



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:35 AM UTC

PDB ID : 2BHW / pdb_00002bhw
Title : PEA LIGHT-HARVESTING COMPLEX II AT 2.5 ANGSTROM RESOLUTION
Authors : Standfuss, J.; Terwisscha van Scheltinga, A.C.; Lamborghini, M.; Kuehlbrandt, W.
Deposited on : 2005-01-19
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

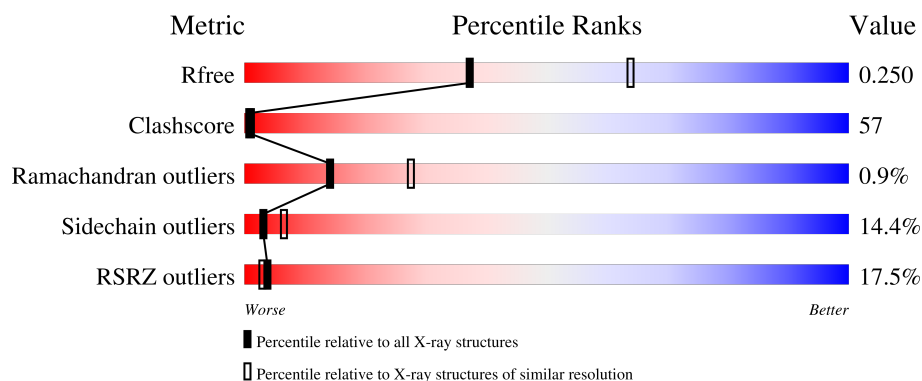
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	232	
1	B	232	
1	C	232	

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
2	LUX	A	501	X	-	X	-
2	LUX	A	502	X	-	-	-
2	LUX	B	501	X	-	X	-
2	LUX	B	502	X	X	-	-
2	LUX	C	501	X	-	X	-
2	LUX	C	502	X	-	-	-
4	XAT	A	504	X	-	-	-
4	XAT	B	504	X	-	-	-
4	XAT	C	504	X	-	-	-
5	CLA	A	601	X	-	-	-
5	CLA	A	602	X	-	-	-
5	CLA	A	603	X	-	-	-
5	CLA	A	604	X	-	-	-
5	CLA	A	605	X	-	-	-
5	CLA	A	606	X	-	-	-
5	CLA	A	607	X	-	-	-
5	CLA	A	608	X	-	-	-
5	CLA	B	601	X	-	X	-
5	CLA	B	602	X	-	-	-
5	CLA	B	603	X	-	X	-
5	CLA	B	604	X	-	X	-
5	CLA	B	605	X	-	X	-
5	CLA	B	606	X	-	-	-
5	CLA	B	607	X	-	-	-
5	CLA	B	608	X	-	X	-
5	CLA	C	601	X	-	X	-
5	CLA	C	602	X	-	-	-
5	CLA	C	603	X	-	-	-
5	CLA	C	604	X	-	-	-
5	CLA	C	605	X	-	-	-
5	CLA	C	606	X	-	-	-
5	CLA	C	607	X	-	-	-
5	CLA	C	608	X	-	-	-
6	CHL	A	609	X	-	X	-
6	CHL	A	610	X	-	X	-
6	CHL	A	611	X	-	-	-
6	CHL	A	612	X	-	-	-
6	CHL	A	613	X	-	-	-
6	CHL	A	614	X	-	-	-
6	CHL	B	609	X	-	X	-
6	CHL	B	610	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CHL	B	611	X	-	X	-
6	CHL	B	612	X	-	X	-
6	CHL	B	613	X	-	-	-
6	CHL	B	614	X	-	-	-
6	CHL	C	609	X	-	X	-
6	CHL	C	610	X	-	X	-
6	CHL	C	611	X	-	X	-
6	CHL	C	612	X	-	X	-
6	CHL	C	613	X	-	-	-
6	CHL	C	614	X	-	-	-
8	DGD	A	802	X	-	-	-
8	DGD	B	802	X	-	-	-
8	DGD	C	802	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8373 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.

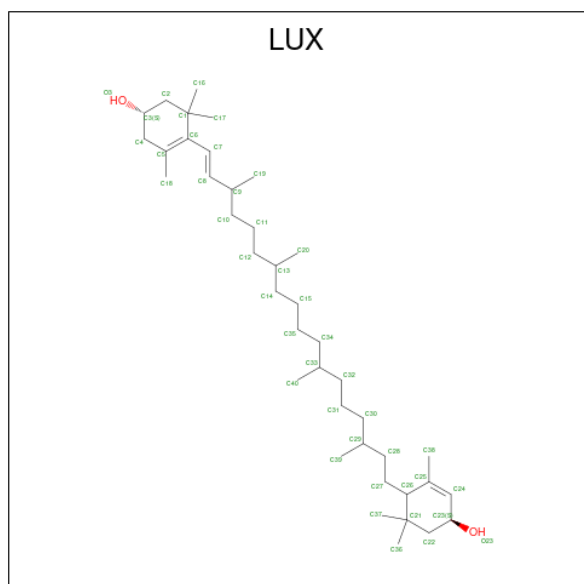
- Molecule 1 is a protein called CHLOROPHYLL A-B BINDING PROTEIN AB80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			
1	B	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			
1	C	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			

There are 3 discrepancies between the modelled and reference sequences:

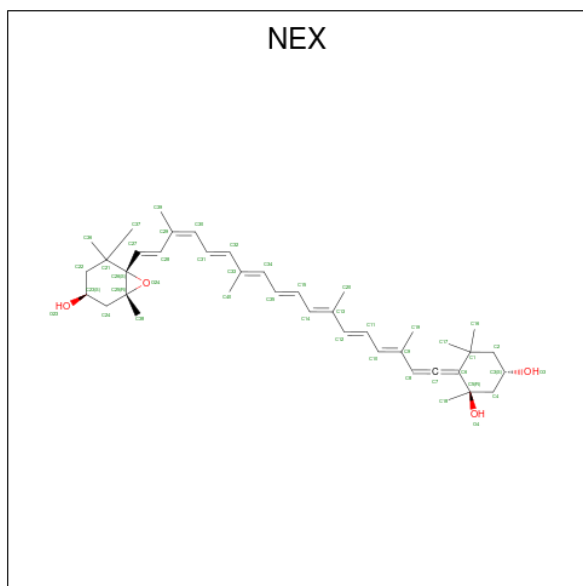
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	SER	CYS	conflict	UNP P07371
B	79	SER	CYS	conflict	UNP P07371
C	79	SER	CYS	conflict	UNP P07371

- Molecule 2 is (3R,3'R,6'S,9R,9'R,13R,13'S)-4',5'-DIDEHYDRO-5',6',7',8',9,9',10,10',11,11',12,12',13,13',14,14',15,15'-OCTADECALYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUX) (formula: C₄₀H₇₂O₂).



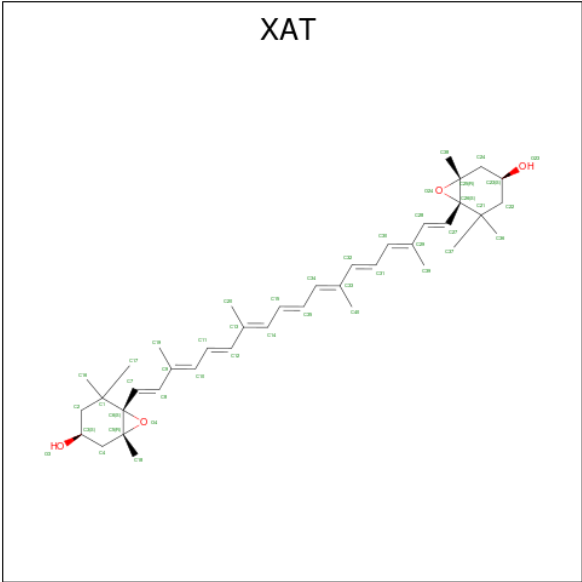
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			42	40	2		
2	A	1	Total	C	O	0	0
			42	40	2		
2	B	1	Total	C	O	0	0
			42	40	2		
2	B	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		

- Molecule 3 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



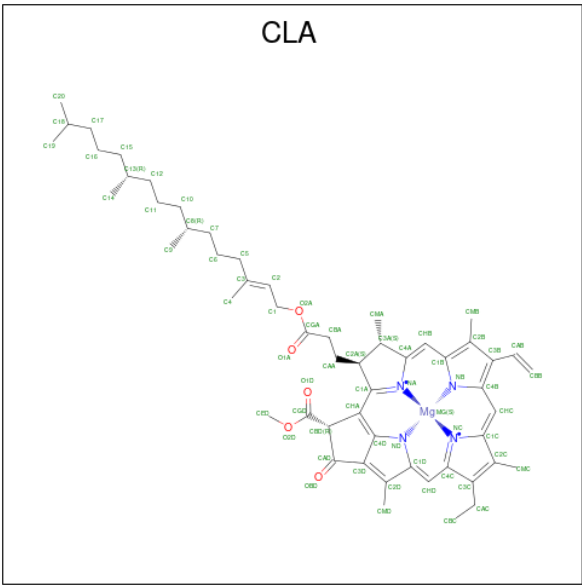
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			44	40	4		
3	B	1	Total	C	O	0	0
			44	40	4		
3	C	1	Total	C	O	0	0
			44	40	4		

- Molecule 4 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			44	40	4		
4	B	1	Total	C	O	0	0
			44	40	4		
4	C	1	Total	C	O	0	0
			44	40	4		

- Molecule 5 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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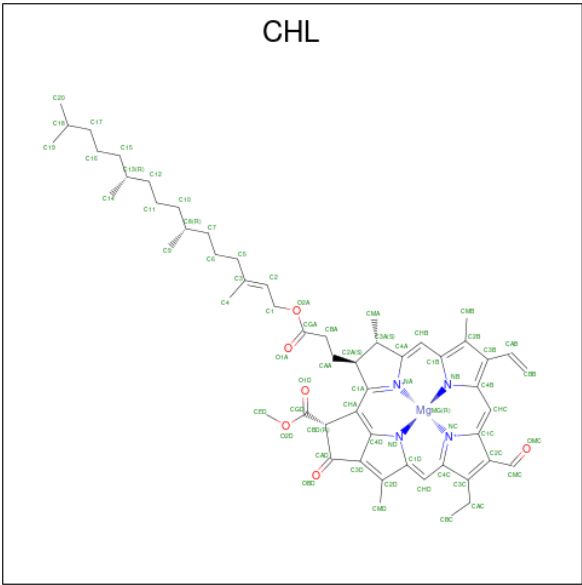
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
5	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	A	1	Total 57	C 47	Mg 1	N 4	O 5	0	0
5	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	A	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
5	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
5	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	B	1	Total 57	C 47	Mg 1	N 4	O 5	0	0
5	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	B	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
5	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	C	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
5	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
5	C	1	Total 57	C 47	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		

- Molecule 6 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



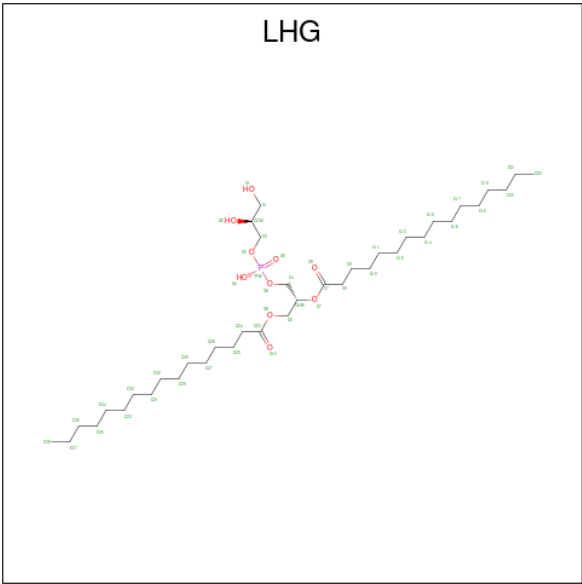
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



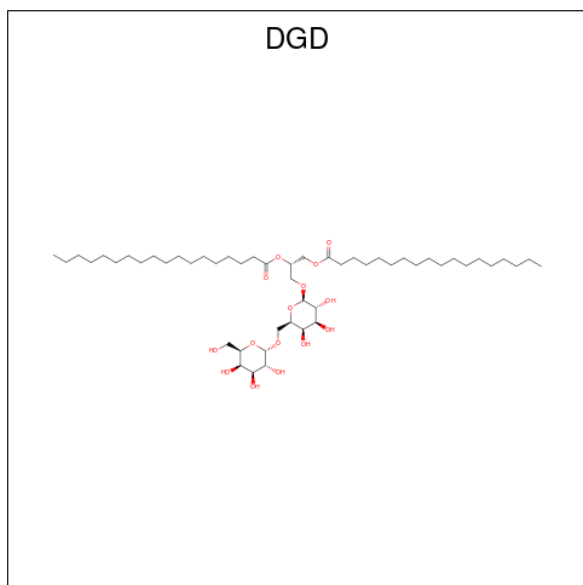
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			49	38	10	1		
7	B	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 8 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			38	25	13		
8	B	1	Total	C	O	0	0
			38	25	13		
8	C	1	Total	C	O	0	0
			38	25	13		

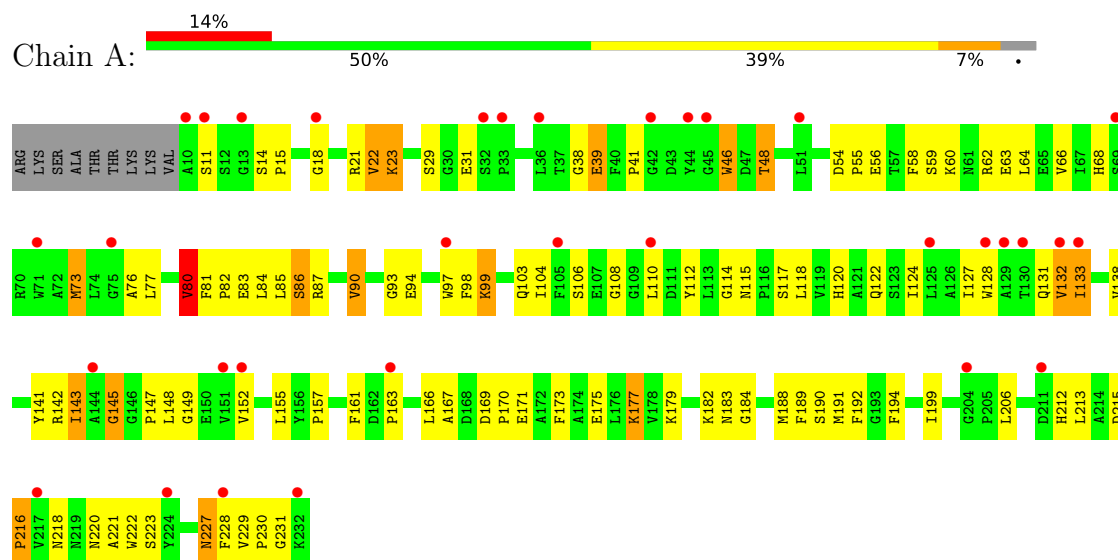
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	9	Total	O	0	0
			9	9		
9	B	7	Total	O	0	0
			7	7		
9	C	5	Total	O	0	0
			5	5		

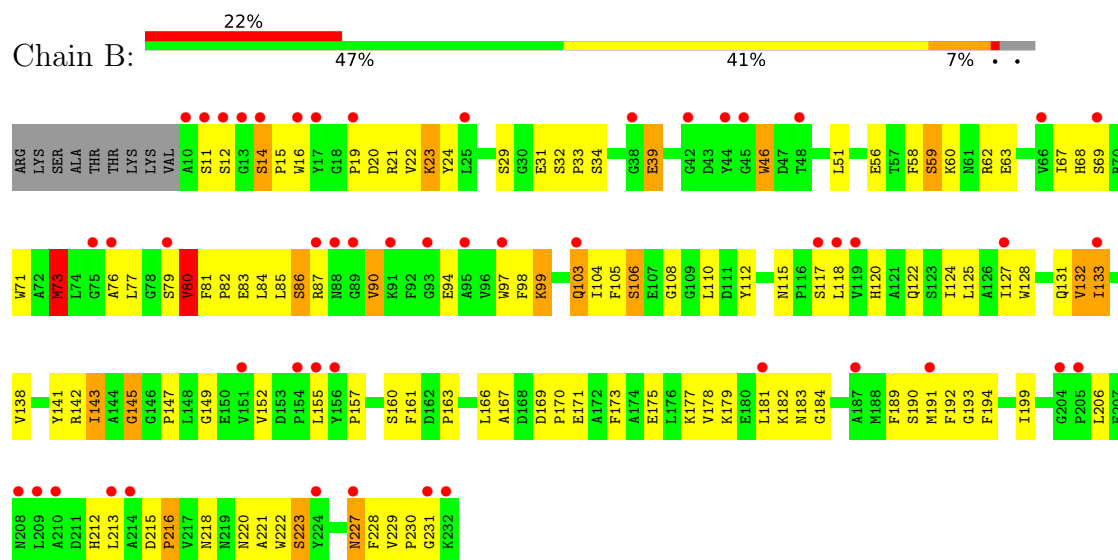
3 Residue-property plots

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: CHLOROPHYLL A-B BINDING PROTEIN AB80

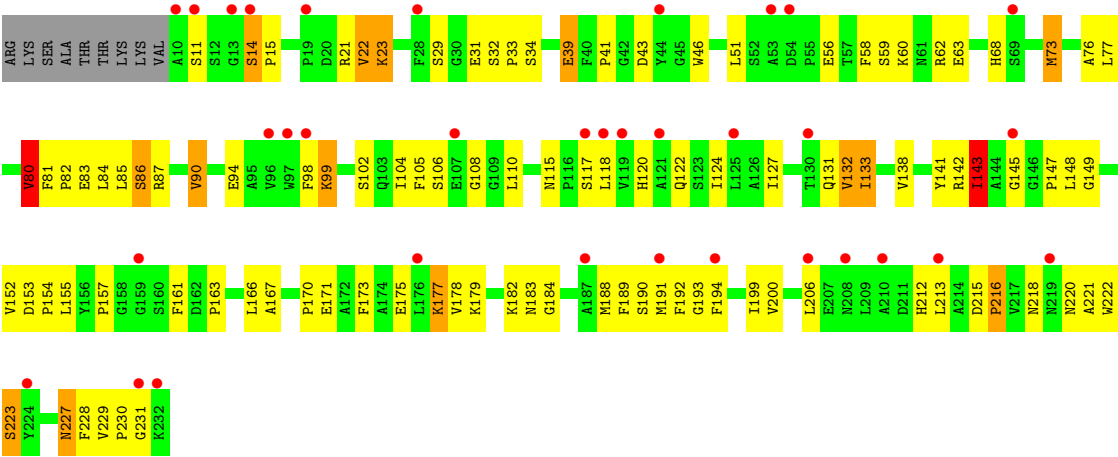


• Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80



• Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.40Å 128.00Å 62.00Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 85.7 (50.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.51Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.220 , 0.241 0.232 , 0.250	Depositor DCC
R_{free} test set	990 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å ²)	92.5	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 105.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8373	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, NEX, CHL, CLA, XAT, DGD, LUX

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	0.68	1/1735 (0.1%)	1.07	10/2363 (0.4%)
1	B	0.74	1/1735 (0.1%)	1.09	10/2363 (0.4%)
1	C	0.71	1/1735 (0.1%)	1.07	7/2363 (0.3%)
All	All	0.71	3/5205 (0.1%)	1.07	27/7089 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	MET	SD-CE	-8.90	1.57	1.79
1	B	73	MET	SD-CE	-7.88	1.59	1.79
1	A	73	MET	SD-CE	-6.99	1.62	1.79

