	B	1226	CLA	C4-C3-C5-C6
22	K	7047	LMU	C4-C5-C6-C7
22	R	7022	LMU	C2-C3-C4-C5
22	4	7008	LMU	C2-C3-C4-C5
19	A	1117	CLA	C16-C17-C18-C20
19	A	1138	CLA	C16-C17-C18-C19
19	B	1235	CLA	C16-C17-C18-C20
19	B	1239	CLA	CBA-CGA-O2A-C1
22	R	7014	LMU	O1'-C1-C2-C3
19	H	1145	CLA	C13-C15-C16-C17
19	3	3013	CLA	C15-C16-C17-C18
22	H	7002	LMU	C4-C5-C6-C7
22	H	7002	LMU	C9-C10-C11-C12
22	H	7043	LMU	C9-C10-C11-C12
19	2	2014	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	A	1135	CLA	C2-C1-O2A-CGA
19	J	1311	CLA	C2-C1-O2A-CGA
22	N	7049	LMU	C5'-C4'-O1B-C1B
19	A	1123	CLA	C3-C5-C6-C7
22	3	7003	LMU	C2-C3-C4-C5
22	3	7003	LMU	C9-C10-C11-C12
22	G	7026	LMU	C4B-C5B-C6B-O6B
19	A	1132	CLA	C10-C11-C12-C13
19	B	1224	CLA	C5-C6-C7-C8
22	G	7039	LMU	C4-C5-C6-C7
22	2	7031	LMU	C9-C10-C11-C12
19	A	1120	CLA	CBA-CGA-O2A-C1
19	B	1219	CLA	CBA-CGA-O2A-C1
19	K	3009	CLA	CBA-CGA-O2A-C1
19	4	4002	CLA	CBA-CGA-O2A-C1
19	B	1209	CLA	C6-C7-C8-C9
19	3	3013	CLA	C16-C17-C18-C19
22	K	7041	LMU	O1'-C1-C2-C3
22	3	7003	LMU	C4B-C5B-C6B-O6B
19	A	1109	CLA	O1A-CGA-O2A-C1
22	G	7039	LMU	C5'-C4'-O1B-C1B
19	A	1103	CLA	C5-C6-C7-C8
21	B	6005	BCR	C20-C21-C22-C23
22	F	7036	LMU	C2'-C1'-O1'-C1
22	R	7022	LMU	C2'-C1'-O1'-C1
19	A	1101	CLA	CAA-CBA-CGA-O2A
19	3	3008	CLA	CAA-CBA-CGA-O2A
22	A	7045	LMU	C1-C2-C3-C4
22	E	7037	LMU	C9-C10-C11-C12
19	A	1106	CLA	C15-C16-C17-C18
19	A	9022	CLA	C15-C16-C17-C18
19	A	1129	CLA	O1A-CGA-O2A-C1
19	B	1238	CLA	O1A-CGA-O2A-C1
19	K	3009	CLA	O1A-CGA-O2A-C1
19	B	1225	CLA	C16-C17-C18-C20
22	R	7020	LMU	C9-C10-C11-C12
22	4	7034	LMU	C4B-C5B-C6B-O6B
19	A	1103	CLA	C11-C10-C8-C7
19	A	1109	CLA	C11-C12-C13-C15
19	A	1110	CLA	C2-C3-C5-C6
19	A	1115	CLA	C12-C13-C15-C16
19	A	1123	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	A	1125	CLA	C6-C7-C8-C10
19	A	1126	CLA	C6-C7-C8-C10
19	A	1132	CLA	C11-C12-C13-C15
19	A	1138	CLA	C12-C13-C15-C16
19	A	1141	CLA	C11-C10-C8-C7
19	A	9013	CLA	C6-C7-C8-C10
19	A	9013	CLA	C12-C13-C15-C16
19	B	1203	CLA	C12-C13-C15-C16
19	B	1205	CLA	C11-C10-C8-C7
19	B	1206	CLA	C11-C10-C8-C7
19	B	1206	CLA	C12-C13-C15-C16
19	B	1216	CLA	C11-C12-C13-C15
19	B	1222	CLA	C11-C10-C8-C7
19	B	1226	CLA	C2-C3-C5-C6
19	B	1226	CLA	C6-C7-C8-C10
19	B	1234	CLA	C6-C7-C8-C10
19	B	1239	CLA	C12-C13-C15-C16
19	B	9010	CLA	C11-C10-C8-C7
19	H	1145	CLA	C12-C13-C15-C16
19	H	1207	CLA	C12-C13-C15-C16
19	J	1311	CLA	C11-C12-C13-C15
19	K	3009	CLA	C11-C10-C8-C7
19	K	3009	CLA	C12-C13-C15-C16
19	R	1150	CLA	C11-C10-C8-C7
19	1	1014	CLA	C11-C12-C13-C15
19	2	2006	CLA	C11-C10-C8-C7
19	2	2007	CLA	C12-C13-C15-C16
19	2	2014	CLA	C11-C10-C8-C7
19	3	3013	CLA	C11-C12-C13-C15
19	3	3016	CLA	C11-C10-C8-C7
19	A	1141	CLA	C3-C5-C6-C7
19	A	1126	CLA	C6-C7-C8-C9
19	A	1128	CLA	C11-C10-C8-C9
19	A	9013	CLA	C6-C7-C8-C9
19	A	9013	CLA	C14-C13-C15-C16
19	B	1203	CLA	C6-C7-C8-C9
19	B	1203	CLA	C14-C13-C15-C16
19	B	1206	CLA	C14-C13-C15-C16
19	B	1216	CLA	C11-C10-C8-C9
19	B	1225	CLA	C6-C7-C8-C9
19	B	1225	CLA	C11-C12-C13-C14
19	B	1226	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	9010	CLA	C14-C13-C15-C16
19	H	1207	CLA	C14-C13-C15-C16
19	J	1311	CLA	C6-C7-C8-C9
19	K	3009	CLA	C11-C10-C8-C9
19	K	3009	CLA	C11-C12-C13-C14
19	2	2006	CLA	C11-C12-C13-C14
19	2	2014	CLA	C11-C10-C8-C9
19	2	2014	CLA	C11-C12-C13-C14
19	3	3011	CLA	C11-C10-C8-C9
19	3	3013	CLA	C11-C12-C13-C14
21	B	6006	BCR	C19-C20-C21-C22
22	G	7039	LMU	C3'-C4'-O1B-C1B
19	H	1145	CLA	CBA-CGA-O2A-C1
19	B	1223	CLA	C13-C15-C16-C17
19	B	9010	CLA	C8-C10-C11-C12
22	K	7047	LMU	C9-C10-C11-C12
22	4	7034	LMU	C6-C7-C8-C9
19	A	1132	CLA	O1A-CGA-O2A-C1
21	A	6002	BCR	C7-C8-C9-C34
21	I	6018	BCR	C36-C18-C19-C20
21	I	6021	BCR	C7-C8-C9-C34
22	H	7030	LMU	C7-C8-C9-C10
21	A	6002	BCR	C7-C8-C9-C10
21	I	6018	BCR	C11-C12-C13-C14
21	I	6018	BCR	C17-C18-C19-C20
21	I	6021	BCR	C7-C8-C9-C10
21	1	6023	BCR	C7-C8-C9-C10
19	R	1150	CLA	C3-C5-C6-C7
19	1	1007	CLA	C3-C5-C6-C7
22	B	7012	LMU	C4B-C5B-C6B-O6B
22	R	7021	LMU	C4'-C5'-C6'-O6'
19	A	9023	CLA	CBA-CGA-O2A-C1
19	1	1002	CLA	CBA-CGA-O2A-C1
22	4	7033	LMU	C9-C10-C11-C12
19	2	2006	CLA	C10-C11-C12-C13
22	R	7014	LMU	C9-C10-C11-C12
22	H	7032	LMU	C4B-C5B-C6B-O6B
19	B	1220	CLA	C5-C6-C7-C8
19	B	1226	CLA	C13-C15-C16-C17
19	B	1209	CLA	C2-C3-C5-C6
22	B	7040	LMU	C5-C6-C7-C8
19	2	2007	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	1	1007	CLA	C14-C13-C15-C16
22	A	7044	LMU	C1-C2-C3-C4
19	A	1149	CLA	CAA-CBA-CGA-O2A
22	A	7045	LMU	C4-C5-C6-C7
22	C	7015	LMU	C3-C4-C5-C6
22	3	7003	LMU	C5-C6-C7-C8
19	A	1110	CLA	C3A-C2A-CAA-CBA
19	A	1120	CLA	C3A-C2A-CAA-CBA
19	A	1134	CLA	C3A-C2A-CAA-CBA
19	B	1202	CLA	C3A-C2A-CAA-CBA
19	B	1222	CLA	C3A-C2A-CAA-CBA
19	L	1503	CLA	C3A-C2A-CAA-CBA
22	A	7045	LMU	C9-C10-C11-C12
22	C	7015	LMU	C9-C10-C11-C12
22	R	7014	LMU	C5-C6-C7-C8
22	2	7046	LMU	C9-C10-C11-C12
22	A	7016	LMU	C2-C1-O1'-C1'
22	E	7048	LMU	C2-C1-O1'-C1'
22	G	7039	LMU	C2-C1-O1'-C1'
22	H	7011	LMU	C2-C1-O1'-C1'
22	H	7017	LMU	C2-C1-O1'-C1'
22	K	7042	LMU	C2-C1-O1'-C1'
22	L	7029	LMU	C2-C1-O1'-C1'
22	N	7049	LMU	C2-C1-O1'-C1'
22	R	7021	LMU	C2-C1-O1'-C1'
22	R	7025	LMU	C2-C1-O1'-C1'
22	2	7006	LMU	C2-C1-O1'-C1'
22	2	7046	LMU	C2-C1-O1'-C1'
22	3	7005	LMU	C2-C1-O1'-C1'
22	4	7019	LMU	C2-C1-O1'-C1'
22	4	7052	LMU	C2-C1-O1'-C1'
22	1	7013	LMU	C9-C10-C11-C12
19	A	1103	CLA	C16-C17-C18-C20
19	4	1306	CLA	C6-C7-C8-C9
19	A	1127	CLA	O1D-CGD-O2D-CED
19	2	2012	CLA	O1D-CGD-O2D-CED
22	F	7036	LMU	C5-C6-C7-C8
22	R	7024	LMU	C3'-C4'-O1B-C1B
19	1	1014	CLA	C8-C10-C11-C12
22	1	7004	LMU	O5'-C5'-C6'-O6'
22	3	7003	LMU	O5B-C5B-C6B-O6B
19	A	1120	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	4	7018	LMU	C4B-C5B-C6B-O6B
22	A	7023	LMU	O5B-C1B-O1B-C4'
19	B	1230	CLA	O2A-C1-C2-C3
19	A	1132	CLA	C5-C6-C7-C8
22	E	7048	LMU	C6-C7-C8-C9
22	R	7021	LMU	C4-C5-C6-C7
19	3	3011	CLA	C10-C11-C12-C13
19	A	1124	CLA	C16-C17-C18-C20
22	4	7052	LMU	C4'-C5'-C6'-O6'
22	R	7022	LMU	C9-C10-C11-C12
22	H	7043	LMU	O5'-C5'-C6'-O6'
19	A	1138	CLA	C16-C17-C18-C20
22	E	7037	LMU	C5-C6-C7-C8
24	B	7101	LMG	C41-C42-C43-C44
22	G	7026	LMU	C2B-C1B-O1B-C4'
22	A	7044	LMU	C6-C7-C8-C9
19	A	1109	CLA	C13-C15-C16-C17
19	B	1203	CLA	C5-C6-C7-C8
22	R	7025	LMU	C1-C2-C3-C4
19	B	1219	CLA	O1A-CGA-O2A-C1
19	B	1239	CLA	O1A-CGA-O2A-C1
22	A	7035	LMU	C5-C6-C7-C8
22	R	7020	LMU	C7-C8-C9-C10
19	A	1106	CLA	C13-C15-C16-C17
19	A	1140	CLA	C15-C16-C17-C18
19	A	1103	CLA	C16-C17-C18-C19
19	A	1119	CLA	C16-C17-C18-C20
19	A	9022	CLA	C16-C17-C18-C20
19	B	1225	CLA	C16-C17-C18-C19
19	A	1102	CLA	C2-C1-O2A-CGA
19	A	1106	CLA	C2-C1-O2A-CGA
19	A	1237	CLA	C2-C1-O2A-CGA
19	4	4001	CLA	C2-C1-O2A-CGA
22	4	7019	LMU	C4'-C5'-C6'-O6'
19	A	9023	CLA	O1A-CGA-O2A-C1
19	A	1124	CLA	C10-C11-C12-C13
19	A	1126	CLA	C11-C12-C13-C14
19	A	1132	CLA	C11-C12-C13-C14
19	B	1202	CLA	C11-C10-C8-C9
19	B	1214	CLA	C11-C10-C8-C9
19	B	1216	CLA	C11-C12-C13-C14
19	B	1234	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	2	2006	CLA	C6-C7-C8-C9
19	4	1304	CLA	C11-C12-C13-C14
22	3	7003	LMU	O1'-C1-C2-C3
19	B	1238	CLA	C5-C6-C7-C8
19	4	4003	CLA	C5-C6-C7-C8
19	B	1233	CLA	C4-C3-C5-C6
19	1	1303	CLA	C4-C3-C5-C6
19	4	4002	CLA	O1A-CGA-O2A-C1
22	A	7023	LMU	C1-C2-C3-C4
19	A	1127	CLA	C2A-CAA-CBA-CGA
19	A	9022	CLA	C2A-CAA-CBA-CGA
19	A	1106	CLA	C16-C17-C18-C20
19	A	1131	CLA	C16-C17-C18-C19
19	4	1304	CLA	C16-C17-C18-C20
19	B	1225	CLA	C3-C5-C6-C7
21	B	6005	BCR	C23-C24-C25-C26
21	B	6017	BCR	C23-C24-C25-C30
21	I	6021	BCR	C5-C6-C7-C8
21	A	6002	BCR	C36-C18-C19-C20
21	1	6023	BCR	C7-C8-C9-C34
21	A	6007	BCR	C11-C12-C13-C14
19	A	9012	CLA	C5-C6-C7-C8
19	1	1002	CLA	O1A-CGA-O2A-C1
22	B	7038	LMU	C7-C8-C9-C10
22	R	7021	LMU	C9-C10-C11-C12
22	4	7052	LMU	C2-C3-C4-C5
19	2	2014	CLA	C14-C13-C15-C16
19	A	9011	CLA	C13-C15-C16-C17
22	R	7007	LMU	O1'-C1-C2-C3
19	A	1103	CLA	C11-C12-C13-C15
19	A	1106	CLA	C11-C10-C8-C7
19	A	1117	CLA	C12-C13-C15-C16
19	A	1128	CLA	C6-C7-C8-C10
19	A	1131	CLA	C11-C10-C8-C7
19	A	1132	CLA	C12-C13-C15-C16
19	A	1136	CLA	C12-C13-C15-C16
19	A	9013	CLA	C11-C10-C8-C7
19	B	1202	CLA	C6-C7-C8-C10
19	B	1203	CLA	C6-C7-C8-C10
19	B	1211	CLA	C6-C7-C8-C10
19	B	1214	CLA	C11-C10-C8-C7
19	B	1216	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	B	1220	CLA	C6-C7-C8-C10
19	B	1223	CLA	C11-C12-C13-C15
19	B	1225	CLA	C6-C7-C8-C10
19	B	1225	CLA	C11-C12-C13-C15
19	B	1238	CLA	C11-C10-C8-C7
19	B	1239	CLA	C11-C12-C13-C15
19	K	3009	CLA	C11-C12-C13-C15
19	2	2006	CLA	C11-C12-C13-C15
19	2	2007	CLA	C11-C10-C8-C7
19	2	4009	CLA	C12-C13-C15-C16
19	3	3013	CLA	C11-C10-C8-C7
21	A	6008	BCR	C19-C20-C21-C22
21	F	6016	BCR	C19-C20-C21-C22
19	J	1308	CLA	C6-C7-C8-C9
19	1	1014	CLA	CBA-CGA-O2A-C1
22	K	7041	LMU	C9-C10-C11-C12
19	A	1124	CLA	C5-C6-C7-C8
19	4	1004	CLA	C5-C6-C7-C8
19	A	1116	CLA	C4C-C3C-CAC-CBC
19	A	1137	CLA	C4C-C3C-CAC-CBC
19	A	1149	CLA	C4C-C3C-CAC-CBC
19	A	9013	CLA	C4C-C3C-CAC-CBC
19	B	1234	CLA	C4C-C3C-CAC-CBC
19	B	1238	CLA	C4C-C3C-CAC-CBC
19	K	1146	CLA	C4C-C3C-CAC-CBC
19	1	1001	CLA	C4C-C3C-CAC-CBC
19	1	1010	CLA	C4C-C3C-CAC-CBC
19	2	2007	CLA	C4C-C3C-CAC-CBC
21	I	6018	BCR	C11-C10-C9-C34
22	R	7022	LMU	C5-C6-C7-C8
22	1	7004	LMU	C3'-C4'-O1B-C1B
22	2	7046	LMU	C3'-C4'-O1B-C1B
19	B	1223	CLA	C5-C6-C7-C8
19	A	1111	CLA	CBA-CGA-O2A-C1
19	A	1119	CLA	CBA-CGA-O2A-C1
19	J	1311	CLA	C12-C13-C15-C16
19	1	1007	CLA	C12-C13-C15-C16
22	H	7043	LMU	C11-C10-C9-C8
19	A	1102	CLA	CAD-CBD-CGD-O2D
19	B	1213	CLA	CAD-CBD-CGD-O2D
19	B	1233	CLA	CAD-CBD-CGD-O2D
19	B	1236	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	1238	CLA	CAD-CBD-CGD-O2D
19	K	1146	CLA	CAD-CBD-CGD-O2D
19	L	1503	CLA	CAD-CBD-CGD-O2D
19	R	1150	CLA	CAD-CBD-CGD-O2D
19	1	1003	CLA	CAD-CBD-CGD-O2D
19	2	2002	CLA	CAD-CBD-CGD-O2D
19	2	2006	CLA	CAD-CBD-CGD-O2D
19	3	2009	CLA	CAD-CBD-CGD-O2D
19	3	3007	CLA	CAD-CBD-CGD-O2D
24	B	7101	LMG	C9-C8-O7-C10
22	B	7040	LMU	C2-C3-C4-C5
19	3	1147	CLA	O1A-CGA-O2A-C1
22	R	7021	LMU	C3-C4-C5-C6
22	A	7010	LMU	O5B-C1B-O1B-C4'
19	4	1004	CLA	CBA-CGA-O2A-C1
19	B	1215	CLA	C4-C3-C5-C6
19	B	1220	CLA	C16-C17-C18-C20
22	C	7015	LMU	C4'-C5'-C6'-O6'
19	1	1014	CLA	O1A-CGA-O2A-C1
19	B	1211	CLA	C15-C16-C17-C18
19	H	1207	CLA	C13-C15-C16-C17
22	K	7047	LMU	C3-C4-C5-C6
19	A	1151	CLA	C2A-CAA-CBA-CGA
19	B	1206	CLA	C2A-CAA-CBA-CGA
19	B	1236	CLA	C2A-CAA-CBA-CGA
22	A	7035	LMU	C9-C10-C11-C12
22	2	7031	LMU	C1-C2-C3-C4
19	A	1106	CLA	CHA-CBD-CGD-O1D
19	A	1106	CLA	CHA-CBD-CGD-O2D
19	A	1115	CLA	CHA-CBD-CGD-O1D
19	A	1132	CLA	CHA-CBD-CGD-O1D
19	A	1132	CLA	CHA-CBD-CGD-O2D
19	A	1138	CLA	CHA-CBD-CGD-O1D
19	A	1237	CLA	CHA-CBD-CGD-O1D
19	A	1237	CLA	CHA-CBD-CGD-O2D
19	A	9011	CLA	CHA-CBD-CGD-O1D
19	A	9011	CLA	CHA-CBD-CGD-O2D
19	A	9012	CLA	CHA-CBD-CGD-O1D
19	A	9012	CLA	CHA-CBD-CGD-O2D
19	B	1218	CLA	CHA-CBD-CGD-O1D
19	B	1218	CLA	CHA-CBD-CGD-O2D
19	B	1220	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	1232	CLA	CHA-CBD-CGD-O1D
19	B	1232	CLA	CHA-CBD-CGD-O2D
19	B	9010	CLA	CHA-CBD-CGD-O1D
19	B	9010	CLA	CHA-CBD-CGD-O2D
19	1	1001	CLA	CHA-CBD-CGD-O1D
19	1	1001	CLA	CHA-CBD-CGD-O2D
19	2	2013	CLA	CHA-CBD-CGD-O1D
19	2	4009	CLA	CHA-CBD-CGD-O1D
19	2	4009	CLA	CHA-CBD-CGD-O2D
19	4	1306	CLA	CHA-CBD-CGD-O1D
19	4	1306	CLA	CHA-CBD-CGD-O2D
19	4	4003	CLA	CHA-CBD-CGD-O1D
19	H	1145	CLA	O1A-CGA-O2A-C1
21	I	6018	BCR	C11-C10-C9-C8
22	G	7039	LMU	C2'-C1'-O1'-C1
19	A	1138	CLA	C5-C6-C7-C8
22	H	7028	LMU	C1-C2-C3-C4
19	A	1125	CLA	C5-C6-C7-C8
19	B	9010	CLA	C4-C3-C5-C6
19	H	1207	CLA	C4-C3-C5-C6
22	A	7010	LMU	O1'-C1-C2-C3
19	H	1207	CLA	C2-C3-C5-C6
19	A	1141	CLA	CBA-CGA-O2A-C1
22	4	7053	LMU	O5B-C1B-O1B-C4'
19	A	1136	CLA	C14-C13-C15-C16
19	B	1202	CLA	C6-C7-C8-C9
19	B	1211	CLA	C6-C7-C8-C9
19	B	1238	CLA	C11-C10-C8-C9
19	J	1311	CLA	C11-C10-C8-C9
19	2	2007	CLA	C11-C10-C8-C9
22	H	7017	LMU	C5-C6-C7-C8
22	G	7039	LMU	O5B-C5B-C6B-O6B
19	A	1119	CLA	O1A-CGA-O2A-C1
19	B	1210	CLA	C13-C15-C16-C17
19	2	4009	CLA	C13-C15-C16-C17
21	B	6020	BCR	C7-C8-C9-C34
22	K	7001	LMU	C3'-C4'-O1B-C1B
22	G	7026	LMU	C7-C8-C9-C10
22	A	7023	LMU	C2B-C1B-O1B-C4'
21	B	6010	BCR	C17-C18-C19-C20
19	B	1234	CLA	C1A-C2A-CAA-CBA
19	3	3017	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	4	4002	CLA	C1A-C2A-CAA-CBA
20	A	5001	PQN	C26-C27-C28-C29
19	B	1212	CLA	C10-C11-C12-C13
22	E	7048	LMU	C1-C2-C3-C4
19	A	1133	CLA	C2-C1-O2A-CGA
19	B	1206	CLA	C2-C1-O2A-CGA
19	B	1228	CLA	C2-C1-O2A-CGA
21	A	6008	BCR	C13-C14-C15-C16
21	B	6017	BCR	C19-C20-C21-C22
19	A	1137	CLA	O1D-CGD-O2D-CED
22	A	7023	LMU	C5-C6-C7-C8
19	A	1115	CLA	C3-C5-C6-C7
19	B	1229	CLA	C3-C5-C6-C7
19	1	1007	CLA	C2-C3-C5-C6
22	G	7051	LMU	C3-C4-C5-C6
19	J	1308	CLA	C6-C7-C8-C10
19	A	1127	CLA	CBA-CGA-O2A-C1
22	3	7003	LMU	C3-C4-C5-C6
19	B	1224	CLA	C3-C5-C6-C7
19	L	1148	CLA	C3-C5-C6-C7
22	H	7043	LMU	O5B-C5B-C6B-O6B
22	1	7004	LMU	C6-C7-C8-C9
19	A	1119	CLA	C16-C17-C18-C19
19	A	1132	CLA	C16-C17-C18-C19
19	A	1140	CLA	C16-C17-C18-C20
19	B	1219	CLA	C6-C7-C8-C9
19	L	1130	CLA	C16-C17-C18-C20
19	A	1120	CLA	C2-C3-C5-C6
19	A	1126	CLA	CAD-CBD-CGD-O1D
19	A	1133	CLA	CAD-CBD-CGD-O1D
19	A	9012	CLA	CAD-CBD-CGD-O1D
19	A	9022	CLA	CAD-CBD-CGD-O1D
19	B	1203	CLA	CAD-CBD-CGD-O1D
19	B	1232	CLA	CAD-CBD-CGD-O1D
19	B	1234	CLA	CAD-CBD-CGD-O1D
19	F	1302	CLA	CAD-CBD-CGD-O1D
19	1	1013	CLA	C2-C3-C5-C6
19	2	2001	CLA	C2-C3-C5-C6
19	2	2007	CLA	CAD-CBD-CGD-O1D
19	4	1004	CLA	CAD-CBD-CGD-O1D
19	4	4003	CLA	CAD-CBD-CGD-O1D
19	4	4014	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	7040	LMU	C3-C4-C5-C6
19	A	1127	CLA	O1A-CGA-O2A-C1
22	R	7020	LMU	C4-C5-C6-C7
19	B	1205	CLA	C3-C5-C6-C7
19	1	1303	CLA	CBA-CGA-O2A-C1
22	4	7053	LMU	C2B-C1B-O1B-C4'
19	4	1304	CLA	C16-C17-C18-C19
19	J	1311	CLA	C4-C3-C5-C6
19	A	1124	CLA	C11-C10-C8-C7
19	A	1135	CLA	C3A-C2A-CAA-CBA
19	A	1138	CLA	C11-C10-C8-C7
19	A	9012	CLA	C6-C7-C8-C10
19	A	9013	CLA	C11-C12-C13-C15
19	A	9023	CLA	C12-C13-C15-C16
19	B	1202	CLA	C11-C12-C13-C15
19	B	1210	CLA	C11-C10-C8-C7
19	B	1220	CLA	C12-C13-C15-C16
19	B	1226	CLA	C11-C12-C13-C15
19	B	1226	CLA	C12-C13-C15-C16
19	B	1229	CLA	C11-C10-C8-C7
19	B	1235	CLA	C11-C10-C8-C7
19	H	1145	CLA	C11-C12-C13-C15
19	I	1204	CLA	C11-C10-C8-C7
19	K	3009	CLA	C6-C7-C8-C10
19	1	1002	CLA	C3A-C2A-CAA-CBA
19	2	2006	CLA	C6-C7-C8-C10
19	3	3011	CLA	C11-C12-C13-C15
19	4	1304	CLA	C11-C12-C13-C15
19	4	4015	CLA	C3A-C2A-CAA-CBA
20	A	5001	PQN	C21-C22-C23-C25
20	A	5001	PQN	C22-C23-C25-C26
22	C	7015	LMU	C2-C1-O1'-C1'
19	4	4003	CLA	CAA-CBA-CGA-O2A
19	A	1131	CLA	C8-C10-C11-C12
19	A	1111	CLA	O1A-CGA-O2A-C1
22	A	7016	LMU	C9-C10-C11-C12
19	B	1212	CLA	C11-C12-C13-C14
22	2	7006	LMU	O5B-C5B-C6B-O6B
19	4	1004	CLA	O1A-CGA-O2A-C1
24	B	7101	LMG	O1-C7-C8-O7
22	1	7004	LMU	C5'-C4'-O1B-C1B
19	3	3011	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	D	7050	LMU	C4-C5-C6-C7
22	4	7019	LMU	C9-C10-C11-C12
19	B	1206	CLA	C3-C5-C6-C7
19	A	1141	CLA	O1A-CGA-O2A-C1
19	B	1229	CLA	CBA-CGA-O2A-C1
19	4	4003	CLA	CBA-CGA-O2A-C1
22	H	7030	LMU	O1'-C1-C2-C3
22	N	7049	LMU	C3-C4-C5-C6
19	B	1215	CLA	C2-C3-C5-C6
22	4	7018	LMU	C6-C7-C8-C9
19	A	1103	CLA	C11-C12-C13-C14
19	A	1106	CLA	C6-C7-C8-C9
19	A	1117	CLA	C14-C13-C15-C16
19	A	1131	CLA	C11-C10-C8-C9
19	B	1211	CLA	C11-C10-C8-C9
19	B	1215	CLA	C6-C7-C8-C9
19	B	1239	CLA	C11-C12-C13-C14
19	I	1204	CLA	C11-C10-C8-C9
19	K	3009	CLA	C6-C7-C8-C9
19	3	3013	CLA	C11-C10-C8-C9
22	R	7020	LMU	C5-C6-C7-C8
22	4	7052	LMU	C7-C8-C9-C10
22	4	7053	LMU	C4-C5-C6-C7
19	F	1305	CLA	C5-C6-C7-C8
19	4	4003	CLA	O1A-CGA-O2A-C1
19	A	1123	CLA	C8-C10-C11-C12
21	A	6011	BCR	C18-C19-C20-C21
21	B	6010	BCR	C18-C19-C20-C21
21	1	6023	BCR	C18-C19-C20-C21
21	F	6014	BCR	C7-C8-C9-C34
19	A	1126	CLA	C10-C11-C12-C13
19	B	1229	CLA	O1A-CGA-O2A-C1
22	C	7015	LMU	C5'-C4'-O1B-C1B
19	A	1131	CLA	C16-C17-C18-C20
21	B	6010	BCR	C21-C22-C23-C24
19	A	9022	CLA	C5-C6-C7-C8
19	B	1224	CLA	CAA-CBA-CGA-O2A
19	B	9010	CLA	C2-C3-C5-C6
19	4	1004	CLA	C6-C7-C8-C10
22	H	7032	LMU	C3-C4-C5-C6
22	2	7027	LMU	O5B-C1B-O1B-C4'
19	A	1126	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	B	1235	CLA	C3-C5-C6-C7
19	A	9012	CLA	C2A-CAA-CBA-CGA
19	A	1151	CLA	C2-C1-O2A-CGA
19	A	9012	CLA	C2-C1-O2A-CGA
19	B	1223	CLA	C2-C1-O2A-CGA
19	B	1230	CLA	C2-C1-O2A-CGA
19	B	1235	CLA	C2-C1-O2A-CGA
19	H	1207	CLA	C2-C1-O2A-CGA
19	R	1144	CLA	C2-C1-O2A-CGA
19	2	2014	CLA	C2-C1-O2A-CGA
19	B	1210	CLA	CAA-CBA-CGA-O2A
22	3	7005	LMU	C4'-C5'-C6'-O6'
19	B	1238	CLA	CBD-CGD-O2D-CED
21	B	6017	BCR	C15-C16-C17-C18
22	L	7029	LMU	C3-C4-C5-C6
19	L	1130	CLA	C16-C17-C18-C19
22	K	7001	LMU	C4-C5-C6-C7
21	B	6005	BCR	C23-C24-C25-C30
21	L	6019	BCR	C23-C24-C25-C30
19	A	1141	CLA	C13-C15-C16-C17
19	B	1213	CLA	CAA-CBA-CGA-O2A
22	2	7031	LMU	O5B-C1B-O1B-C4'
22	H	7028	LMU	O5'-C1'-O1'-C1
19	A	1137	CLA	C2A-CAA-CBA-CGA
19	1	1014	CLA	C2A-CAA-CBA-CGA
21	F	6014	BCR	C11-C10-C9-C8
22	K	7042	LMU	C2'-C1'-O1'-C1
22	H	7011	LMU	C4-C5-C6-C7
22	A	7023	LMU	C9-C10-C11-C12
19	A	1131	CLA	CBA-CGA-O2A-C1
19	B	1222	CLA	CBA-CGA-O2A-C1
19	A	1102	CLA	C6-C7-C8-C10
19	B	1215	CLA	C6-C7-C8-C10
19	B	1238	CLA	C6-C7-C8-C10
19	B	9010	CLA	C12-C13-C15-C16
19	B	1222	CLA	O1A-CGA-O2A-C1
19	A	1106	CLA	C11-C10-C8-C9
19	A	1106	CLA	C14-C13-C15-C16
19	A	1124	CLA	C11-C10-C8-C9
19	A	1128	CLA	C6-C7-C8-C9
19	A	9011	CLA	C14-C13-C15-C16
19	A	9013	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B	1210	CLA	C11-C10-C8-C9
19	B	1235	CLA	C11-C10-C8-C9
19	B	1239	CLA	C14-C13-C15-C16
21	A	6003	BCR	C19-C20-C21-C22
21	B	6004	BCR	C19-C20-C21-C22
19	A	1115	CLA	C16-C17-C18-C19
19	A	9013	CLA	C16-C17-C18-C20
19	A	1131	CLA	O1A-CGA-O2A-C1
22	B	7038	LMU	C4-C5-C6-C7
22	H	7011	LMU	C3'-C4'-O1B-C1B
19	A	1103	CLA	CBD-CGD-O2D-CED
22	2	7006	LMU	C3-C4-C5-C6
22	A	7035	LMU	C2-C3-C4-C5
21	F	6014	BCR	C7-C8-C9-C10
19	A	1102	CLA	C4-C3-C5-C6
19	A	1237	CLA	C4-C3-C5-C6
19	A	1140	CLA	C16-C17-C18-C19
19	A	1124	CLA	CBA-CGA-O2A-C1
22	A	7035	LMU	O1'-C1-C2-C3
19	B	9010	CLA	CAA-CBA-CGA-O2A
19	A	1136	CLA	C13-C15-C16-C17
19	A	9022	CLA	C10-C11-C12-C13
19	A	1124	CLA	O1A-CGA-O2A-C1
19	1	1303	CLA	O1A-CGA-O2A-C1
21	A	6007	BCR	C13-C14-C15-C16
21	F	6014	BCR	C13-C14-C15-C16
22	4	7052	LMU	C11-C10-C9-C8
22	4	7019	LMU	C4-C5-C6-C7
19	B	1227	CLA	CAA-CBA-CGA-O2A
19	A	1109	CLA	C4-C3-C5-C6
19	A	9011	CLA	C4-C3-C5-C6
22	4	7019	LMU	C2-C3-C4-C5
19	J	1308	CLA	CAA-CBA-CGA-O2A
19	A	1107	CLA	C2-C1-O2A-CGA
19	B	1226	CLA	C2-C1-O2A-CGA
19	F	1305	CLA	C2-C1-O2A-CGA
22	C	7015	LMU	C3'-C4'-O1B-C1B
22	H	7032	LMU	O5B-C5B-C6B-O6B
19	B	1224	CLA	C2A-CAA-CBA-CGA
19	L	1501	CLA	C2A-CAA-CBA-CGA
22	H	7017	LMU	C3'-C4'-O1B-C1B
19	A	1138	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	K	1146	CLA	C3A-C2A-CAA-CBA
19	1	1005	CLA	C3A-C2A-CAA-CBA
19	3	3008	CLA	C3A-C2A-CAA-CBA
19	3	3017	CLA	C3A-C2A-CAA-CBA
21	A	6011	BCR	C13-C14-C15-C16
22	K	7001	LMU	C2-C3-C4-C5
19	B	1210	CLA	C4-C3-C5-C6
19	J	1311	CLA	C2-C3-C5-C6
19	H	1145	CLA	CAA-CBA-CGA-O2A
19	A	1103	CLA	C14-C13-C15-C16
19	A	1131	CLA	C6-C7-C8-C9
19	B	1206	CLA	C6-C7-C8-C9
19	B	1220	CLA	C6-C7-C8-C9
19	B	1238	CLA	C14-C13-C15-C16
19	B	1226	CLA	C10-C11-C12-C13
19	H	1207	CLA	C10-C11-C12-C13
21	A	6011	BCR	C35-C13-C14-C15
21	F	6014	BCR	C20-C21-C22-C37
21	F	6016	BCR	C16-C17-C18-C36
19	B	1225	CLA	CBD-CGD-O2D-CED
19	3	1147	CLA	C2A-CAA-CBA-CGA
19	H	1145	CLA	C10-C11-C12-C13
22	4	7034	LMU	C4'-C5'-C6'-O6'
22	G	7051	LMU	C5-C6-C7-C8
19	A	9013	CLA	C16-C17-C18-C19
19	4	4003	CLA	C6-C7-C8-C9
22	A	7035	LMU	O5'-C1'-O1'-C1
22	G	7039	LMU	O5'-C1'-O1'-C1
22	H	7032	LMU	C9-C10-C11-C12
19	A	1104	CLA	C1A-C2A-CAA-CBA
19	A	1110	CLA	C1A-C2A-CAA-CBA
19	A	1120	CLA	C1A-C2A-CAA-CBA
19	A	1141	CLA	C1A-C2A-CAA-CBA
19	B	1222	CLA	C1A-C2A-CAA-CBA
19	K	1146	CLA	C1A-C2A-CAA-CBA
19	3	3016	CLA	C1A-C2A-CAA-CBA
19	4	1304	CLA	CBA-CGA-O2A-C1
19	A	1109	CLA	C11-C10-C8-C7
19	A	1125	CLA	C11-C10-C8-C7
19	A	1128	CLA	C11-C10-C8-C7
19	B	1211	CLA	C11-C12-C13-C15
19	B	1212	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	H	1207	CLA	C11-C10-C8-C7
19	4	1304	CLA	C6-C7-C8-C10
22	4	7033	LMU	C3-C4-C5-C6
19	B	1223	CLA	C10-C11-C12-C13
22	4	7033	LMU	C7-C8-C9-C10
22	H	7002	LMU	C3-C4-C5-C6
22	K	7001	LMU	O1'-C1-C2-C3
24	B	7101	LMG	C38-C39-C40-C41
22	B	7040	LMU	C9-C10-C11-C12
22	H	7011	LMU	C7-C8-C9-C10
22	1	7004	LMU	C9-C10-C11-C12
22	G	7026	LMU	O5B-C5B-C6B-O6B
22	R	7021	LMU	C11-C10-C9-C8
19	A	9013	CLA	C2A-CAA-CBA-CGA
19	I	1204	CLA	C2A-CAA-CBA-CGA
19	1	1007	CLA	C2A-CAA-CBA-CGA
22	H	7030	LMU	C6-C7-C8-C9
22	R	7014	LMU	C1-C2-C3-C4
24	B	7101	LMG	C14-C15-C16-C17
19	A	1132	CLA	C16-C17-C18-C20
22	B	7038	LMU	C2-C3-C4-C5
19	B	1212	CLA	C4-C3-C5-C6
19	A	9011	CLA	C2-C3-C5-C6
19	B	1210	CLA	C2-C3-C5-C6
22	C	7015	LMU	O1'-C1-C2-C3
22	H	7043	LMU	C1-C2-C3-C4
19	2	2007	CLA	O1D-CGD-O2D-CED
21	A	6011	BCR	C12-C13-C14-C15
21	F	6014	BCR	C20-C21-C22-C23
21	F	6016	BCR	C16-C17-C18-C19
19	A	1131	CLA	C10-C11-C12-C13
19	R	1150	CLA	CAA-CBA-CGA-O2A
21	J	6012	BCR	C15-C16-C17-C18
22	G	7039	LMU	C4B-C5B-C6B-O6B
19	A	9011	CLA	C16-C17-C18-C19
22	R	7025	LMU	C2-C3-C4-C5
19	A	1122	CLA	O1A-CGA-O2A-C1
19	A	9012	CLA	C8-C10-C11-C12
19	B	1225	CLA	C4-C3-C5-C6
22	D	7050	LMU	C3-C4-C5-C6
19	B	1227	CLA	C2-C1-O2A-CGA
19	3	3016	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	A	1149	CLA	C2-C1-O2A-CGA
24	B	7101	LMG	C28-C29-C30-C31
19	A	1237	CLA	C6-C7-C8-C9
19	B	1202	CLA	C14-C13-C15-C16
19	B	9010	CLA	C6-C7-C8-C9
22	2	7046	LMU	C5-C6-C7-C8
19	1	1013	CLA	C4-C3-C5-C6
19	2	2001	CLA	C4-C3-C5-C6
19	A	1101	CLA	CAA-CBA-CGA-O1A
22	R	7021	LMU	C6-C7-C8-C9
22	4	7034	LMU	O5'-C5'-C6'-O6'
19	A	1119	CLA	C2A-CAA-CBA-CGA
19	4	4014	CLA	C2A-CAA-CBA-CGA
19	A	1122	CLA	CBA-CGA-O2A-C1
22	4	7009	LMU	O5B-C1B-O1B-C4'
21	I	6021	BCR	C1-C6-C7-C8
21	I	6021	BCR	C23-C24-C25-C30
19	B	1221	CLA	O1D-CGD-O2D-CED
19	B	1202	CLA	CAA-CBA-CGA-O2A
21	B	6004	BCR	C13-C14-C15-C16
19	4	4007	CLA	C4-C3-C5-C6
19	A	1125	CLA	C10-C11-C12-C13
19	A	1237	CLA	C2-C3-C5-C6
19	B	1223	CLA	C16-C17-C18-C20
22	H	7011	LMU	C2-C3-C4-C5
19	2	2006	CLA	CAA-CBA-CGA-O2A
19	J	1311	CLA	C3-C5-C6-C7
19	A	1125	CLA	C16-C17-C18-C20
22	H	7032	LMU	O5B-C1B-O1B-C4'
19	A	1102	CLA	C2-C3-C5-C6
19	A	1126	CLA	C11-C12-C13-C15
19	A	9011	CLA	C11-C10-C8-C7
19	B	1238	CLA	C12-C13-C15-C16
19	J	1311	CLA	C11-C10-C8-C7
19	4	1304	CLA	C11-C10-C8-C7
19	A	1128	CLA	C10-C11-C12-C13
22	F	7036	LMU	C4-C5-C6-C7
22	1	7004	LMU	C4-C5-C6-C7
19	3	3008	CLA	CAA-CBA-CGA-O1A
22	K	7041	LMU	C1-C2-C3-C4
19	A	1149	CLA	CAA-CBA-CGA-O1A
22	G	7026	LMU	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	A	1117	CLA	C8-C10-C11-C12
22	R	7022	LMU	C6-C7-C8-C9
19	A	1124	CLA	C8-C10-C11-C12
22	D	7050	LMU	C7-C8-C9-C10
22	K	7001	LMU	C4'-C5'-C6'-O6'
19	A	1107	CLA	C4C-C3C-CAC-CBC
19	A	1109	CLA	C4C-C3C-CAC-CBC
19	A	1132	CLA	C4C-C3C-CAC-CBC
19	A	1141	CLA	C4C-C3C-CAC-CBC
19	B	1201	CLA	C4C-C3C-CAC-CBC
19	F	1302	CLA	C4C-C3C-CAC-CBC
19	J	1311	CLA	C4C-C3C-CAC-CBC
19	1	1008	CLA	C4C-C3C-CAC-CBC
19	4	4015	CLA	C4C-C3C-CAC-CBC
21	B	6010	BCR	C20-C21-C22-C37
21	B	6017	BCR	C20-C21-C22-C37
19	A	1138	CLA	CAA-CBA-CGA-O2A
19	A	9011	CLA	CAA-CBA-CGA-O2A
19	B	1217	CLA	CAA-CBA-CGA-O2A
19	B	1223	CLA	CAA-CBA-CGA-O2A
19	A	1126	CLA	C4-C3-C5-C6
19	A	9023	CLA	C4-C3-C5-C6
19	4	1304	CLA	C4-C3-C5-C6
19	B	1236	CLA	C2-C1-O2A-CGA
22	4	7053	LMU	O1'-C1-C2-C3
19	A	1237	CLA	C5-C6-C7-C8
19	L	1130	CLA	CBA-CGA-O2A-C1
19	H	1505	CLA	CAA-CBA-CGA-O2A
19	I	1204	CLA	CAA-CBA-CGA-O2A
22	H	7011	LMU	C3-C4-C5-C6
19	B	1226	CLA	C11-C12-C13-C14
19	B	1238	CLA	C6-C7-C8-C9
19	H	1145	CLA	C11-C12-C13-C14
19	3	3011	CLA	C11-C12-C13-C14
20	A	5001	PQN	C24-C23-C25-C26
19	A	1103	CLA	O1D-CGD-O2D-CED
19	A	1122	CLA	C3A-C2A-CAA-CBA
19	A	1141	CLA	C3A-C2A-CAA-CBA
19	B	1234	CLA	C3A-C2A-CAA-CBA
19	2	2004	CLA	C3A-C2A-CAA-CBA
19	3	3016	CLA	C3A-C2A-CAA-CBA
19	4	1304	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	1103	CLA	CAA-CBA-CGA-O2A
19	A	1139	CLA	CAA-CBA-CGA-O2A
19	B	1218	CLA	CAA-CBA-CGA-O2A
19	4	4015	CLA	CAA-CBA-CGA-O2A
19	A	1101	CLA	CAD-CBD-CGD-O2D
19	A	1111	CLA	CAD-CBD-CGD-O2D
19	A	1119	CLA	CAD-CBD-CGD-O2D
19	A	1123	CLA	CAD-CBD-CGD-O2D
19	A	1135	CLA	CAD-CBD-CGD-O2D
19	B	1209	CLA	CAD-CBD-CGD-O2D
19	B	1221	CLA	CAD-CBD-CGD-O2D
19	B	1222	CLA	CAD-CBD-CGD-O2D
19	B	1225	CLA	CAD-CBD-CGD-O2D
19	H	1207	CLA	CAD-CBD-CGD-O2D
19	K	1142	CLA	CAD-CBD-CGD-O2D
19	1	1013	CLA	CAD-CBD-CGD-O2D
19	2	2013	CLA	CAD-CBD-CGD-O2D
22	4	7009	LMU	C2-C1-O1'-C1'
19	B	1220	CLA	C2-C1-O2A-CGA
22	A	7023	LMU	C11-C10-C9-C8
19	K	3009	CLA	CAA-CBA-CGA-O2A
19	B	1229	CLA	C4-C3-C5-C6
19	A	9023	CLA	C16-C17-C18-C20
19	A	1109	CLA	C2-C3-C5-C6
19	4	4007	CLA	C2-C3-C5-C6
19	4	1304	CLA	CAA-CBA-CGA-O2A
21	A	6002	BCR	C17-C18-C19-C20
21	B	6006	BCR	C17-C18-C19-C20
21	B	6020	BCR	C7-C8-C9-C10
19	A	1103	CLA	C2C-C3C-CAC-CBC
19	A	1138	CLA	C2C-C3C-CAC-CBC
19	A	1141	CLA	C2C-C3C-CAC-CBC
19	B	1210	CLA	C2C-C3C-CAC-CBC
19	F	1302	CLA	C2C-C3C-CAC-CBC
19	G	1242	CLA	C2C-C3C-CAC-CBC
19	J	1311	CLA	C2C-C3C-CAC-CBC
19	1	1010	CLA	C2C-C3C-CAC-CBC
19	4	4015	CLA	C2C-C3C-CAC-CBC
22	4	7008	LMU	C3'-C4'-O1B-C1B
19	A	1110	CLA	C6-C7-C8-C9
19	B	1233	CLA	CAA-CBA-CGA-O2A
19	1	1002	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	A	1116	CLA	O2A-C1-C2-C3
19	A	9023	CLA	O2A-C1-C2-C3
19	B	1222	CLA	O2A-C1-C2-C3
19	4	4001	CLA	O2A-C1-C2-C3
22	4	7008	LMU	C6-C7-C8-C9
19	1	1007	CLA	CAA-CBA-CGA-O2A
19	A	1109	CLA	C15-C16-C17-C18
19	4	4003	CLA	C6-C7-C8-C10
19	A	1103	CLA	CHA-CBD-CGD-O1D
19	A	1112	CLA	CHA-CBD-CGD-O2D
19	A	1115	CLA	CHA-CBD-CGD-O2D
19	A	1127	CLA	CHA-CBD-CGD-O1D
19	A	1127	CLA	CHA-CBD-CGD-O2D
19	A	1136	CLA	CHA-CBD-CGD-O1D
19	A	1136	CLA	CHA-CBD-CGD-O2D
19	A	1138	CLA	CHA-CBD-CGD-O2D
19	B	1202	CLA	CHA-CBD-CGD-O1D
19	B	1202	CLA	CHA-CBD-CGD-O2D
19	B	1205	CLA	CHA-CBD-CGD-O1D
19	B	1205	CLA	CHA-CBD-CGD-O2D
19	B	1212	CLA	CHA-CBD-CGD-O1D
19	B	1212	CLA	CHA-CBD-CGD-O2D
19	B	1216	CLA	CHA-CBD-CGD-O1D
19	B	1235	CLA	CHA-CBD-CGD-O1D
19	B	1239	CLA	CHA-CBD-CGD-O1D
19	B	1239	CLA	CHA-CBD-CGD-O2D
19	J	1308	CLA	CHA-CBD-CGD-O1D
19	J	1308	CLA	CHA-CBD-CGD-O2D
19	L	1502	CLA	CHA-CBD-CGD-O1D
19	L	1502	CLA	CHA-CBD-CGD-O2D
19	2	2013	CLA	CHA-CBD-CGD-O2D
19	2	2014	CLA	CHA-CBD-CGD-O2D
19	3	3011	CLA	CHA-CBD-CGD-O1D
19	3	3011	CLA	CHA-CBD-CGD-O2D
19	3	3016	CLA	CHA-CBD-CGD-O1D
19	3	3016	CLA	CHA-CBD-CGD-O2D
19	4	4003	CLA	CHA-CBD-CGD-O2D
19	4	4006	CLA	CHA-CBD-CGD-O1D
19	4	4006	CLA	CHA-CBD-CGD-O2D
19	4	4014	CLA	CHA-CBD-CGD-O1D
19	4	4014	CLA	CHA-CBD-CGD-O2D
19	A	1141	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	A	7045	LMU	C3'-C4'-O1B-C1B
22	4	7053	LMU	C7-C8-C9-C10
19	3	3016	CLA	C10-C11-C12-C13
21	B	6010	BCR	C20-C21-C22-C23
21	B	6017	BCR	C20-C21-C22-C23
21	F	6016	BCR	C20-C21-C22-C23
19	2	2013	CLA	CAA-CBA-CGA-O2A
22	L	7029	LMU	C5-C6-C7-C8
19	A	1111	CLA	CAA-CBA-CGA-O2A
19	A	1125	CLA	CAA-CBA-CGA-O2A
19	4	4001	CLA	C2A-CAA-CBA-CGA
19	A	1125	CLA	C16-C17-C18-C19
19	B	1221	CLA	C4-C3-C5-C6
19	B	9010	CLA	C11-C12-C13-C15
19	3	1147	CLA	CAA-CBA-CGA-O2A
19	3	3013	CLA	CAA-CBA-CGA-O2A
22	A	7010	LMU	C11-C10-C9-C8
19	A	1140	CLA	C6-C7-C8-C9
19	A	9011	CLA	C6-C7-C8-C9
19	B	1202	CLA	C11-C12-C13-C14
19	B	1212	CLA	C11-C10-C8-C9
19	H	1145	CLA	C14-C13-C15-C16
19	H	1207	CLA	C11-C10-C8-C9
21	I	6018	BCR	C15-C16-C17-C18
22	B	7012	LMU	C2-C1-O1'-C1'
19	A	1140	CLA	CAA-CBA-CGA-O2A
19	1	1002	CLA	CAA-CBA-CGA-O2A
19	A	9011	CLA	C16-C17-C18-C20
22	G	7026	LMU	C11-C10-C9-C8
22	G	7039	LMU	O1'-C1-C2-C3
19	A	1138	CLA	CAA-CBA-CGA-O1A
19	B	1223	CLA	CAA-CBA-CGA-O1A
19	B	1233	CLA	CAA-CBA-CGA-O1A
19	1	1007	CLA	CAA-CBA-CGA-O1A
19	4	1304	CLA	CAA-CBA-CGA-O1A
19	A	1138	CLA	C1A-C2A-CAA-CBA
19	B	1218	CLA	C1A-C2A-CAA-CBA
19	B	1220	CLA	C1A-C2A-CAA-CBA
19	B	1232	CLA	C1A-C2A-CAA-CBA
19	H	1505	CLA	C1A-C2A-CAA-CBA
19	K	1142	CLA	C1A-C2A-CAA-CBA
19	1	1008	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	2	2004	CLA	C1A-C2A-CAA-CBA
22	E	7037	LMU	C2-C3-C4-C5
19	A	1103	CLA	CAA-CBA-CGA-O1A
19	I	1204	CLA	CAA-CBA-CGA-O1A
22	1	7004	LMU	C4B-C5B-C6B-O6B
19	B	1213	CLA	C2A-CAA-CBA-CGA
19	B	1233	CLA	C2A-CAA-CBA-CGA
19	A	9011	CLA	CAA-CBA-CGA-O1A
19	B	1218	CLA	CAA-CBA-CGA-O1A
19	H	1505	CLA	CAA-CBA-CGA-O1A
22	1	7013	LMU	C7-C8-C9-C10
19	A	1139	CLA	CAA-CBA-CGA-O1A
19	A	1125	CLA	CAA-CBA-CGA-O1A
19	B	1217	CLA	CAA-CBA-CGA-O1A
19	K	3009	CLA	CAA-CBA-CGA-O1A
21	F	6016	BCR	C5-C6-C7-C8
21	3	6022	BCR	C23-C24-C25-C26
21	3	6022	BCR	C23-C24-C25-C30
19	A	1123	CLA	C13-C15-C16-C17
19	B	1239	CLA	C8-C10-C11-C12
19	2	2013	CLA	CAA-CBA-CGA-O1A
19	4	4015	CLA	CAA-CBA-CGA-O1A
19	4	4007	CLA	CAA-CBA-CGA-O2A
19	A	1140	CLA	CAA-CBA-CGA-O1A
22	H	7002	LMU	C2-C3-C4-C5
19	A	1106	CLA	C10-C11-C12-C13
19	3	3011	CLA	C15-C16-C17-C18
22	R	7007	LMU	C3-C4-C5-C6
19	A	1102	CLA	CAD-CBD-CGD-O1D
19	A	1103	CLA	CAD-CBD-CGD-O1D
19	A	1106	CLA	CAD-CBD-CGD-O1D
19	A	1132	CLA	CAD-CBD-CGD-O1D
19	A	9013	CLA	CAD-CBD-CGD-O1D
19	B	1201	CLA	CAD-CBD-CGD-O1D
19	B	1235	CLA	CAD-CBD-CGD-O1D
19	H	1505	CLA	CAD-CBD-CGD-O1D
19	4	4001	CLA	CAD-CBD-CGD-O1D
19	4	4015	CLA	CAD-CBD-CGD-O1D
19	L	1130	CLA	O1A-CGA-O2A-C1
19	A	1111	CLA	CAA-CBA-CGA-O1A
19	A	1141	CLA	CAA-CBA-CGA-O1A
22	H	7017	LMU	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
19	B	1211	CLA	C11-C12-C13-C14
19	1	1014	CLA	C6-C7-C8-C9
19	2	2014	CLA	C6-C7-C8-C9
22	K	7042	LMU	C2-C3-C4-C5
19	2	2002	CLA	C3-C5-C6-C7
19	B	1208	CLA	C6-C7-C8-C10
19	B	1219	CLA	CAA-CBA-CGA-O2A
19	2	2007	CLA	CAA-CBA-CGA-O2A
19	3	3017	CLA	CAA-CBA-CGA-O2A
22	H	7032	LMU	C2-C3-C4-C5
19	A	1109	CLA	CAA-CBA-CGA-O2A
19	A	1115	CLA	CAA-CBA-CGA-O2A
19	B	1235	CLA	CAA-CBA-CGA-O2A
19	A	1111	CLA	C4-C3-C5-C6
19	A	1124	CLA	C4-C3-C5-C6
19	A	1137	CLA	C3A-C2A-CAA-CBA
19	A	1237	CLA	C6-C7-C8-C10
19	A	9011	CLA	C6-C7-C8-C10
19	A	9012	CLA	C12-C13-C15-C16
19	B	1212	CLA	C2-C3-C5-C6
19	B	1220	CLA	C11-C10-C8-C7
19	J	1308	CLA	C3A-C2A-CAA-CBA
19	R	1150	CLA	C3A-C2A-CAA-CBA
19	2	2014	CLA	C6-C7-C8-C10
19	A	1109	CLA	CAA-CBA-CGA-O1A
19	A	1131	CLA	CAA-CBA-CGA-O1A
19	A	1131	CLA	CAA-CBA-CGA-O2A
21	B	6005	BCR	C17-C18-C19-C20
21	B	6006	BCR	C7-C8-C9-C10
19	3	3017	CLA	CAA-CBA-CGA-O1A
21	B	6004	BCR	C15-C16-C17-C18
21	F	6014	BCR	C15-C16-C17-C18
22	4	7033	LMU	C2-C1-O1'-C1'
19	A	9023	CLA	CAA-CBA-CGA-O2A
19	A	9022	CLA	C8-C10-C11-C12
19	4	4007	CLA	CAA-CBA-CGA-O1A
19	B	1215	CLA	C5-C6-C7-C8
19	H	1241	CLA	CAA-CBA-CGA-O2A
22	4	7052	LMU	C4-C5-C6-C7
22	4	7018	LMU	O1'-C1-C2-C3
19	A	1123	CLA	CAA-CBA-CGA-O2A
19	1	1303	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

234 monomers are involved in 3097 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	H	7002	LMU	3	0
22	E	7048	LMU	17	0
19	B	1201	CLA	11	0
19	B	1230	CLA	21	0
22	H	7030	LMU	4	0
19	A	1110	CLA	3	0
19	2	2004	CLA	18	0
19	A	1125	CLA	65	0
19	4	4010	CLA	2	0
21	A	6007	BCR	32	0
19	A	1120	CLA	10	0
21	I	6018	BCR	15	0
22	B	7038	LMU	7	0
19	B	1235	CLA	62	0
22	E	7037	LMU	7	0
19	3	3006	CLA	9	0
19	A	1136	CLA	24	0
23	C	8002	SF4	6	0
19	A	1128	CLA	21	0
19	3	3012	CLA	11	0
19	A	1103	CLA	19	0
19	B	1202	CLA	31	0
19	3	3004	CLA	7	0
21	B	6017	BCR	42	0
19	B	1215	CLA	10	0
19	A	1101	CLA	15	0
19	A	1137	CLA	8	0
19	L	1502	CLA	27	0
19	3	3011	CLA	12	0
22	B	7012	LMU	1	0
22	G	7039	LMU	4	0
22	K	7047	LMU	5	2
19	A	1106	CLA	27	0
19	A	1123	CLA	29	0
19	B	1219	CLA	13	0
19	L	1501	CLA	17	0
19	B	1209	CLA	14	0
19	L	1504	CLA	21	0
19	A	1108	CLA	7	0
19	B	1222	CLA	43	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	H	1241	CLA	11	0
19	B	1217	CLA	9	0
21	B	6004	BCR	6	0
19	H	1505	CLA	3	0
19	3	3003	CLA	7	0
19	A	1112	CLA	31	0
19	3	3016	CLA	14	0
19	A	1138	CLA	29	0
19	A	1134	CLA	20	0
22	H	7017	LMU	2	0
19	A	1127	CLA	16	0
19	A	1139	CLA	31	0
19	B	1218	CLA	20	0
21	A	6003	BCR	14	0
22	4	7034	LMU	36	0
23	A	8001	SF4	2	0
22	4	7019	LMU	1	0
21	F	6016	BCR	37	0
19	L	1148	CLA	21	0
19	1	1011	CLA	6	0
19	J	1308	CLA	31	0
22	A	7016	LMU	12	0
19	A	1109	CLA	18	0
19	1	1002	CLA	10	0
21	1	6023	BCR	6	0
19	B	1220	CLA	44	0
19	A	9011	CLA	13	0
19	1	1010	CLA	8	0
19	4	4002	CLA	23	0
22	R	7007	LMU	5	0
19	A	1119	CLA	43	0
22	4	7008	LMU	3	0
22	1	7013	LMU	4	0
19	L	1503	CLA	9	0
19	B	1301	CLA	6	0
19	3	3010	CLA	5	0
19	2	2011	CLA	1	0
22	R	7022	LMU	5	0
19	B	1231	CLA	16	0
19	4	1304	CLA	23	0
19	1	1007	CLA	19	0
19	4	4001	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	8003	SF4	3	0
22	A	7045	LMU	2	0
19	2	2001	CLA	13	0
19	3	3007	CLA	2	0
19	A	9013	CLA	29	0
19	4	1306	CLA	19	0
19	A	1113	CLA	9	0
19	A	1102	CLA	19	0
22	A	7023	LMU	6	0
19	J	1311	CLA	20	0
19	B	1223	CLA	38	0
19	B	1212	CLA	14	0
19	A	1140	CLA	47	0
19	A	1115	CLA	76	0
22	K	7001	LMU	11	0
19	B	1203	CLA	19	0
19	4	1004	CLA	33	0
19	B	1210	CLA	21	0
19	3	1147	CLA	15	0
19	B	9010	CLA	17	0
19	1	1005	CLA	5	0
19	4	4014	CLA	8	0
22	R	7025	LMU	1	0
22	R	7021	LMU	9	0
19	A	1149	CLA	7	0
19	A	1104	CLA	15	0
22	4	7009	LMU	3	0
19	4	4003	CLA	2	0
19	B	1236	CLA	24	0
19	L	1130	CLA	29	0
22	R	7020	LMU	10	0
19	B	1211	CLA	19	0
22	4	7052	LMU	36	0
19	3	3005	CLA	9	0
22	K	7041	LMU	6	0
22	B	7040	LMU	3	0
19	2	2003	CLA	1	0
22	D	7050	LMU	21	0
19	B	1239	CLA	22	0
19	A	9023	CLA	53	0
19	A	9022	CLA	39	0
19	3	3017	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1015	CLA	3	0
19	1	1008	CLA	8	1
22	A	7010	LMU	6	0
19	A	1133	CLA	31	0
20	A	5001	PQN	9	0
22	N	7049	LMU	9	0
19	B	1221	CLA	21	0
22	4	7053	LMU	13	0
19	1	1303	CLA	10	0
21	B	6020	BCR	24	0
19	K	1146	CLA	7	0
19	A	1126	CLA	43	0
19	F	1302	CLA	10	0
22	A	7044	LMU	1	0
19	B	1229	CLA	20	0
19	B	1208	CLA	6	0
19	1	1012	CLA	2	0
19	1	1014	CLA	17	0
19	2	2007	CLA	18	0
19	3	2009	CLA	37	0
19	B	1224	CLA	19	0
19	B	1213	CLA	19	0
19	B	1214	CLA	23	0
19	B	1227	CLA	11	0
19	2	2014	CLA	35	0
19	A	1122	CLA	24	0
19	2	4009	CLA	6	0
22	2	7031	LMU	2	0
19	B	1234	CLA	11	0
19	3	3013	CLA	18	0
19	G	1242	CLA	9	0
22	G	7051	LMU	1	0
22	R	7014	LMU	4	0
19	A	1121	CLA	8	0
19	B	1228	CLA	14	0
19	K	1142	CLA	15	1
22	L	7029	LMU	11	0
19	K	3009	CLA	3	7
19	A	1107	CLA	40	0
19	B	1216	CLA	15	0
19	A	1151	CLA	18	0
19	B	1238	CLA	24	0

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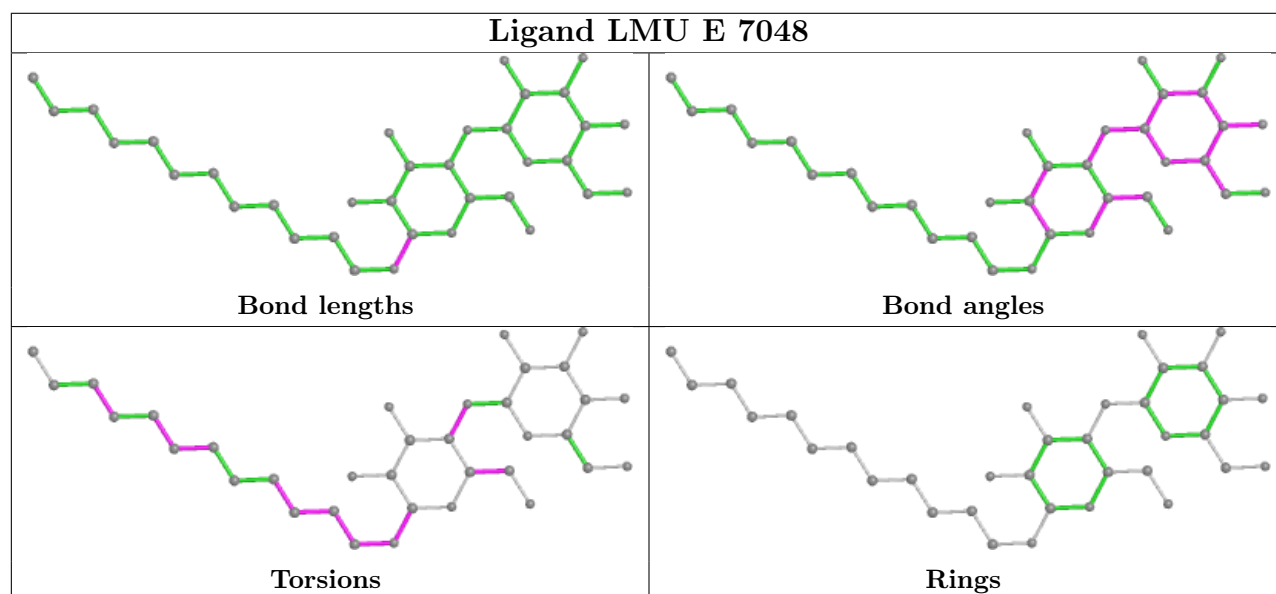
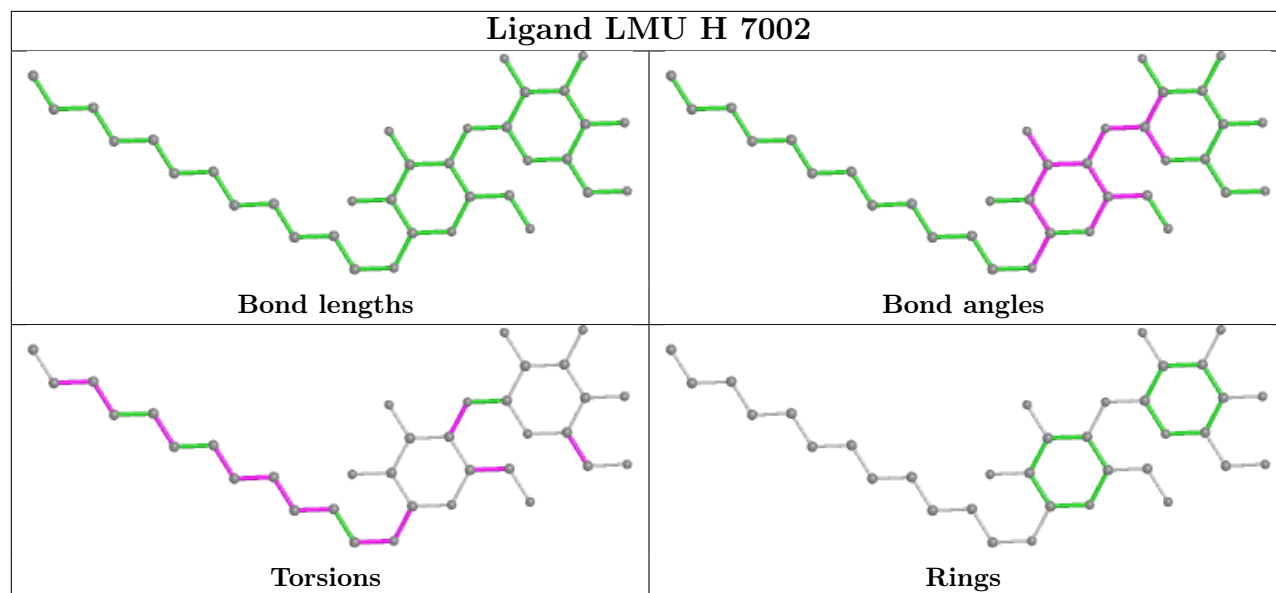
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22	F	7036	LMU	12	0
19	4	4004	CLA	2	0
19	A	1237	CLA	31	0
21	B	6006	BCR	14	0
19	I	1204	CLA	7	0
19	4	4015	CLA	4	0
21	A	6008	BCR	27	0
19	R	1144	CLA	10	0
19	4	1009	CLA	3	0
19	4	4006	CLA	11	0
19	A	1111	CLA	21	0
22	2	7046	LMU	1	0
22	K	7042	LMU	16	0
19	1	1001	CLA	11	0
21	B	6010	BCR	23	0
19	B	1233	CLA	6	0
21	B	6005	BCR	7	0
22	H	7011	LMU	15	0
22	3	7005	LMU	38	0
19	A	1117	CLA	27	0
19	3	3008	CLA	15	0
19	1	1013	CLA	13	0
20	B	5002	PQN	22	0
19	H	1207	CLA	25	0
21	F	6014	BCR	24	0
19	A	1129	CLA	8	0
19	A	1132	CLA	18	0
19	A	1135	CLA	23	0
19	2	2013	CLA	5	0
19	2	2006	CLA	7	0
19	4	4011	CLA	2	0
22	4	7033	LMU	7	0
22	H	7032	LMU	11	0
19	B	1226	CLA	21	0
19	2	2012	CLA	20	0
19	4	4012	CLA	7	0
19	H	1145	CLA	22	0
19	1	1006	CLA	15	0
19	A	1131	CLA	36	0
19	B	1206	CLA	20	0
21	L	6019	BCR	34	0
21	J	6012	BCR	32	0

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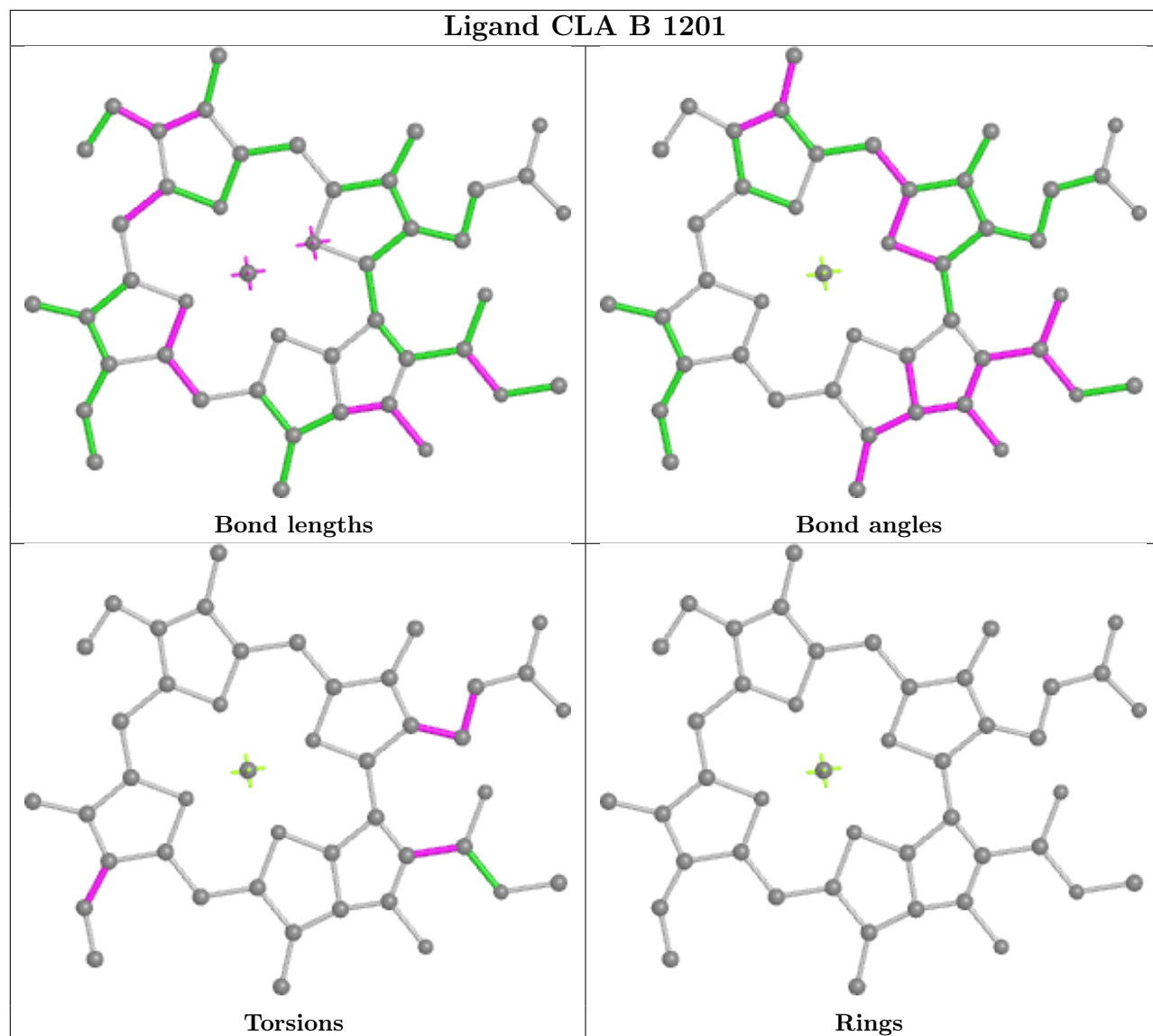
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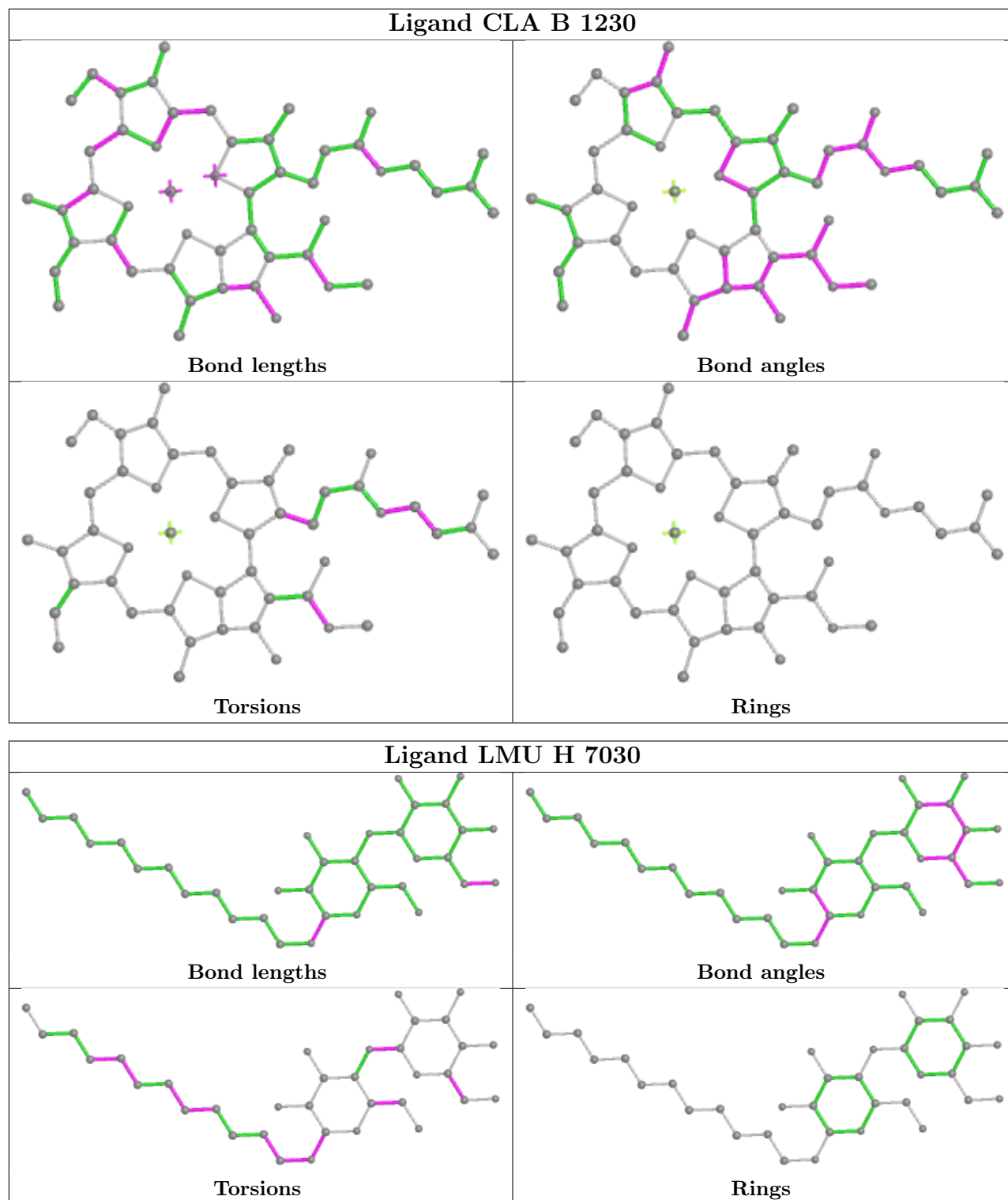
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	6011	BCR	46	0
19	A	9012	CLA	39	0
24	B	7101	LMG	19	0
19	2	2002	CLA	19	0
19	B	1232	CLA	18	0
19	B	1205	CLA	25	0
19	B	1225	CLA	28	0
19	R	1150	CLA	3	0
21	A	6002	BCR	43	0
22	1	7004	LMU	6	0
21	3	6022	BCR	6	0
19	4	4013	CLA	11	0
19	A	1141	CLA	29	0
22	2	7006	LMU	8	0
22	3	7003	LMU	20	0
19	A	1124	CLA	59	0
21	I	6021	BCR	32	0
19	F	1305	CLA	13	0
19	1	1003	CLA	5	0
22	H	7028	LMU	2	0
19	A	1105	CLA	26	0
22	G	7026	LMU	9	0
22	2	7027	LMU	3	0
22	H	7043	LMU	3	0
19	A	1116	CLA	9	0
19	K	1143	CLA	29	0

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

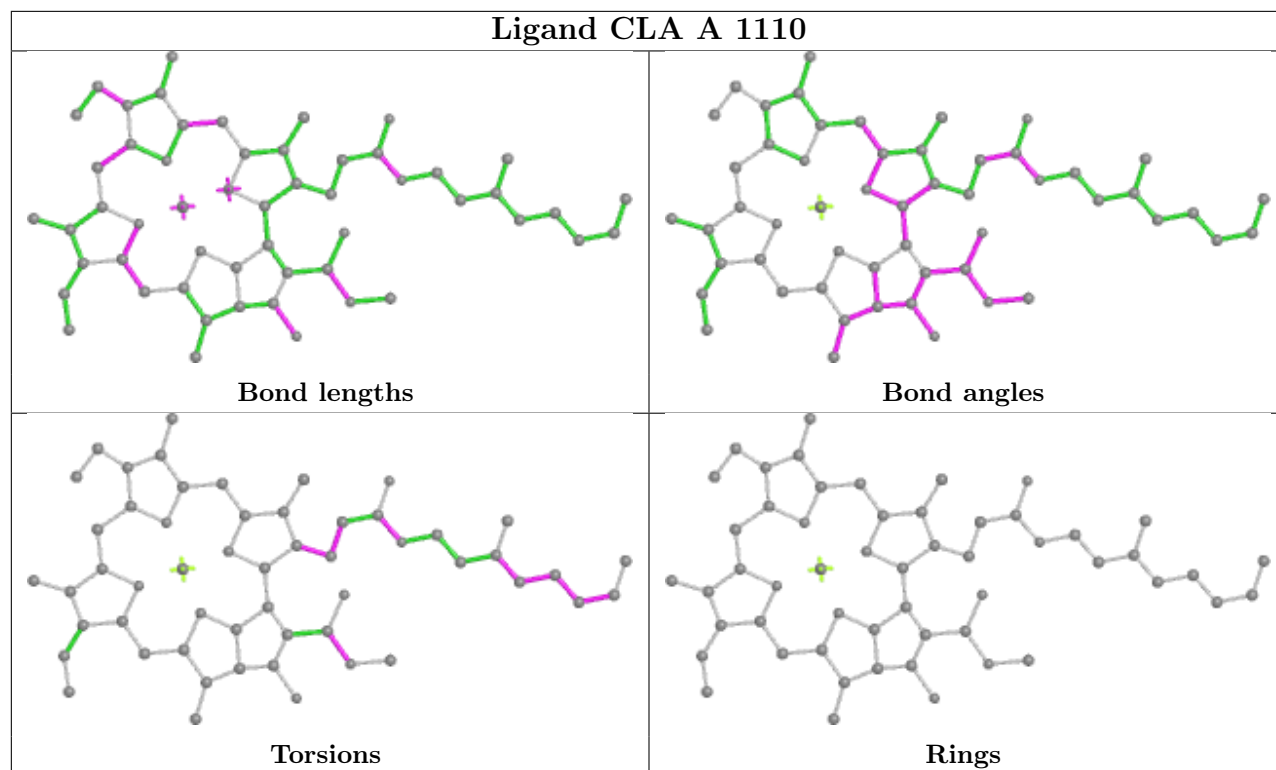


Ligand CLA B 1201

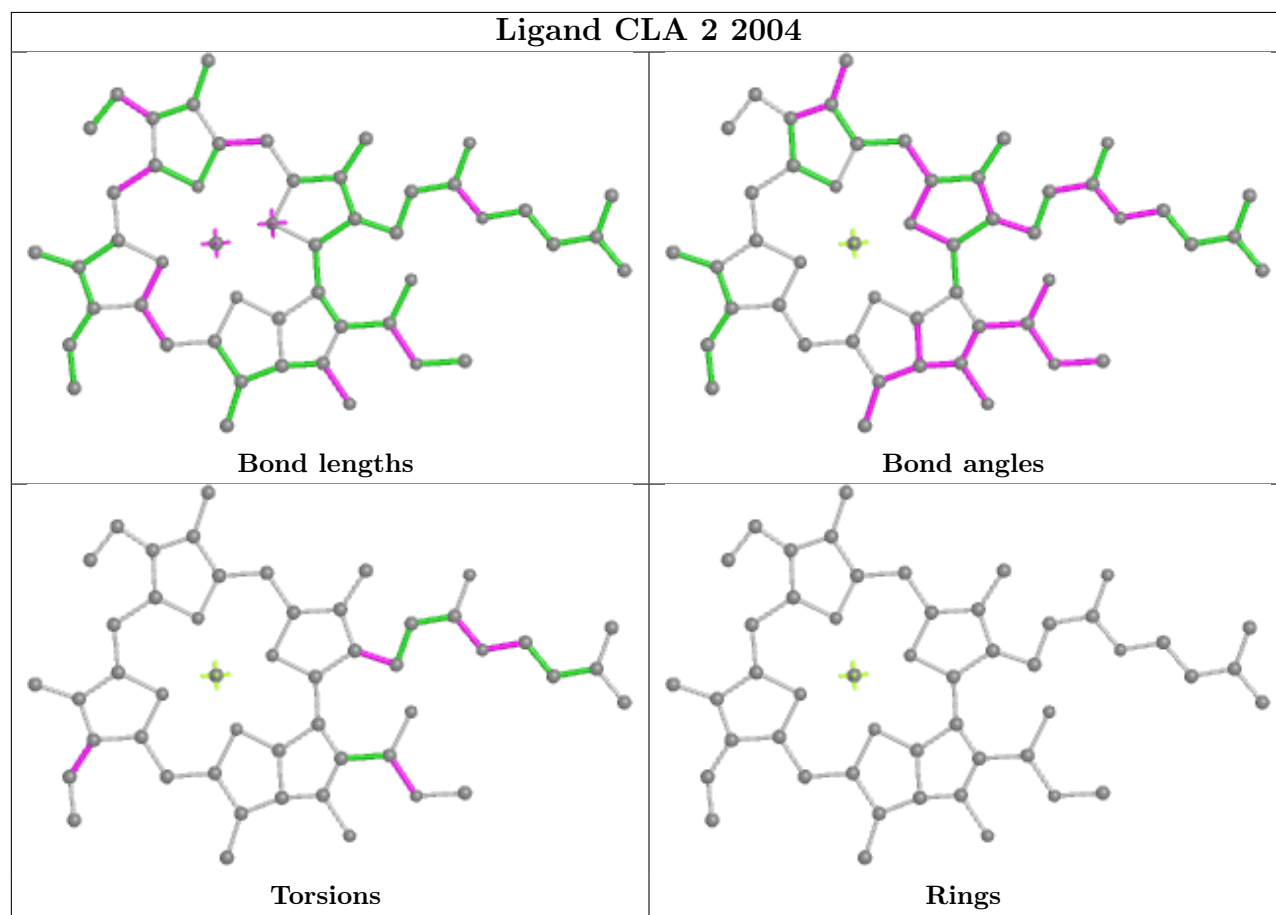


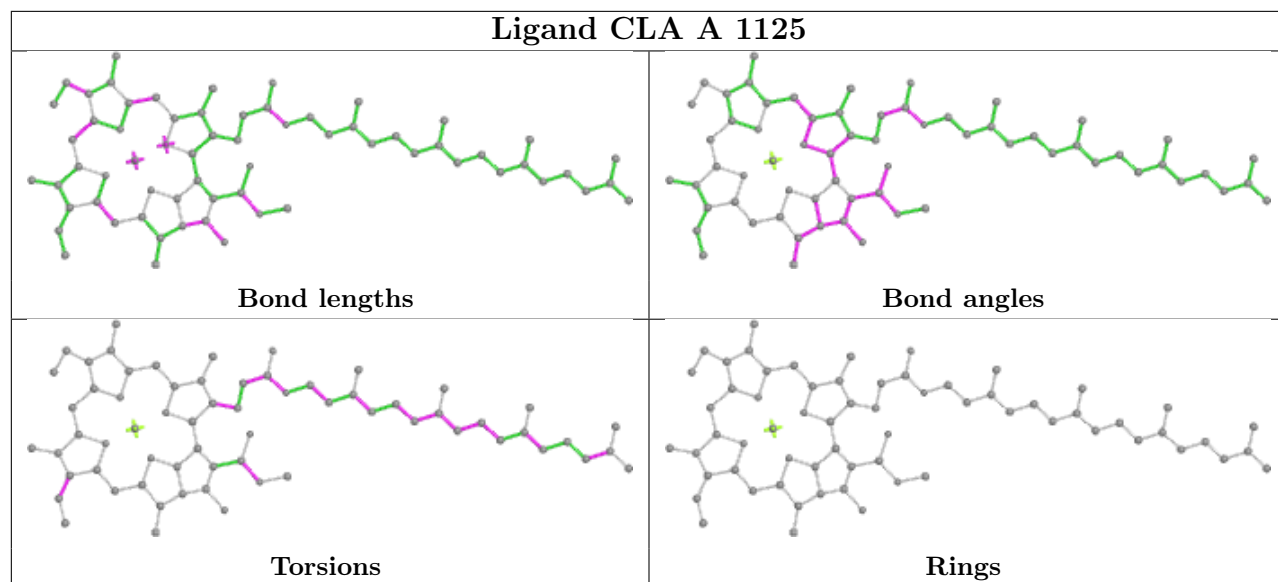


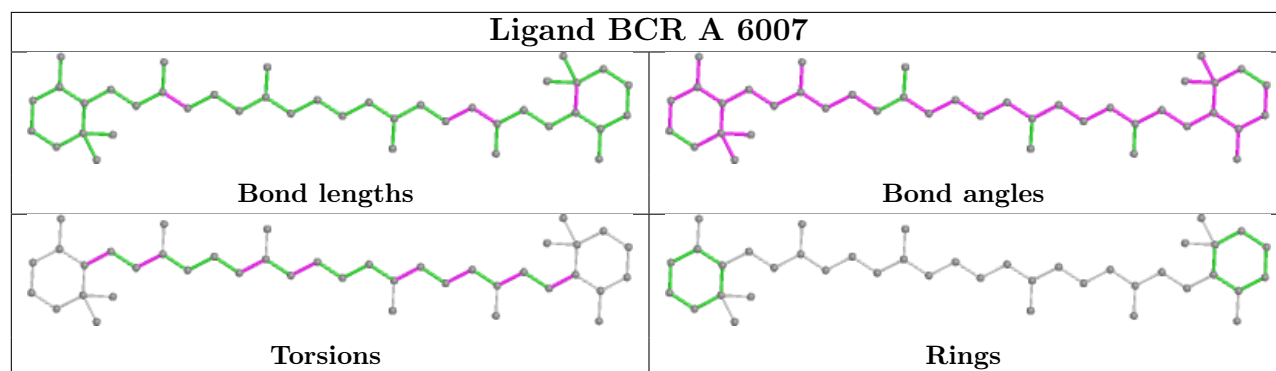
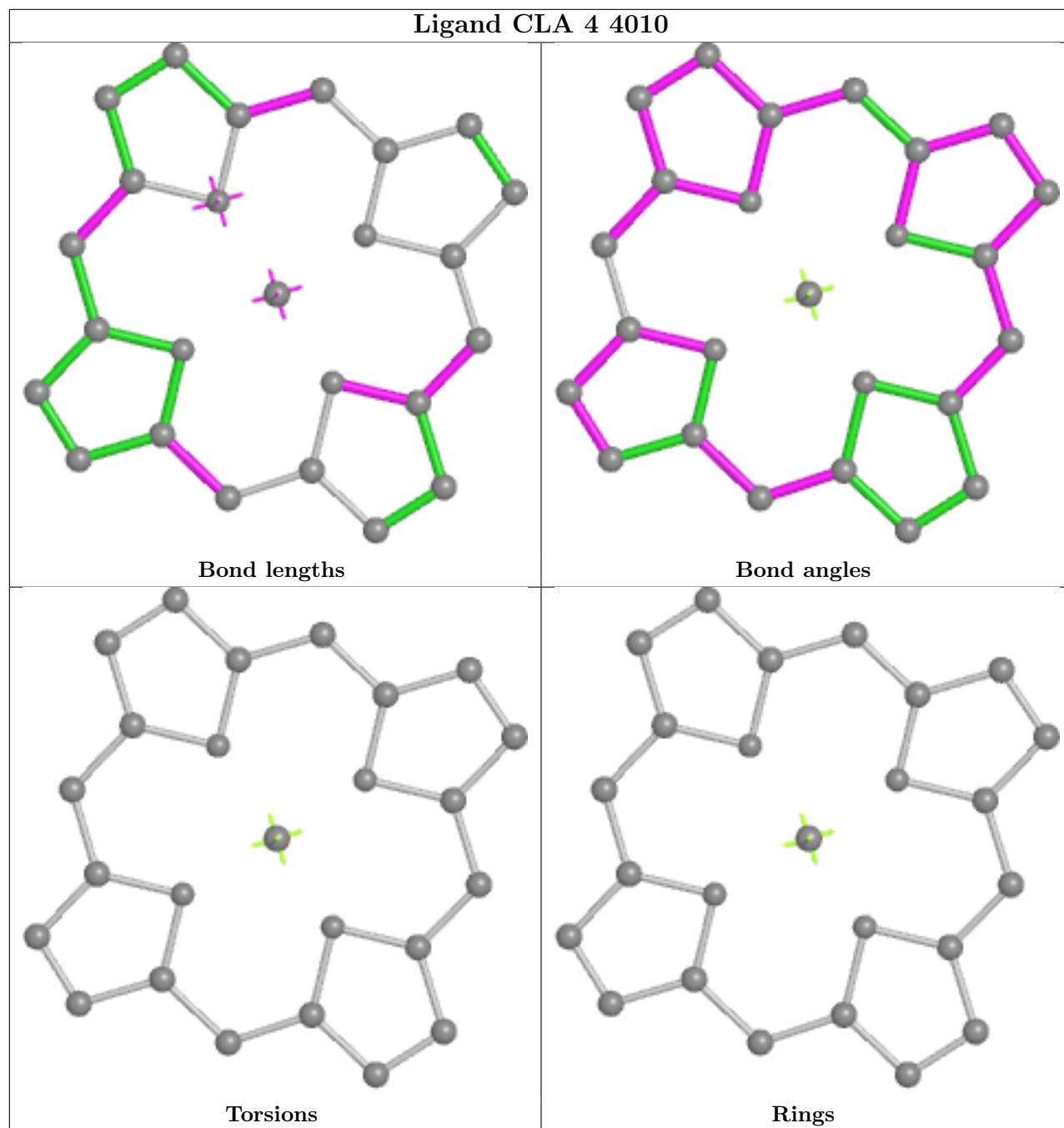
Ligand CLA A 1110



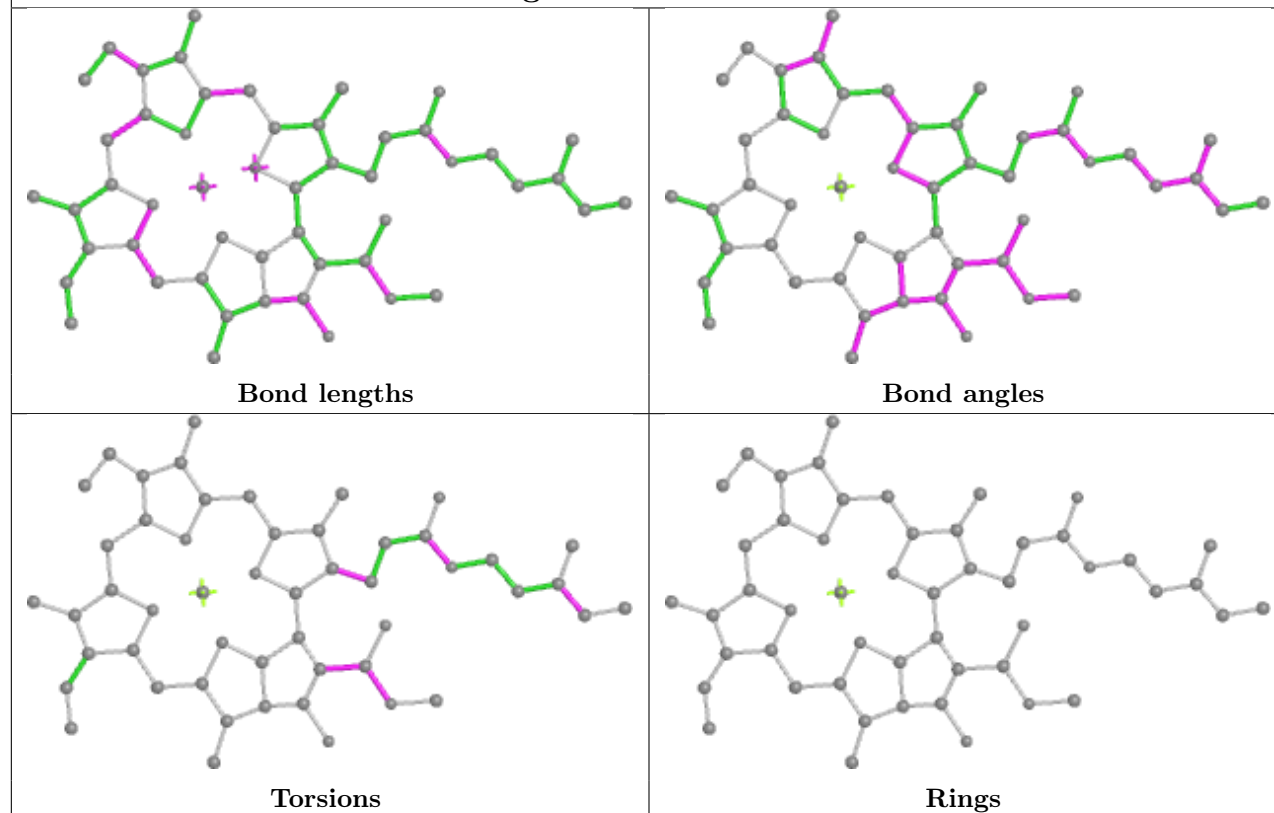
Ligand CLA 2 2004



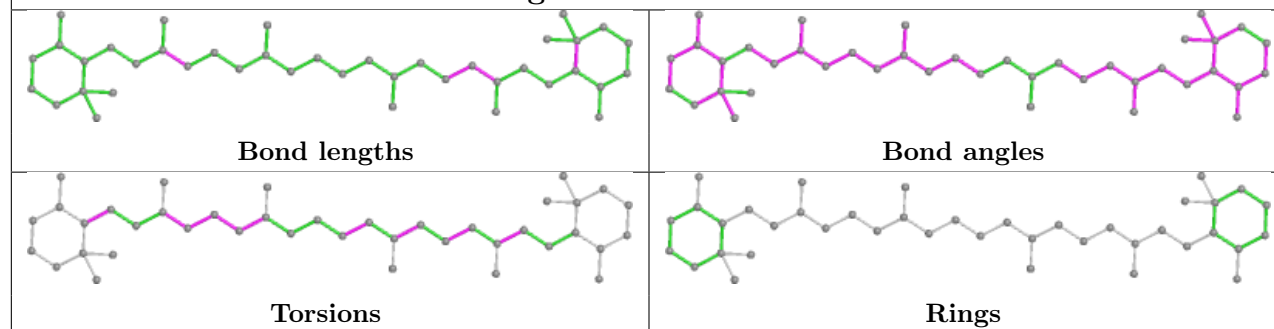


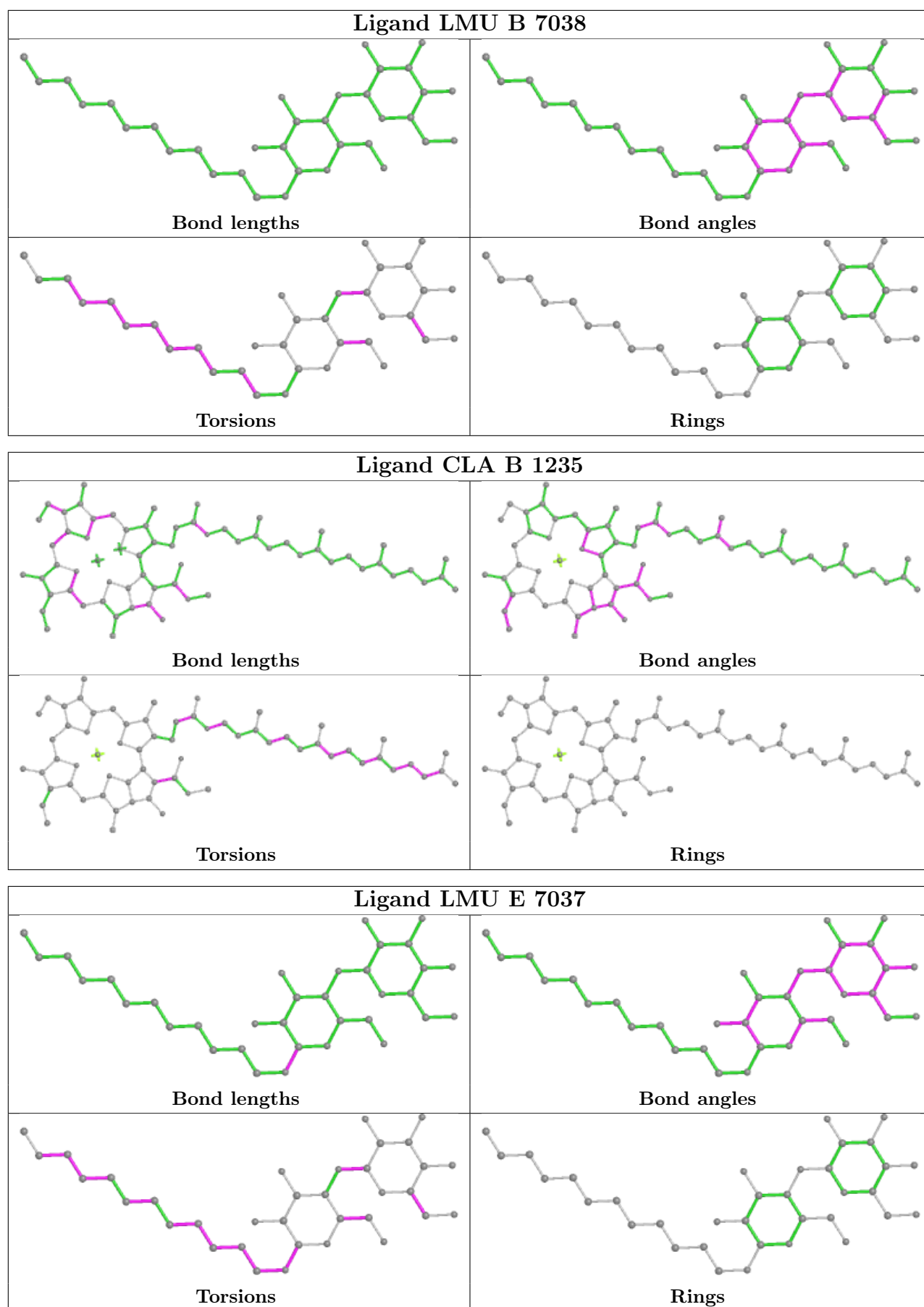


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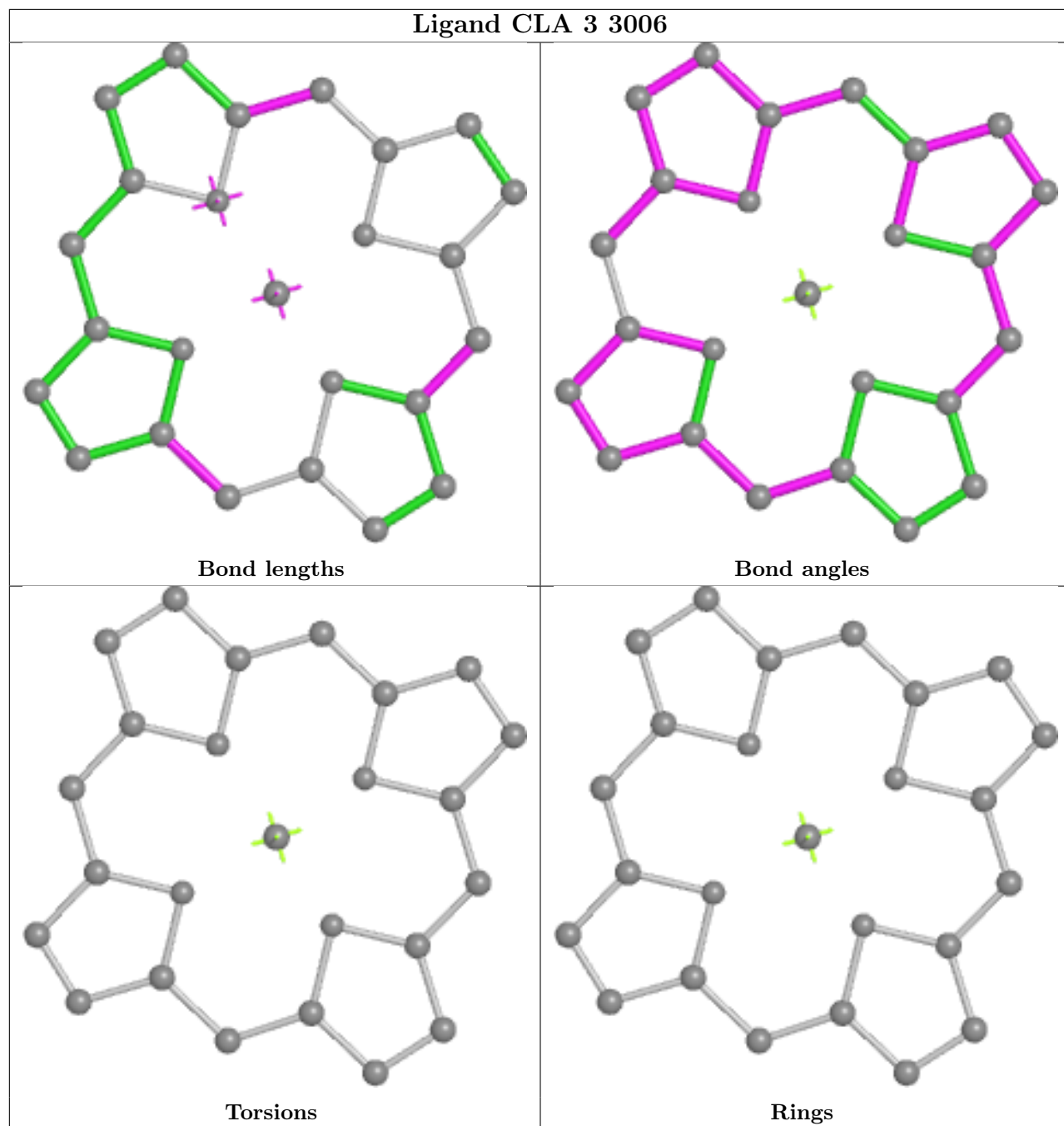


Ligand BCR I 6018

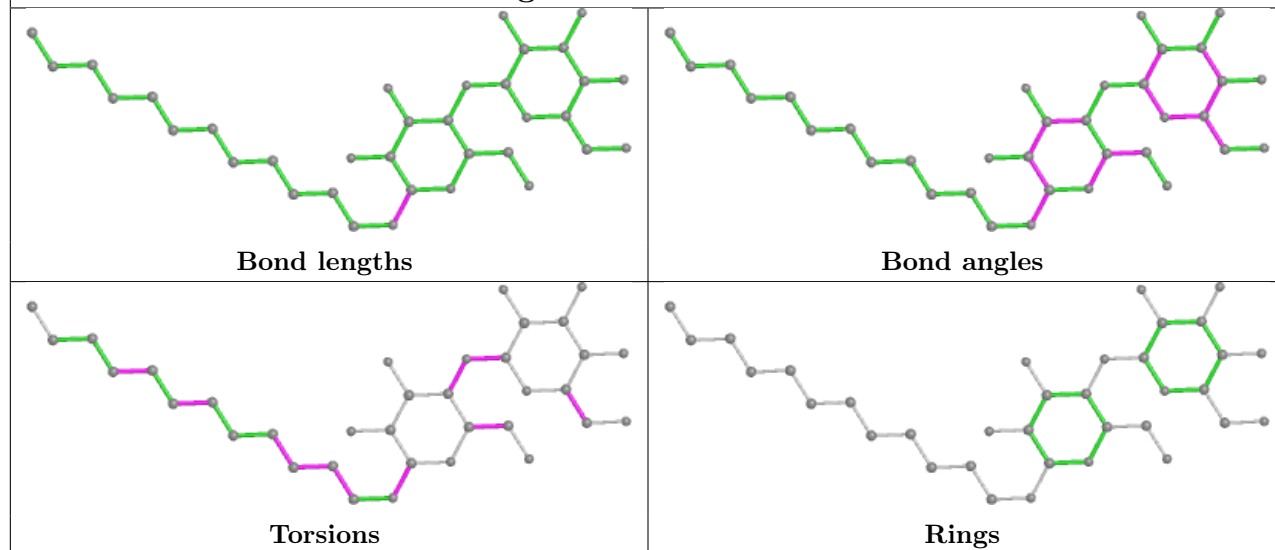




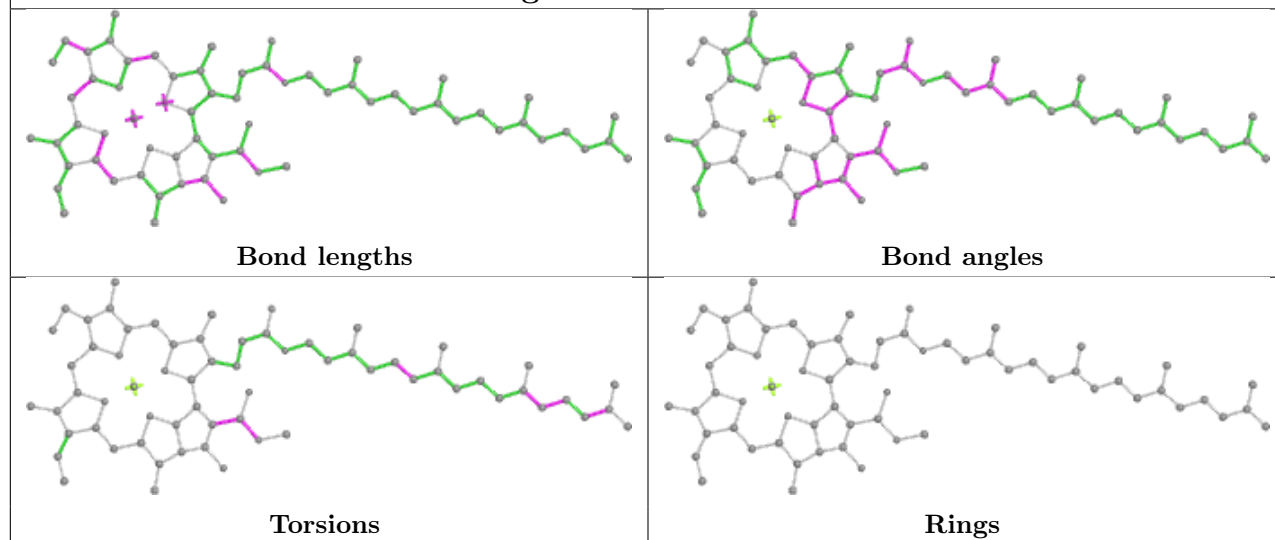
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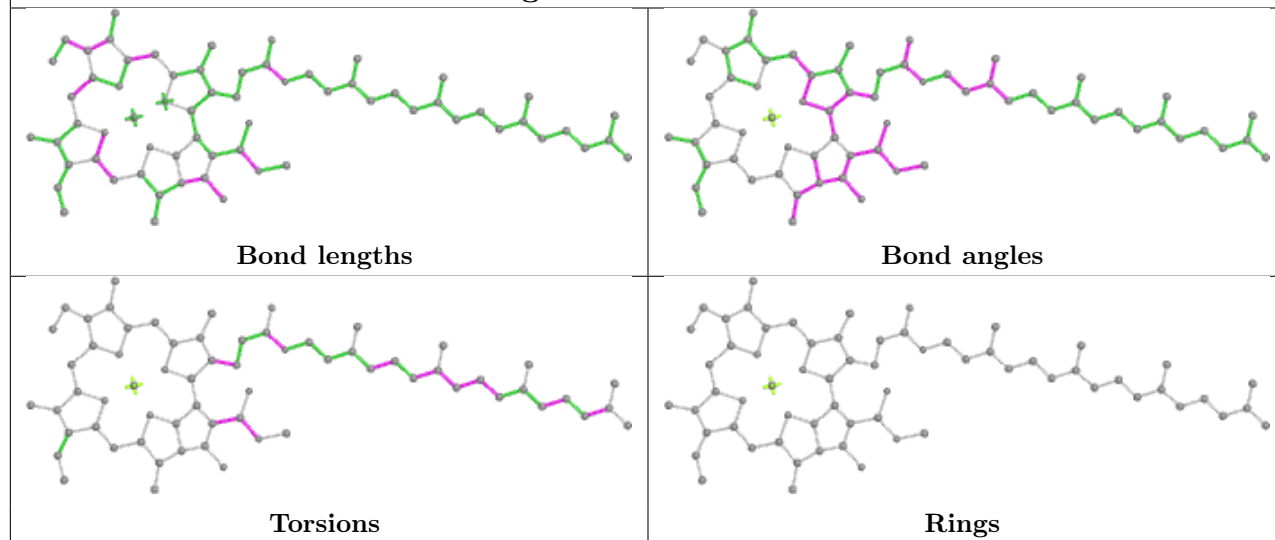
Ligand LMU R 7024



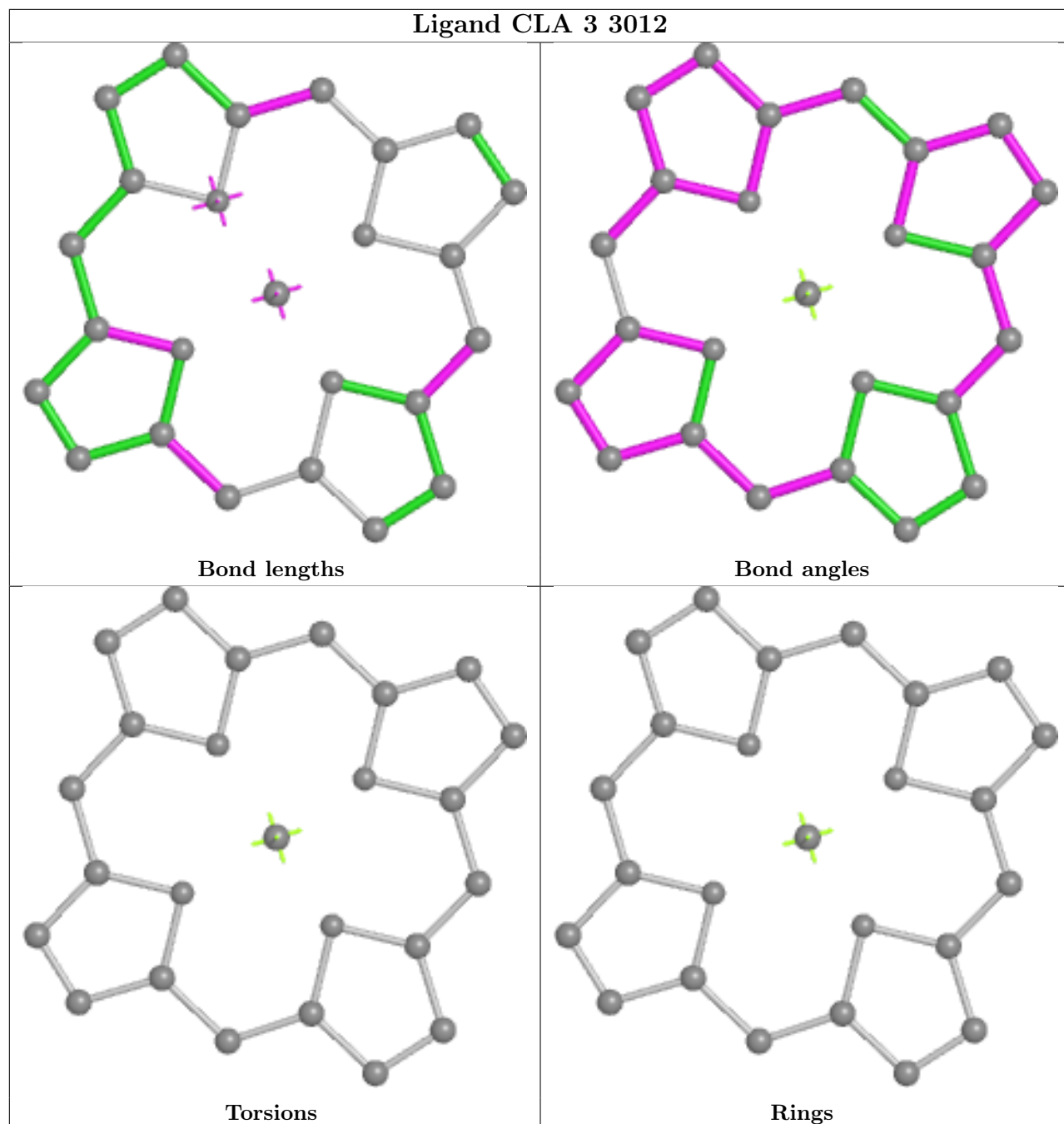
Ligand CLA A 1136

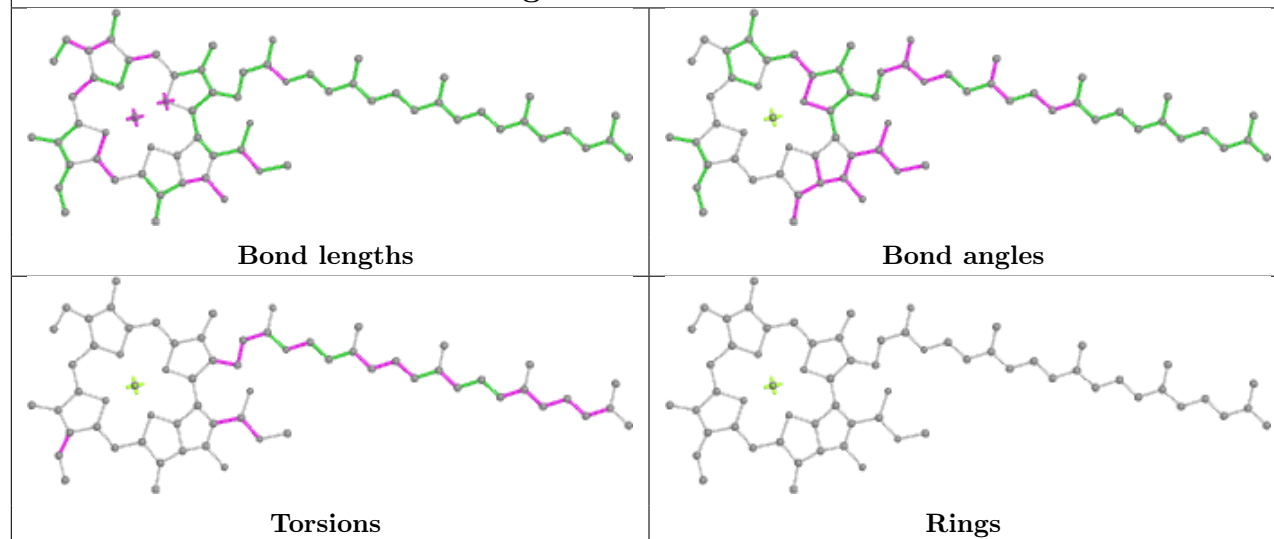
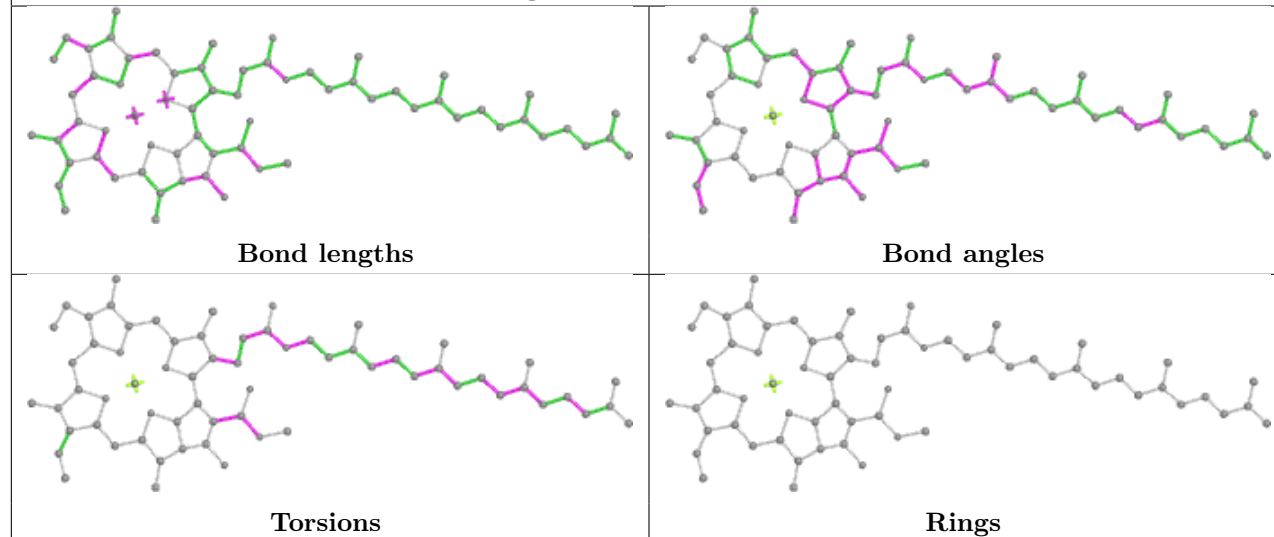


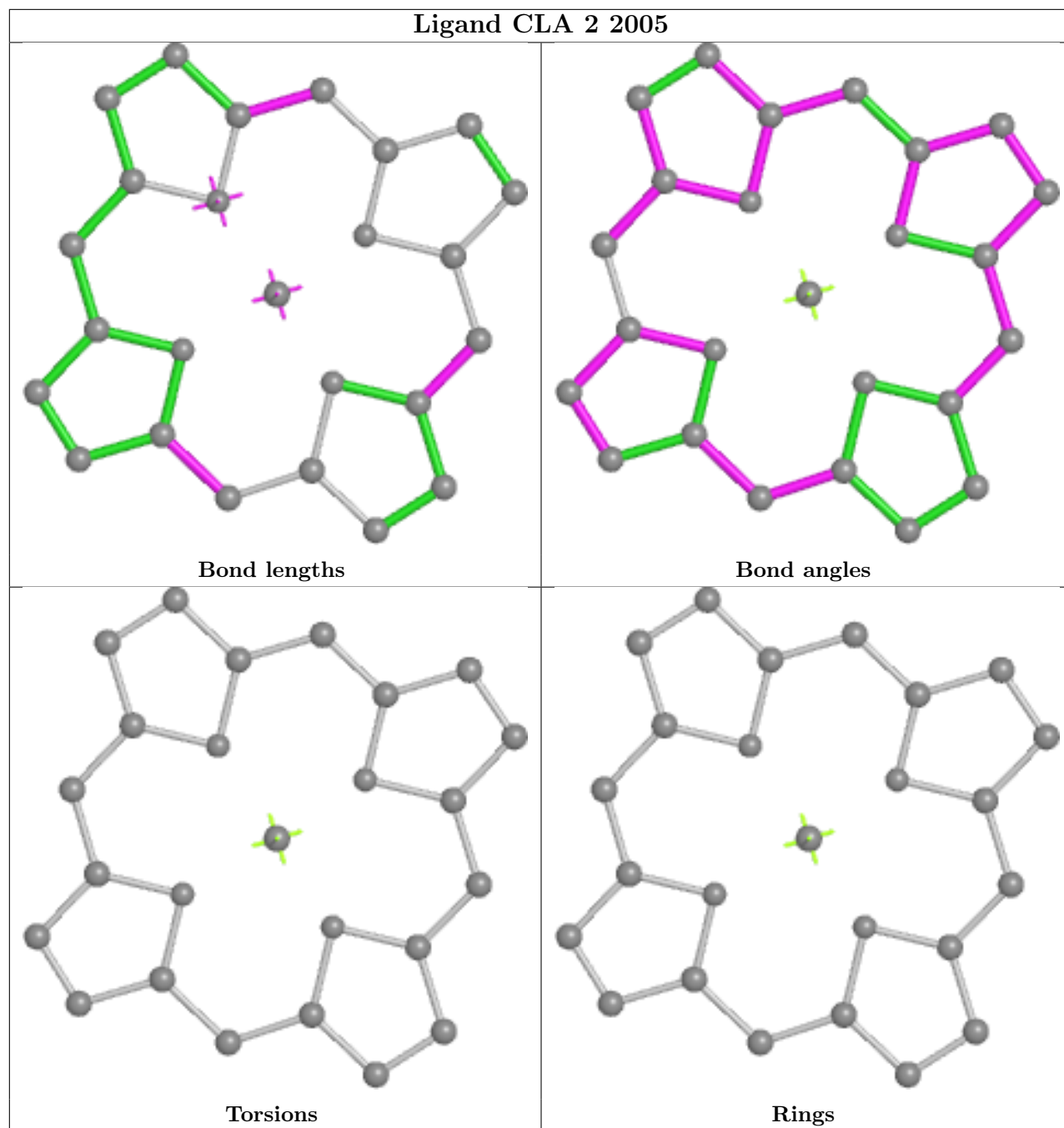
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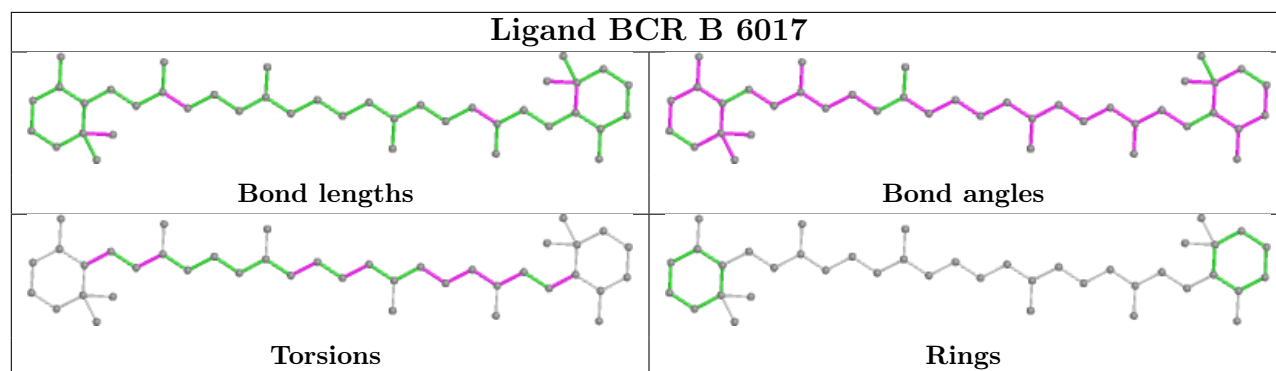
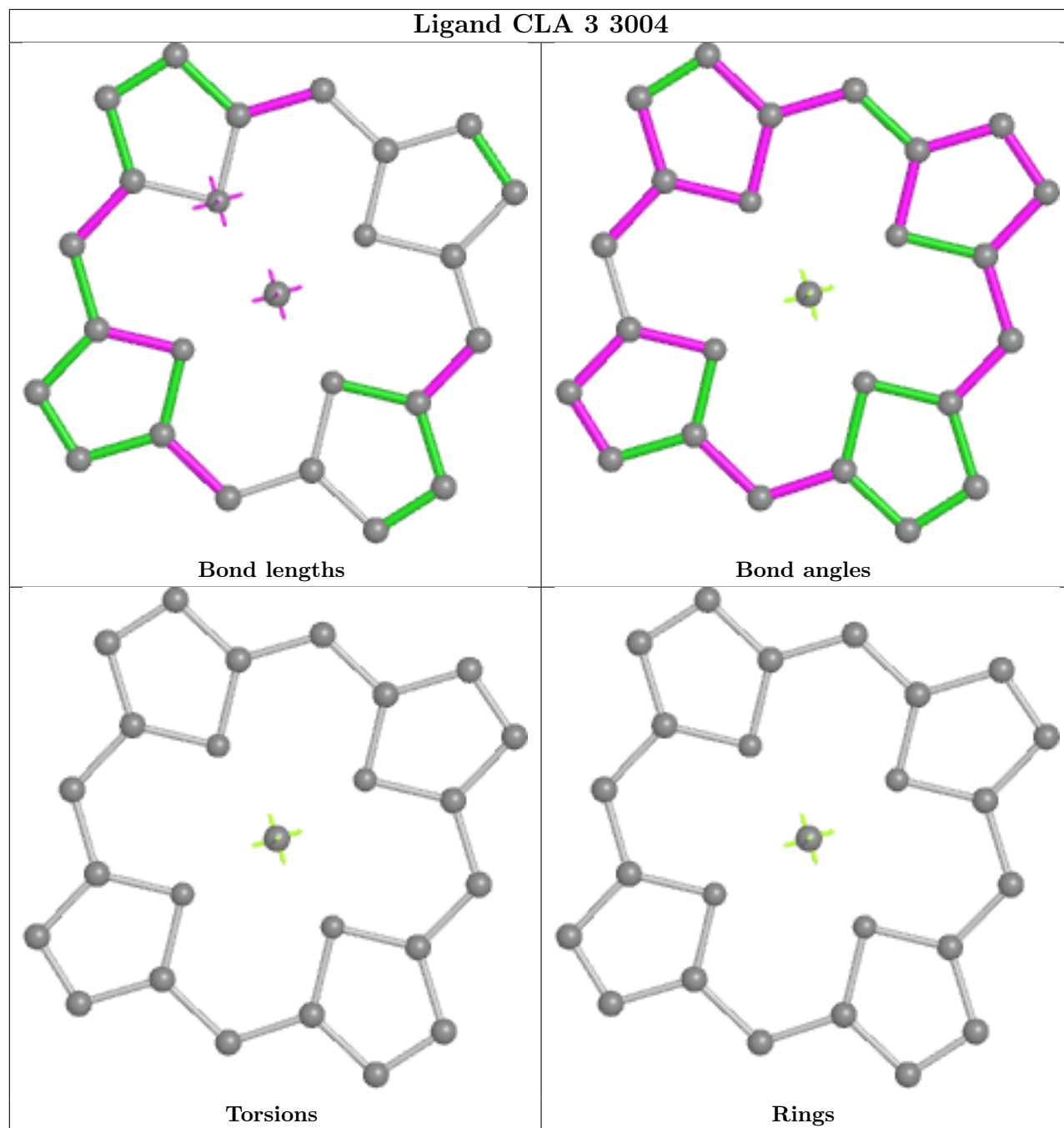


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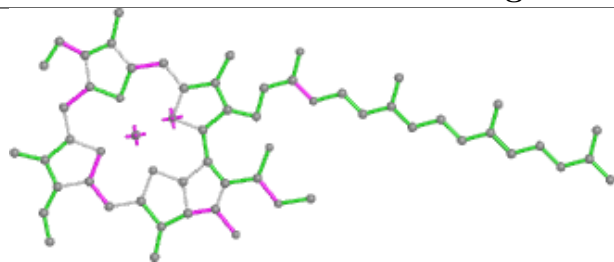


Ligand CLA A 1103**Ligand CLA B 1202**

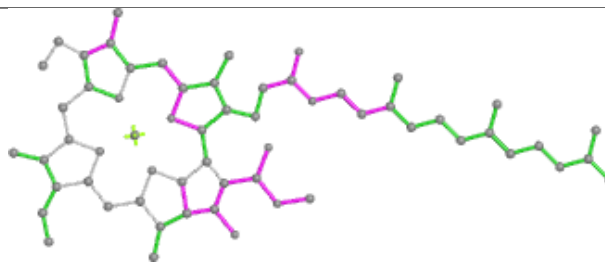




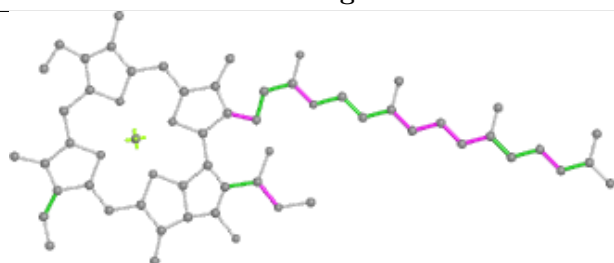
Ligand CLA B 1215



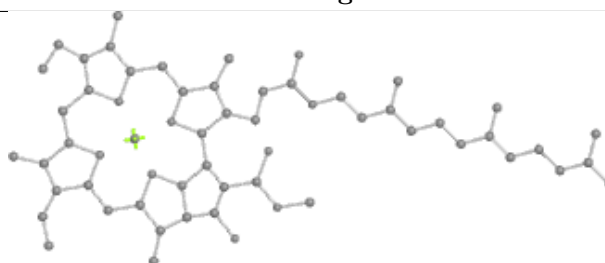
Bond lengths



Bond angles

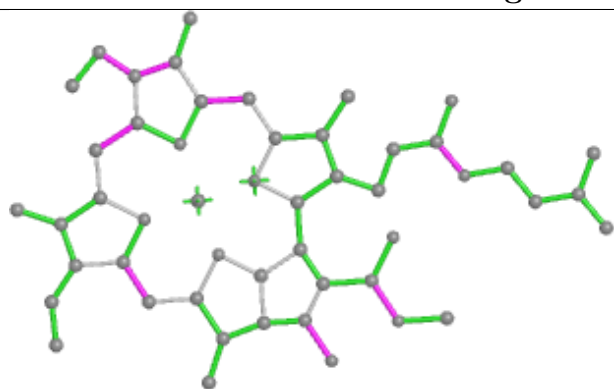


Torsions

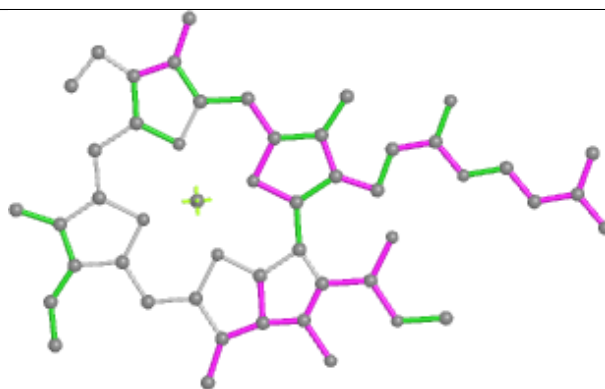


Rings

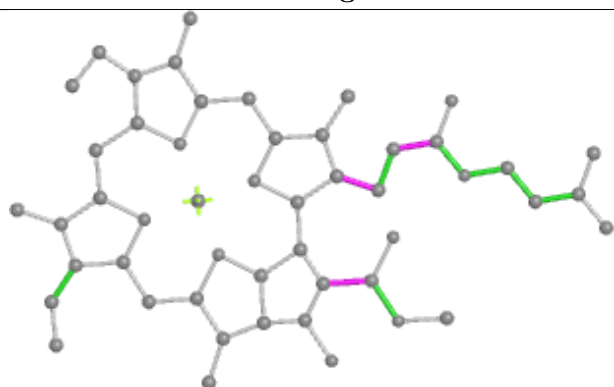
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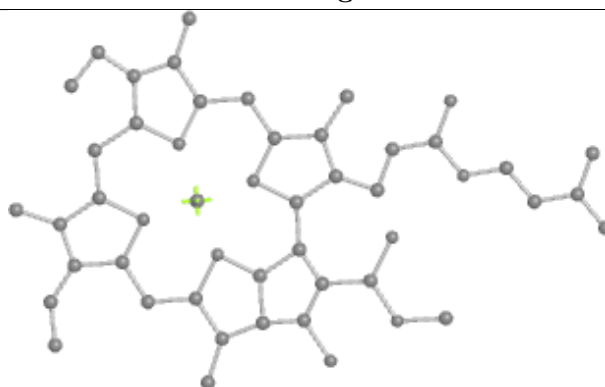
Bond lengths



Bond angles

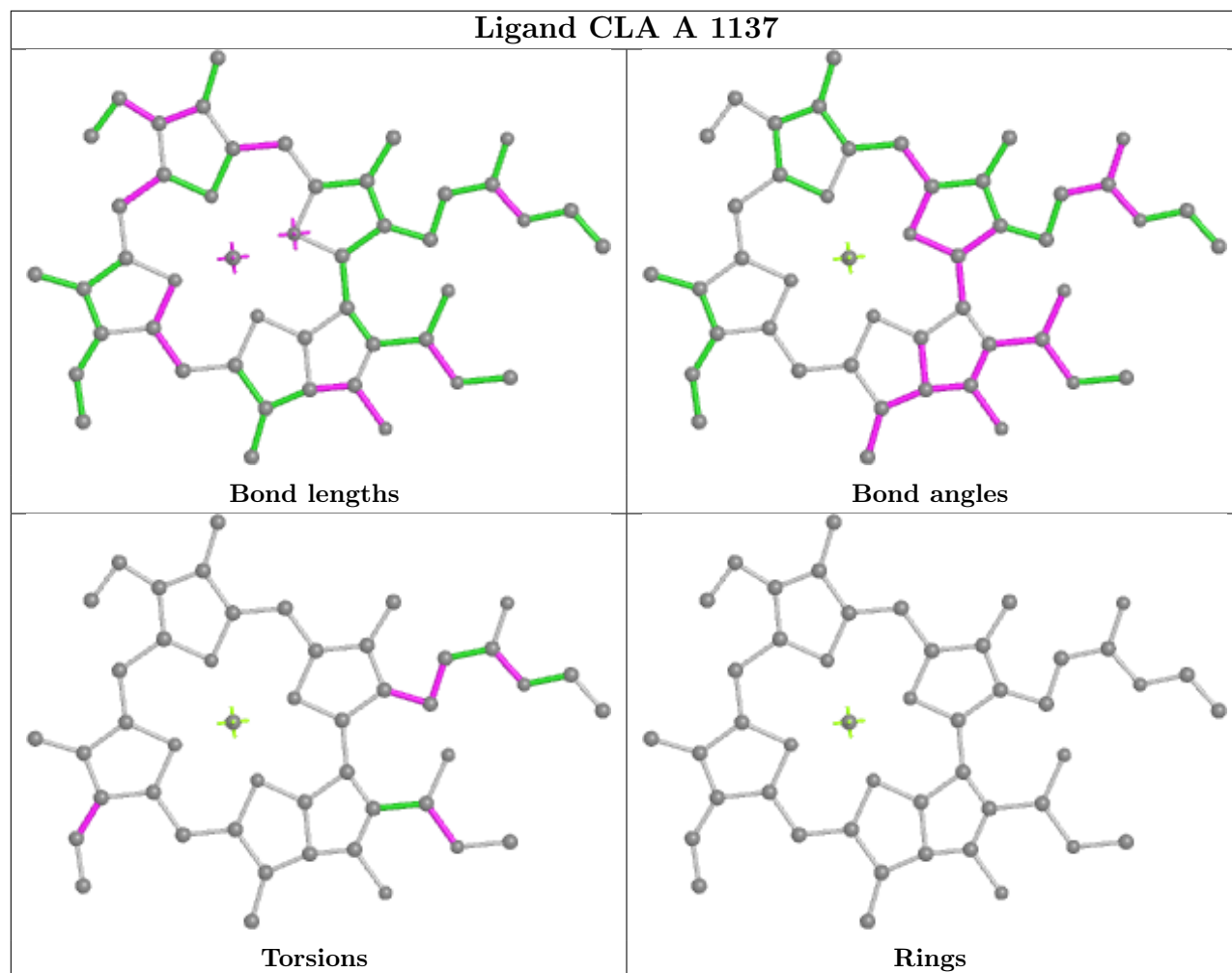


Torsions

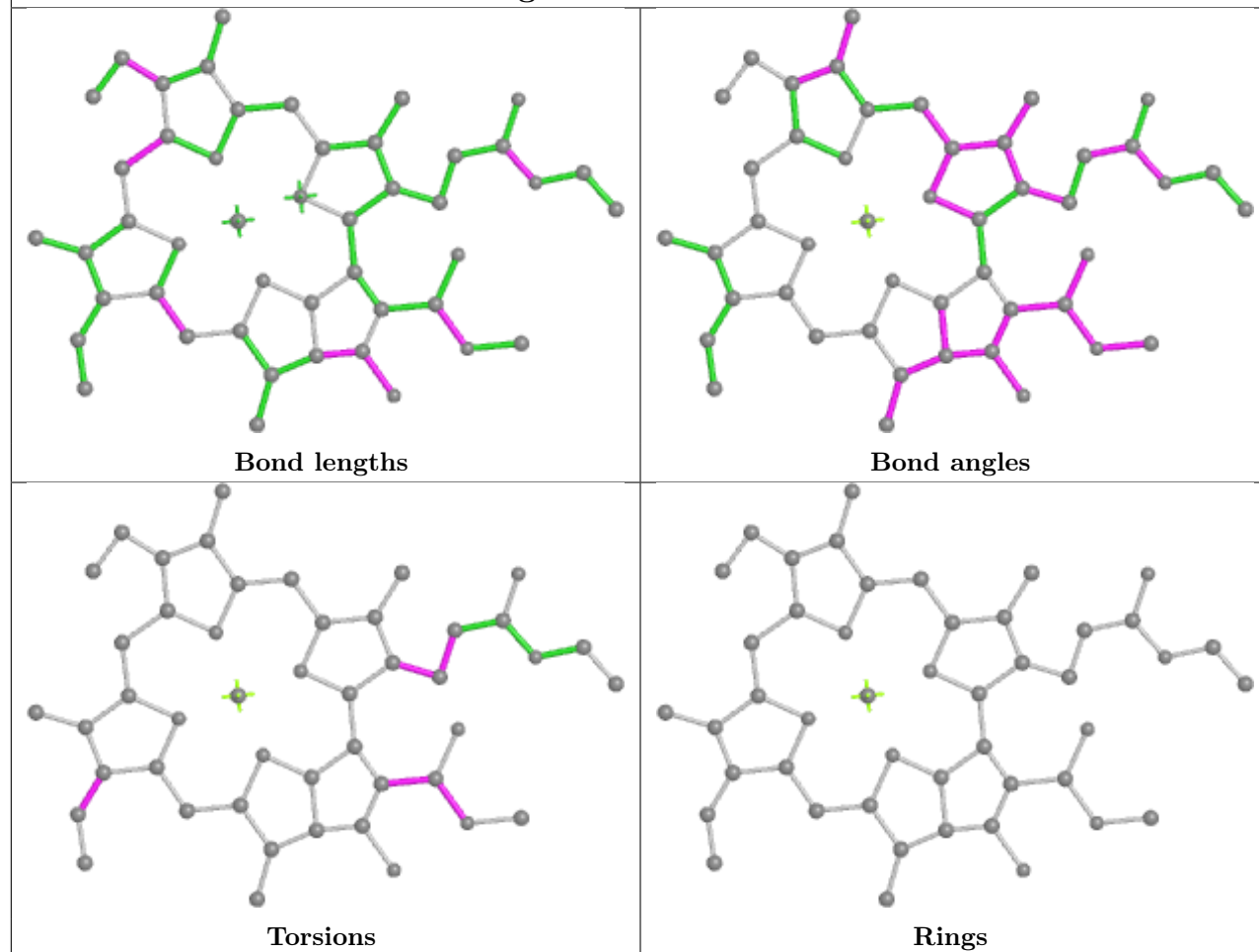


Rings

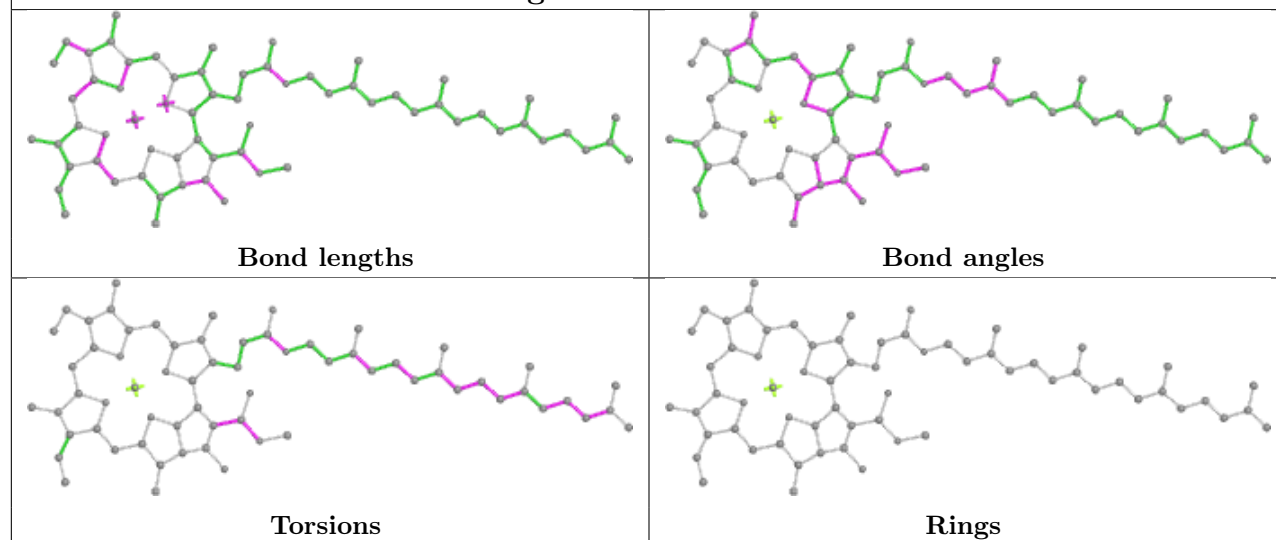
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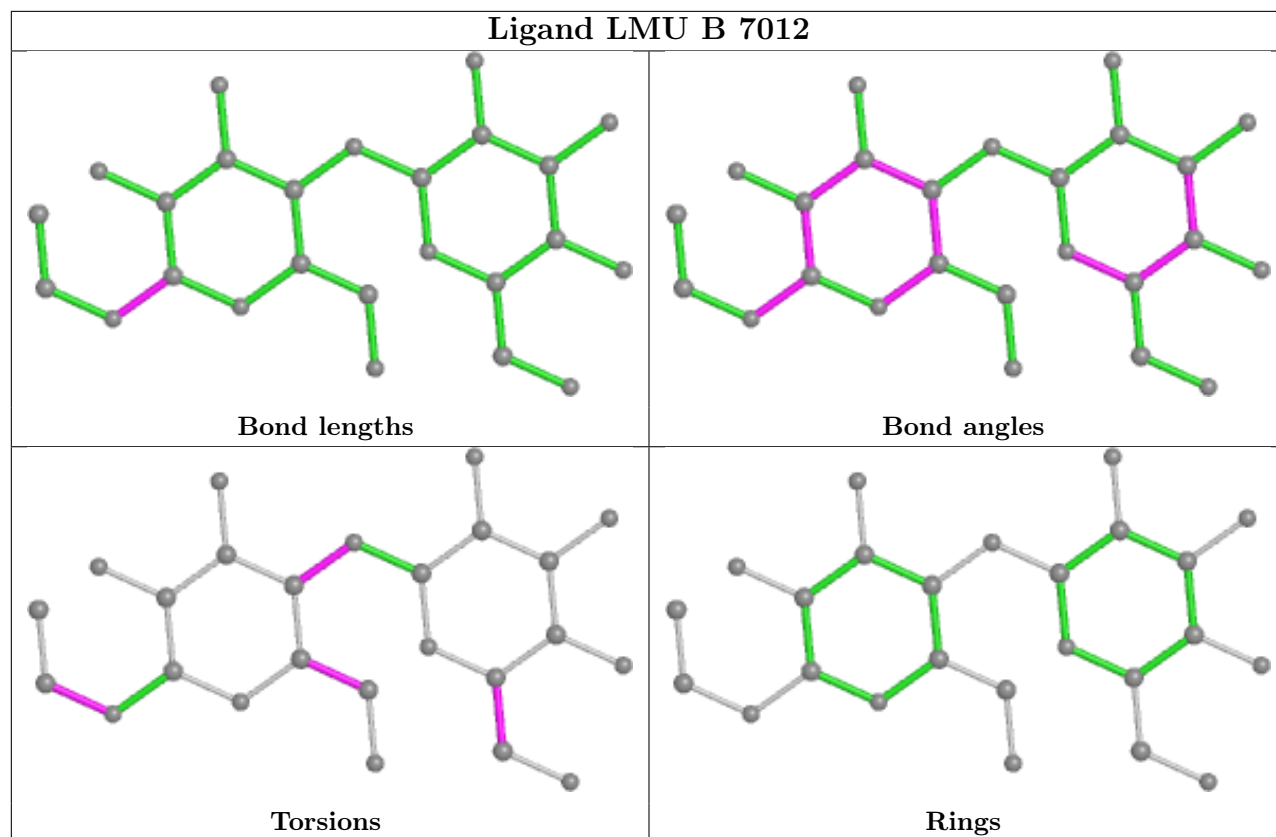
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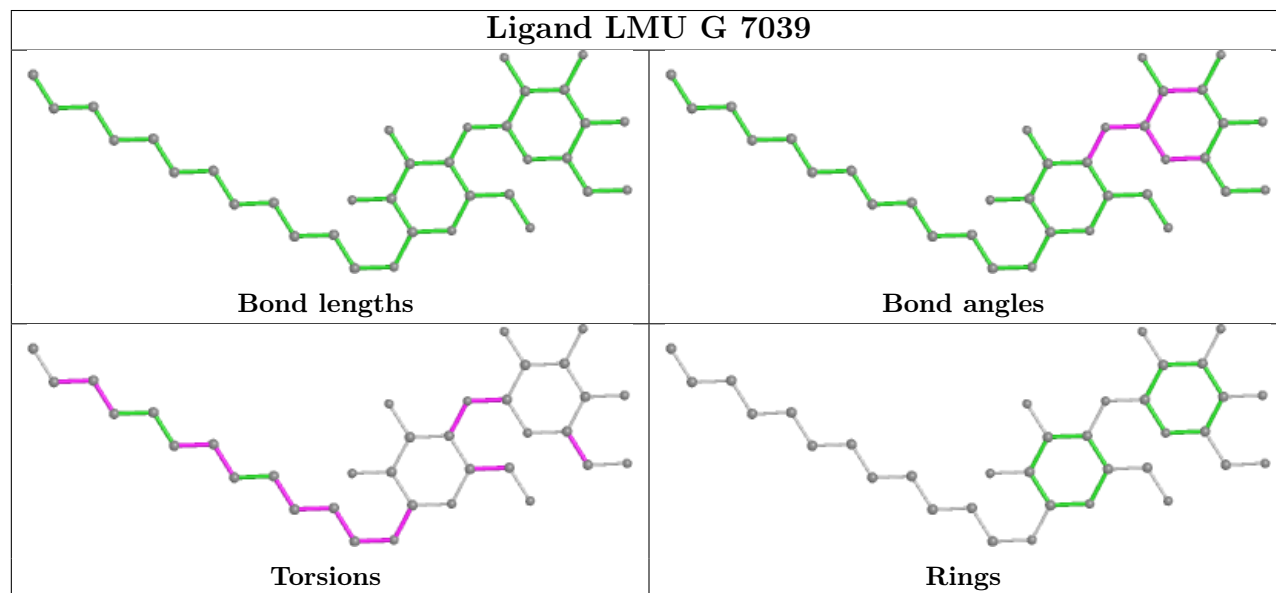
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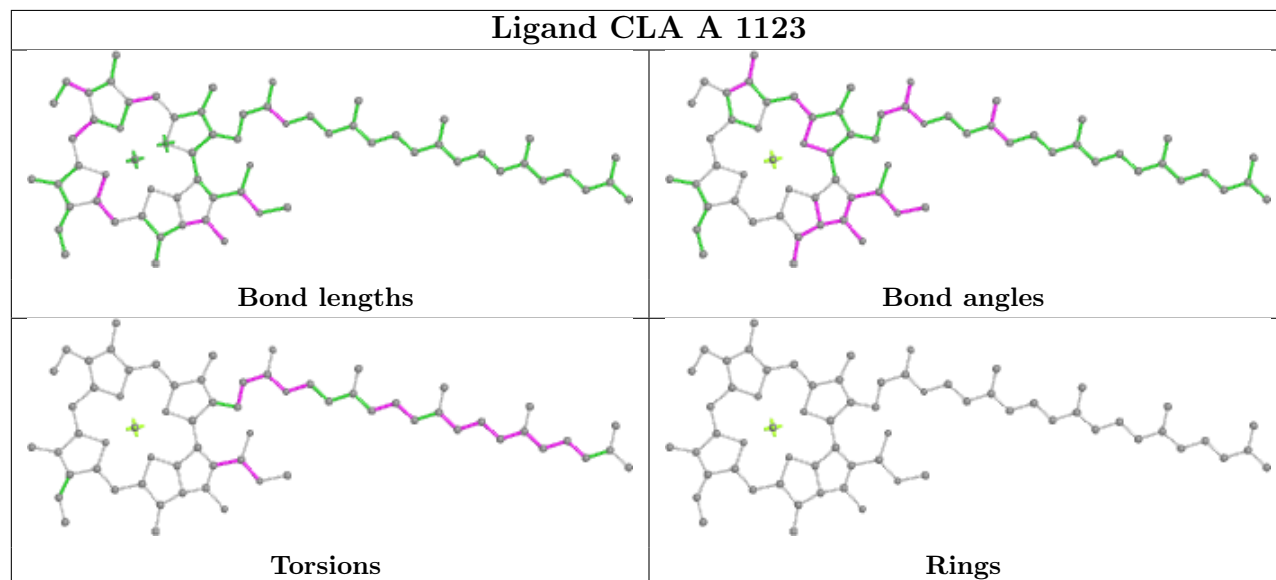
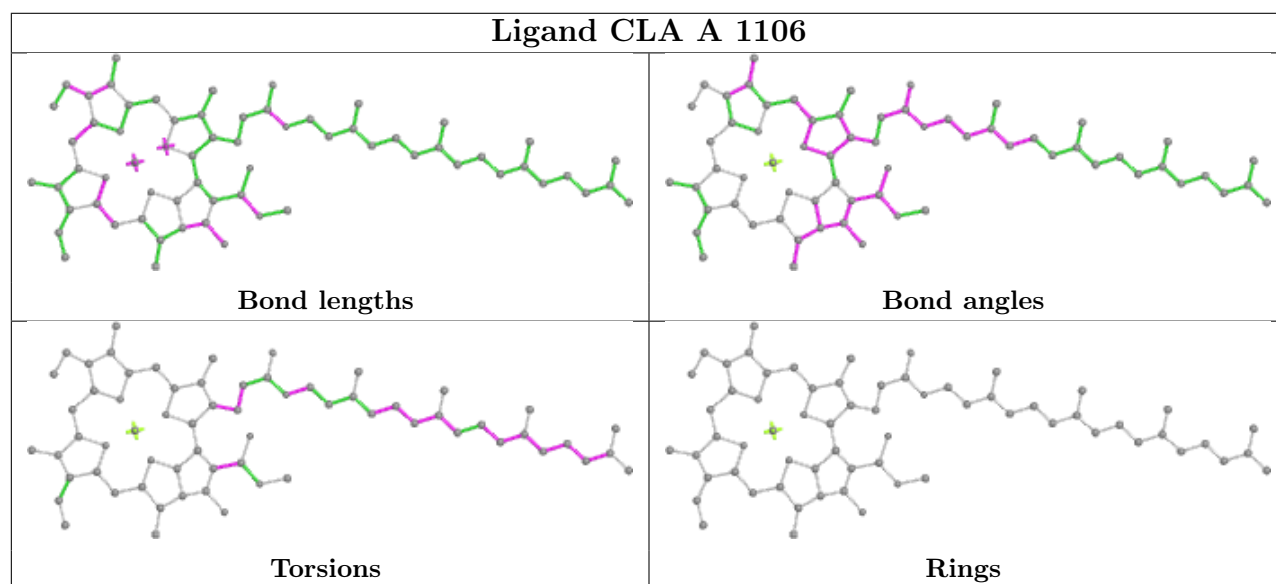
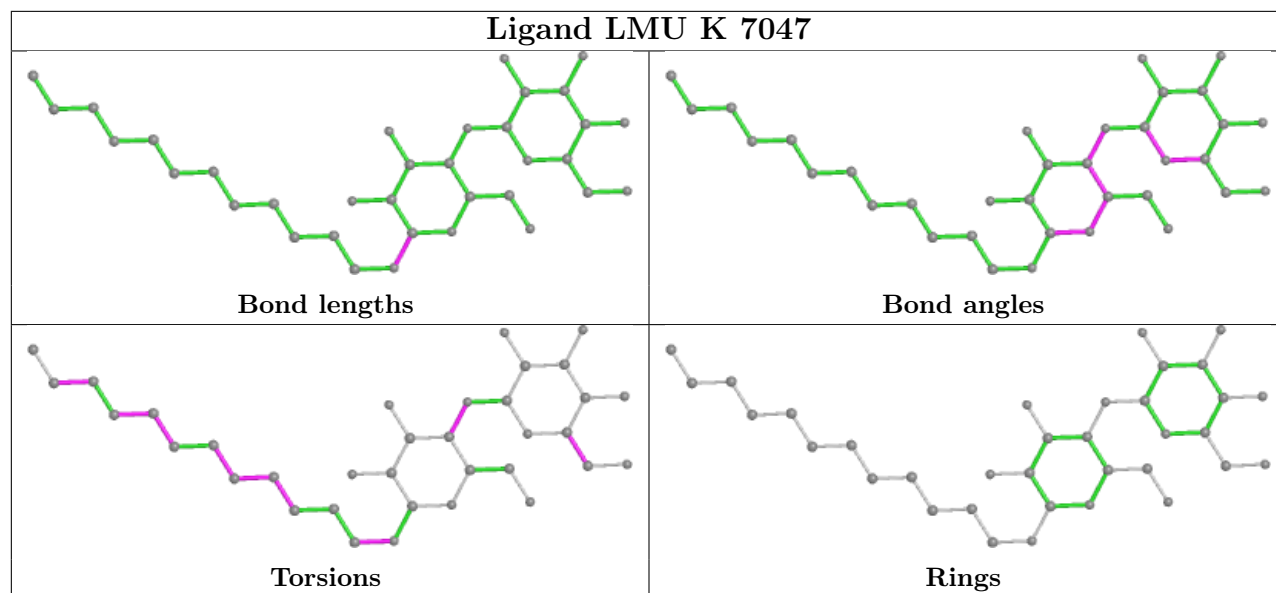