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	GLY	N-CA-C	-9.39	102.08	111.56
1	A	80	VAL	N-CA-C	7.22	117.83	110.82
1	B	24	TYR	N-CA-C	6.71	120.56	112.38
1	A	145	GLY	N-CA-C	-6.63	103.89	111.85
1	B	145	GLY	N-CA-C	-6.62	103.90	111.85
1	B	80	VAL	N-CA-C	6.49	117.11	110.82
1	C	80	VAL	N-CA-C	6.37	117.00	110.82
1	B	227	ASN	N-CA-C	-6.31	102.03	110.55
1	B	105	PHE	N-CA-C	-6.18	105.68	113.72
1	C	105	PHE	N-CA-C	-6.05	105.86	113.72
1	C	145	GLY	N-CA-C	-5.96	104.70	111.85
1	A	97	TRP	N-CA-C	5.94	118.52	111.33
1	B	97	TRP	N-CA-C	5.91	118.20	111.11
1	B	58	PHE	N-CA-C	-5.87	104.79	111.07
1	B	143	ILE	N-CA-C	5.85	117.78	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	ASN	N-CA-C	-5.84	102.67	110.55
1	C	58	PHE	N-CA-C	-5.80	104.87	111.14
1	B	46	TRP	N-CA-C	5.71	117.96	108.20
1	A	58	PHE	N-CA-C	-5.70	104.97	111.07
1	A	68	HIS	N-CA-C	-5.63	105.22	111.36
1	A	93	GLY	N-CA-C	-5.63	105.68	112.49
1	A	46	TRP	N-CA-C	5.60	117.78	108.20
1	C	143	ILE	N-CA-C	5.24	116.71	111.00
1	C	68	HIS	N-CA-C	-5.20	105.69	111.36
1	A	227	ASN	N-CA-C	-5.14	103.74	110.53
1	B	68	HIS	N-CA-C	-5.14	105.76	111.36
1	A	143	ILE	N-CA-C	5.07	116.52	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1683	0	1601	128	0
1	B	1683	0	1601	145	0
1	C	1683	0	1601	137	0
2	A	84	0	134	44	0
2	B	84	0	134	45	0
2	C	84	0	134	46	0
3	A	44	0	56	3	0
3	B	44	0	56	3	0
3	C	44	0	56	3	0
4	A	44	0	56	18	0
4	B	44	0	56	16	0
4	C	44	0	56	16	0
5	A	490	0	508	119	0
5	B	490	0	508	139	0
5	C	490	0	508	124	0
6	A	352	0	338	109	0
6	B	352	0	338	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	352	0	338	112	0
7	A	49	0	74	12	0
7	B	49	0	74	13	0
7	C	49	0	74	13	0
8	A	38	0	40	4	0
8	B	38	0	40	2	0
8	C	38	0	40	4	0
9	A	9	0	0	1	0
9	B	7	0	0	1	0
9	C	5	0	0	1	0
All	All	8373	0	8421	964	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (964) 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)
1:A:220:ASN:HB2	5:A:608:CLA:HED1	1.24	1.14
5:A:607:CLA:H121	5:A:607:CLA:H91	1.29	1.14
5:A:605:CLA:H41	5:C:605:CLA:H51	1.29	1.13
6:A:610:CHL:H92	6:A:612:CHL:H162	1.31	1.12
5:C:602:CLA:H121	5:C:602:CLA:H91	1.21	1.11
5:C:607:CLA:H91	5:C:607:CLA:H121	1.26	1.11
5:B:602:CLA:H121	5:B:602:CLA:H91	1.19	1.09
1:C:73:MET:HG2	2:C:501:LUX:H352	1.34	1.09
5:A:602:CLA:H91	5:A:602:CLA:H121	1.22	1.08
5:B:607:CLA:H121	5:B:607:CLA:H91	1.30	1.08
1:B:220:ASN:HB2	5:B:608:CLA:HED1	1.31	1.05
6:C:610:CHL:H92	6:C:612:CHL:H162	1.36	1.05
5:A:605:CLA:H51	5:B:605:CLA:H41	1.39	1.04
5:B:605:CLA:H51	5:C:605:CLA:H41	1.39	1.04
1:A:73:MET:HG2	2:A:501:LUX:H352	1.38	1.03
6:B:612:CHL:H192	6:B:612:CHL:H152	1.40	1.03
6:B:610:CHL:H92	6:B:612:CHL:H162	1.37	1.03
1:A:118:LEU:HA	6:A:614:CHL:CED	1.89	1.03
1:B:73:MET:HG2	2:B:501:LUX:H352	1.40	1.02
5:C:606:CLA:HBB1	5:C:606:CLA:HMB1	1.41	1.01
5:A:605:CLA:H52	5:B:604:CLA:H91	1.43	1.00
1:C:83:GLU:HB3	1:C:206:LEU:HD12	1.42	1.00
1:A:194:PHE:CZ	2:A:501:LUX:H383	1.96	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:HB3	1:A:206:LEU:HD12	1.43	1.00
6:A:612:CHL:H192	6:A:612:CHL:H152	1.41	1.00
1:C:194:PHE:HZ	2:C:501:LUX:H383	1.24	1.00
1:C:194:PHE:CZ	2:C:501:LUX:H383	1.97	1.00
5:B:605:CLA:H52	5:C:604:CLA:H91	1.41	0.99
5:B:601:CLA:HBB1	5:B:601:CLA:HMB1	1.43	0.99
5:A:606:CLA:HMB1	5:A:606:CLA:HBB1	1.44	0.99
1:C:118:LEU:HA	6:C:614:CHL:CED	1.92	0.98
1:B:118:LEU:HA	6:B:614:CHL:CED	1.93	0.98
1:C:220:ASN:HB2	5:C:608:CLA:HED1	1.45	0.98
6:A:610:CHL:H142	6:A:612:CHL:H72	1.43	0.98
6:A:610:CHL:HBA1	1:B:229:VAL:HG22	1.45	0.97
1:C:132:VAL:HG12	1:C:133:ILE:HD13	1.46	0.97
6:C:612:CHL:H192	6:C:612:CHL:H152	1.42	0.97
5:B:604:CLA:HBB1	5:B:604:CLA:HMB1	1.47	0.97
1:B:83:GLU:HB3	1:B:206:LEU:HD12	1.42	0.97
5:B:606:CLA:HMB1	5:B:606:CLA:HBB1	1.43	0.97
1:B:132:VAL:HG12	1:B:133:ILE:HD13	1.45	0.96
1:B:194:PHE:HZ	2:B:501:LUX:H383	1.29	0.96
5:C:604:CLA:HBB1	5:C:604:CLA:HMB1	1.48	0.96
1:B:194:PHE:CZ	2:B:501:LUX:H383	2.01	0.96
1:A:194:PHE:HZ	2:A:501:LUX:H383	1.25	0.95
5:B:602:CLA:H141	5:B:607:CLA:H112	1.48	0.95
5:A:604:CLA:H91	5:C:605:CLA:H52	1.48	0.95
6:A:610:CHL:H201	6:B:609:CHL:H62	1.48	0.95
5:A:604:CLA:HMB1	5:A:604:CLA:HBB1	1.47	0.95
5:B:602:CLA:H121	5:B:602:CLA:C9	1.95	0.94
5:C:602:CLA:H121	5:C:602:CLA:C9	1.97	0.94
6:C:611:CHL:H151	6:C:611:CHL:H192	1.50	0.94
5:A:603:CLA:HBB1	5:A:603:CLA:HMB1	1.48	0.93
1:C:14:SER:HB2	1:C:15:PRO:HD2	1.47	0.93
6:B:610:CHL:H142	6:B:612:CHL:H72	1.46	0.93
6:B:610:CHL:HBA1	1:C:229:VAL:HG22	1.48	0.93
6:B:611:CHL:H151	6:B:611:CHL:H192	1.52	0.92
2:C:501:LUX:H373	5:C:603:CLA:C2B	2.00	0.92
5:B:607:CLA:H92	5:B:607:CLA:H52	1.48	0.91
2:A:501:LUX:H373	5:A:603:CLA:C2B	2.01	0.91
5:C:603:CLA:HBB1	5:C:603:CLA:HMB1	1.50	0.91
6:A:609:CHL:H62	6:C:610:CHL:H201	1.52	0.91
6:C:610:CHL:H142	6:C:612:CHL:H72	1.50	0.91
5:A:602:CLA:H121	5:A:602:CLA:C9	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PHE:HB3	1:A:82:PRO:HD3	1.53	0.90
5:A:607:CLA:H92	5:A:607:CLA:H52	1.53	0.89
6:A:613:CHL:HMB1	6:A:613:CHL:HBB1	1.52	0.89
5:C:607:CLA:H92	5:C:607:CLA:H52	1.51	0.89
1:B:14:SER:HB2	1:B:15:PRO:HD2	1.53	0.89
6:B:613:CHL:HBB1	6:B:613:CHL:HMB1	1.52	0.89
2:B:501:LUX:H373	5:B:603:CLA:C2B	2.02	0.89
6:C:611:CHL:H192	6:C:611:CHL:HAA2	1.54	0.89
6:C:613:CHL:HBB1	6:C:613:CHL:HMB1	1.53	0.88
1:A:14:SER:HB2	1:A:15:PRO:HD2	1.55	0.88
5:A:601:CLA:HBB1	5:A:601:CLA:HMB1	1.53	0.88
8:B:802:DGD:HD61	8:B:802:DGD:O2E	1.73	0.88
1:A:220:ASN:CB	5:A:608:CLA:HED1	2.03	0.87
5:B:607:CLA:H91	5:B:607:CLA:C12	2.05	0.87
1:A:73:MET:HE3	1:A:184:GLY:N	1.90	0.87
6:A:610:CHL:C9	6:A:612:CHL:H162	2.05	0.87
1:C:163:PRO:HD2	2:C:501:LUX:H3	1.55	0.87
5:A:607:CLA:H91	5:A:607:CLA:C12	2.06	0.86
1:C:81:PHE:HB3	1:C:82:PRO:HD3	1.58	0.86
5:A:605:CLA:C19	6:A:612:CHL:H71	2.06	0.86
1:B:104:ILE:HD12	1:B:127:ILE:HD12	1.54	0.86
1:A:132:VAL:HG12	1:A:133:ILE:HD13	1.58	0.86
5:C:607:CLA:H121	5:C:607:CLA:C9	2.05	0.85
8:A:802:DGD:O2E	8:A:802:DGD:HD61	1.73	0.85
1:B:220:ASN:CB	5:B:608:CLA:HED1	2.06	0.85
1:A:229:VAL:HG22	6:C:610:CHL:HBA1	1.57	0.85
5:B:603:CLA:HBB1	5:B:603:CLA:HMB1	1.56	0.85
6:B:610:CHL:H201	6:C:609:CHL:H62	1.59	0.85
5:A:602:CLA:HHC	5:A:602:CLA:HBB1	1.59	0.84
1:A:118:LEU:HA	6:A:614:CHL:HED1	1.59	0.84
5:C:601:CLA:HBB1	5:C:601:CLA:HMB1	1.58	0.84
1:B:163:PRO:HD2	2:B:501:LUX:H3	1.58	0.84
1:B:118:LEU:HA	6:B:614:CHL:HED2	1.59	0.84
5:B:602:CLA:HHC	5:B:602:CLA:HBB1	1.59	0.84
6:A:611:CHL:H151	6:A:611:CHL:H192	1.59	0.84
6:C:610:CHL:C9	6:C:612:CHL:H162	2.07	0.84
1:A:104:ILE:HD12	1:A:127:ILE:HD12	1.60	0.84
5:A:602:CLA:H141	5:A:607:CLA:H112	1.58	0.84
1:B:192:PHE:CE2	5:B:604:CLA:H171	2.13	0.84
5:C:607:CLA:H91	5:C:607:CLA:C12	2.08	0.84
1:C:104:ILE:HD12	1:C:127:ILE:HD12	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:610:CHL:C9	6:B:612:CHL:H162	2.07	0.83
1:A:163:PRO:HD2	2:A:501:LUX:H3	1.61	0.83
1:B:14:SER:HB2	1:B:15:PRO:CD	2.07	0.83
8:C:802:DGD:O2E	8:C:802:DGD:HD61	1.76	0.83
1:A:14:SER:HB2	1:A:15:PRO:CD	2.08	0.82
1:C:14:SER:HB2	1:C:15:PRO:CD	2.07	0.82
1:B:81:PHE:HB3	1:B:82:PRO:HD3	1.62	0.82
1:C:85:LEU:HB3	1:C:90:VAL:HG21	1.61	0.82
1:C:73:MET:HE3	1:C:184:GLY:N	1.94	0.82
1:C:118:LEU:HD13	5:C:606:CLA:C12	2.10	0.82
5:A:605:CLA:H191	6:A:612:CHL:H71	1.63	0.81
5:B:604:CLA:HBB1	5:B:604:CLA:CMB	2.10	0.81
5:B:605:CLA:C19	6:B:612:CHL:H71	2.11	0.81
5:C:604:CLA:HBB1	5:C:604:CLA:CMB	2.11	0.81
6:B:609:CHL:H141	6:B:609:CHL:H172	1.62	0.80
6:A:610:CHL:CBA	1:B:229:VAL:HG22	2.11	0.80
5:A:604:CLA:HBB1	5:A:604:CLA:CMB	2.12	0.80
1:B:122:GLN:HB2	6:B:614:CHL:CBB	2.12	0.80
1:C:118:LEU:HA	6:C:614:CHL:HED2	1.62	0.80
6:A:611:CHL:H192	6:A:611:CHL:HAA2	1.62	0.80
1:C:117:SER:O	6:C:614:CHL:HED2	1.82	0.80
5:C:606:CLA:HBB1	5:C:606:CLA:CMB	2.10	0.79
1:A:118:LEU:HA	6:A:614:CHL:HED2	1.62	0.79
1:B:73:MET:HE3	1:B:184:GLY:N	1.98	0.79
4:B:504:XAT:O4	6:B:609:CHL:H192	1.82	0.79
5:C:602:CLA:HHC	5:C:602:CLA:HBB1	1.63	0.79
4:A:504:XAT:O4	6:A:609:CHL:H192	1.82	0.79
1:B:132:VAL:HG12	1:B:133:ILE:CD1	2.12	0.79
5:B:601:CLA:HBB1	5:B:601:CLA:CMB	2.12	0.79
1:A:117:SER:O	6:A:614:CHL:HED2	1.83	0.79
5:A:607:CLA:H121	5:A:607:CLA:C9	2.09	0.79
5:B:605:CLA:H191	6:B:612:CHL:H71	1.65	0.79
1:C:220:ASN:CB	5:C:608:CLA:HED1	2.13	0.79
5:B:606:CLA:HBB1	5:B:606:CLA:CMB	2.12	0.79
1:A:85:LEU:HB3	1:A:90:VAL:HG21	1.66	0.78
1:A:192:PHE:CD2	5:A:604:CLA:H18	2.18	0.78
6:A:609:CHL:H141	6:A:609:CHL:H172	1.66	0.78
5:B:601:CLA:C9	5:B:601:CLA:H122	2.14	0.78
6:B:611:CHL:H192	6:B:611:CHL:HAA2	1.65	0.78
1:C:192:PHE:CD2	5:C:604:CLA:H18	2.19	0.78
1:C:118:LEU:HA	6:C:614:CHL:HED1	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:HB3	1:B:90:VAL:HG21	1.66	0.77
5:C:605:CLA:C19	6:C:612:CHL:H71	2.15	0.77
5:A:603:CLA:HBB1	5:A:603:CLA:CMB	2.14	0.77
5:B:602:CLA:OBD	5:B:607:CLA:HBA2	1.84	0.77
1:C:192:PHE:CE2	5:C:604:CLA:H171	2.20	0.77
1:A:229:VAL:HG22	6:C:610:CHL:CBA	2.15	0.76
2:B:502:LUX:H362	5:B:606:CLA:HMB3	1.67	0.76
6:B:613:CHL:HBB1	6:B:613:CHL:CMB	2.16	0.76
2:C:502:LUX:H362	5:C:606:CLA:HMB3	1.68	0.76
4:C:504:XAT:O4	6:C:609:CHL:H192	1.86	0.76
6:C:613:CHL:HBB1	6:C:613:CHL:CMB	2.16	0.76
2:A:502:LUX:H362	5:A:606:CLA:HMB3	1.68	0.75
1:A:118:LEU:HD13	5:A:606:CLA:C12	2.16	0.75
2:A:501:LUX:H373	5:A:603:CLA:CMB	2.16	0.75
5:C:603:CLA:HBB1	5:C:603:CLA:CMB	2.15	0.75
6:A:613:CHL:HBB1	6:A:613:CHL:CMB	2.15	0.75
6:C:609:CHL:H172	6:C:609:CHL:H141	1.67	0.75
1:B:118:LEU:HD13	5:B:606:CLA:C12	2.17	0.75
5:B:608:CLA:HHC	5:B:608:CLA:HBB1	1.69	0.75
1:C:132:VAL:HG12	1:C:133:ILE:CD1	2.16	0.75
5:B:601:CLA:H92	5:B:601:CLA:C12	2.17	0.74
5:B:605:CLA:H92	5:B:605:CLA:H121	1.70	0.74
6:B:610:CHL:CBA	1:C:229:VAL:HG22	2.17	0.74
5:A:606:CLA:HBB1	5:A:606:CLA:CMB	2.14	0.74
5:A:601:CLA:C9	5:A:601:CLA:H122	2.17	0.74
4:B:504:XAT:H242	6:B:609:CHL:CMC	2.18	0.74
4:B:504:XAT:H361	7:B:801:LHG:HC92	1.69	0.74
6:C:611:CHL:HHC	6:C:611:CHL:HBB1	1.67	0.74
6:A:610:CHL:H201	6:B:609:CHL:C6	2.17	0.74
6:B:612:CHL:HHC	6:B:612:CHL:HBB1	1.69	0.74
5:C:602:CLA:OBD	5:C:607:CLA:HBA2	1.87	0.74
1:B:192:PHE:CD2	5:B:604:CLA:H18	2.22	0.74
2:B:501:LUX:C28	2:B:501:LUX:H381	2.17	0.74
5:A:601:CLA:HBB1	5:A:601:CLA:CMB	2.17	0.73
6:A:609:CHL:HBC2	6:A:609:CHL:HHD	1.70	0.73
6:C:611:CHL:H151	6:C:611:CHL:C19	2.17	0.73
1:B:118:LEU:HA	6:B:614:CHL:HED1	1.71	0.73
6:B:609:CHL:HHC	6:B:609:CHL:HBB1	1.70	0.73
2:C:501:LUX:H122	5:C:601:CLA:HHC	1.71	0.73
2:B:501:LUX:H122	5:B:601:CLA:HHC	1.71	0.73
4:C:504:XAT:H242	6:C:609:CHL:CMC	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:601:CLA:H122	5:B:601:CLA:H92	1.71	0.73
1:C:73:MET:HG2	2:C:501:LUX:C35	2.13	0.73
1:B:73:MET:HG2	2:B:501:LUX:C35	2.18	0.72
1:A:192:PHE:CE2	5:A:604:CLA:H171	2.24	0.72
1:A:73:MET:HG2	2:A:501:LUX:C35	2.18	0.72
2:A:501:LUX:H122	5:A:601:CLA:HHC	1.72	0.72
4:A:504:XAT:H242	6:A:609:CHL:CMC	2.20	0.72
1:A:222:TRP:CH2	6:C:610:CHL:HBC2	2.25	0.71
1:A:122:GLN:HB2	6:A:614:CHL:CBB	2.20	0.71
2:A:501:LUX:C28	2:A:501:LUX:H381	2.19	0.71
6:C:609:CHL:H142	6:C:609:CHL:H101	1.72	0.71
5:A:603:CLA:CHB	5:A:608:CLA:HMD3	2.20	0.71
6:B:611:CHL:HHC	6:B:611:CHL:HBB1	1.72	0.71
5:A:605:CLA:H121	5:A:605:CLA:H92	1.71	0.71
5:B:602:CLA:C14	5:B:607:CLA:H112	2.19	0.71
5:B:603:CLA:H172	5:B:608:CLA:HBA1	1.71	0.71
5:C:605:CLA:H191	6:C:612:CHL:H71	1.72	0.71
2:A:502:LUX:C36	5:A:606:CLA:HMB3	2.20	0.71
2:C:501:LUX:H373	5:C:603:CLA:CMB	2.19	0.71
2:C:502:LUX:H373	5:C:606:CLA:C2B	2.20	0.71
6:A:609:CHL:H101	6:A:609:CHL:H142	1.72	0.71
6:A:611:CHL:HHC	6:A:611:CHL:HBB1	1.72	0.71
1:B:117:SER:O	6:B:614:CHL:HED2	1.90	0.71
1:C:94:GLU:HG2	1:C:99:LYS:HB3	1.70	0.71
5:A:607:CLA:C12	5:A:607:CLA:C9	2.68	0.71
6:A:610:CHL:C14	6:A:612:CHL:H72	2.21	0.70
2:B:501:LUX:H373	5:B:603:CLA:CMB	2.21	0.70
5:A:602:CLA:OBD	5:A:607:CLA:HBA2	1.90	0.70
1:A:167:ALA:HB1	1:A:173:PHE:CD1	2.26	0.70
1:B:73:MET:HE3	1:B:183:ASN:C	2.16	0.70
1:B:166:LEU:HD12	2:B:501:LUX:O3	1.92	0.70
6:B:611:CHL:H151	6:B:611:CHL:C19	2.22	0.70
2:C:501:LUX:C28	2:C:501:LUX:H381	2.21	0.70
5:C:607:CLA:HHC	5:C:607:CLA:HBB1	1.73	0.70
6:A:609:CHL:C6	6:C:610:CHL:H201	2.22	0.70
5:B:603:CLA:HBB1	5:B:603:CLA:CMB	2.21	0.70
5:B:605:CLA:HHC	5:B:605:CLA:HBB1	1.74	0.70
6:A:612:CHL:HHC	6:A:612:CHL:HBB1	1.73	0.70
5:A:602:CLA:OBD	5:A:607:CLA:HBD	1.91	0.70
5:A:605:CLA:C4	5:C:605:CLA:H51	2.16	0.70
5:C:601:CLA:C9	5:C:601:CLA:H122	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HD22	5:B:606:CLA:C12	2.22	0.69
5:A:601:CLA:H92	5:A:601:CLA:C12	2.23	0.69
1:C:167:ALA:HB1	1:C:173:PHE:CD1	2.27	0.69
1:A:73:MET:HE3	1:A:183:ASN:C	2.18	0.69
1:C:142:ARG:NH2	6:C:612:CHL:O1D	2.24	0.69
5:B:607:CLA:C12	5:B:607:CLA:C9	2.68	0.69
2:C:501:LUX:C24	2:C:501:LUX:H363	2.22	0.69
2:A:501:LUX:H363	2:A:501:LUX:C24	2.21	0.69
2:B:502:LUX:C36	5:B:606:CLA:HMB3	2.23	0.69
1:A:142:ARG:NH2	6:A:612:CHL:O1D	2.19	0.69
5:A:602:CLA:H91	5:A:602:CLA:C12	2.12	0.69
1:C:131:GLN:HE22	6:C:610:CHL:HMC	1.58	0.69
2:C:502:LUX:C36	5:C:606:CLA:HMB3	2.22	0.69
1:A:132:VAL:HG12	1:A:133:ILE:CD1	2.22	0.69
5:B:604:CLA:H41	5:B:605:CLA:HBA1	1.75	0.69
1:C:73:MET:HE3	1:C:183:ASN:C	2.18	0.68
1:A:86:SER:HA	1:A:90:VAL:O	1.93	0.68
3:A:503:NEX:H403	6:A:613:CHL:O1A	1.93	0.68
6:C:609:CHL:HHC	6:C:609:CHL:HBB1	1.75	0.68
5:B:601:CLA:C9	5:B:601:CLA:C12	2.72	0.68
5:B:602:CLA:OBD	5:B:607:CLA:HBD	1.94	0.68
1:C:122:GLN:HB2	6:C:614:CHL:CBB	2.24	0.68
5:C:601:CLA:C12	5:C:601:CLA:H92	2.24	0.68
1:A:131:GLN:HE22	6:A:610:CHL:HMC	1.59	0.68
5:A:602:CLA:C14	5:A:607:CLA:H112	2.23	0.68
5:C:605:CLA:H121	5:C:605:CLA:H92	1.76	0.68
1:C:166:LEU:HD12	2:C:501:LUX:O3	1.94	0.68
2:B:501:LUX:H363	2:B:501:LUX:C24	2.24	0.67
1:A:213:LEU:HD21	5:A:608:CLA:CHC	2.25	0.67
4:A:504:XAT:H361	7:A:801:LHG:HC92	1.75	0.67
4:C:504:XAT:H361	7:C:801:LHG:HC92	1.74	0.67
5:C:605:CLA:C15	5:C:605:CLA:H192	2.25	0.67
5:B:604:CLA:H41	5:B:605:CLA:CBA	2.24	0.67
5:B:607:CLA:HHC	5:B:607:CLA:HBB1	1.76	0.67
5:C:607:CLA:H92	5:C:607:CLA:C5	2.24	0.67
1:B:131:GLN:HE22	6:B:610:CHL:HMC	1.59	0.67
5:B:605:CLA:H152	5:B:605:CLA:H192	1.77	0.67
6:B:609:CHL:H101	6:B:609:CHL:H142	1.77	0.67
5:A:605:CLA:HHC	5:A:605:CLA:HBB1	1.75	0.67
1:B:131:GLN:HE22	6:B:610:CHL:CMC	2.07	0.67
1:B:63:GLU:HA	1:B:155:LEU:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:609:CHL:HBC2	6:C:609:CHL:HHD	1.77	0.67
5:A:601:CLA:H122	5:A:601:CLA:H92	1.77	0.66
6:A:610:CHL:HHC	6:A:610:CHL:HBB1	1.76	0.66
1:C:131:GLN:HE22	6:C:610:CHL:CMC	2.07	0.66
1:A:63:GLU:HA	1:A:155:LEU:HD11	1.77	0.66
6:B:610:CHL:C14	6:B:612:CHL:H72	2.24	0.66
1:C:22:VAL:CG2	6:C:609:CHL:HBC3	2.26	0.66
5:B:605:CLA:H192	5:B:605:CLA:C15	2.25	0.66
5:C:602:CLA:H141	5:C:607:CLA:H112	1.77	0.66
6:B:610:CHL:H201	6:C:609:CHL:H8	1.77	0.66
2:B:502:LUX:H373	5:B:606:CLA:C2B	2.26	0.66
5:C:603:CLA:H172	5:C:608:CLA:HBA1	1.77	0.66
6:C:612:CHL:HHC	6:C:612:CHL:HBB1	1.77	0.66
1:B:22:VAL:CG2	6:B:609:CHL:HBC3	2.26	0.66
1:B:142:ARG:NH2	6:B:612:CHL:O1D	2.22	0.66
5:B:602:CLA:H91	5:B:602:CLA:C12	2.13	0.66
6:B:610:CHL:H201	6:C:609:CHL:C6	2.26	0.66
5:C:603:CLA:CHB	5:C:608:CLA:HMD3	2.26	0.66
3:C:503:NEX:H403	6:C:613:CHL:O1A	1.95	0.66
1:A:131:GLN:HE22	6:A:610:CHL:CMC	2.09	0.65
5:C:601:CLA:HBB1	5:C:601:CLA:CMB	2.25	0.65
1:B:80:VAL:HG12	1:B:81:PHE:N	2.11	0.65
6:A:609:CHL:HHC	6:A:609:CHL:HBB1	1.78	0.65
6:B:610:CHL:HBC2	1:C:222:TRP:CH2	2.31	0.65
1:C:73:MET:HE2	1:C:183:ASN:HB3	1.78	0.65
5:C:608:CLA:HHC	5:C:608:CLA:HBB1	1.77	0.65
6:A:610:CHL:HBA1	1:B:229:VAL:CG2	2.23	0.65
3:B:503:NEX:H403	6:B:613:CHL:O1A	1.96	0.65
6:B:612:CHL:HBC1	6:B:613:CHL:HBB2	1.78	0.65
1:A:80:VAL:HG12	1:A:81:PHE:N	2.11	0.65
5:A:607:CLA:H92	5:A:607:CLA:C5	2.25	0.65
5:B:605:CLA:C12	5:B:605:CLA:C9	2.75	0.65
6:C:612:CHL:H192	6:C:612:CHL:C15	2.21	0.65
6:A:609:CHL:H41	7:A:801:LHG:H162	1.79	0.65
1:B:167:ALA:HB1	1:B:173:PHE:CD1	2.31	0.65
6:C:610:CHL:C14	6:C:612:CHL:H72	2.26	0.65
1:B:104:ILE:CD1	1:B:127:ILE:HD12	2.25	0.64
5:A:601:CLA:C9	5:A:601:CLA:C12	2.74	0.64
1:A:213:LEU:HD11	5:A:608:CLA:HMC2	1.78	0.64
1:B:149:GLY:O	6:B:611:CHL:HMC	1.97	0.64
5:A:607:CLA:HHC	5:A:607:CLA:HBB1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:608:CLA:HHC	5:A:608:CLA:HBB1	1.79	0.64
6:B:612:CHL:H192	6:B:612:CHL:C15	2.24	0.64
4:C:504:XAT:H403	7:C:801:LHG:H121	1.79	0.64
5:C:601:CLA:H111	5:C:601:CLA:H162	1.80	0.64
6:C:610:CHL:HBB2	6:C:612:CHL:HBC1	1.78	0.64
5:B:606:CLA:HMB1	5:B:606:CLA:CBB	2.26	0.64
5:C:601:CLA:H122	5:C:601:CLA:H92	1.80	0.64
1:A:104:ILE:HD12	1:A:127:ILE:CD1	2.28	0.63
2:A:502:LUX:H193	5:A:604:CLA:H141	1.80	0.63
1:B:73:MET:HG2	2:B:501:LUX:H142	1.80	0.63
5:C:605:CLA:HHC	5:C:605:CLA:HBB1	1.80	0.63
1:B:213:LEU:HD21	5:B:608:CLA:CHC	2.27	0.63
6:B:610:CHL:HHC	6:B:610:CHL:HBB1	1.80	0.63
4:C:504:XAT:H3	6:C:609:CHL:C19	2.29	0.63
2:A:502:LUX:H321	5:A:605:CLA:HMC2	1.80	0.63
4:B:504:XAT:H371	7:B:801:LHG:H362	1.81	0.63
6:C:610:CHL:HHC	6:C:610:CHL:HBB1	1.80	0.63
5:B:603:CLA:CHB	5:B:608:CLA:HMD3	2.29	0.63
1:A:118:LEU:HD22	5:A:606:CLA:C12	2.29	0.62
1:B:115:ASN:HB3	1:B:118:LEU:HD12	1.80	0.62
2:C:501:LUX:H101	5:C:601:CLA:H72	1.80	0.62
1:B:94:GLU:HG2	1:B:99:LYS:HB3	1.80	0.62
2:B:502:LUX:C24	2:B:502:LUX:H363	2.29	0.62
5:B:605:CLA:H92	5:B:605:CLA:C12	2.29	0.62
5:C:602:CLA:OBD	5:C:607:CLA:HBD	1.99	0.62
2:B:502:LUX:H102	5:B:604:CLA:CHC	2.29	0.62
1:C:213:LEU:HD21	5:C:608:CLA:CHC	2.28	0.62
1:A:166:LEU:HD12	2:A:501:LUX:O3	2.00	0.62
1:C:94:GLU:HG2	1:C:99:LYS:CB	2.30	0.62
1:A:115:ASN:HB3	1:A:118:LEU:HD12	1.81	0.62
1:C:133:ILE:HD13	1:C:133:ILE:N	2.15	0.62
5:C:605:CLA:H192	5:C:605:CLA:H152	1.81	0.62
1:C:84:LEU:CD2	5:C:607:CLA:H191	2.30	0.62
2:C:502:LUX:H381	2:C:502:LUX:C28	2.30	0.62
1:C:21:ARG:HG2	1:C:21:ARG:HH11	1.64	0.62
5:A:605:CLA:H192	5:A:605:CLA:C15	2.30	0.61
1:C:86:SER:HA	1:C:90:VAL:O	2.00	0.61
5:C:601:CLA:C9	5:C:601:CLA:C12	2.77	0.61
2:A:501:LUX:H101	5:A:601:CLA:H72	1.83	0.61
5:B:604:CLA:HMB1	5:B:604:CLA:CBB	2.27	0.61
1:A:81:PHE:HB3	1:A:82:PRO:CD	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:604:CLA:HMB1	5:A:604:CLA:CBB	2.27	0.61
1:B:94:GLU:HG2	1:B:99:LYS:CB	2.30	0.61
5:C:602:CLA:C9	5:C:602:CLA:C12	2.78	0.61
5:C:605:CLA:C12	5:C:605:CLA:C9	2.78	0.61
5:B:601:CLA:H162	5:B:601:CLA:H111	1.82	0.61
5:C:607:CLA:C9	5:C:607:CLA:C12	2.70	0.61
6:A:611:CHL:H151	6:A:611:CHL:C19	2.28	0.61
5:C:605:CLA:H92	5:C:605:CLA:C12	2.30	0.61
1:A:229:VAL:CG2	6:C:610:CHL:HBA1	2.29	0.61
2:A:502:LUX:H363	2:A:502:LUX:C24	2.30	0.61
5:A:605:CLA:C12	5:A:605:CLA:C9	2.78	0.61
5:B:604:CLA:H142	5:B:604:CLA:H101	1.82	0.61
5:B:606:CLA:H102	6:B:614:CHL:CED	2.30	0.61
5:B:608:CLA:HBC2	5:B:608:CLA:HHD	1.83	0.61
1:A:222:TRP:HH2	6:C:610:CHL:HBC2	1.63	0.61
2:A:501:LUX:H381	2:A:501:LUX:H281	1.82	0.61
2:A:501:LUX:H101	5:A:601:CLA:H52	1.82	0.61
6:A:610:CHL:HBC2	1:B:222:TRP:CH2	2.35	0.61
1:A:73:MET:HE2	1:A:183:ASN:HB3	1.82	0.60
2:A:502:LUX:C28	2:A:502:LUX:H381	2.32	0.60
2:A:502:LUX:H373	5:A:606:CLA:C2B	2.31	0.60
1:C:81:PHE:HB3	1:C:82:PRO:CD	2.31	0.60
4:A:504:XAT:H371	7:A:801:LHG:H362	1.84	0.60
5:A:605:CLA:H192	5:A:605:CLA:H152	1.83	0.60
5:B:607:CLA:H92	5:B:607:CLA:C5	2.25	0.60
1:B:133:ILE:HD13	1:B:133:ILE:N	2.16	0.60
1:C:149:GLY:O	6:C:611:CHL:HMC	2.02	0.60
4:A:504:XAT:H3	6:A:609:CHL:C19	2.31	0.60
5:B:601:CLA:HMB1	5:B:601:CLA:CBB	2.25	0.60
1:C:63:GLU:HA	1:C:155:LEU:HD11	1.81	0.60
1:C:83:GLU:CD	1:C:206:LEU:HB2	2.26	0.60
1:C:80:VAL:HG12	1:C:81:PHE:N	2.17	0.59
1:A:73:MET:HE2	1:A:183:ASN:CB	2.32	0.59
1:A:216:PRO:HB3	5:A:608:CLA:C1B	2.32	0.59
5:C:606:CLA:H102	6:C:614:CHL:HED1	1.84	0.59
1:B:73:MET:CG	2:B:501:LUX:H352	2.23	0.59
1:B:104:ILE:HD12	1:B:127:ILE:CD1	2.28	0.59
1:A:98:PHE:HB2	6:A:610:CHL:HMA1	1.84	0.59
1:B:86:SER:HA	1:B:90:VAL:O	2.03	0.59
5:B:602:CLA:C9	5:B:602:CLA:C12	2.76	0.59
5:C:606:CLA:H91	6:C:614:CHL:O2D	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:602:CLA:HMD3	5:A:607:CLA:C4D	2.33	0.59
6:B:610:CHL:HBA1	1:C:229:VAL:CG2	2.27	0.59
1:B:108:GLY:O	1:B:122:GLN:NE2	2.32	0.59
1:C:73:MET:HE2	1:C:183:ASN:CB	2.32	0.59
1:B:182:LYS:HE2	5:B:607:CLA:O1D	2.03	0.59
6:A:610:CHL:H72	6:A:612:CHL:H172	1.84	0.58
1:B:84:LEU:CD2	5:B:607:CLA:H191	2.33	0.58
5:C:604:CLA:H101	5:C:604:CLA:H142	1.85	0.58
5:A:604:CLA:H101	5:A:604:CLA:H142	1.86	0.58
1:A:22:VAL:CG2	6:A:609:CHL:HBC3	2.33	0.58
5:A:603:CLA:H172	5:A:608:CLA:HBA1	1.84	0.58
6:C:611:CHL:HAA2	6:C:611:CHL:C19	2.28	0.58
1:A:94:GLU:HG2	1:A:99:LYS:HB3	1.84	0.58
2:C:502:LUX:H363	2:C:502:LUX:C24	2.34	0.58
1:A:83:GLU:CD	1:A:206:LEU:HB2	2.27	0.58
5:C:604:CLA:HMB1	5:C:604:CLA:CBB	2.27	0.58
1:A:84:LEU:CD2	5:A:607:CLA:H191	2.34	0.58
1:A:104:ILE:CD1	1:A:127:ILE:HD12	2.33	0.58
1:A:182:LYS:NZ	7:A:801:LHG:O4	2.31	0.58
5:B:606:CLA:H91	6:B:614:CHL:O2D	2.04	0.58
1:C:104:ILE:CD1	1:C:127:ILE:HD12	2.32	0.58
5:C:606:CLA:HMB1	5:C:606:CLA:CBB	2.24	0.58
6:C:610:CHL:H72	6:C:612:CHL:H172	1.86	0.58
5:A:605:CLA:H92	5:A:605:CLA:C12	2.32	0.58
2:B:501:LUX:H381	2:B:501:LUX:H281	1.84	0.58
6:B:609:CHL:HBC2	6:B:609:CHL:HHD	1.86	0.58
6:B:610:CHL:HBB2	6:B:612:CHL:HBC1	1.86	0.58
1:C:115:ASN:HB3	1:C:118:LEU:HD12	1.86	0.58
2:C:502:LUX:H122	5:C:604:CLA:HHC	1.86	0.58
4:B:504:XAT:H3	6:B:609:CHL:C19	2.34	0.57
6:A:611:CHL:HAA2	6:A:611:CHL:C19	2.33	0.57
1:A:133:ILE:HD13	1:A:133:ILE:N	2.18	0.57
1:B:21:ARG:HH11	1:B:21:ARG:HG2	1.68	0.57
5:A:602:CLA:C9	5:A:602:CLA:C12	2.78	0.57
5:B:601:CLA:HBC1	6:B:611:CHL:H201	1.86	0.57
1:C:220:ASN:CG	5:C:608:CLA:HED1	2.29	0.57
5:B:603:CLA:H172	5:B:608:CLA:CBA	2.35	0.57
1:C:98:PHE:HB2	6:C:610:CHL:HMA1	1.86	0.57
5:B:606:CLA:H102	6:B:614:CHL:HED1	1.85	0.57
1:B:73:MET:HG2	2:B:501:LUX:C15	2.34	0.57
5:C:607:CLA:C4C	7:C:801:LHG:HC61	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HB3	1:A:90:VAL:CG2	2.34	0.57
1:A:149:GLY:O	6:A:611:CHL:HMC	2.04	0.57
6:B:610:CHL:HBC2	1:C:222:TRP:HH2	1.69	0.57
6:A:610:CHL:HBB2	6:A:612:CHL:HBC1	1.86	0.57
1:A:194:PHE:CE1	2:A:501:LUX:H383	2.38	0.56
6:A:610:CHL:H201	6:B:609:CHL:H8	1.87	0.56
2:B:502:LUX:C28	2:B:502:LUX:H381	2.35	0.56
2:B:502:LUX:H193	5:B:604:CLA:H141	1.86	0.56
6:B:613:CHL:HMB1	6:B:613:CHL:CBB	2.31	0.56
6:B:610:CHL:H201	6:C:609:CHL:C8	2.34	0.56
2:A:502:LUX:H122	5:A:604:CLA:HHC	1.88	0.56
5:A:605:CLA:H51	5:B:605:CLA:C4	2.26	0.56
1:B:147:PRO:HG2	6:B:611:CHL:HBB2	1.88	0.56
2:B:501:LUX:H101	5:B:601:CLA:H52	1.87	0.56
2:B:501:LUX:H101	5:B:601:CLA:H72	1.86	0.56
5:C:606:CLA:H102	6:C:614:CHL:CED	2.35	0.56
1:C:22:VAL:HG22	6:C:609:CHL:HBC3	1.87	0.56
1:C:73:MET:HG2	2:C:501:LUX:C15	2.35	0.56
2:C:501:LUX:H381	2:C:501:LUX:H281	1.86	0.56
1:A:22:VAL:HG22	6:A:609:CHL:HBC3	1.88	0.56
5:B:607:CLA:C4C	7:B:801:LHG:HC61	2.35	0.56
1:C:85:LEU:HB3	1:C:90:VAL:CG2	2.33	0.56
2:C:502:LUX:H102	5:C:604:CLA:CHC	2.36	0.56
1:B:216:PRO:HB3	5:B:608:CLA:C1B	2.36	0.56
2:C:502:LUX:H373	5:C:606:CLA:C3B	2.36	0.56
2:A:502:LUX:H102	5:A:604:CLA:CHC	2.35	0.55
6:B:609:CHL:H41	7:B:801:LHG:H162	1.88	0.55
1:C:147:PRO:HG2	6:C:611:CHL:HBB2	1.88	0.55
1:C:182:LYS:NZ	7:C:801:LHG:O4	2.35	0.55
5:A:606:CLA:H91	6:A:614:CHL:O2D	2.06	0.55
6:A:613:CHL:HMB1	6:A:613:CHL:CBB	2.32	0.55
1:B:98:PHE:HB2	6:B:610:CHL:HMA1	1.88	0.54
4:B:504:XAT:H403	7:B:801:LHG:H121	1.88	0.54
1:C:118:LEU:HD22	5:C:606:CLA:C12	2.37	0.54
1:A:221:ALA:HB3	4:A:504:XAT:H193	1.89	0.54
1:B:83:GLU:CD	1:B:206:LEU:HB2	2.33	0.54
6:B:614:CHL:HHC	6:B:614:CHL:HBB1	1.88	0.54
5:B:602:CLA:HMD3	5:B:607:CLA:C4D	2.37	0.54
1:B:179:LYS:HD3	5:B:602:CLA:HAA2	1.90	0.54
2:B:501:LUX:H381	2:B:501:LUX:H282	1.86	0.54
1:A:215:ASP:CG	1:A:218:ASN:HD22	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:610:CHL:C20	6:C:609:CHL:H8	2.37	0.54
4:C:504:XAT:H3	6:C:609:CHL:H191	1.89	0.54
5:C:604:CLA:H41	5:C:605:CLA:HBA1	1.89	0.54
6:C:614:CHL:HHC	6:C:614:CHL:HBB1	1.88	0.54
5:A:606:CLA:H102	6:A:614:CHL:CED	2.38	0.54
1:C:108:GLY:O	1:C:122:GLN:NE2	2.36	0.54
1:C:216:PRO:HB3	5:C:608:CLA:C1B	2.38	0.54
1:A:147:PRO:HB2	6:A:611:CHL:HBB2	1.90	0.54
1:B:22:VAL:HG21	6:B:609:CHL:CBC	2.38	0.54
5:B:601:CLA:CBC	6:B:611:CHL:H201	2.37	0.54
1:A:94:GLU:HG2	1:A:99:LYS:CB	2.37	0.54
6:A:609:CHL:H8	6:C:610:CHL:H201	1.90	0.54
1:B:85:LEU:HB3	1:B:90:VAL:CG2	2.35	0.53
4:A:504:XAT:H3	6:A:609:CHL:H191	1.91	0.53
5:B:606:CLA:H91	6:B:614:CHL:CED	2.38	0.53
1:A:73:MET:HE3	1:A:184:GLY:CA	2.37	0.53
1:B:118:LEU:HD23	6:B:614:CHL:CED	2.38	0.53
5:C:605:CLA:OBD	6:C:612:CHL:HBA2	2.08	0.53
1:B:23:LYS:HB3	1:B:29:SER:OG	2.08	0.53
2:B:502:LUX:H373	5:B:606:CLA:C3B	2.39	0.53
2:B:502:LUX:H122	5:B:604:CLA:HHC	1.90	0.53
6:B:610:CHL:H142	6:B:612:CHL:C7	2.31	0.53
6:B:611:CHL:C19	6:B:611:CHL:C15	2.87	0.53
1:A:108:GLY:O	1:A:122:GLN:NE2	2.36	0.53
6:A:610:CHL:HBC2	1:B:222:TRP:HH2	1.74	0.53
6:B:612:CHL:H152	6:B:612:CHL:C19	2.25	0.53
1:C:161:PHE:O	2:C:501:LUX:H4C2	2.08	0.53
1:B:19:PRO:HD2	1:B:20:ASP:H	1.73	0.53
1:B:22:VAL:CG2	6:B:609:CHL:CBC	2.87	0.53
1:B:192:PHE:HD2	5:B:603:CLA:HMC1	1.73	0.53
6:C:609:CHL:H41	7:C:801:LHG:H162	1.91	0.53
5:A:601:CLA:H162	5:A:601:CLA:H111	1.91	0.53
5:B:603:CLA:HBB2	7:B:801:LHG:H292	1.89	0.53
5:A:605:CLA:OBD	6:A:612:CHL:HBA2	2.10	0.52
1:B:22:VAL:HG22	6:B:609:CHL:HBC3	1.91	0.52
5:B:605:CLA:OBD	6:B:612:CHL:HBA2	2.10	0.52
1:C:22:VAL:CG2	6:C:609:CHL:CBC	2.87	0.52
1:C:73:MET:HE3	1:C:184:GLY:CA	2.39	0.52
1:C:118:LEU:HD23	6:C:614:CHL:CED	2.40	0.52
6:C:611:CHL:H192	6:C:611:CHL:CAA	2.34	0.52
6:B:609:CHL:H172	6:B:609:CHL:C14	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:602:CLA:C14	5:C:607:CLA:H112	2.39	0.52
1:A:39:GLU:HG3	1:A:39:GLU:O	2.08	0.52
6:A:609:CHL:H172	6:A:609:CHL:C14	2.38	0.52
1:B:81:PHE:HB3	1:B:82:PRO:CD	2.37	0.52
6:C:613:CHL:HMB1	6:C:613:CHL:CBB	2.32	0.52
1:A:76:ALA:HB2	1:A:191:MET:HE1	1.91	0.52
6:B:610:CHL:H203	6:C:609:CHL:H101	1.91	0.52
5:C:606:CLA:H91	6:C:614:CHL:CED	2.40	0.52
6:C:609:CHL:H142	6:C:609:CHL:C10	2.38	0.52
2:A:502:LUX:H202	5:A:604:CLA:H202	1.92	0.52
6:A:611:CHL:C19	6:A:611:CHL:C15	2.88	0.52
1:C:115:ASN:HB3	1:C:118:LEU:CD1	2.40	0.52
5:C:601:CLA:HBC1	6:C:611:CHL:H201	1.91	0.52
5:C:608:CLA:HBC2	5:C:608:CLA:HHD	1.92	0.52
6:C:611:CHL:C19	6:C:611:CHL:CAA	2.88	0.52
1:A:115:ASN:HB3	1:A:118:LEU:CD1	2.40	0.52
1:B:215:ASP:CG	1:B:218:ASN:HD22	2.18	0.52
5:A:606:CLA:H102	6:A:614:CHL:HED1	1.92	0.51
2:A:501:LUX:H381	2:A:501:LUX:H282	1.91	0.51
6:A:609:CHL:H142	6:A:609:CHL:C10	2.39	0.51
6:A:614:CHL:HHC	6:A:614:CHL:HBB1	1.92	0.51
1:A:118:LEU:HD23	6:A:614:CHL:CED	2.40	0.51
2:A:502:LUX:C20	5:A:604:CLA:H202	2.41	0.51
4:A:504:XAT:H403	7:A:801:LHG:H121	1.92	0.51
5:A:603:CLA:HMB1	5:A:603:CLA:CBB	2.31	0.51
5:B:601:CLA:H122	5:B:601:CLA:H91	1.93	0.51
5:B:601:CLA:H92	5:B:601:CLA:H121	1.91	0.51
5:B:604:CLA:H3A	5:B:604:CLA:CGA	2.41	0.51
6:B:610:CHL:H201	6:C:609:CHL:C7	2.40	0.51
1:C:73:MET:HG2	2:C:501:LUX:H142	1.93	0.51
6:A:612:CHL:H192	6:A:612:CHL:C15	2.24	0.51
5:A:606:CLA:H91	6:A:614:CHL:CED	2.41	0.51
1:B:59:SER:O	1:B:63:GLU:HG3	2.11	0.51
1:B:133:ILE:CD1	1:B:133:ILE:N	2.73	0.51
1:C:73:MET:CE	1:C:183:ASN:CB	2.89	0.51
1:A:56:GLU:O	1:A:60:LYS:HG2	2.10	0.51
1:A:118:LEU:O	1:A:120:HIS:N	2.38	0.51
1:B:227:ASN:O	1:B:228:PHE:HB2	2.11	0.51
2:C:501:LUX:H101	5:C:601:CLA:H52	1.93	0.51
6:C:611:CHL:C19	6:C:611:CHL:C15	2.84	0.51
5:A:603:CLA:C1B	5:A:608:CLA:HMD3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:610:CHL:H201	6:B:609:CHL:C8	2.40	0.51
5:B:608:CLA:HBC2	5:B:608:CLA:CHD	2.41	0.51
6:A:609:CHL:HBC2	6:A:609:CHL:CHD	2.40	0.51
2:B:502:LUX:H321	5:B:605:CLA:HMC1	1.92	0.51
5:B:605:CLA:H51	5:C:605:CLA:C4	2.28	0.51
1:C:179:LYS:HD3	5:C:602:CLA:HAA2	1.93	0.51
1:B:147:PRO:CG	6:B:611:CHL:HBB2	2.41	0.50
5:B:607:CLA:C3C	7:B:801:LHG:HC61	2.40	0.50
1:A:73:MET:HG2	2:A:501:LUX:C15	2.39	0.50
1:B:194:PHE:CE1	2:B:501:LUX:H383	2.46	0.50
1:C:22:VAL:HG21	6:C:609:CHL:CBC	2.42	0.50
1:C:102:SER:HB3	6:C:610:CHL:HED2	1.93	0.50
1:A:189:PHE:HE1	6:A:609:CHL:HED2	1.75	0.50
1:A:182:LYS:HE2	5:A:607:CLA:O1D	2.12	0.50
1:A:212:HIS:O	1:A:216:PRO:N	2.44	0.50
1:B:15:PRO:O	1:B:22:VAL:HG12	2.11	0.50
2:C:501:LUX:H101	5:C:601:CLA:C7	2.41	0.50
2:C:501:LUX:C37	5:C:603:CLA:CMB	2.90	0.50
6:A:609:CHL:C7	6:C:610:CHL:H201	2.41	0.50
1:B:22:VAL:HG21	6:B:609:CHL:HBC1	1.94	0.50
1:B:115:ASN:HB3	1:B:118:LEU:CD1	2.41	0.50
2:B:501:LUX:C37	5:B:603:CLA:CMB	2.89	0.50
1:A:104:ILE:HG12	1:A:104:ILE:O	2.11	0.50
1:B:212:HIS:O	1:B:216:PRO:N	2.45	0.50
1:B:83:GLU:O	1:B:87:ARG:HG3	2.11	0.50
1:C:215:ASP:CG	1:C:218:ASN:HD22	2.19	0.50
1:A:179:LYS:HD3	5:A:602:CLA:HAA2	1.93	0.50
6:A:610:CHL:H203	6:B:609:CHL:H101	1.93	0.50
1:C:192:PHE:CZ	5:C:604:CLA:H171	2.47	0.50
1:C:220:ASN:O	1:C:223:SER:OG	2.29	0.50
2:A:501:LUX:C37	5:A:603:CLA:CMB	2.89	0.49
4:B:504:XAT:H363	7:B:801:LHG:C7	2.42	0.49
1:C:77:LEU:HG	5:C:606:CLA:HMC1	1.94	0.49
1:C:148:LEU:HD12	1:C:161:PHE:CZ	2.47	0.49
1:C:227:ASN:O	1:C:228:PHE:HB2	2.12	0.49
5:C:605:CLA:C9	5:C:605:CLA:H122	2.42	0.49
1:A:133:ILE:CD1	1:A:133:ILE:N	2.75	0.49
1:C:21:ARG:HD2	1:C:43:ASP:O	2.11	0.49
1:C:147:PRO:CG	6:C:611:CHL:HBB2	2.42	0.49
1:A:148:LEU:HD12	1:A:161:PHE:CZ	2.47	0.49
5:A:601:CLA:HMB1	5:A:601:CLA:CBB	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:609:CHL:C8	6:C:610:CHL:H201	2.42	0.49
2:B:501:LUX:H102	5:B:601:CLA:CHC	2.43	0.49
6:B:610:CHL:H72	6:B:612:CHL:H172	1.94	0.49
5:C:603:CLA:HMB1	5:C:603:CLA:CBB	2.33	0.49
5:A:606:CLA:CHA	5:A:606:CLA:HBA1	2.42	0.49
1:A:191:MET:HG2	2:A:502:LUX:H322	1.93	0.49
6:A:610:CHL:H2	8:A:802:DGD:C4B	2.42	0.49
1:C:157:PRO:HB3	6:C:611:CHL:HBC2	1.94	0.49
2:A:501:LUX:H101	5:A:601:CLA:C7	2.42	0.49
1:B:39:GLU:O	1:B:39:GLU:HG3	2.12	0.49
6:B:610:CHL:H141	6:B:610:CHL:H172	1.93	0.49
1:C:191:MET:HG2	2:C:502:LUX:H322	1.93	0.49
1:C:194:PHE:CE1	2:C:501:LUX:H383	2.46	0.49
1:C:229:VAL:HG12	1:C:230:PRO:O	2.12	0.49
5:C:601:CLA:H92	5:C:601:CLA:H121	1.94	0.49
5:A:601:CLA:H92	5:A:601:CLA:H121	1.94	0.49
6:A:610:CHL:H142	6:A:612:CHL:C7	2.29	0.49
6:A:611:CHL:H192	6:A:611:CHL:CAA	2.40	0.49
6:B:609:CHL:H142	6:B:609:CHL:C10	2.43	0.49
1:C:133:ILE:CD1	1:C:133:ILE:N	2.75	0.49
1:B:213:LEU:HD21	5:B:608:CLA:HHC	1.94	0.49
1:B:221:ALA:HB3	4:B:504:XAT:H193	1.95	0.49
1:C:190:SER:OG	2:C:501:LUX:H392	2.13	0.49
6:A:611:CHL:C19	6:A:611:CHL:CAA	2.91	0.49
1:B:192:PHE:CZ	5:B:604:CLA:H171	2.47	0.49
1:A:46:TRP:CZ2	6:A:609:CHL:HBA2	2.47	0.49
1:B:190:SER:OG	2:B:501:LUX:H392	2.13	0.49
1:C:56:GLU:O	1:C:60:LYS:HG2	2.12	0.49
1:A:22:VAL:CG2	6:A:609:CHL:CBC	2.91	0.48
1:B:73:MET:HE2	1:B:183:ASN:CB	2.43	0.48
1:B:108:GLY:C	1:B:122:GLN:HE22	2.21	0.48
5:B:604:CLA:H101	5:B:604:CLA:C14	2.42	0.48
3:C:503:NEX:H401	3:C:503:NEX:H35	1.58	0.48
1:B:147:PRO:HB2	6:B:611:CHL:HBB2	1.94	0.48
1:B:191:MET:O	1:B:194:PHE:HB2	2.13	0.48
5:B:605:CLA:C9	5:B:605:CLA:H122	2.43	0.48
2:C:502:LUX:C37	5:C:606:CLA:C2B	2.91	0.48
6:C:610:CHL:H142	6:C:612:CHL:H101	1.94	0.48
1:A:118:LEU:CA	6:A:614:CHL:HED1	2.39	0.48
5:B:606:CLA:CHA	5:B:606:CLA:HBA1	2.38	0.48
1:C:83:GLU:O	1:C:87:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:610:CHL:H142	6:C:612:CHL:C7	2.35	0.48
1:C:104:ILE:HD12	1:C:127:ILE:CD1	2.39	0.48
5:C:603:CLA:C1B	5:C:608:CLA:HMD3	2.44	0.48
6:C:611:CHL:HHC	6:C:611:CHL:OMC	2.13	0.48
1:A:83:GLU:O	1:A:87:ARG:HG3	2.13	0.48
1:B:138:VAL:HB	9:B:2002:HOH:O	2.12	0.48
4:B:504:XAT:H3	6:B:609:CHL:H191	1.95	0.48
5:B:603:CLA:HMB1	5:B:603:CLA:CBB	2.37	0.48
1:C:76:ALA:HB2	1:C:191:MET:HE1	1.95	0.48
1:C:161:PHE:C	1:C:163:PRO:HD3	2.38	0.48
6:C:609:CHL:H143	7:C:801:LHG:H211	1.95	0.48
1:B:69:SER:HB3	1:B:184:GLY:HA3	1.95	0.48
6:C:612:CHL:HBC1	6:C:613:CHL:HBB2	1.95	0.48
1:B:182:LYS:NZ	7:B:801:LHG:O4	2.39	0.48
1:B:220:ASN:CG	5:B:608:CLA:HED1	2.38	0.48
5:B:607:CLA:H121	5:B:607:CLA:C9	2.09	0.48
1:A:161:PHE:C	1:A:163:PRO:HD3	2.39	0.48
4:A:504:XAT:H34	5:A:603:CLA:H122	1.95	0.48
5:A:604:CLA:H101	5:A:604:CLA:C14	2.44	0.48
1:B:32:SER:HB3	1:B:33:PRO:HD2	1.95	0.48
5:B:603:CLA:H92	5:B:608:CLA:CMD	2.43	0.48
1:C:104:ILE:HD13	1:C:124:ILE:HB	1.95	0.48
6:A:610:CHL:H203	6:B:609:CHL:C10	2.44	0.47
1:B:56:GLU:O	1:B:60:LYS:HG2	2.14	0.47
1:B:131:GLN:NE2	6:B:610:CHL:HMC	2.28	0.47
5:C:601:CLA:HMB1	5:C:601:CLA:CBB	2.38	0.47
6:C:611:CHL:H162	6:C:611:CHL:H141	1.64	0.47
5:A:601:CLA:H122	5:A:601:CLA:H91	1.94	0.47
2:B:501:LUX:H27	2:B:501:LUX:H372	1.07	0.47
5:B:601:CLA:H111	5:B:601:CLA:C16	2.44	0.47
6:B:610:CHL:H142	6:B:612:CHL:H101	1.95	0.47
1:C:182:LYS:HE2	5:C:607:CLA:O1D	2.14	0.47
4:A:504:XAT:O4	6:A:609:CHL:H162	2.14	0.47
5:B:603:CLA:H161	5:B:608:CLA:C3D	2.44	0.47
6:B:611:CHL:H61	6:B:611:CHL:H2	1.60	0.47
4:A:504:XAT:O23	7:A:801:LHG:HC12	2.14	0.47
6:A:610:CHL:H201	6:B:609:CHL:C7	2.43	0.47
1:B:118:LEU:HD23	6:B:614:CHL:HED2	1.95	0.47
1:A:48:THR:HG21	6:C:612:CHL:HAA1	1.97	0.47
1:A:161:PHE:O	2:A:501:LUX:H4C2	2.15	0.47
2:A:502:LUX:H373	5:A:606:CLA:C3B	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASN:O	1:A:228:PHE:HB2	2.15	0.47
2:A:501:LUX:H102	5:A:601:CLA:CHC	2.45	0.47
6:A:611:CHL:HHC	6:A:611:CHL:OMC	2.15	0.47
1:B:73:MET:HE3	1:B:184:GLY:CA	2.44	0.47
1:B:192:PHE:CD2	5:B:604:CLA:H171	2.50	0.47
1:C:39:GLU:HG3	1:C:39:GLU:O	2.14	0.47
1:C:46:TRP:CZ2	6:C:609:CHL:HBA2	2.49	0.47
2:C:502:LUX:H381	2:C:502:LUX:H281	1.95	0.47
5:C:607:CLA:C3C	7:C:801:LHG:HC61	2.45	0.47
5:A:601:CLA:O1D	5:A:601:CLA:H2A	2.14	0.47
6:A:609:CHL:H101	6:C:610:CHL:H203	1.97	0.47
1:B:73:MET:CE	1:B:183:ASN:CB	2.93	0.47
2:C:502:LUX:H122	5:C:604:CLA:HAB	1.97	0.47
1:B:161:PHE:O	2:B:501:LUX:H4C2	2.15	0.47
1:A:147:PRO:HG2	6:A:611:CHL:HBB2	1.97	0.47
1:B:73:MET:CE	1:B:183:ASN:HB2	2.45	0.47
2:C:502:LUX:C20	5:C:604:CLA:H202	2.45	0.47
2:A:502:LUX:H381	2:A:502:LUX:H281	1.96	0.46
6:A:612:CHL:HBC1	6:A:613:CHL:HBB2	1.95	0.46
1:B:189:PHE:HE1	6:B:609:CHL:HED2	1.80	0.46
6:B:611:CHL:H8	6:B:611:CHL:H52	1.38	0.46
1:C:131:GLN:NE2	6:C:610:CHL:HMC	2.28	0.46
5:B:603:CLA:H151	5:B:608:CLA:HBA2	1.97	0.46
6:B:610:CHL:C20	6:C:609:CHL:C8	2.93	0.46
6:C:611:CHL:H2	6:C:611:CHL:H61	1.47	0.46
5:A:604:CLA:H41	5:A:605:CLA:HBA1	1.97	0.46
6:A:610:CHL:C20	6:B:609:CHL:H8	2.44	0.46
1:B:73:MET:HE2	1:B:183:ASN:HB3	1.96	0.46
6:B:610:CHL:H203	6:C:609:CHL:C10	2.46	0.46
2:B:502:LUX:C20	5:B:604:CLA:H202	2.45	0.46
1:C:32:SER:HB3	1:C:33:PRO:HD2	1.98	0.46
1:C:73:MET:CG	2:C:501:LUX:H352	2.25	0.46
5:C:601:CLA:O1A	5:C:601:CLA:H3A	2.16	0.46
1:C:22:VAL:HG21	6:C:609:CHL:HBC1	1.97	0.46
5:A:606:CLA:HMB1	5:A:606:CLA:CBB	2.27	0.46
1:B:112:TYR:O	1:B:118:LEU:HD12	2.16	0.46
5:C:603:CLA:C1A	5:C:603:CLA:CGA	2.94	0.46
5:C:606:CLA:CHA	5:C:606:CLA:HBA1	2.43	0.46
1:A:41:PRO:HG3	1:A:177:LYS:HD2	1.98	0.46
4:A:504:XAT:H363	7:A:801:LHG:C7	2.46	0.46
1:B:104:ILE:HG12	1:B:104:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:MET:HG2	2:A:502:LUX:H352	1.97	0.46
5:A:601:CLA:HBC1	6:A:611:CHL:H201	1.97	0.46
1:B:63:GLU:O	1:B:67:ILE:HG12	2.16	0.46
1:B:84:LEU:HD23	5:B:607:CLA:H191	1.98	0.46
4:B:504:XAT:H34	5:B:603:CLA:H122	1.98	0.46
1:A:73:MET:CE	1:A:183:ASN:CB	2.94	0.45
5:A:607:CLA:C4C	7:A:801:LHG:HC61	2.46	0.45
5:B:605:CLA:H12	1:C:51:LEU:HD21	1.98	0.45
1:C:147:PRO:HB2	6:C:611:CHL:HBB2	1.99	0.45
4:C:504:XAT:H371	7:C:801:LHG:H362	1.98	0.45
1:A:23:LYS:HB3	1:A:29:SER:OG	2.15	0.45
6:B:611:CHL:HHC	6:B:611:CHL:OMC	2.16	0.45
1:C:23:LYS:HB3	1:C:29:SER:OG	2.15	0.45
2:C:501:LUX:H102	5:C:601:CLA:CHC	2.46	0.45
5:C:603:CLA:H92	5:C:608:CLA:CMD	2.46	0.45
6:C:609:CHL:HBC2	6:C:609:CHL:CHD	2.46	0.45
1:A:190:SER:OG	2:A:501:LUX:H392	2.15	0.45
3:A:503:NEX:H401	3:A:503:NEX:H35	1.70	0.45
5:A:603:CLA:CGA	5:A:603:CLA:C1A	2.94	0.45
1:B:128:TRP:NE1	4:C:504:XAT:C20	2.78	0.45
2:C:502:LUX:H381	2:C:502:LUX:H282	1.99	0.45
5:C:607:CLA:H52	5:C:607:CLA:C9	2.36	0.45
6:A:609:CHL:HED3	7:A:801:LHG:H142	1.99	0.45
1:B:191:MET:HE2	1:B:191:MET:HB2	1.42	0.45
5:B:603:CLA:C1B	5:B:608:CLA:HMD3	2.46	0.45
5:B:604:CLA:H41	5:B:605:CLA:HBA2	1.99	0.45
7:B:801:LHG:HC62	7:B:801:LHG:H242	1.72	0.45
1:C:115:ASN:HB3	1:C:118:LEU:HG	1.98	0.45
1:C:191:MET:O	1:C:194:PHE:HB2	2.15	0.45
2:C:502:LUX:H111	5:C:604:CLA:HMC2	1.97	0.45
5:C:605:CLA:H191	6:C:612:CHL:H51	1.98	0.45
1:A:104:ILE:HD13	1:A:124:ILE:HB	1.98	0.45
6:A:609:CHL:H8	6:C:610:CHL:C20	2.46	0.45
1:B:76:ALA:HB2	1:B:191:MET:HE1	1.99	0.45
3:B:503:NEX:H35	3:B:503:NEX:H401	1.63	0.45
1:C:118:LEU:HD23	6:C:614:CHL:HED2	1.96	0.45
4:C:504:XAT:H10	7:C:801:LHG:H223	1.98	0.45
1:A:131:GLN:NE2	6:A:610:CHL:HMC	2.30	0.45
2:B:501:LUX:H101	5:B:601:CLA:C7	2.45	0.45
2:B:502:LUX:H202	5:B:604:CLA:H202	1.99	0.45
1:C:191:MET:HB2	1:C:191:MET:HE2	1.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:608:CLA:HBC2	5:C:608:CLA:CHD	2.47	0.45
6:A:610:CHL:C20	6:B:609:CHL:H62	2.33	0.45
1:B:132:VAL:HG12	1:B:133:ILE:N	2.32	0.45
6:B:612:CHL:CBC	6:B:613:CHL:CBB	2.95	0.45
6:B:612:CHL:HAC1	6:B:613:CHL:HBB1	1.98	0.45
2:C:501:LUX:H381	2:C:501:LUX:H282	1.96	0.45
1:A:112:TYR:O	1:A:118:LEU:HD12	2.17	0.45
5:A:605:CLA:C9	5:A:605:CLA:H122	2.47	0.45
1:B:77:LEU:HG	5:B:606:CLA:HMC1	1.97	0.45
5:B:604:CLA:C4	5:B:605:CLA:HBA2	2.47	0.45
1:C:192:PHE:CD2	5:C:604:CLA:C18	2.96	0.45
3:C:503:NEX:H371	6:C:611:CHL:H171	1.98	0.45
4:C:504:XAT:H11	4:C:504:XAT:H191	1.81	0.45
5:A:601:CLA:O1A	5:A:601:CLA:H3A	2.17	0.45
1:B:213:LEU:HD11	5:B:608:CLA:HMC2	1.98	0.45
4:B:504:XAT:C37	7:B:801:LHG:H362	2.47	0.45
5:B:603:CLA:C9	5:B:608:CLA:HMD2	2.47	0.45
5:C:603:CLA:H172	5:C:608:CLA:CBA	2.46	0.45
1:B:16:TRP:CZ3	1:B:22:VAL:HG11	2.52	0.44
5:B:601:CLA:CMB	5:B:601:CLA:CBB	2.84	0.44
5:B:603:CLA:H18	5:B:608:CLA:ND	2.33	0.44
1:C:213:LEU:HD11	5:C:608:CLA:HMC2	1.99	0.44
1:A:21:ARG:HD3	1:A:38:GLY:HA3	1.99	0.44
1:B:46:TRP:CD1	1:B:46:TRP:C	2.92	0.44
1:B:141:TYR:HA	1:B:145:GLY:O	2.17	0.44
1:A:192:PHE:CZ	5:A:604:CLA:H171	2.50	0.44
4:A:504:XAT:H35	4:A:504:XAT:H401	1.63	0.44
4:A:504:XAT:H201	4:A:504:XAT:H15	1.75	0.44
1:B:73:MET:HG2	2:B:501:LUX:C14	2.47	0.44
1:B:138:VAL:HA	1:B:141:TYR:CD1	2.52	0.44
2:C:502:LUX:H27	2:C:502:LUX:H372	1.34	0.44
1:A:21:ARG:HG2	1:A:21:ARG:HH11	1.81	0.44
3:A:503:NEX:H371	6:A:611:CHL:H171	1.98	0.44
1:C:41:PRO:HG3	1:C:177:LYS:HD2	2.00	0.44
1:C:178:VAL:O	1:C:182:LYS:HG3	2.17	0.44
1:A:213:LEU:HD21	5:A:608:CLA:HHC	2.00	0.44
1:A:229:VAL:HG12	1:A:230:PRO:O	2.18	0.44
6:A:611:CHL:H2	6:A:611:CHL:H61	1.49	0.44
6:A:612:CHL:H152	6:A:612:CHL:C19	2.27	0.44
1:B:192:PHE:CD2	5:B:604:CLA:C18	2.96	0.44
1:B:206:LEU:HD23	1:B:206:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:504:XAT:H10	7:B:801:LHG:H223	1.99	0.44
1:C:118:LEU:O	1:C:120:HIS:N	2.47	0.44
1:C:166:LEU:CD1	2:C:501:LUX:H173	2.48	0.44
1:C:189:PHE:HE1	6:C:609:CHL:HED2	1.83	0.44
1:C:212:HIS:O	1:C:216:PRO:N	2.50	0.44
1:A:191:MET:O	1:A:194:PHE:HB2	2.18	0.44
5:A:605:CLA:H12	1:B:51:LEU:HD21	1.99	0.44
1:B:169:ASP:HA	1:B:170:PRO:HD3	1.82	0.44
5:C:602:CLA:HMD3	5:C:607:CLA:C4D	2.48	0.44
6:C:610:CHL:H141	6:C:610:CHL:H172	2.00	0.44
6:A:609:CHL:C10	6:C:610:CHL:H203	2.48	0.44
2:B:502:LUX:H381	2:B:502:LUX:H281	1.99	0.44
5:B:606:CLA:H102	6:B:614:CHL:HED3	1.99	0.44
1:C:188:MET:HB3	2:C:502:LUX:H142	2.00	0.44
5:C:604:CLA:H41	5:C:605:CLA:CBA	2.47	0.44
1:A:138:VAL:HA	1:A:141:TYR:CD1	2.52	0.44
1:C:143:ILE:HD11	6:C:612:CHL:HMA1	1.99	0.44
4:C:504:XAT:H35	4:C:504:XAT:H401	1.76	0.44
2:A:501:LUX:H27	2:A:501:LUX:H372	1.05	0.43
6:B:610:CHL:H143	6:B:610:CHL:H112	1.87	0.43
1:C:73:MET:CE	1:C:183:ASN:HB2	2.48	0.43
1:B:118:LEU:O	1:B:120:HIS:N	2.43	0.43
4:C:504:XAT:H363	7:C:801:LHG:C7	2.48	0.43
1:A:118:LEU:HD23	6:A:614:CHL:HED2	2.00	0.43
2:A:502:LUX:H381	2:A:502:LUX:H282	2.00	0.43
2:B:502:LUX:H122	5:B:604:CLA:HAB	1.99	0.43
5:B:603:CLA:C9	5:B:608:CLA:CMD	2.96	0.43
1:C:84:LEU:HD23	5:C:607:CLA:H191	2.01	0.43
1:A:22:VAL:HG21	6:A:609:CHL:HBC1	2.00	0.43
1:B:124:ILE:HG23	1:B:125:LEU:N	2.32	0.43
1:B:181:LEU:HD23	1:B:181:LEU:HA	1.84	0.43
1:C:221:ALA:HB3	4:C:504:XAT:H193	2.01	0.43
2:C:501:LUX:H27	2:C:501:LUX:H372	1.17	0.43
6:C:612:CHL:C15	6:C:612:CHL:C19	2.91	0.43
1:A:147:PRO:CG	6:A:611:CHL:HBB2	2.48	0.43
5:A:606:CLA:H112	5:A:606:CLA:H61	2.00	0.43
7:A:801:LHG:H242	7:A:801:LHG:HC62	1.77	0.43
1:B:128:TRP:HE1	4:C:504:XAT:C20	2.31	0.43
6:B:611:CHL:HAA2	6:B:611:CHL:C19	2.40	0.43
1:C:102:SER:HB3	6:C:610:CHL:CED	2.49	0.43
1:C:200:VAL:O	8:C:802:DGD:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG21	6:A:609:CHL:CBC	2.49	0.43
1:B:160:SER:O	6:B:611:CHL:C6	2.67	0.43
1:B:193:GLY:HA2	5:B:603:CLA:C3C	2.49	0.43
6:B:612:CHL:CBC	6:B:613:CHL:HBB2	2.47	0.43
2:C:502:LUX:H321	5:C:605:CLA:HMC1	1.99	0.43
1:A:169:ASP:HA	1:A:170:PRO:HD3	1.86	0.43
4:B:504:XAT:H403	7:B:801:LHG:C12	2.49	0.43
5:B:605:CLA:HBC1	6:B:612:CHL:CBC	2.48	0.43
5:C:601:CLA:CBC	6:C:611:CHL:H201	2.49	0.43
6:C:611:CHL:HBA2	6:C:611:CHL:HBD	2.01	0.43
5:A:607:CLA:C3C	7:A:801:LHG:HC61	2.49	0.43
1:B:166:LEU:CD1	2:B:501:LUX:H173	2.48	0.43
6:C:609:CHL:HED3	7:C:801:LHG:H142	2.00	0.43
7:C:801:LHG:H242	7:C:801:LHG:HC62	1.71	0.43
4:A:504:XAT:H11	4:A:504:XAT:H191	1.68	0.43
1:B:94:GLU:HG2	1:B:99:LYS:HB2	2.01	0.43
4:B:504:XAT:H15	4:B:504:XAT:H201	1.62	0.43
5:C:607:CLA:C9	5:C:607:CLA:C5	2.93	0.43
1:A:66:VAL:HB	1:A:155:LEU:HD13	2.00	0.43
1:A:166:LEU:CD1	2:A:501:LUX:H173	2.49	0.43
8:A:802:DGD:HE3	8:A:802:DGD:HD62	2.01	0.43
1:B:23:LYS:HB3	1:B:29:SER:CB	2.49	0.43
2:B:502:LUX:C37	5:B:606:CLA:C2B	2.96	0.43
6:C:610:CHL:CBB	6:C:612:CHL:HBC1	2.47	0.43
1:A:142:ARG:HG3	6:A:611:CHL:C1D	2.50	0.42
2:A:502:LUX:H162	2:A:502:LUX:H3	1.69	0.42
6:A:610:CHL:C20	6:B:609:CHL:C8	2.97	0.42
6:A:611:CHL:H8	6:A:611:CHL:H52	1.41	0.42
8:B:802:DGD:C1E	1:C:231:GLY:H	2.32	0.42
1:C:157:PRO:HD2	5:C:601:CLA:OBD	2.18	0.42
1:A:138:VAL:HG23	9:A:2003:HOH:O	2.20	0.42
1:B:71:TRP:CD1	6:B:611:CHL:HED2	2.54	0.42
5:B:606:CLA:C10	6:B:614:CHL:HED1	2.47	0.42
1:C:213:LEU:HD21	5:C:608:CLA:HHC	2.02	0.42
6:C:609:CHL:H172	6:C:609:CHL:C14	2.43	0.42
4:C:504:XAT:H201	4:C:504:XAT:H15	1.75	0.42
5:C:601:CLA:H111	5:C:601:CLA:C16	2.46	0.42
6:A:610:CHL:H172	6:A:610:CHL:H141	2.02	0.42
5:B:601:CLA:H3A	5:B:601:CLA:O1A	2.20	0.42
1:A:120:HIS:CE1	1:A:122:GLN:NE2	2.87	0.42
5:B:601:CLA:HBC2	6:B:611:CHL:O1A	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:605:CLA:H122	5:B:605:CLA:H91	2.01	0.42
1:C:15:PRO:O	1:C:22:VAL:HG12	2.19	0.42
1:C:115:ASN:HB3	1:C:118:LEU:CG	2.50	0.42
1:B:128:TRP:NE1	4:C:504:XAT:H202	2.34	0.42
6:B:613:CHL:HAA2	6:B:613:CHL:HBD	2.01	0.42
6:C:611:CHL:H52	6:C:611:CHL:H8	1.58	0.42
5:A:603:CLA:H161	5:A:608:CLA:C3D	2.49	0.42
5:A:605:CLA:H121	5:A:605:CLA:C9	2.42	0.42
1:B:157:PRO:HG2	5:B:601:CLA:OBD	2.20	0.42
1:A:18:GLY:O	1:A:21:ARG:HG2	2.19	0.42
1:A:54:ASP:HA	1:A:55:PRO:HD3	1.92	0.42
1:B:103:GLN:O	1:B:106:SER:HB3	2.20	0.42
5:A:601:CLA:CBC	6:A:611:CHL:H201	2.50	0.41
1:B:213:LEU:CD2	5:B:608:CLA:CHC	2.97	0.41
5:C:601:CLA:H3A	5:C:601:CLA:CGA	2.49	0.41
1:A:128:TRP:NE1	4:B:504:XAT:C20	2.83	0.41
2:A:502:LUX:H122	5:A:604:CLA:HAB	2.02	0.41
5:A:603:CLA:H18	5:A:608:CLA:ND	2.35	0.41
1:B:19:PRO:CD	1:B:20:ASP:H	2.33	0.41
1:B:161:PHE:C	1:B:163:PRO:HD3	2.45	0.41
1:B:178:VAL:O	1:B:182:LYS:HG3	2.20	0.41
1:B:191:MET:HG2	2:B:502:LUX:H322	2.01	0.41
5:B:601:CLA:H122	5:B:601:CLA:H161	1.88	0.41
6:B:611:CHL:H192	6:B:611:CHL:CAA	2.43	0.41
5:C:604:CLA:H3A	5:C:604:CLA:CGA	2.50	0.41
1:C:120:HIS:CE1	1:C:122:GLN:NE2	2.87	0.41
1:C:138:VAL:HB	9:C:2001:HOH:O	2.20	0.41
1:A:221:ALA:CB	4:A:504:XAT:H193	2.51	0.41
5:A:604:CLA:H3A	5:A:604:CLA:CGA	2.50	0.41
6:A:610:CHL:H142	6:A:612:CHL:H101	2.01	0.41
1:C:161:PHE:C	1:C:163:PRO:CD	2.93	0.41
5:C:601:CLA:CGA	5:C:601:CLA:C3A	2.98	0.41
5:B:603:CLA:H2	5:B:603:CLA:H61	1.85	0.41
8:C:802:DGD:HB52	8:C:802:DGD:HB21	1.91	0.41
1:A:161:PHE:C	1:A:163:PRO:CD	2.93	0.41
6:A:609:CHL:C8	6:C:610:CHL:C20	2.98	0.41
6:A:613:CHL:HAA2	6:A:613:CHL:HBD	2.01	0.41
4:B:504:XAT:H35	4:B:504:XAT:H401	1.65	0.41
2:A:501:LUX:C10	5:A:601:CLA:H72	2.50	0.41
1:B:169:ASP:OD2	1:B:170:PRO:HD2	2.20	0.41
1:B:229:VAL:HG12	1:B:230:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:LUX:H271	2:B:501:LUX:H371	1.68	0.41
1:A:157:PRO:HB3	6:A:611:CHL:HBC2	2.03	0.41
8:A:802:DGD:C1E	1:B:231:GLY:H	2.33	0.41
1:C:104:ILE:HG12	1:C:104:ILE:O	2.21	0.41
1:C:153:ASP:HA	1:C:154:PRO:HD3	1.92	0.41
8:C:802:DGD:HE3	8:C:802:DGD:HD62	2.01	0.41
1:A:115:ASN:HB3	1:A:118:LEU:HG	2.01	0.41
5:A:606:CLA:H93	6:A:614:CHL:OBD	2.21	0.41
5:A:608:CLA:HBC2	5:A:608:CLA:HHD	2.02	0.41
2:B:501:LUX:H111	5:B:601:CLA:HMC2	2.02	0.41
6:B:611:CHL:C19	6:B:611:CHL:CAA	2.99	0.41
6:B:611:CHL:HBA2	6:B:611:CHL:CHA	2.51	0.41
1:C:157:PRO:HG2	5:C:601:CLA:OBD	2.21	0.41
1:C:193:GLY:HA2	5:C:603:CLA:C3C	2.51	0.41
5:C:606:CLA:H61	5:C:606:CLA:H112	2.03	0.41
1:A:64:LEU:HD13	5:A:605:CLA:CAA	2.51	0.41
1:A:192:PHE:CD2	5:A:604:CLA:C18	2.97	0.41
5:A:602:CLA:HBB1	5:A:602:CLA:CHC	2.40	0.41
1:C:138:VAL:HA	1:C:141:TYR:CD1	2.56	0.41
5:C:604:CLA:H101	5:C:604:CLA:C14	2.49	0.41
6:C:611:CHL:HBA2	6:C:611:CHL:CHA	2.51	0.40
1:A:15:PRO:O	1:A:22:VAL:HG12	2.21	0.40
1:A:141:TYR:HA	1:A:145:GLY:O	2.21	0.40
4:A:504:XAT:C5	6:A:609:CHL:H192	2.51	0.40
5:C:605:CLA:H122	5:C:605:CLA:H91	2.03	0.40
1:A:77:LEU:HG	5:A:606:CLA:HMC1	2.03	0.40
1:A:112:TYR:C	1:A:114:GLY:N	2.78	0.40
1:A:229:VAL:HA	1:A:230:PRO:HD3	1.89	0.40
2:A:502:LUX:H193	5:A:604:CLA:C14	2.50	0.40
1:B:220:ASN:O	1:B:223:SER:OG	2.38	0.40
3:B:503:NEX:H11	3:B:503:NEX:H191	1.88	0.40
5:B:603:CLA:CGA	5:B:603:CLA:C1A	2.99	0.40
1:C:118:LEU:CD2	6:C:614:CHL:CED	3.00	0.40
1:C:132:VAL:HG12	1:C:133:ILE:N	2.35	0.40
5:C:601:CLA:H2A	5:C:601:CLA:O1D	2.21	0.40
4:A:504:XAT:C37	7:A:801:LHG:H362	2.51	0.40
1:C:194:PHE:HZ	2:C:501:LUX:C38	2.13	0.40
2:C:502:LUX:C36	5:C:606:CLA:CMB	2.98	0.40
7:C:801:LHG:H312	7:C:801:LHG:H282	1.85	0.40

There are no symmetry-related clashes.

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	221/232 (95%)	210 (95%)	10 (4%)	1 (0%)	24	43
1	B	221/232 (95%)	210 (95%)	9 (4%)	2 (1%)	14	27
1	C	221/232 (95%)	208 (94%)	10 (4%)	3 (1%)	9	17
All	All	663/696 (95%)	628 (95%)	29 (4%)	6 (1%)	14	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	SER
1	C	14	SER
1	A	216	PRO
1	B	216	PRO
1	C	216	PRO
1	C	170	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	169/181 (93%)	145 (86%)	24 (14%)	3	7
1	B	169/181 (93%)	143 (85%)	26 (15%)	2	5
1	C	169/181 (93%)	146 (86%)	23 (14%)	3	8
All	All	507/543 (93%)	434 (86%)	73 (14%)	3	6

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	22	VAL
1	A	23	LYS
1	A	31	GLU
1	A	39	GLU
1	A	48	THR
1	A	59	SER
1	A	62	ARG
1	A	80	VAL
1	A	86	SER
1	A	90	VAL
1	A	99	LYS
1	A	103	GLN
1	A	106	SER
1	A	110	LEU
1	A	132	VAL
1	A	133	ILE
1	A	143	ILE
1	A	152	VAL
1	A	171	GLU
1	A	175	GLU
1	A	177	LYS
1	A	199	ILE
1	A	223	SER
1	B	11	SER
1	B	12	SER
1	B	23	LYS
1	B	31	GLU
1	B	34	SER
1	B	39	GLU
1	B	59	SER
1	B	62	ARG
1	B	73	MET
1	B	79	SER
1	B	80	VAL
1	B	86	SER
1	B	90	VAL
1	B	99	LYS
1	B	103	GLN
1	B	106	SER
1	B	110	LEU
1	B	132	VAL

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Mol	Chain	Res	Type
1	B	133	ILE
1	B	143	ILE
1	B	152	VAL
1	B	171	GLU
1	B	175	GLU
1	B	177	LYS
1	B	199	ILE
1	B	223	SER
1	C	11	SER
1	C	22	VAL
1	C	23	LYS
1	C	31	GLU
1	C	34	SER
1	C	39	GLU
1	C	59	SER
1	C	62	ARG
1	C	80	VAL
1	C	86	SER
1	C	90	VAL
1	C	99	LYS
1	C	106	SER
1	C	110	LEU
1	C	132	VAL
1	C	133	ILE
1	C	143	ILE
1	C	152	VAL
1	C	171	GLU
1	C	175	GLU
1	C	177	LYS
1	C	199	ILE
1	C	223	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	122	GLN
1	A	131	GLN
1	A	197	GLN
1	A	208	ASN
1	A	218	ASN
1	B	122	GLN

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Mol	Chain	Res	Type
1	B	131	GLN
1	B	197	GLN
1	B	208	ASN
1	B	218	ASN
1	C	122	GLN
1	C	131	GLN
1	C	197	GLN
1	C	208	ASN
1	C	218	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

60 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	$\# Z > 2$
5	CLA	C	601	1	69,73,73	1.32	9 (13%)	82,113,113	1.78	11 (13%)
5	CLA	B	604	1	69,73,73	1.27	6 (8%)	82,113,113	1.56	13 (15%)
5	CLA	B	605	1	69,73,73	1.22	7 (10%)	82,113,113	1.60	8 (9%)
6	CHL	A	613	-	40,54,74	2.44	11 (27%)	34,90,114	3.05	17 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	LHG	A	801	5	48,48,48	1.75	6 (12%)	51,54,54	1.35	4 (7%)
2	LUX	A	502	-	43,43,43	4.78	26 (60%)	53,60,60	3.73	31 (58%)
6	CHL	A	614	1	36,50,74	2.60	11 (30%)	29,85,114	3.37	15 (51%)
5	CLA	C	606	-	61,65,73	1.23	5 (8%)	72,103,113	1.70	11 (15%)
5	CLA	A	602	1	64,68,73	1.24	7 (10%)	76,107,113	1.57	9 (11%)
5	CLA	B	608	1	52,56,73	1.34	6 (11%)	61,92,113	1.74	13 (21%)
6	CHL	C	614	1	36,50,74	2.62	9 (25%)	29,85,114	3.46	15 (51%)
6	CHL	C	609	1	60,74,74	2.01	16 (26%)	58,114,114	2.41	16 (27%)
5	CLA	B	607	7	69,73,73	1.40	8 (11%)	82,113,113	1.76	10 (12%)
3	NEX	B	503	-	40,46,46	2.71	12 (30%)	50,70,70	2.55	12 (24%)
5	CLA	C	603	1	69,73,73	1.13	7 (10%)	82,113,113	1.61	9 (10%)
6	CHL	B	613	-	40,54,74	2.46	12 (30%)	34,90,114	2.99	18 (52%)
6	CHL	B	614	1	36,50,74	2.53	9 (25%)	29,85,114	3.50	15 (51%)
5	CLA	B	602	1	64,68,73	1.32	8 (12%)	76,107,113	1.68	10 (13%)
6	CHL	B	612	1	60,74,74	1.87	12 (20%)	58,114,114	2.50	19 (32%)
3	NEX	C	503	-	40,46,46	2.58	10 (25%)	50,70,70	2.56	14 (28%)
5	CLA	B	601	1	69,73,73	1.17	9 (13%)	82,113,113	1.72	15 (18%)
5	CLA	C	605	1	69,73,73	1.18	8 (11%)	82,113,113	1.65	8 (9%)
6	CHL	A	611	9	60,74,74	1.91	13 (21%)	58,114,114	2.53	21 (36%)
5	CLA	A	606	-	61,65,73	1.18	6 (9%)	72,103,113	1.71	11 (15%)
2	LUX	C	502	-	43,43,43	4.71	26 (60%)	53,60,60	3.80	30 (56%)
5	CLA	A	603	1	69,73,73	1.14	7 (10%)	82,113,113	1.60	10 (12%)
5	CLA	A	605	1	69,73,73	1.17	5 (7%)	82,113,113	1.66	10 (12%)
3	NEX	A	503	-	40,46,46	2.68	11 (27%)	50,70,70	2.45	12 (24%)
6	CHL	A	612	1	60,74,74	1.94	13 (21%)	58,114,114	2.53	17 (29%)
5	CLA	A	608	1	52,56,73	1.51	9 (17%)	61,92,113	1.91	11 (18%)
2	LUX	C	501	-	43,43,43	4.84	26 (60%)	53,60,60	3.68	30 (56%)
7	LHG	C	801	5	48,48,48	1.72	6 (12%)	51,54,54	1.33	4 (7%)
8	DGD	B	802	-	39,39,67	1.32	4 (10%)	51,51,81	1.92	9 (17%)
4	XAT	A	504	-	41,47,47	2.52	16 (39%)	54,74,74	2.82	19 (35%)
6	CHL	C	612	1	60,74,74	2.04	14 (23%)	58,114,114	2.49	18 (31%)
2	LUX	A	501	-	43,43,43	4.83	26 (60%)	53,60,60	3.60	28 (52%)
5	CLA	A	607	7	69,73,73	1.38	8 (11%)	82,113,113	1.73	10 (12%)
6	CHL	B	611	9	60,74,74	1.90	12 (20%)	58,114,114	2.55	21 (36%)
8	DGD	C	802	-	39,39,67	1.41	5 (12%)	51,51,81	1.96	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CLA	B	606	-	61,65,73	1.23	7 (11%)	72,103,113	1.67	10 (13%)
5	CLA	C	608	1	52,56,73	1.31	5 (9%)	61,92,113	1.96	11 (18%)
5	CLA	C	602	1	64,68,73	1.31	7 (10%)	76,107,113	1.60	9 (11%)
5	CLA	A	601	1	69,73,73	1.25	7 (10%)	82,113,113	1.69	14 (17%)
6	CHL	B	609	1	60,74,74	2.06	14 (23%)	58,114,114	2.48	18 (31%)
6	CHL	A	610	9	60,74,74	1.98	13 (21%)	58,114,114	2.37	16 (27%)
5	CLA	C	604	1	69,73,73	1.10	6 (8%)	82,113,113	1.59	11 (13%)
5	CLA	B	603	1	69,73,73	1.17	9 (13%)	82,113,113	1.65	11 (13%)
2	LUX	B	501	-	43,43,43	4.90	26 (60%)	53,60,60	3.69	30 (56%)
6	CHL	C	611	9	60,74,74	1.88	15 (25%)	58,114,114	2.49	21 (36%)
6	CHL	C	610	9	60,74,74	2.03	15 (25%)	58,114,114	2.41	18 (31%)
8	DGD	A	802	-	39,39,67	1.32	3 (7%)	51,51,81	1.94	9 (17%)
4	XAT	B	504	-	41,47,47	2.51	15 (36%)	54,74,74	2.85	20 (37%)
2	LUX	B	502	-	43,43,43	4.85	26 (60%)	53,60,60	3.79	32 (60%)
4	XAT	C	504	-	41,47,47	2.48	13 (31%)	54,74,74	2.66	19 (35%)
5	CLA	A	604	1	69,73,73	1.21	6 (8%)	82,113,113	1.53	9 (10%)
7	LHG	B	801	5	48,48,48	1.70	6 (12%)	51,54,54	1.37	5 (9%)
6	CHL	A	609	1	60,74,74	1.94	13 (21%)	58,114,114	2.51	16 (27%)
6	CHL	B	610	9	60,74,74	2.00	14 (23%)	58,114,114	2.34	20 (34%)
5	CLA	C	607	7	69,73,73	1.28	8 (11%)	82,113,113	1.71	11 (13%)
6	CHL	C	613	-	40,54,74	2.37	10 (25%)	34,90,114	3.03	18 (52%)

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
5	CLA	C	601	1	2/2/15/20	13/39/115/115	-
5	CLA	B	604	1	2/2/15/20	14/39/115/115	-
5	CLA	B	605	1	2/2/15/20	13/39/115/115	-
6	CHL	A	613	-	3/3/16/26	0/15/113/137	-
7	LHG	A	801	5	-	22/53/53/53	-
2	LUX	A	502	-	5/5/12/15	10/29/67/67	0/2/2/2
6	CHL	A	614	1	3/3/15/26	0/10/108/137	-
5	CLA	C	606	-	2/2/13/20	10/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	A	602	1	1/1/14/20	12/33/109/115	-
5	CLA	B	608	1	1/1/11/20	7/19/95/115	-
6	CHL	C	614	1	3/3/15/26	0/10/108/137	-
6	CHL	C	609	1	4/4/20/26	13/39/137/137	-
5	CLA	B	607	7	1/1/15/20	15/39/115/115	-
3	NEX	B	503	-	-	2/27/83/83	0/3/3/3
5	CLA	C	603	1	2/2/15/20	12/39/115/115	-
6	CHL	B	613	-	3/3/16/26	1/15/113/137	-
6	CHL	B	614	1	3/3/15/26	0/10/108/137	-
5	CLA	B	602	1	1/1/14/20	12/33/109/115	-
6	CHL	B	612	1	3/3/20/26	15/39/137/137	-
5	CLA	B	601	1	2/2/15/20	12/39/115/115	-
5	CLA	C	605	1	2/2/15/20	12/39/115/115	-
3	NEX	C	503	-	-	2/27/83/83	0/3/3/3
6	CHL	A	611	9	4/4/20/26	14/39/137/137	-
5	CLA	A	606	-	2/2/13/20	10/30/106/115	-
2	LUX	C	502	-	5/5/12/15	11/29/67/67	0/2/2/2
5	CLA	A	603	1	2/2/15/20	11/39/115/115	-
5	CLA	A	605	1	2/2/15/20	12/39/115/115	-
6	CHL	A	612	1	3/3/20/26	16/39/137/137	-
3	NEX	A	503	-	-	2/27/83/83	0/3/3/3
5	CLA	A	608	1	1/1/11/20	5/19/95/115	-
2	LUX	C	501	-	5/5/12/15	12/29/67/67	0/2/2/2
7	LHG	C	801	5	-	21/53/53/53	-
8	DGD	B	802	-	1/1/11/13	17/24/64/95	0/2/2/2
4	XAT	A	504	-	2/2/12/26	1/31/93/93	0/4/4/4
6	CHL	C	612	1	3/3/20/26	16/39/137/137	-
2	LUX	A	501	-	5/5/12/15	12/29/67/67	0/2/2/2
5	CLA	A	607	7	1/1/15/20	16/39/115/115	-
6	CHL	B	611	9	4/4/20/26	15/39/137/137	-
8	DGD	C	802	-	1/1/11/13	17/24/64/95	0/2/2/2
5	CLA	B	606	-	2/2/13/20	10/30/106/115	-
5	CLA	C	608	1	1/1/11/20	7/19/95/115	-
5	CLA	C	602	1	1/1/14/20	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	A	601	1	2/2/15/20	12/39/115/115	-
6	CHL	B	609	1	4/4/20/26	13/39/137/137	-
6	CHL	A	610	9	4/4/20/26	12/39/137/137	-
5	CLA	C	604	1	2/2/15/20	14/39/115/115	-
5	CLA	B	603	1	2/2/15/20	11/39/115/115	-
2	LUX	B	501	-	5/5/12/15	12/29/67/67	0/2/2/2
6	CHL	C	611	9	4/4/20/26	15/39/137/137	-
6	CHL	C	610	9	4/4/20/26	12/39/137/137	-
8	DGD	A	802	-	1/1/11/13	16/24/64/95	0/2/2/2
4	XAT	B	504	-	2/2/12/26	2/31/93/93	0/4/4/4
2	LUX	B	502	-	5/5/12/15	12/29/67/67	0/2/2/2
4	XAT	C	504	-	2/2/12/26	3/31/93/93	0/4/4/4
5	CLA	A	604	1	2/2/15/20	14/39/115/115	-
7	LHG	B	801	5	-	21/53/53/53	-
6	CHL	A	609	1	4/4/20/26	13/39/137/137	-
6	CHL	B	610	9	4/4/20/26	12/39/137/137	-
5	CLA	C	607	7	1/1/15/20	15/39/115/115	-
6	CHL	C	613	-	3/3/16/26	0/15/113/137	-

All (659) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	LUX	C24-C25	20.52	1.57	1.33
2	B	502	LUX	C24-C25	19.41	1.56	1.33
2	A	501	LUX	C24-C25	19.24	1.56	1.33
2	B	501	LUX	C24-C25	19.09	1.55	1.33
2	A	502	LUX	C24-C25	19.07	1.55	1.33
2	C	502	LUX	C24-C25	18.27	1.54	1.33
2	B	501	LUX	C21-C26	-14.84	1.41	1.55
2	A	501	LUX	C21-C26	-14.05	1.42	1.55
2	C	501	LUX	C21-C26	-13.43	1.42	1.55
2	A	502	LUX	C21-C26	-13.33	1.42	1.55
2	B	502	LUX	C21-C26	-13.08	1.42	1.55
2	C	502	LUX	C21-C26	-12.29	1.43	1.55
3	B	503	NEX	O24-C25	-9.19	1.34	1.46
3	C	503	NEX	O24-C25	-8.64	1.35	1.46
3	A	503	NEX	O24-C25	-8.51	1.35	1.46
4	A	504	XAT	C26-C27	-7.96	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	XAT	C26-C27	-7.91	1.37	1.50
7	A	801	LHG	P-O5	7.71	1.77	1.50
3	A	503	NEX	C26-C27	-7.58	1.37	1.50
6	A	614	CHL	C3B-C4B	7.57	1.48	1.41
4	C	504	XAT	C26-C27	-7.57	1.37	1.50
7	C	801	LHG	P-O5	7.50	1.76	1.50
7	B	801	LHG	P-O5	7.43	1.76	1.50
4	C	504	XAT	O24-C25	-7.40	1.36	1.46
6	C	614	CHL	C3B-C4B	7.32	1.48	1.41
2	B	502	LUX	C28-C27	-7.30	1.33	1.53
4	A	504	XAT	O24-C25	-7.28	1.36	1.46
4	B	504	XAT	O24-C25	-7.25	1.36	1.46
2	B	501	LUX	C27-C26	-7.14	1.38	1.54
2	B	502	LUX	C5-C6	7.11	1.46	1.34
6	B	613	CHL	C3B-C4B	7.02	1.48	1.41
6	C	613	CHL	C3B-C4B	7.02	1.48	1.41
3	C	503	NEX	C26-C27	-6.98	1.38	1.50
2	C	502	LUX	C27-C26	-6.93	1.38	1.54
3	B	503	NEX	C26-C27	-6.83	1.38	1.50
2	A	501	LUX	C28-C27	-6.76	1.34	1.53
6	B	614	CHL	C3B-C4B	6.67	1.47	1.41
2	A	502	LUX	C27-C26	-6.67	1.39	1.54
2	A	502	LUX	C5-C6	6.66	1.45	1.34
6	A	613	CHL	C1D-C2D	6.61	1.47	1.39
6	B	610	CHL	C3B-C4B	6.58	1.47	1.41
6	C	614	CHL	C1D-C2D	6.55	1.47	1.39
2	B	502	LUX	C10-C9	-6.55	1.35	1.54
2	B	501	LUX	C5-C6	6.53	1.45	1.34
6	B	614	CHL	C1D-C2D	6.47	1.46	1.39
2	A	502	LUX	C28-C27	-6.44	1.35	1.53
2	A	502	LUX	C10-C9	-6.44	1.35	1.54
6	C	612	CHL	C3B-C4B	6.43	1.47	1.41
2	C	502	LUX	C28-C27	-6.43	1.35	1.53
2	C	502	LUX	C5-C6	6.34	1.45	1.34
2	C	501	LUX	C5-C6	6.32	1.45	1.34
6	A	614	CHL	C1D-C2D	6.31	1.46	1.39
6	B	613	CHL	C1D-C2D	6.29	1.46	1.39
3	B	503	NEX	C12-C13	-6.28	1.32	1.46
2	C	502	LUX	C10-C9	-6.27	1.35	1.54
2	A	501	LUX	C10-C9	-6.24	1.35	1.54
6	A	609	CHL	C3B-C4B	6.24	1.47	1.41
6	C	612	CHL	C1D-C2D	6.22	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	612	CHL	CMC-C2C	6.20	1.57	1.44
6	B	611	CHL	C1D-C2D	6.20	1.46	1.39
5	B	607	CLA	MG-NA	6.15	2.20	2.06
2	B	502	LUX	C27-C26	-6.15	1.40	1.54
2	B	501	LUX	C10-C9	-6.13	1.36	1.54
6	C	610	CHL	C3B-C4B	6.12	1.47	1.41
6	C	614	CHL	CMC-C2C	6.08	1.57	1.44
3	A	503	NEX	C12-C13	-6.05	1.33	1.46
6	B	609	CHL	C1D-C2D	6.04	1.46	1.39
6	C	609	CHL	CMC-C2C	6.04	1.57	1.44
2	B	501	LUX	C28-C27	-6.03	1.36	1.53
6	A	610	CHL	C3B-C4B	6.01	1.47	1.41
6	B	609	CHL	C3B-C4B	6.00	1.47	1.41
2	B	501	LUX	C26-C25	-5.98	1.34	1.52
5	A	607	CLA	MG-NA	5.95	2.20	2.06
2	C	501	LUX	C10-C9	-5.94	1.36	1.54
6	A	613	CHL	CMC-C2C	5.94	1.57	1.44
6	B	609	CHL	CMC-C2C	5.92	1.57	1.44
6	B	612	CHL	CMC-C2C	5.87	1.57	1.44
2	A	501	LUX	C27-C26	-5.81	1.41	1.54
2	B	502	LUX	C26-C25	-5.79	1.34	1.52
6	B	613	CHL	CMC-C2C	5.77	1.56	1.44
2	C	502	LUX	C26-C25	-5.77	1.34	1.52
6	C	611	CHL	C1D-C2D	5.75	1.46	1.39
6	C	609	CHL	C3B-C4B	5.74	1.47	1.41
6	A	610	CHL	CMC-C2C	5.73	1.56	1.44
2	A	502	LUX	C9-C8	-5.70	1.34	1.51
6	A	611	CHL	C1D-C2D	5.70	1.46	1.39
6	A	612	CHL	CMC-C2C	5.66	1.56	1.44
6	A	613	CHL	C3B-C4B	5.64	1.46	1.41
2	A	501	LUX	C26-C25	-5.63	1.35	1.52
6	C	613	CHL	CMC-C2C	5.63	1.56	1.44
6	B	612	CHL	C1D-C2D	5.62	1.45	1.39
2	A	501	LUX	C5-C6	5.62	1.43	1.34
6	B	611	CHL	C3B-C4B	5.61	1.46	1.41
2	C	502	LUX	C9-C8	-5.60	1.35	1.51
6	A	611	CHL	C3B-C4B	5.59	1.46	1.41
6	A	612	CHL	C3B-C4B	5.54	1.46	1.41
2	C	501	LUX	C28-C27	-5.54	1.38	1.53
6	C	609	CHL	C1D-C2D	5.53	1.45	1.39
6	C	614	CHL	C1B-C2B	5.51	1.45	1.39
3	C	503	NEX	C12-C13	-5.48	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	610	CHL	C1D-C2D	5.43	1.45	1.39
6	A	611	CHL	CMC-C2C	5.43	1.56	1.44
2	A	502	LUX	C26-C25	-5.43	1.35	1.52
6	B	614	CHL	CMC-C2C	5.42	1.56	1.44
2	C	501	LUX	C26-C25	-5.42	1.35	1.52
6	C	613	CHL	C1D-C2D	5.40	1.45	1.39
6	A	614	CHL	CMC-C2C	5.32	1.55	1.44
6	B	609	CHL	C1B-C2B	5.29	1.45	1.39
6	C	611	CHL	C3B-C4B	5.29	1.46	1.41
6	B	610	CHL	CMC-C2C	5.26	1.55	1.44
2	C	501	LUX	C9-C8	-5.23	1.36	1.51
3	A	503	NEX	C32-C33	-5.22	1.34	1.46
6	A	609	CHL	C1D-C2D	5.21	1.45	1.39
6	B	614	CHL	C1B-C2B	5.15	1.45	1.39
2	B	502	LUX	C9-C8	-5.15	1.36	1.51
6	B	610	CHL	C1B-C2B	5.13	1.45	1.39
7	A	801	LHG	P-O3	5.13	1.79	1.59
6	C	610	CHL	C1B-C2B	5.12	1.45	1.39
3	B	503	NEX	C32-C33	-5.12	1.35	1.46
2	C	502	LUX	C18-C5	-5.10	1.42	1.50
6	A	612	CHL	C1D-C2D	5.08	1.45	1.39
6	A	609	CHL	C1B-C2B	5.06	1.45	1.39
4	A	504	XAT	C32-C33	-5.04	1.35	1.46
6	B	611	CHL	CMC-C2C	5.04	1.55	1.44
7	C	801	LHG	P-O3	5.01	1.79	1.59
6	C	610	CHL	CMC-C2C	4.99	1.55	1.44
2	A	501	LUX	C9-C8	-4.97	1.36	1.51
6	C	611	CHL	CMC-C2C	4.97	1.55	1.44
6	A	614	CHL	C1B-C2B	4.93	1.45	1.39
5	B	604	CLA	O2D-CGD	4.93	1.45	1.33
7	B	801	LHG	P-O3	4.92	1.78	1.59
6	A	609	CHL	CMC-C2C	4.90	1.55	1.44
4	C	504	XAT	C32-C33	-4.89	1.35	1.46
6	A	613	CHL	C1B-C2B	4.88	1.45	1.39
6	A	612	CHL	C1B-C2B	4.87	1.45	1.39
2	C	501	LUX	C27-C26	-4.85	1.43	1.54
2	B	501	LUX	C9-C8	-4.80	1.37	1.51
6	A	610	CHL	C1D-C2D	4.79	1.45	1.39
6	B	613	CHL	C1B-C2B	4.75	1.44	1.39
4	A	504	XAT	C12-C13	-4.75	1.35	1.46
5	A	608	CLA	O2D-CGD	4.71	1.44	1.33
4	B	504	XAT	C32-C33	-4.70	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	612	CHL	C3B-C4B	4.69	1.46	1.41
5	C	607	CLA	MG-NA	4.65	2.17	2.06
6	A	610	CHL	C3B-C2B	-4.64	1.34	1.40
6	C	609	CHL	C1B-C2B	4.61	1.44	1.39
4	A	504	XAT	C28-C29	-4.55	1.36	1.46
3	C	503	NEX	C28-C29	-4.53	1.36	1.46
6	B	610	CHL	C1D-C2D	4.50	1.44	1.39
5	B	605	CLA	O2D-CGD	4.46	1.44	1.33
5	A	601	CLA	O2D-CGD	4.46	1.44	1.33
6	A	610	CHL	O2D-CGD	4.41	1.44	1.33
4	C	504	XAT	C28-C29	-4.41	1.36	1.46
6	B	609	CHL	CHA-CBD	4.41	1.56	1.51
4	B	504	XAT	C12-C13	-4.40	1.36	1.46
6	C	613	CHL	C1B-C2B	4.39	1.44	1.39
2	C	501	LUX	C15-C14	-4.38	1.33	1.52
6	C	612	CHL	C1B-C2B	4.36	1.44	1.39
6	C	611	CHL	O2D-CGD	4.36	1.43	1.33
2	A	502	LUX	C31-C30	-4.35	1.34	1.52
6	A	611	CHL	C1B-C2B	4.34	1.44	1.39
2	B	501	LUX	C31-C30	-4.34	1.34	1.52
6	C	610	CHL	O2D-CGD	4.32	1.43	1.33
5	C	605	CLA	O2D-CGD	4.32	1.43	1.33
6	B	610	CHL	O2D-CGD	4.31	1.43	1.33
5	C	603	CLA	O2D-CGD	4.30	1.43	1.33
2	A	502	LUX	C11-C12	-4.30	1.34	1.52
5	A	605	CLA	O2D-CGD	4.28	1.43	1.33
5	A	602	CLA	O2D-CGD	4.28	1.43	1.33
3	C	503	NEX	C32-C33	-4.27	1.36	1.46
2	A	502	LUX	C31-C32	-4.24	1.34	1.52
6	B	611	CHL	O2D-CGD	4.22	1.43	1.33
5	C	602	CLA	O2D-CGD	4.21	1.43	1.33
2	B	502	LUX	C11-C12	-4.21	1.34	1.52
5	B	602	CLA	O2D-CGD	4.20	1.43	1.33
2	B	502	LUX	C31-C32	-4.20	1.34	1.52
6	B	612	CHL	C1B-C2B	4.20	1.44	1.39
4	B	504	XAT	C28-C29	-4.19	1.37	1.46
5	B	603	CLA	O2D-CGD	4.18	1.43	1.33
2	C	502	LUX	C15-C14	-4.17	1.34	1.52
8	C	802	DGD	O5D-C1E	4.15	1.47	1.40
7	A	801	LHG	P-O6	4.10	1.75	1.59
3	B	503	NEX	C7-C6	4.10	1.35	1.30
2	A	501	LUX	C15-C14	-4.10	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	LUX	C11-C12	-4.08	1.35	1.52
3	B	503	NEX	C28-C29	-4.06	1.37	1.46
6	C	614	CHL	O2D-CGD	4.06	1.43	1.33
5	A	603	CLA	O2D-CGD	4.06	1.43	1.33
2	B	502	LUX	C31-C30	-4.05	1.35	1.52
2	A	501	LUX	C4-C5	-4.05	1.44	1.51
2	C	502	LUX	C31-C30	-4.04	1.35	1.52
6	B	614	CHL	O2D-CGD	4.01	1.43	1.33
6	A	614	CHL	O2D-CGD	3.98	1.43	1.33
2	A	501	LUX	C31-C30	-3.98	1.35	1.52
6	B	610	CHL	C3B-C2B	-3.95	1.35	1.40
3	C	503	NEX	C7-C6	3.94	1.35	1.30
7	B	801	LHG	O8-C23	3.92	1.44	1.33
2	A	501	LUX	C35-C34	-3.92	1.35	1.52
7	A	801	LHG	O8-C23	3.91	1.44	1.33
5	B	602	CLA	MG-NA	3.90	2.15	2.06
3	A	503	NEX	C7-C6	3.90	1.35	1.30
2	B	502	LUX	C32-C33	-3.90	1.33	1.52
2	B	501	LUX	C11-C12	-3.89	1.35	1.52
6	C	611	CHL	C1B-C2B	3.89	1.44	1.39
2	B	501	LUX	C35-C34	-3.89	1.35	1.52
4	C	504	XAT	C12-C13	-3.89	1.37	1.46
2	C	501	LUX	C35-C34	-3.88	1.36	1.52
2	C	502	LUX	C11-C10	-3.87	1.36	1.52
6	B	612	CHL	O2D-CGD	3.87	1.42	1.33
5	C	608	CLA	O2D-CGD	3.84	1.42	1.33
6	A	613	CHL	O2D-CGD	3.84	1.42	1.33
2	C	502	LUX	C31-C32	-3.83	1.36	1.52
2	B	501	LUX	C15-C14	-3.82	1.36	1.52
6	A	609	CHL	CHA-CBD	3.79	1.56	1.51
2	C	502	LUX	C32-C33	-3.78	1.34	1.52
2	A	502	LUX	C15-C14	-3.77	1.36	1.52
2	A	501	LUX	C11-C12	-3.77	1.36	1.52
3	A	503	NEX	C28-C29	-3.76	1.37	1.46
5	C	601	CLA	O2D-CGD	3.76	1.42	1.33
7	C	801	LHG	P-O6	3.76	1.74	1.59
5	A	607	CLA	O2D-CGD	3.74	1.42	1.33
6	C	610	CHL	C3B-C2B	-3.74	1.35	1.40
5	C	606	CLA	O2D-CGD	3.72	1.42	1.33
7	C	801	LHG	O8-C23	3.71	1.44	1.33
6	A	612	CHL	CHA-CBD	3.69	1.56	1.51
2	B	501	LUX	C30-C29	-3.68	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	LUX	C32-C33	-3.68	1.34	1.52
8	A	802	DGD	O5D-C1E	3.68	1.46	1.40
2	A	501	LUX	C31-C32	-3.68	1.36	1.52
5	B	608	CLA	O2D-CGD	3.67	1.42	1.33
2	B	502	LUX	C11-C10	-3.67	1.36	1.52
5	C	602	CLA	MG-NA	3.67	2.15	2.06
6	A	609	CHL	O2D-CGD	3.67	1.42	1.33
3	A	503	NEX	C11-C10	-3.66	1.31	1.43
2	B	501	LUX	C11-C10	-3.66	1.36	1.52
5	C	604	CLA	O2D-CGD	3.66	1.42	1.33
2	C	501	LUX	C4-C5	-3.66	1.45	1.51
2	B	501	LUX	C31-C32	-3.65	1.36	1.52
2	B	502	LUX	C12-C13	-3.64	1.34	1.52
6	C	609	CHL	O2D-CGD	3.62	1.42	1.33
6	B	613	CHL	CHA-CBD	3.62	1.55	1.51
5	A	608	CLA	CMC-C2C	3.61	1.58	1.50
6	B	611	CHL	C1B-C2B	3.60	1.43	1.39
2	B	502	LUX	C35-C34	-3.60	1.37	1.52
5	C	607	CLA	O2D-CGD	3.60	1.42	1.33
2	C	502	LUX	C35-C34	-3.59	1.37	1.52
5	A	606	CLA	O2D-CGD	3.59	1.42	1.33
2	A	502	LUX	C12-C13	-3.59	1.35	1.52
2	A	502	LUX	C32-C33	-3.58	1.35	1.52
2	C	501	LUX	C18-C5	-3.57	1.45	1.50
6	C	613	CHL	O2D-CGD	3.57	1.42	1.33
8	B	802	DGD	O5D-C1E	3.57	1.46	1.40
2	A	502	LUX	C11-C10	-3.56	1.37	1.52
2	B	501	LUX	C14-C13	-3.56	1.35	1.52
6	B	609	CHL	O2D-CGD	3.56	1.42	1.33
7	B	801	LHG	P-O6	3.55	1.73	1.59
5	B	606	CLA	O2D-CGD	3.54	1.41	1.33
6	A	611	CHL	O2D-CGD	3.54	1.41	1.33
2	C	501	LUX	C31-C30	-3.54	1.37	1.52
2	C	502	LUX	C14-C13	-3.54	1.35	1.52
4	B	504	XAT	C8-C9	-3.53	1.38	1.46
2	A	501	LUX	C14-C13	-3.53	1.35	1.52
6	C	612	CHL	O2D-CGD	3.51	1.41	1.33
2	C	502	LUX	C34-C33	-3.51	1.35	1.52
6	A	610	CHL	C1B-C2B	3.50	1.43	1.39
2	C	501	LUX	C30-C29	-3.50	1.35	1.52
5	C	601	CLA	CMC-C2C	3.50	1.57	1.50
2	C	501	LUX	C11-C12	-3.50	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	LUX	C31-C32	-3.48	1.37	1.52
5	B	607	CLA	O2D-CGD	3.48	1.41	1.33
6	A	612	CHL	O2D-CGD	3.47	1.41	1.33
6	B	613	CHL	O2D-CGD	3.47	1.41	1.33
2	C	501	LUX	C28-C29	-3.45	1.35	1.52
2	B	502	LUX	C14-C13	-3.45	1.35	1.52
6	C	609	CHL	CHA-CBD	3.42	1.55	1.51
2	B	502	LUX	C28-C29	-3.42	1.36	1.52
2	A	501	LUX	C11-C10	-3.41	1.37	1.52
2	A	501	LUX	C30-C29	-3.40	1.36	1.52
5	A	604	CLA	O2D-CGD	3.40	1.41	1.33
2	B	502	LUX	C18-C5	-3.39	1.45	1.50
6	B	612	CHL	C3B-C2B	-3.39	1.35	1.40
6	B	609	CHL	C3B-C2B	-3.39	1.35	1.40
6	A	612	CHL	C3B-C2B	-3.38	1.35	1.40
3	C	503	NEX	C15-C14	-3.38	1.32	1.43
2	C	501	LUX	C14-C13	-3.37	1.36	1.52
6	C	609	CHL	C3B-C2B	-3.37	1.35	1.40
6	A	613	CHL	CHA-CBD	3.37	1.55	1.51
2	B	502	LUX	C15-C14	-3.36	1.38	1.52
5	C	601	CLA	MG-ND	-3.35	1.99	2.05
2	B	501	LUX	C32-C33	-3.33	1.36	1.52
6	A	610	CHL	CHA-CBD	3.33	1.55	1.51
2	A	501	LUX	C28-C29	-3.32	1.36	1.52
2	B	502	LUX	C34-C33	-3.31	1.36	1.52
2	C	502	LUX	C30-C29	-3.31	1.36	1.52
2	C	501	LUX	C12-C13	-3.30	1.36	1.52
6	C	610	CHL	CHA-CBD	3.30	1.55	1.51
2	A	502	LUX	C35-C34	-3.30	1.38	1.52
5	A	601	CLA	CMC-C2C	3.30	1.57	1.50
6	C	612	CHL	CHA-CBD	3.28	1.55	1.51
6	C	610	CHL	O1D-CGD	3.28	1.29	1.21
2	B	501	LUX	C18-C5	-3.26	1.45	1.50
2	A	501	LUX	C12-C13	-3.26	1.36	1.52
2	C	502	LUX	C12-C13	-3.25	1.36	1.52
2	A	502	LUX	C30-C29	-3.24	1.36	1.52
6	A	614	CHL	MG-NB	3.23	2.12	2.05
5	B	601	CLA	O1D-CGD	3.21	1.29	1.21
2	A	501	LUX	C18-C5	-3.21	1.45	1.50
2	B	501	LUX	C12-C13	-3.20	1.37	1.52
3	B	503	NEX	C15-C14	-3.20	1.33	1.43
6	B	614	CHL	MG-NB	3.18	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	CLA	O1D-CGD	3.18	1.29	1.21
5	B	604	CLA	O1D-CGD	3.18	1.29	1.21
6	C	613	CHL	CHA-CBD	3.18	1.55	1.51
2	C	501	LUX	C11-C10	-3.17	1.38	1.52
2	A	501	LUX	C34-C33	-3.16	1.37	1.52
5	A	608	CLA	MG-NB	3.15	2.12	2.05
6	B	612	CHL	O2A-CGA	3.15	1.42	1.33
2	C	501	LUX	C35-C15	-3.13	1.36	1.51
6	A	614	CHL	C3B-C2B	-3.13	1.36	1.40
5	B	607	CLA	O2A-CGA	3.12	1.42	1.33
2	A	502	LUX	C14-C13	-3.12	1.37	1.52
2	C	502	LUX	C28-C29	-3.11	1.37	1.52
6	C	613	CHL	MG-NB	3.10	2.11	2.05
6	B	610	CHL	CHA-CBD	3.10	1.55	1.51
2	A	501	LUX	C32-C33	-3.09	1.37	1.52
6	A	613	CHL	C3A-C2A	-3.09	1.52	1.54
6	C	611	CHL	O1D-CGD	3.09	1.29	1.21
3	B	503	NEX	C11-C10	-3.08	1.33	1.43
2	A	502	LUX	C28-C29	-3.08	1.37	1.52
5	A	602	CLA	CMC-C2C	3.08	1.57	1.50
5	B	604	CLA	MG-NC	3.07	2.13	2.06
6	A	610	CHL	C3D-C2D	-3.07	1.34	1.39
5	C	602	CLA	O1D-CGD	3.07	1.29	1.21
6	A	614	CHL	CHA-CBD	3.06	1.55	1.51
2	B	501	LUX	C34-C33	-3.06	1.37	1.52
6	A	611	CHL	C3B-C2B	-3.05	1.36	1.40
5	A	603	CLA	O1D-CGD	3.05	1.28	1.21
2	B	501	LUX	C28-C29	-3.05	1.37	1.52
2	A	502	LUX	C7-C6	-3.04	1.34	1.45
6	B	614	CHL	O1D-CGD	3.04	1.28	1.21
6	B	614	CHL	CHA-CBD	3.04	1.55	1.51
6	C	611	CHL	C3B-C2B	-3.03	1.36	1.40
2	B	501	LUX	C35-C15	-3.03	1.36	1.51
2	C	501	LUX	C34-C33	-3.01	1.38	1.52
5	B	608	CLA	O1D-CGD	3.01	1.28	1.21
2	B	501	LUX	C4-C5	-3.01	1.46	1.51
2	A	501	LUX	C35-C15	-3.01	1.36	1.51
4	C	504	XAT	C4-C3	3.00	1.56	1.52
3	C	503	NEX	C11-C10	-2.99	1.33	1.43
6	A	612	CHL	O2A-CGA	2.99	1.42	1.33
5	A	604	CLA	MG-NC	2.99	2.13	2.06
2	A	502	LUX	C34-C33	-2.97	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	608	CLA	MG-NC	2.96	2.13	2.06
5	B	602	CLA	O1D-CGD	2.96	1.28	1.21
5	B	604	CLA	CMC-C2C	2.95	1.56	1.50
6	A	610	CHL	O1D-CGD	2.95	1.28	1.21
6	C	612	CHL	C3B-C2B	-2.94	1.36	1.40
3	A	503	NEX	C15-C14	-2.94	1.34	1.43
6	B	611	CHL	CHA-CBD	2.93	1.55	1.51
2	B	502	LUX	C30-C29	-2.92	1.38	1.52
5	C	607	CLA	O2A-CGA	2.91	1.41	1.33
2	B	502	LUX	C16-C1	-2.91	1.48	1.53
5	A	601	CLA	MG-ND	-2.91	2.00	2.05
6	C	612	CHL	O2A-CGA	2.90	1.41	1.33
7	C	801	LHG	O7-C7	2.89	1.42	1.34
3	C	503	NEX	C35-C34	-2.89	1.34	1.43
2	A	501	LUX	C17-C1	-2.88	1.48	1.53
6	B	612	CHL	CHA-CBD	2.88	1.55	1.51
5	C	601	CLA	O1D-CGD	2.88	1.28	1.21
6	B	610	CHL	C2-C3	2.88	1.39	1.33
5	C	605	CLA	CMC-C2C	2.88	1.56	1.50
2	C	502	LUX	C35-C15	-2.87	1.37	1.51
4	C	504	XAT	C8-C9	-2.87	1.39	1.46
5	A	607	CLA	O2A-CGA	2.87	1.41	1.33
5	A	604	CLA	MG-ND	-2.87	2.00	2.05
5	B	605	CLA	CMC-C2C	2.86	1.56	1.50
2	A	501	LUX	C7-C6	-2.85	1.35	1.45
6	B	609	CHL	MG-NB	2.85	2.11	2.05
6	A	614	CHL	O1D-CGD	2.85	1.28	1.21
6	C	614	CHL	MG-NB	2.85	2.11	2.05
5	A	604	CLA	O1D-CGD	2.85	1.28	1.21
5	A	605	CLA	CMC-C2C	2.84	1.56	1.50
5	A	606	CLA	CMC-C2C	2.84	1.56	1.50
6	B	611	CHL	C3B-C2B	-2.84	1.36	1.40
6	A	613	CHL	MG-NB	2.84	2.11	2.05
5	B	601	CLA	C2-C3	2.84	1.39	1.33
5	C	604	CLA	CMC-C2C	2.84	1.56	1.50
5	C	606	CLA	CMC-C2C	2.83	1.56	1.50
5	B	602	CLA	CMC-C2C	2.82	1.56	1.50
6	A	613	CHL	O2A-CGA	2.82	1.40	1.30
5	C	601	CLA	MG-NC	2.82	2.13	2.06
2	B	502	LUX	C4-C5	-2.81	1.46	1.51
2	C	502	LUX	O23-C23	-2.81	1.38	1.43
5	C	602	CLA	CMC-C2C	2.81	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	612	CHL	C1A-CHA	2.80	1.43	1.40
6	C	614	CHL	O1D-CGD	2.80	1.28	1.21
2	C	501	LUX	C7-C6	-2.79	1.35	1.45
8	A	802	DGD	O3G-C1D	2.79	1.44	1.40
5	C	605	CLA	O1D-CGD	2.78	1.28	1.21
5	C	602	CLA	MG-ND	-2.78	2.00	2.05
5	B	605	CLA	O1D-CGD	2.78	1.28	1.21
5	A	601	CLA	O2A-CGA	2.77	1.41	1.33
2	A	502	LUX	C18-C5	-2.77	1.46	1.50
6	A	613	CHL	O1D-CGD	2.76	1.28	1.21
6	C	609	CHL	OMC-CMC	2.76	1.28	1.22
5	C	601	CLA	C1B-NB	-2.76	1.34	1.37
4	C	504	XAT	C15-C14	-2.75	1.34	1.43
5	C	608	CLA	O2A-CGA	2.75	1.41	1.33
6	C	613	CHL	O2A-CGA	2.75	1.39	1.30
2	B	502	LUX	C7-C6	-2.74	1.35	1.45
2	B	501	LUX	C7-C6	-2.73	1.35	1.45
6	C	610	CHL	C2-C3	2.72	1.39	1.33
5	A	608	CLA	MG-NC	2.72	2.12	2.06
6	C	609	CHL	MG-NB	2.72	2.11	2.05
4	B	504	XAT	C4-C3	2.71	1.56	1.52
5	B	607	CLA	MG-NB	2.70	2.11	2.05
6	A	610	CHL	C2-C3	2.70	1.39	1.33
5	B	608	CLA	MG-NB	2.70	2.11	2.05
6	C	610	CHL	O2A-CGA	2.70	1.41	1.33
5	A	604	CLA	CMC-C2C	2.69	1.56	1.50
6	B	610	CHL	O2A-CGA	2.69	1.41	1.33
5	B	606	CLA	CMC-C2C	2.69	1.56	1.50
6	B	609	CHL	O1D-CGD	2.69	1.28	1.21
6	A	610	CHL	MG-ND	-2.68	2.00	2.05
6	C	614	CHL	CHA-CBD	2.68	1.54	1.51
6	A	610	CHL	O2A-CGA	2.68	1.41	1.33
5	C	606	CLA	MG-NC	2.68	2.12	2.06
5	C	601	CLA	MG-NB	2.68	2.11	2.05
5	B	601	CLA	O2D-CGD	2.68	1.39	1.33
2	A	502	LUX	C35-C15	-2.68	1.38	1.51
6	C	613	CHL	O1D-CGD	2.68	1.28	1.21
6	B	613	CHL	MG-NB	2.67	2.11	2.05
2	B	502	LUX	C35-C15	-2.67	1.38	1.51
6	B	611	CHL	MG-ND	-2.66	2.00	2.05
6	A	610	CHL	CAC-C3C	2.66	1.56	1.51
5	B	608	CLA	O2A-CGA	2.66	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	604	CLA	O1D-CGD	2.65	1.27	1.21
5	B	603	CLA	CMC-C2C	2.65	1.56	1.50
6	C	612	CHL	C2-C3	2.65	1.39	1.33
6	B	613	CHL	O2A-CGA	2.64	1.39	1.30
7	B	801	LHG	O7-C5	-2.64	1.40	1.46
4	A	504	XAT	C15-C14	-2.63	1.35	1.43
5	B	607	CLA	CMC-C2C	2.63	1.56	1.50
5	A	608	CLA	O2A-CGA	2.63	1.41	1.33
4	A	504	XAT	C4-C5	2.63	1.55	1.52
4	C	504	XAT	C11-C10	-2.62	1.35	1.43
6	A	611	CHL	O1D-CGD	2.61	1.27	1.21
6	A	612	CHL	C2-C3	2.60	1.39	1.33
2	C	502	LUX	C7-C6	-2.60	1.36	1.45
5	C	603	CLA	O1D-CGD	2.60	1.27	1.21
5	B	606	CLA	MG-NC	2.60	2.12	2.06
6	A	611	CHL	MG-ND	-2.60	2.00	2.05
5	C	603	CLA	CMC-C2C	2.59	1.56	1.50
6	B	610	CHL	O1D-CGD	2.59	1.27	1.21
5	C	606	CLA	O1D-CGD	2.58	1.27	1.21
6	A	612	CHL	MG-NB	2.58	2.10	2.05
4	B	504	XAT	C4-C5	2.58	1.55	1.52
5	C	608	CLA	O1D-CGD	2.58	1.27	1.21
3	B	503	NEX	C31-C30	-2.58	1.35	1.43
8	C	802	DGD	O3G-C1D	2.58	1.44	1.40
7	A	801	LHG	O7-C7	2.58	1.41	1.34
8	C	802	DGD	O6D-C1D	2.58	1.48	1.41
6	C	609	CHL	CBD-CGD	2.57	1.55	1.52
5	A	603	CLA	MG-NA	2.57	2.12	2.06
5	A	601	CLA	MG-NB	2.57	2.10	2.05
5	A	608	CLA	O1D-CGD	2.57	1.27	1.21
6	B	613	CHL	C3A-C2A	-2.57	1.52	1.54
5	B	606	CLA	MG-NB	2.54	2.10	2.05
5	C	607	CLA	CMC-C2C	2.54	1.56	1.50
5	A	607	CLA	CMC-C2C	2.53	1.56	1.50
5	B	608	CLA	CMC-C2C	2.53	1.56	1.50
6	C	609	CHL	O1D-CGD	2.52	1.27	1.21
5	B	607	CLA	C2-C3	2.51	1.38	1.33
6	A	611	CHL	C1-C2	-2.50	1.42	1.49
8	B	802	DGD	C4E-C3E	2.50	1.58	1.52
6	B	609	CHL	CBD-CGD	2.50	1.55	1.52
3	A	503	NEX	C37-C21	-2.50	1.49	1.53
4	C	504	XAT	C16-C1	-2.49	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	610	CHL	C3D-C2D	-2.49	1.35	1.39
6	C	609	CHL	O2A-CGA	2.49	1.40	1.33
5	B	601	CLA	MG-NB	2.49	2.10	2.05
5	C	602	CLA	O2A-CGA	2.49	1.40	1.33
3	A	503	NEX	C31-C30	-2.49	1.35	1.43
3	B	503	NEX	C37-C21	-2.49	1.49	1.53
6	B	609	CHL	CAC-C3C	2.49	1.56	1.51
6	B	612	CHL	C2-C3	2.48	1.38	1.33
2	C	502	LUX	C16-C1	-2.48	1.49	1.53
6	B	611	CHL	O1D-CGD	2.48	1.27	1.21
5	C	604	CLA	MG-NC	2.48	2.12	2.06
5	A	607	CLA	C2-C3	2.46	1.38	1.33
5	B	602	CLA	O2A-CGA	2.46	1.40	1.33
4	C	504	XAT	C4-C5	2.46	1.55	1.52
2	A	502	LUX	C16-C1	-2.45	1.49	1.53
5	B	602	CLA	C2-C3	2.45	1.38	1.33
6	B	610	CHL	MG-NB	2.43	2.10	2.05
6	B	613	CHL	O1D-CGD	2.43	1.27	1.21
2	A	501	LUX	C16-C1	-2.43	1.49	1.53
5	A	603	CLA	CMC-C2C	2.43	1.55	1.50
3	B	503	NEX	C35-C34	-2.42	1.35	1.43
6	C	611	CHL	MG-ND	-2.42	2.01	2.05
5	A	607	CLA	MG-NB	2.42	2.10	2.05
4	A	504	XAT	C8-C9	-2.42	1.40	1.46
8	A	802	DGD	O6D-C1D	2.42	1.48	1.41
6	C	610	CHL	C3D-C2D	-2.42	1.35	1.39
5	A	602	CLA	C2-C3	2.41	1.38	1.33
6	C	612	CHL	C2C-C3C	2.41	1.38	1.36
5	B	603	CLA	MG-NC	2.41	2.12	2.06
6	B	611	CHL	C1-C2	-2.41	1.42	1.49
4	A	504	XAT	C2-C1	-2.41	1.50	1.54
5	C	606	CLA	MG-NB	2.40	2.10	2.05
5	B	605	CLA	C2-C3	2.40	1.38	1.33
6	C	612	CHL	MG-NB	2.39	2.10	2.05
6	C	609	CHL	C2C-C3C	2.39	1.38	1.36
2	C	502	LUX	C4-C5	-2.39	1.47	1.51
5	C	607	CLA	C2-C3	2.39	1.38	1.33
4	B	504	XAT	C20-C13	-2.37	1.46	1.50
6	A	611	CHL	C3D-C4D	2.37	1.45	1.41
5	A	602	CLA	O2A-CGA	2.36	1.40	1.33
6	C	611	CHL	MG-NB	2.36	2.10	2.05
5	C	608	CLA	MG-NB	2.36	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	613	CHL	OBD-CAD	2.36	1.25	1.22
5	A	606	CLA	MG-NB	2.35	2.10	2.05
5	B	603	CLA	O2A-CGA	2.35	1.40	1.33
5	A	605	CLA	O1D-CGD	2.35	1.27	1.21
5	A	603	CLA	O2A-CGA	2.35	1.40	1.33
5	A	605	CLA	C2-C3	2.35	1.38	1.33
6	B	611	CHL	C3D-C4D	2.34	1.45	1.41
7	C	801	LHG	O7-C5	-2.34	1.41	1.46
5	B	607	CLA	CHC-C1C	2.34	1.43	1.38
3	A	503	NEX	C35-C34	-2.34	1.35	1.43
4	B	504	XAT	C31-C30	-2.32	1.36	1.43
5	A	607	CLA	O1D-CGD	2.31	1.27	1.21
5	C	605	CLA	MG-NB	2.31	2.10	2.05
6	A	612	CHL	C2C-C3C	2.31	1.38	1.36
6	A	613	CHL	OBD-CAD	2.31	1.25	1.22
5	A	601	CLA	O1D-CGD	2.31	1.27	1.21
6	A	611	CHL	MG-NB	2.31	2.10	2.05
5	A	602	CLA	MG-NC	2.30	2.11	2.06
4	B	504	XAT	C15-C14	-2.30	1.36	1.43
5	B	601	CLA	CMC-C2C	2.29	1.55	1.50
6	B	609	CHL	MG-ND	-2.29	2.01	2.05
5	B	605	CLA	O2A-CGA	2.29	1.40	1.33
5	A	608	CLA	CHD-C4C	2.28	1.44	1.39
5	B	606	CLA	O2A-CGA	2.28	1.40	1.33
6	A	609	CHL	OBD-CAD	2.27	1.25	1.22
6	A	609	CHL	C3B-C2B	-2.27	1.37	1.40
5	B	606	CLA	O1D-CGD	2.27	1.27	1.21
6	C	612	CHL	CBA-CGA	2.26	1.57	1.50
7	A	801	LHG	O7-C5	-2.26	1.41	1.46
6	C	614	CHL	C3B-C2B	-2.26	1.37	1.40
5	C	605	CLA	O2A-CGA	2.26	1.39	1.33
5	A	605	CLA	O2A-CGA	2.25	1.39	1.33
6	B	614	CHL	C3B-C2B	-2.25	1.37	1.40
6	B	610	CHL	CHC-C1C	2.25	1.43	1.39
5	C	607	CLA	MG-NB	2.24	2.10	2.05
2	A	502	LUX	C17-C1	-2.24	1.49	1.53
5	B	603	CLA	O1D-CGD	2.24	1.26	1.21
5	B	605	CLA	MG-NA	2.24	2.11	2.06
5	B	604	CLA	MG-ND	-2.24	2.01	2.05
8	C	802	DGD	O6E-C1E	2.23	1.47	1.41
6	A	614	CHL	CHC-C4B	2.23	1.43	1.39
5	B	601	CLA	MG-NC	2.23	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	610	CHL	MG-NB	2.23	2.10	2.05
4	C	504	XAT	C31-C30	-2.23	1.36	1.43
4	A	504	XAT	C24-C25	-2.22	1.49	1.52
5	A	602	CLA	MG-ND	-2.22	2.01	2.05
6	A	609	CHL	MG-NB	2.22	2.10	2.05
5	B	601	CLA	MG-NA	2.22	2.11	2.06
6	A	614	CHL	C1A-CHA	2.21	1.42	1.40
5	C	601	CLA	O2A-CGA	2.21	1.39	1.33
3	C	503	NEX	C31-C30	-2.21	1.36	1.43
6	B	611	CHL	MG-NB	2.21	2.10	2.05
7	B	801	LHG	O7-C7	2.20	1.40	1.34
2	B	501	LUX	C17-C1	-2.20	1.49	1.53
6	B	610	CHL	C3D-CAD	-2.20	1.43	1.47
5	C	605	CLA	C2-C3	2.20	1.38	1.33
8	B	802	DGD	O6E-C1E	2.20	1.47	1.41
5	B	603	CLA	C1B-NB	-2.20	1.35	1.37
6	A	609	CHL	O2A-CGA	2.19	1.39	1.33
6	C	611	CHL	CHA-CBD	2.19	1.54	1.51
5	A	606	CLA	MG-NC	2.19	2.11	2.06
5	A	601	CLA	C2-C3	2.19	1.38	1.33
8	B	802	DGD	O6D-C1D	2.19	1.47	1.41
6	A	611	CHL	C5-C3	2.19	1.55	1.51
4	A	504	XAT	C35-C34	-2.19	1.36	1.43
5	B	605	CLA	MG-NC	2.17	2.11	2.06
5	A	607	CLA	CHD-C1D	2.17	1.42	1.38
5	C	602	CLA	C2-C3	2.17	1.38	1.33
6	C	609	CHL	MG-ND	-2.17	2.01	2.05
2	A	502	LUX	C4-C5	-2.17	1.47	1.51
5	B	606	CLA	C2-C3	2.16	1.38	1.33
5	B	603	CLA	MG-ND	-2.16	2.01	2.05
6	C	611	CHL	C4-C3	2.16	1.56	1.50
5	C	607	CLA	MG-NC	2.16	2.11	2.06
5	C	605	CLA	MG-NC	2.16	2.11	2.06
5	B	602	CLA	MG-NB	2.16	2.10	2.05
4	A	504	XAT	C31-C30	-2.16	1.36	1.43
6	B	612	CHL	C3D-C2D	-2.15	1.36	1.39
6	B	612	CHL	CBA-CGA	2.15	1.56	1.50
5	A	608	CLA	C3B-C2B	-2.14	1.33	1.41
6	C	611	CHL	C3D-C4D	2.14	1.44	1.41
5	C	603	CLA	C2-C3	2.13	1.38	1.33
4	B	504	XAT	C16-C1	-2.13	1.49	1.53
6	C	610	CHL	CAC-C3C	2.13	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	603	CLA	C2-C3	2.13	1.38	1.33
2	C	501	LUX	C23-C24	2.13	1.53	1.50
5	A	606	CLA	O1D-CGD	2.12	1.26	1.21
5	B	608	CLA	MG-NC	2.12	2.11	2.06
5	C	603	CLA	MG-NB	2.12	2.10	2.05
6	C	611	CHL	C3A-C2A	-2.12	1.52	1.54
4	B	504	XAT	C35-C34	-2.11	1.36	1.43
5	A	604	CLA	O2A-CGA	2.11	1.39	1.33
4	A	504	XAT	C16-C1	-2.11	1.49	1.53
6	A	609	CHL	O1D-CGD	2.11	1.26	1.21
4	A	504	XAT	C17-C1	-2.11	1.49	1.53
4	B	504	XAT	C11-C10	-2.11	1.36	1.43
5	C	604	CLA	O2A-CGA	2.11	1.39	1.33
5	B	601	CLA	C5-C3	2.11	1.55	1.51
6	A	609	CHL	C2C-C3C	2.10	1.38	1.36
5	B	601	CLA	O2A-CGA	2.10	1.39	1.33
6	C	609	CHL	C3D-C2D	-2.10	1.36	1.39
4	C	504	XAT	C35-C34	-2.10	1.36	1.43
8	C	802	DGD	C4E-C3E	2.10	1.57	1.52
5	B	604	CLA	O2A-CGA	2.10	1.39	1.33
5	A	603	CLA	MG-NC	2.10	2.11	2.06
5	B	603	CLA	C2-C3	2.10	1.37	1.33
6	C	610	CHL	CHC-C4B	2.10	1.43	1.39
6	B	609	CHL	C1-C2	-2.09	1.43	1.49
6	A	611	CHL	CHA-CBD	2.09	1.54	1.51
6	C	612	CHL	O1D-CGD	2.09	1.26	1.21
6	C	611	CHL	O2A-CGA	2.08	1.39	1.33
6	B	613	CHL	MG-ND	-2.07	2.01	2.05
2	C	501	LUX	C1-C6	-2.07	1.51	1.53
6	A	609	CHL	CAC-C3C	2.06	1.55	1.51
5	C	603	CLA	MG-NC	2.06	2.11	2.06
3	B	503	NEX	C28-C27	2.06	1.37	1.32
6	B	609	CHL	O2A-CGA	2.05	1.39	1.33
6	C	612	CHL	C1A-CHA	2.05	1.42	1.40
5	B	607	CLA	O1D-CGD	2.04	1.26	1.21
5	B	602	CLA	MG-ND	-2.04	2.01	2.05
6	C	610	CHL	MG-ND	-2.04	2.01	2.05
5	C	603	CLA	O2A-CGA	2.04	1.39	1.33
5	C	601	CLA	C2-C3	2.04	1.37	1.33
5	C	607	CLA	O1D-CGD	2.04	1.26	1.21
2	B	502	LUX	C17-C1	-2.04	1.49	1.53
6	B	612	CHL	C5-C3	2.03	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	604	CLA	C1-C2	-2.03	1.43	1.49
5	B	603	CLA	MG-NB	2.03	2.09	2.05
4	A	504	XAT	C8-C7	2.01	1.37	1.32
6	C	613	CHL	CHB-C4A	2.01	1.41	1.38
6	A	612	CHL	O1D-CGD	2.01	1.26	1.21
5	C	605	CLA	MG-ND	-2.01	2.01	2.05
4	B	504	XAT	C8-C7	2.01	1.37	1.32
6	C	611	CHL	OBD-CAD	2.01	1.24	1.22
6	C	609	CHL	OBD-CAD	2.00	1.24	1.22
2	B	501	LUX	C16-C1	-2.00	1.50	1.53
5	A	606	CLA	C2-C3	2.00	1.37	1.33
4	A	504	XAT	C11-C10	-2.00	1.37	1.43
5	A	608	CLA	CHD-C1D	2.00	1.42	1.38