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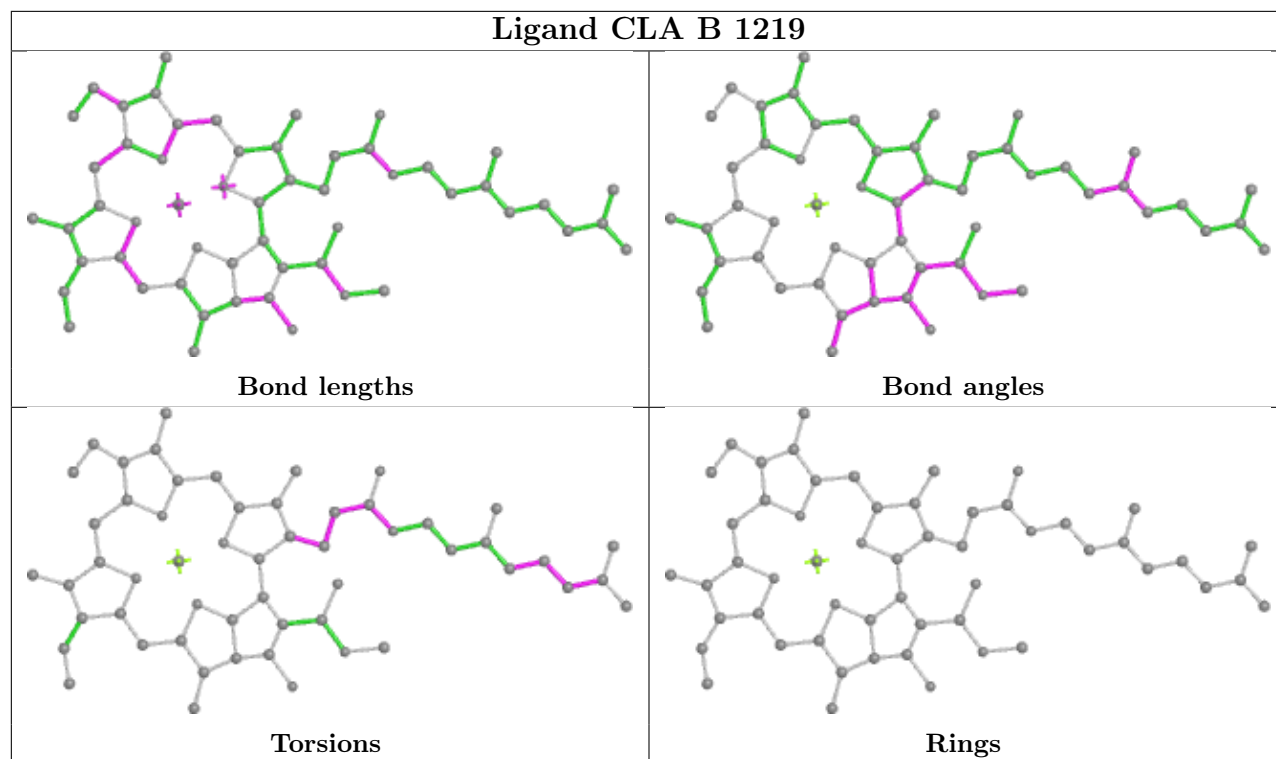


Ligand LMU G 7039

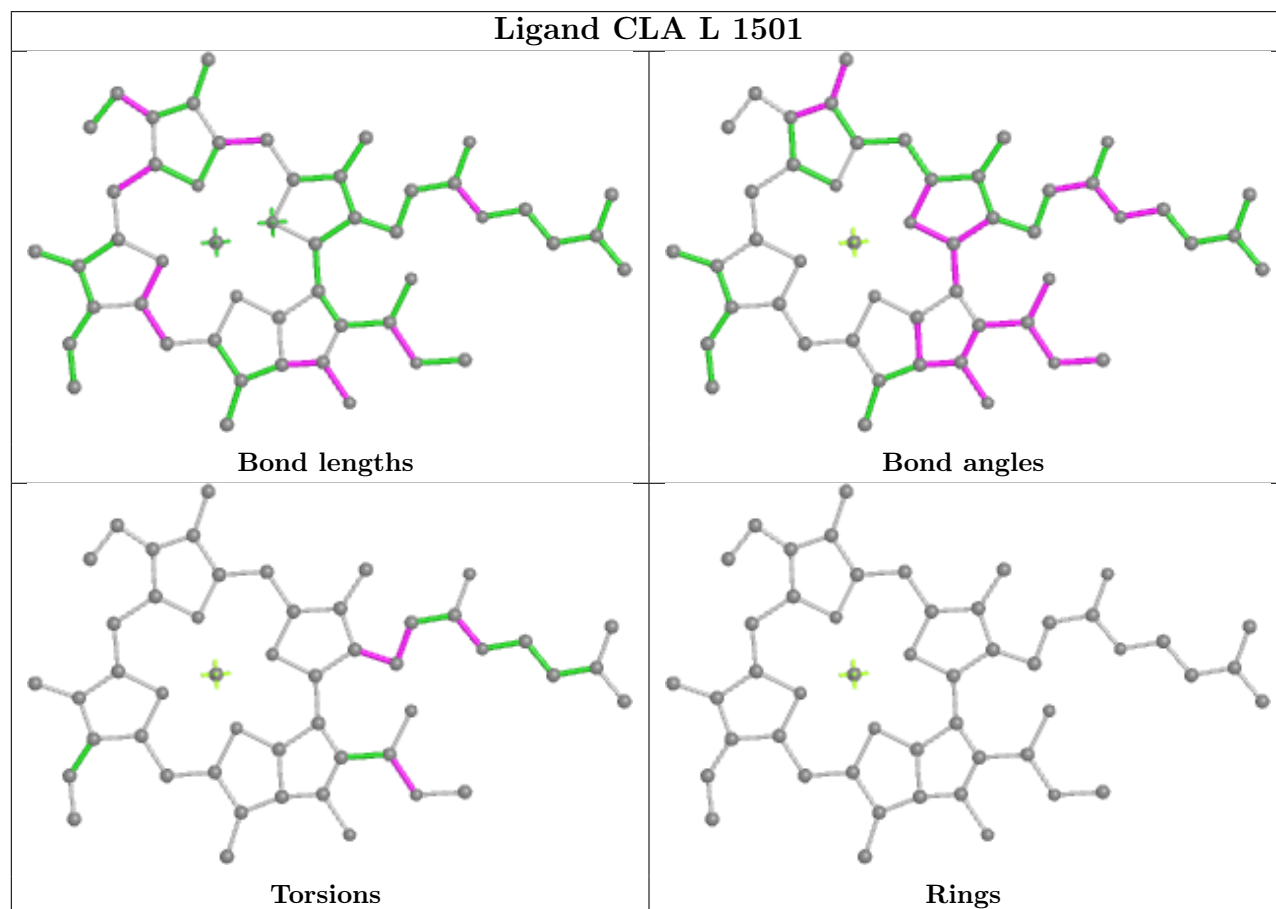




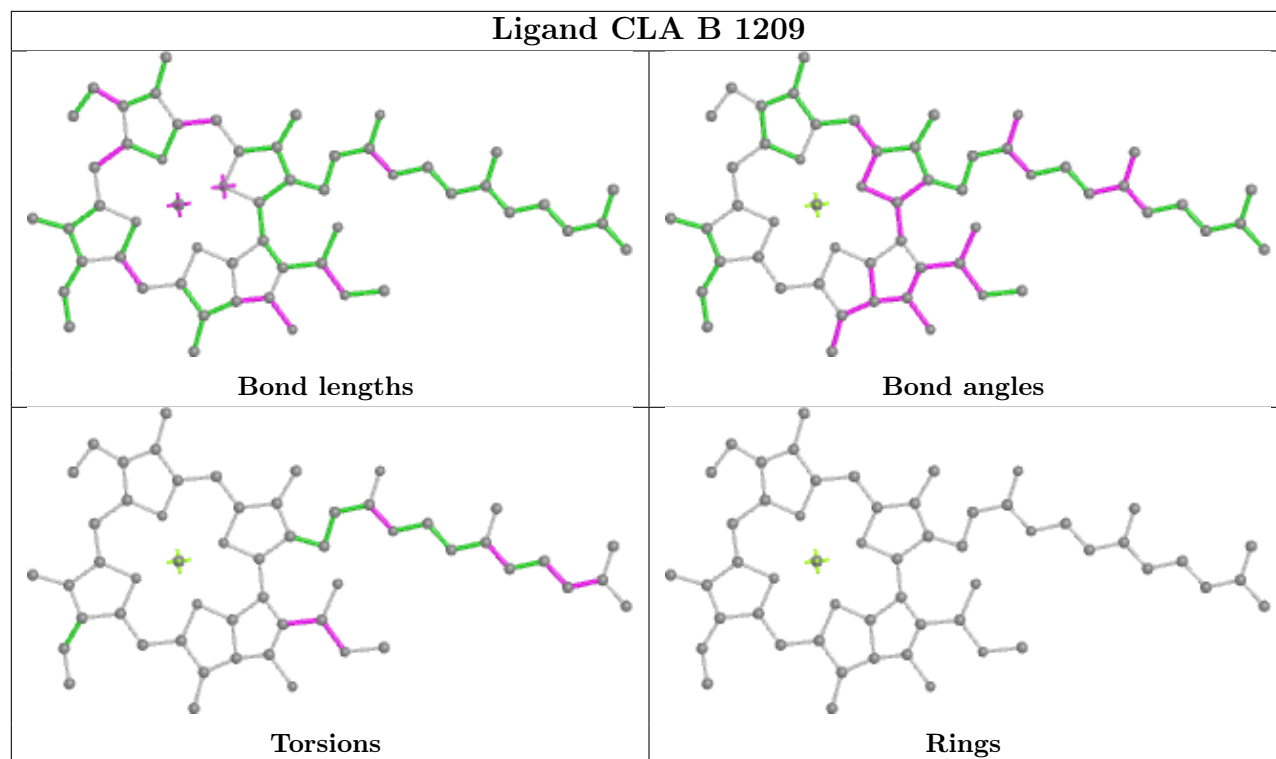
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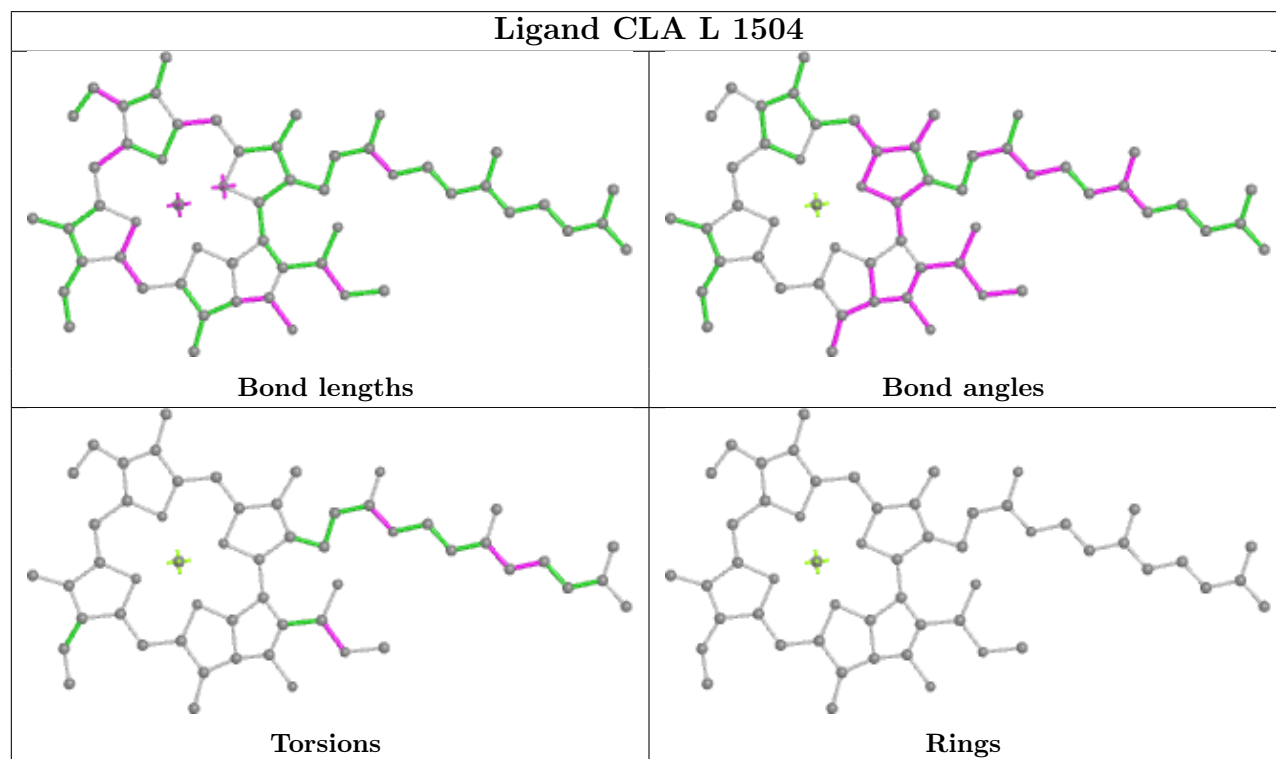
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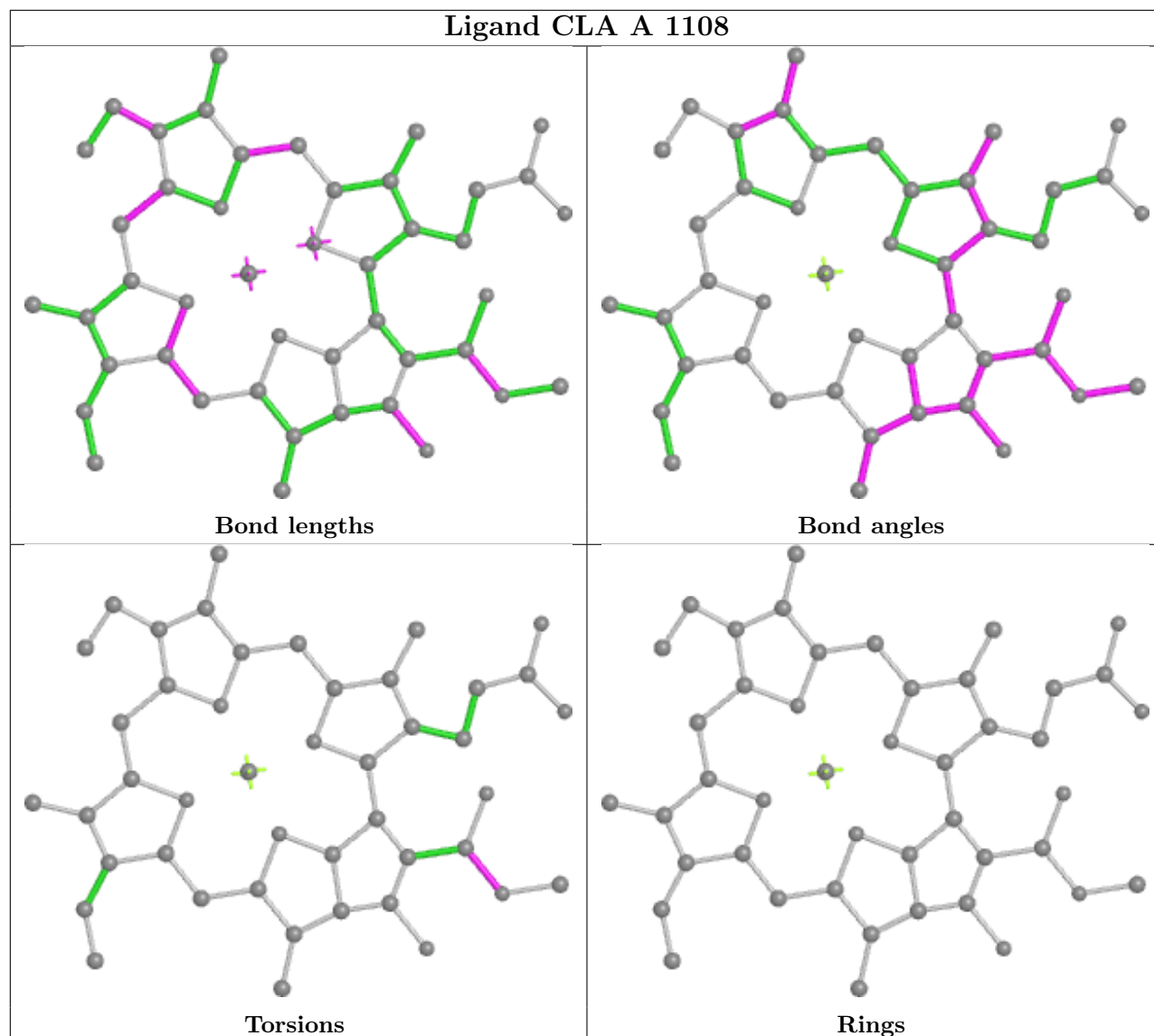
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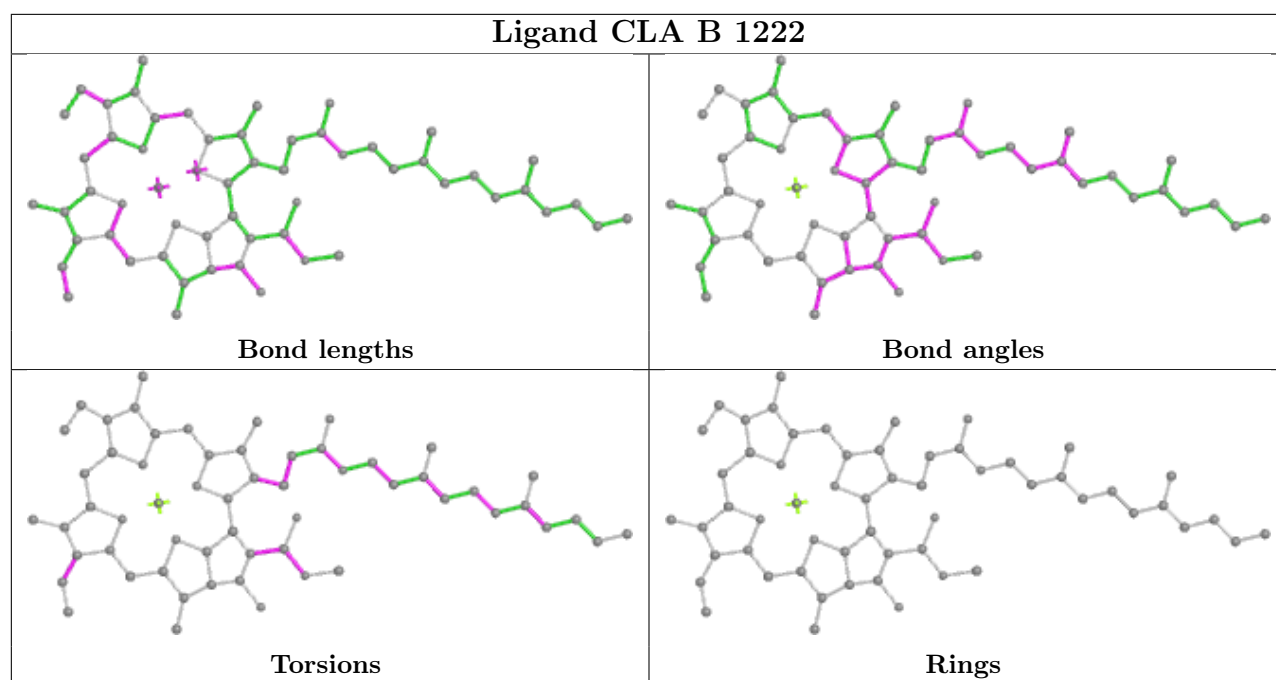


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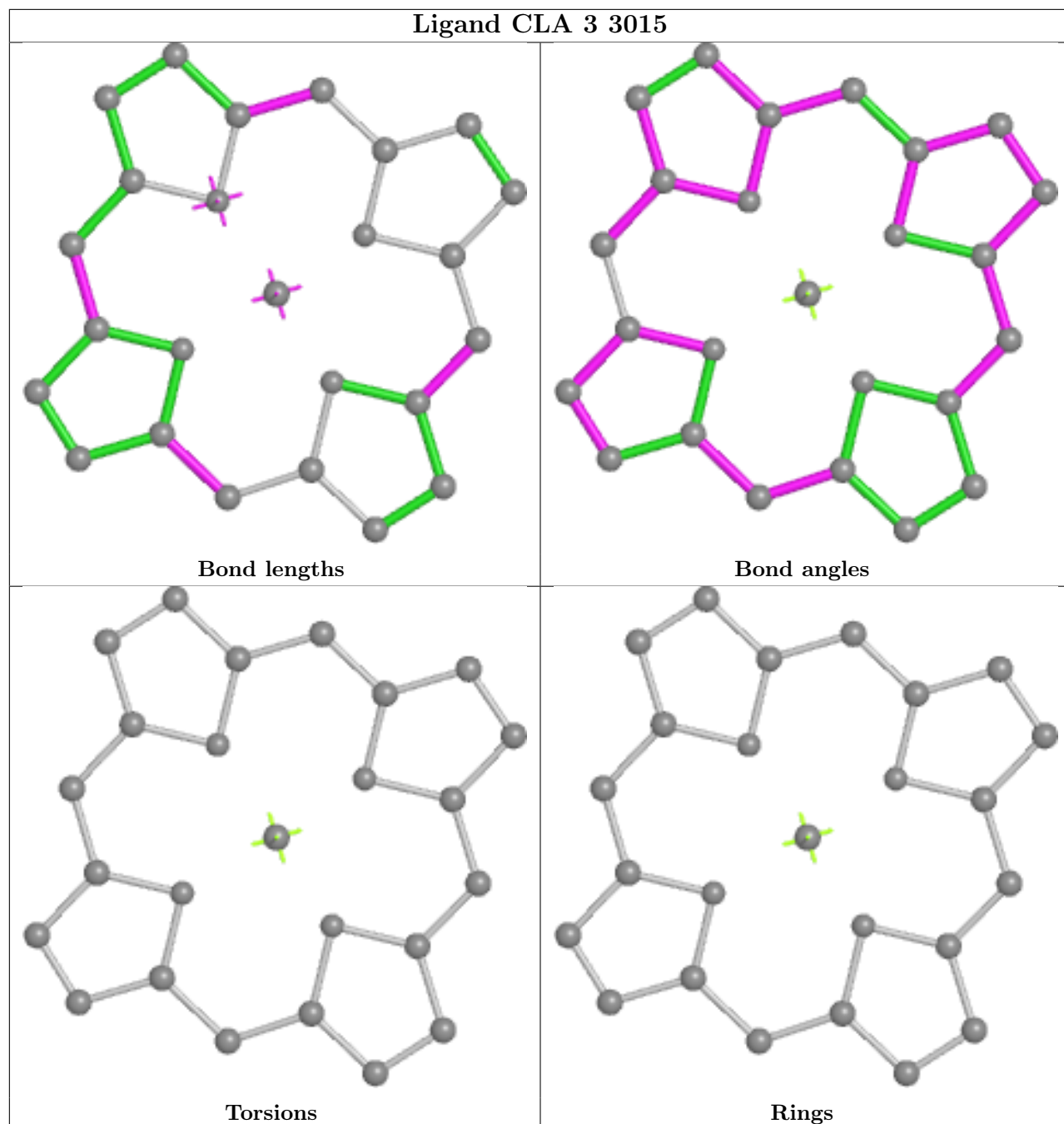


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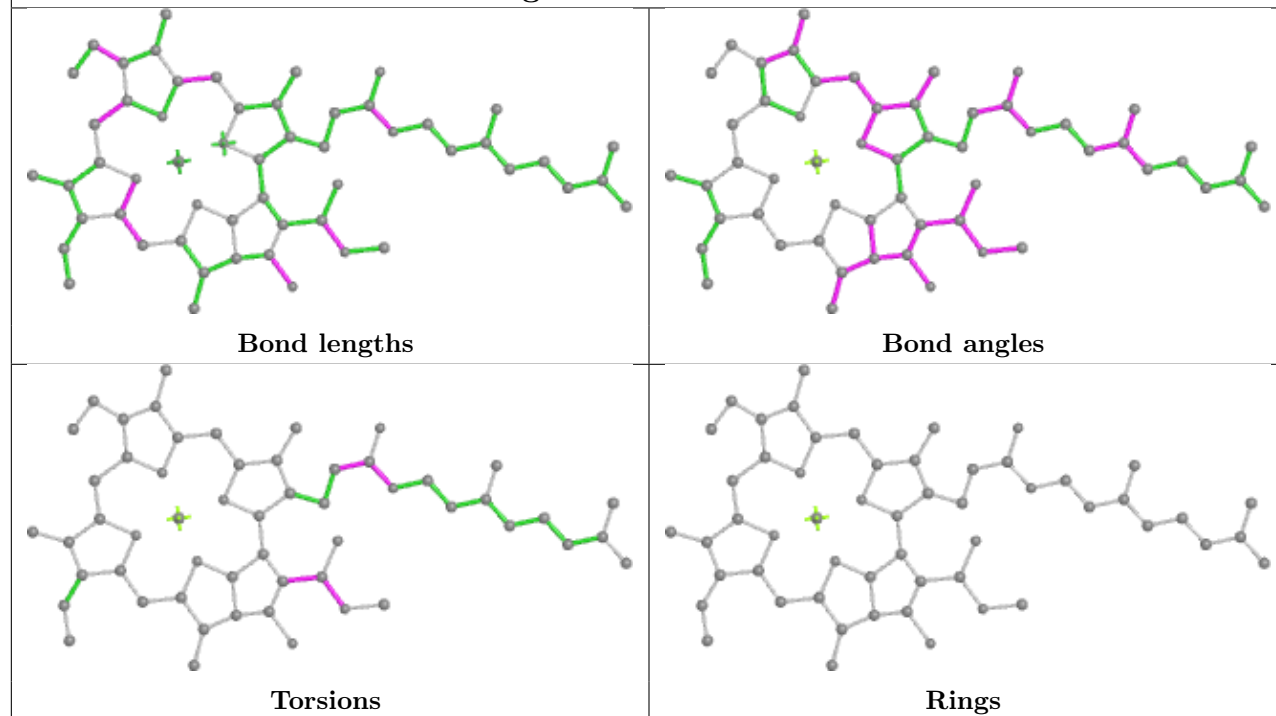




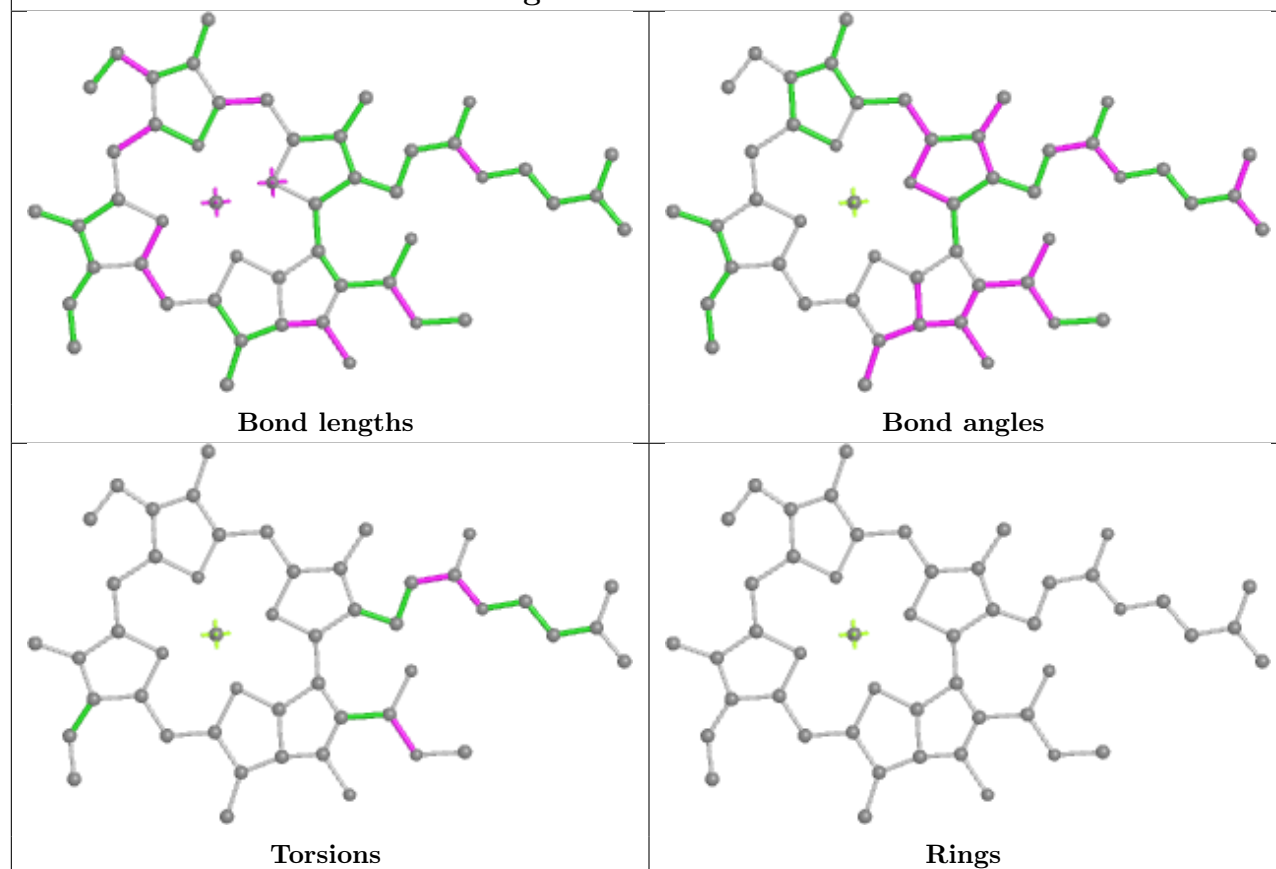
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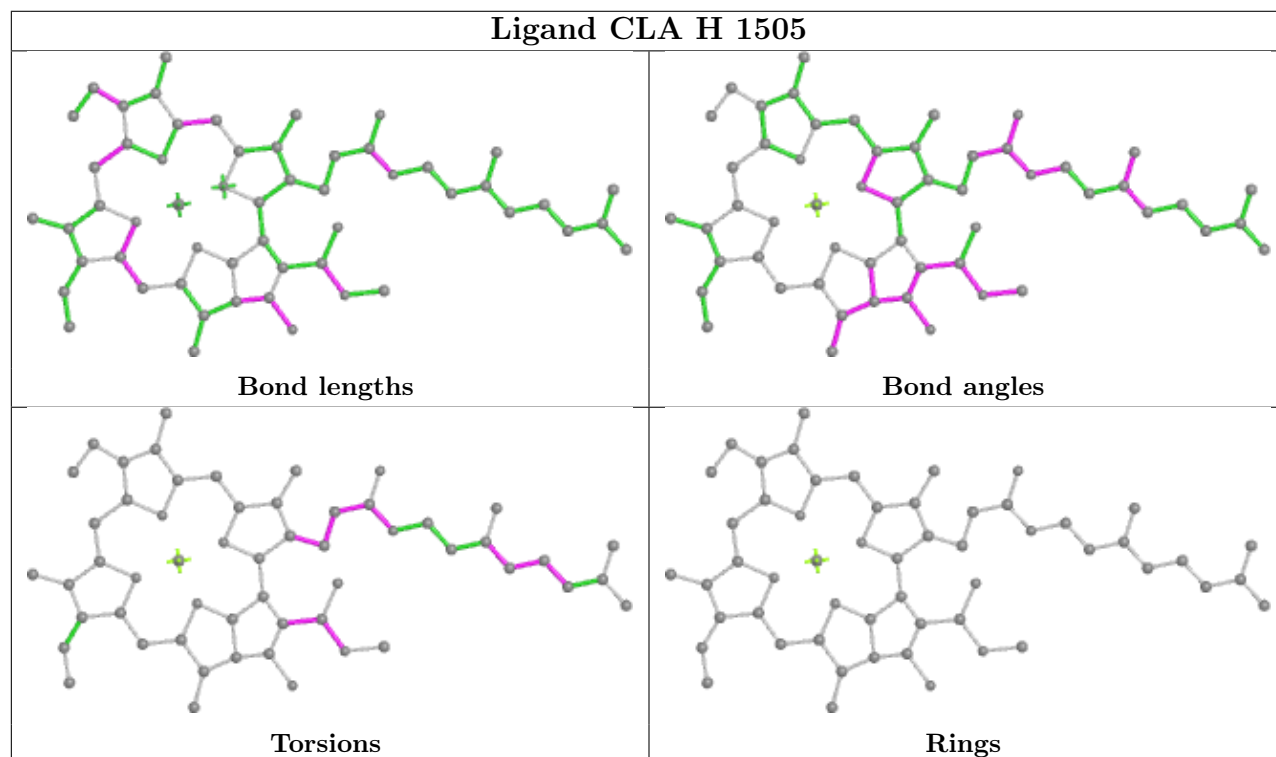
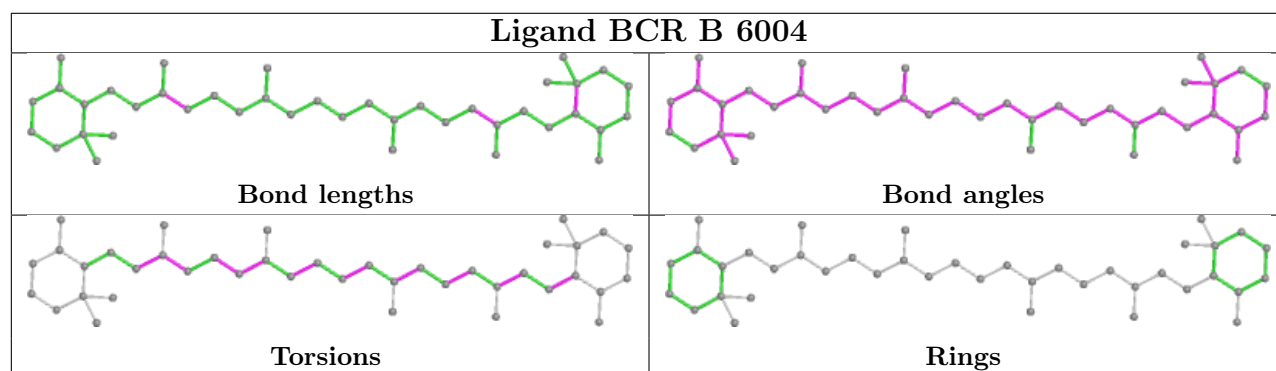
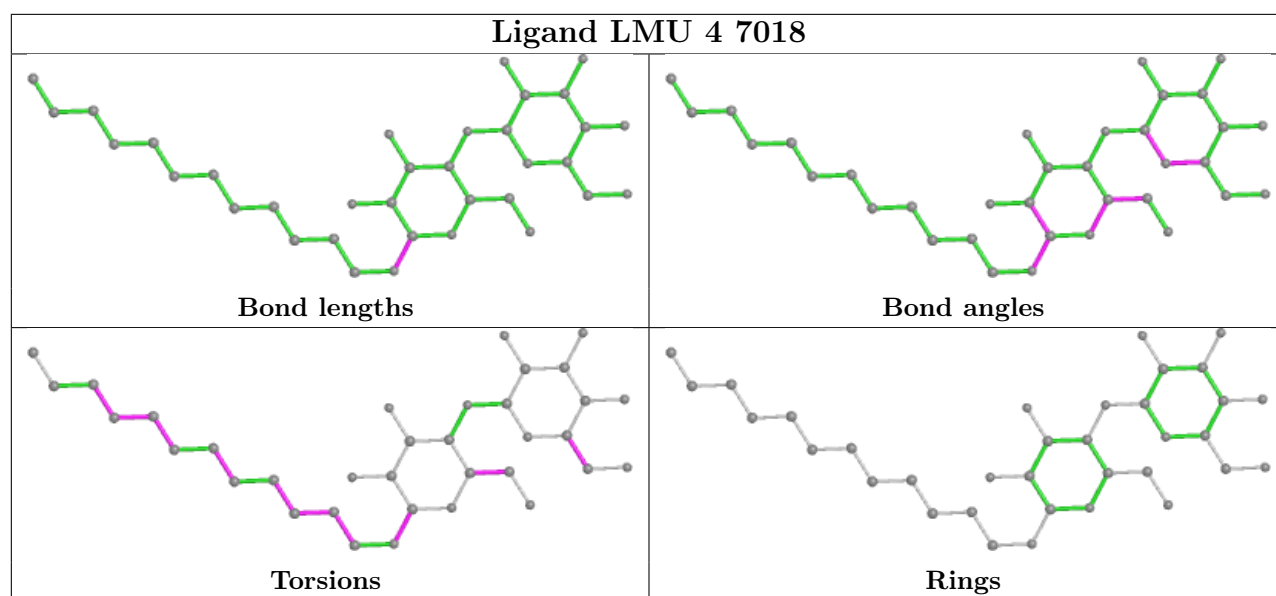


Ligand CLA H 1241

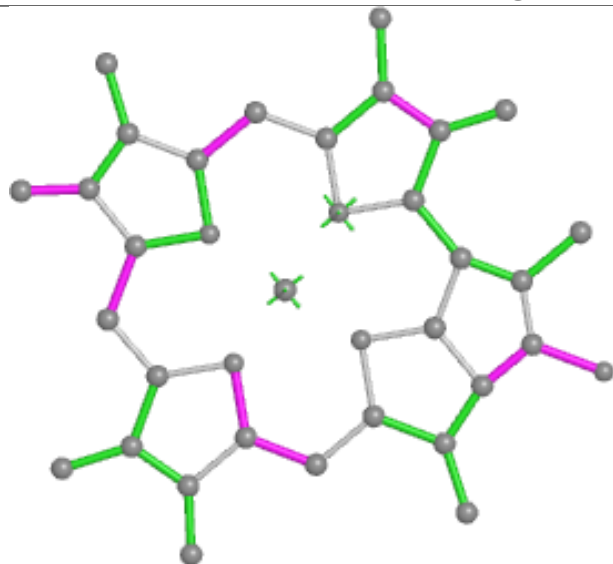


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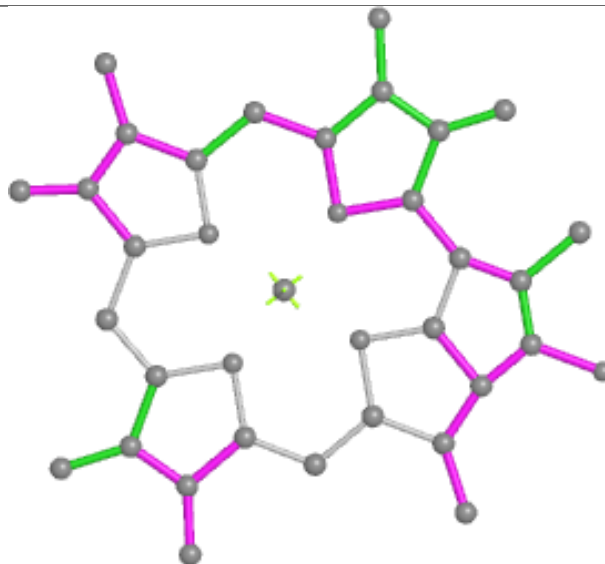




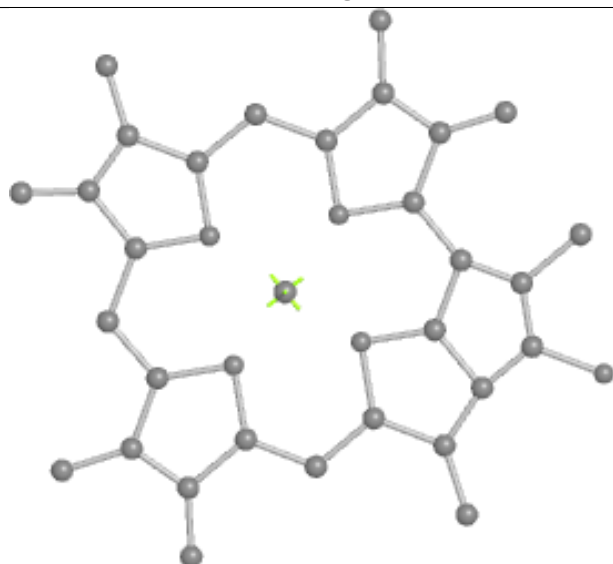
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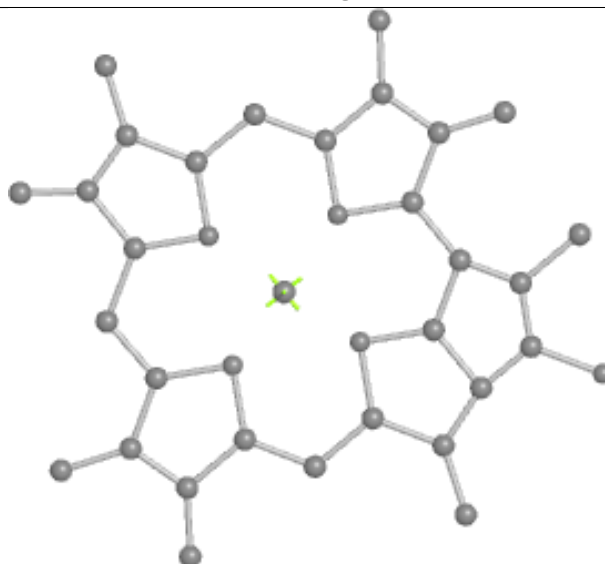
Bond lengths



Bond angles

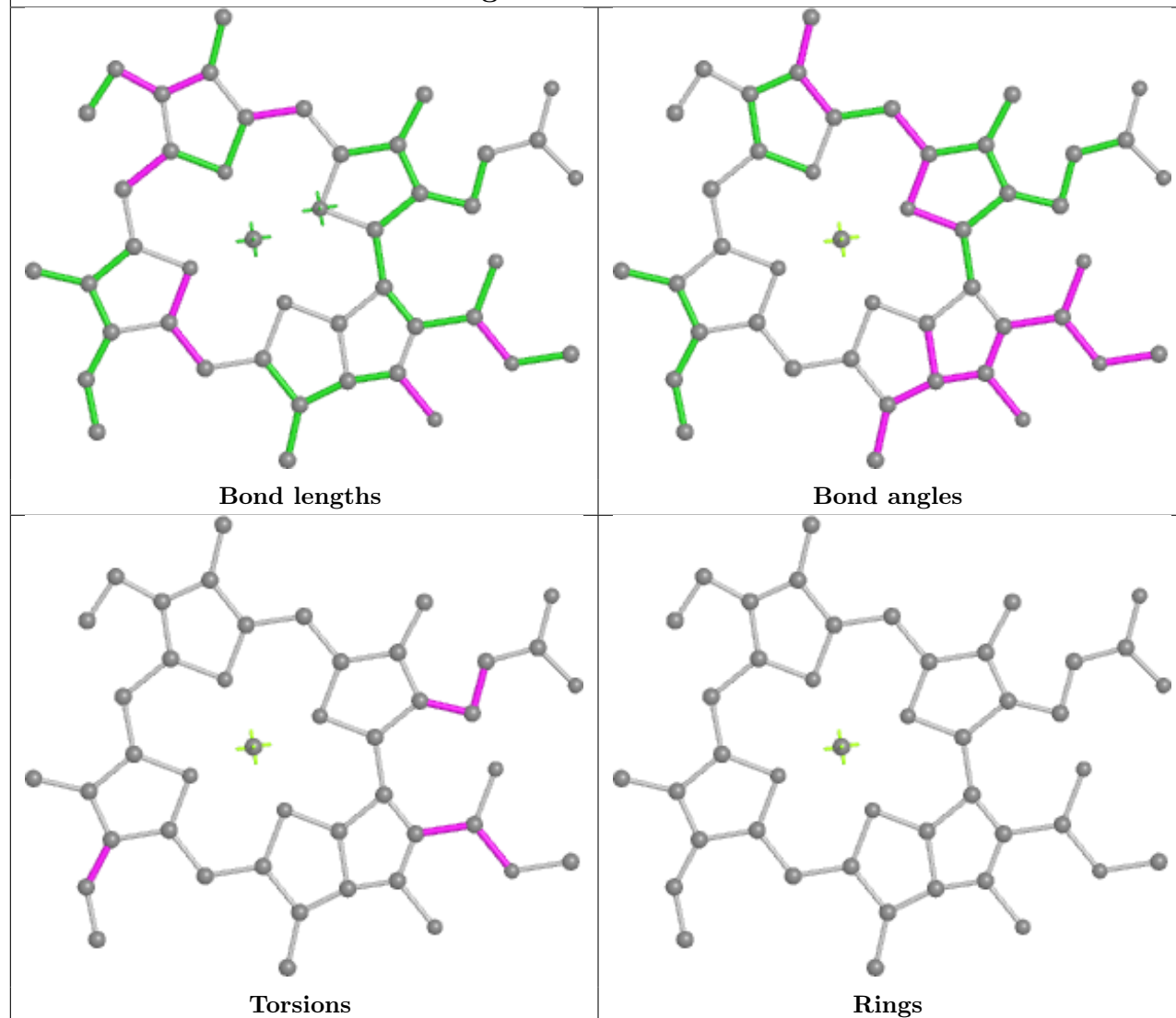


Torsions

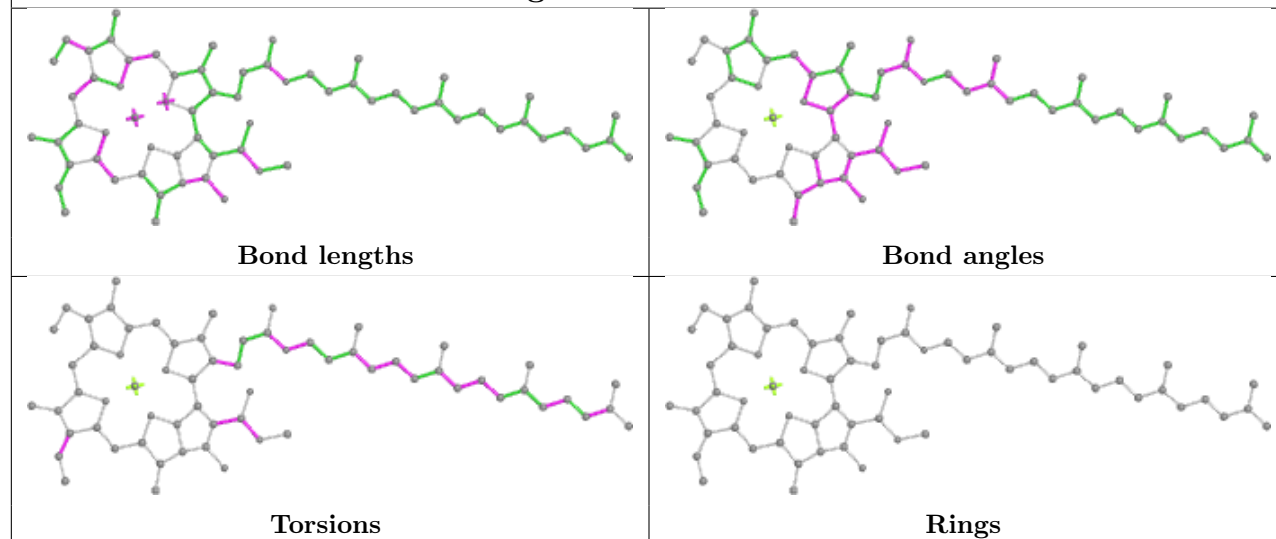


Rings

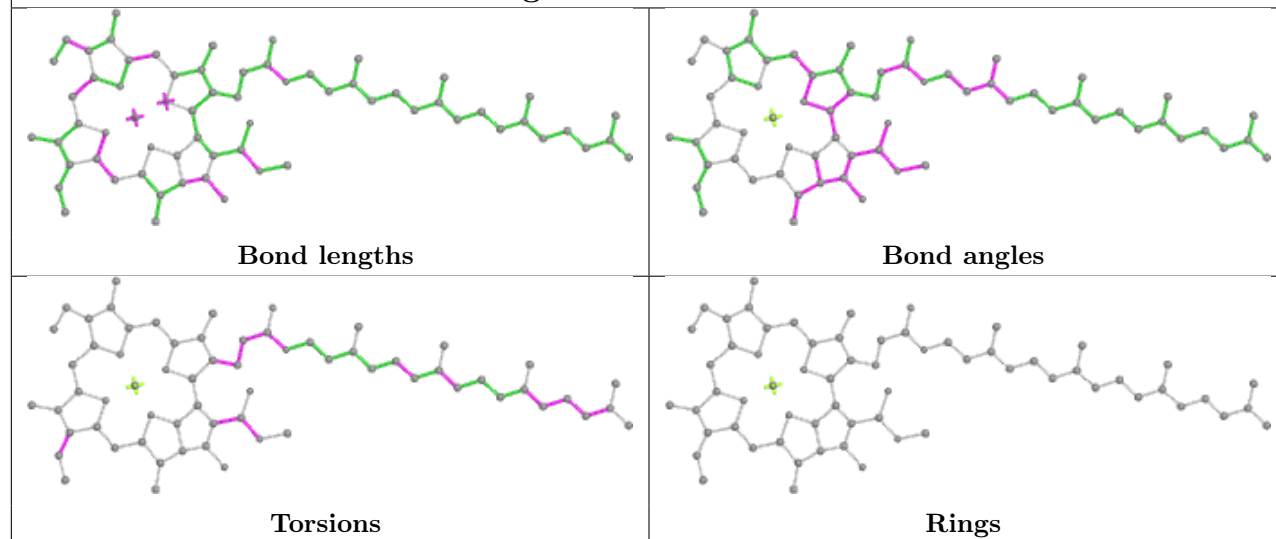
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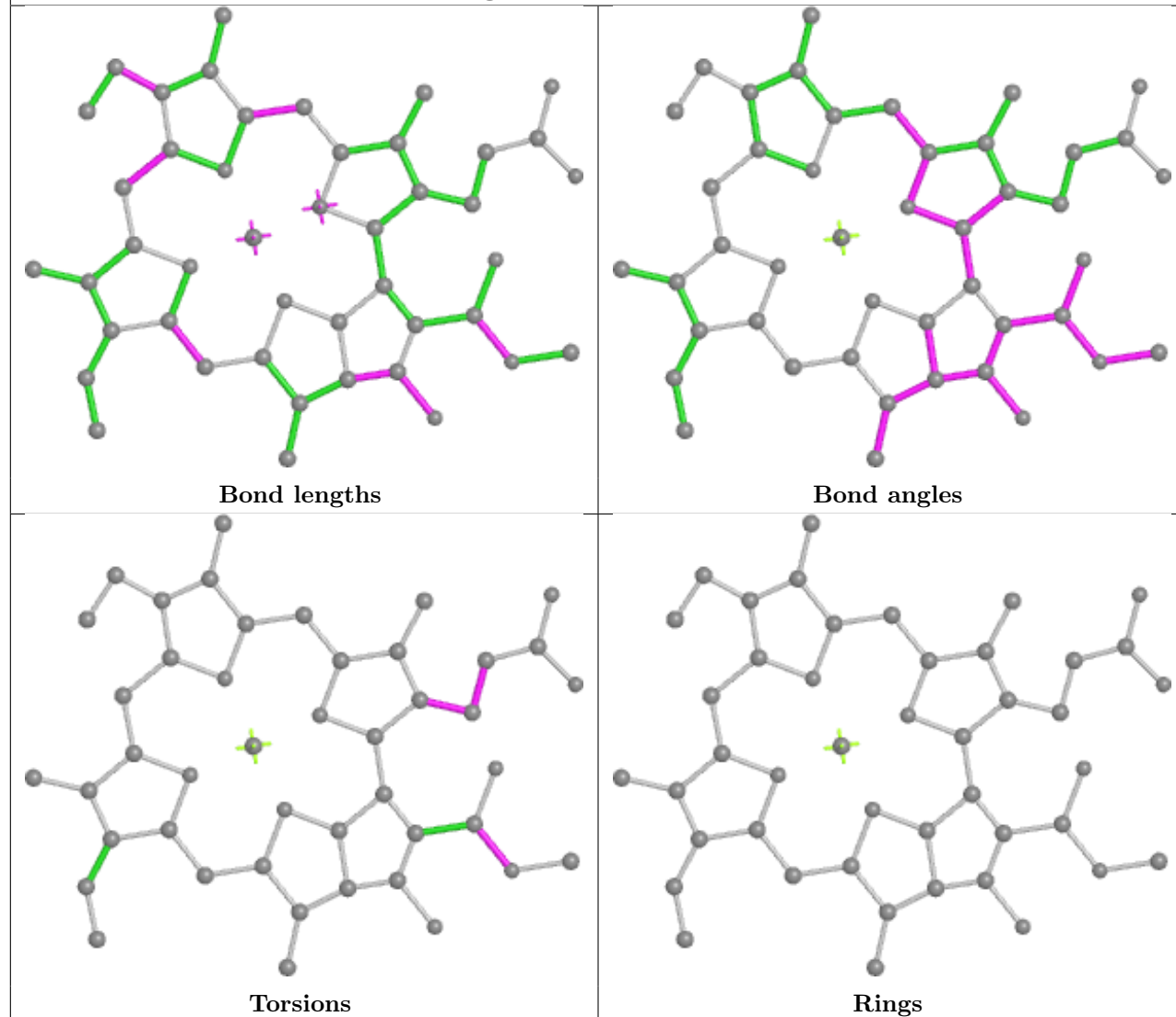
Ligand CLA 3 3016

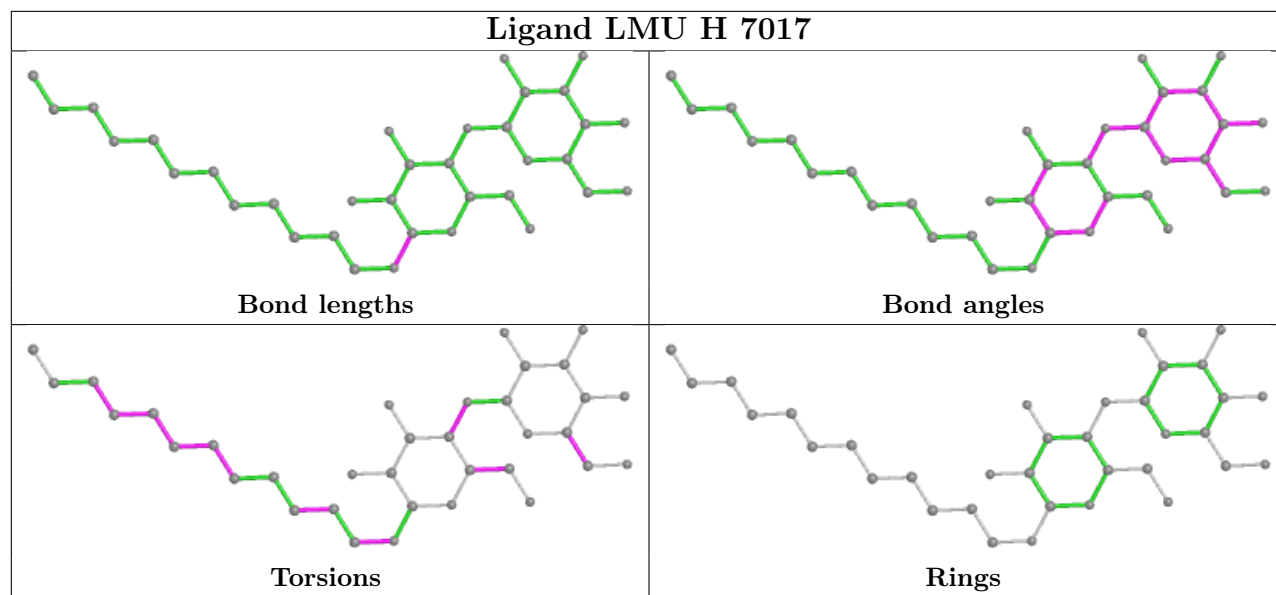


Ligand CLA A 1138

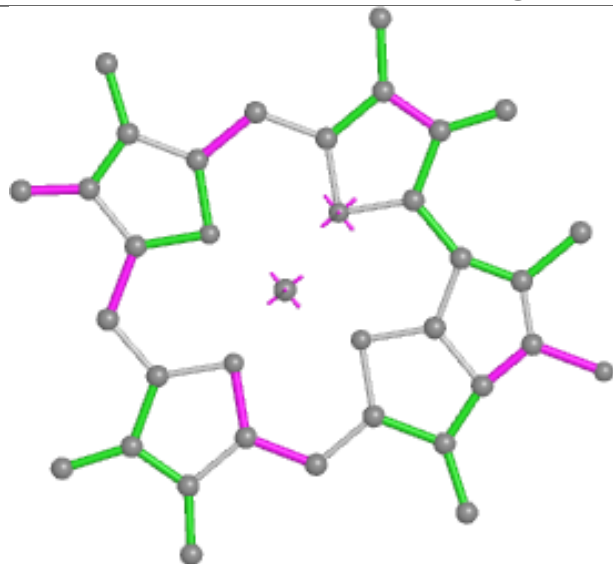


Ligand CLA A 1134

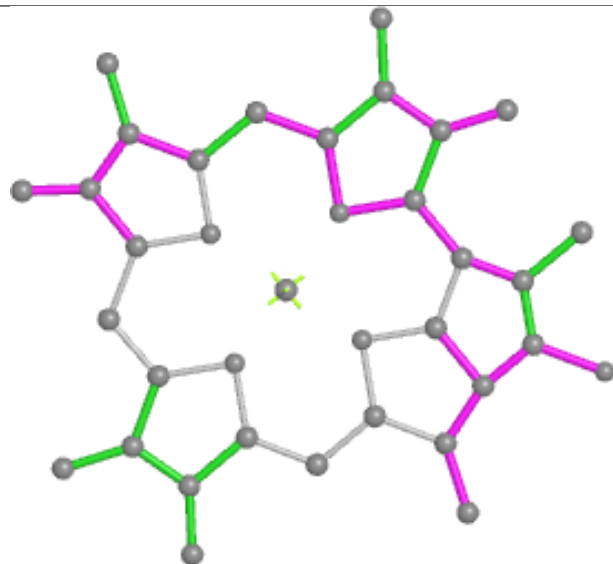




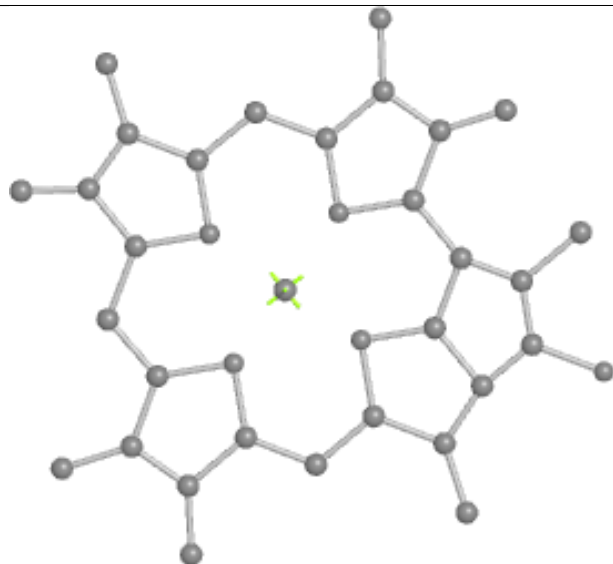
Ligand CLA 3 1118



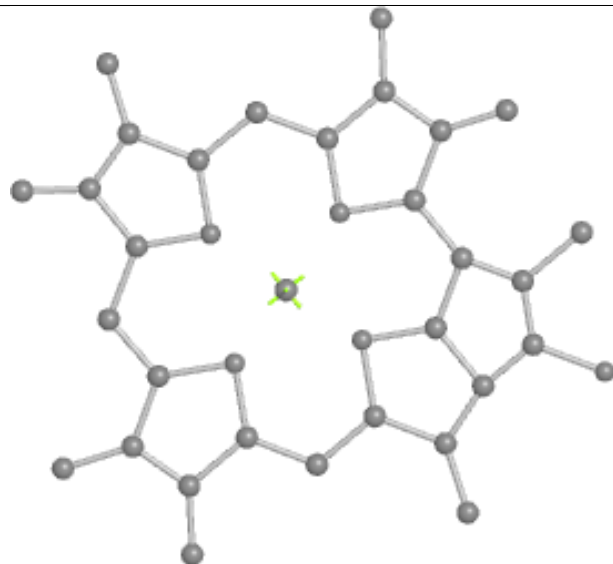
Bond lengths



Bond angles

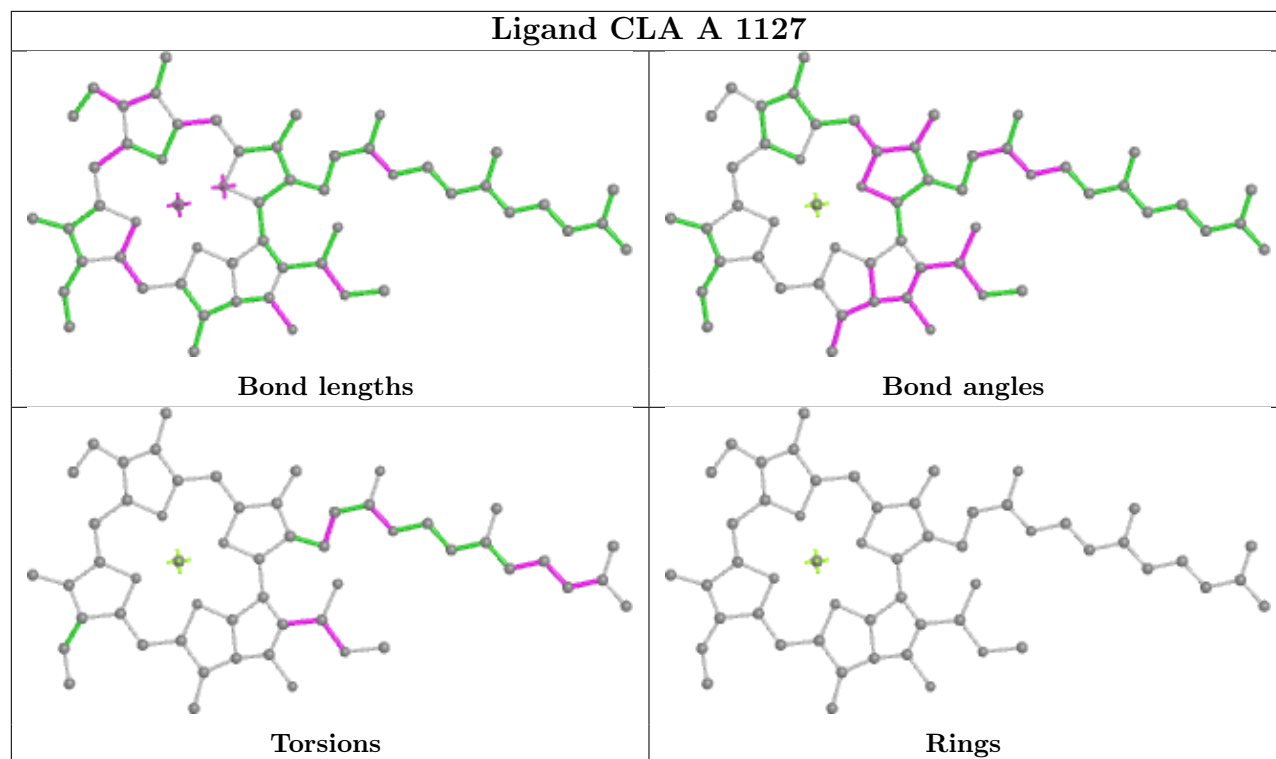


Torsions

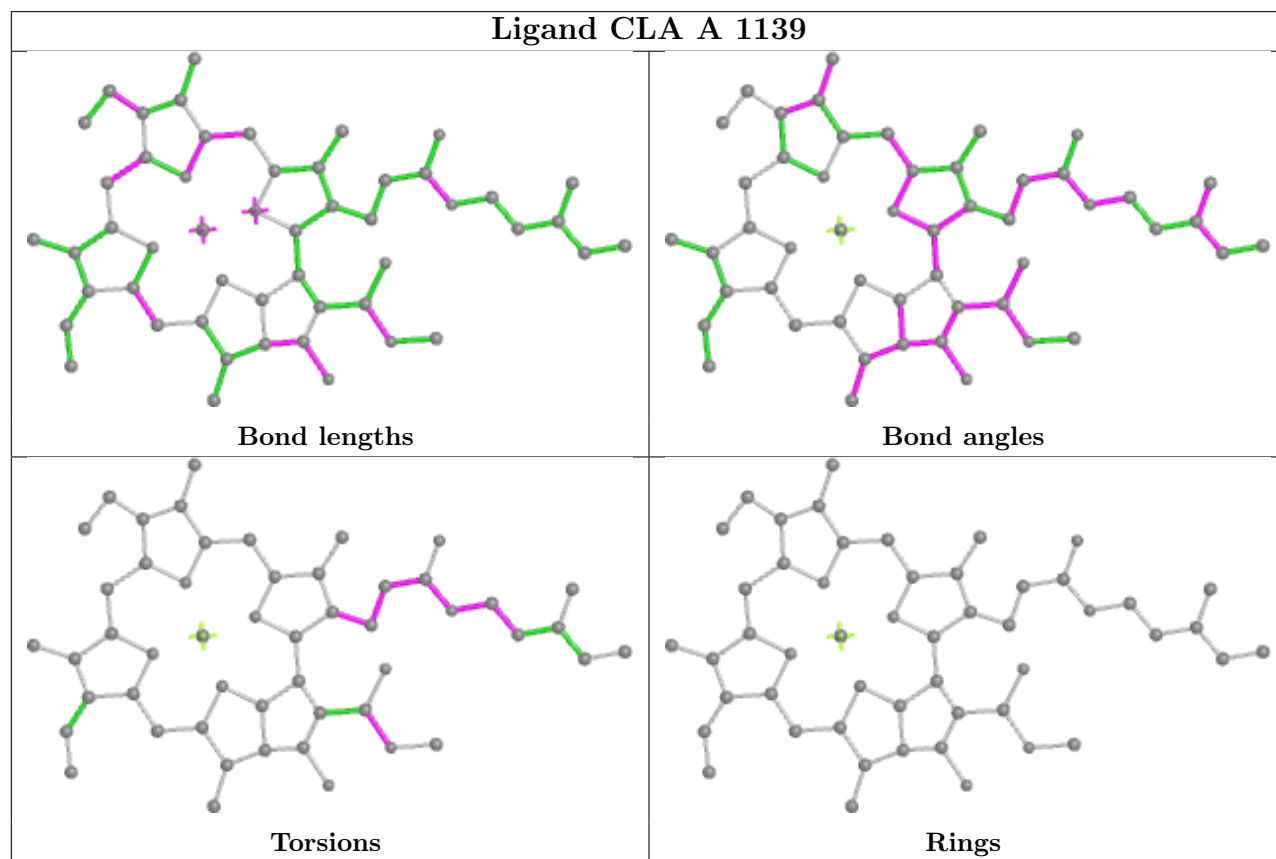


Rings

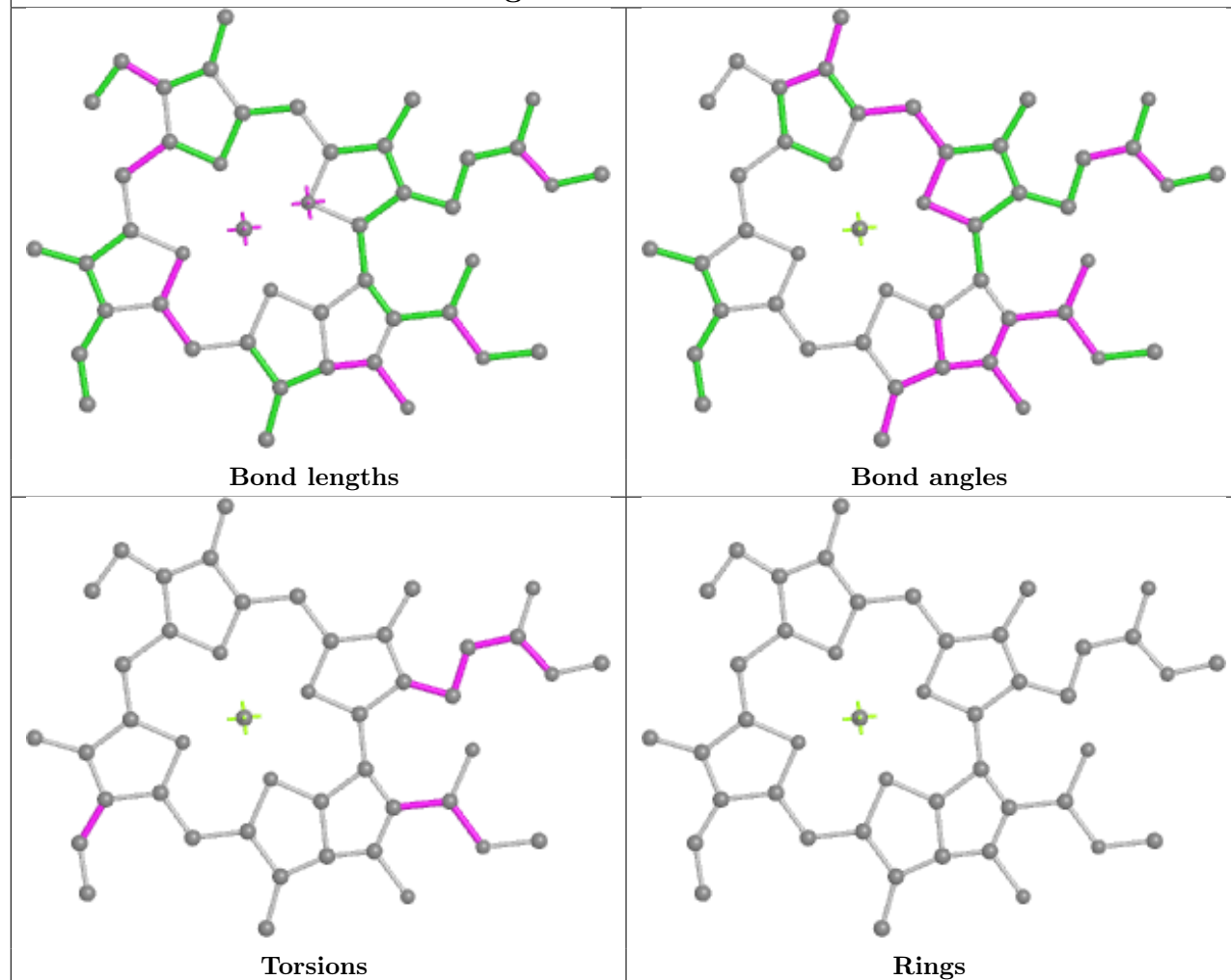
Ligand CLA A 1127



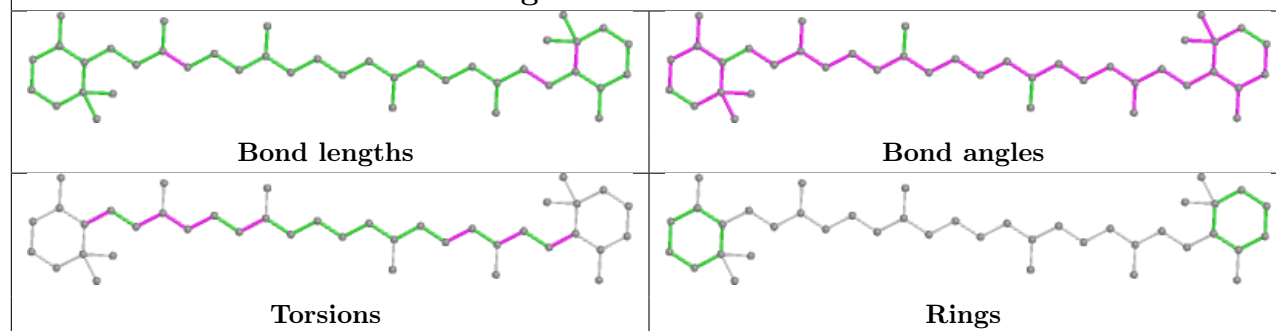
Ligand CLA A 1139

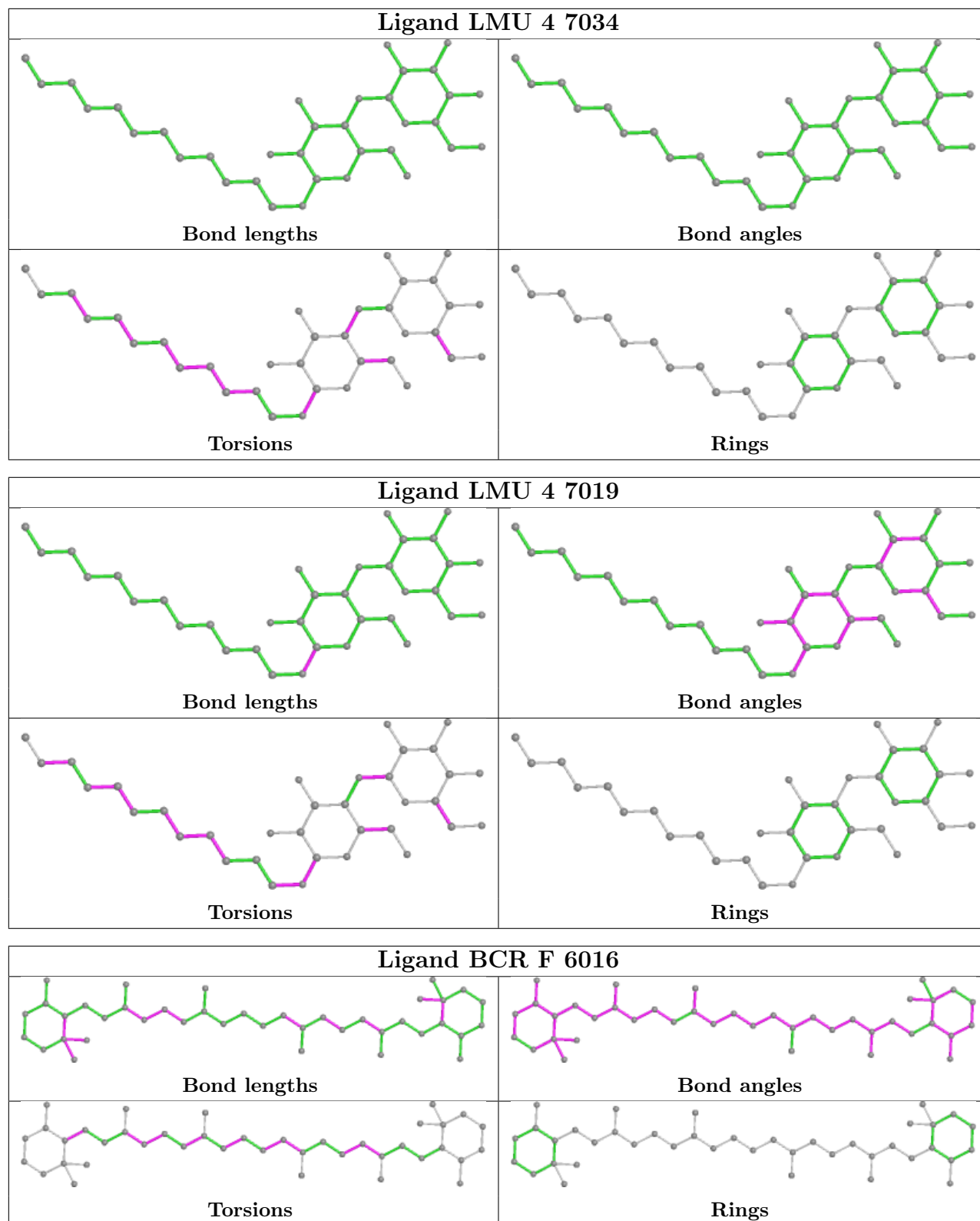


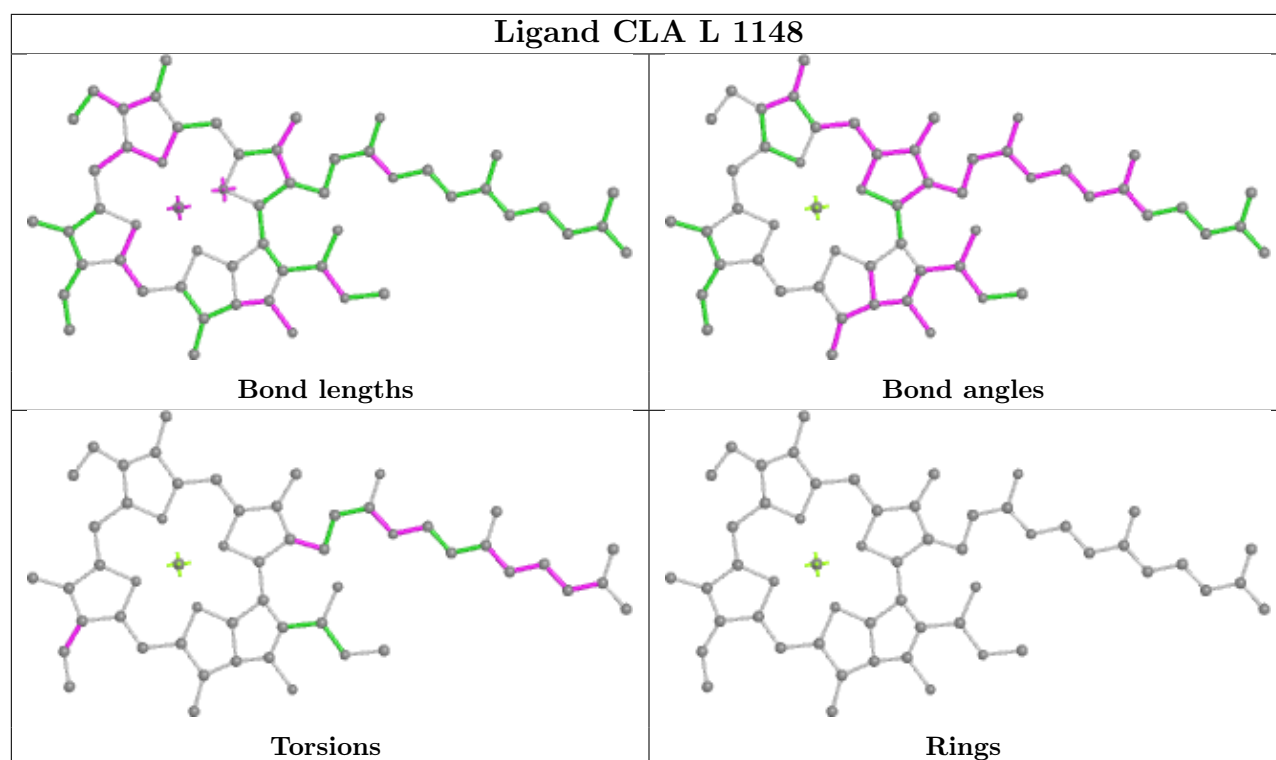
Ligand CLA B 1218

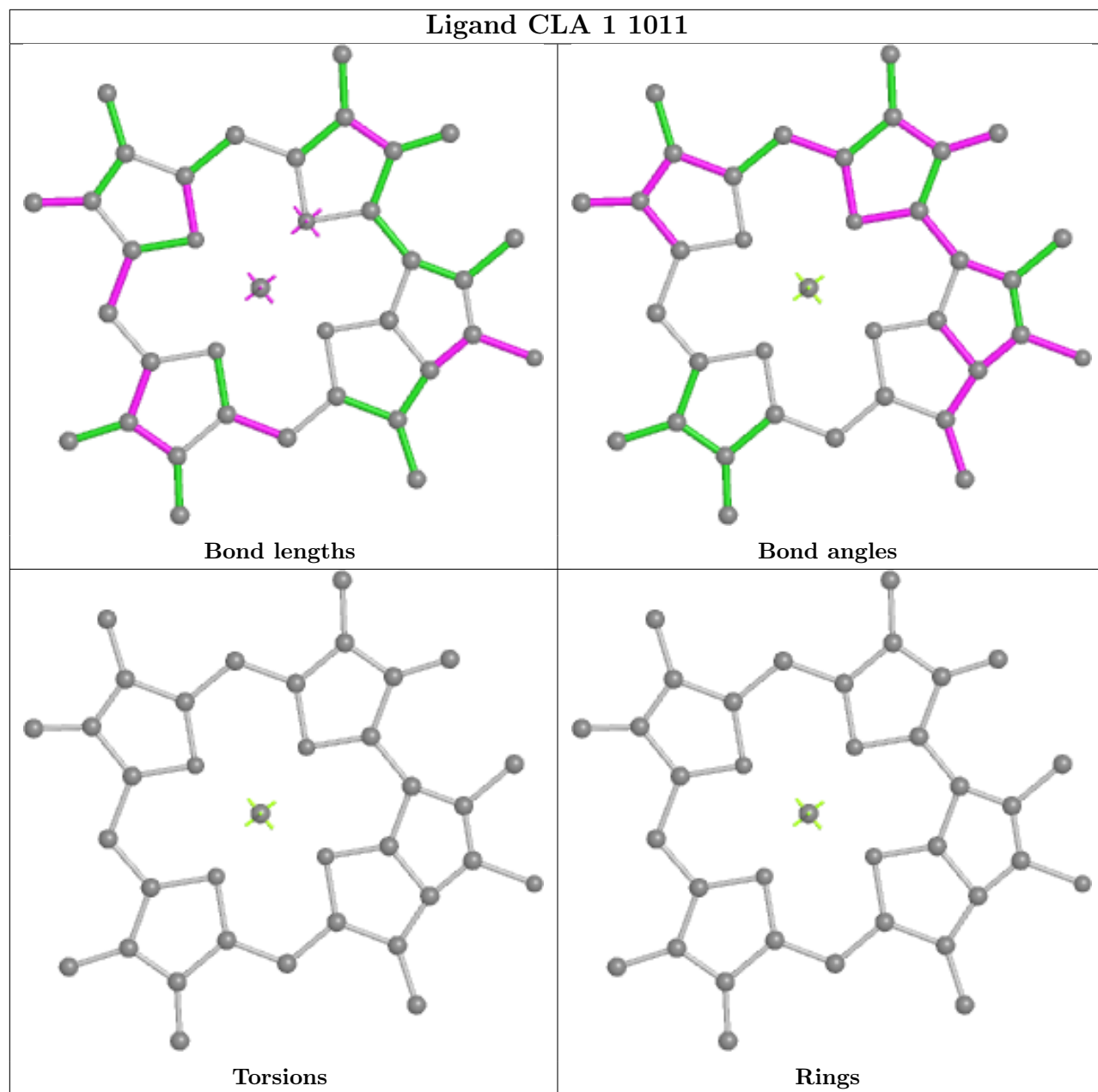


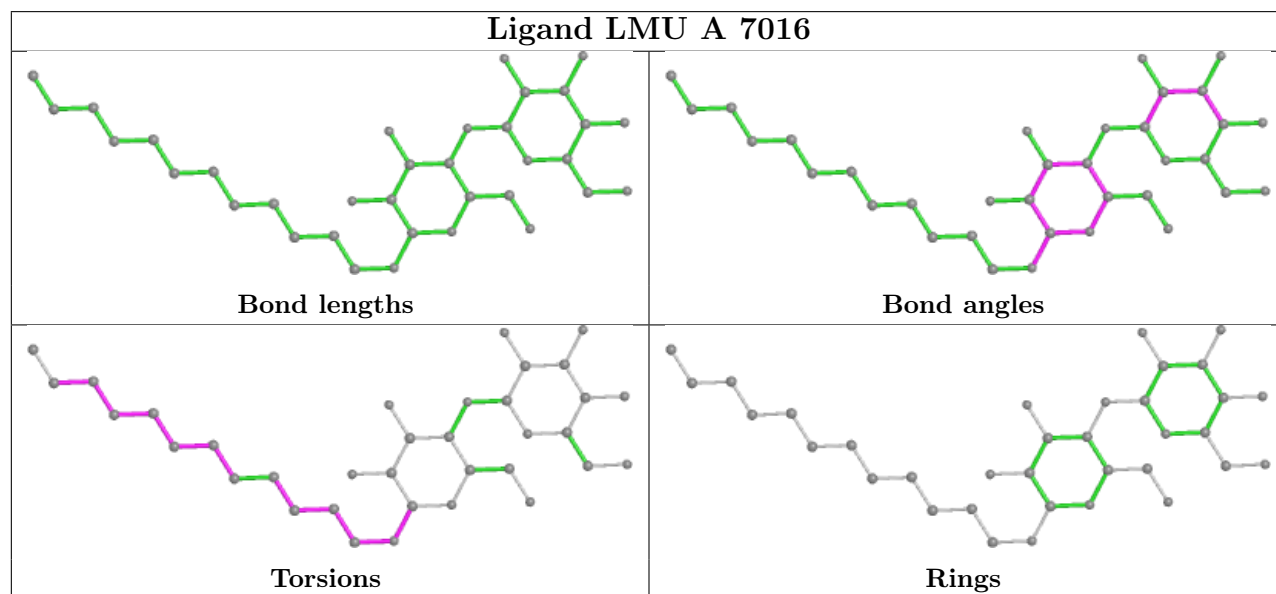
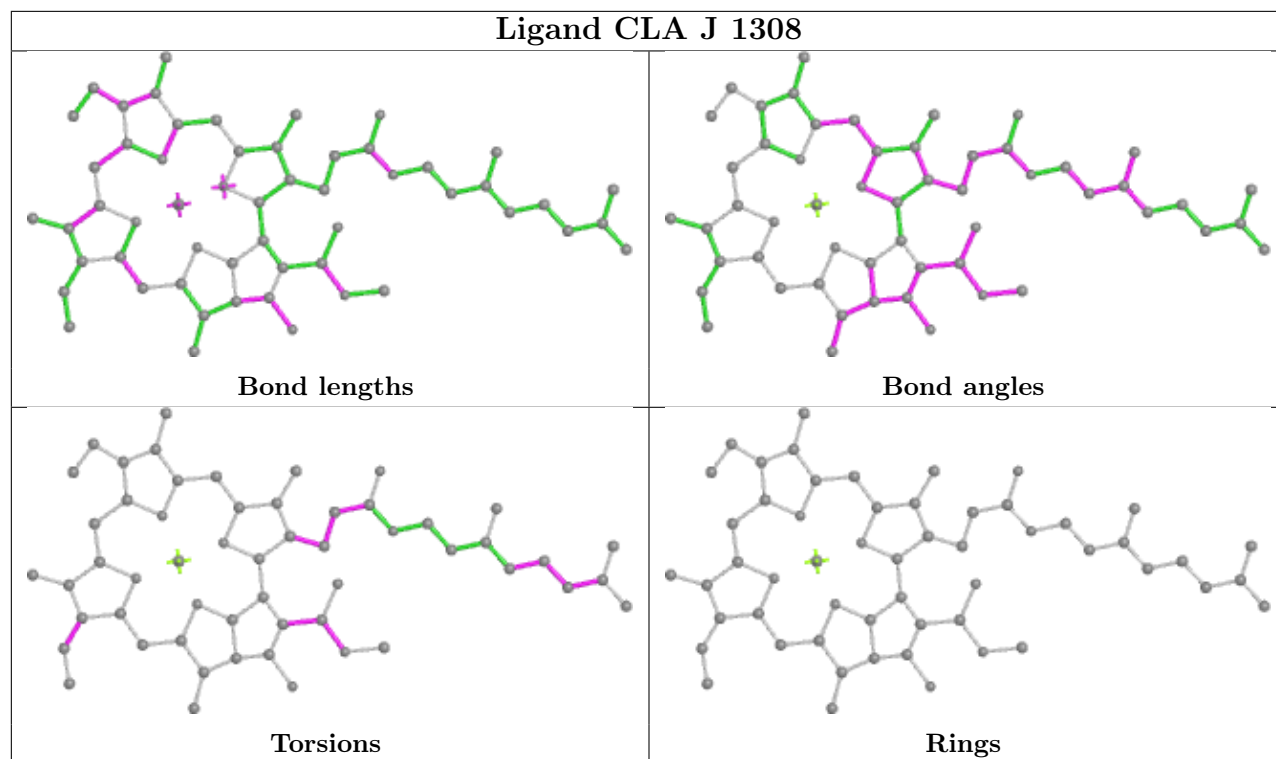
Ligand BCR A 6003



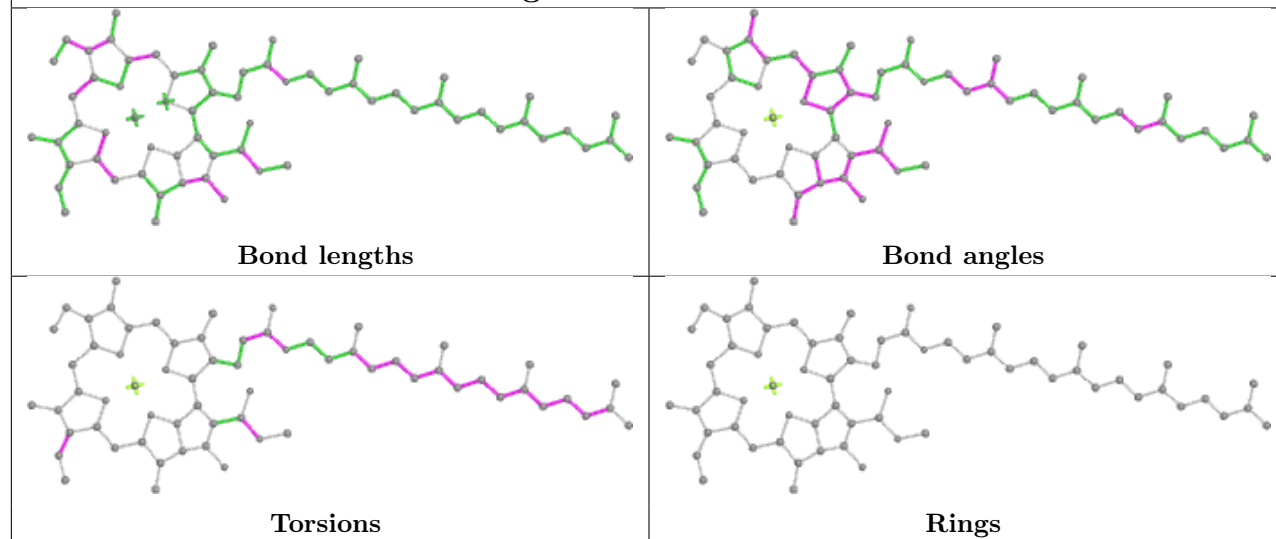




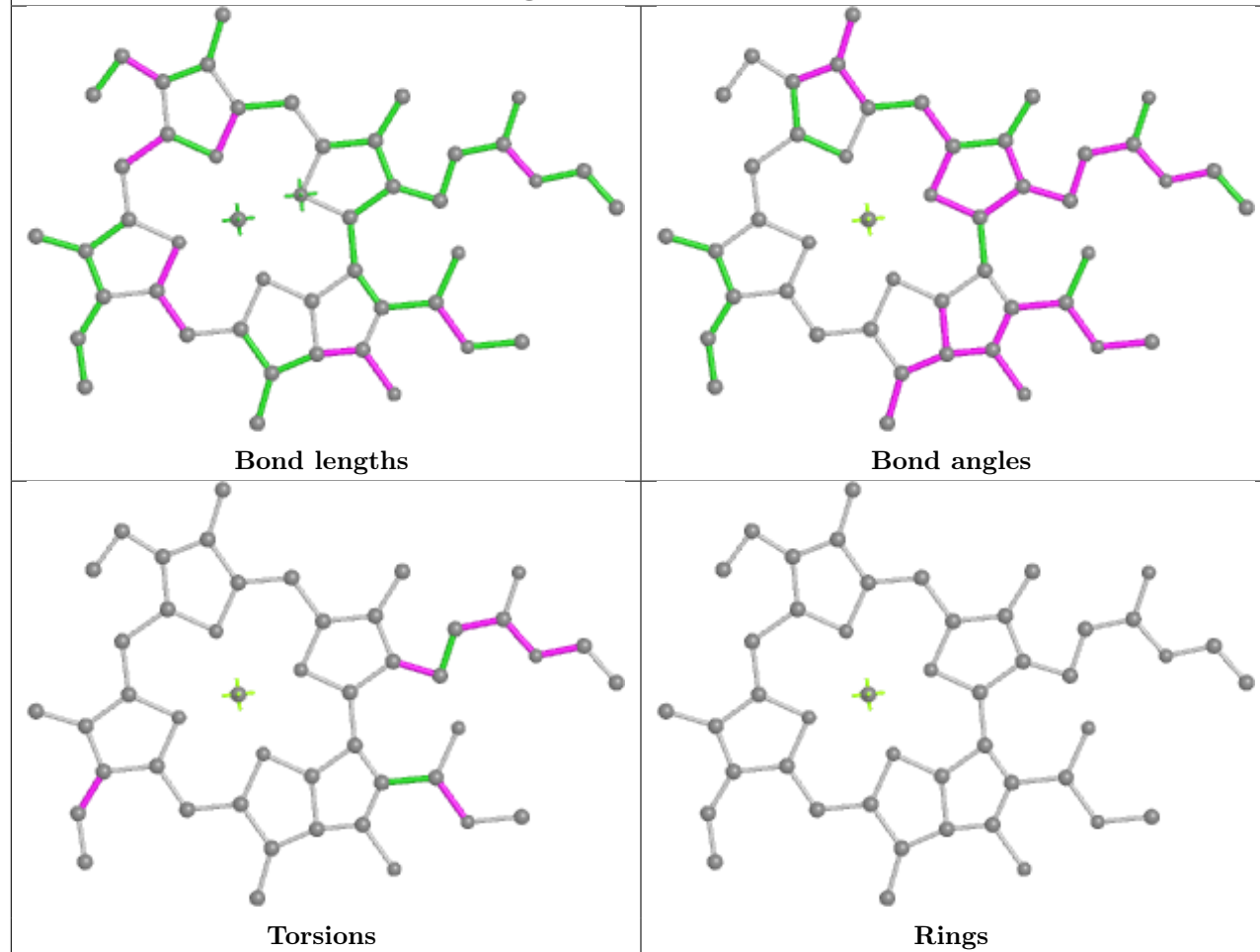


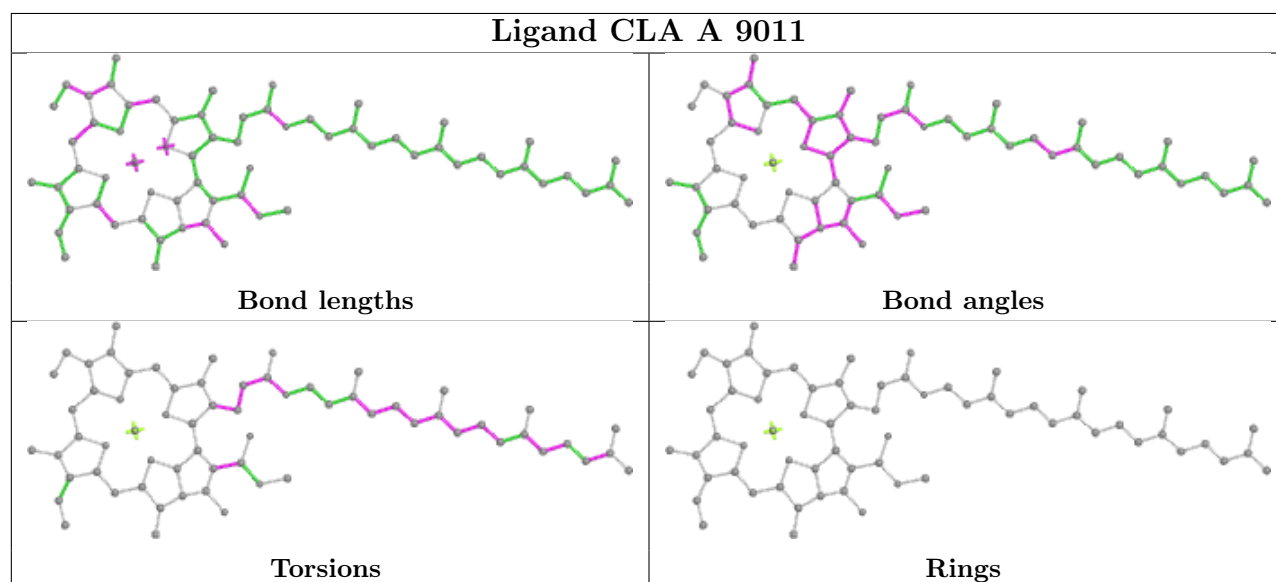
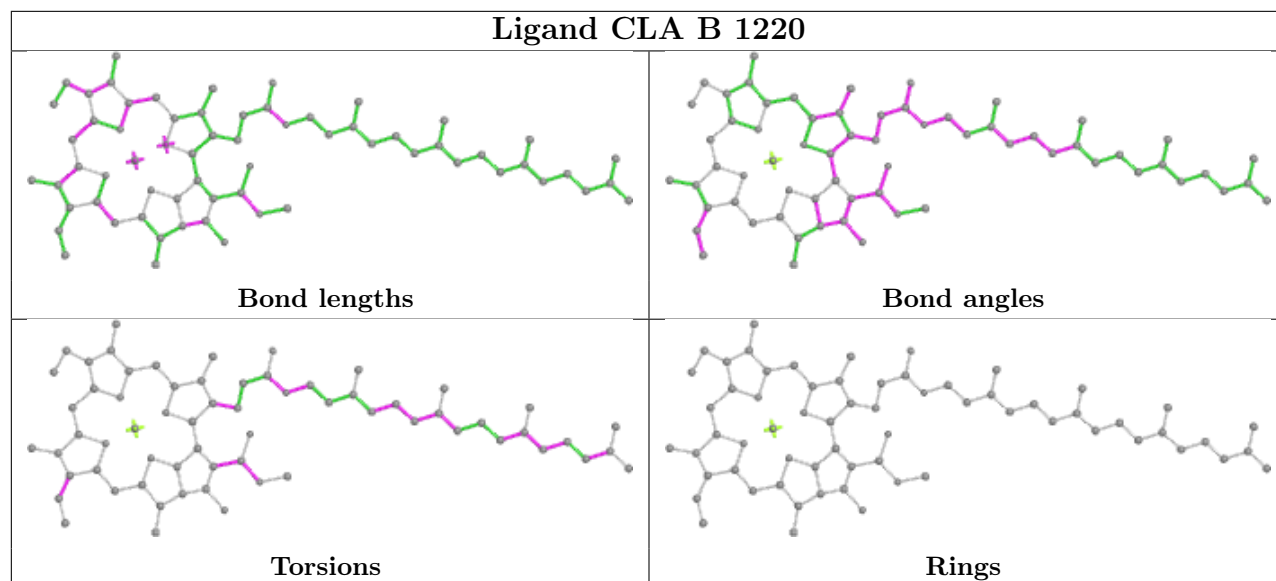
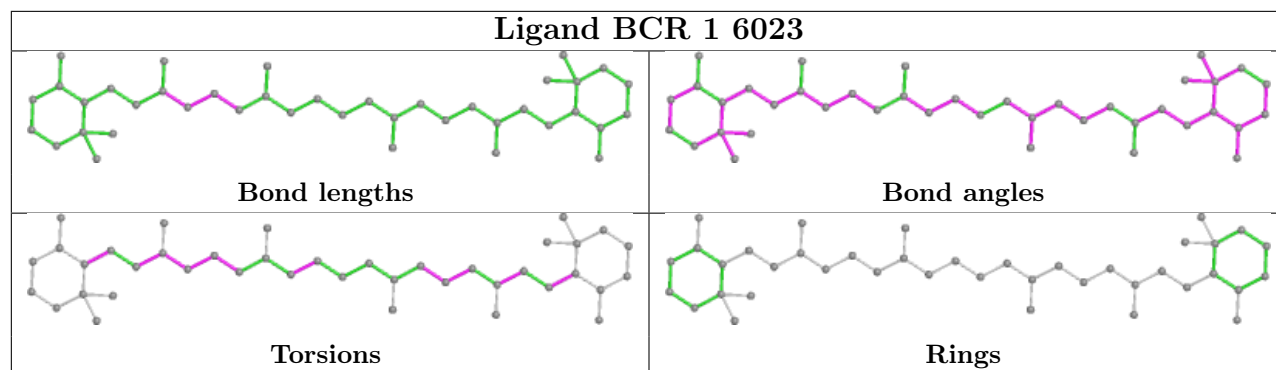


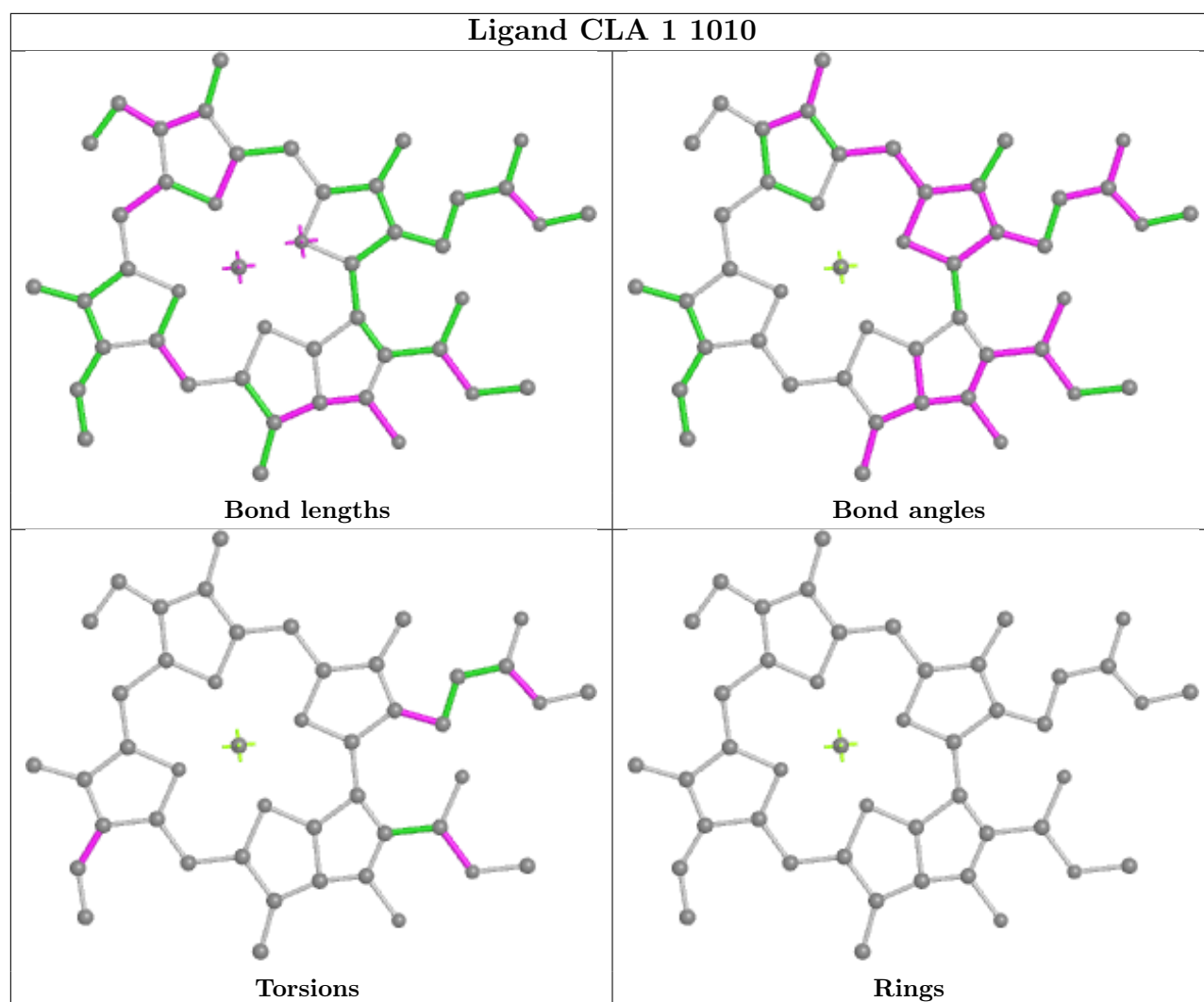
Ligand CLA A 1109

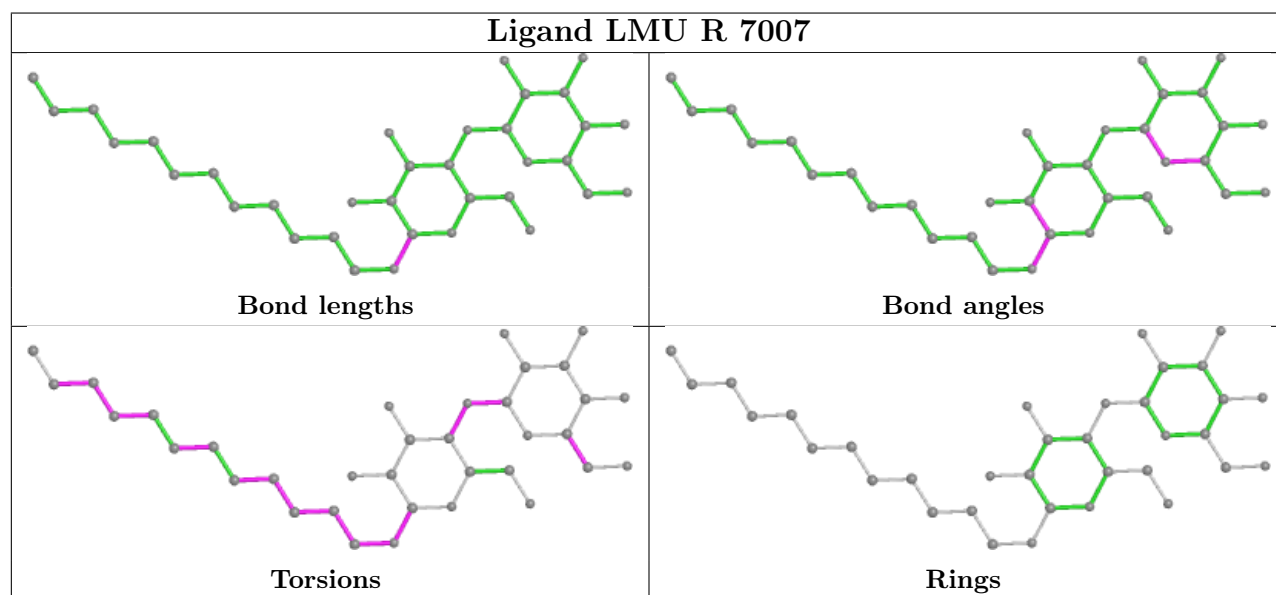
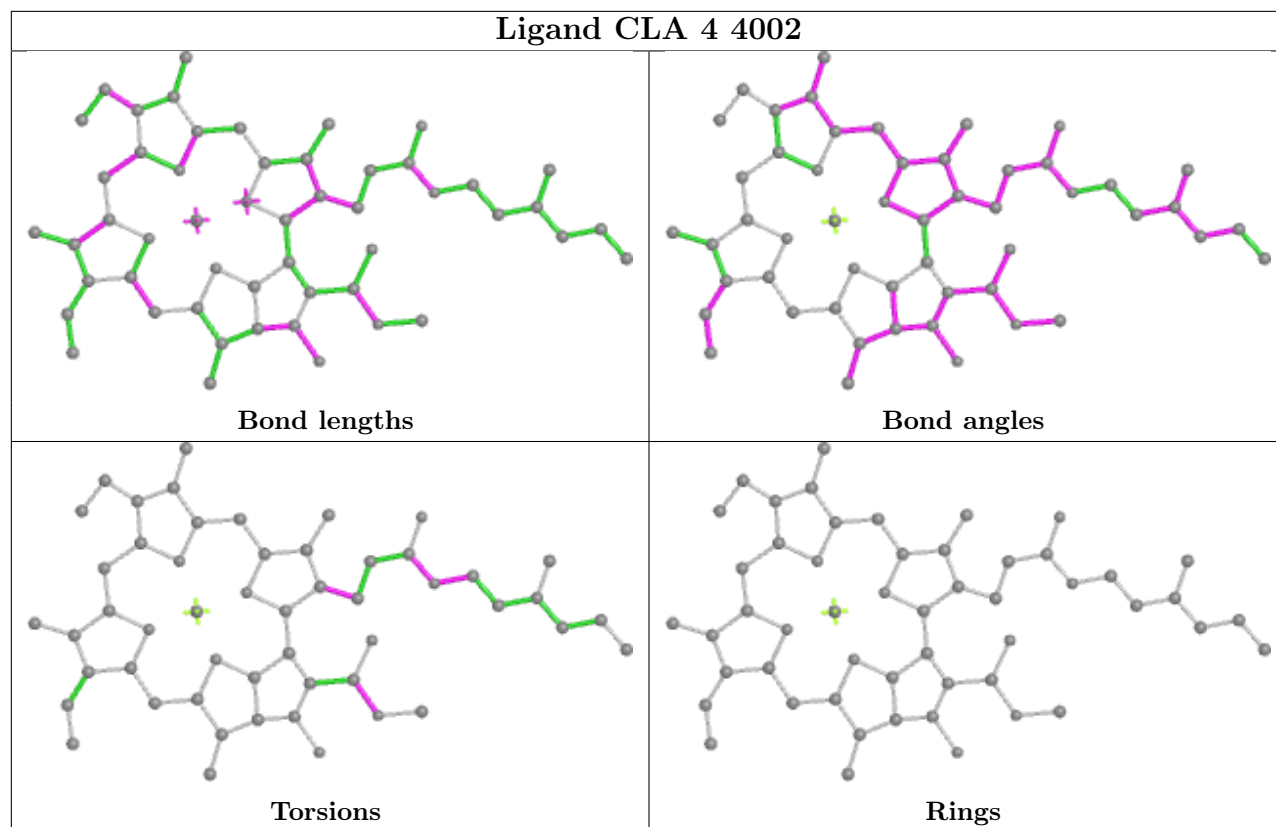


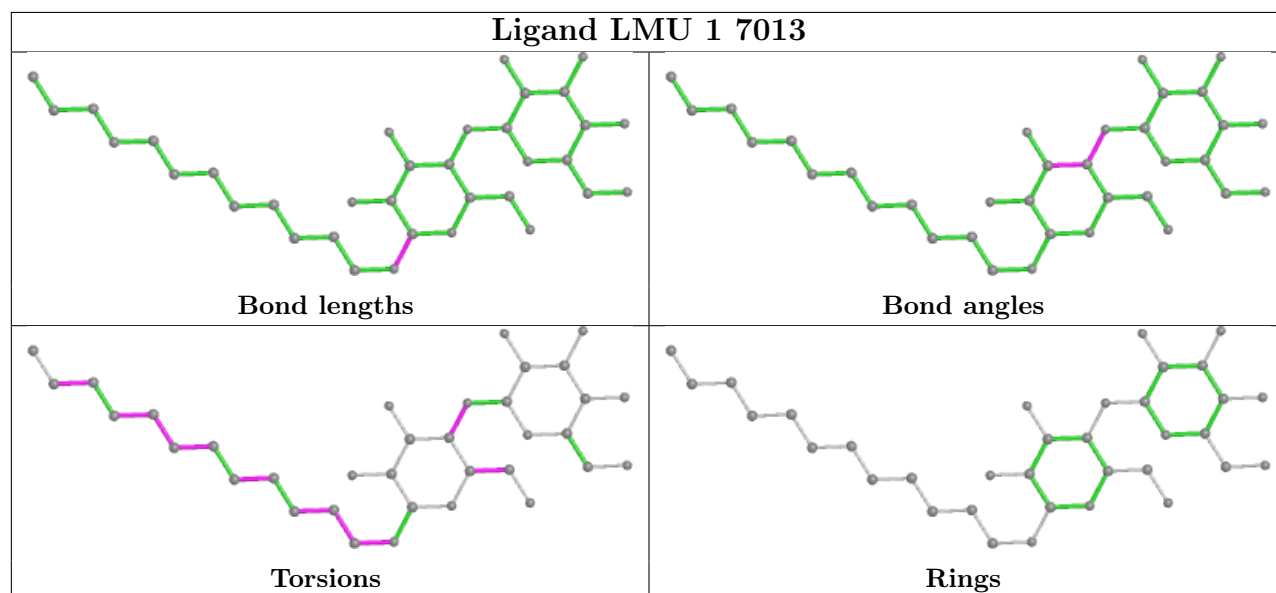
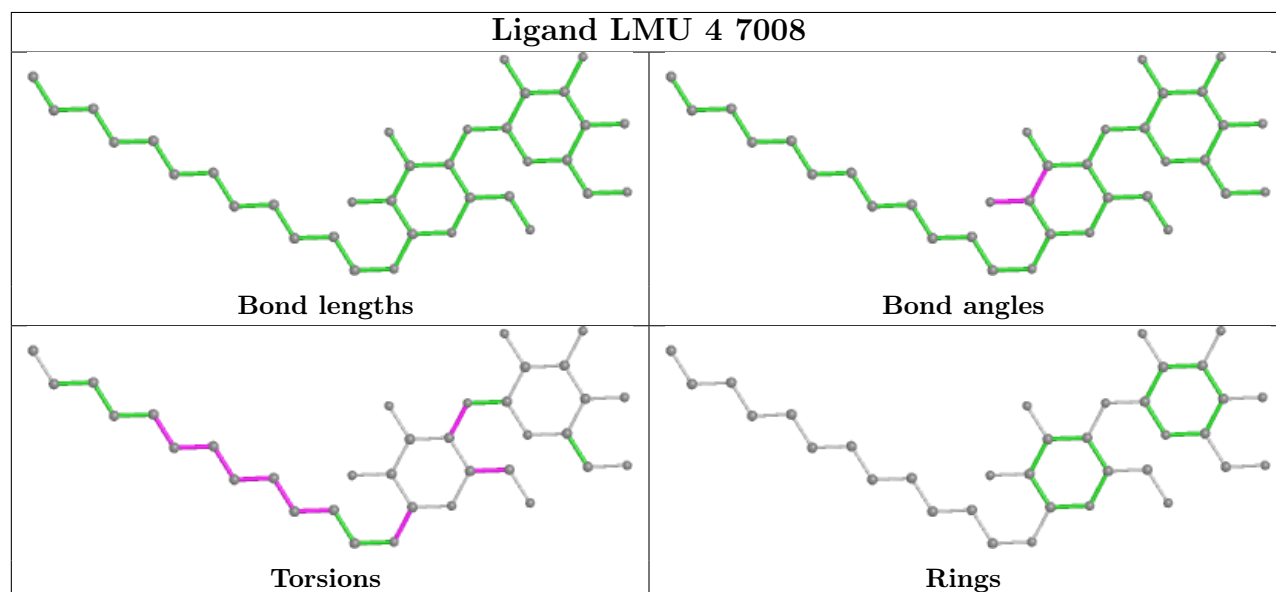
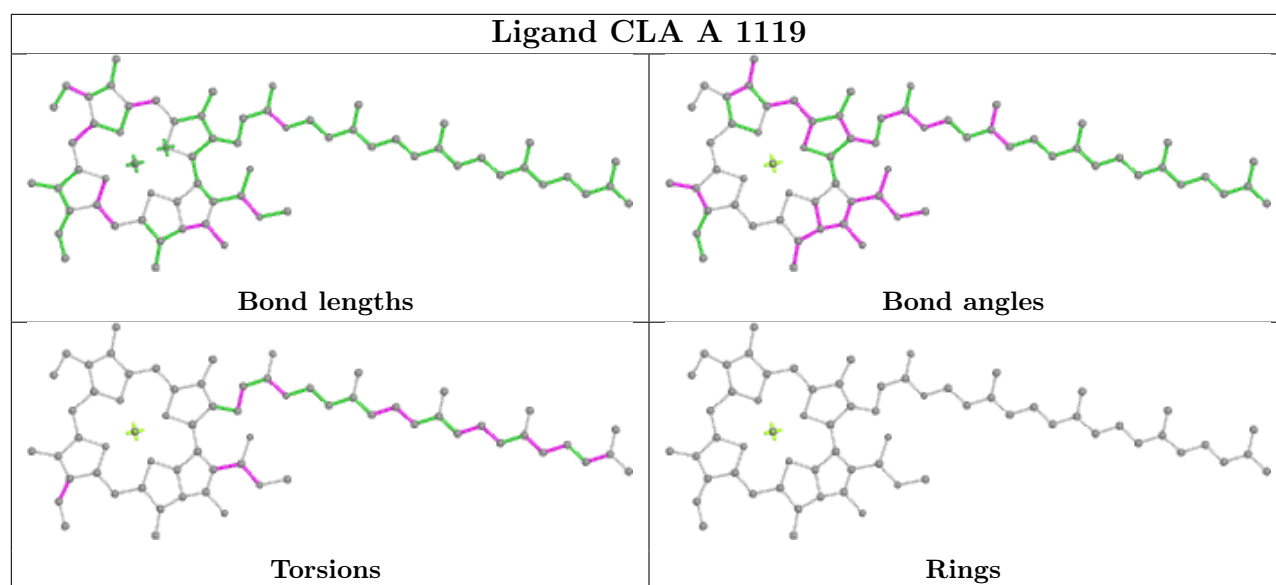
Ligand CLA 1 1002

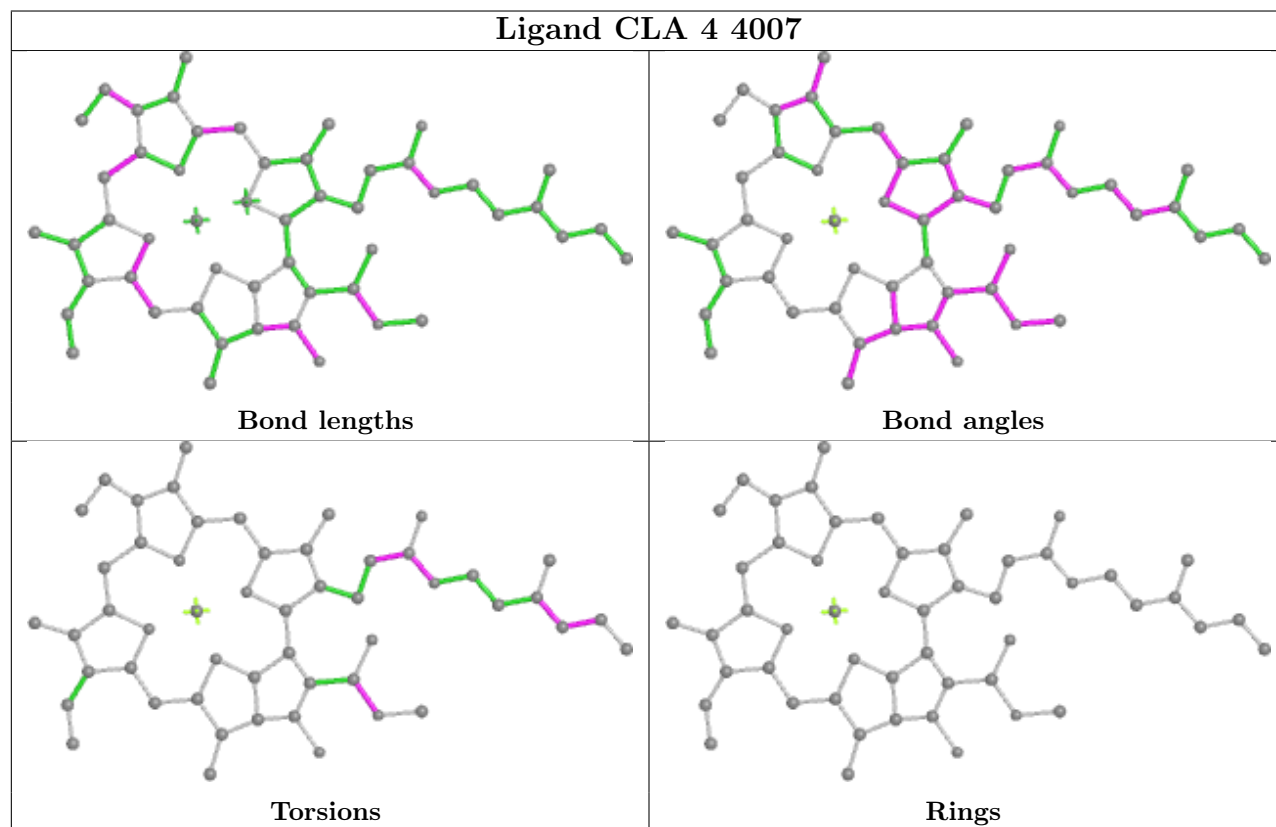
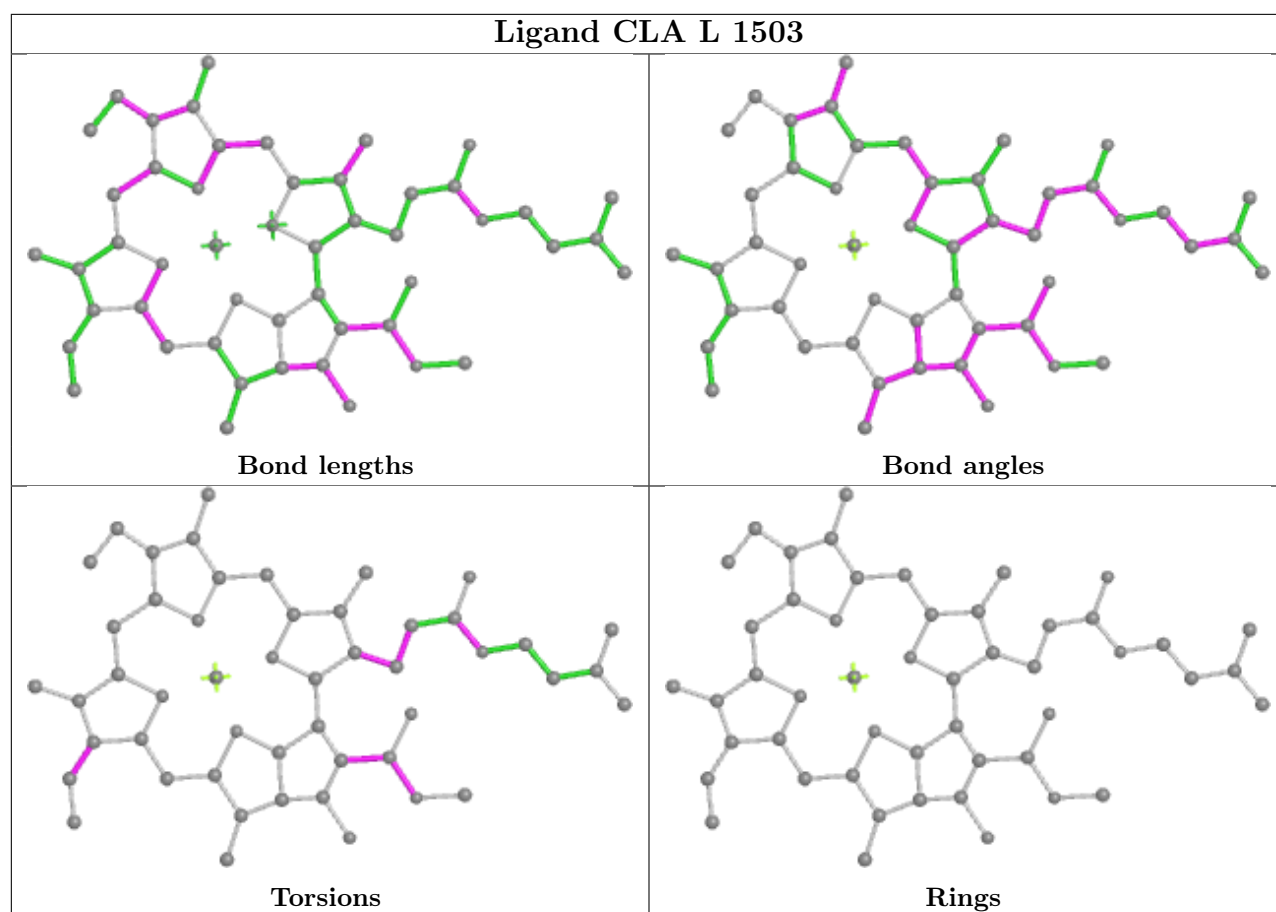




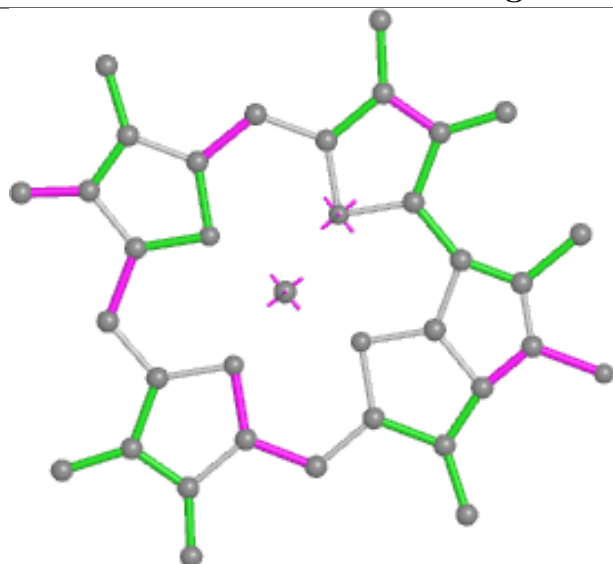




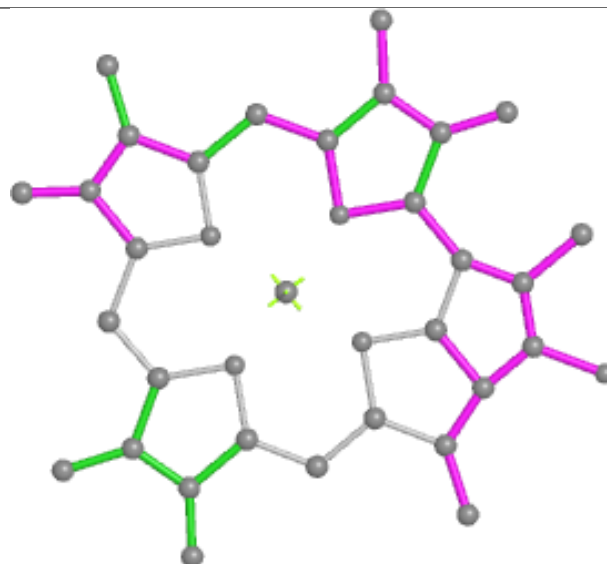




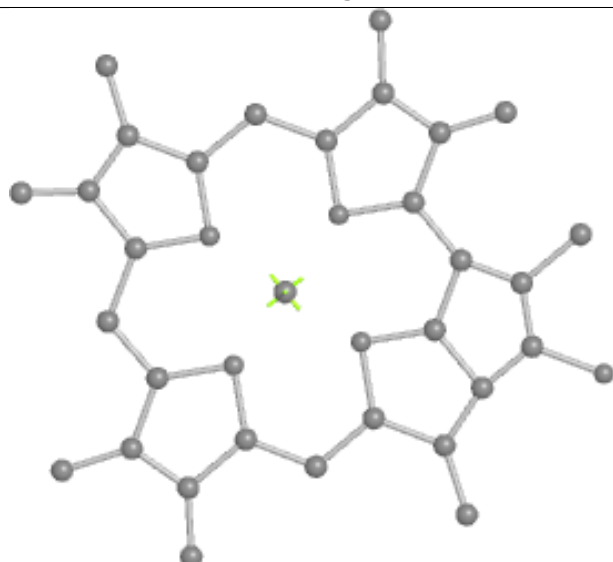
Ligand CLA B 1301



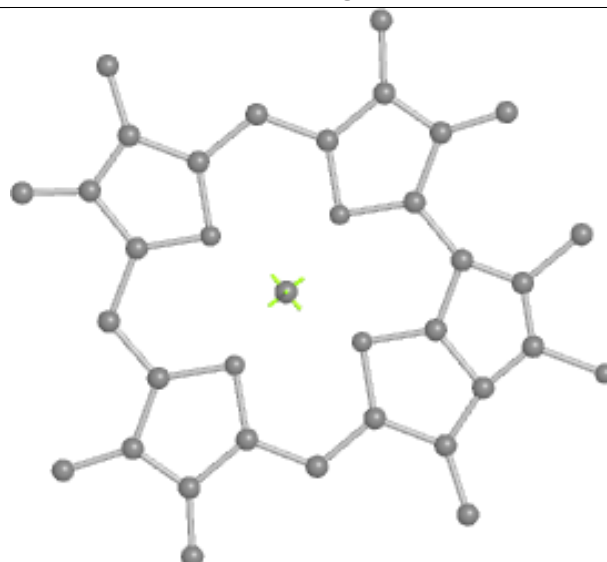
Bond lengths



Bond angles

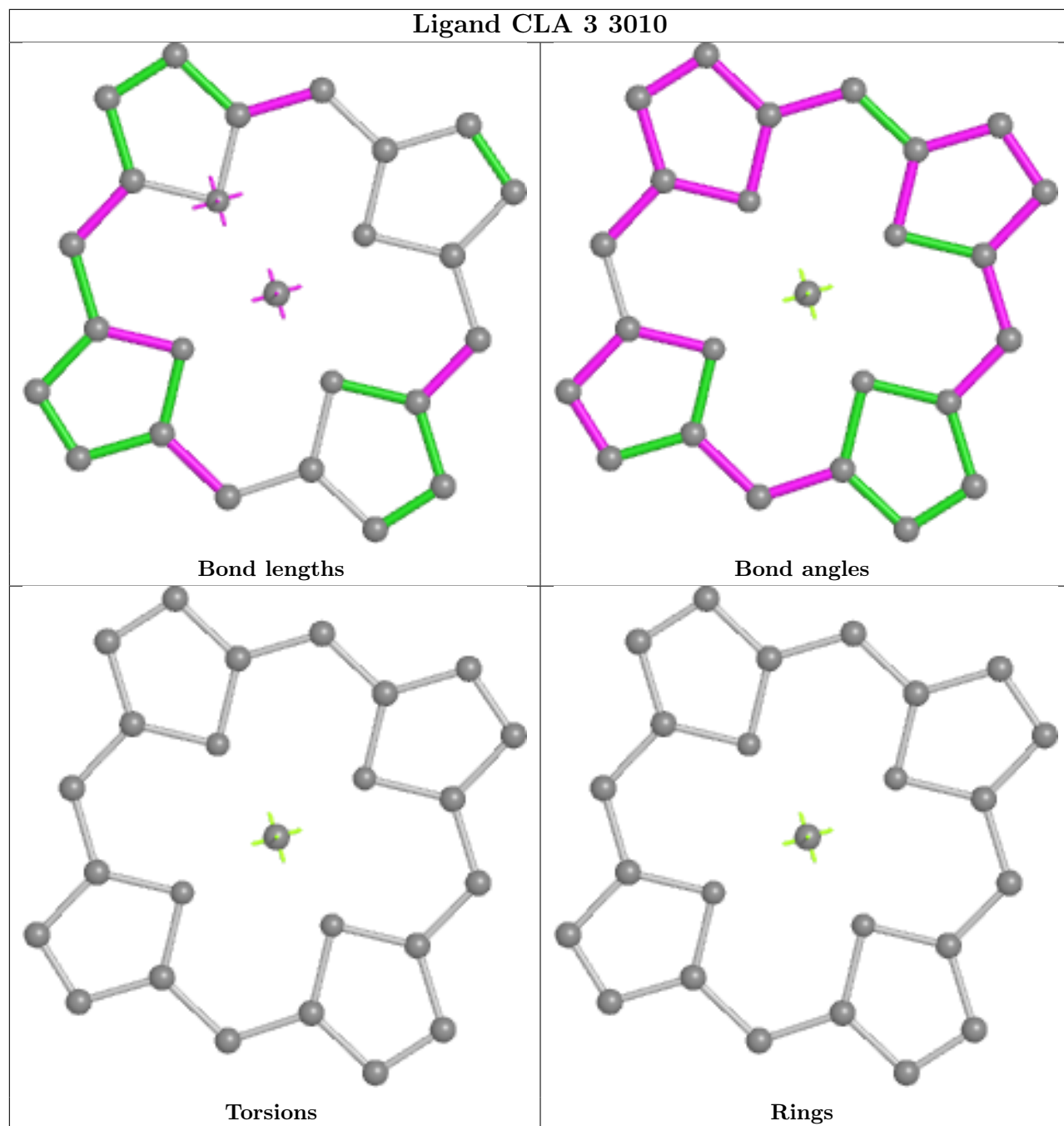


Torsions

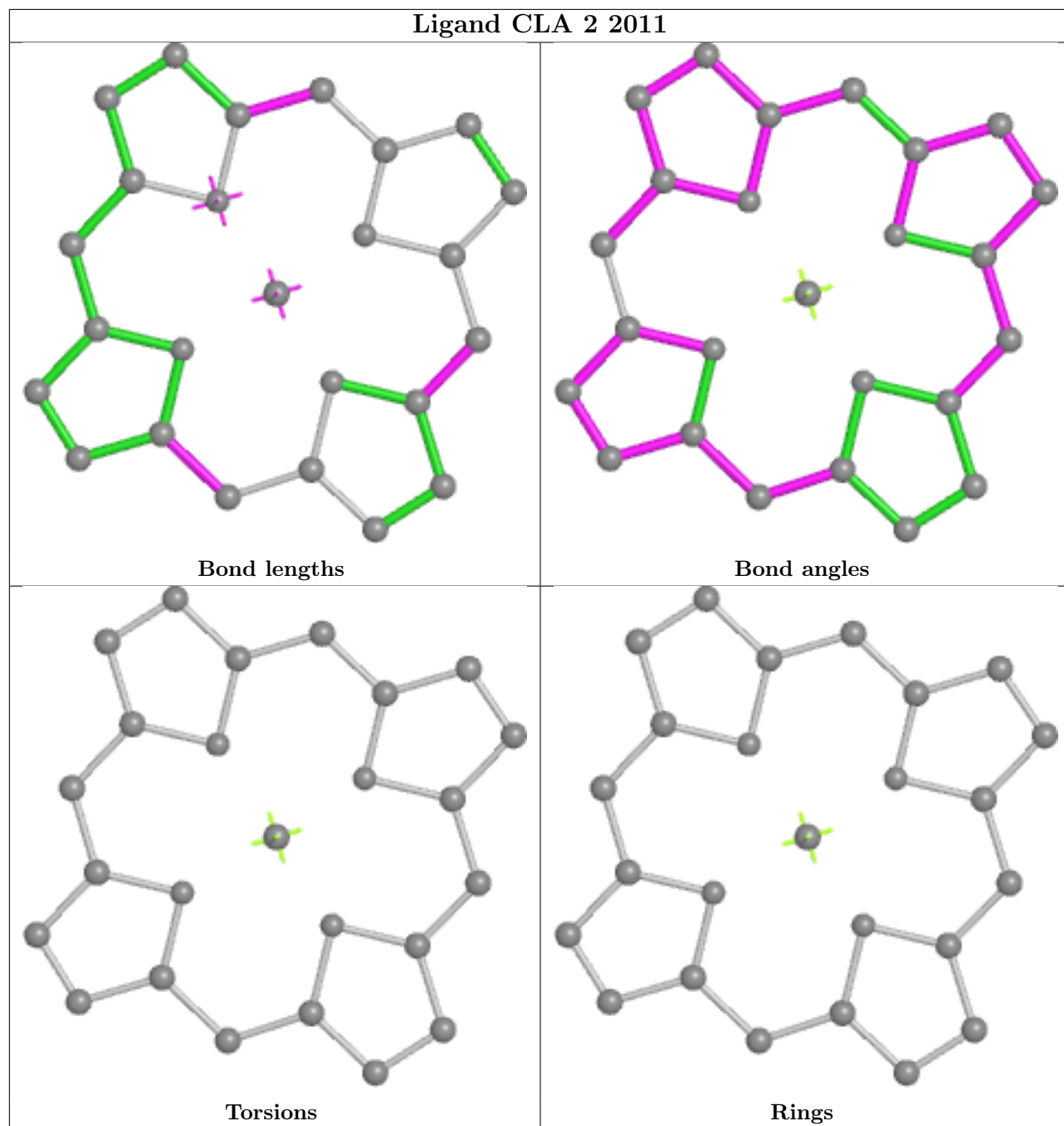


Rings

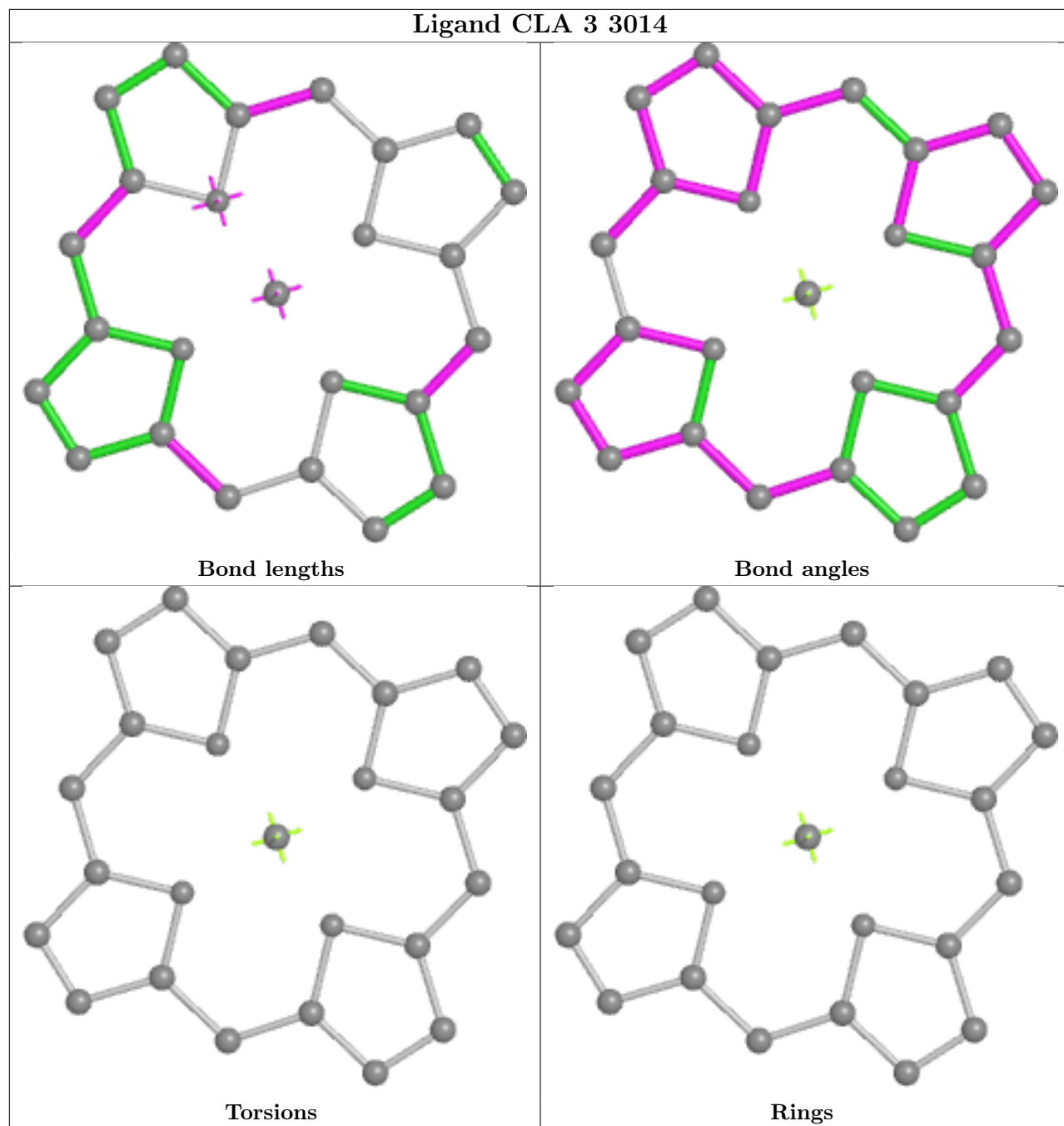
Ligand CLA 3 3010

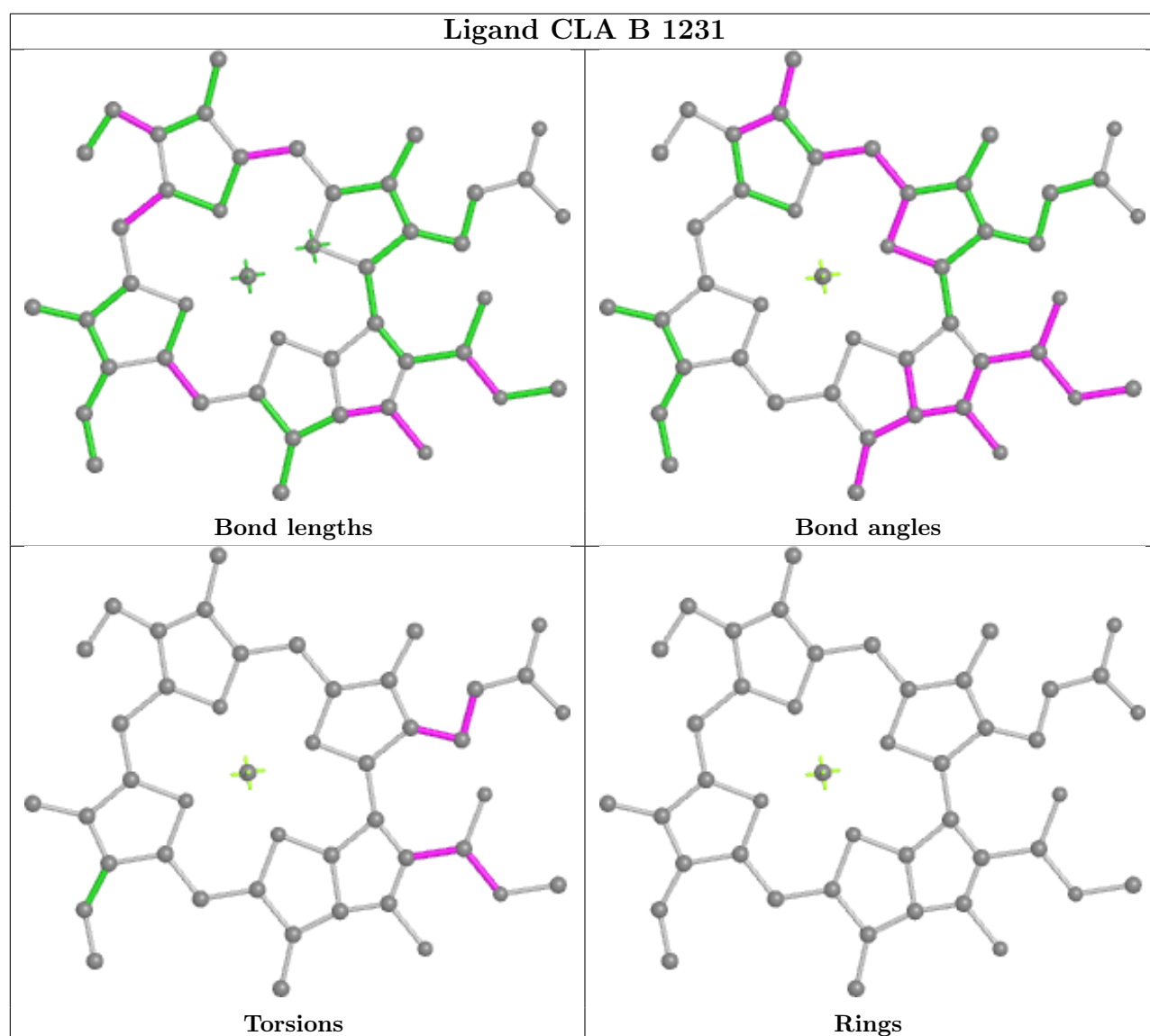
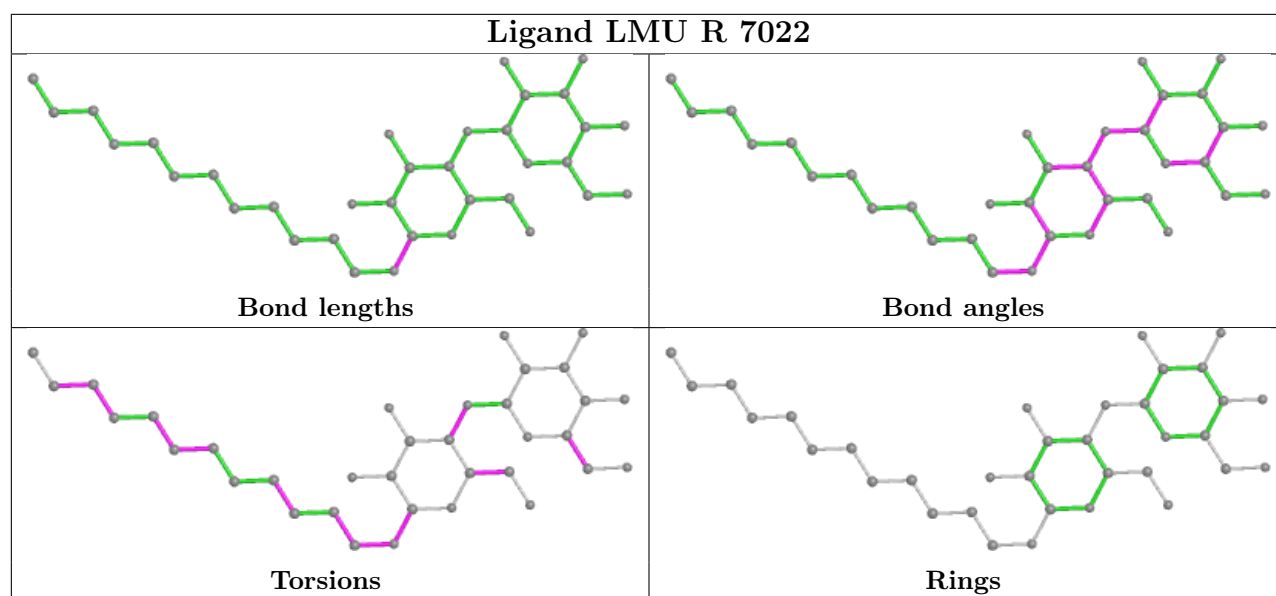