All (891) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LUX	C27-C26-C25	13.26	136.38	111.92
6	B	614	CHL	C1B-CHB-C4A	12.88	129.61	121.32
2	C	501	LUX	C27-C26-C25	12.84	135.60	111.92
2	B	502	LUX	C27-C26-C25	12.51	135.00	111.92
2	B	501	LUX	C27-C26-C25	12.51	134.99	111.92
6	C	614	CHL	C1B-CHB-C4A	12.35	129.26	121.32
2	A	502	LUX	C27-C26-C25	12.28	134.56	111.92
6	A	609	CHL	C1B-CHB-C4A	12.21	129.18	121.32
6	C	612	CHL	C1B-CHB-C4A	12.16	129.14	121.32
6	A	612	CHL	C1B-CHB-C4A	12.06	129.08	121.32
6	C	610	CHL	C1B-CHB-C4A	12.04	129.06	121.32
6	B	612	CHL	C1B-CHB-C4A	11.95	129.01	121.32
6	A	614	CHL	C1B-CHB-C4A	11.88	128.97	121.32
6	B	611	CHL	C1B-CHB-C4A	11.75	128.88	121.32
6	A	610	CHL	C1B-CHB-C4A	11.70	128.85	121.32
6	A	613	CHL	C1B-CHB-C4A	11.63	128.80	121.32
6	B	609	CHL	C1B-CHB-C4A	11.58	128.77	121.32
2	C	502	LUX	C27-C26-C25	11.55	133.22	111.92
6	A	611	CHL	C1B-CHB-C4A	11.45	128.69	121.32
6	C	613	CHL	C1B-CHB-C4A	11.31	128.60	121.32
6	C	609	CHL	C1B-CHB-C4A	11.27	128.57	121.32
6	B	613	CHL	C1B-CHB-C4A	11.16	128.50	121.32
6	C	611	CHL	C1B-CHB-C4A	11.03	128.42	121.32
2	A	502	LUX	C37-C21-C36	10.93	123.78	107.87
3	B	503	NEX	O24-C25-C26	10.46	67.22	58.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	LUX	C37-C21-C36	10.41	123.03	107.87
6	B	610	CHL	C1B-CHB-C4A	10.38	128.00	121.32
4	B	504	XAT	C37-C21-C22	-10.24	90.97	108.97
4	A	504	XAT	C37-C21-C22	-10.21	91.02	108.97
5	C	608	CLA	C4A-NA-C1A	10.14	111.31	106.68
2	B	502	LUX	C37-C21-C36	10.11	122.59	107.87
3	A	503	NEX	O24-C25-C26	9.89	66.77	58.93
5	B	607	CLA	C4A-NA-C1A	9.86	111.18	106.68
2	A	501	LUX	C37-C21-C26	-9.82	92.99	110.49
2	C	501	LUX	C37-C21-C36	9.74	122.05	107.87
3	C	503	NEX	O24-C25-C26	9.73	66.64	58.93
4	C	504	XAT	O24-C25-C26	9.59	66.53	58.93
5	A	607	CLA	C4A-NA-C1A	9.51	111.02	106.68
2	B	501	LUX	C37-C21-C36	9.46	121.64	107.87
5	B	602	CLA	C4A-NA-C1A	9.45	110.99	106.68
5	C	607	CLA	C4A-NA-C1A	9.32	110.93	106.68
2	C	501	LUX	C37-C21-C26	-9.30	93.91	110.49
5	C	605	CLA	C4A-NA-C1A	9.30	110.92	106.68
5	A	608	CLA	C4A-NA-C1A	9.20	110.88	106.68
5	A	606	CLA	C4A-NA-C1A	9.09	110.83	106.68
5	C	602	CLA	C4A-NA-C1A	9.07	110.81	106.68
4	A	504	XAT	O24-C25-C26	9.06	66.11	58.93
5	C	606	CLA	C4A-NA-C1A	9.03	110.80	106.68
4	B	504	XAT	O24-C25-C26	8.98	66.05	58.93
2	A	501	LUX	C37-C21-C36	8.97	120.92	107.87
5	B	605	CLA	C4A-NA-C1A	8.88	110.73	106.68
5	C	601	CLA	C4A-NA-C1A	8.80	110.69	106.68
5	A	603	CLA	C4A-NA-C1A	8.76	110.68	106.68
5	A	605	CLA	C4A-NA-C1A	8.71	110.66	106.68
5	B	606	CLA	C4A-NA-C1A	8.70	110.65	106.68
5	C	603	CLA	C4A-NA-C1A	8.63	110.61	106.68
8	A	802	DGD	O6E-C5E-C4E	8.59	125.18	109.70
5	A	602	CLA	C4A-NA-C1A	8.58	110.59	106.68
5	B	603	CLA	C4A-NA-C1A	8.58	110.59	106.68
2	A	502	LUX	C37-C21-C26	-8.57	95.21	110.49
8	C	802	DGD	O6E-C5E-C4E	8.48	124.97	109.70
8	B	802	DGD	O6E-C5E-C4E	8.46	124.94	109.70
4	C	504	XAT	C37-C21-C22	-8.20	94.55	108.97
2	B	501	LUX	C37-C21-C26	-8.14	95.97	110.49
2	B	502	LUX	C1-C6-C5	-8.13	111.53	122.64
2	C	502	LUX	C18-C5-C6	-7.89	115.87	124.48
5	B	608	CLA	C4A-NA-C1A	7.88	110.27	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	CLA	C4A-NA-C1A	7.79	110.23	106.68
5	C	604	CLA	C4A-NA-C1A	7.49	110.10	106.68
2	C	502	LUX	C28-C27-C26	7.47	128.35	114.23
6	C	614	CHL	O2D-CGD-CBD	7.39	119.07	110.95
2	B	502	LUX	C28-C27-C26	7.35	128.14	114.23
5	A	601	CLA	C4A-NA-C1A	7.35	110.03	106.68
6	B	609	CHL	O2D-CGD-CBD	7.33	119.00	110.95
5	B	604	CLA	C4A-NA-C1A	7.27	110.00	106.68
6	A	609	CHL	O2D-CGD-CBD	7.21	118.87	110.95
2	C	502	LUX	C1-C6-C5	-7.18	112.83	122.64
3	B	503	NEX	C1-C2-C3	7.16	129.31	113.59
2	A	502	LUX	C28-C27-C26	7.16	127.76	114.23
2	B	501	LUX	C28-C27-C26	7.13	127.72	114.23
6	A	614	CHL	O2D-CGD-CBD	7.12	118.77	110.95
6	B	614	CHL	O2D-CGD-CBD	7.09	118.74	110.95
3	C	503	NEX	C1-C2-C3	7.09	129.14	113.59
3	A	503	NEX	C1-C2-C3	7.05	129.06	113.59
2	C	501	LUX	C28-C27-C26	7.03	127.52	114.23
5	A	604	CLA	C4A-NA-C1A	6.99	109.87	106.68
2	B	502	LUX	C37-C21-C26	-6.85	98.28	110.49
6	A	612	CHL	O2D-CGD-CBD	6.73	118.34	110.95
2	C	502	LUX	C37-C21-C26	-6.62	98.69	110.49
6	B	612	CHL	O2D-CGD-CBD	6.54	118.14	110.95
6	C	609	CHL	O2D-CGD-CBD	6.49	118.08	110.95
4	B	504	XAT	O4-C5-C18	-6.30	108.00	115.05
6	C	612	CHL	O2D-CGD-CBD	6.16	117.71	110.95
6	B	610	CHL	O2D-CGD-CBD	6.08	117.62	110.95
2	B	501	LUX	C36-C21-C26	-6.07	99.67	110.49
6	A	613	CHL	O2D-CGD-CBD	6.05	117.60	110.95
6	A	610	CHL	O2D-CGD-CBD	5.89	117.42	110.95
2	B	502	LUX	C36-C21-C22	5.82	120.25	109.41
2	B	501	LUX	O23-C23-C22	5.80	120.33	110.06
2	A	501	LUX	C36-C21-C26	-5.79	100.17	110.49
6	B	613	CHL	O2D-CGD-CBD	5.73	117.24	110.95
2	A	502	LUX	C1-C6-C5	-5.70	114.84	122.64
6	C	613	CHL	O2D-CGD-CBD	5.69	117.19	110.95
2	A	501	LUX	C28-C27-C26	5.65	124.92	114.23
7	A	801	LHG	C25-C24-C23	5.59	134.18	113.69
2	C	502	LUX	C31-C30-C29	5.51	134.26	115.97
2	C	501	LUX	C36-C21-C26	-5.46	100.76	110.49
2	B	501	LUX	C36-C21-C22	5.34	119.36	109.41
2	B	502	LUX	C18-C5-C6	-5.30	118.70	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	610	CHL	O2D-CGD-CBD	5.30	116.77	110.95
5	C	601	CLA	CAA-C2A-C3A	-5.29	98.69	113.00
7	C	801	LHG	C25-C24-C23	5.27	133.00	113.69
8	C	802	DGD	O6D-C5D-C6D	5.24	117.09	106.69
4	C	504	XAT	O4-C6-C7	-5.23	101.89	116.88
8	A	802	DGD	O6D-C5D-C6D	5.22	117.04	106.69
7	B	801	LHG	C25-C24-C23	5.21	132.77	113.69
6	A	611	CHL	O2D-CGD-CBD	5.16	116.61	110.95
2	B	502	LUX	C31-C30-C29	5.12	132.97	115.97
2	C	502	LUX	C36-C21-C22	5.03	118.78	109.41
8	B	802	DGD	O6D-C5D-C6D	4.98	116.56	106.69
6	C	609	CHL	CMA-C3A-C4A	-4.97	103.90	114.61
6	B	611	CHL	O2D-CGD-CBD	4.94	116.38	110.95
2	B	502	LUX	C19-C9-C8	4.92	121.06	110.82
6	A	609	CHL	CMA-C3A-C4A	-4.91	104.02	114.61
2	A	502	LUX	C36-C21-C22	4.90	118.55	109.41
4	B	504	XAT	O4-C6-C7	-4.89	102.86	116.88
6	B	609	CHL	CMA-C3A-C4A	-4.86	104.13	114.61
2	C	501	LUX	O23-C23-C22	4.83	118.62	110.06
4	C	504	XAT	O4-C5-C18	-4.82	109.66	115.05
4	C	504	XAT	C18-C5-C4	4.81	119.65	114.24
3	A	503	NEX	O24-C25-C38	-4.79	109.69	115.05
6	A	611	CHL	C3D-C4D-CHA	4.78	115.81	108.54
6	C	611	CHL	C3D-C4D-CHA	4.76	115.77	108.54
6	B	611	CHL	C4D-CHA-CBD	-4.73	104.20	108.97
6	C	611	CHL	C4D-CHA-CBD	-4.71	104.22	108.97
6	A	611	CHL	C4D-CHA-CBD	-4.69	104.24	108.97
5	B	601	CLA	CAA-C2A-C3A	-4.69	100.34	113.00
4	A	504	XAT	C19-C9-C10	-4.66	115.27	122.82
6	C	611	CHL	O2D-CGD-CBD	4.64	116.05	110.95
2	A	502	LUX	C18-C5-C6	-4.63	119.43	124.48
5	A	605	CLA	O2D-CGD-CBD	4.62	119.30	111.23
6	C	614	CHL	C3D-C4D-CHA	4.60	115.53	108.54
6	B	610	CHL	C3D-C4D-CHA	4.60	115.53	108.54
2	A	502	LUX	C31-C30-C29	4.58	131.18	115.97
6	A	614	CHL	C3D-C4D-CHA	4.57	115.49	108.54
6	A	613	CHL	C3D-C4D-CHA	4.55	115.45	108.54
6	C	613	CHL	C3D-C4D-CHA	4.52	115.42	108.54
5	B	604	CLA	CAA-C2A-C3A	-4.51	100.81	113.00
6	B	614	CHL	C3D-C4D-CHA	4.47	115.33	108.54
6	A	612	CHL	C3D-C4D-CHA	4.46	115.32	108.54
2	B	501	LUX	C19-C9-C8	4.44	120.07	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	802	DGD	O5D-C1E-C2E	4.43	115.01	108.27
6	B	613	CHL	C3D-C4D-CHA	4.43	115.28	108.54
2	A	501	LUX	C36-C21-C22	4.43	117.66	109.41
6	B	611	CHL	C3D-C4D-CHA	4.42	115.26	108.54
4	A	504	XAT	O4-C6-C7	-4.42	104.22	116.88
5	C	607	CLA	O2D-CGD-CBD	4.41	118.93	111.23
4	B	504	XAT	C15-C14-C13	-4.40	121.11	127.28
5	A	607	CLA	O2D-CGD-CBD	4.37	118.88	111.23
4	A	504	XAT	O4-C5-C18	-4.36	110.18	115.05
6	C	612	CHL	C4D-CHA-CBD	-4.35	104.58	108.97
5	A	604	CLA	CAA-C2A-C3A	-4.35	101.24	113.00
6	A	610	CHL	C3D-C4D-CHA	4.34	115.13	108.54
6	B	612	CHL	C3D-C4D-CHA	4.34	115.13	108.54
6	A	614	CHL	C4D-CHA-CBD	-4.33	104.60	108.97
2	C	502	LUX	C19-C9-C8	4.32	119.83	110.82
6	C	610	CHL	C3D-C4D-CHA	4.32	115.11	108.54
6	B	609	CHL	C3D-C4D-CHA	4.32	115.10	108.54
5	B	607	CLA	O2D-CGD-CBD	4.31	118.76	111.23
2	C	501	LUX	C36-C21-C22	4.30	117.42	109.41
7	C	801	LHG	O8-C23-C24	4.30	124.95	111.83
3	B	503	NEX	C39-C29-C30	-4.29	115.86	122.82
3	B	503	NEX	C28-C29-C30	4.25	125.70	119.01
6	C	614	CHL	CBC-CAC-C3C	-4.25	106.79	112.87
6	B	614	CHL	C4D-CHA-CBD	-4.24	104.69	108.97
6	C	612	CHL	C3D-C4D-CHA	4.24	114.98	108.54
5	C	604	CLA	CAA-C2A-C3A	-4.21	101.62	113.00
8	C	802	DGD	C3G-O3G-C1D	-4.21	106.49	113.68
2	A	501	LUX	C31-C30-C29	4.18	129.84	115.97
6	A	612	CHL	C4D-CHA-CBD	-4.17	104.77	108.97
3	C	503	NEX	C40-C33-C34	-4.15	116.09	122.82
7	B	801	LHG	O8-C23-C24	4.15	124.47	111.83
6	B	611	CHL	C1-C2-C3	4.14	132.99	126.20
2	C	502	LUX	C15-C14-C13	4.14	129.72	115.97
6	A	609	CHL	C3D-C4D-CHA	4.13	114.82	108.54
2	A	501	LUX	C19-C9-C8	4.13	119.43	110.82
6	C	609	CHL	C3D-C4D-CHA	4.09	114.76	108.54
6	C	611	CHL	OMC-CMC-C2C	-4.08	118.03	125.12
6	C	614	CHL	C4D-CHA-CBD	-4.08	104.86	108.97
2	B	501	LUX	C31-C30-C29	4.07	129.50	115.97
2	C	501	LUX	C31-C30-C29	4.07	129.50	115.97
6	B	611	CHL	OMC-CMC-C2C	-4.07	118.05	125.12
6	B	610	CHL	C4D-CHA-CBD	-4.05	104.89	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	CLA	O2D-CGD-CBD	4.03	118.28	111.23
2	B	501	LUX	C1-C6-C5	-4.01	117.16	122.64
8	C	802	DGD	O5D-C1E-C2E	4.01	114.36	108.27
3	A	503	NEX	C39-C29-C30	-3.99	116.35	122.82
7	A	801	LHG	O8-C23-C24	3.97	123.93	111.83
5	A	601	CLA	O2A-CGA-CBA	3.96	123.92	111.83
2	C	501	LUX	C22-C23-C24	-3.96	105.31	111.18
2	C	501	LUX	C10-C9-C8	3.94	121.44	110.64
2	C	502	LUX	C36-C21-C26	-3.94	103.47	110.49
5	B	605	CLA	O2D-CGD-CBD	3.94	118.12	111.23
5	A	601	CLA	CAA-C2A-C3A	-3.94	102.36	113.00
2	B	502	LUX	C37-C21-C22	-3.94	102.07	109.41
2	A	502	LUX	C19-C9-C8	3.93	119.00	110.82
6	B	612	CHL	C4D-CHA-CBD	-3.92	105.01	108.97
4	A	504	XAT	C19-C9-C8	3.92	124.08	118.09
6	C	610	CHL	C4D-CHA-CBD	-3.91	105.03	108.97
5	C	604	CLA	O2D-CGD-CBD	3.90	118.05	111.23
5	A	604	CLA	O2D-CGD-CBD	3.90	118.04	111.23
5	A	608	CLA	O2D-CGD-CBD	3.89	118.04	111.23
2	A	502	LUX	C15-C14-C13	3.89	128.88	115.97
3	B	503	NEX	O24-C25-C38	-3.89	110.71	115.05
8	B	802	DGD	C3G-O3G-C1D	-3.88	107.06	113.68
8	B	802	DGD	O5D-C1E-C2E	3.87	114.15	108.27
2	B	502	LUX	C31-C32-C33	3.87	128.81	115.97
5	A	606	CLA	O2D-CGD-CBD	3.86	117.97	111.23
3	A	503	NEX	C28-C29-C30	3.85	125.06	119.01
6	C	610	CHL	OMC-CMC-C2C	-3.85	118.44	125.12
5	C	605	CLA	O2D-CGD-CBD	3.83	117.93	111.23
3	A	503	NEX	C38-C25-C24	3.83	118.55	114.24
3	C	503	NEX	C39-C29-C30	-3.82	116.62	122.82
2	C	502	LUX	C18-C5-C4	3.82	121.44	114.42
2	C	501	LUX	C11-C12-C13	3.80	128.60	115.97
5	C	601	CLA	O2A-CGA-CBA	3.80	123.43	111.83
8	C	802	DGD	O6E-C5E-C6E	3.79	115.83	106.44
5	B	603	CLA	O2D-CGD-CBD	3.78	117.84	111.23
6	B	610	CHL	CMA-C3A-C4A	-3.77	106.48	114.61
2	C	502	LUX	C1-C2-C3	-3.77	105.33	113.59
5	C	606	CLA	O2D-CGD-CBD	3.76	117.80	111.23
4	B	504	XAT	C12-C13-C14	3.75	124.91	119.01
3	B	503	NEX	C35-C34-C33	-3.75	122.02	127.28
6	A	613	CHL	CHA-C1A-C2A	-3.74	124.52	133.31
2	B	502	LUX	C15-C14-C13	3.74	128.40	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	802	DGD	O6E-C5E-C6E	3.74	115.71	106.44
2	A	501	LUX	C10-C9-C8	3.73	120.86	110.64
2	B	501	LUX	C10-C9-C8	3.72	120.82	110.64
5	B	601	CLA	O2A-CGA-CBA	3.71	123.14	111.83
6	C	613	CHL	C4D-CHA-CBD	-3.70	105.23	108.97
6	A	610	CHL	C4D-CHA-CBD	-3.69	105.25	108.97
5	B	601	CLA	C4D-CHA-C1A	3.69	125.64	121.24
6	B	610	CHL	O2A-CGA-CBA	3.68	123.06	111.83
6	A	610	CHL	O2A-CGA-CBA	3.68	123.06	111.83
2	B	501	LUX	C11-C12-C13	3.67	128.18	115.97
8	A	802	DGD	O6E-C5E-C6E	3.66	115.52	106.44
2	A	502	LUX	C11-C12-C13	3.66	128.13	115.97
2	C	501	LUX	O23-C23-C24	3.65	117.85	110.39
2	A	501	LUX	O23-C23-C22	3.65	116.53	110.06
6	B	613	CHL	CHA-C1A-C2A	-3.65	124.75	133.31
5	A	607	CLA	CAA-C2A-C3A	-3.63	103.18	113.00
6	C	609	CHL	OMC-CMC-C2C	-3.63	118.82	125.12
5	B	607	CLA	CAA-C2A-C3A	-3.63	103.19	113.00
6	C	611	CHL	C1-C2-C3	3.63	132.14	126.20
6	C	610	CHL	O2A-CGA-CBA	3.63	122.89	111.83
5	B	608	CLA	O2A-CGA-CBA	3.62	122.89	111.83
4	A	504	XAT	C40-C33-C34	-3.62	116.95	122.82
5	C	605	CLA	C11-C10-C8	3.61	127.95	115.97
4	B	504	XAT	C35-C34-C33	-3.61	122.22	127.28
2	C	502	LUX	C37-C21-C22	-3.60	102.69	109.41
5	A	605	CLA	C11-C10-C8	3.60	127.92	115.97
5	A	601	CLA	O2D-CGD-CBD	3.59	117.50	111.23
5	B	608	CLA	O2D-CGD-CBD	3.58	117.49	111.23
5	C	607	CLA	CAA-C2A-C3A	-3.58	103.32	113.00
5	C	608	CLA	O2A-CGA-CBA	3.58	122.75	111.83
5	B	606	CLA	O2A-CGA-CBA	3.58	122.74	111.83
2	C	501	LUX	C19-C9-C10	3.57	121.12	110.91
6	A	611	CHL	OMC-CMC-C2C	-3.57	118.92	125.12
6	B	612	CHL	OBD-CAD-CBD	-3.56	120.59	125.82
4	A	504	XAT	C35-C34-C33	-3.56	122.28	127.28
5	A	603	CLA	CAA-C2A-C3A	-3.56	103.39	113.00
6	A	611	CHL	CAA-C2A-C3A	-3.56	103.39	113.00
2	A	502	LUX	C31-C32-C33	3.54	127.75	115.97
3	C	503	NEX	C35-C34-C33	-3.54	122.31	127.28
3	A	503	NEX	C35-C34-C33	-3.54	122.32	127.28
4	A	504	XAT	C27-C28-C29	-3.53	120.06	125.53
4	C	504	XAT	O3-C3-C4	3.52	116.95	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	604	CLA	O2A-CGA-CBA	3.52	122.57	111.83
2	A	501	LUX	C11-C12-C13	3.52	127.66	115.97
2	B	501	LUX	C22-C23-C24	-3.51	105.97	111.18
5	C	608	CLA	CBC-CAC-C3C	-3.50	102.92	112.42
2	A	502	LUX	C10-C9-C8	3.50	120.23	110.64
5	B	603	CLA	CAA-C2A-C3A	-3.50	103.55	113.00
6	A	612	CHL	CBC-CAC-C3C	-3.50	107.87	112.87
2	B	502	LUX	C36-C21-C26	-3.49	104.26	110.49
2	C	502	LUX	C10-C9-C8	3.49	120.21	110.64
5	C	606	CLA	O2A-CGA-CBA	3.49	122.47	111.83
5	B	607	CLA	C3B-C4B-NB	-3.48	107.42	110.53
6	B	611	CHL	C1A-CHA-C4D	3.48	124.78	118.98
6	C	613	CHL	CHA-C1A-C2A	-3.47	125.16	133.31
5	B	603	CLA	CBA-CAA-C2A	3.47	124.11	113.79
5	A	606	CLA	O2A-CGA-CBA	3.47	122.40	111.83
5	C	603	CLA	O2A-CGA-CBA	3.46	122.39	111.83
6	A	611	CHL	C1-C2-C3	3.45	131.85	126.20
6	B	611	CHL	CAA-C2A-C3A	-3.45	103.67	113.00
5	B	603	CLA	O2A-CGA-CBA	3.45	122.35	111.83
2	A	502	LUX	C19-C9-C10	3.45	120.76	110.91
6	A	611	CHL	C1A-CHA-C4D	3.44	124.73	118.98
6	C	611	CHL	C1A-CHA-C4D	3.44	124.71	118.98
3	C	503	NEX	C28-C29-C30	3.43	124.40	119.01
6	A	612	CHL	CMA-C3A-C4A	-3.42	107.24	114.61
4	B	504	XAT	C19-C9-C10	-3.42	117.28	122.82
5	A	601	CLA	C4D-CHA-C1A	3.41	125.32	121.24
6	A	611	CHL	OBD-CAD-CBD	-3.41	120.81	125.82
8	A	802	DGD	C3G-O3G-C1D	-3.41	107.85	113.68
5	A	608	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
5	C	602	CLA	C11-C10-C8	3.41	127.30	115.97
3	C	503	NEX	C37-C21-C36	-3.40	102.43	107.37
5	A	608	CLA	O2A-CGA-CBA	3.40	122.21	111.83
6	C	612	CHL	CAA-C2A-C3A	-3.40	103.81	113.00
6	C	613	CHL	OMC-CMC-C2C	-3.40	119.22	125.12
5	C	603	CLA	O2D-CGD-CBD	3.39	117.16	111.23
2	A	501	LUX	C35-C34-C33	3.38	127.22	115.97
6	C	612	CHL	CMA-C3A-C4A	-3.38	107.32	114.61
2	C	501	LUX	C1-C2-C3	3.38	121.01	113.59
5	B	602	CLA	C11-C10-C8	3.38	127.21	115.97
3	B	503	NEX	C38-C25-C24	3.38	118.04	114.24
5	A	604	CLA	O2A-CGA-CBA	3.38	122.14	111.83
5	A	605	CLA	O2A-CGA-CBA	3.37	122.11	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	611	CHL	OBD-CAD-CBD	-3.37	120.88	125.82
5	C	605	CLA	O2A-CGA-CBA	3.37	122.11	111.83
5	C	607	CLA	C3B-C4B-NB	-3.36	107.53	110.53
5	B	604	CLA	O2D-CGD-CBD	3.36	117.10	111.23
5	B	605	CLA	C11-C10-C8	3.35	127.10	115.97
6	B	612	CHL	CAA-C2A-C3A	-3.35	103.94	113.00
2	B	501	LUX	C18-C5-C6	-3.35	120.83	124.48
4	A	504	XAT	C37-C21-C36	3.35	112.23	107.37
4	C	504	XAT	C15-C14-C13	-3.35	122.59	127.28
5	C	601	CLA	C4D-CHA-C1A	3.34	125.23	121.24
2	A	501	LUX	C18-C5-C4	3.34	120.56	114.42
3	C	503	NEX	C16-C1-C6	3.34	113.46	110.47
6	B	611	CHL	CBC-CAC-C3C	-3.33	108.10	112.87
4	C	504	XAT	C27-C28-C29	-3.33	120.36	125.53
5	A	602	CLA	C11-C10-C8	3.33	127.04	115.97
4	B	504	XAT	C17-C1-C2	-3.32	103.13	108.97
5	A	607	CLA	C3B-C4B-NB	-3.32	107.56	110.53
5	A	603	CLA	O2A-CGA-CBA	3.31	121.94	111.83
5	C	603	CLA	CAA-C2A-C3A	-3.30	104.07	113.00
6	A	612	CHL	CAA-C2A-C3A	-3.30	104.08	113.00
6	B	614	CHL	OMC-CMC-C2C	-3.30	119.39	125.12
5	C	608	CLA	O2D-CGD-CBD	3.30	117.00	111.23
3	C	503	NEX	C37-C21-C22	3.30	114.76	108.97
3	B	503	NEX	C40-C33-C34	-3.29	117.48	122.82
2	A	501	LUX	C39-C29-C30	3.28	122.98	111.27
6	C	612	CHL	CBC-CAC-C3C	-3.27	108.19	112.87
6	A	613	CHL	C4D-CHA-CBD	-3.27	105.67	108.97
5	B	602	CLA	O2A-CGA-CBA	3.27	121.80	111.83
2	C	501	LUX	C18-C5-C6	-3.26	120.93	124.48
5	C	603	CLA	CBA-CAA-C2A	3.25	123.46	113.79
2	C	502	LUX	C7-C6-C5	-3.24	114.10	121.56
4	A	504	XAT	C12-C13-C14	3.23	124.10	119.01
2	B	502	LUX	C10-C9-C8	3.23	119.49	110.64
4	C	504	XAT	C38-C25-C24	3.23	117.87	114.24
6	A	609	CHL	CHA-C1A-C2A	-3.23	125.72	133.31
6	B	610	CHL	OMC-CMC-C2C	-3.23	119.51	125.12
5	A	602	CLA	O2A-CGA-CBA	3.23	121.67	111.83
6	A	612	CHL	C1-C2-C3	3.22	131.48	126.20
2	A	502	LUX	C35-C34-C33	3.22	126.68	115.97
2	A	502	LUX	C40-C33-C34	3.22	122.74	111.27
6	B	609	CHL	O2A-CGA-CBA	3.21	121.63	111.83
6	B	609	CHL	CHA-C1A-C2A	-3.21	125.77	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	607	CLA	C1-C2-C3	3.21	131.45	126.20
2	B	502	LUX	C39-C29-C30	3.21	122.70	111.27
6	B	610	CHL	O1D-CGD-CBD	-3.21	119.86	124.72
2	C	502	LUX	C20-C13-C12	3.19	122.66	111.27
2	A	502	LUX	C18-C5-C4	3.19	120.29	114.42
2	A	502	LUX	C36-C21-C26	-3.19	104.80	110.49
2	C	501	LUX	C35-C34-C33	3.19	126.58	115.97
5	C	601	CLA	C11-C10-C8	3.19	126.56	115.97
2	A	502	LUX	C27-C28-C29	3.18	125.89	114.97
2	C	501	LUX	C19-C9-C8	3.17	117.44	110.82
5	C	607	CLA	C11-C10-C8	3.17	126.51	115.97
3	B	503	NEX	C16-C1-C6	3.17	113.31	110.47
6	B	612	CHL	C1-C2-C3	3.17	131.39	126.20
2	C	502	LUX	C19-C9-C10	3.17	119.97	110.91
5	A	605	CLA	C3B-C4B-NB	-3.16	107.71	110.53
5	B	607	CLA	C11-C10-C8	3.16	126.47	115.97
6	B	614	CHL	CBC-CAC-C3C	-3.14	108.37	112.87
5	C	602	CLA	O2A-CGA-CBA	3.14	121.42	111.83
2	B	501	LUX	C20-C13-C12	3.14	122.47	111.27
5	A	603	CLA	CBA-CAA-C2A	3.13	123.12	113.79
6	A	614	CHL	OMC-CMC-C2C	-3.13	119.68	125.12
2	C	502	LUX	C35-C34-C33	3.13	126.37	115.97
4	C	504	XAT	C18-C5-C6	-3.13	117.15	122.30
6	B	612	CHL	O2A-CGA-CBA	3.11	121.33	111.83
6	C	614	CHL	C1A-CHA-C4D	3.11	124.16	118.98
6	B	611	CHL	O2A-CGA-CBA	3.10	121.30	111.83
5	B	605	CLA	O2A-CGA-CBA	3.10	121.29	111.83
5	C	608	CLA	CAA-C2A-C3A	-3.10	104.63	113.00
4	B	504	XAT	C31-C30-C29	-3.10	122.94	127.28
5	A	601	CLA	CMB-C2B-C1B	-3.09	120.71	125.42
5	A	607	CLA	C11-C10-C8	3.09	126.23	115.97
7	B	801	LHG	O7-C7-C8	3.09	118.16	111.48
5	B	604	CLA	O2A-CGA-CBA	3.08	121.24	111.83
6	B	613	CHL	C4D-CHA-CBD	-3.08	105.86	108.97
3	C	503	NEX	C38-C25-C24	3.08	117.70	114.24
6	A	613	CHL	OMC-CMC-C2C	-3.08	119.77	125.12
6	C	612	CHL	C1-C2-C3	3.08	131.24	126.20
2	A	501	LUX	C19-C9-C10	3.08	119.70	110.91
2	A	502	LUX	C20-C13-C12	3.08	122.24	111.27
2	C	502	LUX	C11-C12-C13	3.08	126.19	115.97
6	A	612	CHL	O2A-CGA-CBA	3.07	121.20	111.83
6	C	609	CHL	CHA-C1A-C2A	-3.07	126.10	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LUX	C3-C4-C5	3.06	119.80	112.18
6	A	614	CHL	CBC-CAC-C3C	-3.05	108.50	112.87
6	A	609	CHL	O2A-CGA-CBA	3.05	121.15	111.83
2	A	502	LUX	C3-C4-C5	3.05	119.78	112.18
5	B	601	CLA	C11-C10-C8	3.05	126.10	115.97
6	A	614	CHL	O1D-CGD-CBD	-3.05	120.10	124.72
3	C	503	NEX	C38-C25-C26	-3.04	117.29	122.30
2	A	502	LUX	C37-C21-C22	-3.04	103.73	109.41
6	B	614	CHL	C1A-CHA-C4D	3.04	124.06	118.98
2	C	502	LUX	C31-C32-C33	3.04	126.07	115.97
2	C	502	LUX	C39-C29-C30	3.04	122.11	111.27
6	A	614	CHL	CMA-C3A-C4A	-3.04	108.06	114.61
2	B	501	LUX	C40-C33-C34	3.03	122.08	111.27
2	B	501	LUX	C15-C14-C13	3.03	126.04	115.97
4	B	504	XAT	C40-C33-C34	-3.03	117.91	122.82
2	B	501	LUX	C35-C34-C33	3.03	126.02	115.97
6	C	611	CHL	CAA-C2A-C3A	-3.02	104.83	113.00
2	A	502	LUX	C1-C2-C3	-3.02	106.97	113.59
5	A	603	CLA	O2D-CGD-CBD	3.02	116.50	111.23
5	A	608	CLA	C3A-C2A-C1A	3.02	105.86	101.34
6	A	611	CHL	O2A-CGA-CBA	3.01	121.02	111.83
5	B	602	CLA	O2D-CGD-CBD	3.01	116.49	111.23
6	B	613	CHL	C1C-CHC-C4B	3.00	126.80	116.07
2	B	501	LUX	C27-C28-C29	3.00	125.28	114.97
6	C	611	CHL	O2A-CGA-CBA	3.00	120.97	111.83
4	A	504	XAT	C15-C14-C13	-2.99	123.08	127.28
6	B	613	CHL	OMC-CMC-C2C	-2.99	119.92	125.12
5	A	604	CLA	C2A-C3A-C4A	2.99	106.70	101.87
6	C	610	CHL	C1A-CHA-C4D	2.99	123.97	118.98
6	B	613	CHL	OBD-CAD-CBD	-2.99	121.43	125.82
2	A	502	LUX	C8-C7-C6	-2.99	119.99	125.96
4	B	504	XAT	C38-C25-C24	2.99	117.60	114.24
2	B	502	LUX	C20-C13-C14	2.98	121.90	111.27
6	C	609	CHL	O2A-CGA-CBA	2.98	120.92	111.83
2	B	502	LUX	C19-C9-C10	2.98	119.42	110.91
2	B	501	LUX	C39-C29-C28	2.98	121.89	111.27
6	C	614	CHL	CMA-C3A-C4A	-2.97	108.22	114.61
5	B	601	CLA	C3B-C4B-NB	-2.96	107.88	110.53
6	B	614	CHL	CMA-C3A-C4A	-2.96	108.23	114.61
6	A	611	CHL	CBC-CAC-C3C	-2.96	108.64	112.87
2	C	501	LUX	C40-C33-C34	2.95	121.81	111.27
2	C	501	LUX	C39-C29-C30	2.95	121.81	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	613	CHL	CMB-C2B-C3B	2.95	130.59	124.68
6	A	614	CHL	C1A-CHA-C4D	2.95	123.91	118.98
6	C	613	CHL	C1C-CHC-C4B	2.95	126.63	116.07
6	C	613	CHL	C1A-CHA-C4D	2.95	123.90	118.98
2	B	501	LUX	C18-C5-C4	2.95	119.84	114.42
5	B	608	CLA	CAA-C2A-C3A	-2.94	105.05	113.00
2	C	501	LUX	C3-C4-C5	2.94	119.50	112.18
5	A	601	CLA	C11-C10-C8	2.94	125.72	115.97
5	A	607	CLA	O2A-CGA-CBA	2.93	120.77	111.83
5	B	604	CLA	C2A-C3A-C4A	2.93	106.60	101.87
2	A	501	LUX	C15-C14-C13	2.93	125.70	115.97
5	C	601	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
5	A	602	CLA	O2D-CGD-CBD	2.93	116.35	111.23
3	C	503	NEX	C27-C28-C29	-2.92	121.00	125.53
2	B	502	LUX	C40-C33-C34	2.92	121.67	111.27
6	B	611	CHL	OBD-CAD-CBD	-2.92	121.54	125.82
2	C	502	LUX	C40-C33-C34	2.91	121.66	111.27
2	B	502	LUX	C3-C4-C5	2.91	119.43	112.18
5	B	605	CLA	C3B-C4B-NB	-2.91	107.94	110.53
5	C	601	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
6	B	609	CHL	OBD-CAD-CBD	-2.90	121.57	125.82
6	B	612	CHL	CBC-CAC-C3C	-2.90	108.72	112.87
6	C	612	CHL	O2A-CGA-CBA	2.89	120.66	111.83
6	B	609	CHL	C4D-CHA-CBD	-2.89	106.05	108.97
2	C	502	LUX	C8-C7-C6	-2.89	120.19	125.96
6	B	610	CHL	C1-C2-C3	2.88	130.92	126.20
4	A	504	XAT	O3-C3-C4	2.88	115.63	109.75
6	C	609	CHL	C4D-CHA-CBD	-2.87	106.07	108.97
5	C	607	CLA	C1-C2-C3	2.87	130.91	126.20
5	A	601	CLA	CAA-CBA-CGA	-2.87	105.06	113.21
2	B	501	LUX	C19-C9-C10	2.87	119.11	110.91
6	B	613	CHL	C1A-CHA-C4D	2.87	123.77	118.98
6	C	614	CHL	OMC-CMC-C2C	-2.86	120.16	125.12
5	A	608	CLA	C4D-CHA-C1A	2.86	124.65	121.24
2	A	502	LUX	C39-C29-C30	2.85	121.45	111.27
5	C	607	CLA	O2A-CGA-CBA	2.85	120.53	111.83
6	B	614	CHL	O1D-CGD-CBD	-2.85	120.40	124.72
5	C	601	CLA	CBC-CAC-C3C	-2.85	104.69	112.42
6	C	611	CHL	CHA-C1A-C2A	-2.85	126.62	133.31
5	B	602	CLA	C1-C2-C3	2.85	130.86	126.20
4	C	504	XAT	C19-C9-C10	-2.85	118.20	122.82
6	A	609	CHL	CBC-CAC-C3C	-2.84	108.80	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	613	CHL	OBD-CAD-CBD	-2.84	121.65	125.82
6	C	609	CHL	C1C-CHC-C4B	2.84	126.24	116.07
2	B	501	LUX	C3-C4-C5	2.84	119.25	112.18
5	B	603	CLA	C2A-C3A-C4A	2.84	106.46	101.87
2	A	501	LUX	C20-C13-C12	2.84	121.40	111.27
5	A	607	CLA	C1-C2-C3	2.83	130.83	126.20
6	A	613	CHL	OBD-CAD-CBD	-2.83	121.68	125.82
2	A	501	LUX	C22-C23-C24	-2.82	106.99	111.18
5	C	608	CLA	CHD-C1D-ND	-2.82	120.84	124.80
6	C	611	CHL	CBC-CAC-C3C	-2.82	108.84	112.87
6	A	613	CHL	CMB-C2B-C3B	2.82	130.31	124.68
6	A	614	CHL	CAA-C2A-C3A	-2.81	109.78	116.23
4	B	504	XAT	C36-C21-C22	2.81	113.91	108.97
4	B	504	XAT	C18-C5-C4	2.81	117.40	114.24
5	A	606	CLA	C1-C2-C3	2.81	130.80	126.20
2	C	502	LUX	C27-C28-C29	2.81	124.62	114.97
6	B	610	CHL	C1C-CHC-C4B	2.80	126.10	116.07
6	B	609	CHL	C1C-CHC-C4B	2.80	126.10	116.07
4	A	504	XAT	C17-C1-C2	-2.80	104.05	108.97
6	A	614	CHL	C1C-CHC-C4B	2.79	126.07	116.07
6	B	612	CHL	C1A-CHA-C4D	2.79	123.64	118.98
6	C	612	CHL	O1D-CGD-CBD	-2.79	120.49	124.72
6	A	612	CHL	C1A-CHA-C4D	2.79	123.64	118.98
6	A	610	CHL	CMA-C3A-C4A	-2.79	108.60	114.61
3	B	503	NEX	C38-C25-C26	-2.79	117.71	122.30
4	A	504	XAT	C18-C5-C4	2.79	117.37	114.24
5	B	607	CLA	O2A-CGA-CBA	2.78	120.32	111.83
5	C	601	CLA	O2D-CGD-CBD	2.78	116.09	111.23
6	B	612	CHL	CMA-C3A-C4A	-2.78	108.62	114.61
6	C	612	CHL	C4C-CHD-C1D	2.78	126.01	116.07
6	C	610	CHL	C1C-CHC-C4B	2.78	126.00	116.07
2	B	502	LUX	C35-C34-C33	2.78	125.19	115.97
6	A	610	CHL	OMC-CMC-C2C	-2.77	120.30	125.12
6	B	612	CHL	C4C-CHD-C1D	2.77	125.99	116.07
6	A	611	CHL	C17-C16-C15	2.77	125.70	113.28
2	A	501	LUX	C40-C33-C32	2.77	121.16	111.27
2	C	502	LUX	C39-C29-C28	2.77	121.15	111.27
8	C	802	DGD	O6D-C1D-C2D	2.76	116.05	110.37
6	B	612	CHL	CHA-C1A-C2A	-2.75	126.84	133.31
6	A	609	CHL	C4D-CHA-CBD	-2.75	106.19	108.97
6	B	613	CHL	CMB-C2B-C3B	2.75	130.18	124.68
5	B	601	CLA	O2A-CGA-O1A	-2.75	116.75	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	604	CLA	C3B-C4B-NB	-2.75	108.08	110.53
6	C	612	CHL	OBD-CAD-CBD	-2.75	121.80	125.82
2	A	501	LUX	C40-C33-C34	2.74	121.06	111.27
2	A	501	LUX	C27-C28-C29	2.74	124.40	114.97
6	A	610	CHL	C1C-CHC-C4B	2.74	125.88	116.07
8	C	802	DGD	O5D-C6D-C5D	2.74	115.59	109.42
5	C	602	CLA	O2D-CGD-CBD	2.74	116.02	111.23
6	B	611	CHL	C1C-CHC-C4B	2.74	125.86	116.07
6	A	612	CHL	C4C-CHD-C1D	2.74	125.86	116.07
6	B	614	CHL	OBD-CAD-CBD	-2.74	121.81	125.82
6	C	612	CHL	C1A-CHA-C4D	2.73	123.53	118.98
6	A	613	CHL	C1C-CHC-C4B	2.73	125.82	116.07
6	C	612	CHL	C1C-CHC-C4B	2.72	125.81	116.07
6	B	610	CHL	CHA-C1A-C2A	-2.71	126.93	133.31
6	B	612	CHL	O1D-CGD-CBD	-2.71	120.61	124.72
5	C	601	CLA	CED-O2D-CGD	2.71	122.07	115.92
5	A	602	CLA	C1-C2-C3	2.71	130.64	126.20
4	B	504	XAT	O3-C3-C4	2.71	115.29	109.75
5	A	601	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
2	B	502	LUX	C8-C7-C6	-2.71	120.55	125.96
2	B	502	LUX	C11-C12-C13	2.71	124.97	115.97
6	A	612	CHL	C1C-CHC-C4B	2.71	125.76	116.07
2	B	502	LUX	O23-C23-C22	2.71	114.85	110.06
6	B	611	CHL	O1D-CGD-CBD	-2.70	120.62	124.72
4	C	504	XAT	C40-C33-C34	-2.70	118.44	122.82
6	A	610	CHL	CHA-C1A-C2A	-2.70	126.96	133.31
2	C	501	LUX	C31-C32-C33	2.70	124.94	115.97
6	B	613	CHL	CBC-CAC-C3C	-2.70	109.01	112.87
6	A	612	CHL	OMC-CMC-C2C	-2.69	120.45	125.12
5	A	608	CLA	C3B-C4B-NB	-2.69	108.13	110.53
6	C	609	CHL	OBD-CAD-CBD	-2.69	121.88	125.82
6	B	612	CHL	C1C-CHC-C4B	2.68	125.68	116.07
6	C	610	CHL	OBD-CAD-CBD	-2.68	121.88	125.82
4	A	504	XAT	C32-C33-C34	2.68	123.23	119.01
5	A	607	CLA	C4D-CHA-C1A	2.68	124.44	121.24
6	B	613	CHL	O2A-CGA-CBA	2.68	122.46	114.00
4	C	504	XAT	C12-C13-C14	2.68	123.22	119.01
6	B	614	CHL	C4C-CHD-C1D	2.68	125.64	116.07
2	B	502	LUX	C20-C13-C12	2.67	120.80	111.27
6	A	611	CHL	C1C-CHC-C4B	2.67	125.63	116.07
6	C	614	CHL	C1C-CHC-C4B	2.67	125.63	116.07
6	B	614	CHL	C1C-CHC-C4B	2.67	125.62	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	610	CHL	O1D-CGD-CBD	-2.67	120.68	124.72
6	A	611	CHL	CHA-C1A-C2A	-2.67	127.05	133.31
6	A	610	CHL	OBD-CAD-CBD	-2.66	121.91	125.82
5	A	608	CLA	CHD-C1D-ND	-2.66	121.06	124.80
6	A	614	CHL	OBD-CAD-CBD	-2.66	121.92	125.82
6	B	610	CHL	C1A-CHA-C4D	2.66	123.41	118.98
5	C	606	CLA	C1-C2-C3	2.65	130.55	126.20
6	C	614	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
2	A	501	LUX	O23-C23-C24	2.65	115.80	110.39
6	C	610	CHL	CHA-C1A-C2A	-2.64	127.10	133.31
2	B	502	LUX	C18-C5-C4	2.64	119.28	114.42
5	B	603	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
5	C	605	CLA	C3B-C4B-NB	-2.64	108.17	110.53
5	C	602	CLA	C1-C2-C3	2.64	130.52	126.20
5	C	604	CLA	C2A-C3A-C4A	2.64	106.13	101.87
6	B	611	CHL	CHA-C1A-C2A	-2.63	127.12	133.31
6	C	610	CHL	CED-O2D-CGD	2.63	121.88	115.92
4	B	504	XAT	C20-C13-C14	-2.62	118.57	122.82
6	A	610	CHL	CED-O2D-CGD	2.62	121.85	115.92
5	C	603	CLA	C2A-C3A-C4A	2.62	106.09	101.87
7	A	801	LHG	O7-C7-C8	2.61	117.14	111.48
5	C	608	CLA	C4D-CHA-C1A	2.61	124.36	121.24
6	C	611	CHL	C1C-CHC-C4B	2.61	125.41	116.07
3	C	503	NEX	C40-C33-C32	2.61	122.08	118.09
6	A	613	CHL	C1A-CHA-C4D	2.61	123.33	118.98
7	C	801	LHG	O7-C7-C8	2.60	117.11	111.48
6	A	610	CHL	C4C-CHD-C1D	2.60	125.37	116.07
2	B	502	LUX	C27-C28-C29	2.60	123.90	114.97
5	A	601	CLA	CED-O2D-CGD	2.59	121.78	115.92
6	A	612	CHL	OBD-CAD-CBD	-2.58	122.03	125.82
2	B	501	LUX	C1-C2-C3	2.58	119.26	113.59
4	A	504	XAT	C38-C25-C24	2.58	117.14	114.24
6	B	612	CHL	OMC-CMC-C2C	-2.58	120.65	125.12
6	A	609	CHL	C1C-CHC-C4B	2.57	125.27	116.07
5	C	602	CLA	C3B-C4B-NB	-2.57	108.24	110.53
6	C	613	CHL	CBC-CAC-C3C	-2.56	109.20	112.87
6	B	614	CHL	CAA-C2A-C3A	-2.56	110.35	116.23
6	A	609	CHL	C4C-CHD-C1D	2.56	125.23	116.07
2	B	501	LUX	C31-C32-C33	2.56	124.46	115.97
3	A	503	NEX	C38-C25-C26	-2.55	118.11	122.30
5	B	601	CLA	O2D-CGD-CBD	2.54	115.68	111.23
2	C	501	LUX	C15-C14-C13	2.54	124.42	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	610	CHL	C1A-CHA-C4D	2.54	123.22	118.98
5	C	606	CLA	CAA-C2A-C3A	-2.54	106.13	113.00
6	C	614	CHL	C4C-CHD-C1D	2.54	125.15	116.07
5	B	607	CLA	C4D-CHA-C1A	2.54	124.27	121.24
5	A	603	CLA	C2A-C3A-C4A	2.53	105.96	101.87
6	C	613	CHL	O2A-CGA-CBA	2.53	121.99	114.00
5	B	601	CLA	CMA-C3A-C4A	-2.53	104.97	111.77
2	C	501	LUX	C1-C6-C5	-2.53	119.18	122.64
5	C	606	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
6	C	611	CHL	C17-C16-C15	2.52	124.59	113.28
5	C	604	CLA	C3B-C4B-NB	-2.52	108.28	110.53
6	A	609	CHL	OBD-CAD-CBD	-2.52	122.12	125.82
6	B	610	CHL	CED-O2D-CGD	2.52	121.64	115.92
6	B	611	CHL	C17-C16-C15	2.52	124.58	113.28
6	A	612	CHL	CHA-C1A-C2A	-2.52	127.39	133.31
5	C	603	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
5	B	606	CLA	CAA-C2A-C3A	-2.51	106.21	113.00
6	C	614	CHL	OBD-CAD-CBD	-2.51	122.14	125.82
8	B	802	DGD	O6D-C5D-C4D	2.51	114.22	109.70
6	A	613	CHL	O2A-CGA-CBA	2.51	121.93	114.00
6	A	613	CHL	CMA-C3A-C4A	-2.51	109.21	114.61
8	B	802	DGD	O6D-C1D-C2D	2.50	115.51	110.37
6	A	612	CHL	O1D-CGD-CBD	-2.50	120.93	124.72
5	A	604	CLA	C3B-C4B-NB	-2.50	108.30	110.53
2	A	502	LUX	C20-C13-C14	2.50	120.19	111.27
6	A	613	CHL	O1D-CGD-CBD	-2.50	120.93	124.72
5	A	603	CLA	C3B-C4B-NB	-2.50	108.30	110.53
5	A	606	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
5	B	605	CLA	C3A-C2A-C1A	2.49	105.06	101.34
6	C	612	CHL	CHA-C1A-C2A	-2.49	127.47	133.31
5	A	603	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
2	A	502	LUX	C35-C15-C14	2.48	122.97	113.62
6	C	611	CHL	C4C-CHD-C1D	2.48	124.94	116.07
6	A	610	CHL	C1-C2-C3	2.48	130.26	126.20
5	A	606	CLA	CAA-C2A-C3A	-2.48	106.30	113.00
4	B	504	XAT	C32-C33-C34	2.48	122.90	119.01
3	B	503	NEX	C10-C11-C12	-2.47	116.05	123.20
6	C	610	CHL	C4C-CHD-C1D	2.47	124.90	116.07
6	B	611	CHL	C4C-CHD-C1D	2.46	124.88	116.07
2	A	501	LUX	C31-C32-C33	2.46	124.15	115.97
2	B	501	LUX	O3-C3-C2	2.46	114.78	109.75
2	A	502	LUX	C39-C29-C28	2.46	120.04	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	614	CHL	C3C-C4C-NC	-2.46	108.64	114.65
6	A	612	CHL	C3C-C4C-NC	-2.46	108.64	114.65
4	B	504	XAT	C27-C28-C29	-2.45	121.72	125.53
6	A	613	CHL	C4C-CHD-C1D	2.45	124.85	116.07
6	C	610	CHL	CMA-C3A-C4A	-2.45	109.32	114.61
6	B	609	CHL	C1A-CHA-C4D	2.45	123.07	118.98
5	C	604	CLA	C4D-CHA-C1A	2.45	124.16	121.24
6	B	609	CHL	O2D-CGD-O1D	-2.44	119.09	123.85
6	C	611	CHL	OBD-CAD-C3D	2.44	131.70	127.89
2	B	502	LUX	C15-C35-C34	2.44	122.83	113.62
6	C	610	CHL	C1-C2-C3	2.44	130.19	126.20
6	C	609	CHL	C4C-CHD-C1D	2.44	124.78	116.07
6	A	610	CHL	O2A-CGA-O1A	-2.43	117.55	123.63
6	C	609	CHL	CBA-CAA-C2A	2.43	120.93	113.78
2	C	501	LUX	C20-C13-C14	2.43	119.93	111.27
5	B	608	CLA	C3B-C4B-NB	-2.43	108.36	110.53
6	A	611	CHL	C4C-CHD-C1D	2.42	124.74	116.07
6	C	611	CHL	CMA-C3A-C4A	-2.42	109.39	114.61
2	C	501	LUX	C20-C13-C12	2.42	119.89	111.27
6	C	609	CHL	O2D-CGD-O1D	-2.42	119.14	123.85
5	B	601	CLA	CHD-C1D-ND	-2.42	121.40	124.80
5	B	605	CLA	O1D-CGD-CBD	-2.41	119.75	124.52
7	B	801	LHG	O10-C23-C24	-2.41	114.34	123.78
8	A	802	DGD	O2G-C1B-C2B	2.41	119.19	111.83
6	C	613	CHL	C4C-CHD-C1D	2.41	124.68	116.07
5	B	601	CLA	C2A-C3A-C4A	2.41	105.75	101.87
5	C	606	CLA	C3B-C4B-NB	-2.41	108.38	110.53
5	B	602	CLA	CMA-C3A-C4A	-2.40	105.31	111.77
4	C	504	XAT	C32-C33-C34	2.40	122.79	119.01
6	B	609	CHL	OMC-CMC-C2C	-2.40	120.95	125.12
5	B	602	CLA	C3B-C4B-NB	-2.40	108.39	110.53
6	C	614	CHL	CAA-C2A-C3A	-2.40	110.73	116.23
6	B	613	CHL	OBD-CAD-C3D	2.40	131.63	127.89
2	C	501	LUX	C40-C33-C32	2.40	119.81	111.27
6	C	612	CHL	OMC-CMC-C2C	-2.39	120.96	125.12
7	C	801	LHG	O10-C23-C24	-2.39	114.44	123.78
5	C	602	CLA	CMA-C3A-C4A	-2.39	105.36	111.77
6	A	614	CHL	C4C-CHD-C1D	2.39	124.61	116.07
6	B	609	CHL	C4C-CHD-C1D	2.39	124.60	116.07
5	B	608	CLA	CHD-C1D-ND	-2.38	121.46	124.80
8	A	802	DGD	O6D-C1D-C2D	2.37	115.25	110.37
6	B	611	CHL	C3C-C4C-NC	-2.37	108.85	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	802	DGD	C1E-O6E-C5E	2.37	118.35	113.72
6	B	609	CHL	C3C-C4C-NC	-2.37	108.86	114.65
5	B	605	CLA	C2A-C1A-CHA	2.37	127.97	123.87
6	B	611	CHL	CMA-C3A-C4A	-2.36	109.52	114.61
2	C	501	LUX	C18-C5-C4	2.36	118.76	114.42
5	A	608	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
2	B	502	LUX	C22-C23-C24	-2.36	107.68	111.18
6	A	610	CHL	O1D-CGD-CBD	-2.36	121.15	124.72
5	B	601	CLA	CGD-CBD-CAD	2.36	118.47	110.85
6	C	613	CHL	O1D-CGD-CBD	-2.35	121.15	124.72
5	A	602	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
3	C	503	NEX	C10-C11-C12	-2.35	116.39	123.20
5	B	606	CLA	C1-C2-C3	2.35	130.04	126.20
5	A	602	CLA	C3A-C2A-C1A	2.35	104.86	101.34
5	B	604	CLA	CAA-CBA-CGA	-2.35	106.55	113.21
5	B	604	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
5	C	605	CLA	C3A-C2A-C1A	2.34	104.84	101.34
6	A	609	CHL	CBA-CAA-C2A	2.34	120.66	113.78
5	B	606	CLA	C2A-C3A-C4A	2.34	105.65	101.87
2	B	502	LUX	C7-C6-C5	-2.34	116.17	121.56
5	C	603	CLA	CMB-C2B-C1B	-2.33	121.86	125.42
6	C	612	CHL	C3C-C4C-NC	-2.33	108.95	114.65
4	A	504	XAT	C37-C21-C26	2.33	116.34	110.05
6	A	609	CHL	C3C-C4C-NC	-2.33	108.95	114.65
6	A	613	CHL	OBD-CAD-C3D	2.33	131.53	127.89
5	B	608	CLA	C4D-CHA-C1A	2.33	124.02	121.24
5	A	605	CLA	C3A-C2A-C1A	2.33	104.83	101.34
2	A	501	LUX	C18-C5-C6	-2.33	121.94	124.48
6	C	611	CHL	O1D-CGD-CBD	-2.32	121.20	124.72
4	A	504	XAT	C15-C35-C34	-2.32	118.77	123.52
2	B	501	LUX	C35-C15-C14	2.32	122.36	113.62
6	A	609	CHL	O2D-CGD-O1D	-2.32	119.33	123.85
5	C	605	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
8	C	802	DGD	O2G-C1B-C2B	2.31	118.89	111.83
6	A	614	CHL	CMA-C3A-C2A	-2.31	110.93	116.23
3	A	503	NEX	C10-C11-C12	-2.31	116.51	123.20
2	B	502	LUX	C39-C29-C28	2.31	119.50	111.27
8	B	802	DGD	O2G-C1B-C2B	2.31	118.87	111.83
6	B	613	CHL	C4C-CHD-C1D	2.31	124.32	116.07
2	A	502	LUX	C7-C6-C5	-2.30	116.26	121.56
3	A	503	NEX	C40-C33-C34	-2.30	119.09	122.82
5	B	606	CLA	CMA-C3A-C4A	-2.30	105.60	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	LUX	C39-C29-C30	2.30	119.46	111.27
6	B	610	CHL	OBD-CAD-CBD	-2.29	122.46	125.82
5	B	607	CLA	CHB-C1B-NB	2.29	127.49	124.05
2	A	502	LUX	C15-C35-C34	2.29	122.26	113.62
5	C	604	CLA	CAA-CBA-CGA	-2.29	106.71	113.21
5	B	602	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
6	B	612	CHL	C3C-C4C-NC	-2.29	109.06	114.65
6	A	611	CHL	C3C-C4C-NC	-2.29	109.06	114.65
6	C	610	CHL	C3C-C4C-NC	-2.28	109.07	114.65
6	C	610	CHL	O2A-CGA-O1A	-2.28	117.92	123.63
6	C	614	CHL	C3C-C4C-NC	-2.27	109.09	114.65
2	B	502	LUX	C40-C33-C32	2.27	119.35	111.27
5	B	603	CLA	C3B-C4B-NB	-2.26	108.51	110.53
2	C	501	LUX	C8-C7-C6	-2.26	121.45	125.96
6	A	609	CHL	C1A-CHA-C4D	2.26	122.75	118.98
5	B	608	CLA	CMD-C2D-C1D	2.25	128.69	124.73
6	B	610	CHL	C4C-CHD-C1D	2.25	124.13	116.07
6	A	614	CHL	C3C-C4C-NC	-2.25	109.15	114.65
4	C	504	XAT	C35-C34-C33	-2.25	124.13	127.28
5	A	605	CLA	C2A-C1A-CHA	2.24	127.76	123.87
2	C	501	LUX	C27-C28-C29	2.24	122.69	114.97
6	C	613	CHL	CMA-C3A-C4A	-2.24	109.78	114.61
5	A	607	CLA	CHB-C1B-NB	2.24	127.42	124.05
6	B	611	CHL	CMB-C2B-C3B	2.24	129.16	124.68
2	C	502	LUX	C20-C13-C14	2.24	119.25	111.27
5	B	603	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
5	A	601	CLA	C1-C2-C3	2.24	129.86	126.20
5	C	604	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
6	C	612	CHL	O2A-CGA-O1A	-2.23	118.04	123.63
6	B	614	CHL	CMA-C3A-C2A	-2.23	111.11	116.23
6	C	609	CHL	C3C-C4C-NC	-2.22	109.22	114.65
4	B	504	XAT	C37-C21-C26	2.22	116.04	110.05
6	C	611	CHL	C3C-C4C-NC	-2.22	109.23	114.65
3	A	503	NEX	C15-C14-C13	-2.21	124.17	127.28
8	A	802	DGD	C1E-O6E-C5E	2.21	118.04	113.72
5	B	601	CLA	CMA-C3A-C2A	-2.20	105.47	113.98
5	C	608	CLA	C2A-C1A-CHA	2.20	127.68	123.87
6	B	610	CHL	C3C-C4C-NC	-2.20	109.28	114.65
5	A	604	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
4	C	504	XAT	C15-C35-C34	-2.19	119.03	123.52
2	C	502	LUX	C40-C33-C32	2.19	119.08	111.27
2	C	502	LUX	C35-C15-C14	2.19	121.88	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	504	XAT	C36-C21-C22	2.19	112.82	108.97
6	C	614	CHL	CMA-C3A-C2A	-2.19	111.21	116.23
5	C	608	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
6	B	610	CHL	O2A-CGA-O1A	-2.18	118.17	123.63
6	B	612	CHL	OBD-CAD-C3D	2.18	131.30	127.89
5	C	605	CLA	C2A-C1A-CHA	2.18	127.64	123.87
5	B	602	CLA	C3A-C2A-C1A	2.18	104.60	101.34
6	B	613	CHL	O2A-CGA-O1A	-2.17	117.74	123.33
5	A	606	CLA	C2A-C3A-C4A	2.17	105.38	101.87
8	C	802	DGD	C1E-O6E-C5E	2.17	117.96	113.72
5	B	602	CLA	C4D-CHA-C1A	2.17	123.83	121.24
5	B	606	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
5	A	605	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
4	B	504	XAT	C19-C9-C8	2.16	121.39	118.09
5	A	606	CLA	CMB-C2B-C1B	-2.16	122.12	125.42
5	C	607	CLA	C4D-CHA-C1A	2.16	123.82	121.24
5	C	602	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
2	C	501	LUX	C39-C29-C28	2.15	118.95	111.27
5	A	601	CLA	CGD-CBD-CAD	2.15	117.81	110.85
6	B	609	CHL	CBC-CAC-C3C	-2.15	109.80	112.87
5	A	603	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
6	B	609	CHL	CBA-CAA-C2A	2.14	120.09	113.78
6	A	611	CHL	OBD-CAD-C3D	2.14	131.23	127.89
2	B	501	LUX	C27-C26-C21	-2.14	111.28	114.30
6	B	612	CHL	O2A-CGA-O1A	-2.14	118.28	123.63
5	A	604	CLA	CAA-CBA-CGA	-2.14	107.14	113.21
2	A	501	LUX	C20-C13-C14	2.14	118.89	111.27
5	B	604	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
5	C	606	CLA	C2A-C3A-C4A	2.14	105.32	101.87
5	A	604	CLA	CAA-C2A-C1A	2.13	118.97	111.97
3	B	503	NEX	C11-C12-C13	-2.13	120.52	126.36
6	A	611	CHL	O1D-CGD-CBD	-2.13	121.50	124.72
5	A	606	CLA	C2A-C1A-CHA	2.12	127.55	123.87
5	A	603	CLA	C12-C11-C10	-2.12	103.78	113.28
2	B	502	LUX	C27-C26-C21	-2.12	111.31	114.30
5	C	607	CLA	CHB-C1B-NB	2.12	127.22	124.05
6	B	613	CHL	O1D-CGD-CBD	-2.12	121.51	124.72
6	B	610	CHL	C12-C11-C10	-2.11	103.80	113.28
8	A	802	DGD	O5D-C6D-C5D	2.11	114.19	109.42
6	B	611	CHL	O2A-CGA-O1A	-2.11	118.34	123.63
5	A	602	CLA	CED-O2D-CGD	2.11	120.71	115.92
5	C	606	CLA	CHD-C1D-ND	-2.11	121.83	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	609	CHL	C1A-CHA-C4D	2.11	122.50	118.98
7	A	801	LHG	O10-C23-C24	-2.10	115.57	123.78
5	B	608	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
5	A	608	CLA	C2A-C1A-CHA	2.10	127.51	123.87
5	B	608	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
5	B	604	CLA	C12-C11-C10	-2.09	103.90	113.28
6	B	609	CHL	O2A-CGA-O1A	-2.09	118.40	123.63
5	B	607	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
6	B	613	CHL	C3C-C4C-NC	-2.09	109.55	114.65
5	A	608	CLA	CED-O2D-CGD	2.09	120.65	115.92
2	A	501	LUX	C39-C29-C28	2.09	118.71	111.27
6	A	611	CHL	CMA-C3A-C4A	-2.08	110.12	114.61
6	C	610	CHL	C12-C11-C10	-2.08	103.94	113.28
4	C	504	XAT	C17-C1-C2	-2.08	105.31	108.97
6	C	613	CHL	OBD-CAD-C3D	2.08	131.14	127.89
5	A	606	CLA	C3A-C2A-C1A	2.08	104.45	101.34
5	A	602	CLA	C3B-C4B-NB	-2.08	108.67	110.53
6	A	613	CHL	C3C-C4C-NC	-2.08	109.57	114.65
6	C	611	CHL	CMB-C2B-C3B	2.08	128.84	124.68
5	B	604	CLA	CHD-C1D-ND	-2.08	121.88	124.80
5	B	608	CLA	CED-O2D-CGD	2.08	120.63	115.92
5	B	604	CLA	CED-O2D-CGD	2.08	120.63	115.92
2	B	501	LUX	C40-C33-C32	2.08	118.68	111.27
5	C	603	CLA	C12-C11-C10	-2.08	103.97	113.28
5	C	601	CLA	CGD-CBD-CAD	2.07	117.56	110.85
3	A	503	NEX	C8-C7-C6	-2.07	175.22	177.66
5	B	604	CLA	C4D-CHA-C1A	2.07	123.71	121.24
5	C	606	CLA	C3A-C2A-C1A	2.07	104.44	101.34
5	C	604	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
6	B	609	CHL	CMA-C3A-C2A	-2.07	106.14	114.13
5	A	601	CLA	CMB-C2B-C3B	2.07	131.41	126.55
5	B	601	CLA	C5-C3-C2	2.06	125.80	121.17
2	A	501	LUX	C35-C15-C14	2.06	121.40	113.62
5	B	606	CLA	C2A-C1A-CHA	2.06	127.45	123.87
6	A	611	CHL	O2A-CGA-O1A	-2.06	118.47	123.63
5	C	608	CLA	C3A-C2A-C1A	2.06	104.42	101.34
5	B	608	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
2	A	502	LUX	C40-C33-C32	2.06	118.61	111.27
6	C	613	CHL	CMD-C2D-C3D	2.05	128.79	124.68
6	B	611	CHL	C16-C17-C18	2.05	125.11	115.94
5	C	608	CLA	CHD-C4C-NC	2.05	127.41	124.23
5	B	606	CLA	O1D-CGD-CBD	-2.05	120.47	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	608	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
6	C	611	CHL	C11-C10-C8	-2.05	109.16	115.97
4	C	504	XAT	C37-C21-C26	2.05	115.57	110.05
5	A	605	CLA	C1-C2-C3	2.04	129.55	126.20
2	C	502	LUX	C3-C4-C5	2.04	117.27	112.18
6	C	613	CHL	C3C-C4C-NC	-2.04	109.66	114.65
5	C	606	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
5	C	602	CLA	CED-O2D-CGD	2.04	120.55	115.92
6	B	613	CHL	CMA-C3A-C4A	-2.04	110.21	114.61
5	C	604	CLA	CHD-C1D-ND	-2.04	121.93	124.80
6	B	610	CHL	C7-C6-C5	-2.04	107.83	113.26
5	B	603	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
5	C	607	CLA	C2A-C3A-C4A	2.03	105.15	101.87
7	B	801	LHG	O8-C23-O10	-2.03	118.55	123.63
5	A	601	CLA	CHD-C1D-ND	-2.03	121.95	124.80
5	B	603	CLA	CED-O2D-CGD	2.02	120.50	115.92
6	A	611	CHL	CMD-C2D-C3D	2.02	128.72	124.68
5	A	605	CLA	CED-O2D-CGD	2.02	120.50	115.92
6	A	609	CHL	C7-C6-C5	-2.02	107.88	113.26
6	B	610	CHL	CBC-CAC-C3C	-2.02	109.98	112.87
6	C	609	CHL	CBC-CAC-C3C	-2.02	109.98	112.87
5	B	601	CLA	CHD-C4C-NC	2.02	127.36	124.23
5	C	607	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
5	A	607	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
5	A	606	CLA	CHD-C1D-ND	-2.01	121.98	124.80
6	A	613	CHL	O2A-CGA-O1A	-2.00	118.18	123.33

All (141) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	LUX	C9
2	A	501	LUX	C13
2	A	501	LUX	C33
2	A	501	LUX	C26
2	A	501	LUX	C29
2	A	502	LUX	C9
2	A	502	LUX	C13
2	A	502	LUX	C33
2	A	502	LUX	C26
2	A	502	LUX	C29
2	B	501	LUX	C9
2	B	501	LUX	C13

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Mol	Chain	Res	Type	Atom
2	B	501	LUX	C33
2	B	501	LUX	C26
2	B	501	LUX	C29
2	B	502	LUX	C9
2	B	502	LUX	C13
2	B	502	LUX	C33
2	B	502	LUX	C26
2	B	502	LUX	C29
2	C	501	LUX	C9
2	C	501	LUX	C13
2	C	501	LUX	C33
2	C	501	LUX	C26
2	C	501	LUX	C29
2	C	502	LUX	C9
2	C	502	LUX	C13
2	C	502	LUX	C33
2	C	502	LUX	C26
2	C	502	LUX	C29
4	A	504	XAT	C26
4	A	504	XAT	C6
4	B	504	XAT	C26
4	B	504	XAT	C6
4	C	504	XAT	C26
4	C	504	XAT	C6
5	A	601	CLA	C8
5	A	601	CLA	ND
5	A	602	CLA	ND
5	A	603	CLA	C8
5	A	603	CLA	ND
5	A	604	CLA	C8
5	A	604	CLA	ND
5	A	605	CLA	C8
5	A	605	CLA	ND
5	A	606	CLA	C8
5	A	606	CLA	ND
5	A	607	CLA	ND
5	A	608	CLA	ND
5	B	601	CLA	C8
5	B	601	CLA	ND
5	B	602	CLA	ND
5	B	603	CLA	C8
5	B	603	CLA	ND

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Mol	Chain	Res	Type	Atom
5	B	604	CLA	C8
5	B	604	CLA	ND
5	B	605	CLA	C8
5	B	605	CLA	ND
5	B	606	CLA	C8
5	B	606	CLA	ND
5	B	607	CLA	ND
5	B	608	CLA	ND
5	C	601	CLA	C8
5	C	601	CLA	ND
5	C	602	CLA	ND
5	C	603	CLA	C8
5	C	603	CLA	ND
5	C	604	CLA	C8
5	C	604	CLA	ND
5	C	605	CLA	C8
5	C	605	CLA	ND
5	C	606	CLA	C8
5	C	606	CLA	ND
5	C	607	CLA	ND
5	C	608	CLA	ND
6	A	609	CHL	NA
6	A	609	CHL	C8
6	A	609	CHL	ND
6	A	609	CHL	NC
6	A	610	CHL	NA
6	A	610	CHL	C8
6	A	610	CHL	ND
6	A	610	CHL	NC
6	A	611	CHL	NA
6	A	611	CHL	C8
6	A	611	CHL	ND
6	A	611	CHL	NC
6	A	612	CHL	NA
6	A	612	CHL	ND
6	A	612	CHL	NC
6	A	613	CHL	NA
6	A	613	CHL	ND
6	A	613	CHL	NC
6	A	614	CHL	NA
6	A	614	CHL	ND
6	A	614	CHL	NC

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Mol	Chain	Res	Type	Atom
6	B	609	CHL	NA
6	B	609	CHL	C8
6	B	609	CHL	ND
6	B	609	CHL	NC
6	B	610	CHL	NA
6	B	610	CHL	C8
6	B	610	CHL	ND
6	B	610	CHL	NC
6	B	611	CHL	NA
6	B	611	CHL	C8
6	B	611	CHL	ND
6	B	611	CHL	NC
6	B	612	CHL	NA
6	B	612	CHL	ND
6	B	612	CHL	NC
6	B	613	CHL	NA
6	B	613	CHL	ND
6	B	613	CHL	NC
6	B	614	CHL	NA
6	B	614	CHL	ND
6	B	614	CHL	NC
6	C	609	CHL	NA
6	C	609	CHL	C8
6	C	609	CHL	ND
6	C	609	CHL	NC
6	C	610	CHL	NA
6	C	610	CHL	C8
6	C	610	CHL	ND
6	C	610	CHL	NC
6	C	611	CHL	NA
6	C	611	CHL	C8
6	C	611	CHL	ND
6	C	611	CHL	NC
6	C	612	CHL	NA
6	C	612	CHL	ND
6	C	612	CHL	NC
6	C	613	CHL	NA
6	C	613	CHL	ND
6	C	613	CHL	NC
6	C	614	CHL	NA
6	C	614	CHL	ND
6	C	614	CHL	NC

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Mol	Chain	Res	Type	Atom
8	A	802	DGD	C5E
8	B	802	DGD	C5E
8	C	802	DGD	C5E

All (643) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LUX	C11-C10-C9-C19
2	A	501	LUX	C11-C12-C13-C20
2	A	501	LUX	C20-C13-C14-C15
2	A	501	LUX	C25-C26-C27-C28
2	A	501	LUX	C27-C28-C29-C39
2	A	501	LUX	C40-C33-C34-C35
2	A	502	LUX	C5-C6-C7-C8
2	A	502	LUX	C11-C10-C9-C19
2	A	502	LUX	C11-C12-C13-C20
2	A	502	LUX	C25-C26-C27-C28
2	A	502	LUX	C27-C28-C29-C39
2	B	501	LUX	C11-C10-C9-C19
2	B	501	LUX	C11-C12-C13-C20
2	B	501	LUX	C20-C13-C14-C15
2	B	501	LUX	C25-C26-C27-C28
2	B	501	LUX	C31-C32-C33-C40
2	B	501	LUX	C40-C33-C34-C35
2	B	502	LUX	C5-C6-C7-C8
2	B	502	LUX	C11-C10-C9-C19
2	B	502	LUX	C20-C13-C14-C15
2	B	502	LUX	C25-C26-C27-C28
2	B	502	LUX	C27-C28-C29-C39
2	B	502	LUX	C40-C33-C34-C35
2	C	501	LUX	C11-C10-C9-C19
2	C	501	LUX	C11-C12-C13-C20
2	C	501	LUX	C20-C13-C14-C15
2	C	501	LUX	C25-C26-C27-C28
2	C	501	LUX	C27-C28-C29-C39
2	C	501	LUX	C40-C33-C34-C35
2	C	502	LUX	C5-C6-C7-C8
2	C	502	LUX	C11-C10-C9-C19
2	C	502	LUX	C11-C12-C13-C20
2	C	502	LUX	C25-C26-C27-C28
2	C	502	LUX	C27-C28-C29-C39
5	A	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
5	A	604	CLA	CHA-CBD-CGD-O2D
5	A	606	CLA	C1A-C2A-CAA-CBA
5	A	607	CLA	C1A-C2A-CAA-CBA
5	A	607	CLA	C3A-C2A-CAA-CBA
5	A	608	CLA	C1A-C2A-CAA-CBA
5	A	608	CLA	C3A-C2A-CAA-CBA
5	B	603	CLA	C11-C10-C8-C9
5	B	606	CLA	C1A-C2A-CAA-CBA
5	B	607	CLA	C1A-C2A-CAA-CBA
5	B	607	CLA	C3A-C2A-CAA-CBA
5	B	608	CLA	C1A-C2A-CAA-CBA
5	C	603	CLA	C11-C10-C8-C9
5	C	604	CLA	CHA-CBD-CGD-O1D
5	C	604	CLA	CHA-CBD-CGD-O2D
5	C	606	CLA	C1A-C2A-CAA-CBA
5	C	607	CLA	C1A-C2A-CAA-CBA
5	C	607	CLA	C3A-C2A-CAA-CBA
5	C	608	CLA	C1A-C2A-CAA-CBA
5	C	608	CLA	C3A-C2A-CAA-CBA
6	A	609	CHL	C11-C10-C8-C9
6	A	610	CHL	C11-C10-C8-C9
6	A	611	CHL	C1A-C2A-CAA-CBA
6	A	611	CHL	C11-C10-C8-C9
6	A	612	CHL	C1A-C2A-CAA-CBA
6	A	612	CHL	C3A-C2A-CAA-CBA
6	A	612	CHL	C11-C10-C8-C9
6	B	609	CHL	C11-C10-C8-C9
6	B	610	CHL	C11-C10-C8-C9
6	B	611	CHL	C1A-C2A-CAA-CBA
6	B	611	CHL	C11-C10-C8-C9
6	B	611	CHL	C14-C13-C15-C16
6	B	612	CHL	C1A-C2A-CAA-CBA
6	B	612	CHL	C11-C10-C8-C9
6	C	609	CHL	C11-C10-C8-C9
6	C	610	CHL	C11-C10-C8-C9
6	C	611	CHL	C1A-C2A-CAA-CBA
6	C	612	CHL	C1A-C2A-CAA-CBA
6	C	612	CHL	C3A-C2A-CAA-CBA
6	C	612	CHL	C4C-C3C-CAC-CBC
6	C	612	CHL	C11-C10-C8-C9
7	A	801	LHG	C3-O3-P-O4
7	A	801	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
7	A	801	LHG	C3-O3-P-O6
7	A	801	LHG	C4-O6-P-O3
7	A	801	LHG	C4-O6-P-O5
7	A	801	LHG	O10-C23-O8-C6
7	A	801	LHG	C24-C23-O8-C6
7	B	801	LHG	C3-O3-P-O4
7	B	801	LHG	C3-O3-P-O5
7	B	801	LHG	C3-O3-P-O6
7	B	801	LHG	C4-O6-P-O3
7	B	801	LHG	C4-O6-P-O5
7	B	801	LHG	O10-C23-O8-C6
7	B	801	LHG	C24-C23-O8-C6
7	C	801	LHG	C3-O3-P-O4
7	C	801	LHG	C3-O3-P-O5
7	C	801	LHG	C3-O3-P-O6
7	C	801	LHG	C4-O6-P-O3
7	C	801	LHG	C4-O6-P-O5
7	C	801	LHG	O10-C23-O8-C6
7	C	801	LHG	C24-C23-O8-C6
8	A	802	DGD	O6D-C1D-O3G-C3G
8	A	802	DGD	C2E-C1E-O5D-C6D
8	A	802	DGD	O6E-C1E-O5D-C6D
8	B	802	DGD	O6D-C1D-O3G-C3G
8	B	802	DGD	C2E-C1E-O5D-C6D
8	B	802	DGD	O6E-C1E-O5D-C6D
8	C	802	DGD	O6D-C1D-O3G-C3G
8	C	802	DGD	C2E-C1E-O5D-C6D
8	C	802	DGD	O6E-C1E-O5D-C6D
5	A	602	CLA	C8-C10-C11-C12
5	A	605	CLA	C8-C10-C11-C12
5	A	605	CLA	C15-C16-C17-C18
5	A	607	CLA	C5-C6-C7-C8
5	A	607	CLA	C8-C10-C11-C12
5	B	602	CLA	C8-C10-C11-C12
5	B	605	CLA	C8-C10-C11-C12
5	B	605	CLA	C15-C16-C17-C18
5	B	607	CLA	C5-C6-C7-C8
5	B	607	CLA	C8-C10-C11-C12
5	C	601	CLA	C8-C10-C11-C12
5	C	602	CLA	C8-C10-C11-C12
5	C	605	CLA	C8-C10-C11-C12
5	C	605	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
5	C	607	CLA	C5-C6-C7-C8
5	C	607	CLA	C8-C10-C11-C12
6	A	611	CHL	C5-C6-C7-C8
6	A	611	CHL	C15-C16-C17-C18
6	A	612	CHL	C15-C16-C17-C18
6	B	610	CHL	C13-C15-C16-C17
6	B	611	CHL	C5-C6-C7-C8
6	B	611	CHL	C15-C16-C17-C18
6	B	612	CHL	C15-C16-C17-C18
6	C	611	CHL	C5-C6-C7-C8
6	C	612	CHL	C15-C16-C17-C18
8	B	802	DGD	O1B-C1B-O2G-C2G
8	C	802	DGD	O1B-C1B-O2G-C2G
5	A	601	CLA	C8-C10-C11-C12
5	B	601	CLA	C8-C10-C11-C12
6	A	610	CHL	C13-C15-C16-C17
6	C	610	CHL	C13-C15-C16-C17
6	C	611	CHL	C15-C16-C17-C18
5	A	601	CLA	C3-C5-C6-C7
5	A	605	CLA	C3-C5-C6-C7
5	A	606	CLA	C3-C5-C6-C7
5	B	601	CLA	C3-C5-C6-C7
5	B	606	CLA	C3-C5-C6-C7
5	C	601	CLA	C3-C5-C6-C7
6	B	609	CHL	C3-C5-C6-C7
5	C	601	CLA	C4-C3-C5-C6
5	C	601	CLA	C2-C3-C5-C6
6	A	609	CHL	C2A-CAA-CBA-CGA
6	B	609	CHL	C2A-CAA-CBA-CGA
6	C	609	CHL	C2A-CAA-CBA-CGA
8	A	802	DGD	O1B-C1B-O2G-C2G
5	C	605	CLA	C3-C5-C6-C7
5	C	606	CLA	C3-C5-C6-C7
6	A	609	CHL	C3-C5-C6-C7
6	C	609	CHL	C3-C5-C6-C7
6	A	610	CHL	CBA-CGA-O2A-C1
6	B	610	CHL	CBA-CGA-O2A-C1
6	C	610	CHL	CBA-CGA-O2A-C1
8	A	802	DGD	C2B-C1B-O2G-C2G
8	B	802	DGD	C2B-C1B-O2G-C2G
8	C	802	DGD	C2B-C1B-O2G-C2G
6	A	610	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
6	B	610	CHL	O1A-CGA-O2A-C1
6	C	610	CHL	O1A-CGA-O2A-C1
7	A	801	LHG	C33-C34-C35-C36
7	B	801	LHG	C33-C34-C35-C36
8	B	802	DGD	C2B-C3B-C4B-C5B
8	C	802	DGD	C2B-C3B-C4B-C5B
5	B	605	CLA	C3-C5-C6-C7
7	C	801	LHG	C33-C34-C35-C36
8	A	802	DGD	C2B-C3B-C4B-C5B
8	A	802	DGD	O6D-C5D-C6D-O5D
8	B	802	DGD	O6D-C5D-C6D-O5D
8	C	802	DGD	O6D-C5D-C6D-O5D
6	C	611	CHL	C3-C5-C6-C7
8	B	802	DGD	C4E-C5E-C6E-O5E
8	A	802	DGD	C4D-C5D-C6D-O5D
8	A	802	DGD	C4E-C5E-C6E-O5E
8	C	802	DGD	C4E-C5E-C6E-O5E
5	B	605	CLA	CBA-CGA-O2A-C1
8	B	802	DGD	C4D-C5D-C6D-O5D
8	C	802	DGD	C4D-C5D-C6D-O5D
6	B	611	CHL	C3-C5-C6-C7
5	A	605	CLA	CBA-CGA-O2A-C1
5	C	605	CLA	CBA-CGA-O2A-C1
2	A	501	LUX	C39-C29-C30-C31
2	A	501	LUX	C31-C32-C33-C40
2	A	502	LUX	C20-C13-C14-C15
2	A	502	LUX	C39-C29-C30-C31
2	A	502	LUX	C31-C32-C33-C40
2	A	502	LUX	C40-C33-C34-C35
2	B	501	LUX	C27-C28-C29-C39
2	B	501	LUX	C39-C29-C30-C31
2	B	502	LUX	C11-C12-C13-C20
2	B	502	LUX	C39-C29-C30-C31
2	B	502	LUX	C31-C32-C33-C40
2	C	501	LUX	C39-C29-C30-C31
2	C	501	LUX	C31-C32-C33-C40
2	C	502	LUX	C20-C13-C14-C15
2	C	502	LUX	C39-C29-C30-C31
2	C	502	LUX	C31-C32-C33-C40
2	C	502	LUX	C40-C33-C34-C35
5	A	601	CLA	C11-C10-C8-C9
5	A	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
5	A	605	CLA	C11-C10-C8-C9
5	A	607	CLA	C11-C10-C8-C9
5	A	607	CLA	C14-C13-C15-C16
5	B	601	CLA	C11-C10-C8-C9
5	B	602	CLA	C11-C10-C8-C9
5	B	605	CLA	C11-C10-C8-C9
5	B	607	CLA	C11-C10-C8-C9
5	B	607	CLA	C14-C13-C15-C16
5	C	601	CLA	C11-C10-C8-C9
5	C	602	CLA	C11-C10-C8-C9
5	C	605	CLA	C11-C10-C8-C9
5	C	607	CLA	C11-C10-C8-C9
5	C	607	CLA	C14-C13-C15-C16
6	A	609	CHL	C14-C13-C15-C16
6	A	610	CHL	C11-C12-C13-C14
6	A	611	CHL	C14-C13-C15-C16
6	B	609	CHL	C14-C13-C15-C16
6	B	610	CHL	C11-C12-C13-C14
6	C	609	CHL	C14-C13-C15-C16
6	C	610	CHL	C11-C12-C13-C14
6	C	611	CHL	C11-C10-C8-C9
6	C	611	CHL	C14-C13-C15-C16
6	B	610	CHL	C10-C11-C12-C13
7	C	801	LHG	O1-C1-C2-O2
5	A	607	CLA	C11-C12-C13-C15
5	B	607	CLA	C11-C12-C13-C15
5	C	607	CLA	C11-C12-C13-C15
6	A	612	CHL	C12-C13-C15-C16
6	C	612	CHL	C12-C13-C15-C16
6	A	611	CHL	C3-C5-C6-C7
6	A	610	CHL	C10-C11-C12-C13
5	C	605	CLA	O1A-CGA-O2A-C1
6	B	611	CHL	C10-C11-C12-C13
6	C	611	CHL	C10-C11-C12-C13
6	A	609	CHL	C2C-C3C-CAC-CBC
5	B	602	CLA	C10-C11-C12-C13
5	C	602	CLA	C10-C11-C12-C13
5	A	603	CLA	C3-C5-C6-C7
5	C	603	CLA	C13-C15-C16-C17
6	A	611	CHL	C10-C11-C12-C13
6	C	610	CHL	C10-C11-C12-C13
5	A	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
5	A	602	CLA	C10-C11-C12-C13
5	B	608	CLA	O2A-C1-C2-C3
5	B	603	CLA	C13-C15-C16-C17
5	A	603	CLA	C13-C15-C16-C17
5	A	607	CLA	C13-C15-C16-C17
5	B	607	CLA	C13-C15-C16-C17
5	A	606	CLA	C2C-C3C-CAC-CBC
5	C	607	CLA	C13-C15-C16-C17
5	A	601	CLA	C4-C3-C5-C6
8	A	802	DGD	O2G-C2G-C3G-O3G
8	B	802	DGD	O2G-C2G-C3G-O3G
8	C	802	DGD	O2G-C2G-C3G-O3G
5	C	604	CLA	C16-C17-C18-C20
5	B	605	CLA	O1A-CGA-O2A-C1
5	C	604	CLA	C2C-C3C-CAC-CBC
5	A	606	CLA	C2A-CAA-CBA-CGA
5	B	603	CLA	C2A-CAA-CBA-CGA
5	B	606	CLA	C2A-CAA-CBA-CGA
5	C	603	CLA	C2A-CAA-CBA-CGA
7	A	801	LHG	O1-C1-C2-C3
7	B	801	LHG	O1-C1-C2-C3
7	C	801	LHG	O1-C1-C2-C3
5	A	604	CLA	C16-C17-C18-C20
5	B	604	CLA	C16-C17-C18-C20
6	A	610	CHL	C16-C17-C18-C19
6	B	610	CHL	C16-C17-C18-C19
6	C	610	CHL	C16-C17-C18-C19
4	B	504	XAT	C28-C29-C30-C31
4	C	504	XAT	C28-C29-C30-C31
5	C	608	CLA	O2A-C1-C2-C3
5	C	602	CLA	C11-C12-C13-C15
7	C	801	LHG	C11-C10-C9-C8
7	A	801	LHG	O1-C1-C2-O2
7	B	801	LHG	O1-C1-C2-O2
7	A	801	LHG	C13-C14-C15-C16
5	B	607	CLA	C16-C17-C18-C19
6	B	611	CHL	C16-C17-C18-C20
5	C	606	CLA	C2A-CAA-CBA-CGA
7	B	801	LHG	C11-C10-C9-C8
5	A	601	CLA	C11-C10-C8-C7
6	B	612	CHL	C12-C13-C15-C16
7	A	801	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
5	A	602	CLA	O1A-CGA-O2A-C1
5	B	602	CLA	C3-C5-C6-C7
5	C	603	CLA	C3-C5-C6-C7
5	A	606	CLA	C3A-C2A-CAA-CBA
5	B	606	CLA	C3A-C2A-CAA-CBA
5	B	608	CLA	C3A-C2A-CAA-CBA
5	C	606	CLA	C3A-C2A-CAA-CBA
6	A	611	CHL	C3A-C2A-CAA-CBA
6	B	611	CHL	C3A-C2A-CAA-CBA
6	B	612	CHL	C3A-C2A-CAA-CBA
6	C	611	CHL	C3A-C2A-CAA-CBA
5	A	602	CLA	C11-C12-C13-C15
5	A	607	CLA	C16-C17-C18-C19
5	B	604	CLA	C16-C17-C18-C19
5	C	607	CLA	C16-C17-C18-C19
6	A	611	CHL	C16-C17-C18-C20
6	C	611	CHL	C16-C17-C18-C20
6	B	609	CHL	CBA-CGA-O2A-C1
7	A	801	LHG	C26-C27-C28-C29
7	B	801	LHG	C11-C12-C13-C14
5	C	602	CLA	C3-C5-C6-C7
7	C	801	LHG	C13-C14-C15-C16
7	C	801	LHG	C26-C27-C28-C29
6	C	609	CHL	C2C-C3C-CAC-CBC
7	A	801	LHG	C25-C26-C27-C28
7	B	801	LHG	C13-C14-C15-C16
5	B	602	CLA	C11-C12-C13-C15
2	B	501	LUX	C5-C6-C7-C8
2	C	501	LUX	C5-C6-C7-C8
7	B	801	LHG	C19-C20-C21-C22
7	B	801	LHG	C26-C27-C28-C29
7	A	801	LHG	C19-C20-C21-C22
5	A	604	CLA	C2C-C3C-CAC-CBC
7	B	801	LHG	C25-C26-C27-C28
7	A	801	LHG	C11-C12-C13-C14
5	A	601	CLA	C2-C3-C5-C6
7	C	801	LHG	C19-C20-C21-C22
5	A	604	CLA	C16-C17-C18-C19
5	A	607	CLA	C16-C17-C18-C20
5	B	607	CLA	C16-C17-C18-C20
5	C	604	CLA	C16-C17-C18-C19
6	C	611	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
7	C	801	LHG	C25-C26-C27-C28
8	A	802	DGD	C2D-C1D-O3G-C3G
7	C	801	LHG	C15-C16-C17-C18
5	A	602	CLA	C3-C5-C6-C7
6	A	609	CHL	CBA-CGA-O2A-C1
6	A	610	CHL	C16-C17-C18-C20
5	C	606	CLA	C2C-C3C-CAC-CBC
5	B	603	CLA	C3-C5-C6-C7
6	B	612	CHL	C4-C3-C5-C6
6	C	612	CHL	C4-C3-C5-C6
6	C	612	CHL	C2C-C3C-CAC-CBC
5	B	606	CLA	C2C-C3C-CAC-CBC
7	C	801	LHG	C11-C12-C13-C14
5	A	608	CLA	O2A-C1-C2-C3
5	C	607	CLA	C16-C17-C18-C20
6	B	610	CHL	C16-C17-C18-C20
6	C	610	CHL	C16-C17-C18-C20
7	B	801	LHG	C15-C16-C17-C18
5	C	602	CLA	O1A-CGA-O2A-C1
6	B	611	CHL	C13-C15-C16-C17
5	C	602	CLA	C11-C12-C13-C14
6	A	612	CHL	C4-C3-C5-C6
6	C	611	CHL	C16-C17-C18-C19
5	A	601	CLA	C1A-C2A-CAA-CBA
5	A	603	CLA	C1A-C2A-CAA-CBA
5	A	604	CLA	C1A-C2A-CAA-CBA
5	B	601	CLA	C1A-C2A-CAA-CBA
5	B	603	CLA	C1A-C2A-CAA-CBA
5	B	604	CLA	C1A-C2A-CAA-CBA
5	C	601	CLA	C1A-C2A-CAA-CBA
5	C	603	CLA	C1A-C2A-CAA-CBA
5	C	604	CLA	C1A-C2A-CAA-CBA
8	C	802	DGD	C5B-C6B-C7B-C8B
5	A	601	CLA	C6-C7-C8-C10
5	A	601	CLA	C12-C13-C15-C16
5	A	605	CLA	C11-C10-C8-C7
5	B	601	CLA	C6-C7-C8-C10
5	B	601	CLA	C11-C10-C8-C7
5	B	601	CLA	C12-C13-C15-C16
5	B	605	CLA	C11-C10-C8-C7
5	C	601	CLA	C6-C7-C8-C10
5	C	605	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
5	C	605	CLA	C11-C10-C8-C7
6	A	609	CHL	C12-C13-C15-C16
6	A	610	CHL	C11-C10-C8-C7
6	B	609	CHL	C12-C13-C15-C16
6	B	610	CHL	C11-C10-C8-C7
6	B	611	CHL	C11-C10-C8-C7
6	C	609	CHL	C11-C10-C8-C7
6	C	609	CHL	C12-C13-C15-C16
6	C	610	CHL	C11-C10-C8-C7
6	B	612	CHL	C10-C11-C12-C13
8	B	802	DGD	C1B-C2B-C3B-C4B
8	C	802	DGD	C1B-C2B-C3B-C4B
5	B	607	CLA	C2-C3-C5-C6
6	B	612	CHL	C2-C3-C5-C6
5	B	602	CLA	O1A-CGA-O2A-C1
5	A	601	CLA	C6-C7-C8-C9
5	B	601	CLA	C6-C7-C8-C9
5	C	601	CLA	C6-C7-C8-C9
8	A	802	DGD	C5B-C6B-C7B-C8B
8	B	802	DGD	C2D-C1D-O3G-C3G
2	A	501	LUX	C7-C8-C9-C10
2	A	502	LUX	C7-C8-C9-C10
2	B	501	LUX	C7-C8-C9-C10
2	B	502	LUX	C7-C8-C9-C10
2	C	501	LUX	C7-C8-C9-C10
2	C	502	LUX	C7-C8-C9-C10
6	A	612	CHL	CBA-CGA-O2A-C1
6	A	611	CHL	C16-C17-C18-C19
6	B	611	CHL	C16-C17-C18-C19
8	A	802	DGD	C1B-C2B-C3B-C4B
6	A	612	CHL	C2-C3-C5-C6
6	C	612	CHL	C2-C3-C5-C6
8	B	802	DGD	C5B-C6B-C7B-C8B
7	A	801	LHG	C15-C16-C17-C18
6	B	609	CHL	C2C-C3C-CAC-CBC
5	A	604	CLA	C3-C5-C6-C7
5	A	604	CLA	CBA-CGA-O2A-C1
6	C	609	CHL	CBA-CGA-O2A-C1
5	C	604	CLA	C10-C11-C12-C13
5	B	607	CLA	C4-C3-C5-C6
6	C	612	CHL	CBA-CGA-O2A-C1
5	A	604	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
5	C	603	CLA	CBA-CGA-O2A-C1
5	C	607	CLA	C2-C3-C5-C6
5	A	602	CLA	CBA-CGA-O2A-C1
5	A	603	CLA	CBA-CGA-O2A-C1
5	B	604	CLA	C10-C11-C12-C13
5	A	605	CLA	C6-C7-C8-C9
5	C	605	CLA	C6-C7-C8-C9
6	A	612	CHL	C10-C11-C12-C13
5	A	602	CLA	C11-C12-C13-C14
5	B	602	CLA	C11-C12-C13-C14
5	A	605	CLA	C6-C7-C8-C10
5	B	603	CLA	C11-C10-C8-C7
5	B	605	CLA	C6-C7-C8-C10
5	B	607	CLA	C12-C13-C15-C16
5	C	601	CLA	C11-C10-C8-C7
5	C	603	CLA	C11-C10-C8-C7
6	A	609	CHL	C6-C7-C8-C10
6	A	609	CHL	C11-C10-C8-C7
6	A	611	CHL	C11-C10-C8-C7
6	B	609	CHL	C11-C10-C8-C7
6	B	612	CHL	C11-C10-C8-C7
6	C	611	CHL	C11-C10-C8-C7
6	C	612	CHL	C11-C10-C8-C7
6	B	609	CHL	O1A-CGA-O2A-C1
8	B	802	DGD	C6B-C7B-C8B-C9B
6	B	612	CHL	CBA-CGA-O2A-C1
5	A	602	CLA	C4-C3-C5-C6
5	B	602	CLA	C4-C3-C5-C6
5	C	602	CLA	C4-C3-C5-C6
5	C	607	CLA	C4-C3-C5-C6
2	A	501	LUX	C5-C6-C7-C8
5	A	607	CLA	C4-C3-C5-C6
5	A	607	CLA	C2-C3-C5-C6
5	C	602	CLA	C2-C3-C5-C6
5	C	604	CLA	C4C-C3C-CAC-CBC
5	B	605	CLA	C6-C7-C8-C9
6	B	609	CHL	C6-C7-C8-C9
5	B	601	CLA	C13-C15-C16-C17
5	A	602	CLA	C2-C3-C5-C6
5	B	602	CLA	C2-C3-C5-C6
4	B	504	XAT	C39-C29-C30-C31
5	B	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
5	A	606	CLA	C4C-C3C-CAC-CBC
5	C	601	CLA	C13-C15-C16-C17
5	A	603	CLA	C11-C10-C8-C7
5	C	607	CLA	C12-C13-C15-C16
6	A	611	CHL	C12-C13-C15-C16
6	A	612	CHL	C11-C10-C8-C7
6	B	609	CHL	C6-C7-C8-C10
6	B	611	CHL	C12-C13-C15-C16
8	C	802	DGD	C6B-C7B-C8B-C9B
5	C	607	CLA	C10-C11-C12-C13
6	C	612	CHL	C10-C11-C12-C13
6	A	609	CHL	O1A-CGA-O2A-C1
5	A	604	CLA	C2A-CAA-CBA-CGA
5	C	602	CLA	CBA-CGA-O2A-C1
5	B	604	CLA	C3-C5-C6-C7
5	A	603	CLA	C2A-CAA-CBA-CGA
6	A	611	CHL	C13-C15-C16-C17
6	C	612	CHL	C14-C13-C15-C16
8	B	802	DGD	C7B-C8B-C9B-CAB
8	C	802	DGD	C2D-C1D-O3G-C3G
8	A	802	DGD	C6B-C7B-C8B-C9B
6	A	612	CHL	C4C-C3C-CAC-CBC
6	B	612	CHL	C4C-C3C-CAC-CBC
5	A	604	CLA	C4C-C3C-CAC-CBC
6	A	612	CHL	O1A-CGA-O2A-C1
8	A	802	DGD	C8B-C9B-CAB-CBB
5	A	602	CLA	C11-C10-C8-C7
5	A	605	CLA	C12-C13-C15-C16
5	A	607	CLA	C11-C10-C8-C7
5	A	607	CLA	C12-C13-C15-C16
5	B	602	CLA	C11-C10-C8-C7
5	B	607	CLA	C11-C10-C8-C7
5	C	602	CLA	C11-C10-C8-C7
5	C	607	CLA	C11-C10-C8-C7
6	C	609	CHL	C6-C7-C8-C10
6	C	611	CHL	C12-C13-C15-C16
6	A	609	CHL	C6-C7-C8-C9
6	A	612	CHL	C14-C13-C15-C16
6	C	612	CHL	C11-C12-C13-C14
7	A	801	LHG	O7-C5-C6-O8
7	A	801	LHG	C4-C5-C6-O8
5	B	601	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
5	C	604	CLA	C3-C5-C6-C7
5	C	608	CLA	C2C-C3C-CAC-CBC
5	C	608	CLA	O1A-CGA-O2A-C1
6	C	609	CHL	O1A-CGA-O2A-C1
5	C	606	CLA	CBA-CGA-O2A-C1
8	A	802	DGD	C7B-C8B-C9B-CAB
5	A	604	CLA	CHA-CBD-CGD-O1D
5	A	605	CLA	CHA-CBD-CGD-O1D
5	A	605	CLA	CHA-CBD-CGD-O2D
5	B	604	CLA	CHA-CBD-CGD-O1D
5	B	604	CLA	CHA-CBD-CGD-O2D
5	B	605	CLA	CHA-CBD-CGD-O1D
5	B	605	CLA	CHA-CBD-CGD-O2D
5	C	605	CLA	CHA-CBD-CGD-O1D
5	C	605	CLA	CHA-CBD-CGD-O2D
5	C	608	CLA	CHA-CBD-CGD-O2D
6	B	611	CHL	CHA-CBD-CGD-O2D
7	A	801	LHG	C4-O6-P-O4
7	B	801	LHG	C4-O6-P-O4
7	C	801	LHG	C4-O6-P-O4
5	B	601	CLA	C4-C3-C5-C6
5	C	606	CLA	C4C-C3C-CAC-CBC
5	C	604	CLA	C6-C7-C8-C9
6	B	612	CHL	C14-C13-C15-C16
6	C	609	CHL	C6-C7-C8-C9
5	A	606	CLA	C6-C7-C8-C10
5	B	605	CLA	C12-C13-C15-C16
5	B	606	CLA	C4C-C3C-CAC-CBC
5	A	606	CLA	CBA-CGA-O2A-C1
5	B	606	CLA	CBA-CGA-O2A-C1
5	C	604	CLA	CBA-CGA-O2A-C1
5	C	604	CLA	C2A-CAA-CBA-CGA
6	A	610	CHL	C2A-CAA-CBA-CGA
6	B	610	CHL	C2A-CAA-CBA-CGA
5	B	601	CLA	C14-C13-C15-C16
8	C	802	DGD	C8B-C9B-CAB-CBB
5	A	602	CLA	C6-C7-C8-C10
5	C	601	CLA	C12-C13-C15-C16
5	C	602	CLA	C6-C7-C8-C10
5	C	606	CLA	C6-C7-C8-C10
5	A	604	CLA	O1A-CGA-O2A-C1
3	A	503	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
3	B	503	NEX	C39-C29-C30-C31
3	C	503	NEX	C39-C29-C30-C31
5	B	608	CLA	C2C-C3C-CAC-CBC
5	B	604	CLA	C2C-C3C-CAC-CBC
5	A	604	CLA	C6-C7-C8-C9
5	B	604	CLA	C6-C7-C8-C9
6	B	612	CHL	C11-C12-C13-C14
6	C	611	CHL	C11-C12-C13-C14
5	C	604	CLA	C13-C15-C16-C17
5	A	607	CLA	C10-C11-C12-C13
6	C	610	CHL	C2A-CAA-CBA-CGA
3	A	503	NEX	C28-C29-C30-C31
3	C	503	NEX	C28-C29-C30-C31
8	B	802	DGD	C8B-C9B-CAB-CBB
5	A	604	CLA	C12-C13-C15-C16
5	B	602	CLA	C6-C7-C8-C10
5	B	603	CLA	C11-C12-C13-C15
5	B	604	CLA	C12-C13-C15-C16
5	C	604	CLA	C12-C13-C15-C16
5	A	608	CLA	C2A-CAA-CBA-CGA
5	B	604	CLA	C2A-CAA-CBA-CGA
6	A	609	CHL	C4-C3-C5-C6
8	C	802	DGD	C7B-C8B-C9B-CAB
5	A	603	CLA	C6-C7-C8-C9
6	B	609	CHL	C4-C3-C5-C6
6	A	612	CHL	C2C-C3C-CAC-CBC
5	A	608	CLA	O1A-CGA-O2A-C1
7	B	801	LHG	C4-C5-C6-O8
7	C	801	LHG	C4-C5-C6-O8
5	A	601	CLA	C13-C15-C16-C17
4	C	504	XAT	C39-C29-C30-C31
7	B	801	LHG	O7-C5-C6-O8
7	C	801	LHG	O7-C5-C6-O8
5	B	604	CLA	C13-C15-C16-C17
5	C	605	CLA	C12-C13-C15-C16
6	B	610	CHL	C11-C12-C13-C15
6	C	610	CHL	C11-C12-C13-C15
5	B	603	CLA	C14-C13-C15-C16
6	A	611	CHL	C2-C1-O2A-CGA
6	A	612	CHL	C2-C1-O2A-CGA
6	B	611	CHL	C2-C1-O2A-CGA
6	B	612	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
5	B	602	CLA	CBA-CGA-O2A-C1
3	B	503	NEX	C28-C29-C30-C31
5	B	608	CLA	C2A-CAA-CBA-CGA
5	C	608	CLA	C2A-CAA-CBA-CGA
7	A	801	LHG	C27-C28-C29-C30
5	B	607	CLA	C10-C11-C12-C13
5	A	603	CLA	C11-C12-C13-C15
5	B	606	CLA	C6-C7-C8-C10
5	C	603	CLA	C11-C12-C13-C15
6	A	610	CHL	C11-C12-C13-C15
6	B	609	CHL	C11-C12-C13-C15
6	C	609	CHL	C11-C12-C13-C15
6	C	610	CHL	C12-C13-C15-C16
5	A	601	CLA	C2B-C3B-CAB-CBB
5	A	606	CLA	C2B-C3B-CAB-CBB
5	B	606	CLA	C2B-C3B-CAB-CBB
5	C	601	CLA	C2B-C3B-CAB-CBB
5	C	603	CLA	C2B-C3B-CAB-CBB
5	C	606	CLA	C2B-C3B-CAB-CBB
6	C	612	CHL	C2-C1-O2A-CGA
6	C	612	CHL	O1A-CGA-O2A-C1
2	A	501	LUX	C11-C10-C9-C8
2	B	501	LUX	C11-C10-C9-C8
2	B	502	LUX	C11-C10-C9-C8
2	C	501	LUX	C11-C10-C9-C8
5	C	603	CLA	CAA-CBA-CGA-O2A
5	B	608	CLA	C4C-C3C-CAC-CBC
6	A	612	CHL	C11-C12-C13-C14
5	A	603	CLA	CAA-CBA-CGA-O2A
5	A	607	CLA	C4B-C3B-CAB-CBB
5	B	603	CLA	CAA-CBA-CGA-O2A
2	A	501	LUX	C7-C8-C9-C19
2	B	501	LUX	C7-C8-C9-C19
2	B	502	LUX	C7-C8-C9-C19
2	C	501	LUX	C7-C8-C9-C19
2	C	502	LUX	C7-C8-C9-C19
6	C	611	CHL	C2-C1-O2A-CGA
6	A	609	CHL	C11-C12-C13-C15
6	A	610	CHL	C12-C13-C15-C16
6	B	610	CHL	C12-C13-C15-C16
6	B	613	CHL	CAA-CBA-CGA-O2A
6	B	612	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	C	801	LHG	C27-C28-C29-C30
5	B	604	CLA	CBA-CGA-O2A-C1
5	A	606	CLA	CAA-CBA-CGA-O2A
5	A	603	CLA	C14-C13-C15-C16
5	C	603	CLA	C14-C13-C15-C16
7	B	801	LHG	C9-C10-C11-C12
6	C	609	CHL	C4-C3-C5-C6
5	C	606	CLA	CAA-CBA-CGA-O2A
4	A	504	XAT	C21-C26-C27-C28
4	C	504	XAT	C21-C26-C27-C28
5	B	606	CLA	CAA-CBA-CGA-O2A
5	C	601	CLA	C2A-CAA-CBA-CGA
5	B	604	CLA	C4C-C3C-CAC-CBC
5	B	605	CLA	CAD-CBD-CGD-O2D
5	B	608	CLA	CAD-CBD-CGD-O2D
5	C	603	CLA	CAA-CBA-CGA-O1A
7	A	801	LHG	O8-C23-C24-C25
8	B	802	DGD	O2G-C1B-C2B-C3B
8	C	802	DGD	O2G-C1B-C2B-C3B
5	B	603	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

60 monomers are involved in 769 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	CLA	23	0
5	B	604	CLA	22	0
5	B	605	CLA	23	0
6	A	613	CHL	6	0
7	A	801	LHG	12	0
2	A	502	LUX	19	0
6	A	614	CHL	14	0
5	C	606	CLA	18	0
5	A	602	CLA	12	0
5	B	608	CLA	21	0
6	C	614	CHL	13	0
6	C	609	CHL	30	0
5	B	607	CLA	17	0
3	B	503	NEX	3	0
5	C	603	CLA	13	0
6	B	613	CHL	9	0
6	B	614	CHL	14	0

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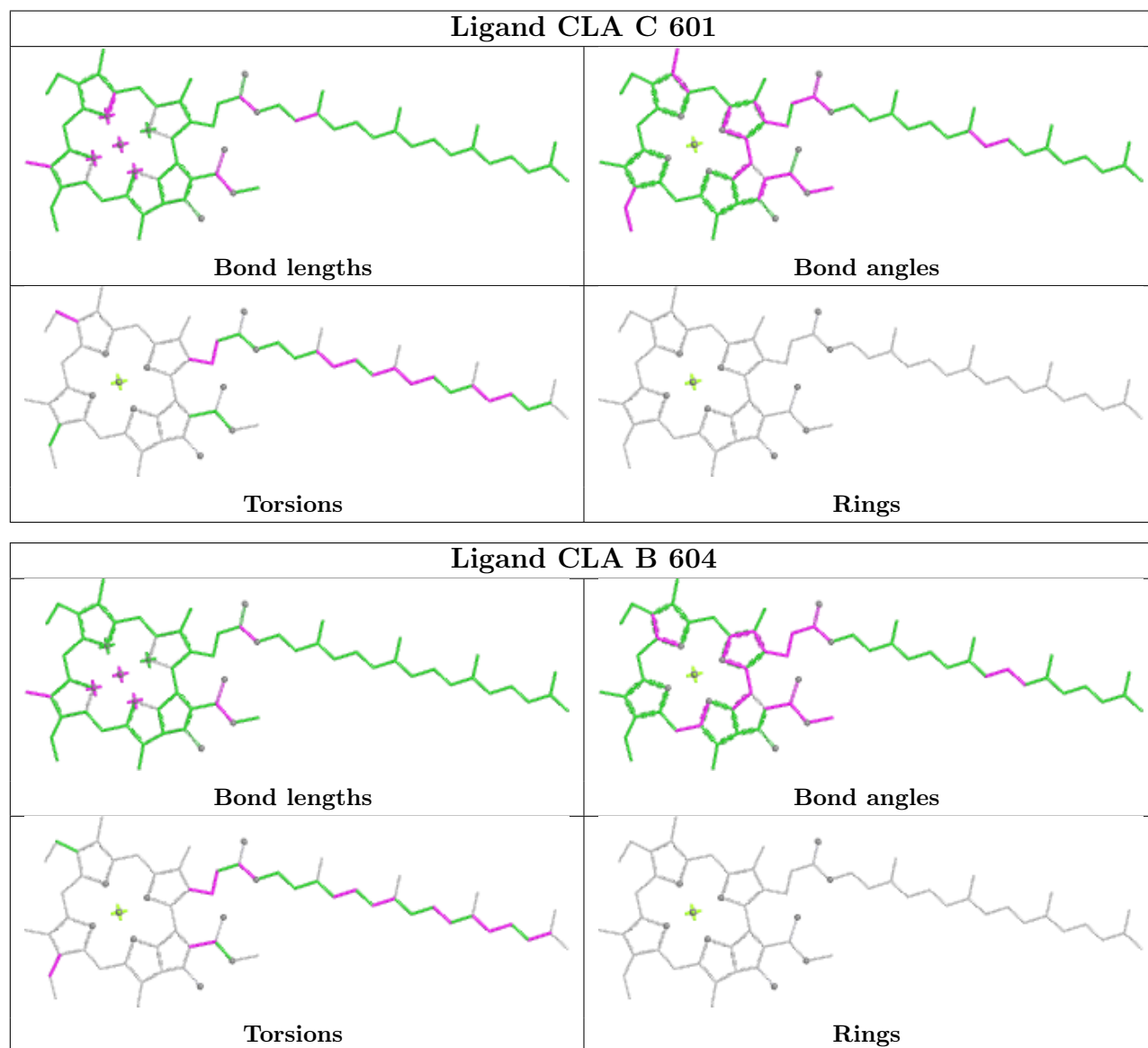
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	602	CLA	11	0
6	B	612	CHL	21	0
3	C	503	NEX	3	0
5	B	601	CLA	24	0
5	C	605	CLA	20	0
6	A	611	CHL	20	0
5	A	606	CLA	17	0
2	C	502	LUX	19	0
5	A	603	CLA	13	0
5	A	605	CLA	20	0
3	A	503	NEX	3	0
6	A	612	CHL	17	0
5	A	608	CLA	13	0
2	C	501	LUX	27	0
7	C	801	LHG	13	0
8	B	802	DGD	2	0
4	A	504	XAT	18	0
6	C	612	CHL	21	0
2	A	501	LUX	25	0
5	A	607	CLA	16	0
6	B	611	CHL	21	0
8	C	802	DGD	4	0
5	B	606	CLA	18	0
5	C	608	CLA	15	0
5	C	602	CLA	10	0
5	A	601	CLA	20	0
6	B	609	CHL	27	0
6	A	610	CHL	30	0
5	C	604	CLA	18	0
5	B	603	CLA	22	0
2	B	501	LUX	29	0
6	C	611	CHL	22	0
6	C	610	CHL	31	0
8	A	802	DGD	4	0
4	B	504	XAT	16	0
2	B	502	LUX	16	0
4	C	504	XAT	16	0
5	A	604	CLA	19	0
7	B	801	LHG	13	0
6	A	609	CHL	31	0
6	B	610	CHL	29	0
5	C	607	CLA	19	0

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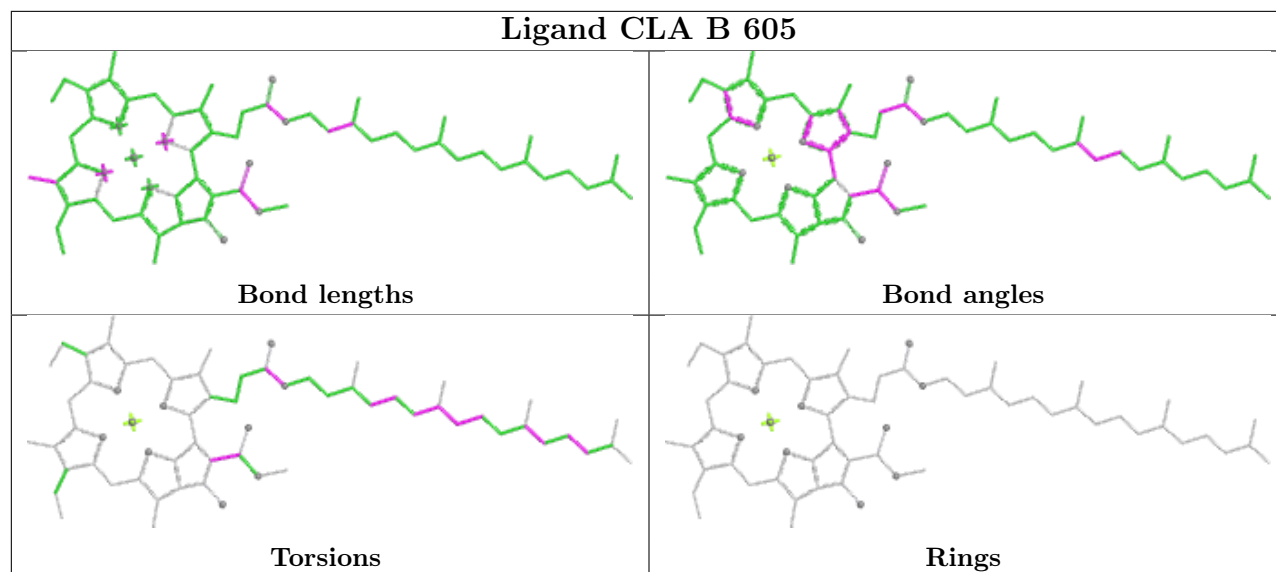
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	613	CHL	5	0

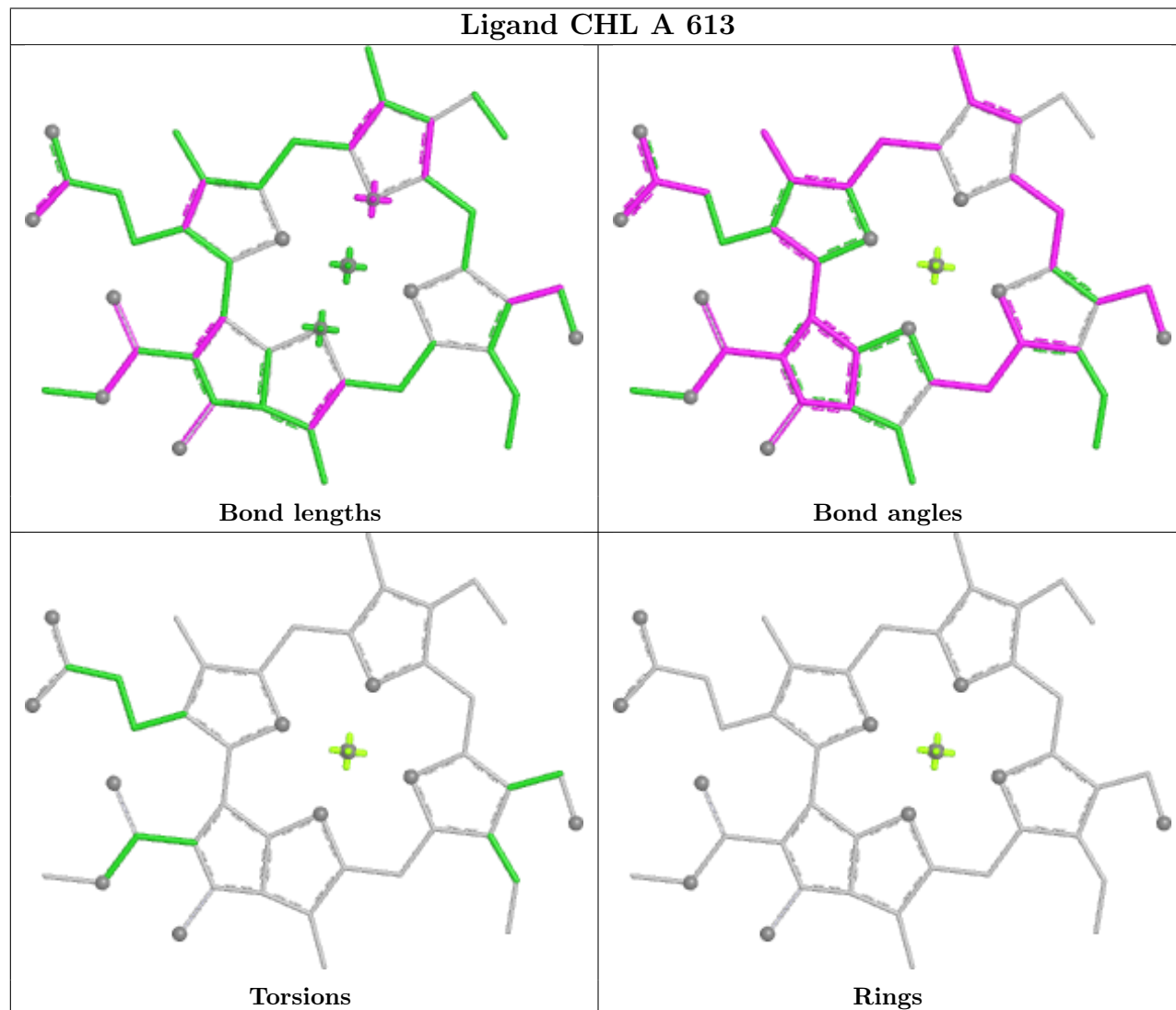
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

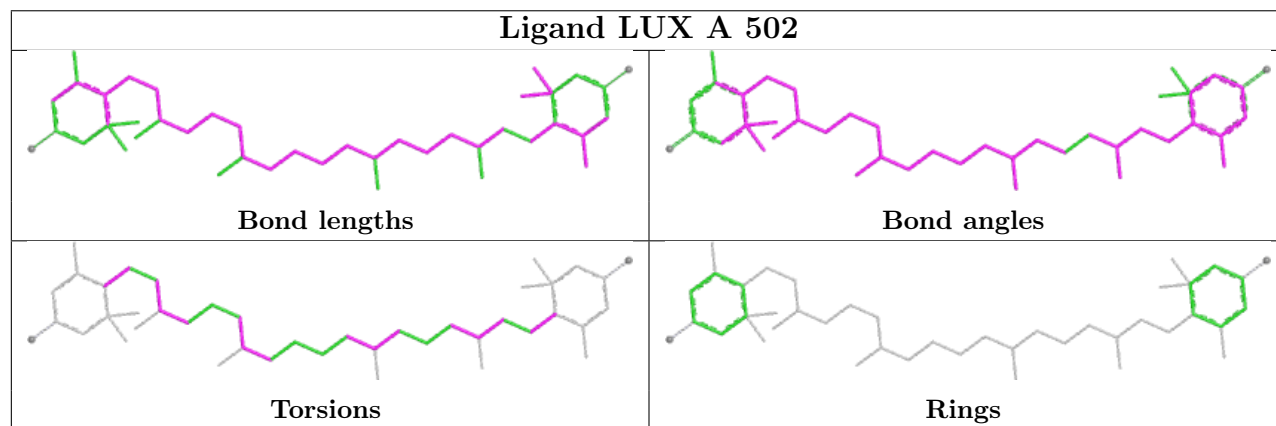
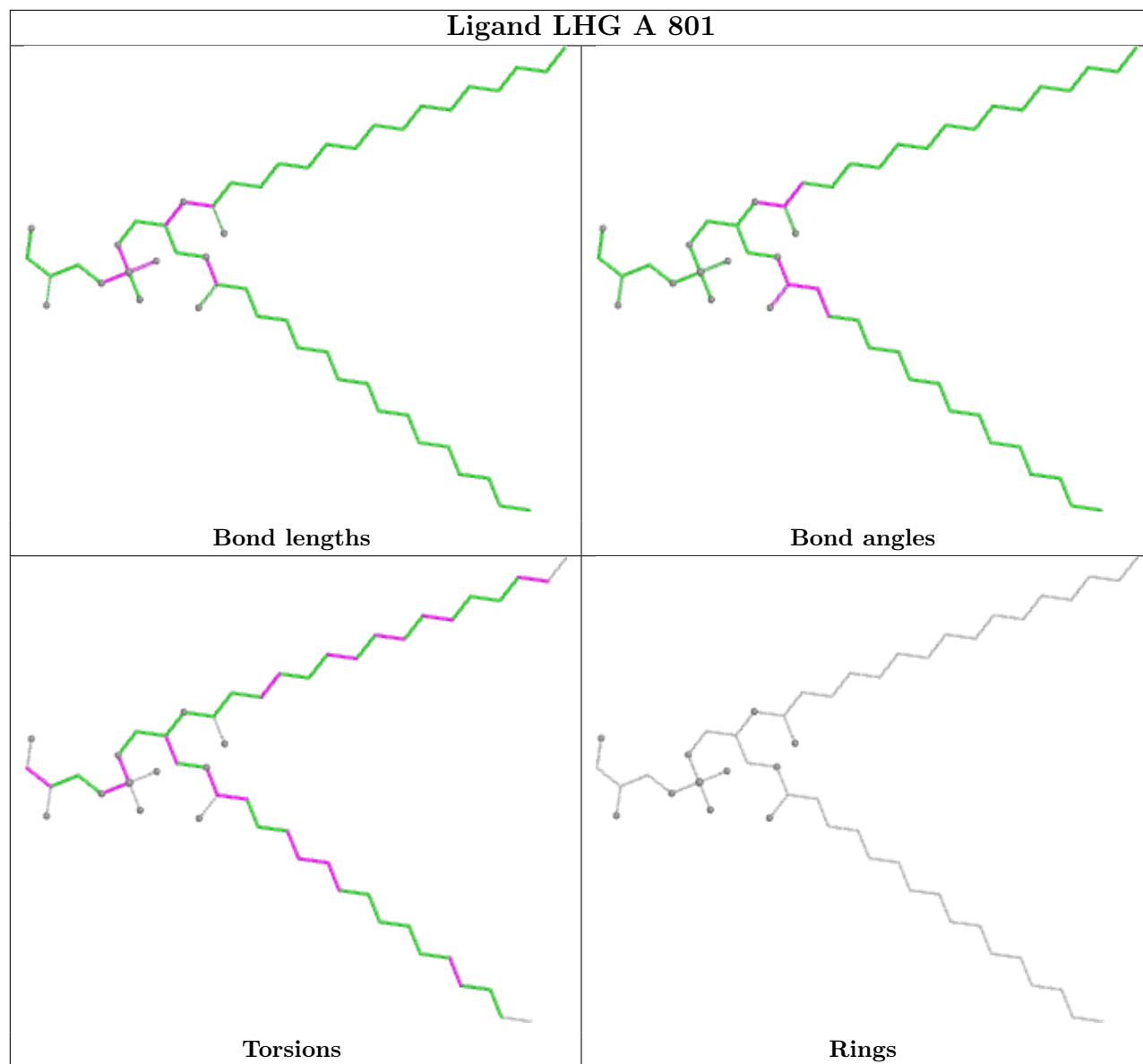


Ligand CLA B 605

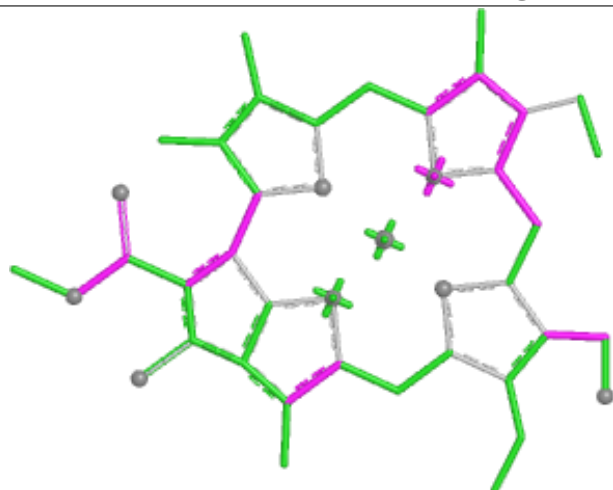


Ligand CHL A 613

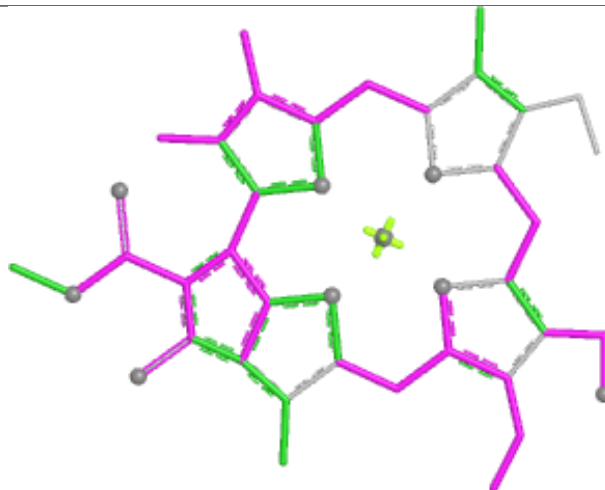




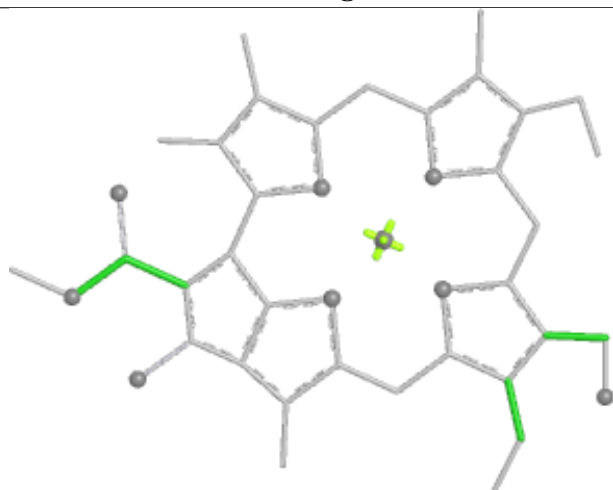
Ligand CHL A 614



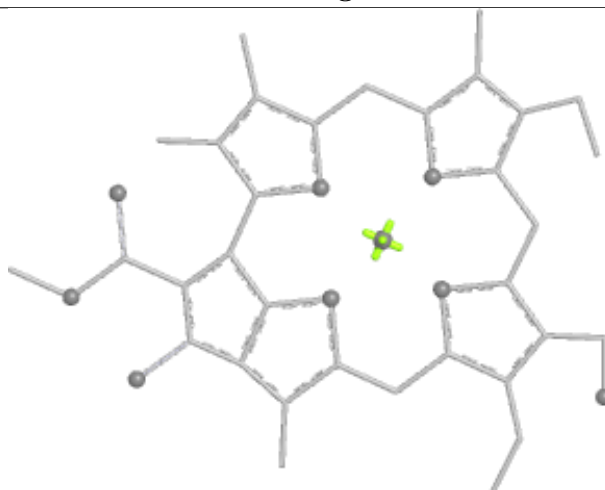
Bond lengths



Bond angles

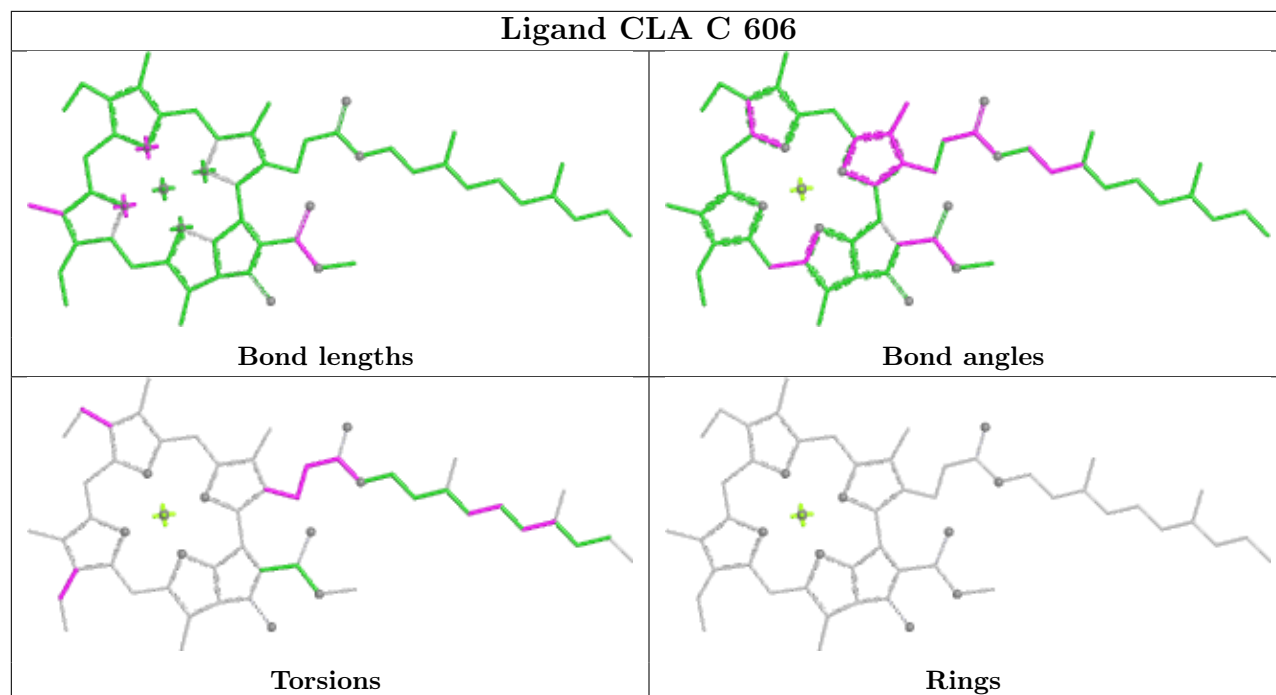


Torsions

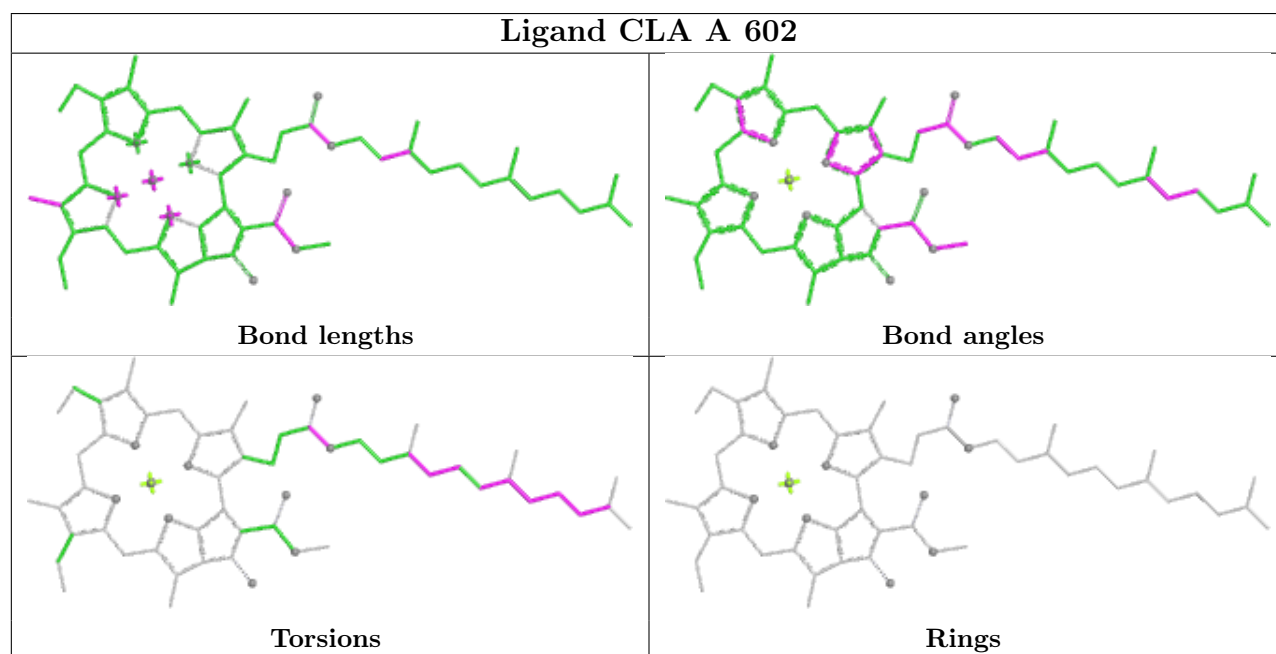


Rings

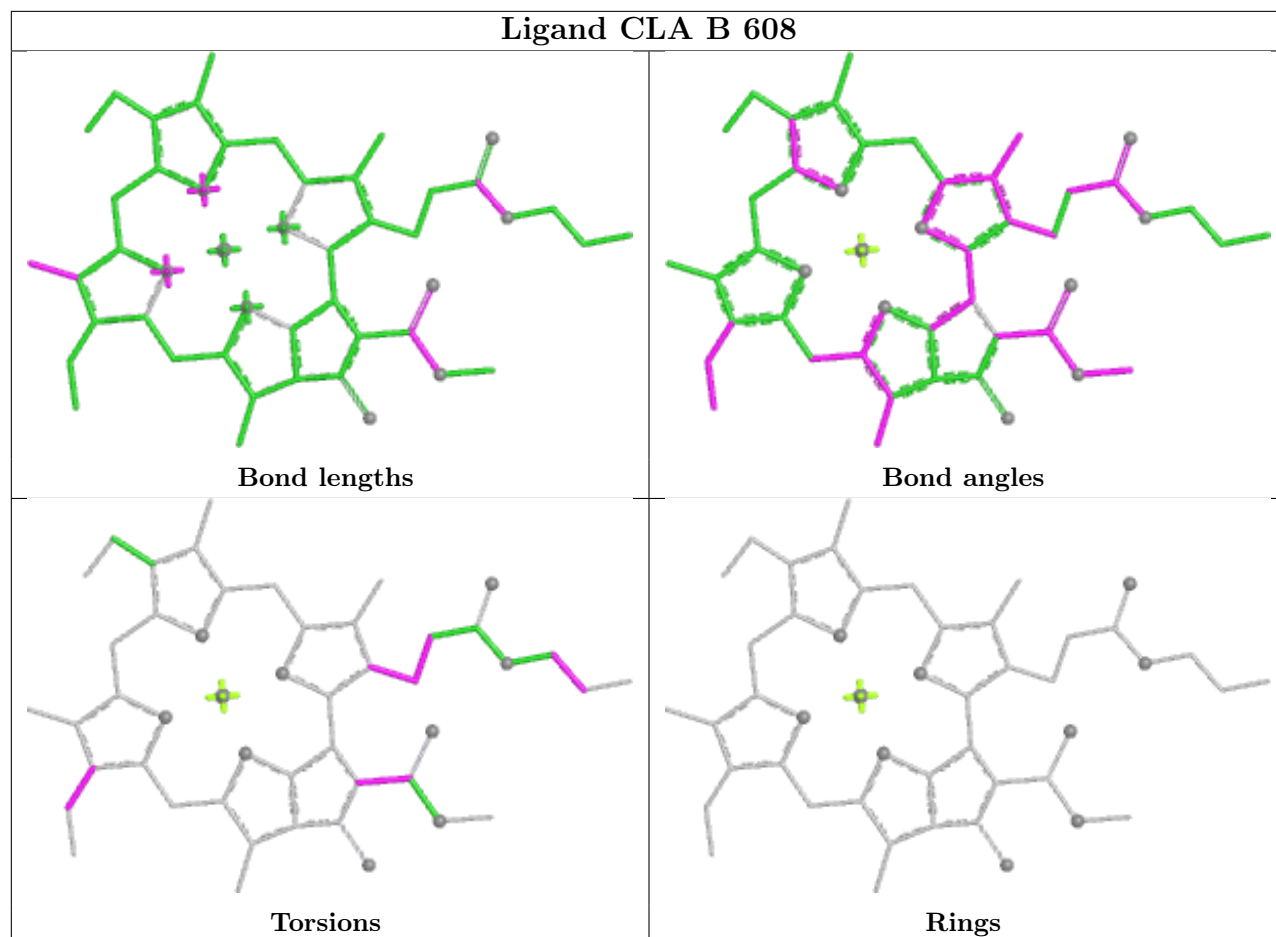
Ligand CLA C 606



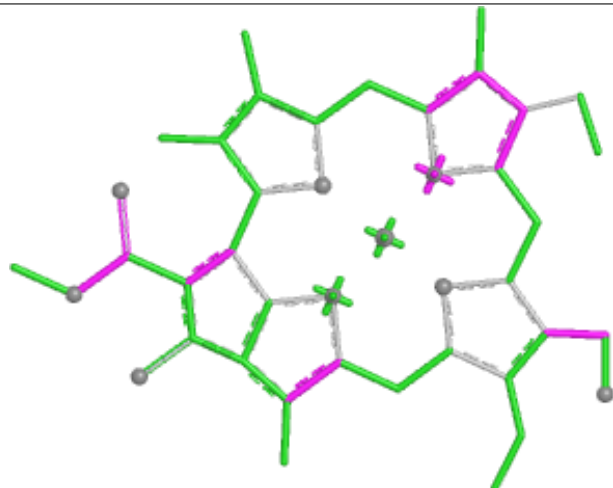
Ligand CLA A 602



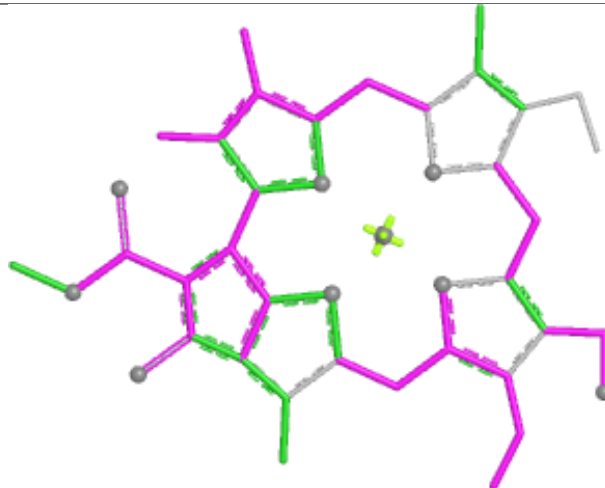
Ligand CLA B 608



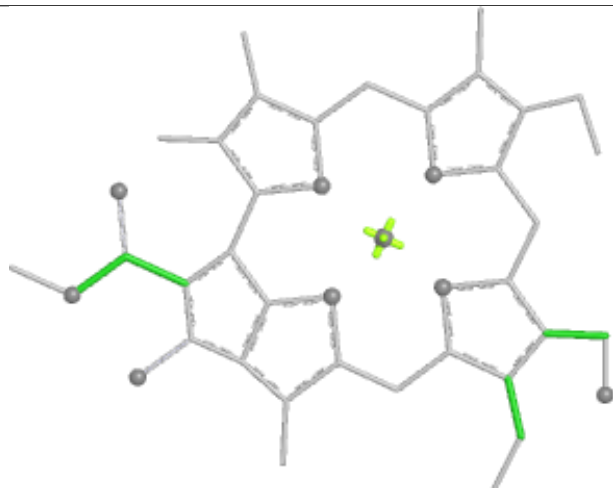
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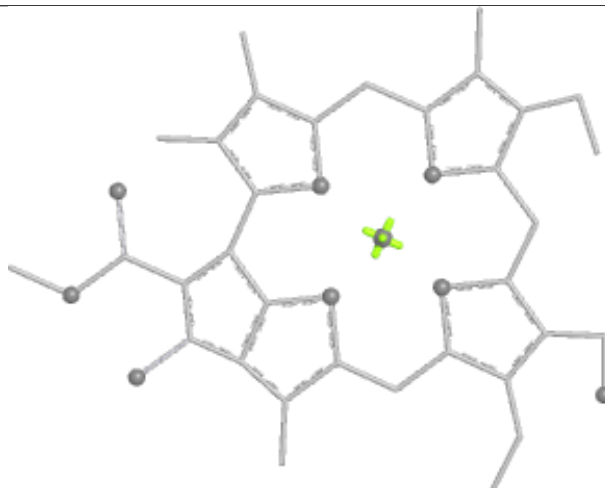
Bond lengths