Ligand CLA 2 2011

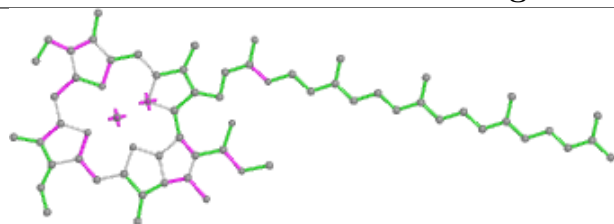


Ligand CLA 3 3014

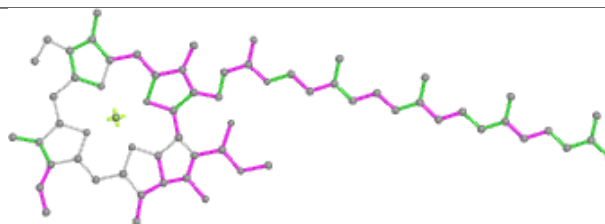




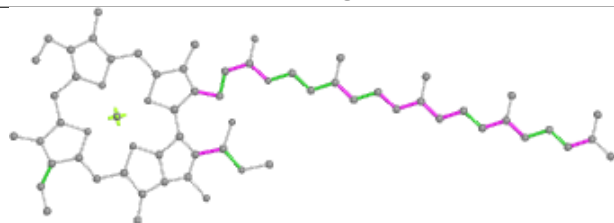
Ligand CLA 4 1304



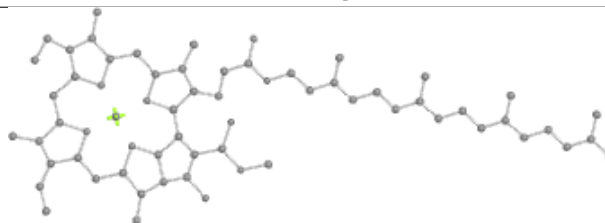
Bond lengths



Bond angles

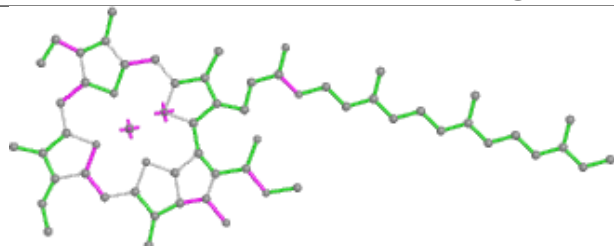


Torsions

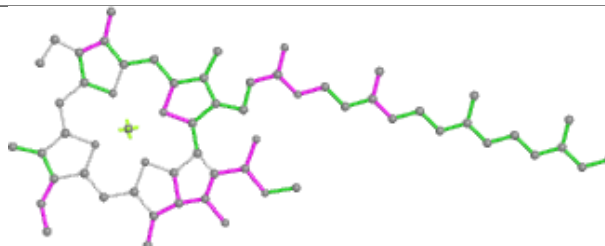


Rings

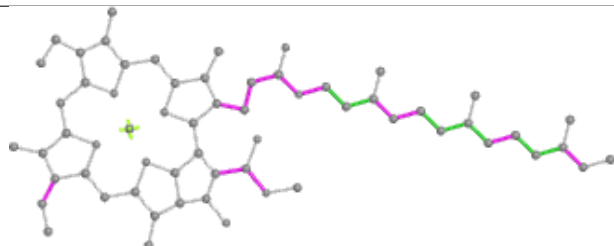
Ligand CLA 1 1007



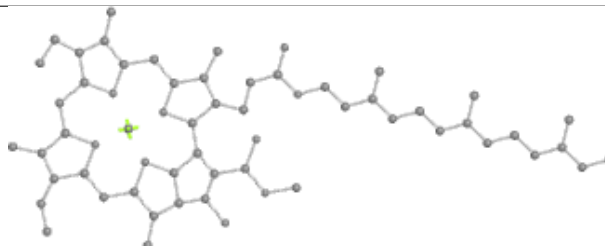
Bond lengths



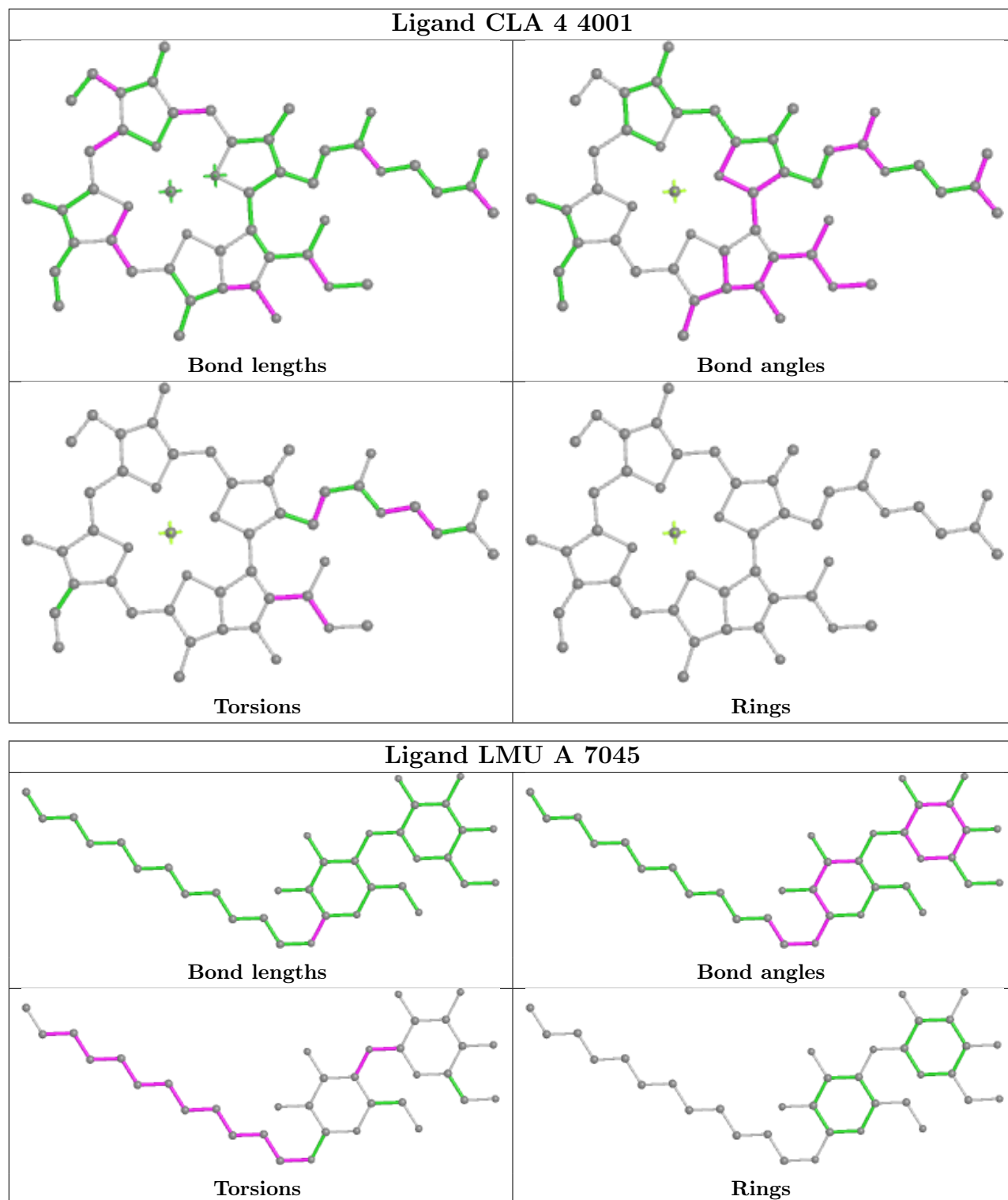
Bond angles

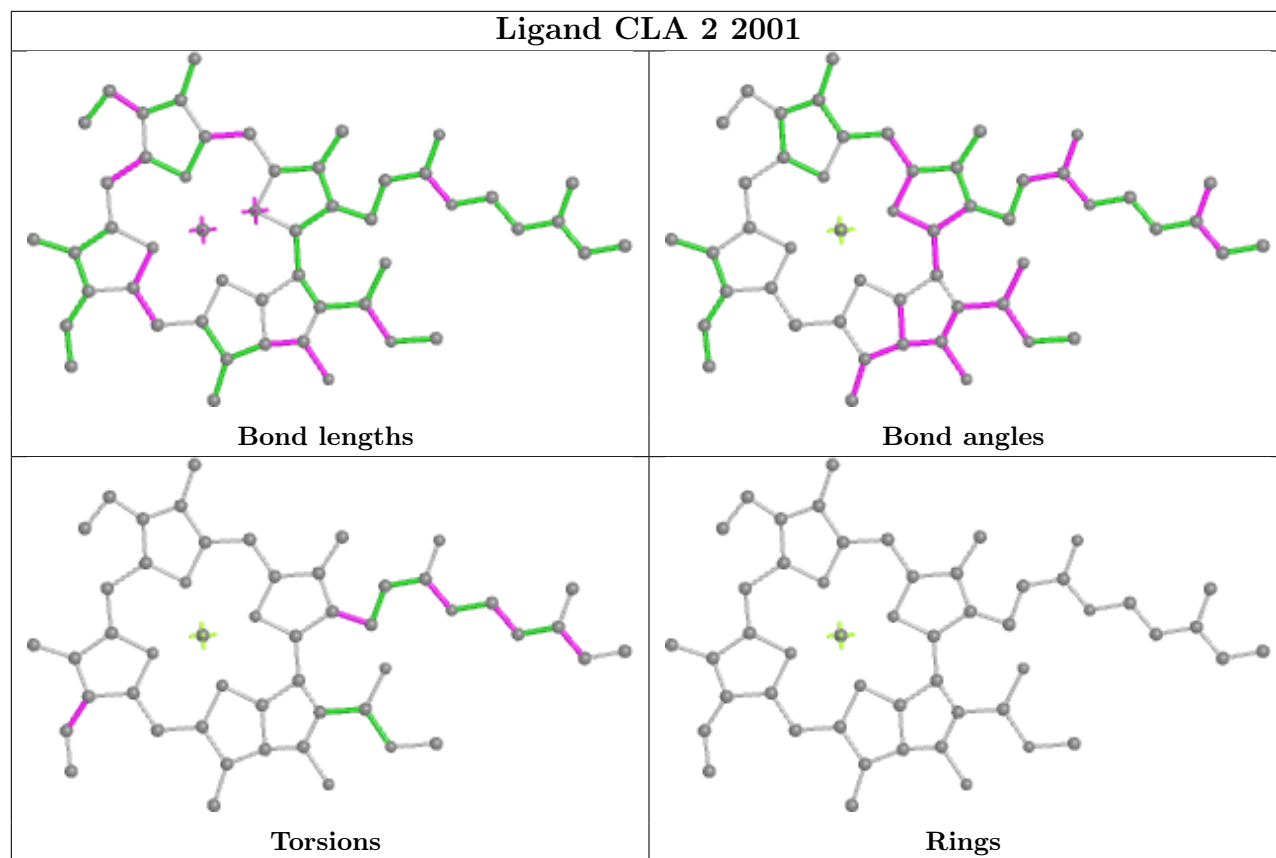


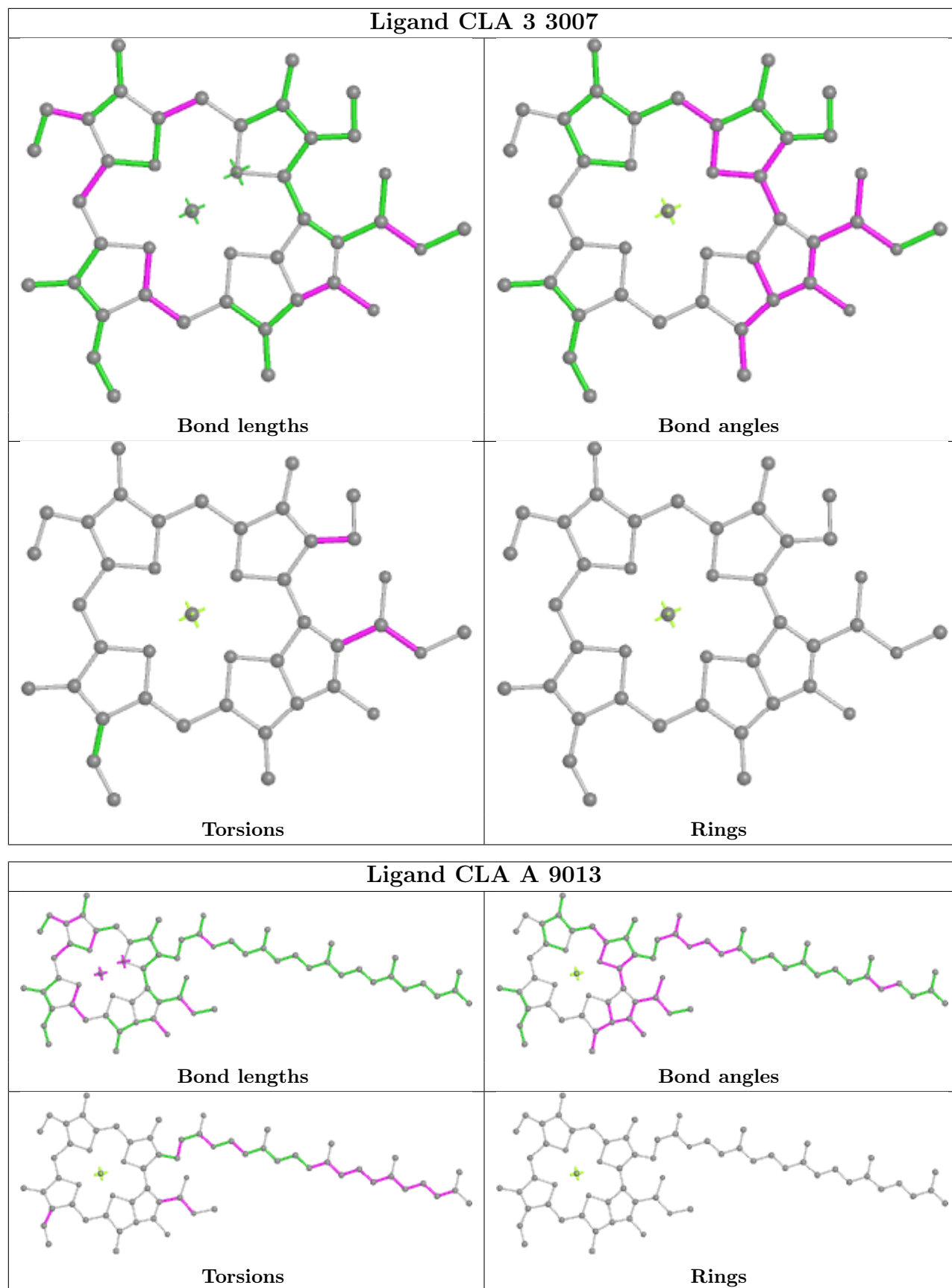
Torsions

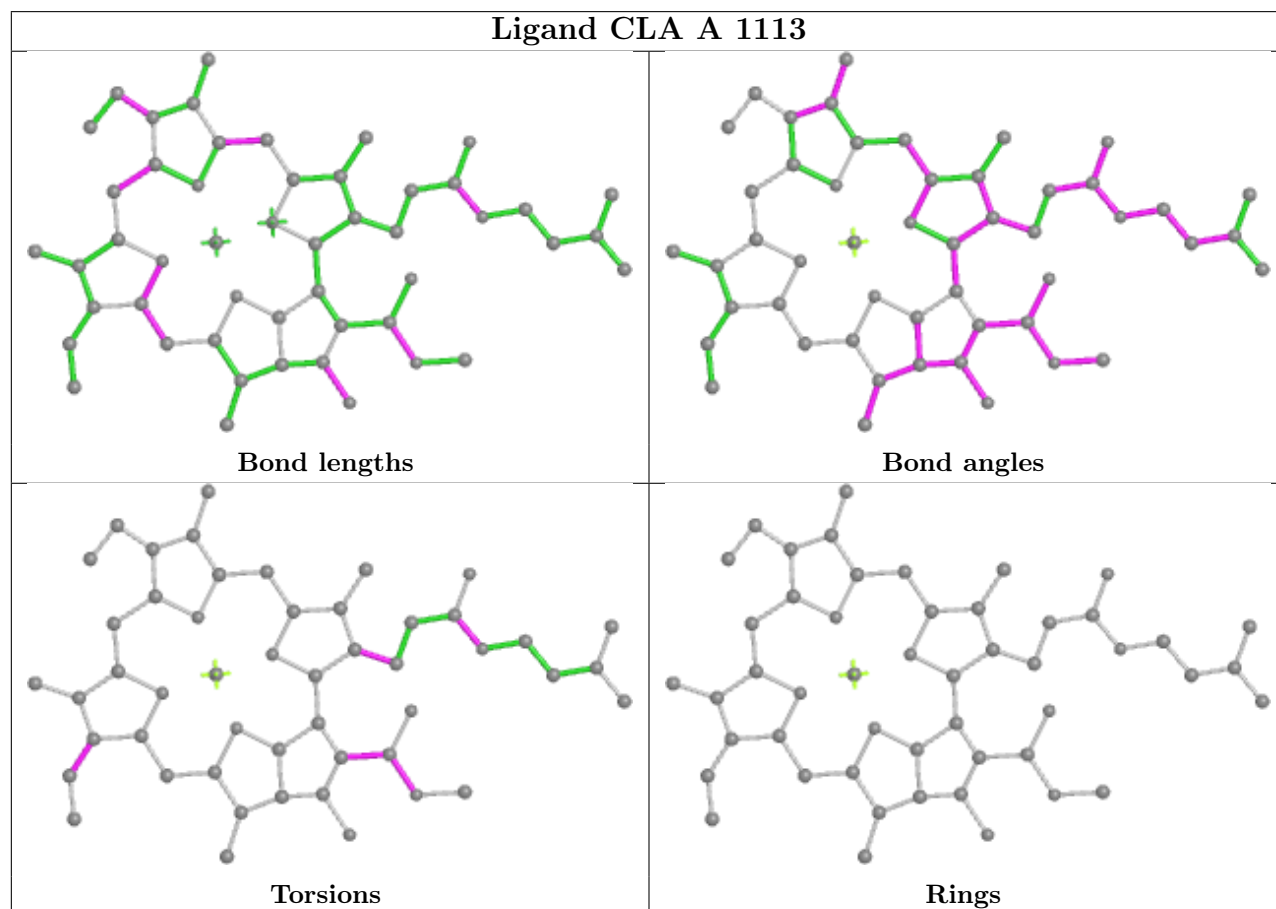
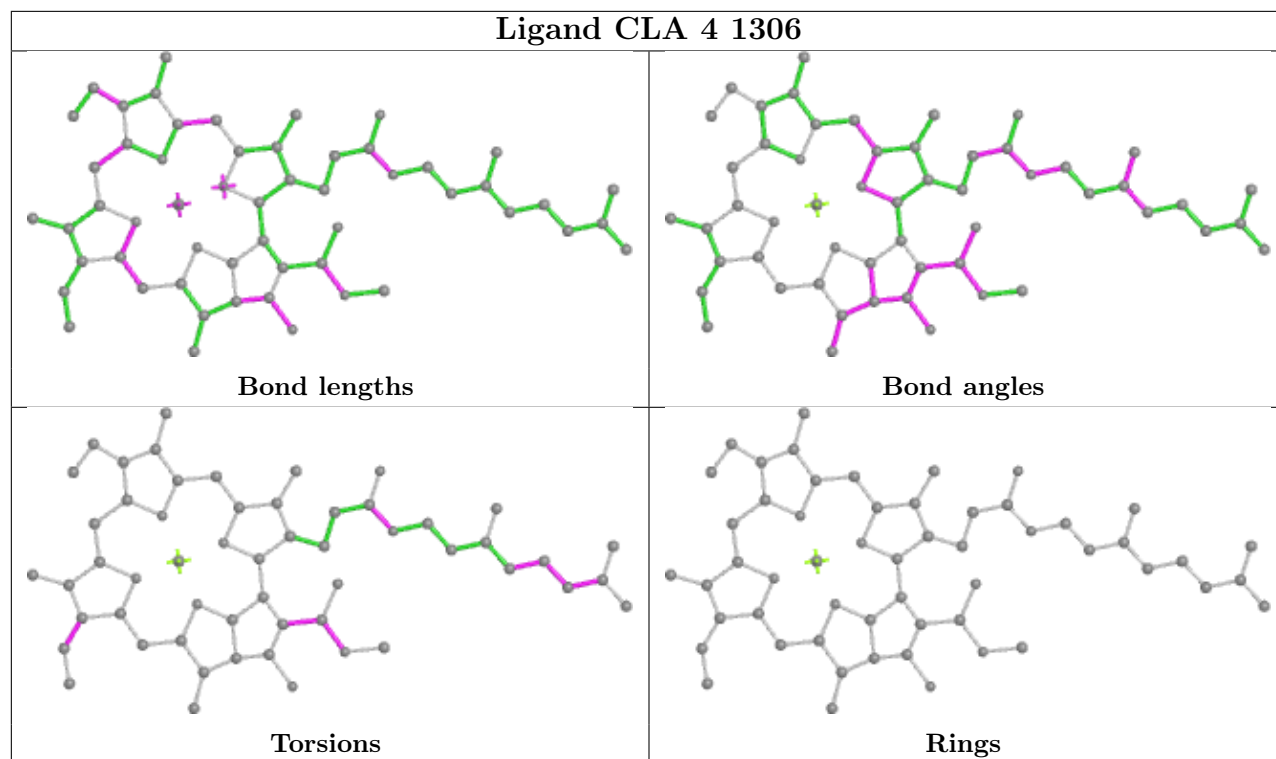


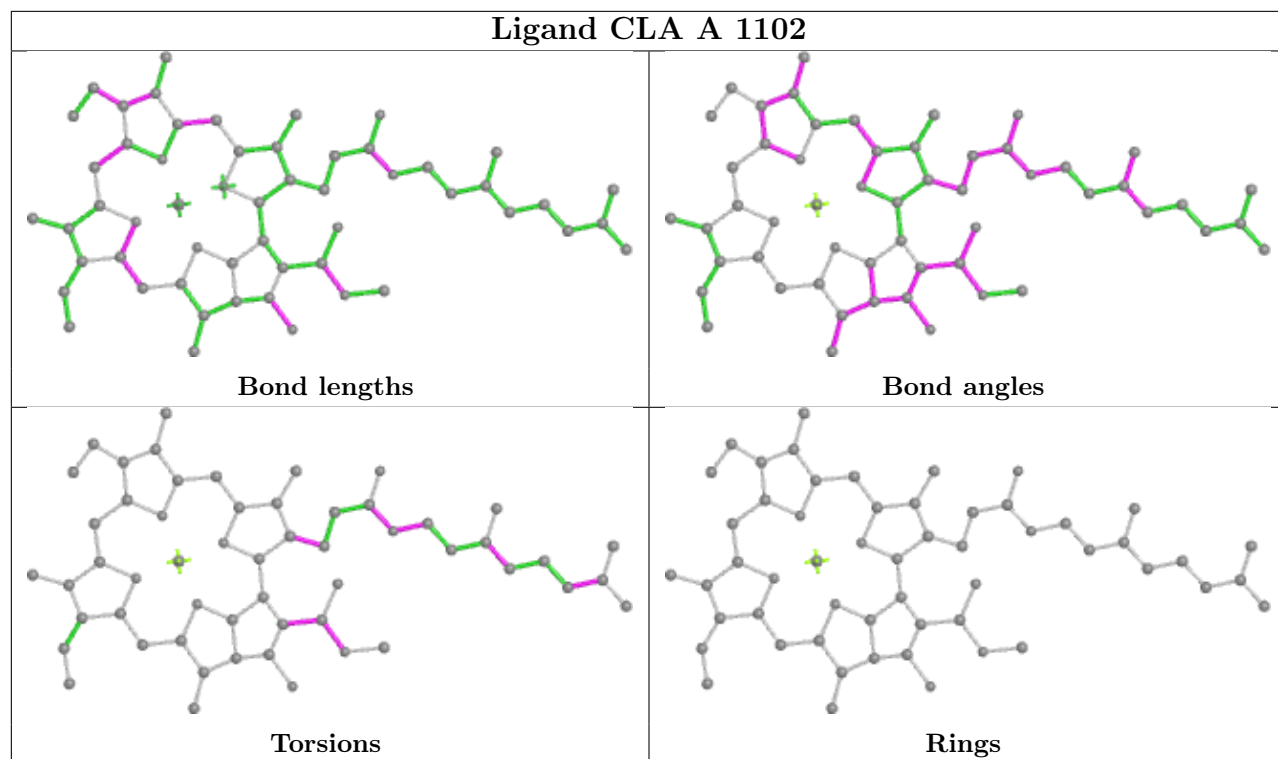
Rings



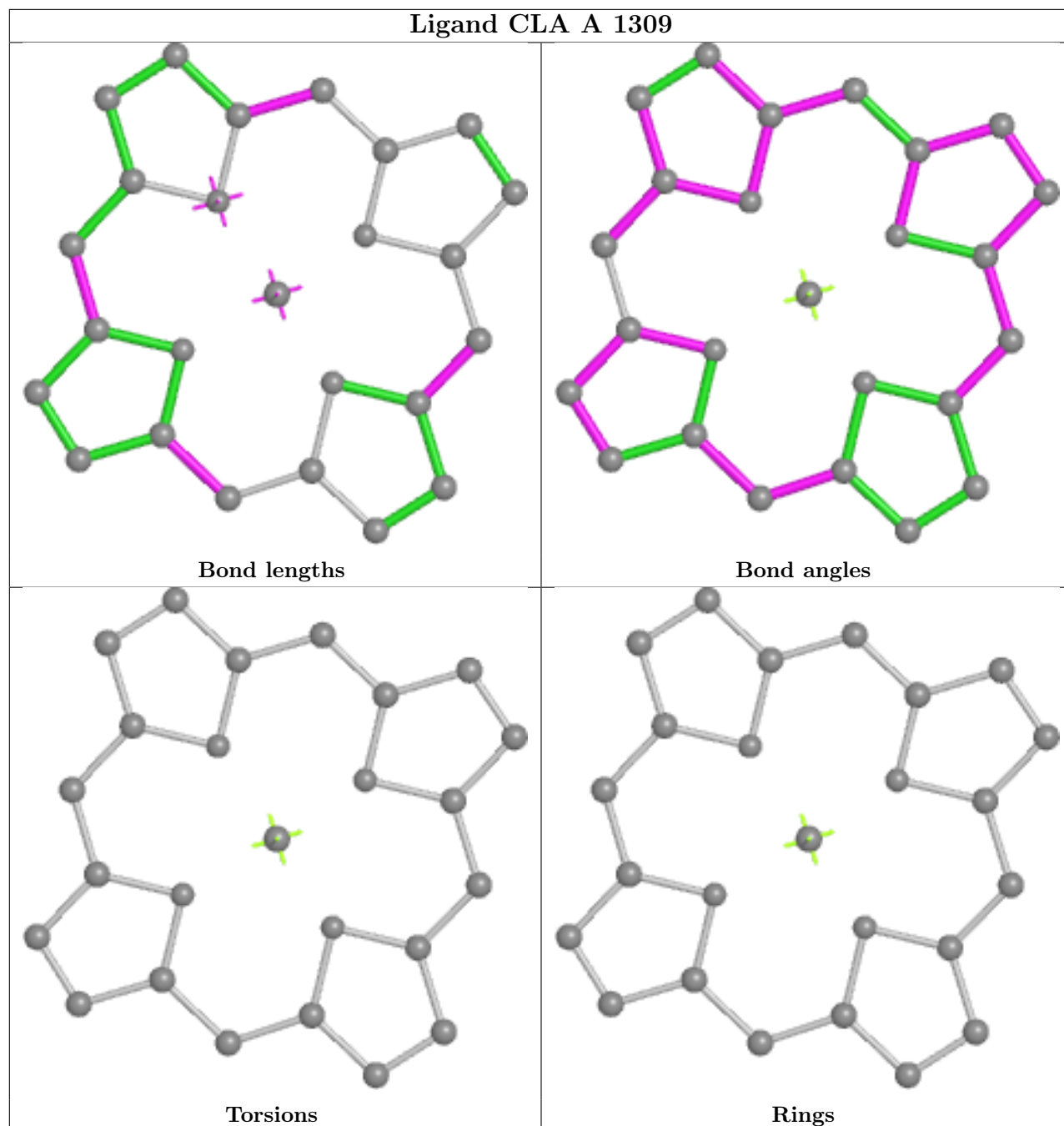


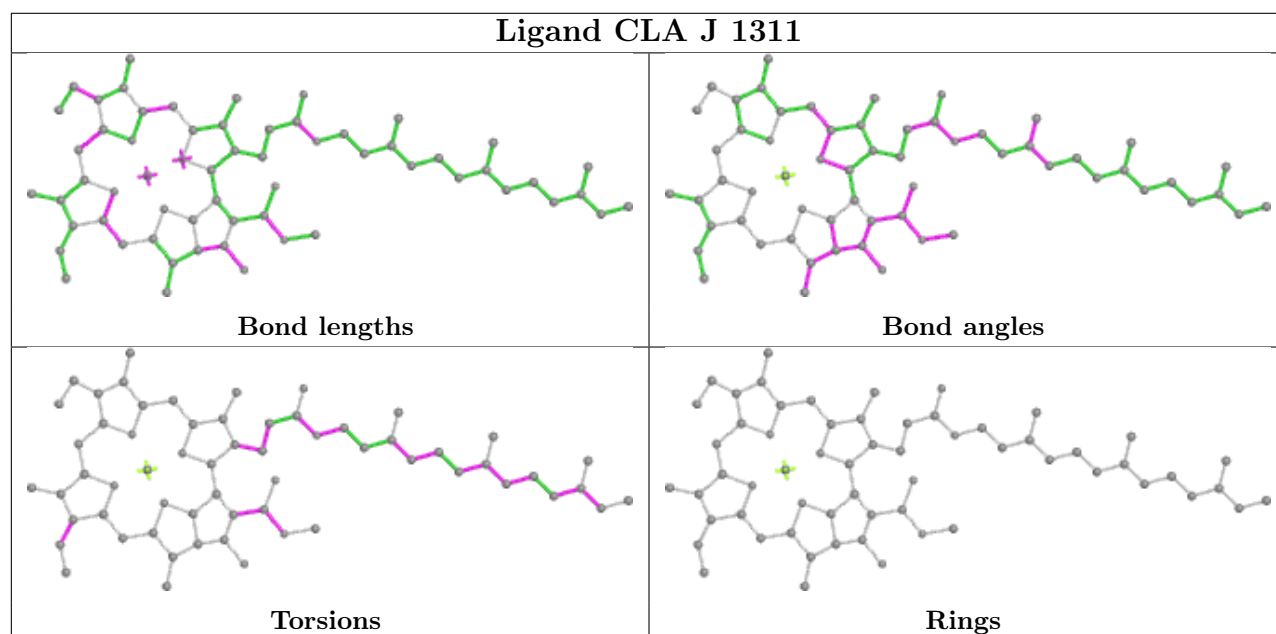
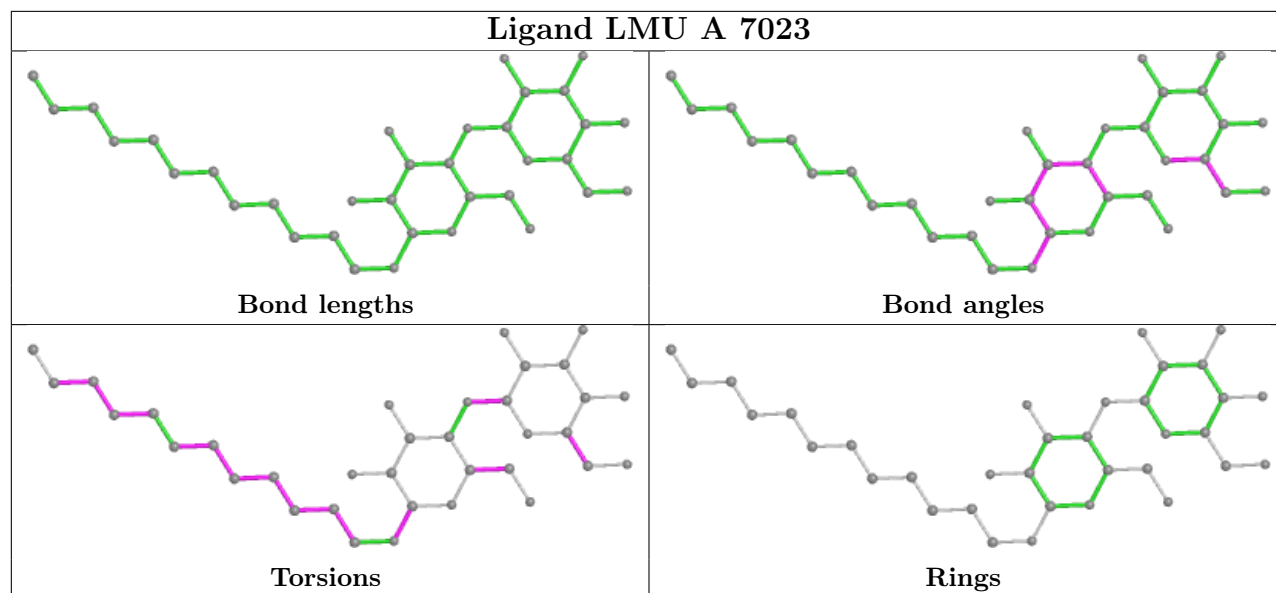




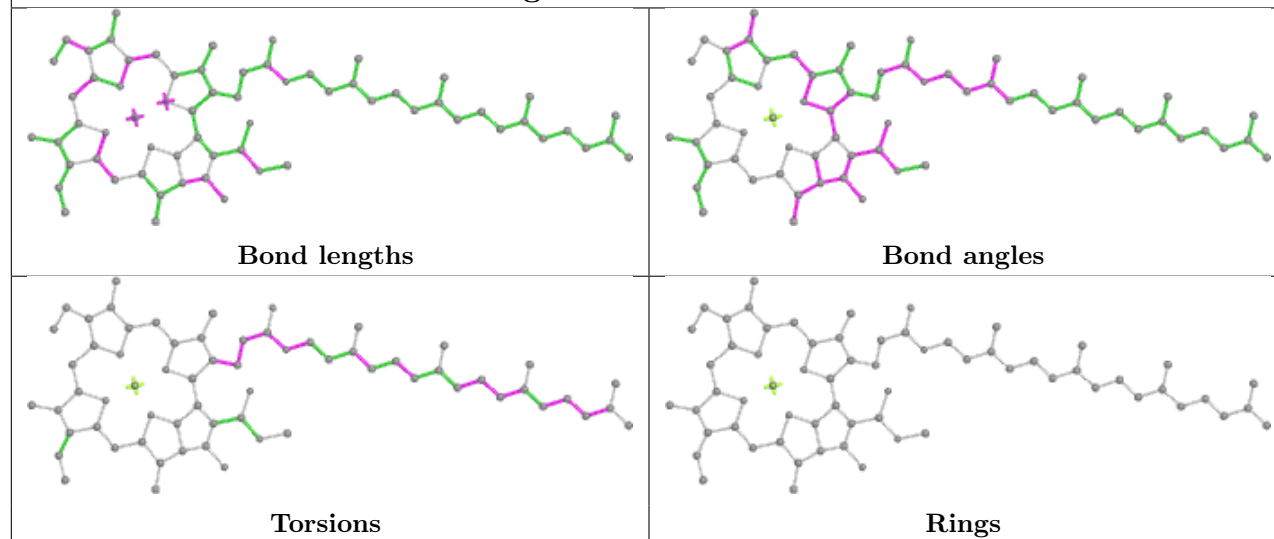


Ligand CLA A 1309

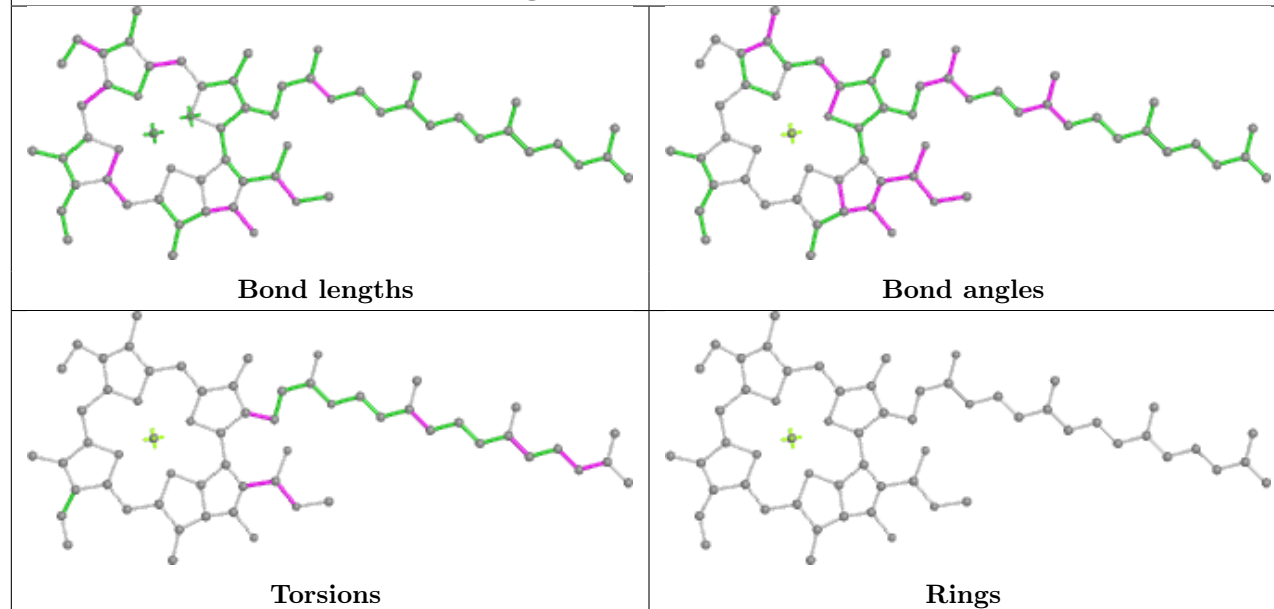




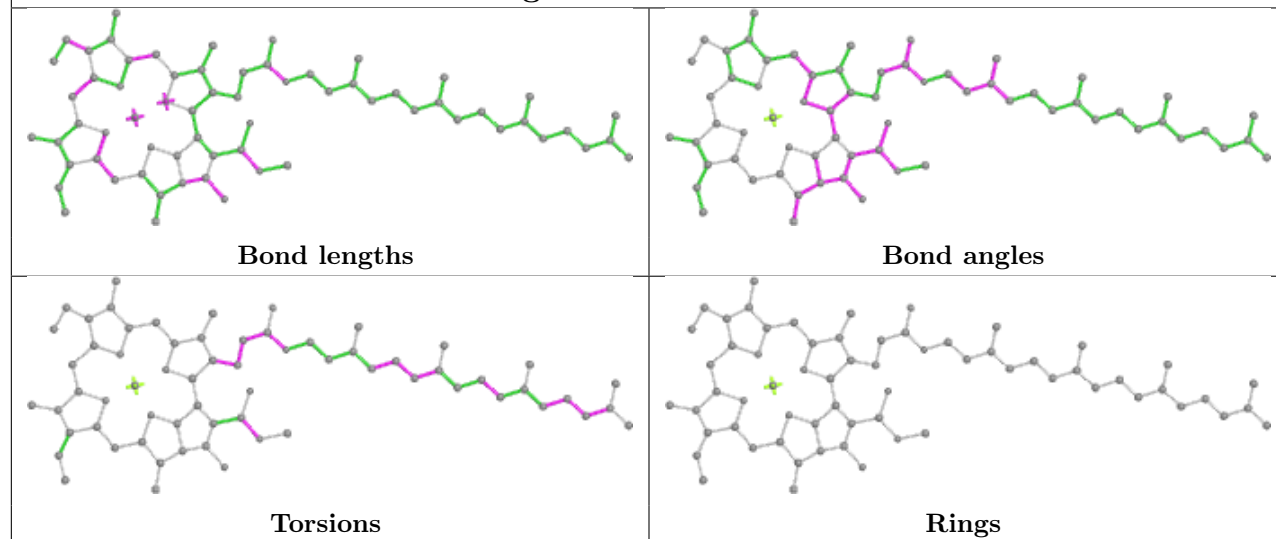
Ligand CLA B 1223



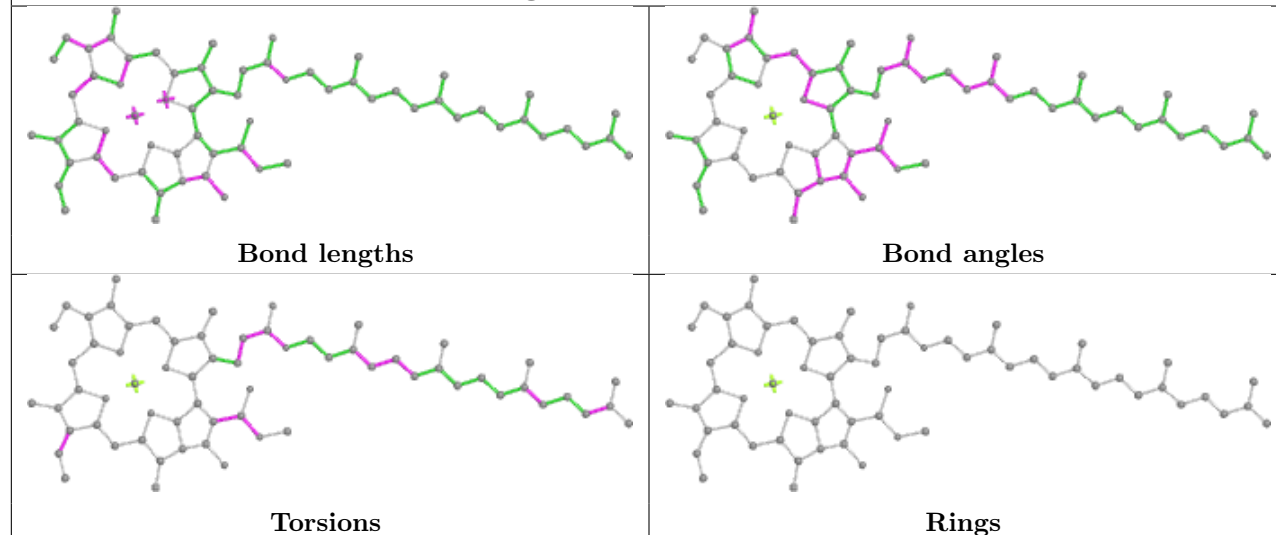
Ligand CLA B 1212



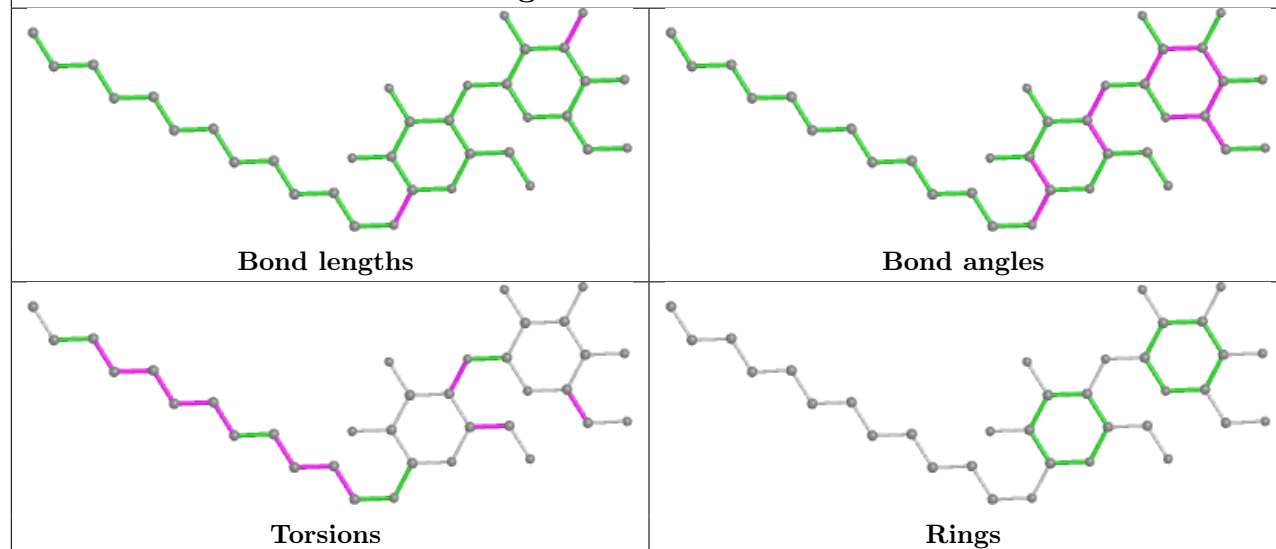
Ligand CLA A 1140



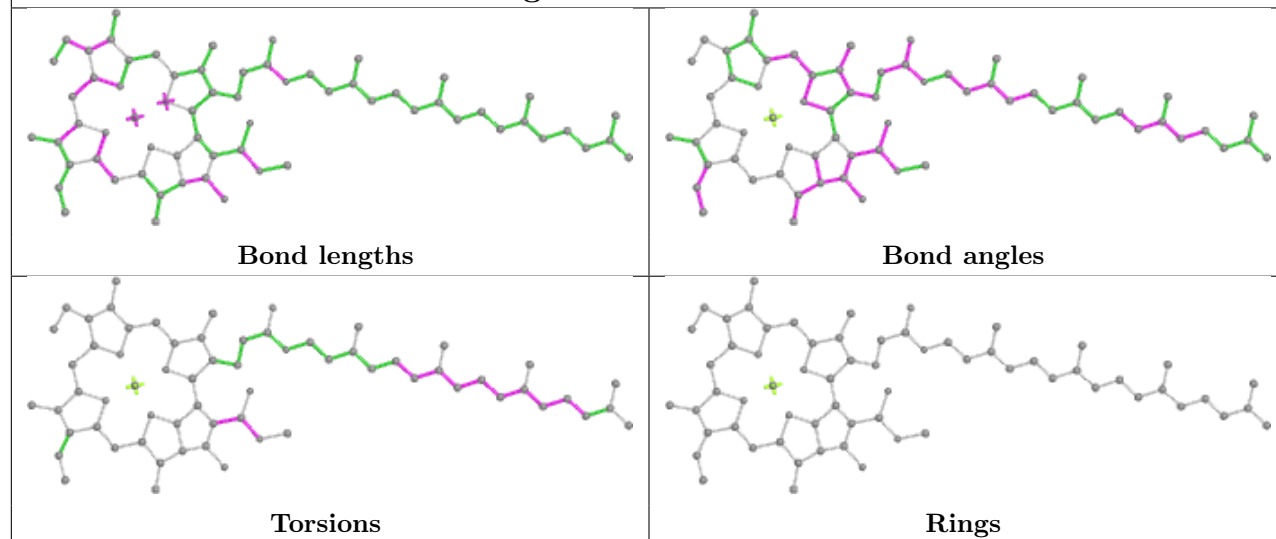
Ligand CLA A 1115



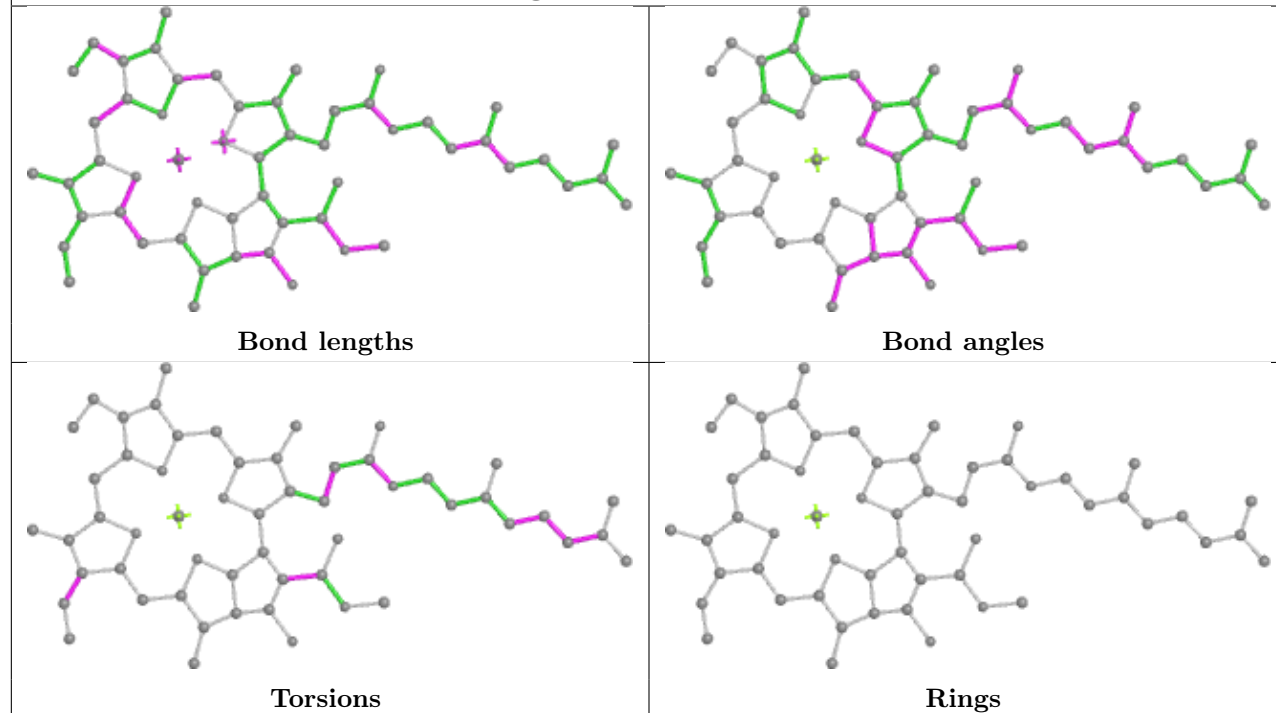
Ligand LMU K 7001



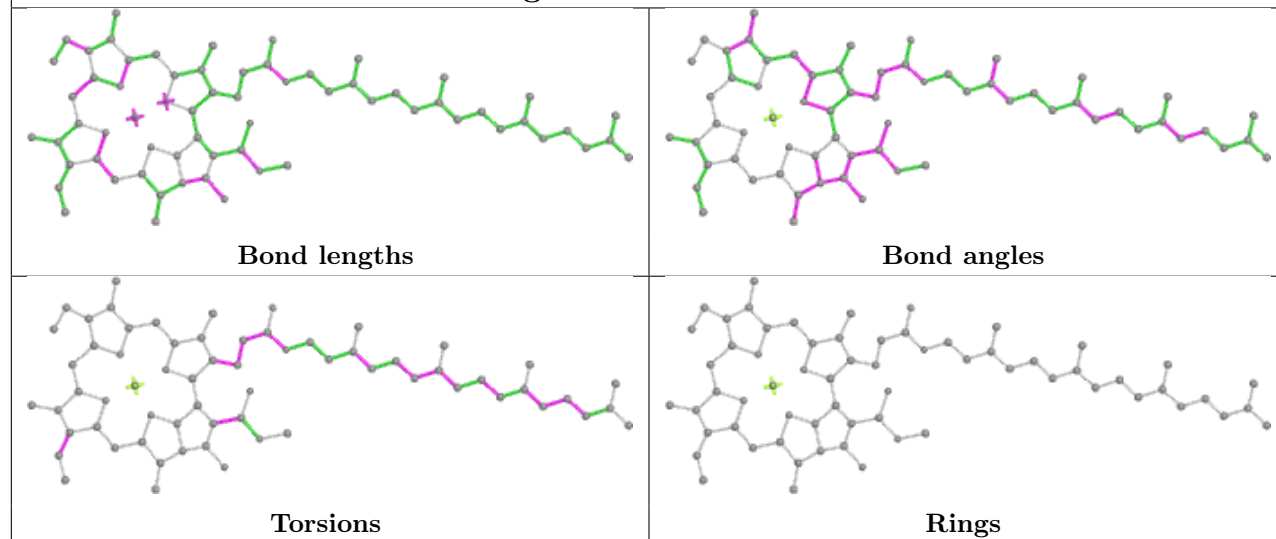
Ligand CLA B 1203



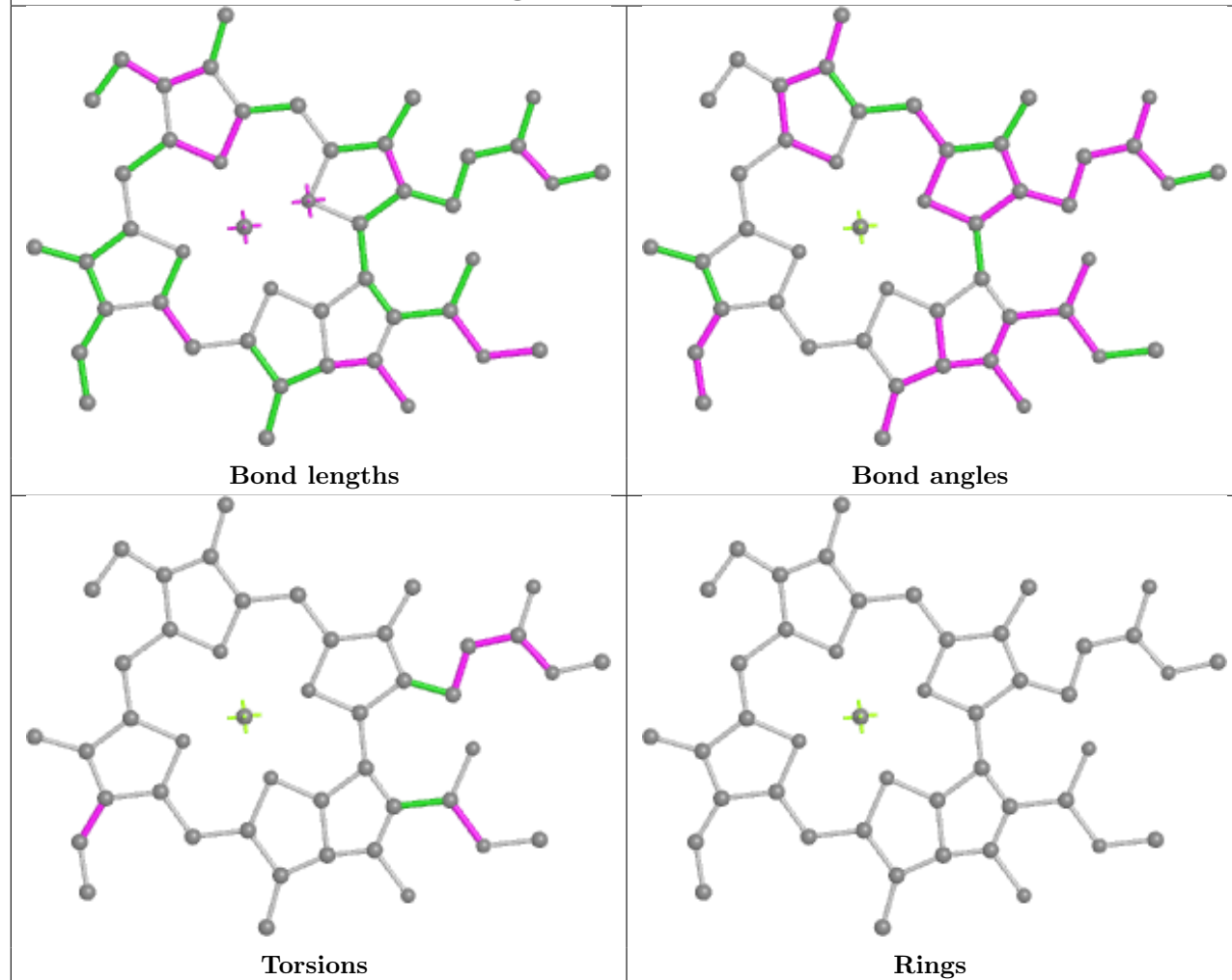
Ligand CLA 4 1004



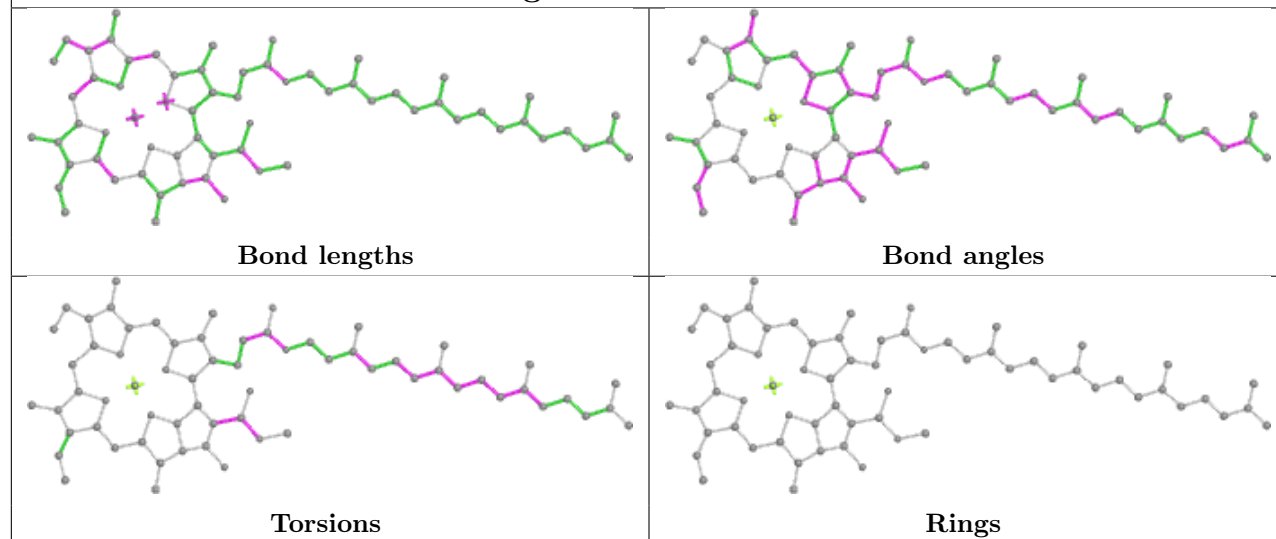
Ligand CLA B 1210



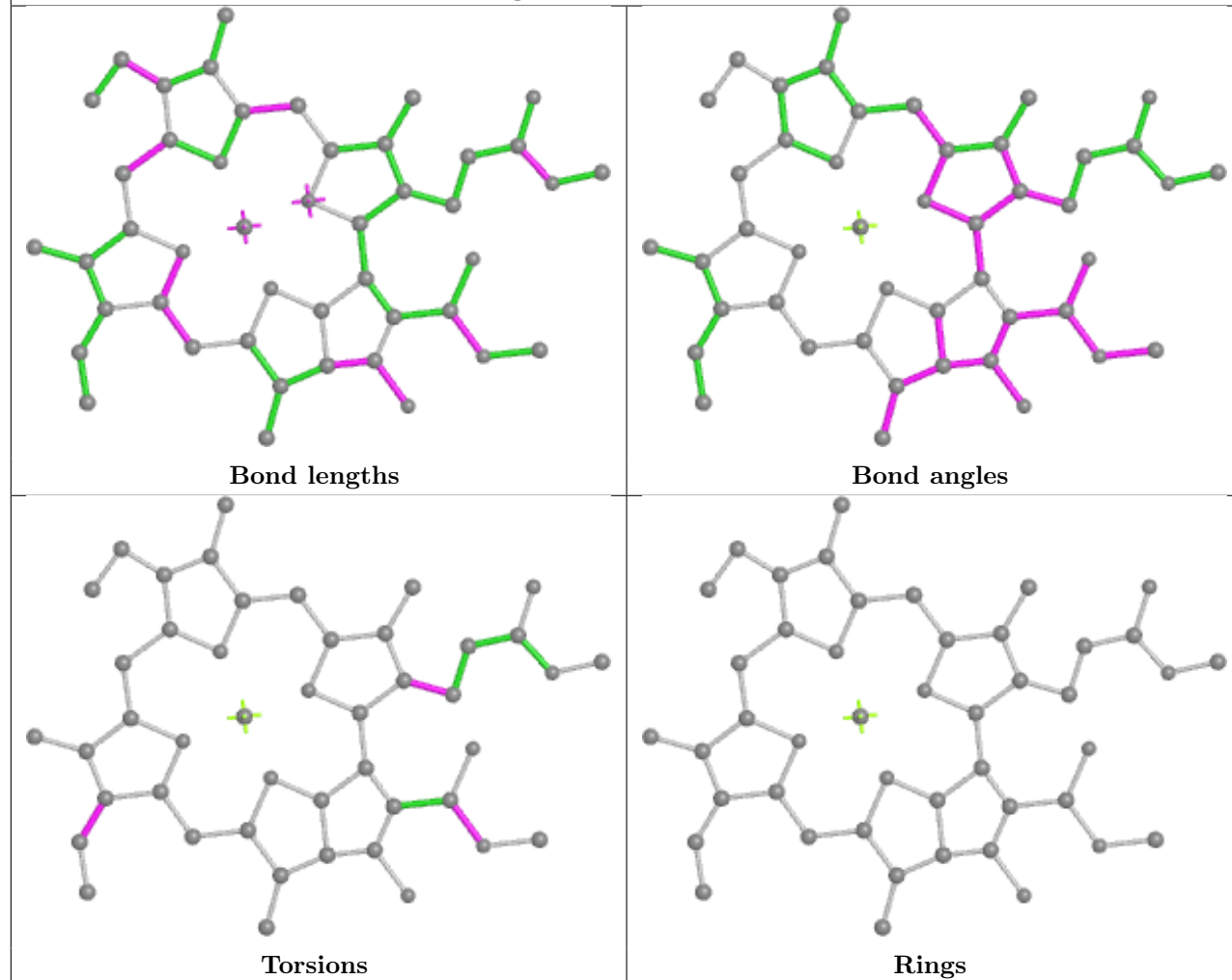
Ligand CLA 3 1147

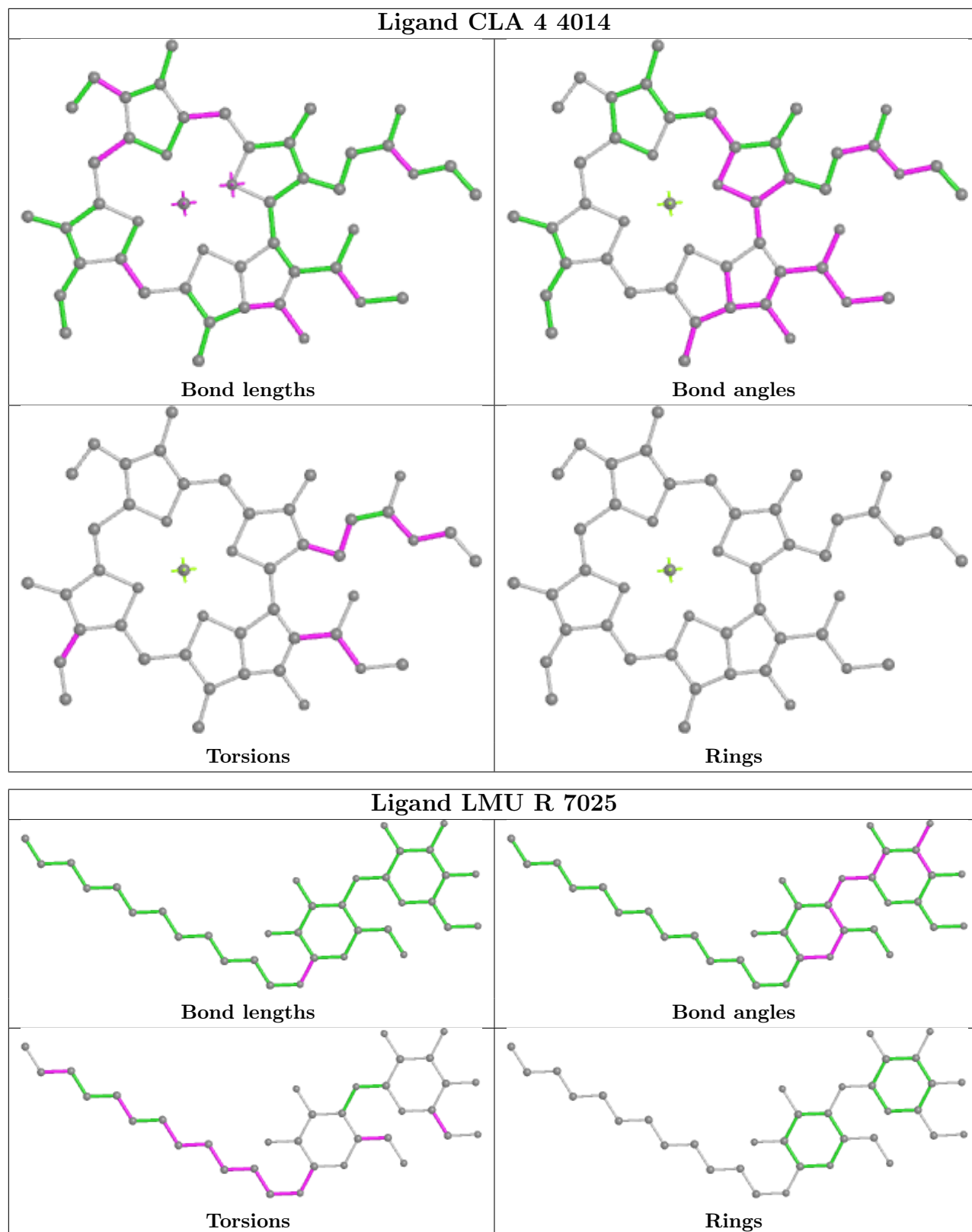


Ligand CLA B 9010

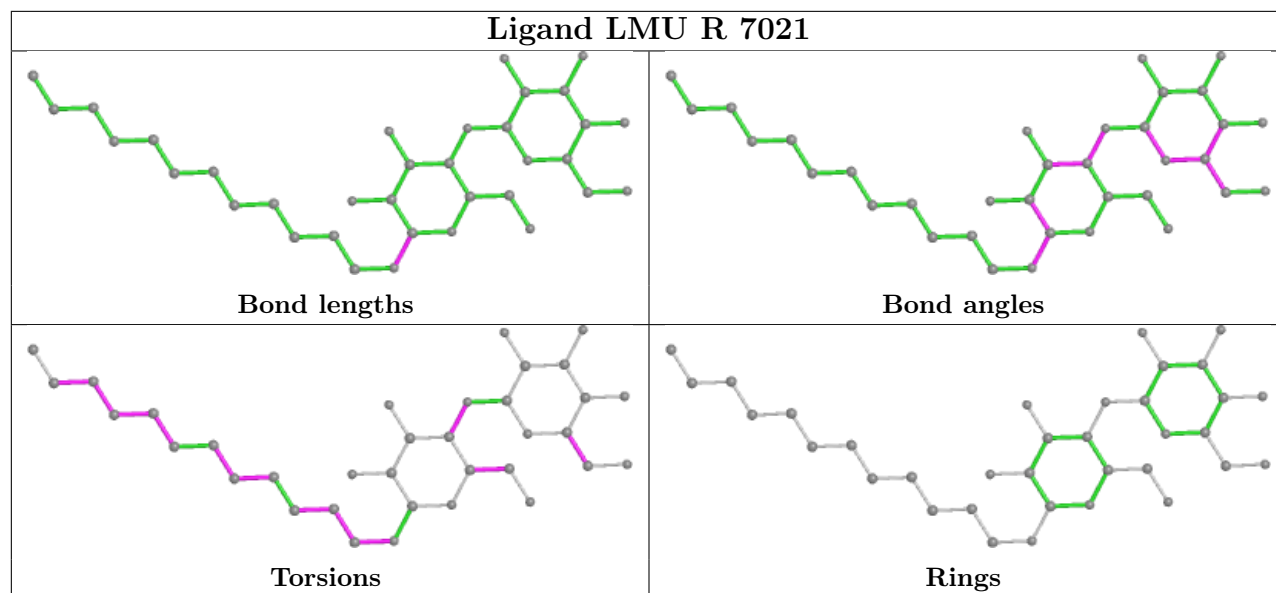


Ligand CLA 1 1005

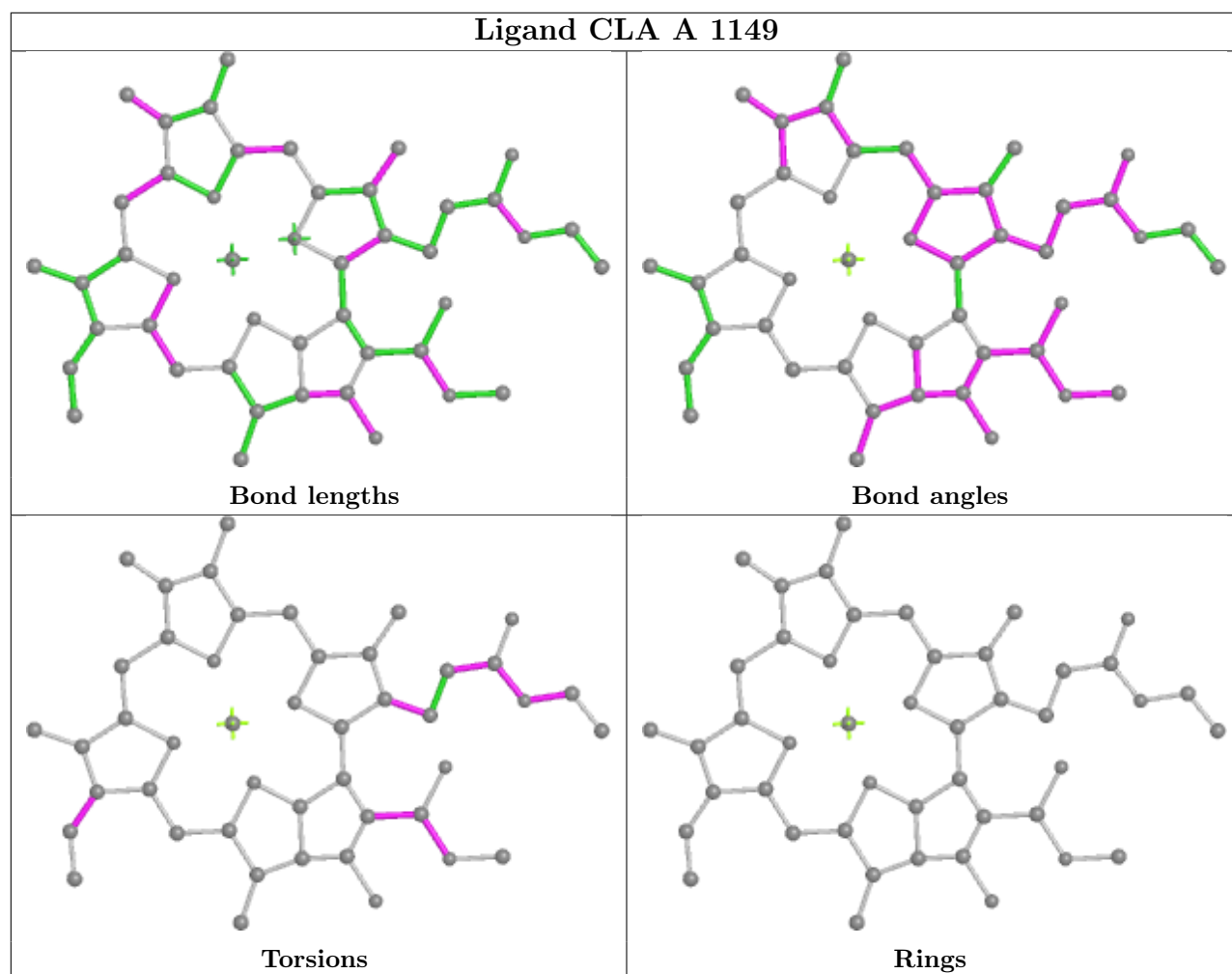


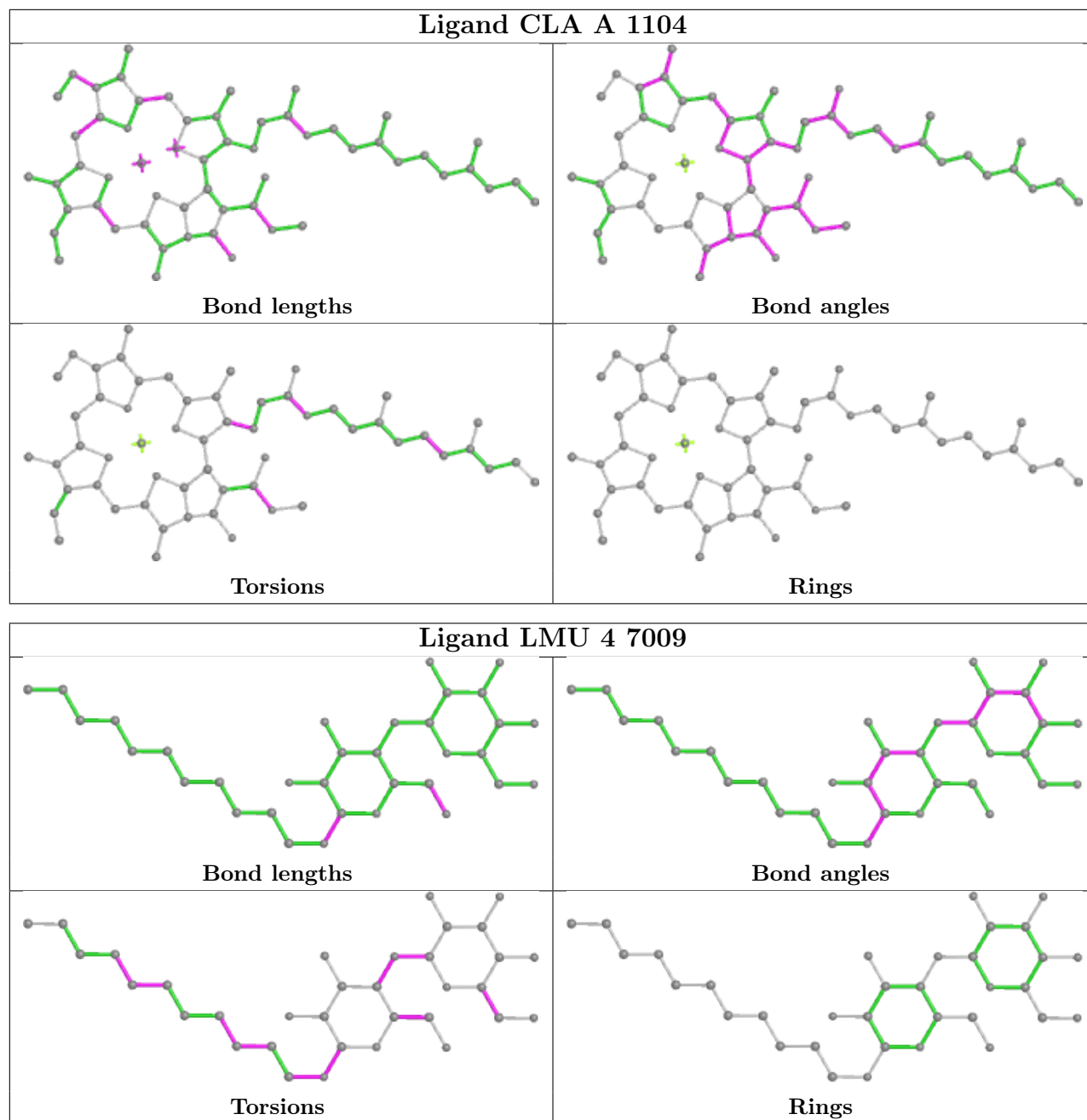


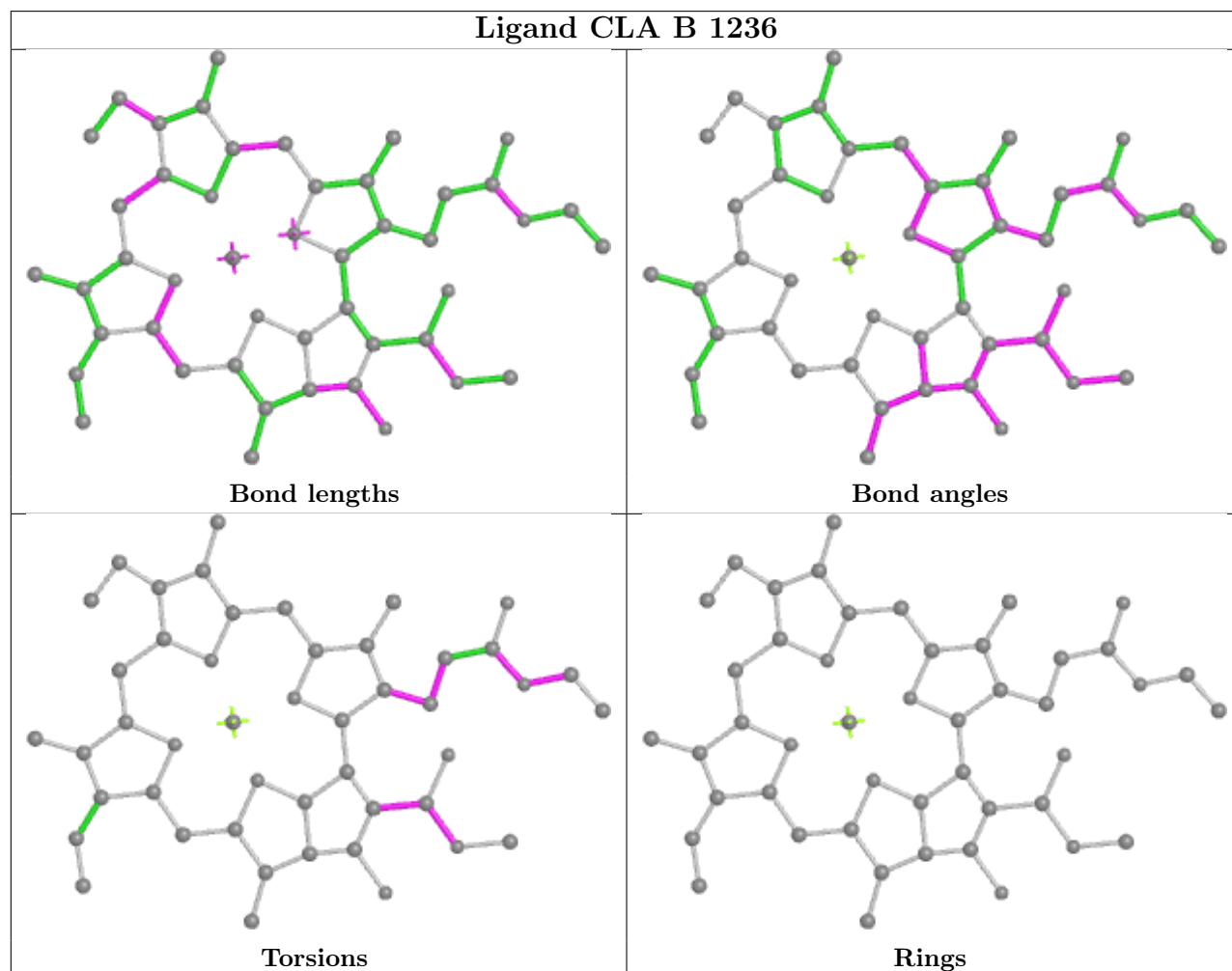
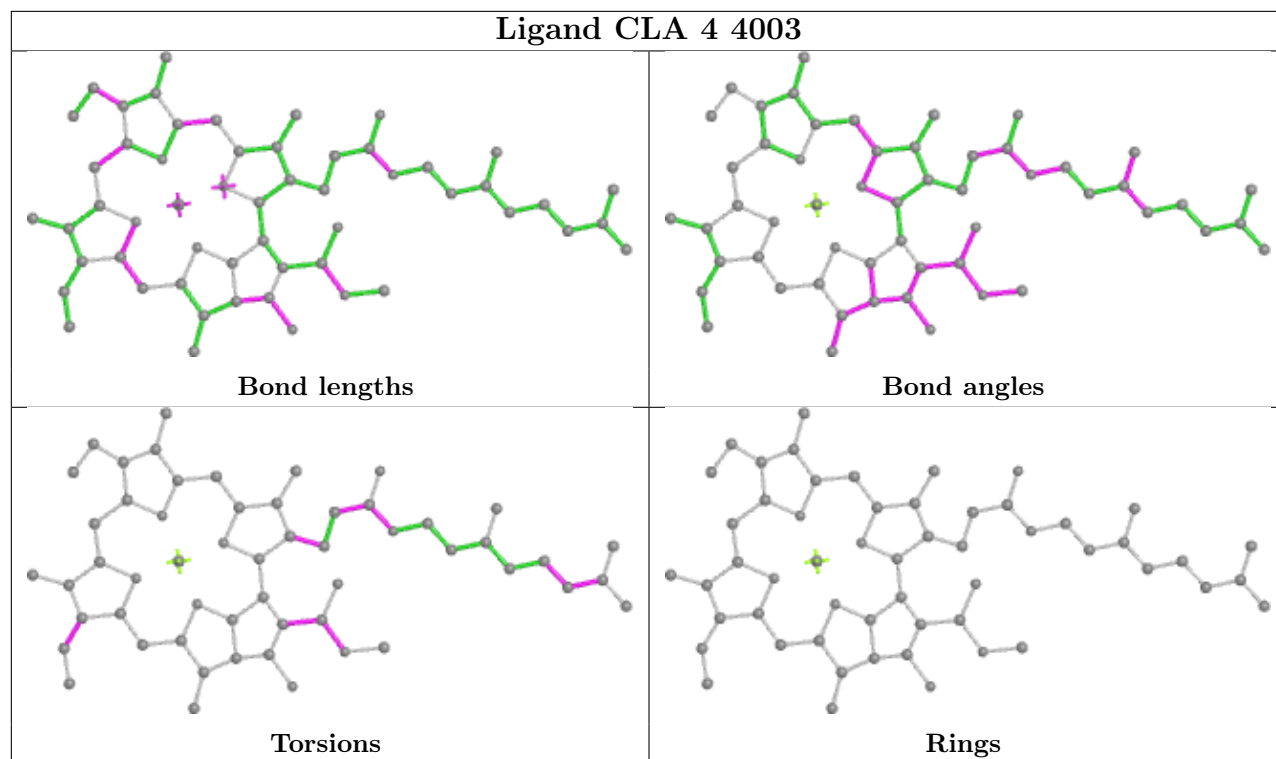
Ligand LMU R 7021

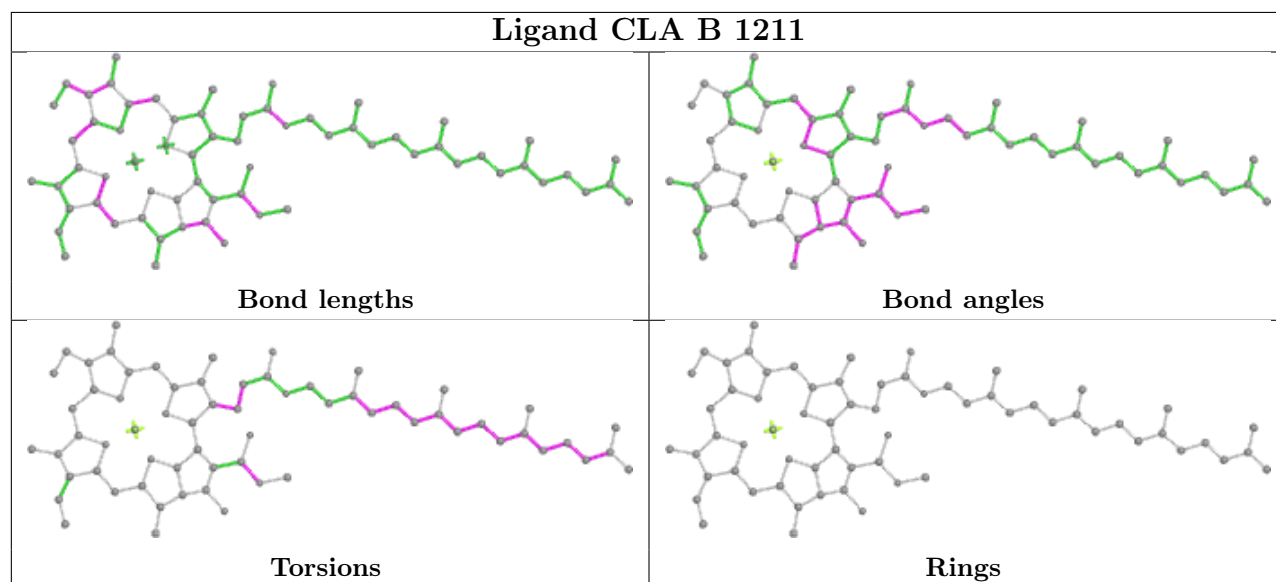
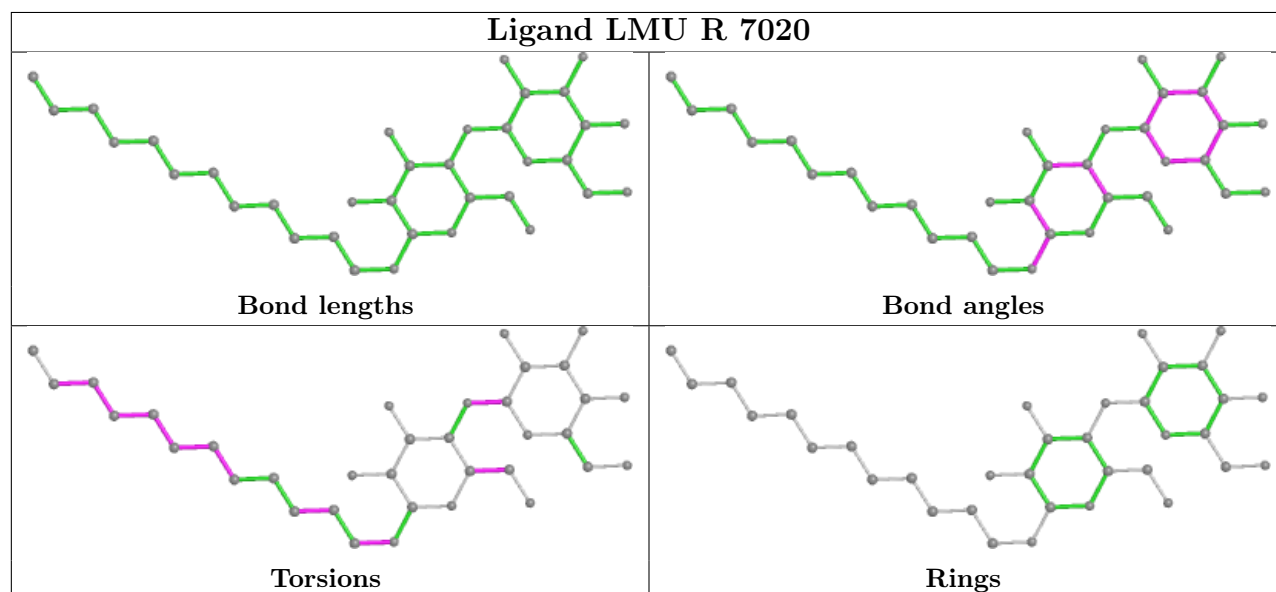
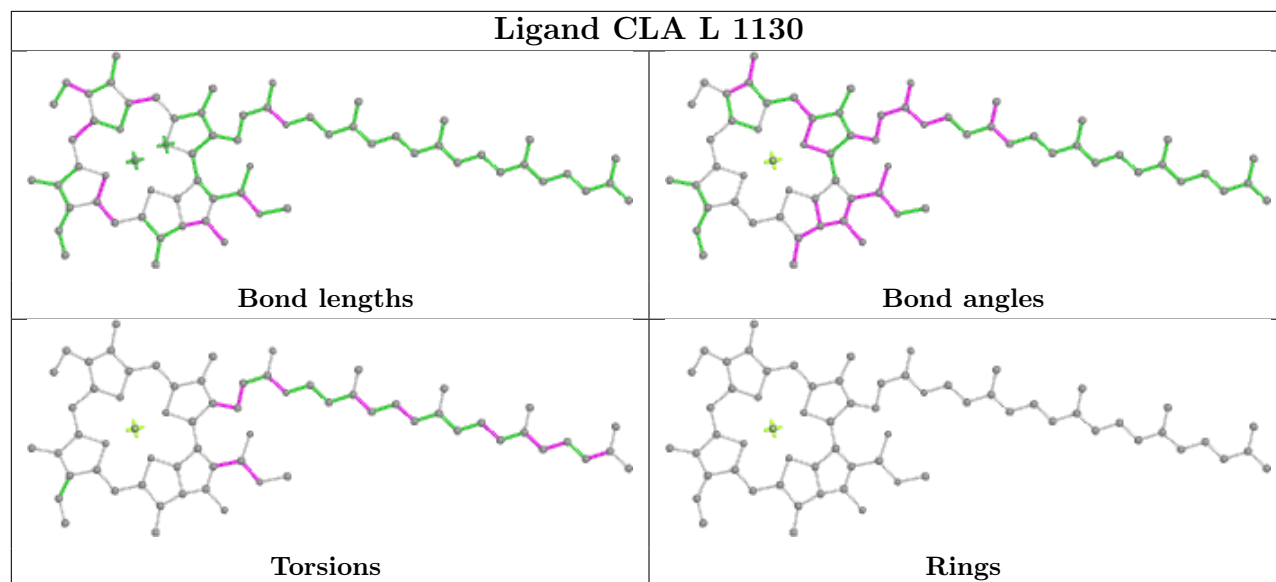


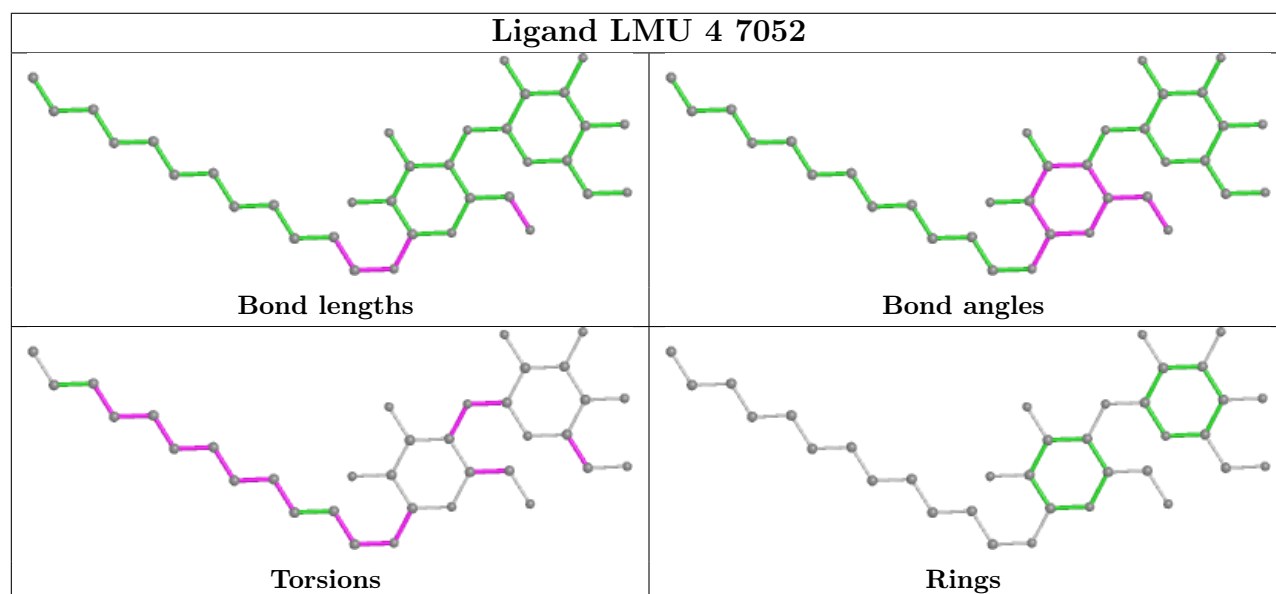
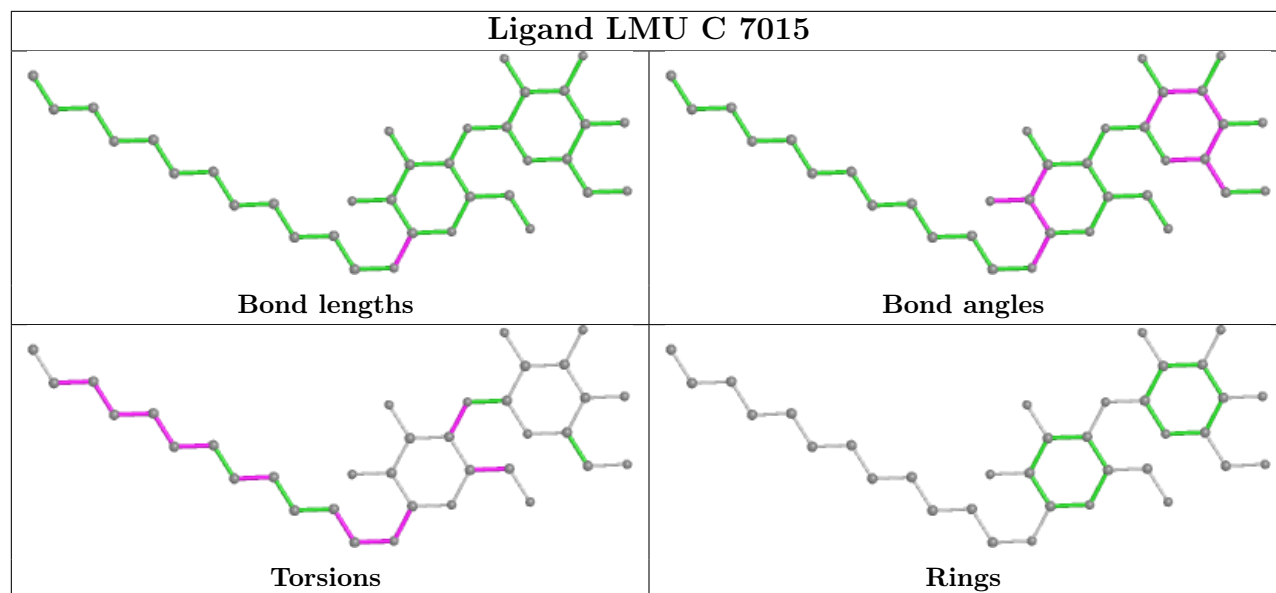
Ligand CLA A 1149

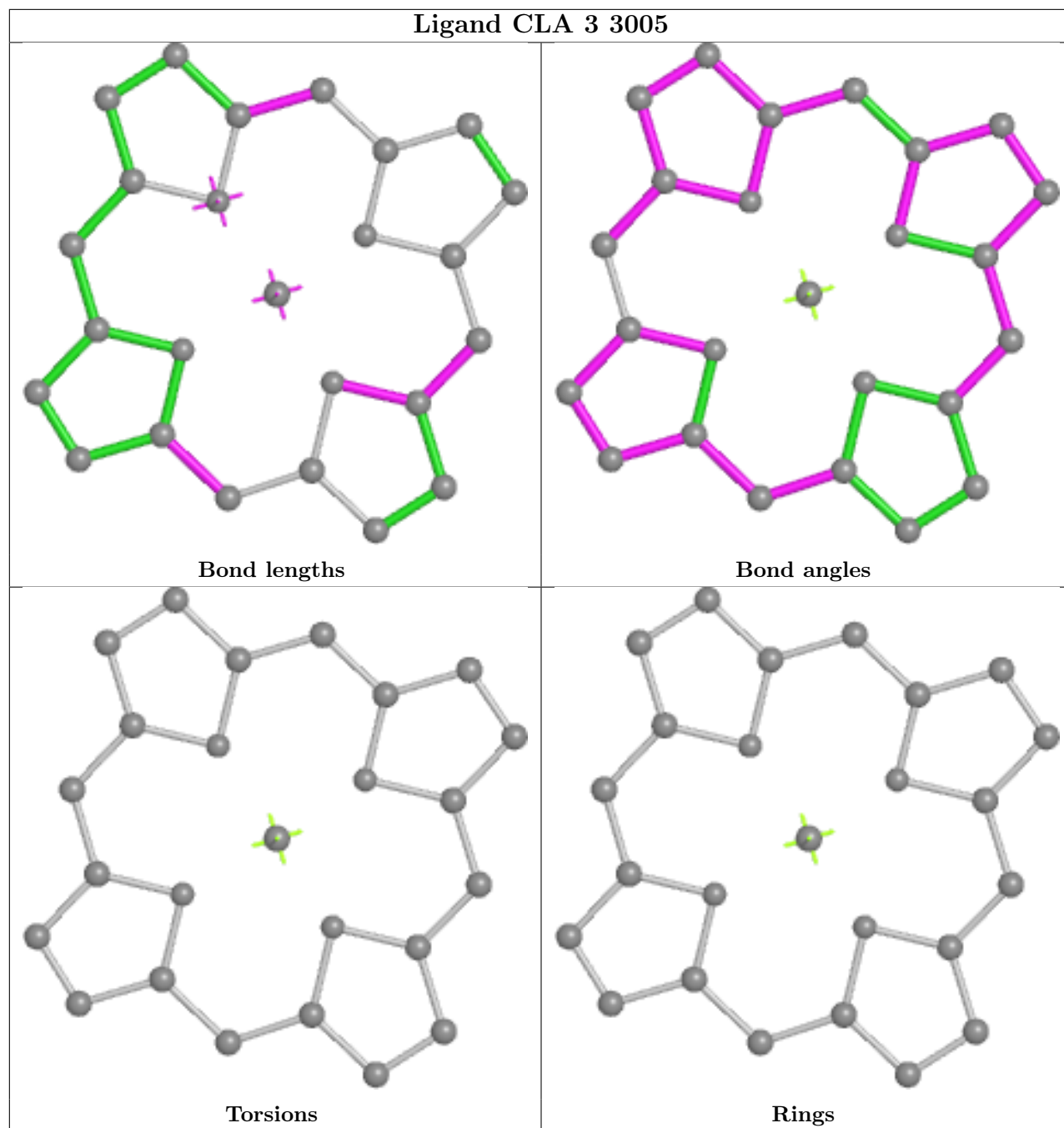


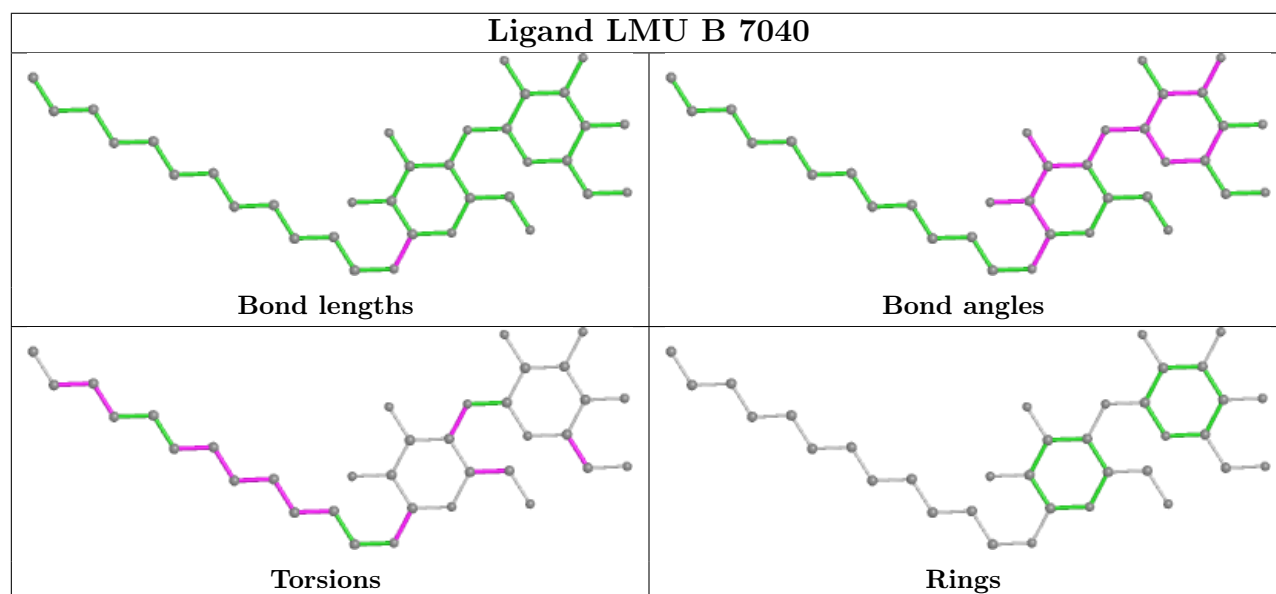
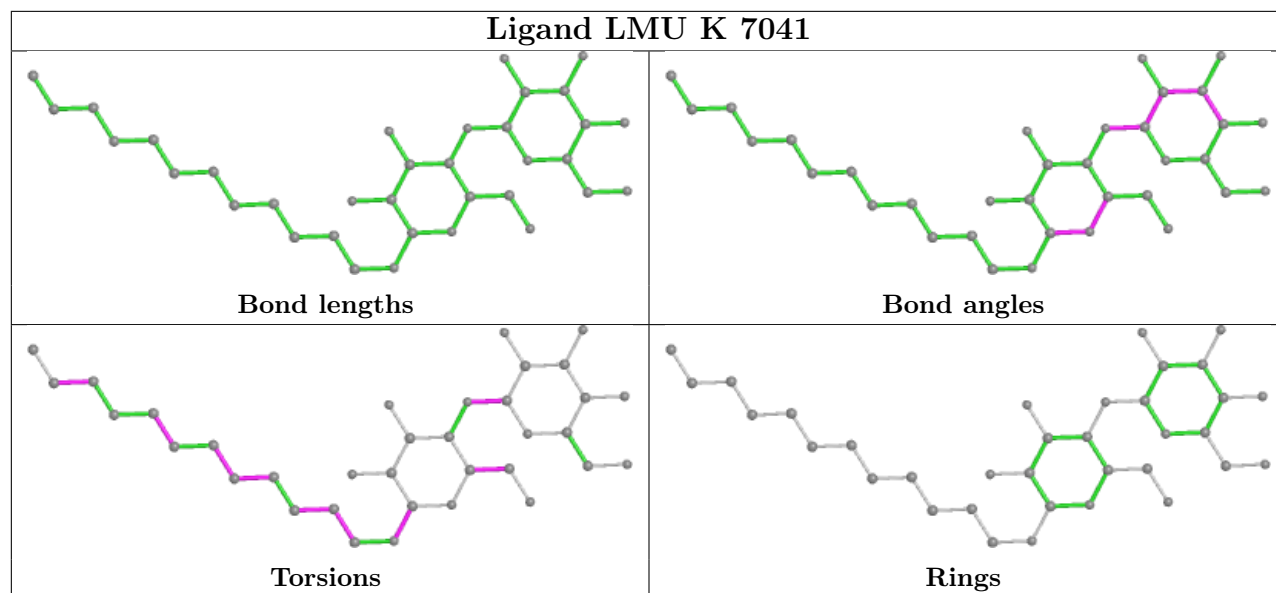


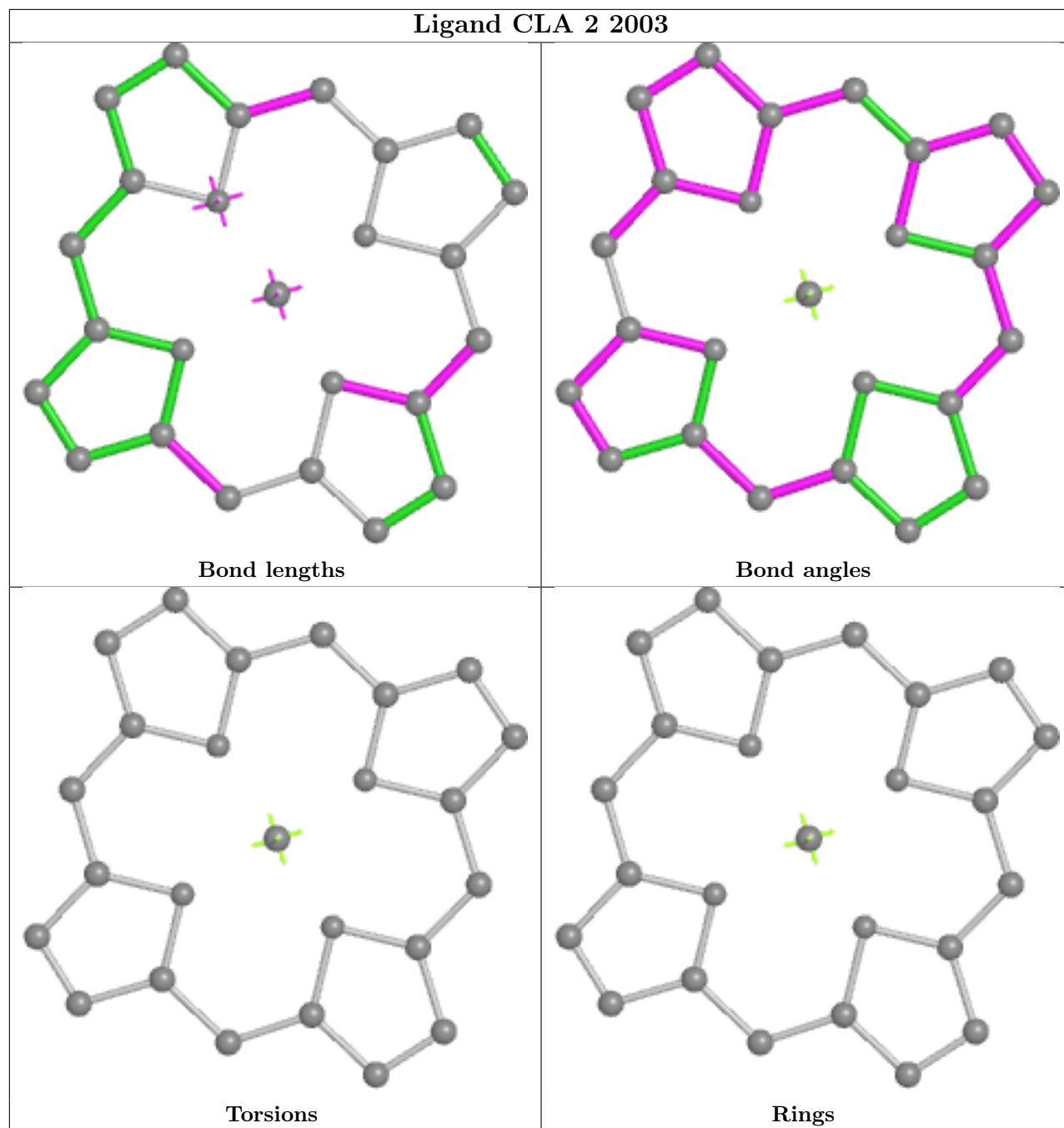


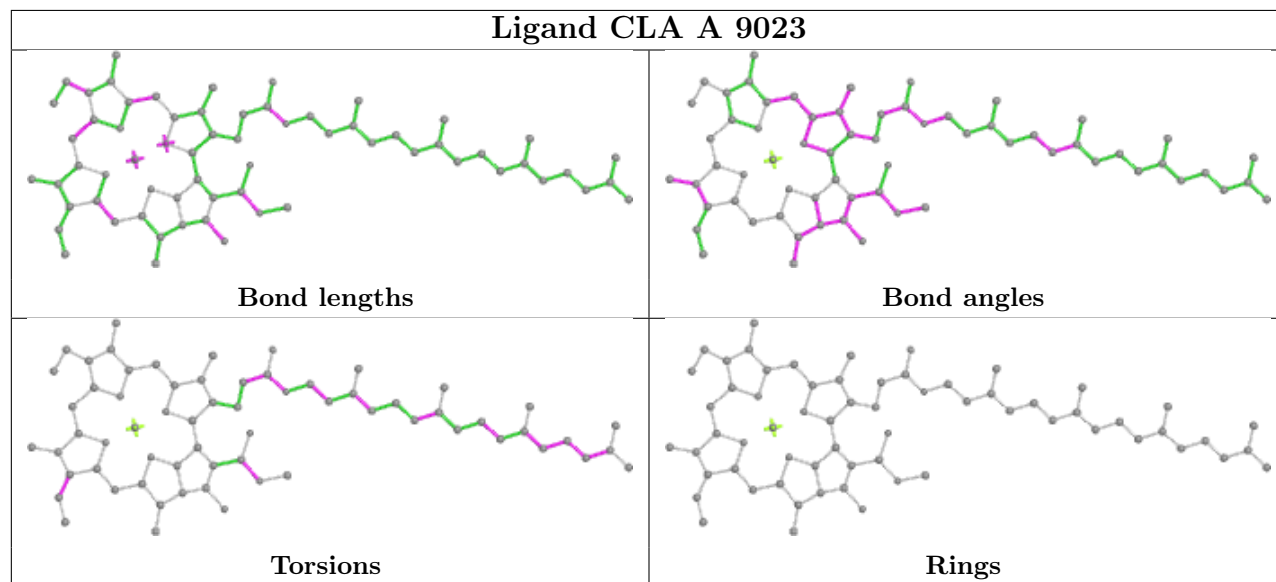
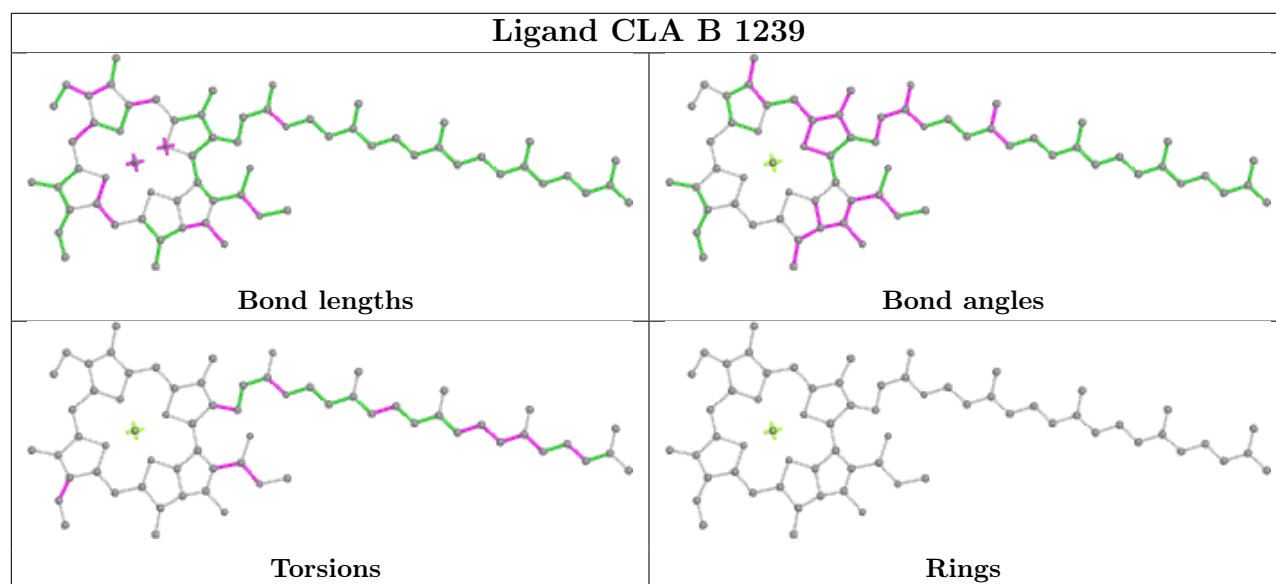
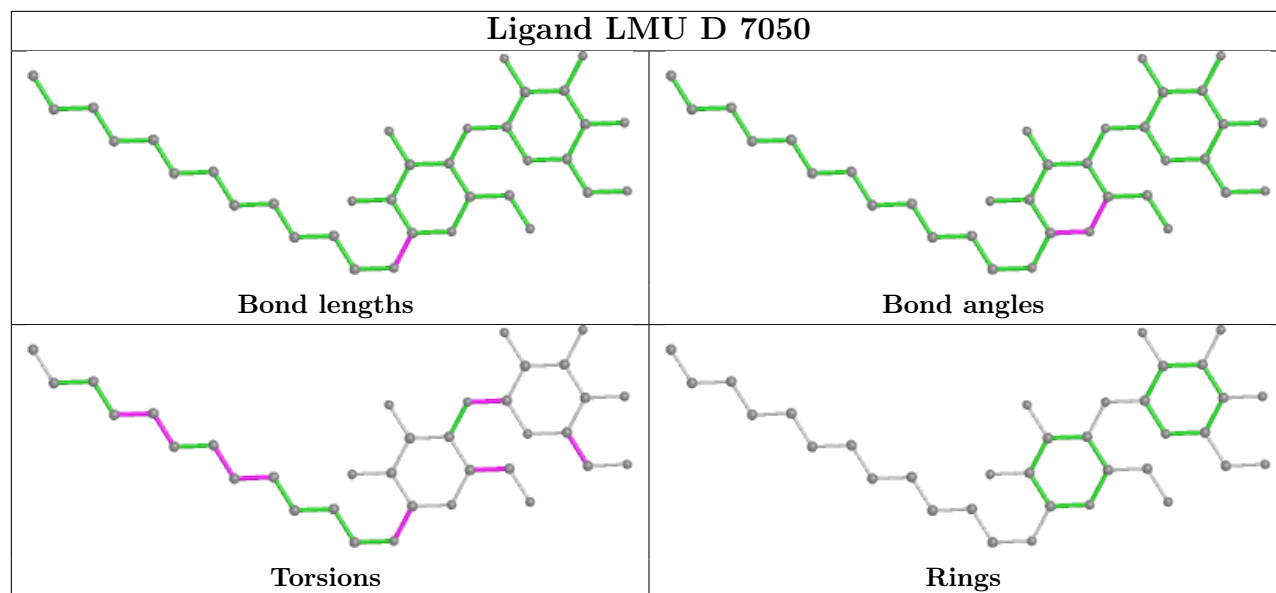




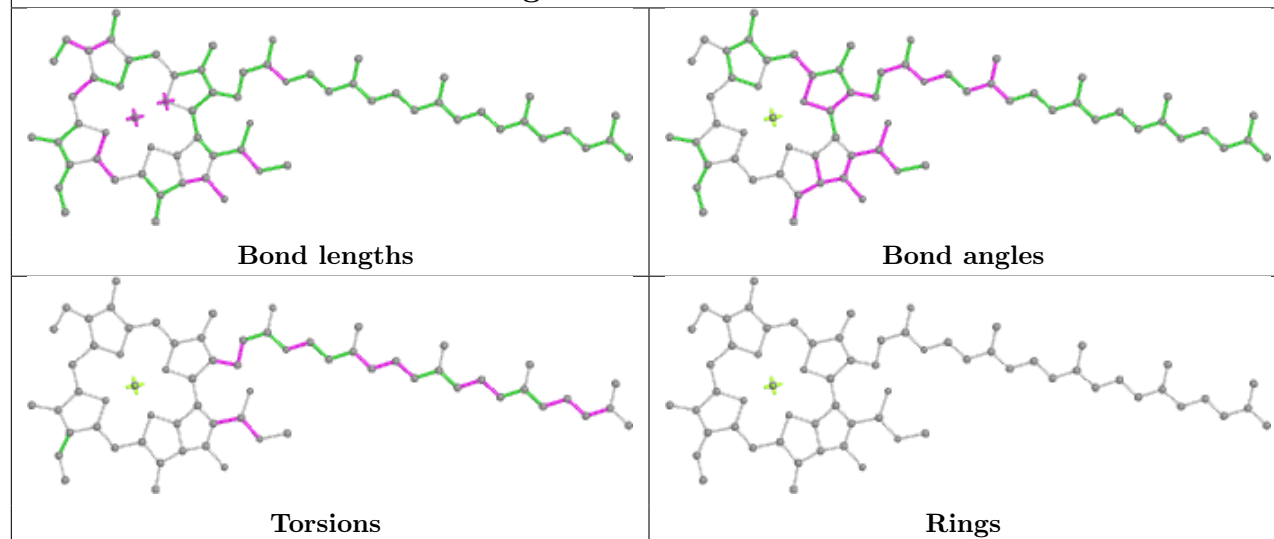




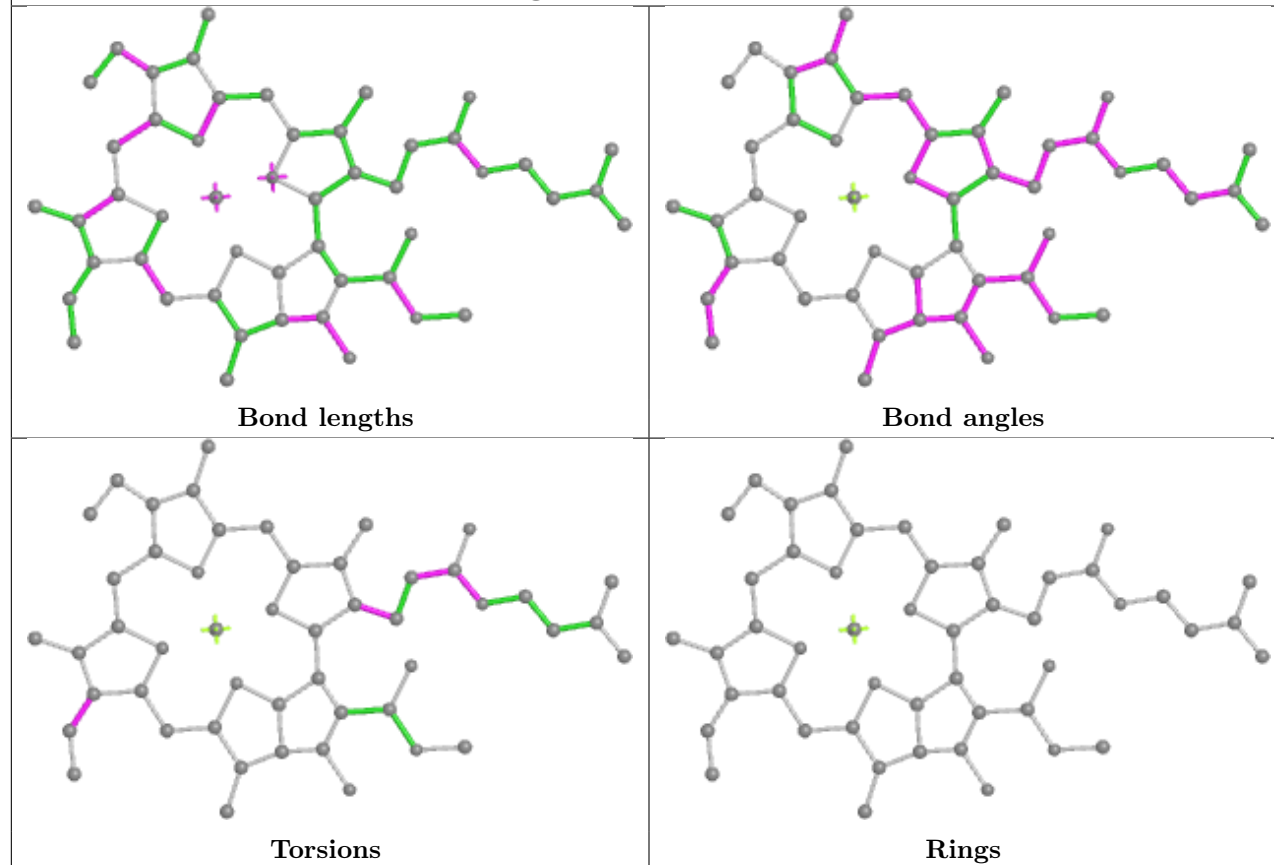




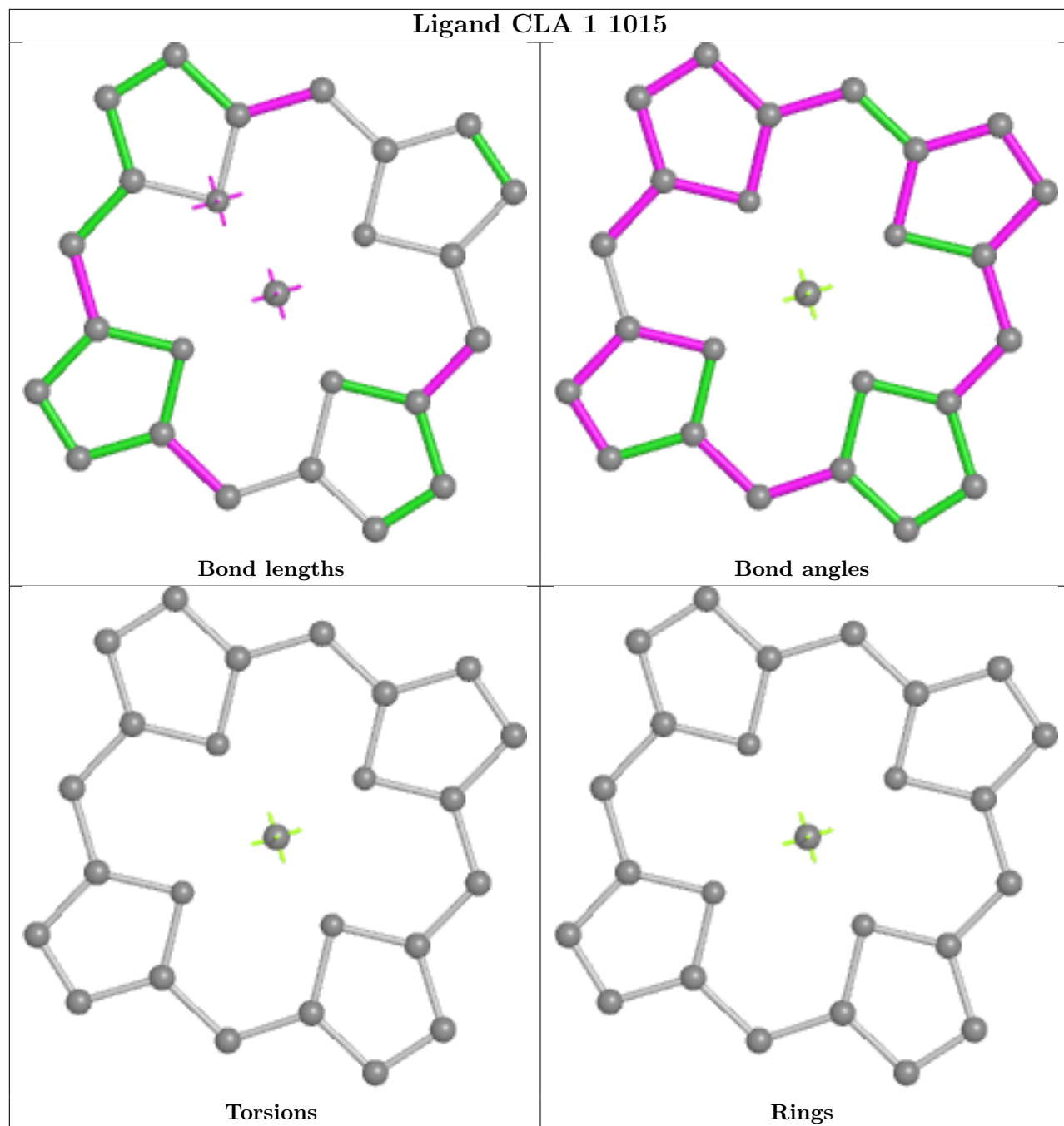
Ligand CLA A 9022

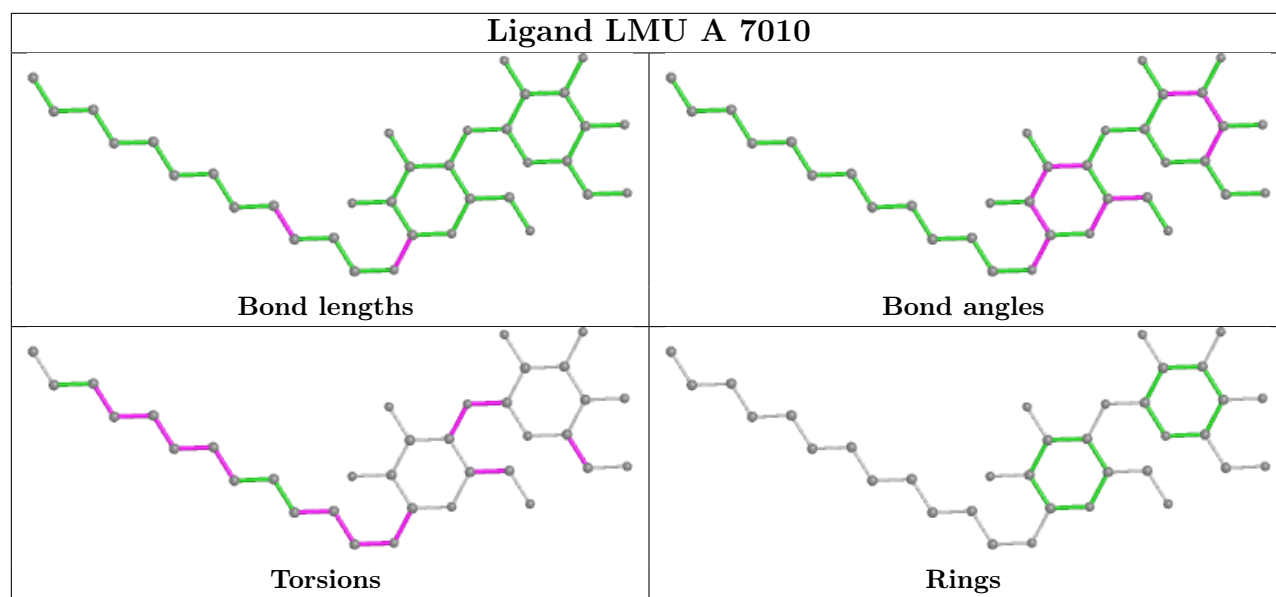
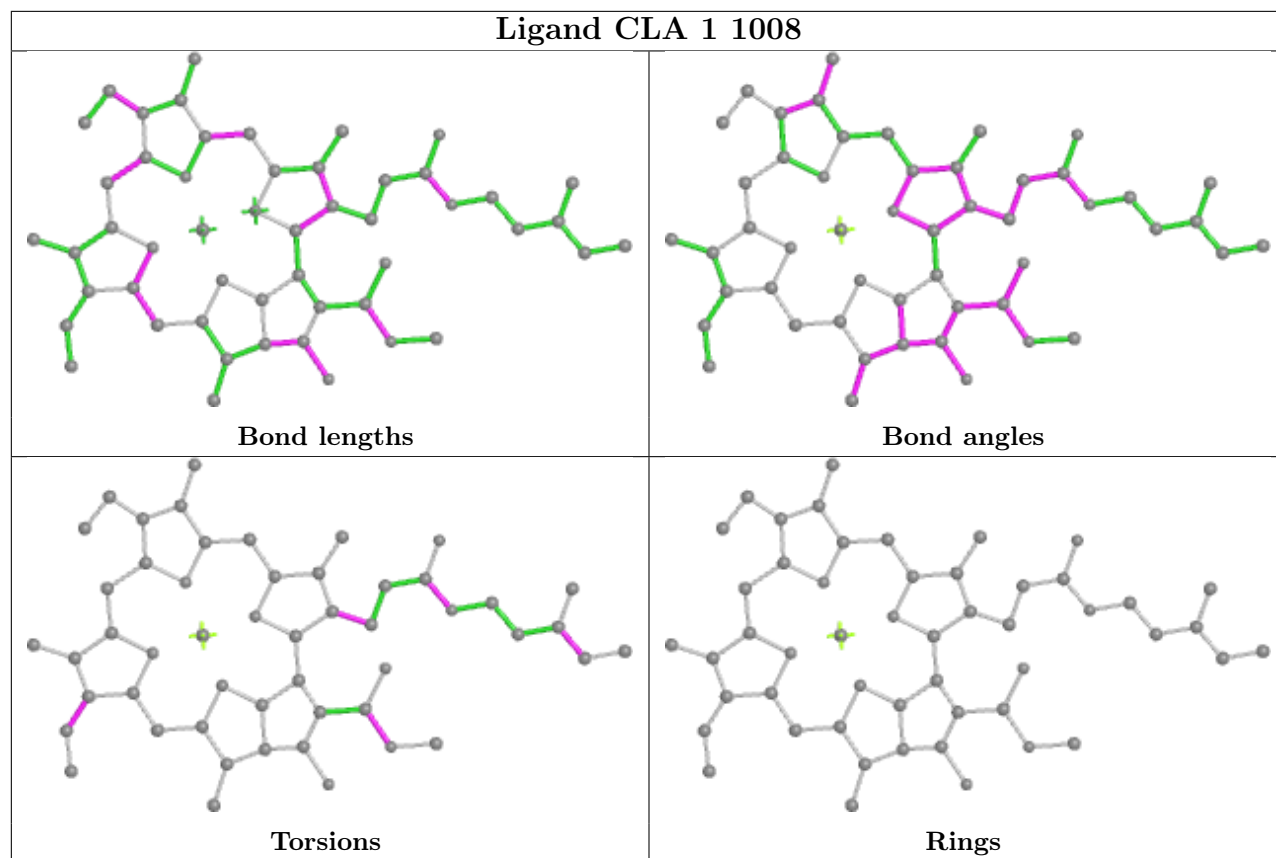


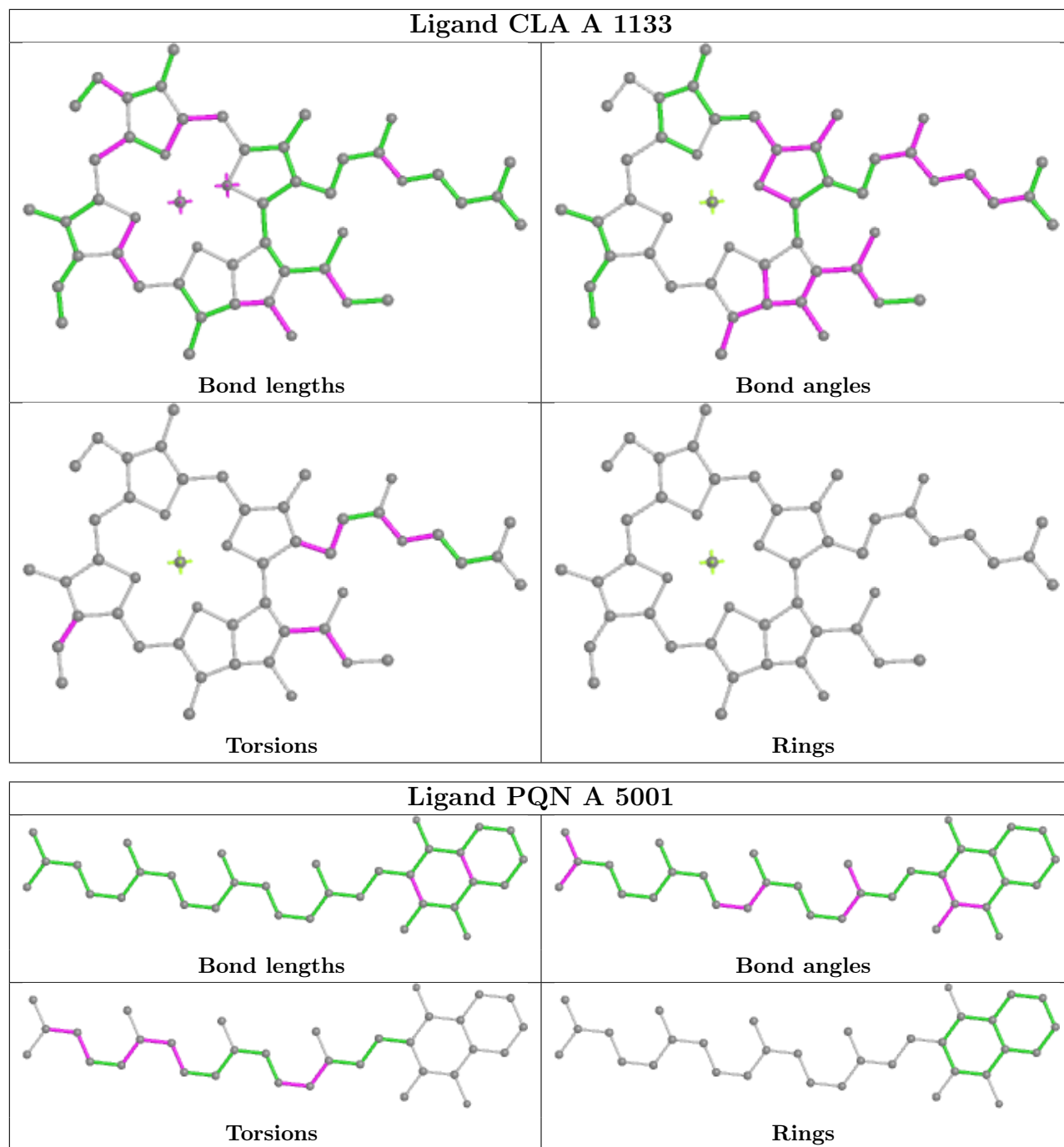
Ligand CLA 3 3017

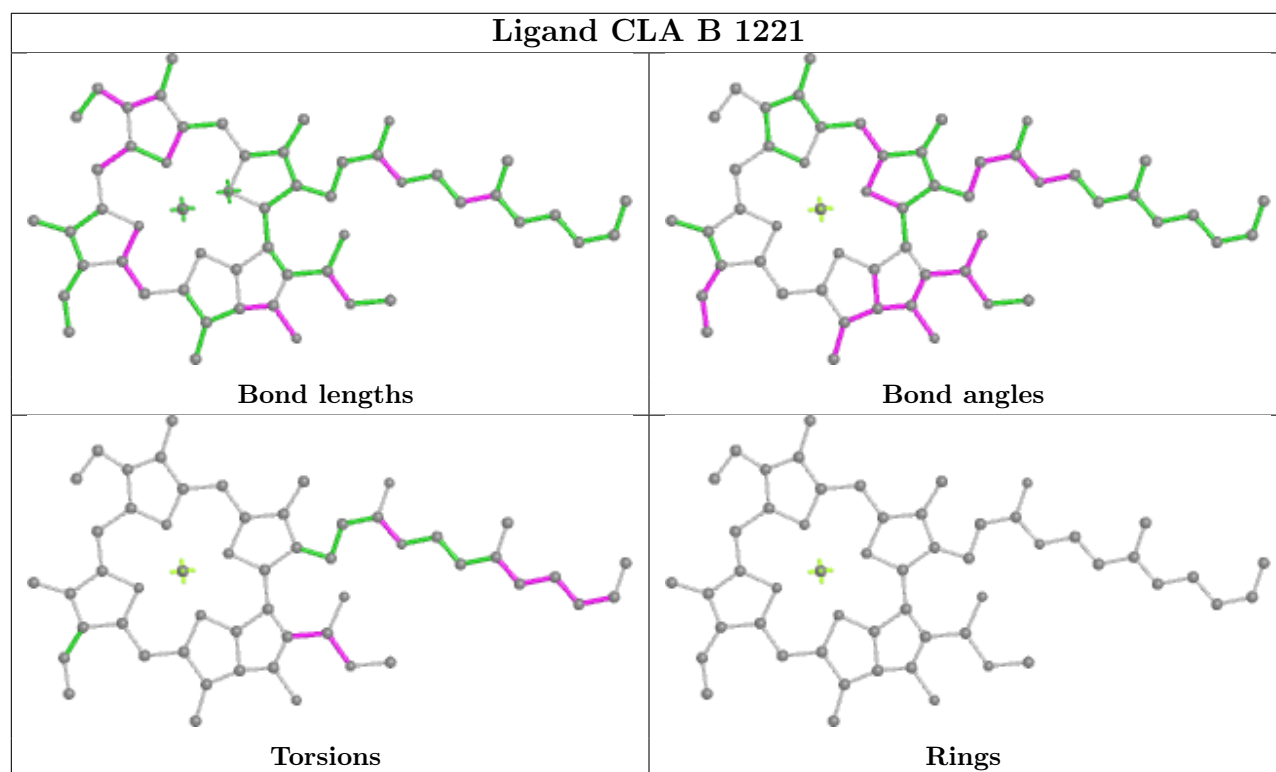
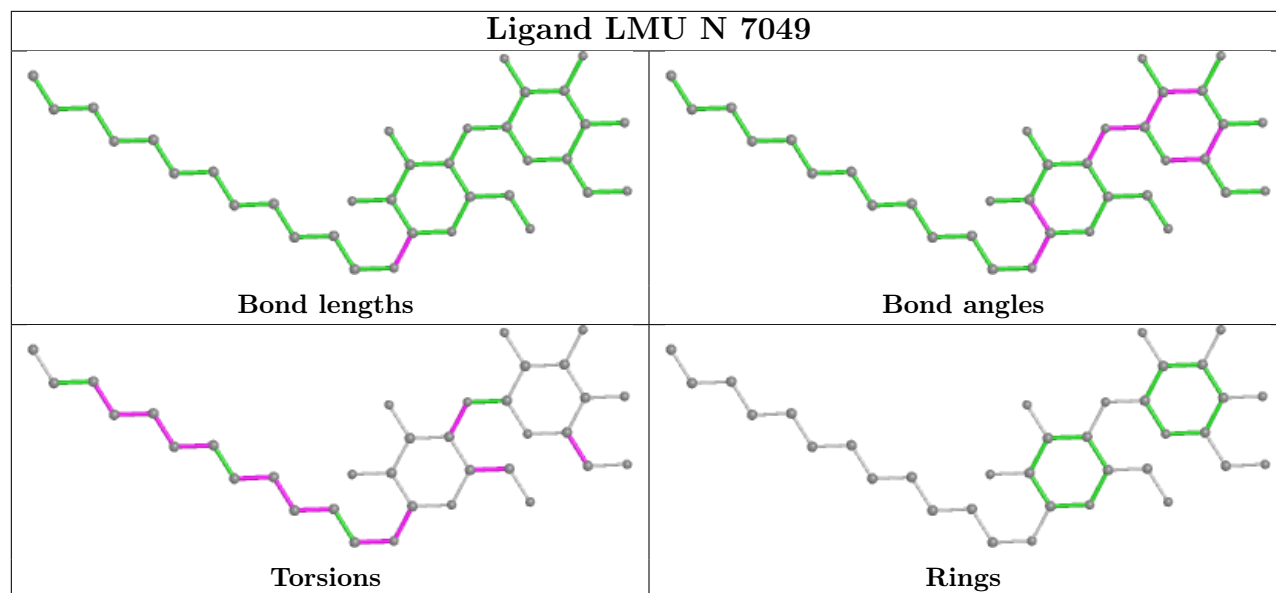


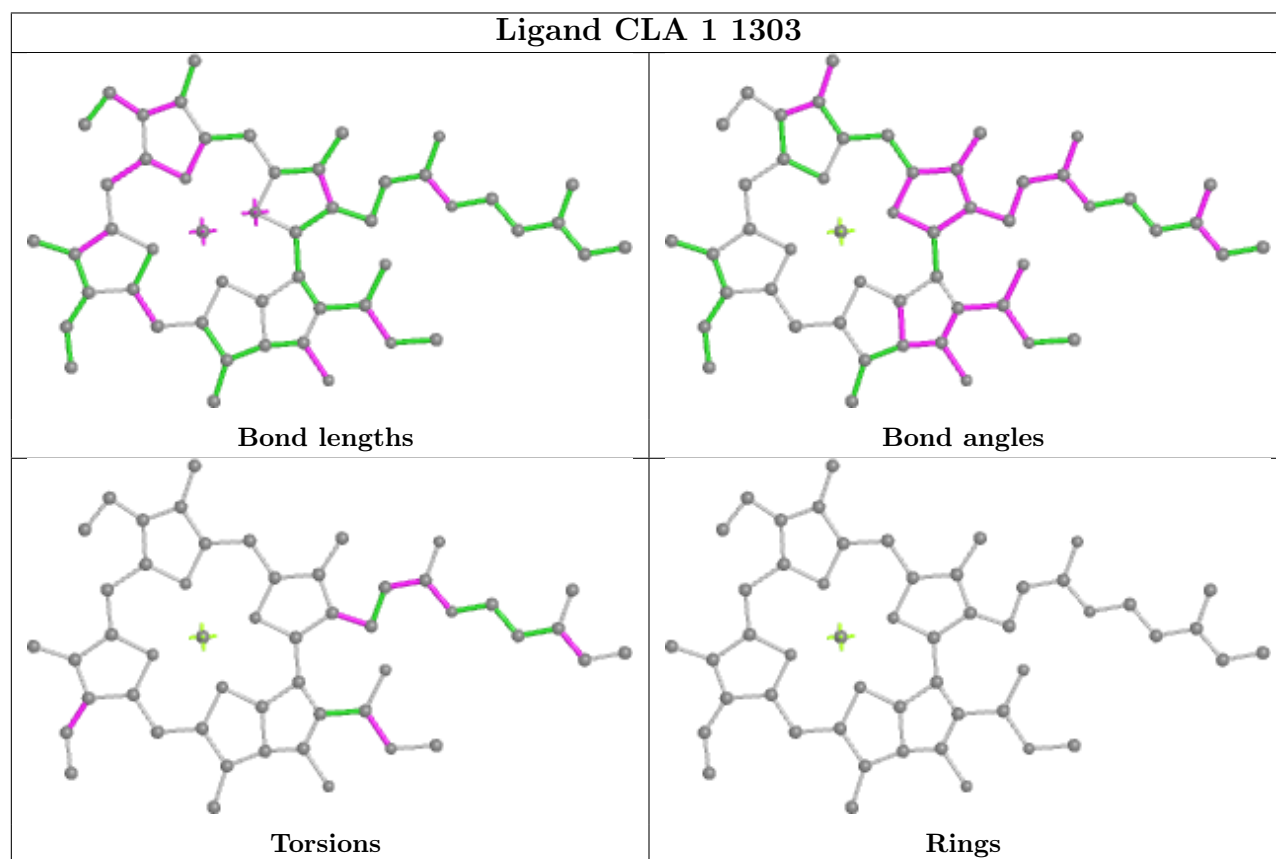
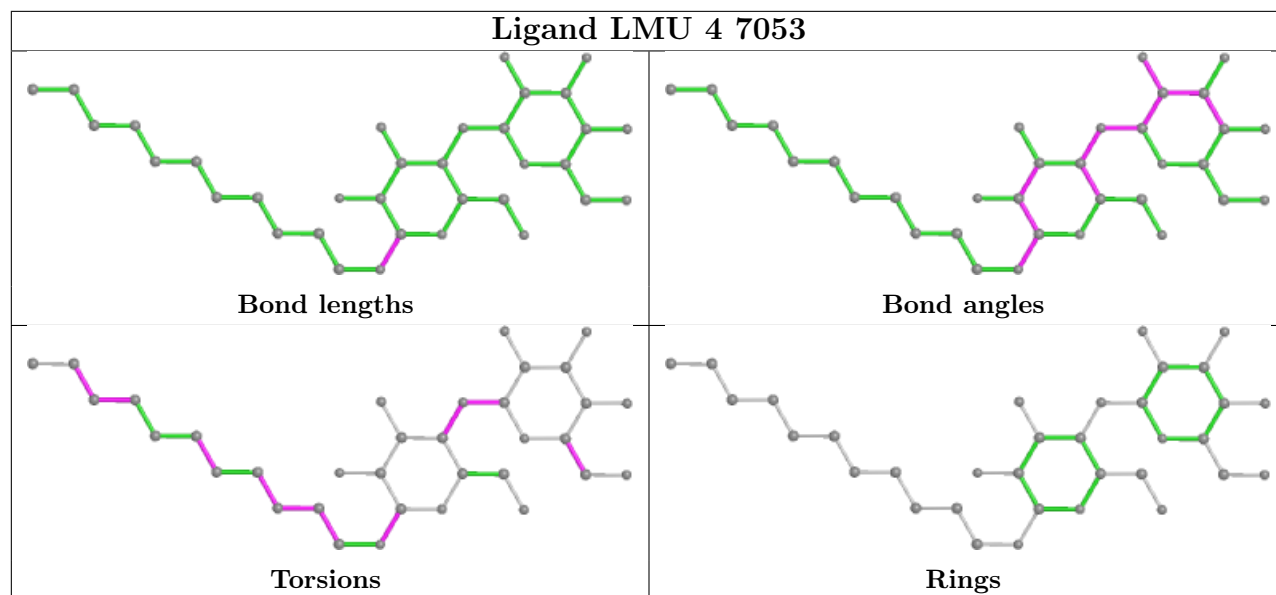
Ligand CLA 1 1015

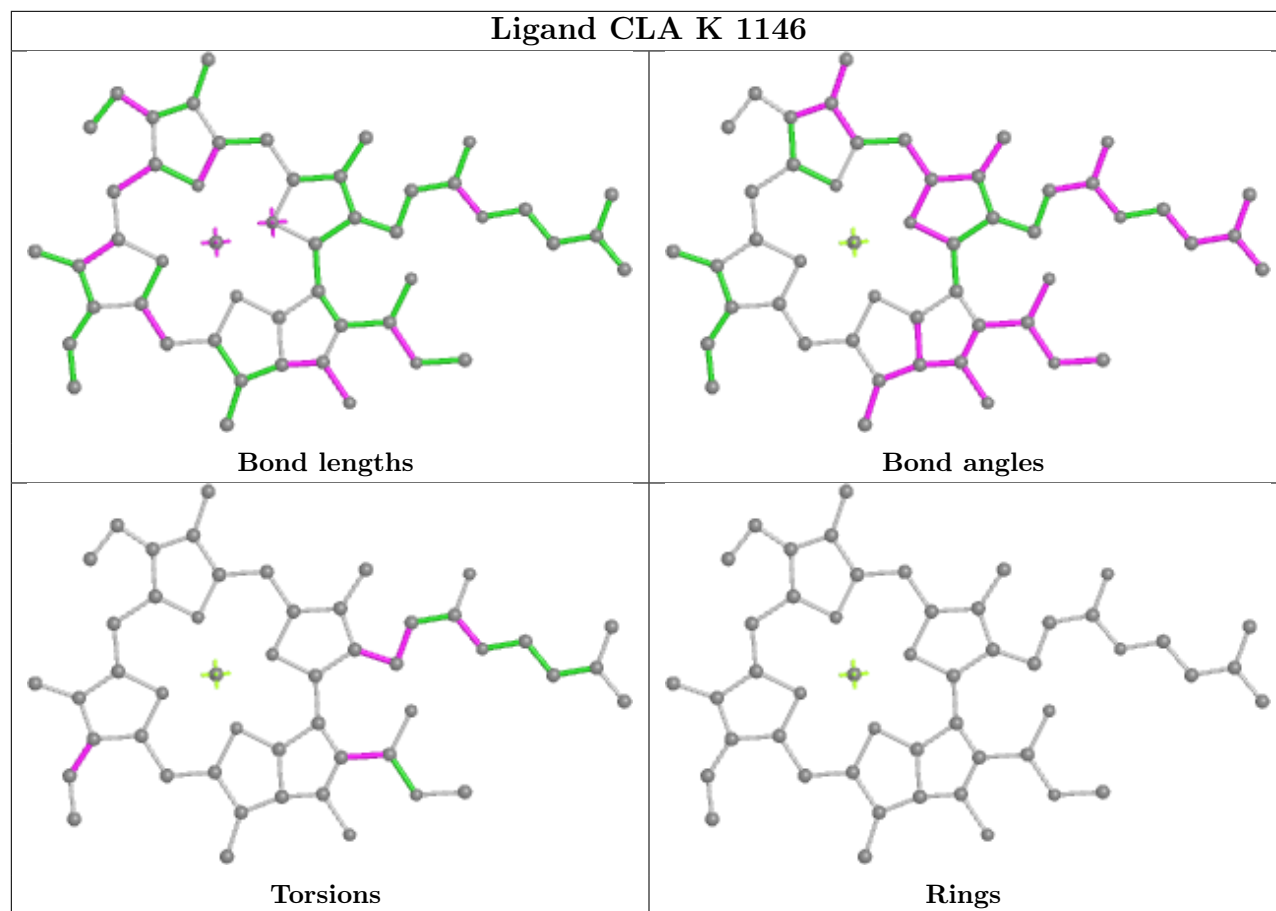
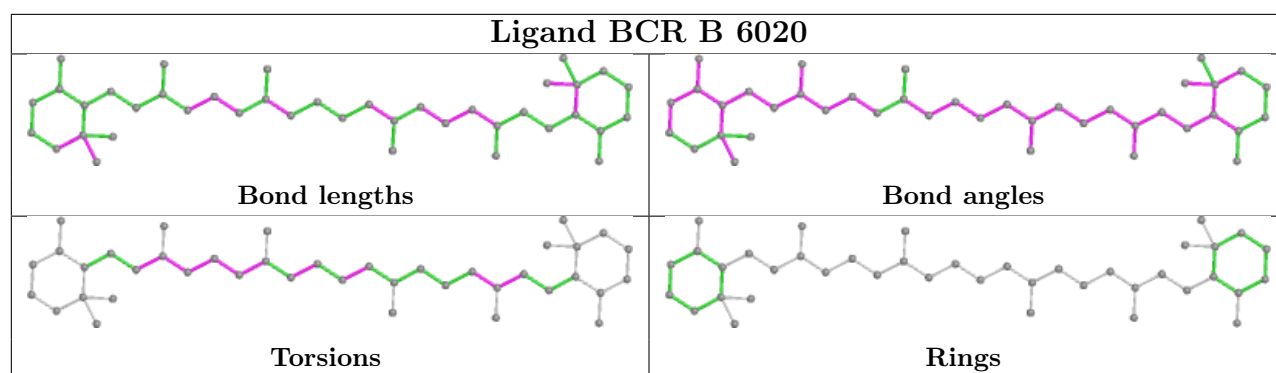




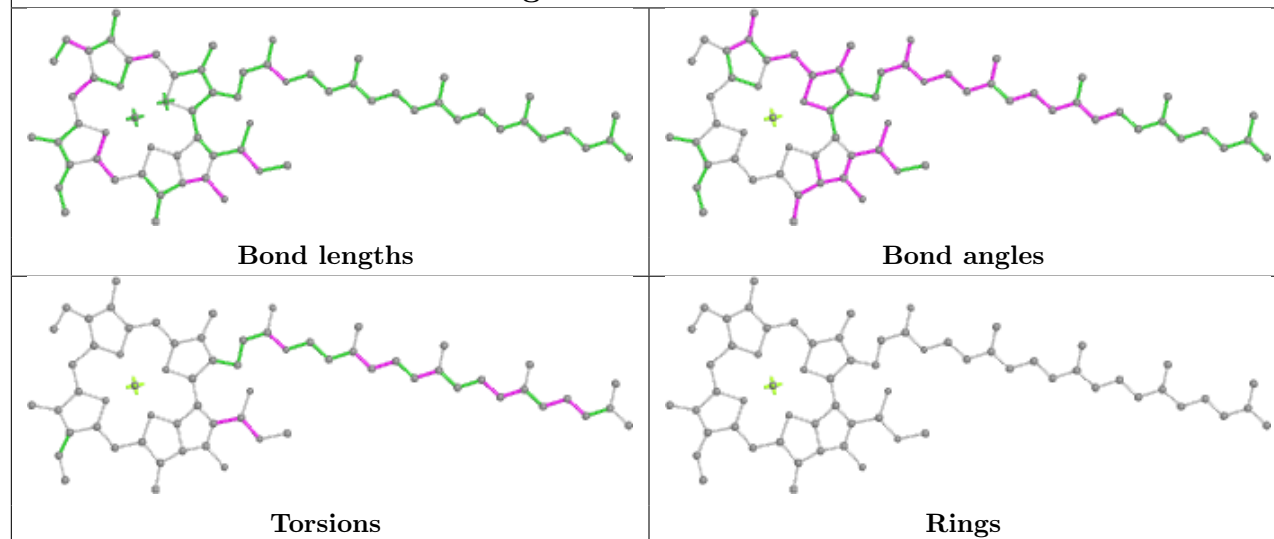




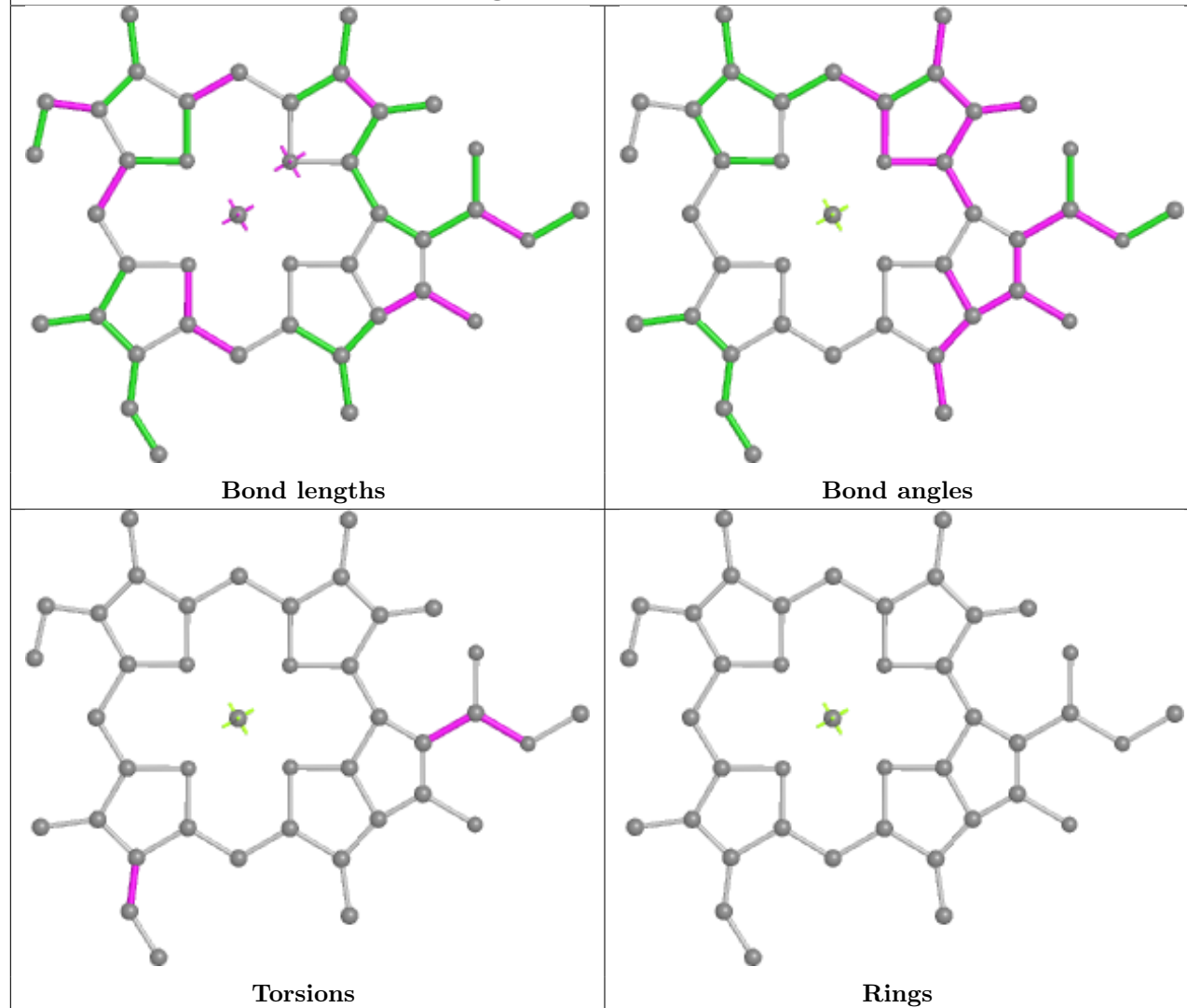


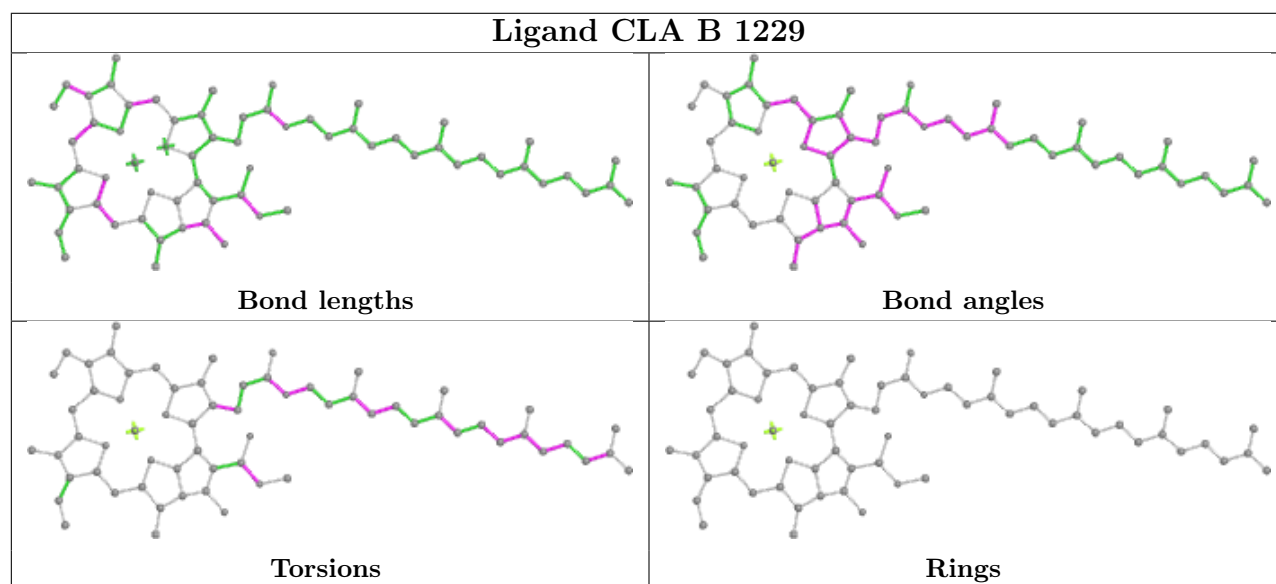
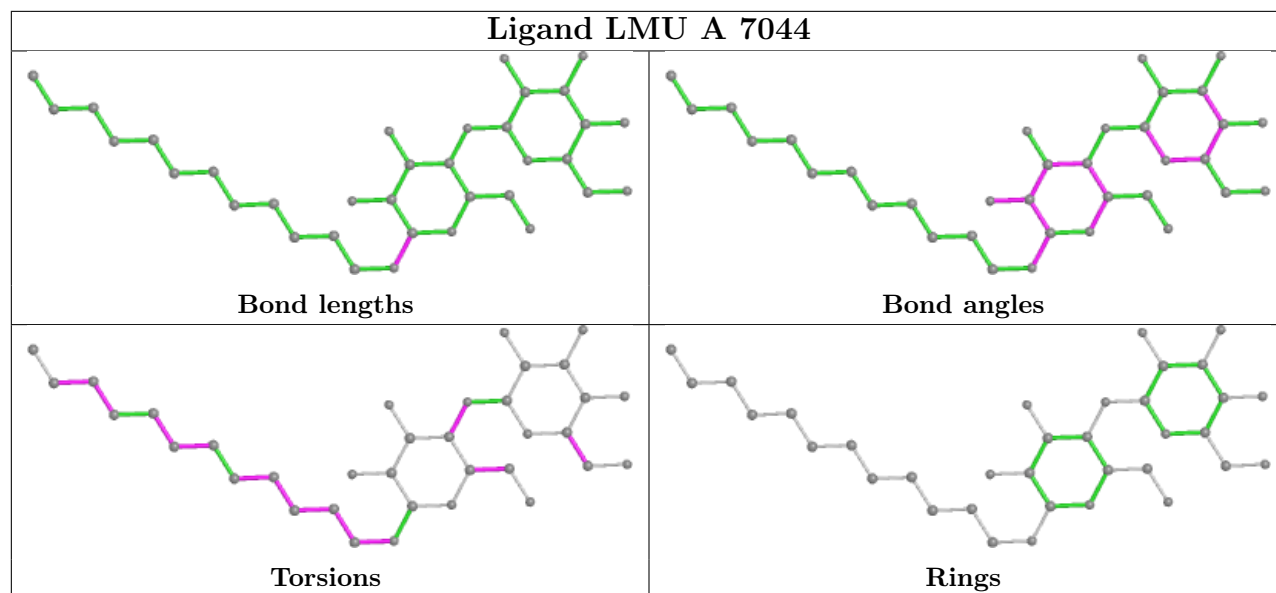