Bond angles

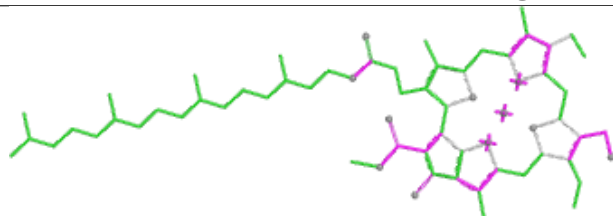


Torsions

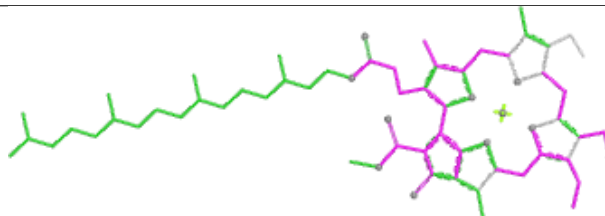


Rings

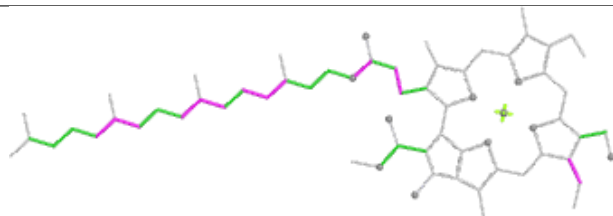
Ligand CHL C 609



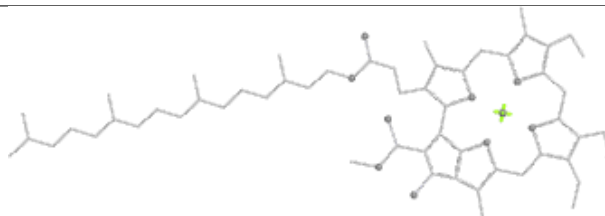
Bond lengths



Bond angles

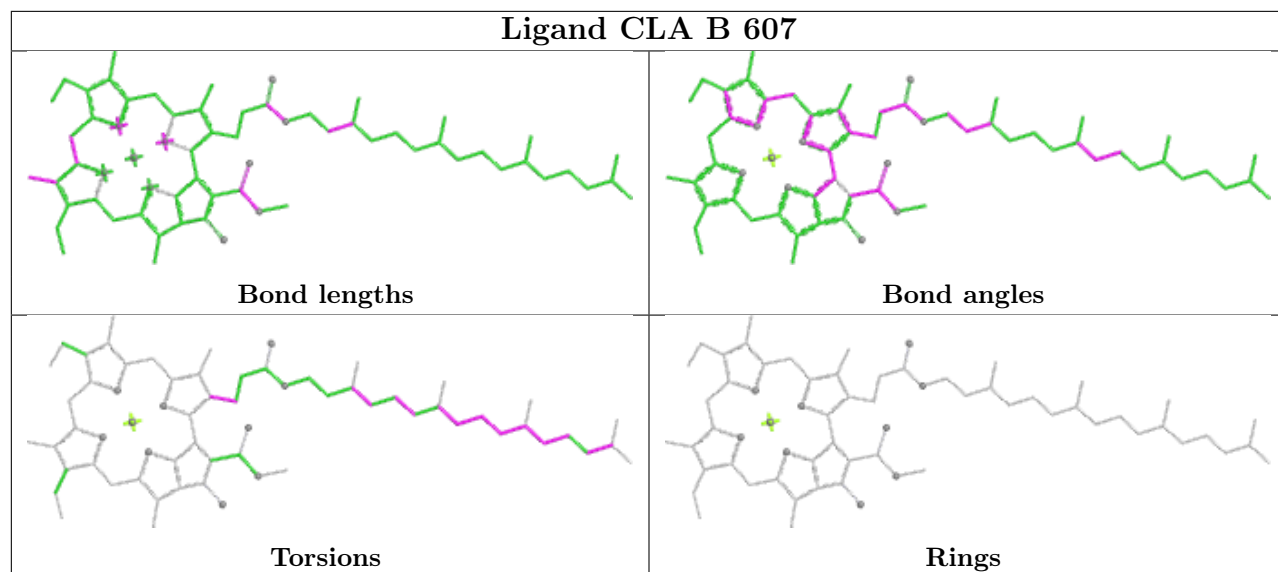


Torsions

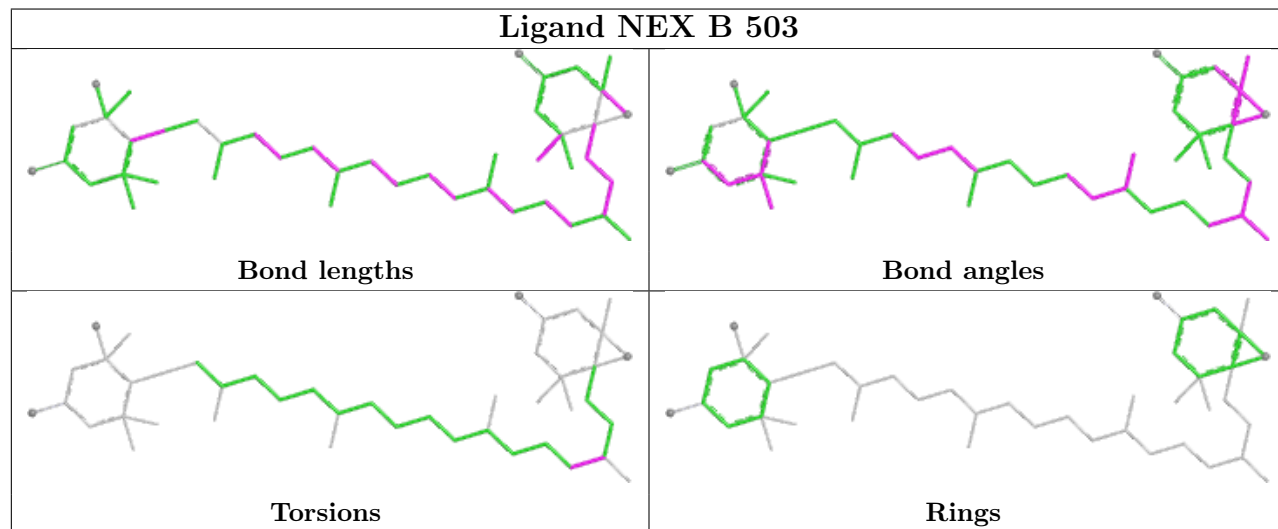


Rings

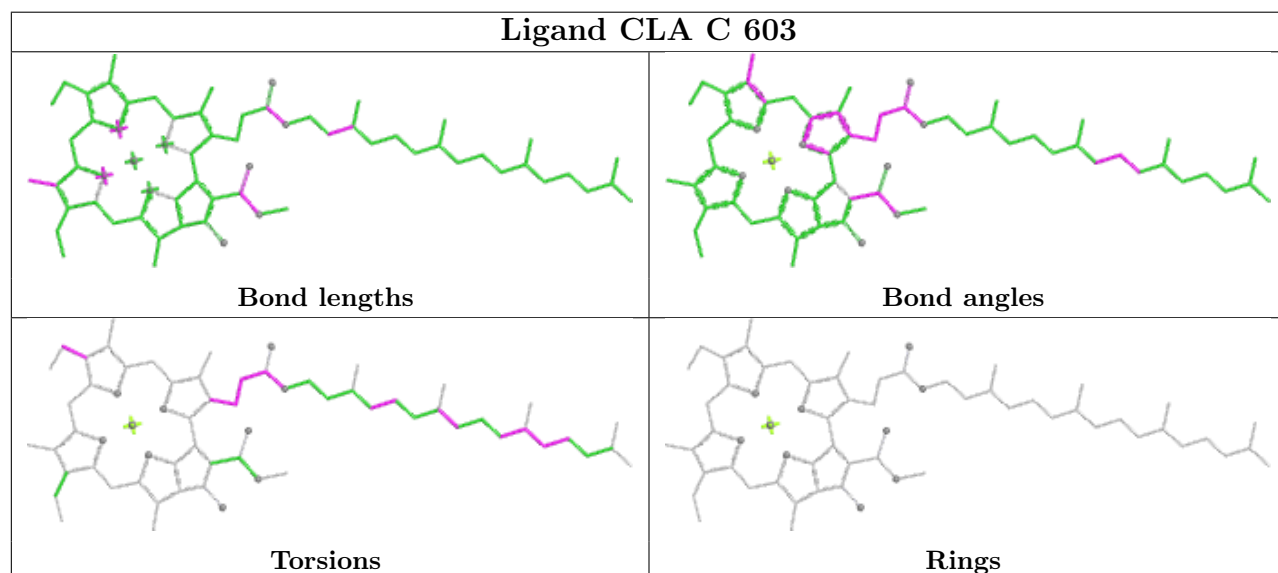
Ligand CLA B 607



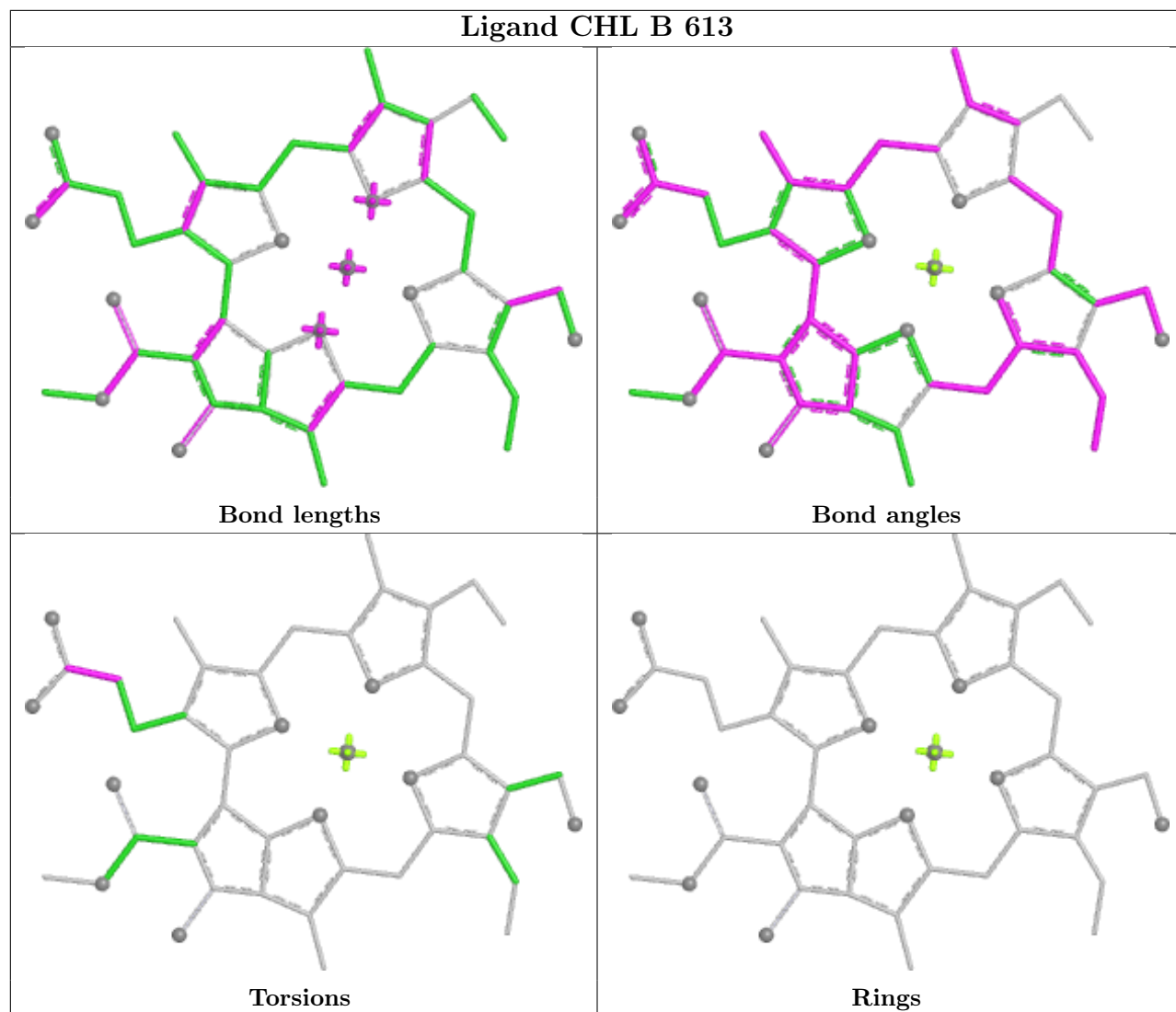
Ligand NEX B 503



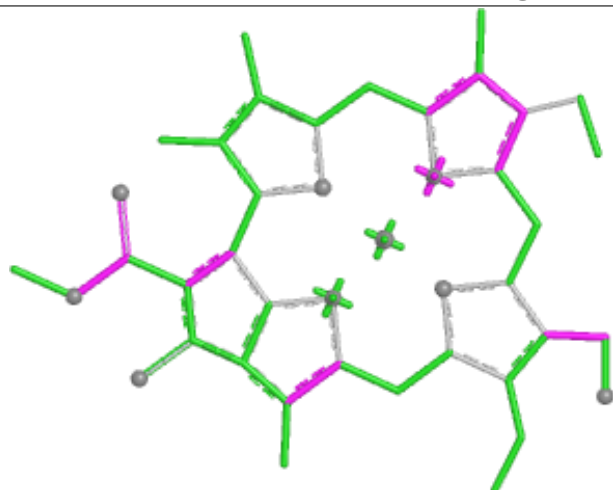
Ligand CLA C 603



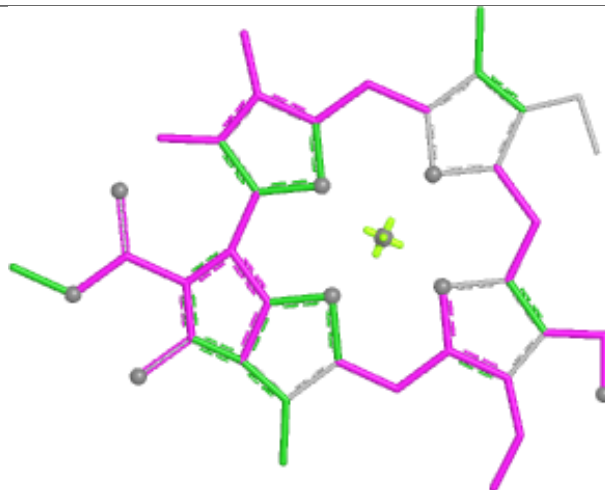
Ligand CHL B 613



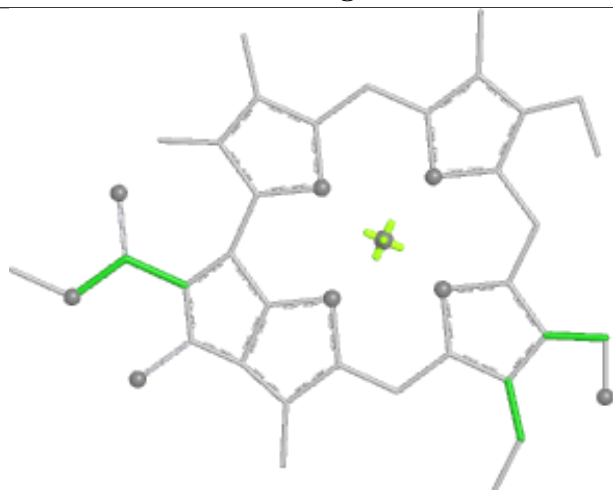
Ligand CHL B 614



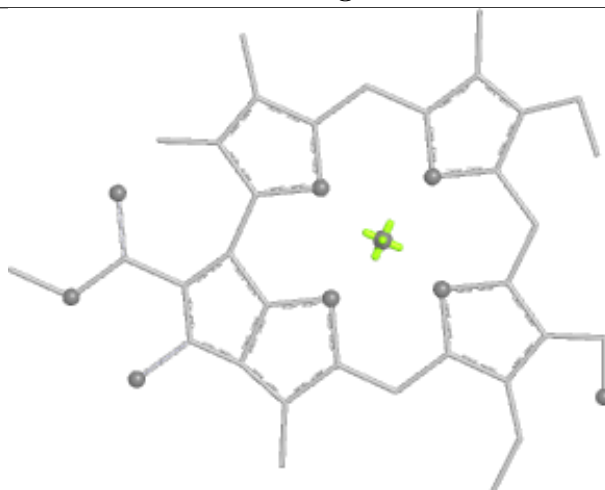
Bond lengths



Bond angles

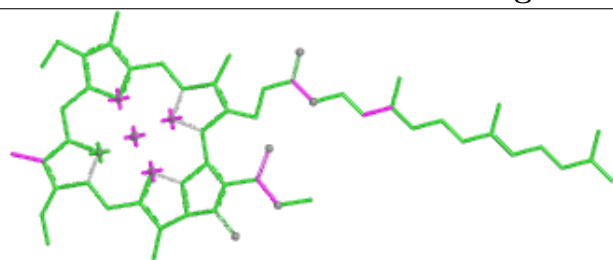


Torsions

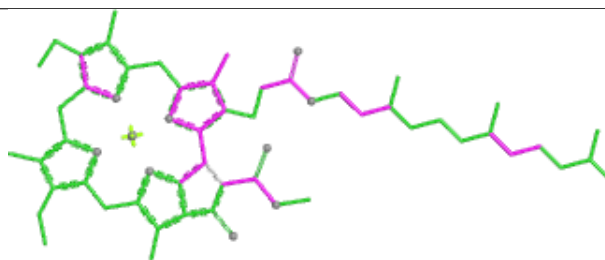


Rings

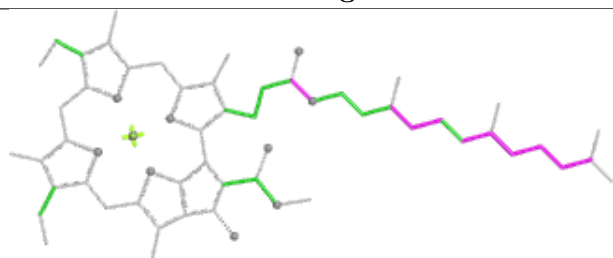
Ligand CLA B 602



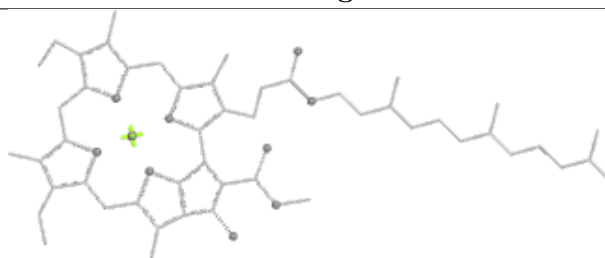
Bond lengths



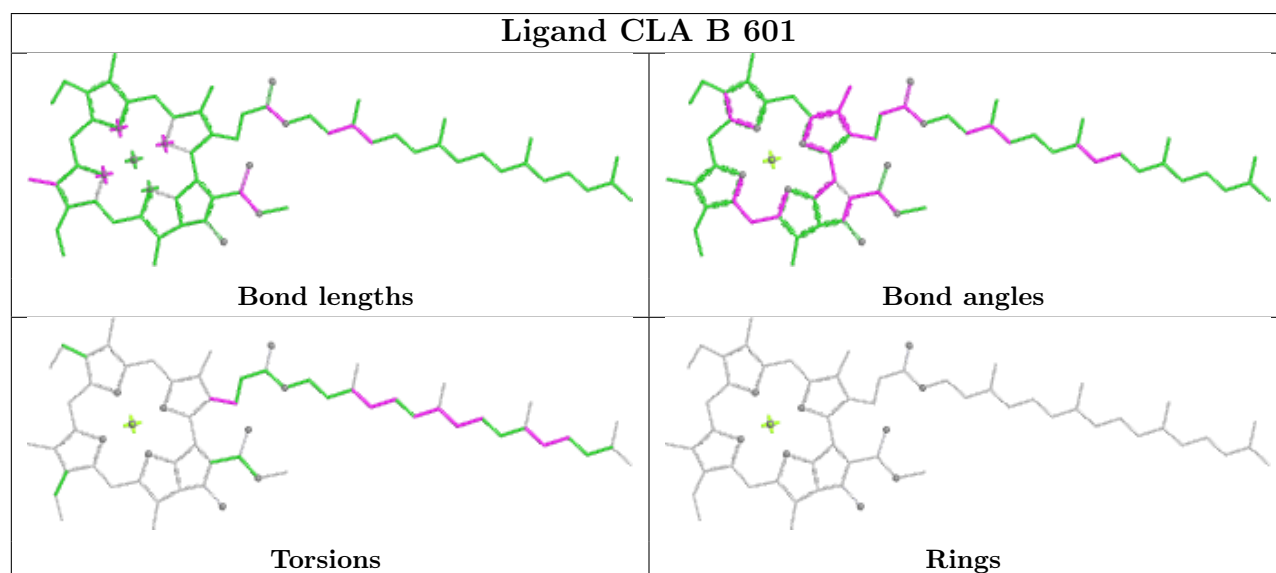
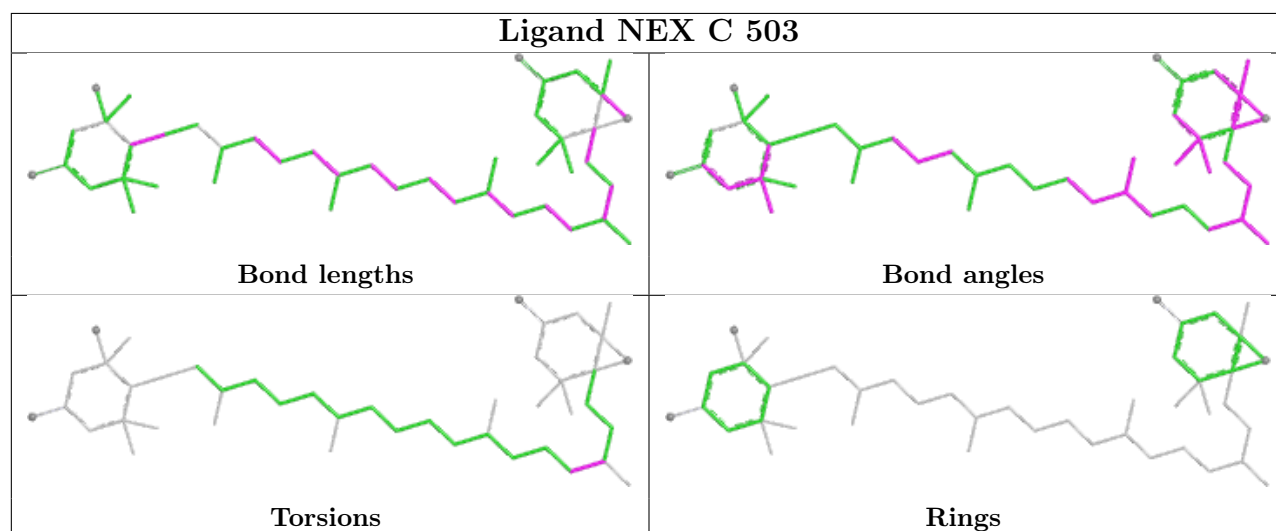
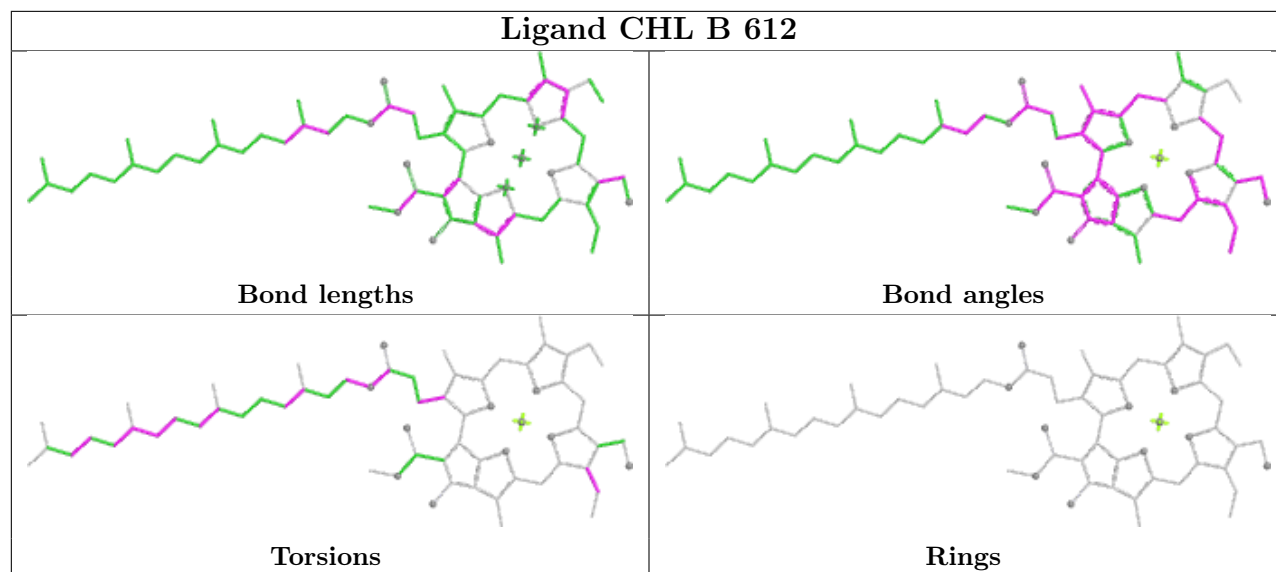
Bond angles

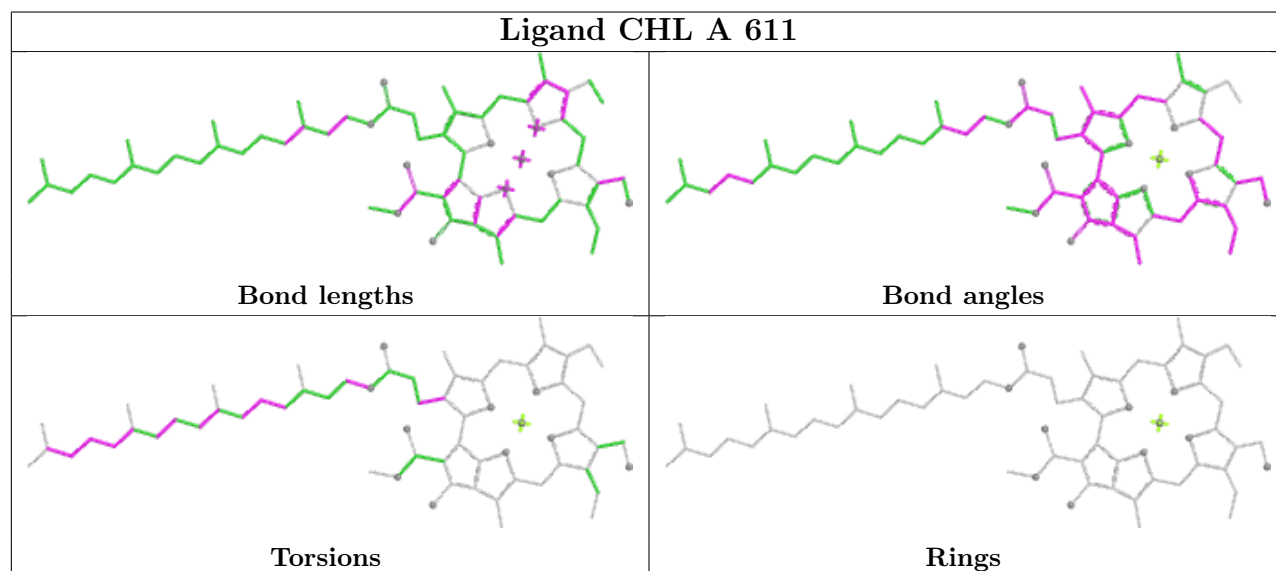
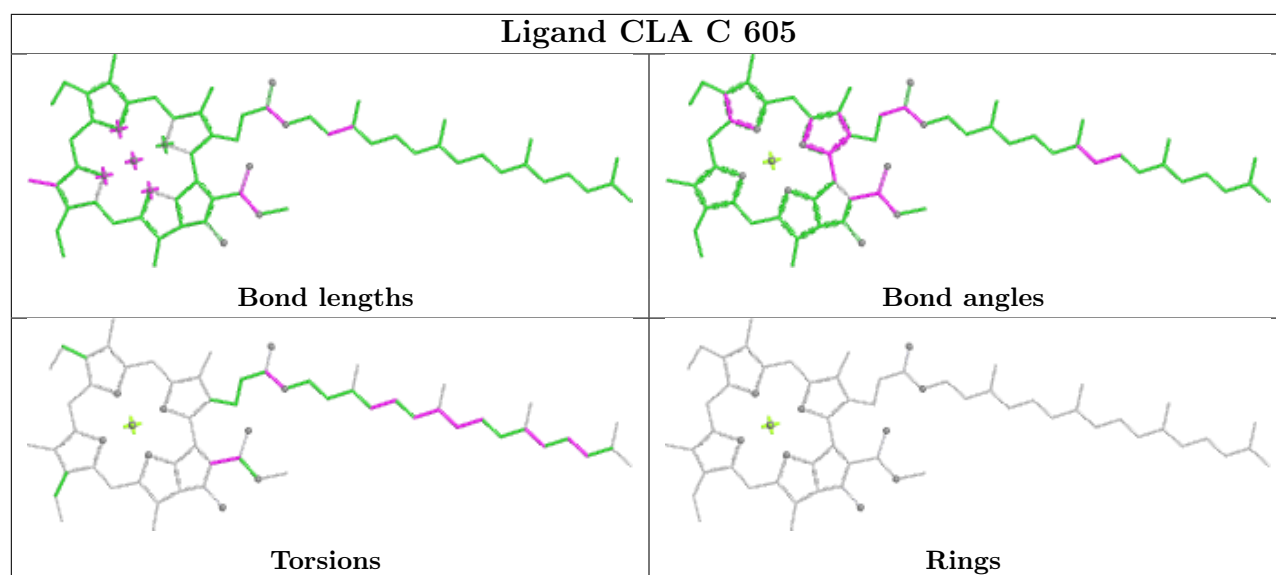


Torsions

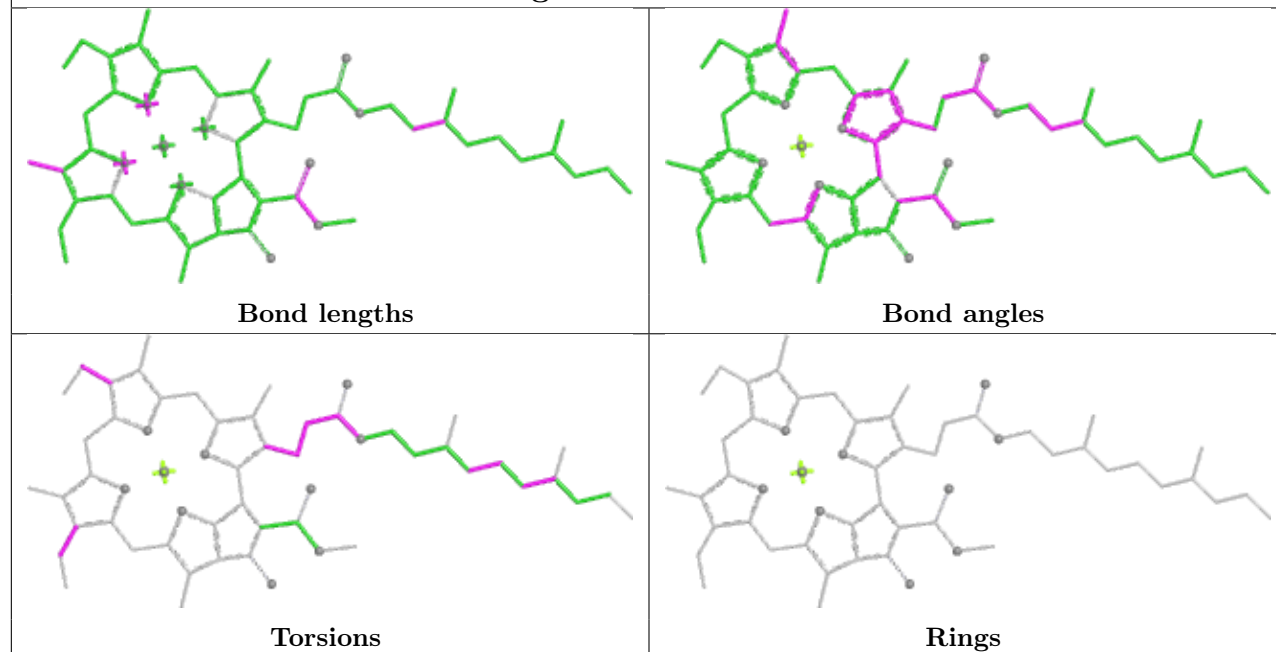


Rings

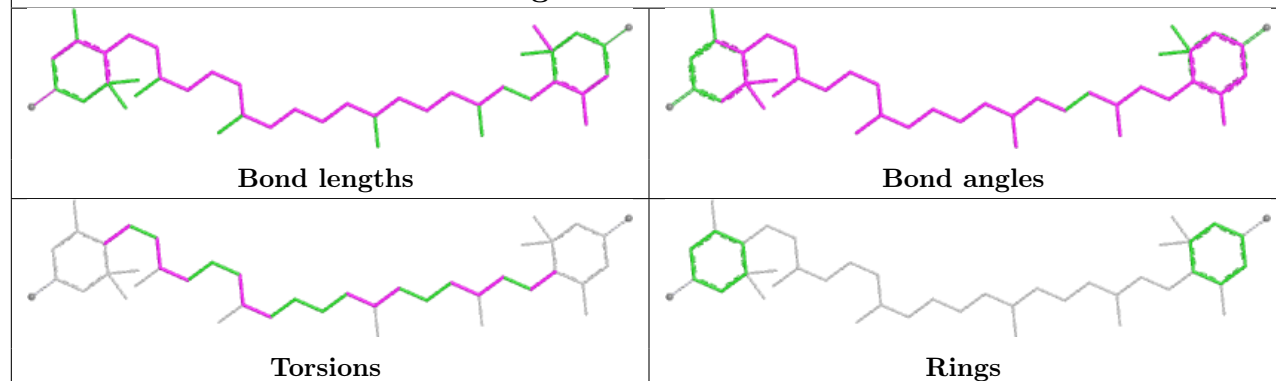




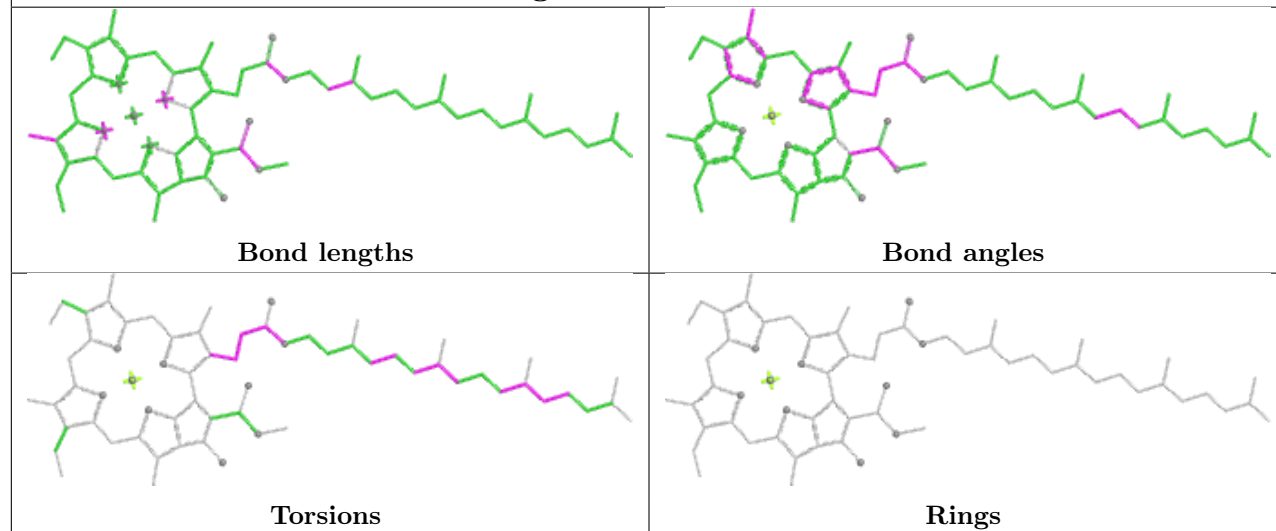
Ligand CLA A 606



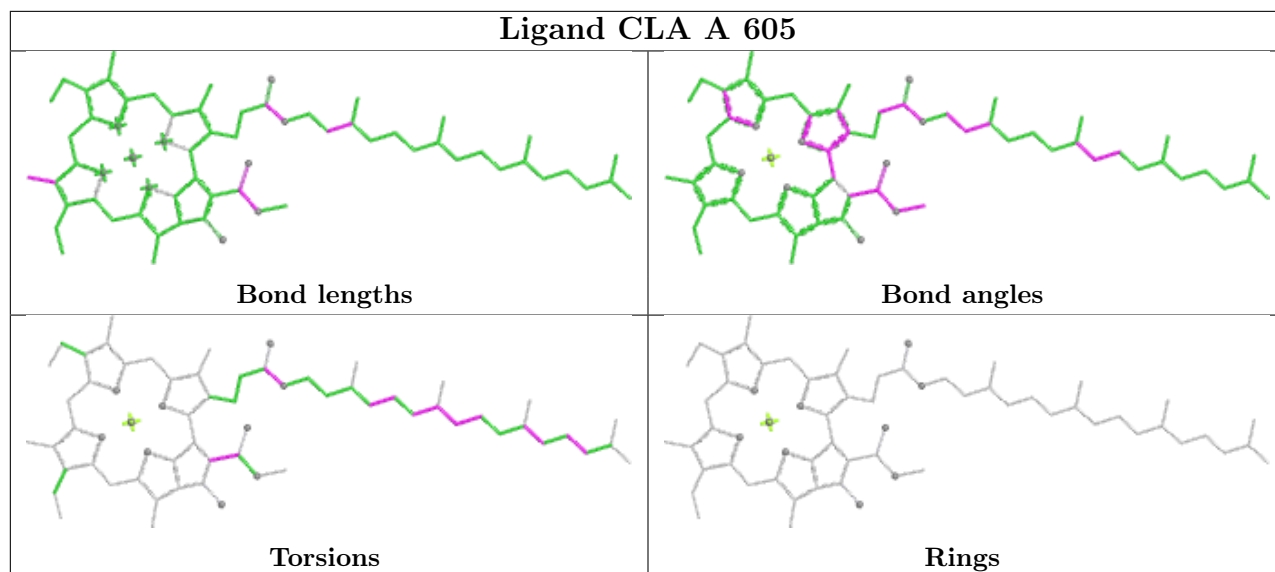
Ligand LUX C 502



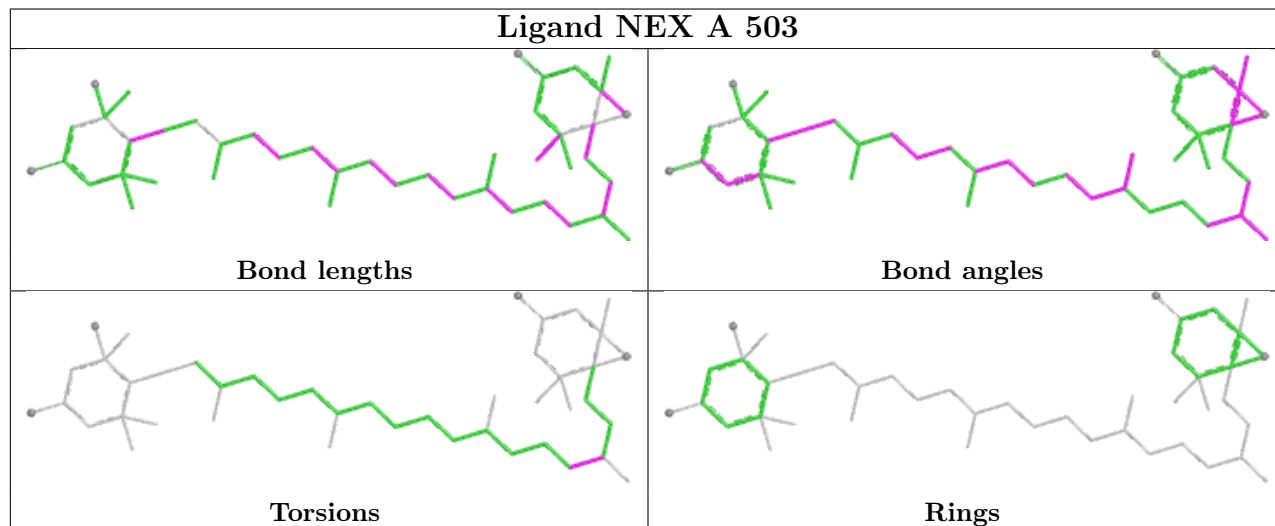
Ligand CLA A 603



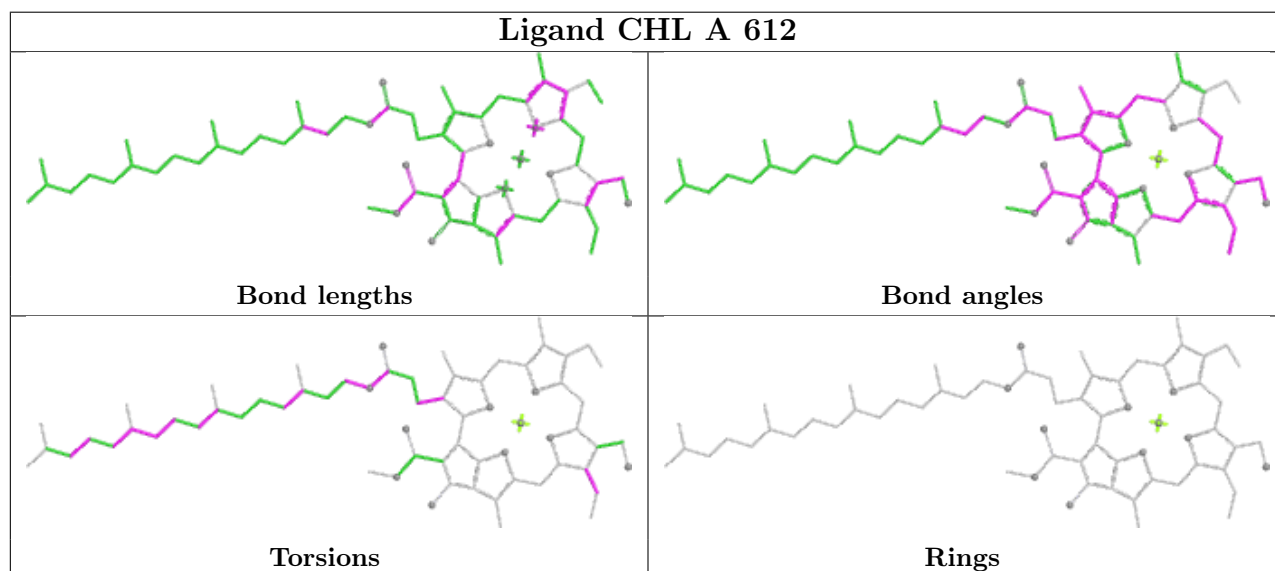
Ligand CLA A 605



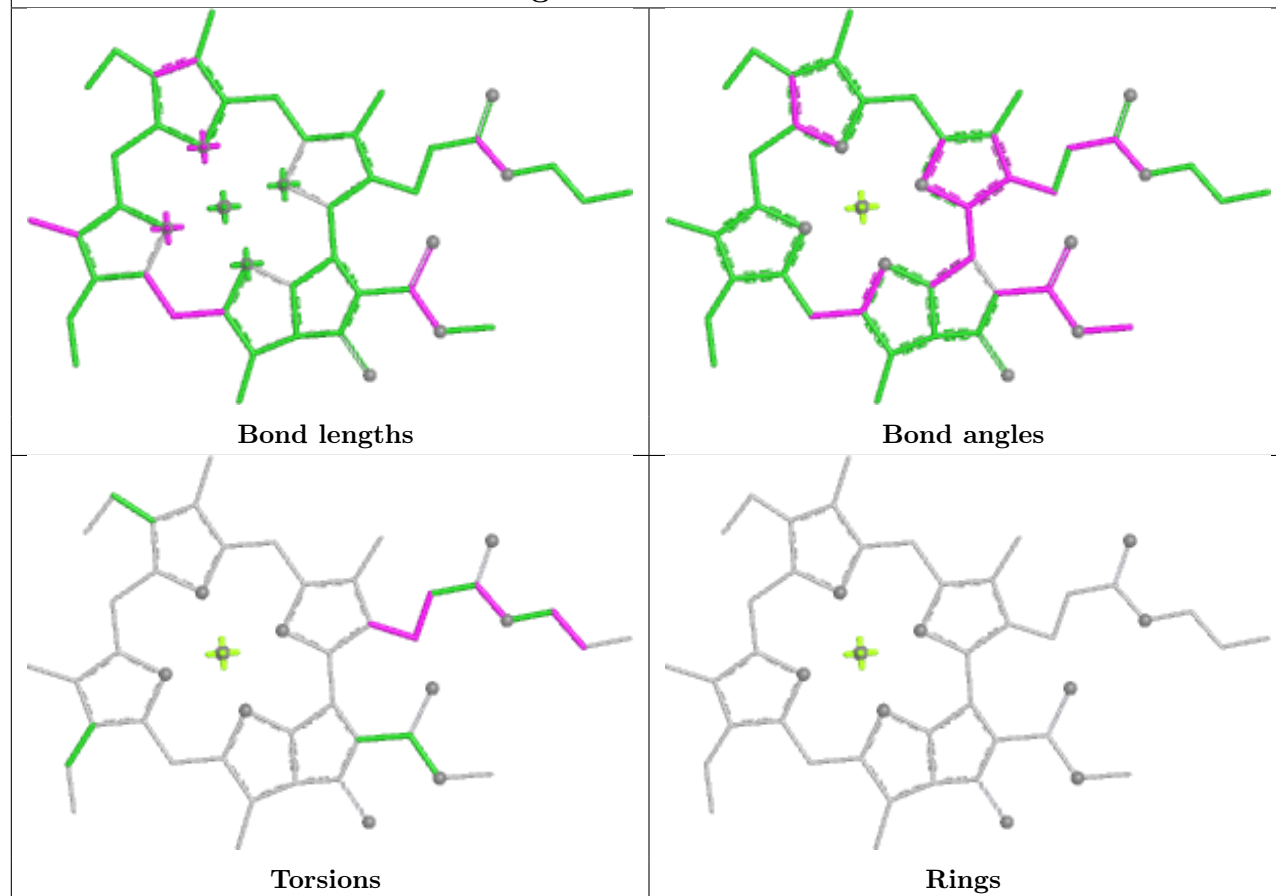
Ligand NEX A 503



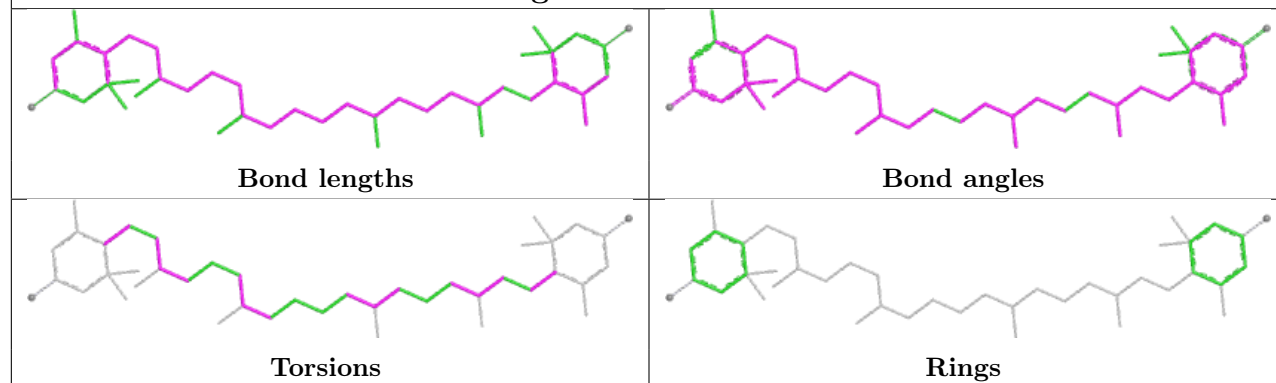
Ligand CHL A 612

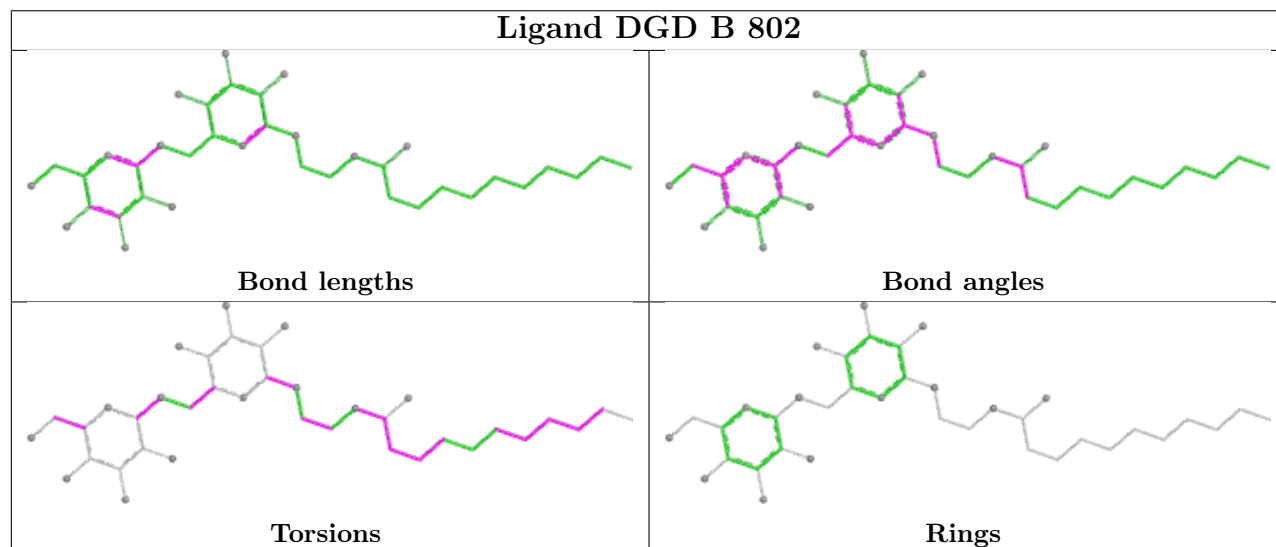
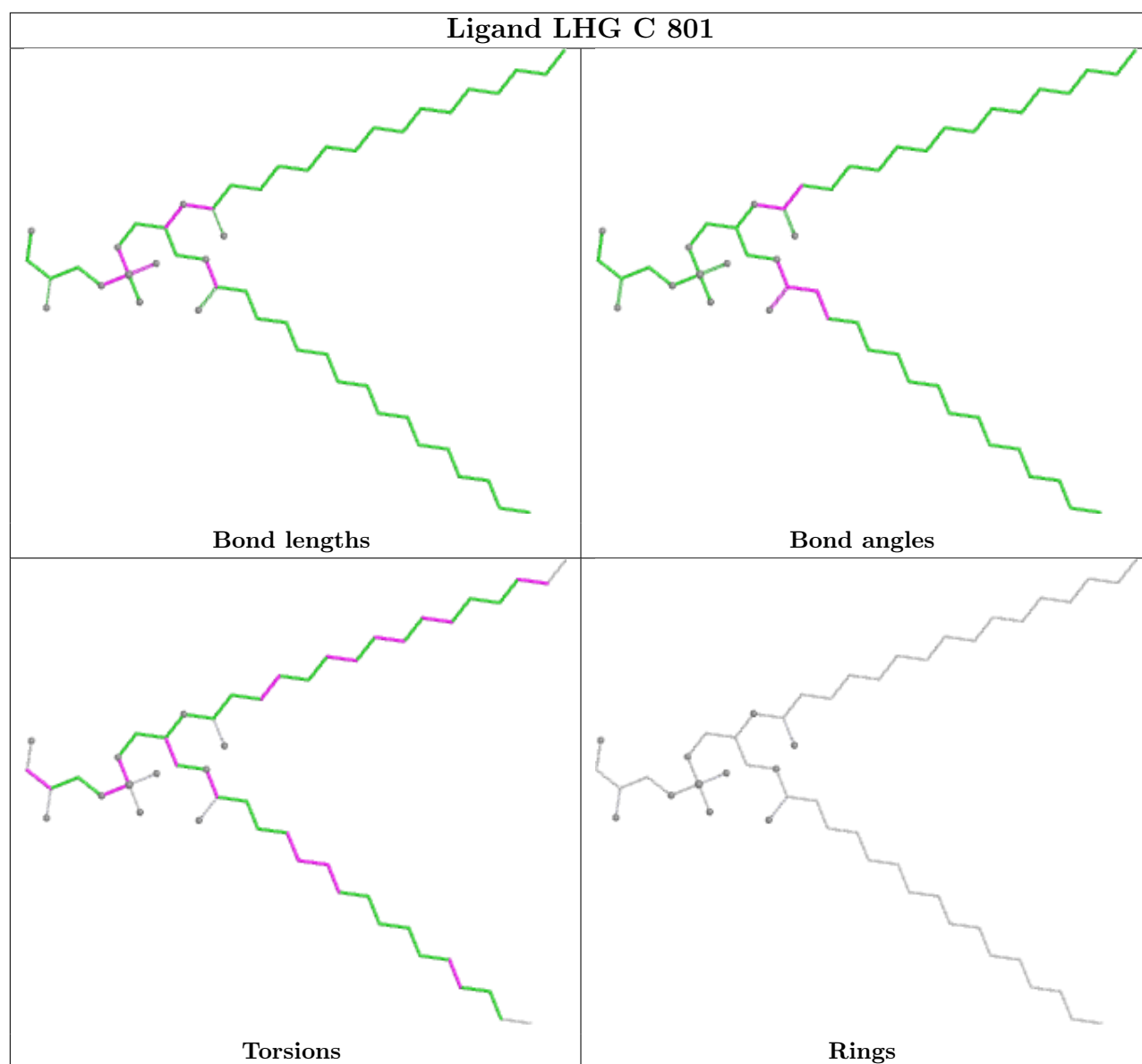


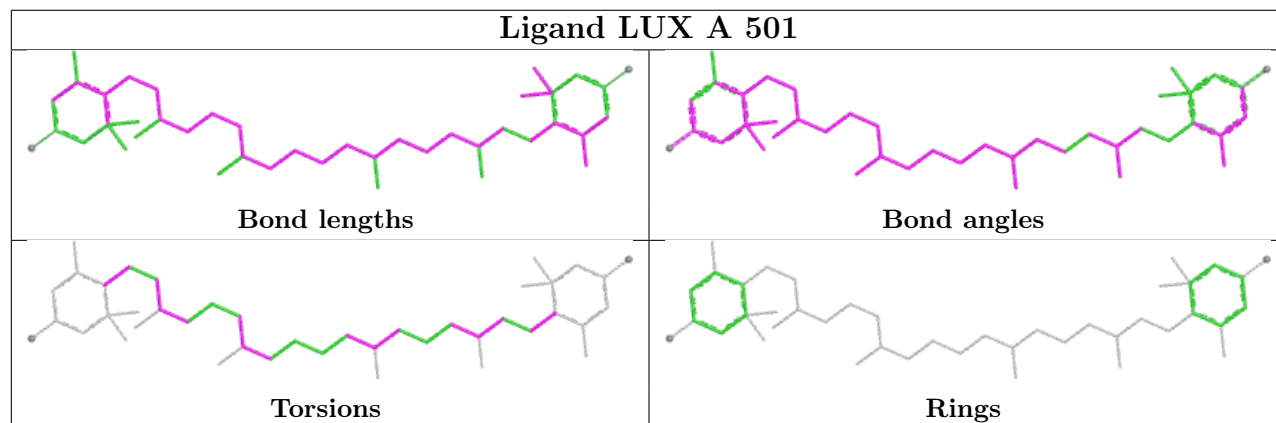
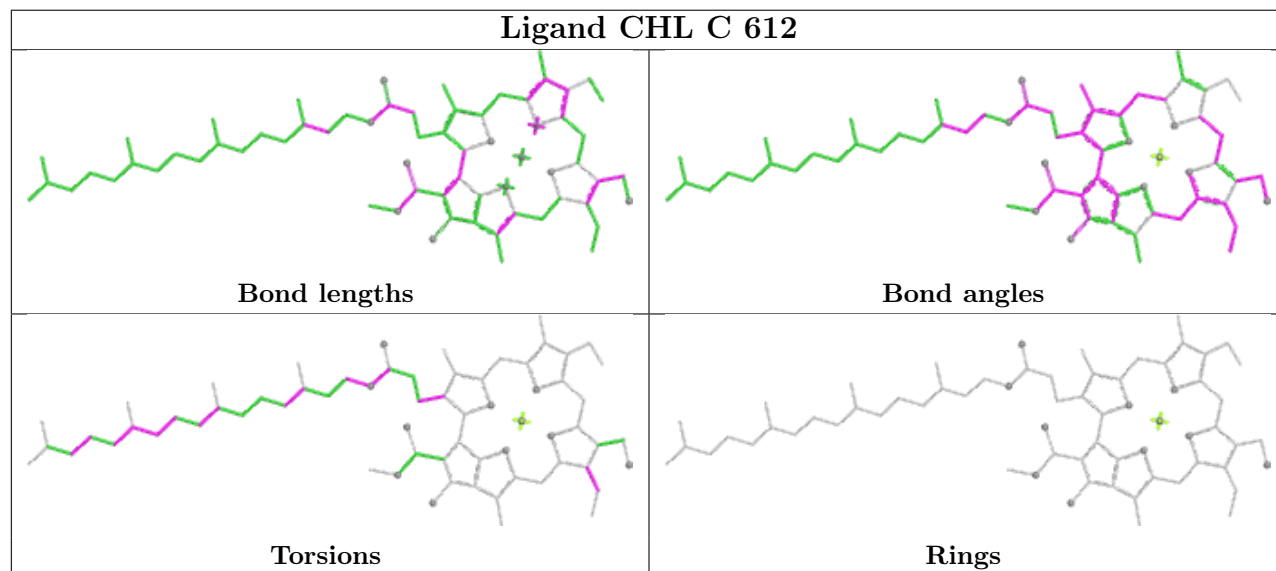
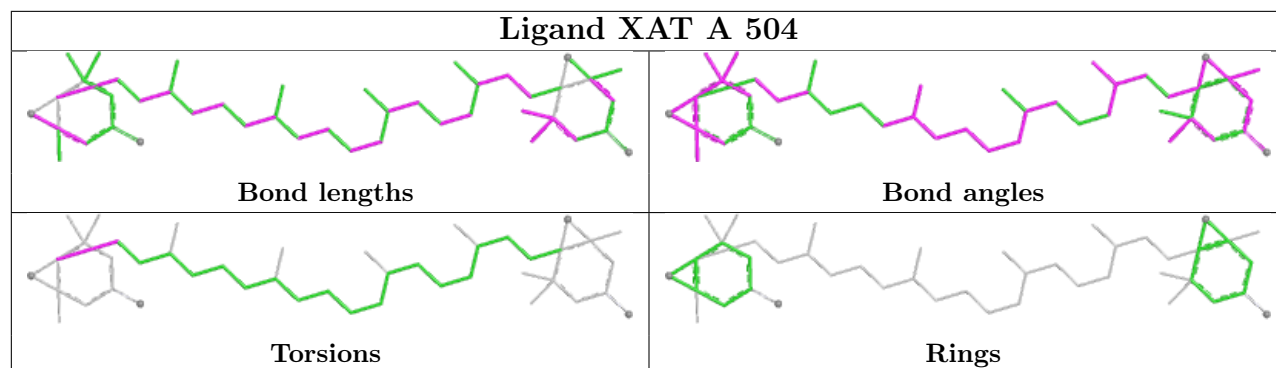
Ligand CLA A 608

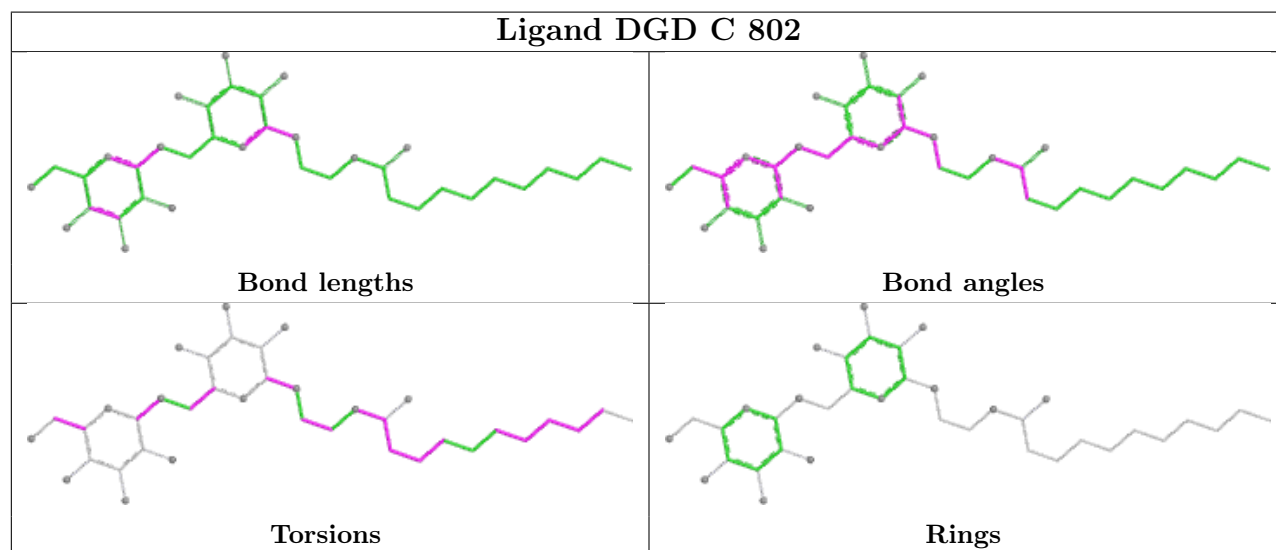
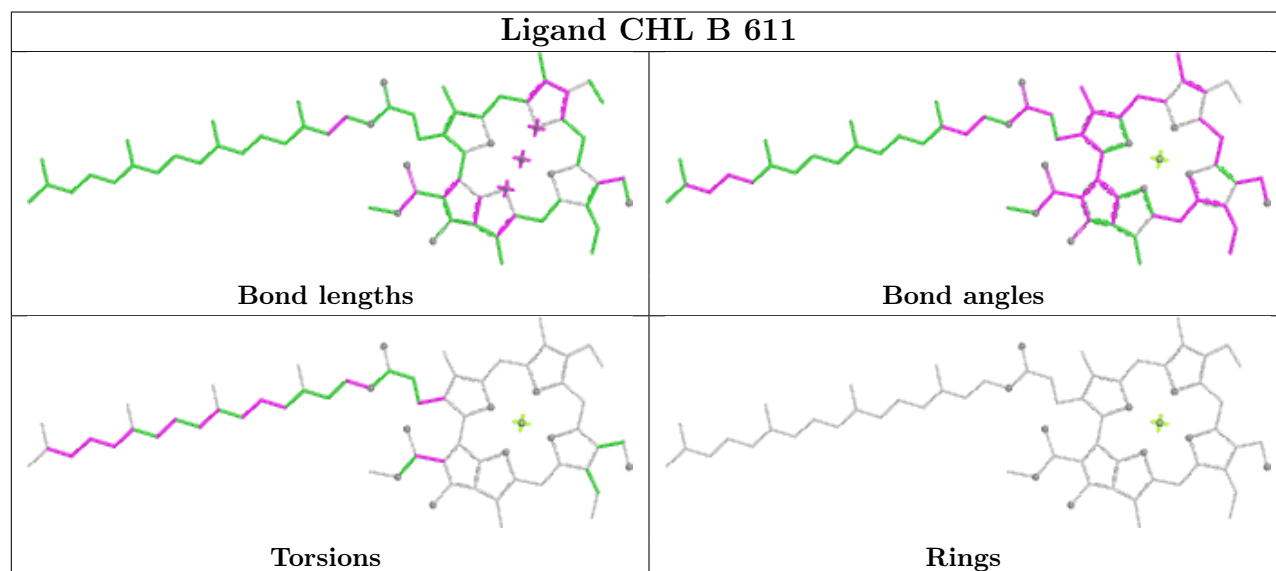
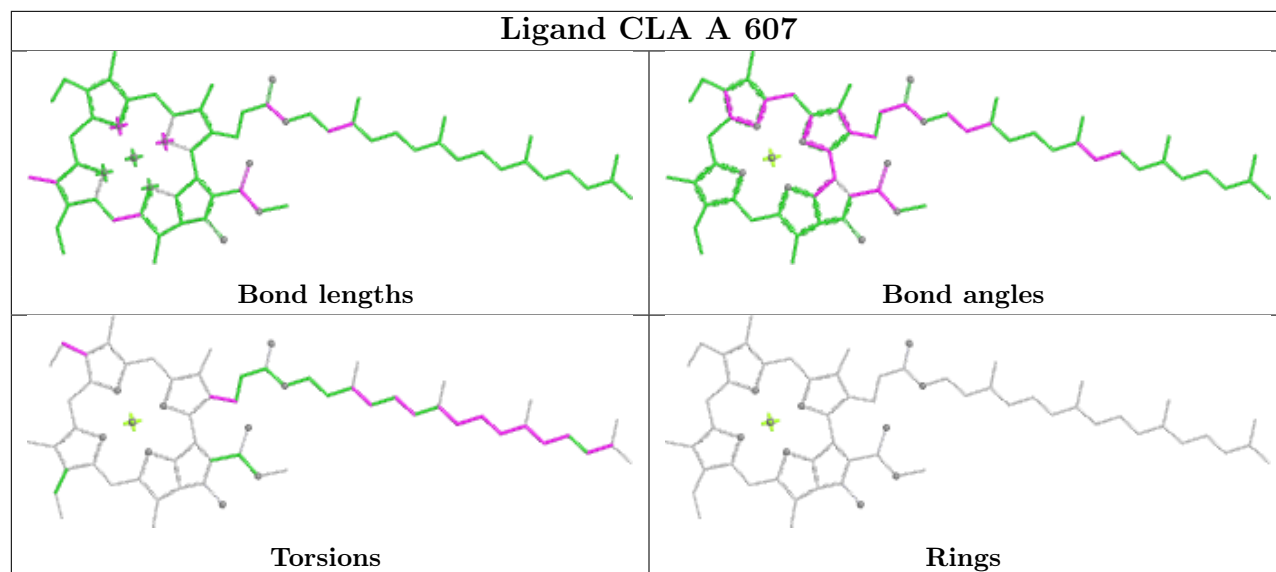


Ligand LUX C 501

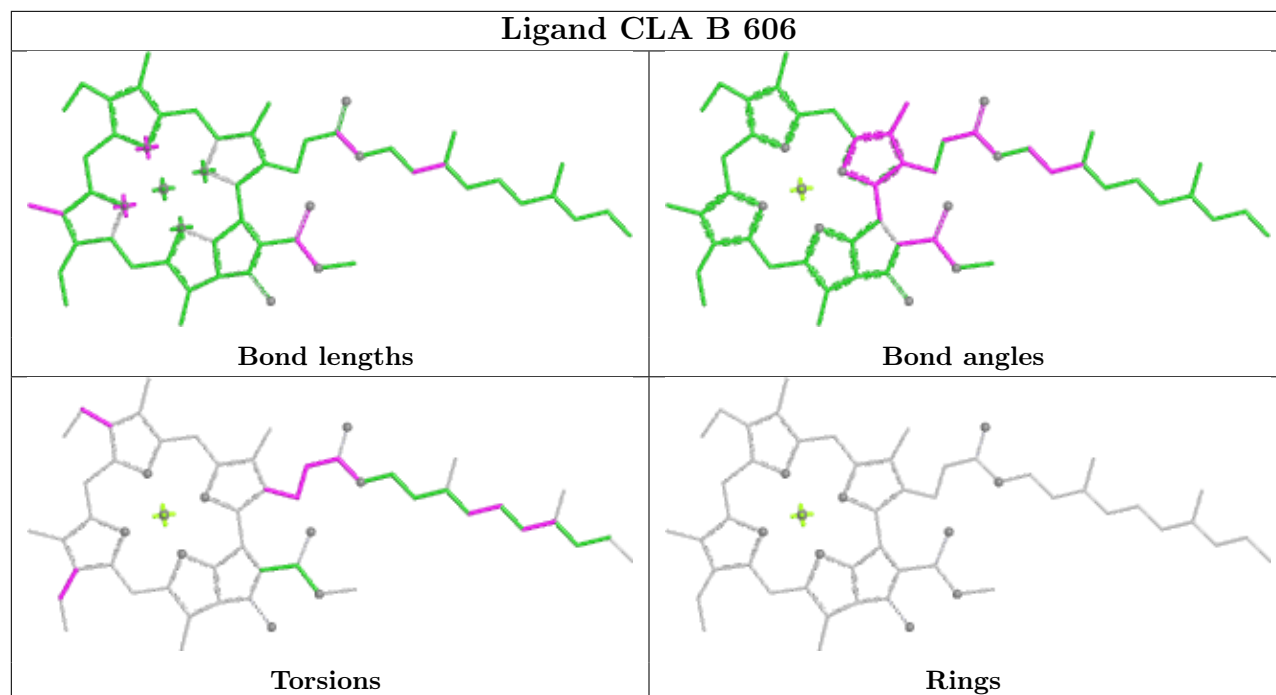




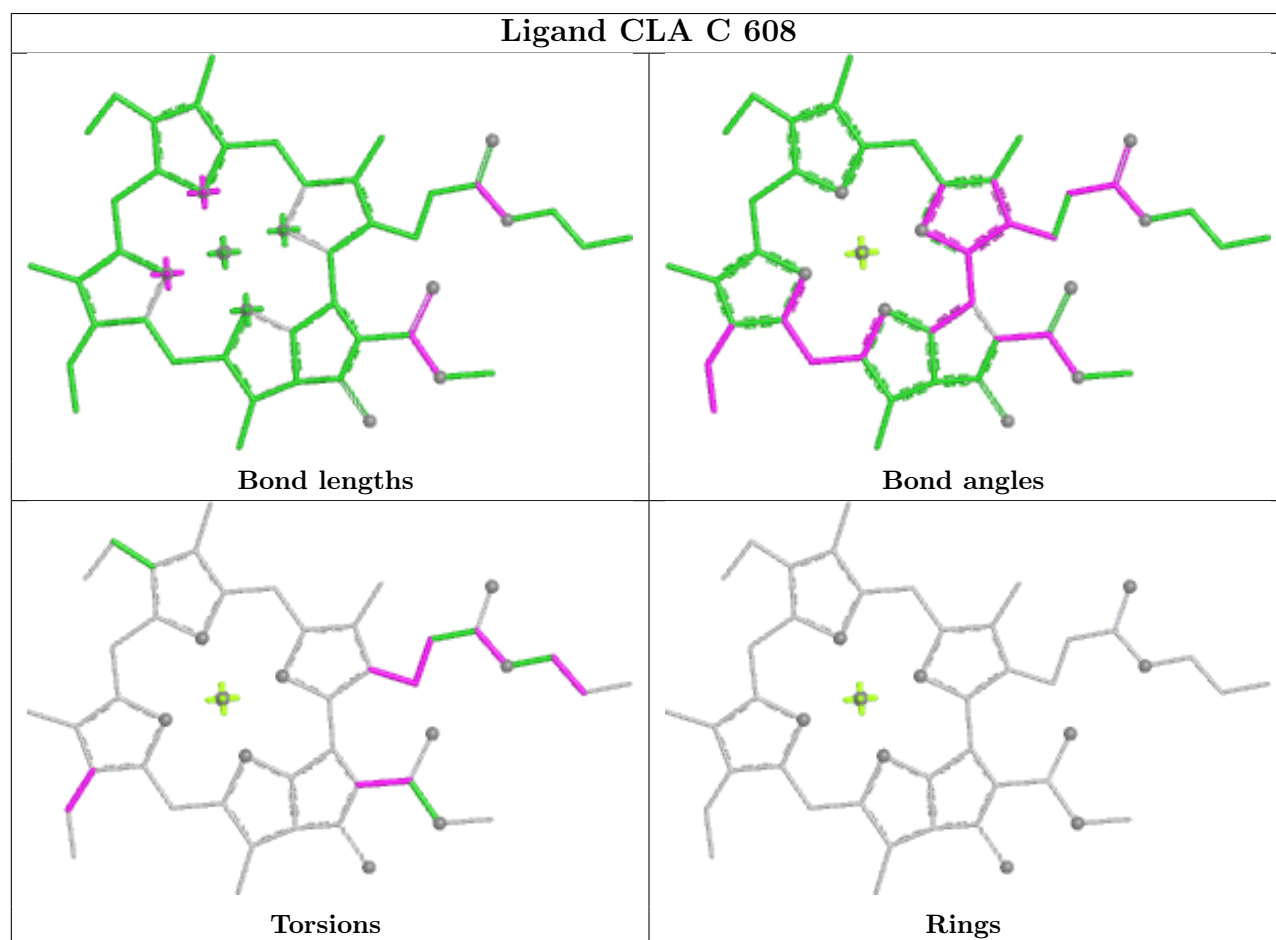




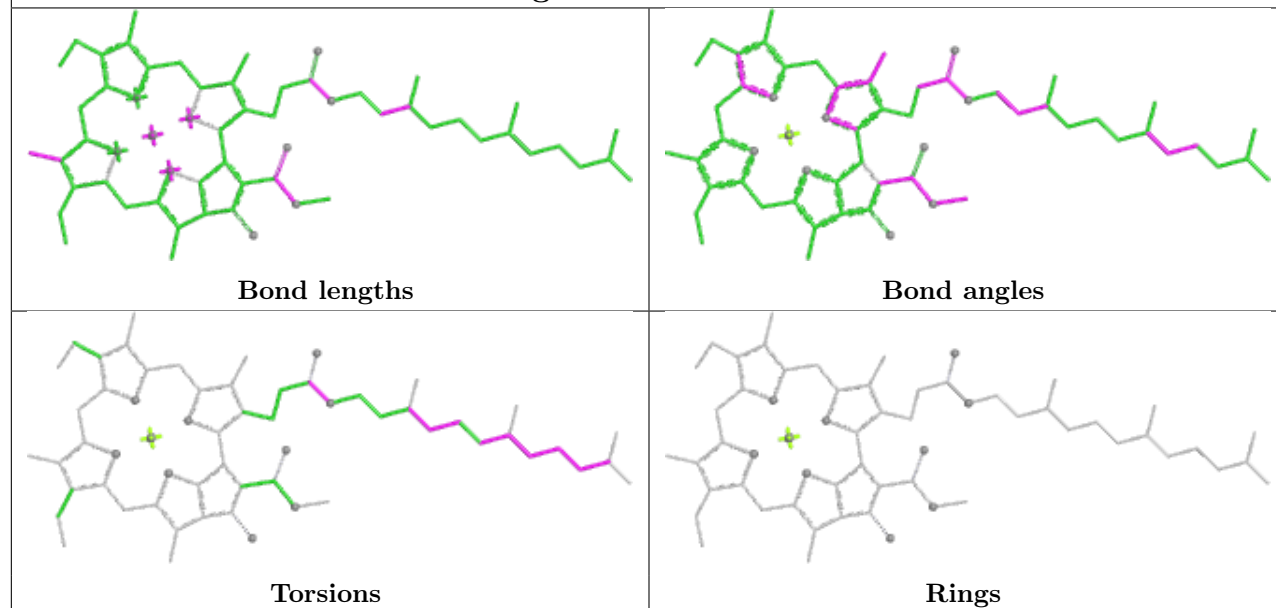
Ligand CLA B 606



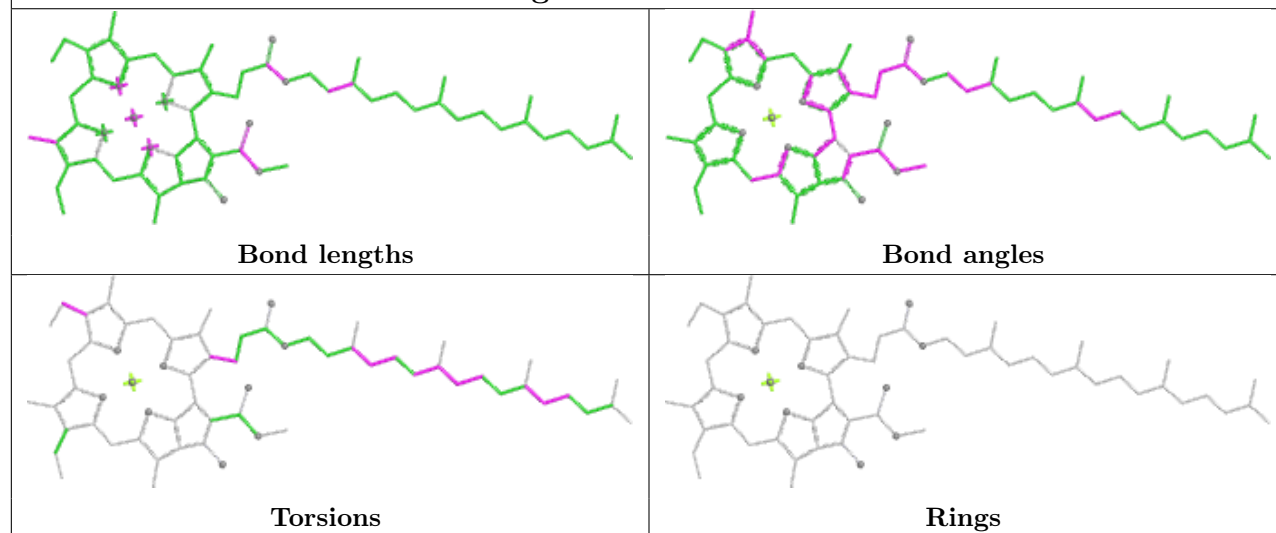
Ligand CLA C 608

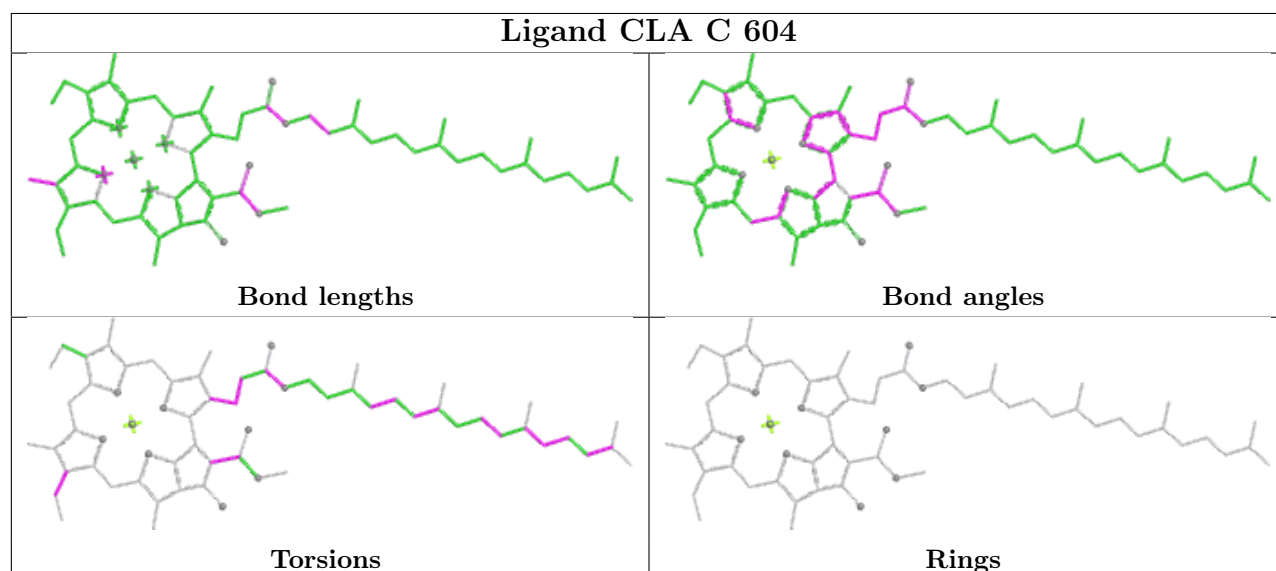
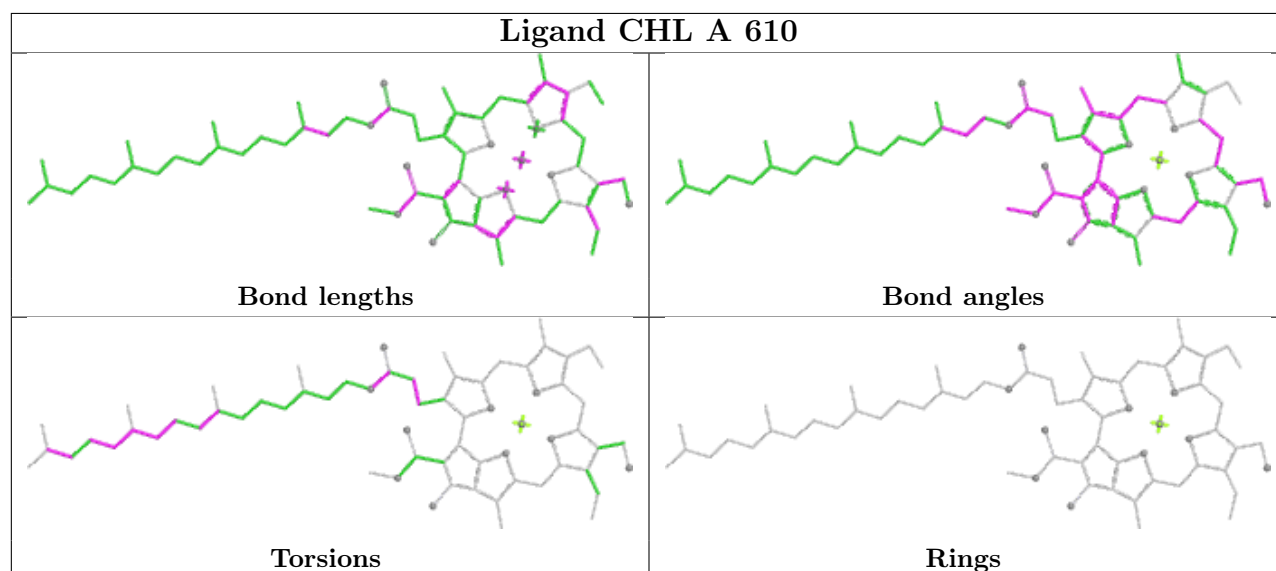
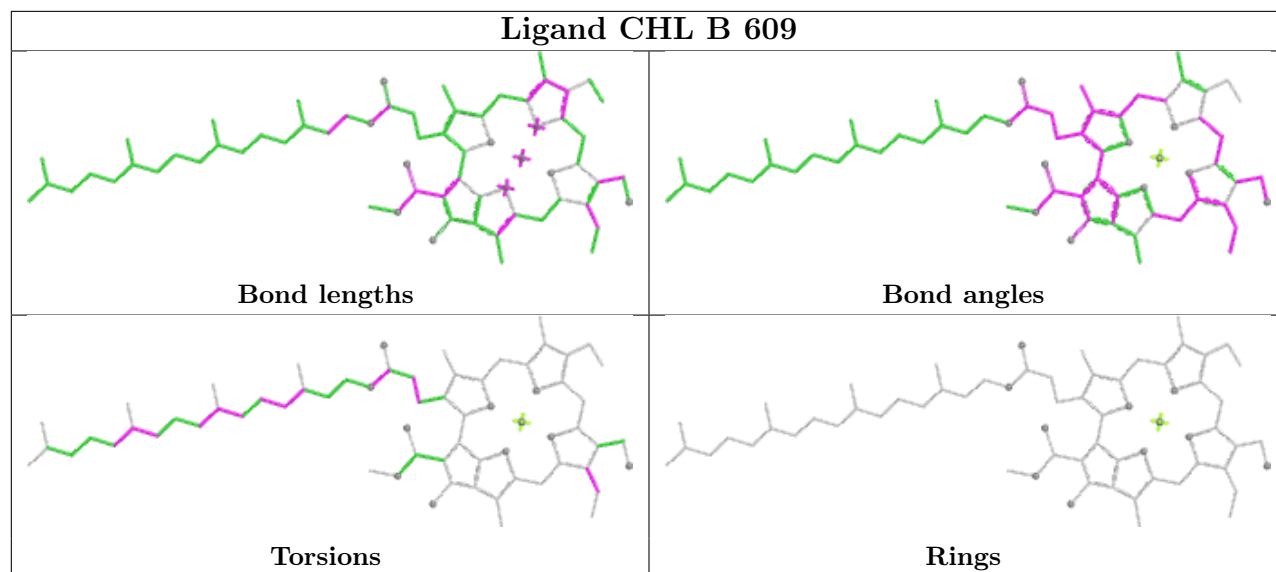


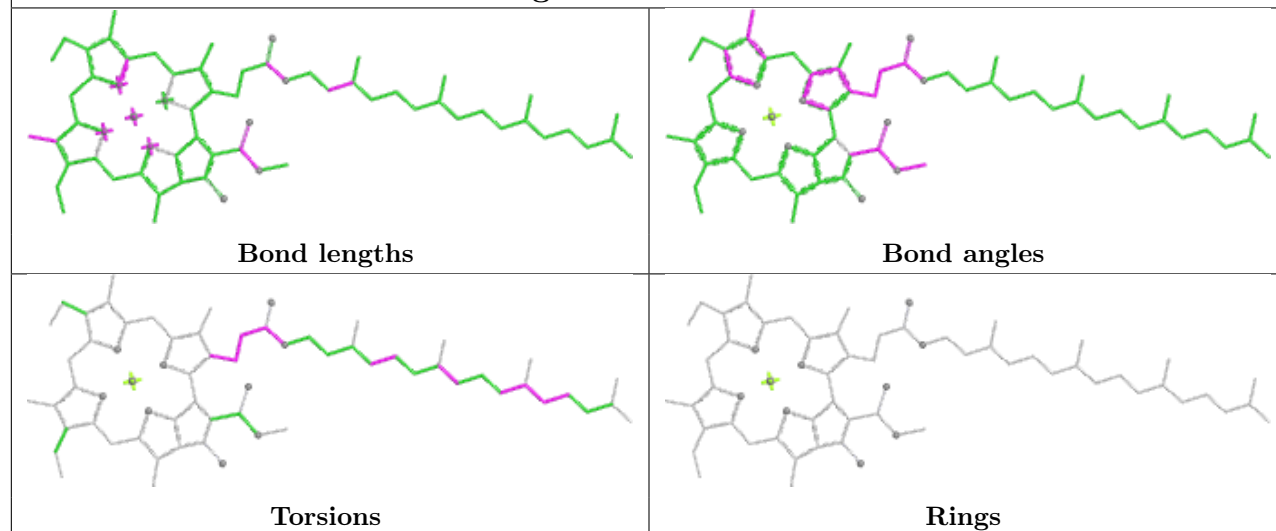
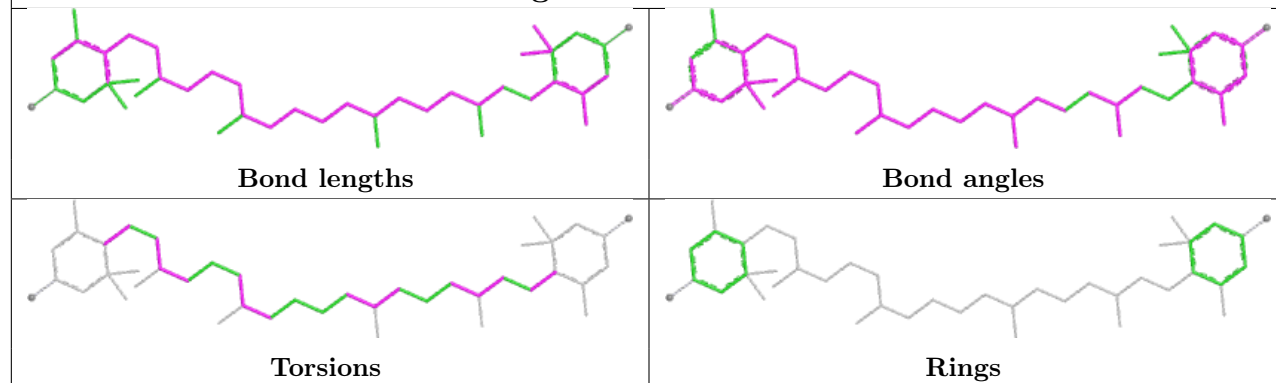
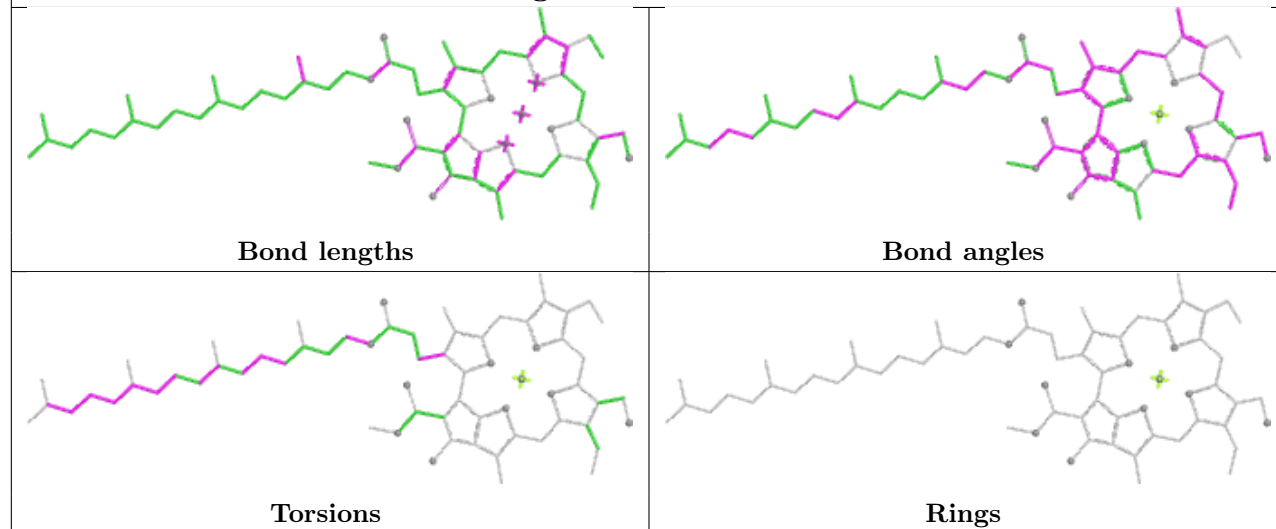
Ligand CLA C 602

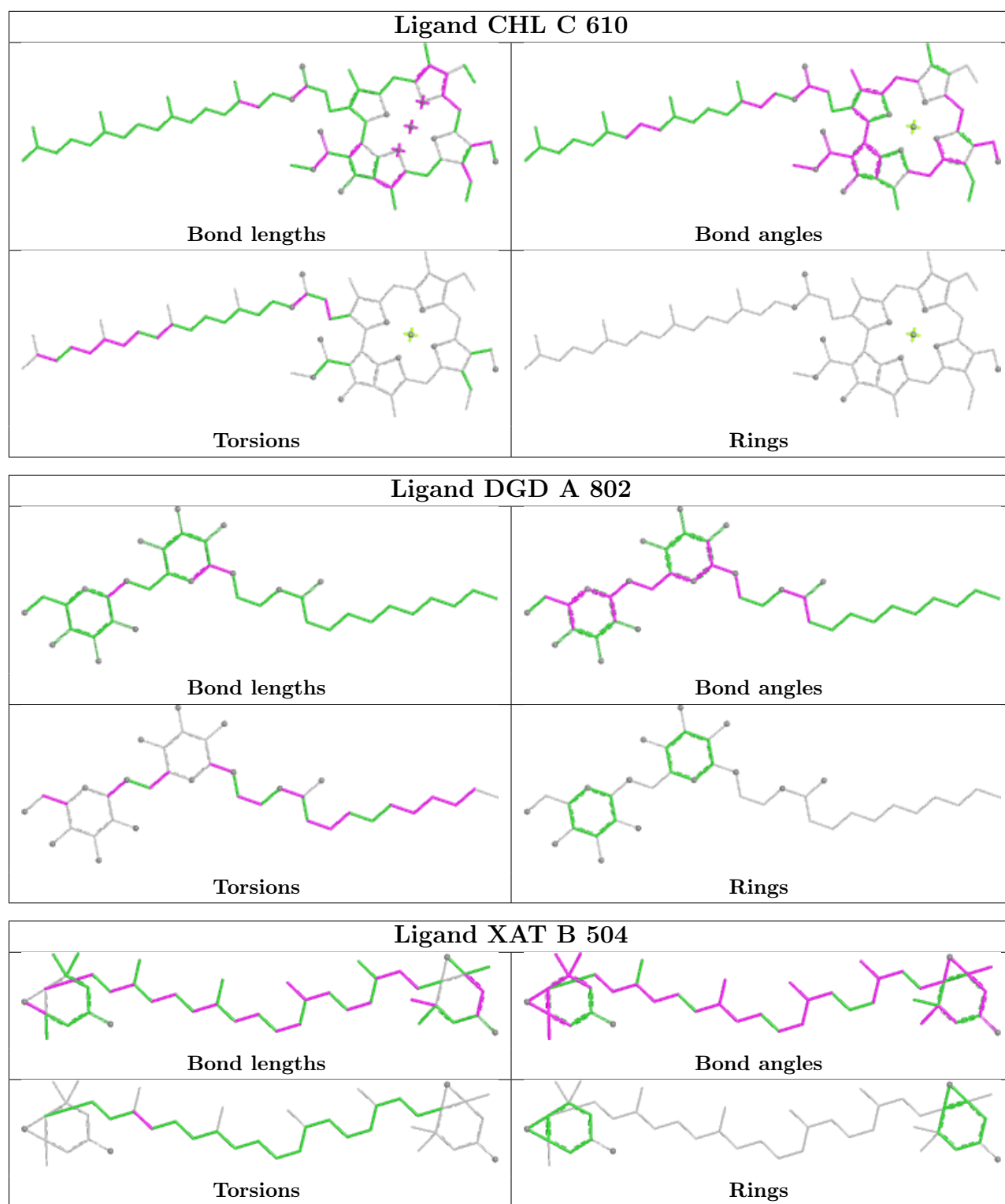


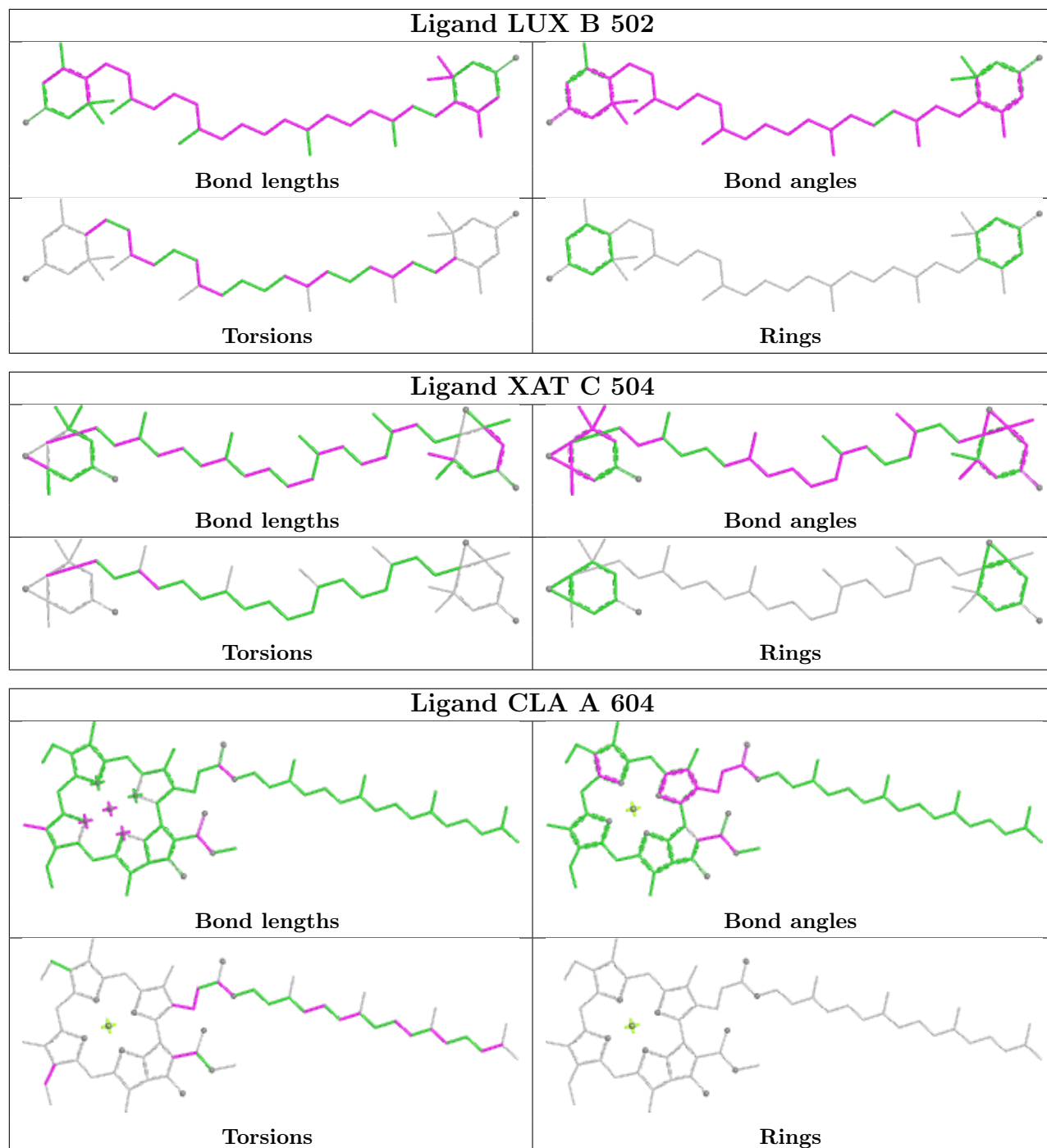
Ligand CLA A 601

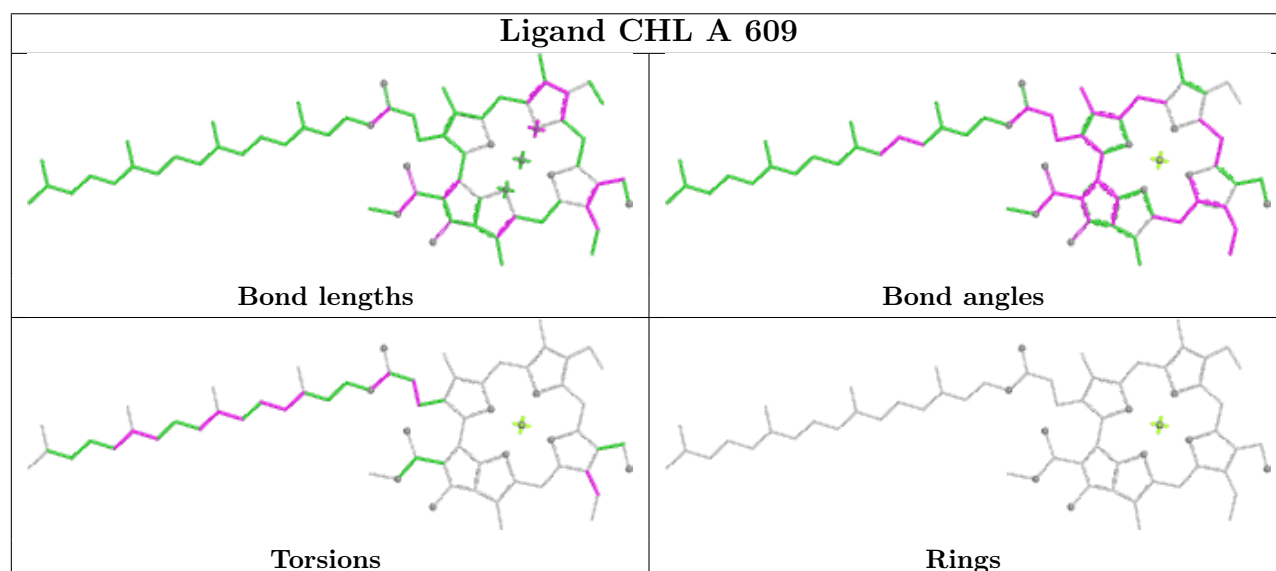
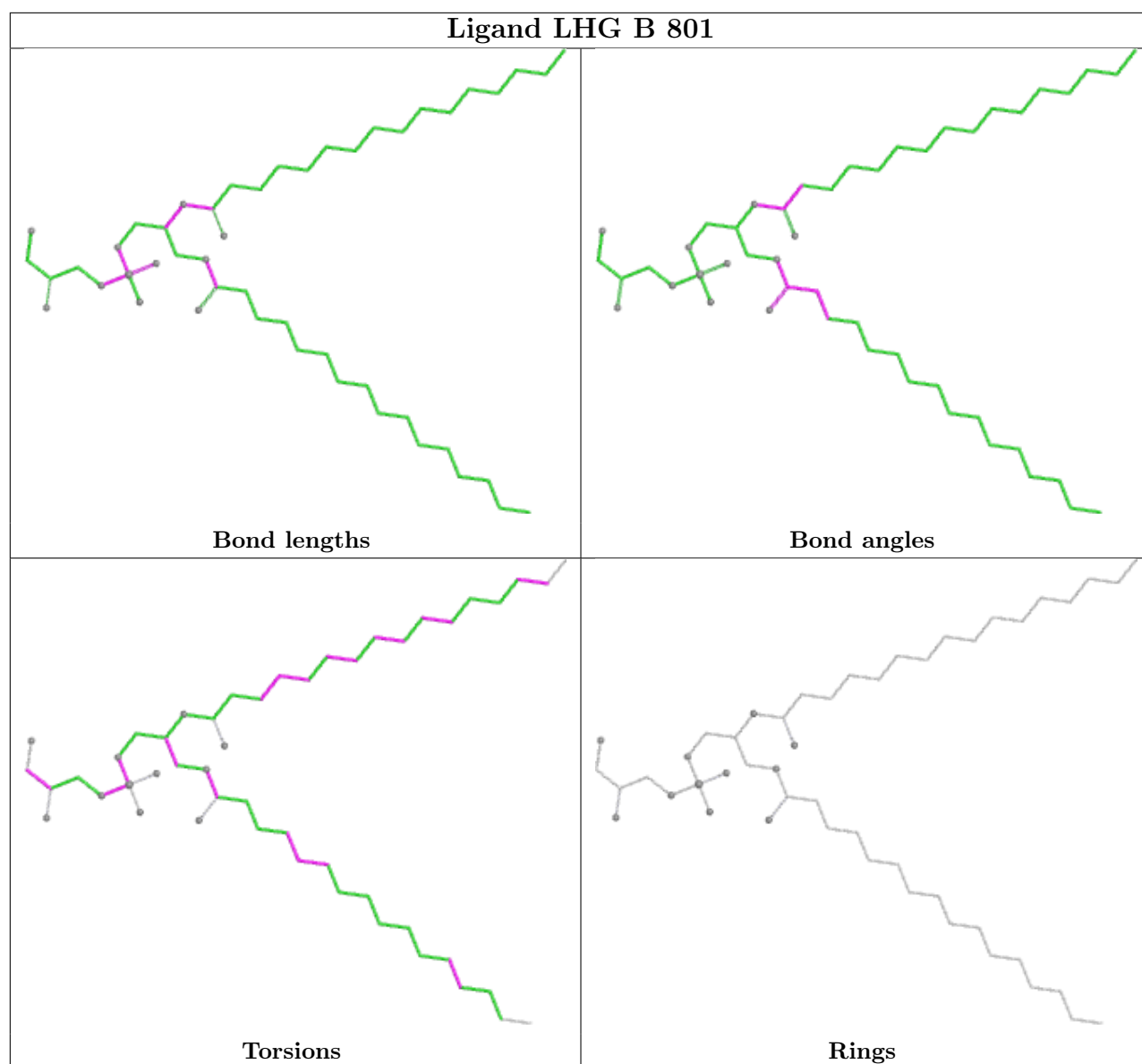




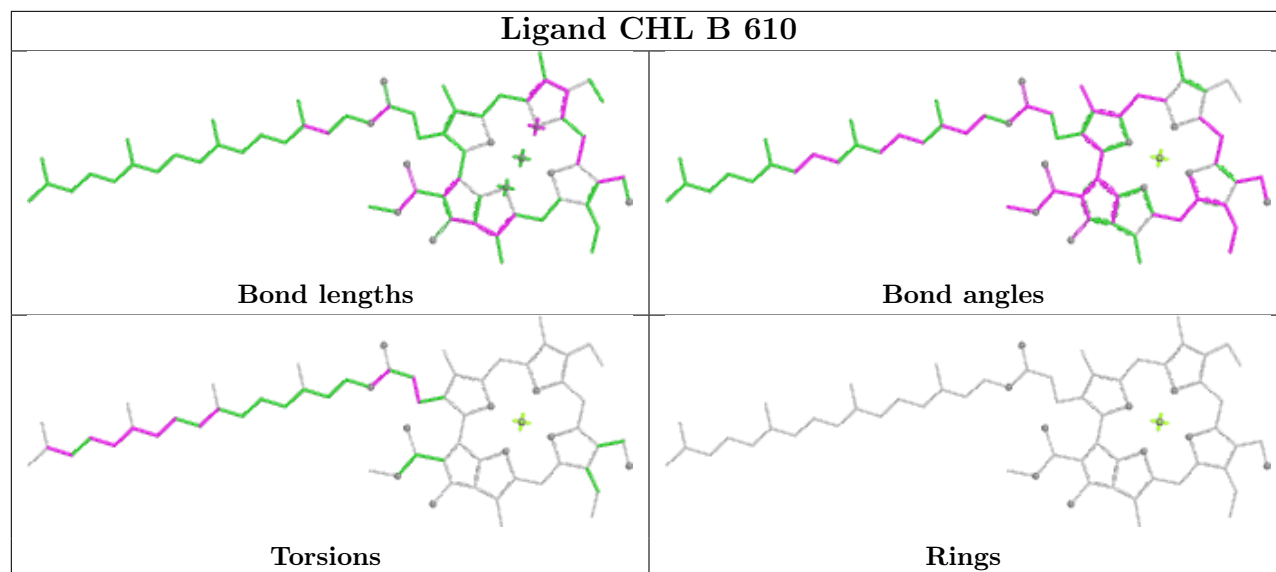
Ligand CLA B 603**Ligand LUX B 501****Ligand CHL C 611**



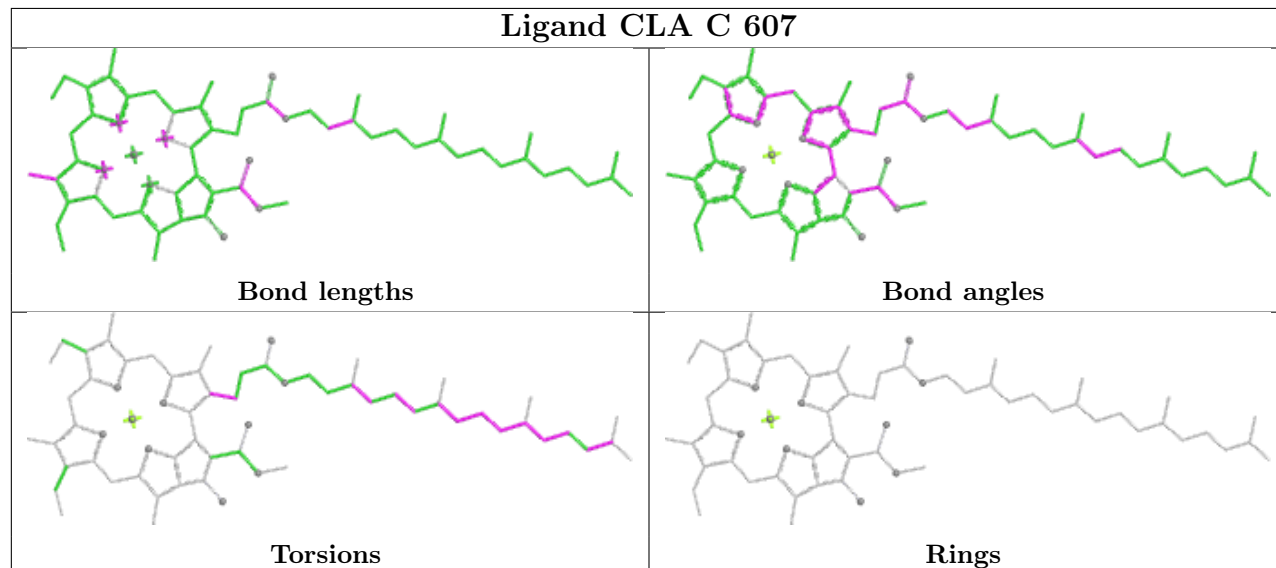


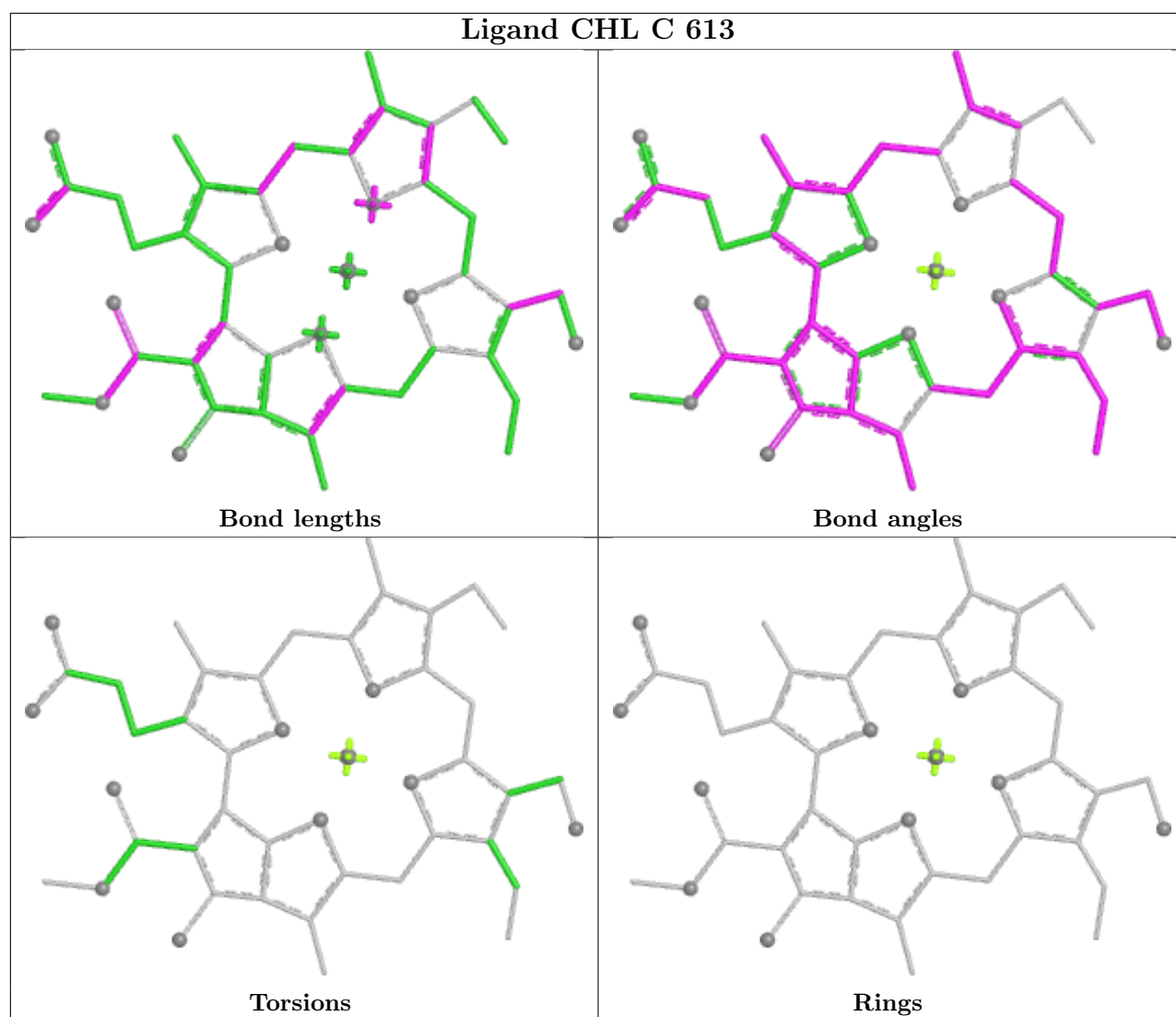


Ligand CHL B 610



Ligand CLA C 607





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	223/232 (96%)	1.07	33 (14%) 5 4	72, 91, 109, 128	0
1	B	223/232 (96%)	1.38	50 (22%) 2 2	70, 89, 107, 126	0
1	C	223/232 (96%)	1.17	34 (15%) 5 4	73, 91, 109, 129	0
All	All	669/696 (96%)	1.21	117 (17%) 4 3	70, 90, 109, 129	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	GLY	7.5
1	B	205	PRO	4.9
1	B	12	SER	4.7
1	A	13	GLY	4.6
1	B	10	ALA	4.5
1	C	13	GLY	4.3
1	B	213	LEU	4.0
1	C	208	ASN	4.0
1	B	11	SER	3.9
1	B	208	ASN	3.9
1	B	44	TYR	3.8
1	A	32	SER	3.8
1	B	97	TRP	3.7
1	C	232	LYS	3.6
1	C	231	GLY	3.6
1	B	232	LYS	3.5
1	A	133	ILE	3.5
1	B	79	SER	3.5
1	B	227	ASN	3.4
1	C	54	ASP	3.3
1	B	204	GLY	3.3
1	C	187	ALA	3.2
1	B	19	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	97	TRP	3.2
1	A	11	SER	3.1
1	A	163	PRO	3.1
1	B	66	VAL	3.1
1	C	121	ALA	3.1
1	A	152	VAL	3.1
1	A	69	SER	3.0
1	B	91	LYS	3.0
1	B	210	ALA	3.0
1	B	95	ALA	3.0
1	C	213	LEU	3.0
1	B	87	ARG	3.0
1	A	42	GLY	3.0
1	C	159	GLY	3.0
1	B	191	MET	2.9
1	C	98	PHE	2.9
1	B	181	LEU	2.9
1	C	118	LEU	2.9
1	C	194	PHE	2.9
1	C	96	VAL	2.8
1	A	97	TRP	2.8
1	C	145	GLY	2.8
1	B	14	SER	2.8
1	C	219	ASN	2.8
1	A	232	LYS	2.7
1	B	88	ASN	2.7
1	A	125	LEU	2.7
1	C	206	LEU	2.6
1	B	45	GLY	2.6
1	B	187	ALA	2.6
1	C	210	ALA	2.6
1	A	45	GLY	2.6
1	C	11	SER	2.6
1	A	71	TRP	2.5
1	B	16	TRP	2.5
1	B	75	GLY	2.5
1	B	127	ILE	2.5
1	B	89	GLY	2.5
1	B	155	LEU	2.5
1	A	130	THR	2.5
1	B	133	ILE	2.4
1	A	36	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	156	TYR	2.4
1	B	151	VAL	2.4
1	C	119	VAL	2.4
1	B	38	GLY	2.4
1	B	17	TYR	2.4
1	C	53	ALA	2.4
1	B	48	THR	2.3
1	B	69	SER	2.3
1	C	14	SER	2.3
1	B	209	LEU	2.3
1	C	176	LEU	2.3
1	C	44	TYR	2.3
1	A	144	ALA	2.3
1	B	154	PRO	2.3
1	B	119	VAL	2.3
1	A	129	ALA	2.3
1	C	10	ALA	2.3
1	B	103	GLN	2.3
1	B	231	GLY	2.3
1	A	33	PRO	2.3
1	C	130	THR	2.2
1	A	18	GLY	2.2
1	A	75	GLY	2.2
1	B	118	LEU	2.2
1	C	125	LEU	2.2
1	A	10	ALA	2.2
1	A	224	TYR	2.2
1	C	224	TYR	2.2
1	A	204	GLY	2.2
1	B	117	SER	2.2
1	C	69	SER	2.2
1	A	128	TRP	2.2
1	C	19	PRO	2.2
1	A	132	VAL	2.1
1	A	110	LEU	2.1
1	C	117	SER	2.1
1	C	28	PHE	2.1
1	A	217	VAL	2.1
1	C	191	MET	2.1
1	A	151	VAL	2.1
1	B	42	GLY	2.1
1	B	214	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	51	LEU	2.1
1	B	93	GLY	2.1
1	A	211	ASP	2.1
1	A	105	PHE	2.0
1	A	44	TYR	2.0
1	B	224	TYR	2.0
1	A	228	PHE	2.0
1	B	25	LEU	2.0
1	B	76	ALA	2.0
1	C	107	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	DGD	B	802	38/66	0.61	0.19	104,118,139,140	0
8	DGD	C	802	38/66	0.73	0.18	106,119,141,141	0
8	DGD	A	802	38/66	0.78	0.17	106,119,140,140	0
5	CLA	B	601	65/65	0.82	0.19	68,77,111,113	0
2	LUX	B	501	42/42	0.85	0.22	59,86,118,134	0
5	CLA	B	608	48/65	0.86	0.17	88,97,115,117	0
2	LUX	C	501	42/42	0.86	0.20	62,88,120,136	0
6	CHL	C	614	42/66	0.87	0.16	99,107,113,137	0
6	CHL	B	611	66/66	0.87	0.17	68,82,115,121	0
5	CLA	B	607	65/65	0.88	0.19	75,88,101,104	0
6	CHL	C	611	66/66	0.88	0.17	69,85,118,124	0
3	NEX	C	503	44/44	0.89	0.16	67,98,128,133	0
2	LUX	A	501	42/42	0.89	0.19	61,87,120,136	0