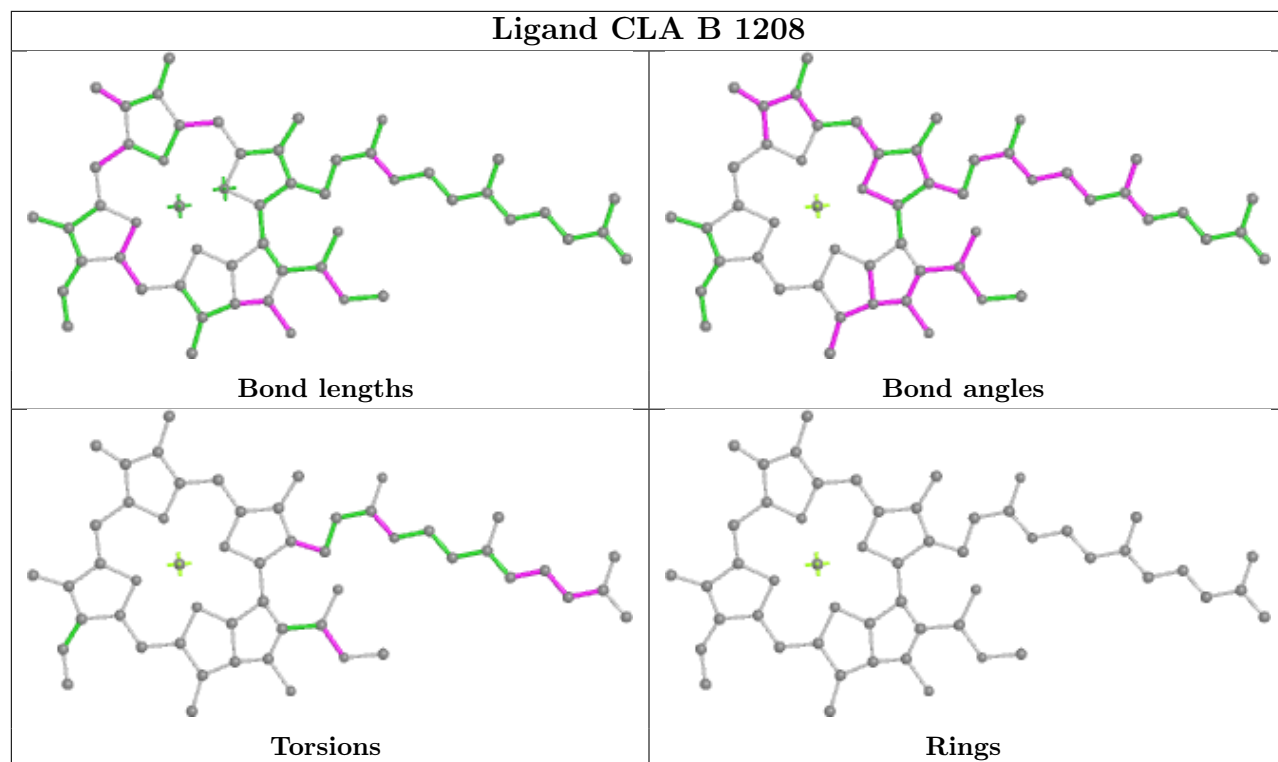
Ligand CLA A 1126



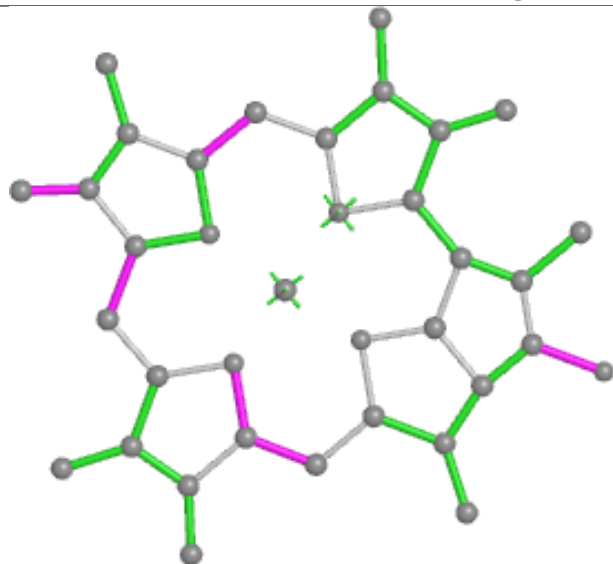
Ligand CLA F 1302



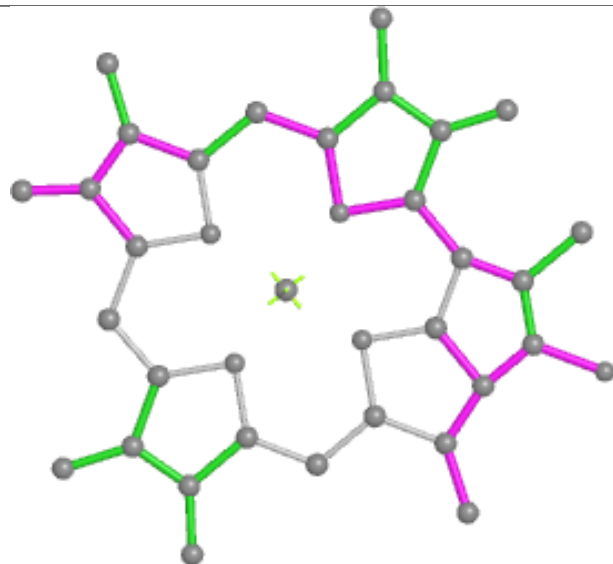




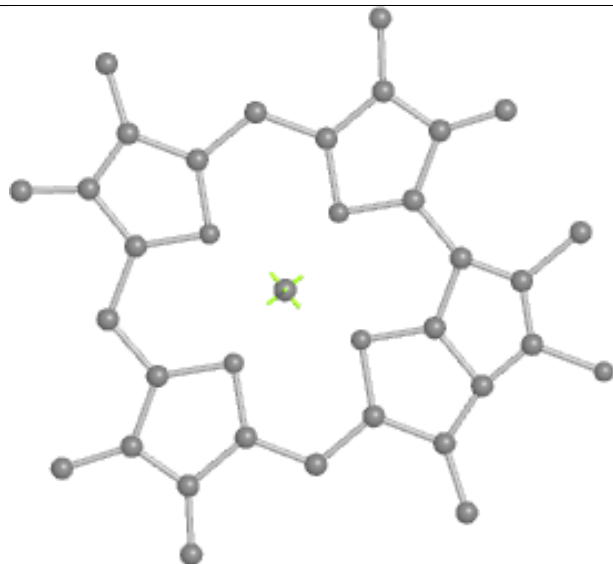
Ligand CLA 1 1012



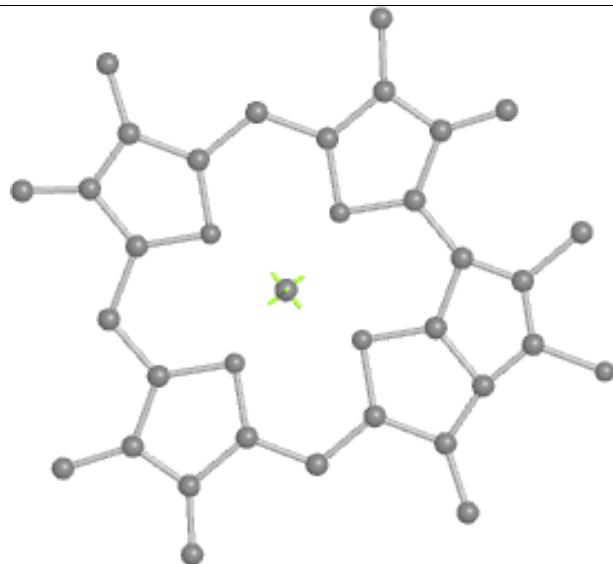
Bond lengths



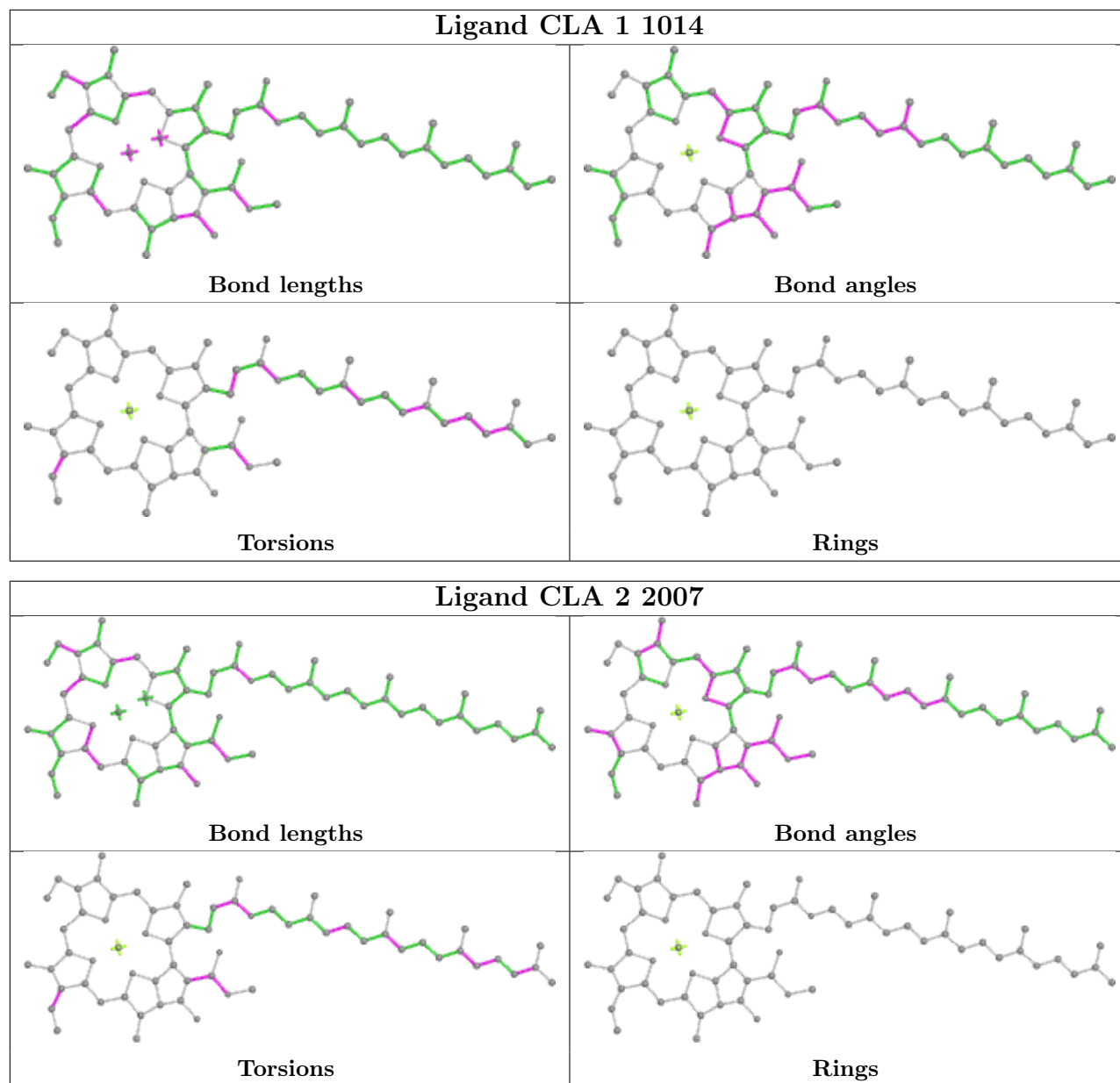
Bond angles

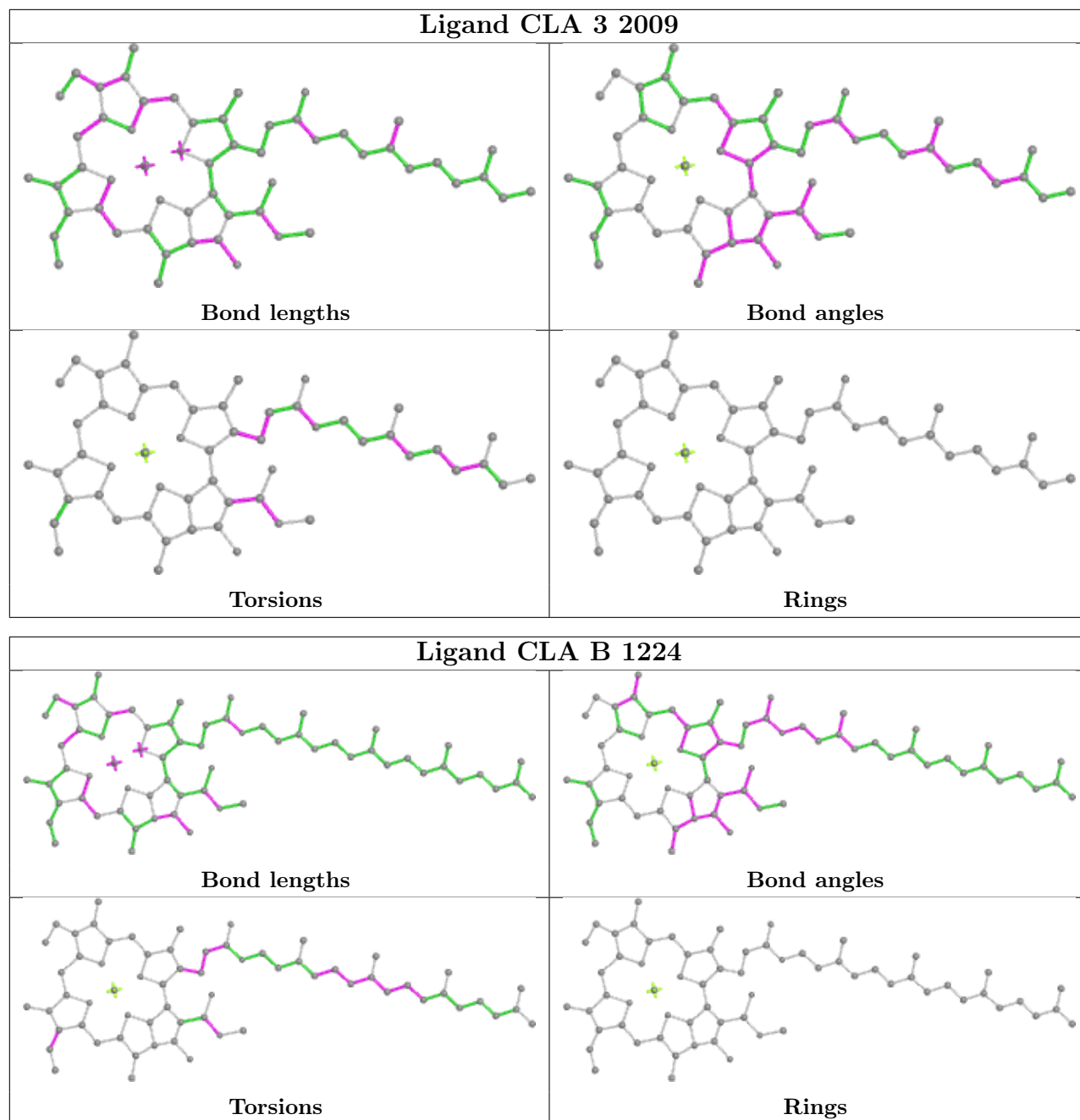


Torsions

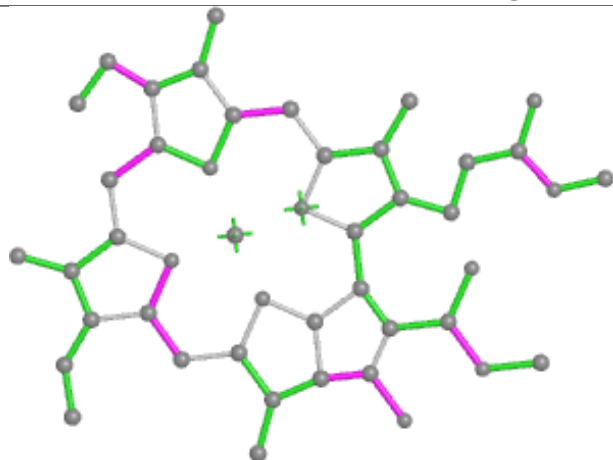


Rings

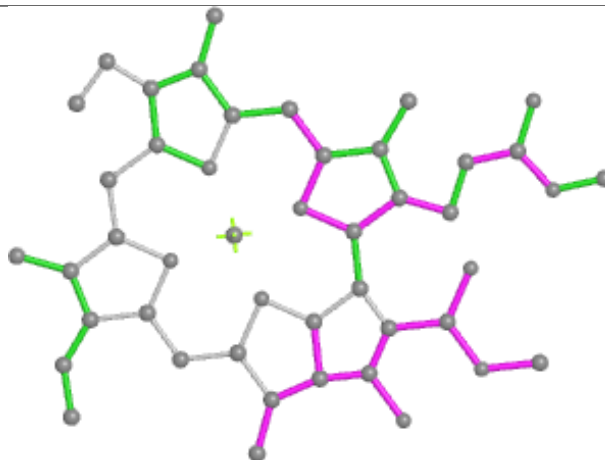




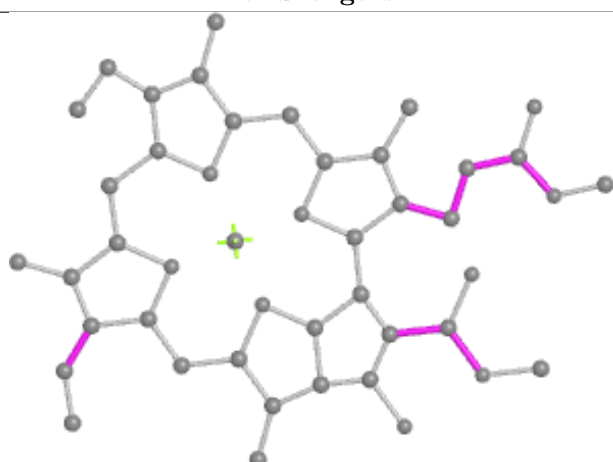
Ligand CLA B 1213



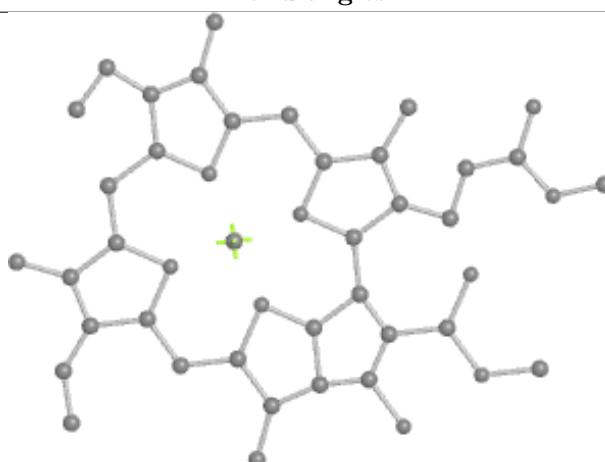
Bond lengths



Bond angles

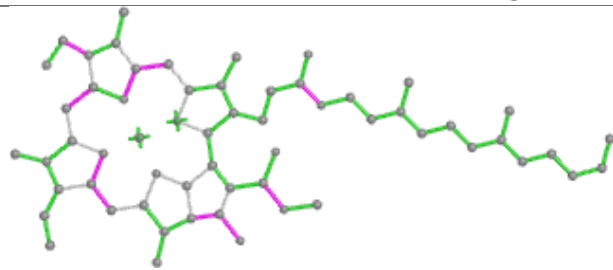


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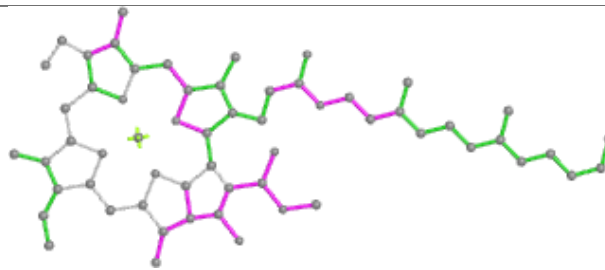


Rings

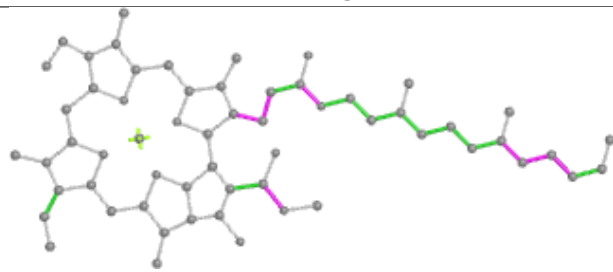
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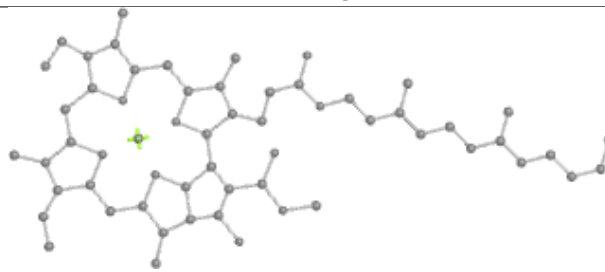
Bond lengths



Bond angles

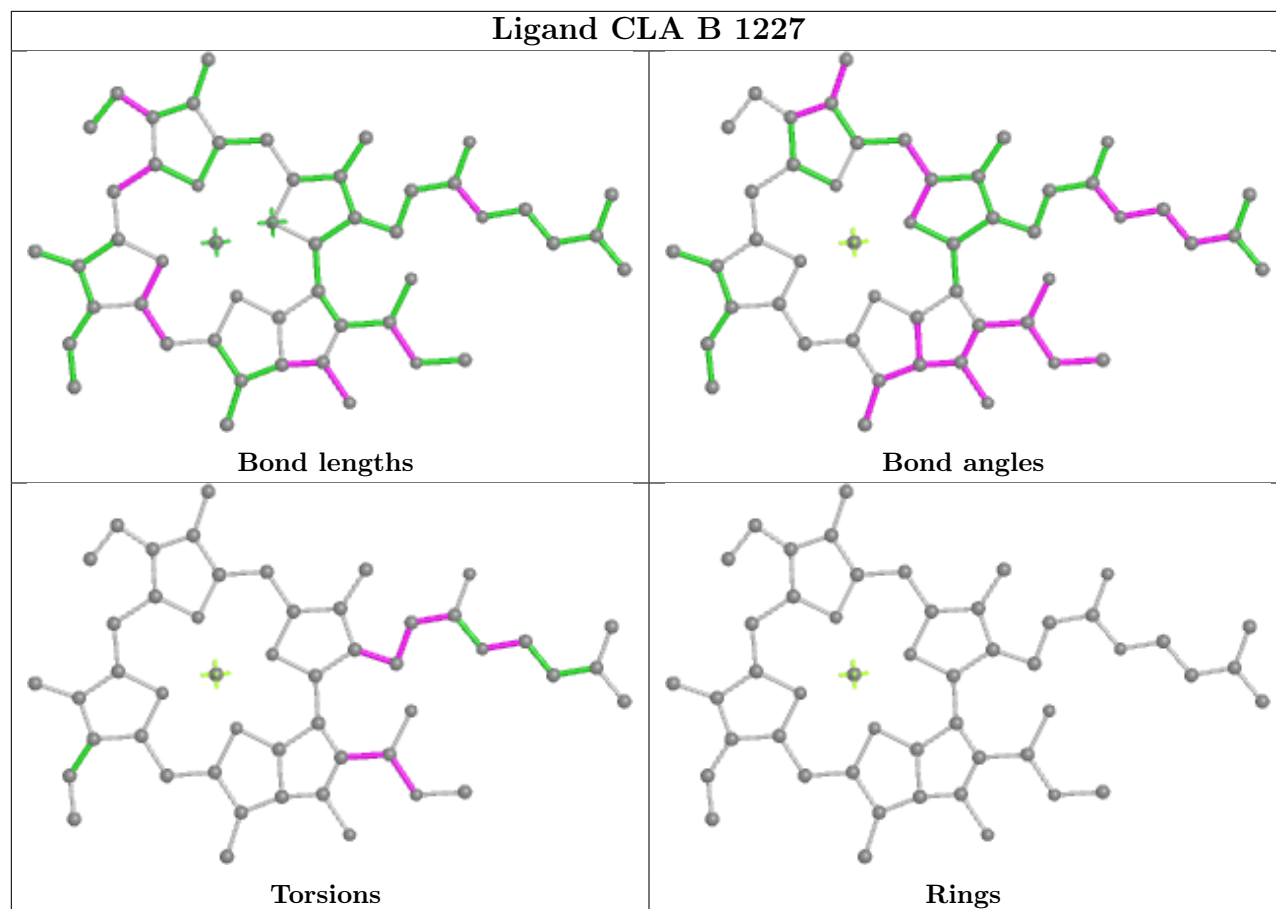


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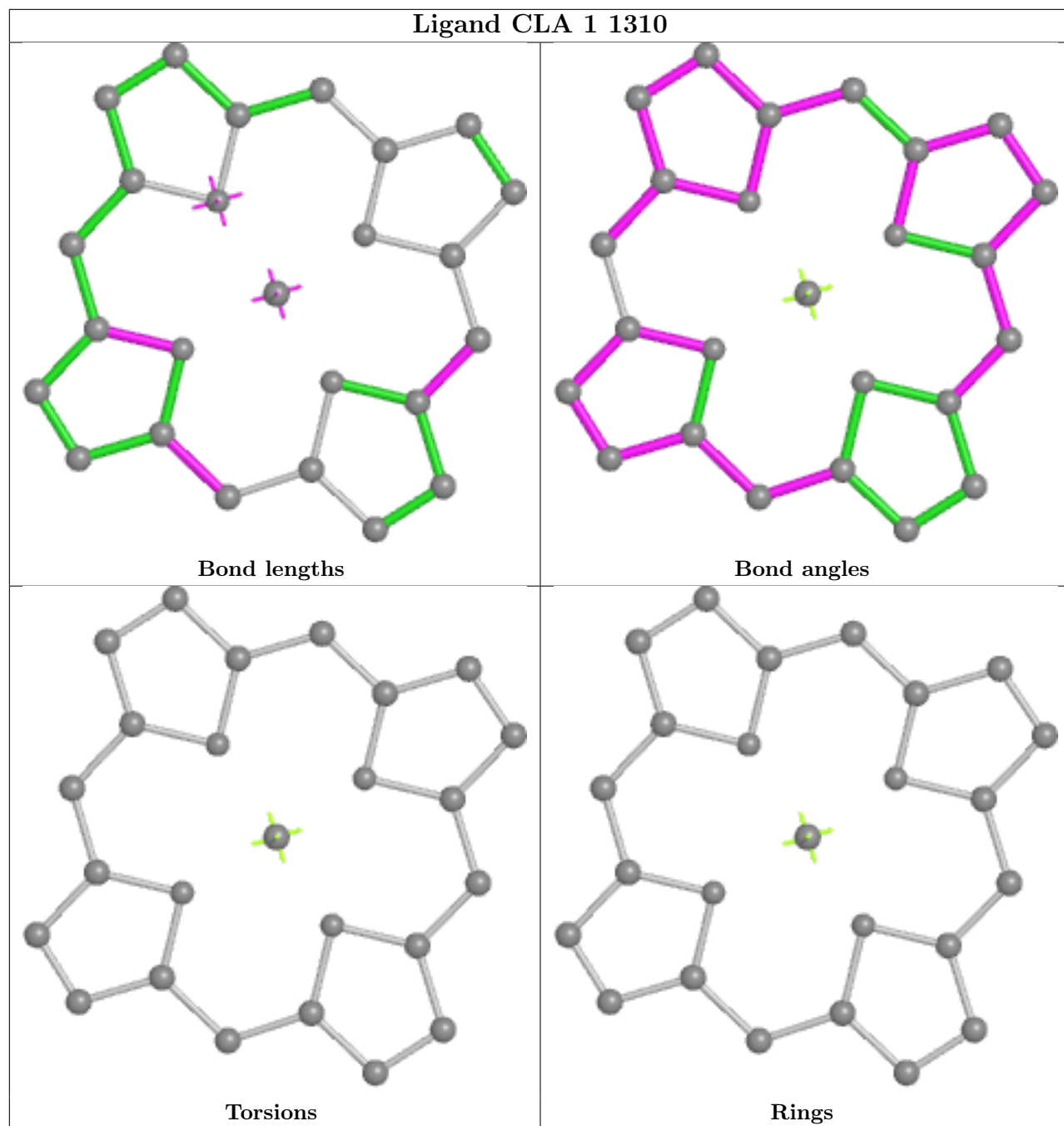


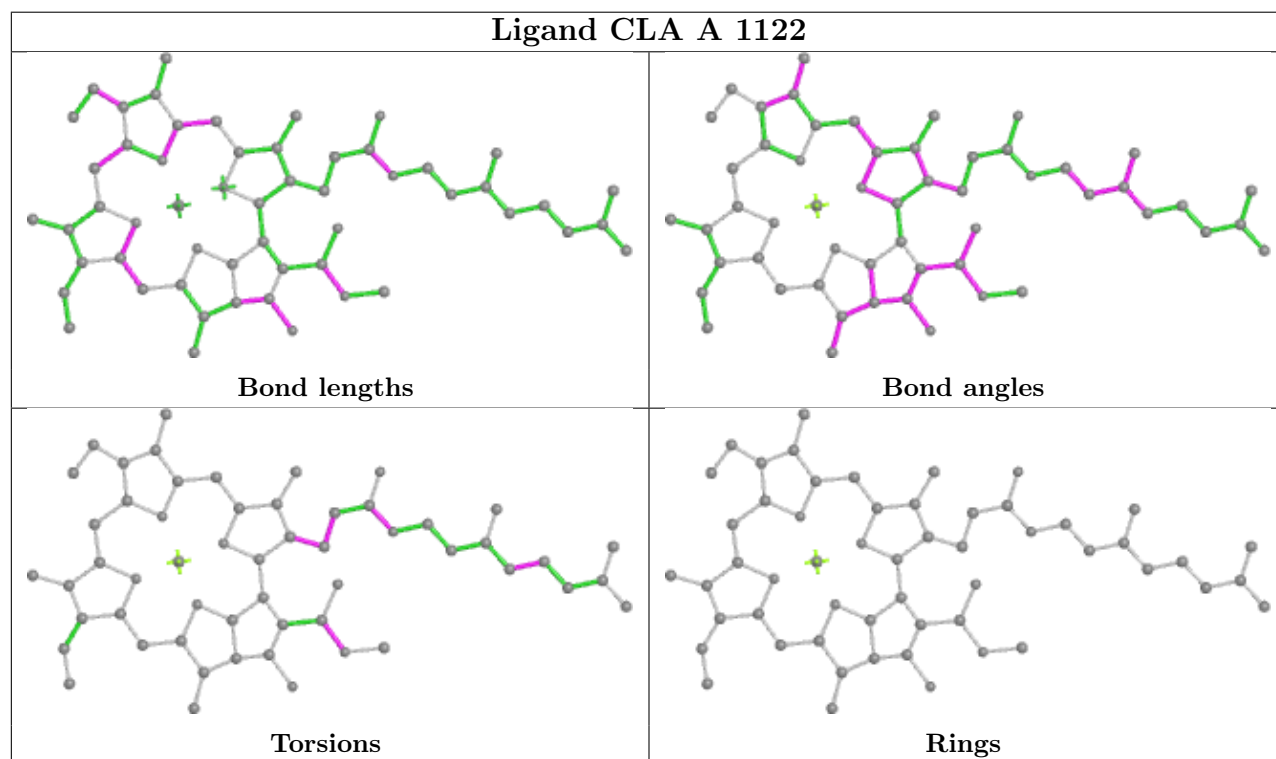
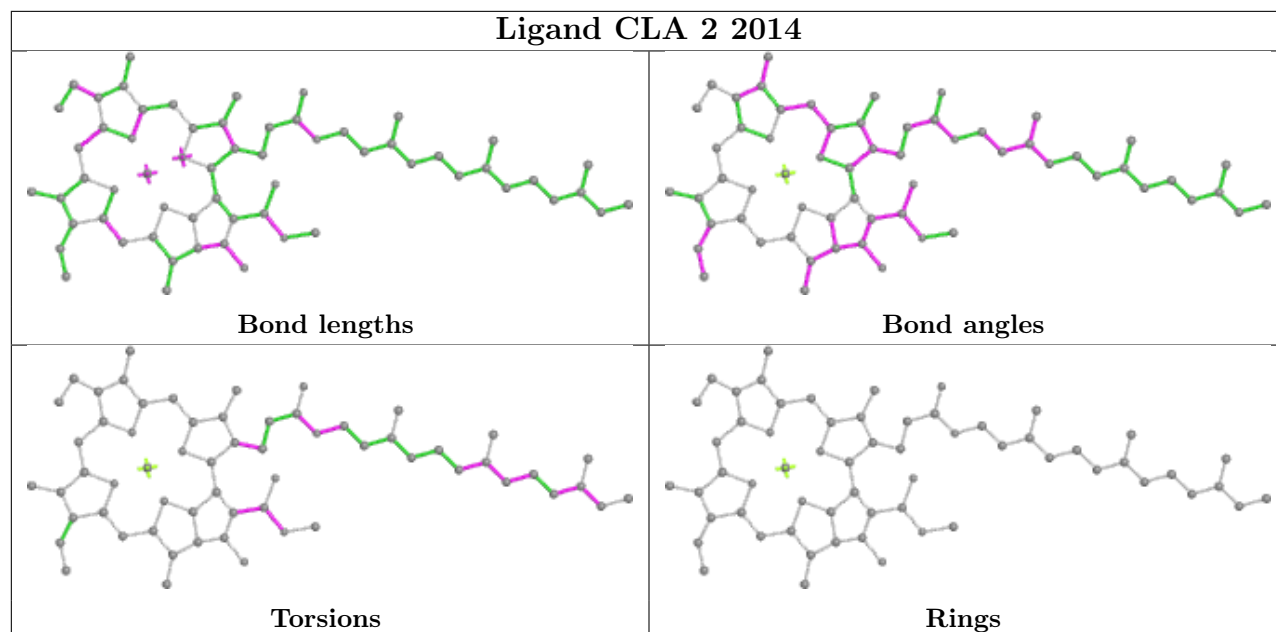
Rings

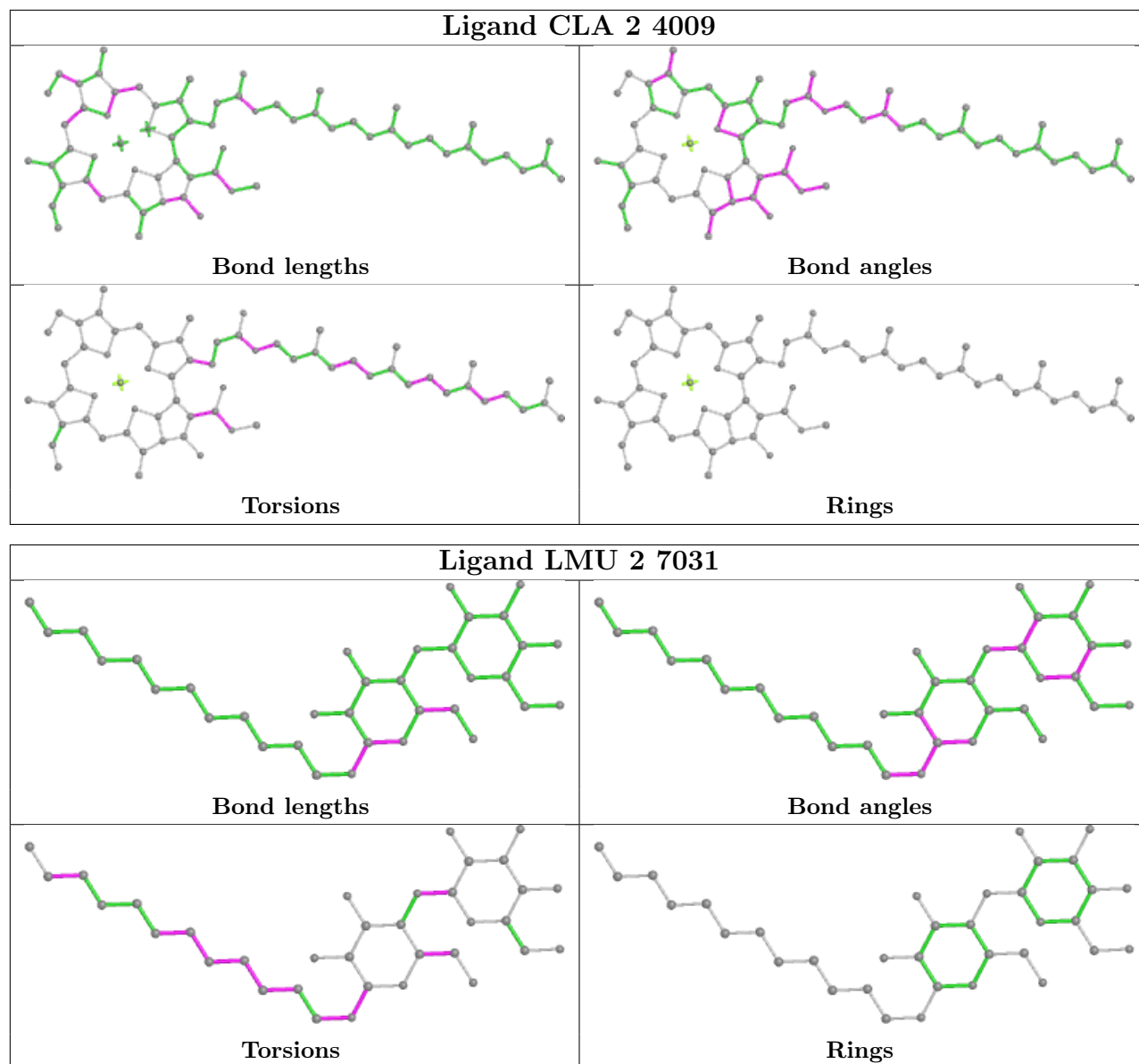
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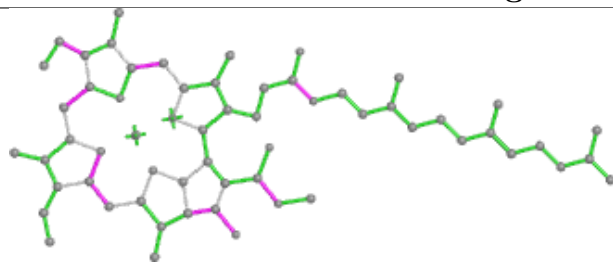
Ligand CLA 1 1310



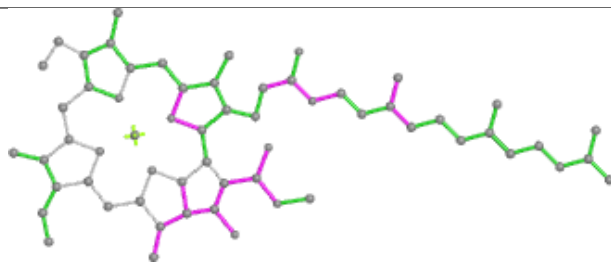




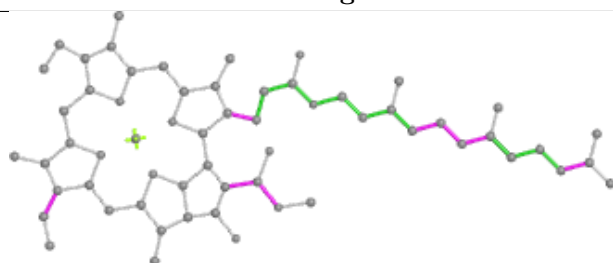
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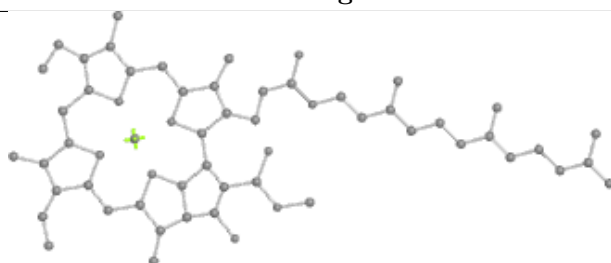
Bond lengths



Bond angles

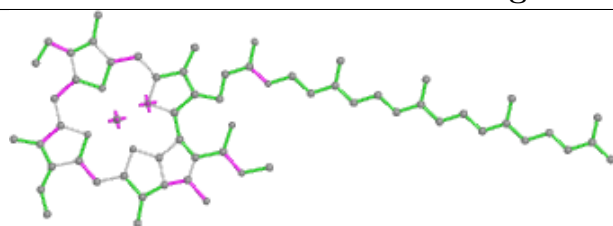


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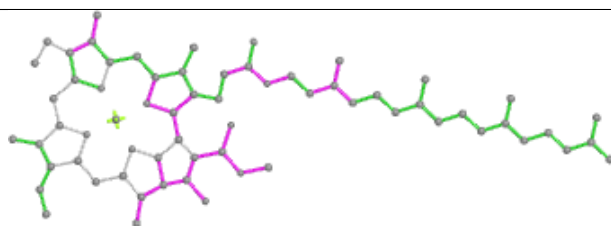


Rings

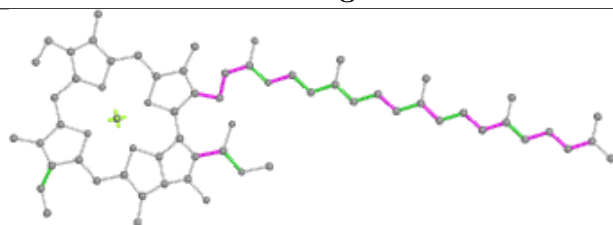
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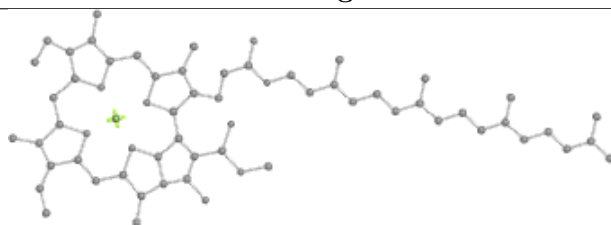
Bond lengths



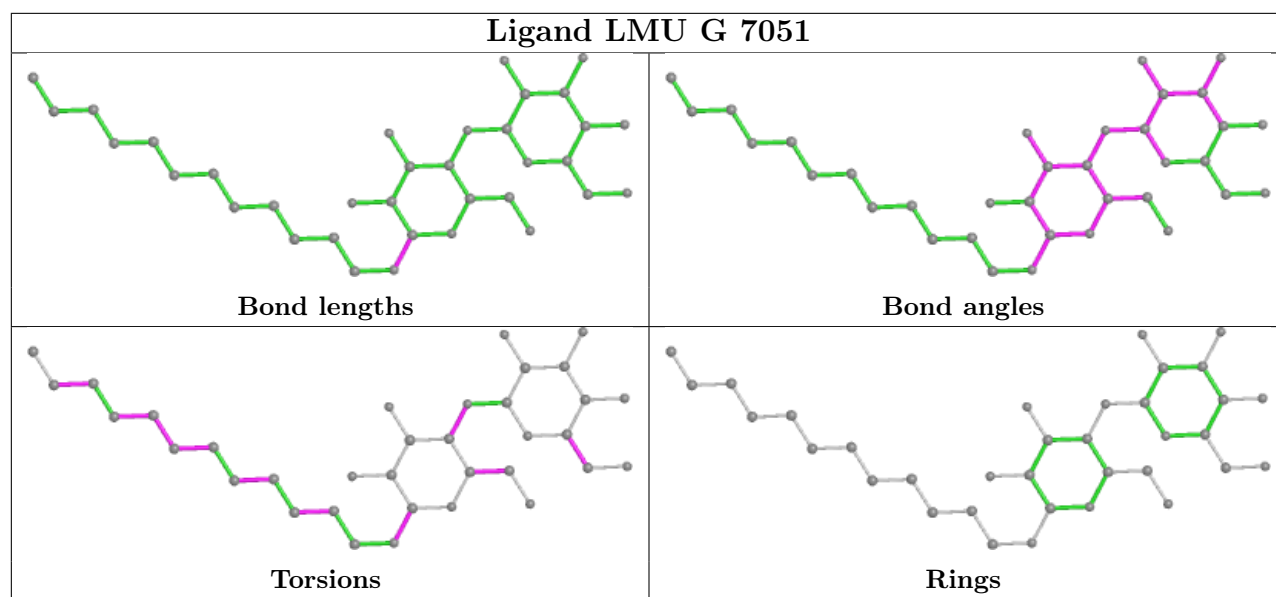
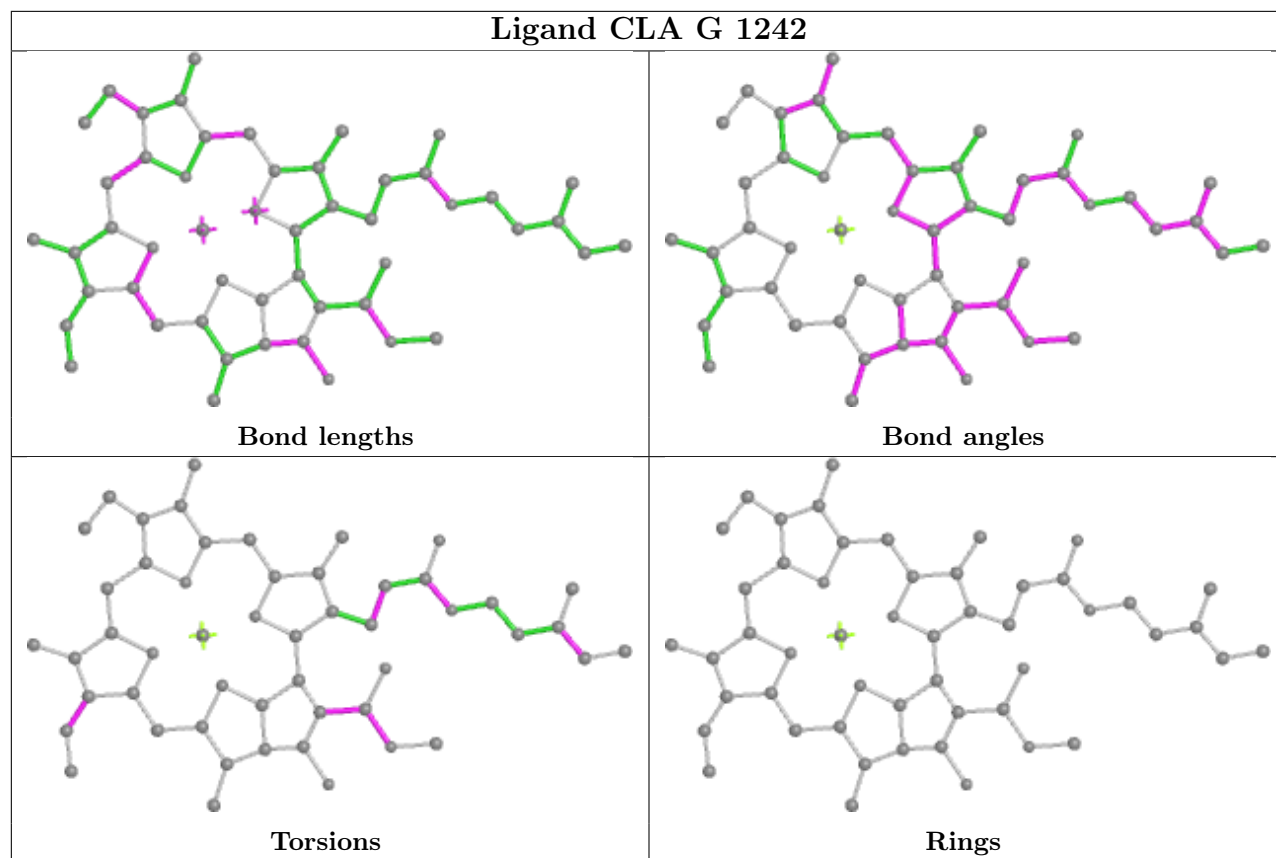
Bond angles

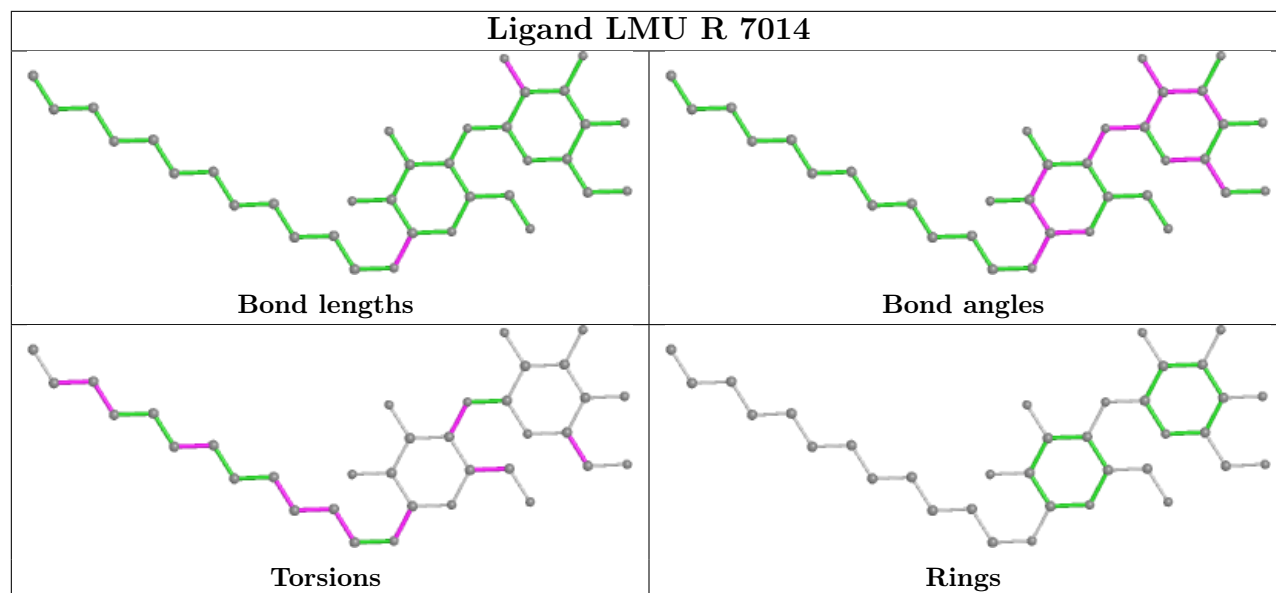


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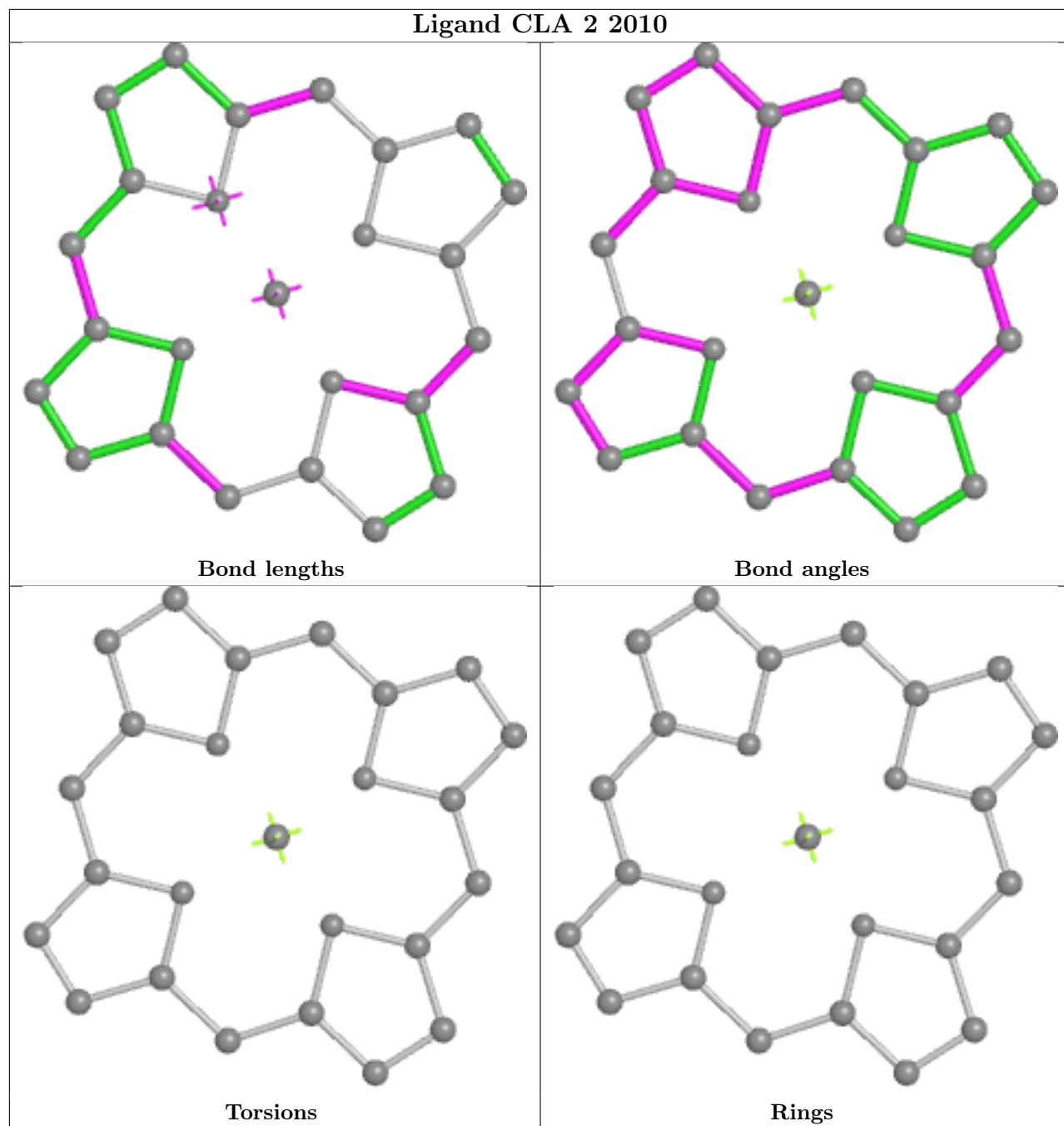


Rings

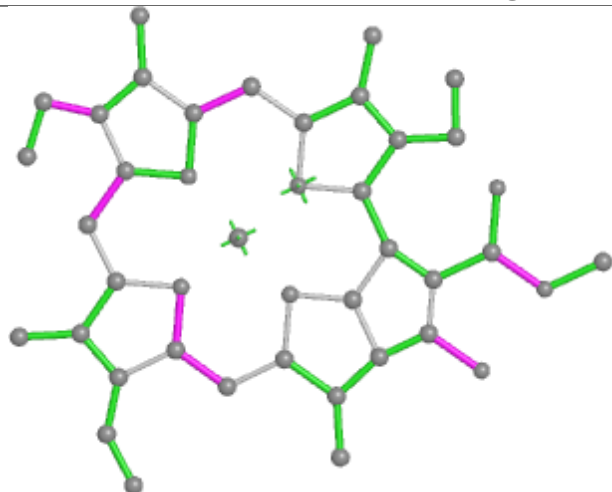




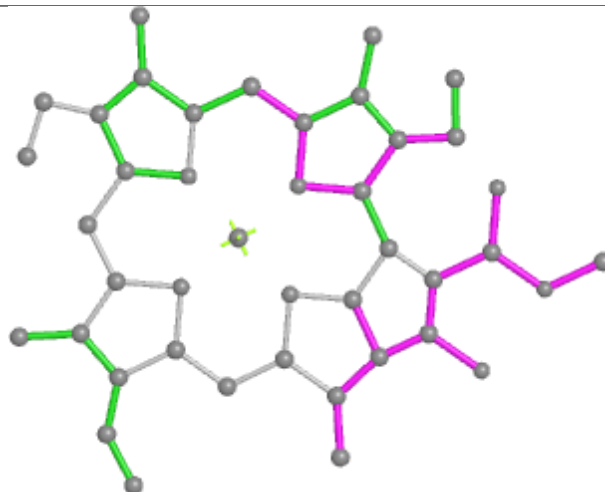
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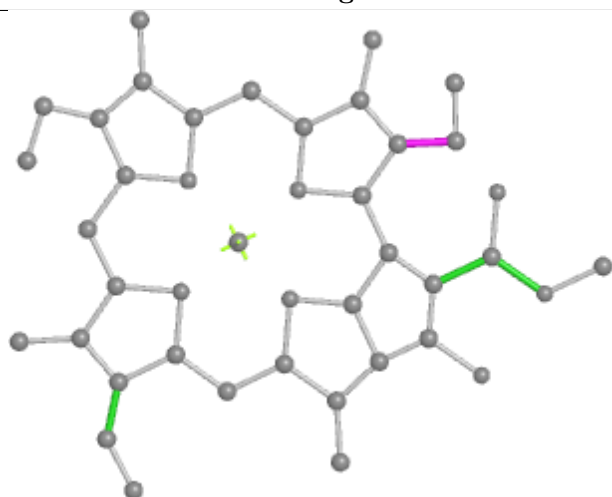
Ligand CLA A 1121



Bond lengths



Bond angles

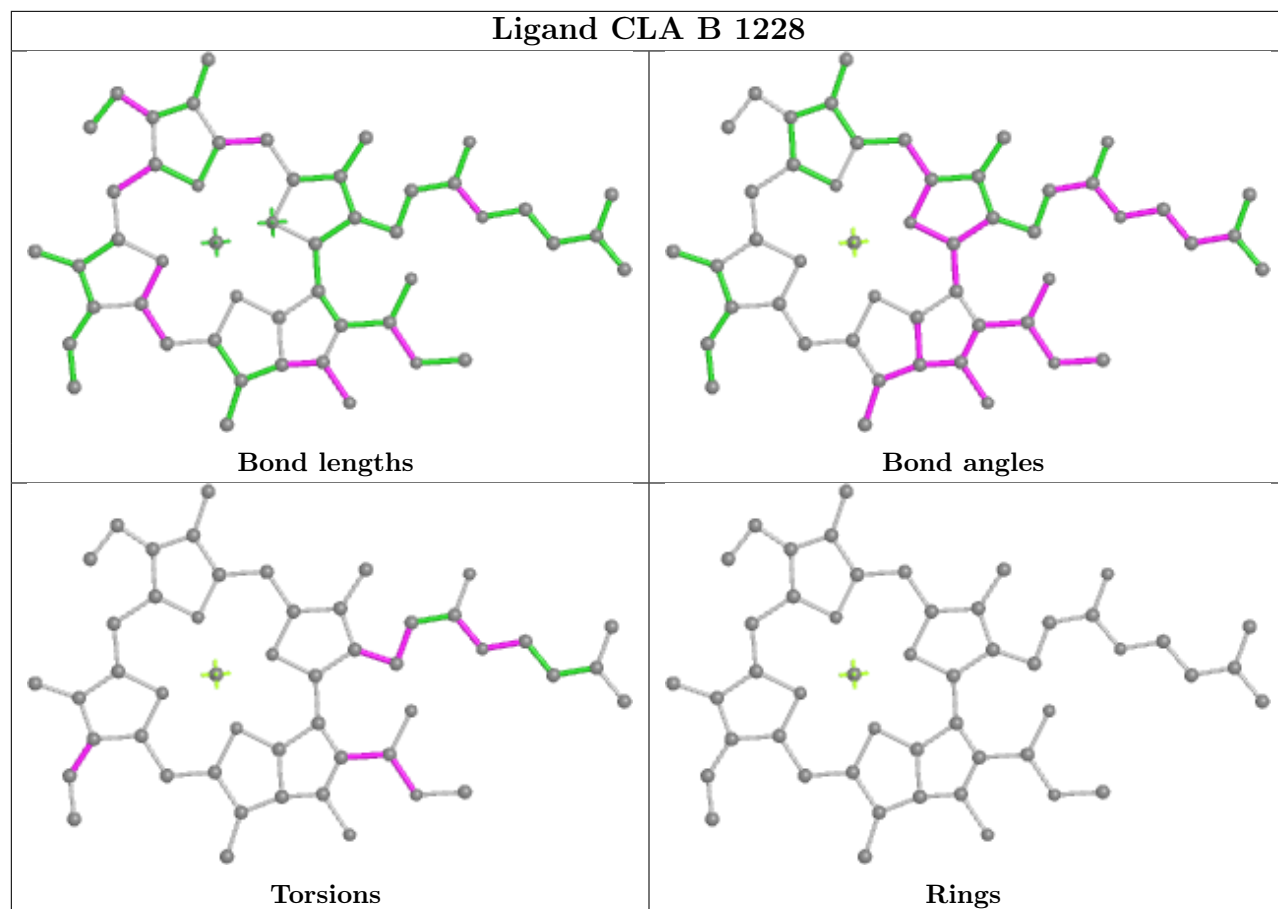


Torsions

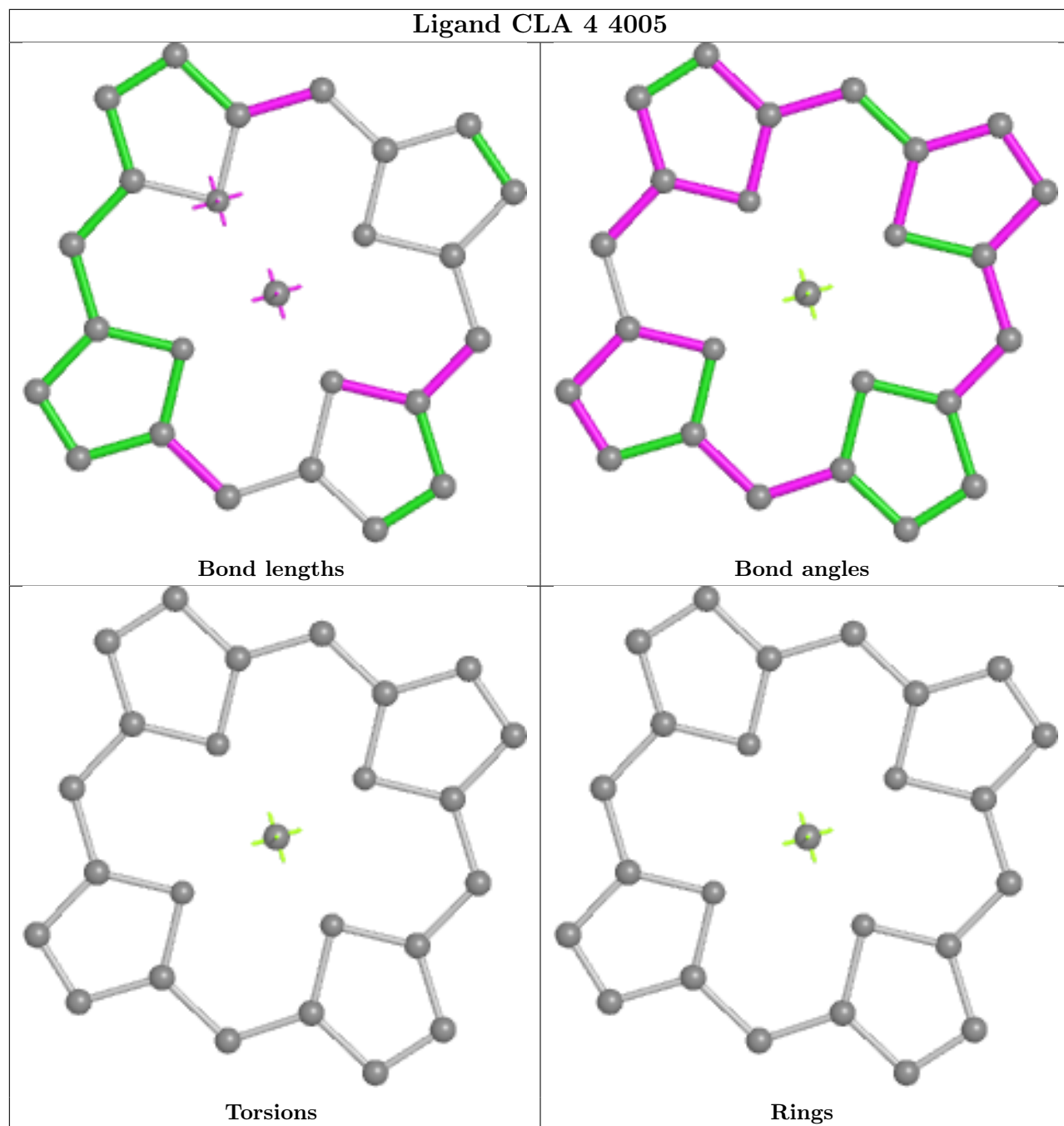


Rings

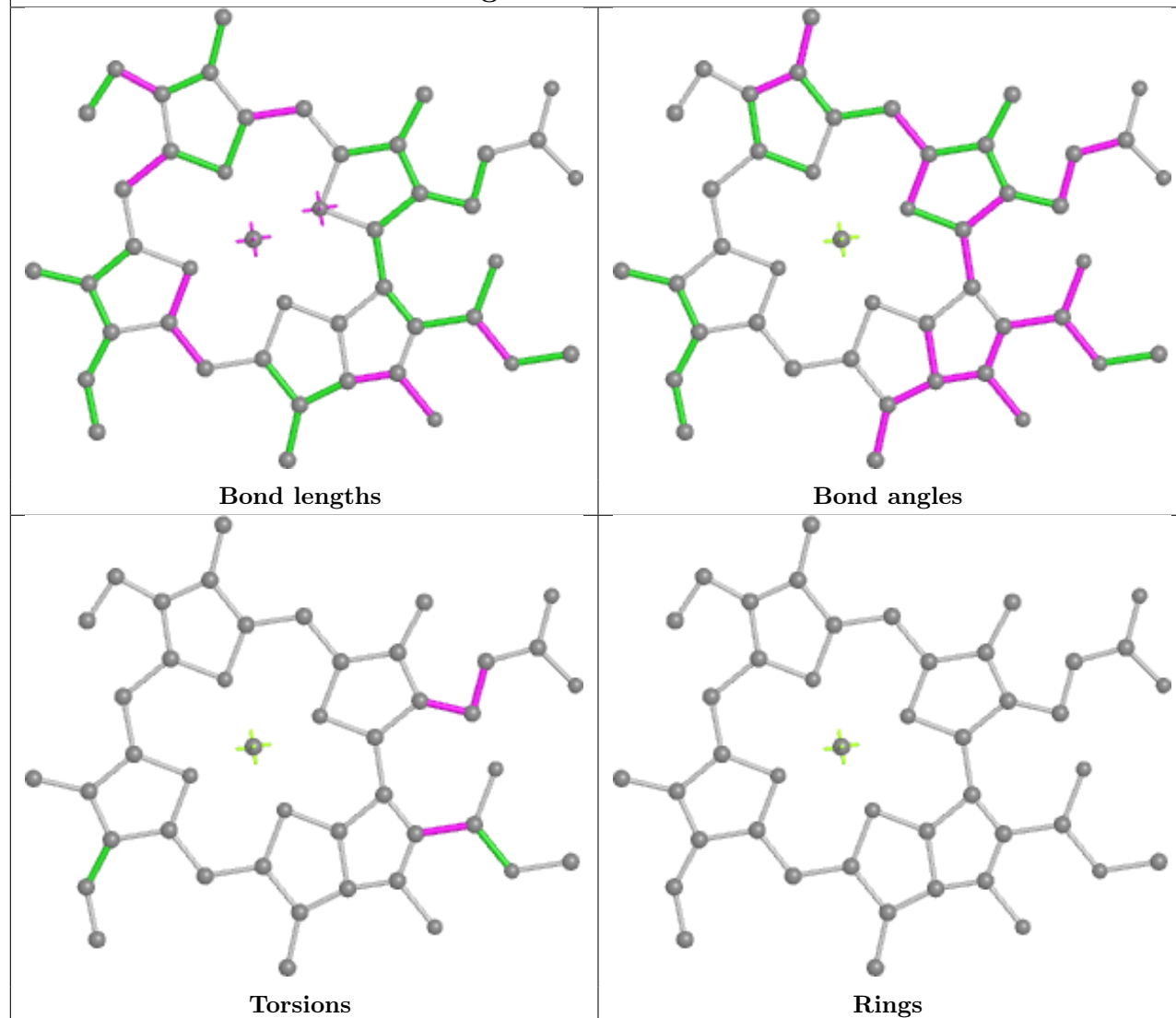
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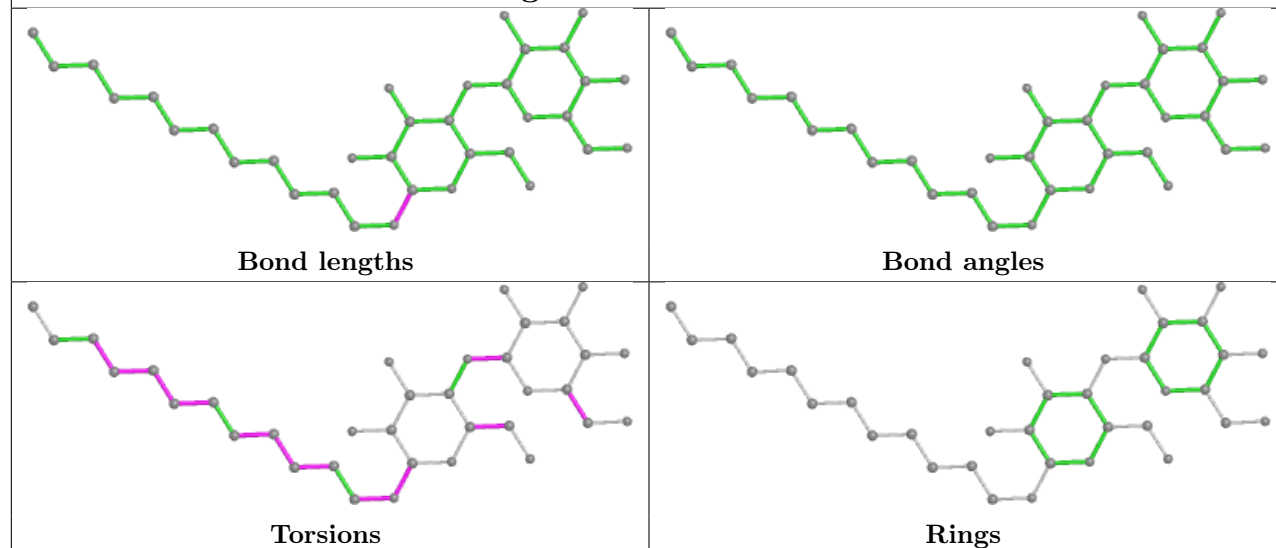
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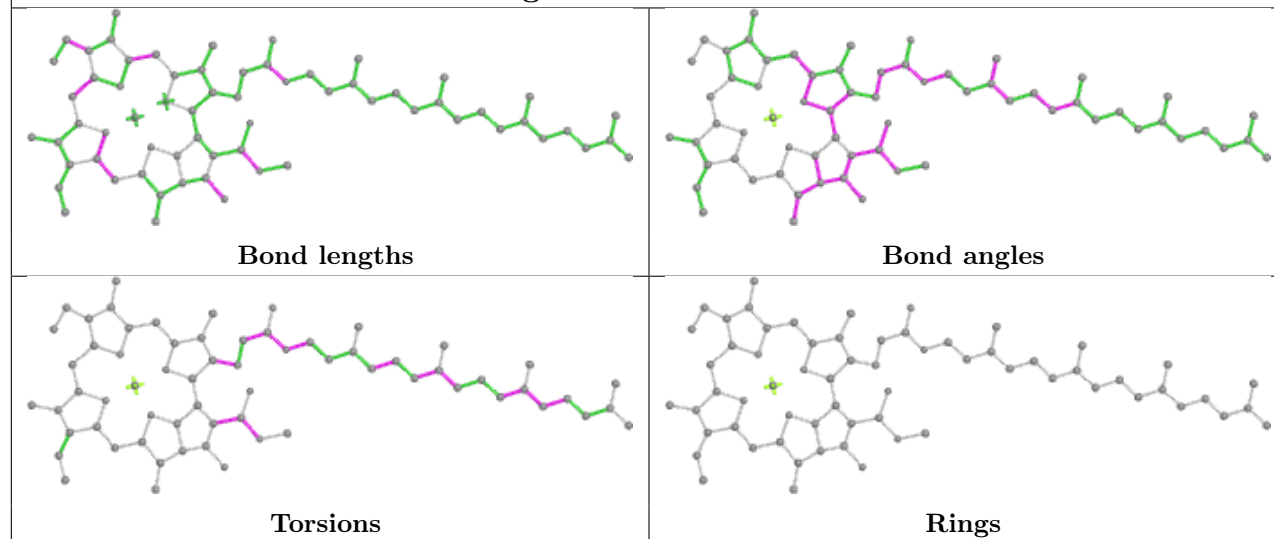
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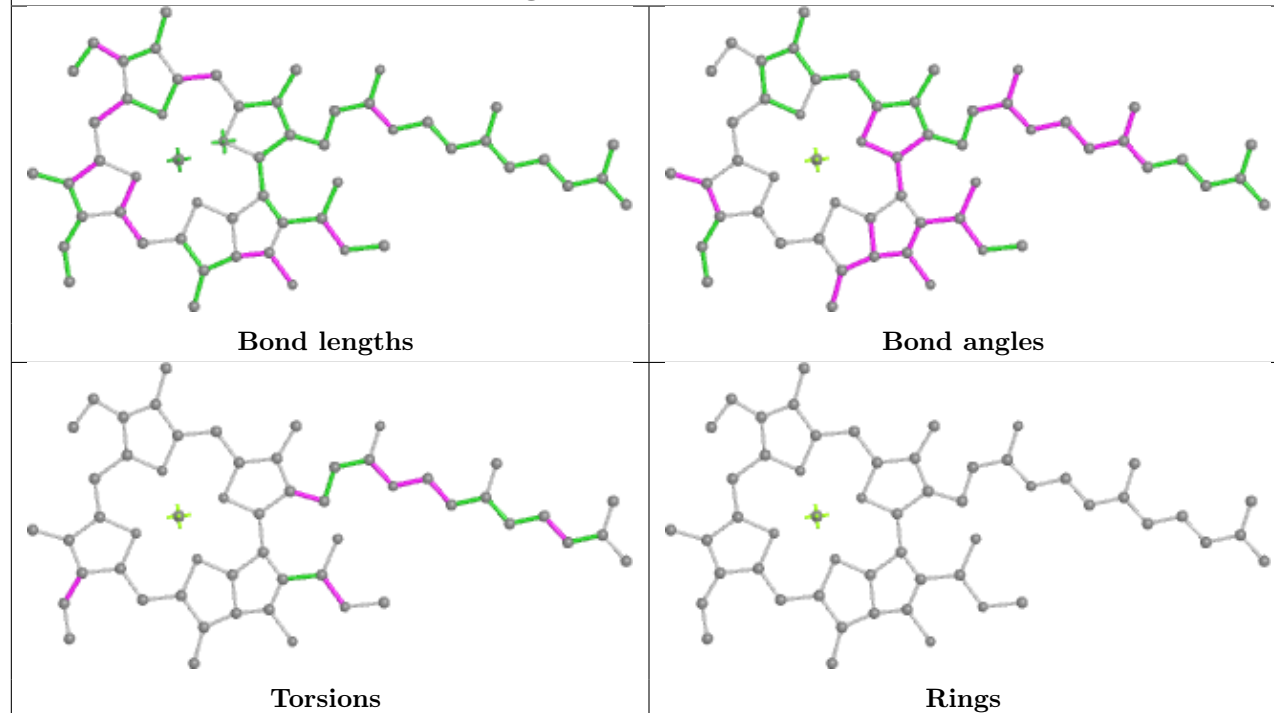
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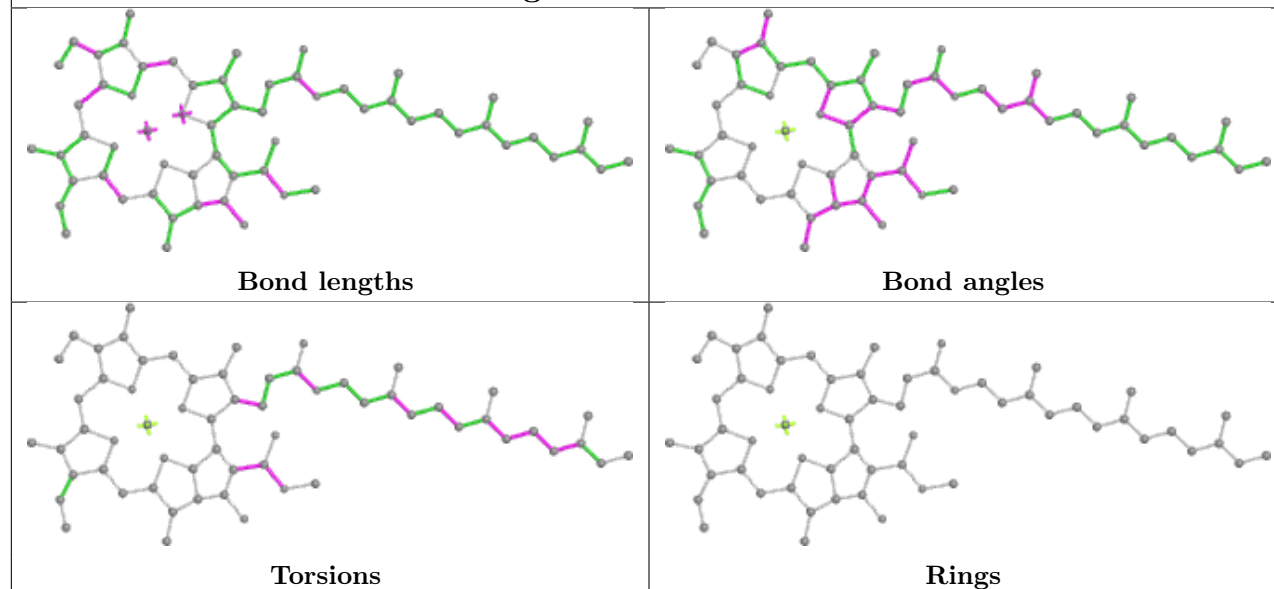
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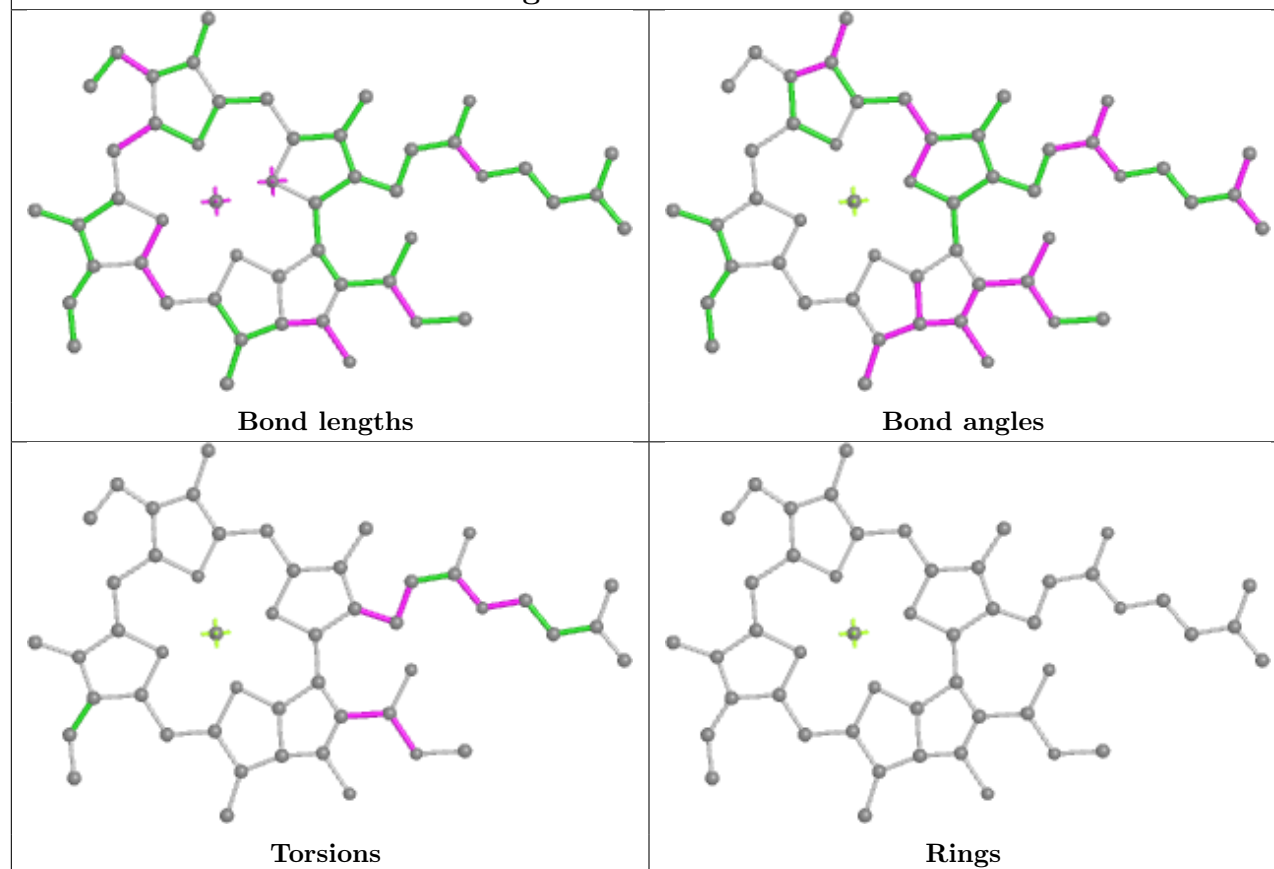
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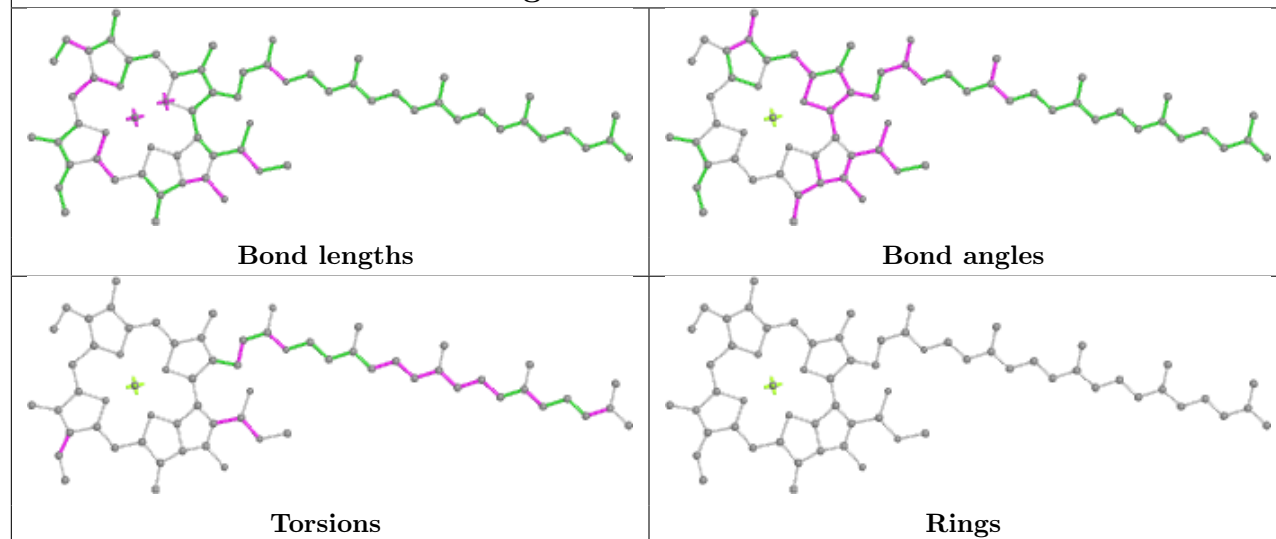
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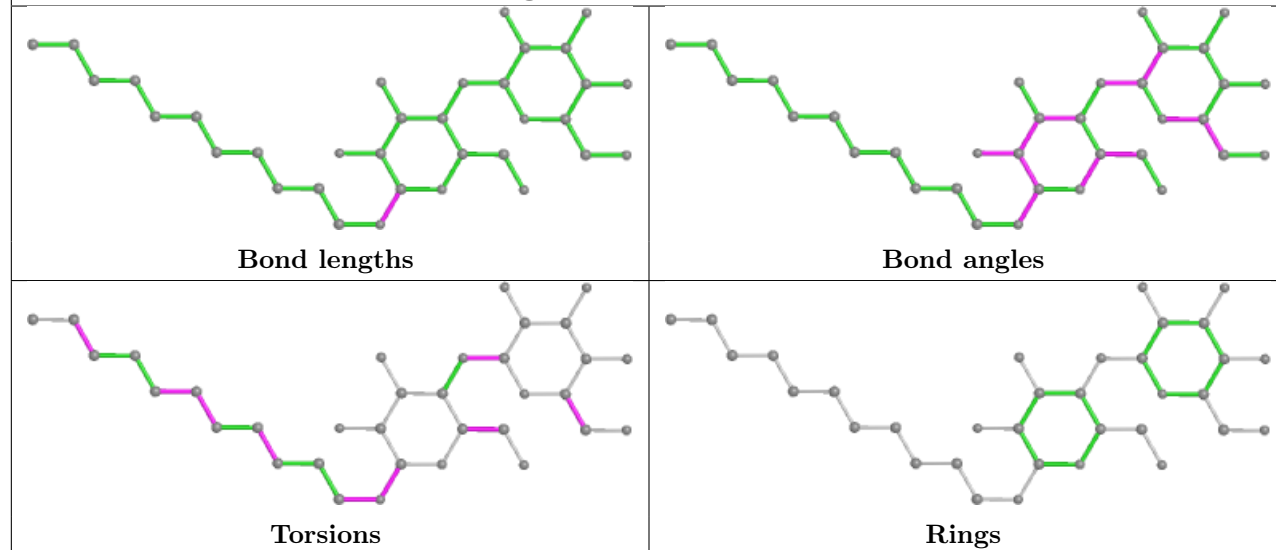
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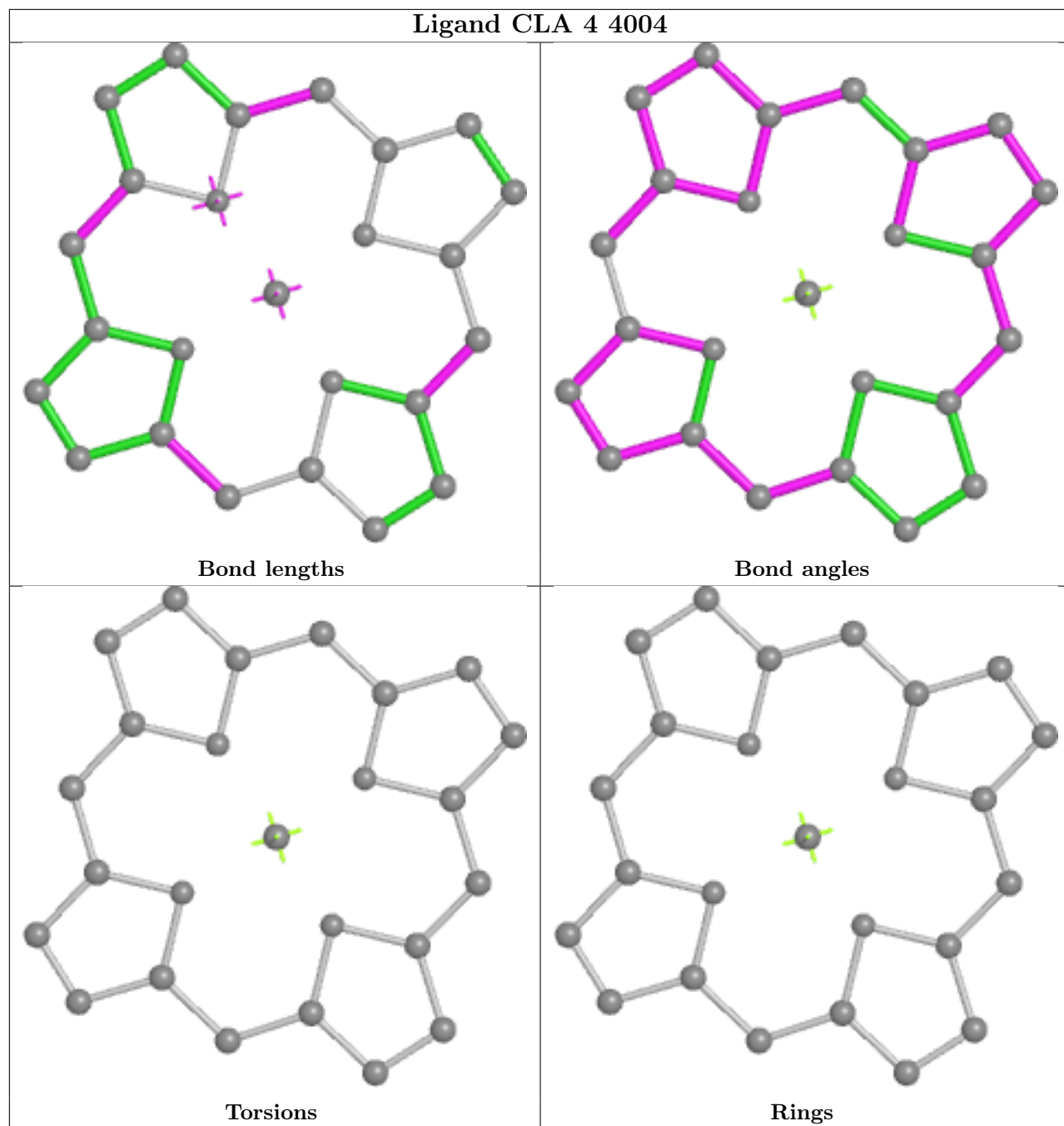
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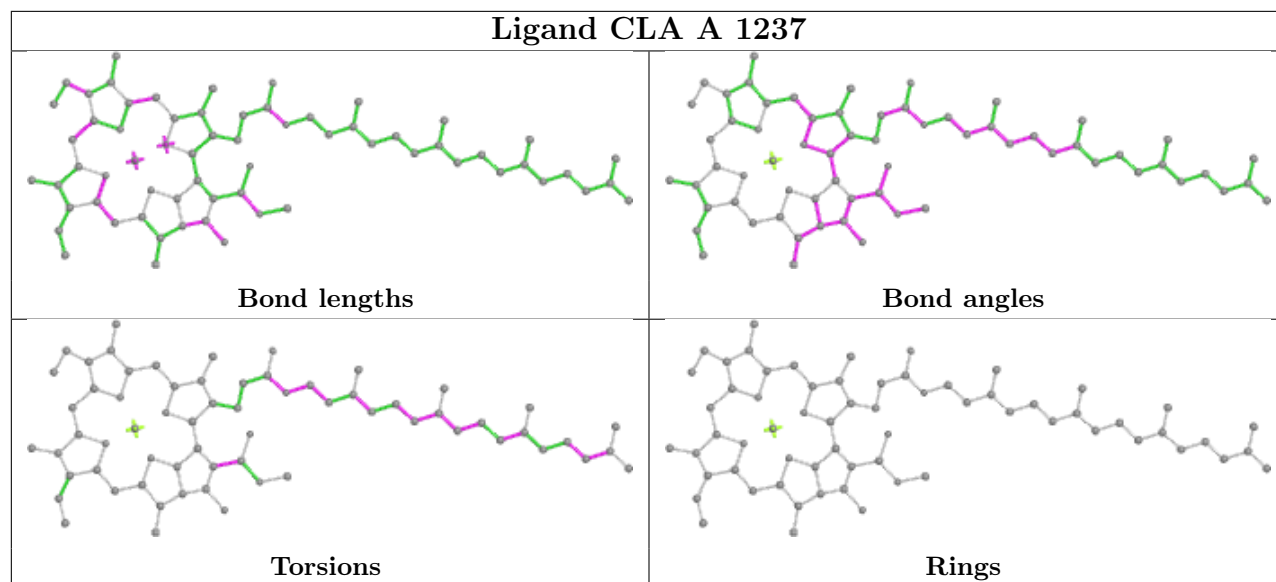
Ligand LMU F 7036



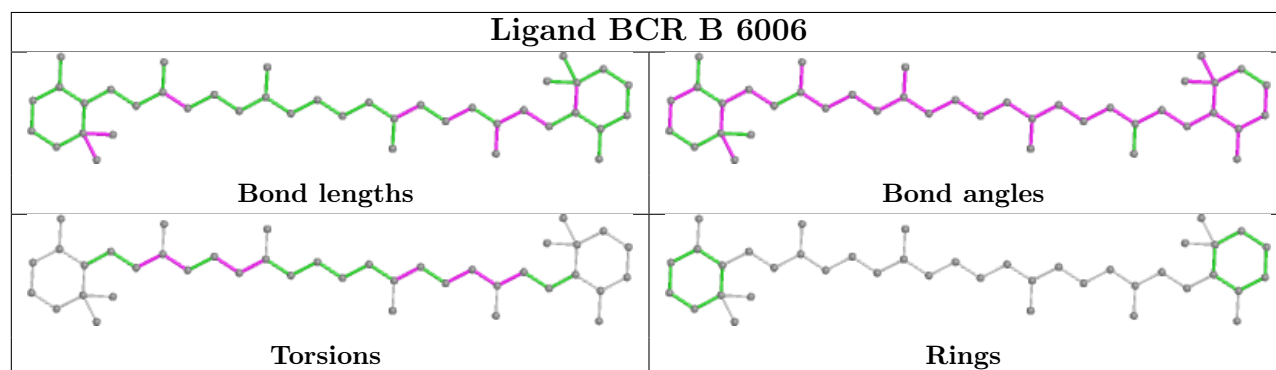
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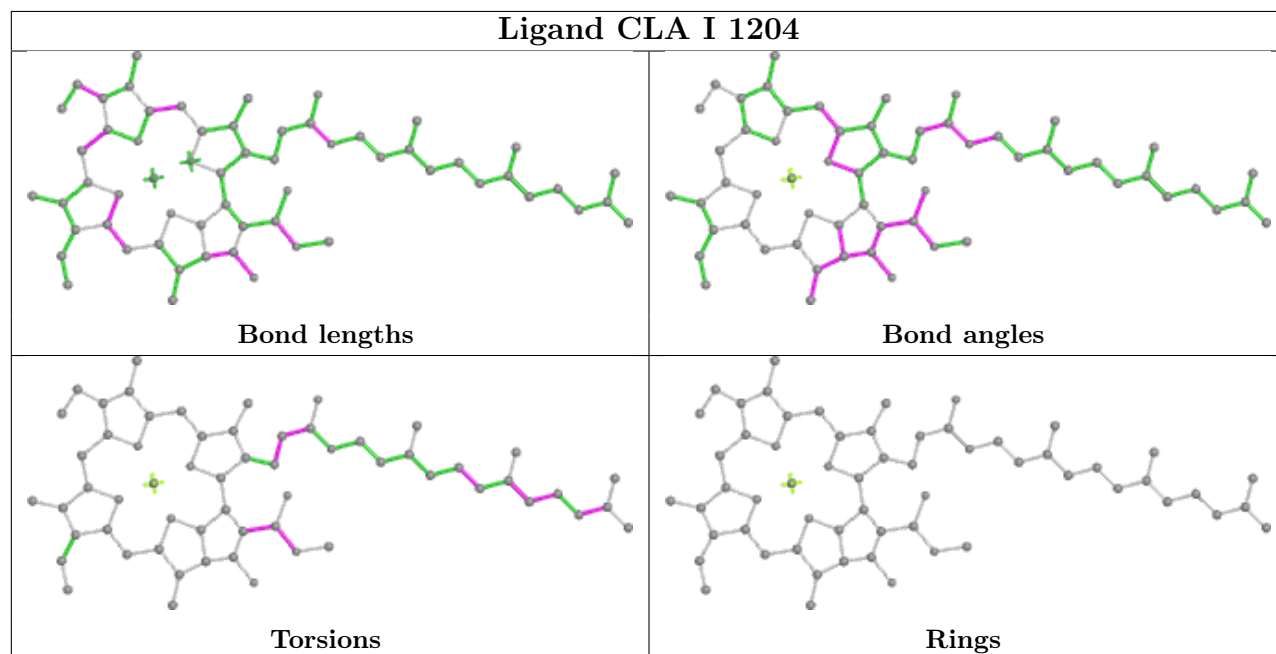
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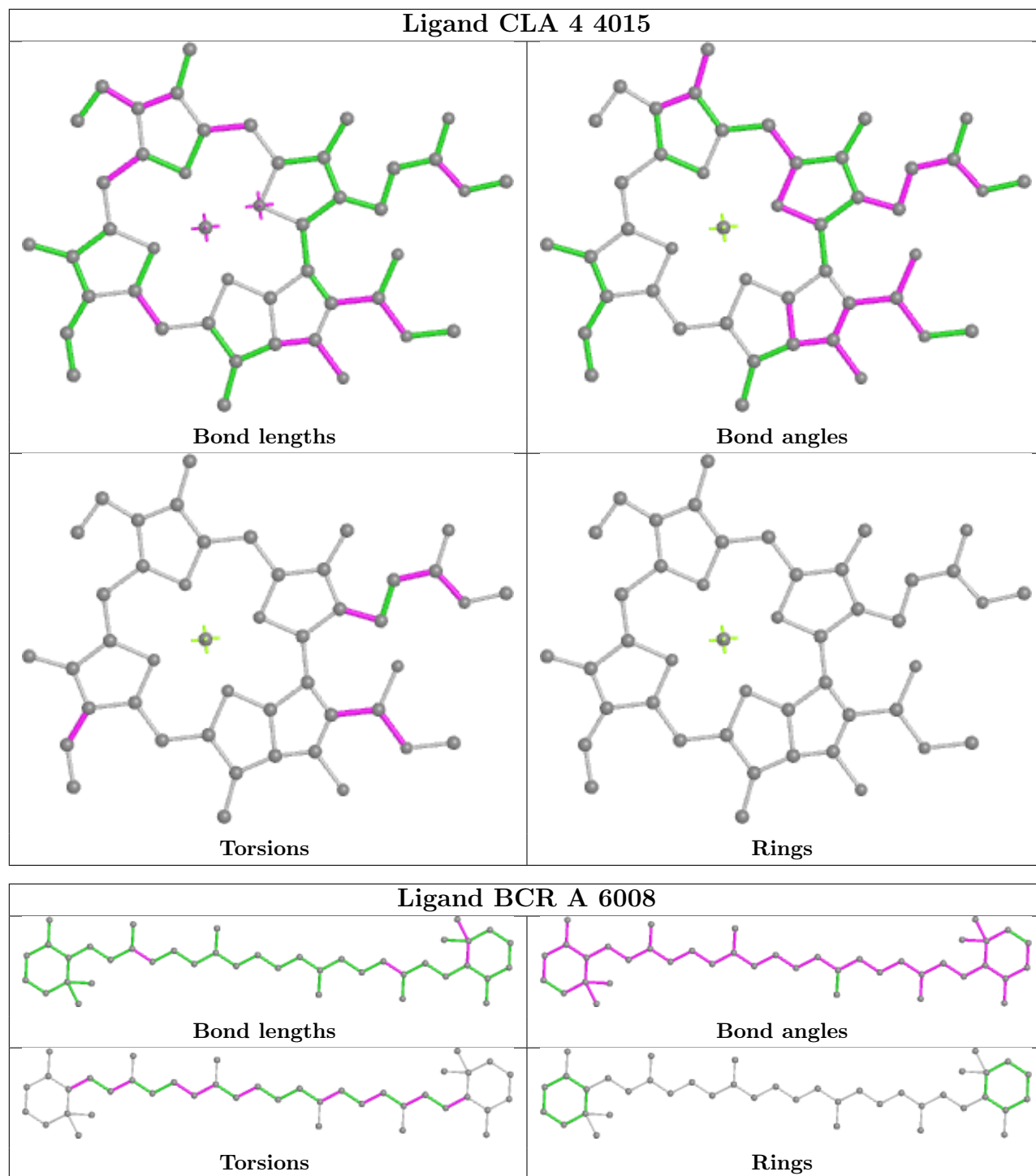


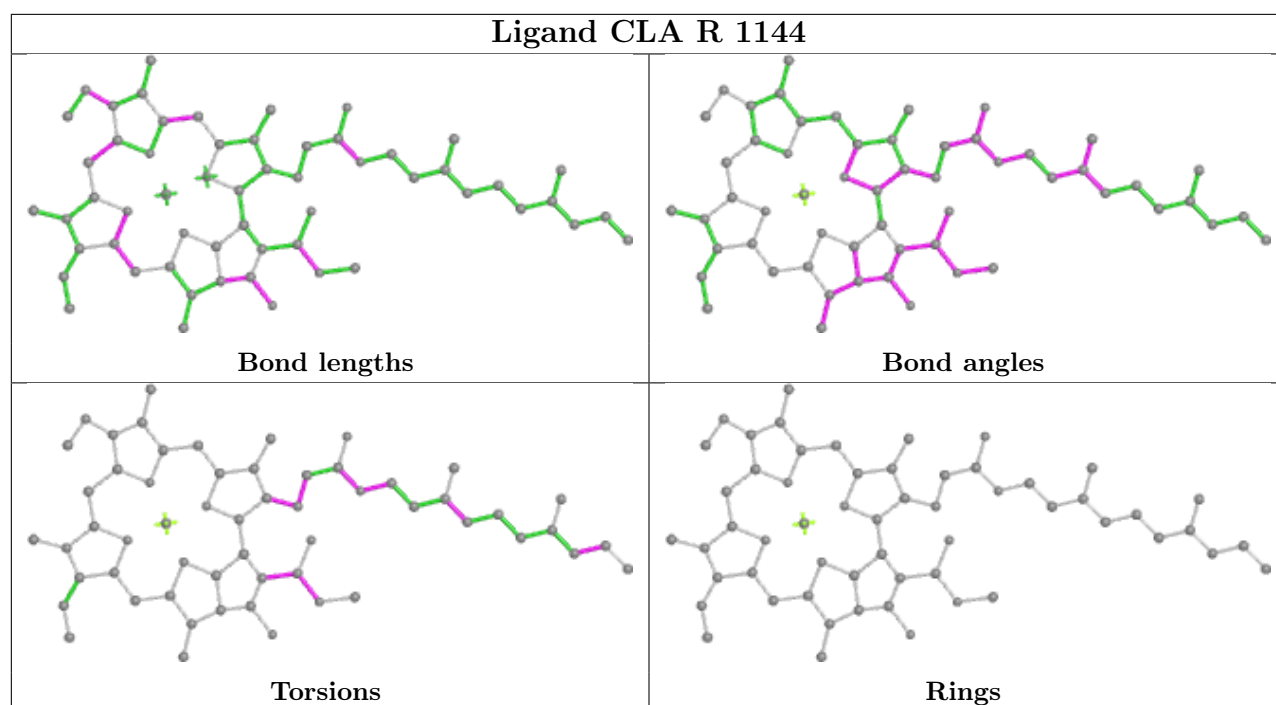
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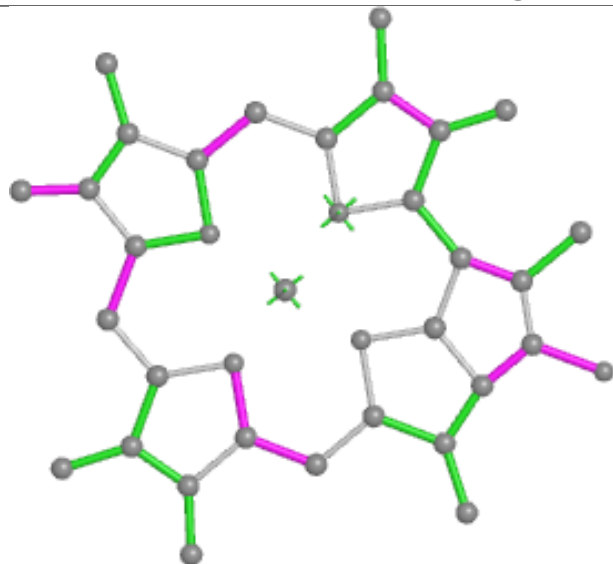
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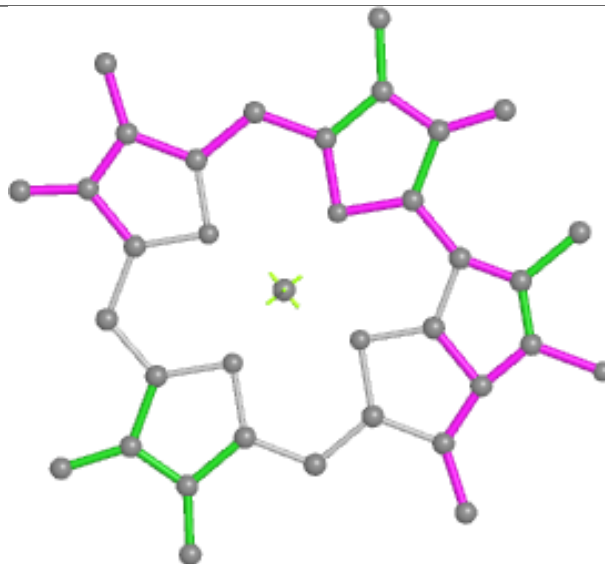




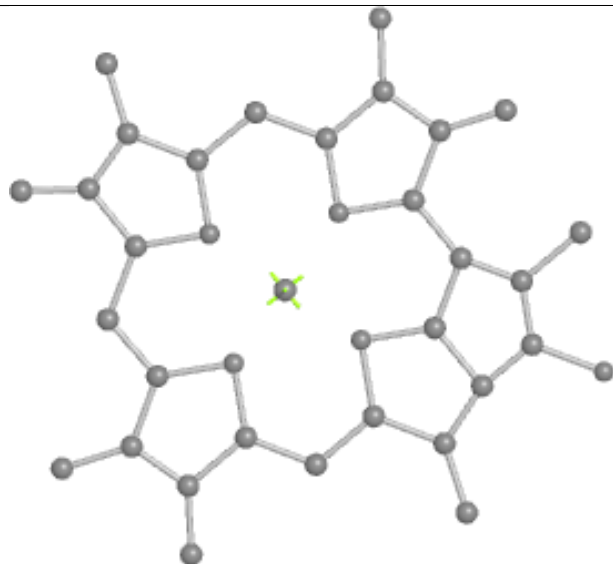
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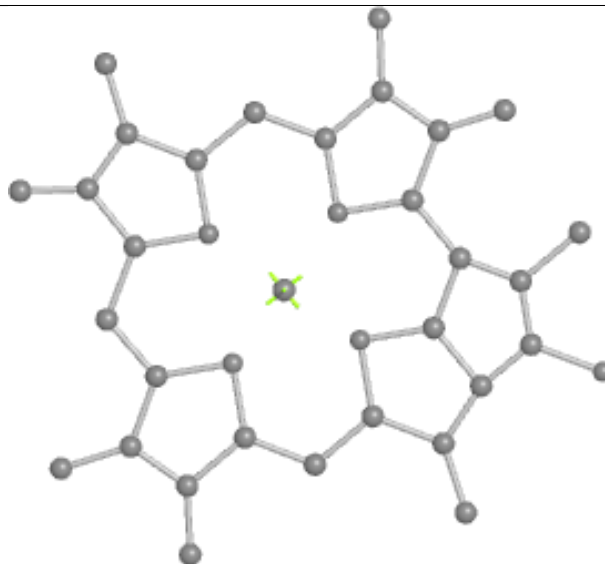
Bond lengths



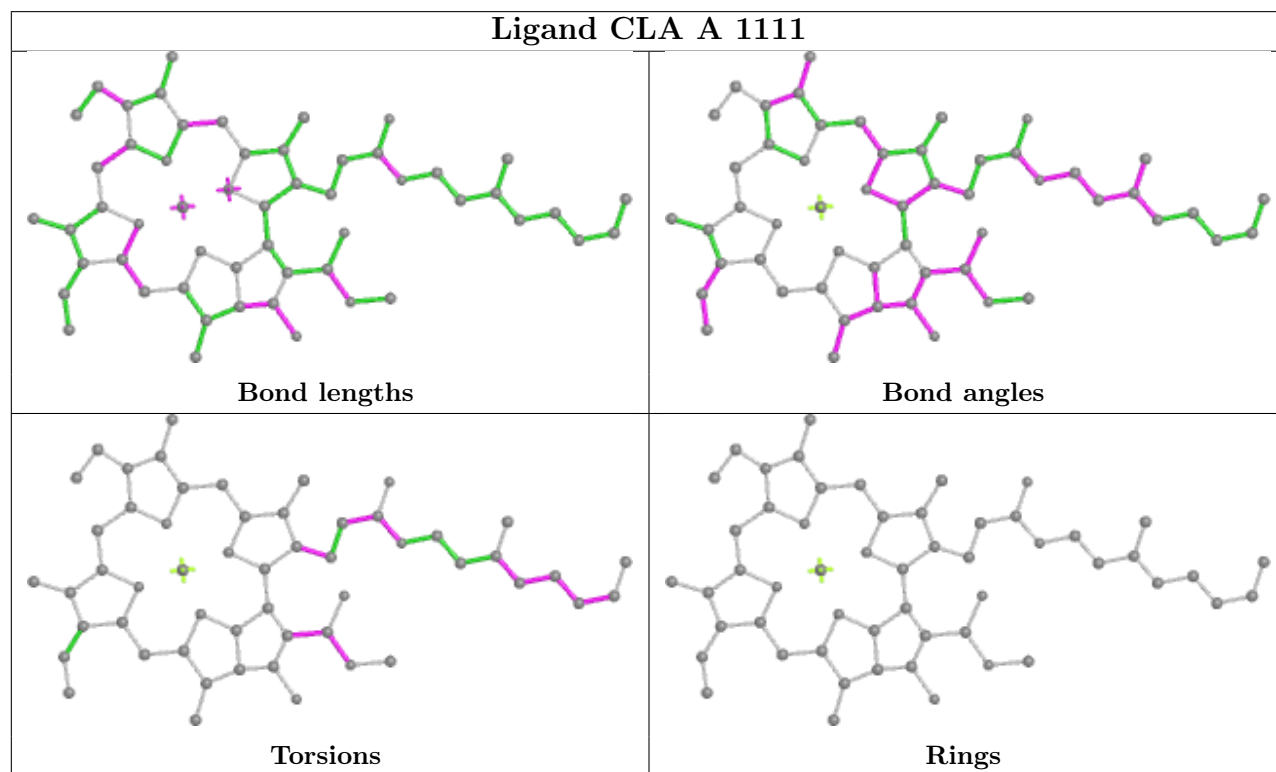
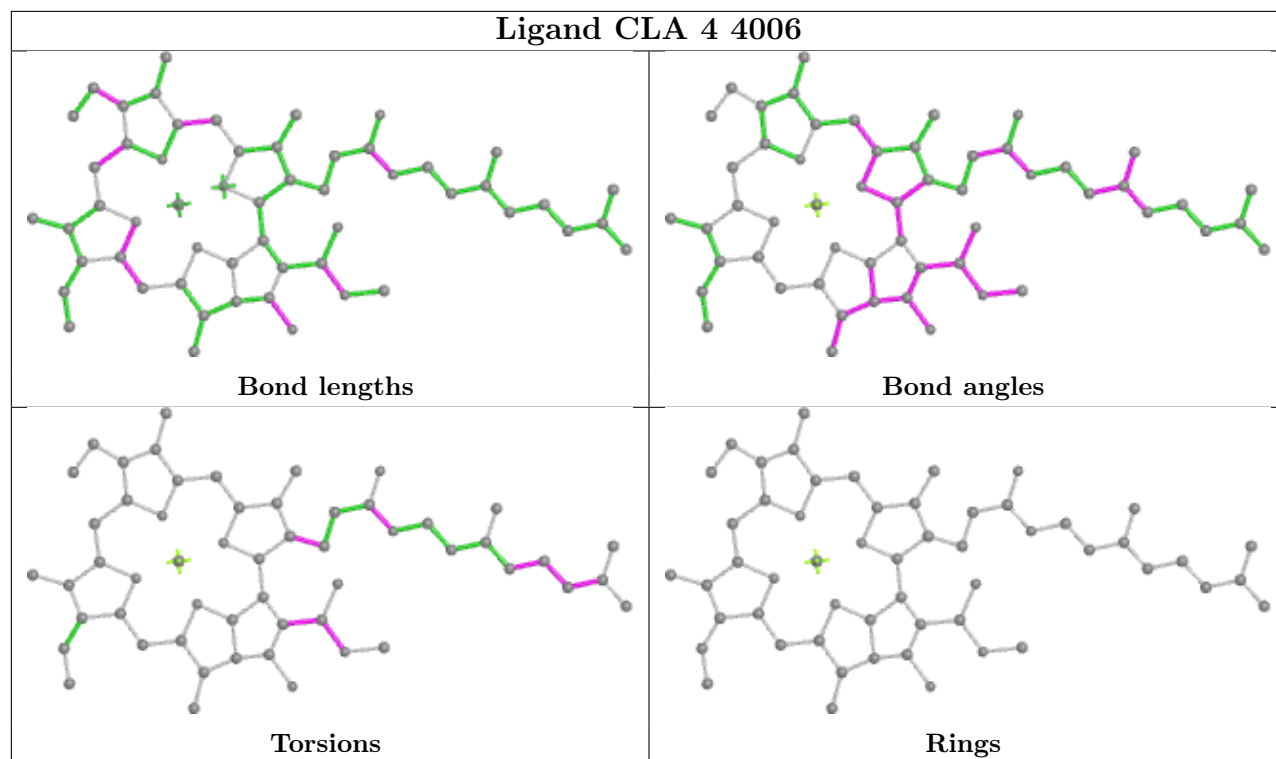
Bond angles



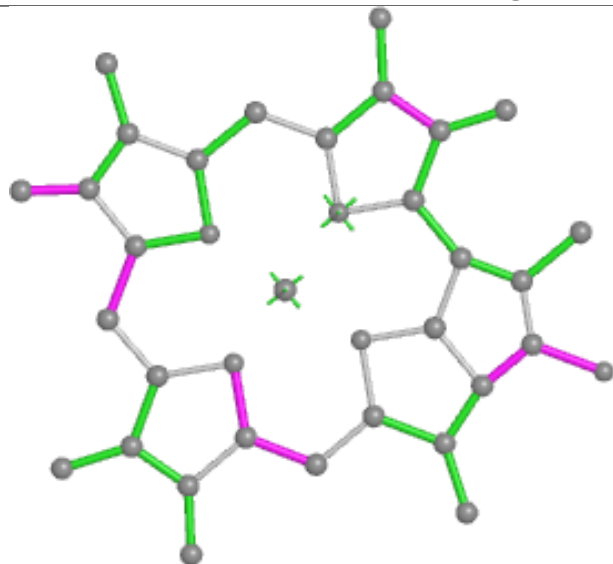
Torsions



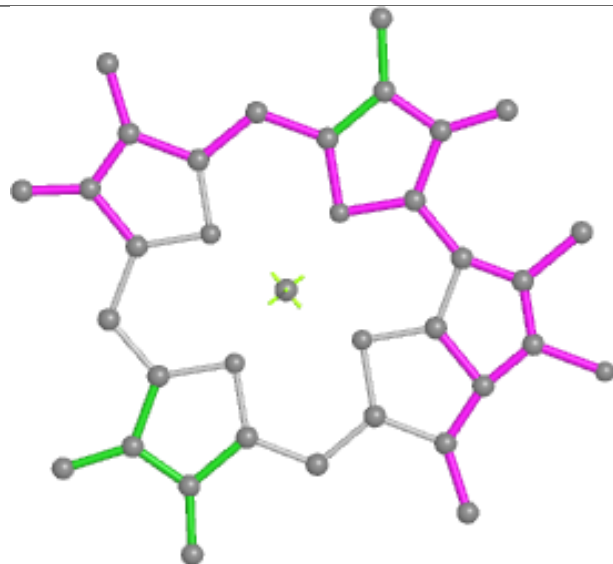
Rings



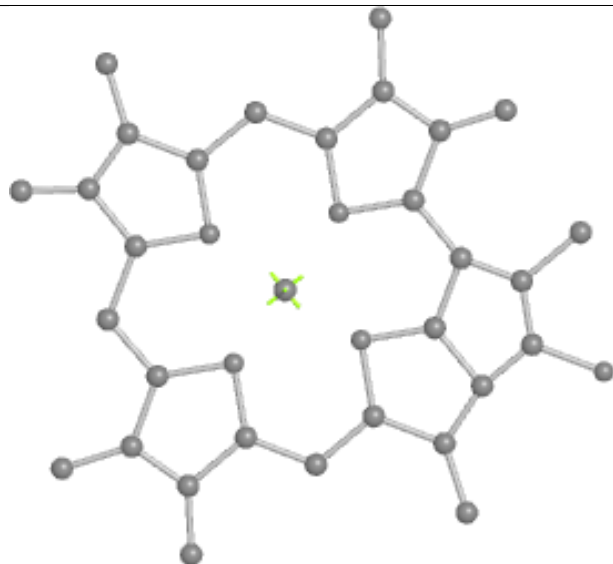
Ligand CLA F 1240



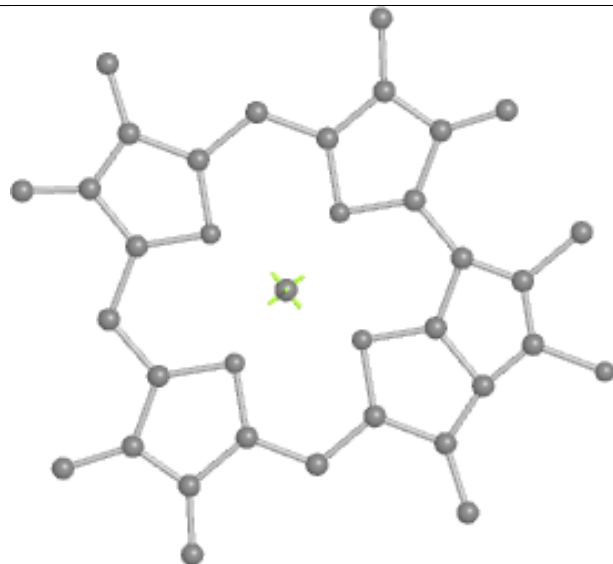
Bond lengths



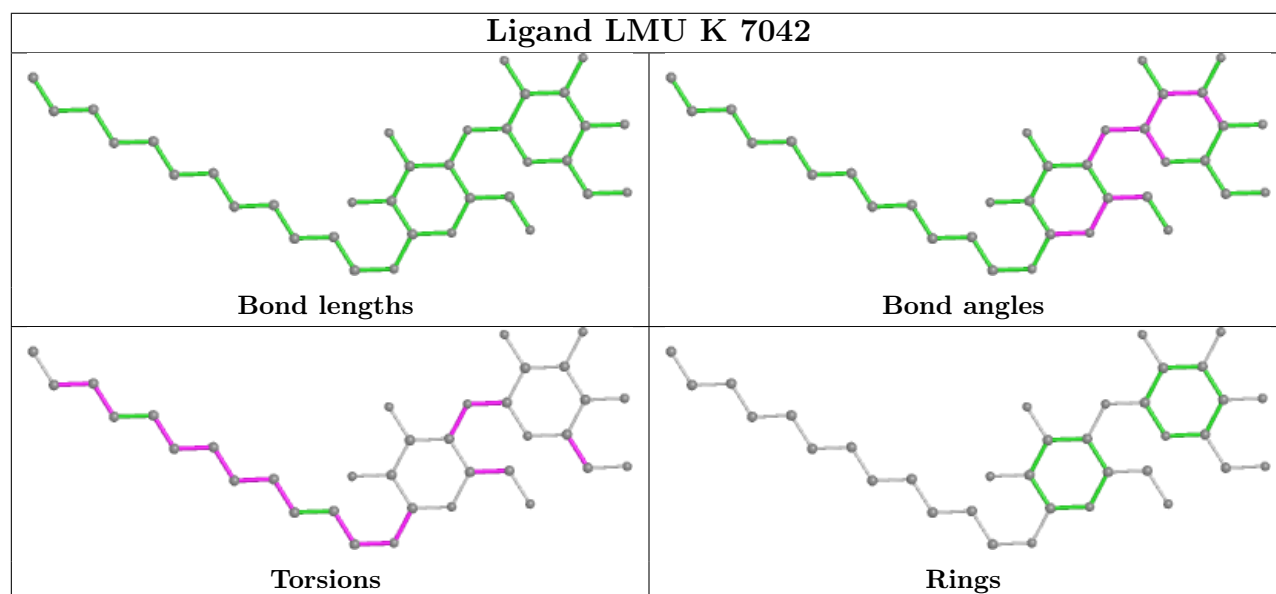
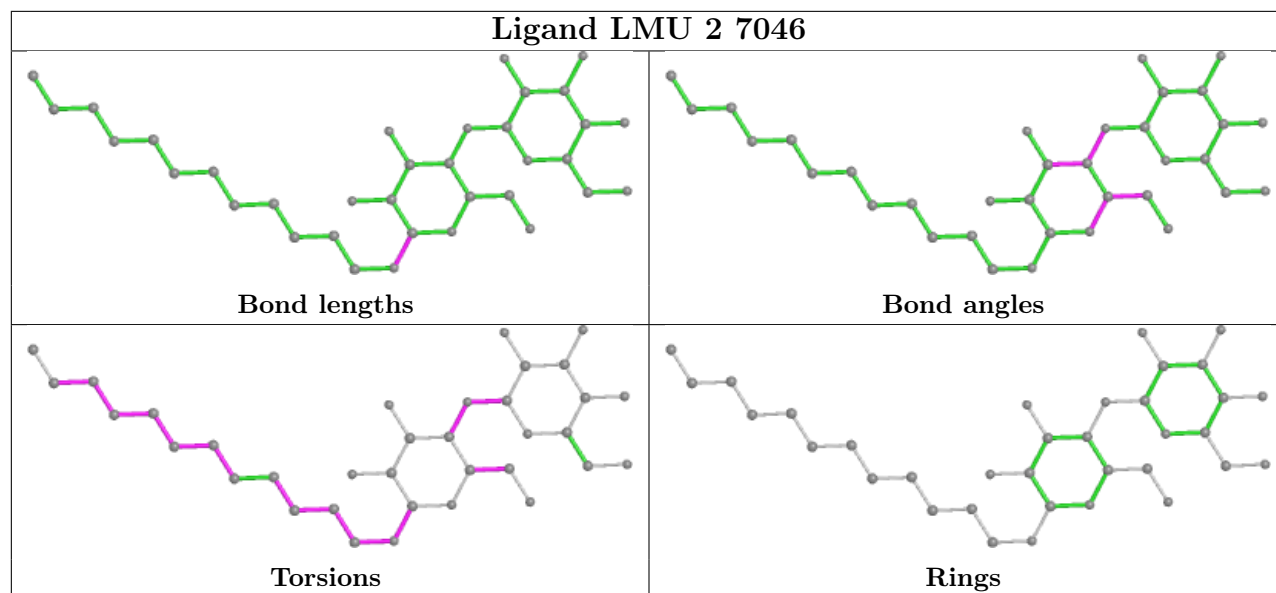
Bond angles



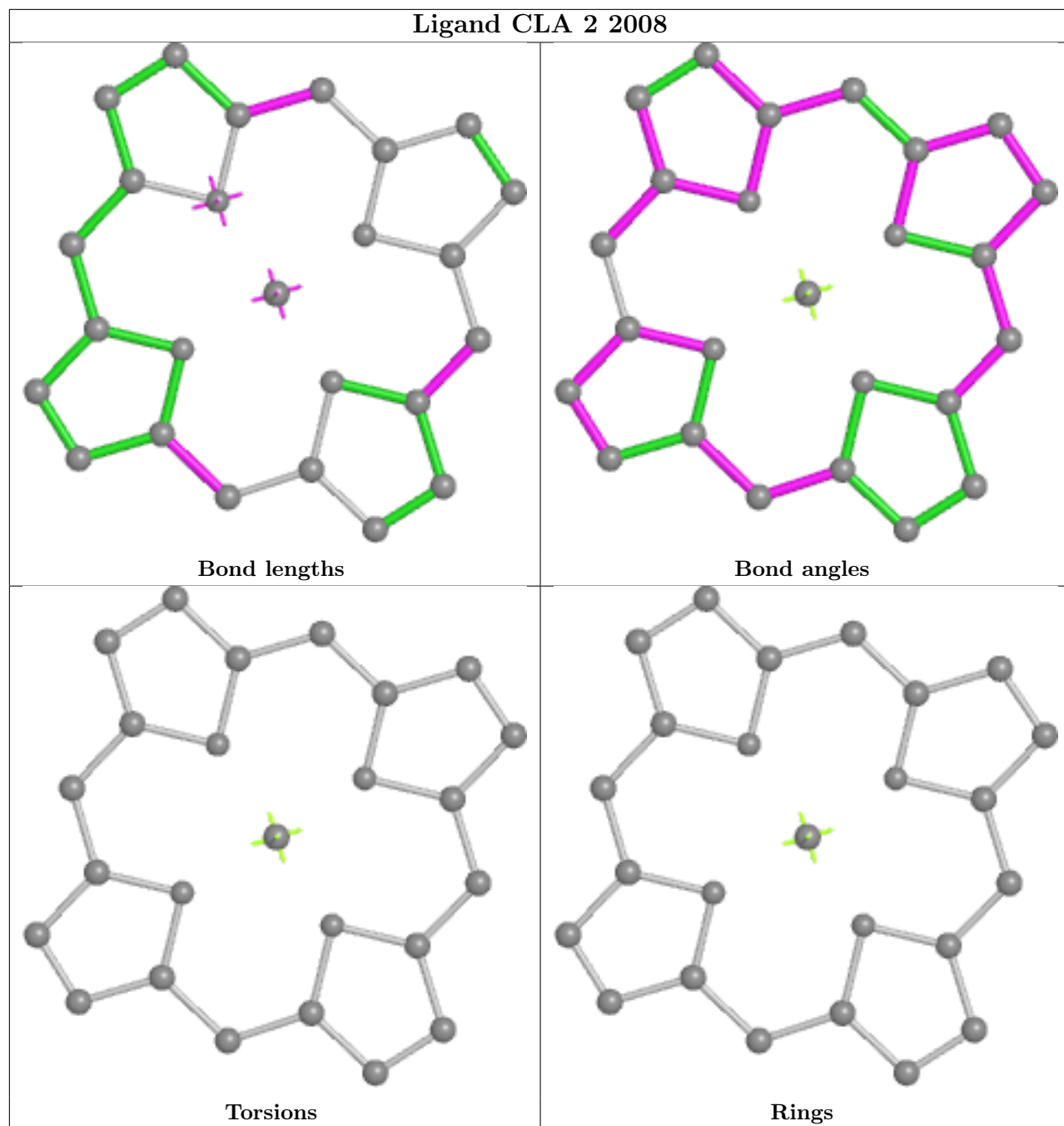
Torsions

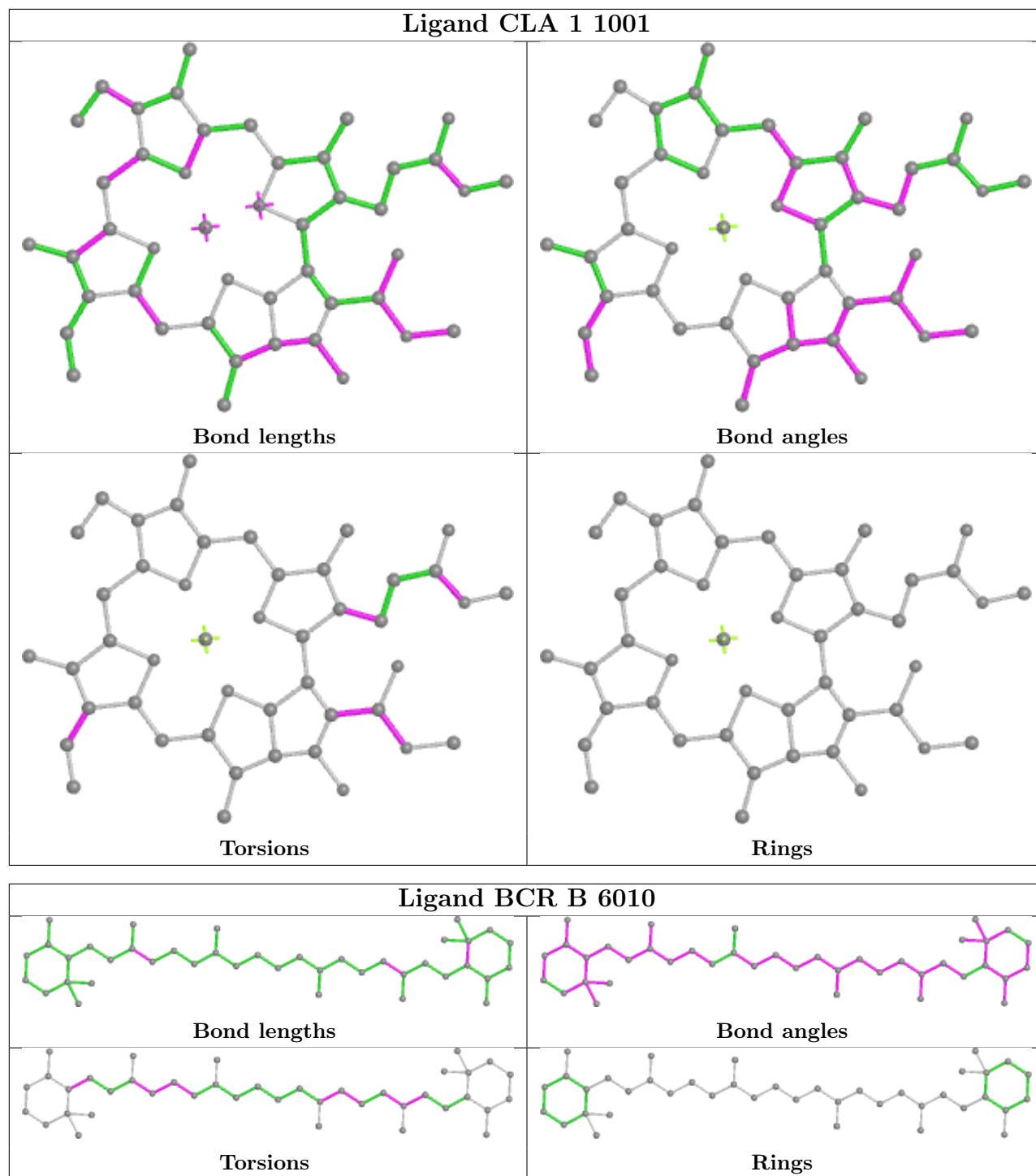


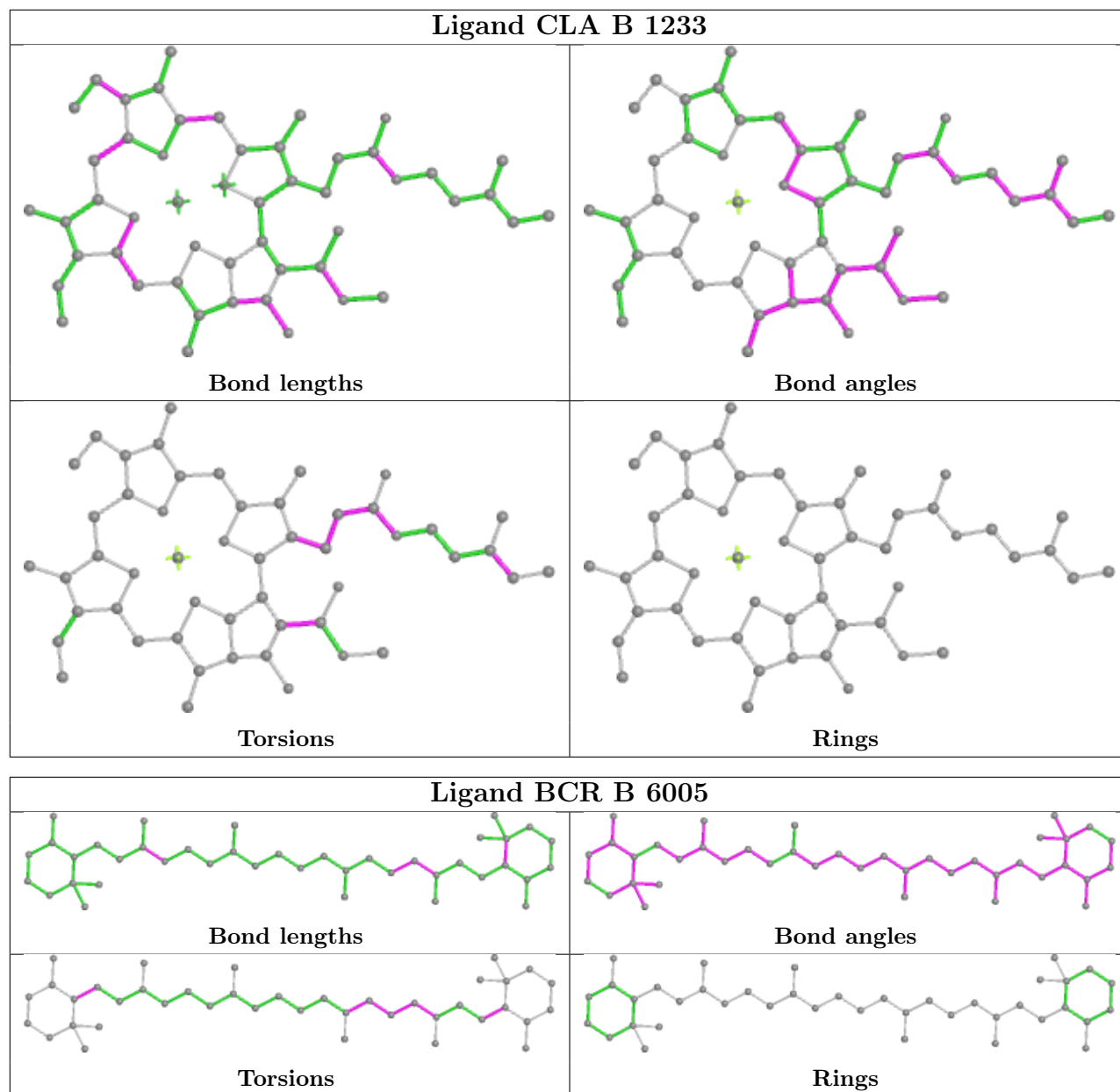
Rings

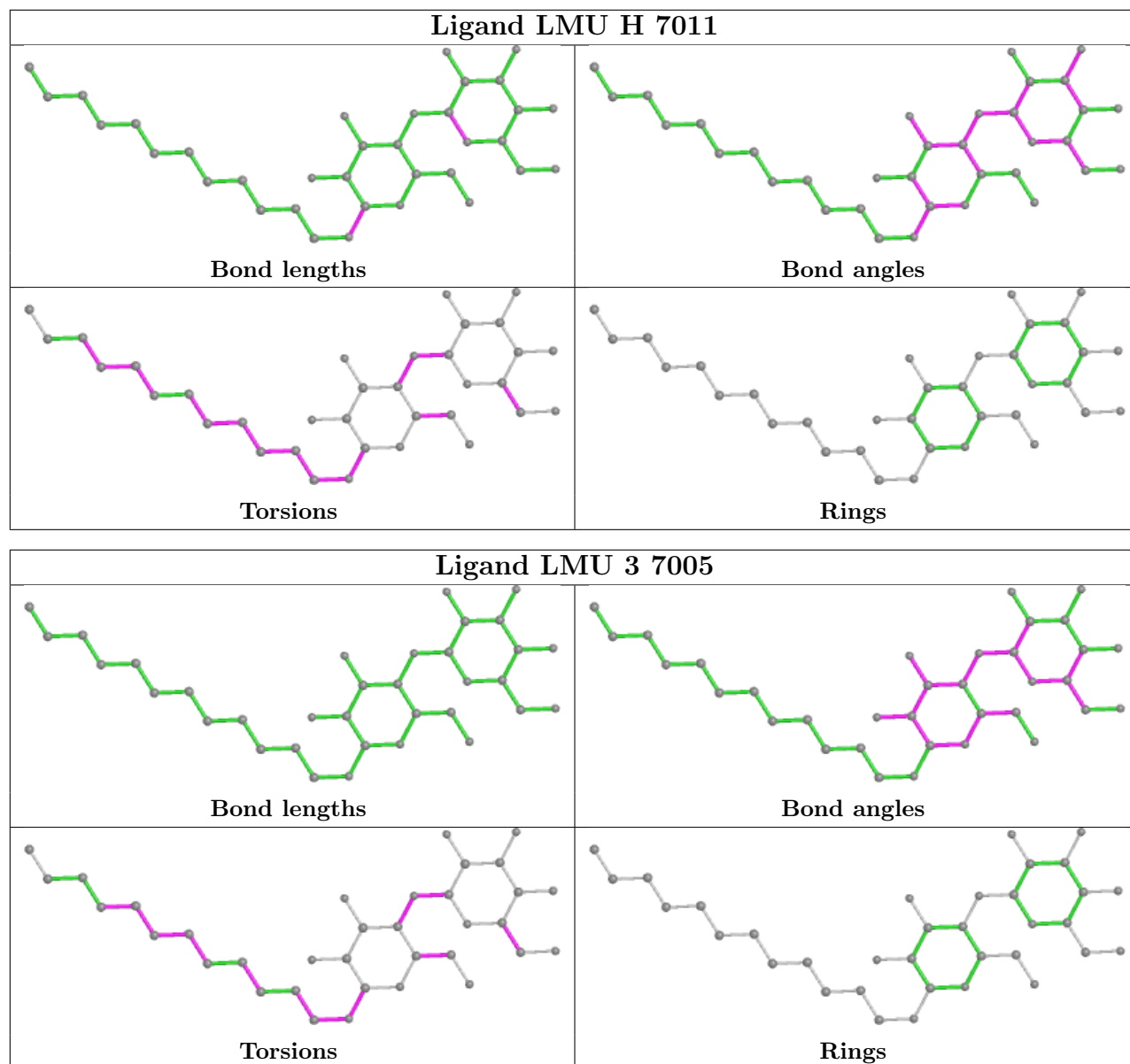


Ligand CLA 2 2008

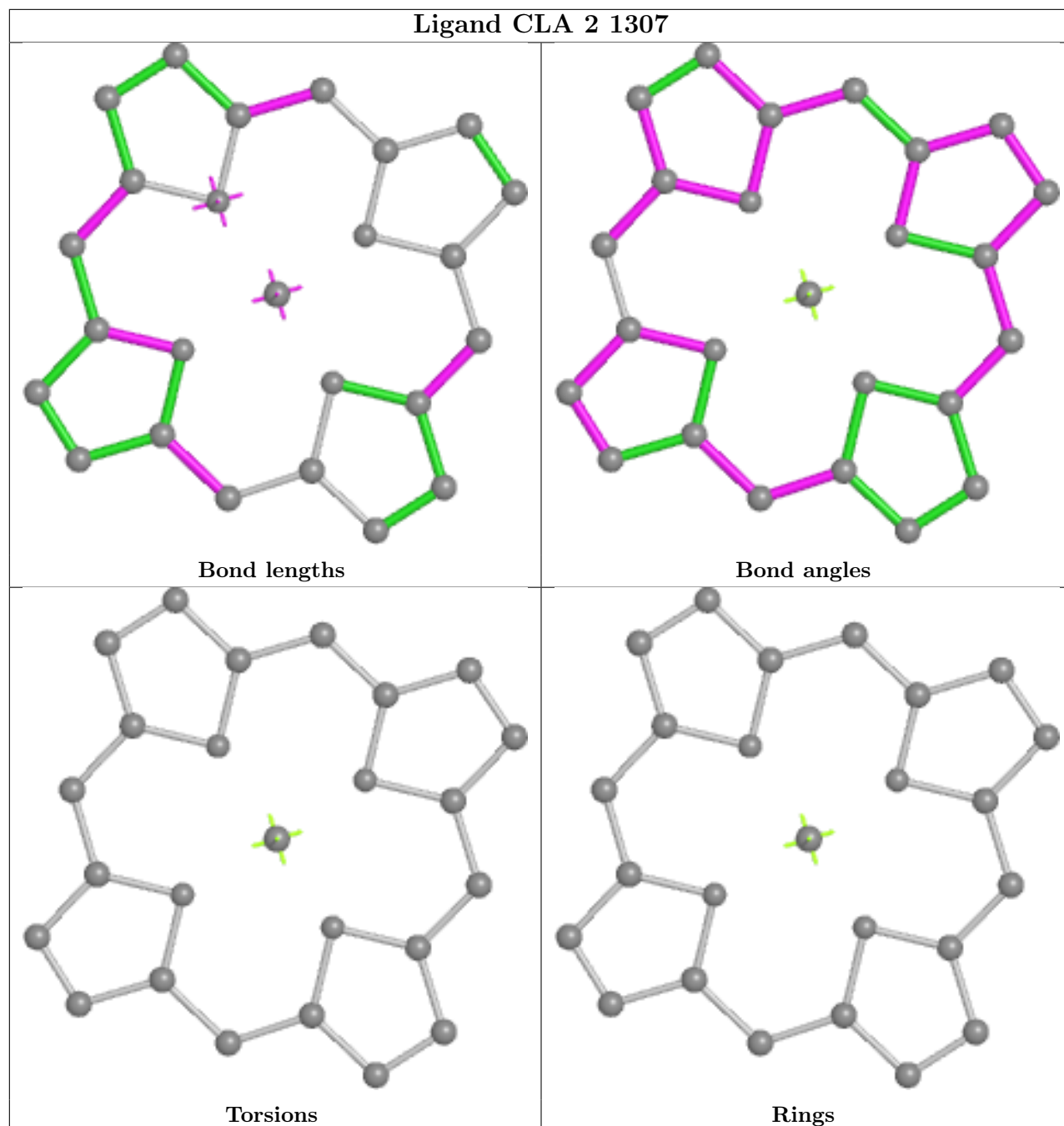




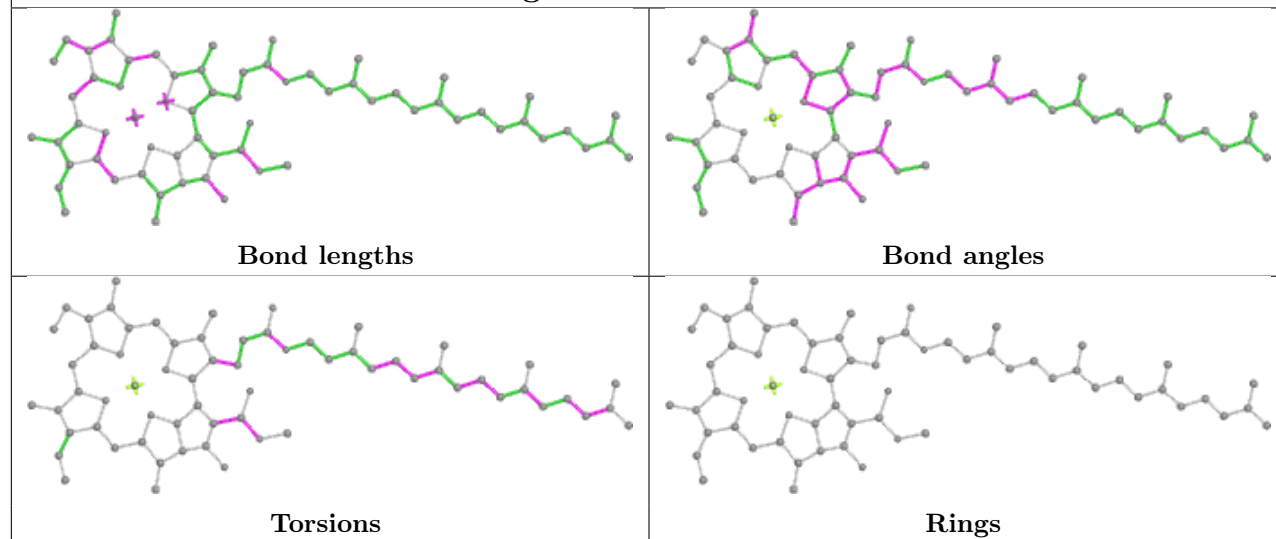




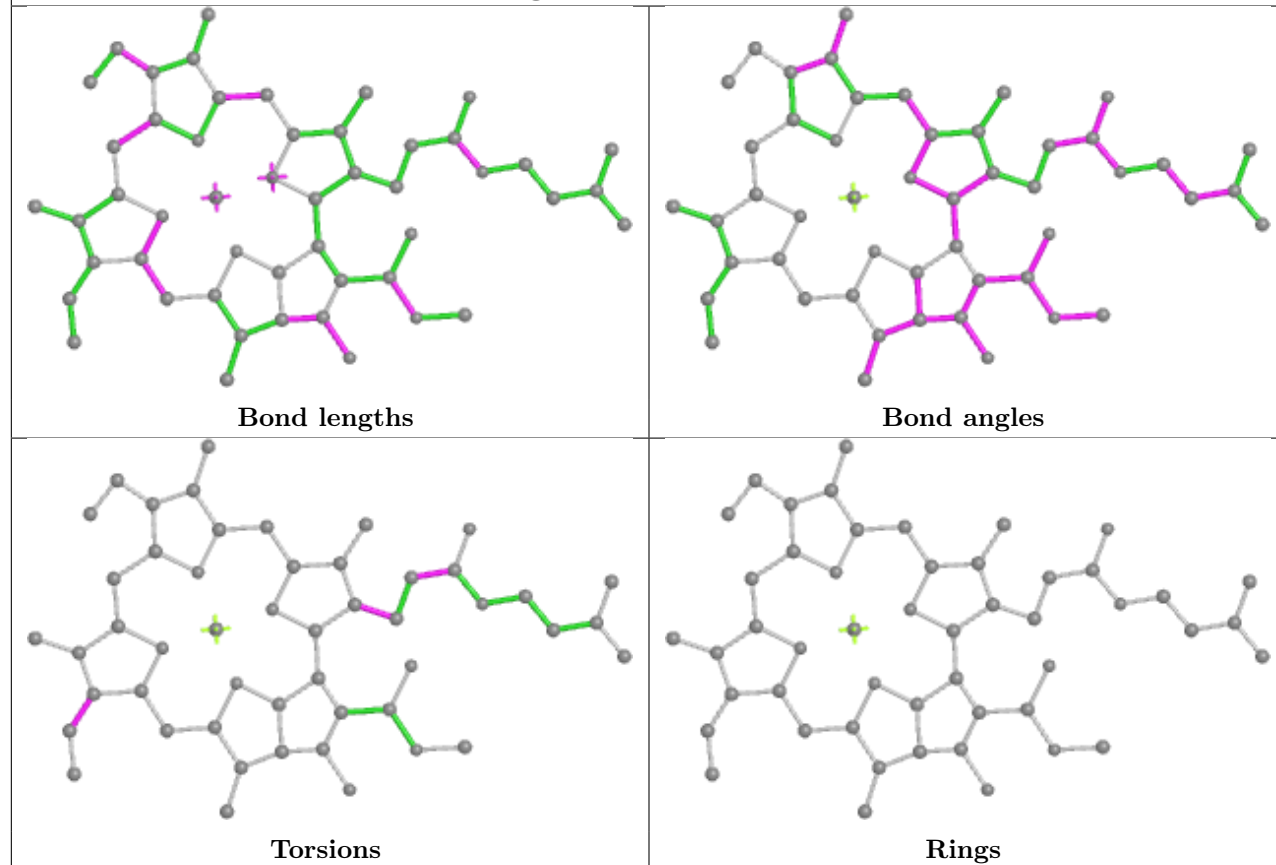
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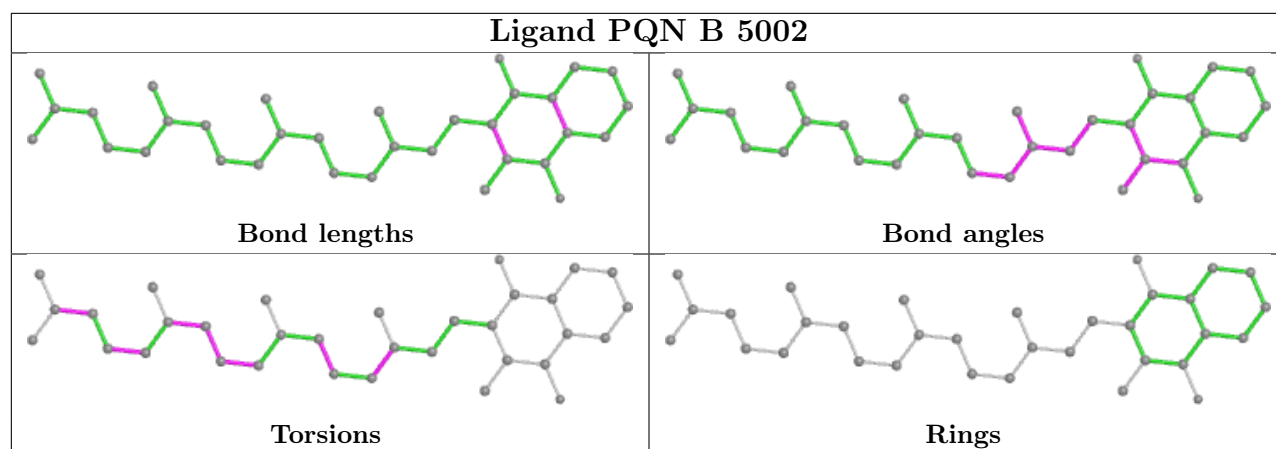
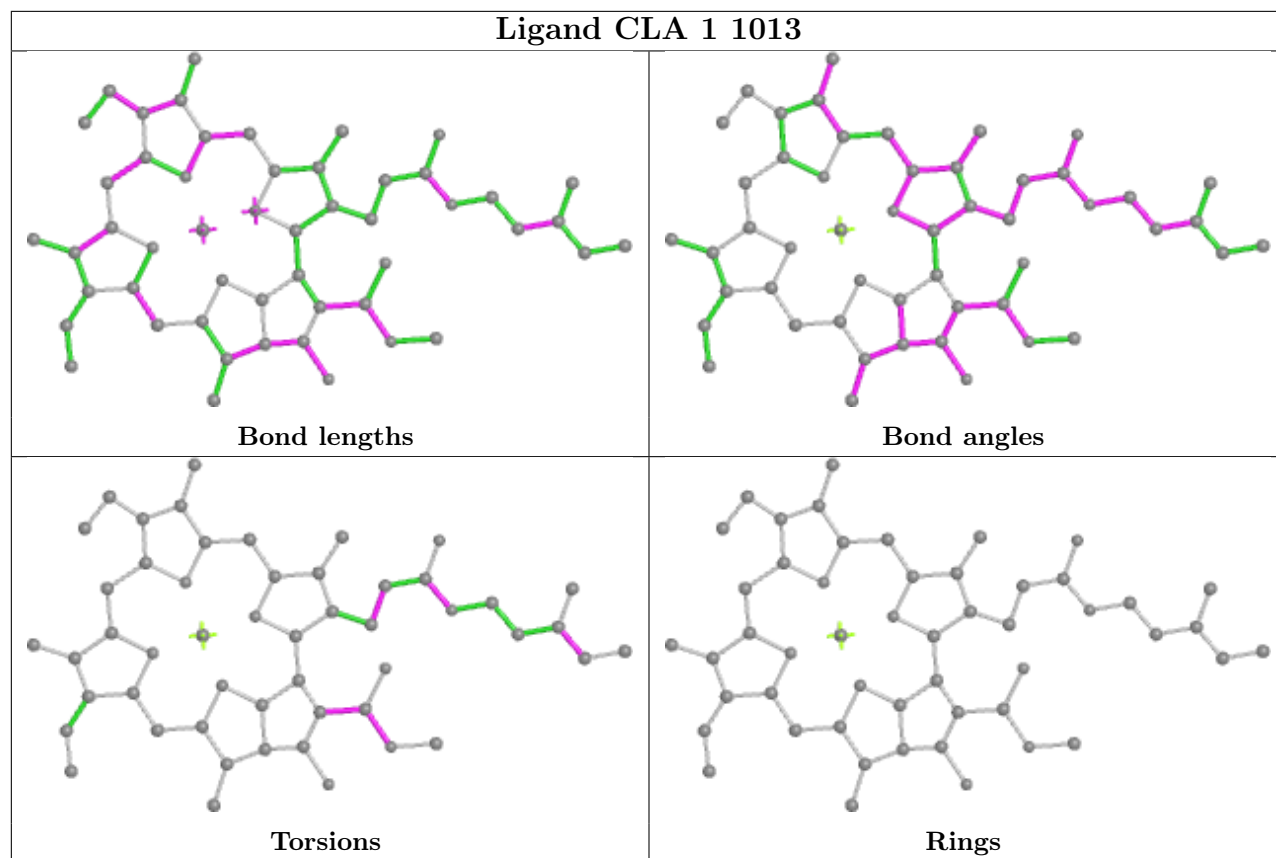


Ligand CLA A 1117

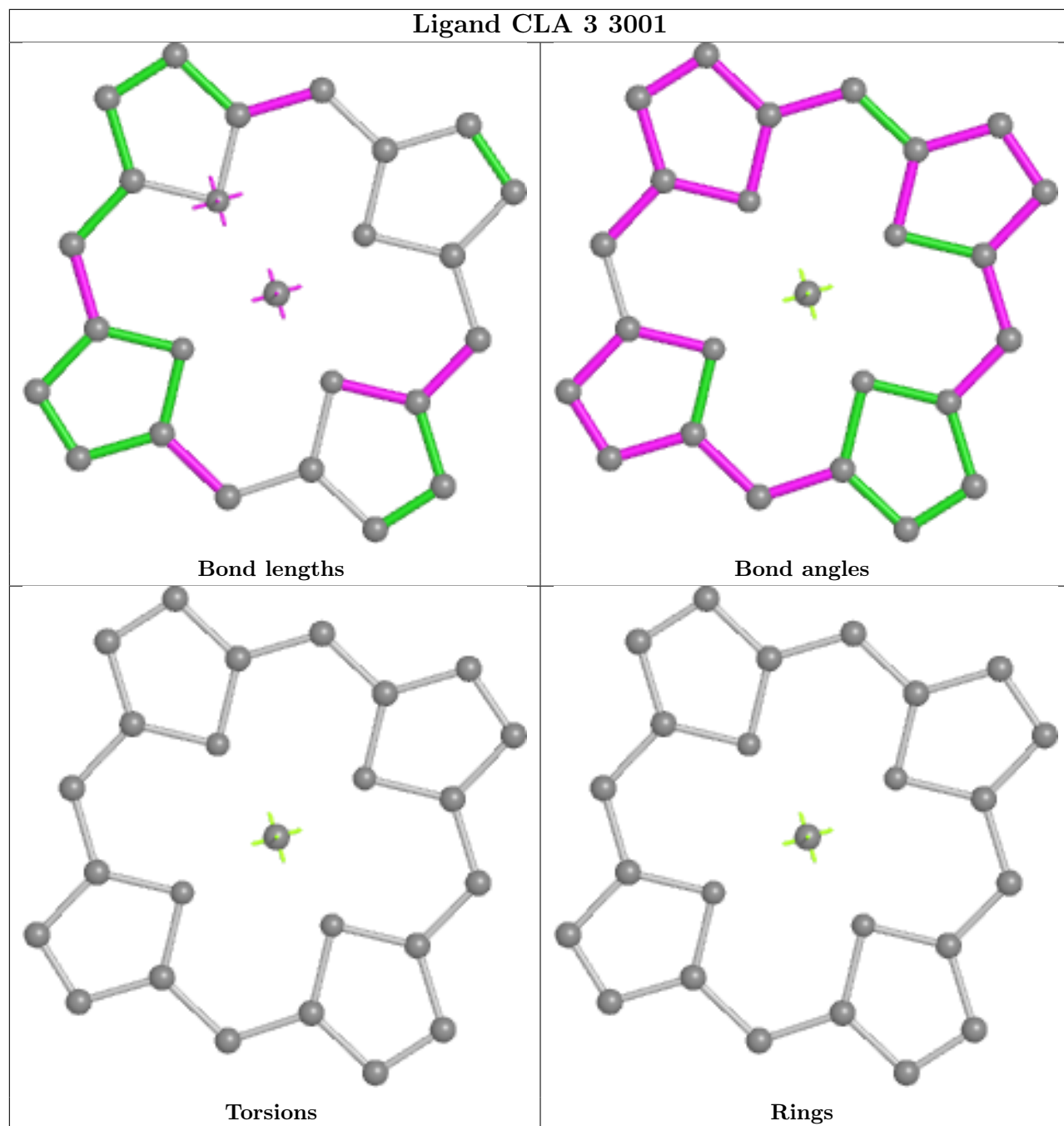


Ligand CLA 3 3008

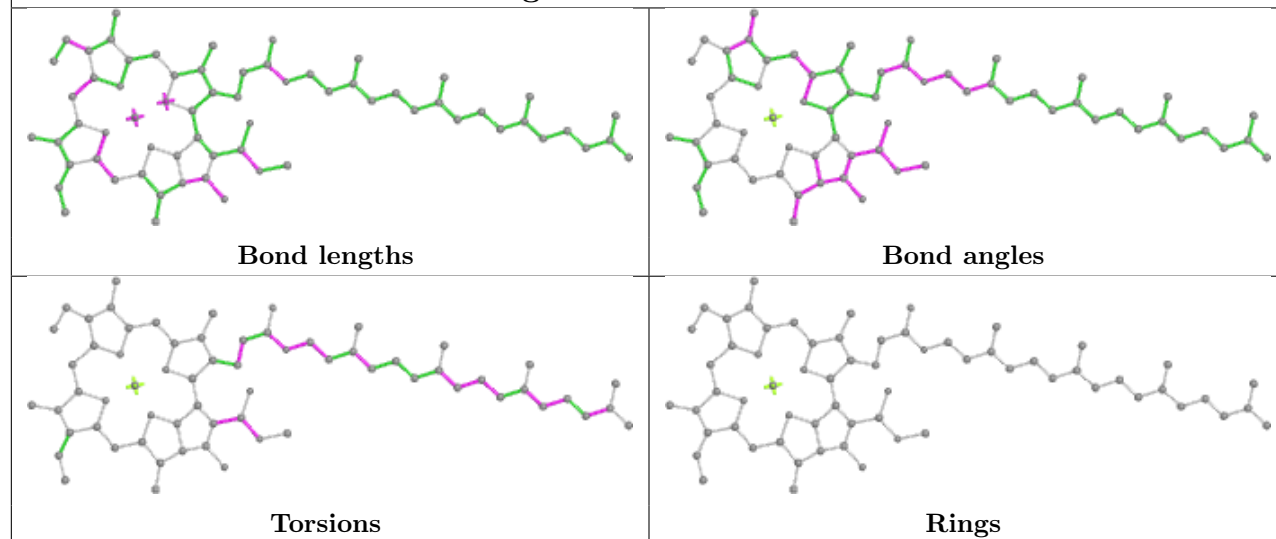




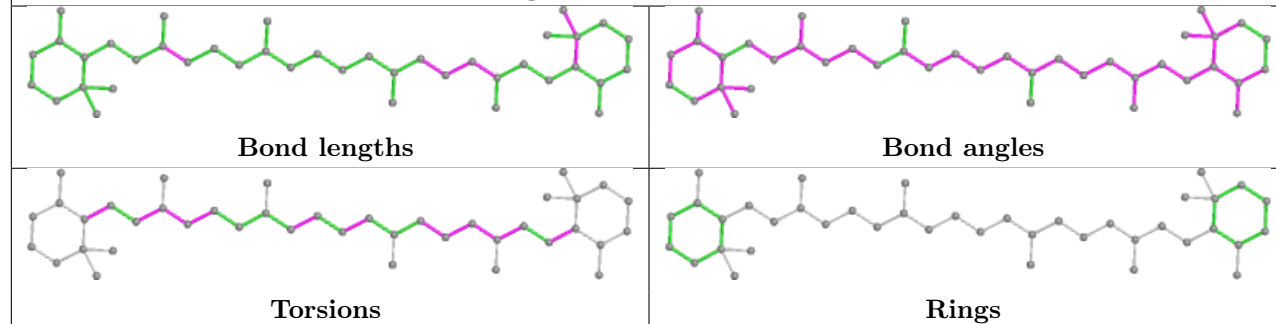
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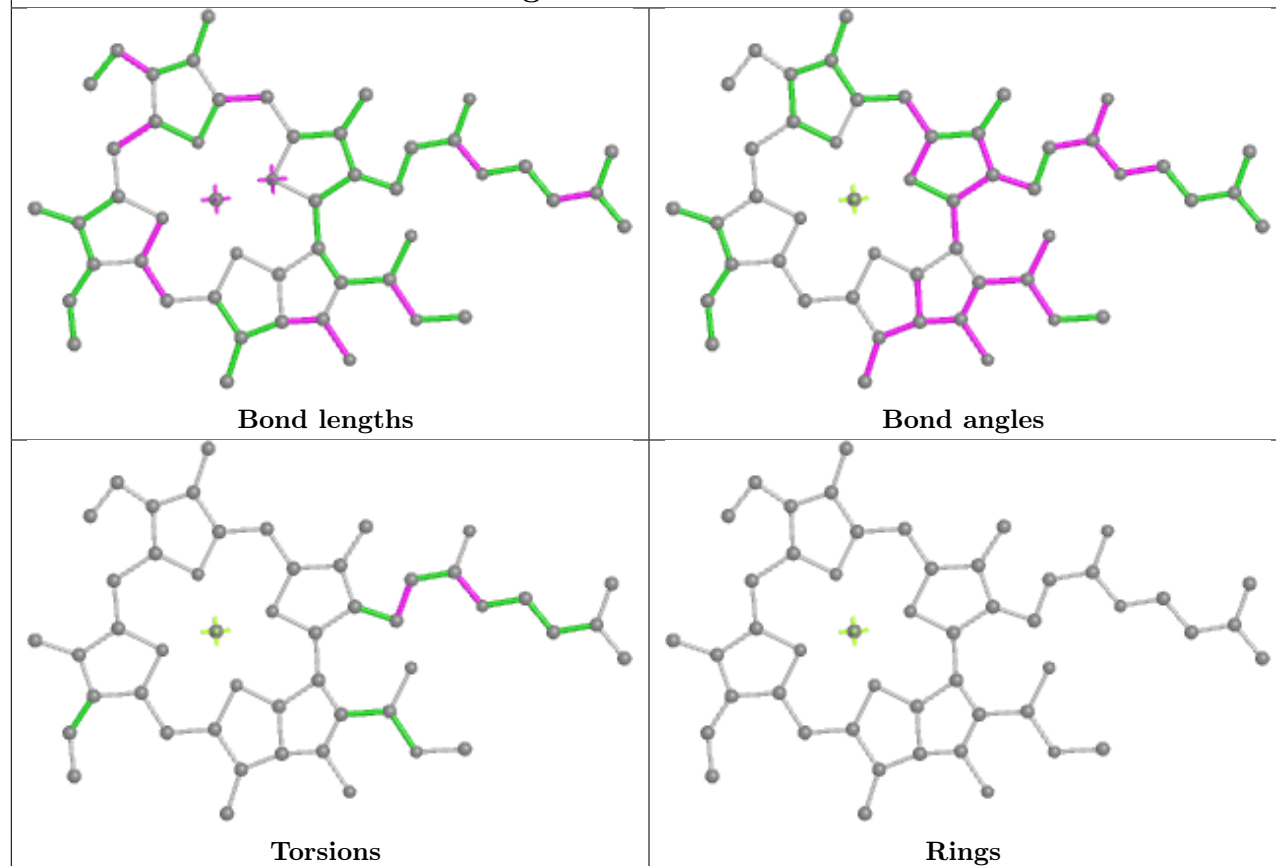
Ligand CLA H 1207



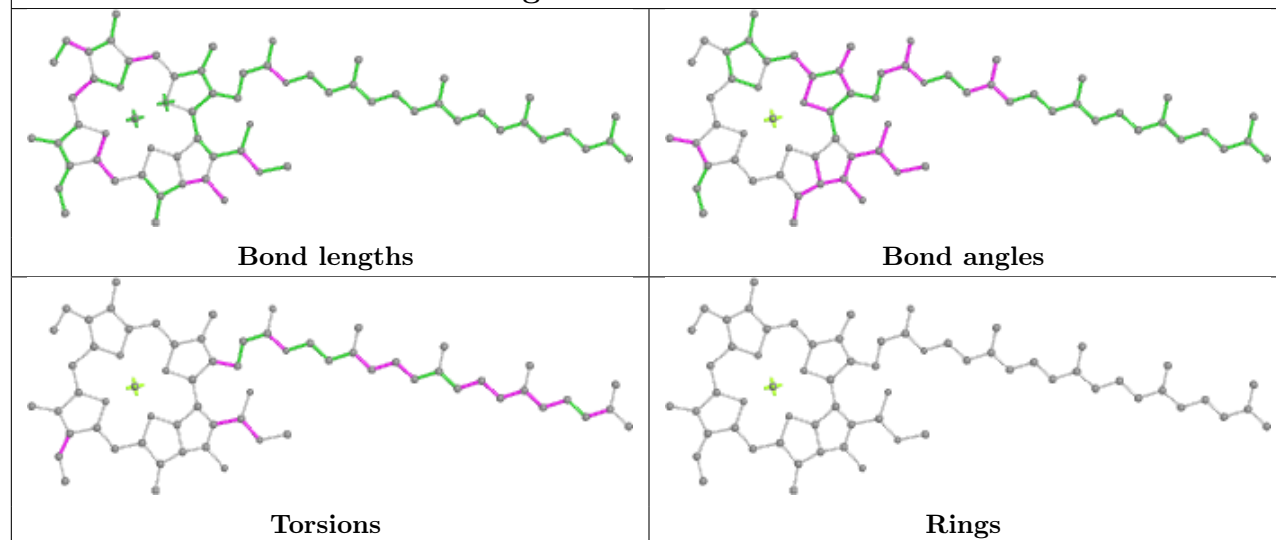
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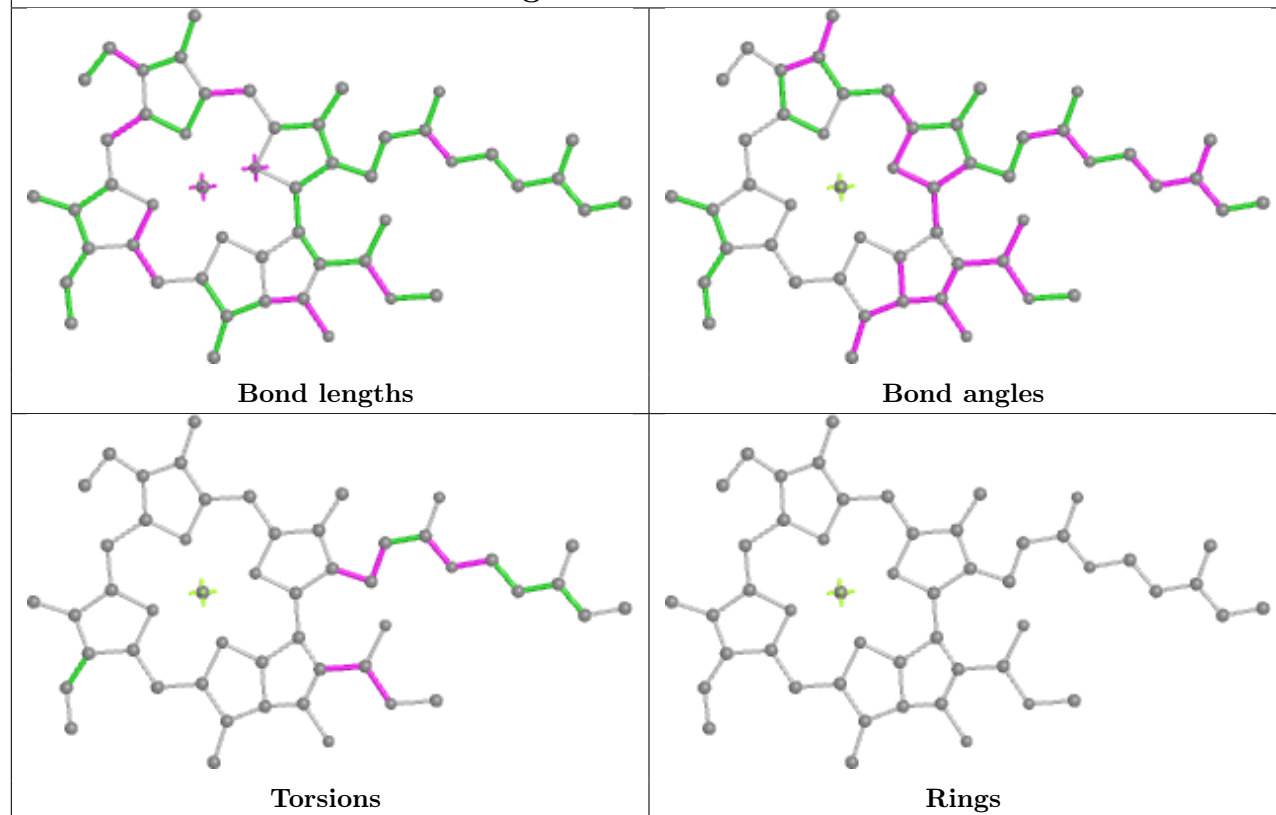
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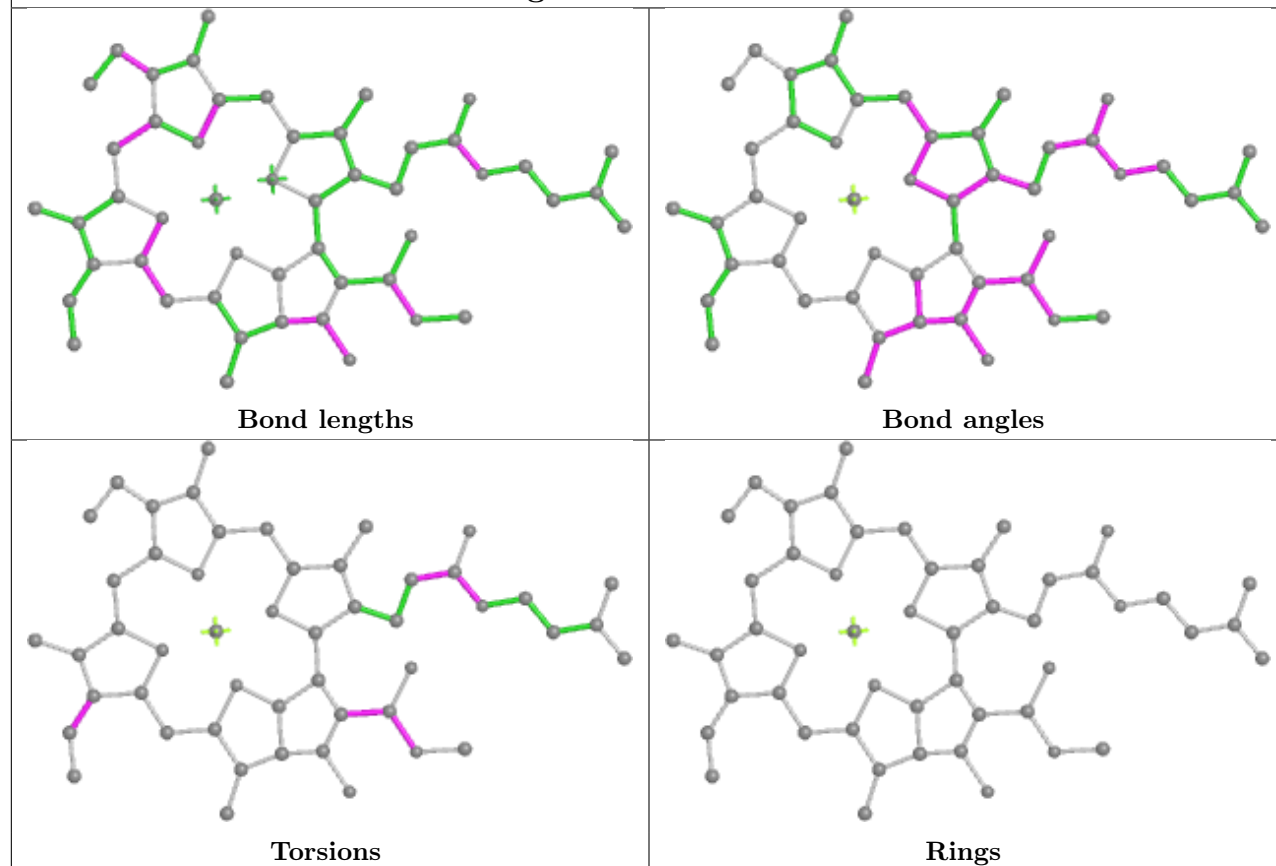
Ligand CLA A 1132

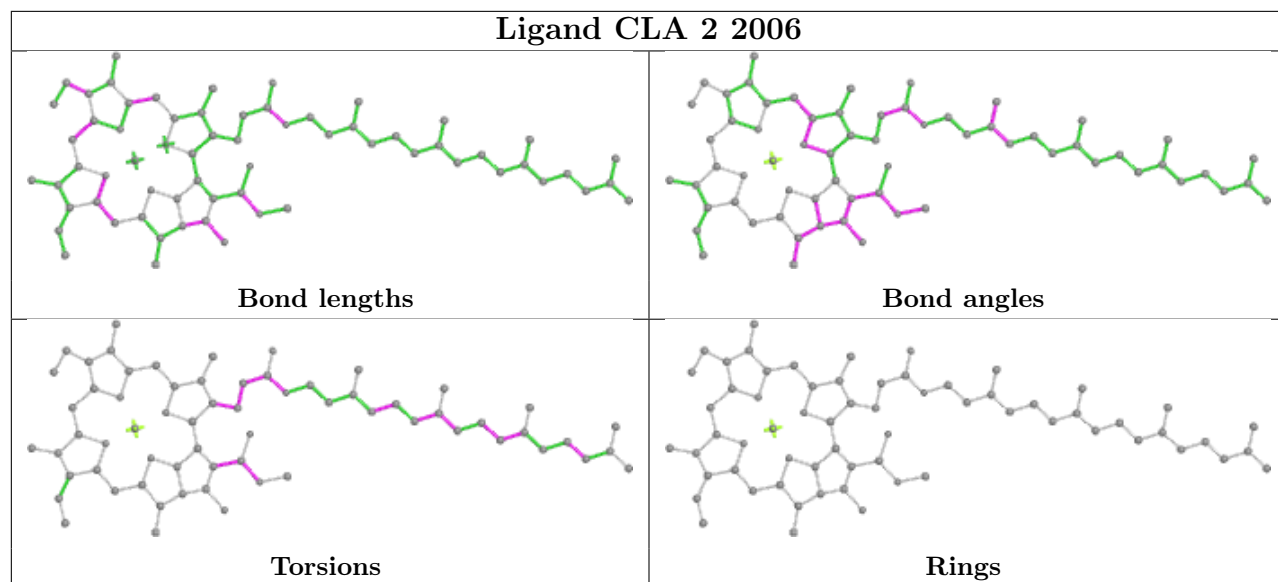


Ligand CLA A 1135

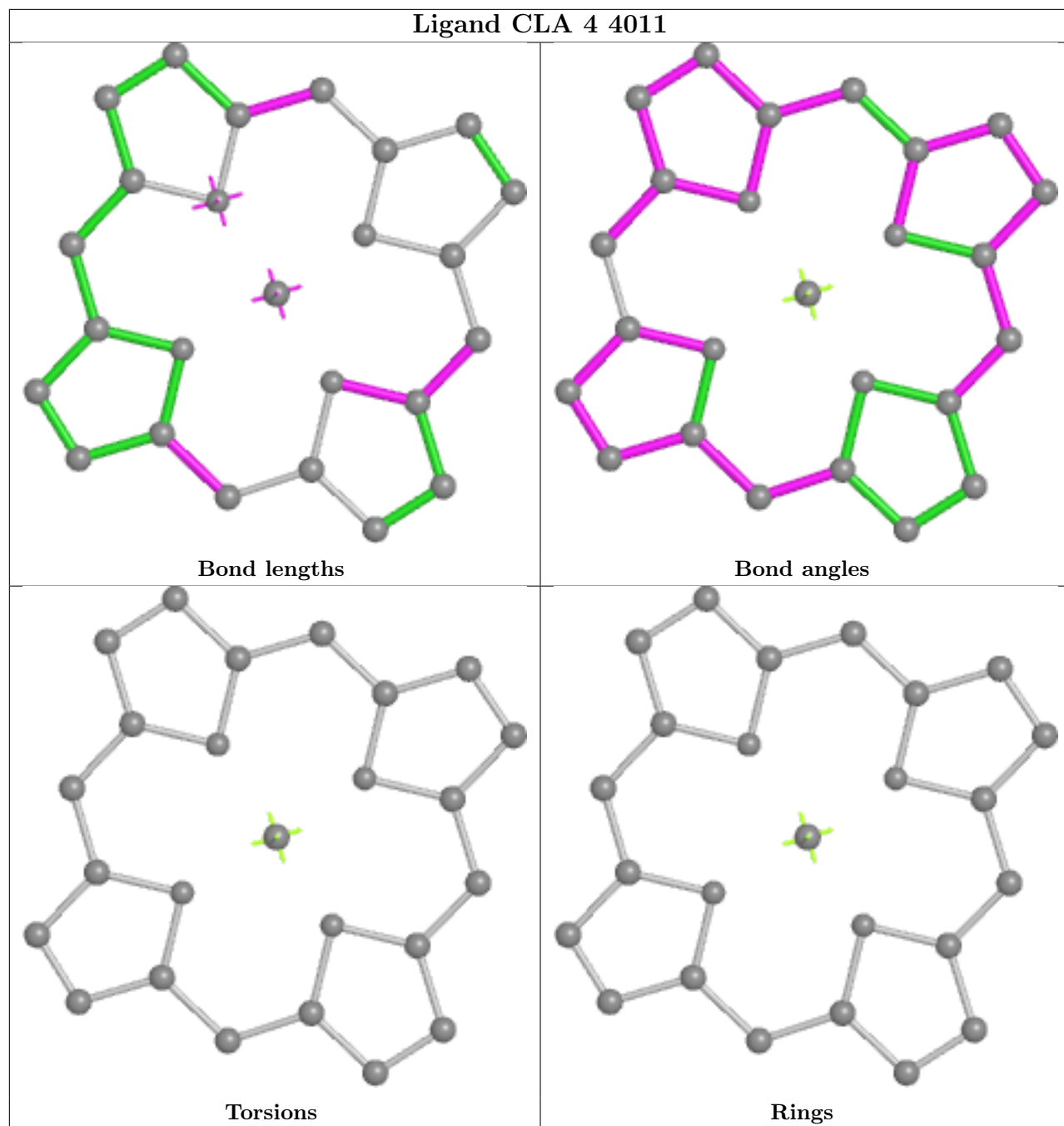


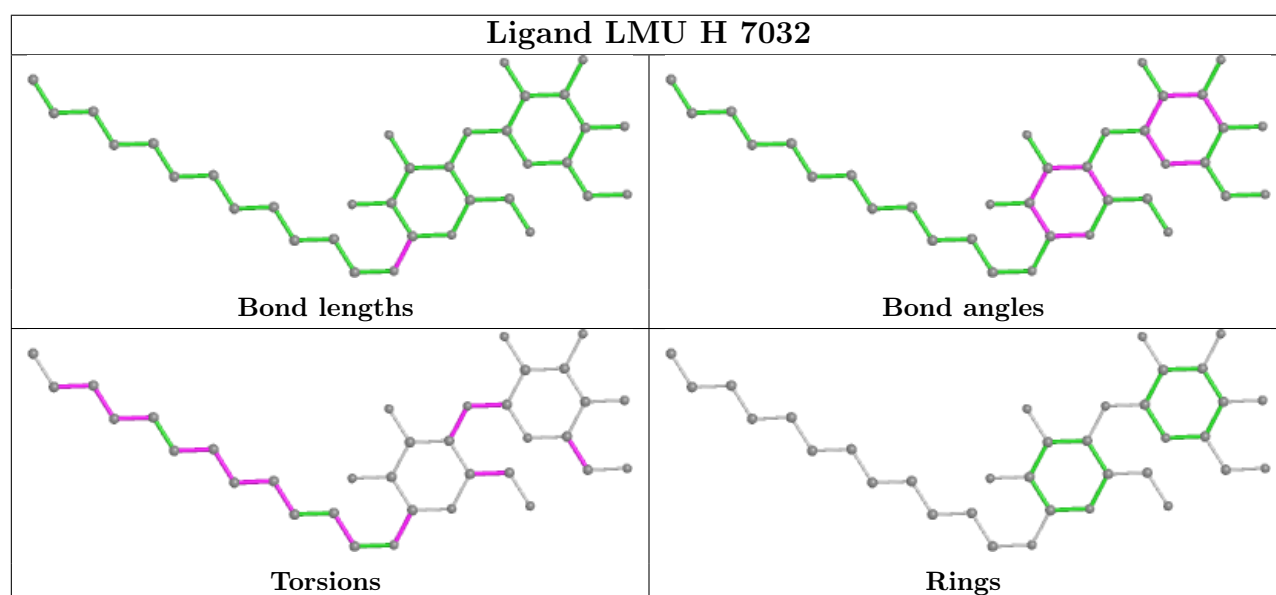
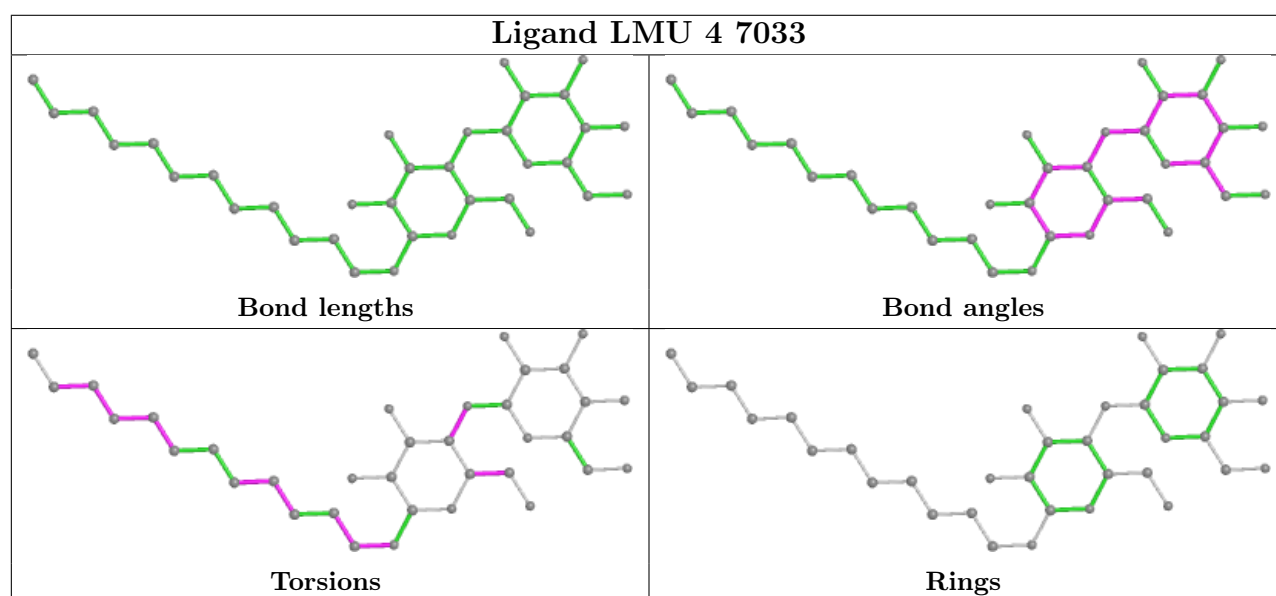
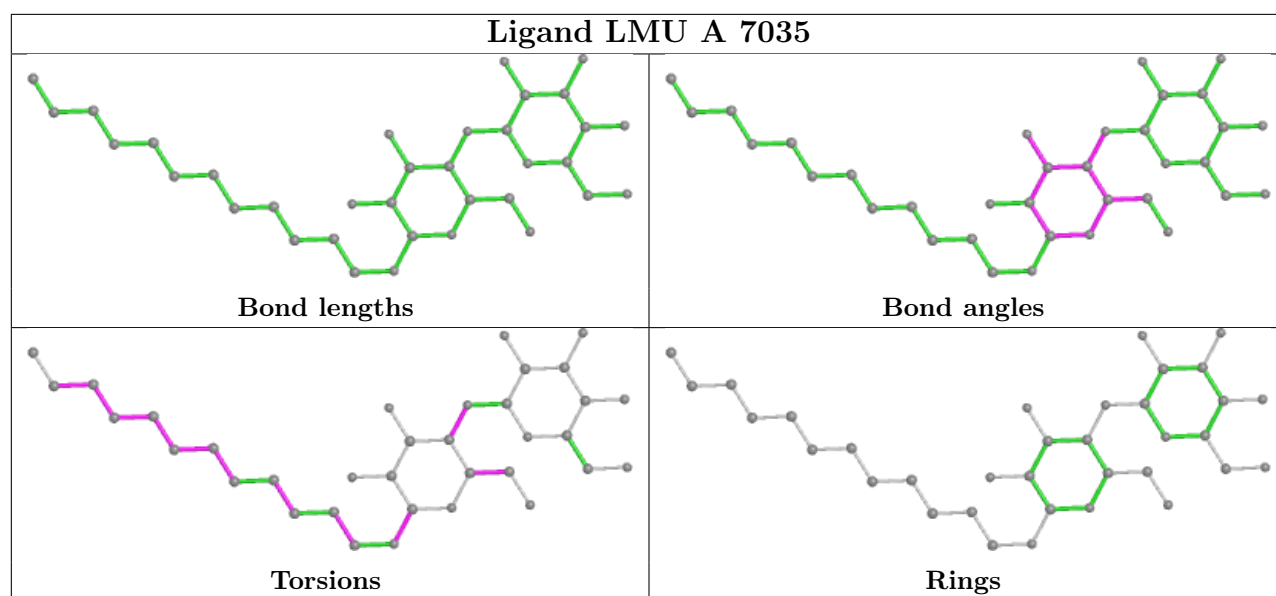
Ligand CLA 2 2013



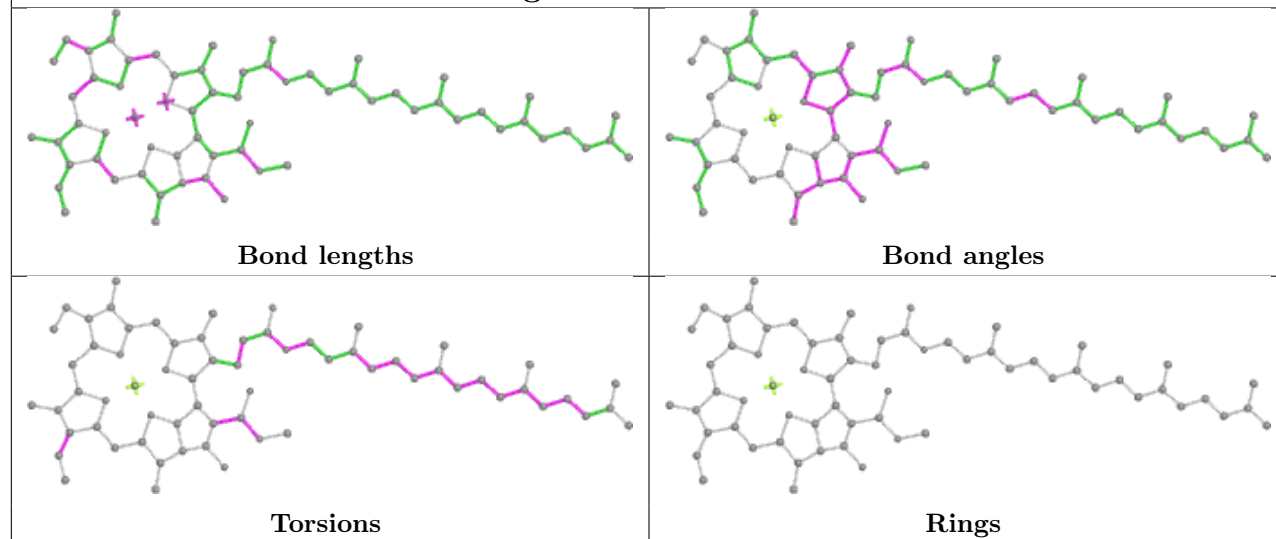


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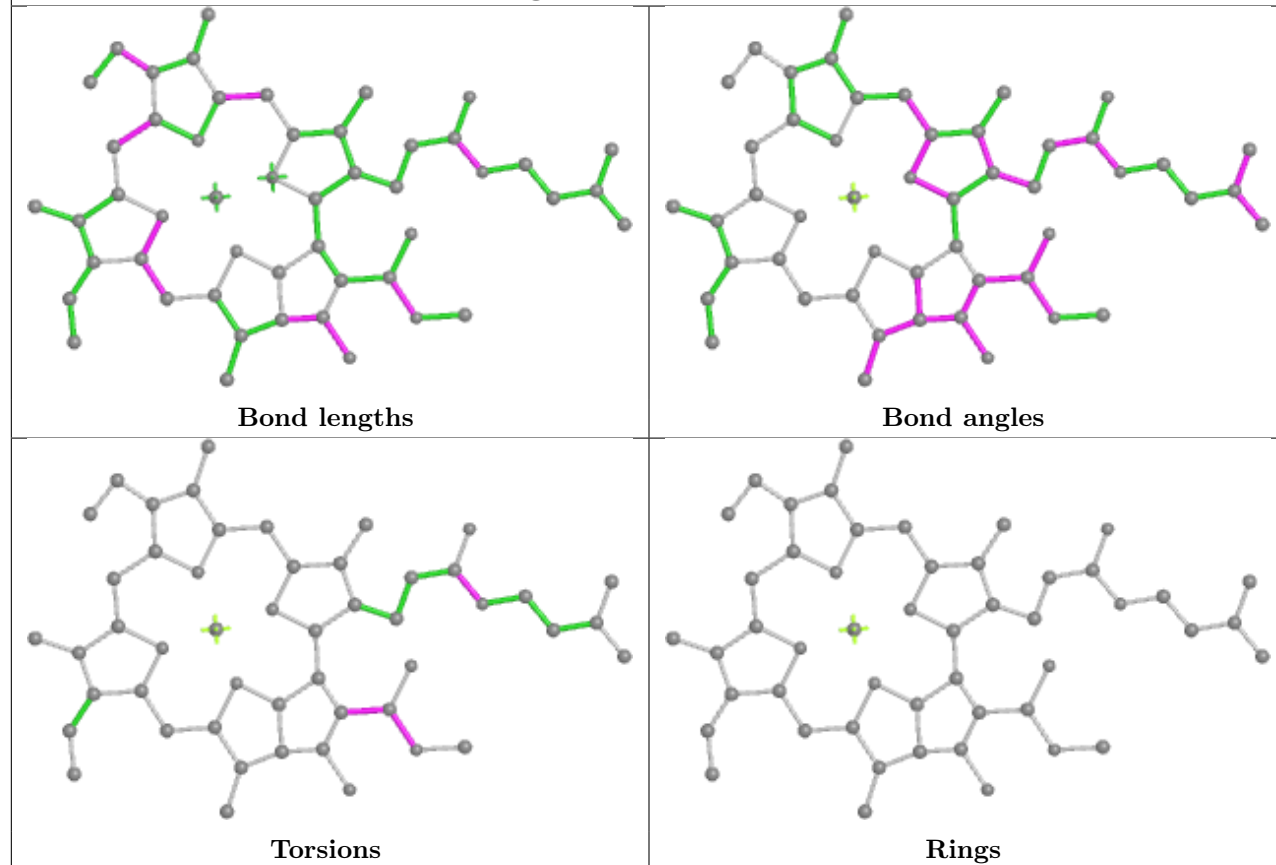


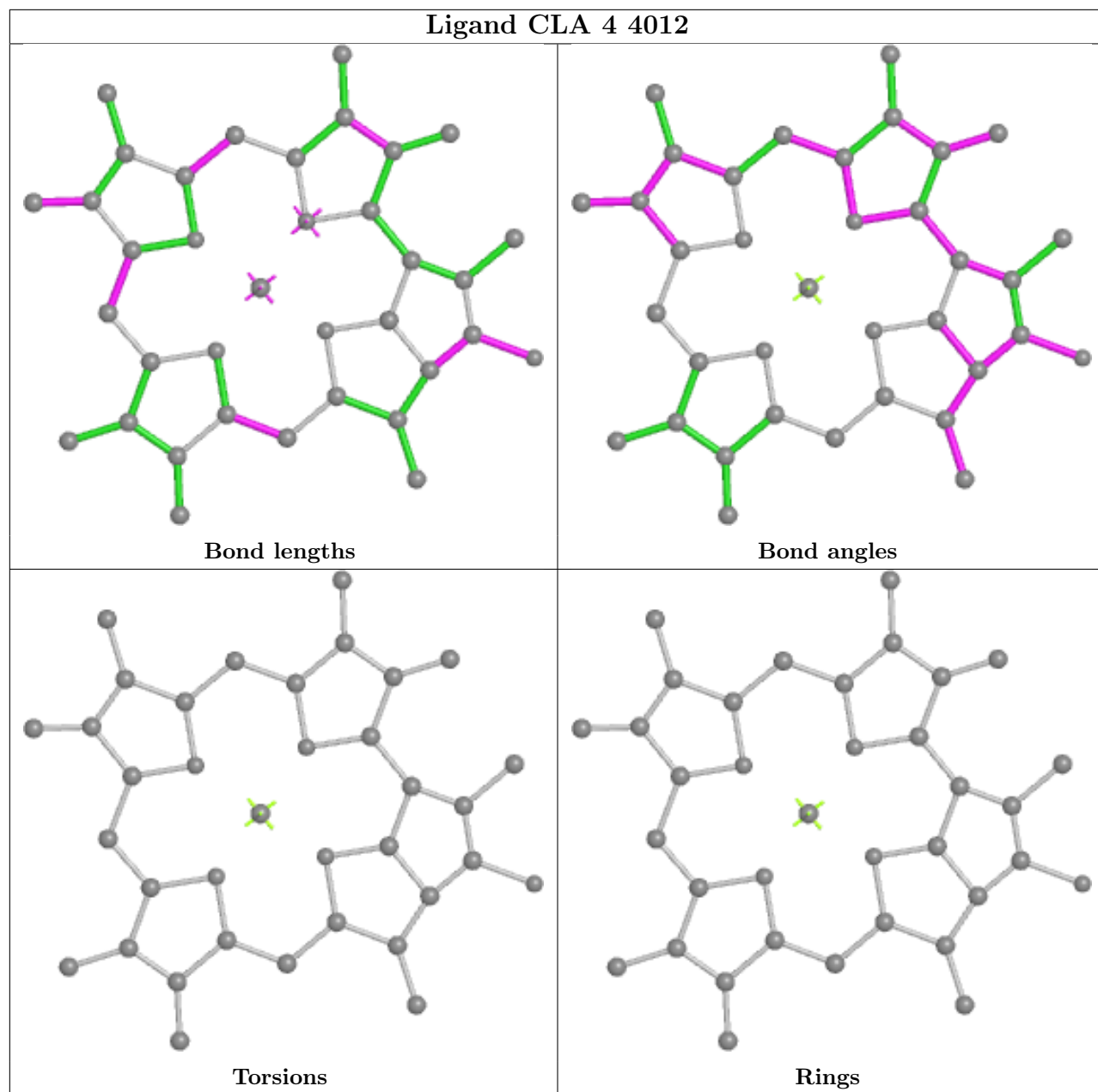


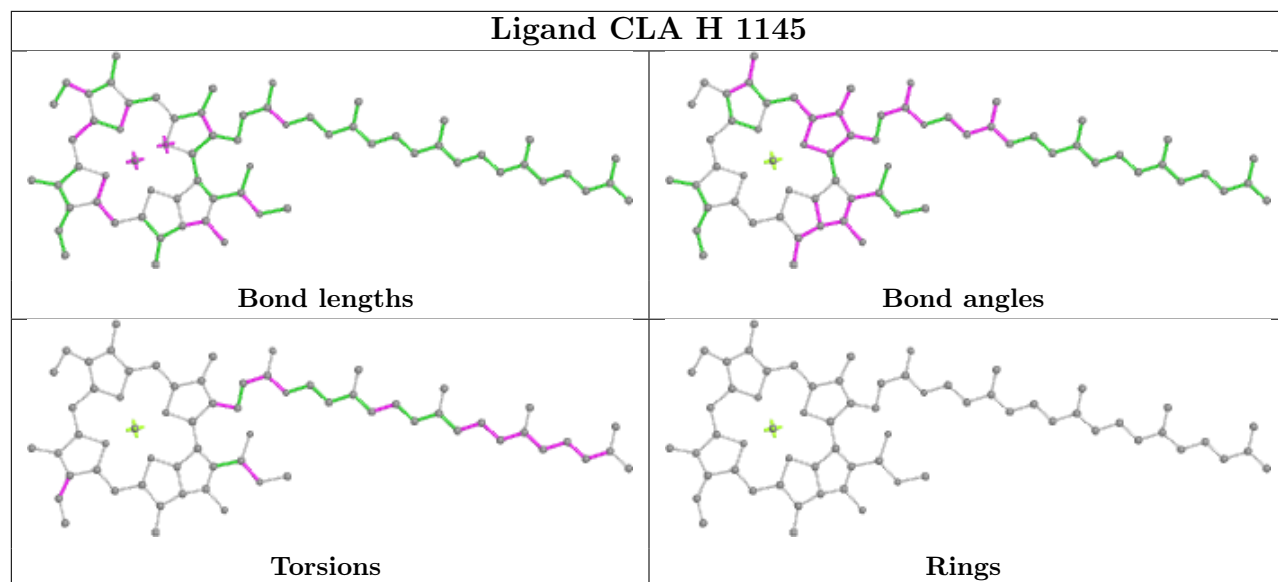
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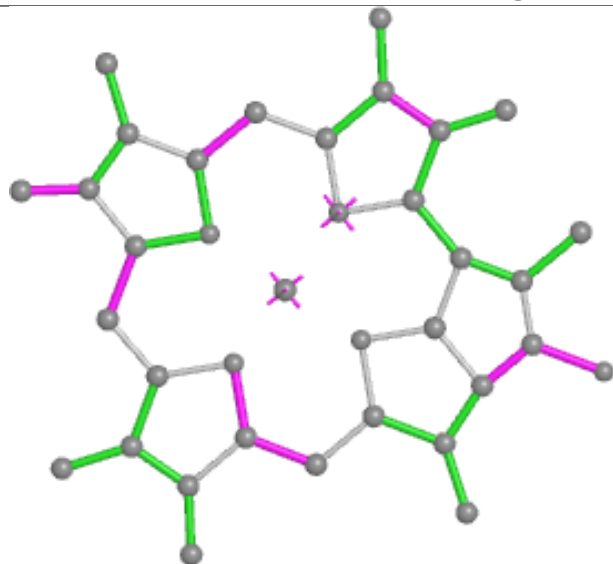
Ligand CLA 2 2012



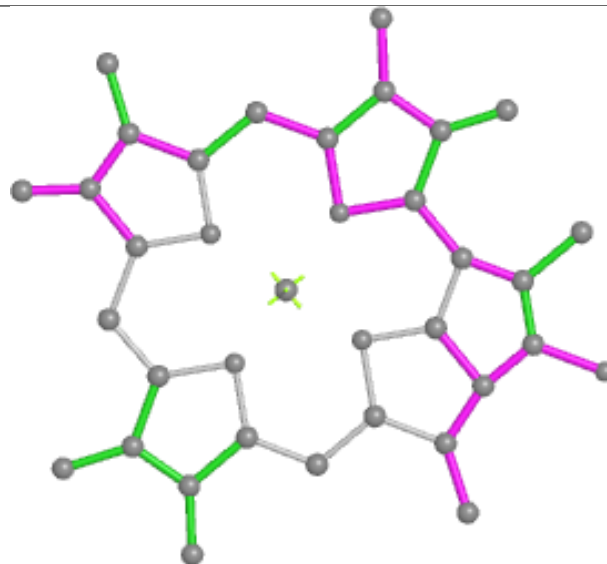




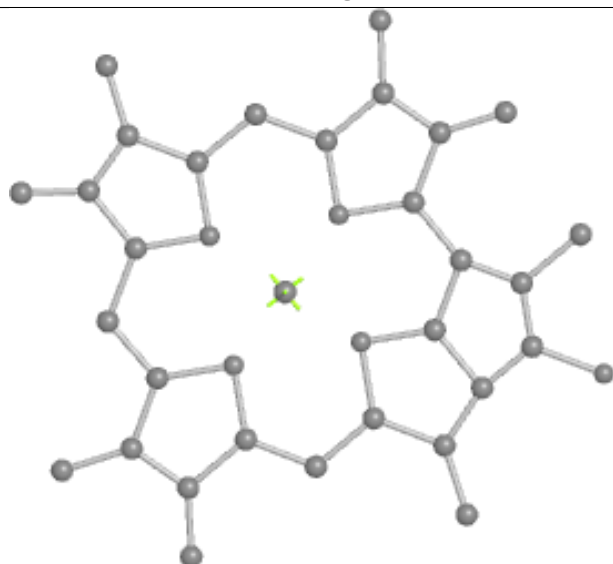
Ligand CLA 1 1006



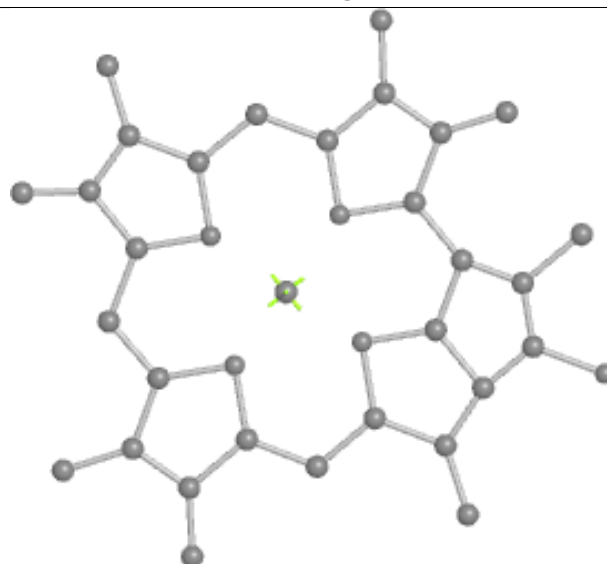
Bond lengths



Bond angles

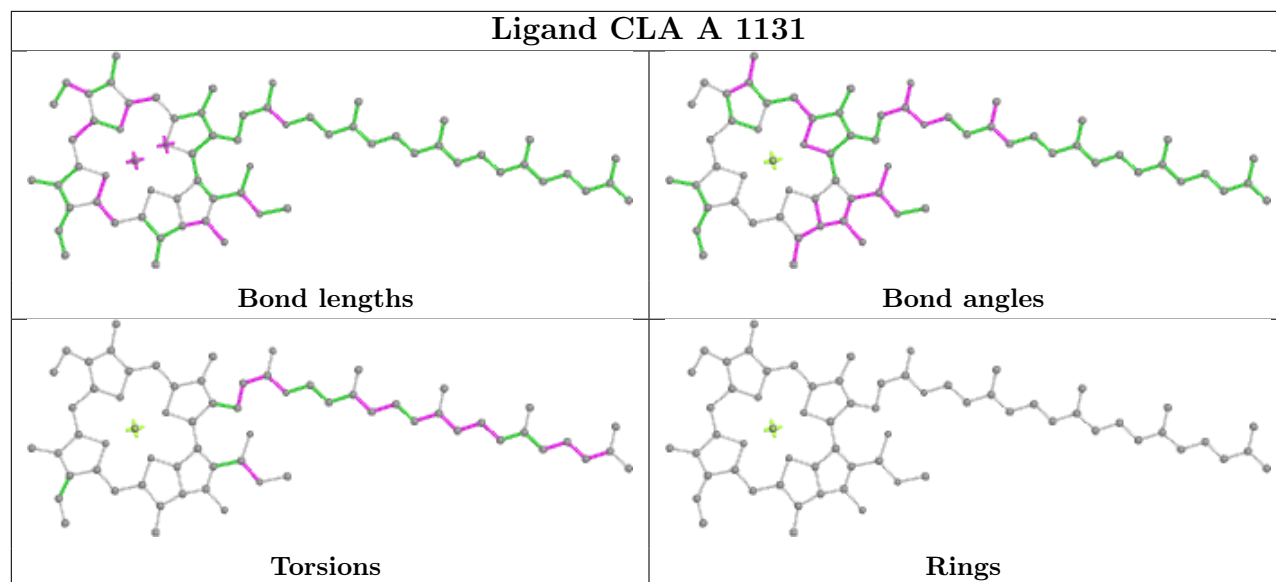


Torsions

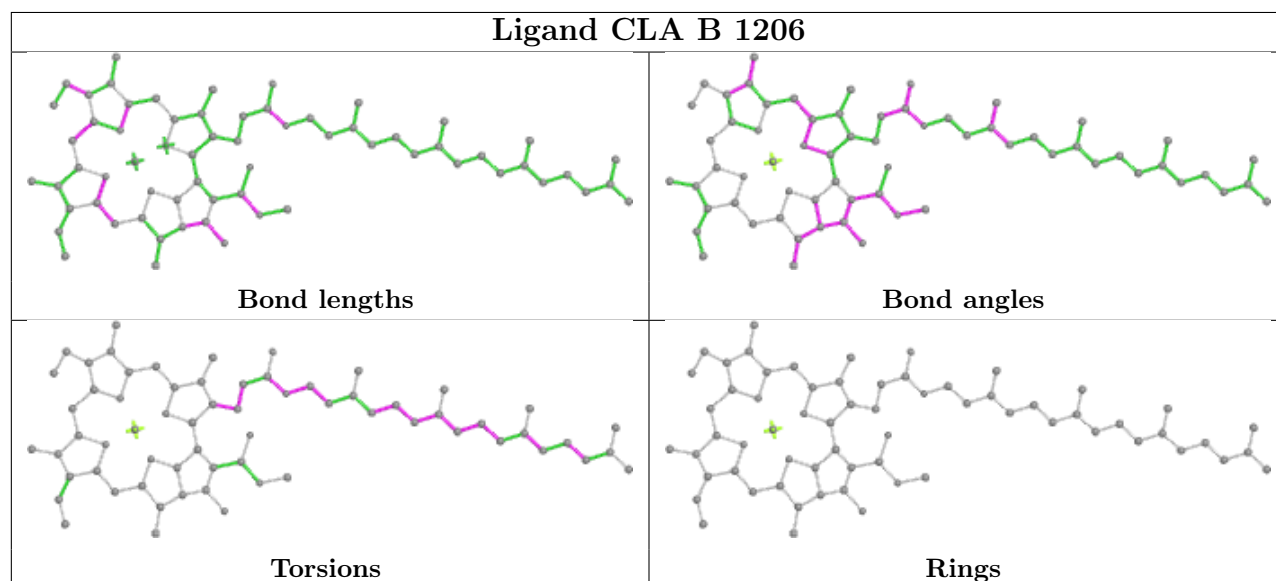


Rings

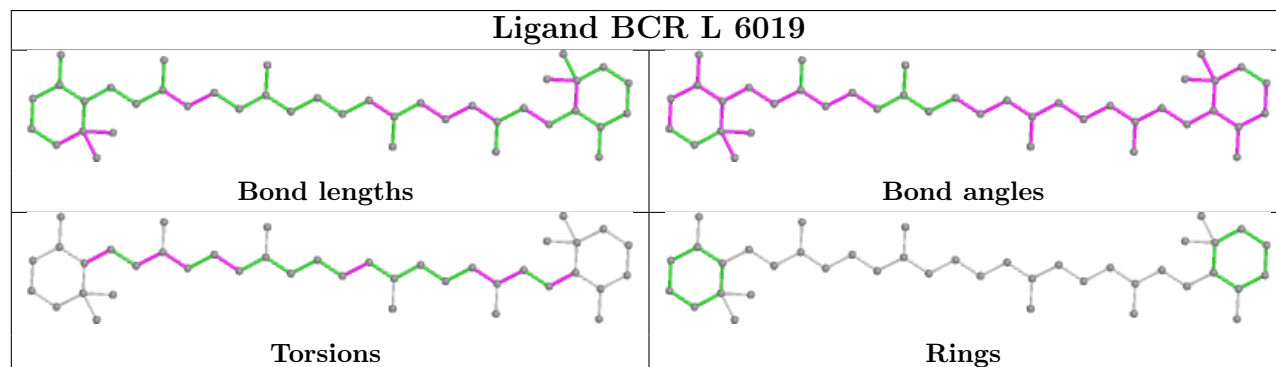
Ligand CLA A 1131

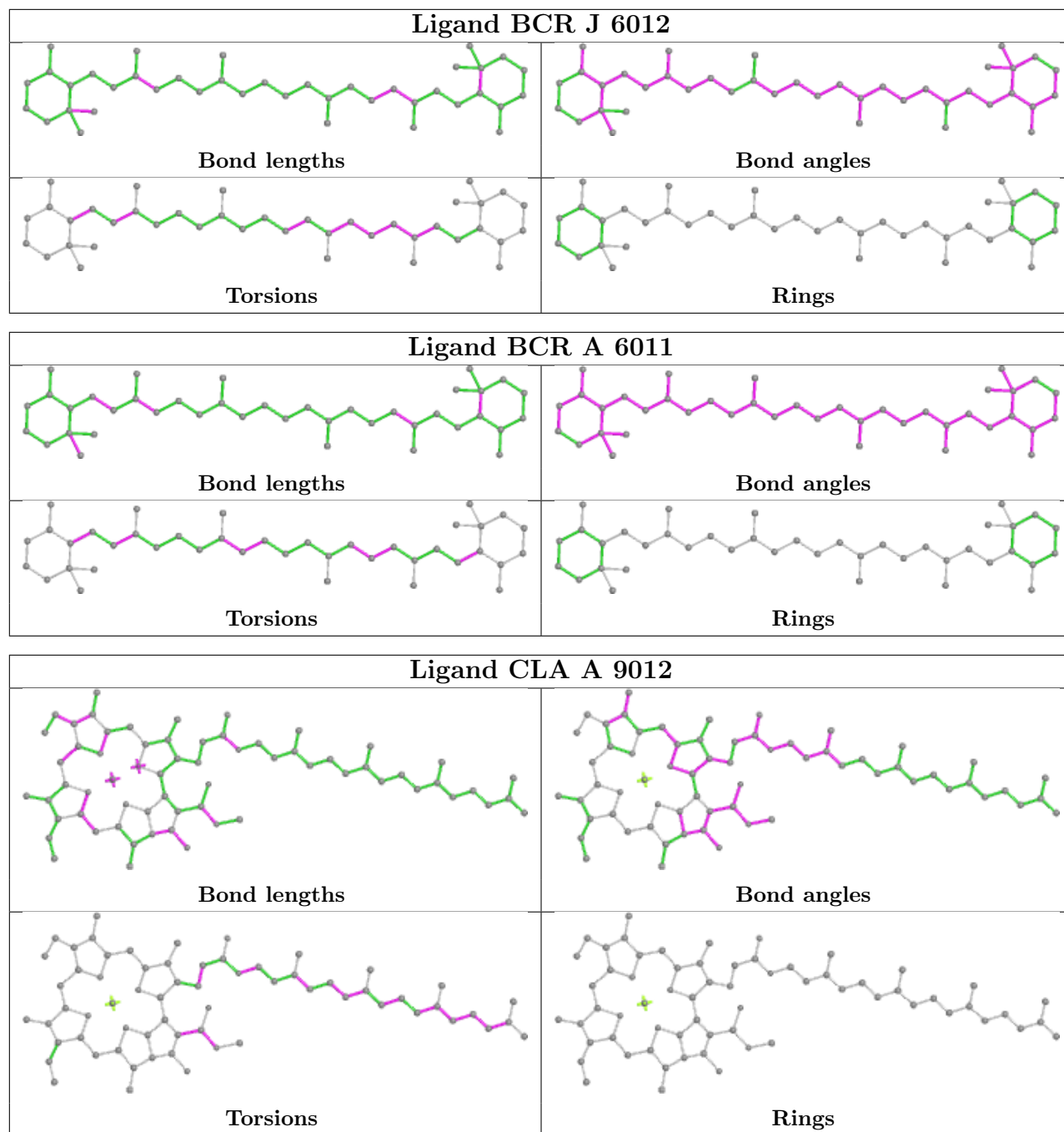


Ligand CLA B 1206

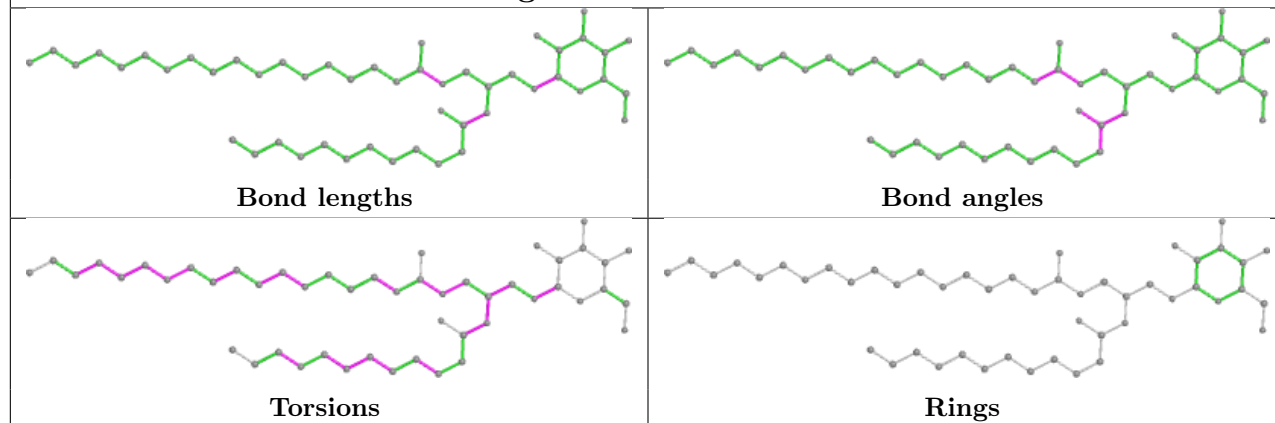


Ligand BCR L 6019

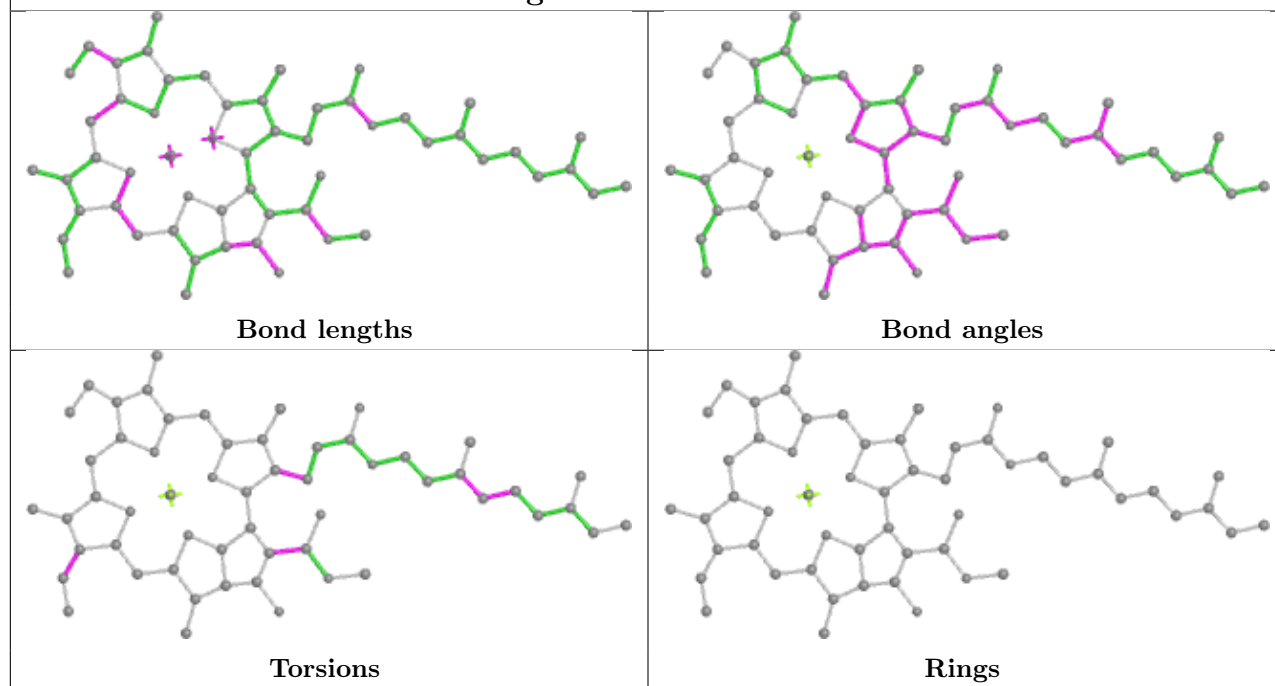




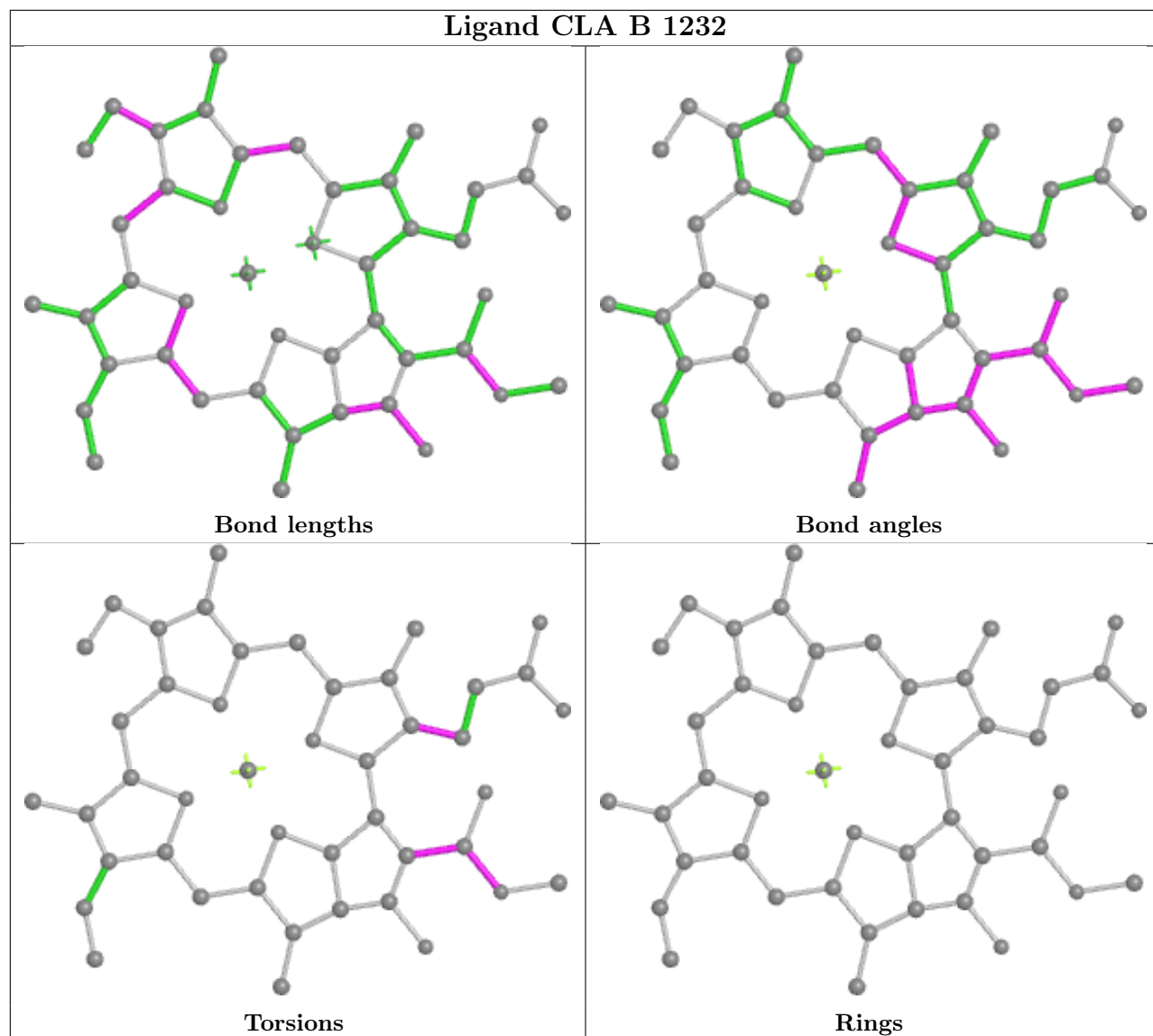
Ligand LMG B 7101

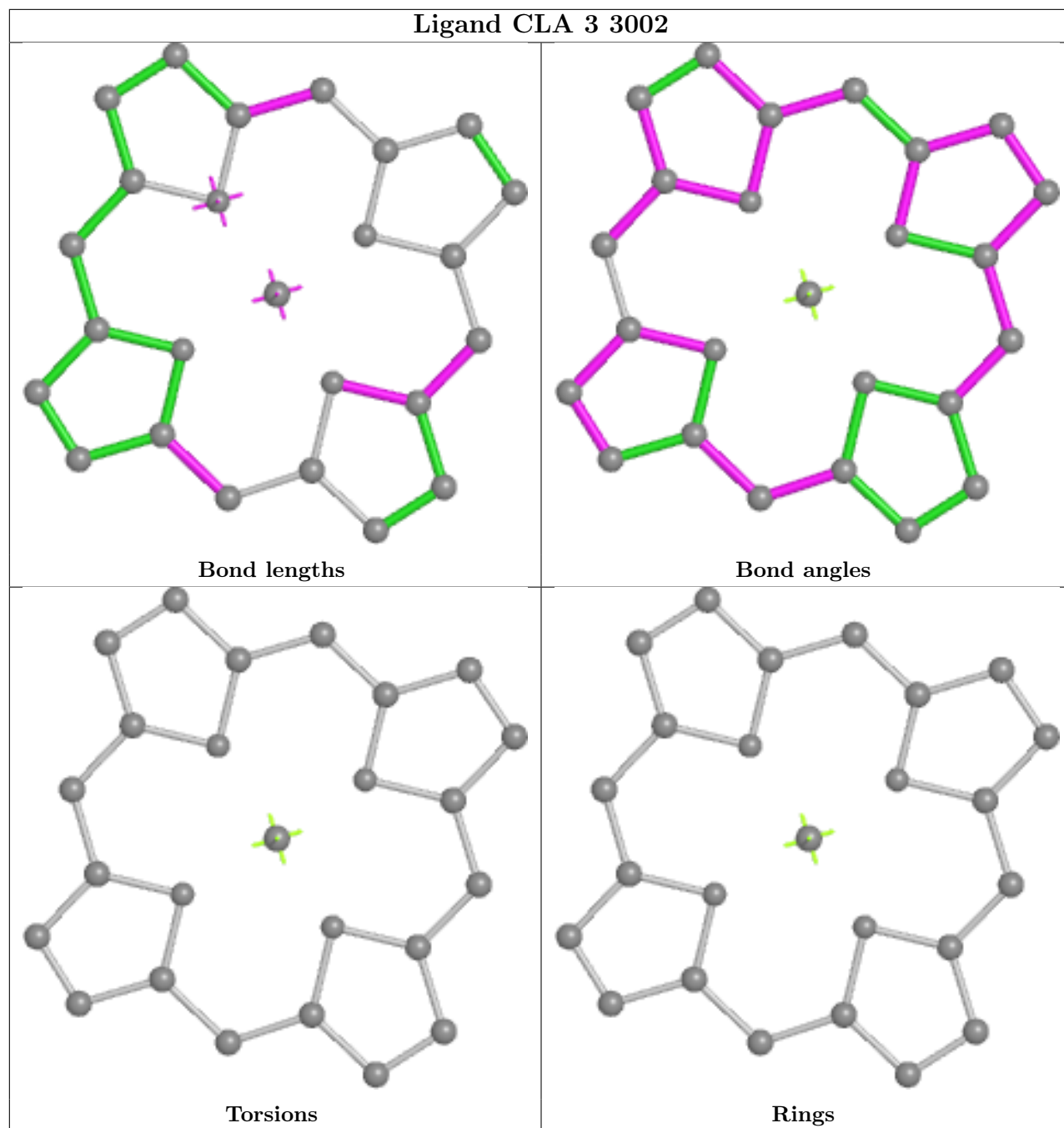


Ligand CLA 2 2002

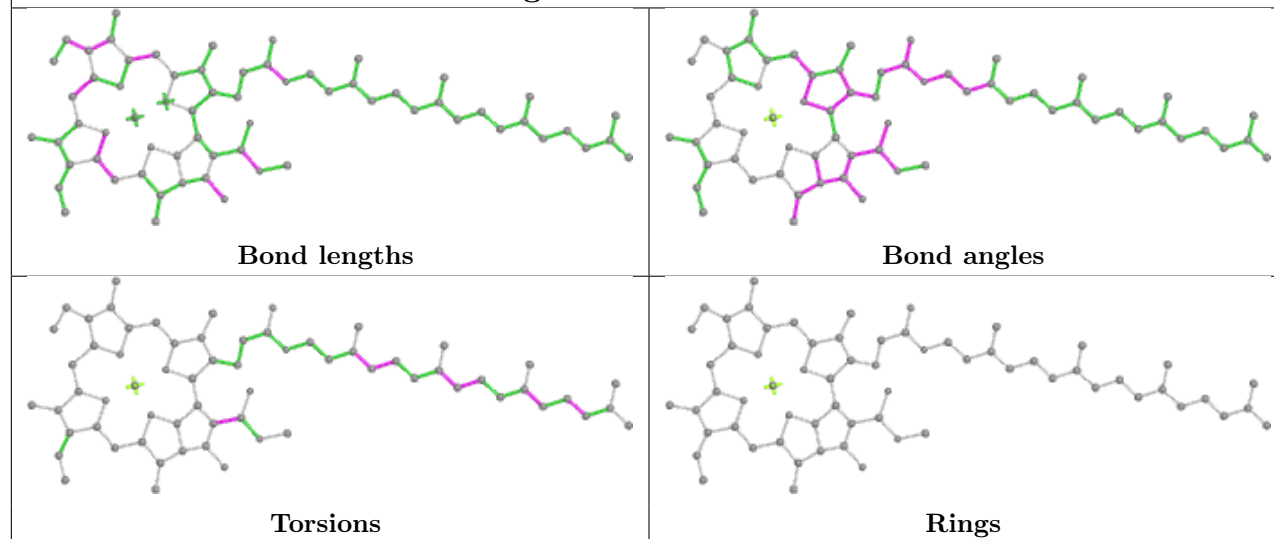


Ligand CLA B 1232

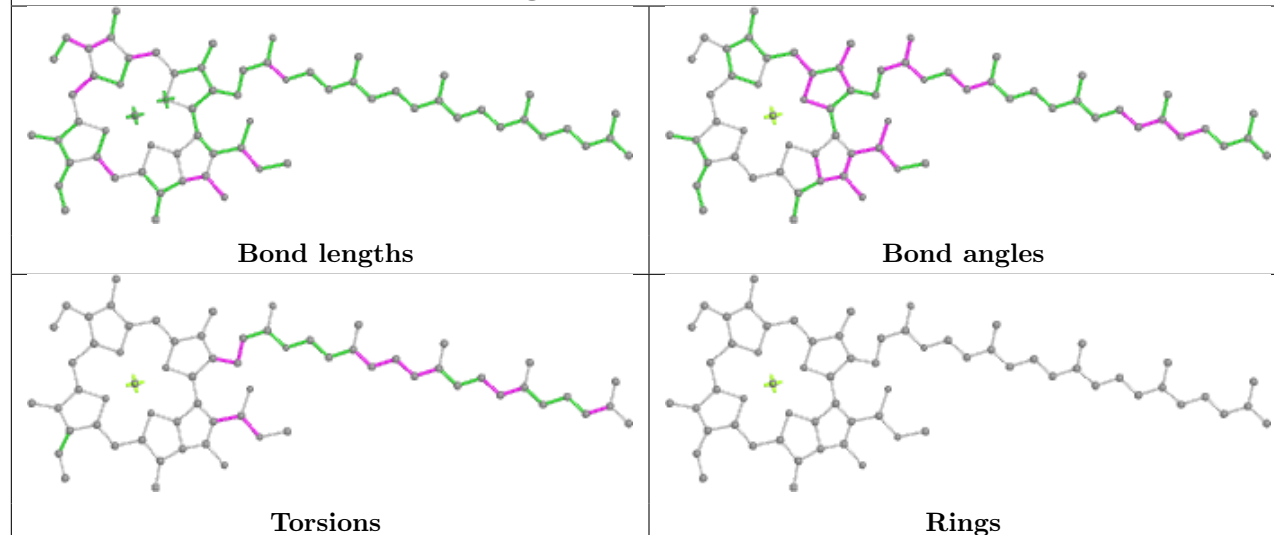




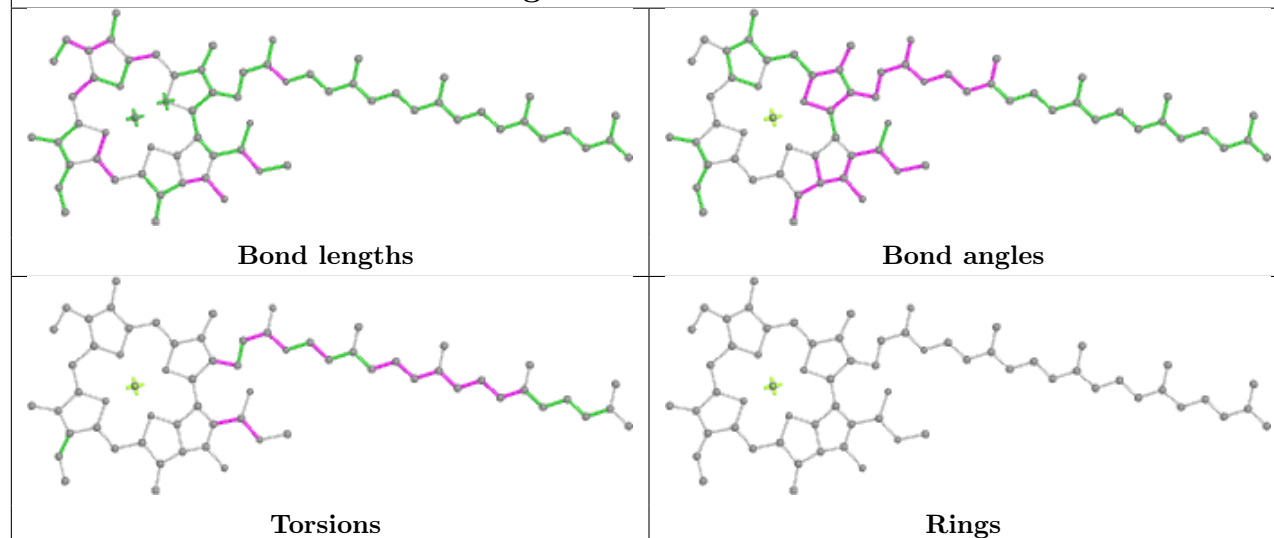
Ligand CLA B 1205



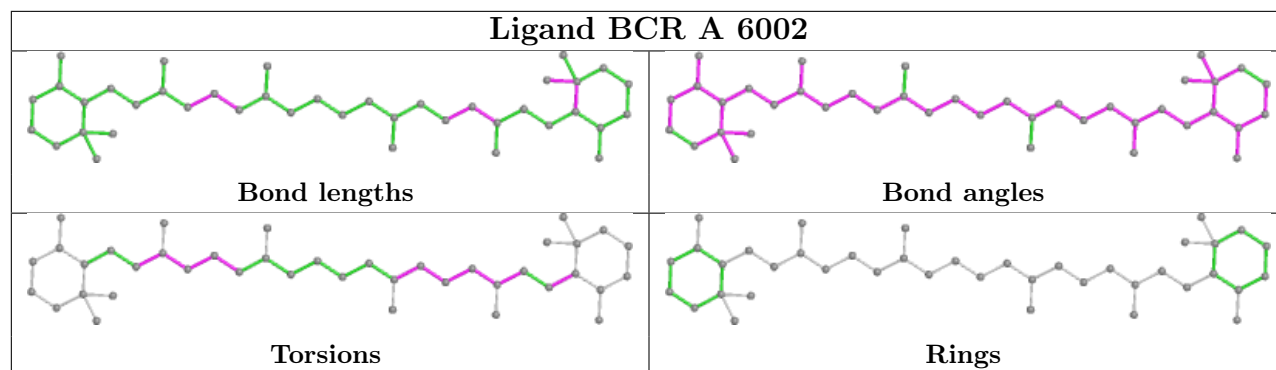
Ligand CLA B 1225



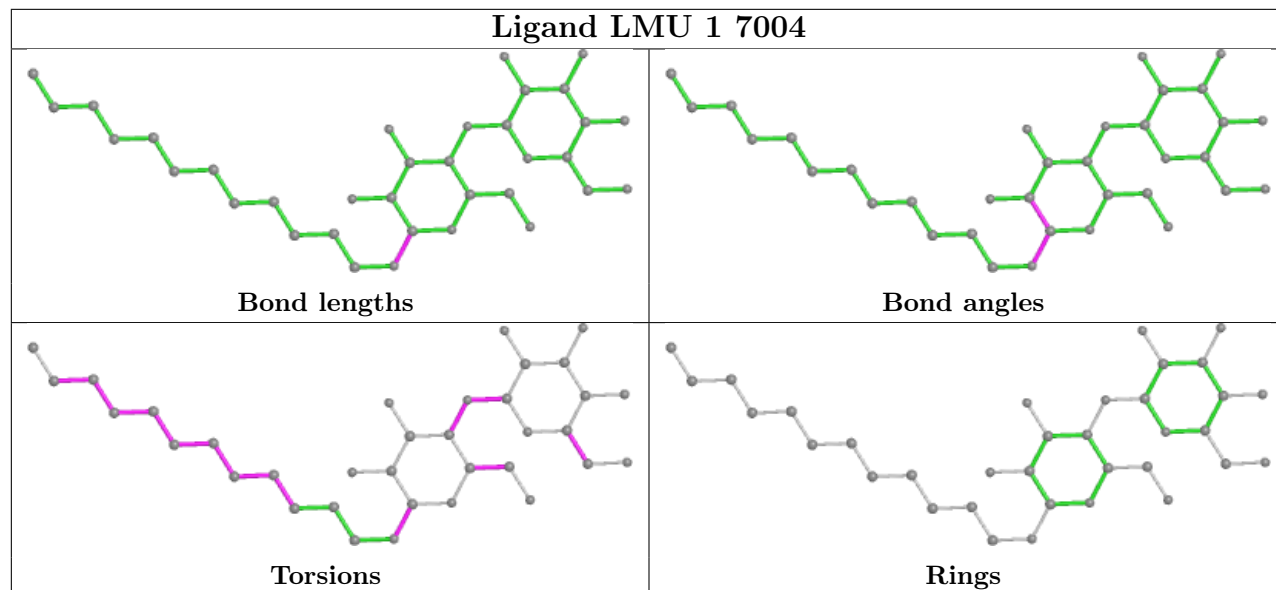
Ligand CLA R 1150



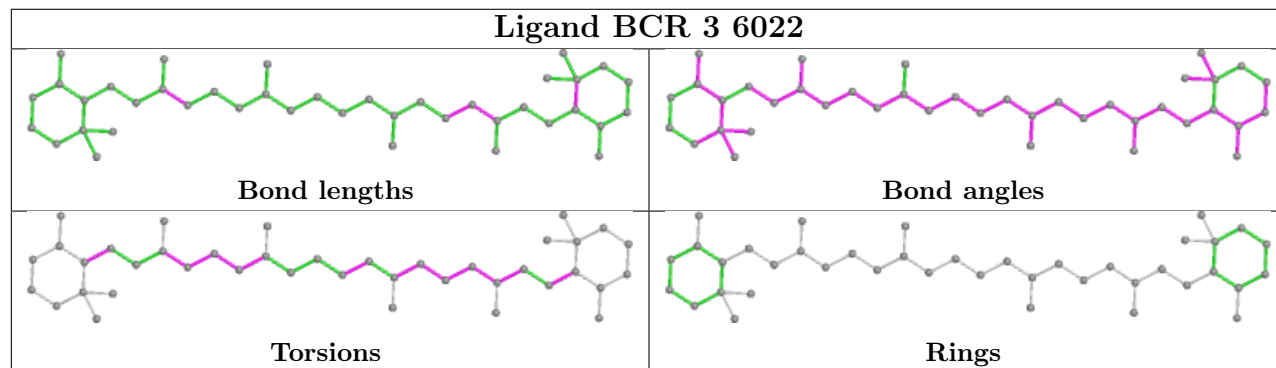
Ligand BCR A 6002



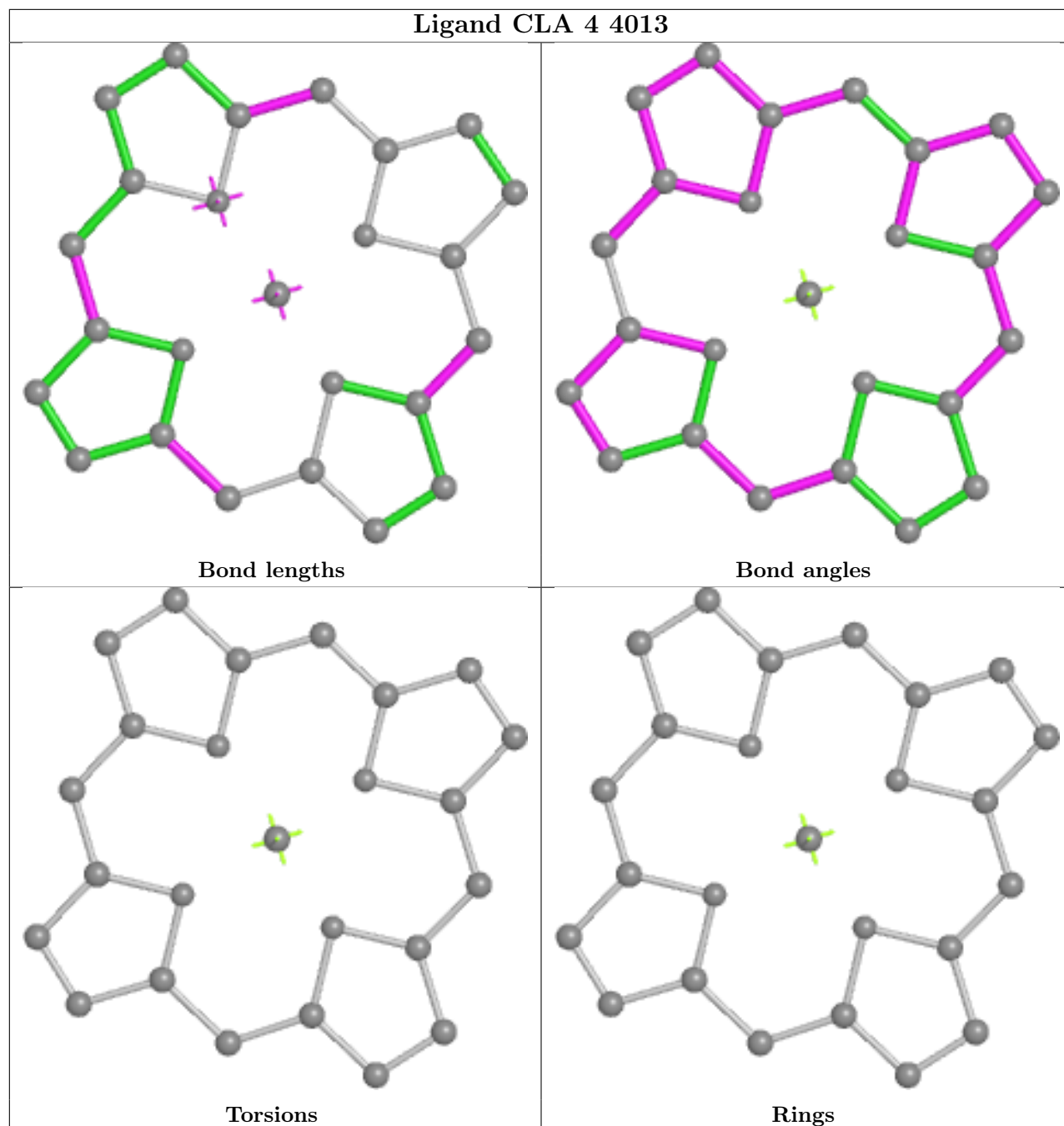
Ligand LMU 1 7004



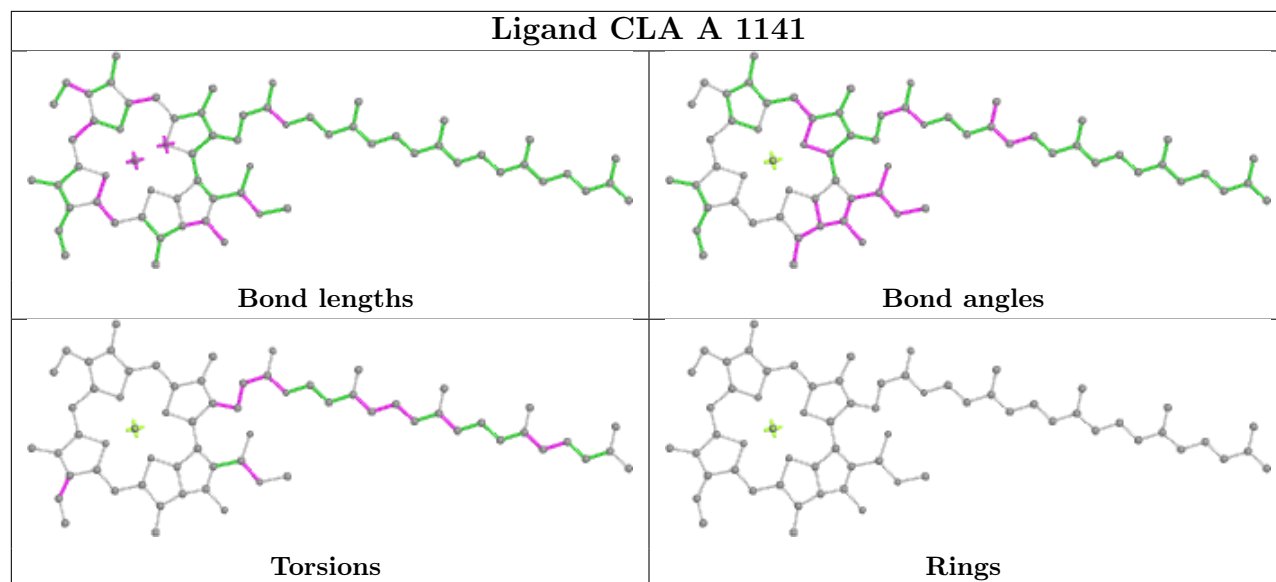
Ligand BCR 3 6022



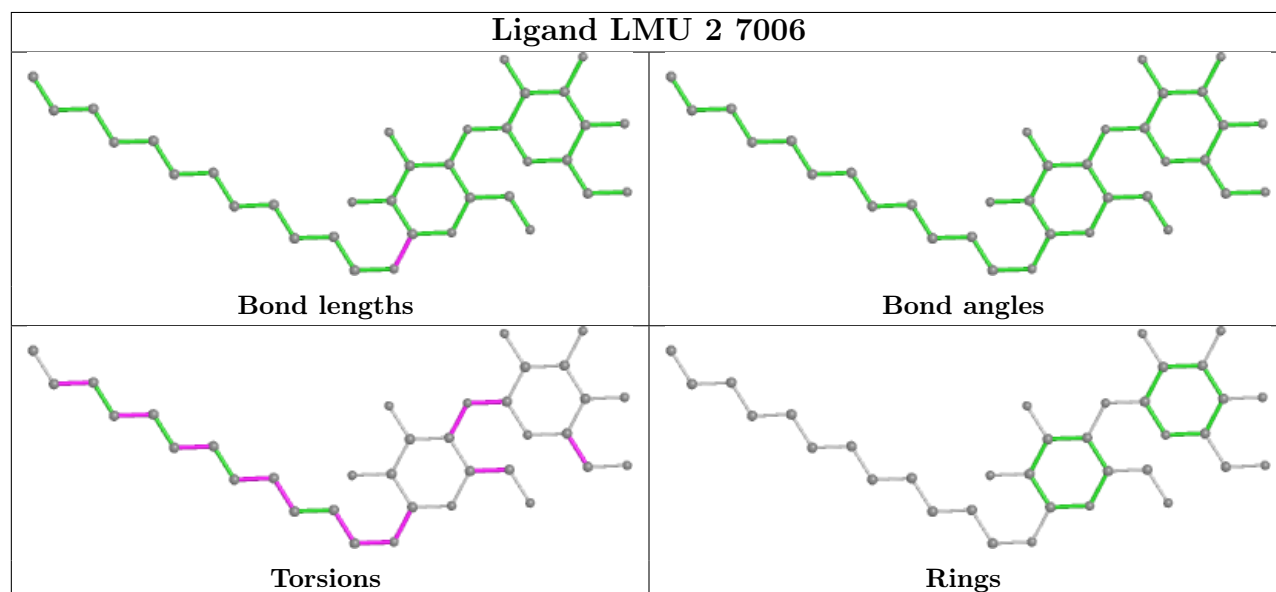
Ligand CLA 4 4013



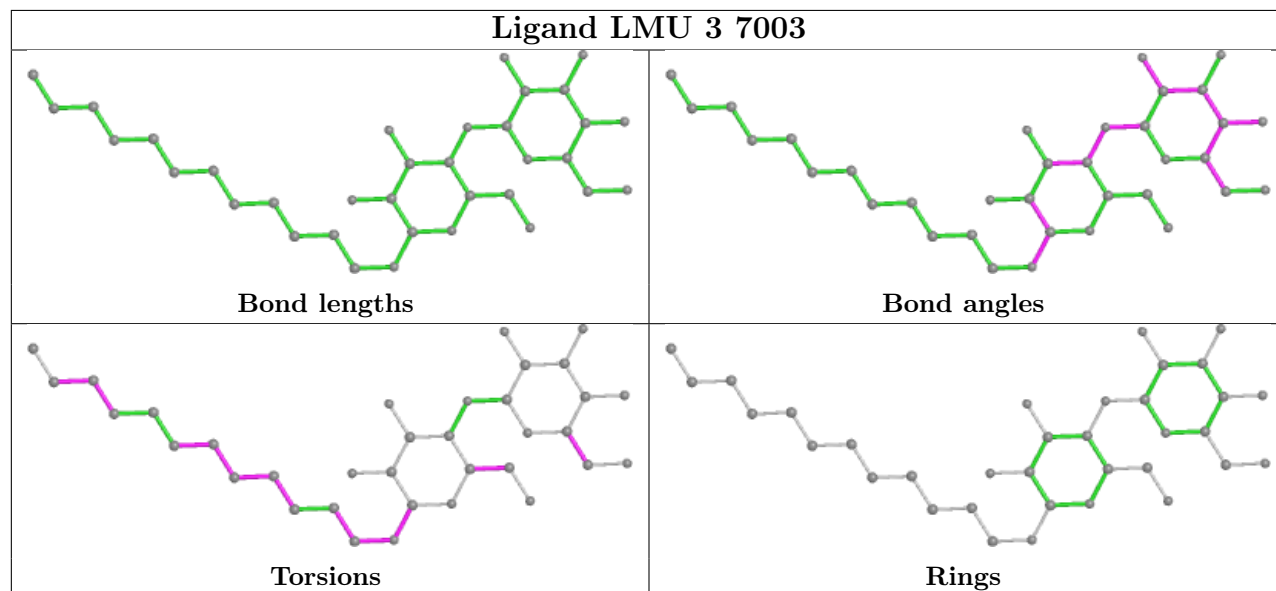
Ligand CLA A 1141



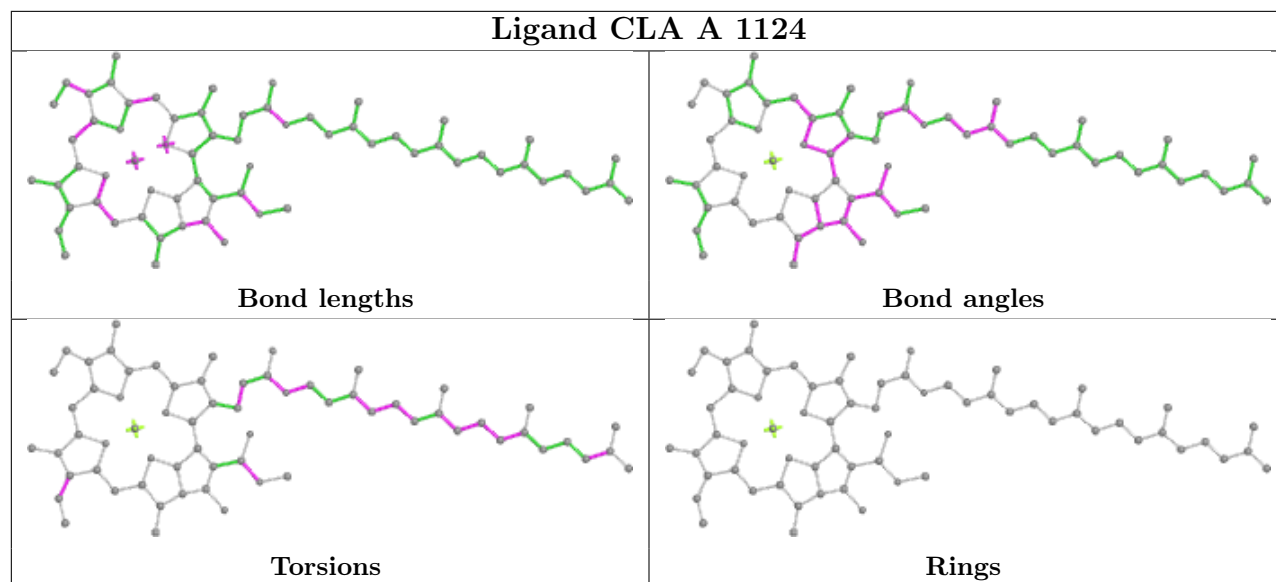
Ligand LMU 2 7006



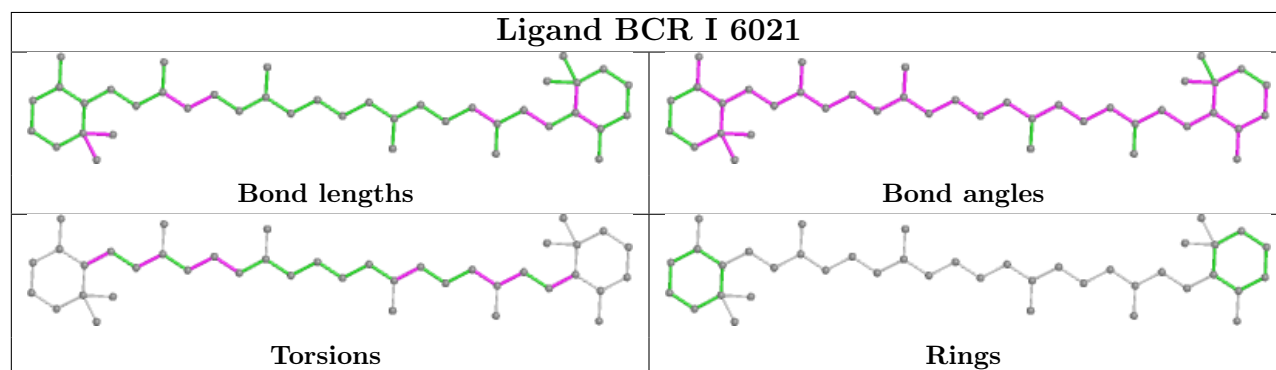
Ligand LMU 3 7003



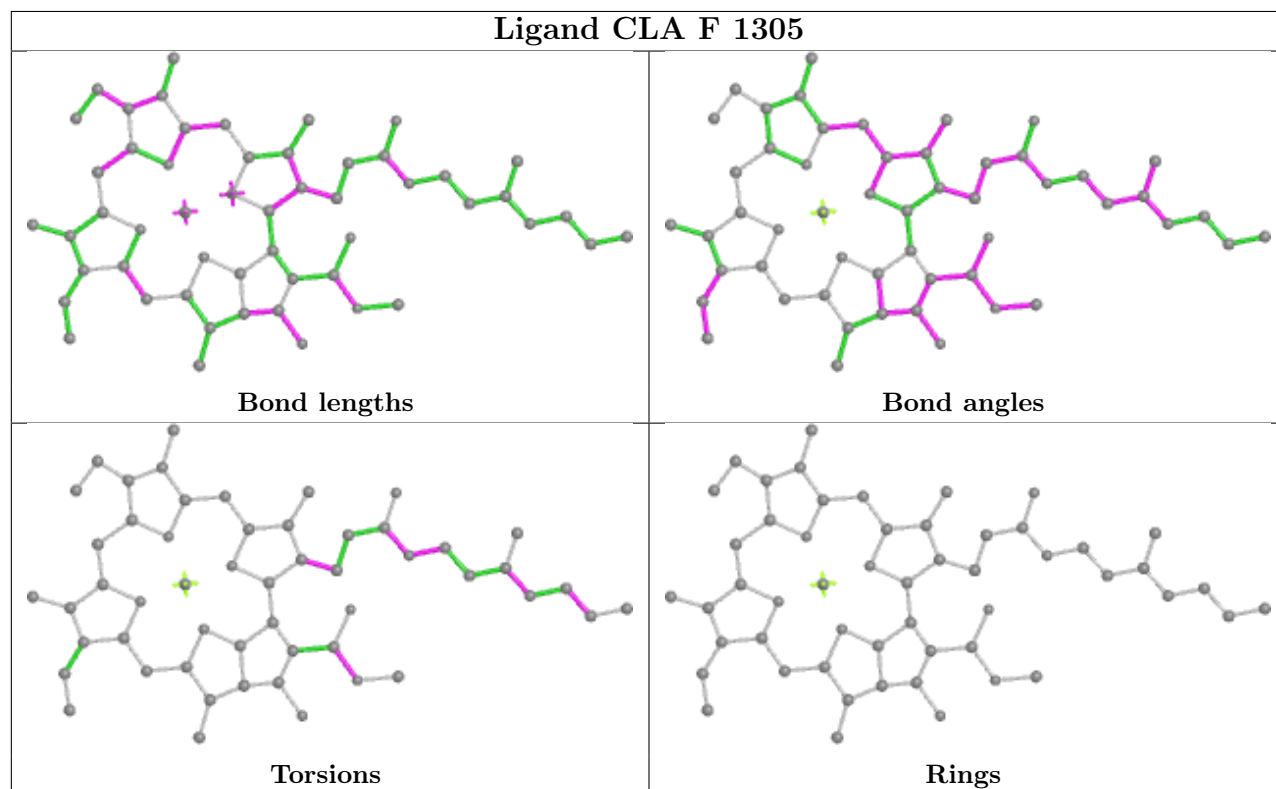
Ligand CLA A 1124

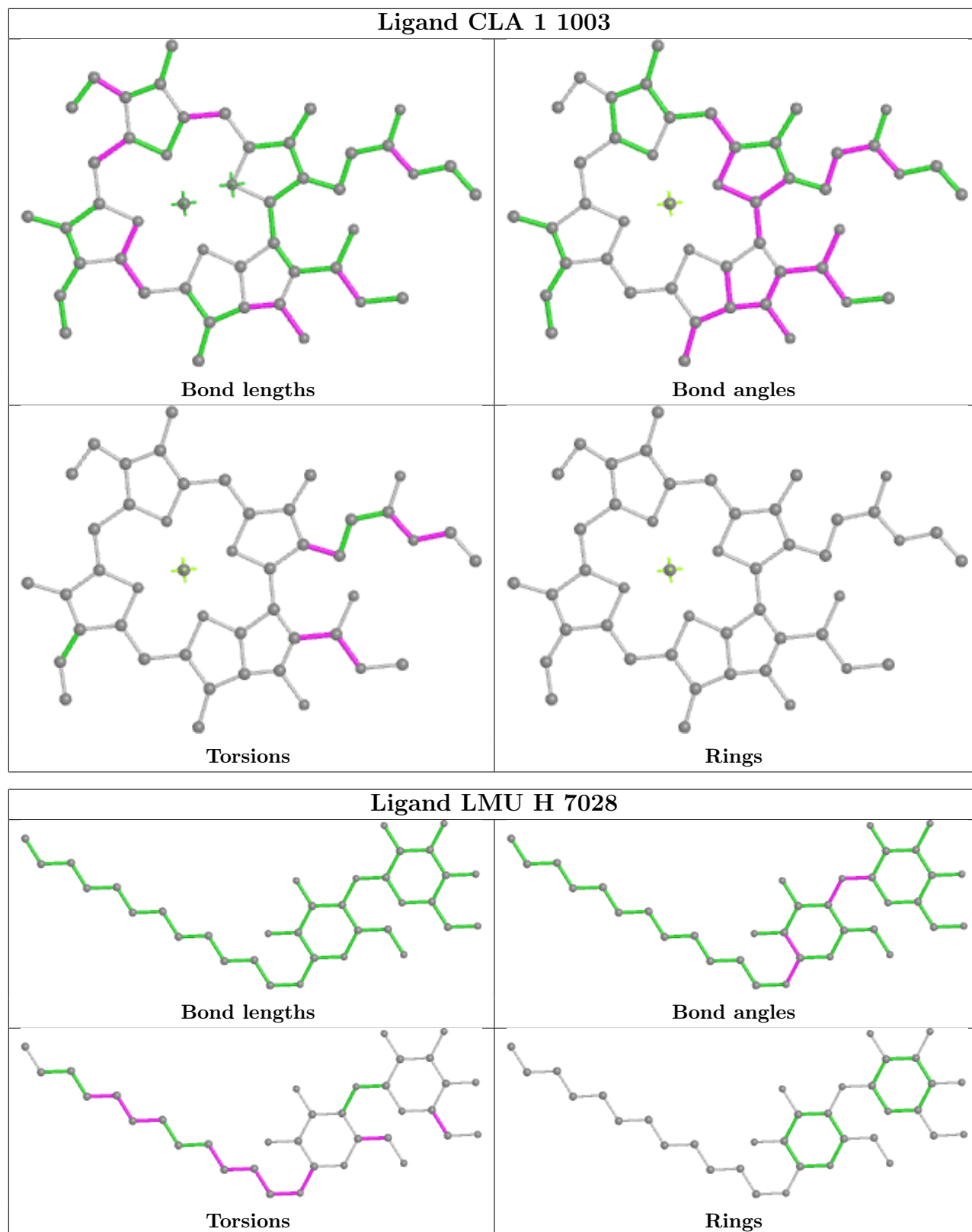


Ligand BCR I 6021

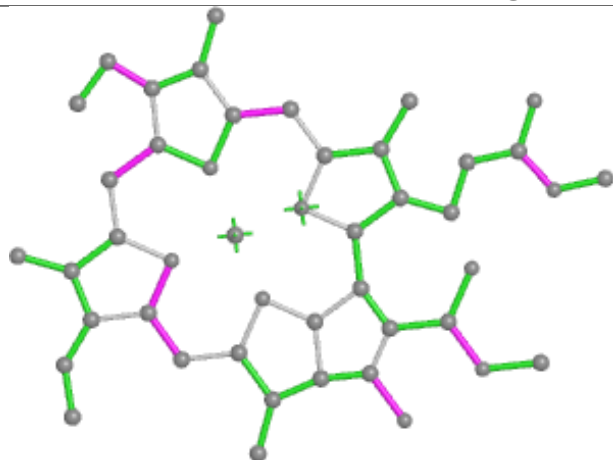


Ligand CLA F 1305

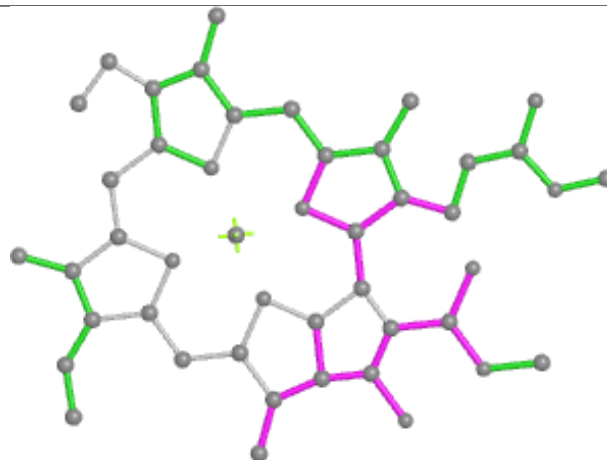




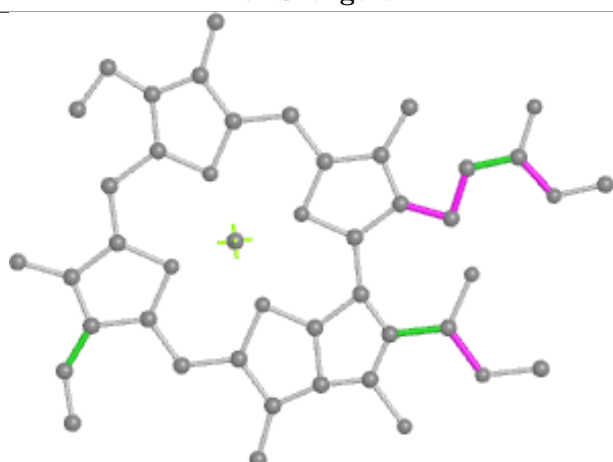
Ligand CLA A 1105



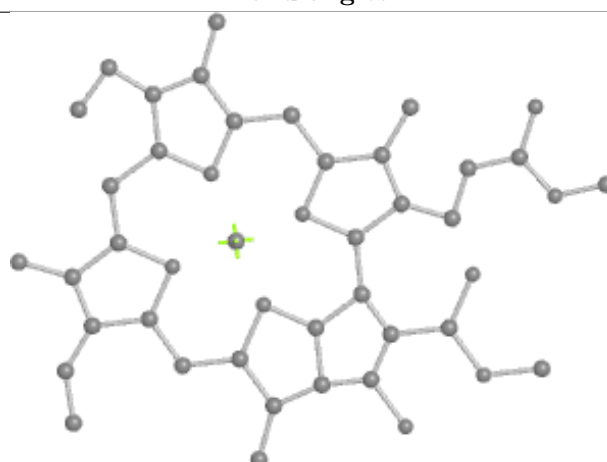
Bond lengths



Bond angles

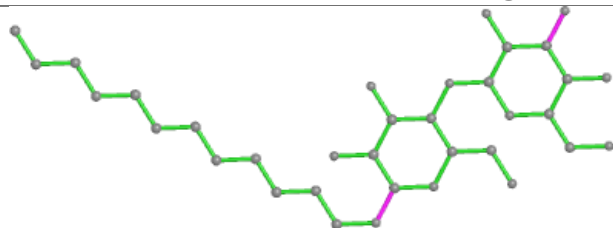


Torsions

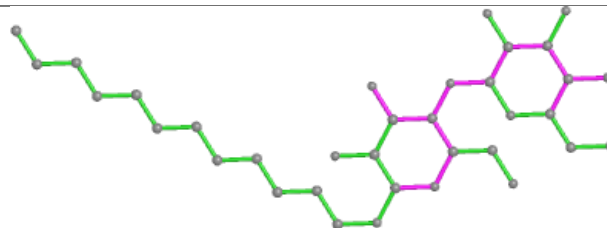


Rings

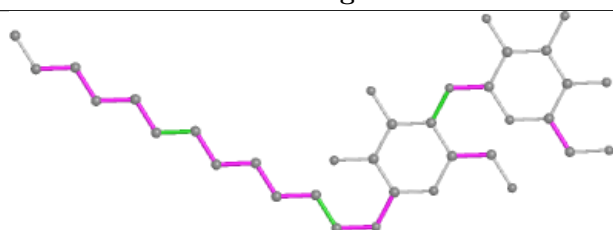
Ligand LMU G 7026



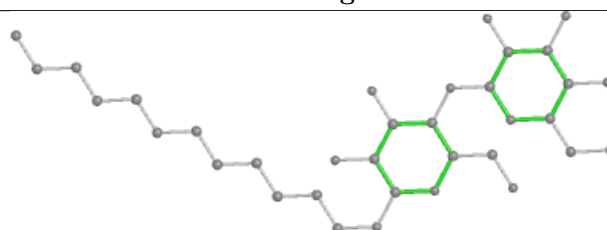
Bond lengths



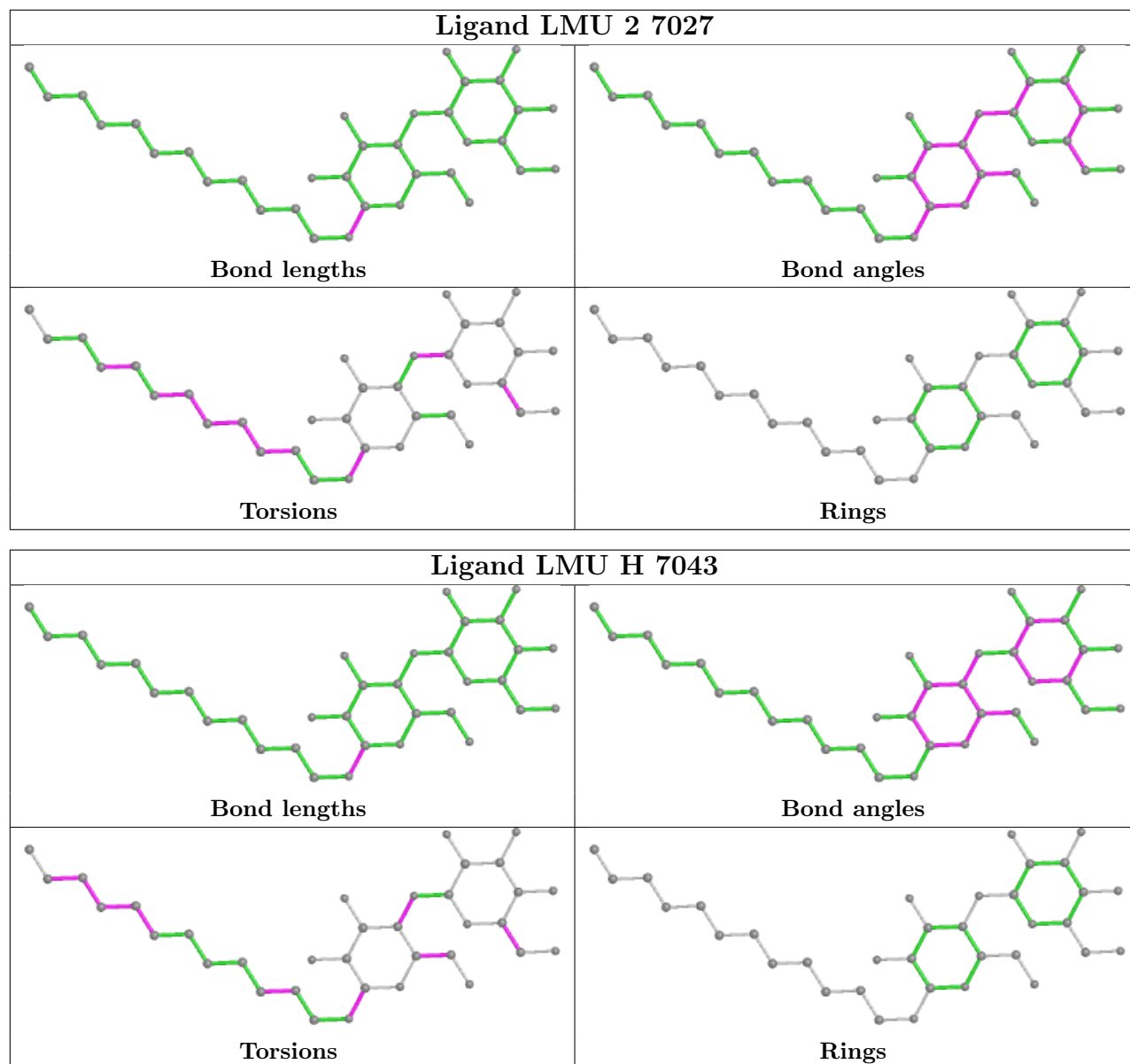
Bond angles



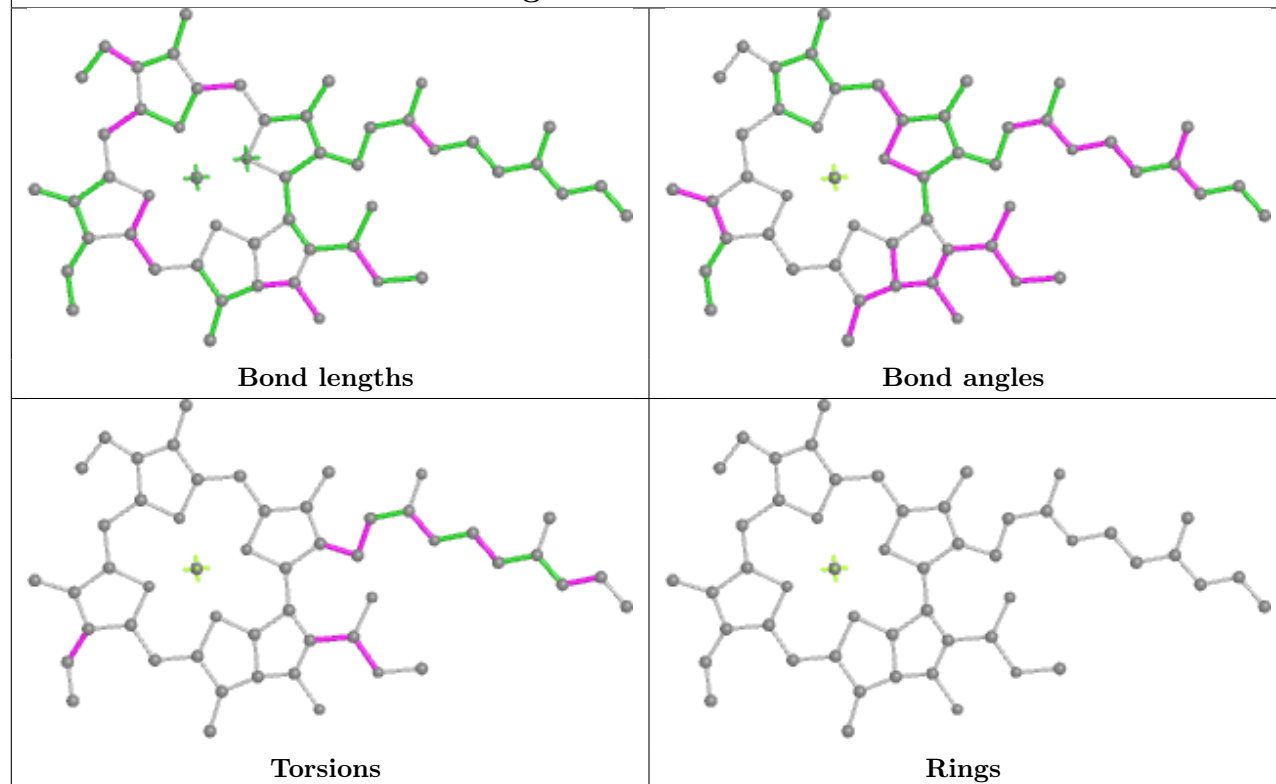
Torsions



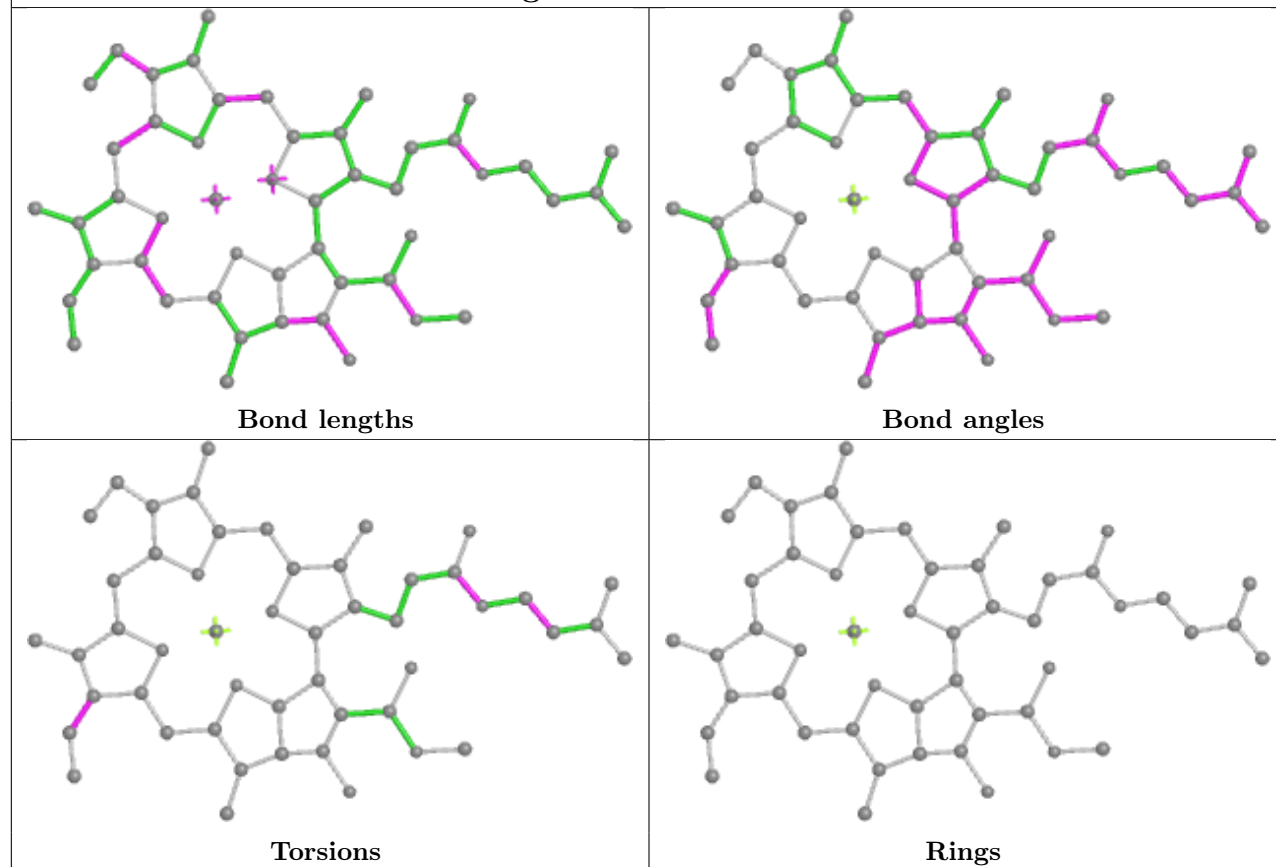
Rings



Ligand CLA A 1116



Ligand CLA K 1143



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	730/738 (98%)	0.15	17 (2%) 60 59	12, 19, 25, 27	0
2	B	733/733 (100%)	0.09	12 (1%) 72 70	8, 18, 26, 28	0
3	C	81/81 (100%)	0.69	10 (12%) 4 3	17, 21, 23, 24	0
4	D	138/138 (100%)	0.24	8 (5%) 23 22	18, 22, 25, 27	0
5	E	64/64 (100%)	0.15	4 (6%) 20 20	17, 21, 24, 25	0
6	F	154/154 (100%)	0.11	7 (4%) 33 32	17, 22, 25, 26	0
7	G	95/95 (100%)	0.41	5 (5%) 26 24	20, 25, 28, 29	0
8	H	69/69 (100%)	0.25	2 (2%) 51 50	22, 24, 29, 30	0
9	I	30/30 (100%)	0.02	2 (6%) 17 17	17, 19, 22, 22	0
10	J	42/42 (100%)	0.24	3 (7%) 16 16	17, 20, 25, 26	0
11	K	84/84 (100%)	1.02	17 (20%) 1 1	24, 27, 29, 30	0
12	L	161/161 (100%)	0.18	7 (4%) 35 34	16, 20, 26, 27	0
13	N	85/85 (100%)	0.13	3 (3%) 44 42	22, 25, 28, 29	0
14	R	0/53	-	-	-	-
15	1	165/170 (97%)	0.36	12 (7%) 15 15	32, 59, 69, 70	0
16	2	176/176 (100%)	0.20	9 (5%) 28 26	32, 52, 63, 66	0
17	3	156/172 (90%)	0.27	8 (5%) 28 26	25, 28, 32, 33	0
18	4	166/166 (100%)	0.27	11 (6%) 18 18	20, 44, 56, 57	0
All	All	3129/3211 (97%)	0.21	137 (4%) 34 33	8, 22, 57, 70	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	62	SER	8.6
16	2	181	PRO	8.3
15	1	132	GLY	8.2

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Mol	Chain	Res	Type	RSRZ
2	B	491	ASN	6.5
6	F	229	ASN	5.2
18	4	118	ILE	5.1
12	L	126	ALA	4.9
12	L	127	GLY	4.8
1	A	251	ASN	4.7
12	L	163	SER	4.4
1	A	505	PRO	4.4
15	1	174	SER	4.4
4	D	170	ASP	4.4
12	L	162	PRO	4.3
15	1	153	SER	4.3
11	K	90	ASP	4.2
13	N	141	LYS	4.2
7	G	130	TRP	4.2
11	K	109	CYS	4.1
3	C	17	CYS	3.8
16	2	197	GLY	3.8
4	D	195	VAL	3.8
15	1	127	ASN	3.8
11	K	68	GLY	3.5
17	3	86	PRO	3.5
1	A	249	ILE	3.5
15	1	212	GLY	3.5
1	A	635	THR	3.4
12	L	130	GLY	3.4
2	B	562	PRO	3.3
11	K	72	LEU	3.3
18	4	230	ASP	3.3
18	4	187	GLY	3.2
7	G	142	LEU	3.2
11	K	105	ASP	3.2
4	D	205	LYS	3.1
18	4	182	VAL	3.1
1	A	391	THR	3.1
4	D	78	THR	3.0
18	4	119	GLY	3.0
7	G	143	ALA	3.0
13	N	162	CYS	3.0
4	D	169	LYS	3.0
17	3	167	PHE	2.9
2	B	502	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
15	1	217	LEU	2.9
1	A	752	ALA	2.9
16	2	180	ASP	2.9
1	A	124	TRP	2.9
18	4	196	PRO	2.8
1	A	66	SER	2.8
16	2	168	TRP	2.8
16	2	268	PRO	2.8
18	4	130	GLY	2.8
6	F	115	PRO	2.8
15	1	218	ALA	2.7
15	1	164	PRO	2.7
3	C	15	THR	2.7
10	J	7	TYR	2.7
3	C	34	CYS	2.7
11	K	71	GLY	2.7
17	3	166	GLY	2.7
5	E	66	ILE	2.7
8	H	60	ASN	2.7
16	2	198	GLY	2.7
10	J	41	PHE	2.6
3	C	37	LYS	2.6
1	A	494	ASN	2.6
17	3	130	GLN	2.6
15	1	154	MET	2.6
2	B	263	PRO	2.6
4	D	86	SER	2.5
18	4	185	PRO	2.5
11	K	67	ALA	2.5
5	E	102	PRO	2.5
15	1	215	GLU	2.5
10	J	4	LEU	2.5
11	K	47	ASP	2.5
1	A	486	PRO	2.5
2	B	484	PRO	2.5
1	A	181	ALA	2.4
1	A	245	PRO	2.4
1	A	487	VAL	2.4
3	C	56	SER	2.4
5	E	68	PRO	2.4
2	B	492	ILE	2.3
6	F	114	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
17	3	135	ALA	2.3
18	4	186	GLY	2.3
11	K	128	GLY	2.3
15	1	116	ALA	2.3
2	B	212	PHE	2.3
3	C	67	VAL	2.3
17	3	84	SER	2.3
16	2	199	LEU	2.3
11	K	80	ALA	2.3
6	F	214	PRO	2.3
16	2	196	PRO	2.3
18	4	242	ASN	2.2
6	F	215	VAL	2.2
9	I	30	LYS	2.2
2	B	479	SER	2.2
12	L	157	ALA	2.2
3	C	50	GLY	2.2
5	E	103	VAL	2.2
11	K	54	ASN	2.2
8	H	54	ASP	2.2
4	D	203	THR	2.1
13	N	164	SER	2.1
15	1	87	CYS	2.1
17	3	194	PHE	2.1
6	F	187	ASP	2.1
1	A	32	GLU	2.1
11	K	51	SER	2.1
2	B	210	ASN	2.1
12	L	161	ALA	2.1
17	3	102	GLU	2.1
4	D	210	LEU	2.1
3	C	80	ALA	2.1
7	G	109	GLU	2.1
11	K	73	ALA	2.1
3	C	60	THR	2.1
18	4	193	ASN	2.0
2	B	260	GLY	2.0
7	G	132	SER	2.0
1	A	101	ALA	2.0
3	C	16	GLN	2.0
9	I	29	GLU	2.0
2	B	487	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	34	TRP	2.0
16	2	231	ALA	2.0
2	B	319	HIS	2.0
6	F	212	SER	2.0
11	K	99	ALA	2.0
11	K	110	GLY	2.0
11	K	101	PHE	2.0
1	A	344	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
19	CLA	3	3014	25/65	0.53	0.52	31,31,32,32	0
22	LMU	1	7013	35/35	0.56	0.33	15,34,47,48	0
19	CLA	L	1504	55/65	0.57	0.42	18,25,27,27	0
19	CLA	3	3012	25/65	0.57	0.28	30,31,31,31	0
19	CLA	A	1309	25/65	0.58	0.56	25,46,54,54	0
22	LMU	E	7048	35/35	0.59	0.30	19,30,44,46	0
19	CLA	3	3005	25/65	0.59	0.28	31,31,31,31	0
22	LMU	4	7053	34/35	0.59	0.30	21,41,47,48	0
21	BCR	1	6023	40/40	0.61	0.40	21,28,29,30	0
22	LMU	1	7004	35/35	0.61	0.49	17,44,50,52	0
19	CLA	3	1118	36/65	0.62	0.33	28,29,30,30	0
19	CLA	1	1006	36/65	0.63	0.42	29,30,30,31	0
19	CLA	4	4003	55/65	0.63	0.29	15,34,47,50	0
22	LMU	L	7029	35/35	0.63	0.31	30,44,53,55	0
19	CLA	H	1505	55/65	0.64	0.39	18,27,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	2	2014	61/65	0.64	0.33	24,26,28,28	0
22	LMU	A	7010	35/35	0.64	0.32	16,38,45,48	0
19	CLA	3	3016	65/65	0.64	0.47	23,26,29,31	0
22	LMU	2	7046	35/35	0.65	0.30	4,27,42,42	0
22	LMU	4	7052	35/35	0.65	0.26	18,30,48,75	0
19	CLA	4	4014	47/65	0.65	0.28	21,35,46,48	0
22	LMU	B	7038	35/35	0.66	0.42	13,35,48,48	0
21	BCR	A	6002	40/40	0.66	0.39	23,27,32,33	0
19	CLA	B	1233	51/65	0.66	0.40	24,27,27,28	0
19	CLA	2	2001	51/65	0.66	0.26	27,28,29,29	0
19	CLA	K	1142	45/65	0.67	0.25	27,29,30,31	0
19	CLA	2	2005	25/65	0.67	0.25	30,31,32,32	0
22	LMU	N	7049	35/35	0.67	0.28	15,28,40,41	0
19	CLA	2	2007	65/65	0.67	0.30	17,25,26,26	0
19	CLA	4	4004	25/65	0.68	0.36	29,30,30,30	0
19	CLA	F	1305	53/65	0.68	0.36	22,23,25,25	0
19	CLA	4	4001	50/65	0.68	0.43	21,23,25,25	0
22	LMU	H	7011	35/35	0.68	0.27	17,32,38,43	0
22	LMU	H	7030	35/35	0.68	0.36	16,29,46,50	0
19	CLA	G	1242	51/65	0.68	0.34	26,28,29,29	0
19	CLA	B	1213	46/65	0.69	0.37	19,21,24,25	0
19	CLA	B	1232	45/65	0.69	0.42	23,26,27,27	0
22	LMU	B	7040	35/35	0.69	0.22	12,26,40,43	0
19	CLA	A	1112	45/65	0.69	0.41	23,26,26,27	0
19	CLA	1	1010	46/65	0.69	0.26	24,25,26,27	0
19	CLA	1	1310	25/65	0.69	0.31	27,28,28,28	0
22	LMU	H	7043	35/35	0.69	0.19	12,31,46,47	0
22	LMU	E	7037	35/35	0.70	0.22	8,21,40,40	0
22	LMU	4	7008	35/35	0.70	0.34	11,29,41,42	0
19	CLA	3	3010	25/65	0.70	0.23	32,32,33,33	0
19	CLA	4	4007	52/65	0.70	0.29	22,26,27,28	0
19	CLA	4	1306	55/65	0.71	0.32	20,26,27,27	0
19	CLA	2	2011	25/65	0.71	0.31	24,25,25,25	0
19	CLA	A	1141	65/65	0.71	0.26	28,30,31,32	0
22	LMU	G	7051	35/35	0.71	0.28	20,32,43,44	0
21	BCR	3	6022	40/40	0.71	0.25	21,22,23,23	0
19	CLA	1	1015	25/65	0.71	0.24	27,28,28,28	0
19	CLA	K	3009	65/65	0.71	0.37	22,25,27,28	0
22	LMU	K	7047	35/35	0.71	0.27	14,33,46,49	0
22	LMU	K	7041	35/35	0.72	0.24	15,31,45,45	0
19	CLA	1	1001	46/65	0.72	0.27	28,29,30,30	0
19	CLA	2	2008	25/65	0.72	0.22	24,24,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	LMU	C	7015	35/35	0.72	0.35	9,22,37,39	0
19	CLA	A	1151	50/65	0.72	0.37	24,27,29,29	0
19	CLA	3	3015	25/65	0.72	0.42	28,28,29,29	0
19	CLA	2	1307	25/65	0.72	0.50	29,30,31,31	0
19	CLA	4	1304	65/65	0.72	0.26	21,23,25,25	0
19	CLA	H	1241	55/65	0.72	0.26	23,25,26,26	0
19	CLA	1	1014	61/65	0.72	0.27	3,31,46,46	0
19	CLA	3	1147	46/65	0.73	0.28	25,27,28,28	0
19	CLA	J	1311	61/65	0.73	0.27	19,26,27,28	0
19	CLA	3	3007	42/65	0.73	0.32	27,30,30,30	0
19	CLA	4	1004	55/65	0.73	0.26	22,25,26,27	0
19	CLA	A	1134	45/65	0.73	0.26	22,26,27,28	0
19	CLA	4	4015	46/65	0.73	0.36	24,25,26,27	0
22	LMU	4	7009	34/35	0.73	0.26	22,44,50,50	0
22	LMU	4	7018	35/35	0.73	0.29	9,23,41,42	0
22	LMU	4	7034	35/35	0.73	0.28	14,30,42,47	0
22	LMU	K	7042	35/35	0.73	0.23	13,23,42,43	0
19	CLA	F	1302	41/65	0.73	0.25	24,26,26,26	0
19	CLA	3	3003	36/65	0.74	0.34	29,30,31,31	0
22	LMU	H	7017	35/35	0.74	0.21	8,23,39,41	0
19	CLA	2	2013	50/65	0.74	0.27	20,22,24,26	0
22	LMU	3	7005	35/35	0.74	0.25	20,32,42,43	0
19	CLA	1	1003	47/65	0.74	0.24	17,19,19,20	0
19	CLA	3	3008	50/65	0.74	0.35	20,26,27,27	0
19	CLA	B	1212	60/65	0.74	0.32	20,23,25,26	0
19	CLA	3	3011	65/65	0.74	0.30	23,25,26,26	0
21	BCR	A	6007	40/40	0.74	0.38	19,23,28,28	0
19	CLA	L	1148	55/65	0.74	0.32	21,25,26,27	0
19	CLA	R	1150	65/65	0.75	0.28	22,24,25,25	0
19	CLA	1	1013	51/65	0.75	0.42	26,27,29,29	0
22	LMU	2	7031	35/35	0.75	0.23	17,37,45,48	0
19	CLA	3	3002	25/65	0.75	0.27	28,28,28,28	0
22	LMU	3	7003	35/35	0.75	0.20	8,25,41,41	0
22	LMU	K	7001	35/35	0.75	0.20	17,34,48,50	0
19	CLA	A	1113	50/65	0.75	0.31	19,22,23,24	0
19	CLA	2	2004	50/65	0.75	0.26	23,25,25,25	0
22	LMU	G	7026	35/35	0.75	0.30	12,35,46,51	0
22	LMU	4	7019	35/35	0.75	0.22	11,25,40,43	0
19	CLA	3	3006	25/65	0.75	0.21	26,27,28,28	0
19	CLA	1	1008	51/65	0.75	0.35	24,26,27,27	0
22	LMU	R	7021	35/35	0.75	0.25	17,28,45,46	0
24	LMG	B	7101	49/55	0.75	0.36	14,18,26,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	LMU	2	7006	35/35	0.76	0.22	22,25,26,27	0
22	LMU	2	7027	35/35	0.76	0.21	6,17,40,40	0
19	CLA	H	1145	65/65	0.76	0.24	12,24,33,39	0
19	CLA	A	1121	42/65	0.76	0.24	26,28,28,28	0
21	BCR	A	6003	40/40	0.76	0.35	21,24,26,26	0
22	LMU	D	7050	35/35	0.76	0.23	14,31,46,46	0
19	CLA	A	1149	46/65	0.76	0.32	22,25,25,25	0
21	BCR	J	6012	40/40	0.76	0.33	19,24,26,26	0
22	LMU	F	7036	34/35	0.76	0.30	19,32,42,45	0
19	CLA	3	3017	50/65	0.76	0.23	26,37,49,52	0
19	CLA	B	1301	36/65	0.76	0.30	27,28,29,29	0
22	LMU	R	7024	35/35	0.76	0.21	6,19,32,40	0
19	CLA	R	1144	57/65	0.76	0.25	24,27,28,28	0
22	LMU	A	7016	35/35	0.76	0.26	10,30,46,46	0
22	LMU	H	7002	35/35	0.77	0.17	16,29,41,43	0
19	CLA	3	3013	65/65	0.77	0.26	20,21,24,25	0
19	CLA	A	1105	46/65	0.77	0.37	22,23,24,24	0
22	LMU	H	7028	35/35	0.77	0.17	7,21,40,40	0
22	LMU	A	7045	35/35	0.77	0.19	11,23,41,43	0
19	CLA	3	3004	25/65	0.77	0.20	27,28,28,28	0
19	CLA	2	2010	25/65	0.77	0.28	23,23,24,24	0
19	CLA	2	2002	56/65	0.77	0.23	21,22,25,25	0
19	CLA	2	2003	25/65	0.77	0.38	23,24,25,25	0
19	CLA	1	1303	51/65	0.77	0.32	23,28,28,29	0
21	BCR	I	6021	40/40	0.77	0.30	16,20,22,22	0
19	CLA	K	1143	50/65	0.77	0.26	24,27,28,28	0
22	LMU	R	7014	35/35	0.77	0.35	9,26,40,44	0
19	CLA	2	2006	65/65	0.77	0.38	18,23,24,25	0
19	CLA	K	1146	50/65	0.77	0.27	25,28,30,30	0
22	LMU	R	7025	35/35	0.77	0.25	5,22,39,42	0
22	LMU	R	7020	35/35	0.78	0.23	7,26,40,44	0
19	CLA	A	1108	45/65	0.78	0.29	19,22,23,24	0
19	CLA	A	1116	52/65	0.78	0.28	24,25,26,26	0
19	CLA	3	2009	56/65	0.78	0.23	13,35,50,50	0
22	LMU	A	7044	35/35	0.78	0.18	8,20,39,40	0
19	CLA	B	1218	46/65	0.78	0.30	20,20,22,23	0
19	CLA	4	4005	25/65	0.78	0.27	20,21,22,22	0
19	CLA	4	4006	55/65	0.78	0.23	16,23,24,24	0
19	CLA	1	1007	61/65	0.78	0.26	14,20,21,22	0
19	CLA	4	4010	25/65	0.78	0.23	26,27,27,27	0
19	CLA	B	1222	58/65	0.79	0.35	18,21,23,24	0
19	CLA	A	1102	55/65	0.79	0.30	13,19,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	BCR	L	6019	40/40	0.79	0.34	15,17,19,19	0
22	LMU	A	7023	35/35	0.79	0.25	6,20,39,41	0
19	CLA	3	3001	25/65	0.79	0.28	24,25,25,25	0
22	LMU	R	7022	35/35	0.79	0.18	5,21,33,35	0
21	BCR	B	6006	40/40	0.80	0.38	15,19,20,21	0
19	CLA	B	1201	45/65	0.80	0.28	19,21,22,22	0
22	LMU	4	7033	35/35	0.80	0.20	12,26,40,41	0
19	CLA	2	4009	65/65	0.80	0.23	18,23,24,24	0
19	CLA	J	1308	55/65	0.80	0.23	12,30,44,45	0
21	BCR	A	6008	40/40	0.80	0.35	21,24,27,27	0
21	BCR	B	6004	40/40	0.80	0.33	18,20,22,22	0
19	CLA	A	1119	65/65	0.81	0.35	13,18,19,20	0
19	CLA	A	1115	65/65	0.81	0.24	10,28,41,42	0
19	CLA	1	1002	47/65	0.81	0.23	22,23,24,24	0
19	CLA	L	1130	65/65	0.81	0.28	13,18,19,20	0
19	CLA	A	1110	54/65	0.81	0.25	19,22,23,23	0
19	CLA	L	1503	50/65	0.81	0.25	19,21,23,24	0
19	CLA	H	1207	65/65	0.81	0.28	15,17,19,20	0
19	CLA	B	1231	45/65	0.81	0.28	19,20,21,21	0
21	BCR	B	6017	40/40	0.81	0.34	15,18,20,20	0
21	BCR	I	6018	40/40	0.81	0.31	14,15,18,18	0
22	LMU	B	7012	25/35	0.81	0.18	22,32,44,49	0
21	BCR	B	6010	40/40	0.82	0.34	13,15,16,16	0
19	CLA	B	1229	65/65	0.82	0.27	8,12,14,15	0
19	CLA	1	1005	46/65	0.82	0.23	19,21,22,22	0
19	CLA	B	1223	65/65	0.82	0.32	13,18,19,20	0
22	LMU	H	7032	35/35	0.82	0.31	8,25,36,45	0
19	CLA	1	1011	36/65	0.82	0.22	27,27,28,28	0
19	CLA	2	2012	50/65	0.82	0.26	20,22,23,23	0
19	CLA	4	4002	52/65	0.83	0.21	21,22,24,25	0
19	CLA	A	1123	65/65	0.83	0.30	12,18,19,20	0
19	CLA	B	1209	55/65	0.83	0.25	18,19,20,21	0
19	CLA	B	1211	65/65	0.83	0.31	17,20,21,21	0
19	CLA	L	1502	47/65	0.83	0.25	17,19,20,20	0
21	BCR	F	6014	40/40	0.83	0.31	9,11,15,15	0
19	CLA	B	1230	50/65	0.83	0.28	17,18,19,20	0
19	CLA	A	1117	65/65	0.84	0.31	10,20,21,22	0
19	CLA	A	1124	65/65	0.84	0.28	18,21,23,24	0
21	BCR	F	6016	40/40	0.84	0.28	13,16,17,17	0
19	CLA	A	1109	65/65	0.84	0.28	13,20,22,23	0
19	CLA	B	1216	61/65	0.84	0.28	12,18,19,20	0
19	CLA	B	1217	50/65	0.84	0.26	19,21,22,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	A	1135	51/65	0.84	0.27	16,19,19,21	0
19	CLA	A	1111	54/65	0.84	0.26	20,24,24,24	0
19	CLA	I	1204	60/65	0.84	0.24	13,17,18,18	0
19	CLA	4	4013	25/65	0.84	0.19	20,21,21,21	0
19	CLA	A	1138	65/65	0.85	0.29	15,18,19,20	0
19	CLA	B	1219	55/65	0.85	0.24	18,18,21,21	0
19	CLA	A	1140	65/65	0.85	0.28	15,18,19,21	0
22	LMU	A	7035	35/35	0.85	0.27	6,18,32,40	0
19	CLA	B	1234	60/65	0.85	0.28	13,14,21,21	0
19	CLA	A	1120	51/65	0.85	0.37	22,24,24,26	0
19	CLA	B	1208	54/65	0.85	0.26	18,18,21,22	0
19	CLA	4	1009	36/65	0.85	0.20	20,22,22,23	0
19	CLA	A	1103	65/65	0.85	0.29	13,14,21,22	0
22	LMU	R	7007	35/35	0.85	0.24	8,21,40,41	0
19	CLA	L	1501	50/65	0.85	0.24	20,20,21,21	0
19	CLA	A	1237	65/65	0.86	0.28	8,17,18,18	0
19	CLA	1	1012	36/65	0.86	0.22	23,24,25,25	0
19	CLA	A	1132	65/65	0.86	0.27	13,17,18,19	0
19	CLA	B	1228	50/65	0.86	0.23	12,14,14,15	0
21	BCR	A	6011	40/40	0.86	0.30	10,15,16,16	0
19	CLA	4	4011	25/65	0.86	0.18	10,11,12,12	0
19	CLA	4	4012	36/65	0.86	0.21	14,15,16,16	0
19	CLA	A	1133	50/65	0.86	0.23	17,19,19,20	0
19	CLA	B	1238	65/65	0.86	0.27	10,14,15,16	0
19	CLA	A	1128	65/65	0.86	0.27	14,16,17,18	0
19	CLA	B	1239	65/65	0.87	0.30	8,11,13,14	0
22	LMU	G	7039	35/35	0.87	0.15	15,30,47,47	0
21	BCR	B	6005	40/40	0.87	0.29	14,16,17,17	0
19	CLA	A	1107	55/65	0.87	0.26	15,16,24,24	0
19	CLA	F	1240	36/65	0.87	0.23	15,16,17,17	0
19	CLA	B	1220	65/65	0.87	0.24	13,15,20,21	0
19	CLA	B	1214	59/65	0.87	0.24	18,20,22,23	0
19	CLA	A	1125	65/65	0.87	0.24	15,17,19,20	0
19	CLA	A	1101	50/65	0.87	0.23	17,18,18,19	0
19	CLA	B	1206	65/65	0.87	0.27	10,12,17,18	0
19	CLA	B	1235	65/65	0.88	0.26	14,15,16,17	0
19	CLA	B	1236	47/65	0.88	0.28	14,15,17,17	0
19	CLA	B	1226	65/65	0.88	0.31	11,12,19,19	0
19	CLA	A	1129	50/65	0.88	0.20	17,19,20,20	0
20	PQN	A	5001	33/33	0.88	0.29	12,13,14,15	0
19	CLA	A	1131	65/65	0.88	0.25	12,14,16,16	0
19	CLA	A	1126	65/65	0.88	0.29	12,14,15,15	0

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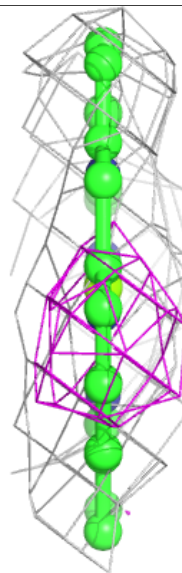
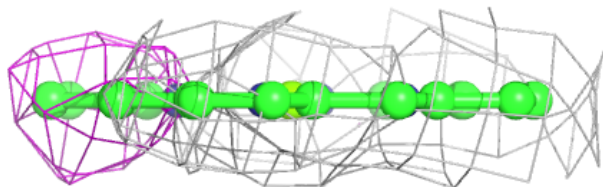
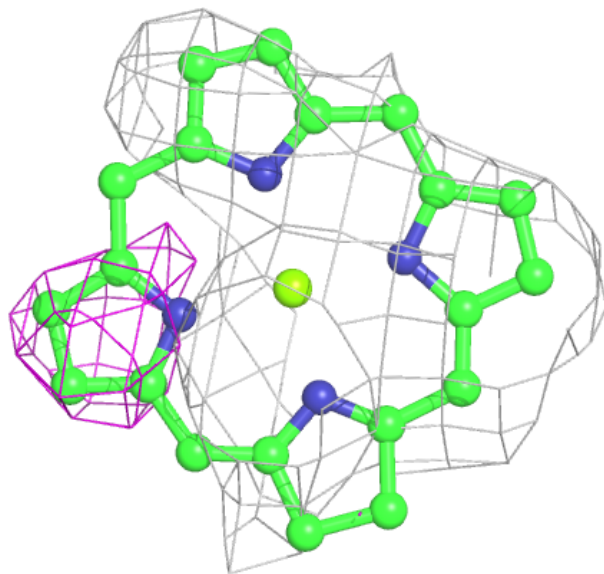
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	A	1139	51/65	0.88	0.23	16,16,17,18	0
19	CLA	A	1122	55/65	0.88	0.22	13,14,18,18	0
19	CLA	B	1224	65/65	0.88	0.27	9,13,14,15	0
19	CLA	B	1225	65/65	0.88	0.29	9,12,13,14	0
19	CLA	A	1136	65/65	0.89	0.27	14,15,16,17	0
19	CLA	B	1202	65/65	0.89	0.25	7,16,16,18	0
19	CLA	B	1215	60/65	0.89	0.27	11,13,15,16	0
19	CLA	B	1205	65/65	0.89	0.26	9,13,14,14	0
19	CLA	B	1227	50/65	0.89	0.23	13,15,16,17	0
19	CLA	A	1127	55/65	0.89	0.25	13,16,17,18	0
19	CLA	A	1104	57/65	0.89	0.27	13,15,18,18	0
19	CLA	B	9010	65/65	0.89	0.25	2,12,34,40	0
19	CLA	A	9012	65/65	0.89	0.25	2,14,28,36	0
21	BCR	B	6020	40/40	0.89	0.25	8,11,12,13	0
19	CLA	A	9013	65/65	0.89	0.25	2,10,29,32	0
19	CLA	A	9023	65/65	0.89	0.27	2,14,29,38	0
19	CLA	A	9022	65/65	0.90	0.28	2,12,26,31	0
19	CLA	A	1137	47/65	0.90	0.24	13,14,15,17	0
19	CLA	B	1210	65/65	0.90	0.23	16,20,21,22	0
19	CLA	A	1106	65/65	0.91	0.29	10,12,13,14	0
20	PQN	B	5002	33/33	0.91	0.26	7,8,14,14	0
19	CLA	A	9011	65/65	0.91	0.26	2,11,30,40	0
19	CLA	B	1203	65/65	0.91	0.24	10,13,14,15	0
19	CLA	B	1221	54/65	0.91	0.22	13,13,16,16	0
23	SF4	C	8002	8/8	0.97	0.08	14,16,24,28	0
23	SF4	C	8003	8/8	0.98	0.07	14,19,21,22	0
23	SF4	A	8001	8/8	0.99	0.09	12,17,19,21	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.

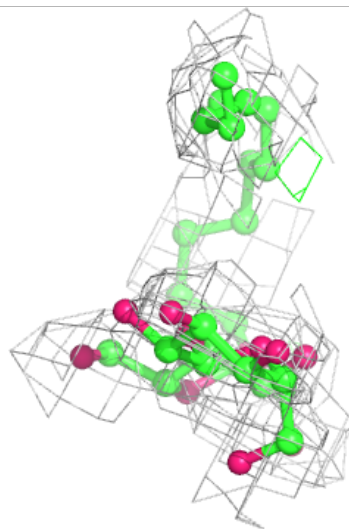
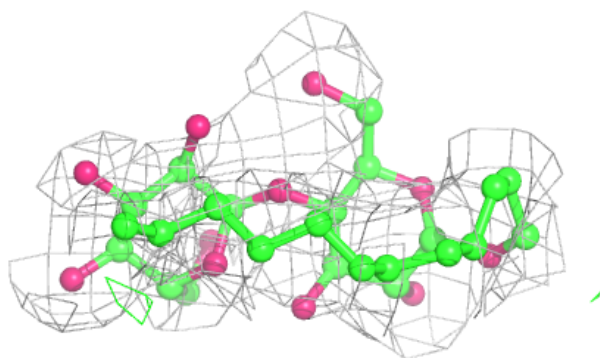
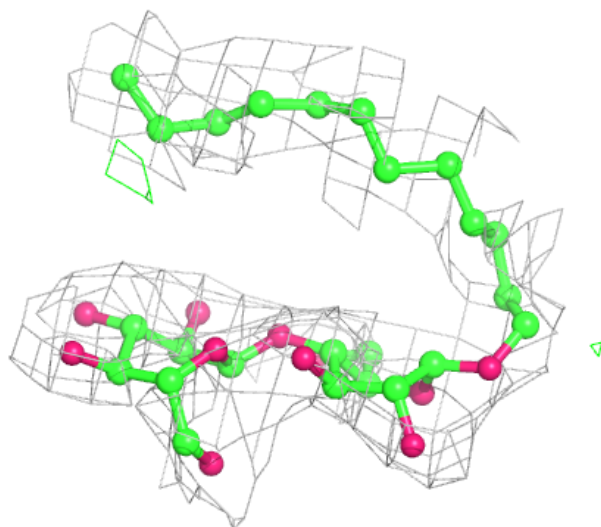
Electron density around CLA 3 3014:

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



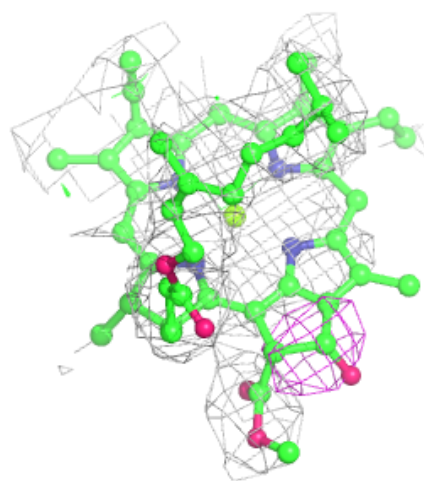
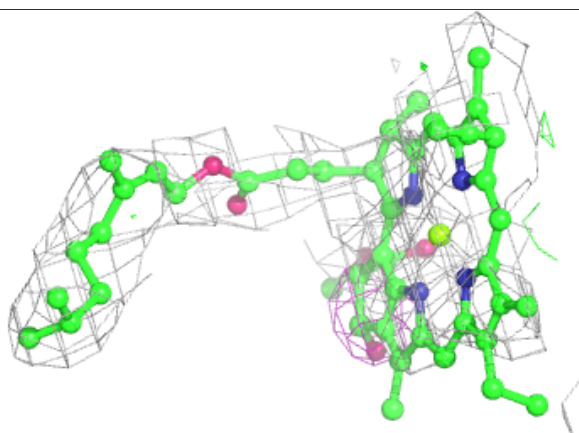
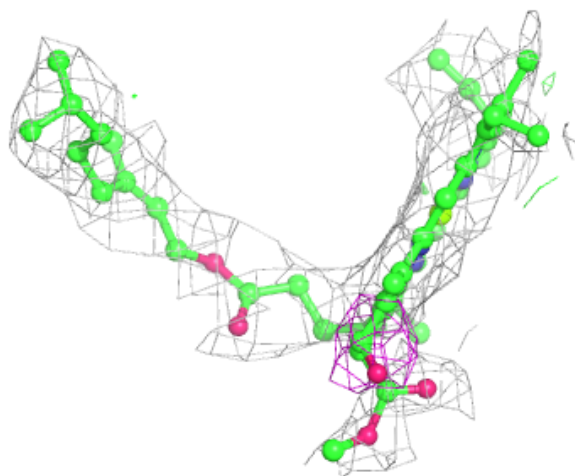
Electron density around LMU 1 7013:

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



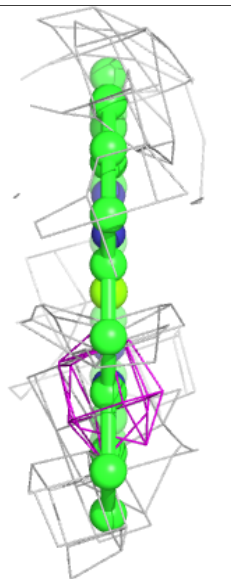
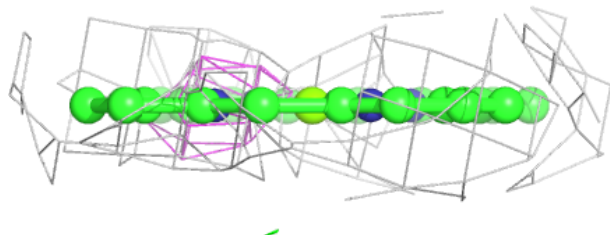
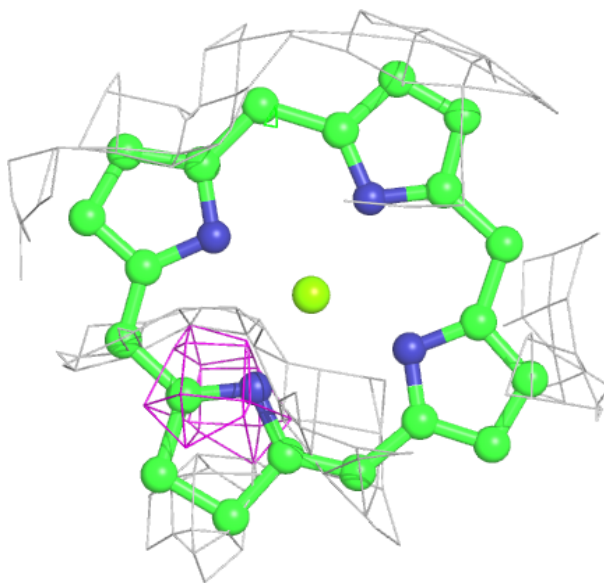
Electron density around CLA L 1504:

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



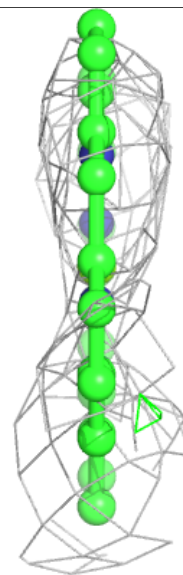
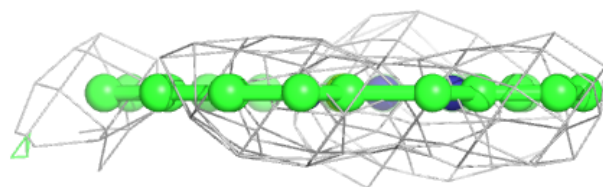
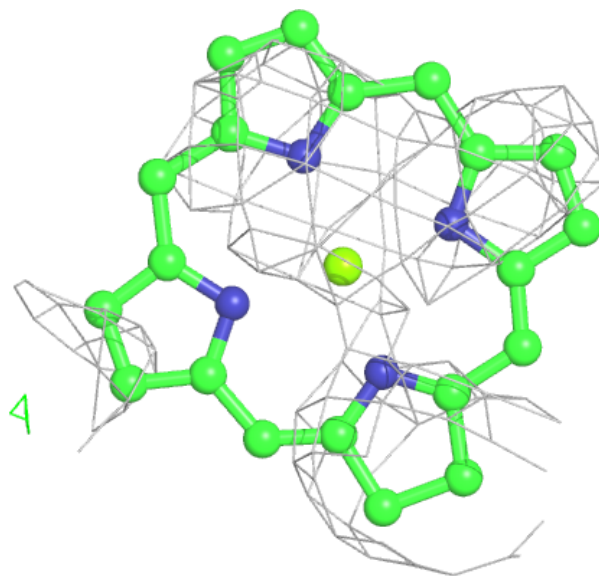
Electron density around CLA 3 3012:

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



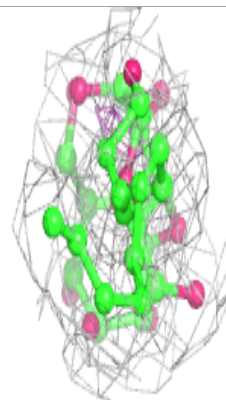
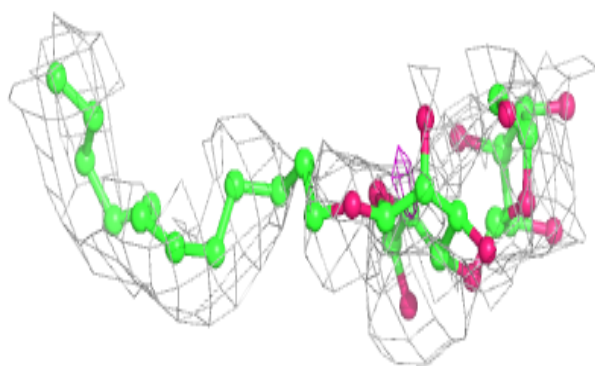
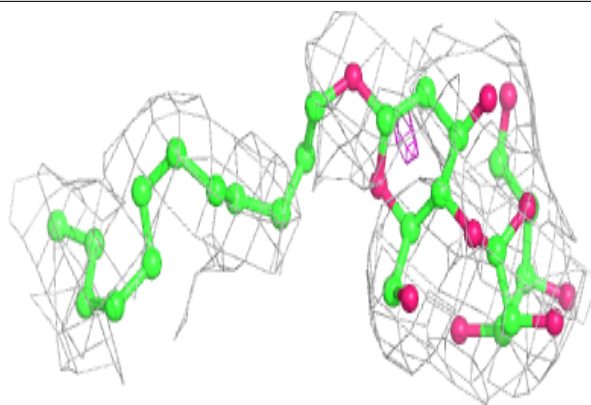
Electron density around CLA A 1309:

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



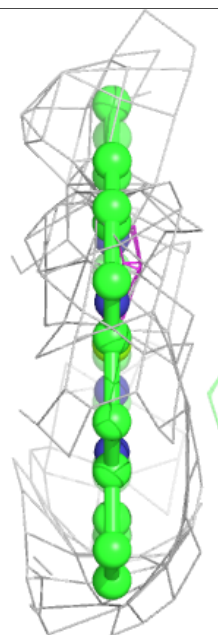
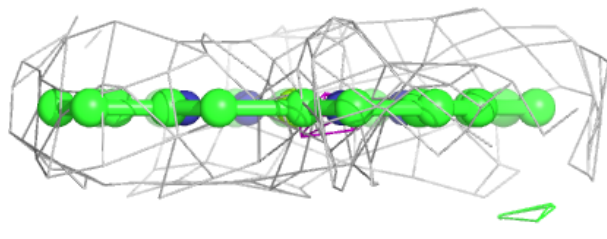
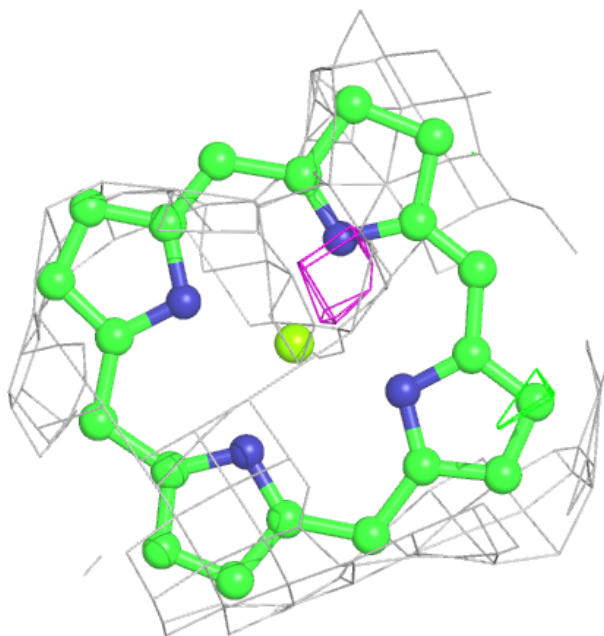
Electron density around LMU E 7048:

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



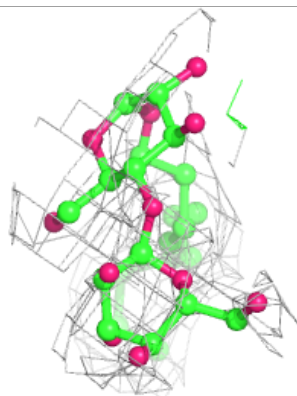
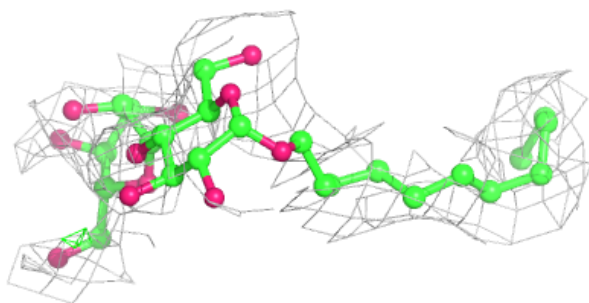
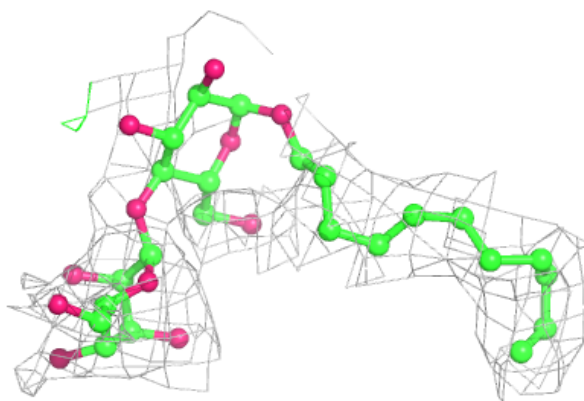
Electron density around CLA 3 3005:

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

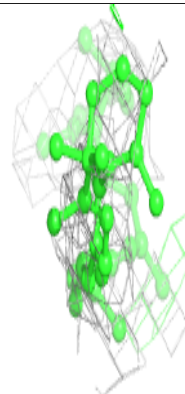
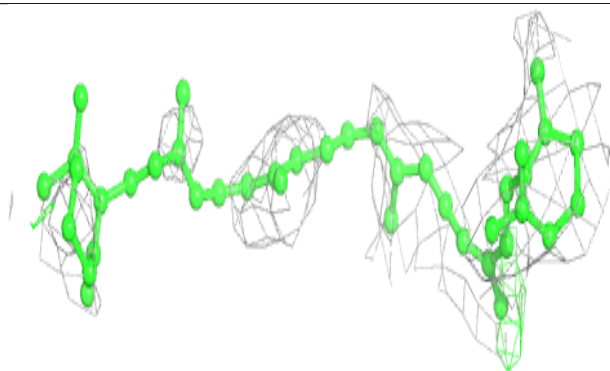
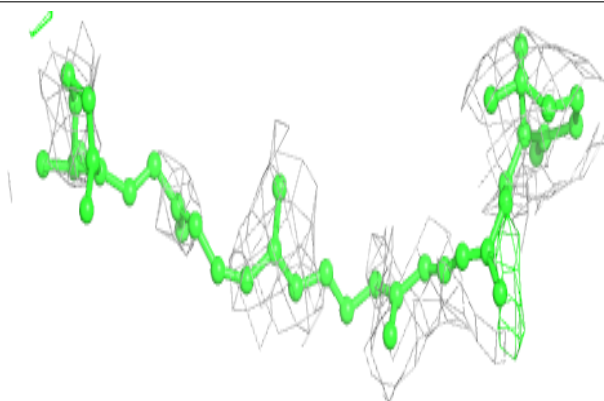


Electron density around LMU 4 7053:

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

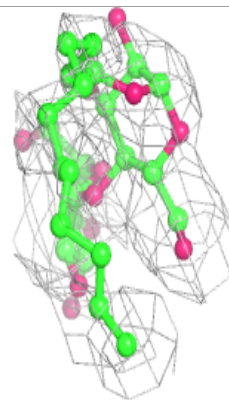
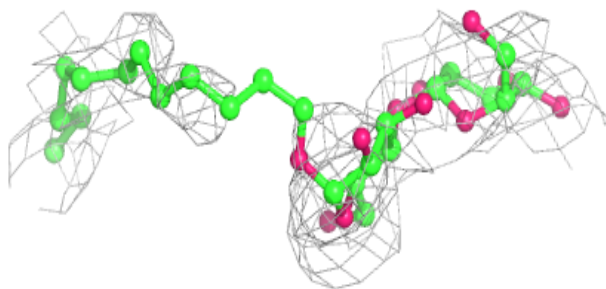
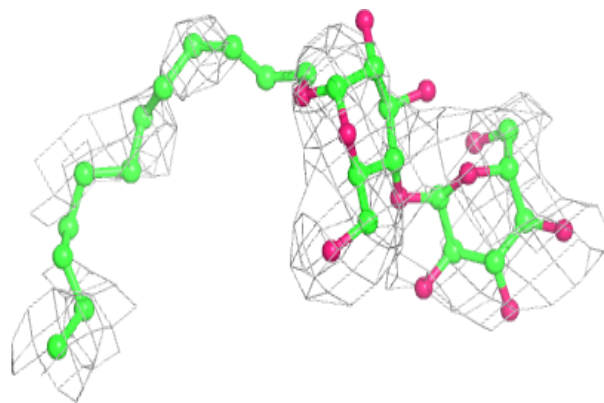
**Electron density around BCR 1 6023:**

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



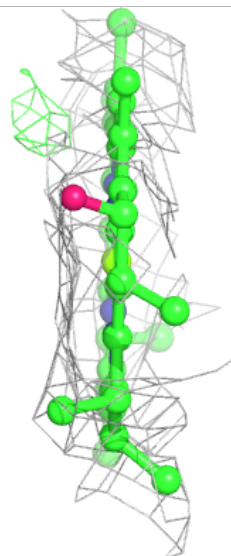
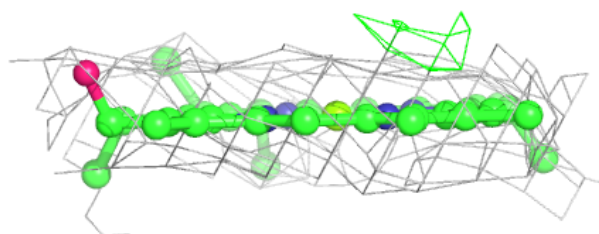
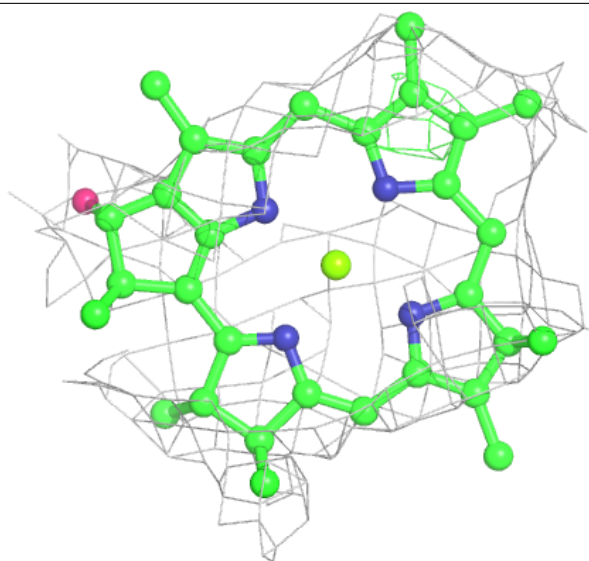
Electron density around LMU 1 7004:

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



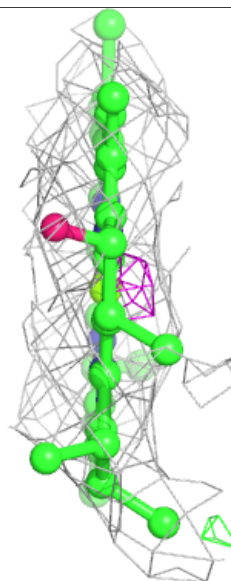
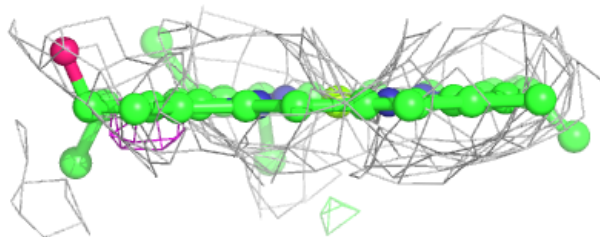
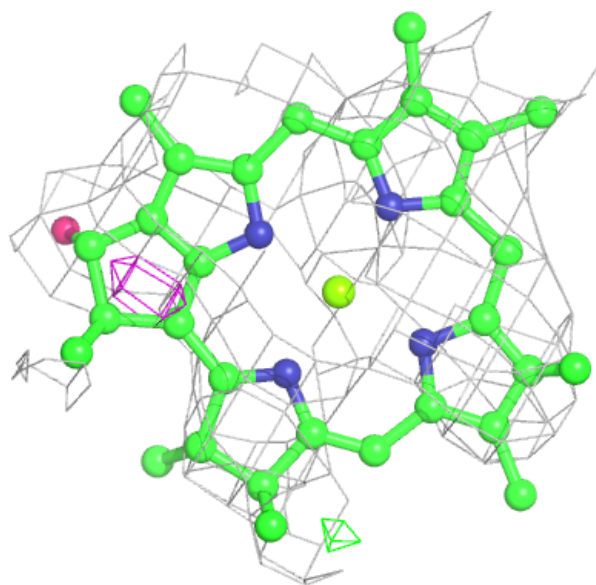
Electron density around CLA 3 1118:

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



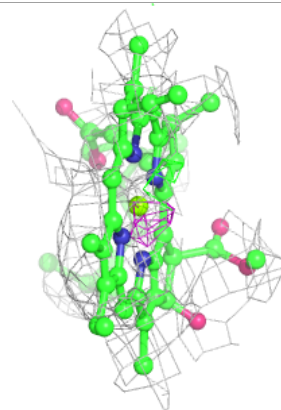
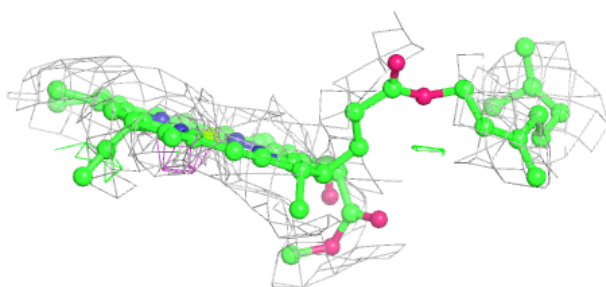
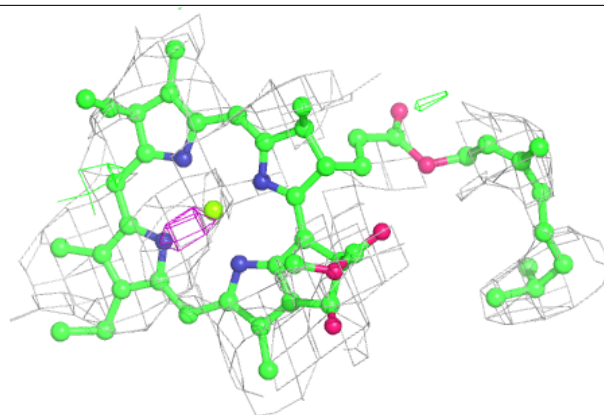
Electron density around CLA 1 1006:

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

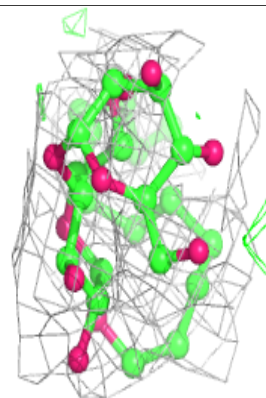
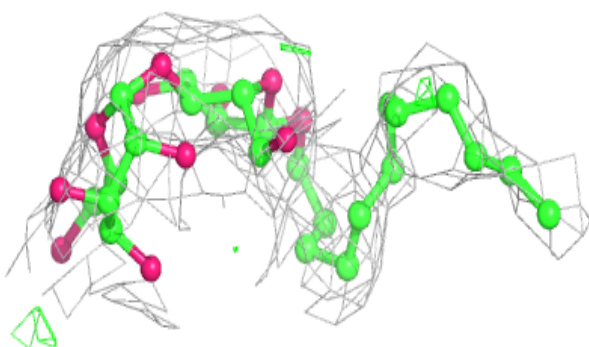
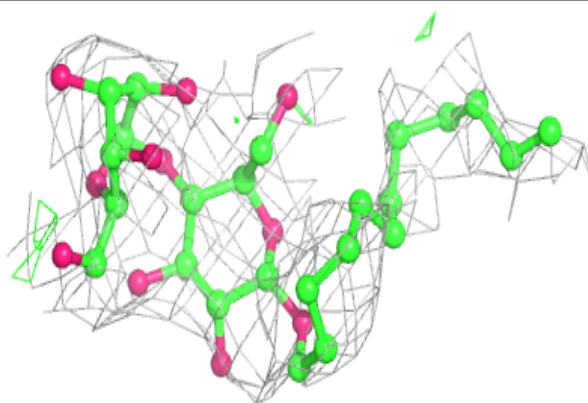


Electron density around CLA 4 4003:

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

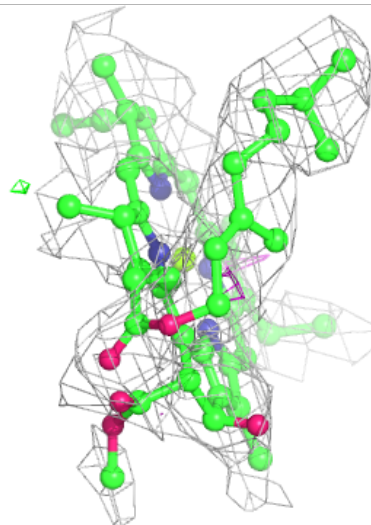
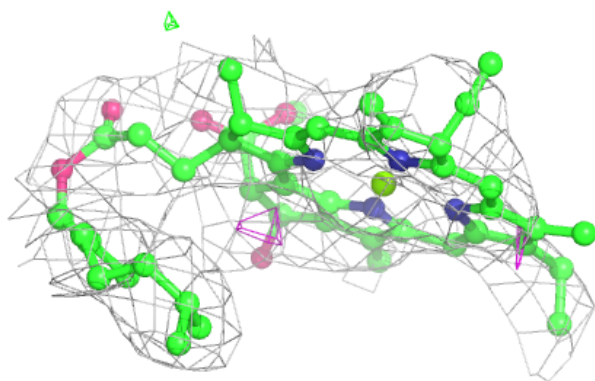
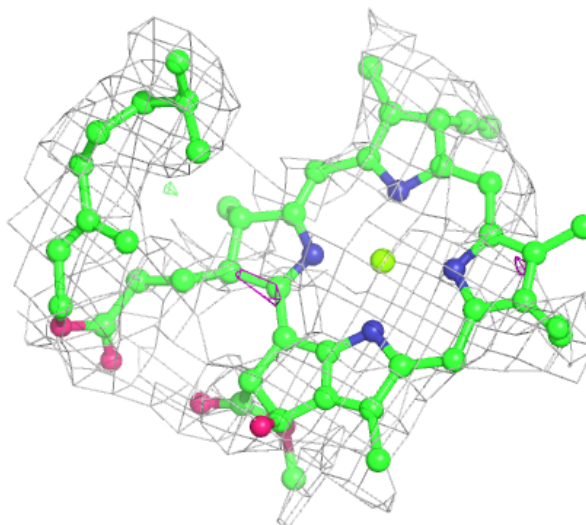
**Electron density around LMU L 7029:**

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



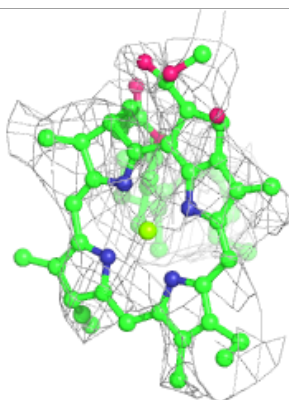
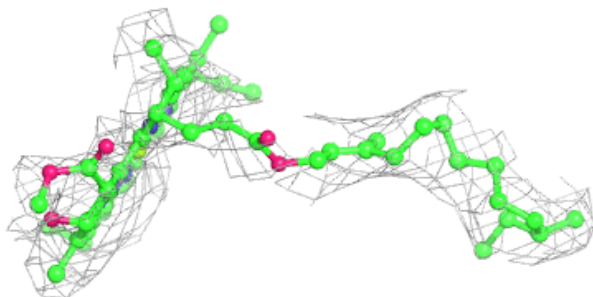
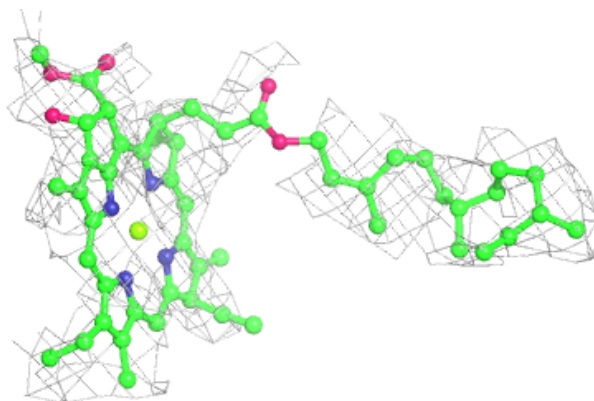
Electron density around CLA H 1505:

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

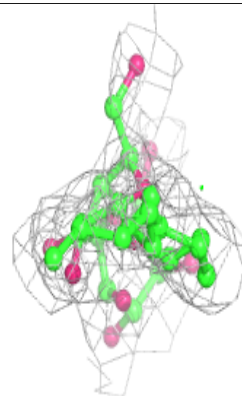
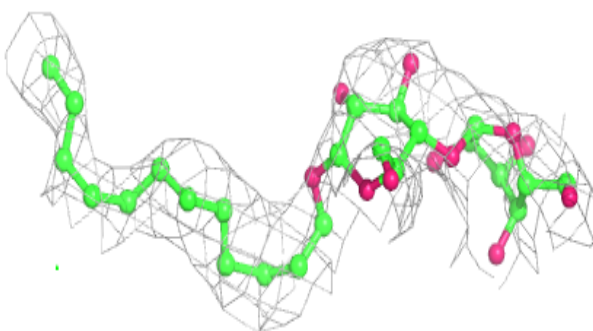
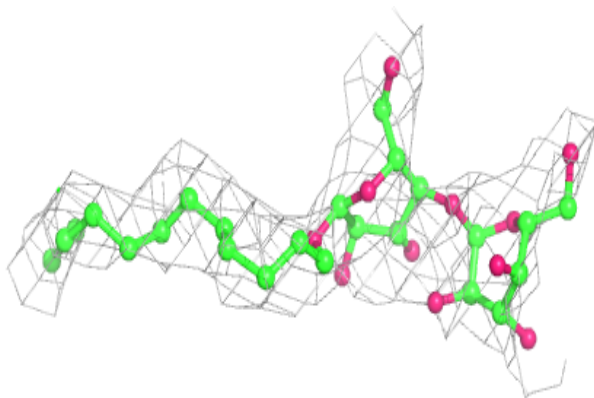


Electron density around CLA 2 2014:

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

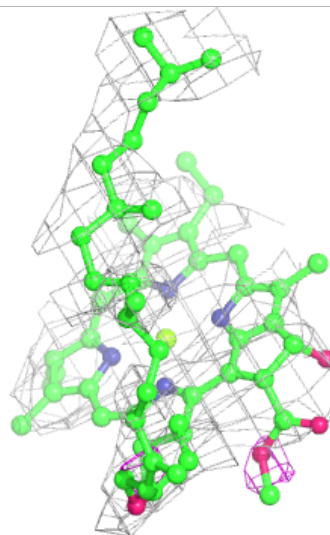
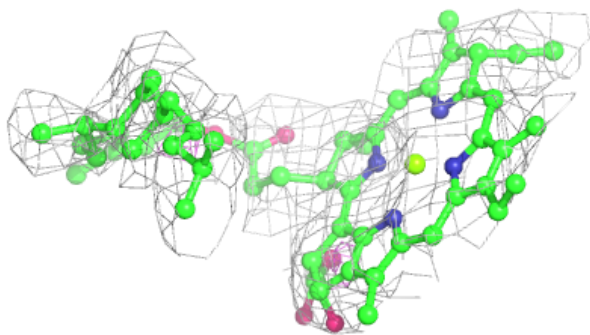
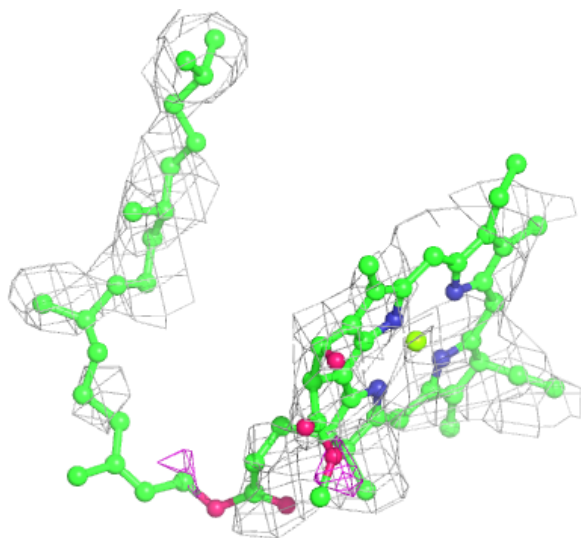
**Electron density around LMU A 7010:**

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



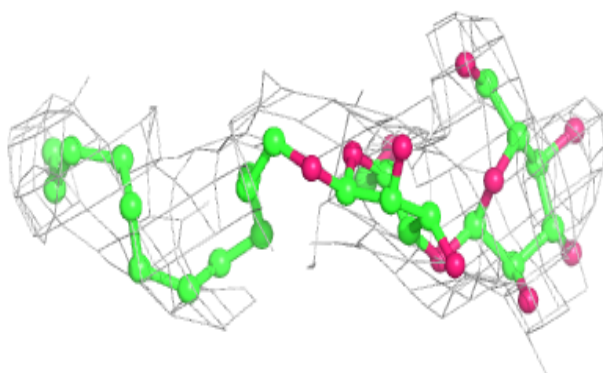
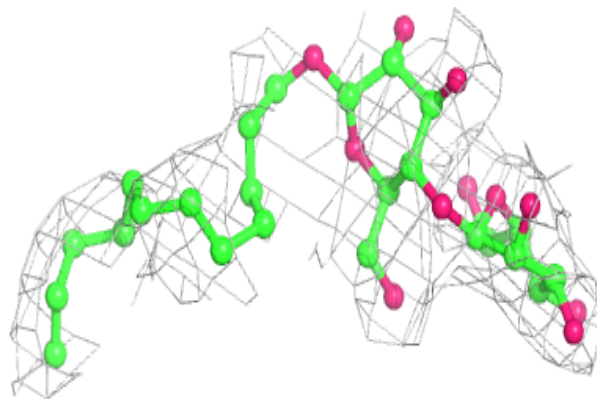
Electron density around CLA 3 3016:

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

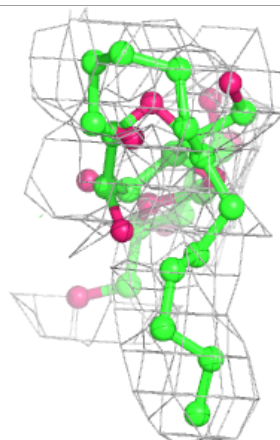
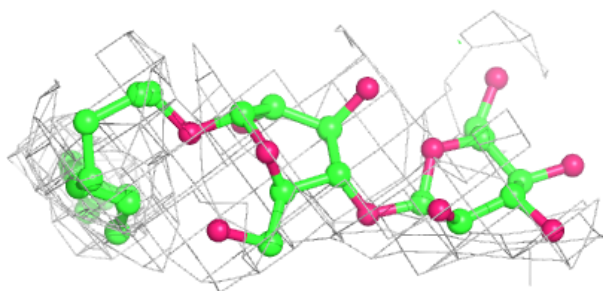
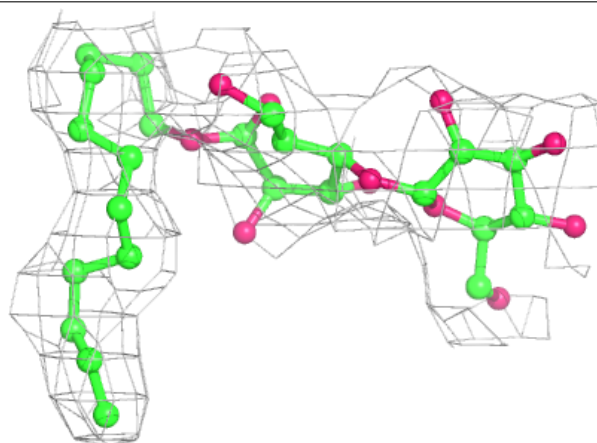


Electron density around LMU 2 7046:

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

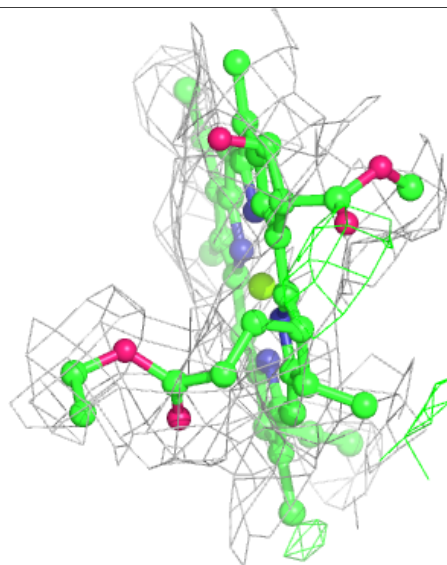
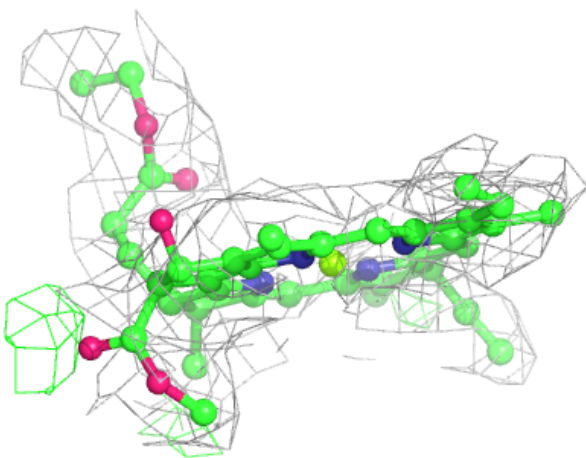
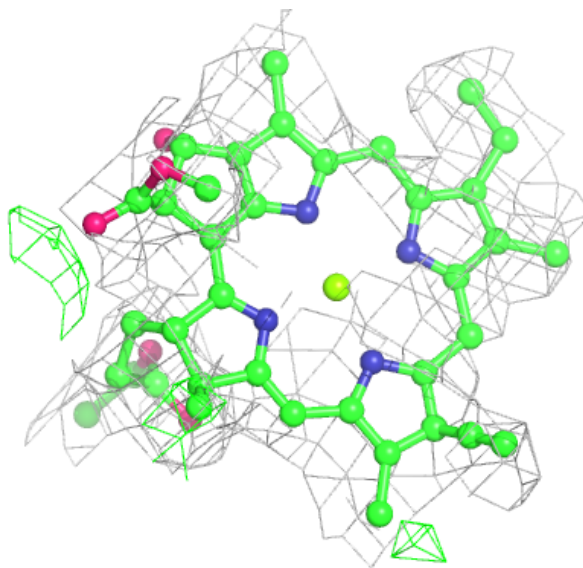
**Electron density around LMU 4 7052:**

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



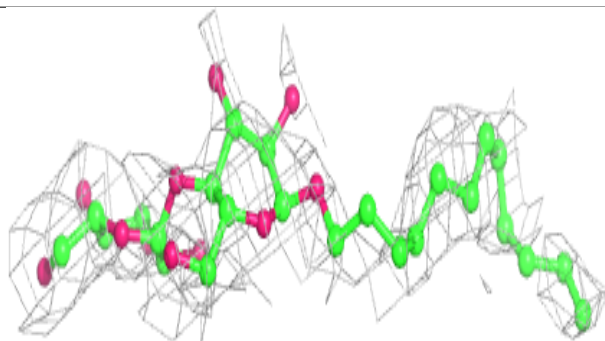
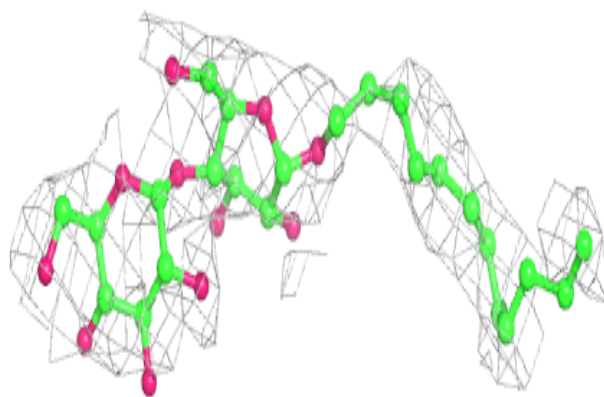
Electron density around CLA 4 4014:

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

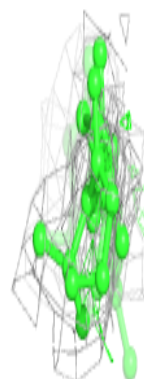
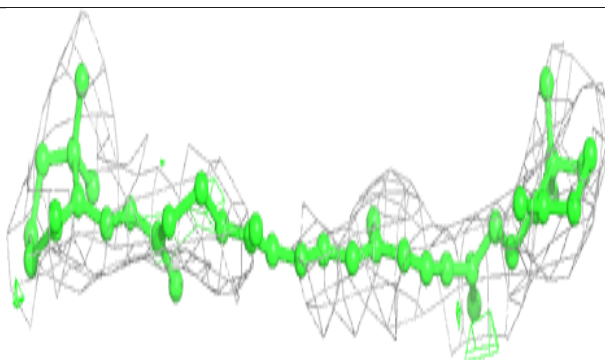
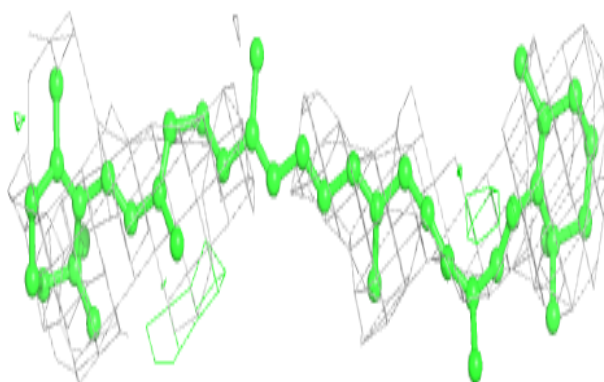


Electron density around LMU B 7038:

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

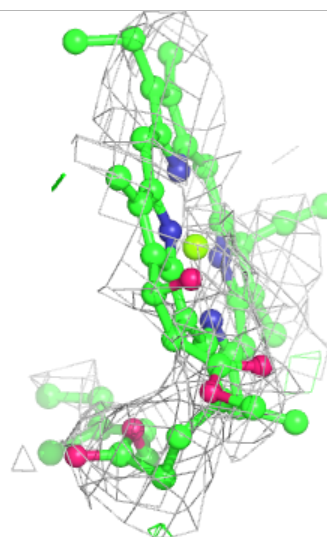
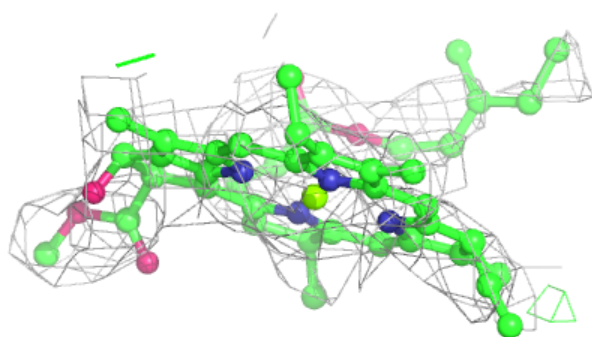
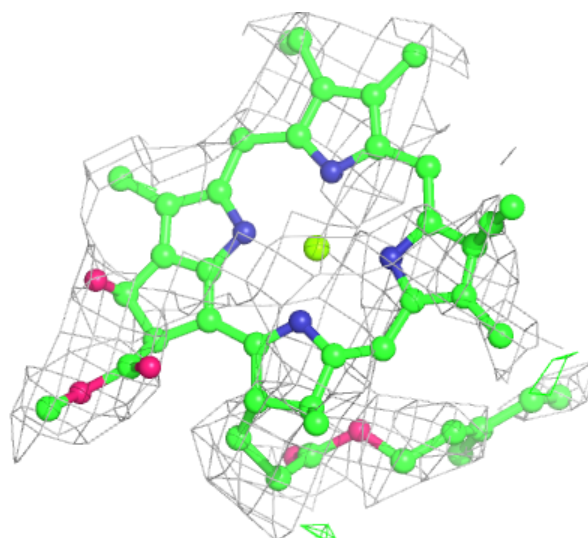
**Electron density around BCR A 6002:**

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



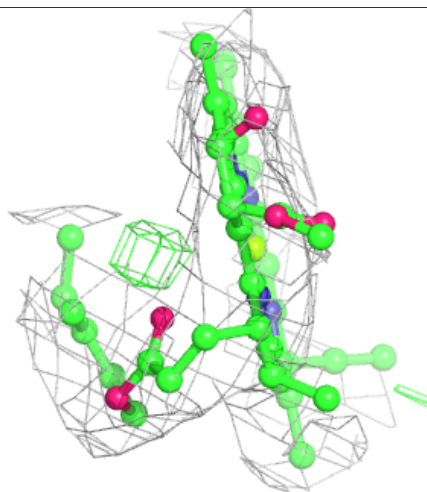
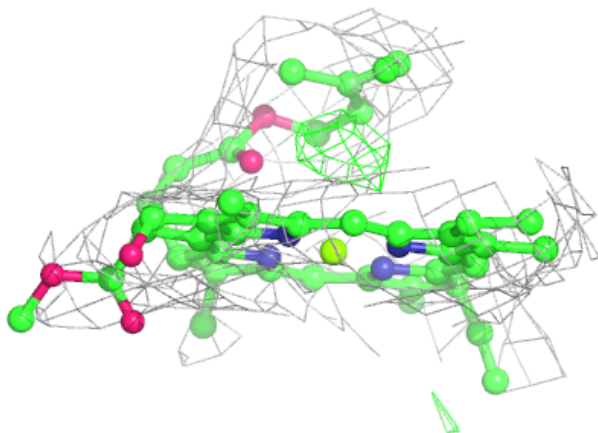
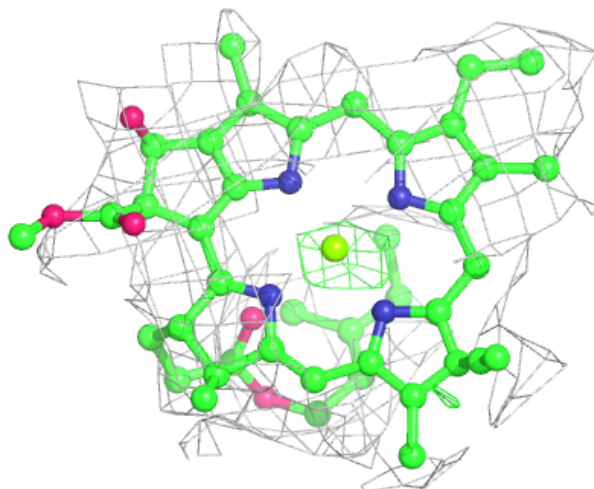
Electron density around CLA B 1233:

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



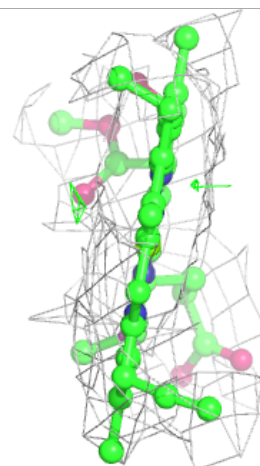
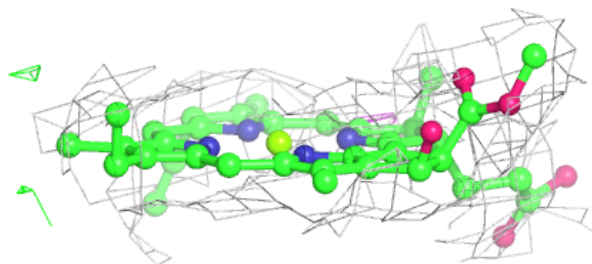
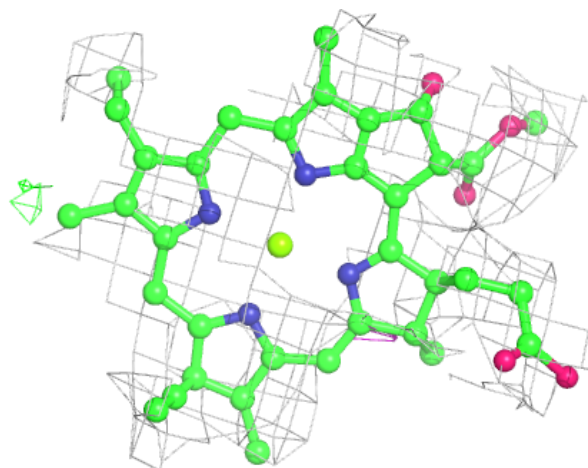
Electron density around CLA 2 2001:

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



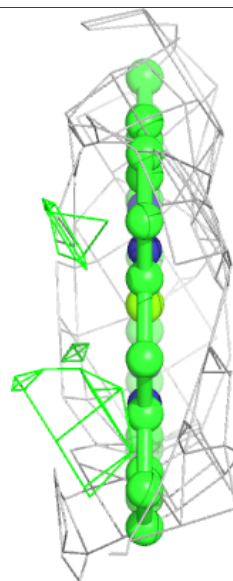
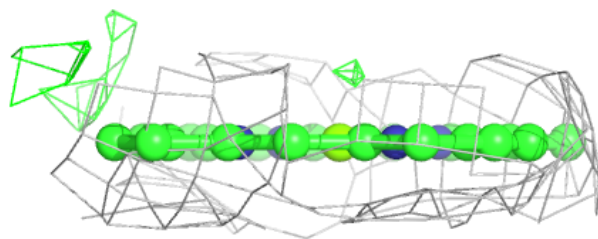
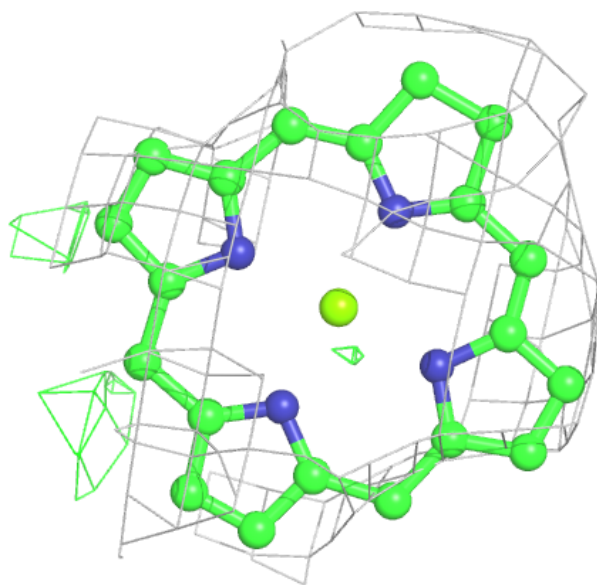
Electron density around CLA K 1142:

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



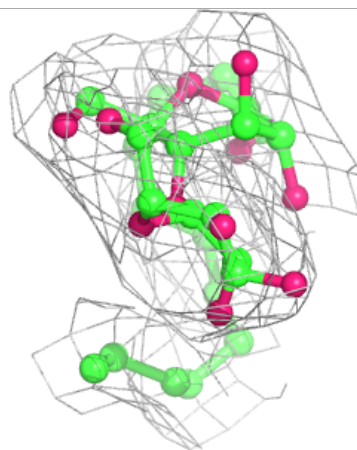
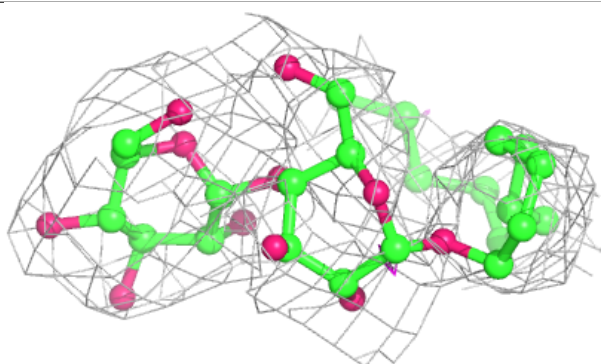
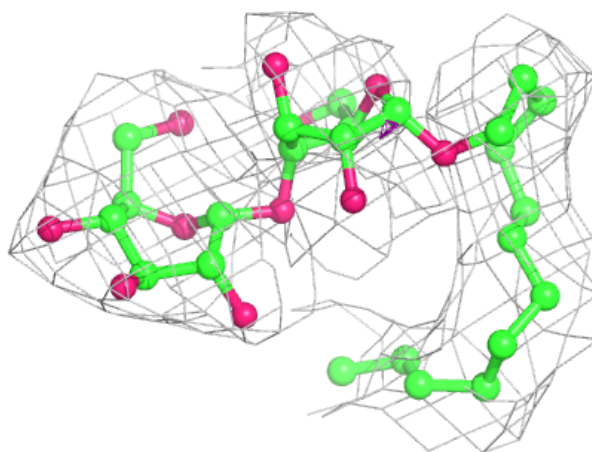
Electron density around CLA 2 2005:

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



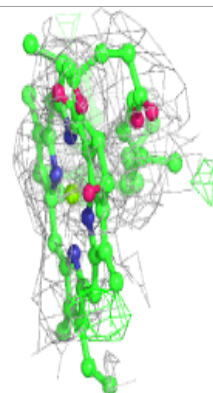
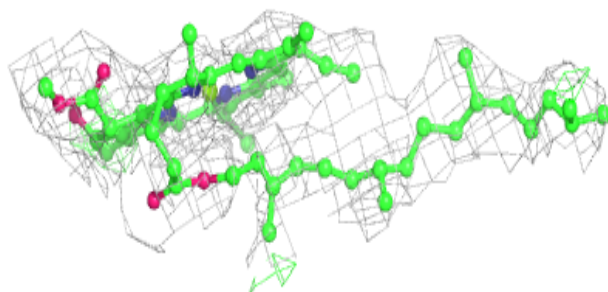
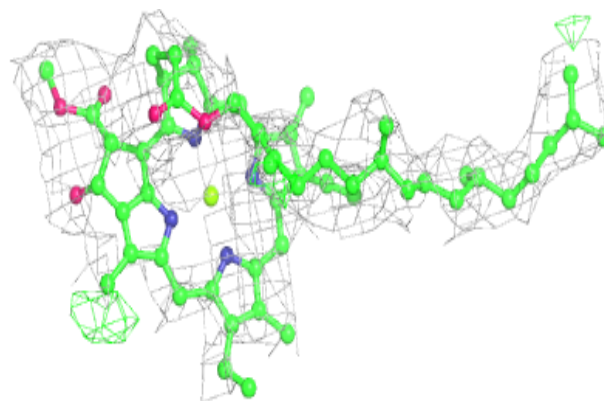
Electron density around LMU N 7049:

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



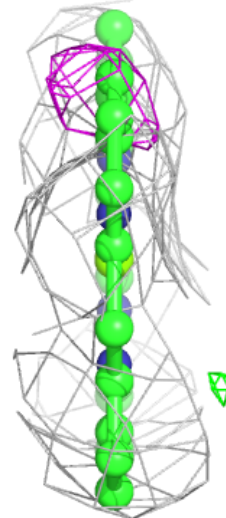
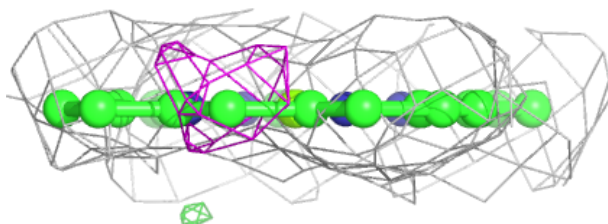
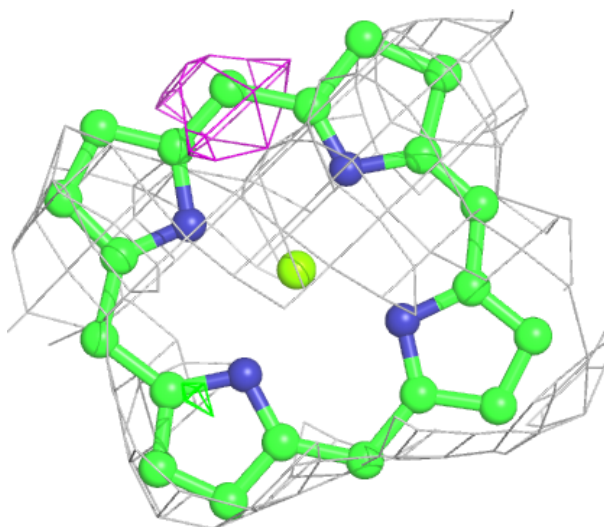
Electron density around CLA 2 2007:

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



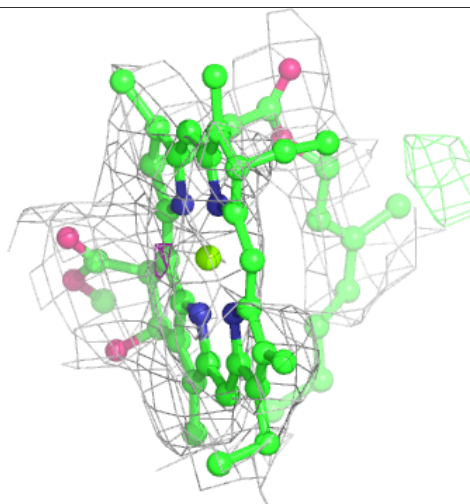
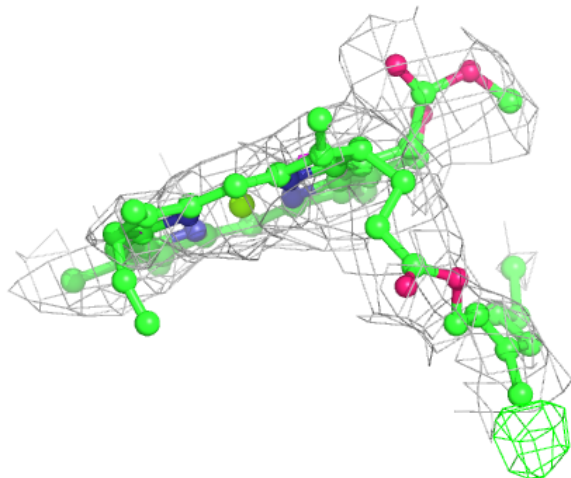
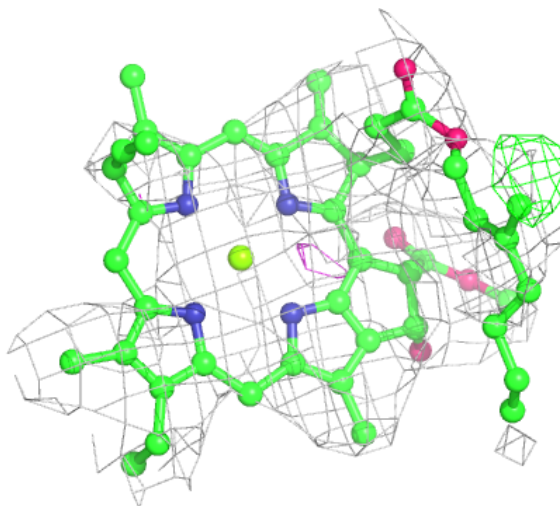
Electron density around CLA 4 4004:

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



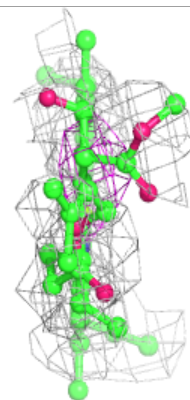
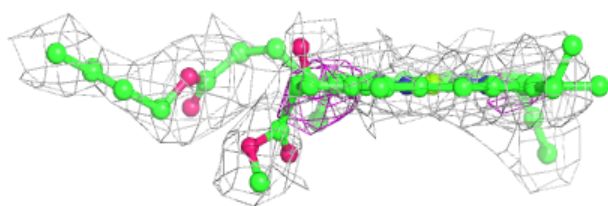
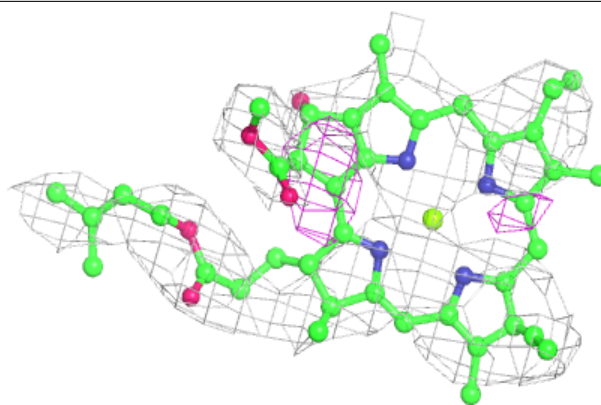
Electron density around CLA F 1305:

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

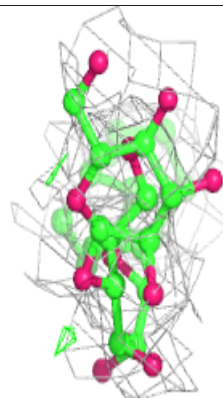
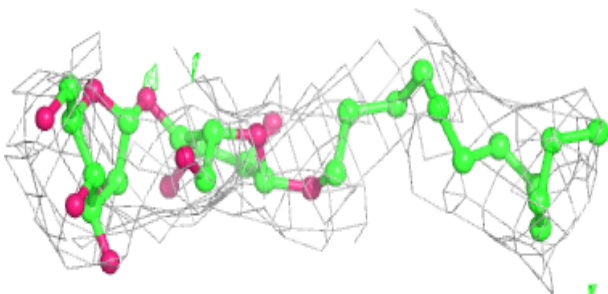
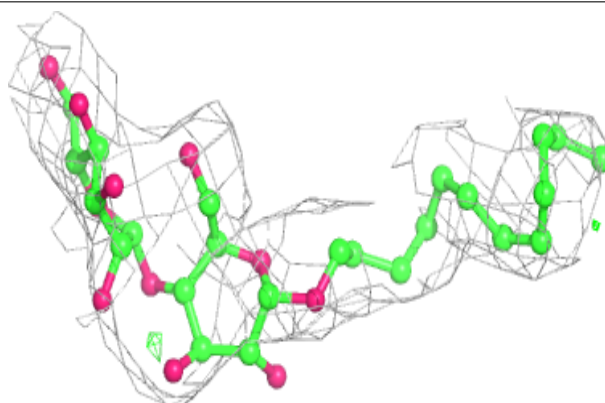


Electron density around CLA 4 4001:

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

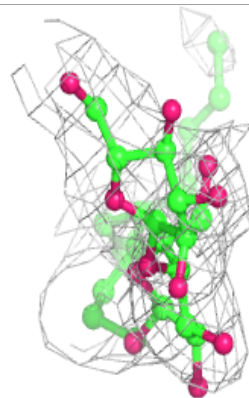
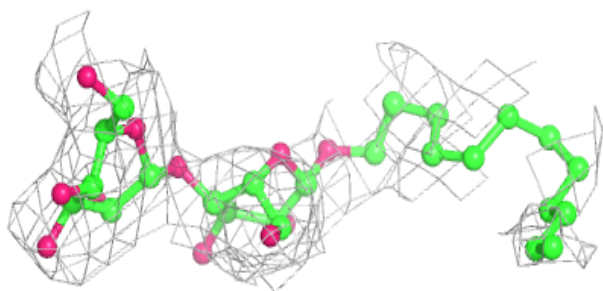
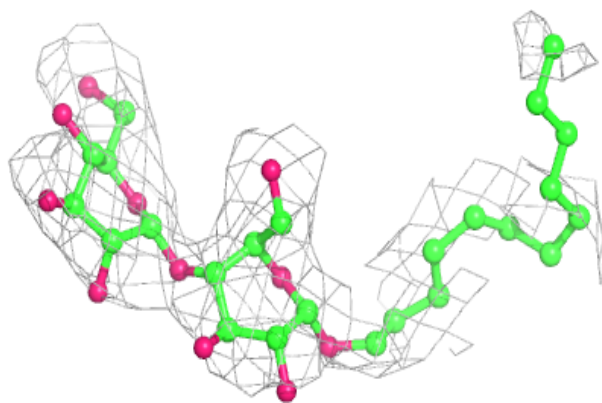
**Electron density around LMU H 7011:**

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



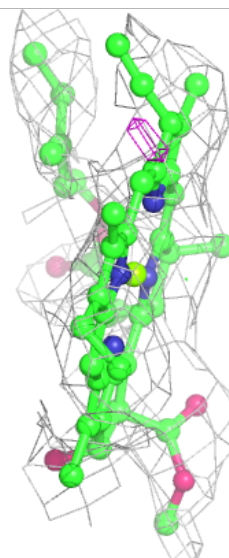
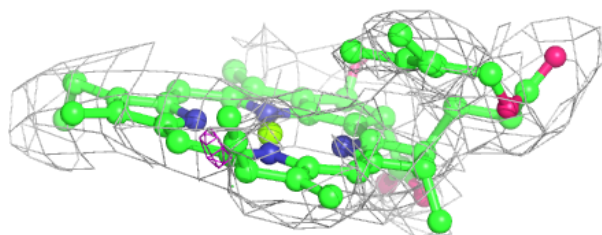
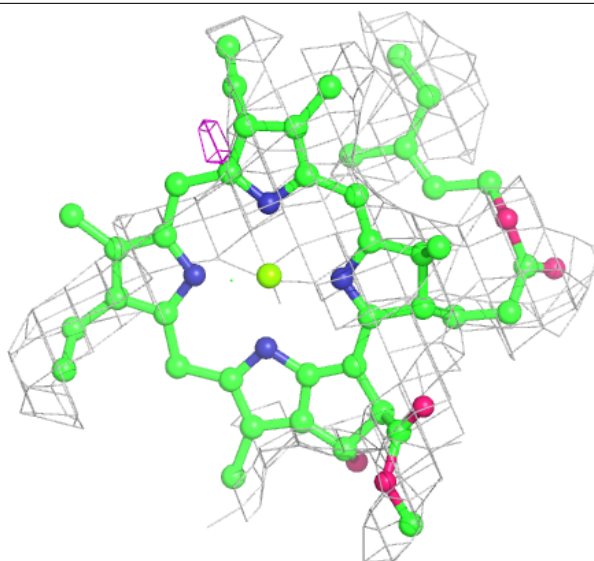
Electron density around LMU H 7030:

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



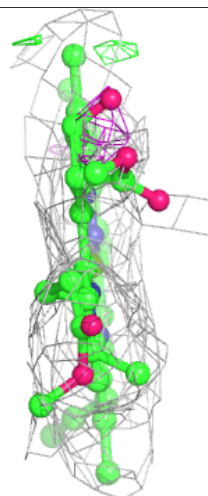
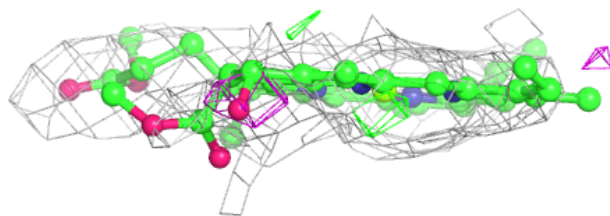
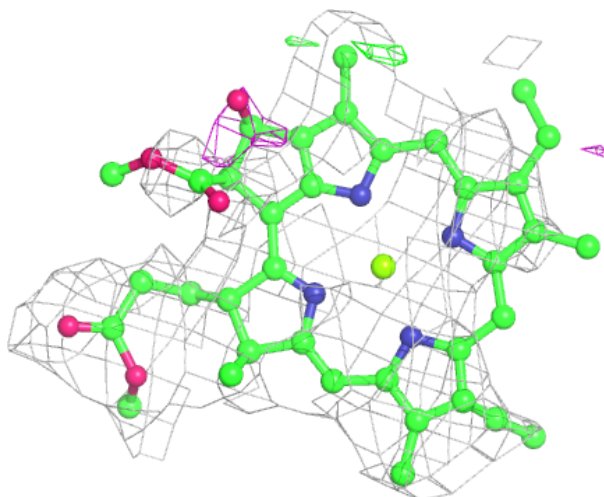
Electron density around CLA G 1242:

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



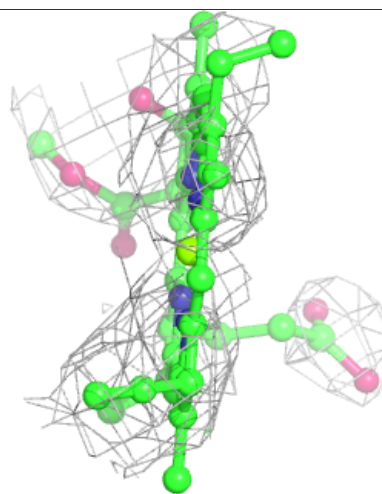
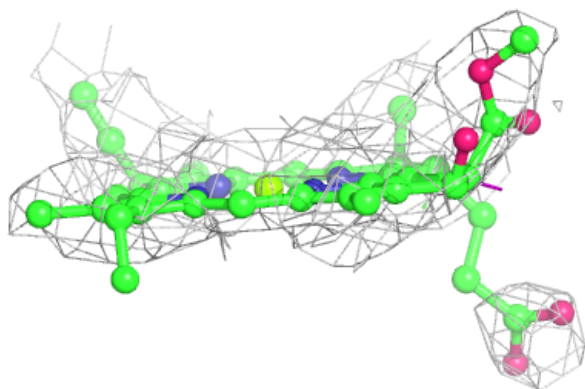
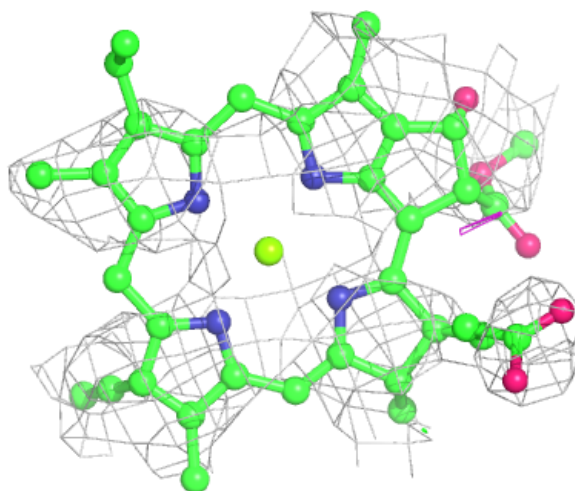
Electron density around CLA B 1213:

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



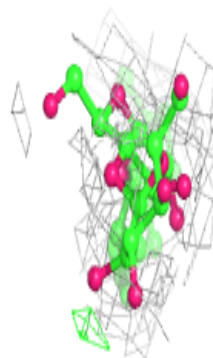
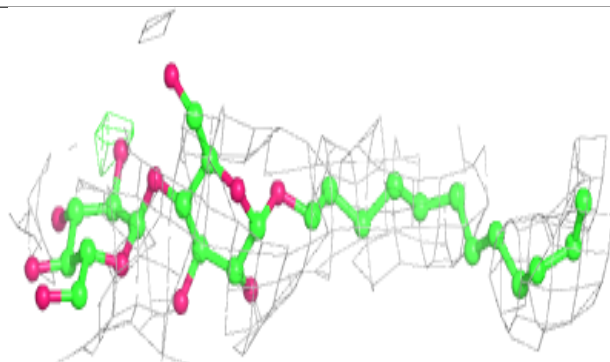
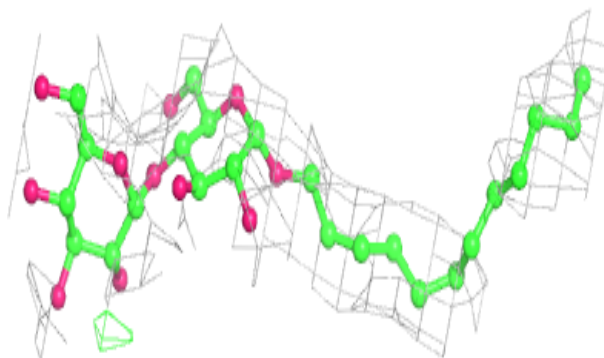
Electron density around CLA B 1232:

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



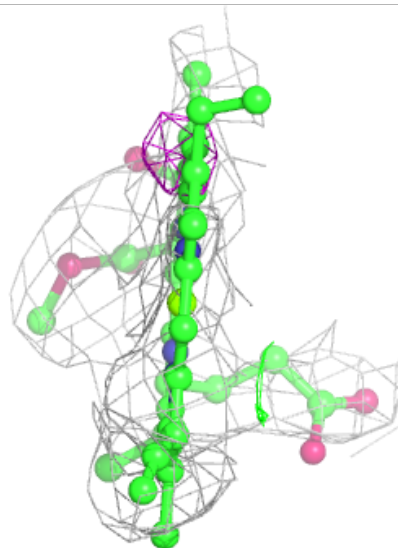
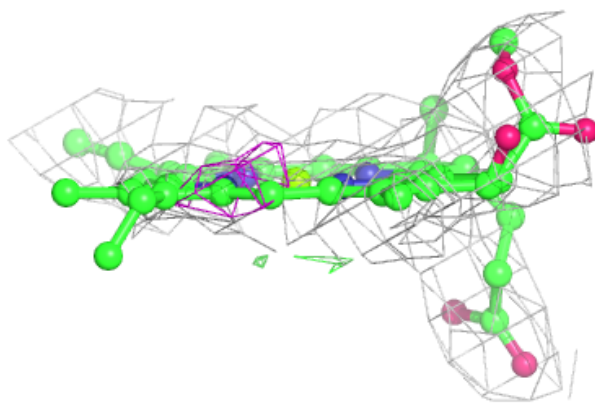
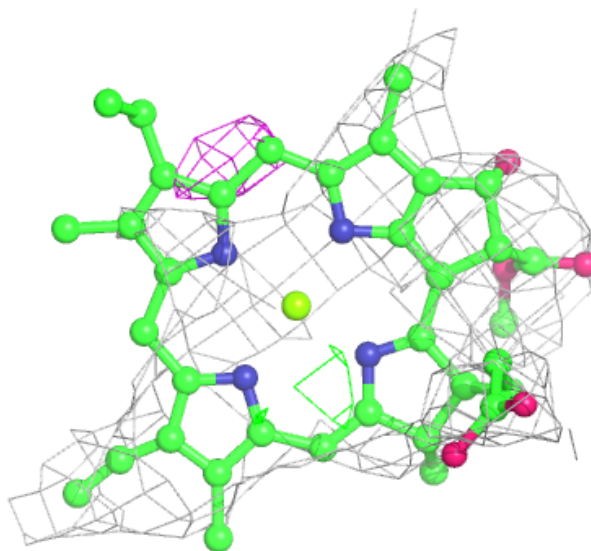
Electron density around LMU B 7040:

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



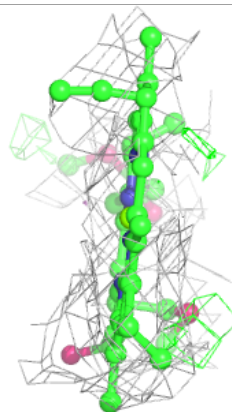
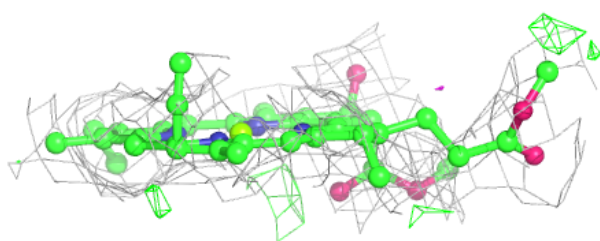
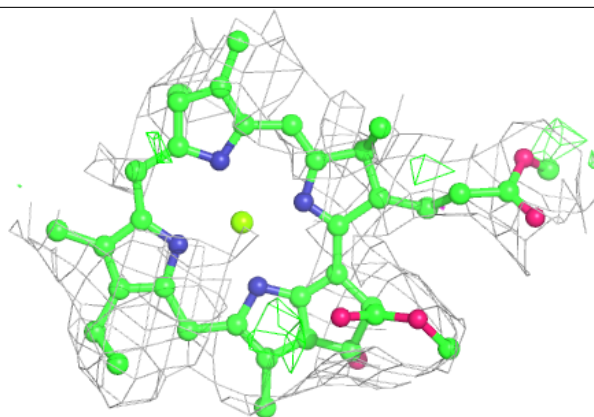
Electron density around CLA A 1112:

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



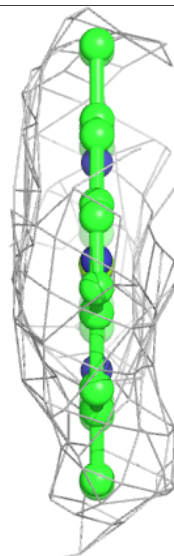
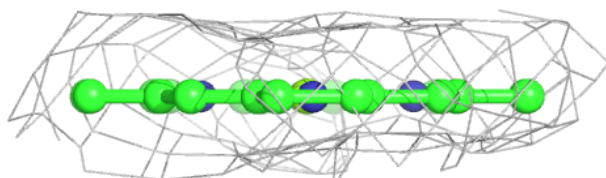
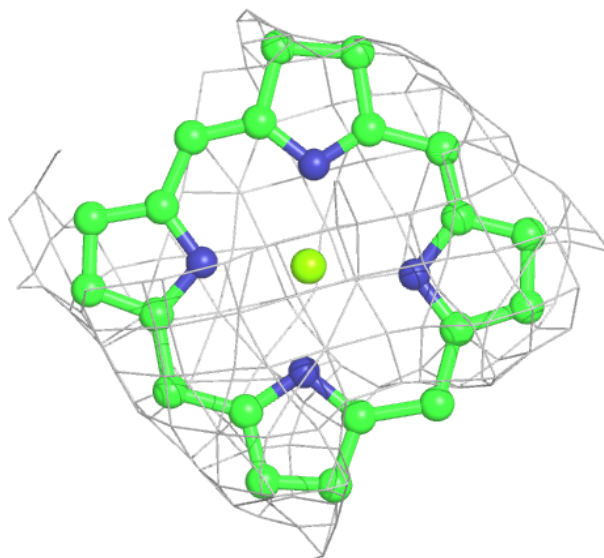
Electron density around CLA 1 1010:

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



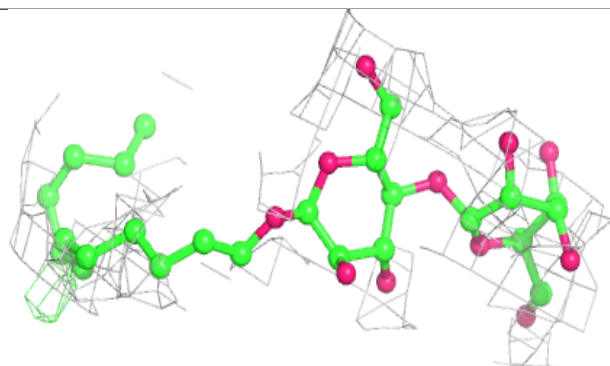
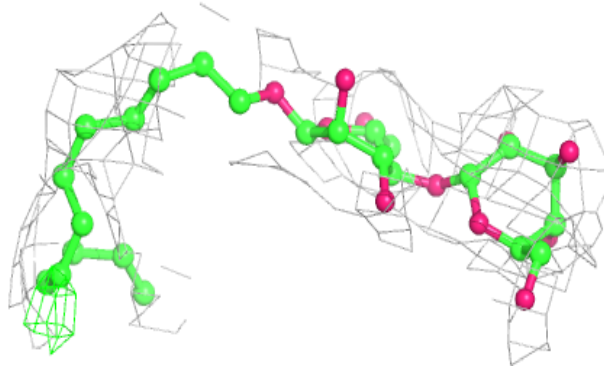
Electron density around CLA 1 1310:

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

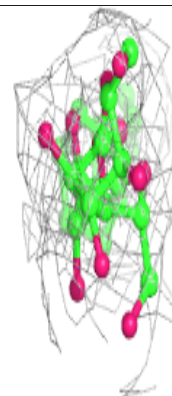
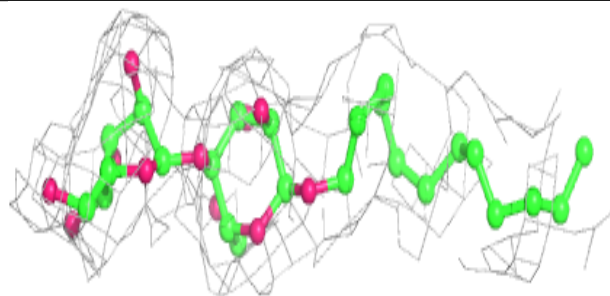
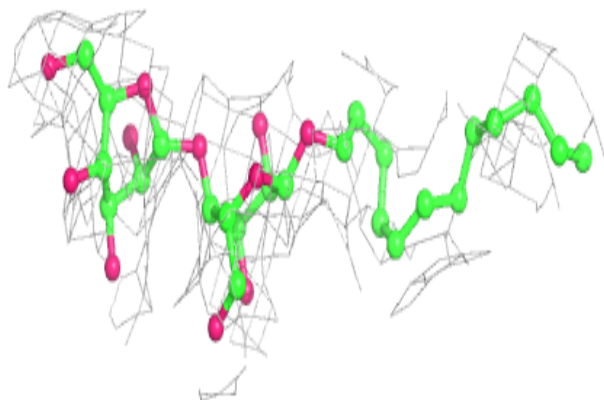


Electron density around LMU H 7043:

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

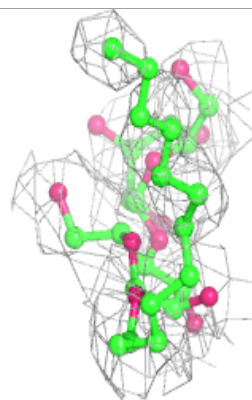
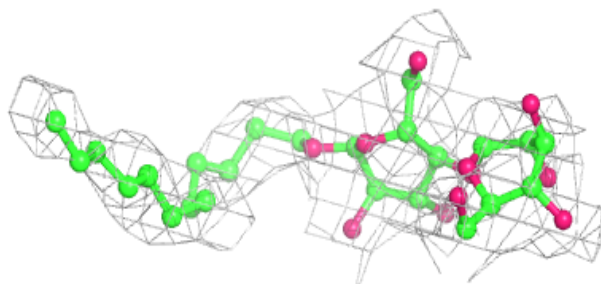
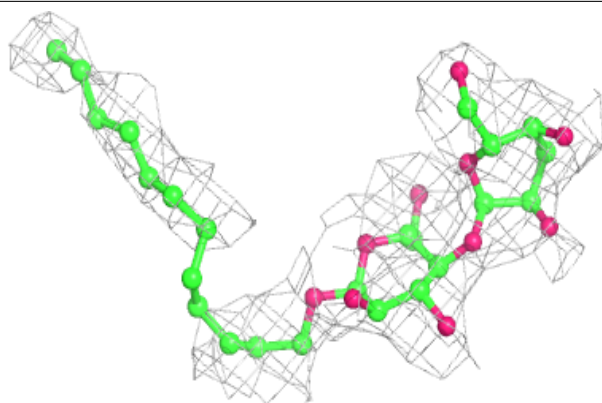
**Electron density around LMU E 7037:**

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



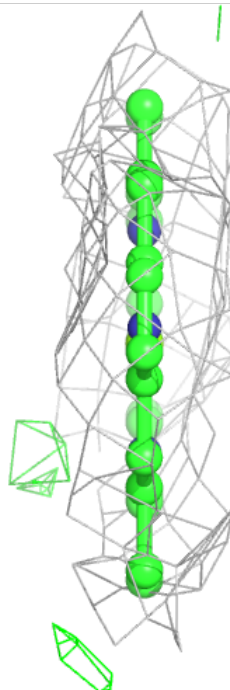
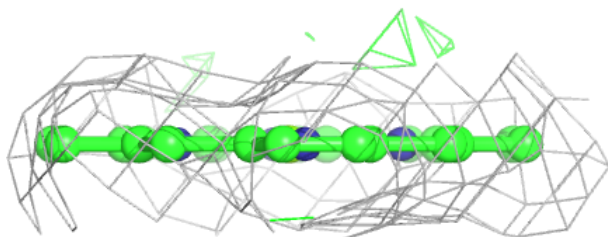
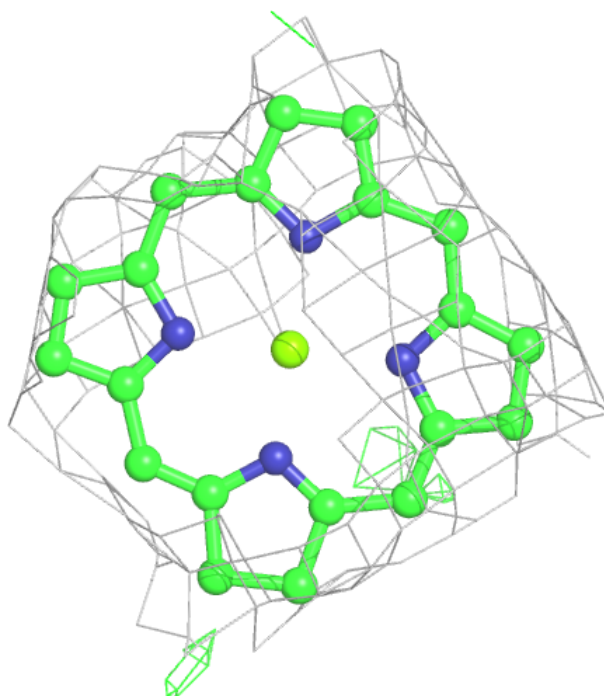
Electron density around LMU 4 7008:

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



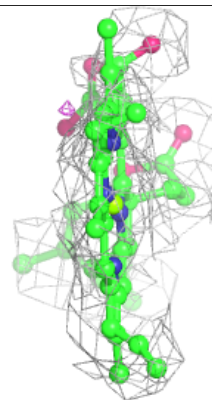
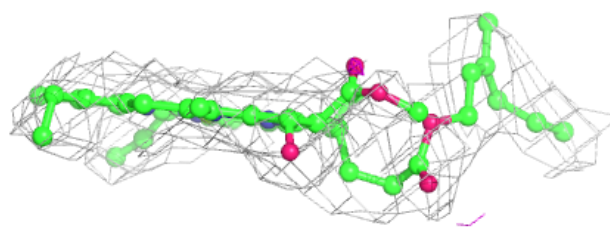
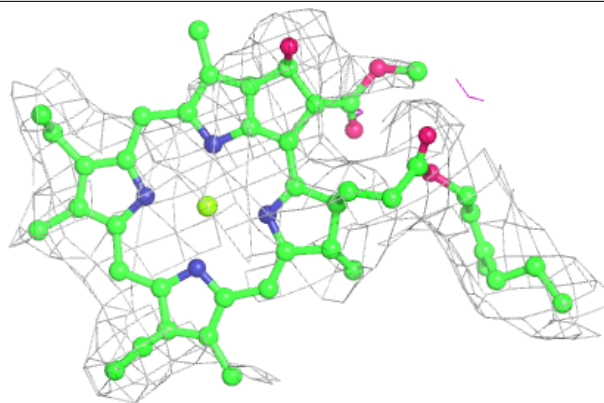
Electron density around CLA 3 3010:

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



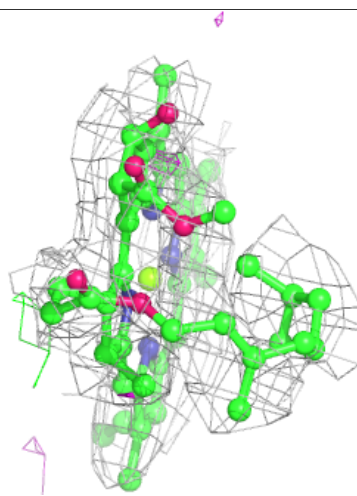
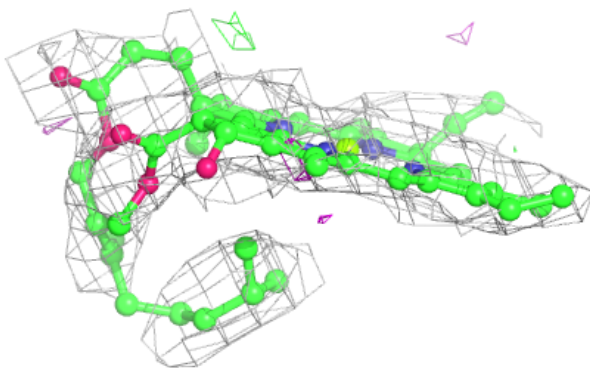
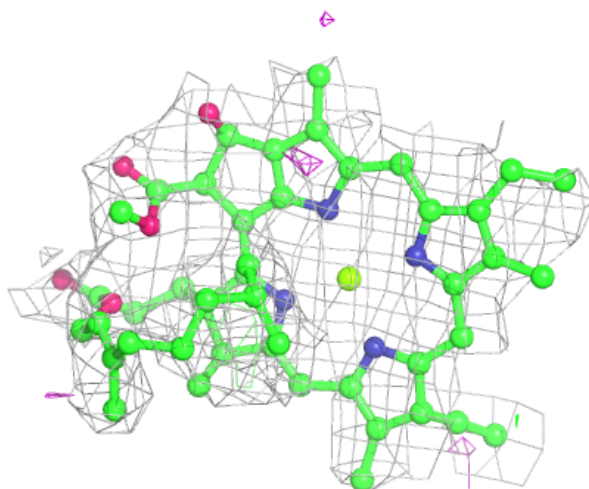
Electron density around CLA 4 4007:

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



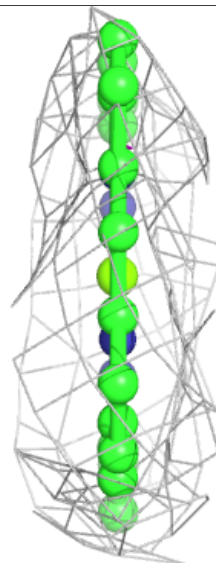
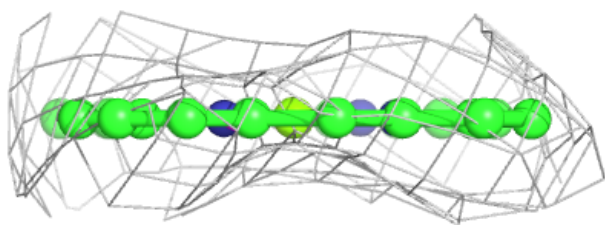
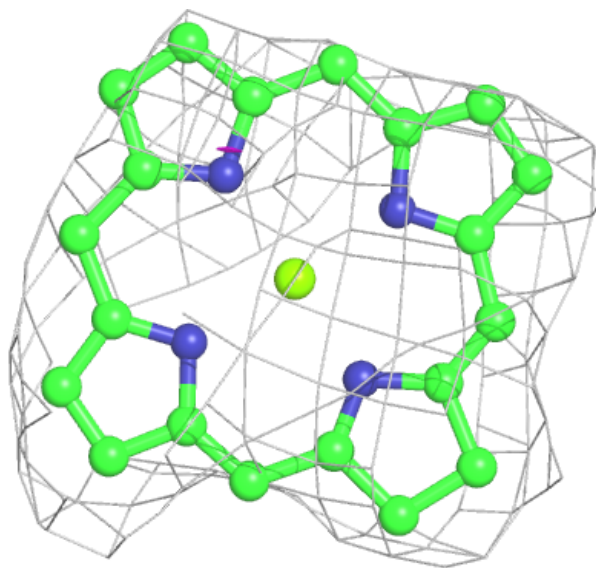
Electron density around CLA 4 1306:

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



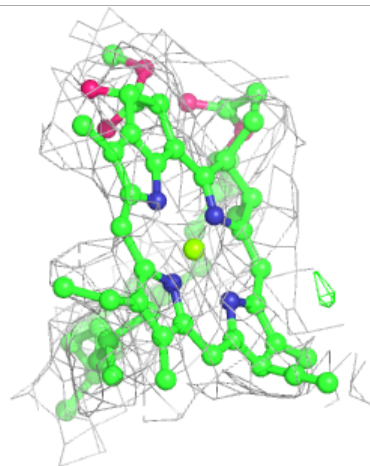
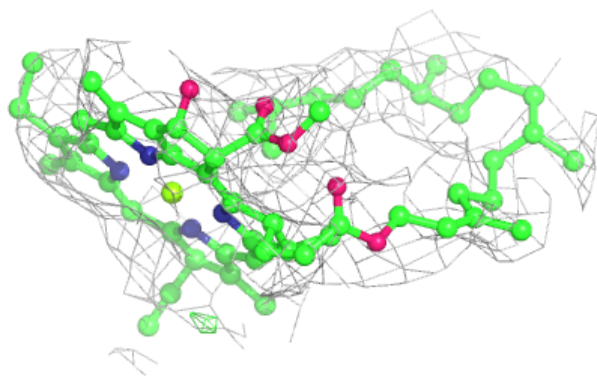
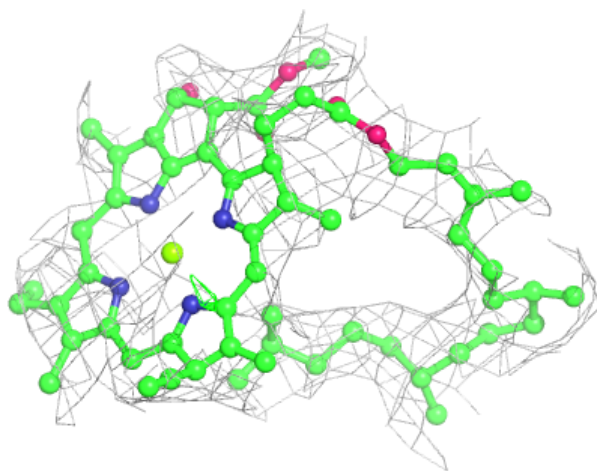
Electron density around CLA 2 2011:

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



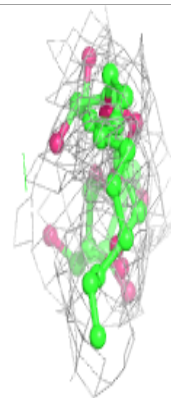
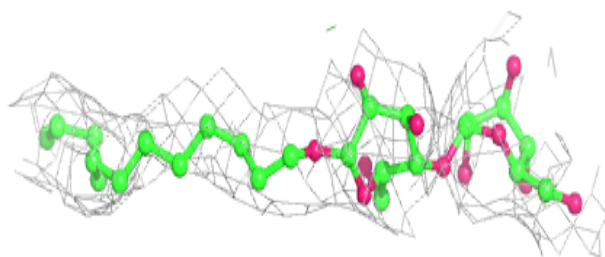
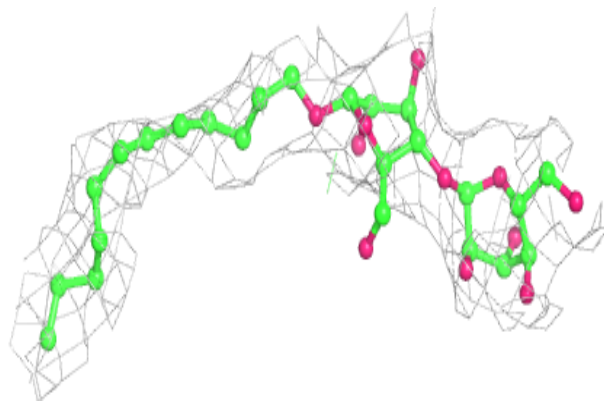
Electron density around CLA A 1141:

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

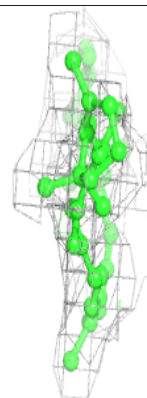
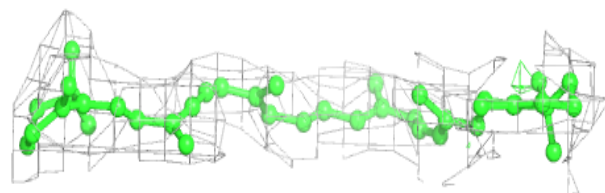
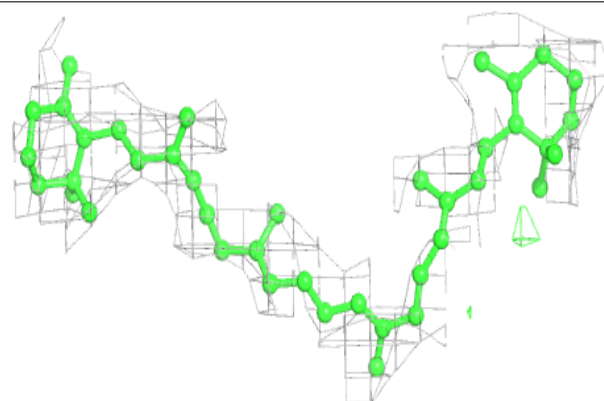


Electron density around LMU G 7051:

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

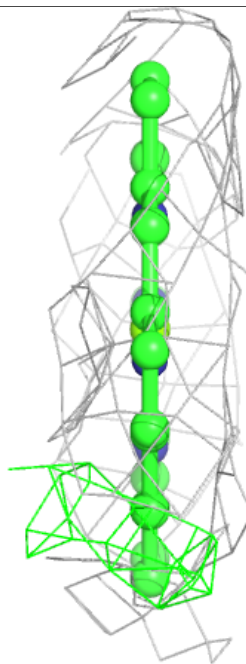
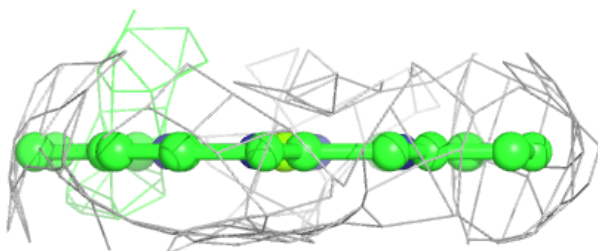
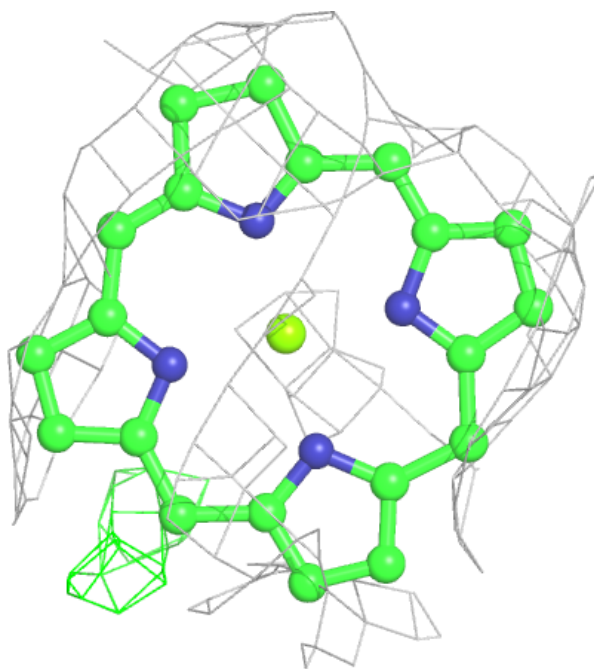
**Electron density around BCR 3 6022:**

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



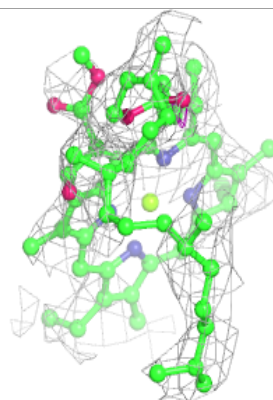
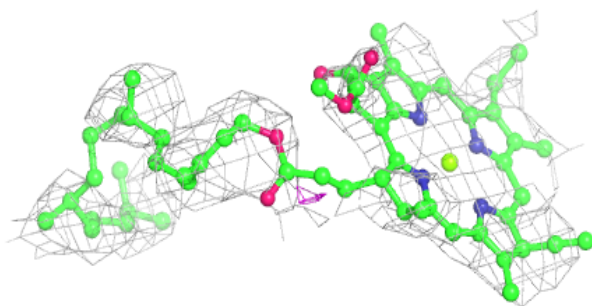
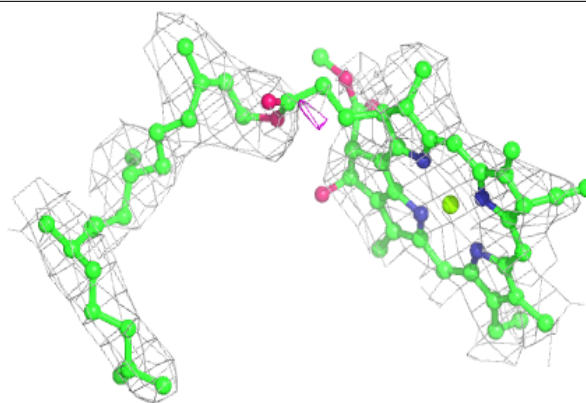
Electron density around CLA 1 1015:

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

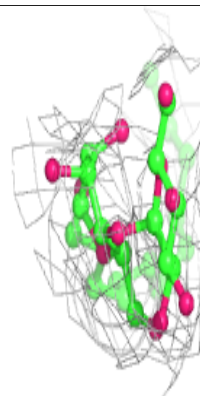
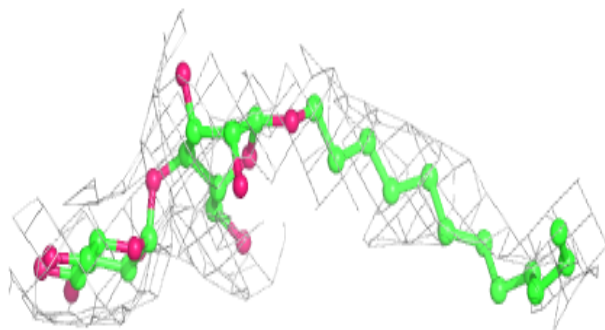
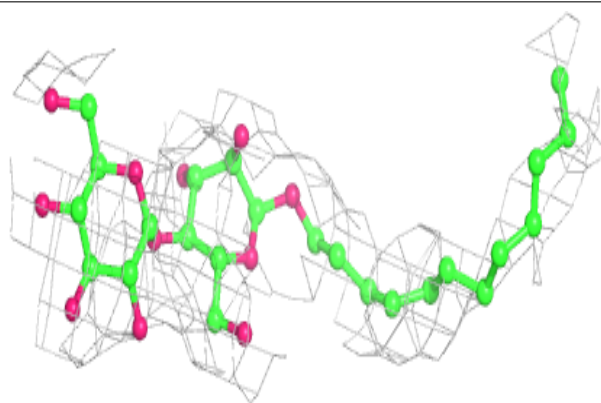


Electron density around CLA K 3009:

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

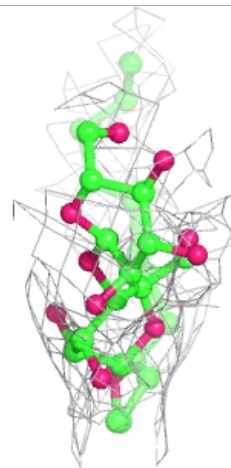
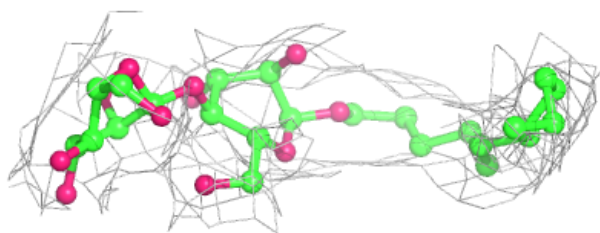
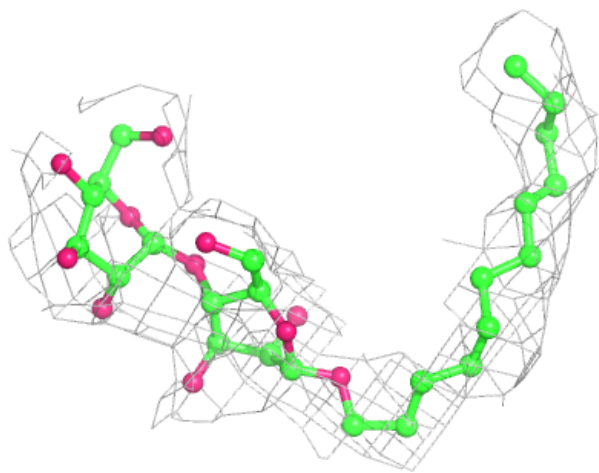
**Electron density around LMU K 7047:**

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



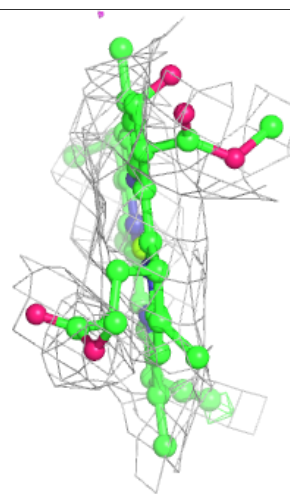
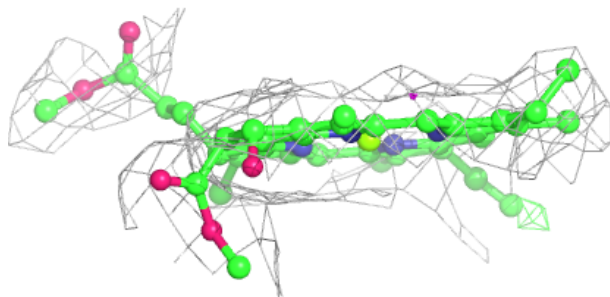
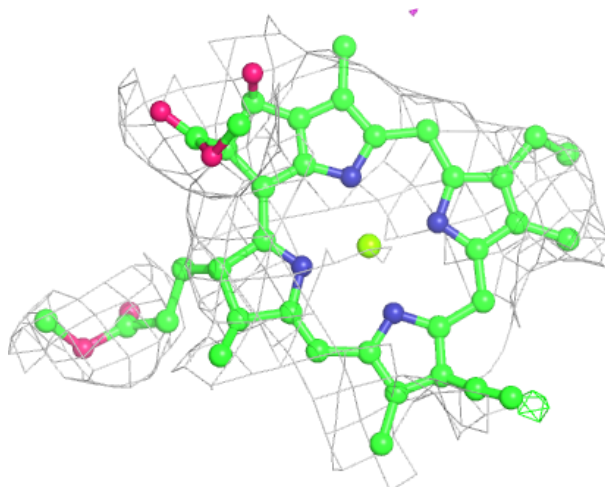
Electron density around LMU K 7041:

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



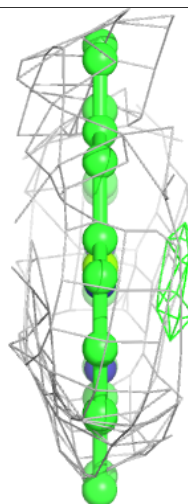
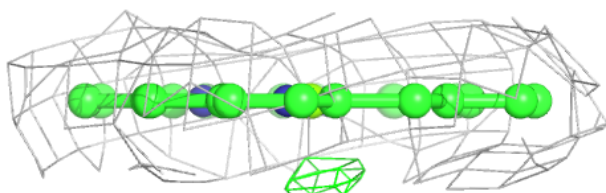
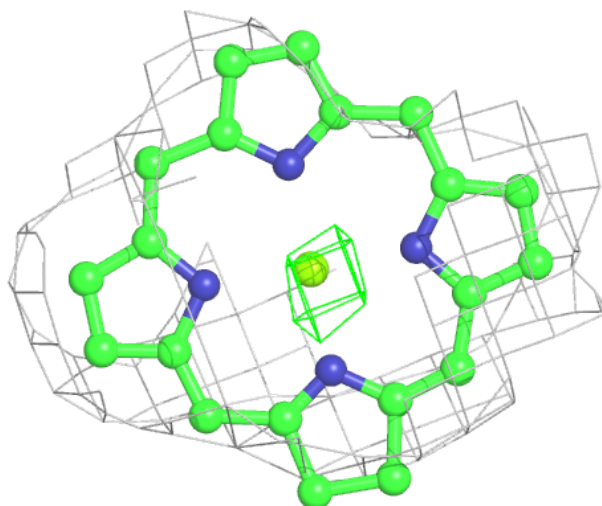
Electron density around CLA 1 1001:

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



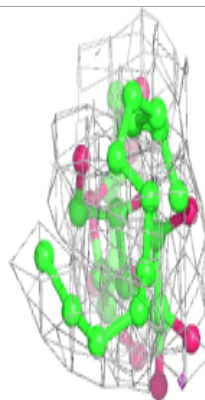
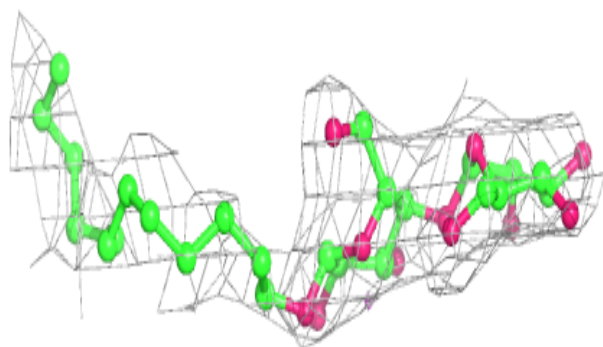
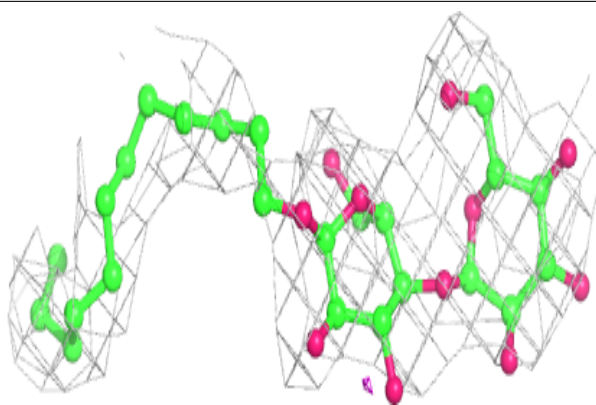
Electron density around CLA 2 2008:

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

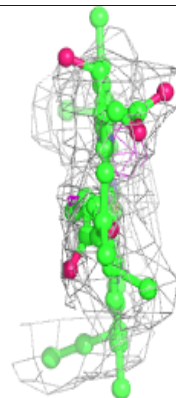
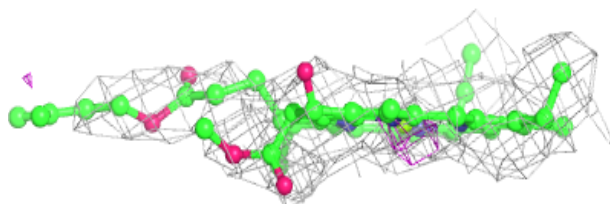
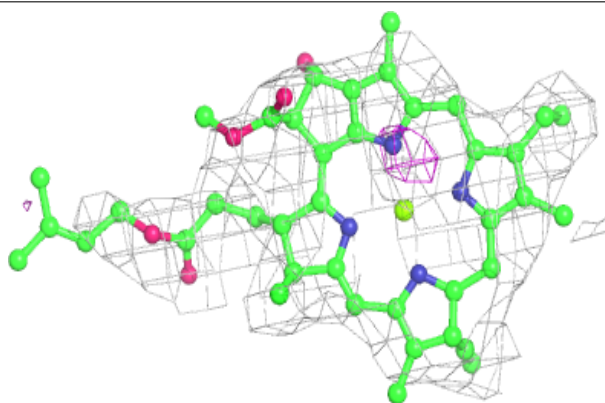


Electron density around LMU C 7015:

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

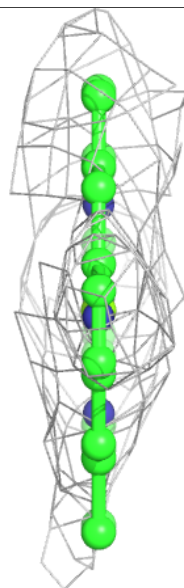
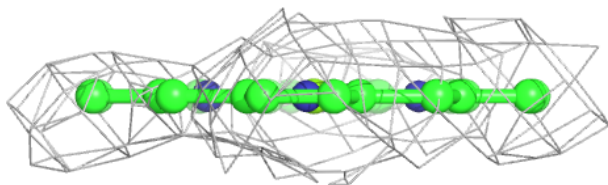
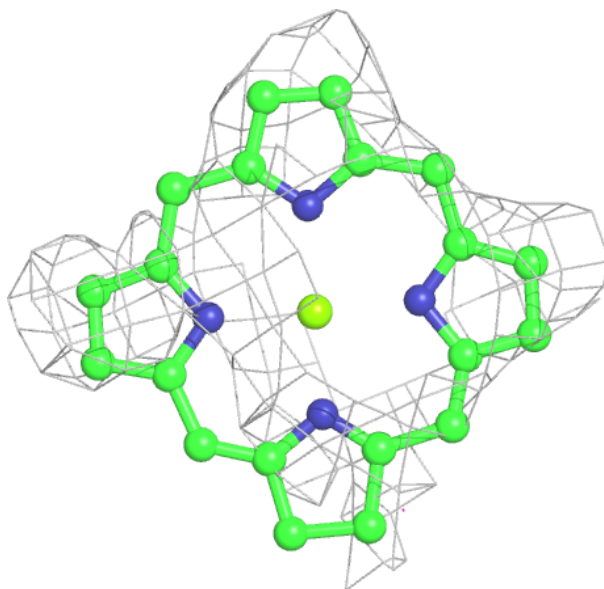
**Electron density around CLA A 1151:**

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



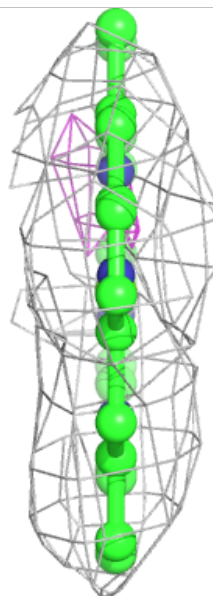
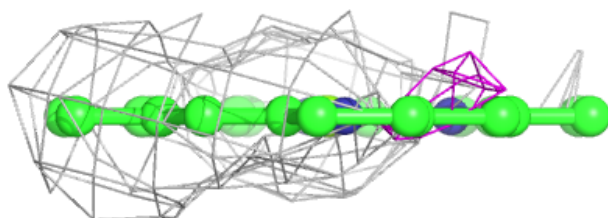
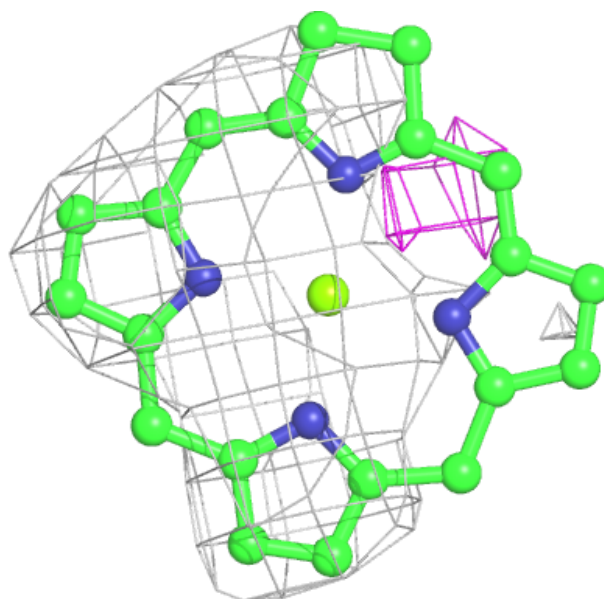
Electron density around CLA 3 3015:

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



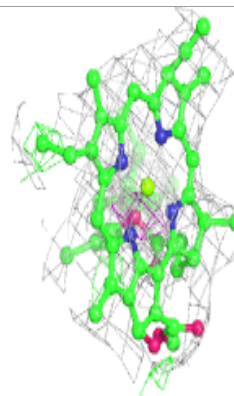
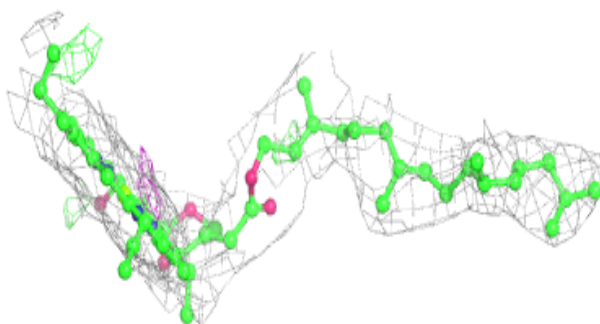
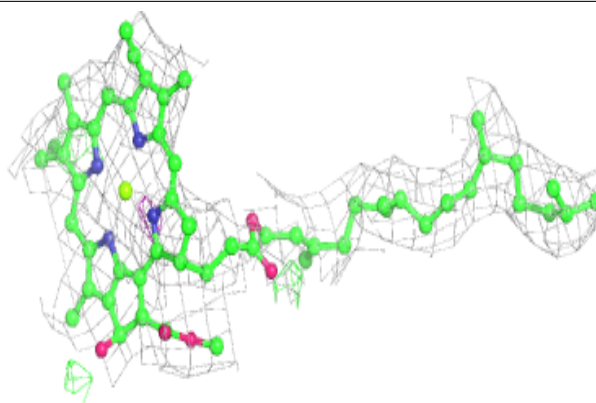
Electron density around CLA 2 1307:

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

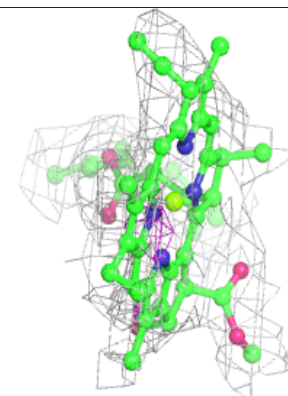
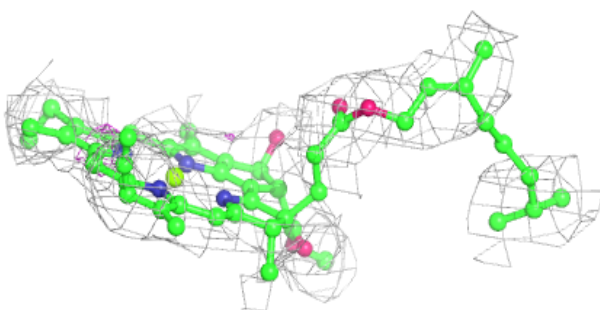
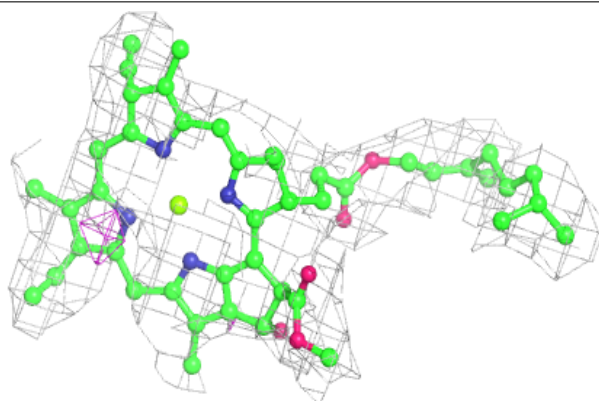


Electron density around CLA 4 1304:

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

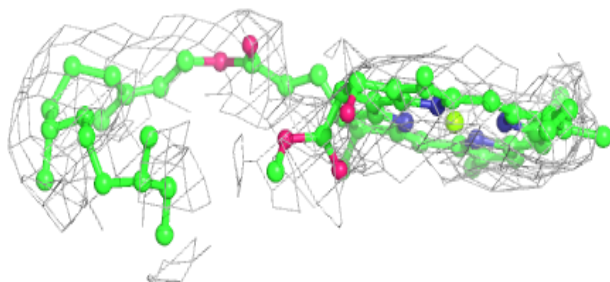
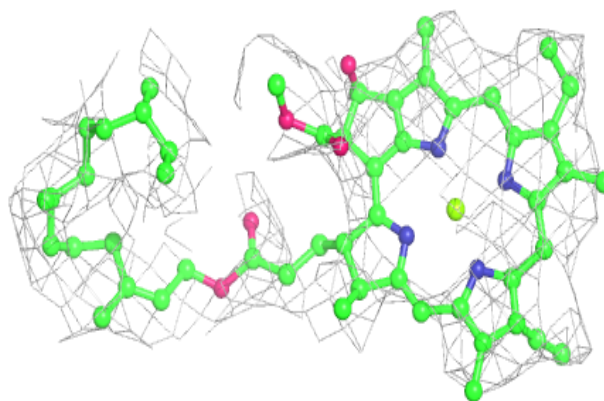
**Electron density around CLA H 1241:**

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

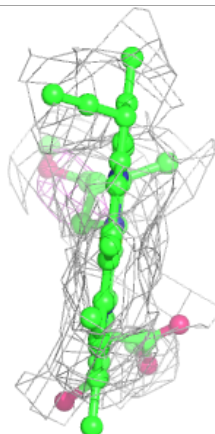
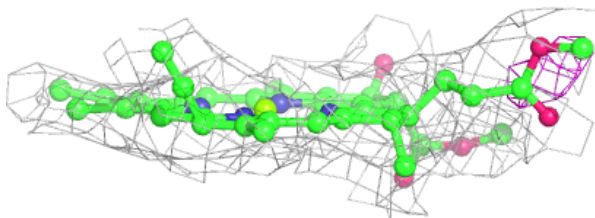
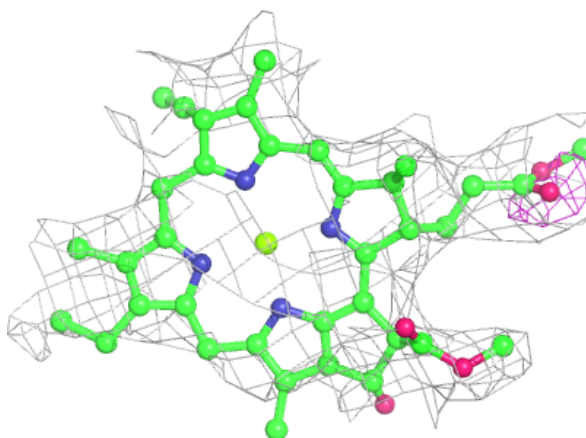


Electron density around CLA 1 1014:

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

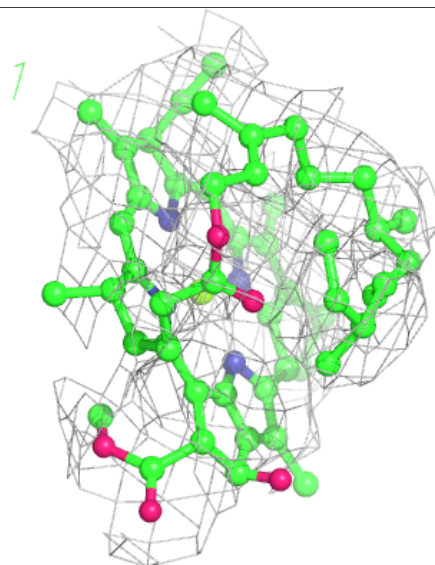
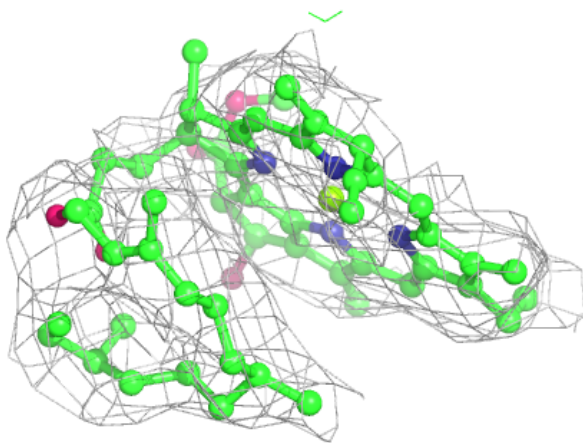
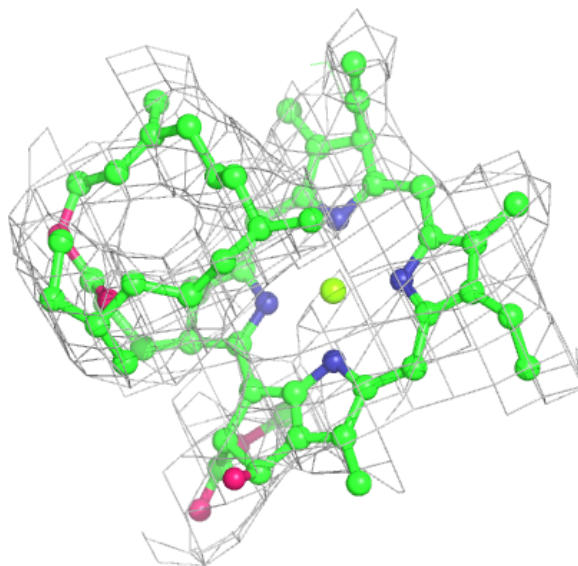
**Electron density around CLA 3 1147:**

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



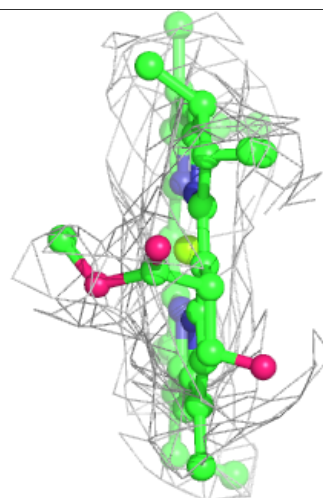
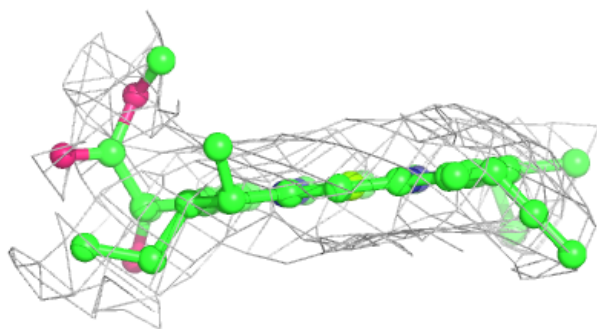
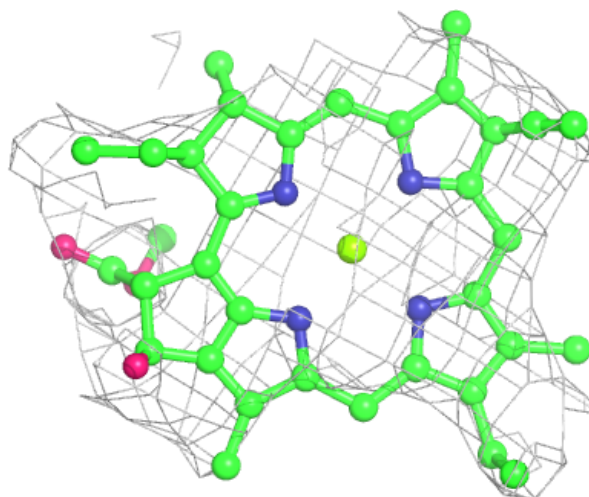
Electron density around CLA J 1311:

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



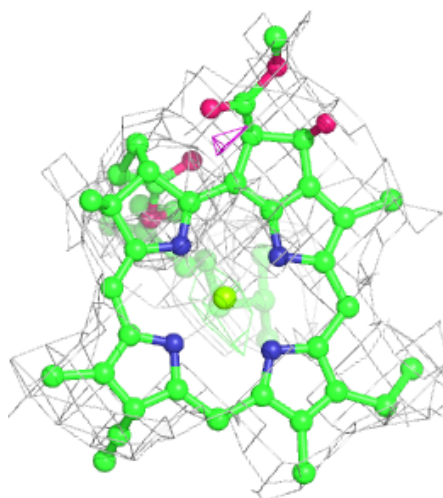
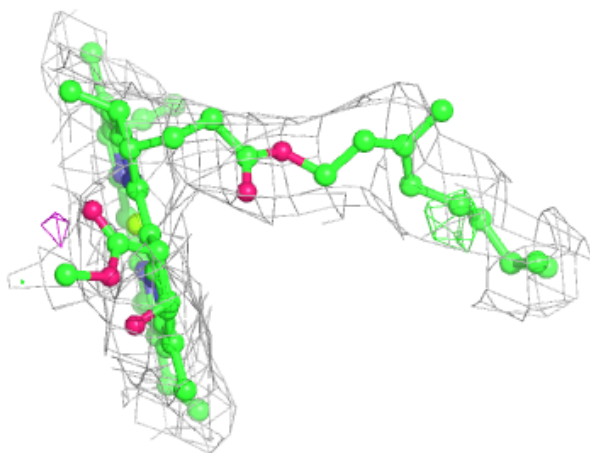
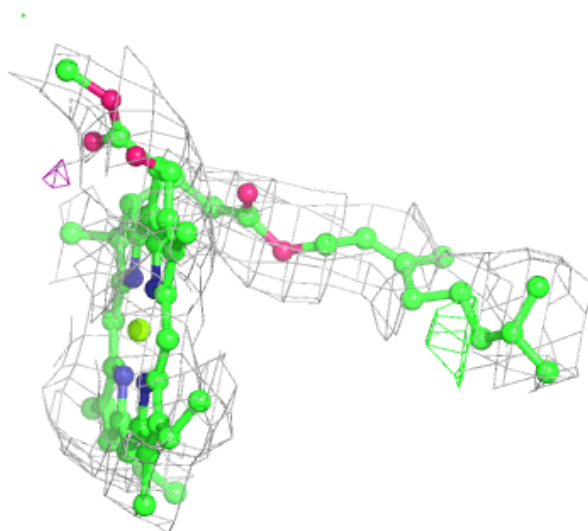
Electron density around CLA 3 3007:

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



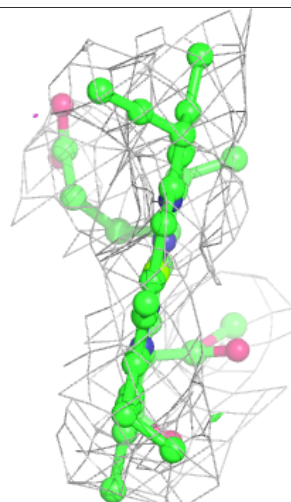
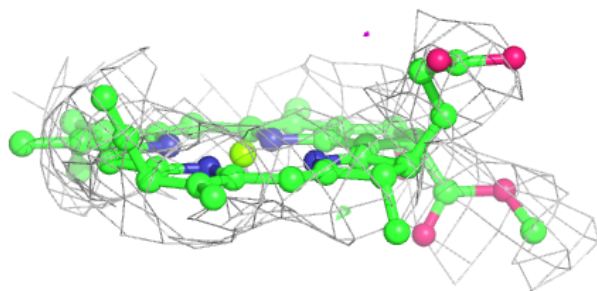
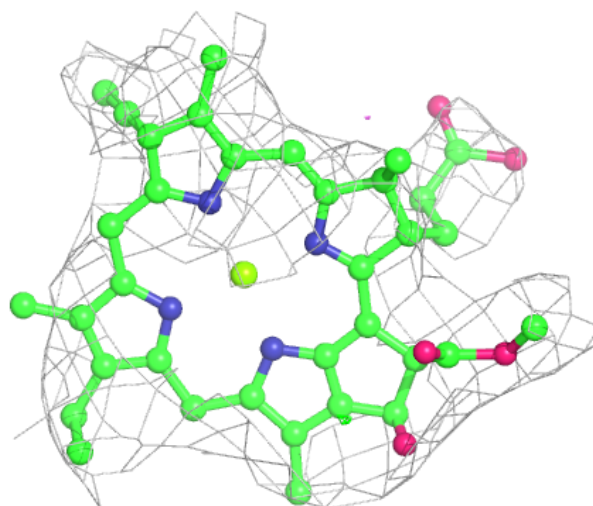
Electron density around CLA 4 1004:

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



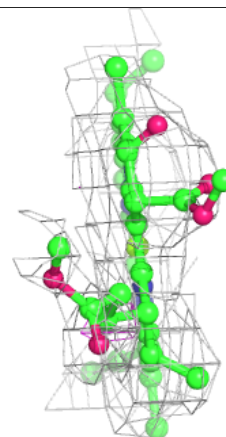
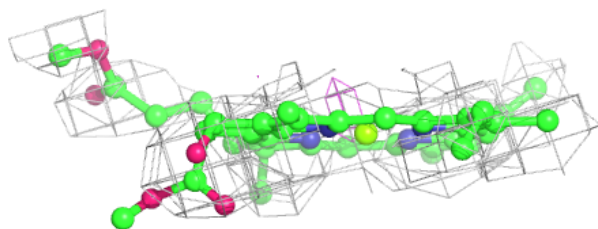
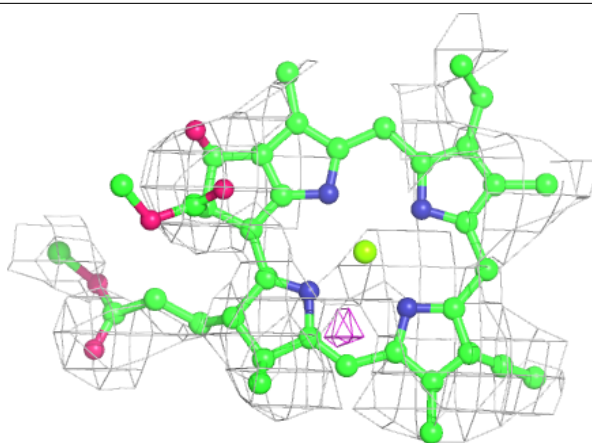
Electron density around CLA A 1134:

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

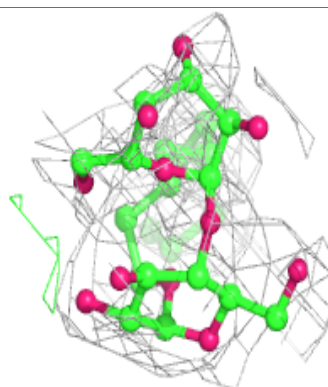
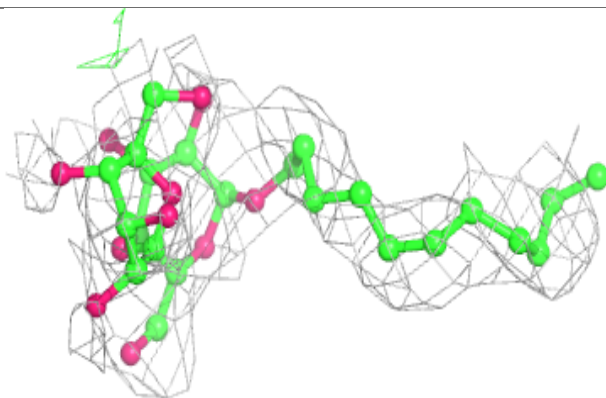
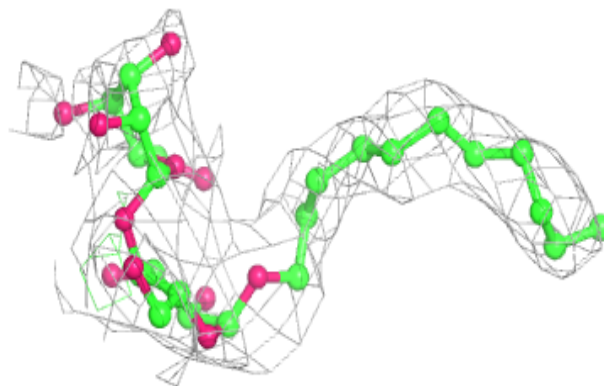


Electron density around CLA 4 4015:

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

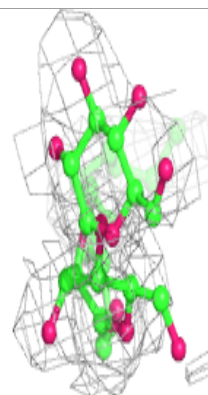
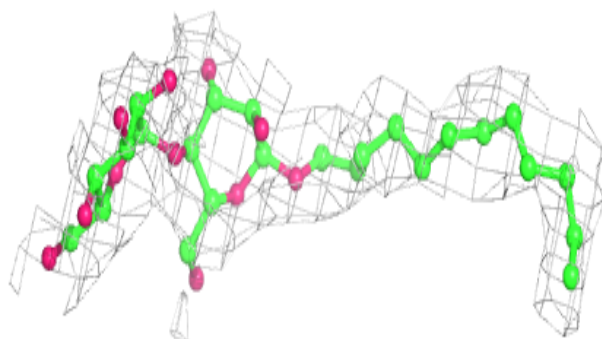
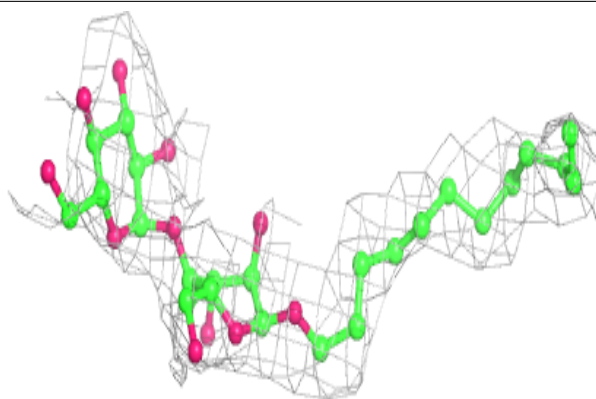
**Electron density around LMU 4 7009:**

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

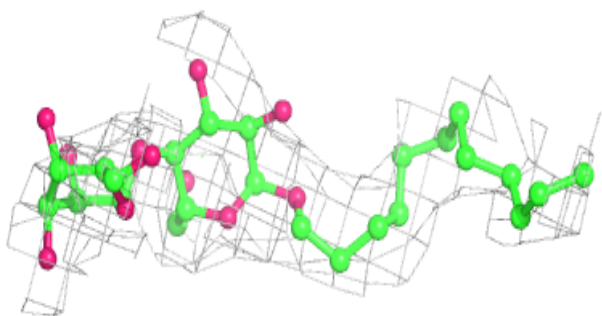
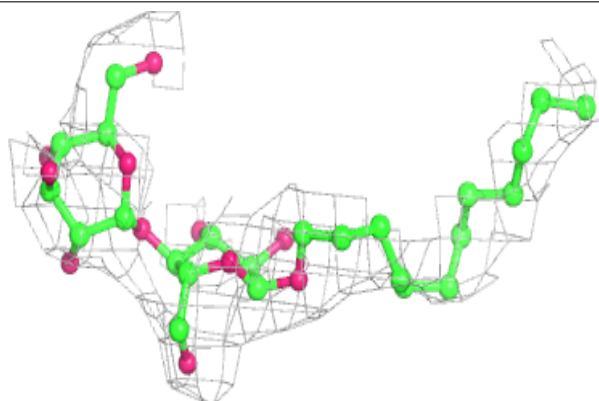


Electron density around LMU 4 7018:

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

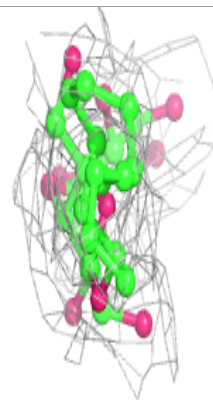
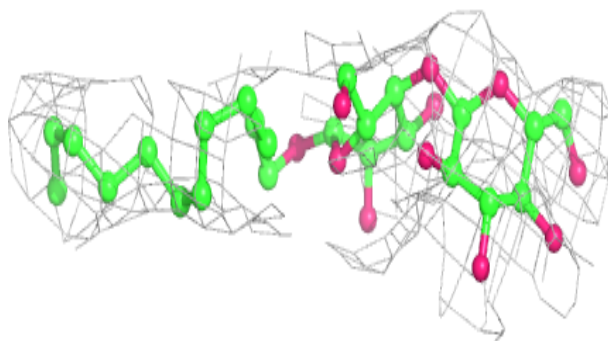
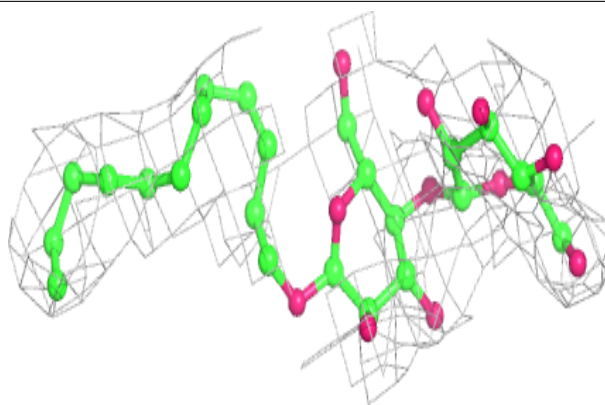
**Electron density around LMU 4 7034:**

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



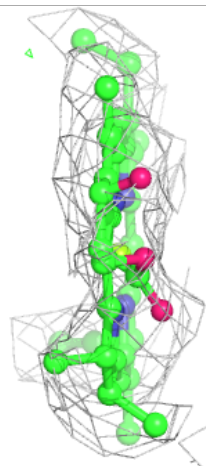
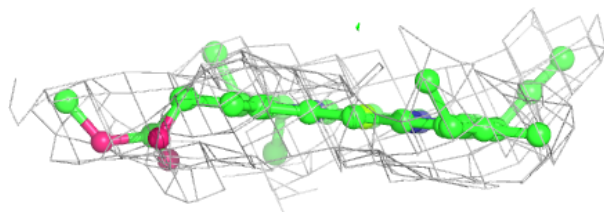
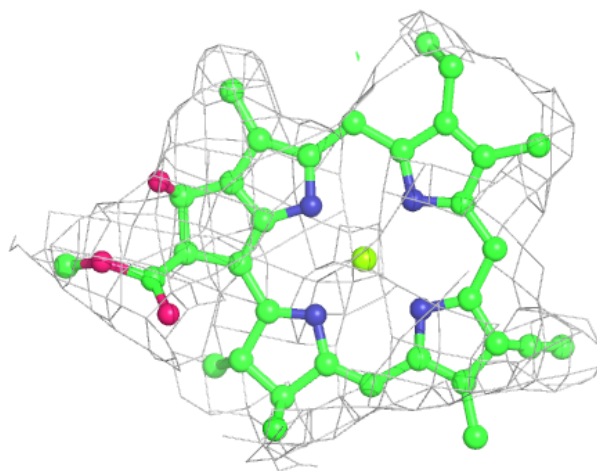
Electron density around LMU K 7042:

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



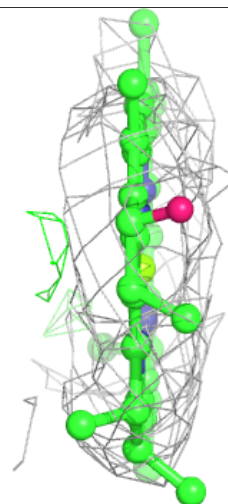
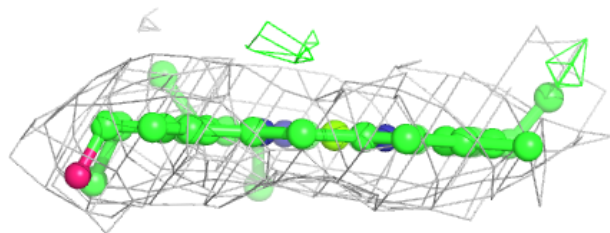
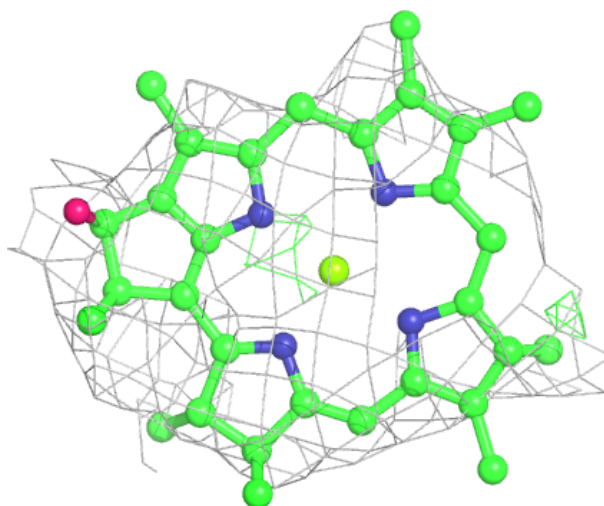
Electron density around CLA F 1302:

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



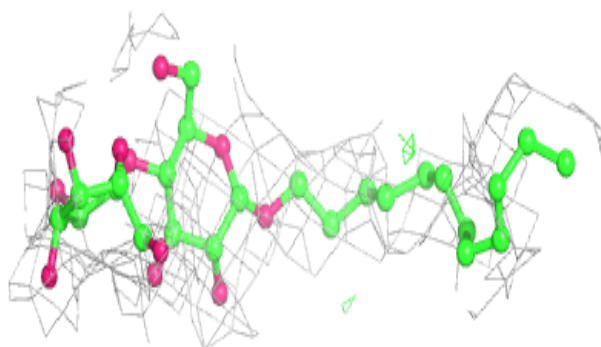
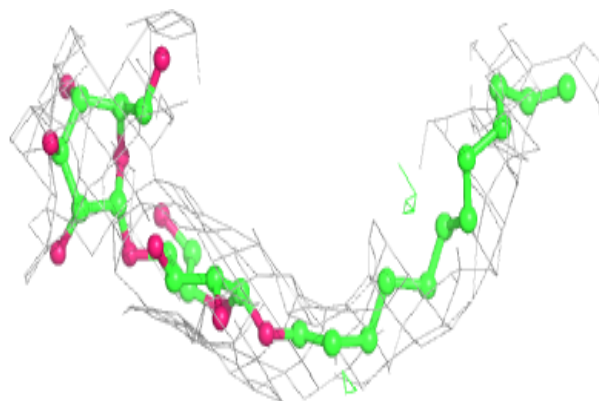
Electron density around CLA 3 3003:

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



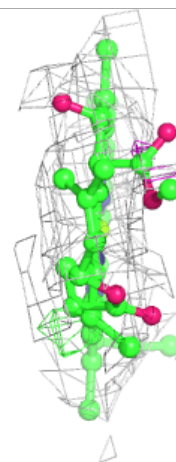
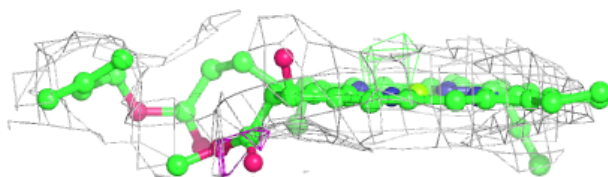
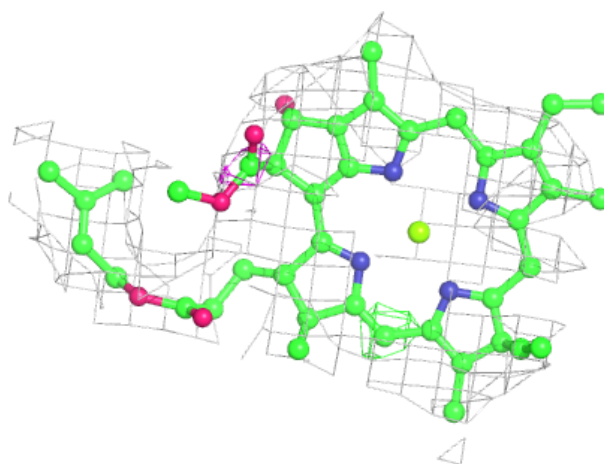
Electron density around LMU H 7017:

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



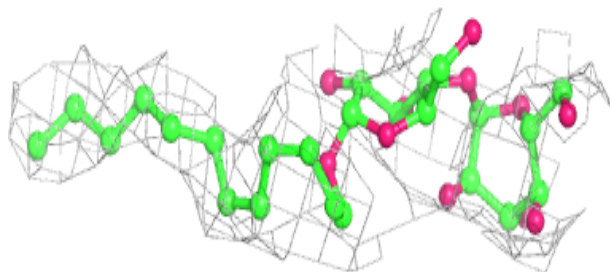
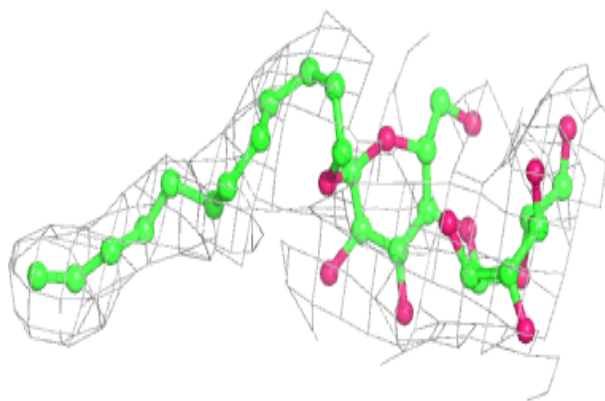
Electron density around CLA 2 2013:

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

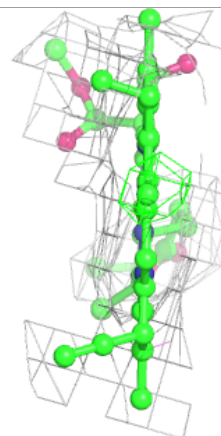
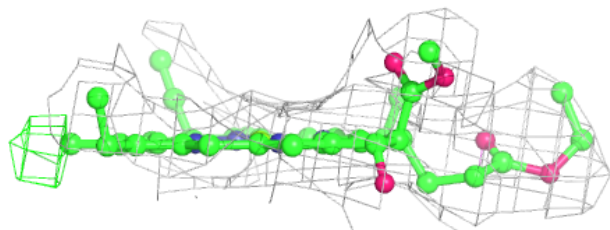
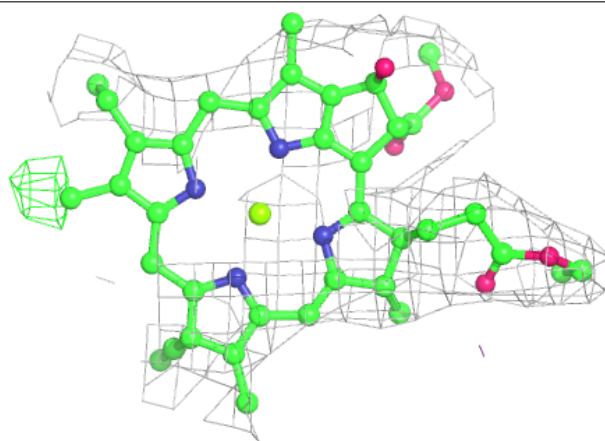


Electron density around LMU 3 7005:

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

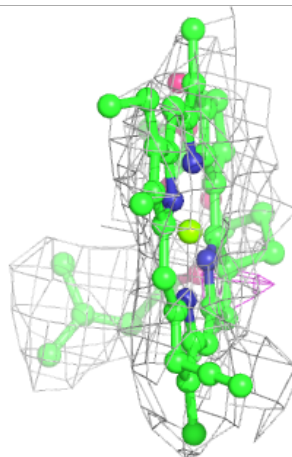
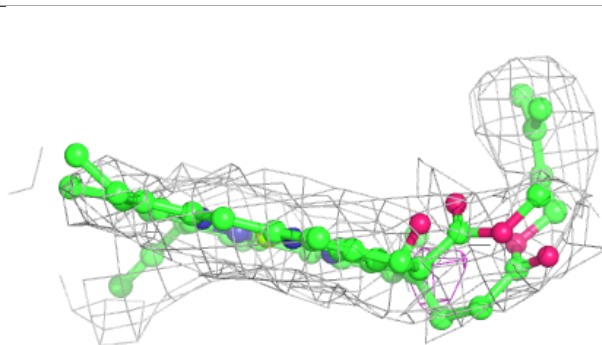
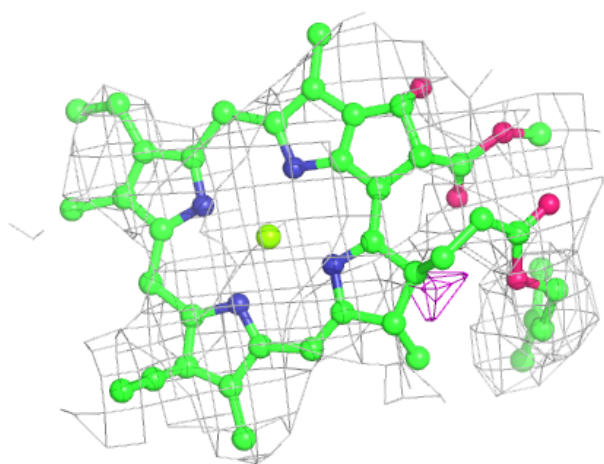
**Electron density around CLA 1 1003:**

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



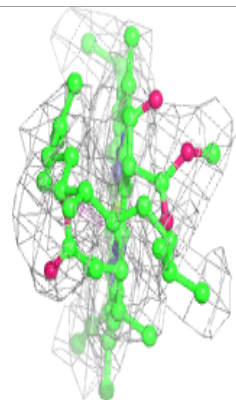
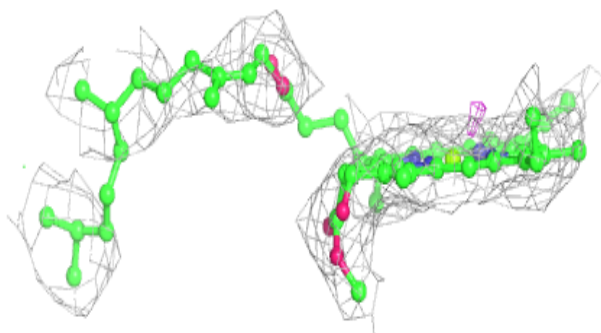
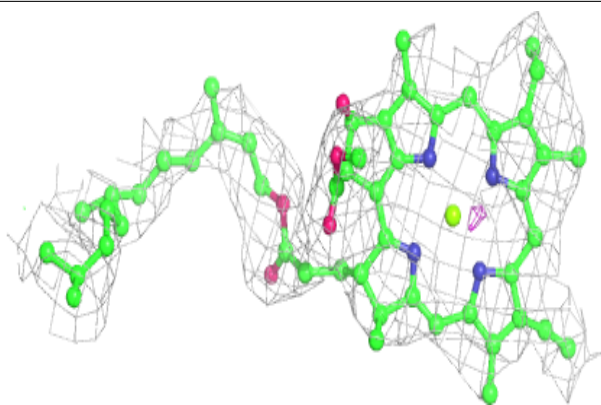
Electron density around CLA 3 3008:

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

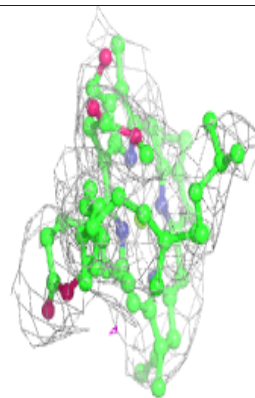
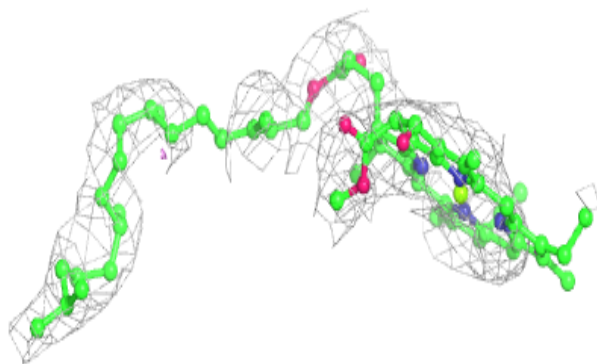
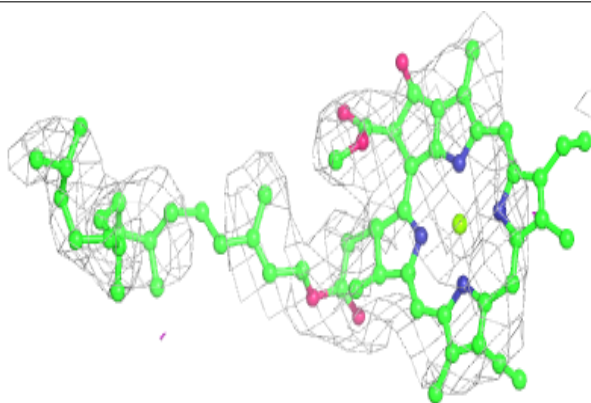


Electron density around CLA B 1212:

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

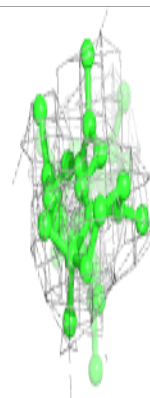
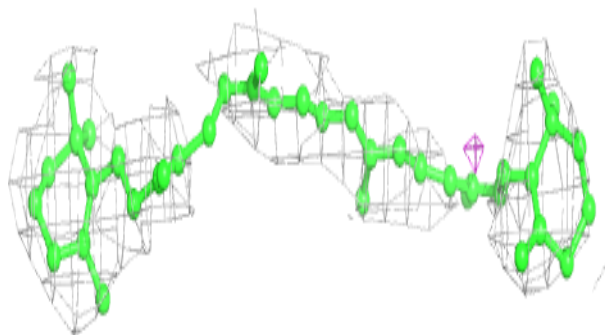
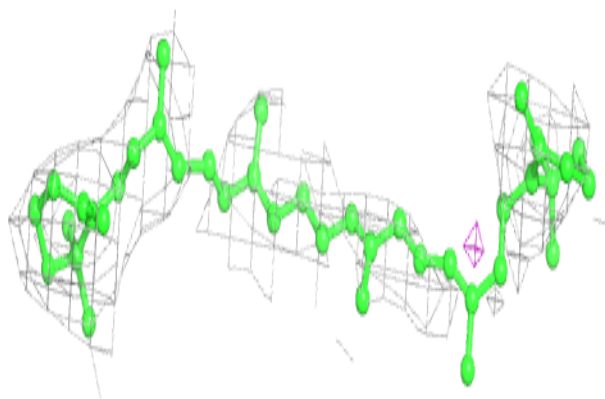
**Electron density around CLA 3 3011:**

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



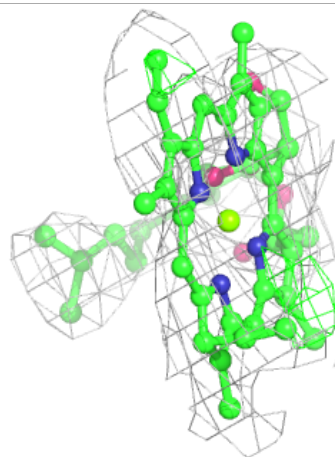
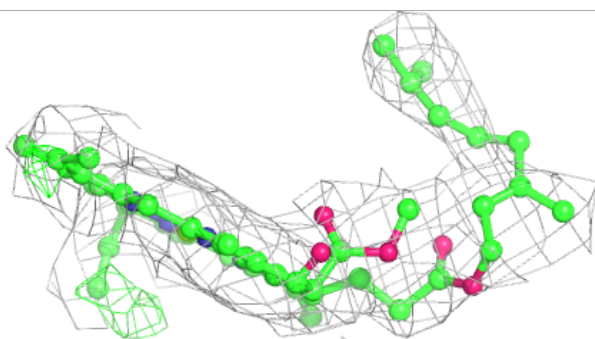
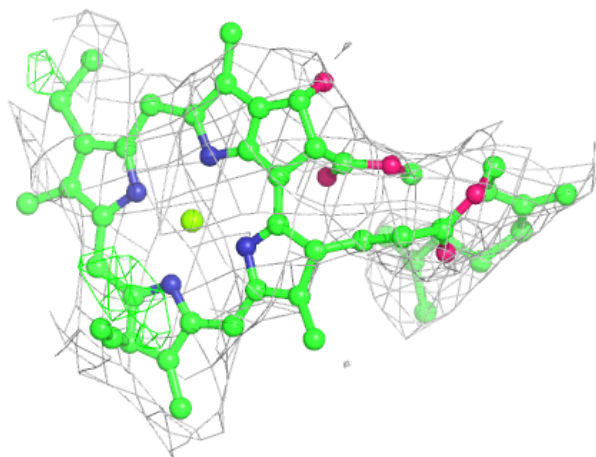
Electron density around BCR A 6007:

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



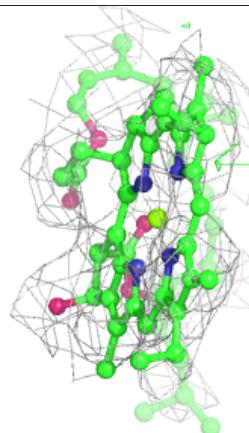
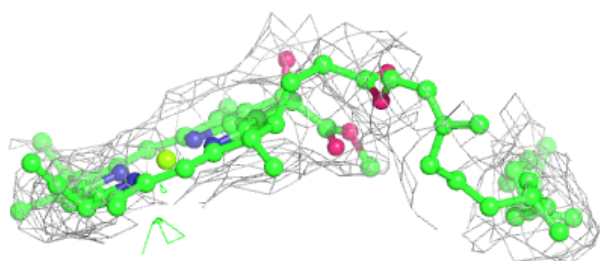
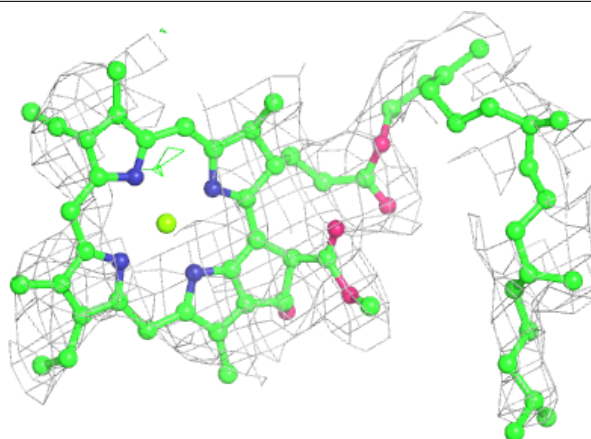
Electron density around CLA L 1148:

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

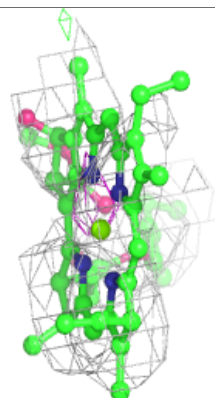
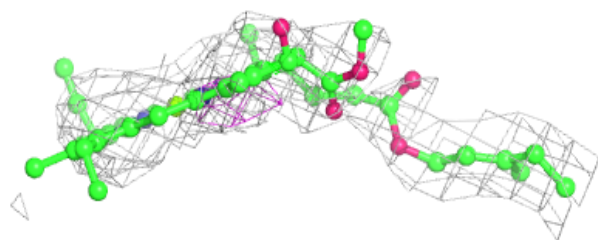
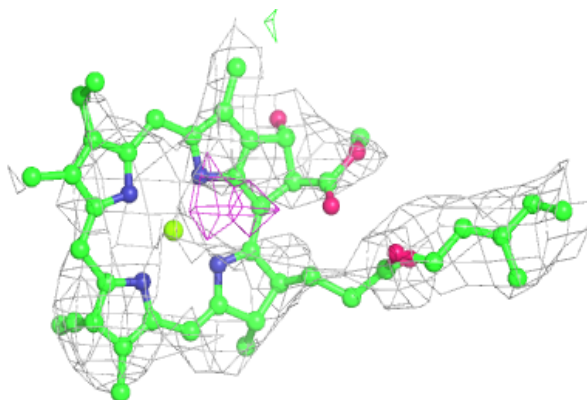


Electron density around CLA R 1150:

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

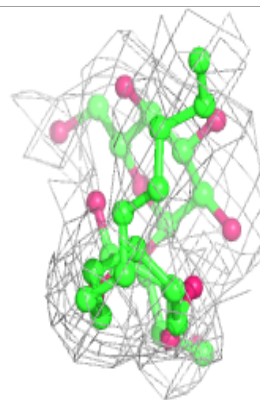
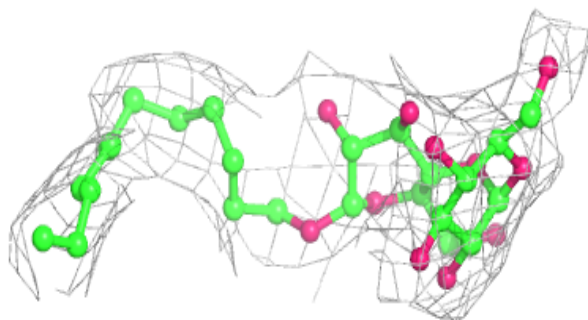
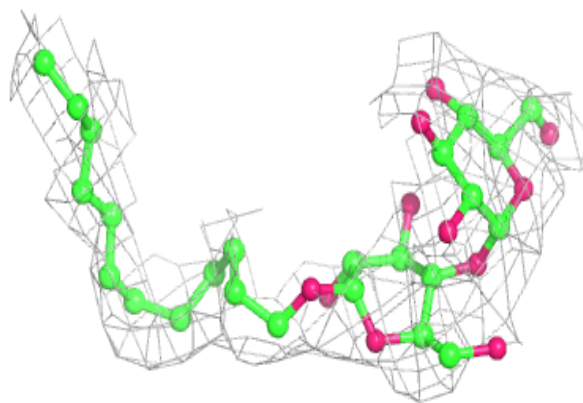
**Electron density around CLA 1 1013:**

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



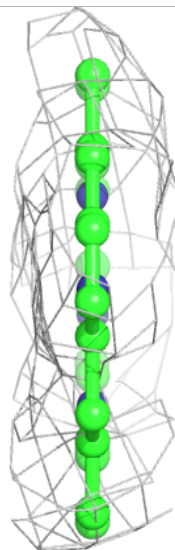
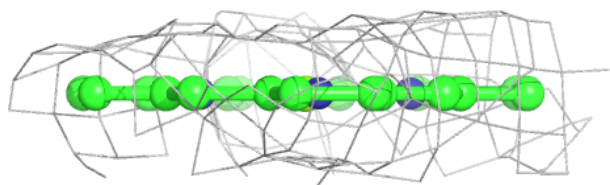
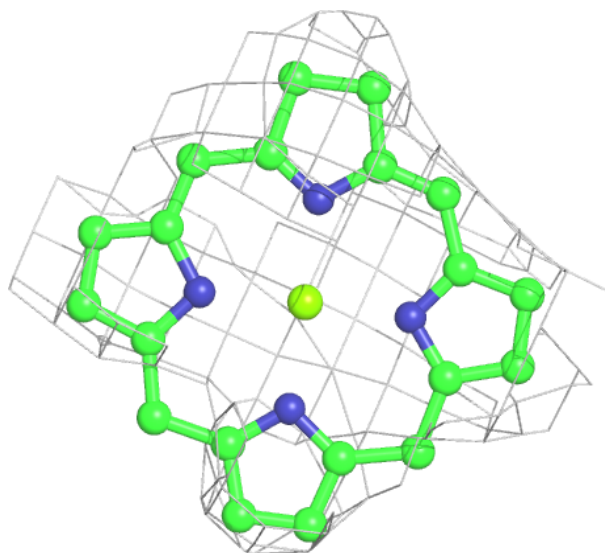
Electron density around LMU 2 7031:

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



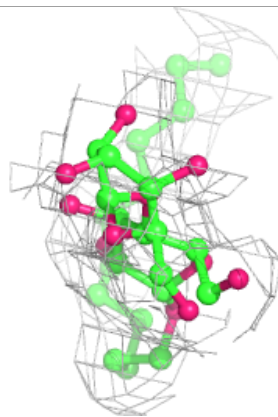
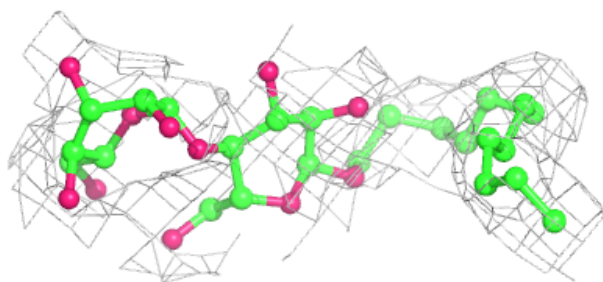
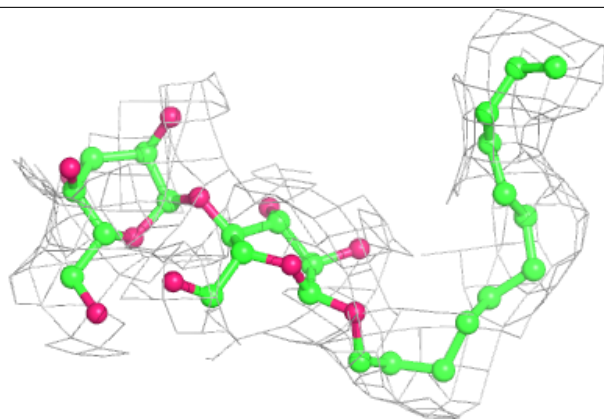
Electron density around CLA 3 3002:

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

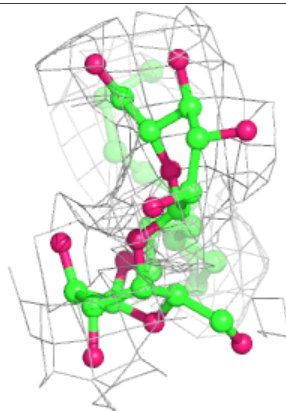
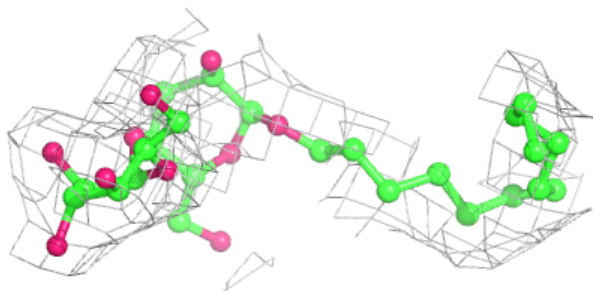
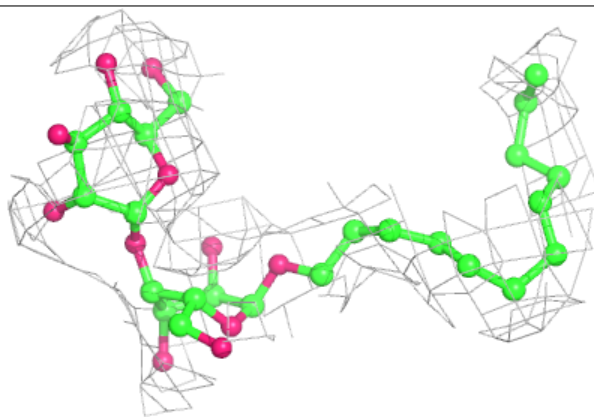


Electron density around LMU 3 7003:

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

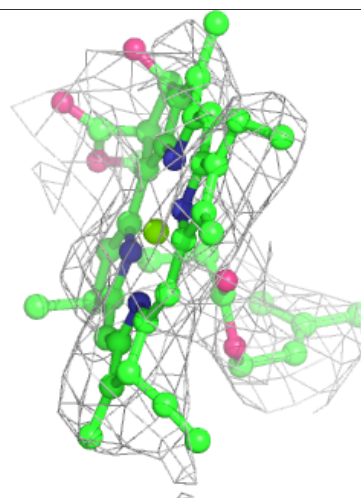
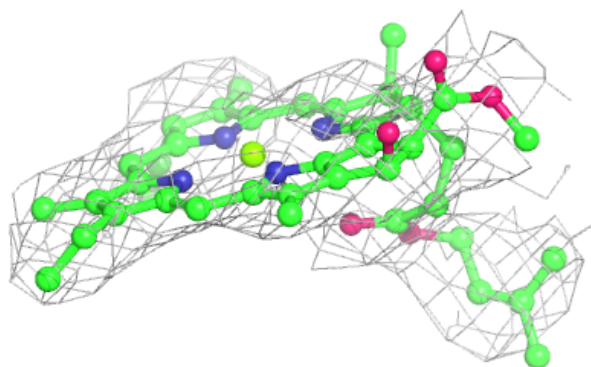
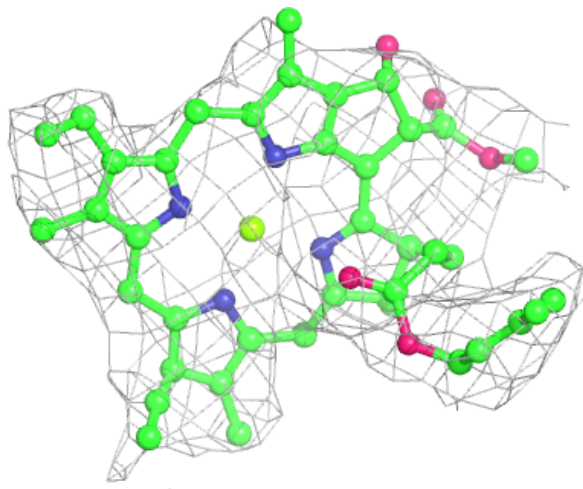
**Electron density around LMU K 7001:**

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



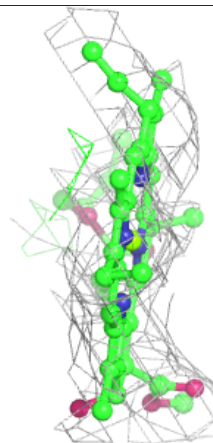
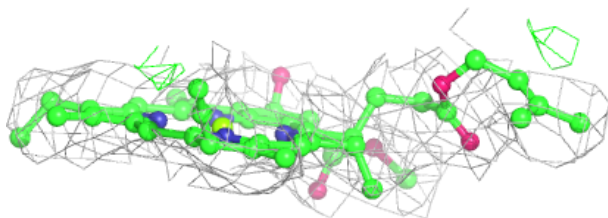
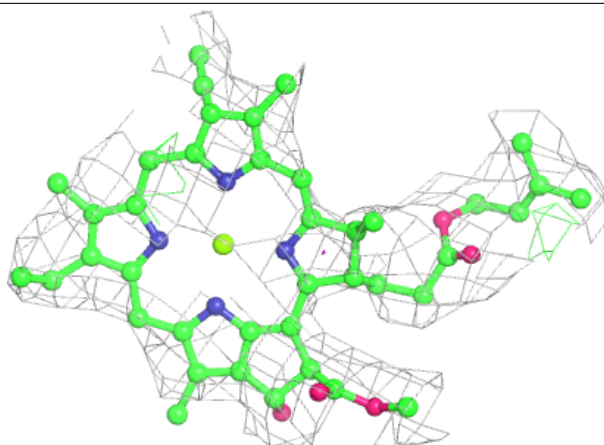
Electron density around CLA A 1113:

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

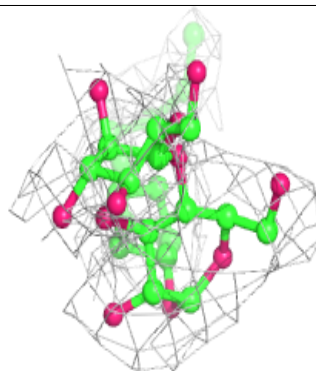
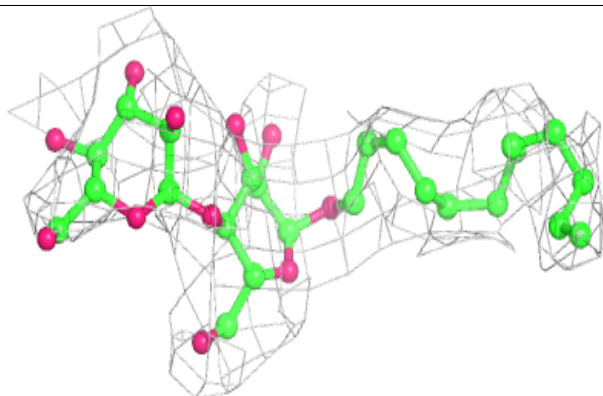
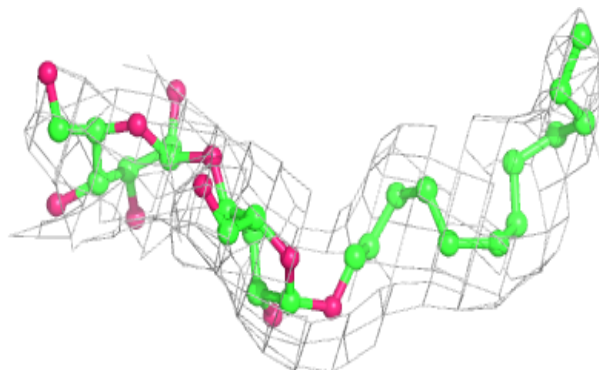


Electron density around CLA 2 2004:

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

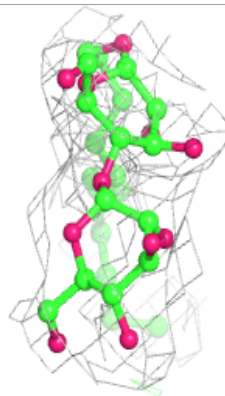
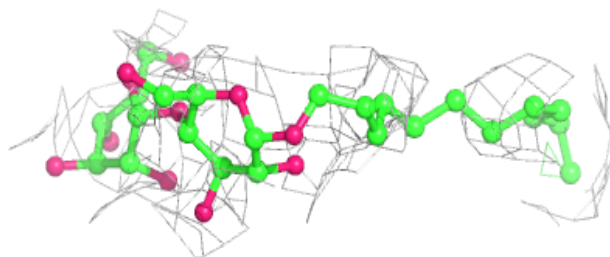
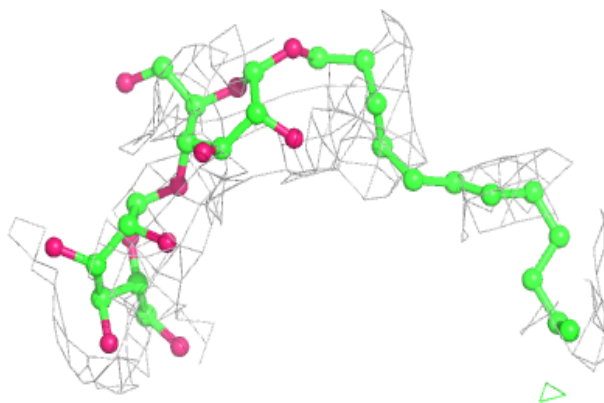
**Electron density around LMU G 7026:**

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



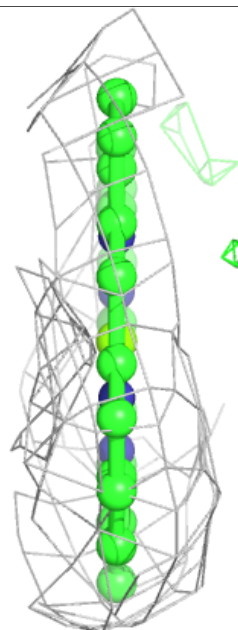
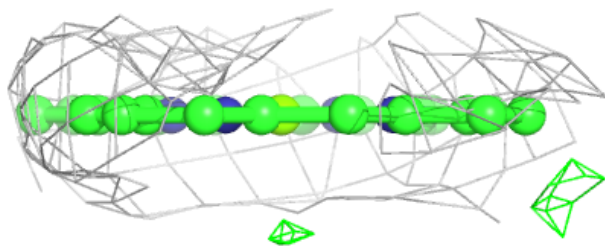
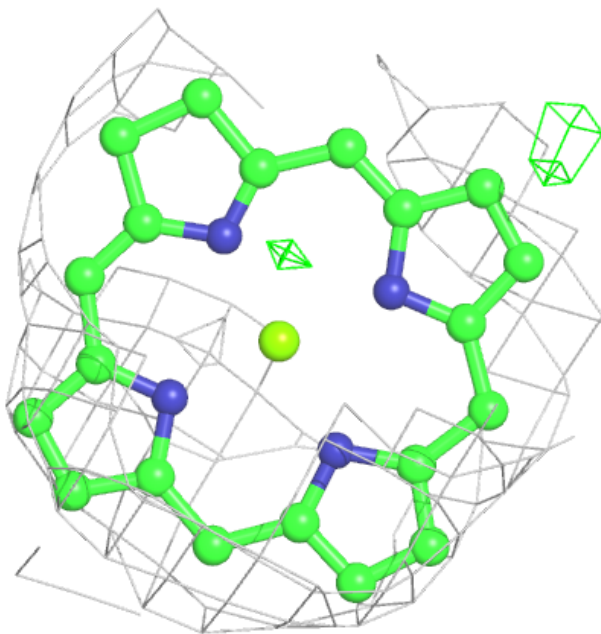
Electron density around LMU 4 7019:

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



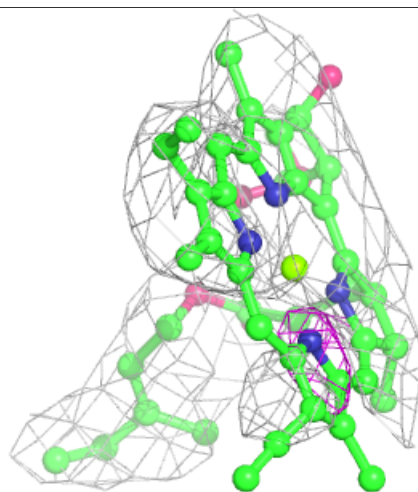
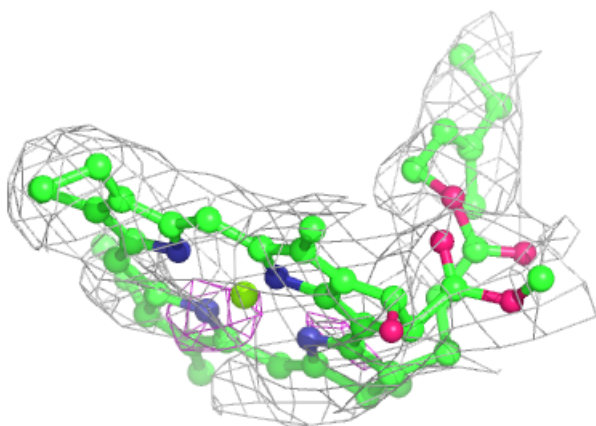
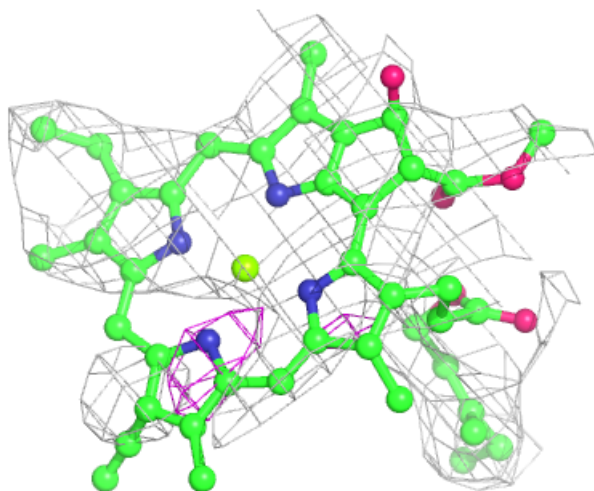
Electron density around CLA 3 3006:

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



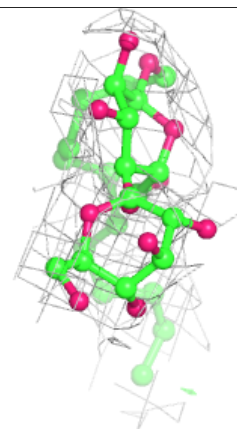
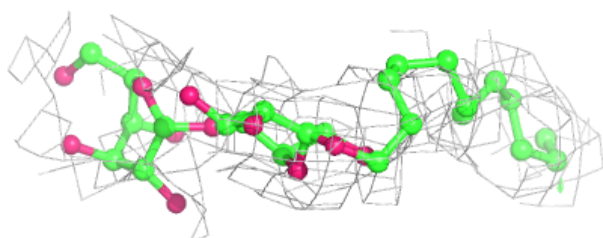
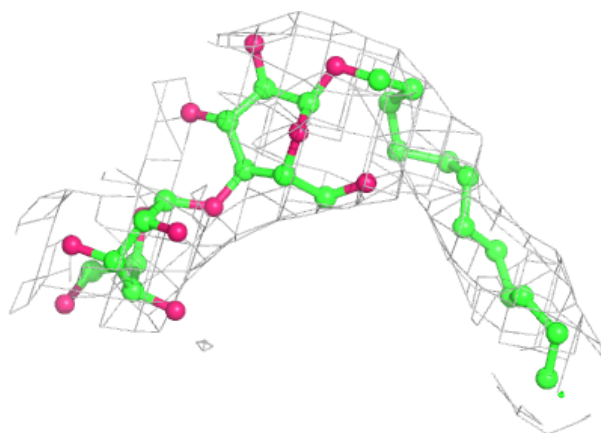
Electron density around CLA 1 1008:

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

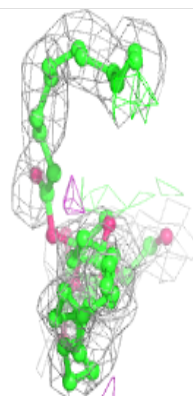
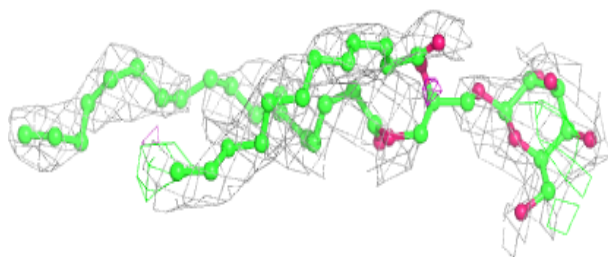
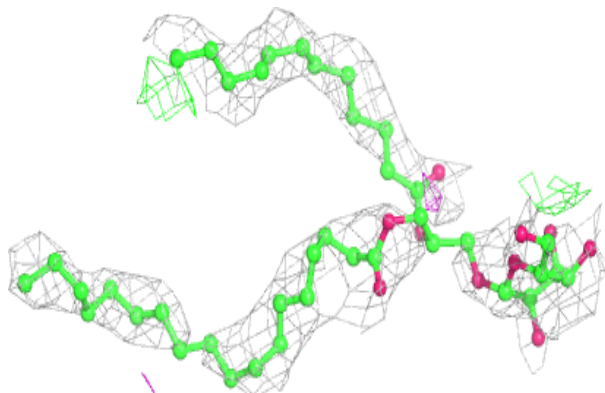


Electron density around LMU R 7021:

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

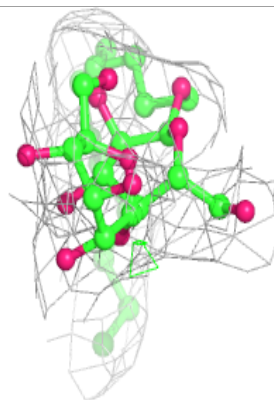
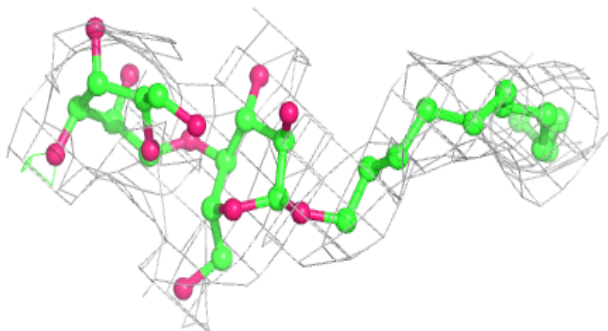
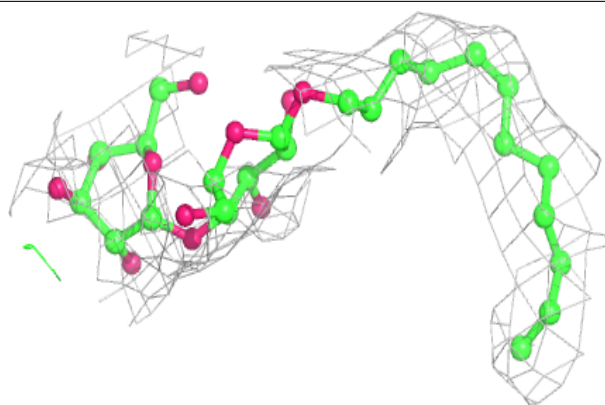
**Electron density around LMG B 7101:**

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

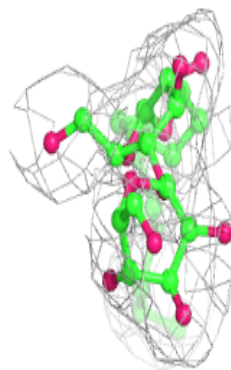
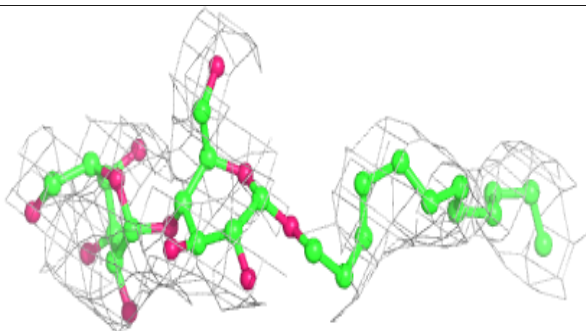
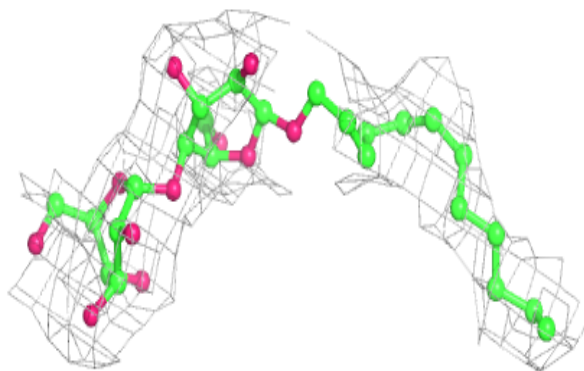


Electron density around LMU 2 7006:

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

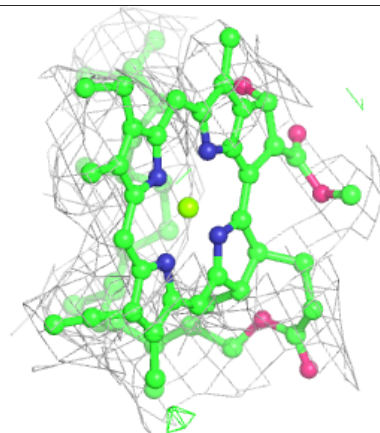
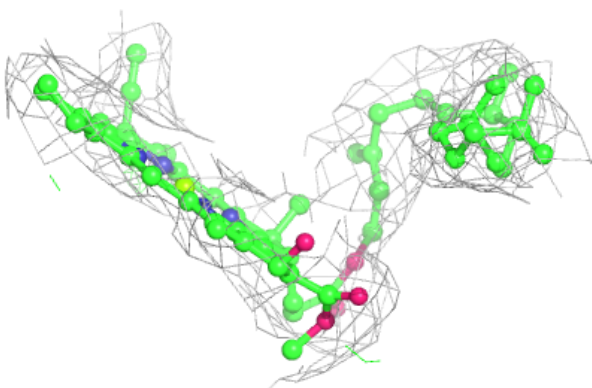
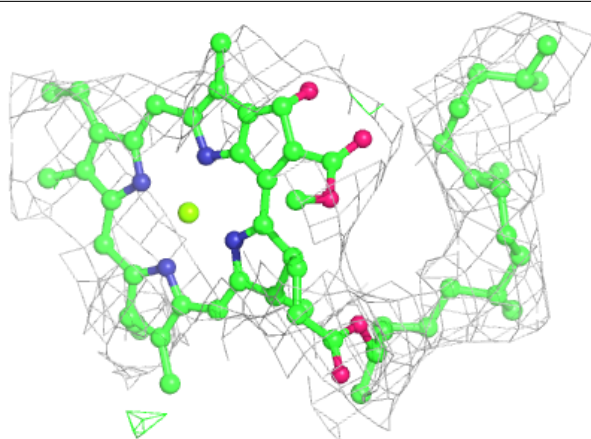
**Electron density around LMU 2 7027:**

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



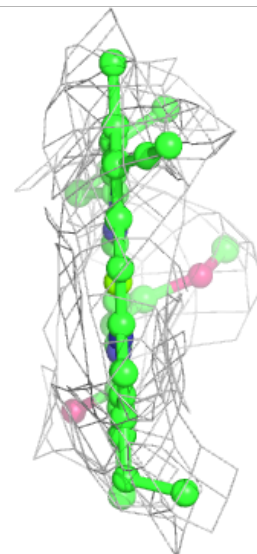
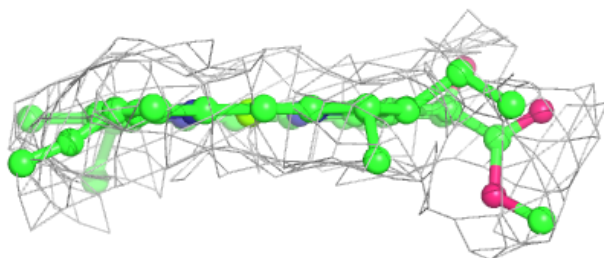
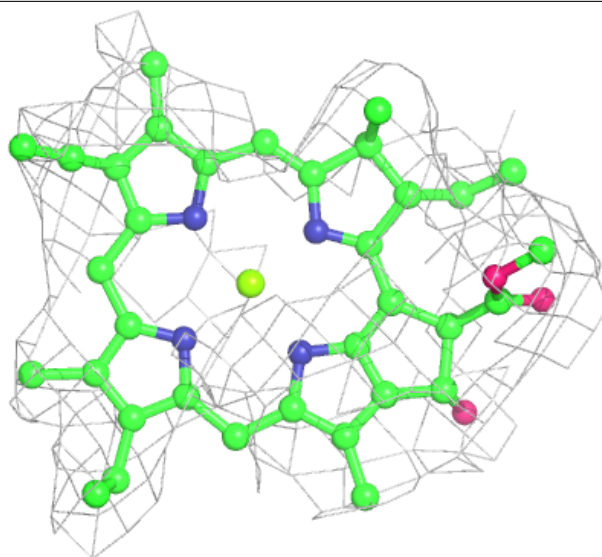
Electron density around CLA H 1145:

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



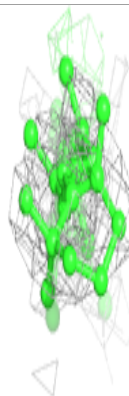
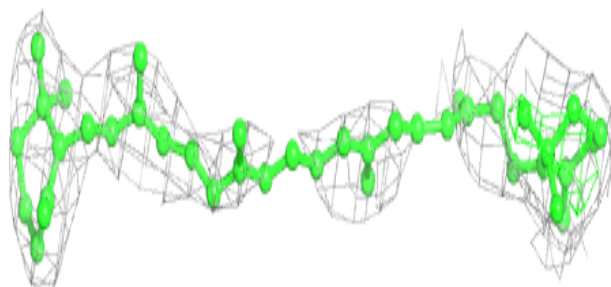
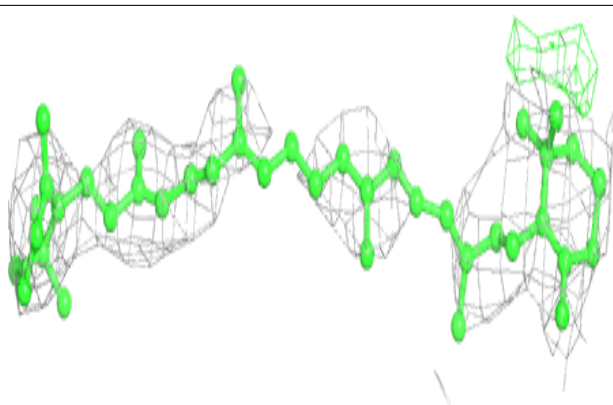
Electron density around CLA A 1121:

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

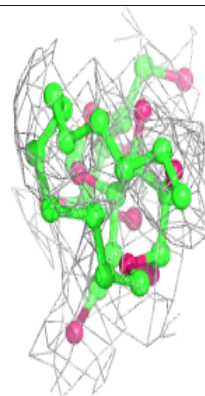
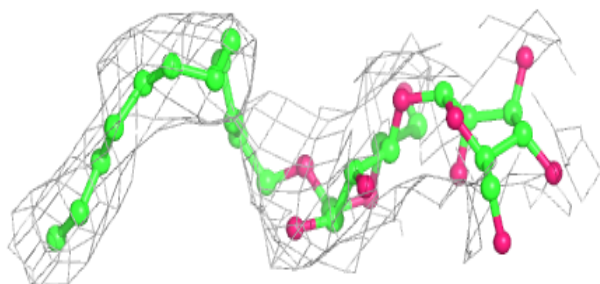
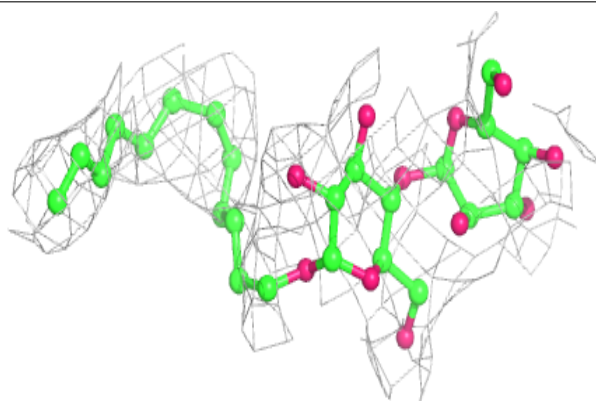


Electron density around BCR A 6003:

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

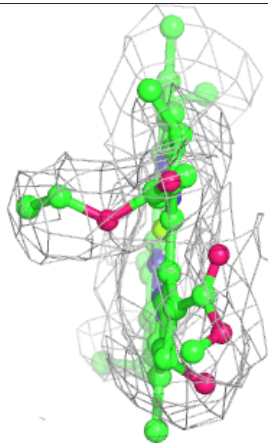
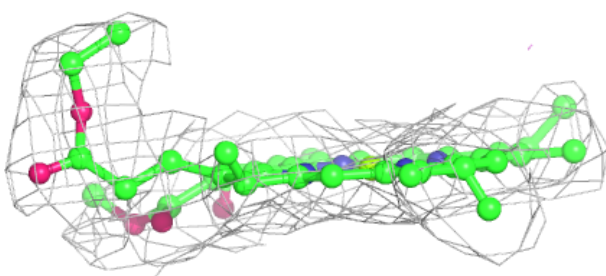
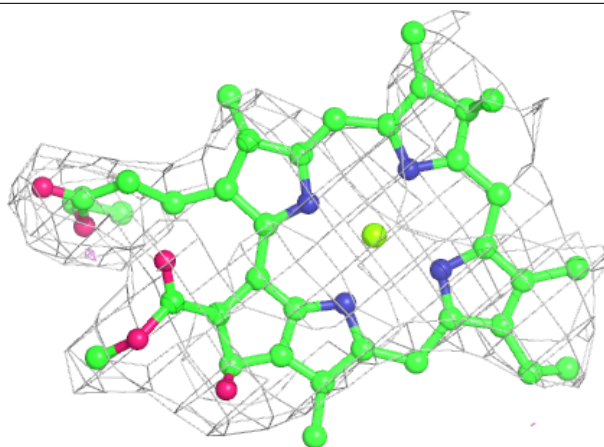
**Electron density around LMU D 7050:**

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

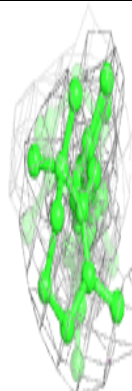
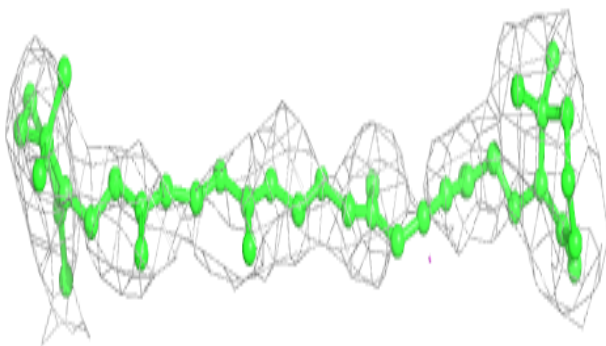
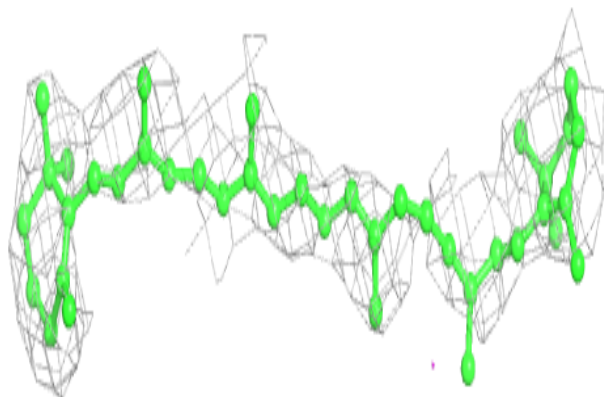


Electron density around CLA A 1149:

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

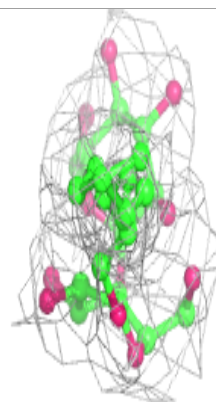
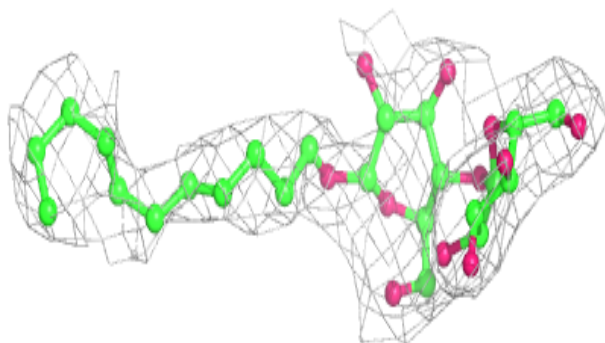
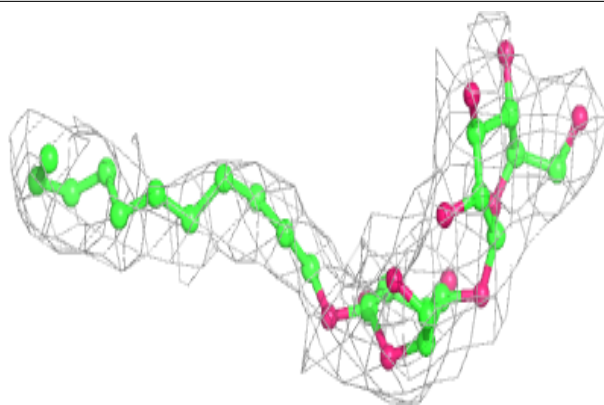
**Electron density around BCR J 6012:**

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



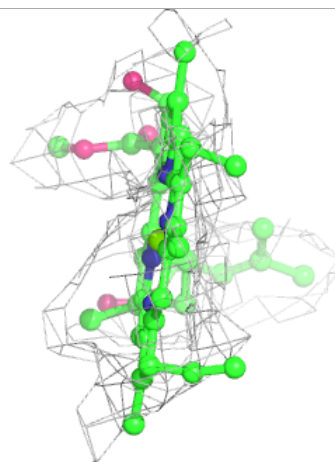
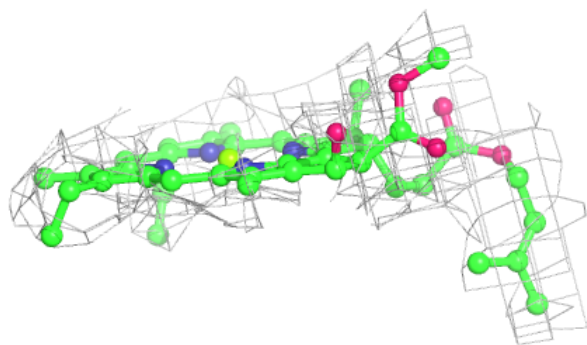
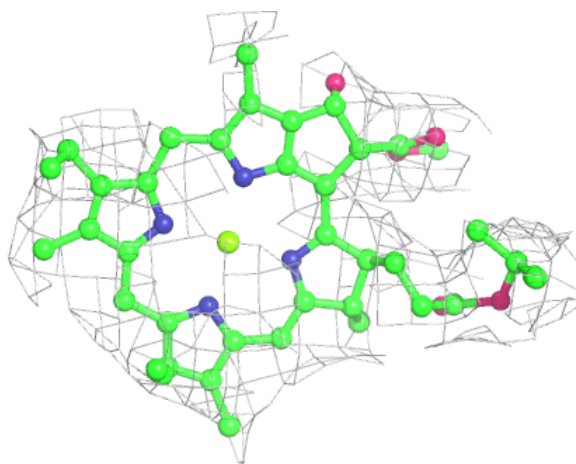
Electron density around LMU F 7036:

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



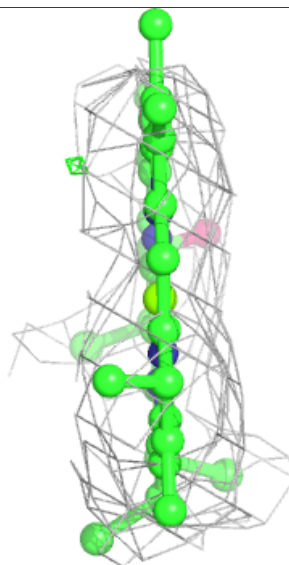
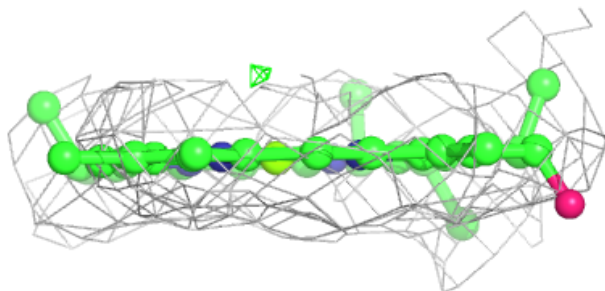
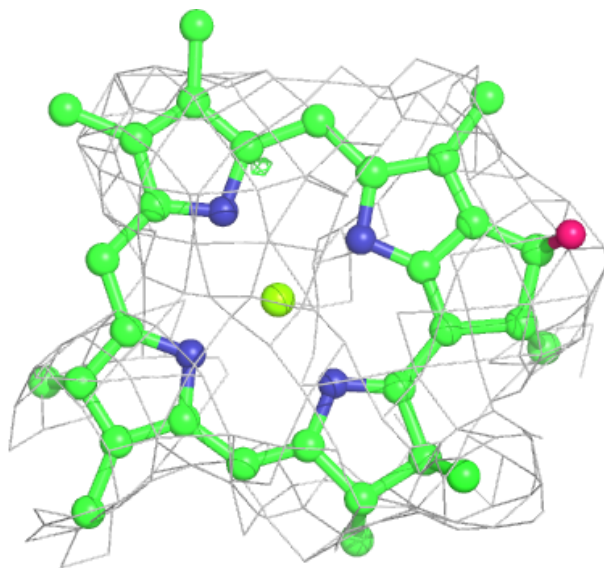
Electron density around CLA 3 3017:

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



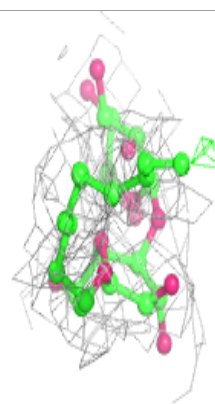
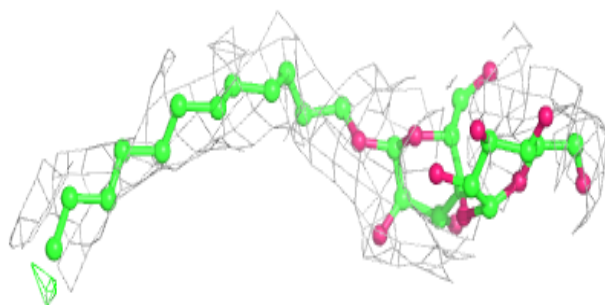
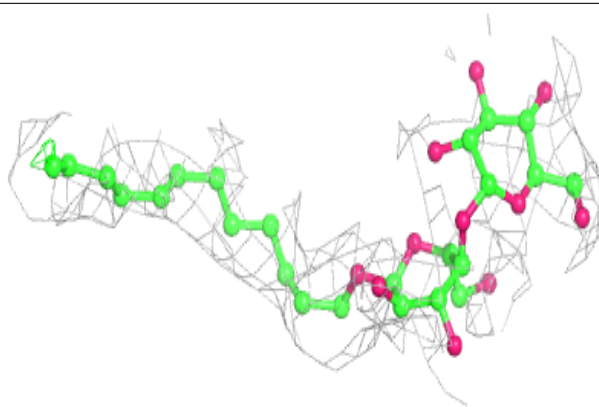
Electron density around CLA B 1301:

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

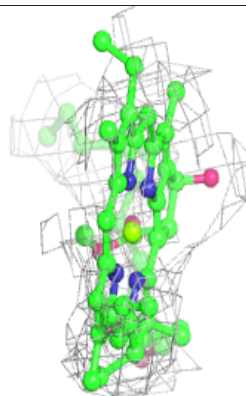
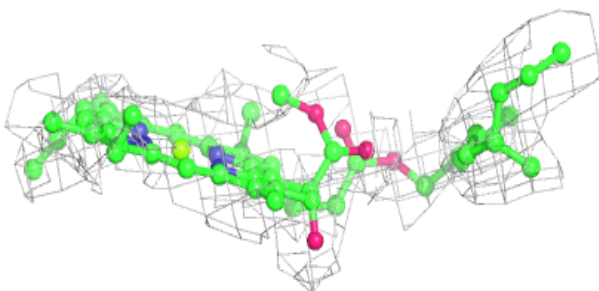
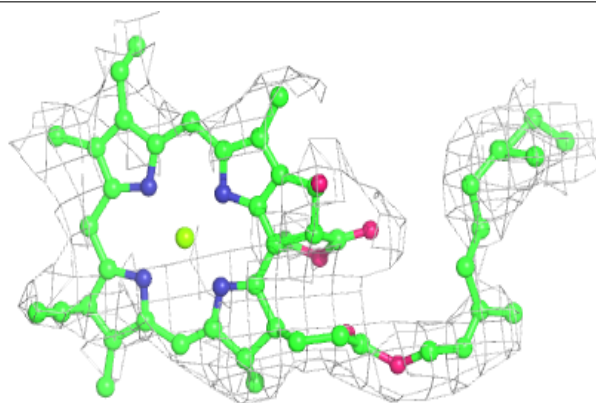


Electron density around LMU R 7024:

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

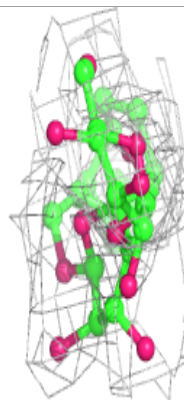
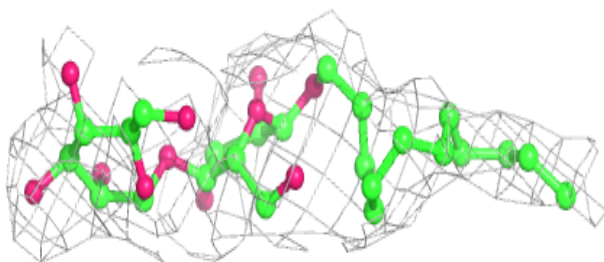
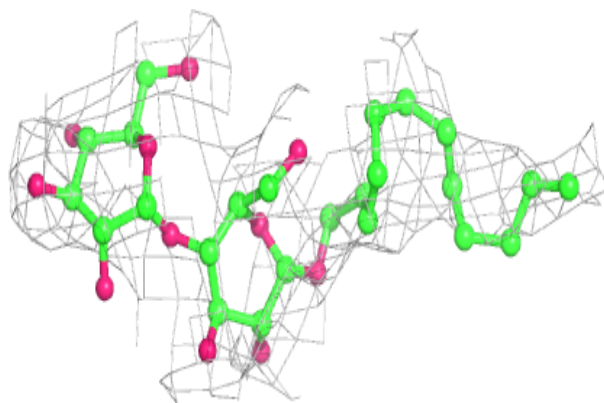
**Electron density around CLA R 1144:**

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

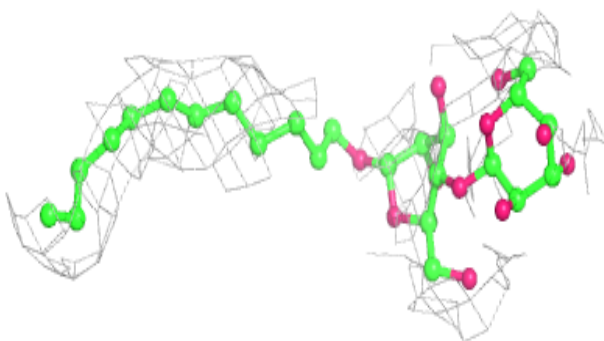
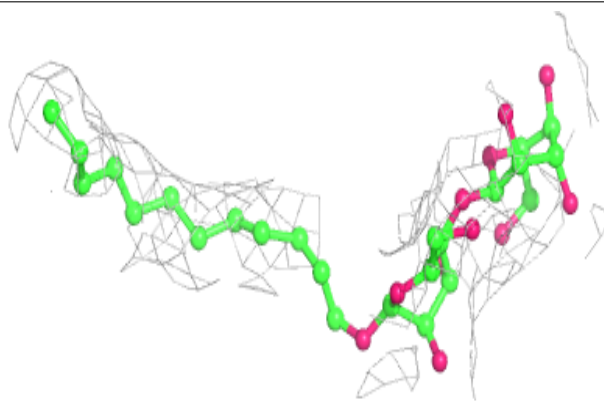


Electron density around LMU A 7016:

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

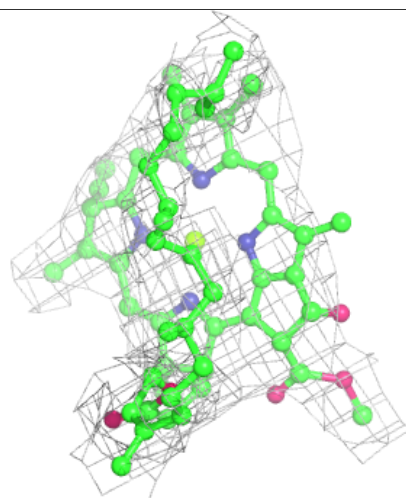
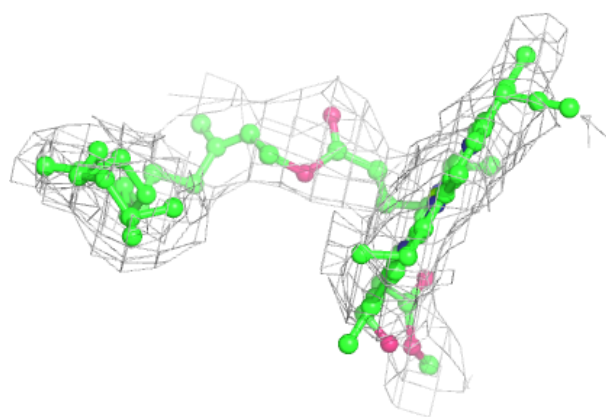
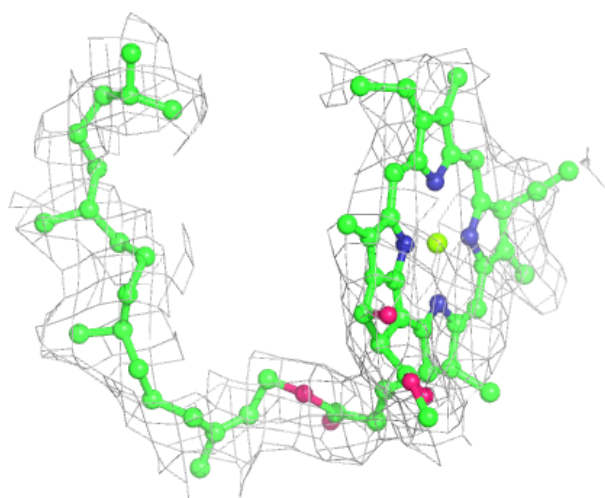
**Electron density around LMU H 7002:**

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



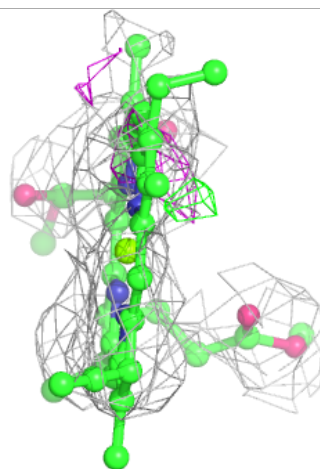
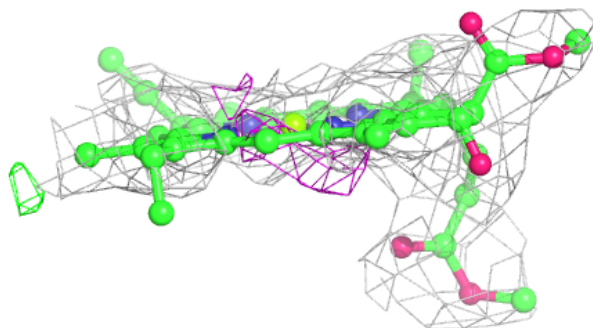
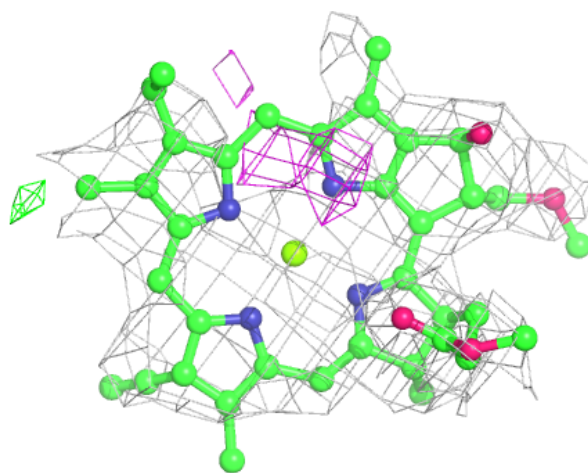
Electron density around CLA 3 3013:

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



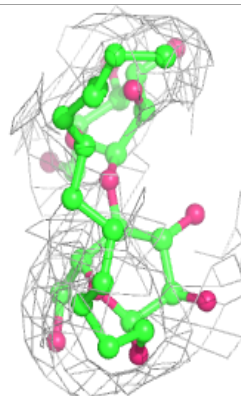
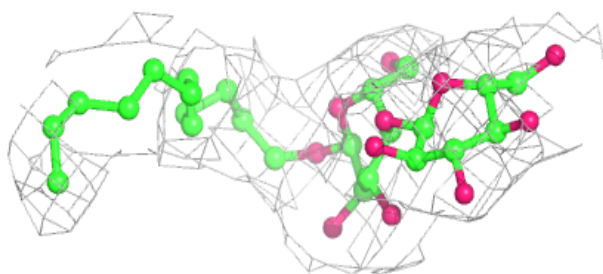
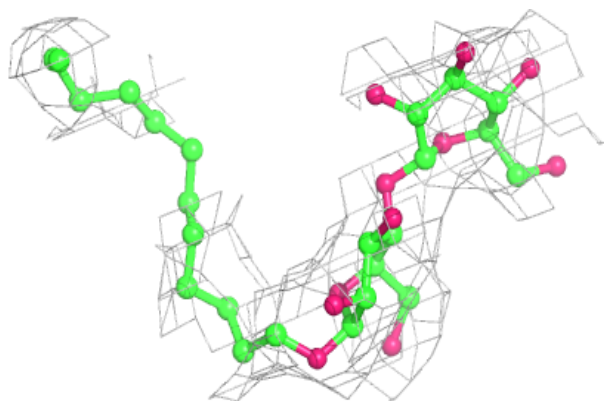
Electron density around CLA A 1105:

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

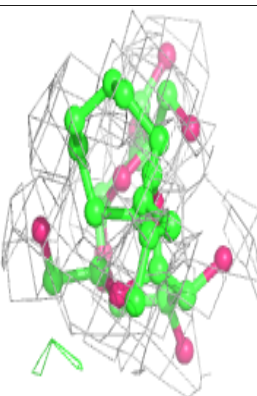
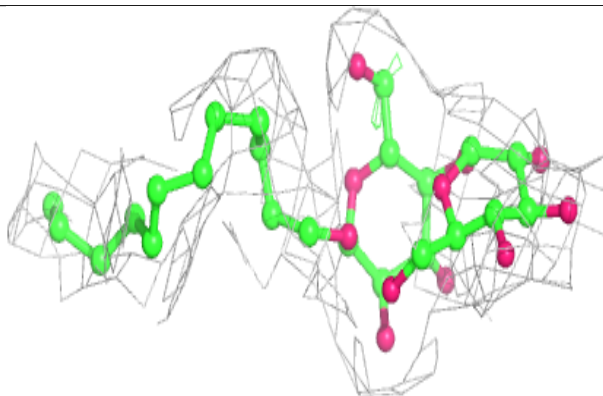
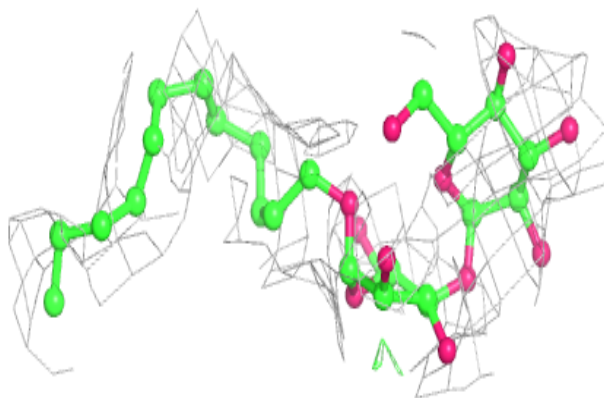


Electron density around LMU H 7028:

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

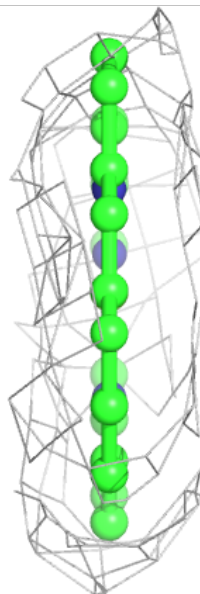
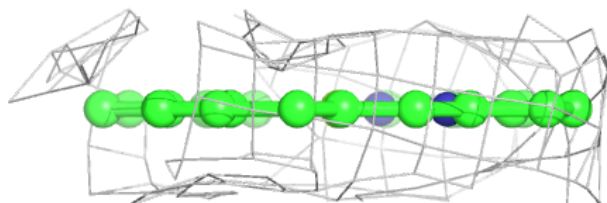
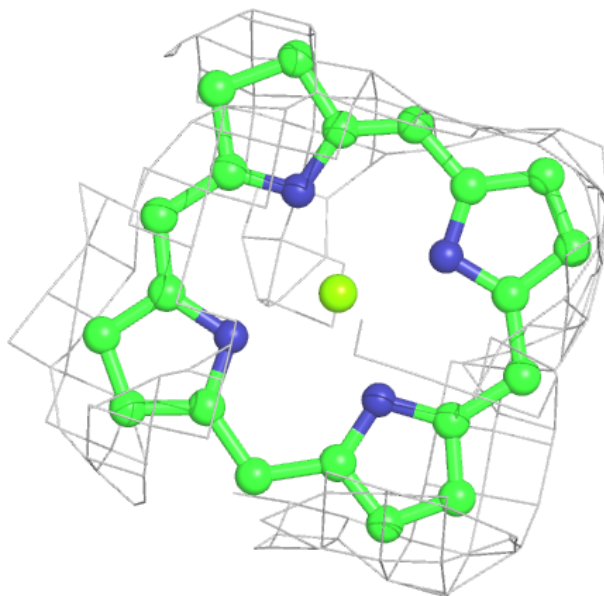
**Electron density around LMU A 7045:**

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



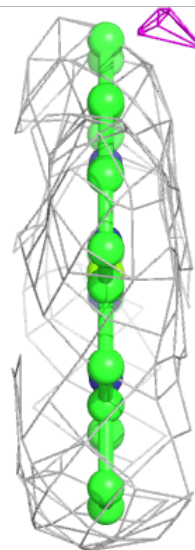
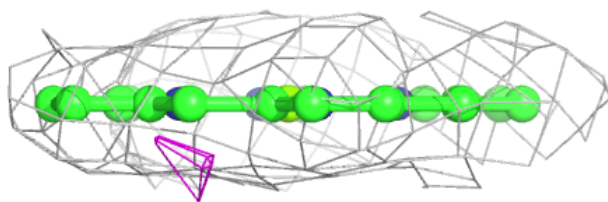
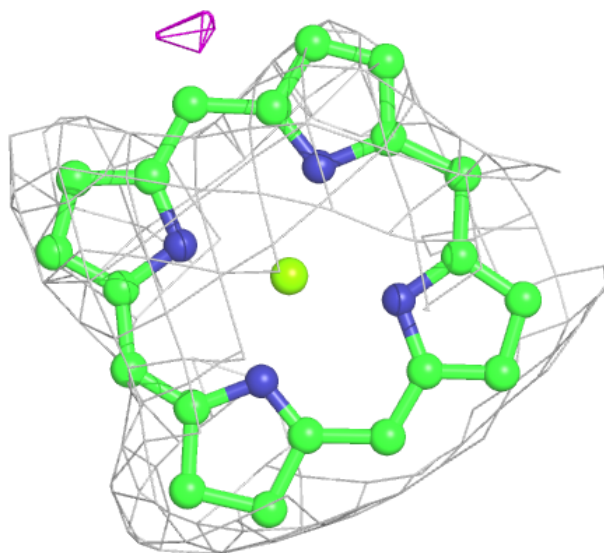
Electron density around CLA 3 3004:

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



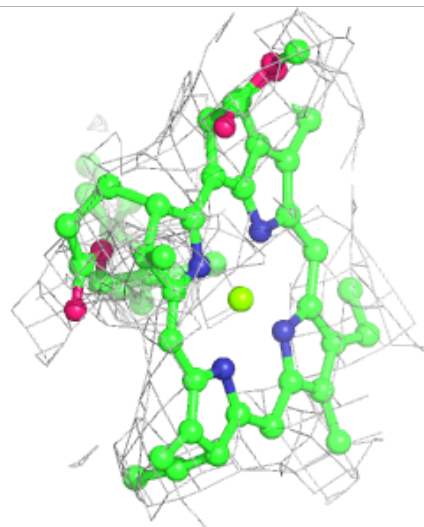
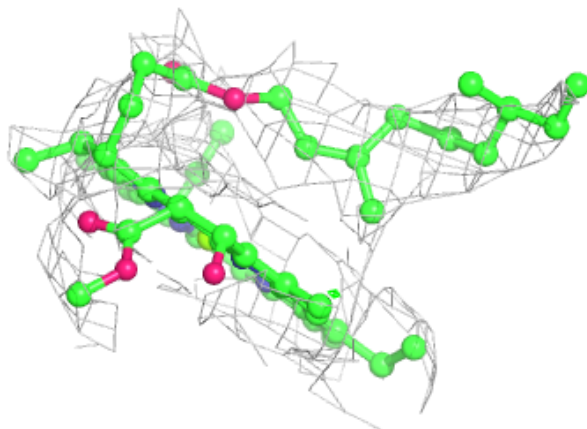
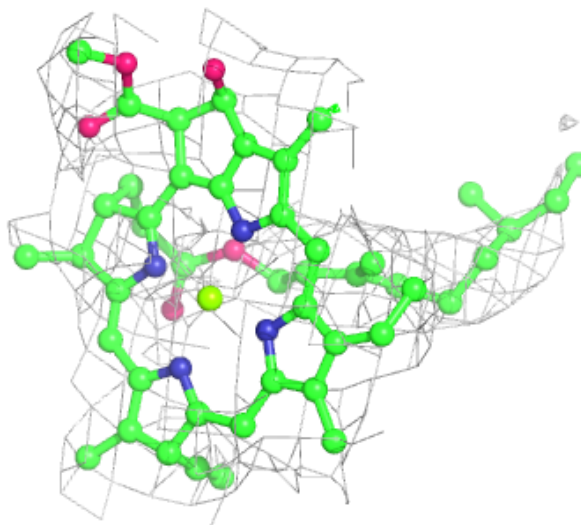
Electron density around CLA 2 2010:

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



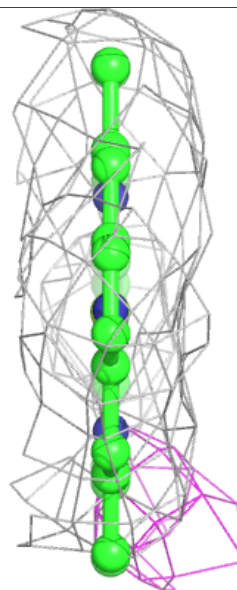
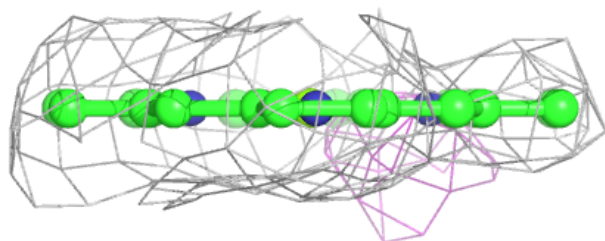
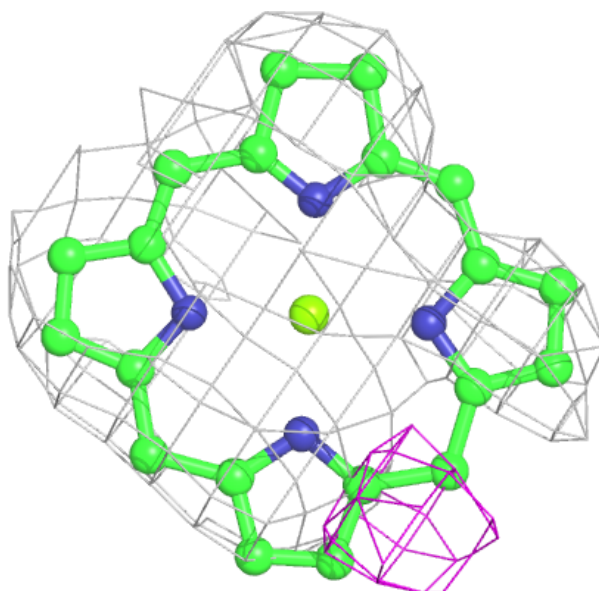
Electron density around CLA 2 2002:

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



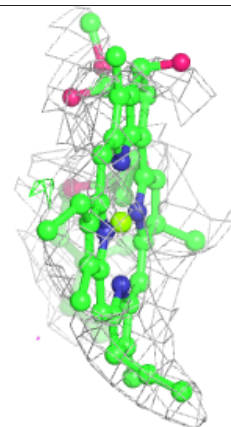
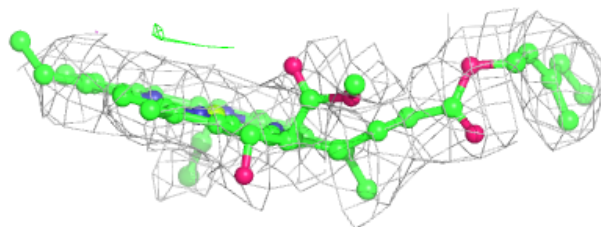
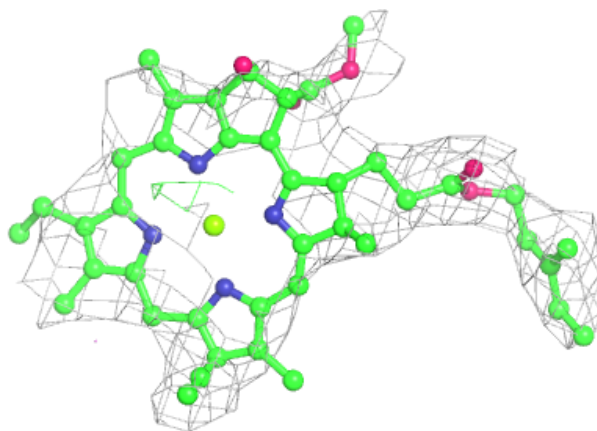
Electron density around CLA 2 2003:

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

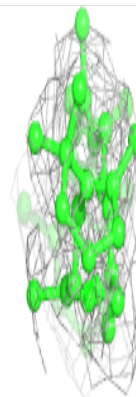
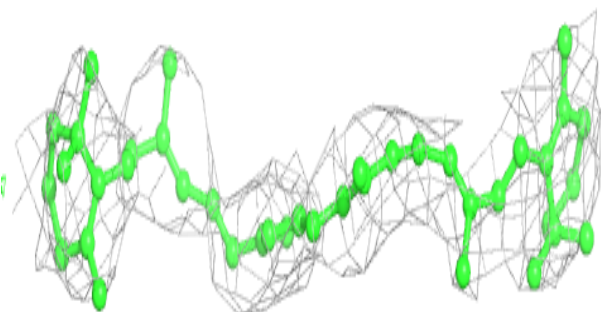
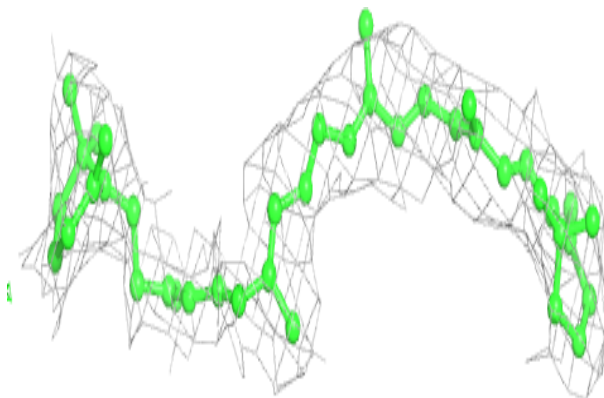


Electron density around CLA 1 1303:

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

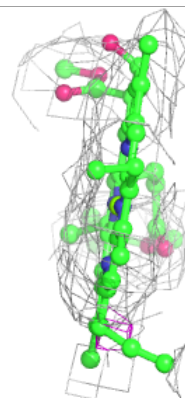
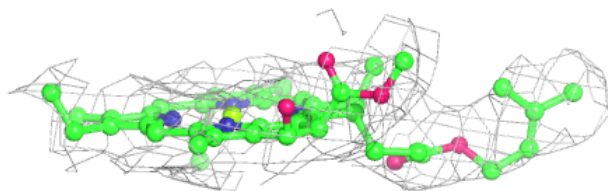
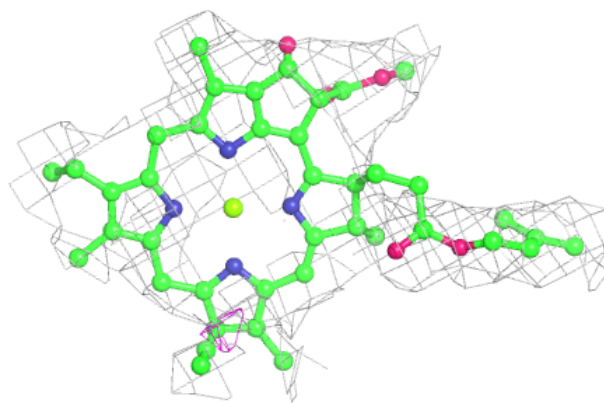
**Electron density around BCR I 6021:**

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



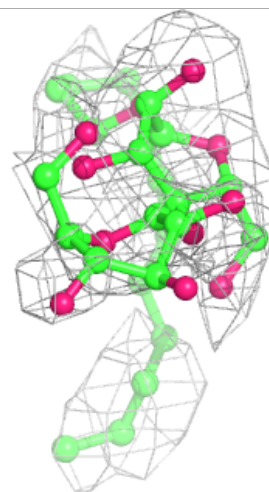
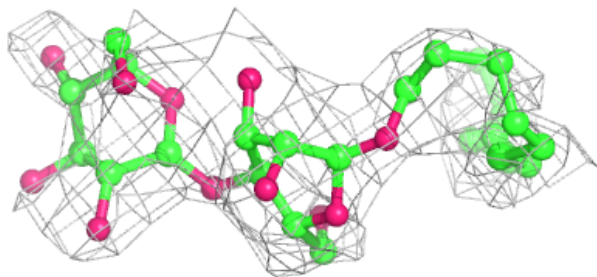
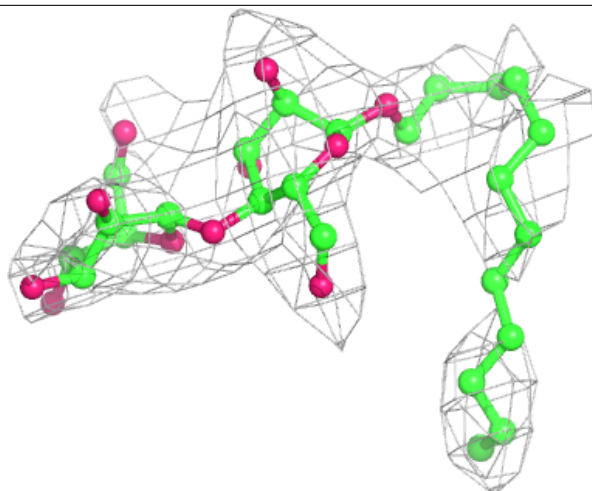
Electron density around CLA K 1143:

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



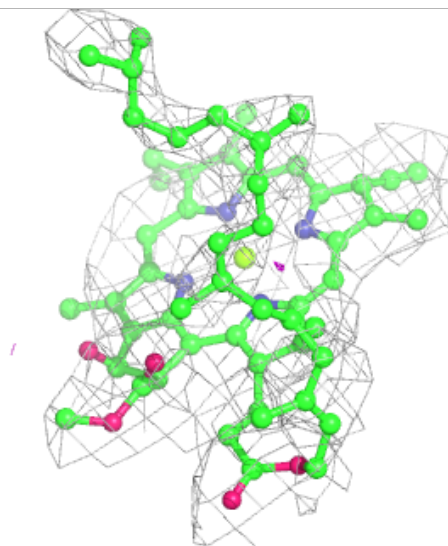
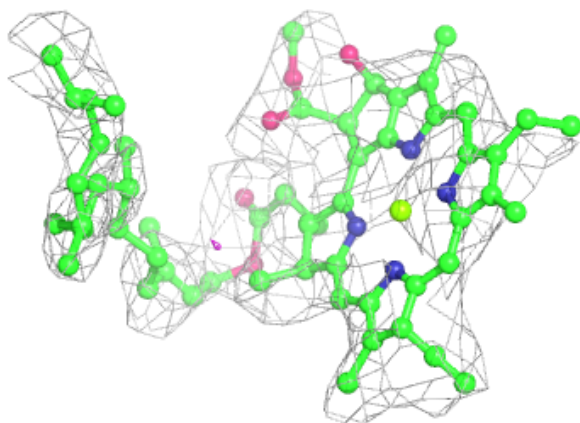
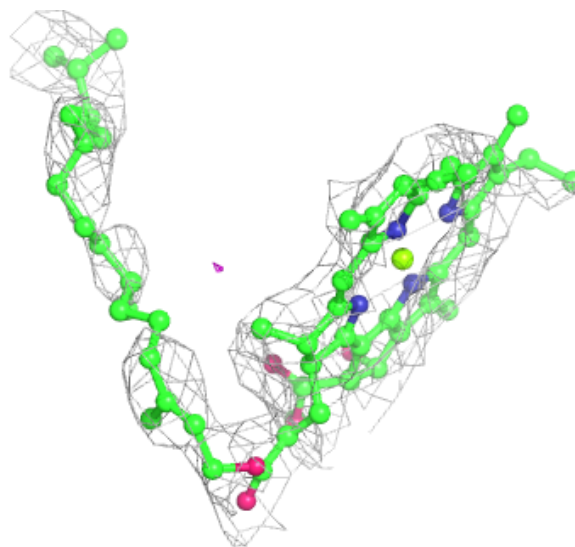
Electron density around LMU R 7014:

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



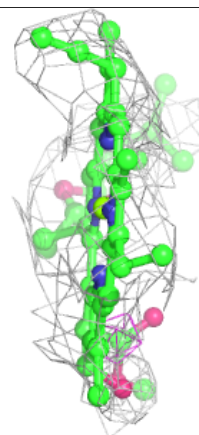
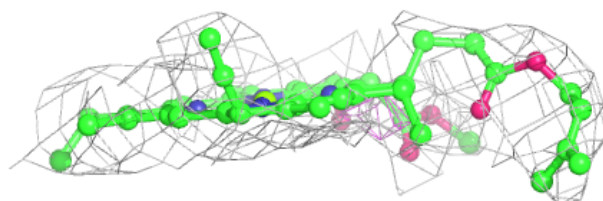
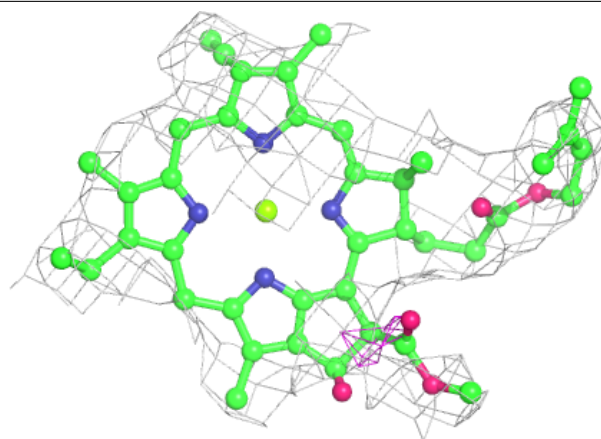
Electron density around CLA 2 2006:

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

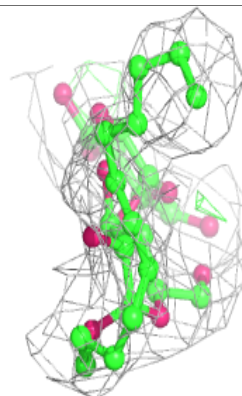
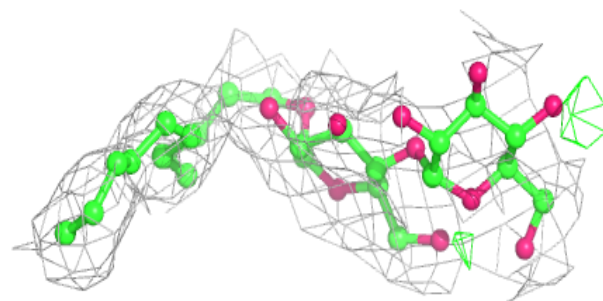
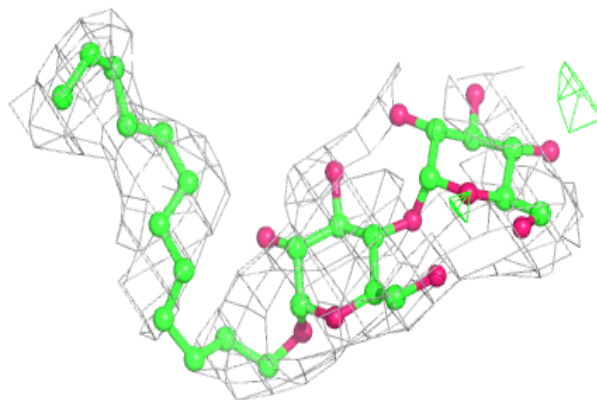


Electron density around CLA K 1146:

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

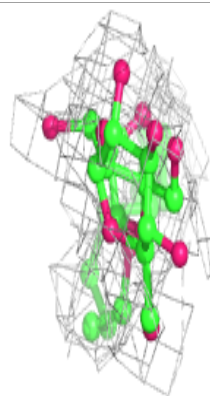
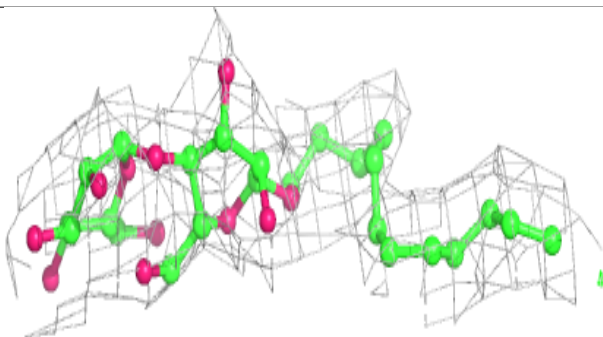
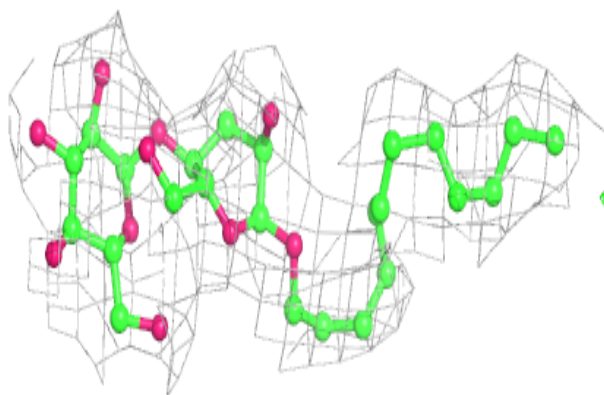
**Electron density around LMU R 7025:**

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



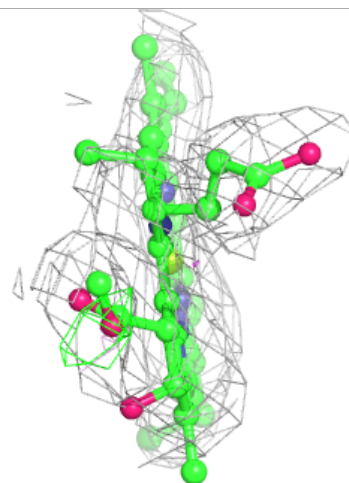
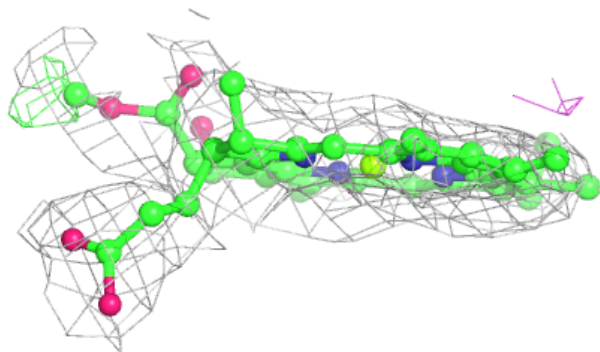
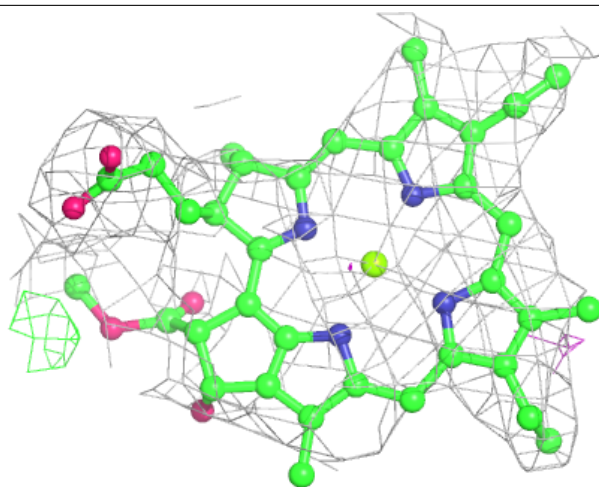
Electron density around LMU R 7020:

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



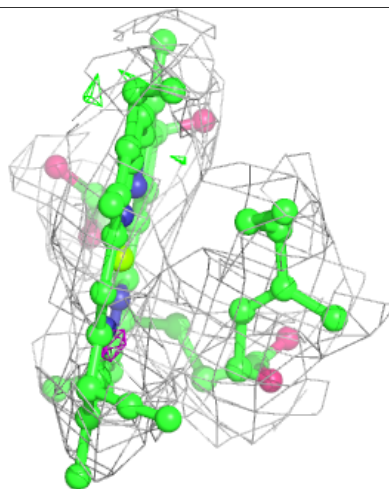
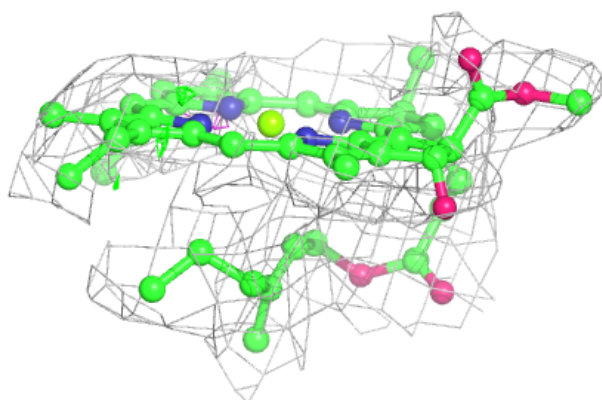
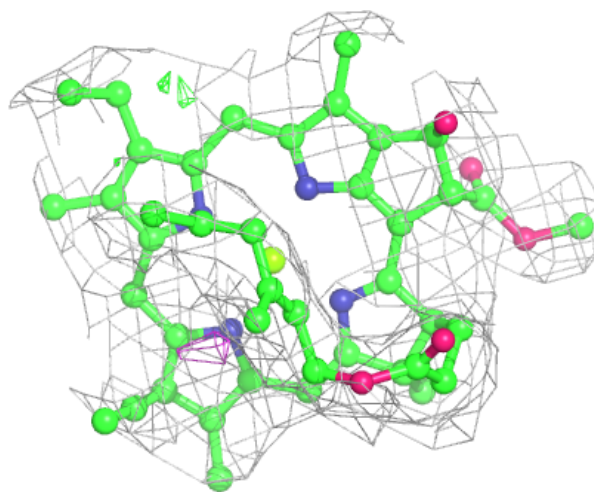
Electron density around CLA A 1108:

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



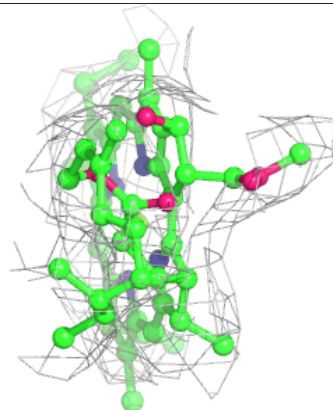
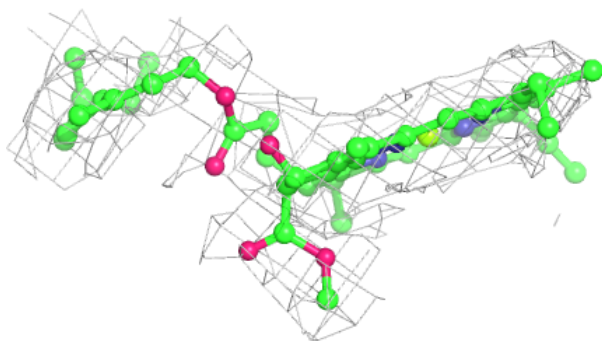
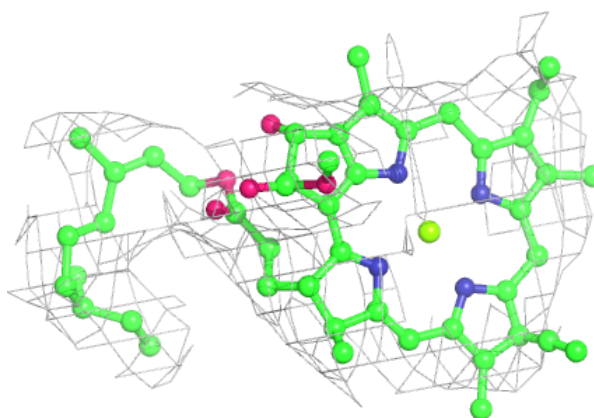
Electron density around CLA A 1116:

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

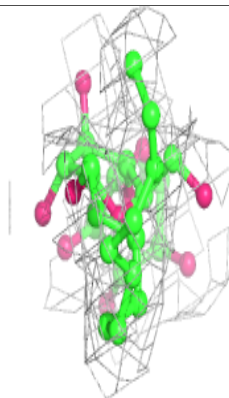
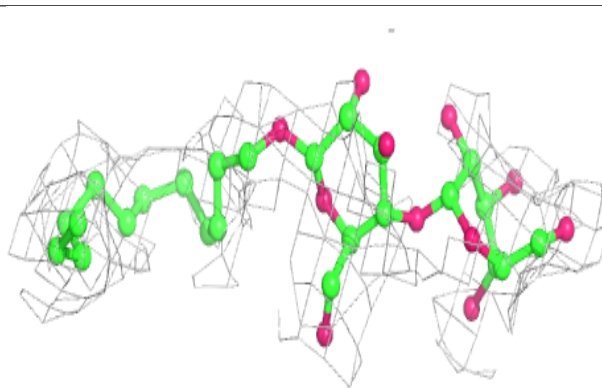
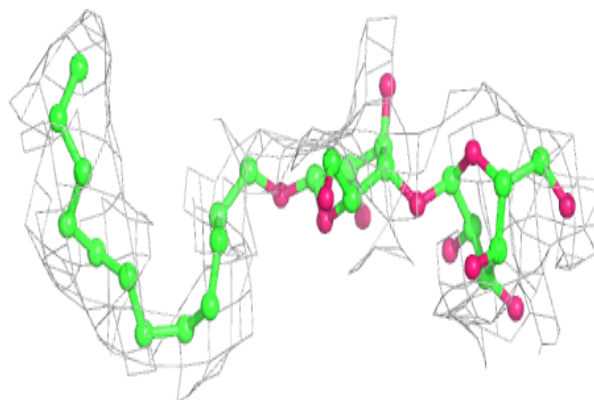


Electron density around CLA 3 2009:

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

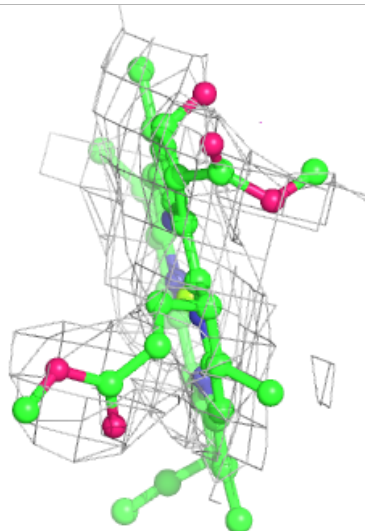
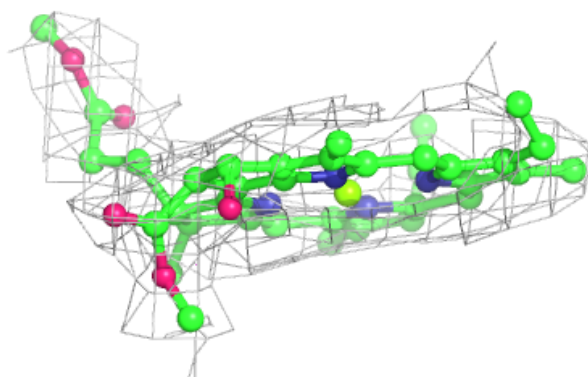
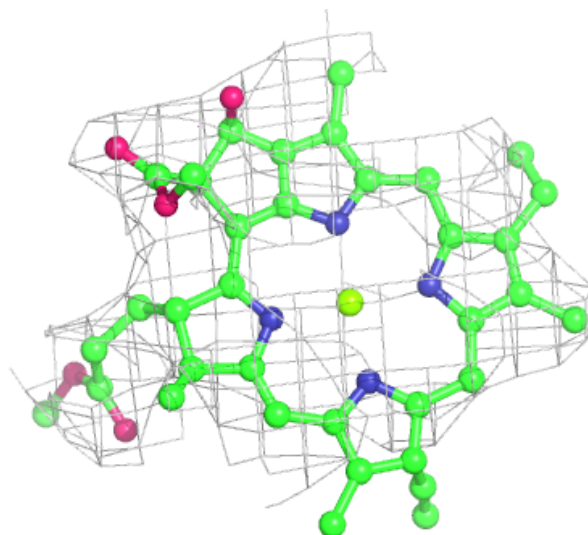
**Electron density around LMU A 7044:**

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



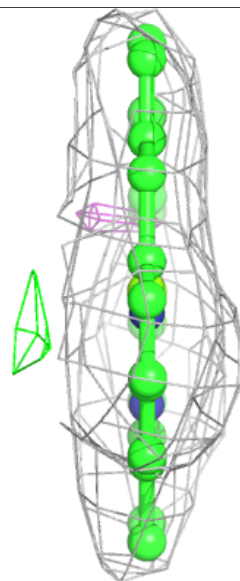
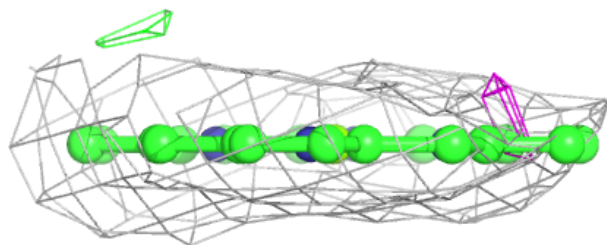
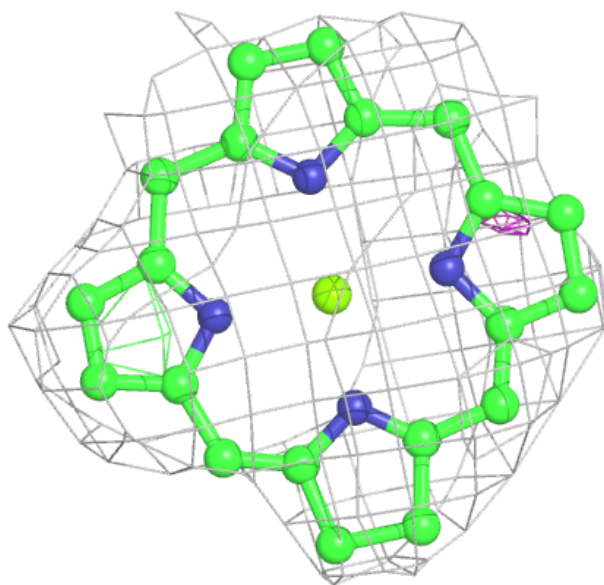
Electron density around CLA B 1218:

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



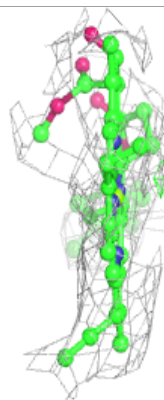
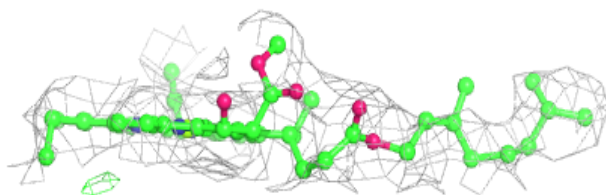
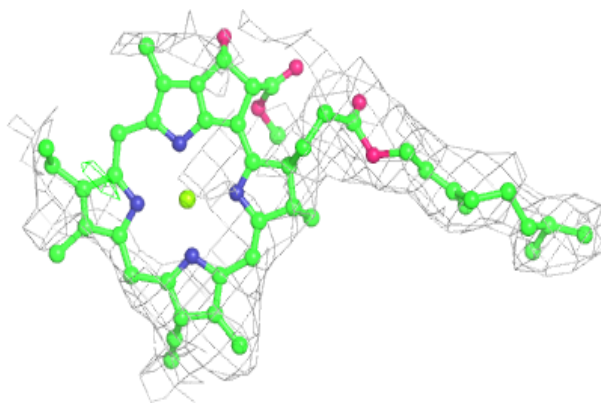
Electron density around CLA 4 4005:

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



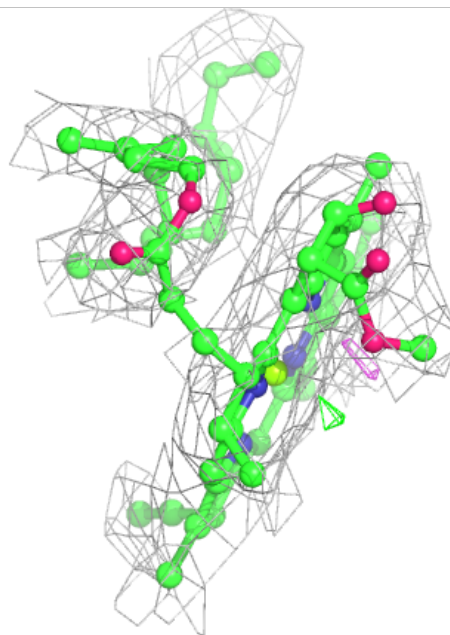
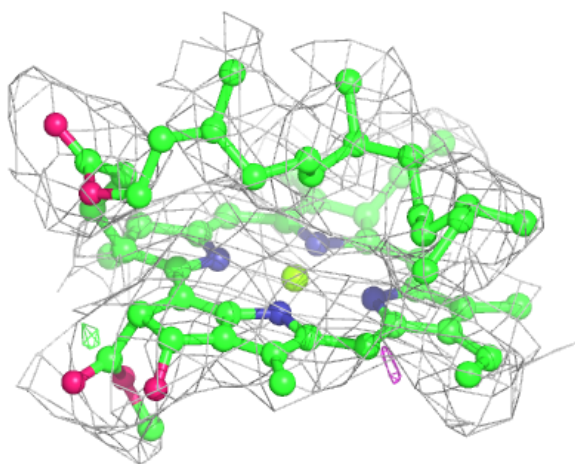
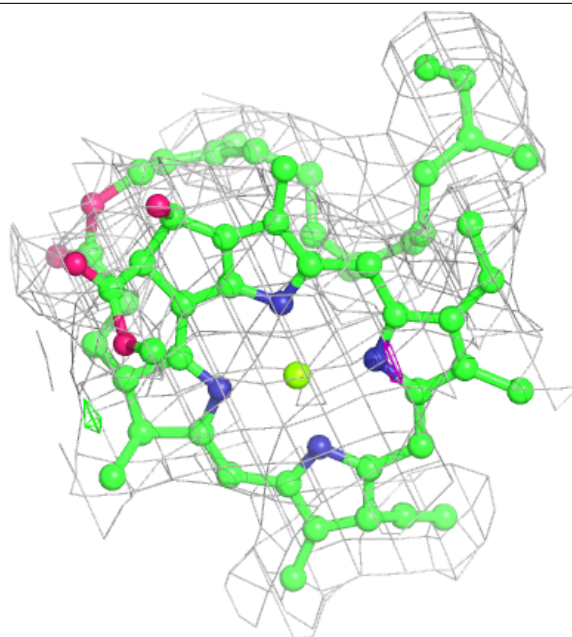
Electron density around CLA 4 4006:

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



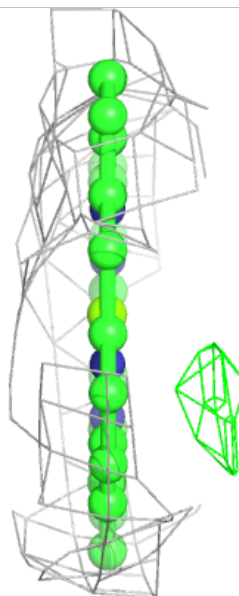
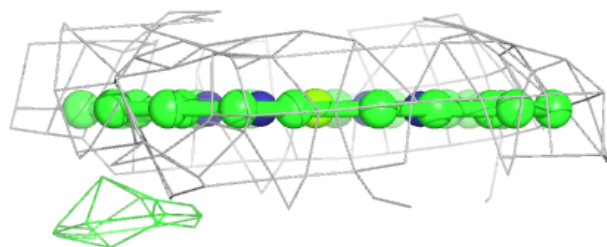
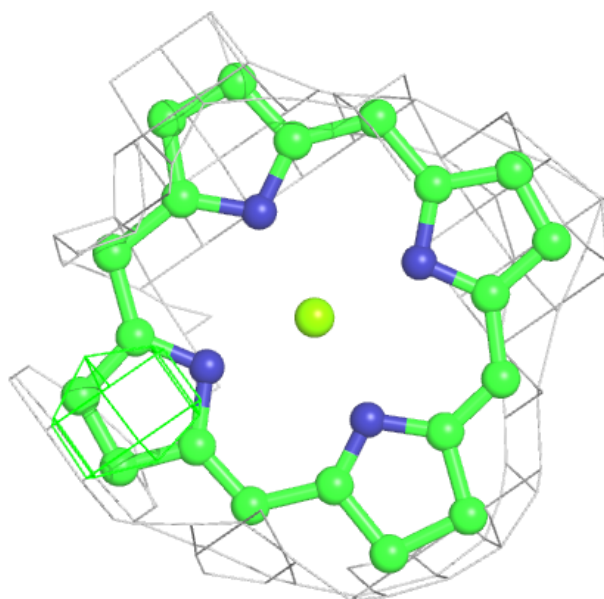
Electron density around CLA 1 1007:

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



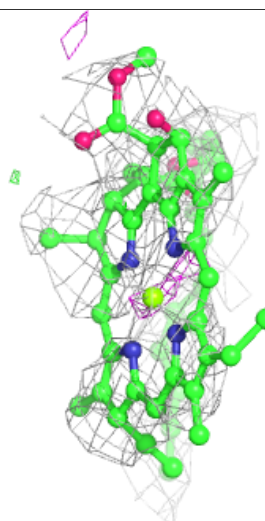
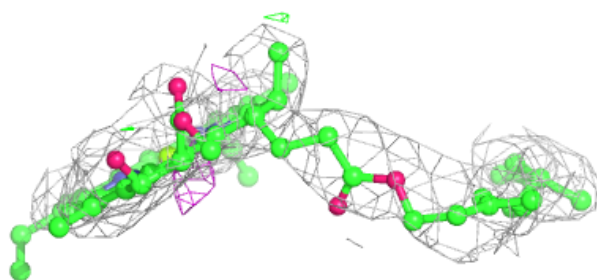
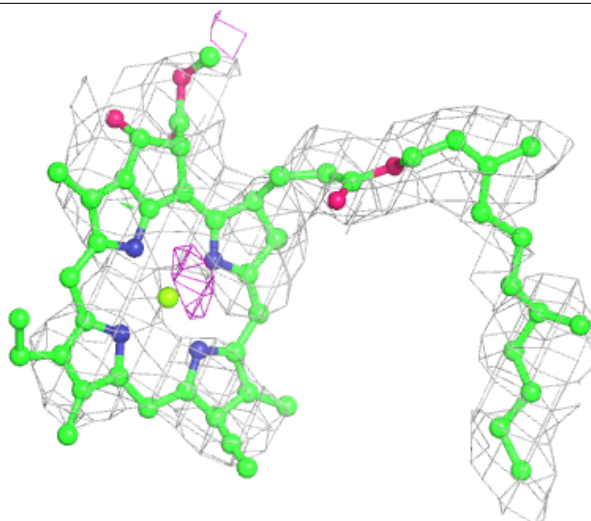
Electron density around CLA 4 4010:

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



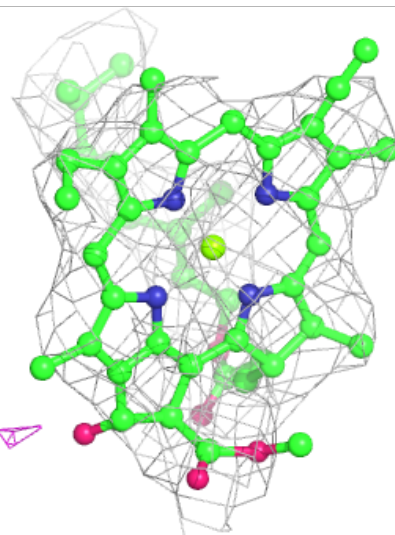
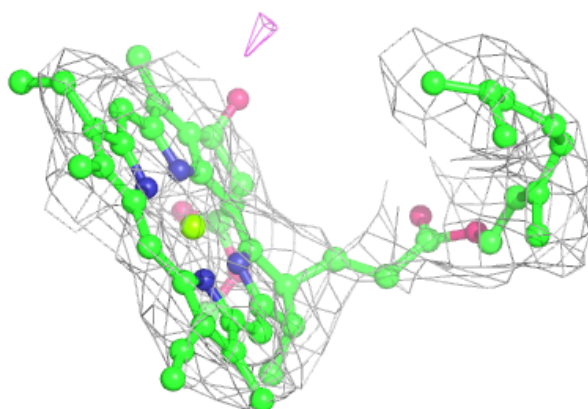
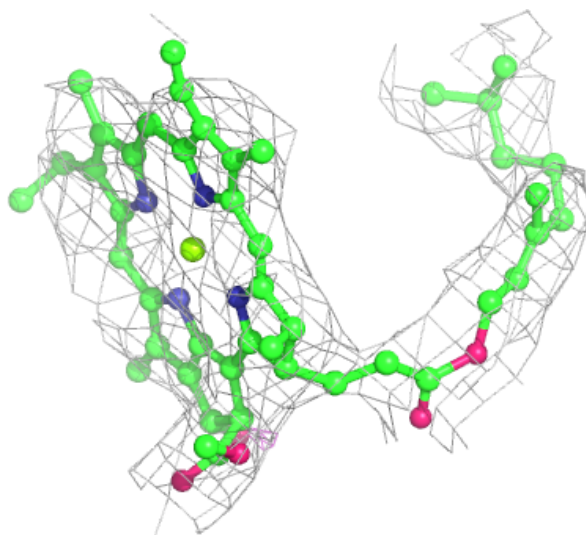
Electron density around CLA B 1222:

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



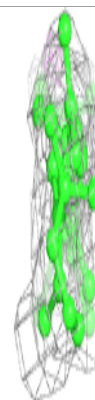
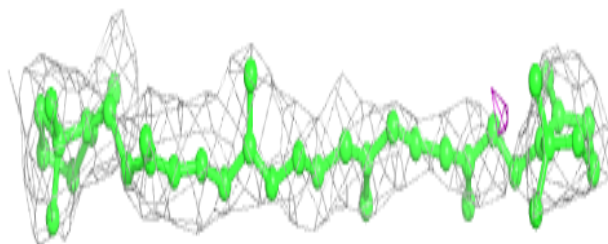
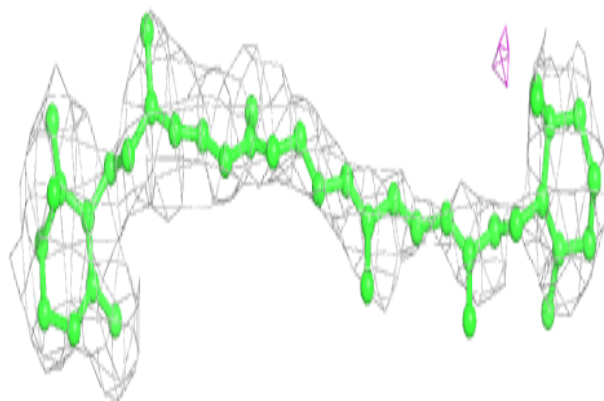
Electron density around CLA A 1102:

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

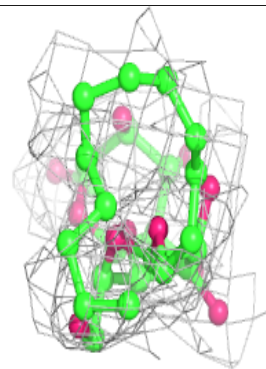
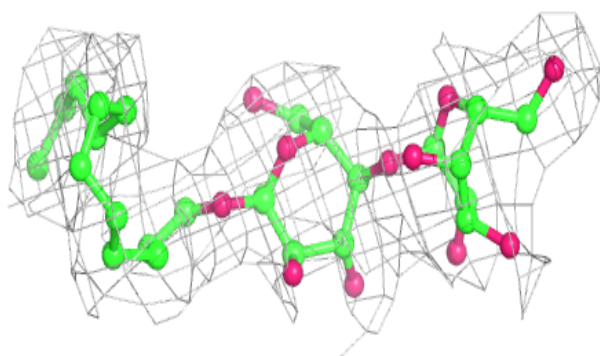
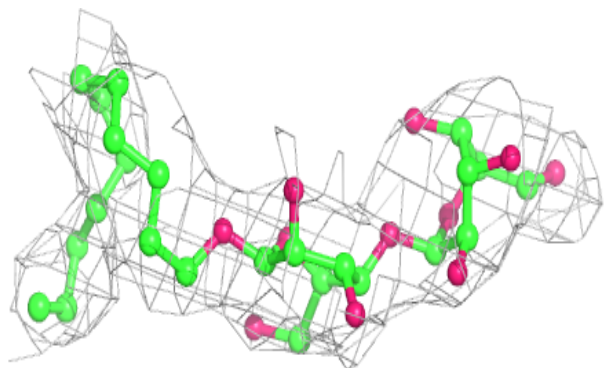


Electron density around BCR L 6019:

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

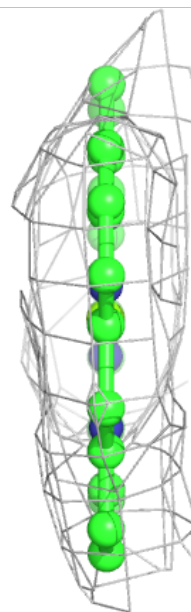
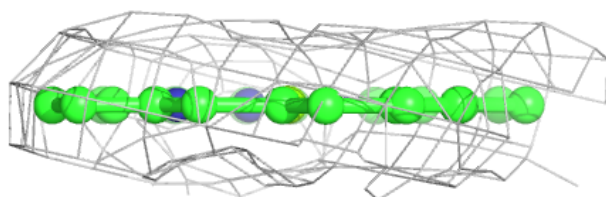
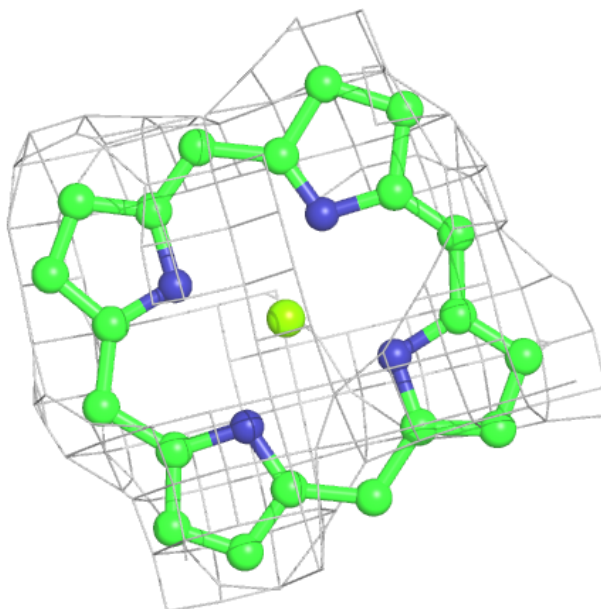
**Electron density around LMU A 7023:**

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



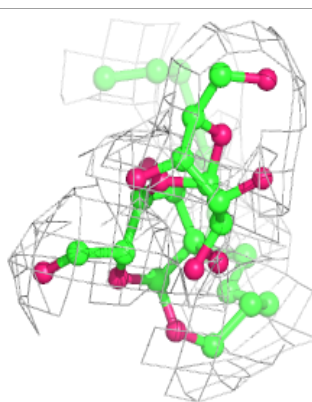
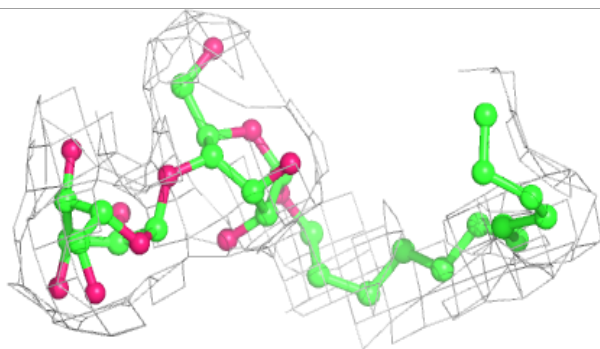
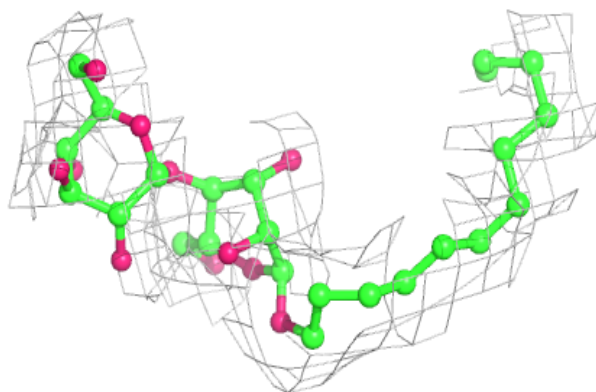
Electron density around CLA 3 3001:

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

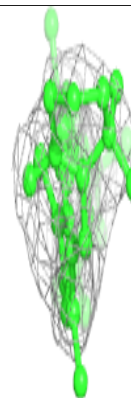
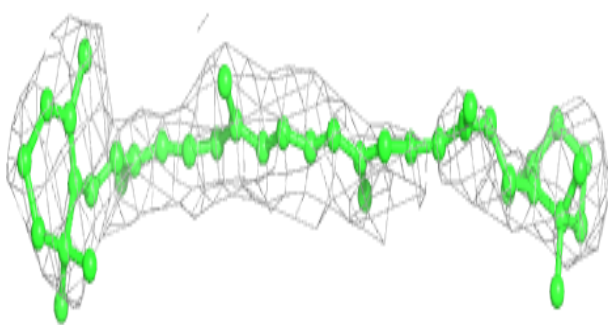
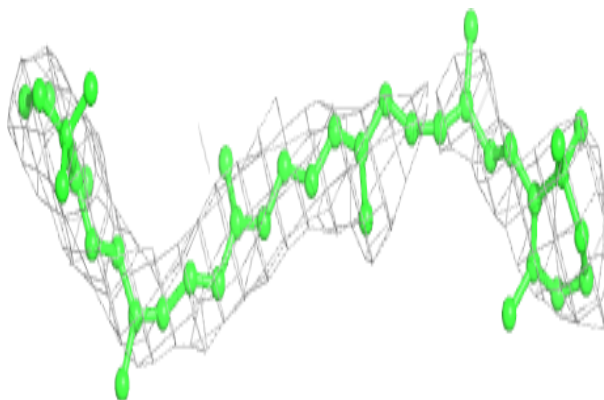


Electron density around LMU R 7022:

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

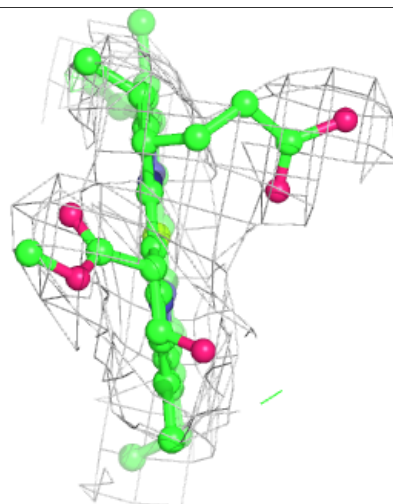
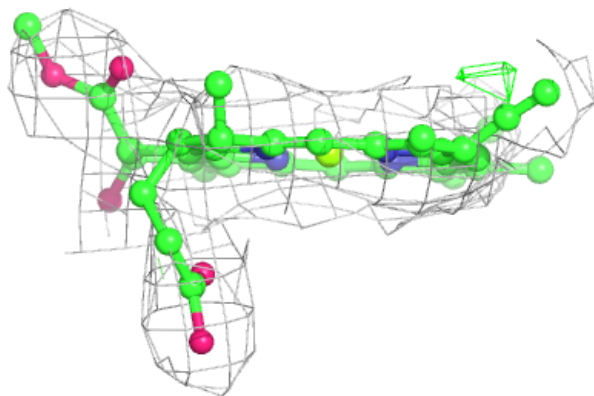
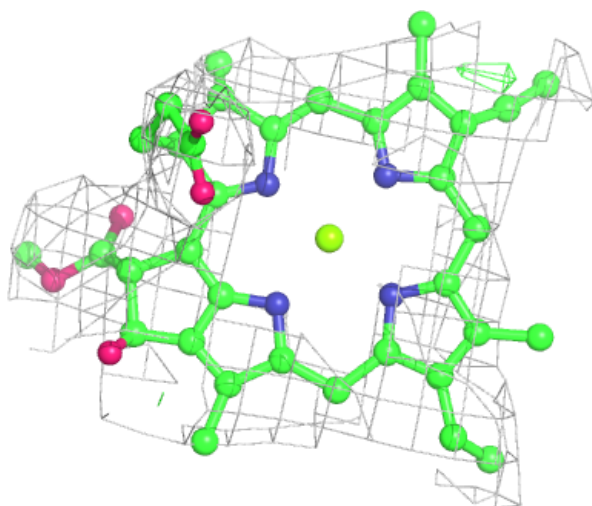
**Electron density around BCR B 6006:**

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



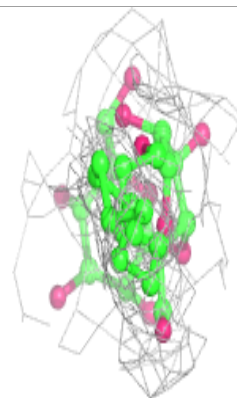
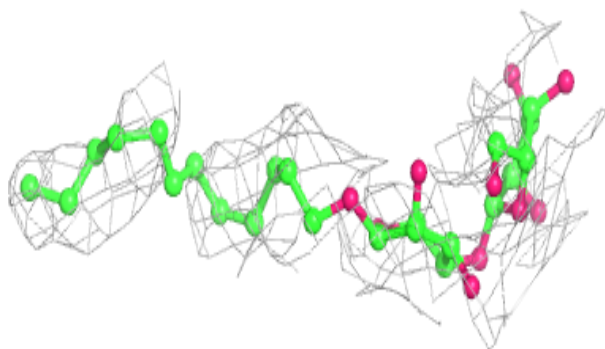
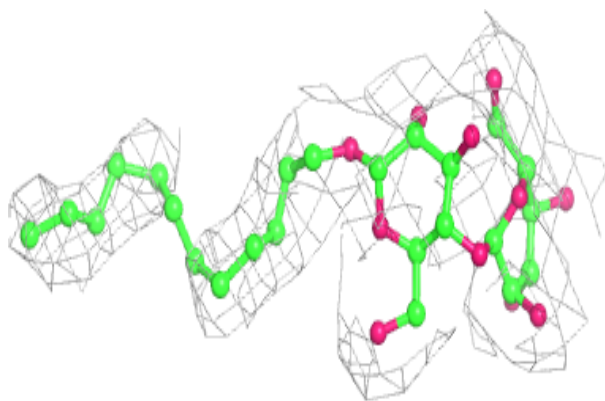
Electron density around CLA B 1201:

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



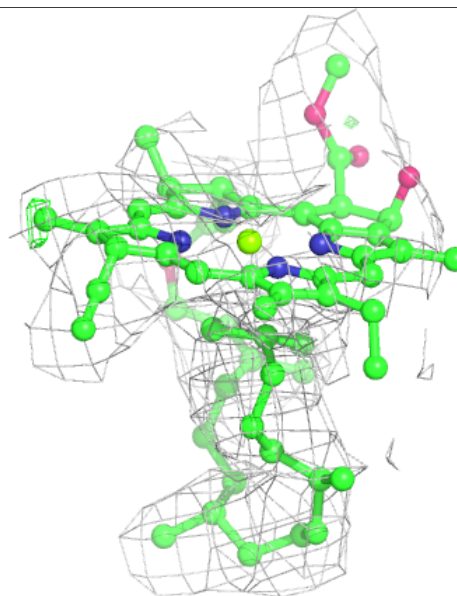
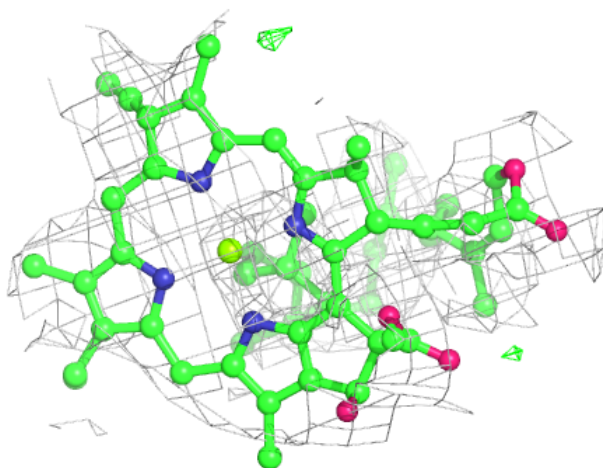
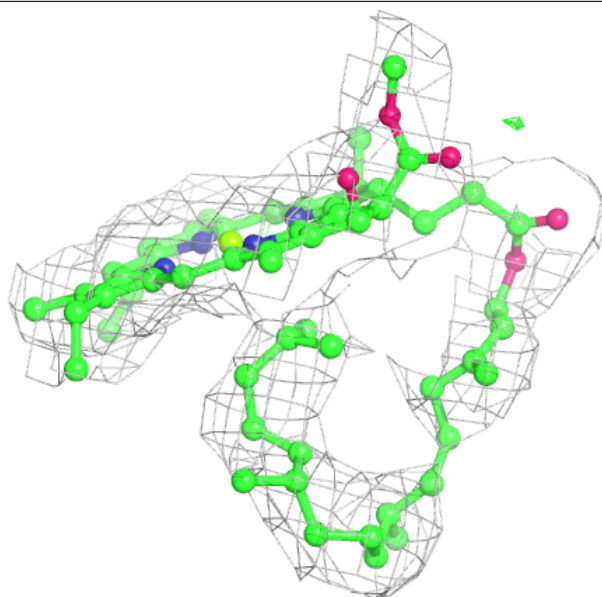
Electron density around LMU 4 7033:

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



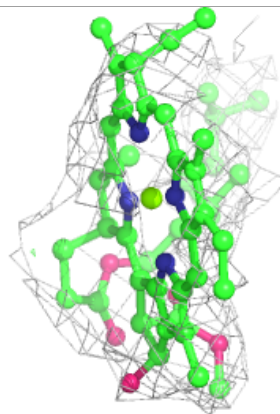
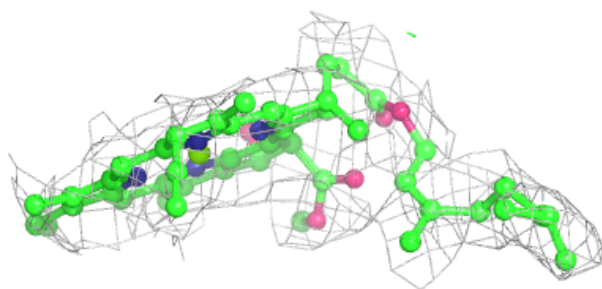
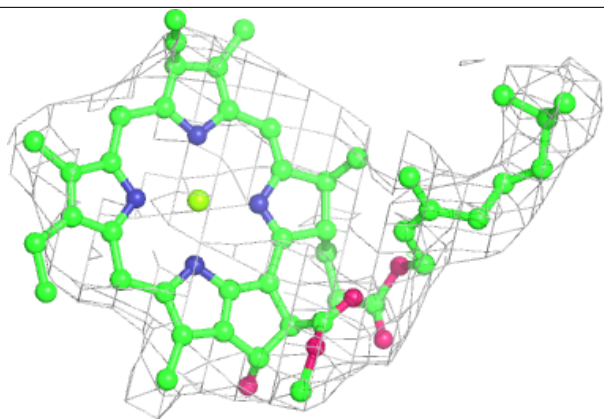
Electron density around CLA 2 4009:

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

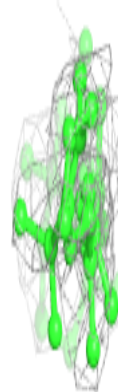
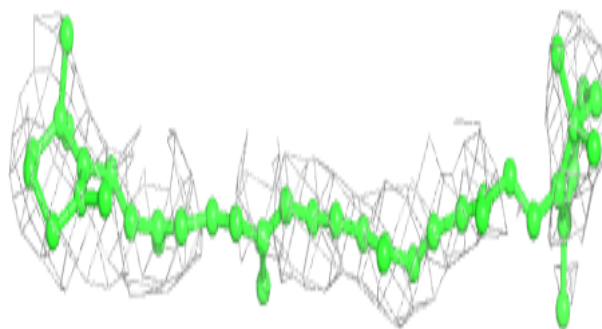
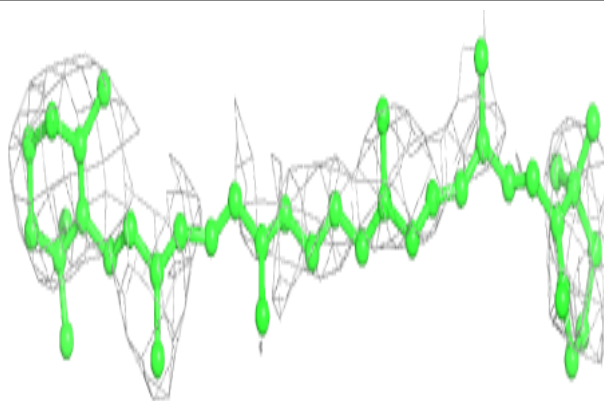


Electron density around CLA J 1308:

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

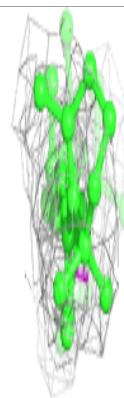
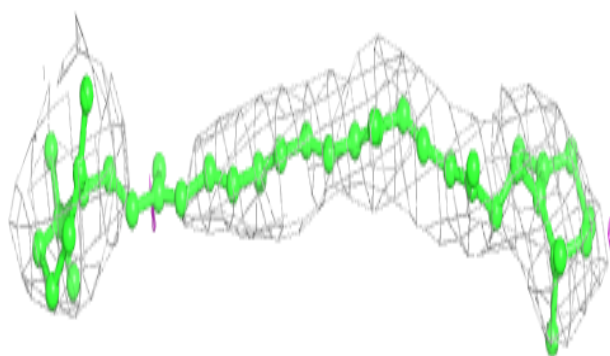
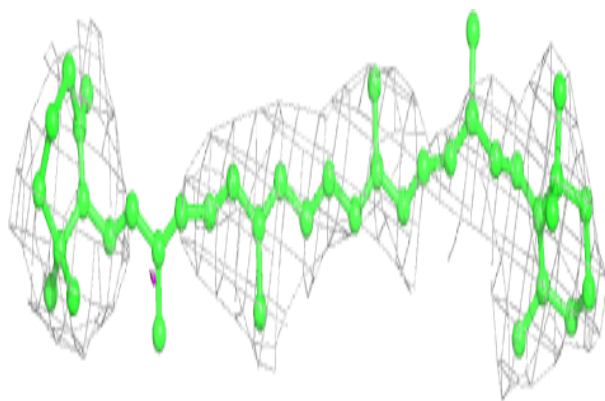
**Electron density around BCR A 6008:**

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

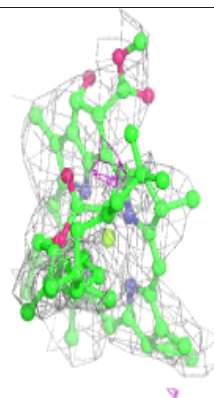
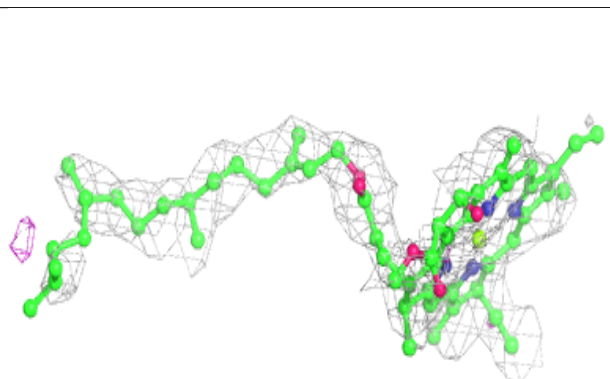
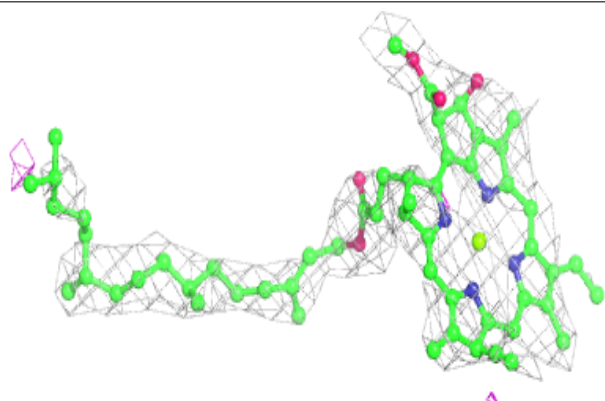


Electron density around BCR B 6004:

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

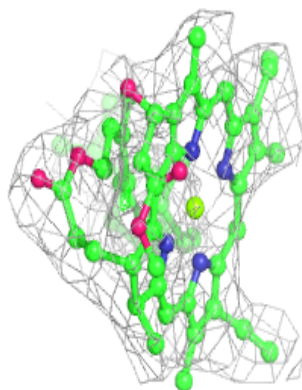
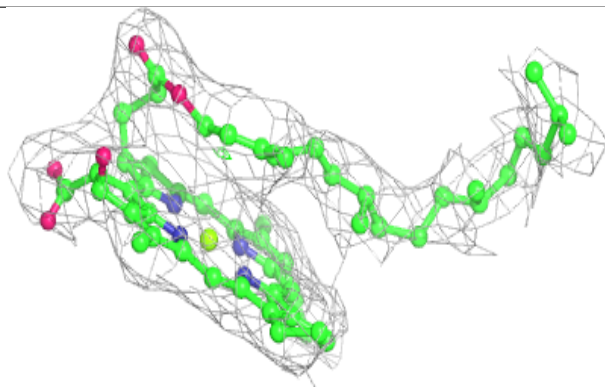
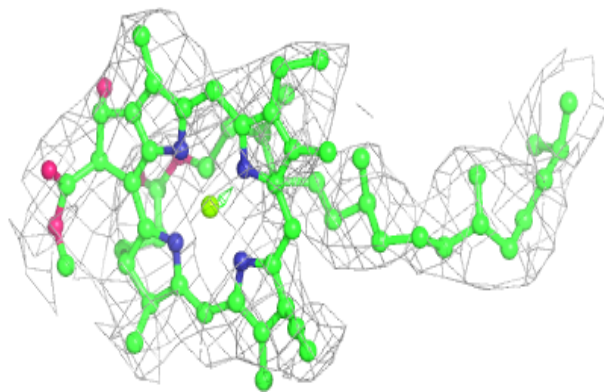
**Electron density around CLA A 1119:**

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



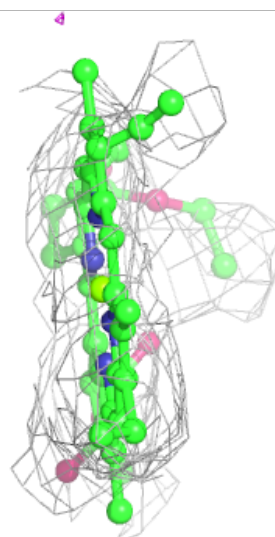
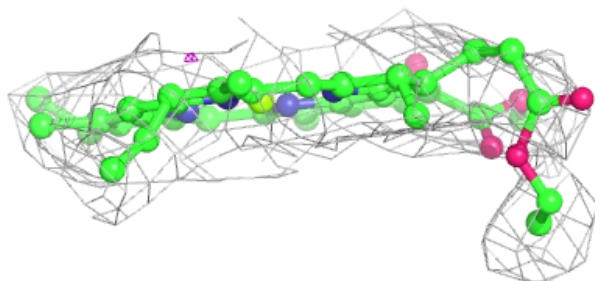
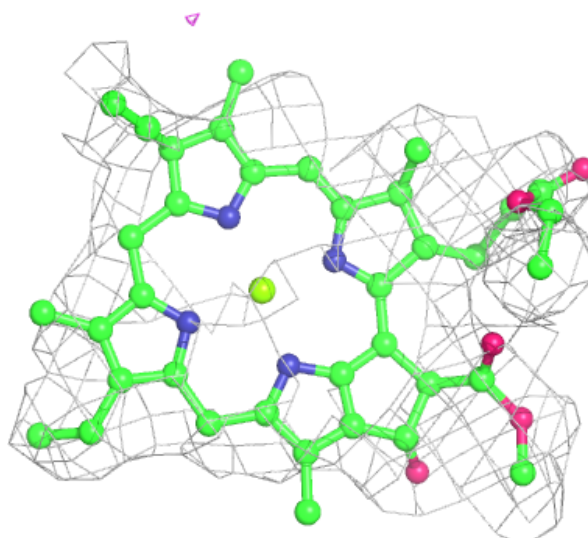
Electron density around CLA A 1115:

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



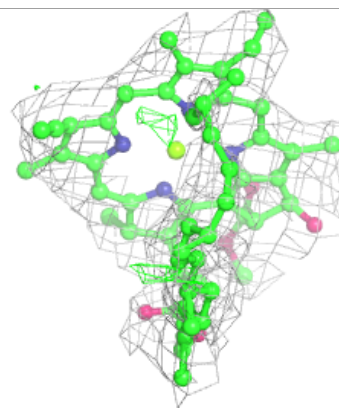
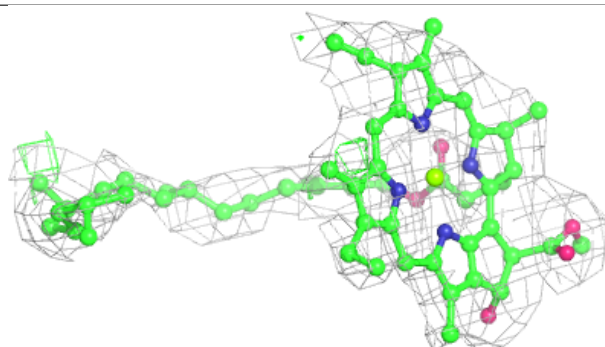
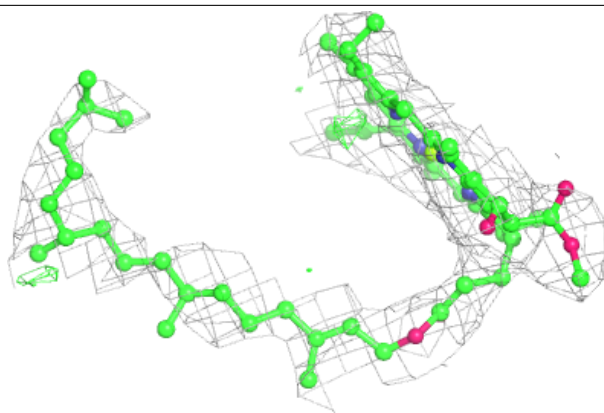
Electron density around CLA 1 1002:

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



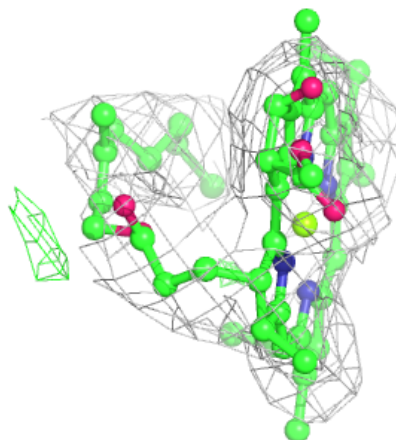
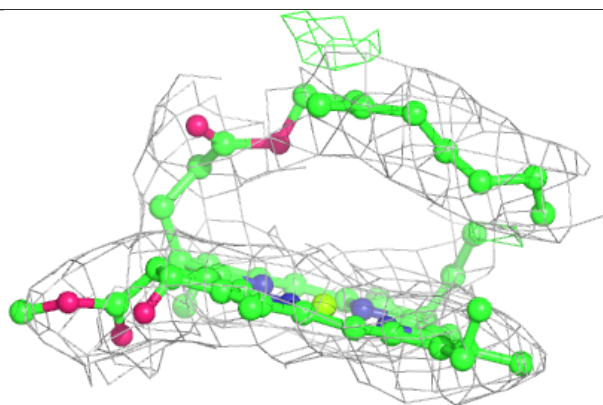
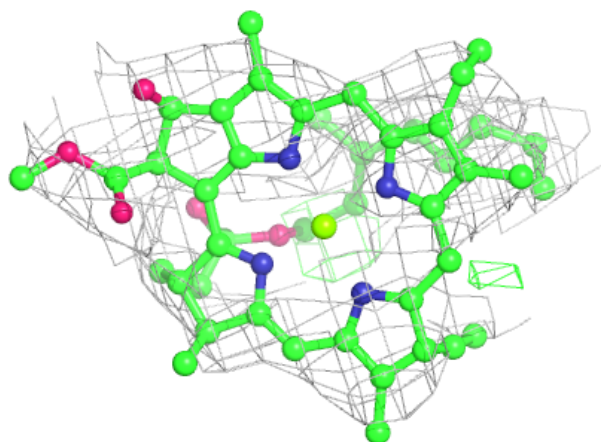
Electron density around CLA L 1130:

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



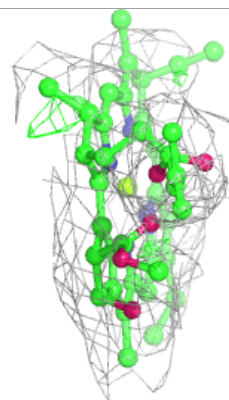
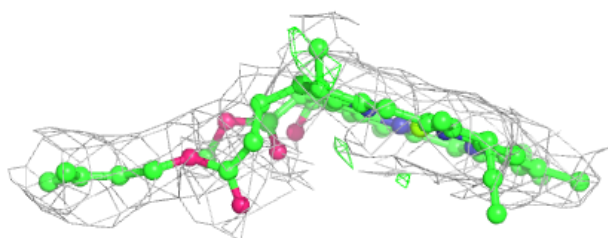
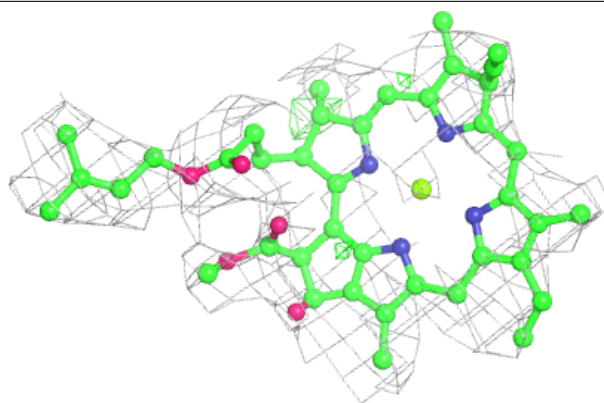
Electron density around CLA A 1110:

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

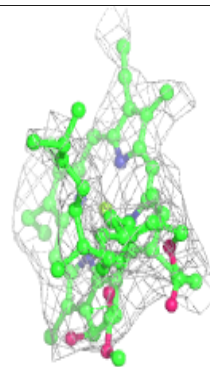
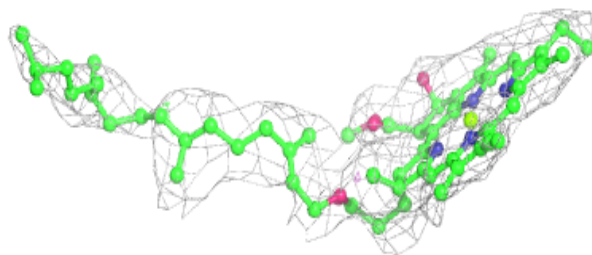
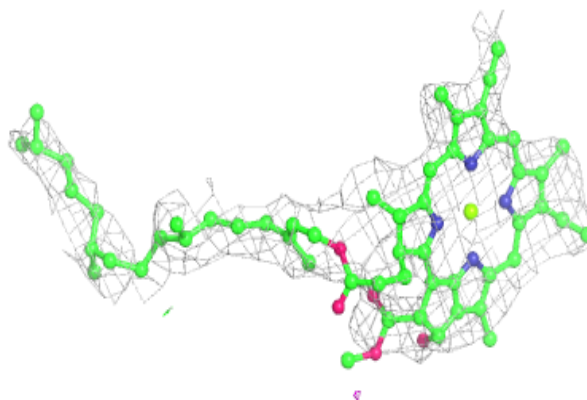


Electron density around CLA L 1503:

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

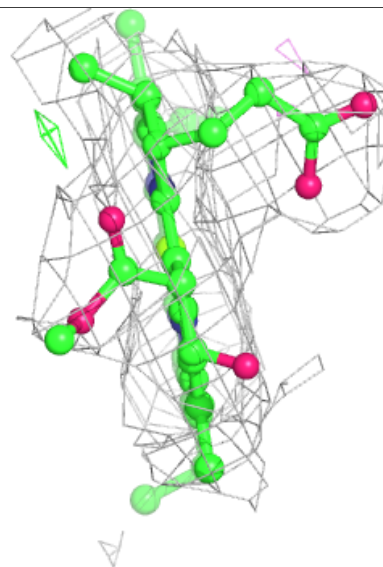
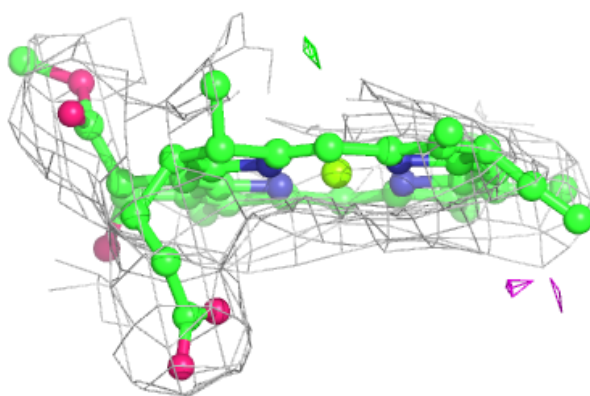
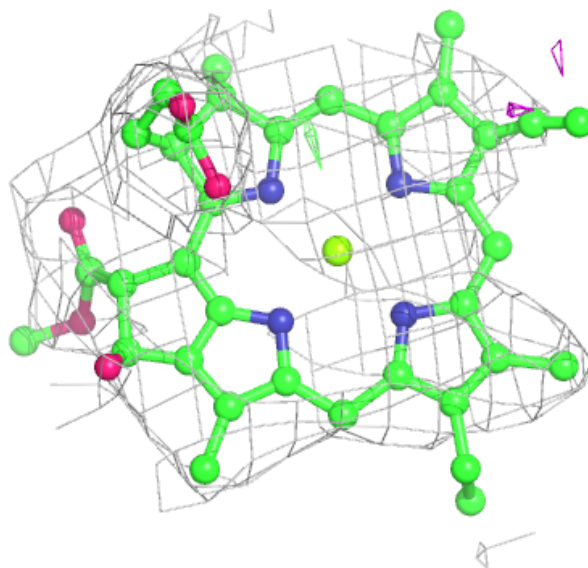
**Electron density around CLA H 1207:**

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



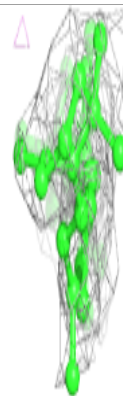
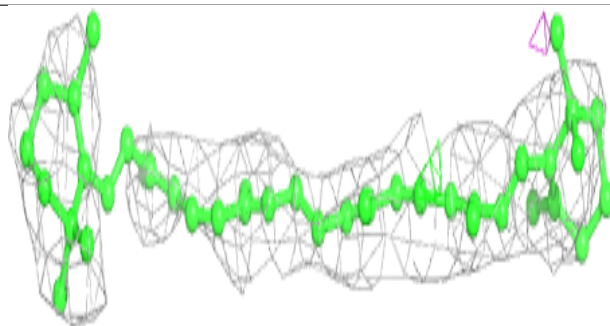
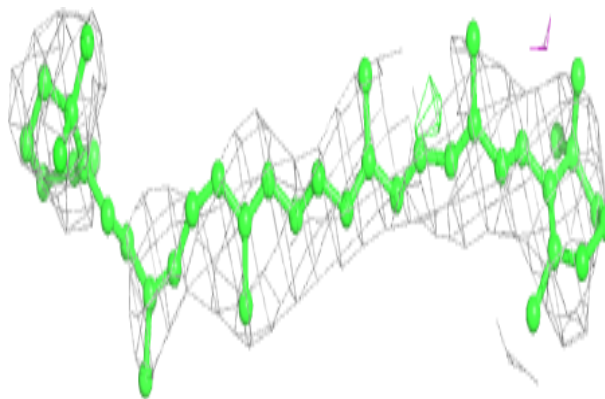
Electron density around CLA B 1231:

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

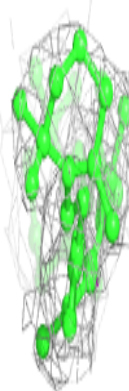
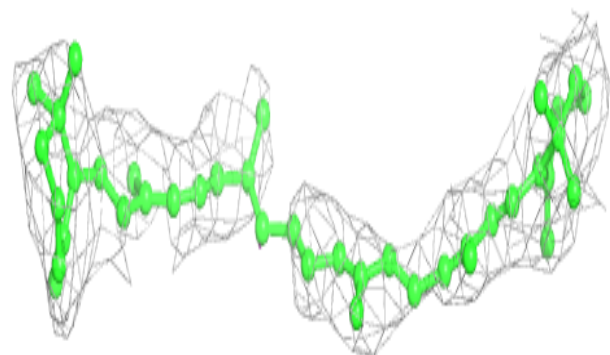
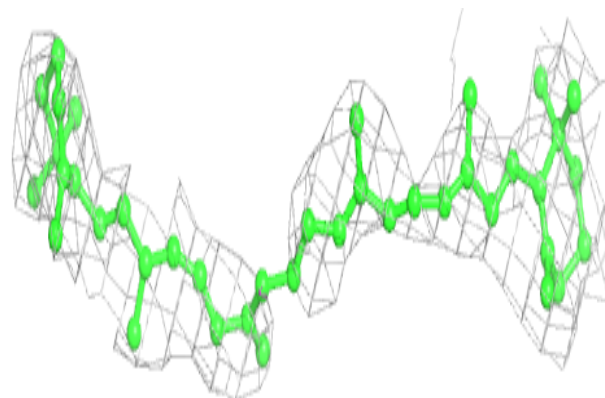


Electron density around BCR B 6017:

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

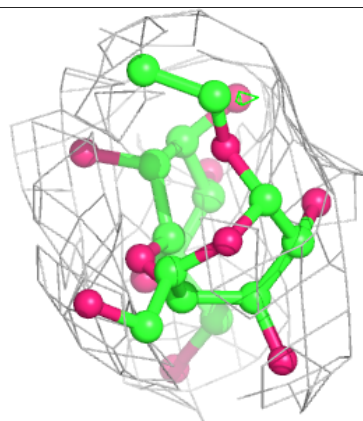
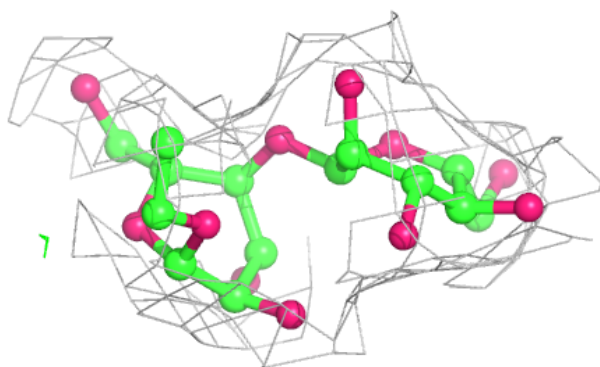
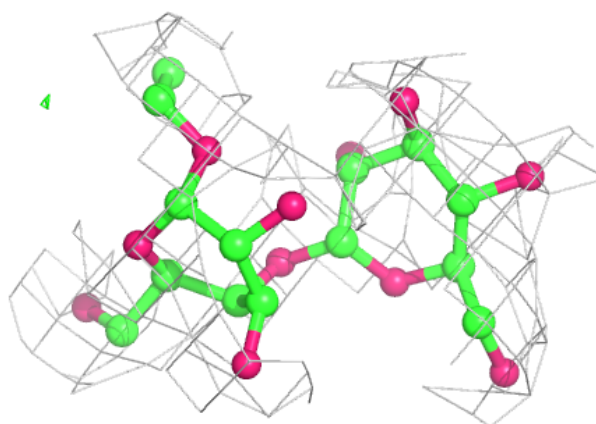
**Electron density around BCR I 6018:**

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

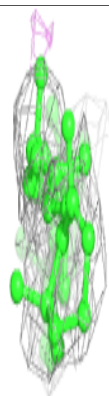
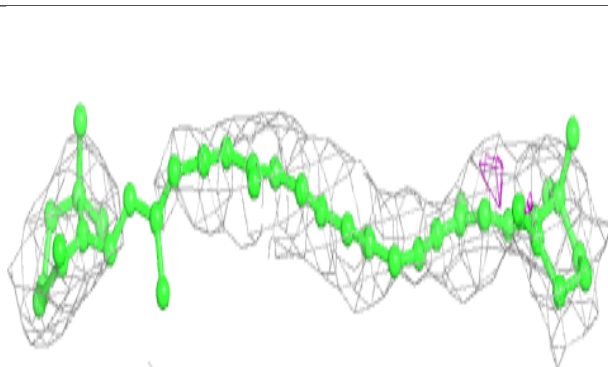
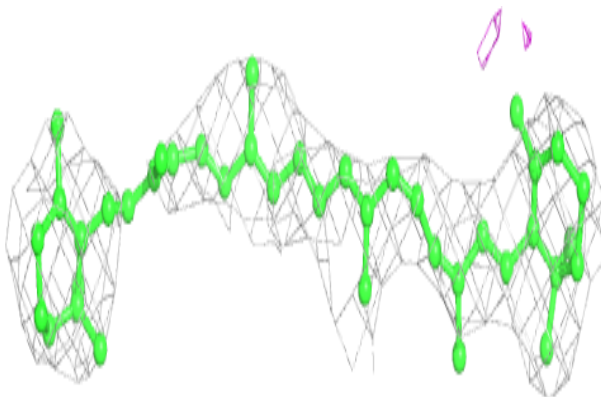


Electron density around LMU B 7012:

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

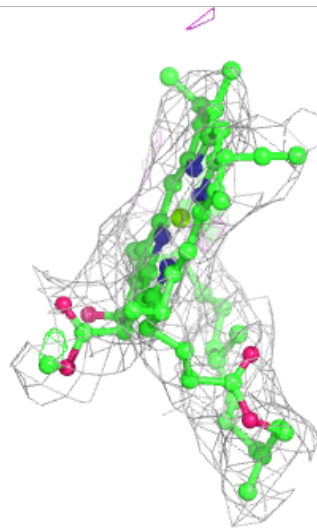
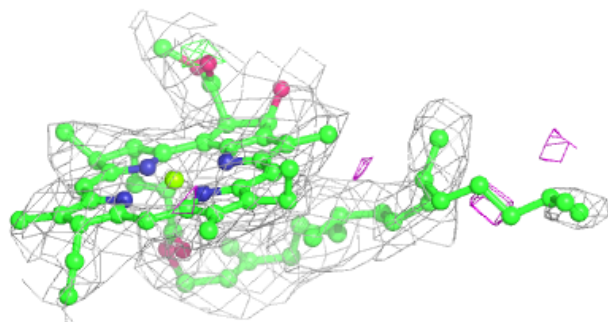
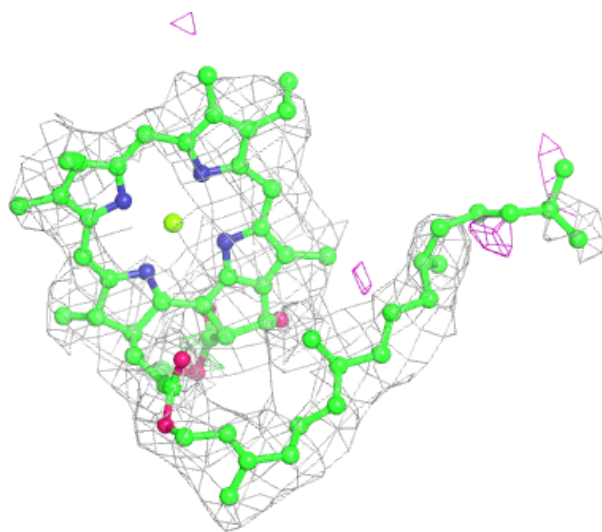
**Electron density around BCR B 6010:**

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



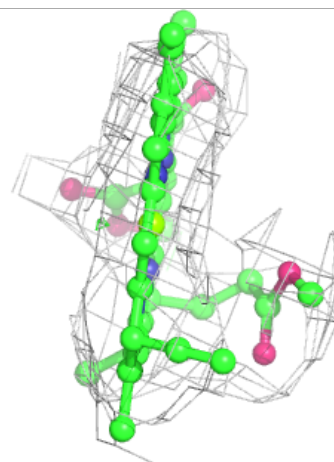
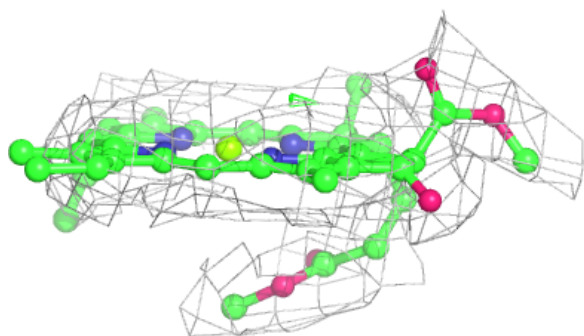
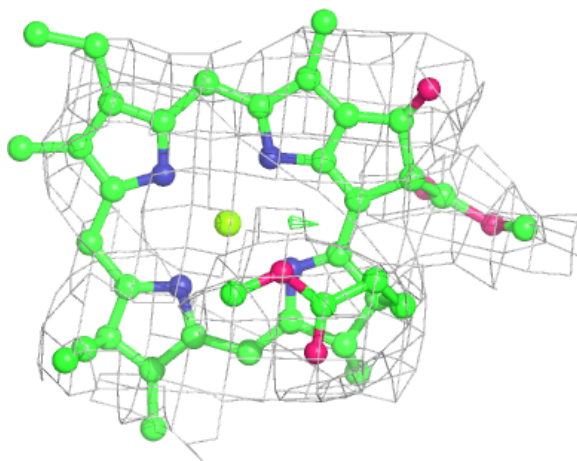
Electron density around CLA B 1229:

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



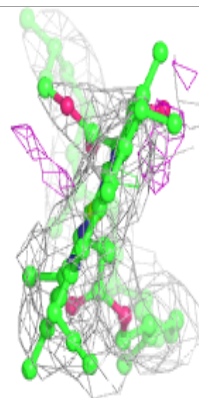
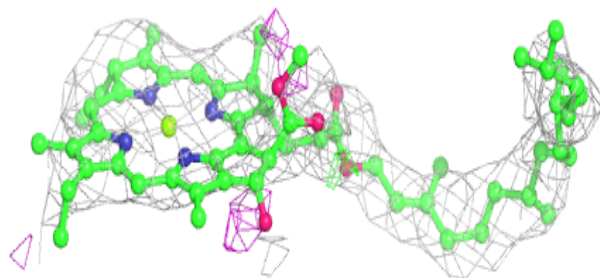
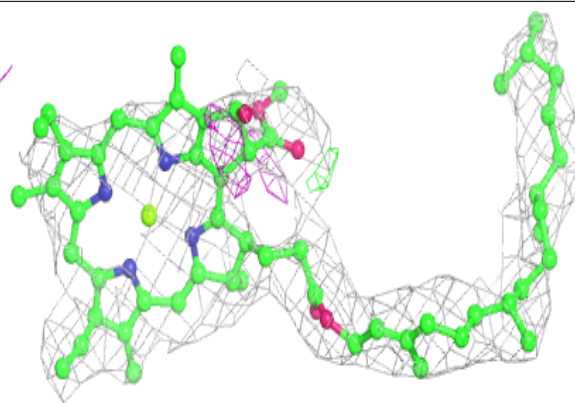
Electron density around CLA 1 1005:

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



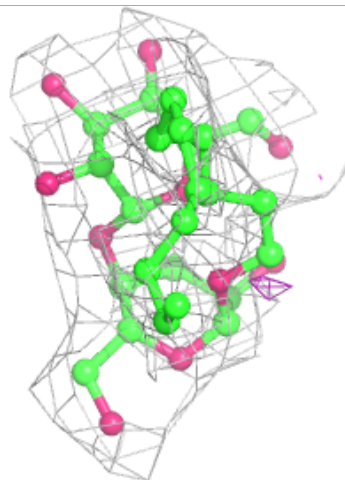
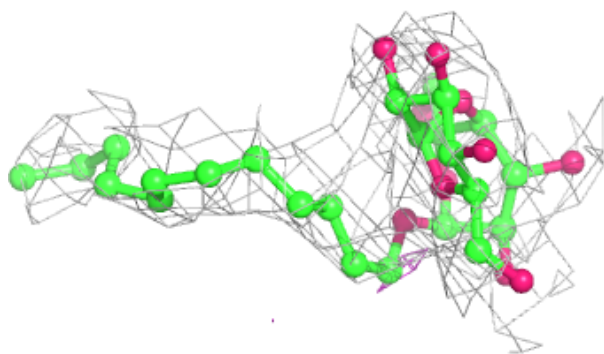
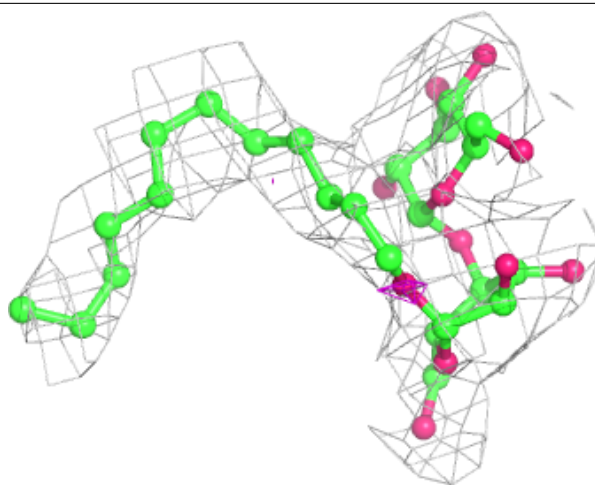
Electron density around CLA B 1223:

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



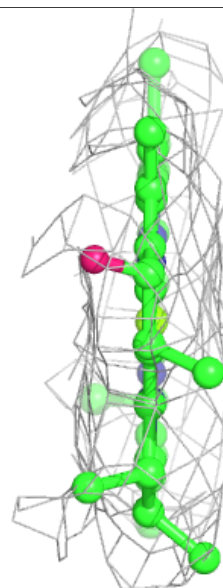
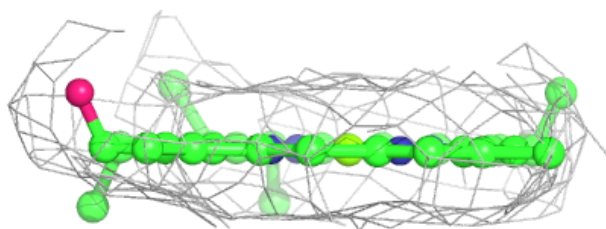
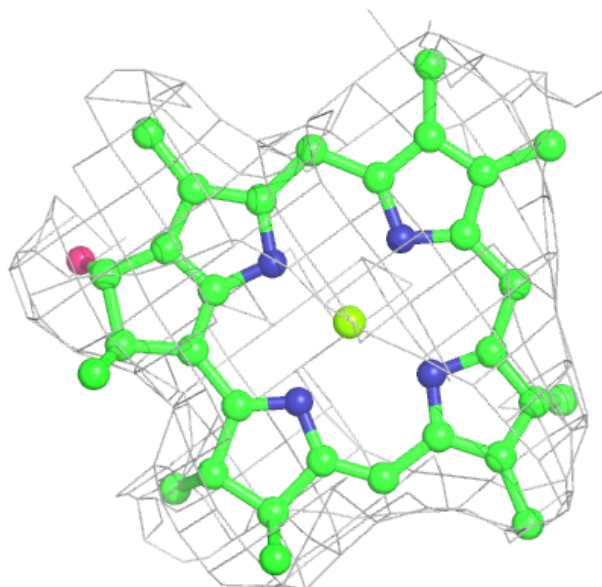
Electron density around LMU H 7032:

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



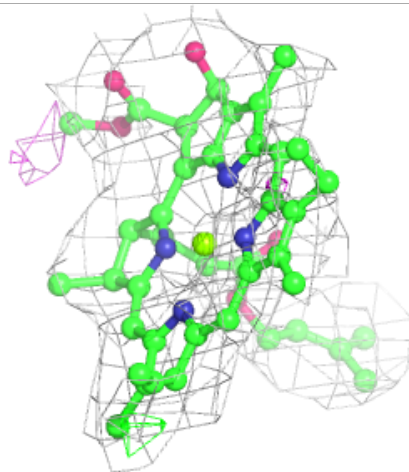
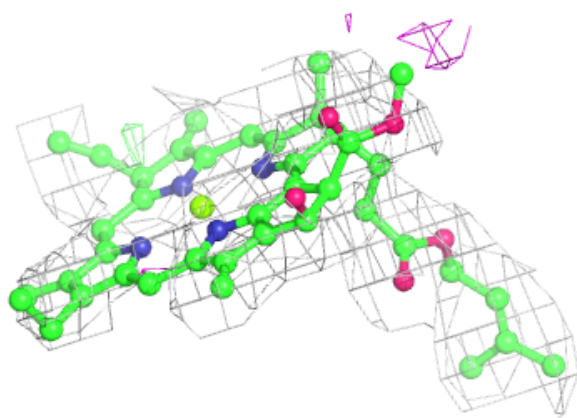
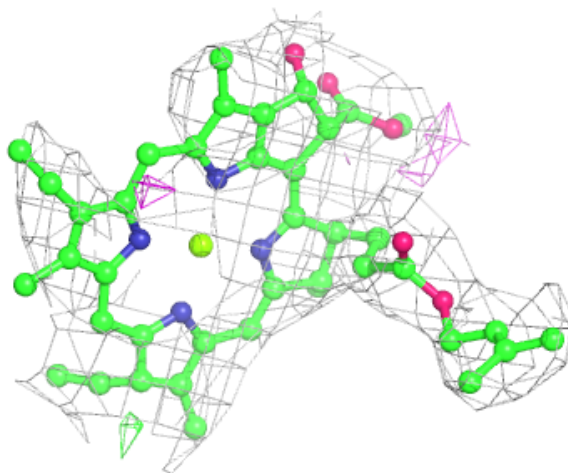
Electron density around CLA 1 1011:

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



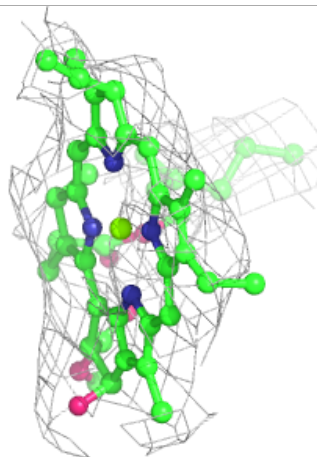
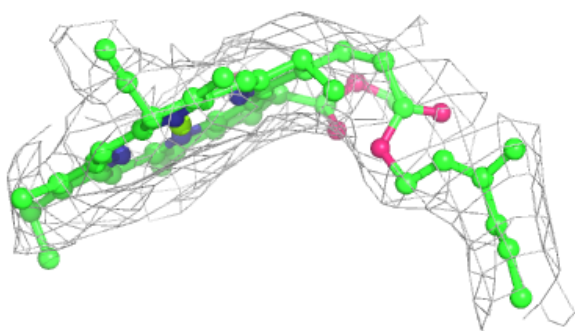
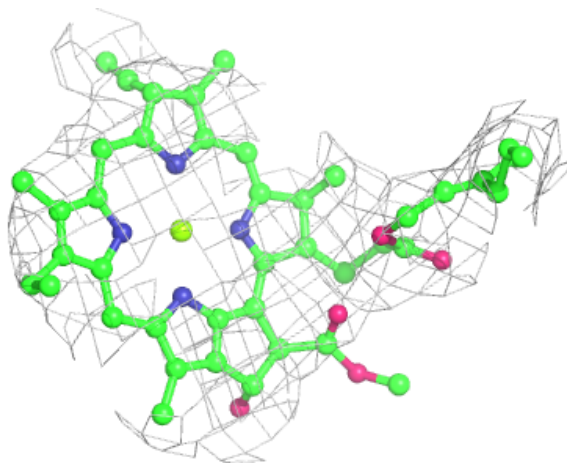
Electron density around CLA 2 2012:

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



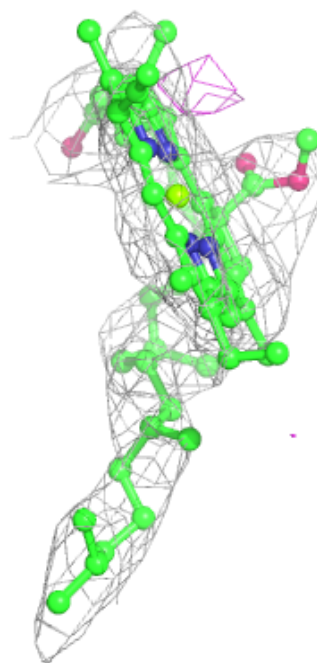
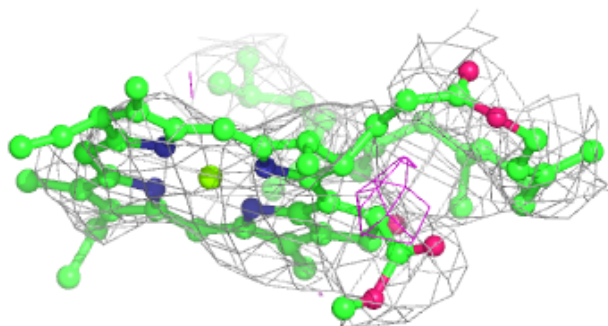
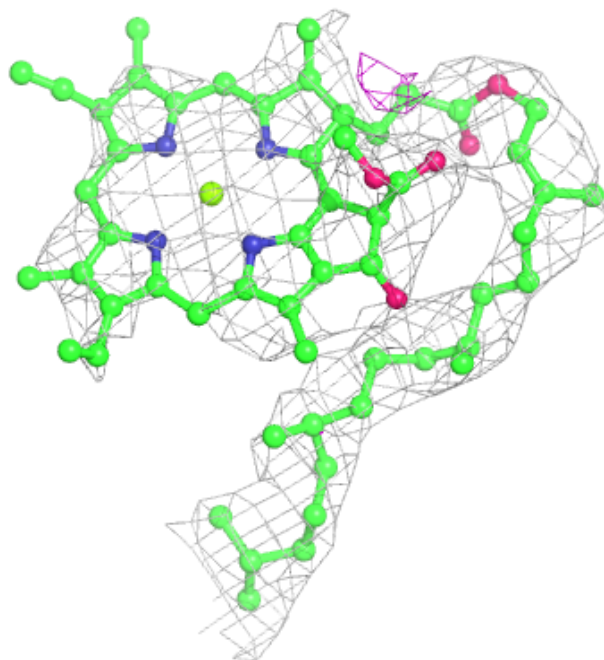
Electron density around CLA 4 4002:

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



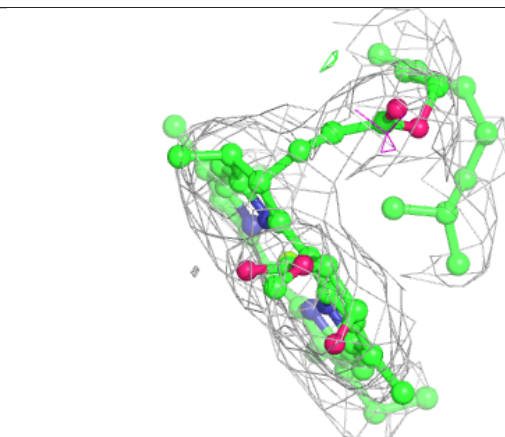
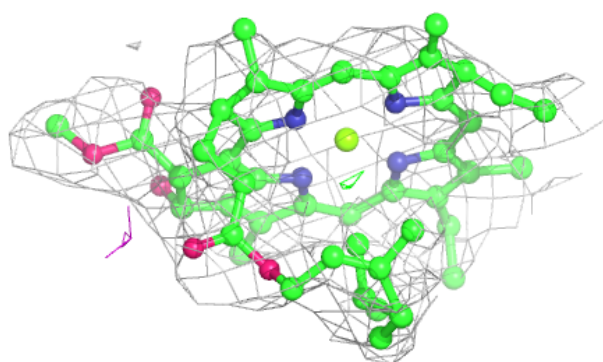
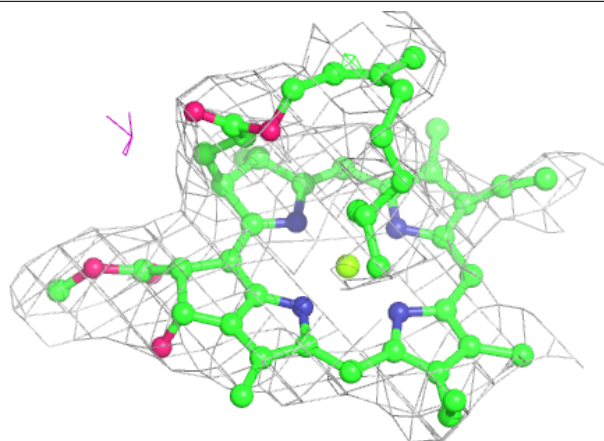
Electron density around CLA A 1123:

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

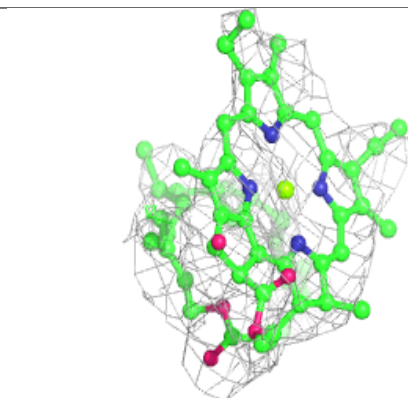
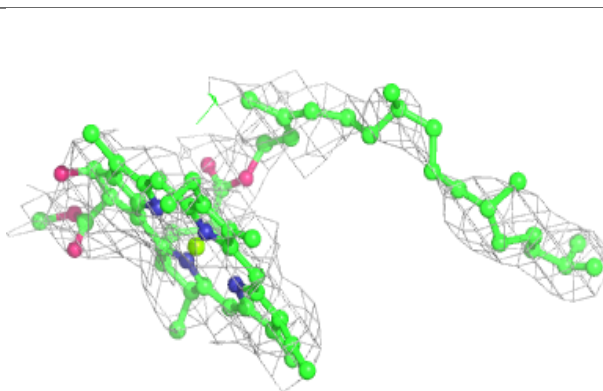
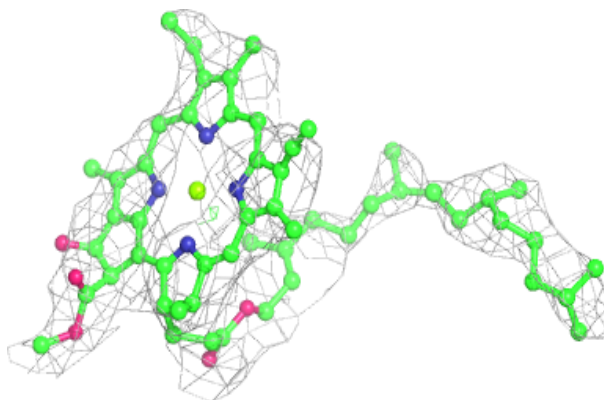


Electron density around CLA B 1209:

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

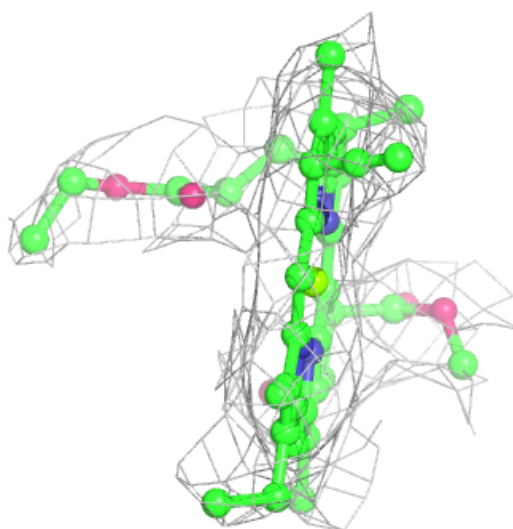
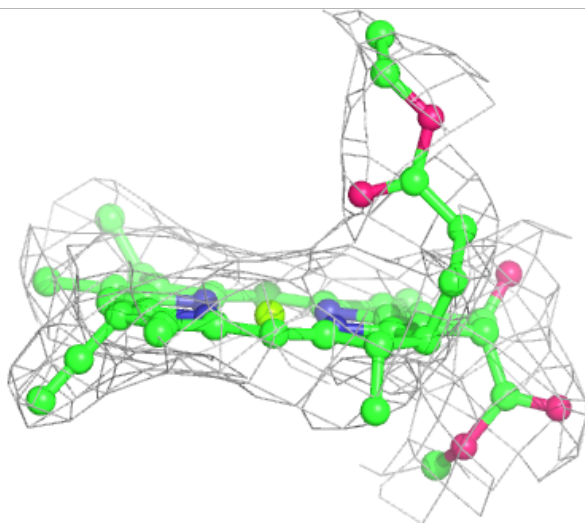
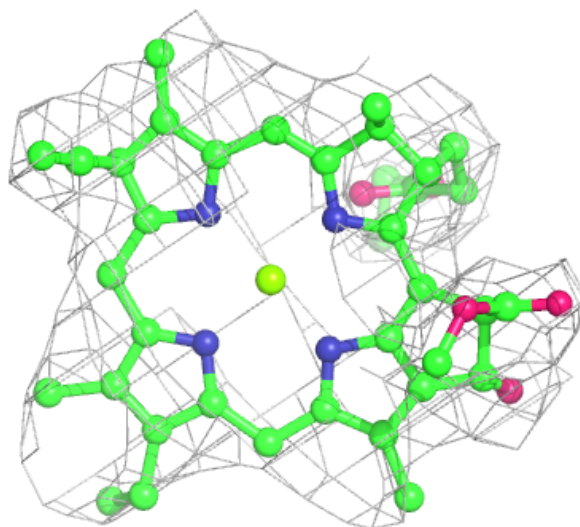
**Electron density around CLA B 1211:**

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



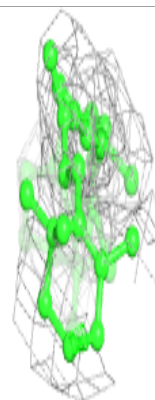
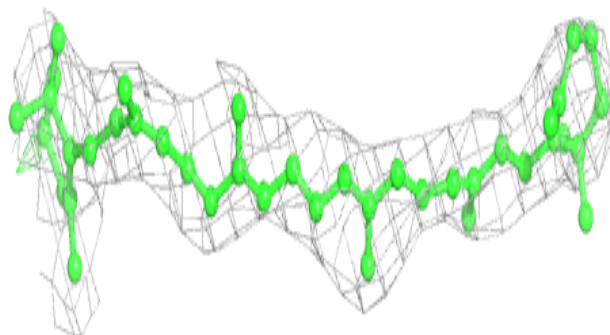
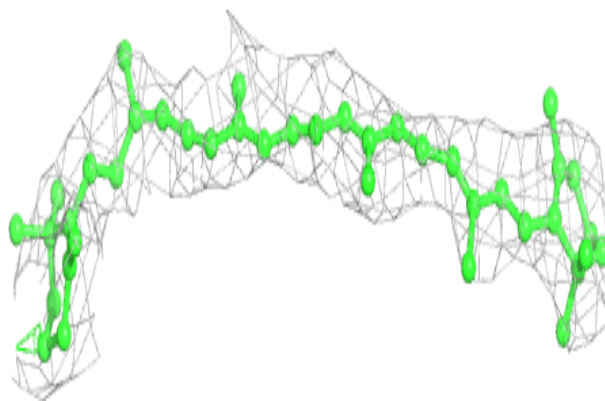
Electron density around CLA L 1502:

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

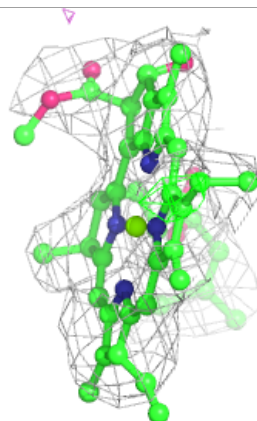
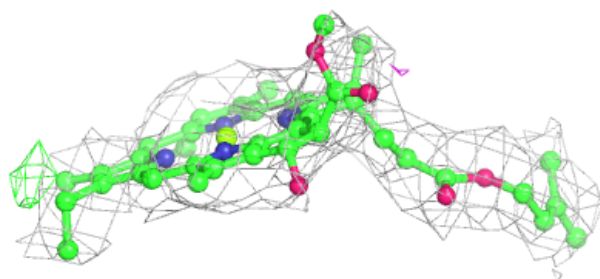
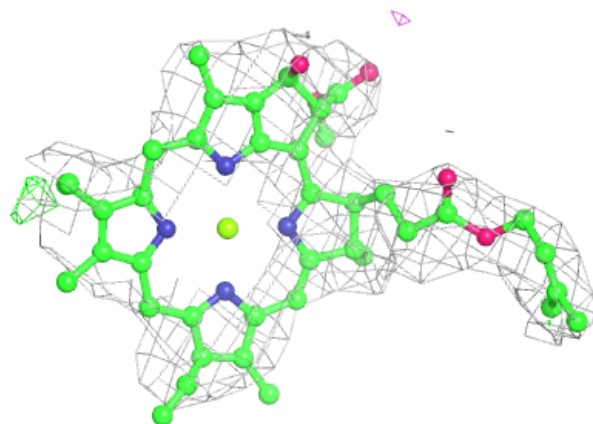


Electron density around BCR F 6014:

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

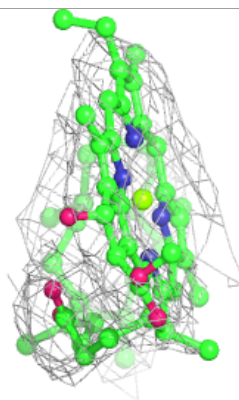
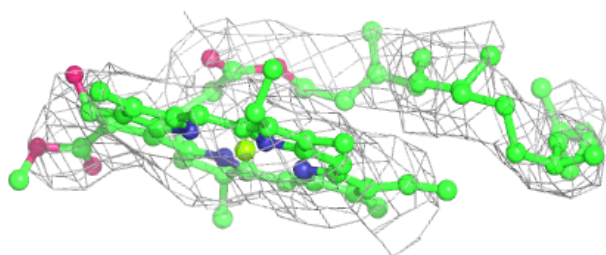
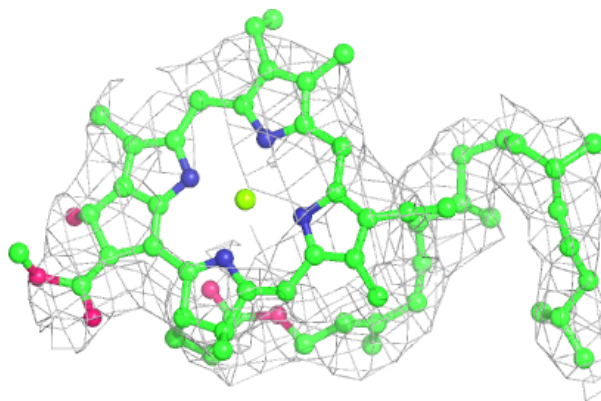
**Electron density around CLA B 1230:**

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

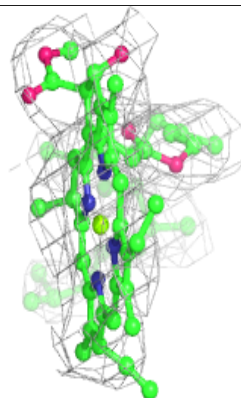
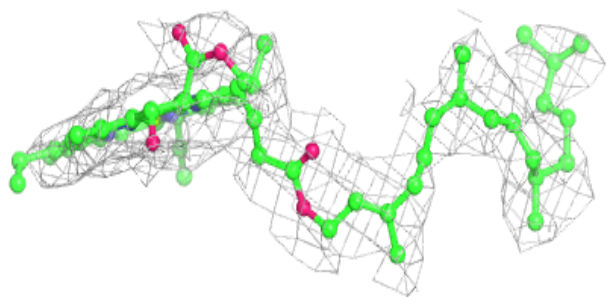
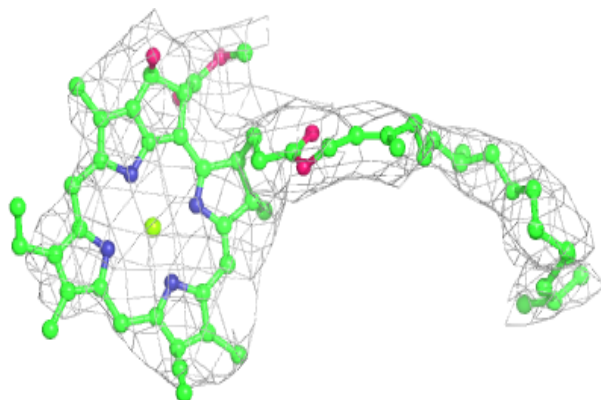


Electron density around CLA A 1117:

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

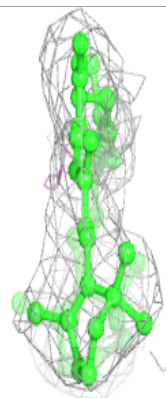
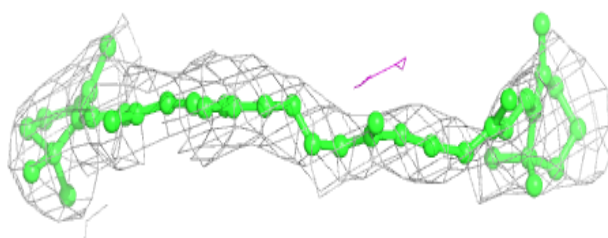
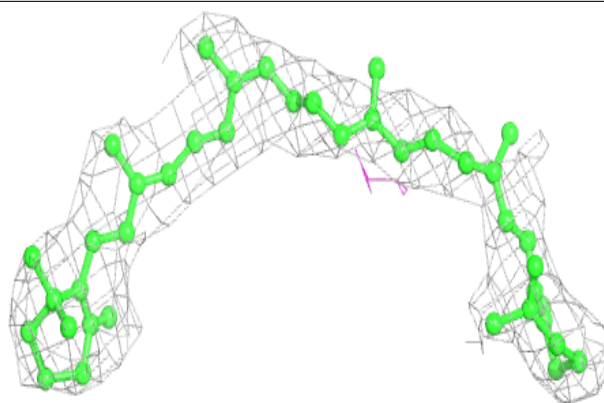
**Electron density around CLA A 1124:**

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

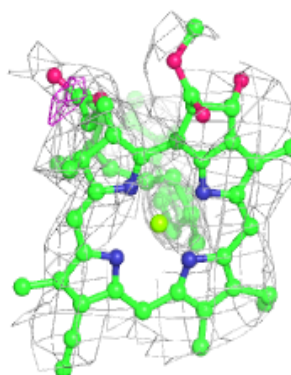
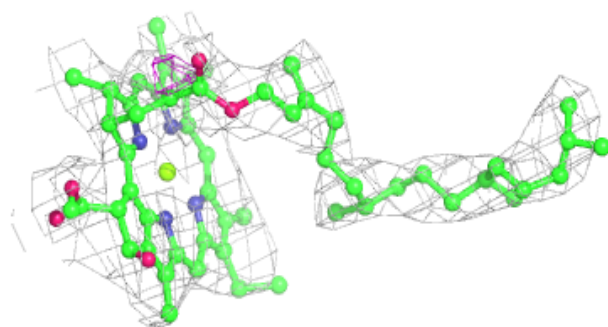
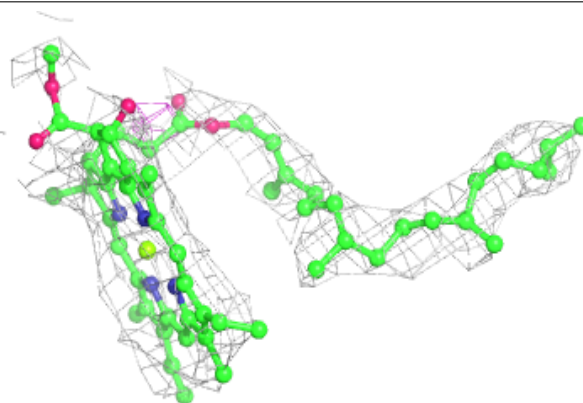


Electron density around BCR F 6016:

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

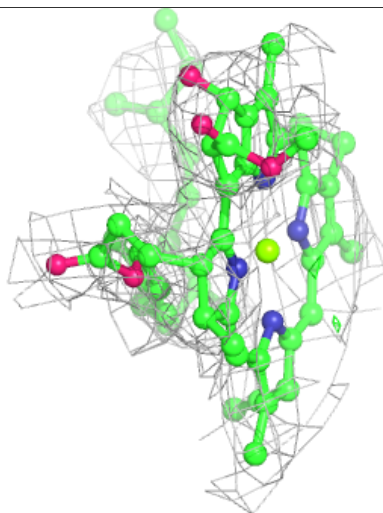
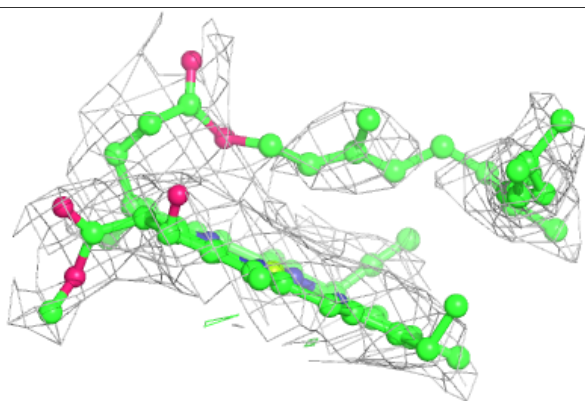
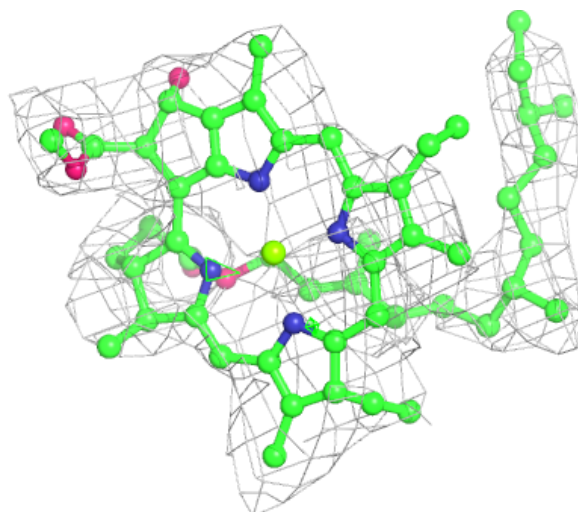
**Electron density around CLA A 1109:**

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



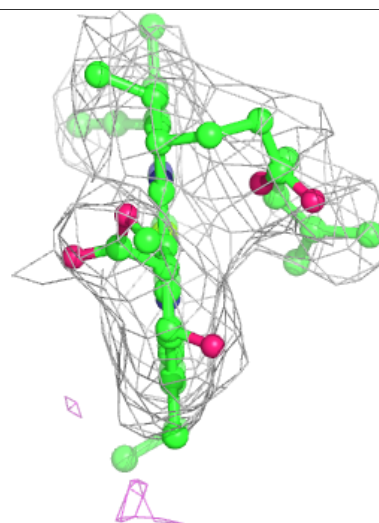
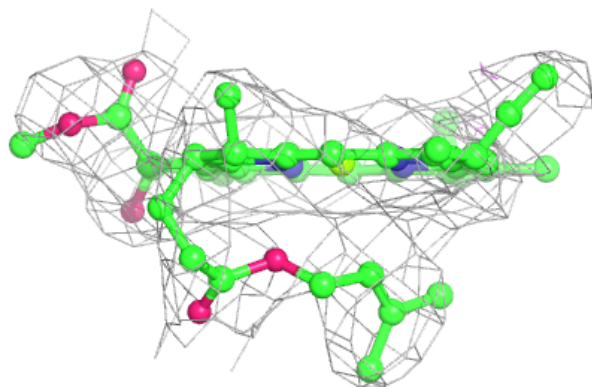
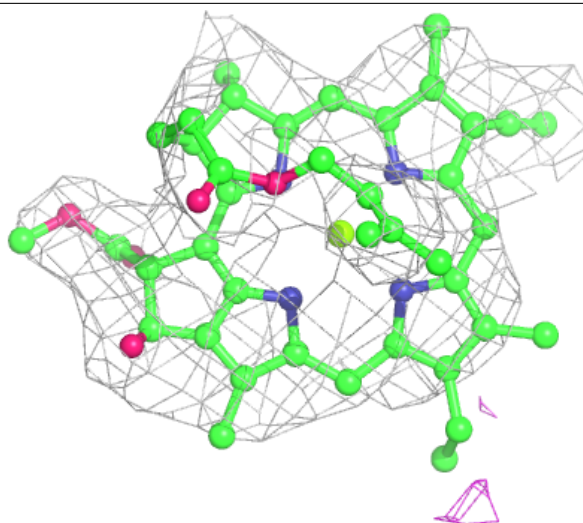
Electron density around CLA B 1216:

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



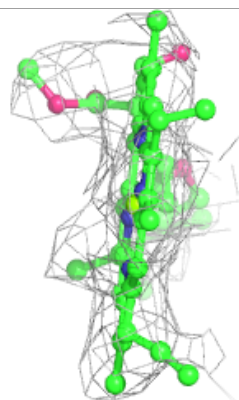
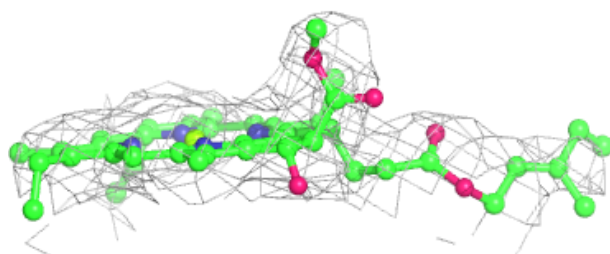
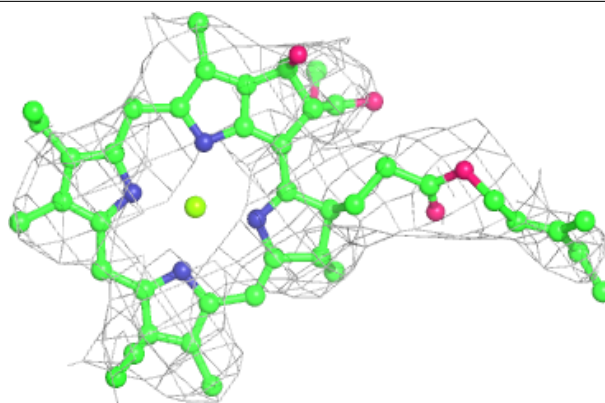
Electron density around CLA B 1217:

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



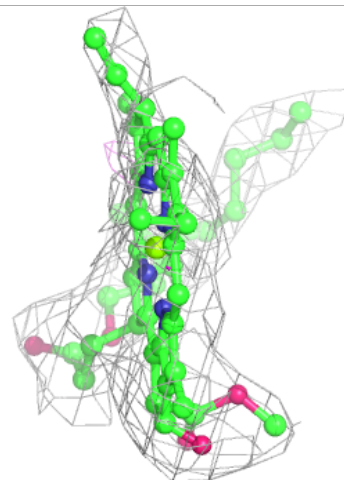
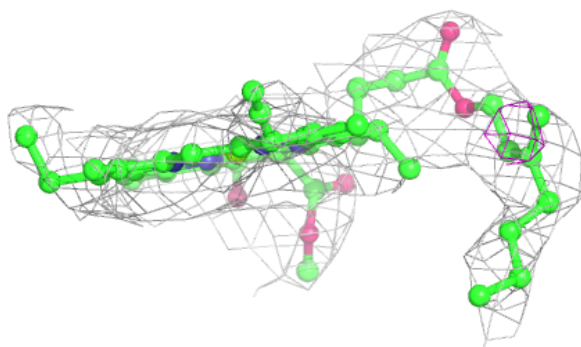
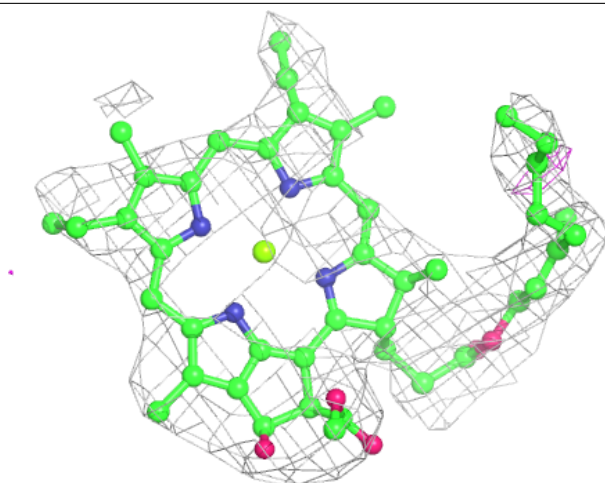
Electron density around CLA A 1135:

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



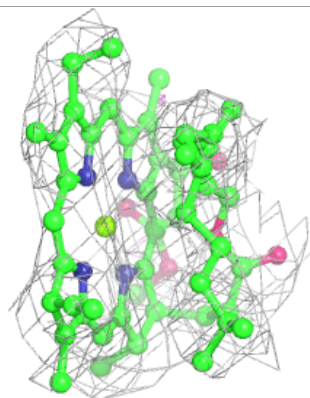
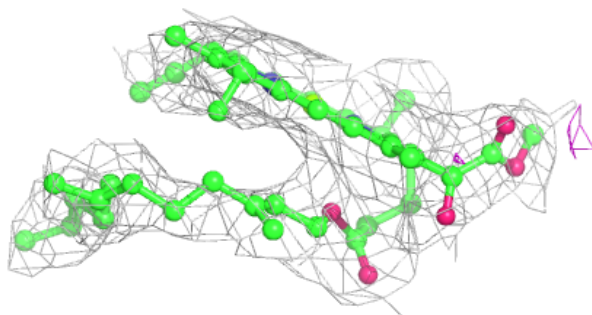
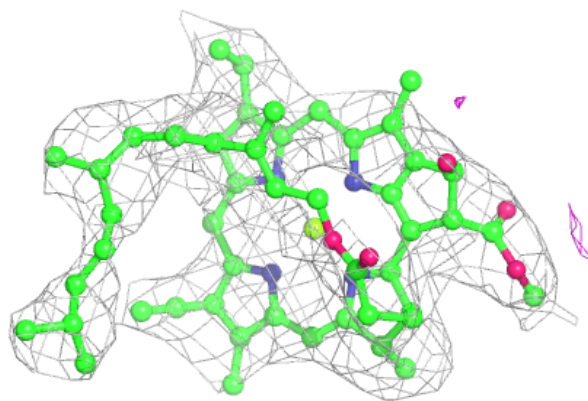
Electron density around CLA A 1111:

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



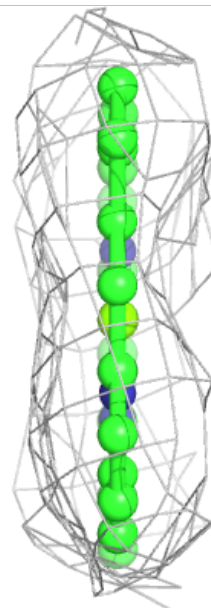
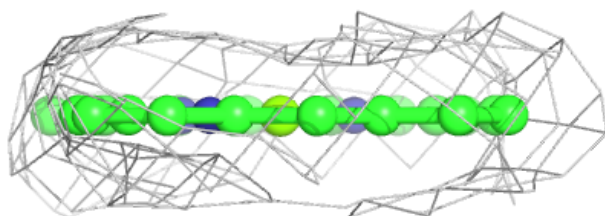
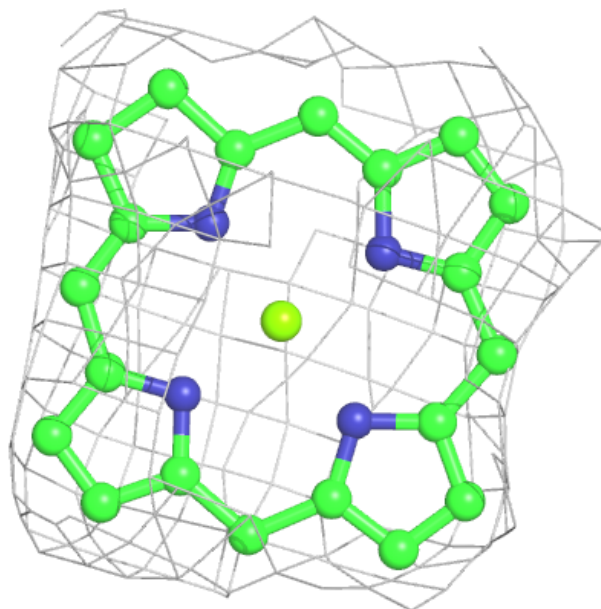
Electron density around CLA I 1204:

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



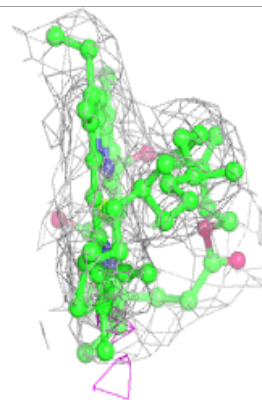
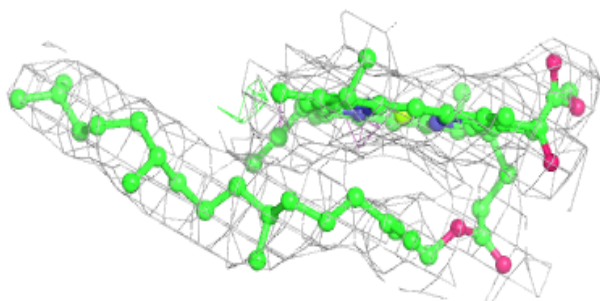
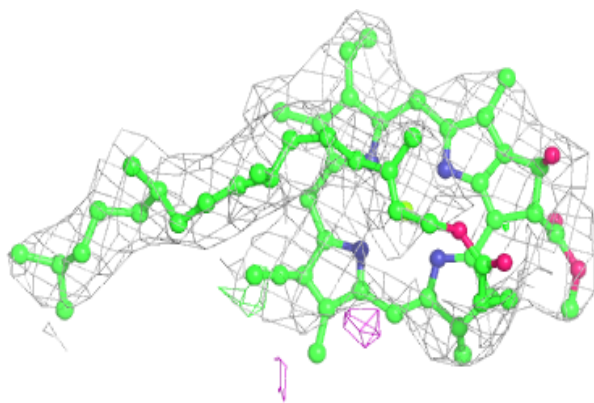
Electron density around CLA 4 4013:

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

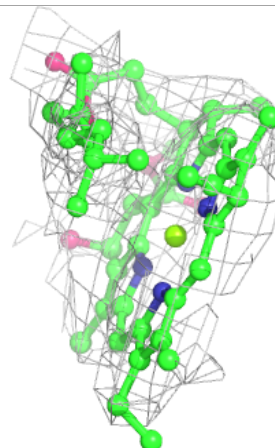
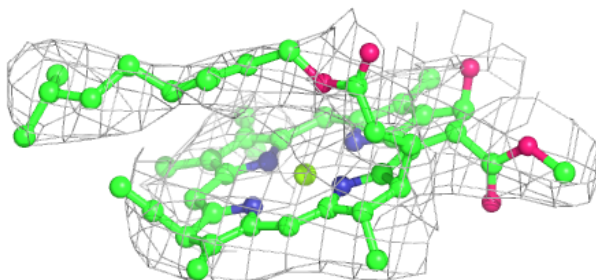
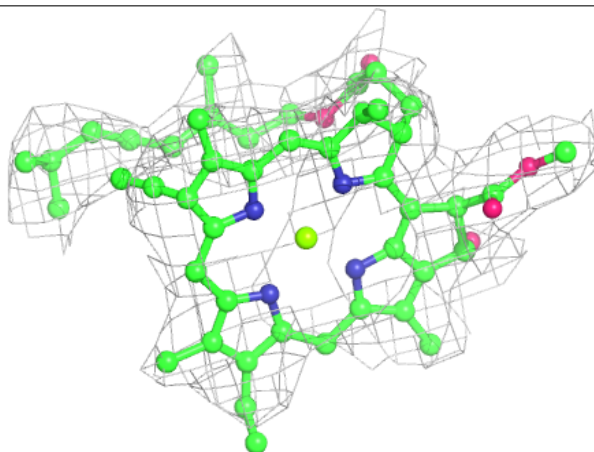


Electron density around CLA A 1138:

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

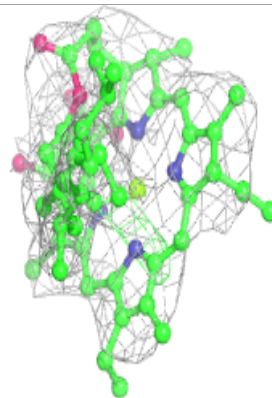
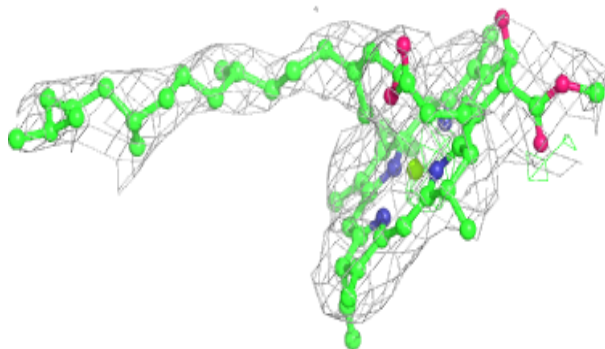
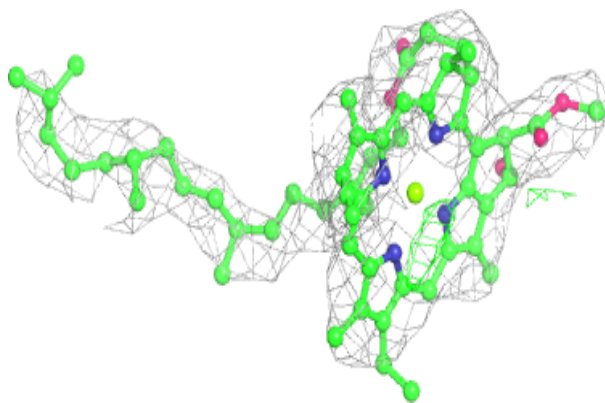
**Electron density around CLA B 1219:**

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

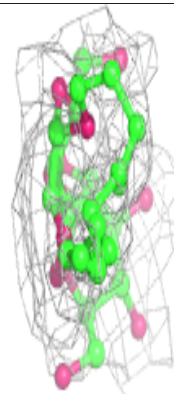
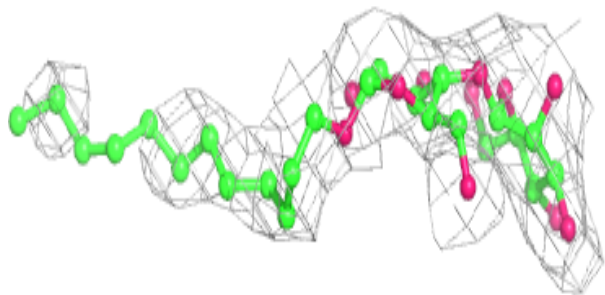
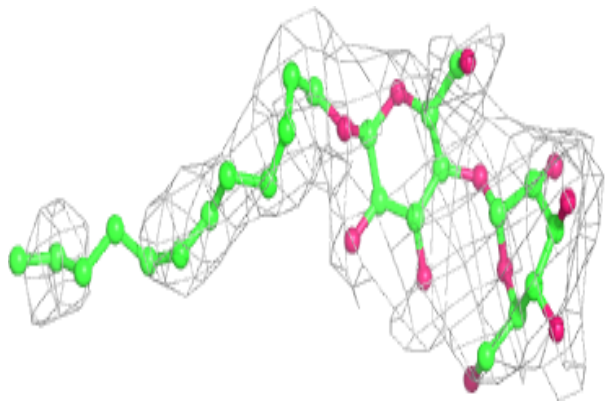


Electron density around CLA A 1140:

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

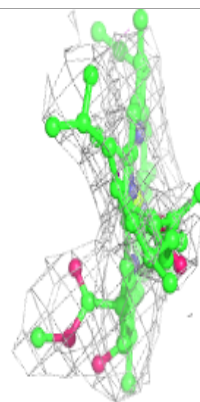
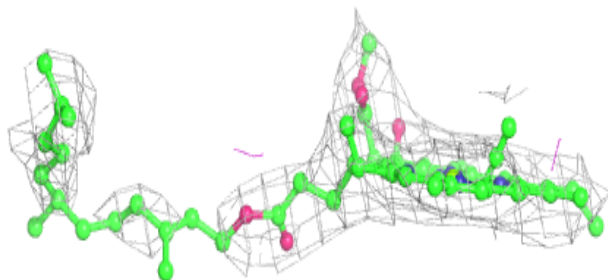
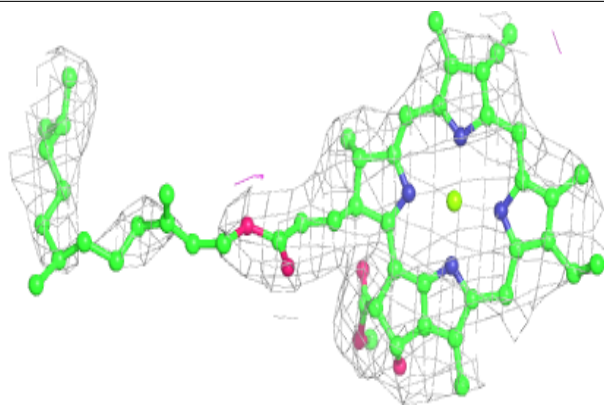
**Electron density around LMU A 7035:**

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



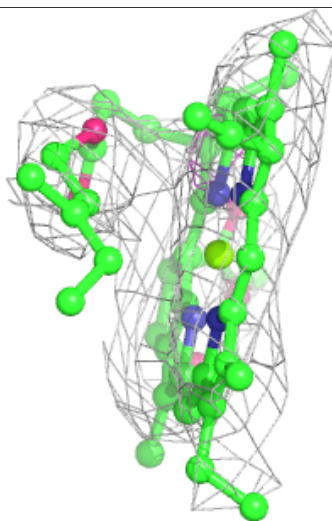
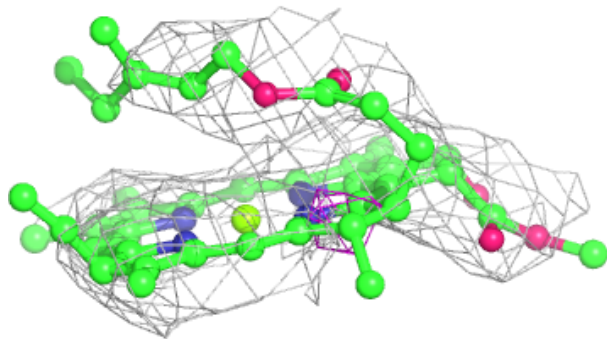
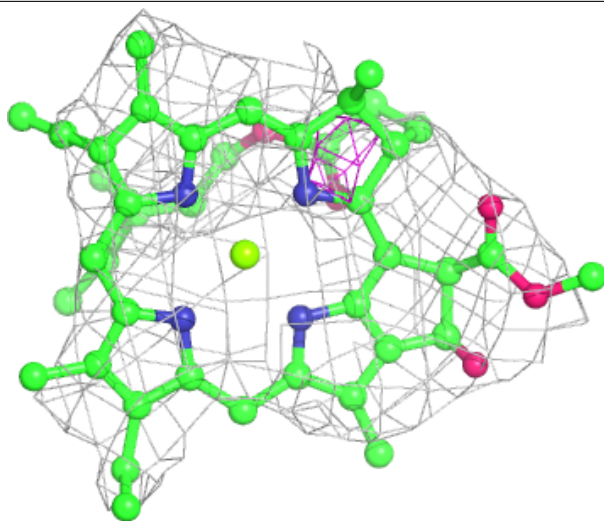
Electron density around CLA B 1234:

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



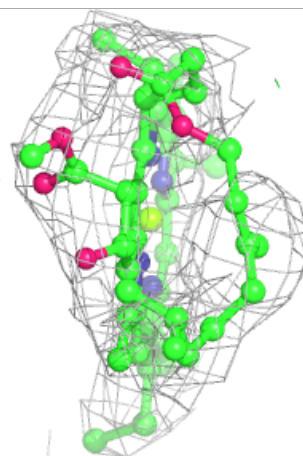
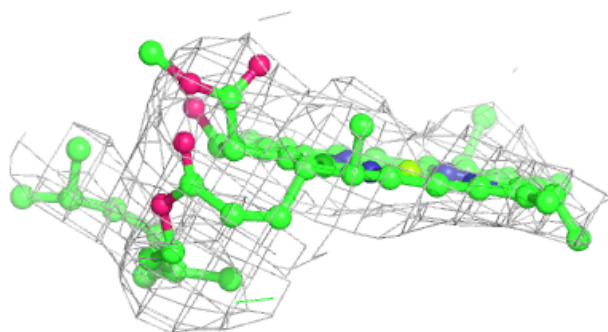
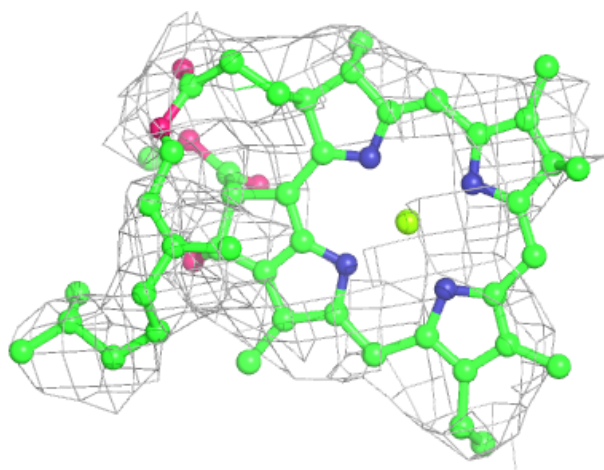
Electron density around CLA A 1120:

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



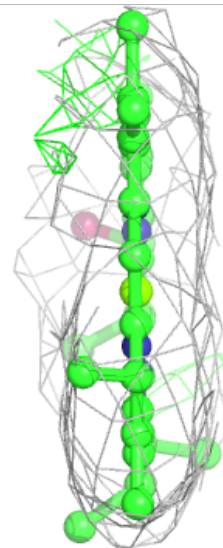
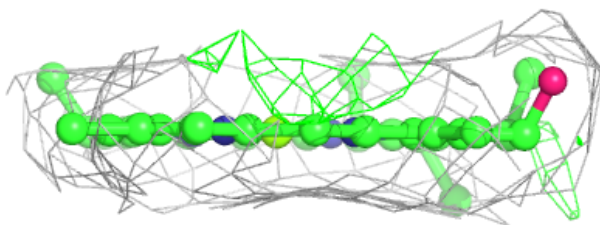
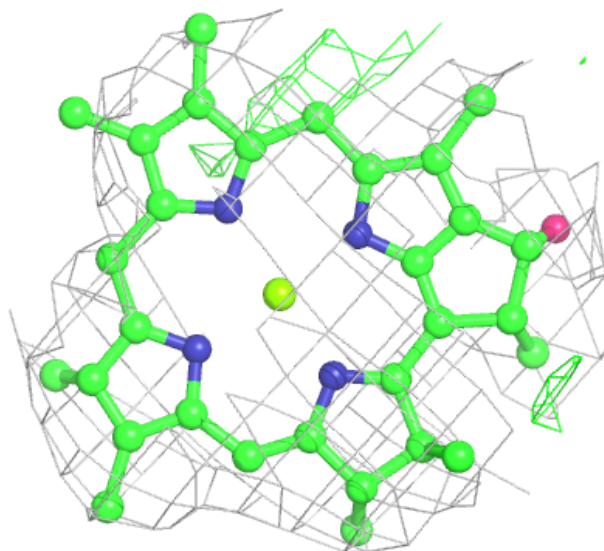
Electron density around CLA B 1208:

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



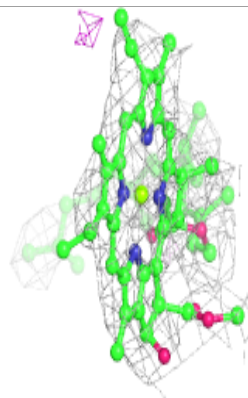
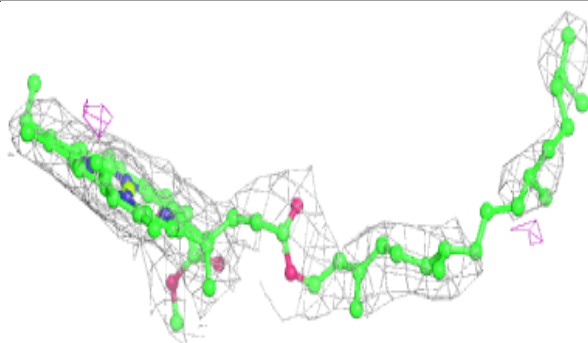
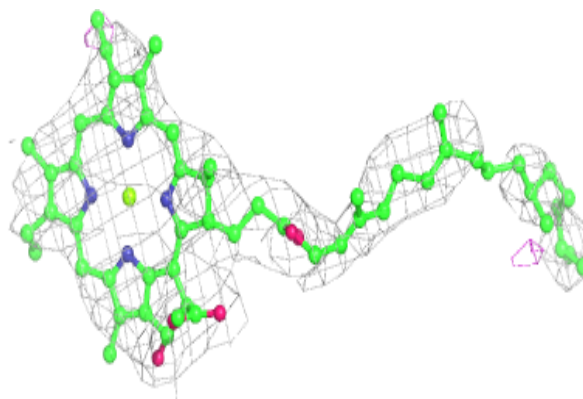
Electron density around CLA 4 1009:

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

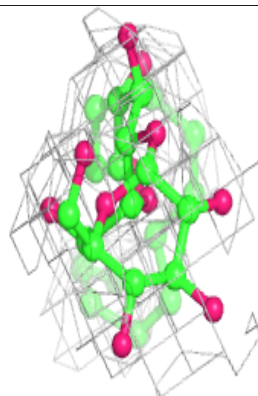
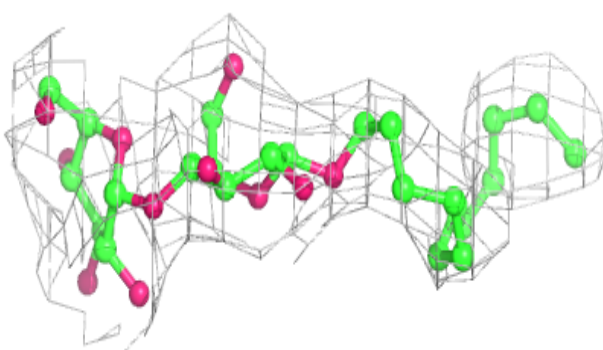
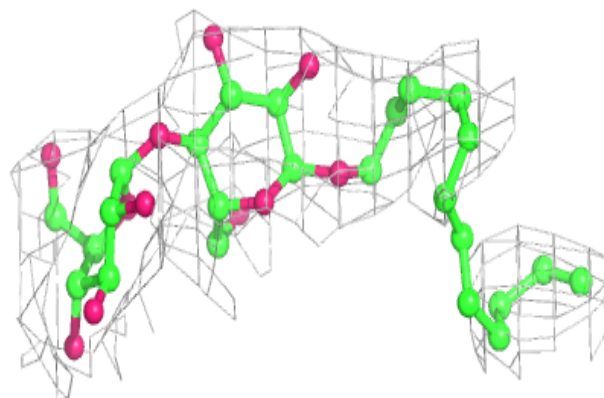


Electron density around CLA A 1103:

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

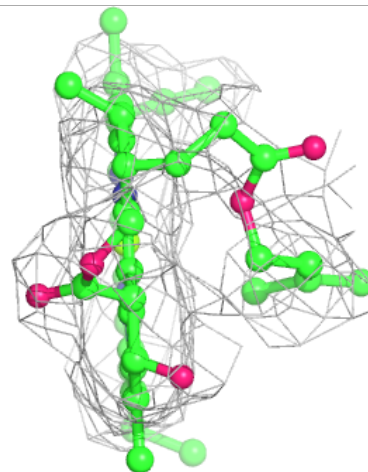
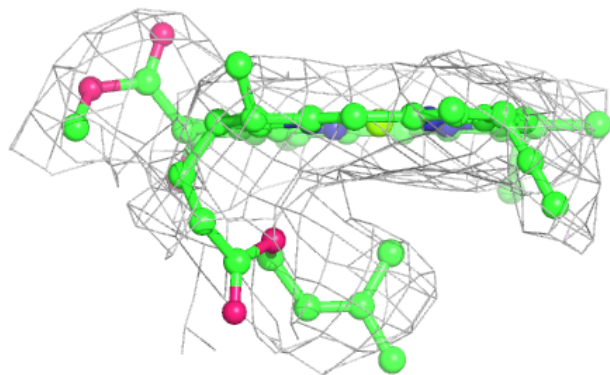
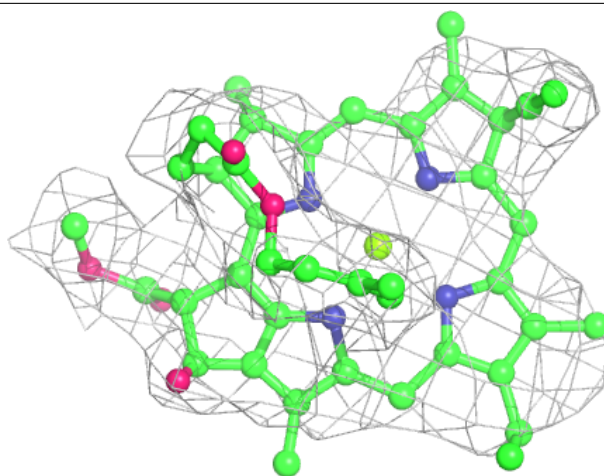
**Electron density around LMU R 7007:**

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



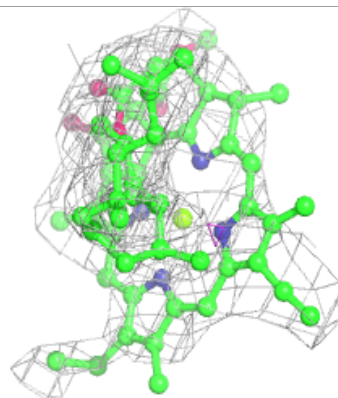
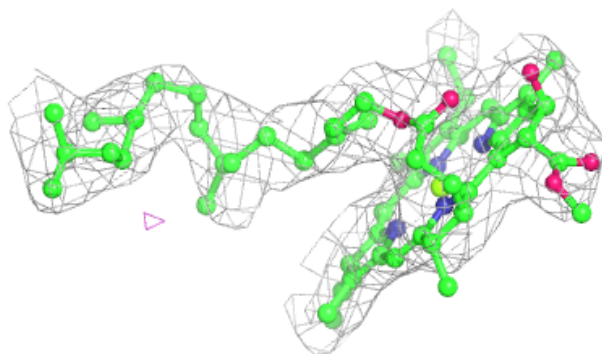
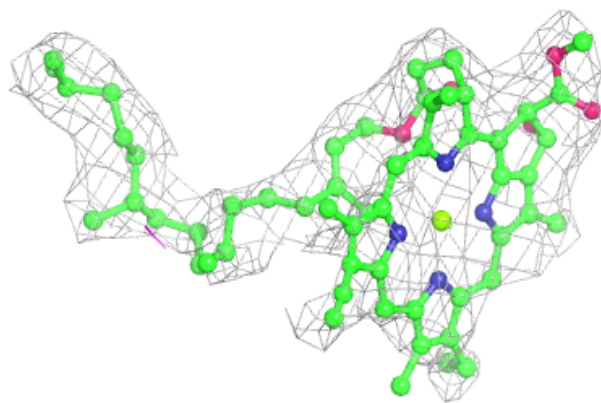
Electron density around CLA L 1501:

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



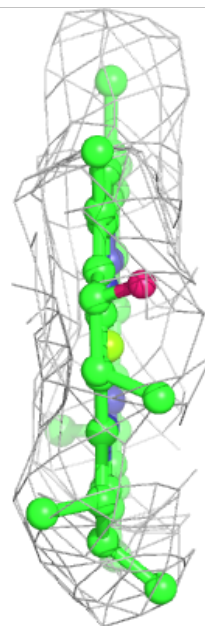
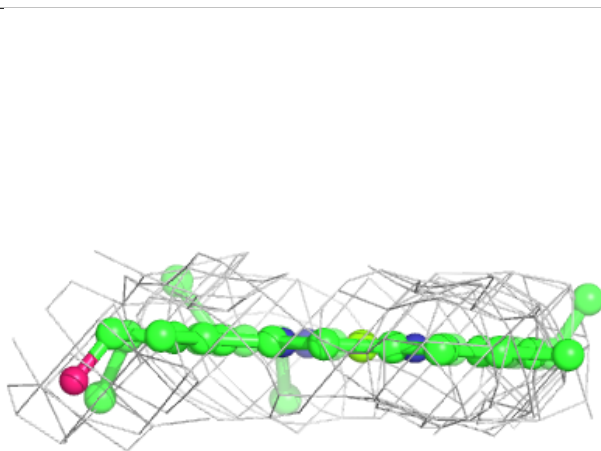
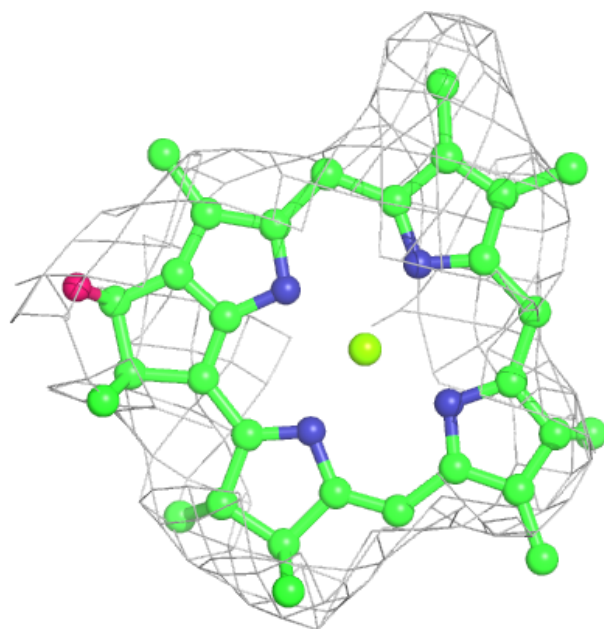
Electron density around CLA A 1237:

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



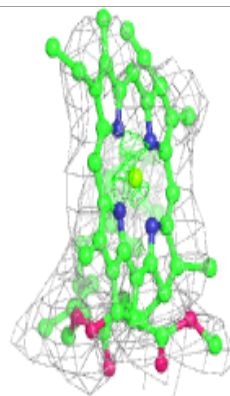
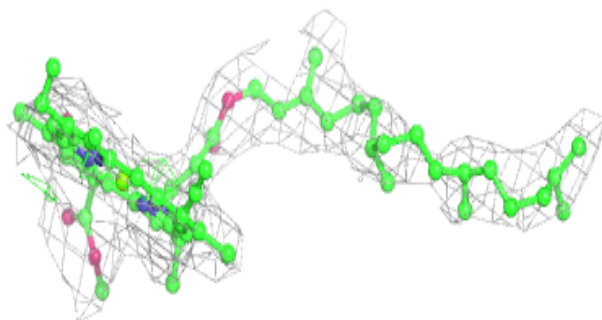
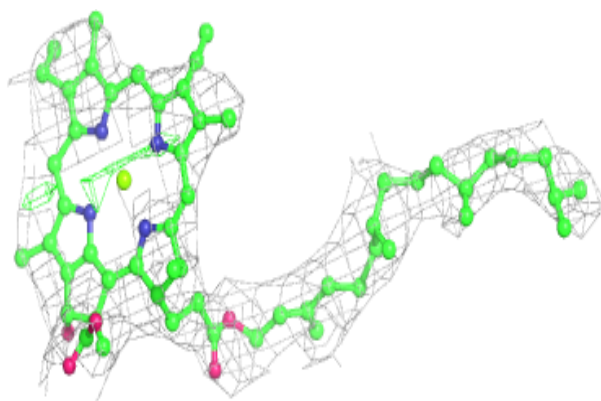
Electron density around CLA 1 1012:

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

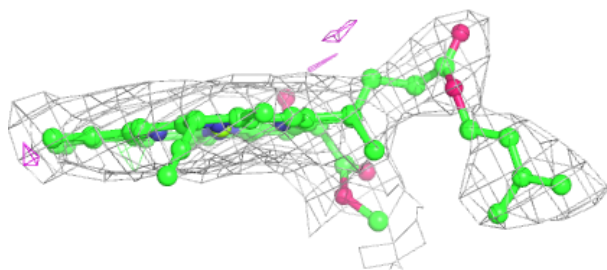
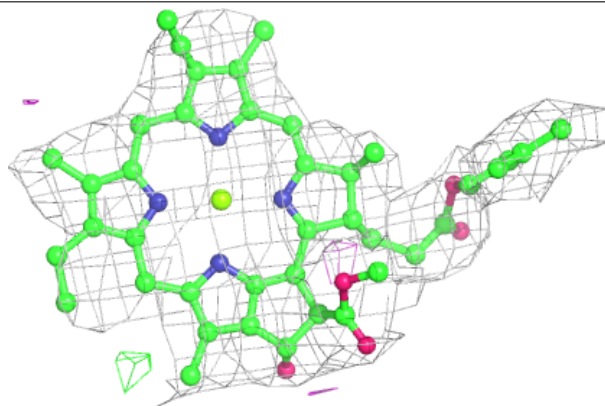


Electron density around CLA A 1132:

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

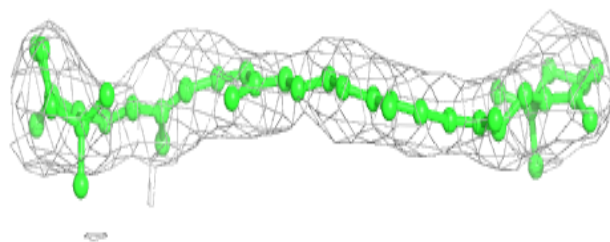
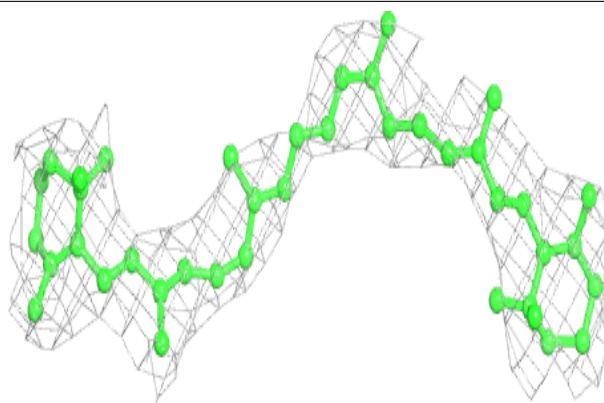
**Electron density around CLA B 1228:**

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



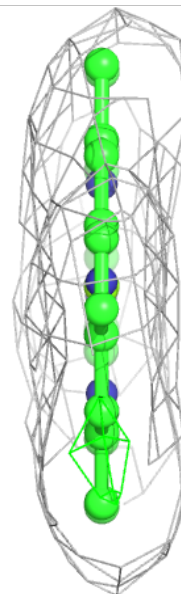
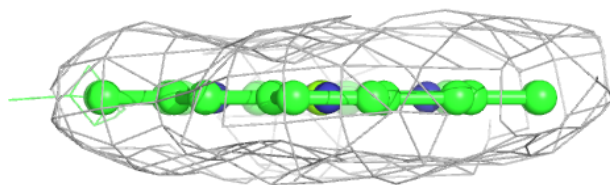
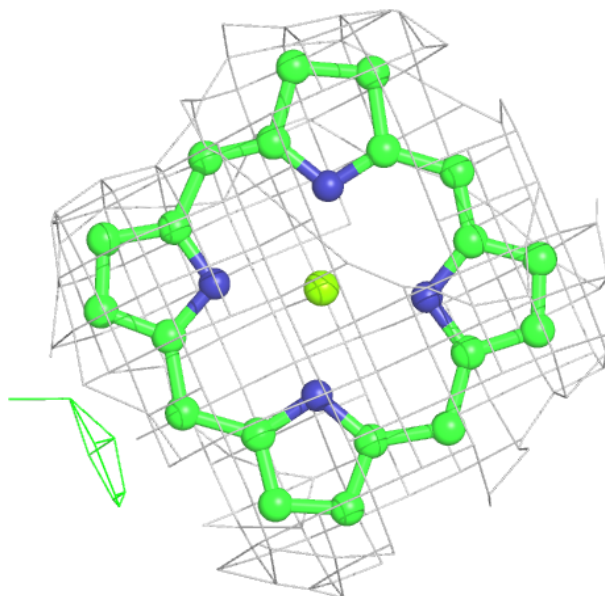
Electron density around BCR A 6011:

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



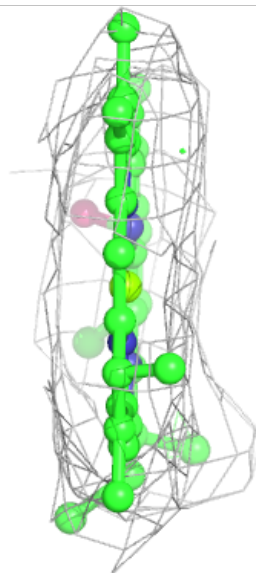
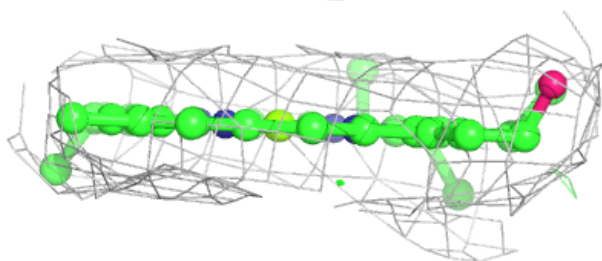
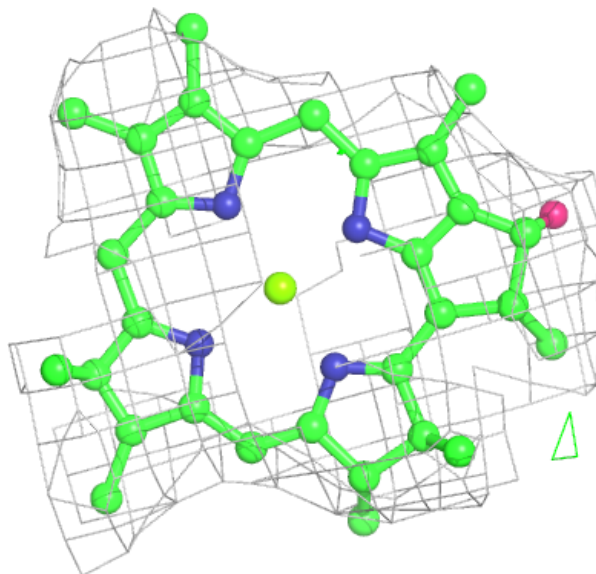
Electron density around CLA 4 4011:

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



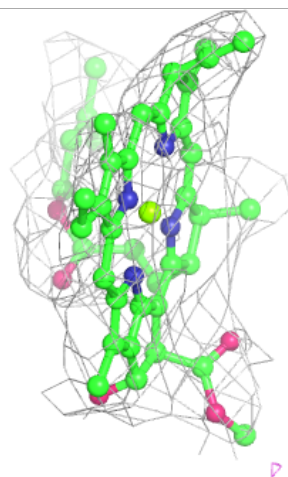
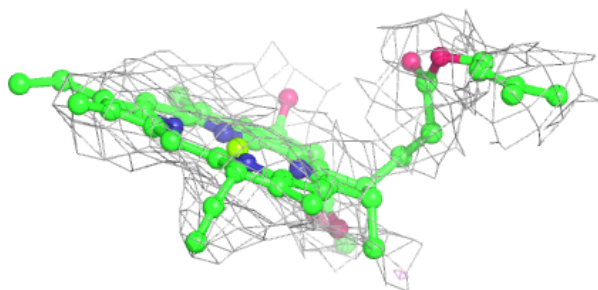
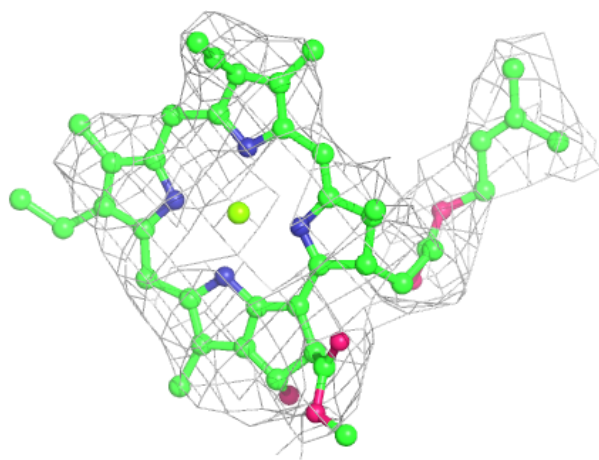
Electron density around CLA 4 4012:

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



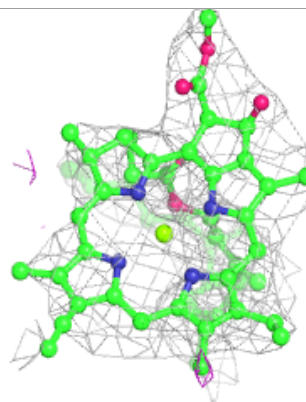
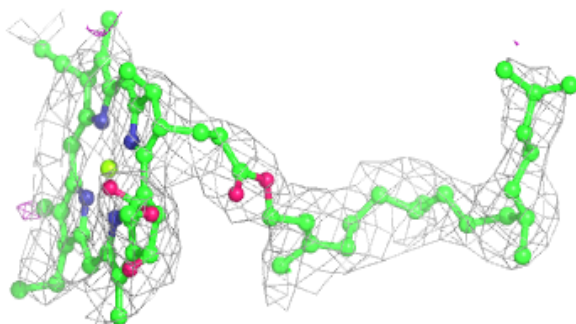
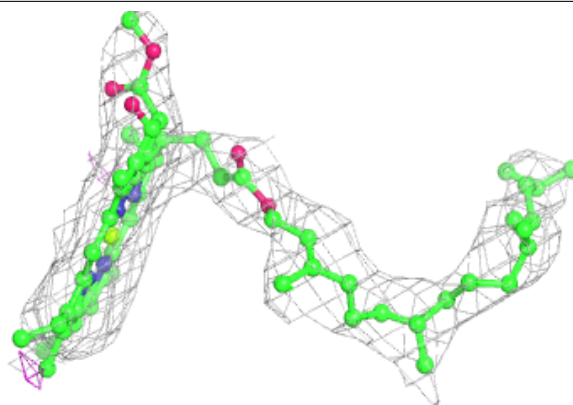
Electron density around CLA A 1133:

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

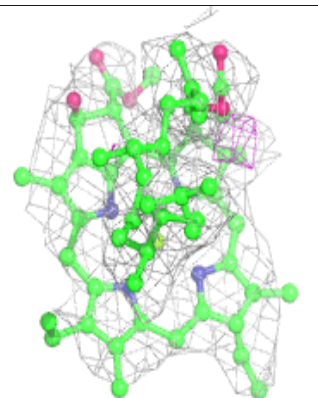
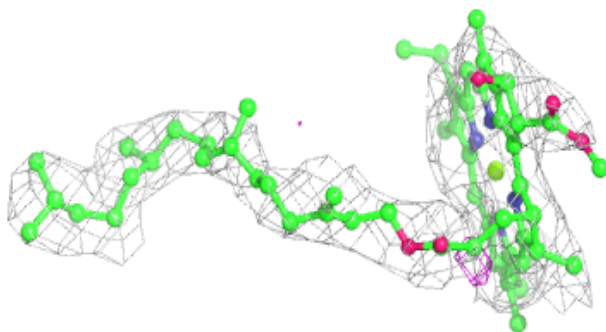
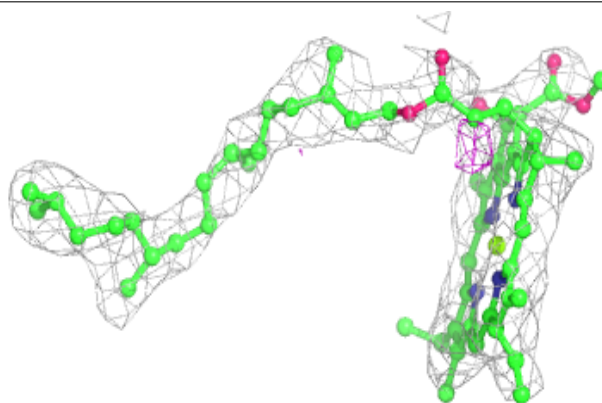


Electron density around CLA B 1238:

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

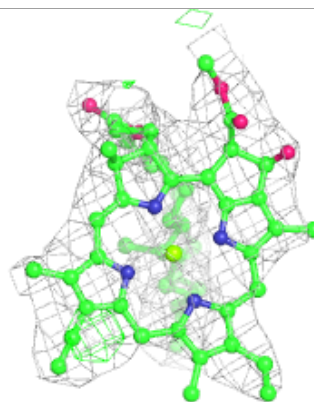
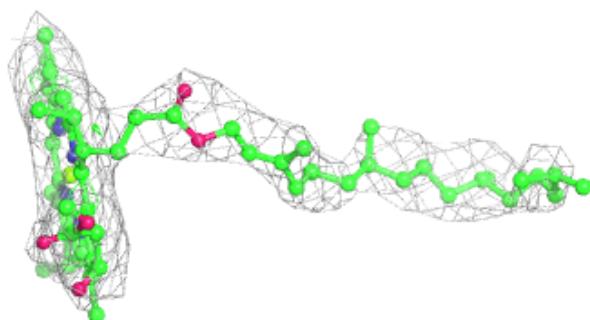
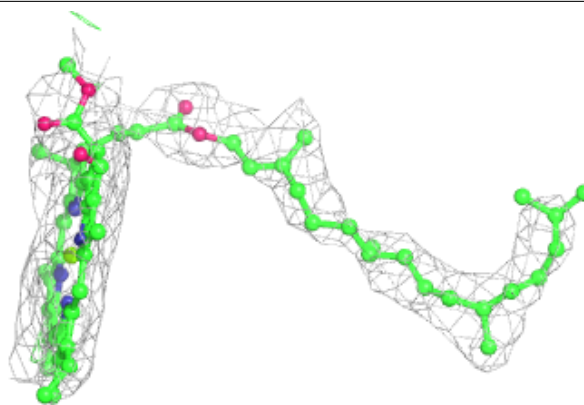
**Electron density around CLA A 1128:**

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

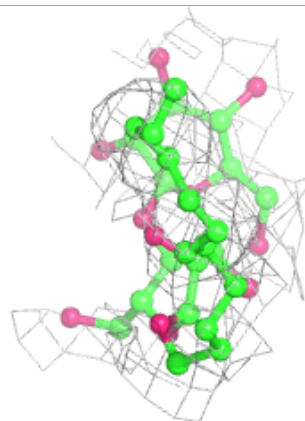
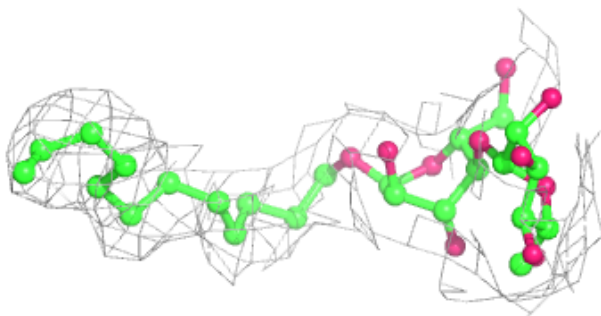
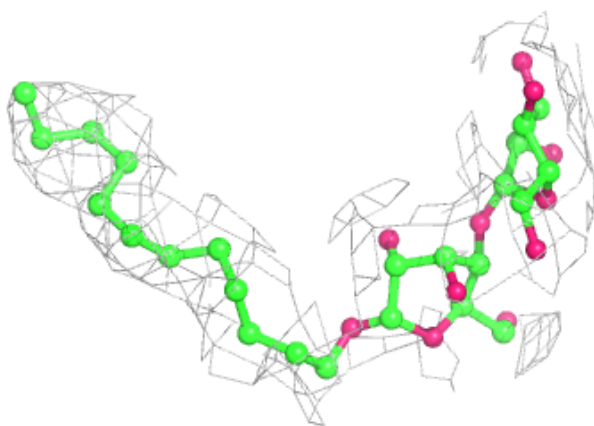


Electron density around CLA B 1239:

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

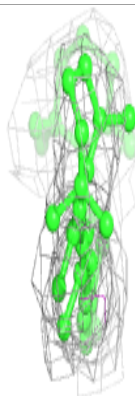
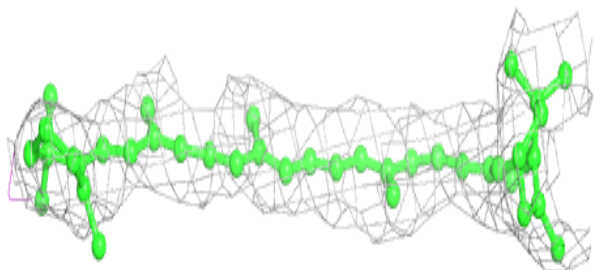
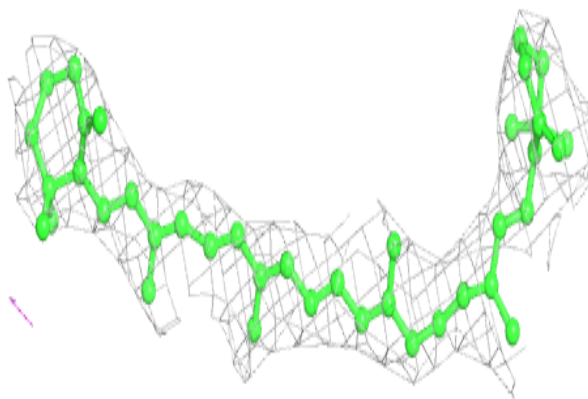
**Electron density around LMU G 7039:**

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

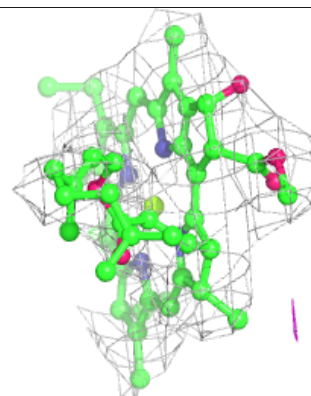
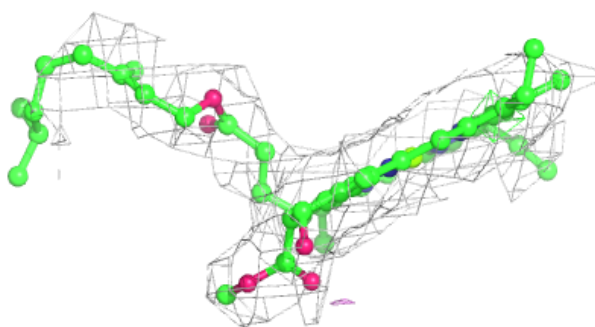
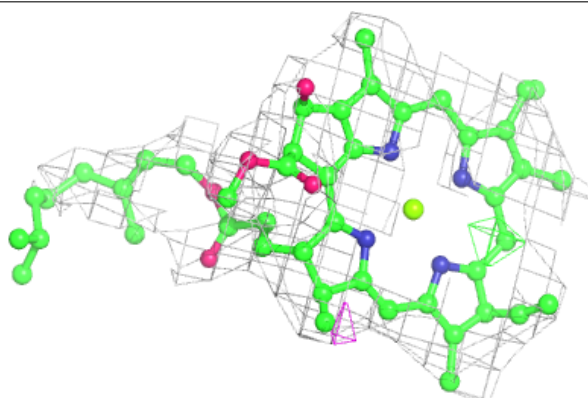


Electron density around BCR B 6005:

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

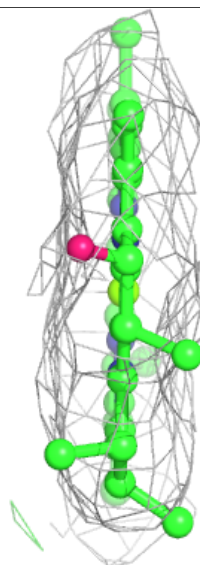
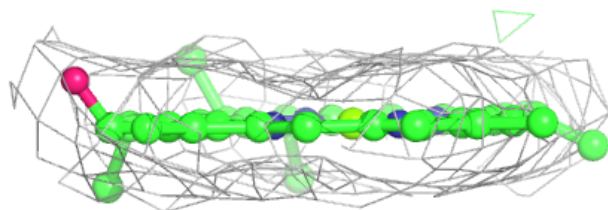
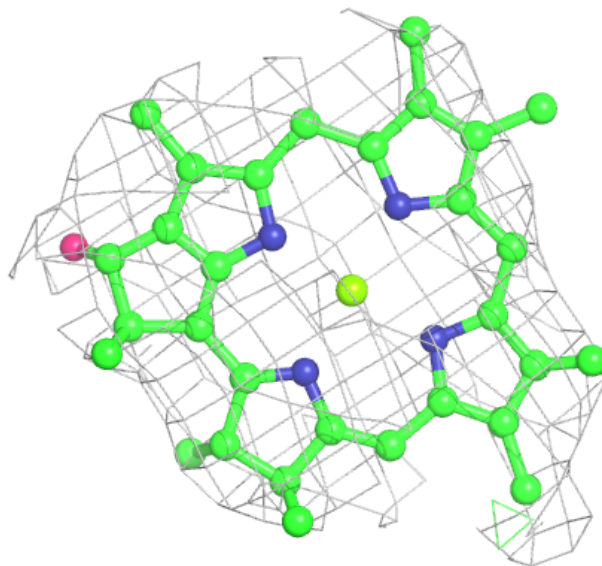
**Electron density around CLA A 1107:**

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



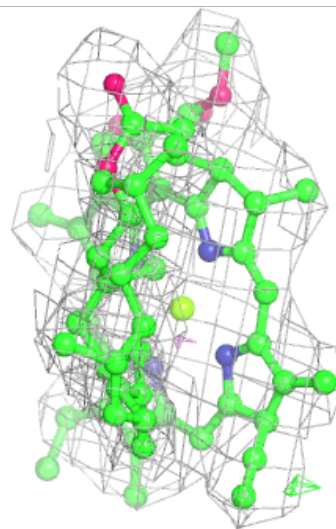
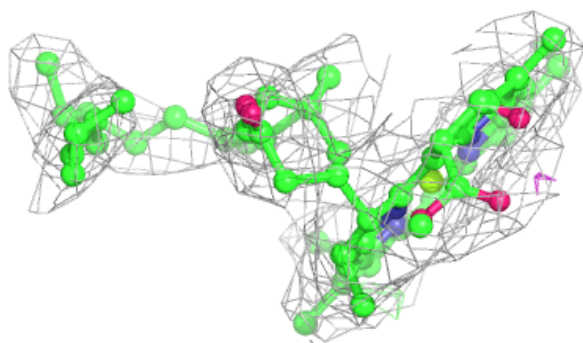
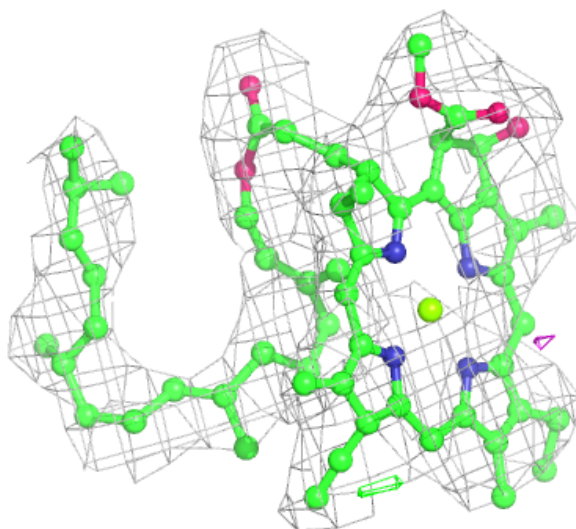
Electron density around CLA F 1240:

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



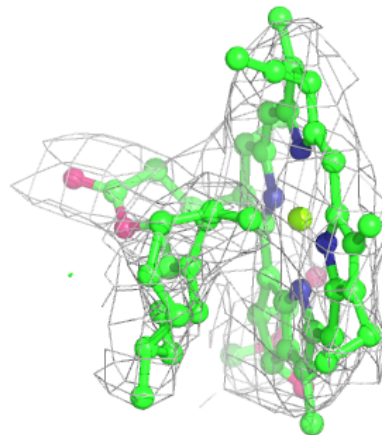
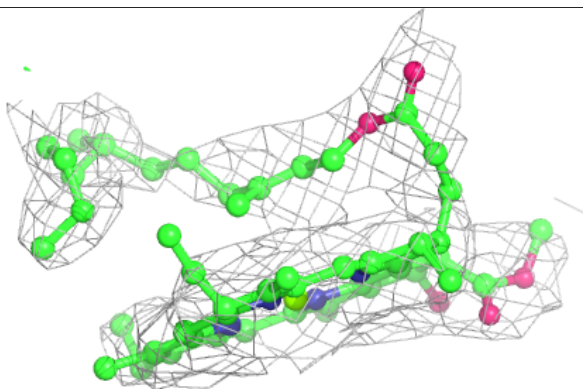
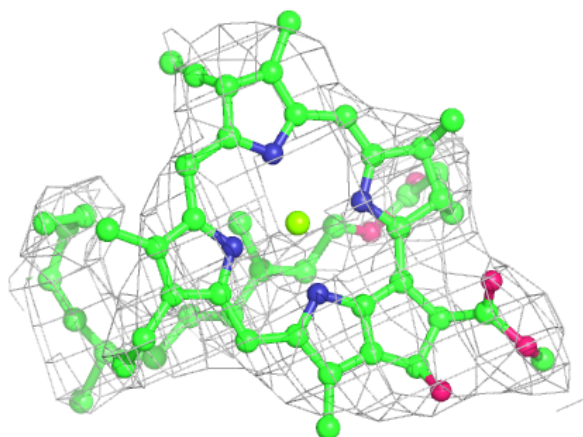
Electron density around CLA B 1220:

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

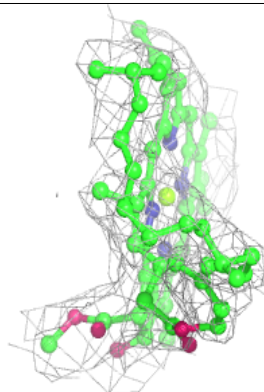
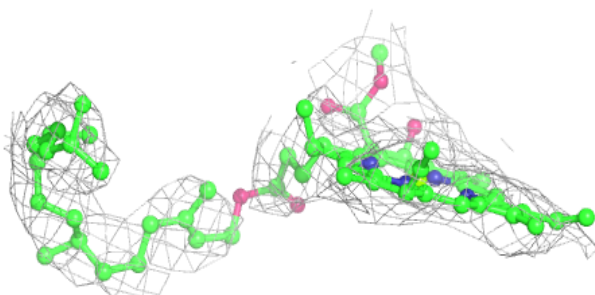
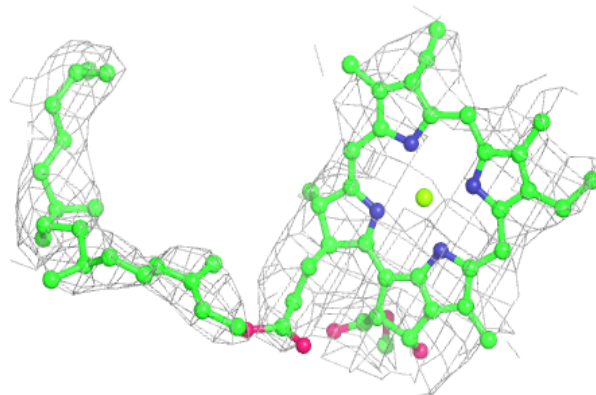


Electron density around CLA B 1214:

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

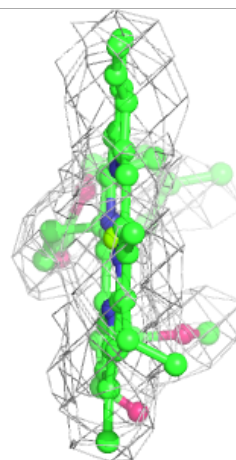
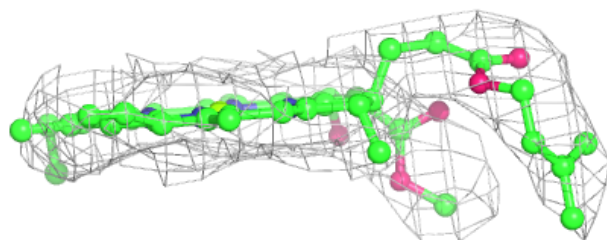
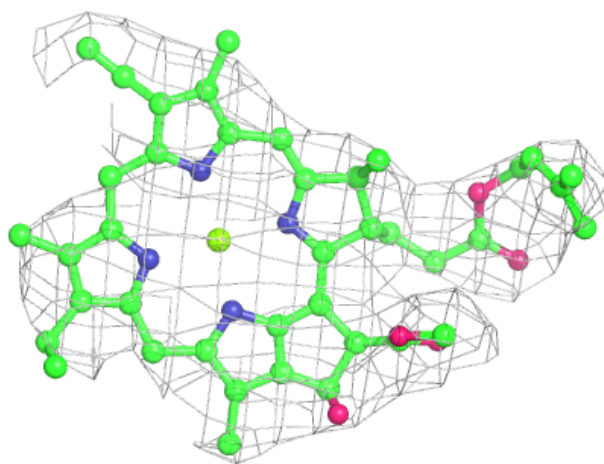
**Electron density around CLA A 1125:**

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



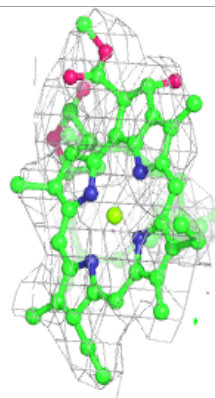
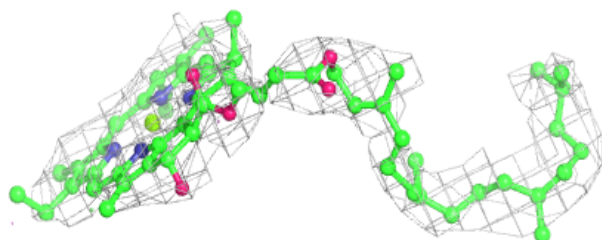
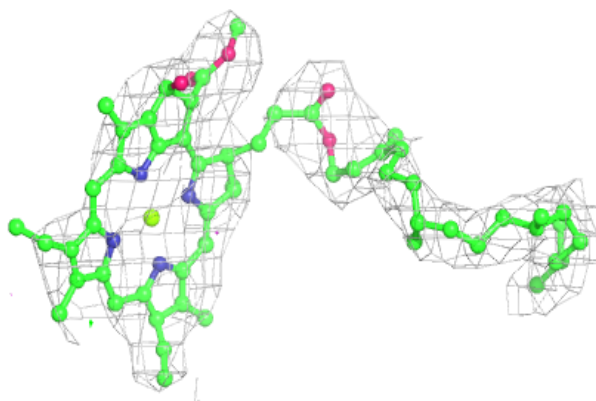
Electron density around CLA A 1101:

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

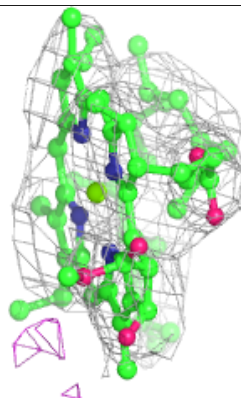
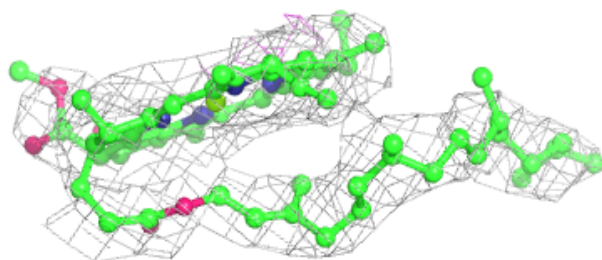
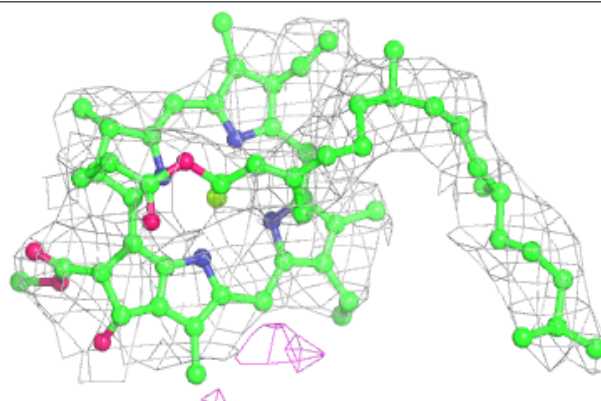


Electron density around CLA B 1206:

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

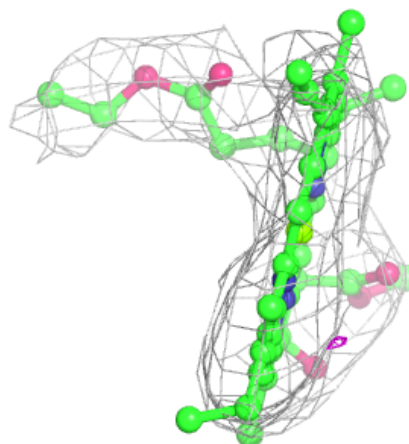
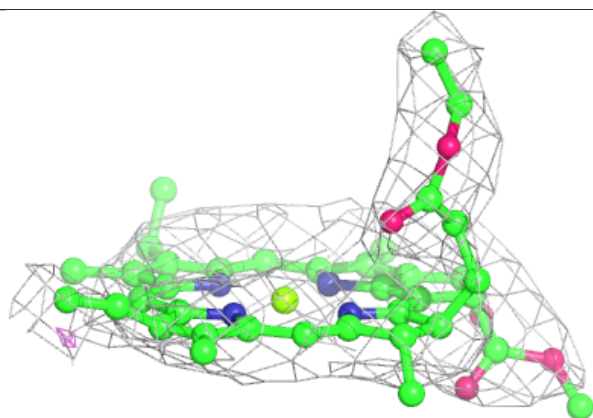
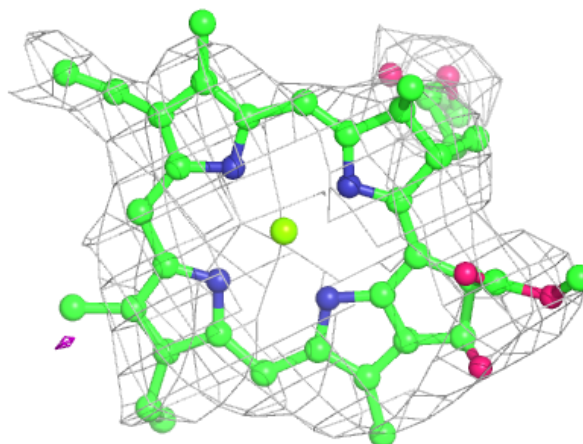
**Electron density around CLA B 1235:**

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



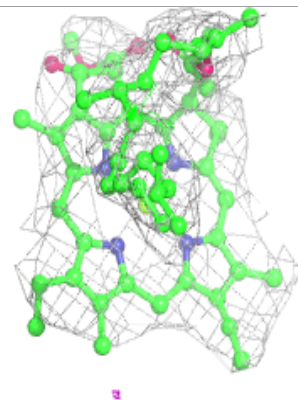
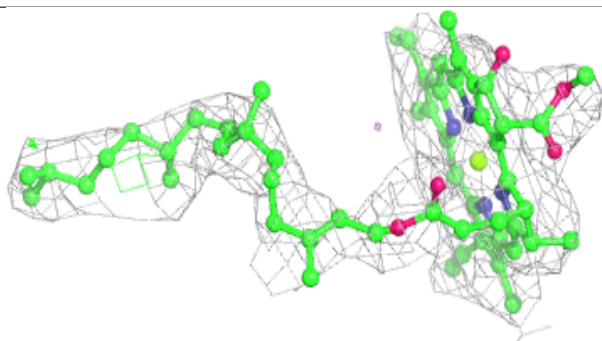
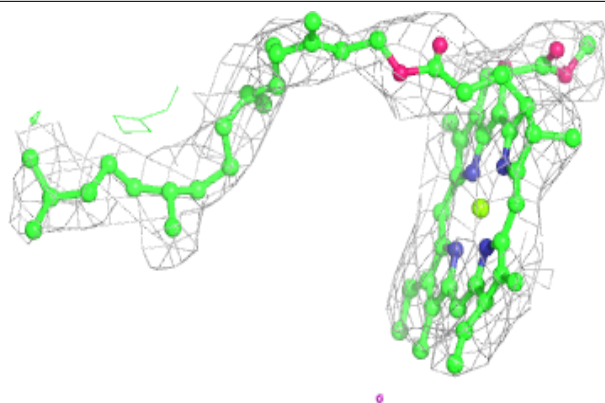
Electron density around CLA B 1236:

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

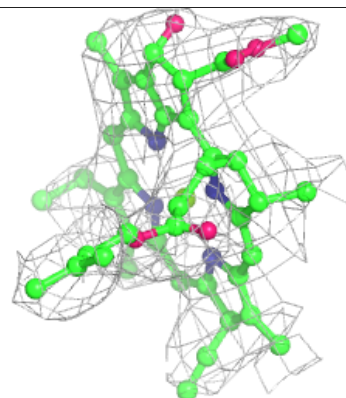
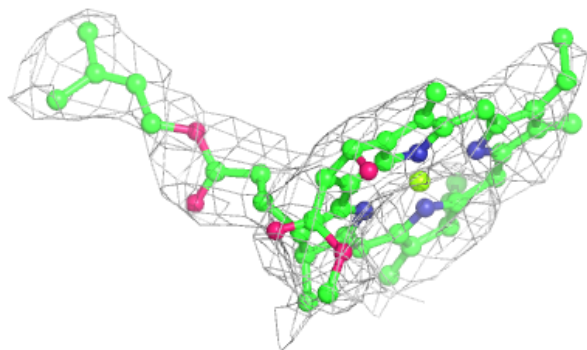
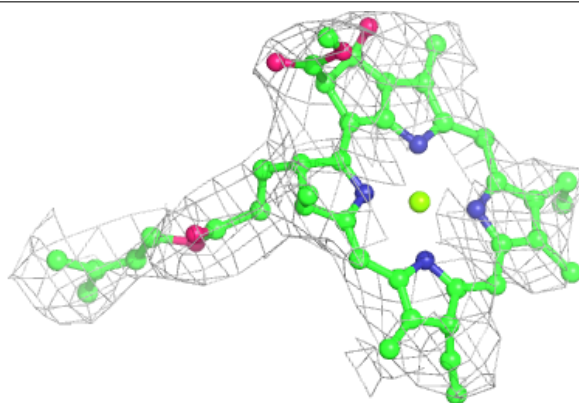


Electron density around CLA B 1226:

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

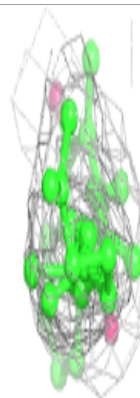
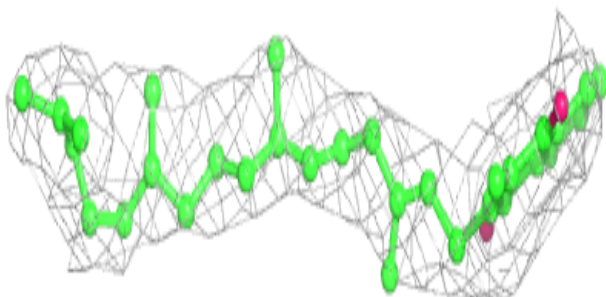
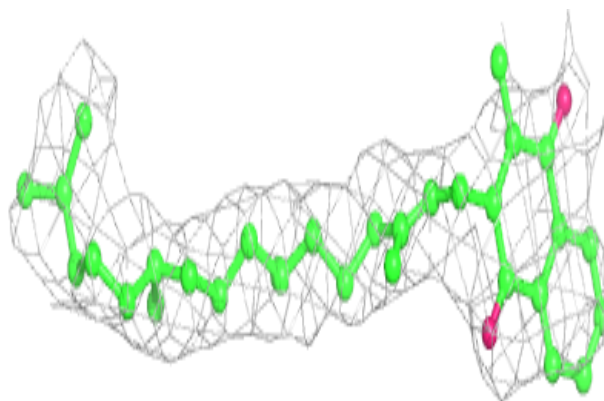
**Electron density around CLA A 1129:**

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

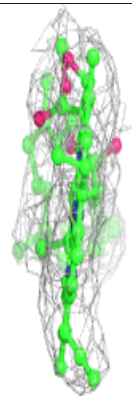
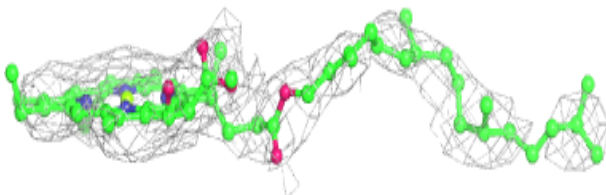
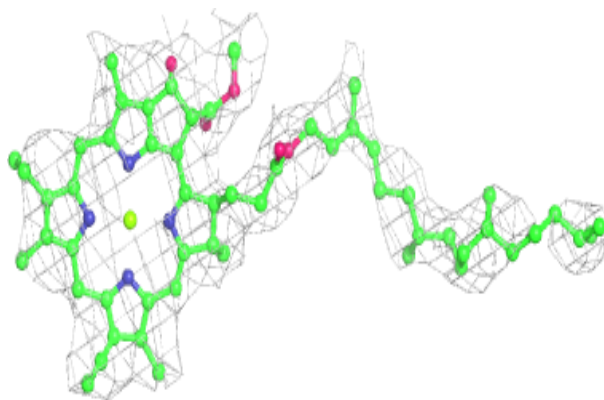


Electron density around PQN A 5001:

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

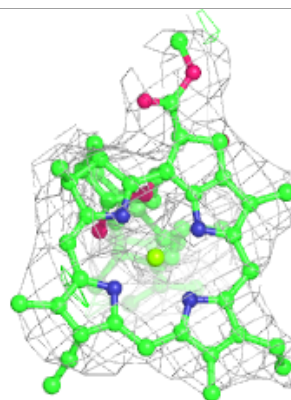
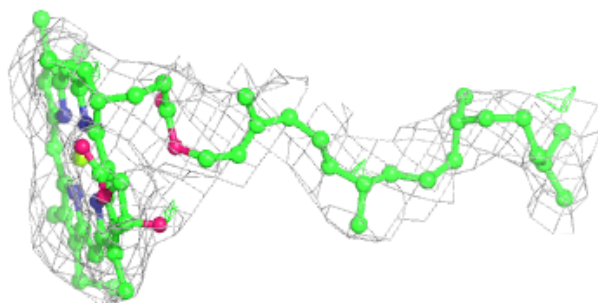
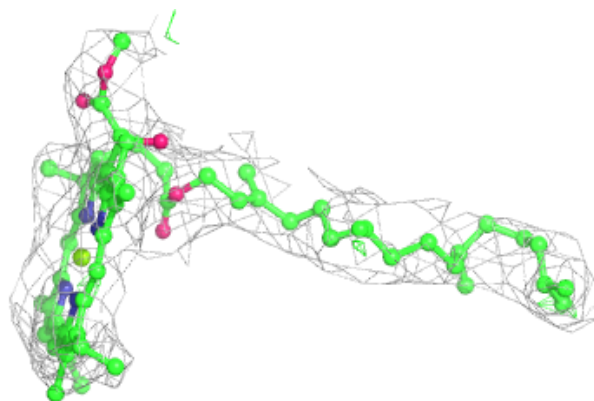
**Electron density around CLA A 1131:**

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

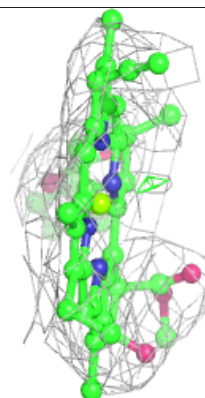
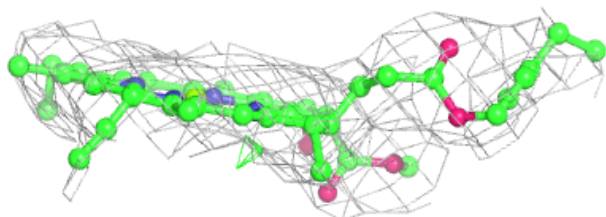
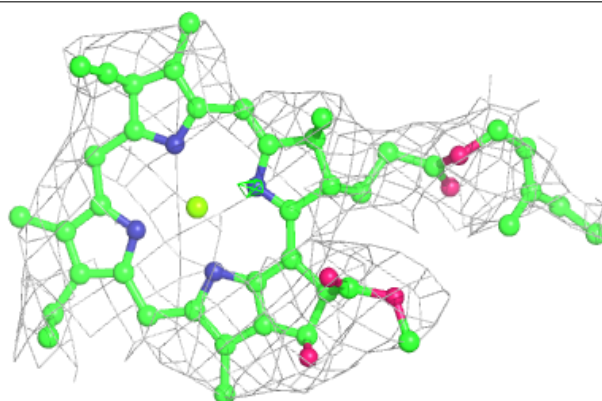


Electron density around CLA A 1126:

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

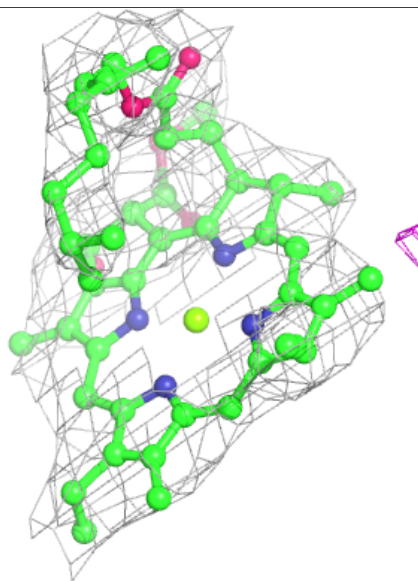
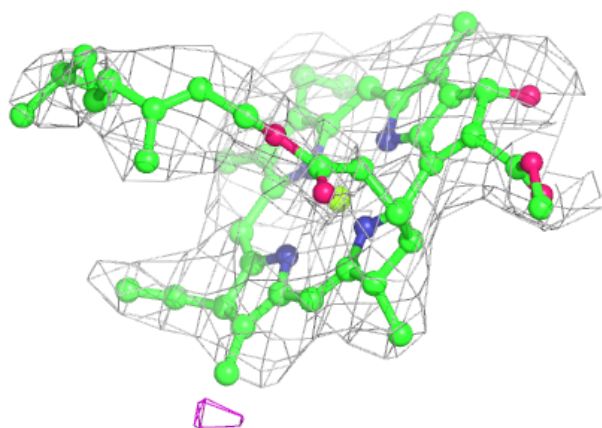
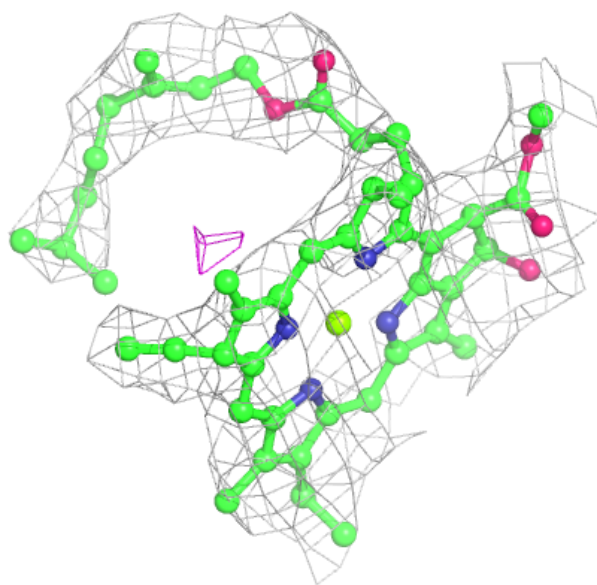
**Electron density around CLA A 1139:**

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



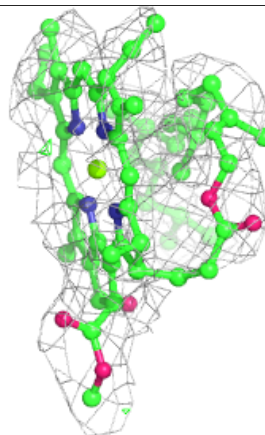
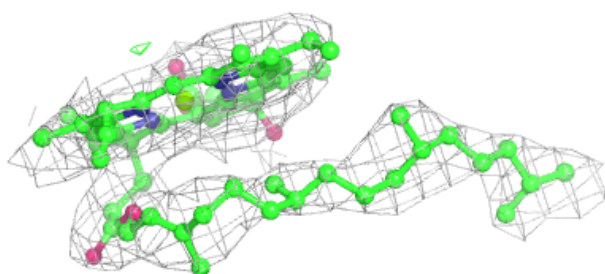
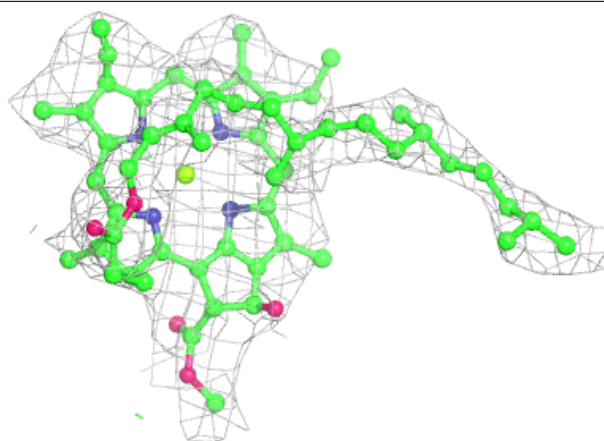
Electron density around CLA A 1122:

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

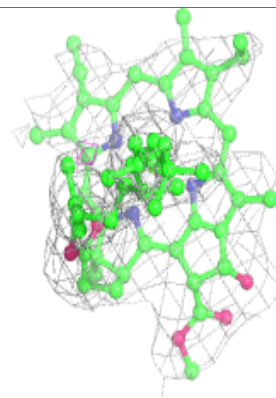
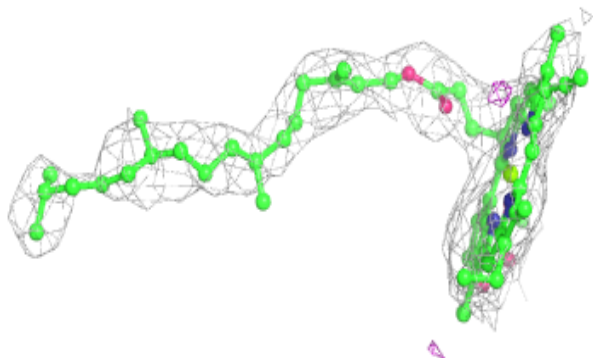
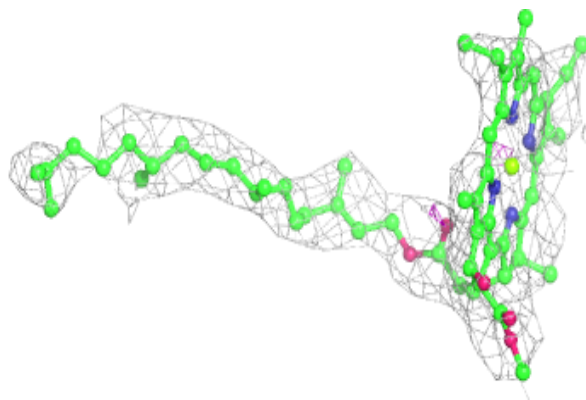


Electron density around CLA B 1224:

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

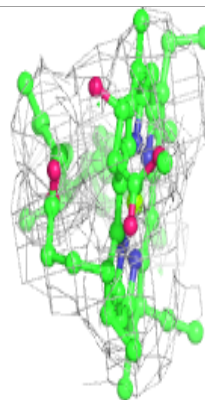
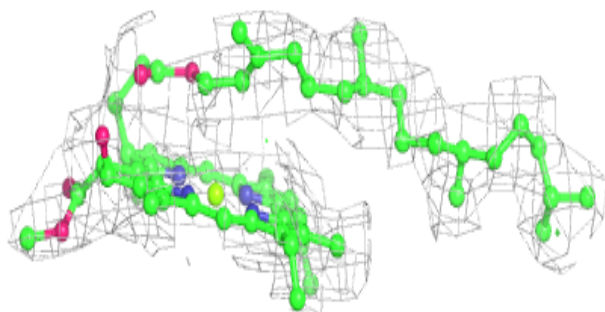
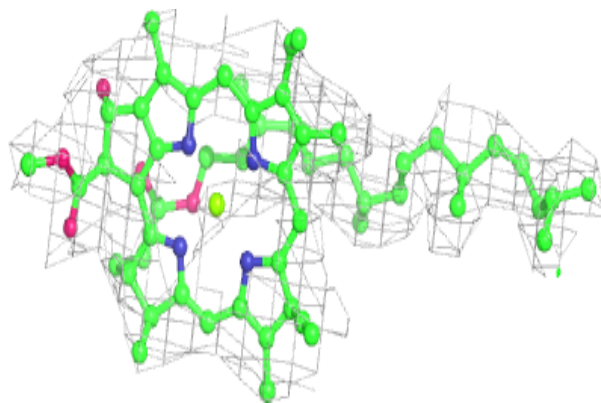
**Electron density around CLA B 1225:**

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



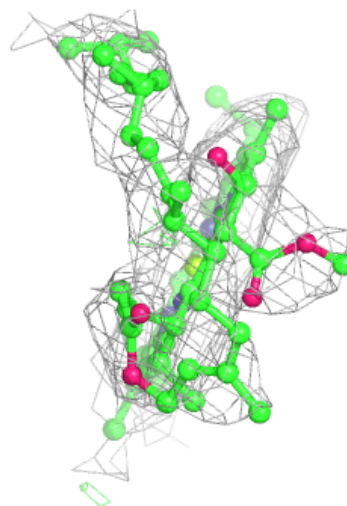
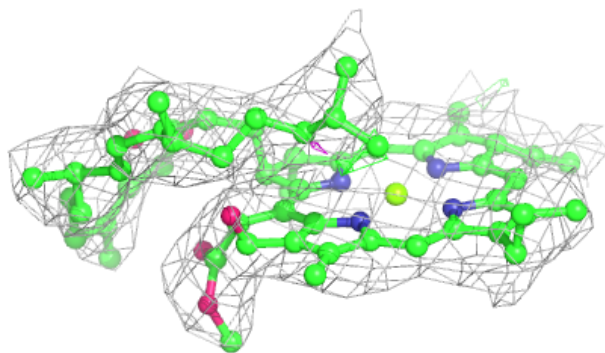
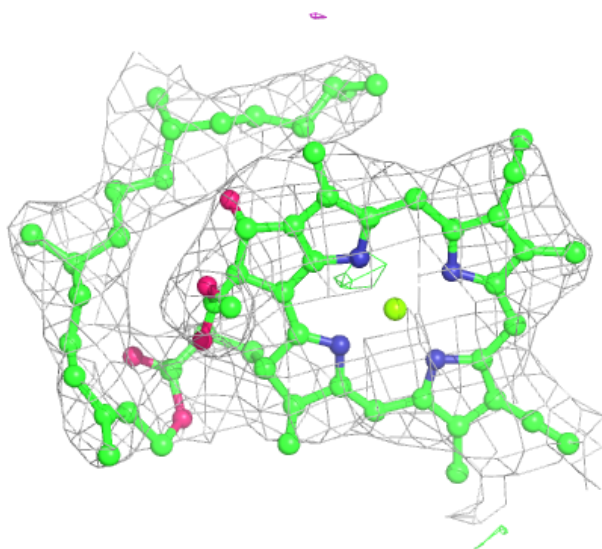
Electron density around CLA A 1136:

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



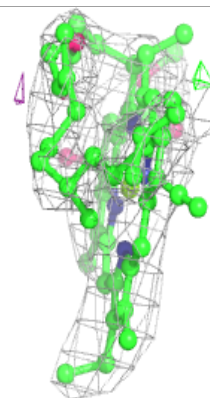
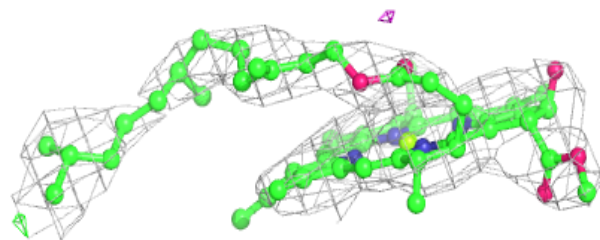
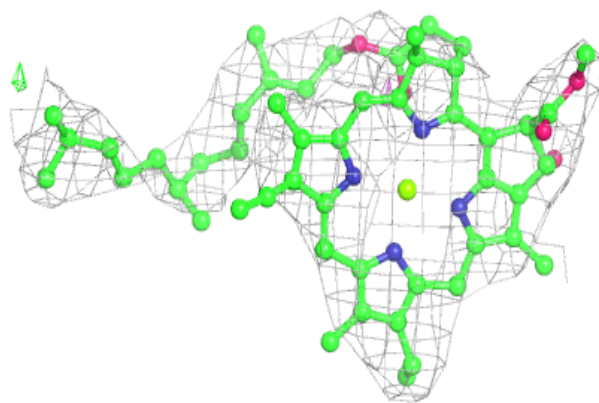
Electron density around CLA B 1202:

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



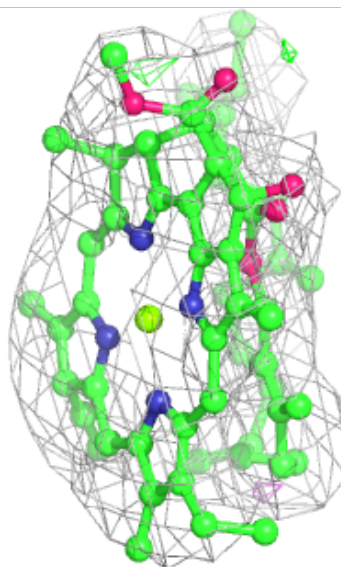
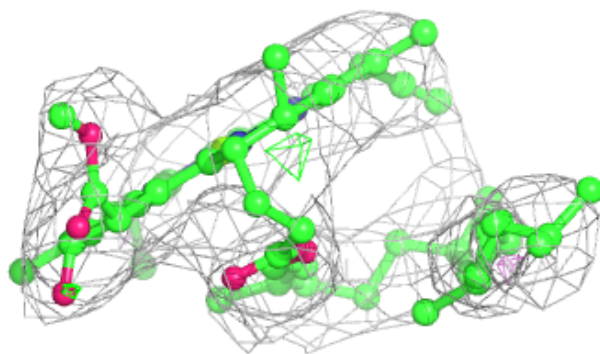
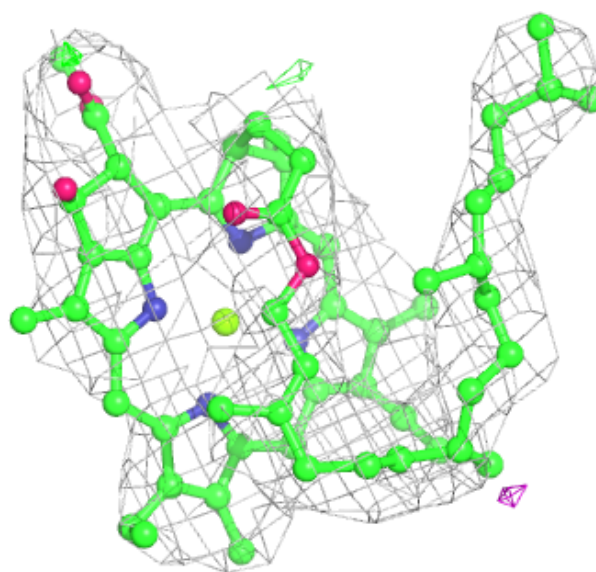
Electron density around CLA B 1215:

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



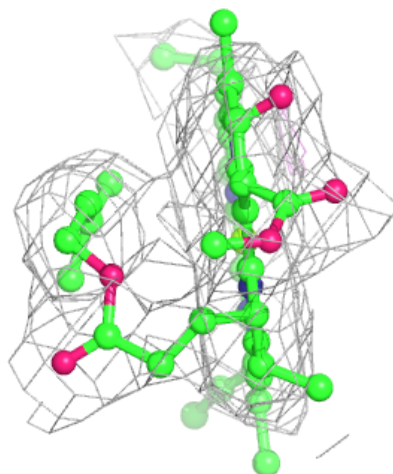
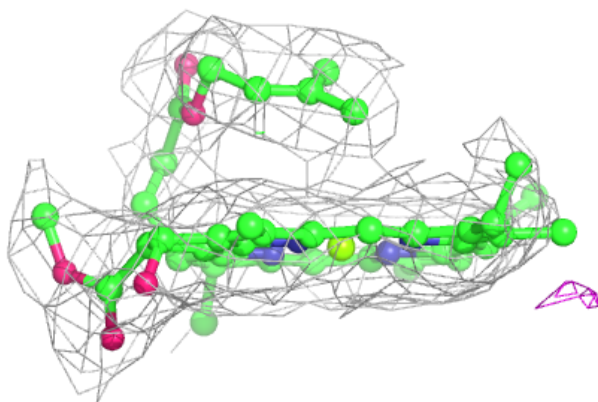
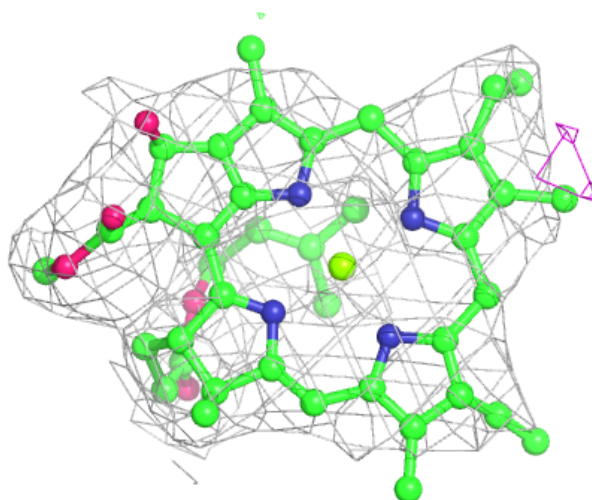
Electron density around CLA B 1205:

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



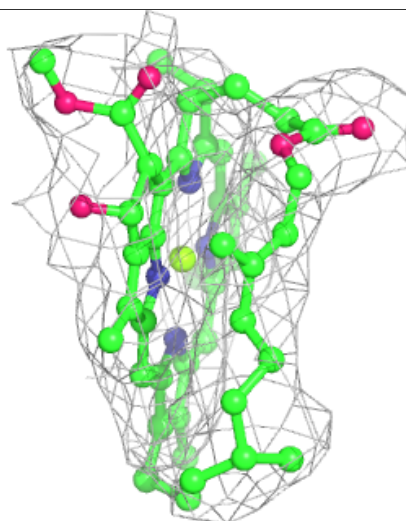
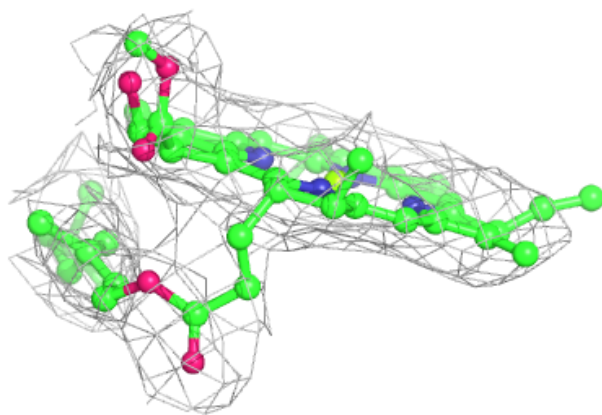
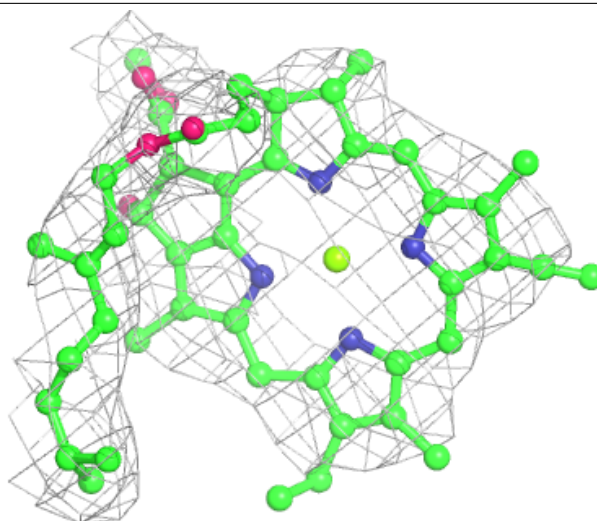
Electron density around CLA B 1227:

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



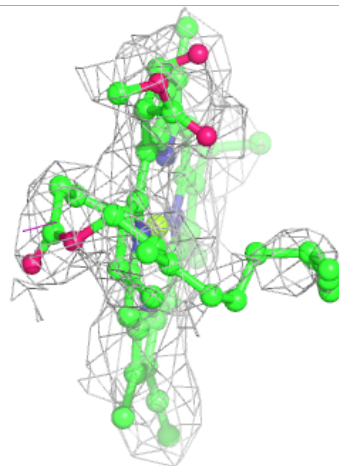
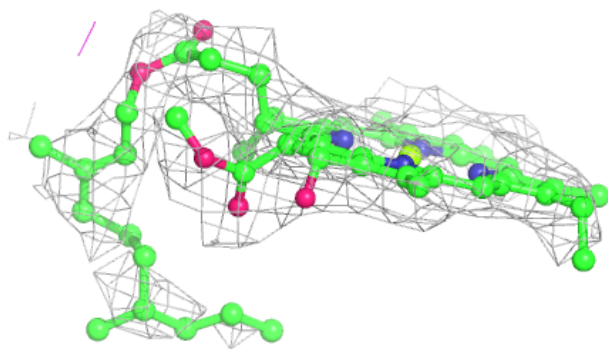
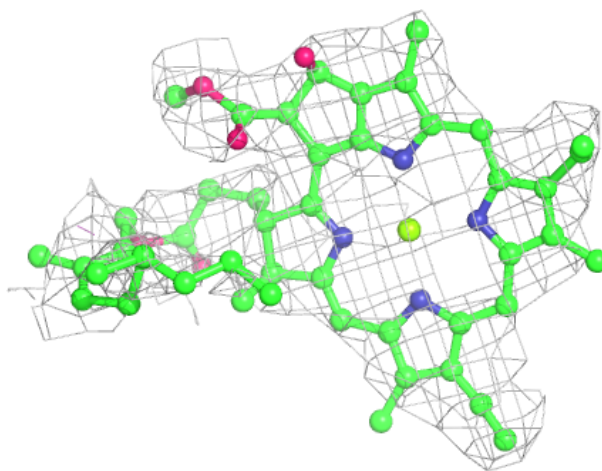
Electron density around CLA A 1127:

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



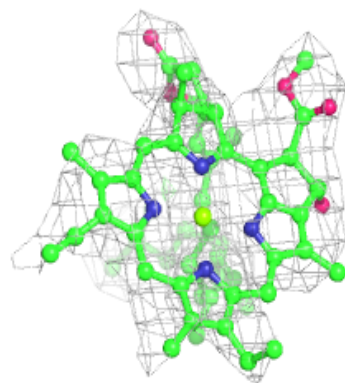
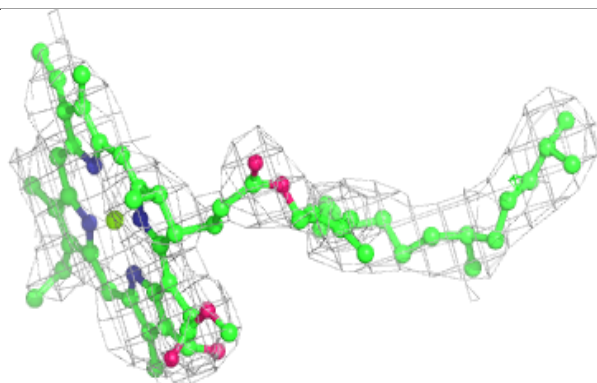
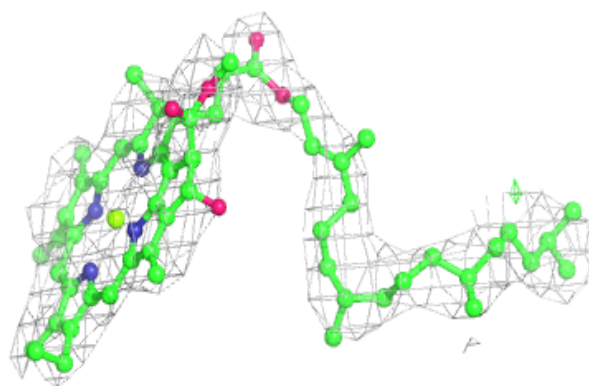
Electron density around CLA A 1104:

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

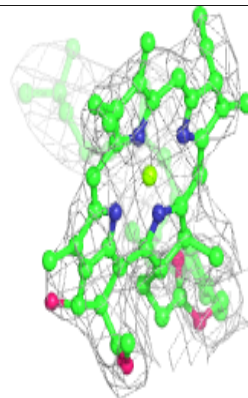
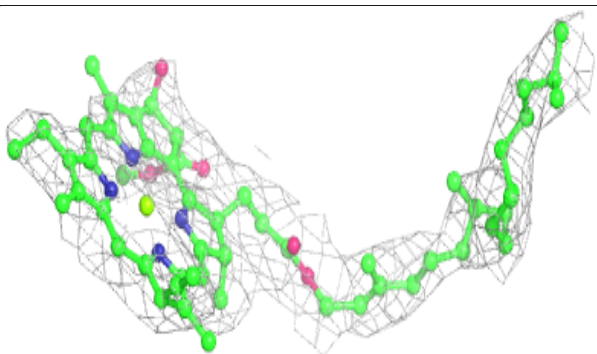
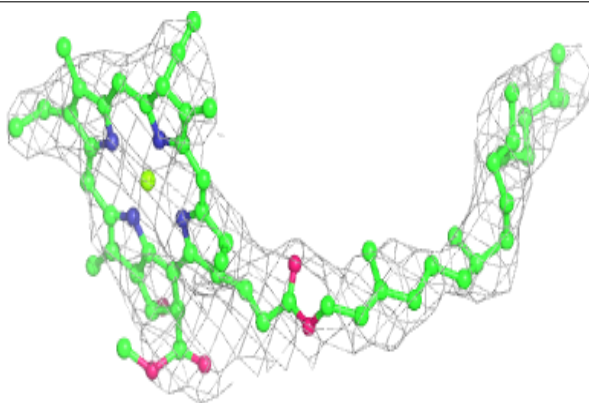


Electron density around CLA B 9010:

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

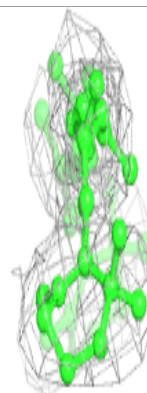
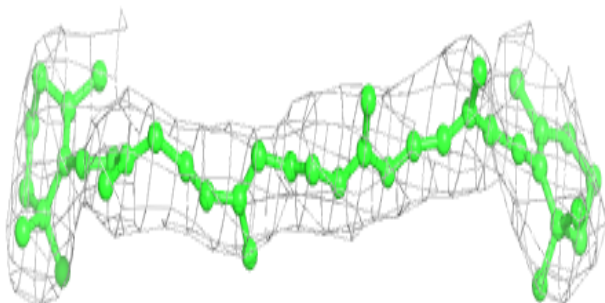
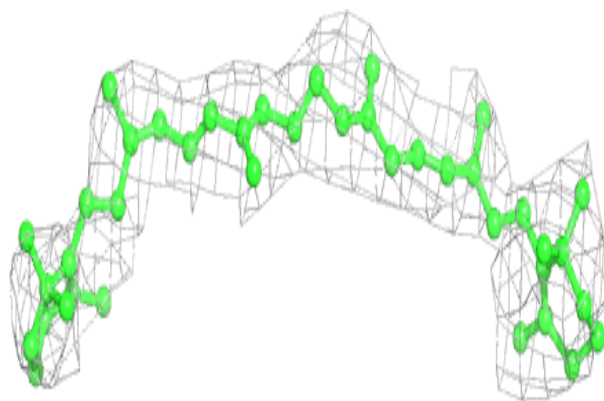
**Electron density around CLA A 9012:**

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

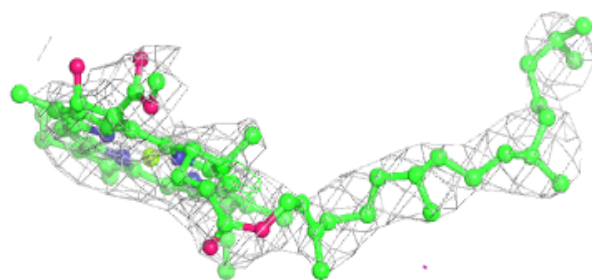
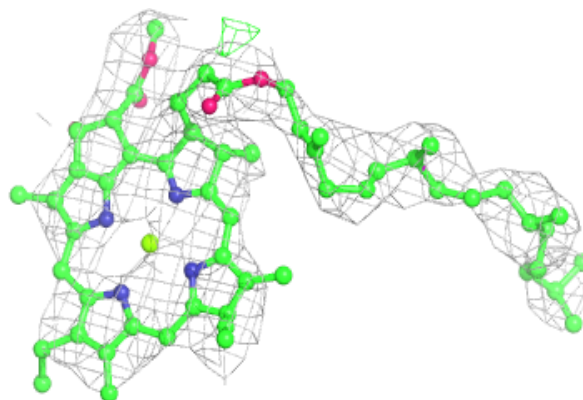


Electron density around BCR B 6020:

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

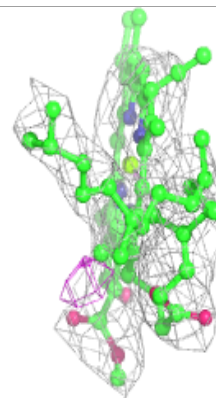
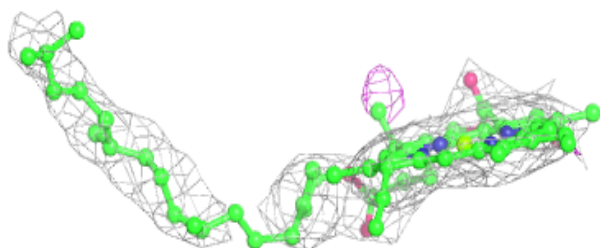
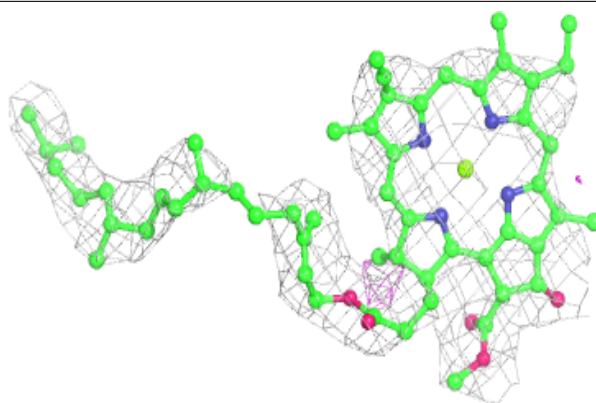
**Electron density around CLA A 9013:**

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

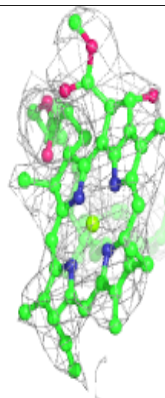
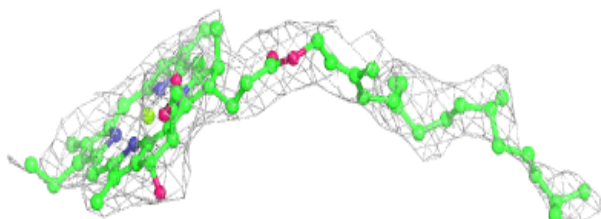
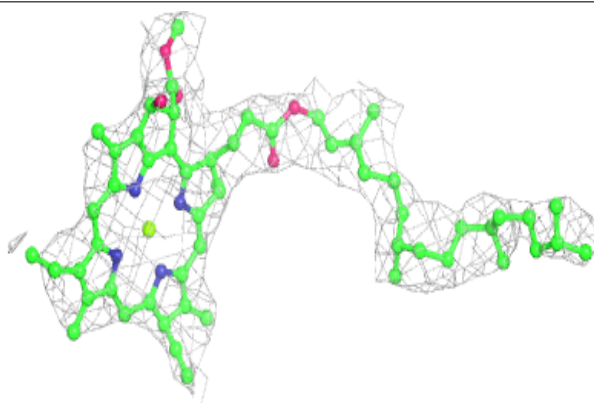


Electron density around CLA A 9023:

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

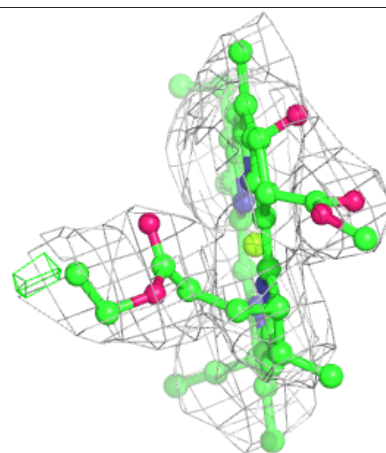
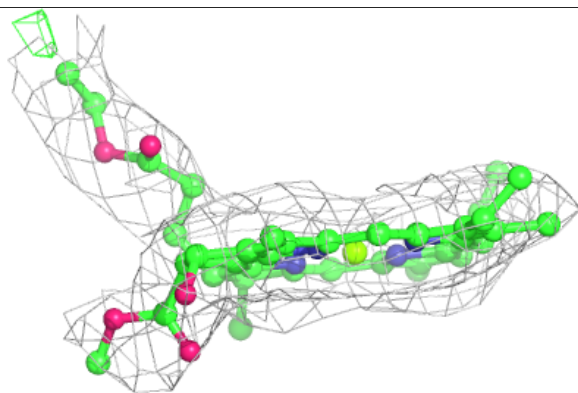
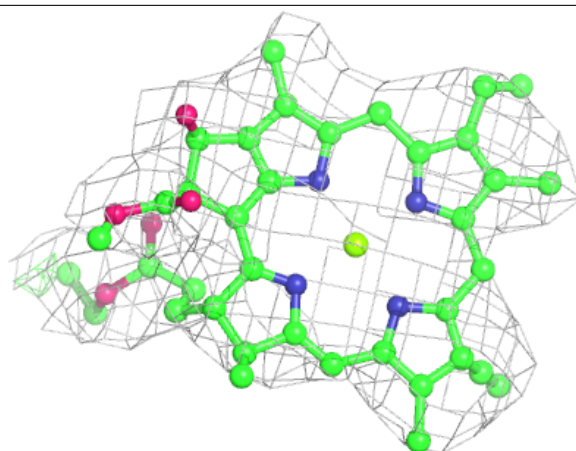
**Electron density around CLA A 9022:**

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

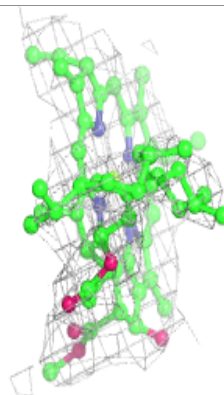
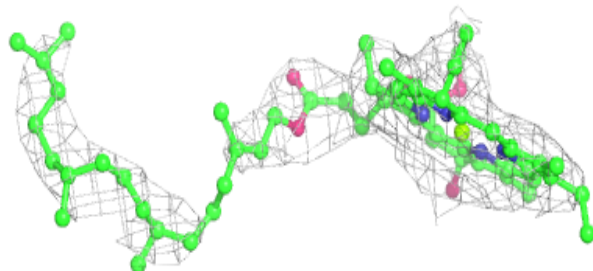
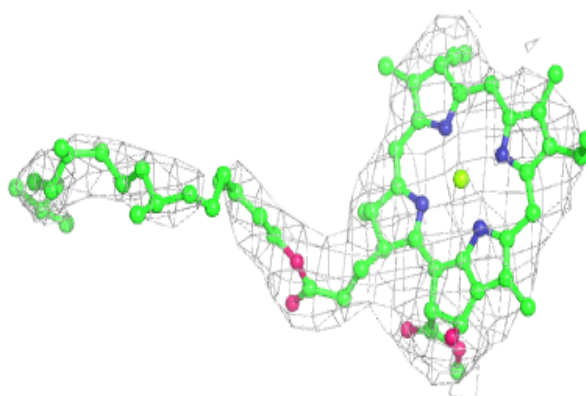


Electron density around CLA A 1137:

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

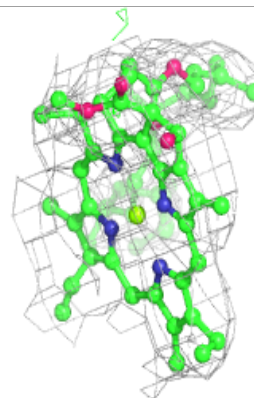
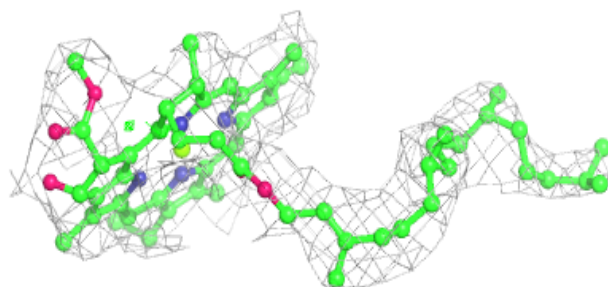
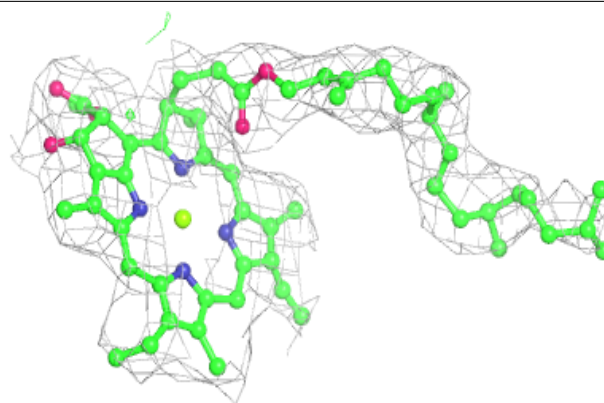
**Electron density around CLA B 1210:**

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

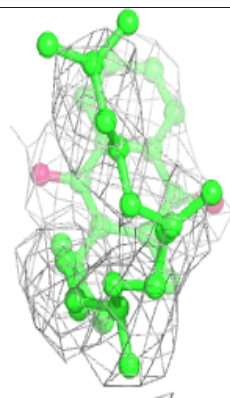
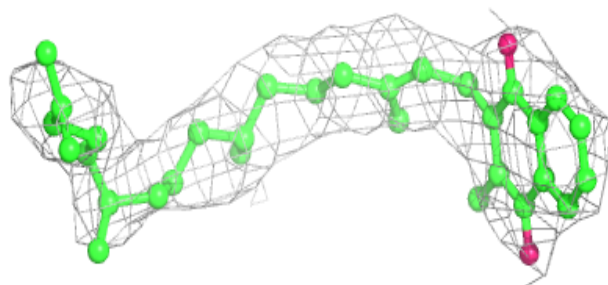
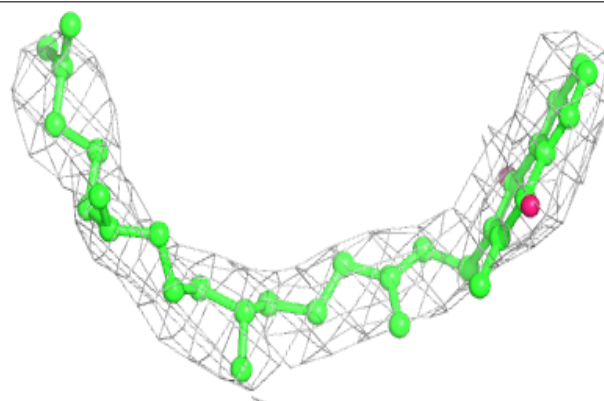


Electron density around CLA A 1106:

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

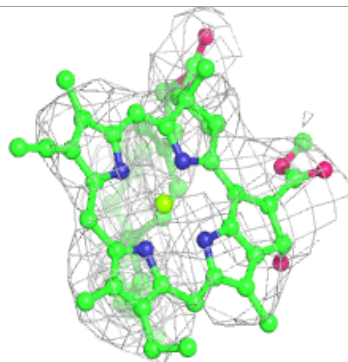
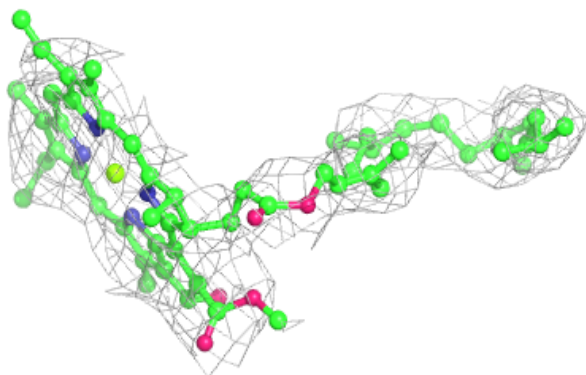
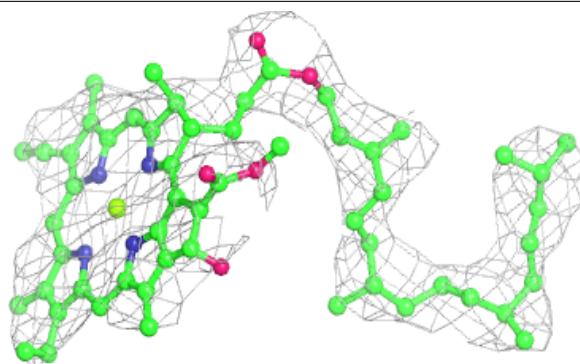
**Electron density around PQN B 5002:**

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

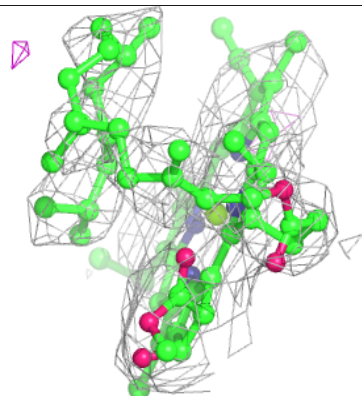
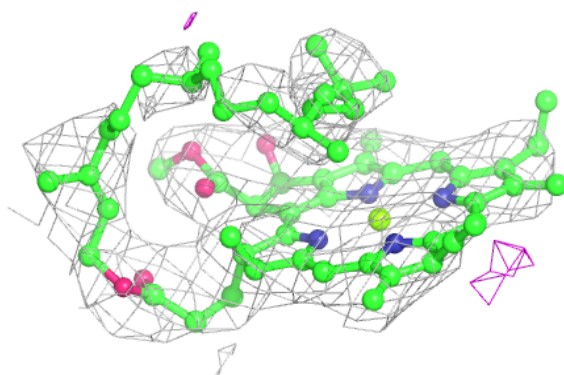
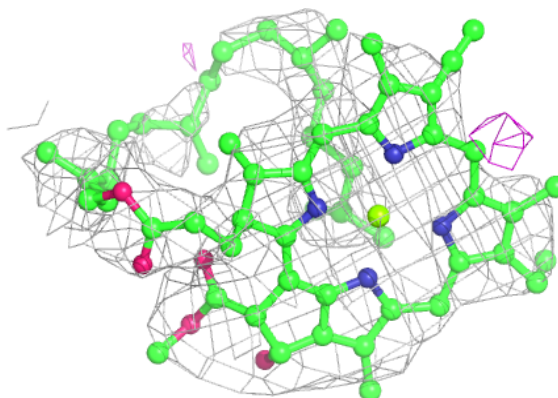


Electron density around CLA A 9011:

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

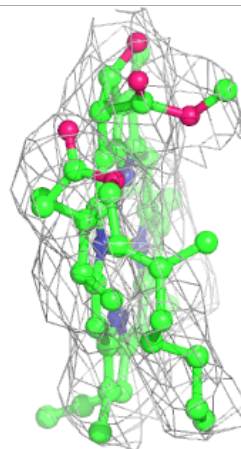
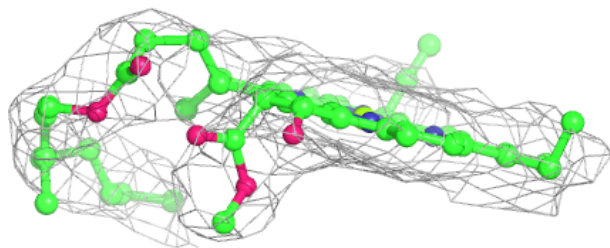
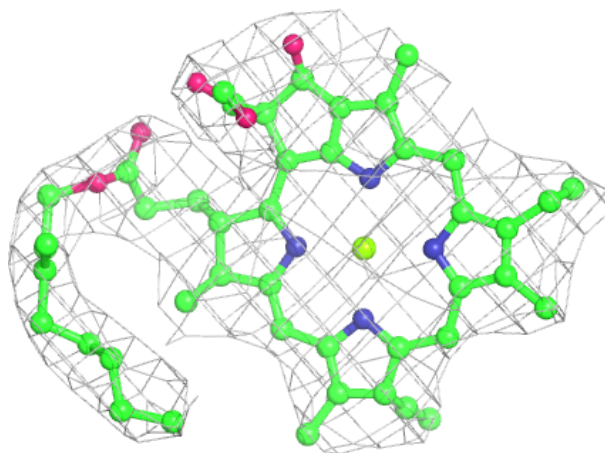
**Electron density around CLA B 1203:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.