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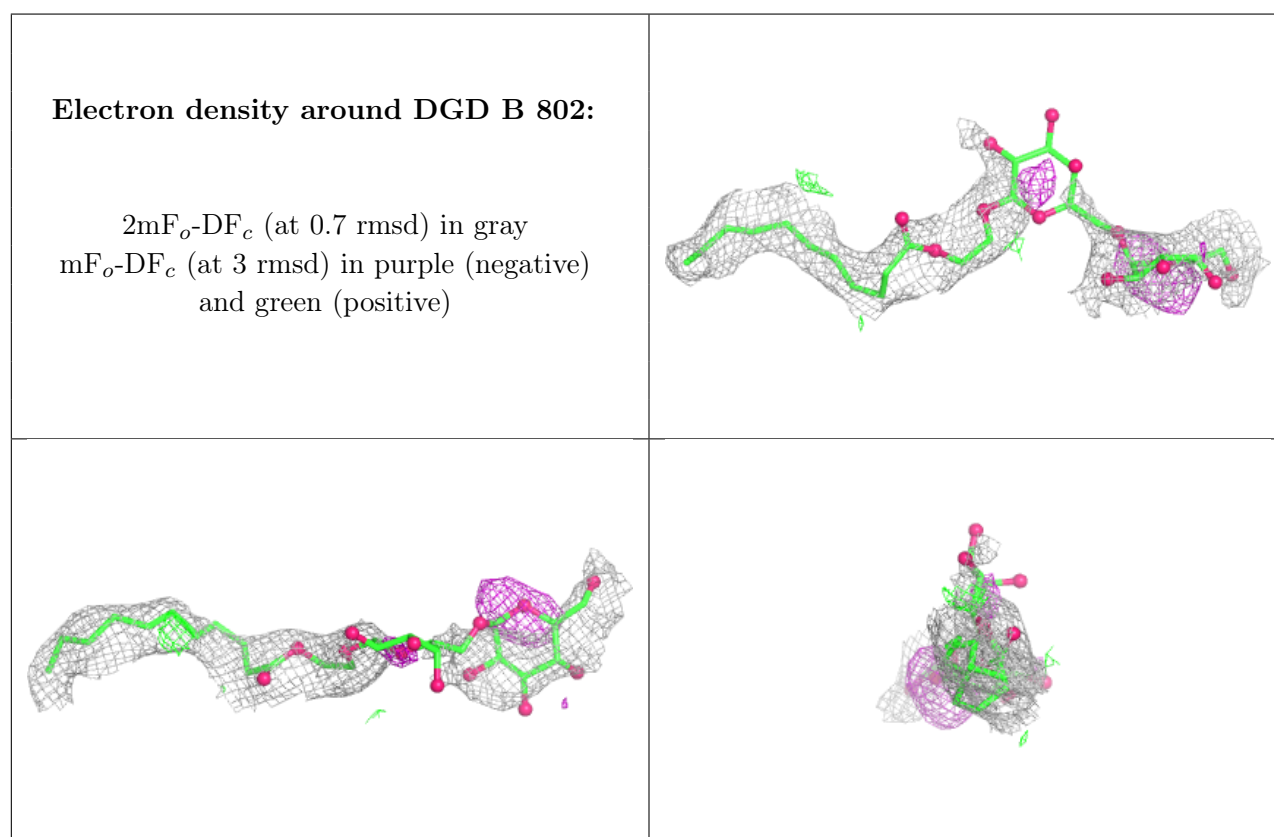
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LUX	B	502	42/42	0.89	0.18	53,76,113,126	0
2	LUX	A	502	42/42	0.89	0.18	57,78,115,128	0
6	CHL	A	611	66/66	0.89	0.17	70,85,117,123	0
6	CHL	A	612	66/66	0.89	0.14	76,85,102,104	0
3	NEX	A	503	44/44	0.90	0.14	66,97,128,132	0
5	CLA	B	602	60/65	0.90	0.15	77,85,114,114	0
4	XAT	A	504	44/44	0.90	0.15	65,91,117,148	0
5	CLA	A	602	60/65	0.90	0.16	79,87,115,116	0
7	LHG	B	801	49/49	0.90	0.18	72,88,109,115	0
5	CLA	C	605	65/65	0.90	0.13	77,86,108,110	0
5	CLA	C	607	65/65	0.90	0.16	77,91,104,106	0
5	CLA	A	605	65/65	0.90	0.15	77,86,107,110	0
5	CLA	B	605	65/65	0.91	0.14	75,84,105,108	0
5	CLA	A	601	65/65	0.91	0.15	69,79,112,115	0
5	CLA	A	606	57/65	0.91	0.16	79,90,107,110	0
6	CHL	C	612	66/66	0.91	0.14	77,85,102,104	0
5	CLA	C	602	60/65	0.91	0.13	80,87,116,117	0
7	LHG	A	801	49/49	0.91	0.18	74,90,110,116	0
5	CLA	A	608	48/65	0.91	0.16	90,99,116,118	0
2	LUX	C	502	42/42	0.91	0.17	58,79,115,128	0
5	CLA	C	608	48/65	0.91	0.14	90,99,117,119	0
5	CLA	A	603	65/65	0.91	0.15	75,85,102,105	0
5	CLA	B	603	65/65	0.92	0.13	74,83,100,103	0
6	CHL	C	613	46/66	0.92	0.13	73,82,107,121	0
5	CLA	C	601	65/65	0.92	0.16	70,79,113,115	0
5	CLA	A	607	65/65	0.92	0.16	77,90,103,106	0
6	CHL	A	614	42/66	0.92	0.13	99,106,113,136	0
7	LHG	C	801	49/49	0.92	0.17	74,90,111,117	0
5	CLA	B	606	57/65	0.92	0.16	78,89,105,109	0
6	CHL	B	614	42/66	0.92	0.14	97,105,111,134	0
3	NEX	B	503	44/44	0.92	0.15	64,96,126,131	0
5	CLA	B	604	65/65	0.93	0.14	56,69,95,100	0
6	CHL	B	610	66/66	0.93	0.13	65,79,106,108	0
6	CHL	A	609	66/66	0.93	0.13	75,85,97,100	0
5	CLA	C	606	57/65	0.93	0.14	80,91,107,111	0
6	CHL	C	609	66/66	0.93	0.14	77,85,98,101	0
6	CHL	C	610	66/66	0.93	0.13	67,81,108,110	0
5	CLA	C	603	65/65	0.93	0.14	75,85,102,105	0
6	CHL	A	613	46/66	0.93	0.11	73,81,107,120	0
5	CLA	C	604	65/65	0.94	0.14	60,72,97,102	0
4	XAT	C	504	44/44	0.94	0.15	65,91,117,149	0
6	CHL	A	610	66/66	0.94	0.14	65,80,108,110	0

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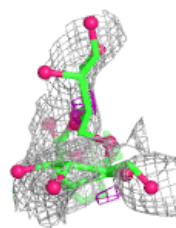
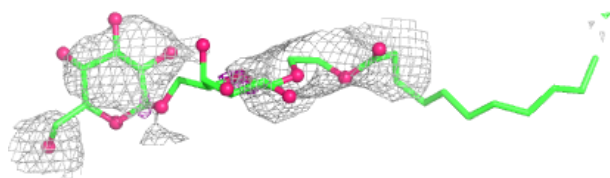
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	XAT	B	504	44/44	0.94	0.13	63,89,115,147	0
6	CHL	B	612	66/66	0.94	0.12	74,83,100,102	0
5	CLA	A	604	65/65	0.94	0.12	59,71,96,101	0
6	CHL	B	613	46/66	0.95	0.10	71,80,106,119	0
6	CHL	B	609	66/66	0.95	0.12	75,83,95,99	0

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

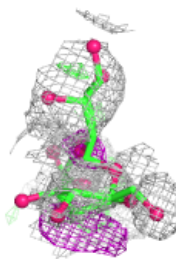
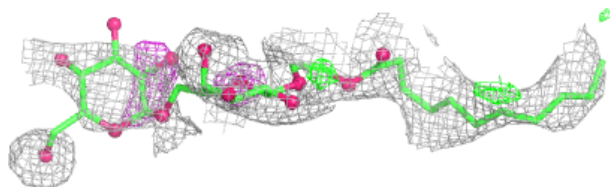
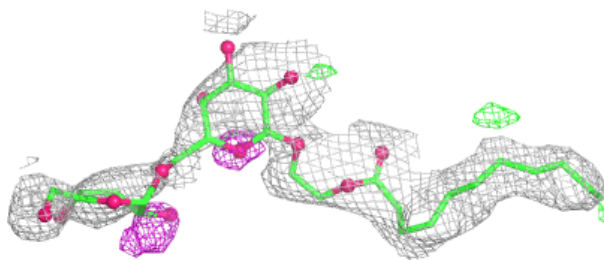


Electron density around DGD C 802:

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

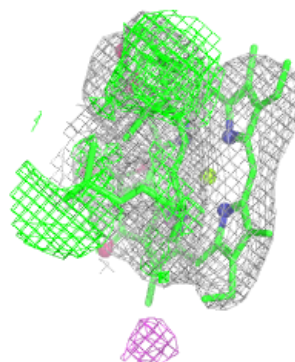
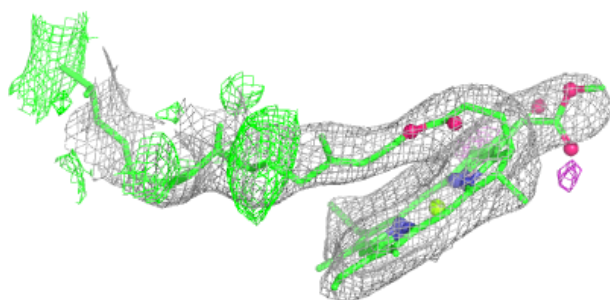
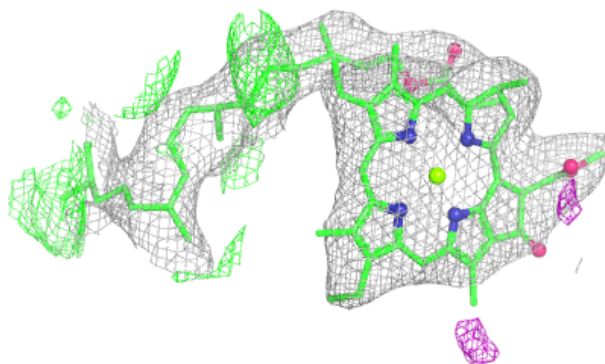
**Electron density around DGD A 802:**

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

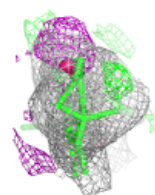
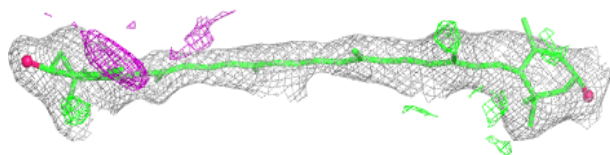
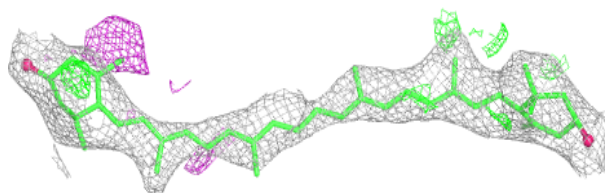


Electron density around CLA B 601:

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

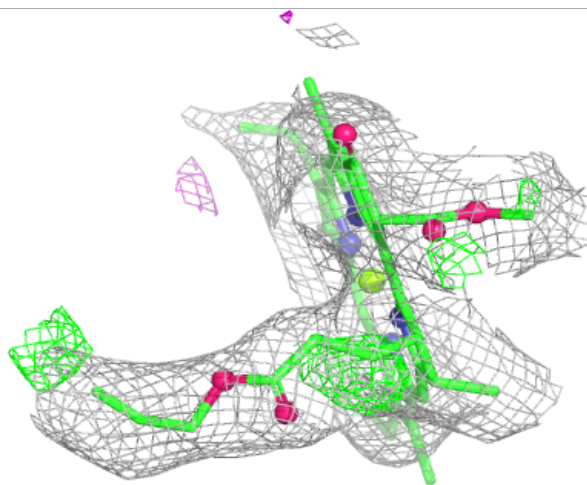
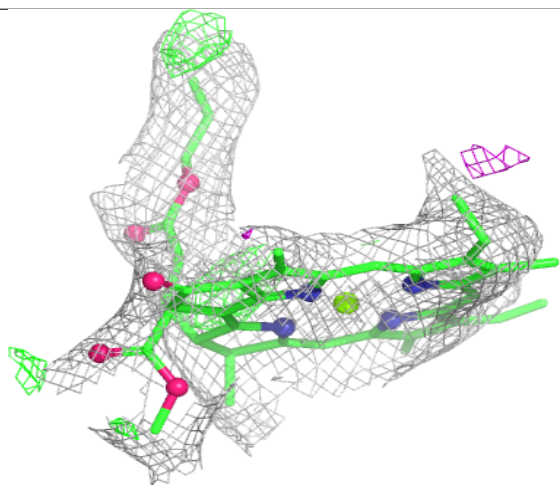
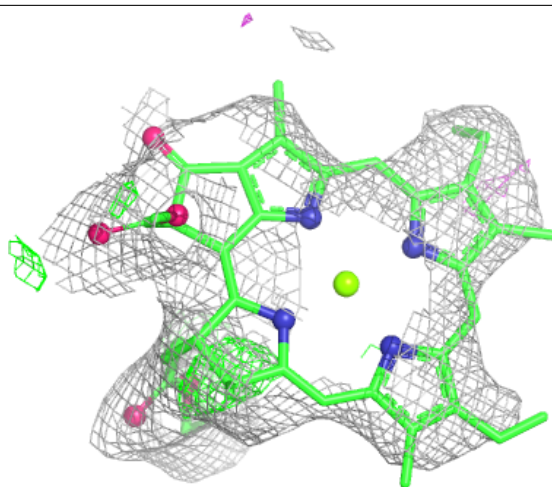
**Electron density around LUX B 501:**

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



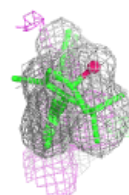
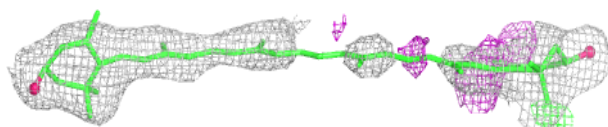
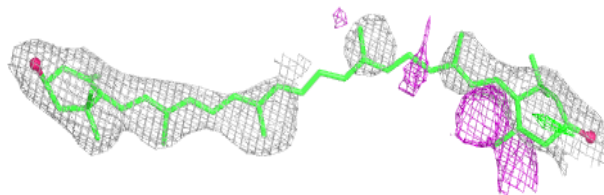
Electron density around CLA B 608:

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

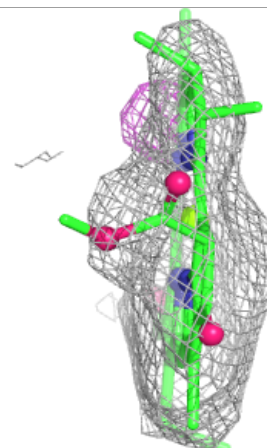
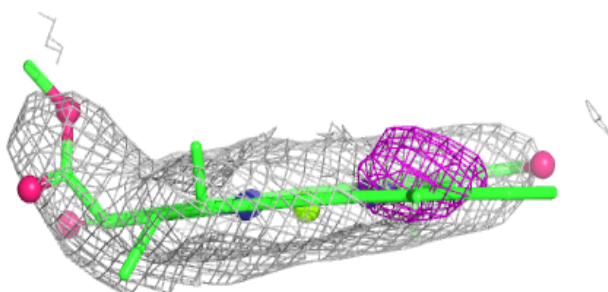
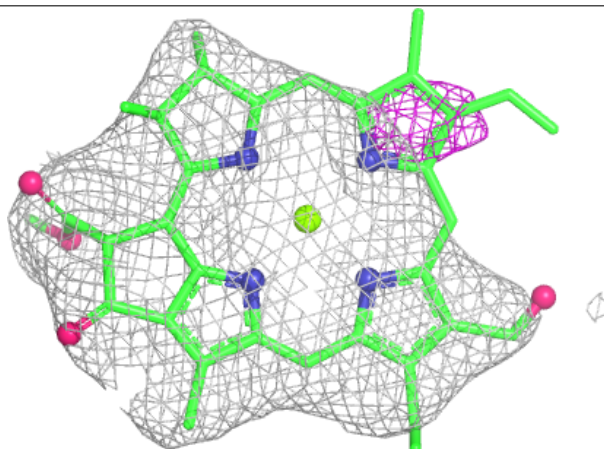


Electron density around LUX C 501:

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

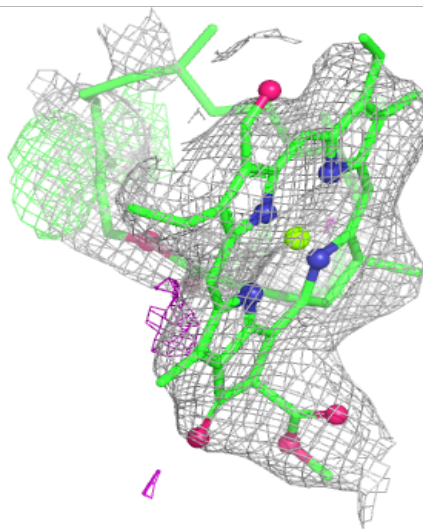
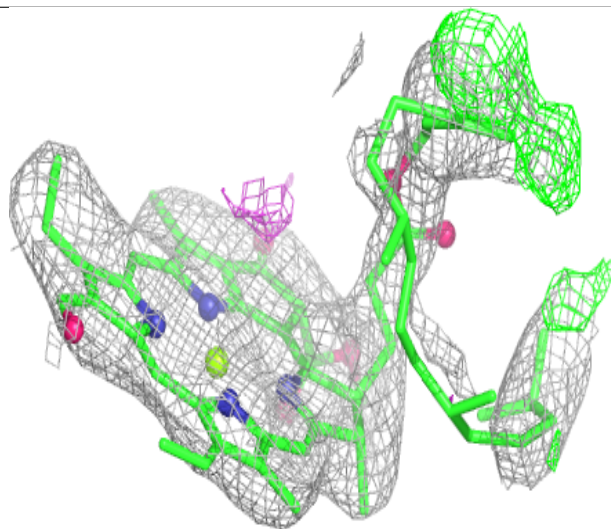
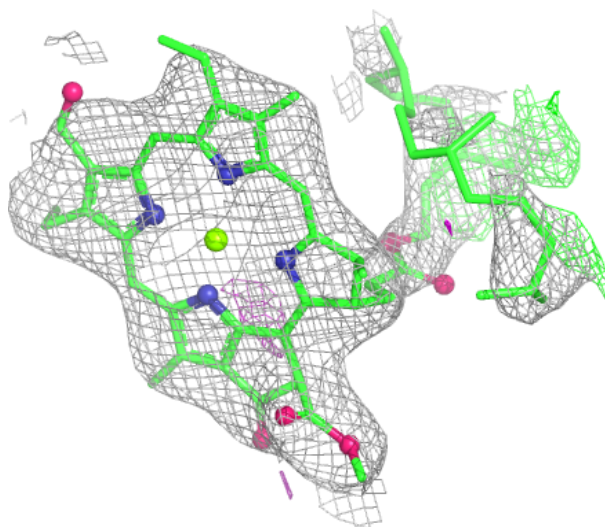
**Electron density around CHL C 614:**

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



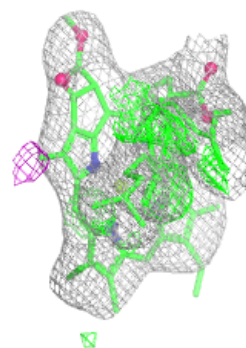
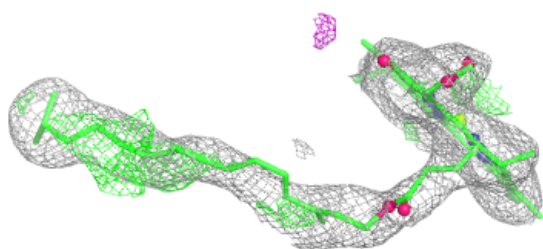
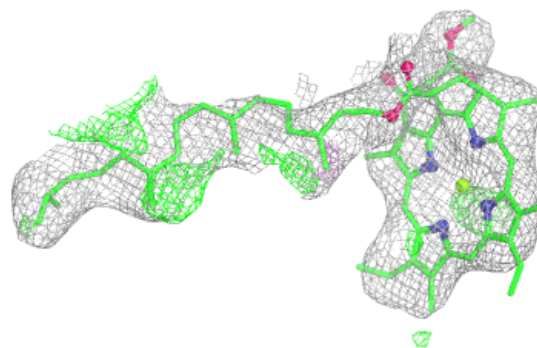
Electron density around CHL B 611:

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



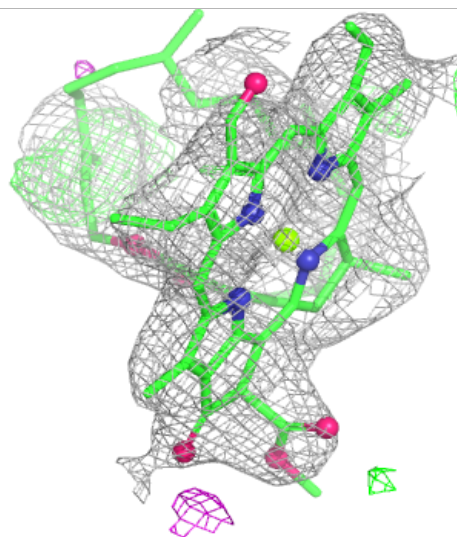
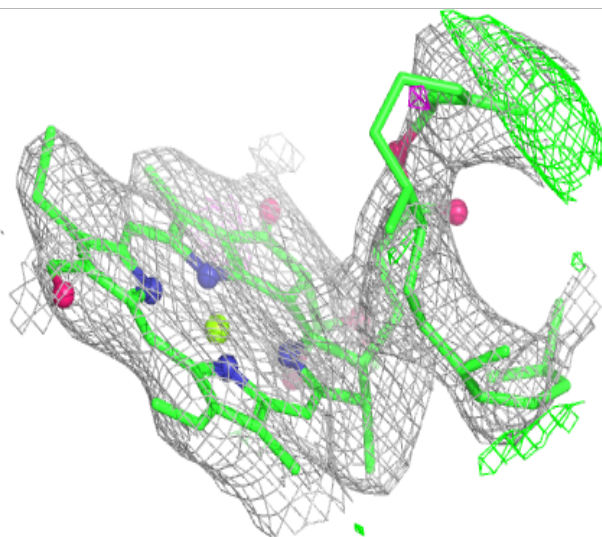
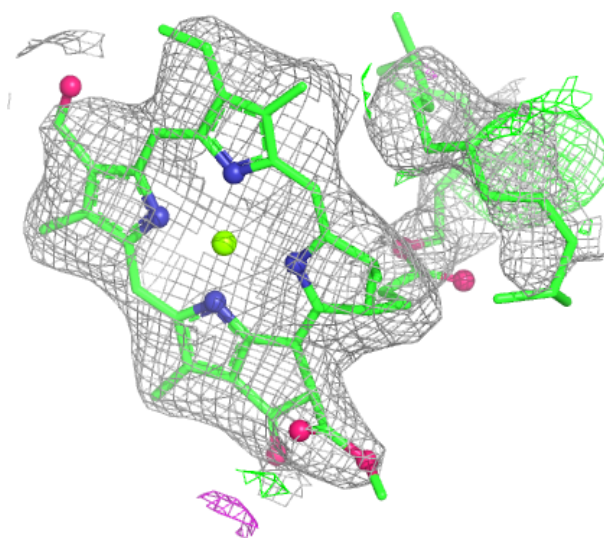
Electron density around CLA B 607:

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



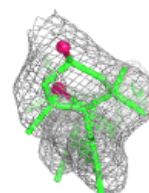
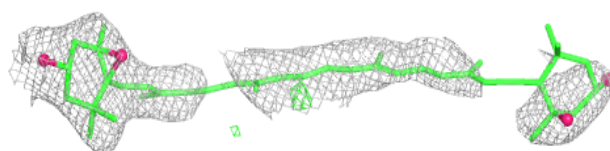
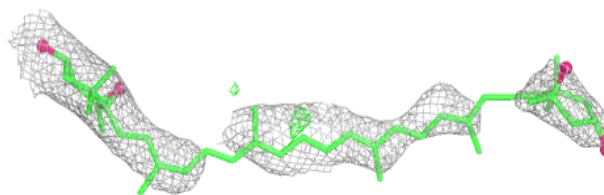
Electron density around CHL C 611:

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

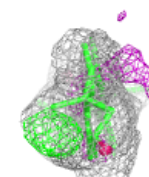
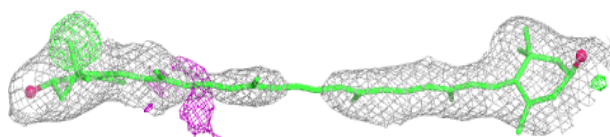
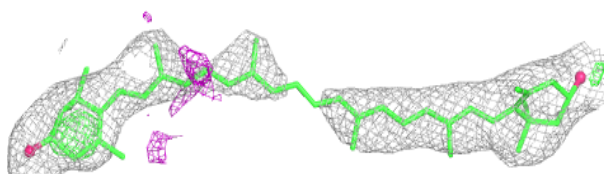


Electron density around NEX C 503:

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

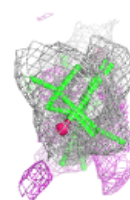
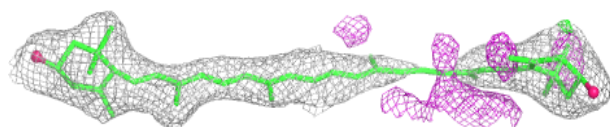
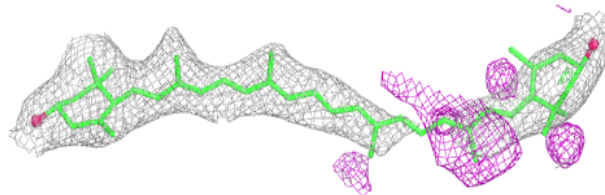
**Electron density around LUX A 501:**

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

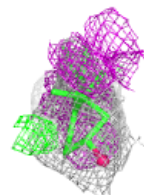
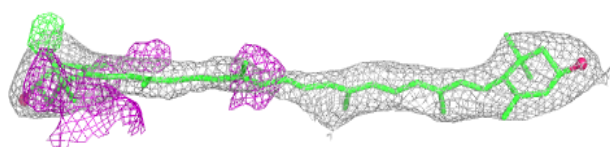
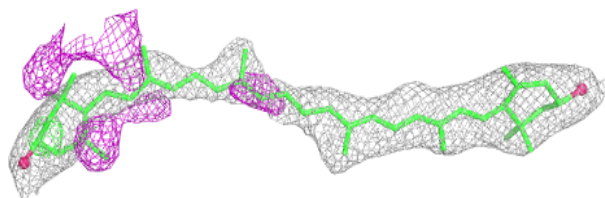


Electron density around LUX B 502:

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

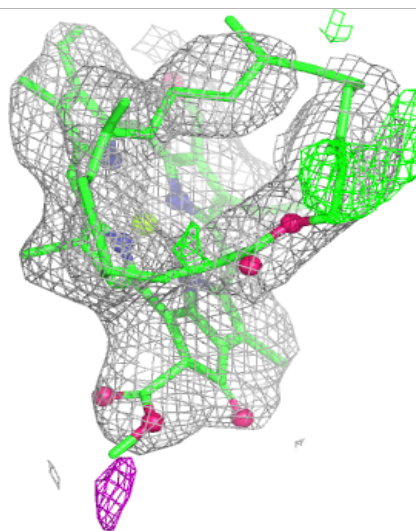
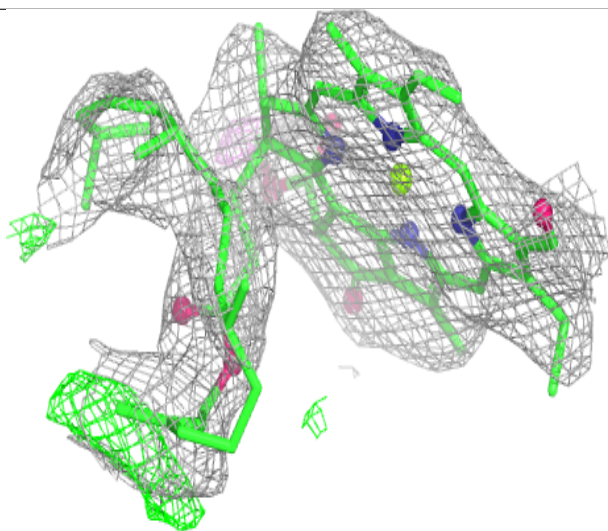
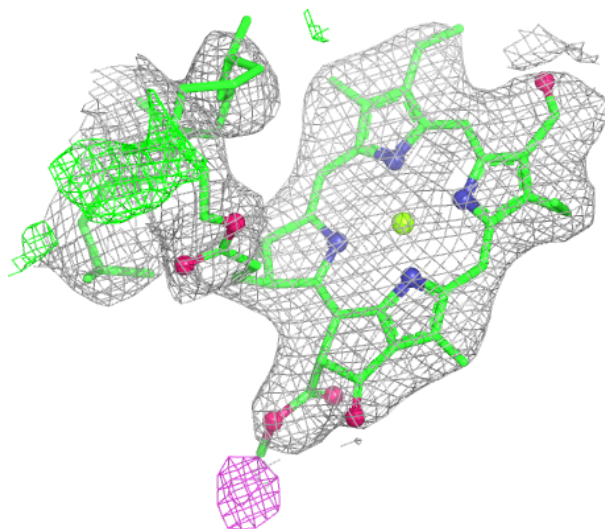
**Electron density around LUX A 502:**

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



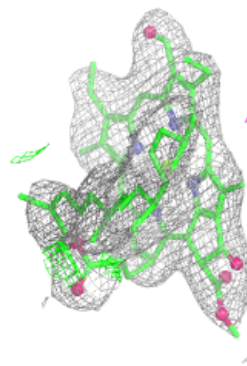
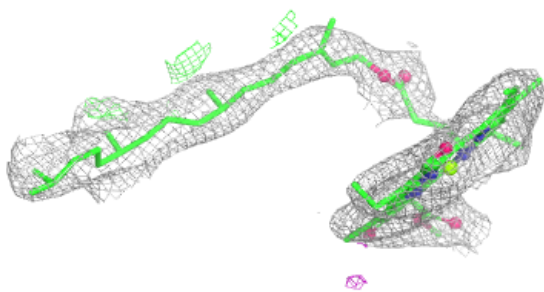
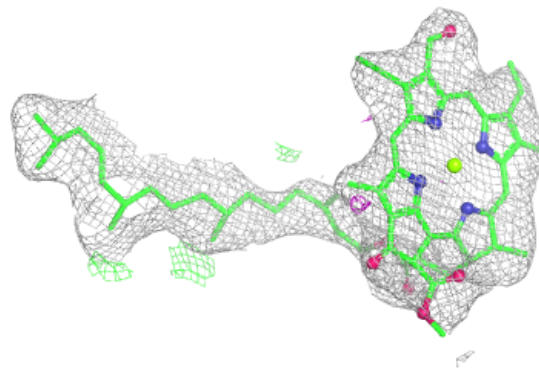
Electron density around CHL A 611:

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

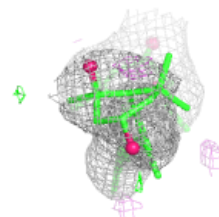
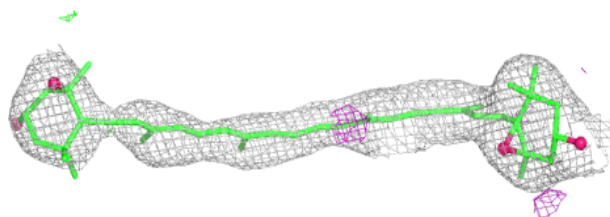
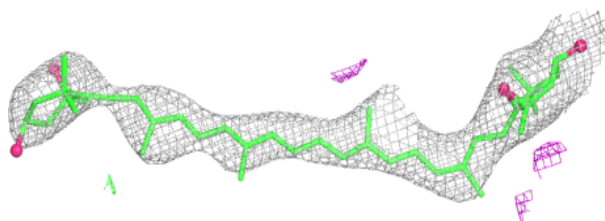


Electron density around CHL A 612:

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

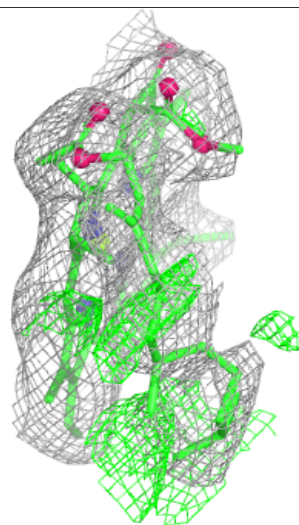
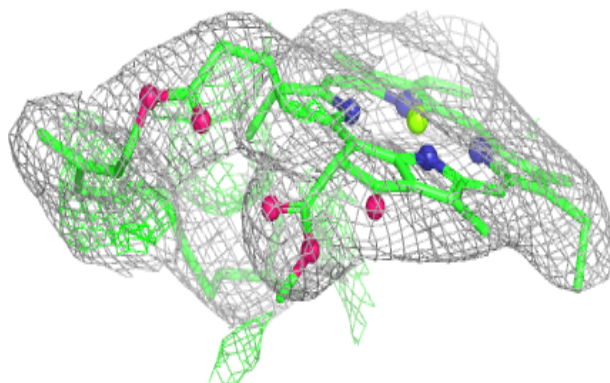
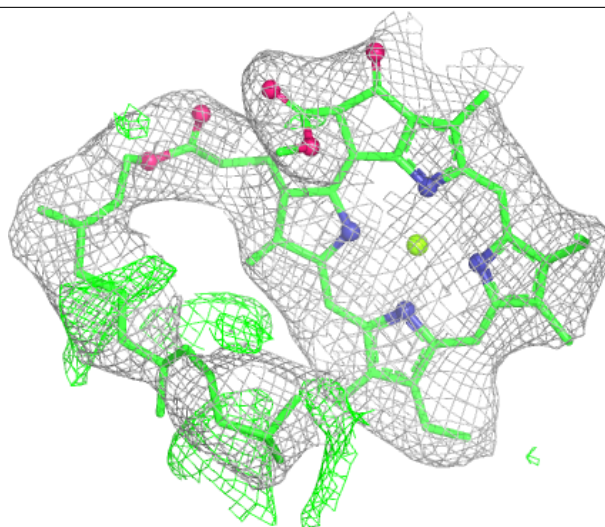
**Electron density around NEX A 503:**

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



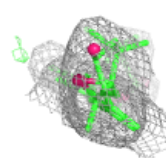
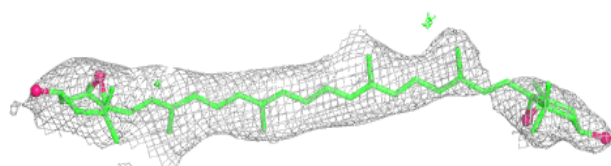
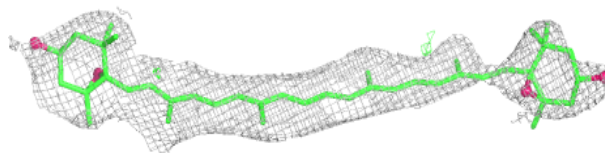
Electron density around CLA B 602:

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



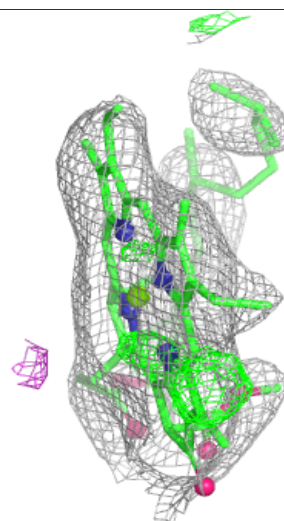
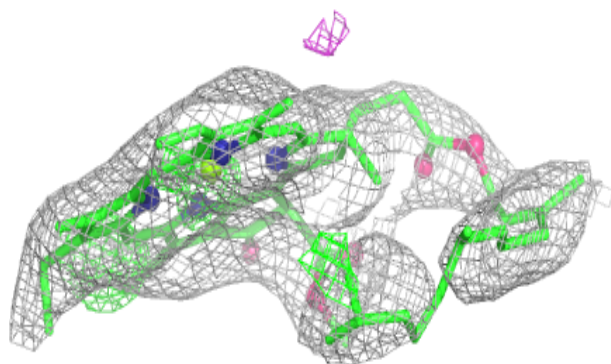
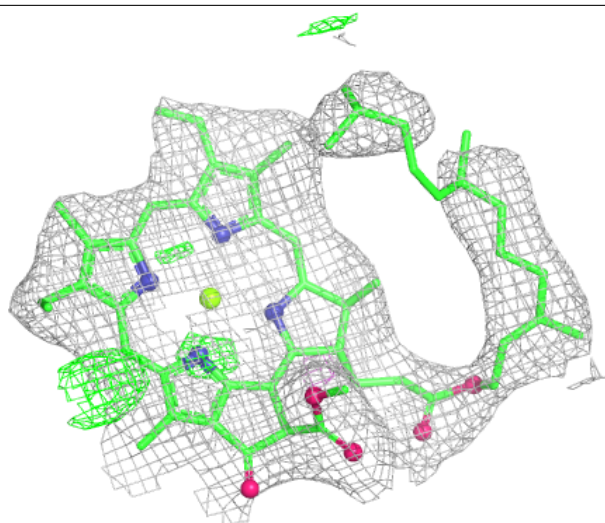
Electron density around XAT A 504:

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



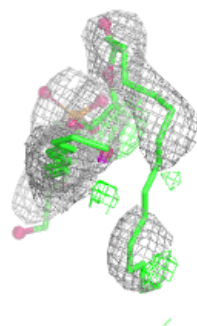
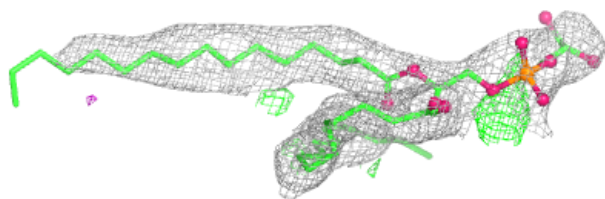
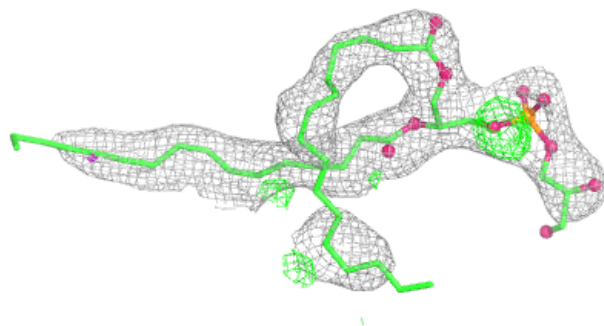
Electron density around CLA A 602:

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



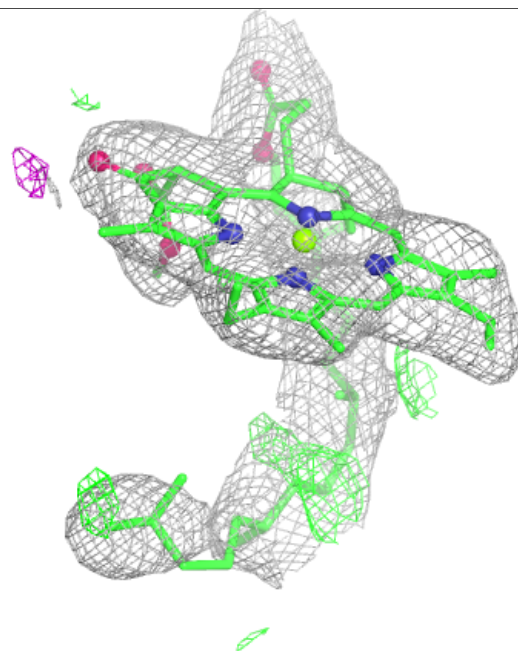
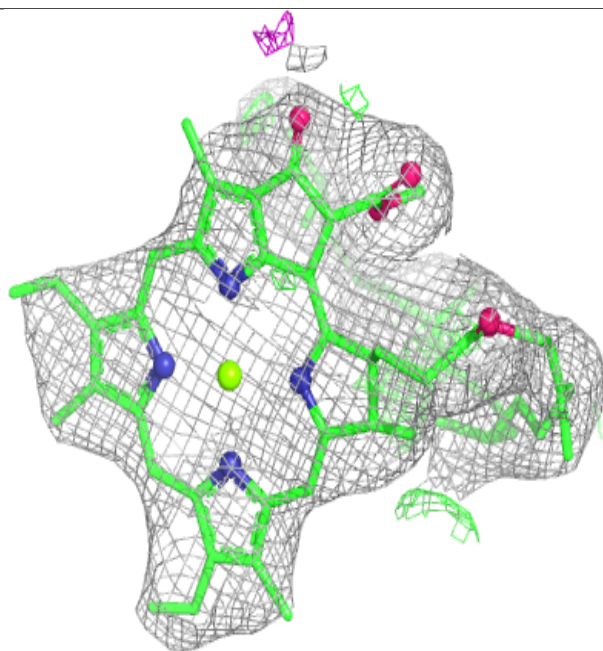
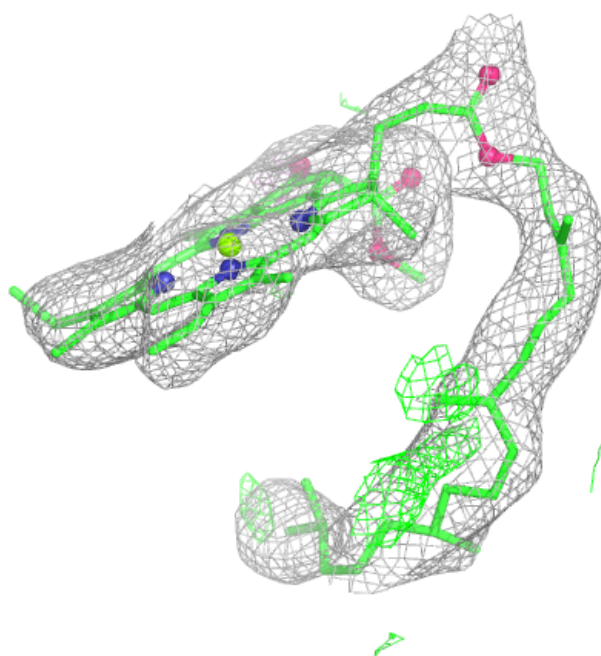
Electron density around LHG B 801:

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



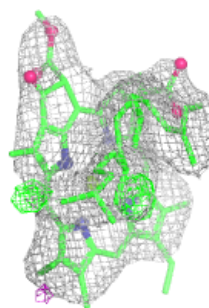
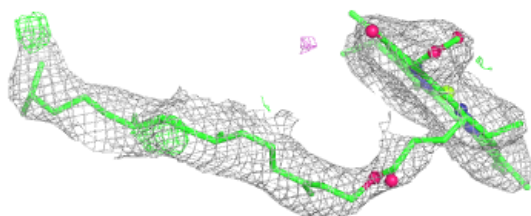
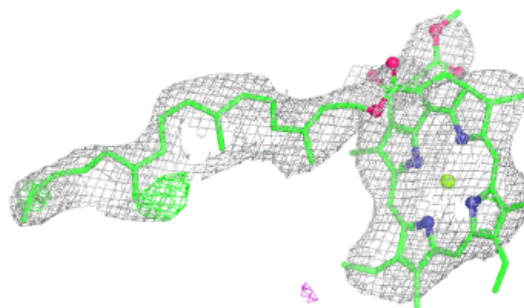
Electron density around CLA C 605:

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



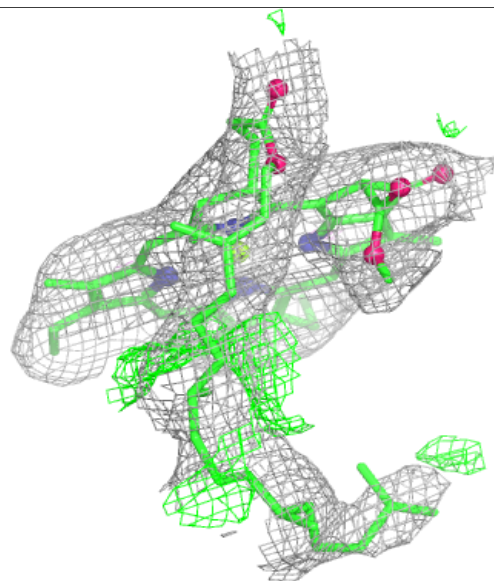
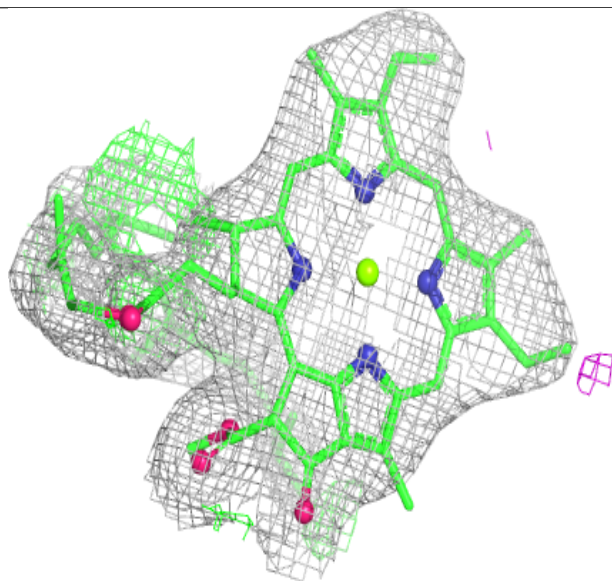
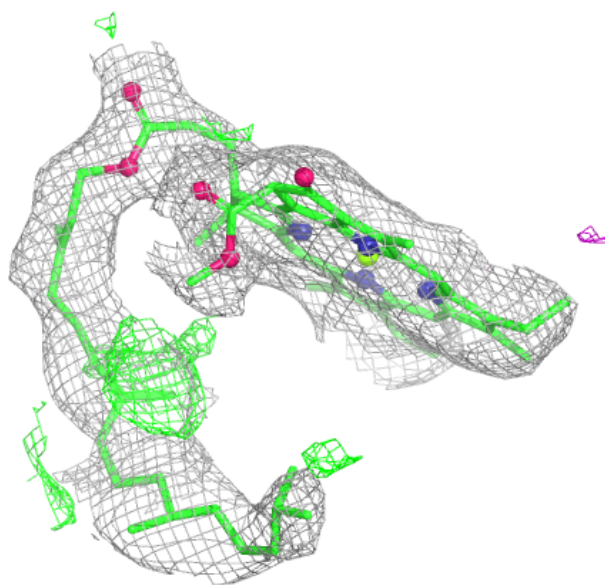
Electron density around CLA C 607:

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



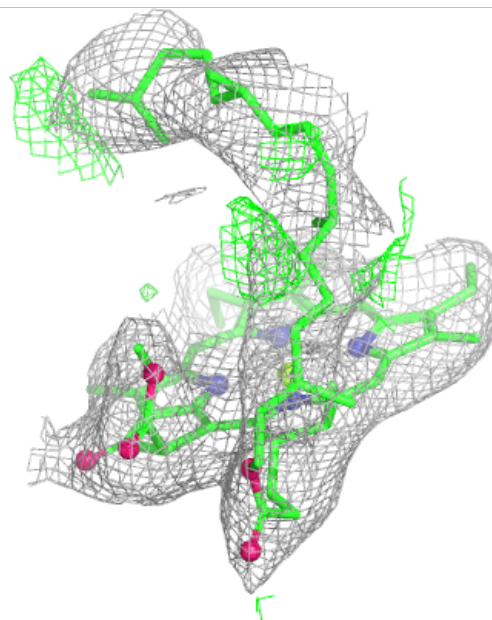
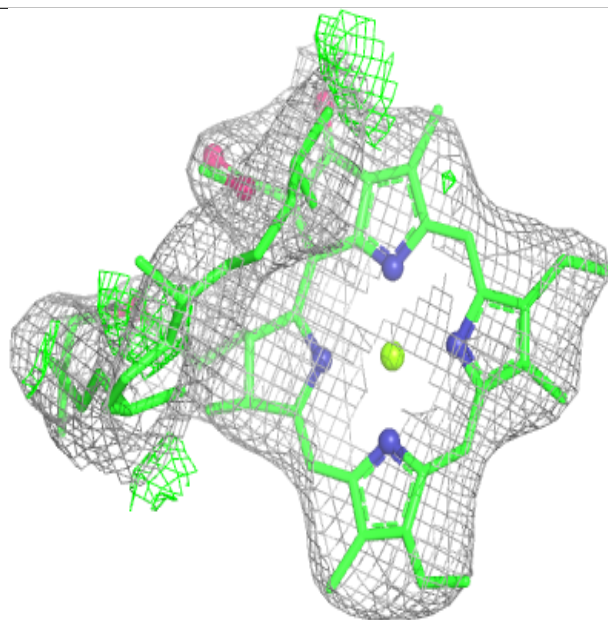
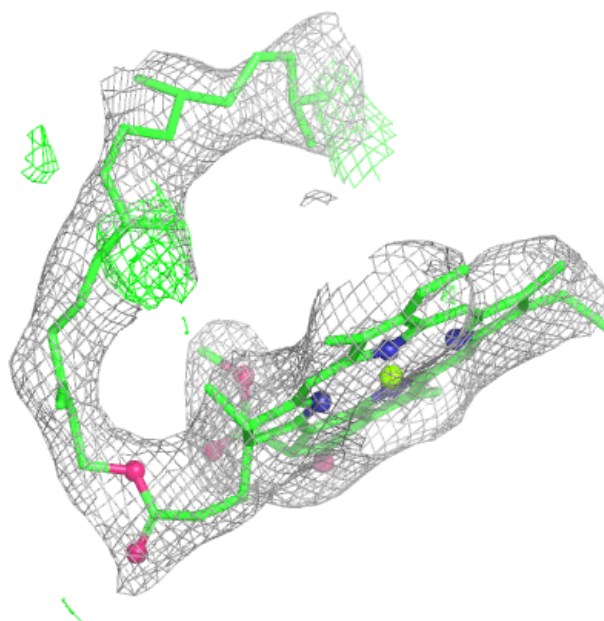
Electron density around CLA A 605:

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



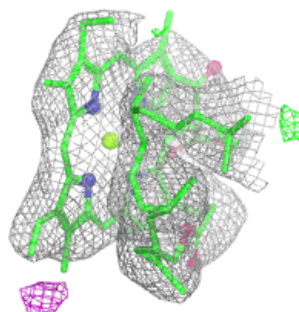
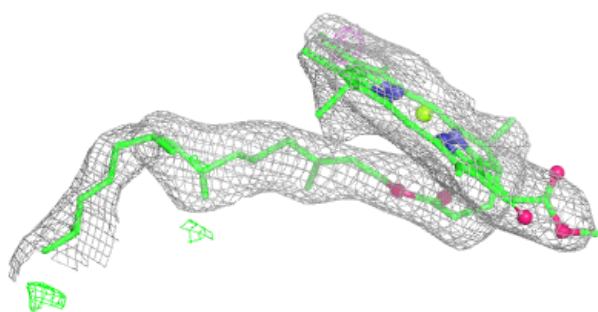
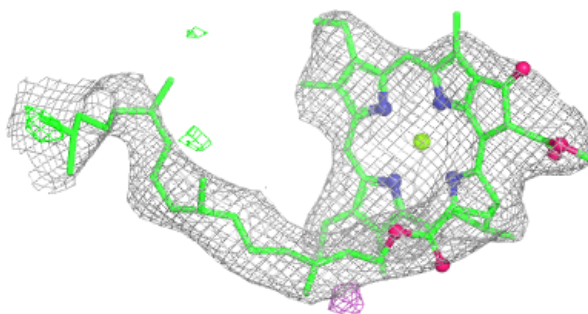
Electron density around CLA B 605:

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

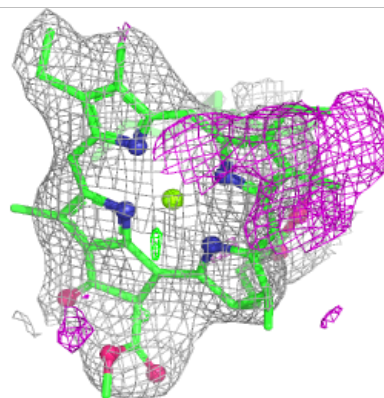
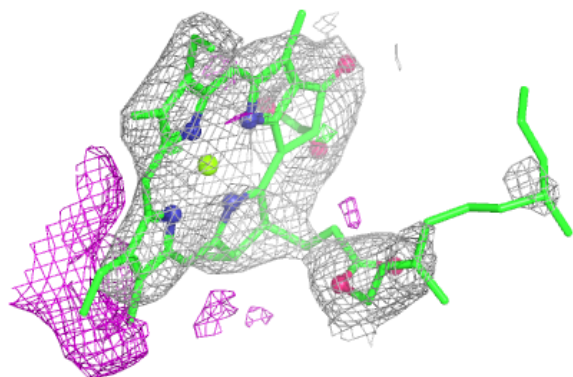
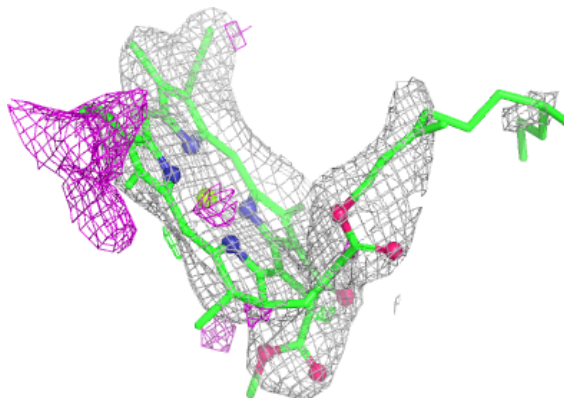


Electron density around CLA A 601:

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

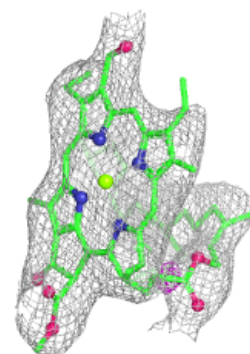
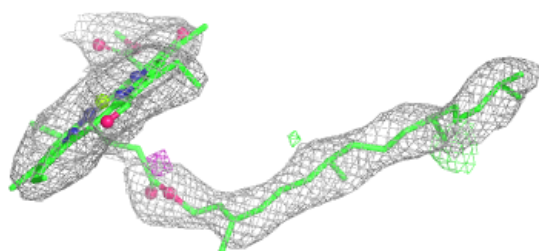
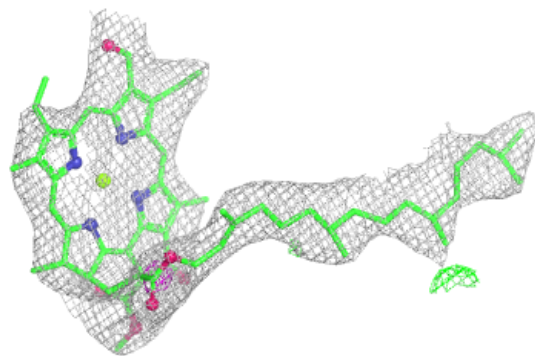
**Electron density around CLA A 606:**

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



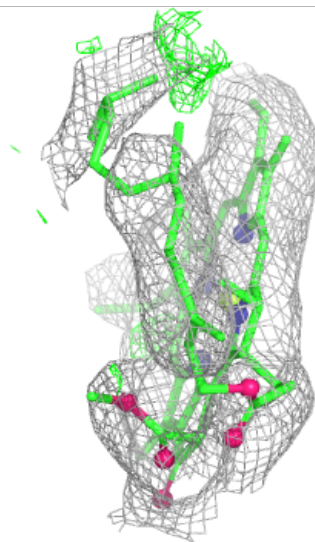
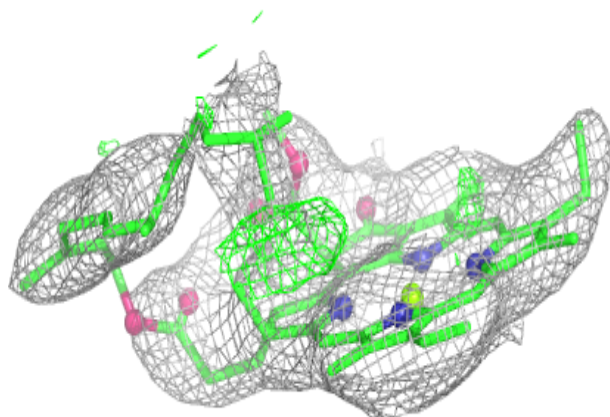
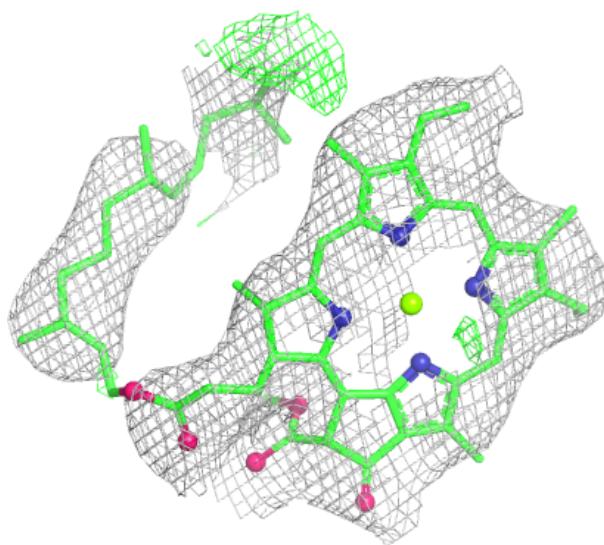
Electron density around CHL C 612:

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



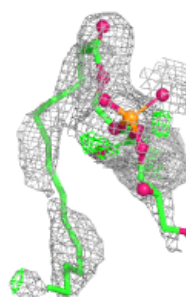
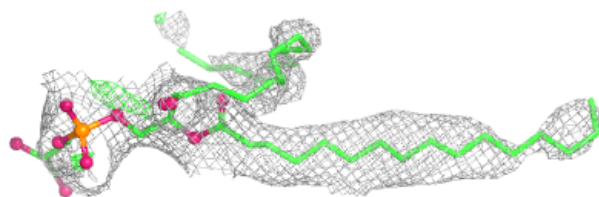
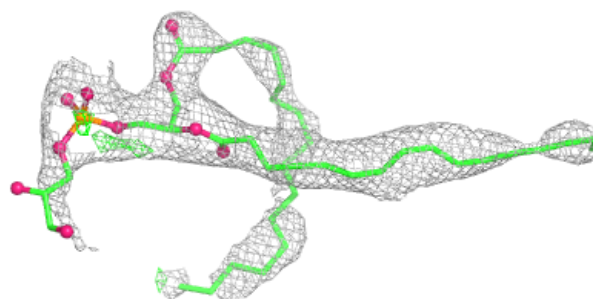
Electron density around CLA C 602:

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



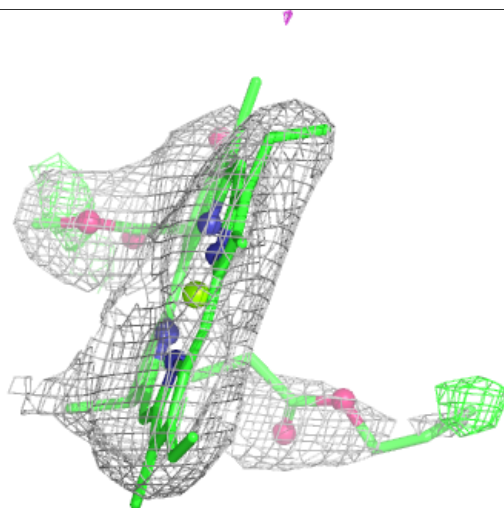
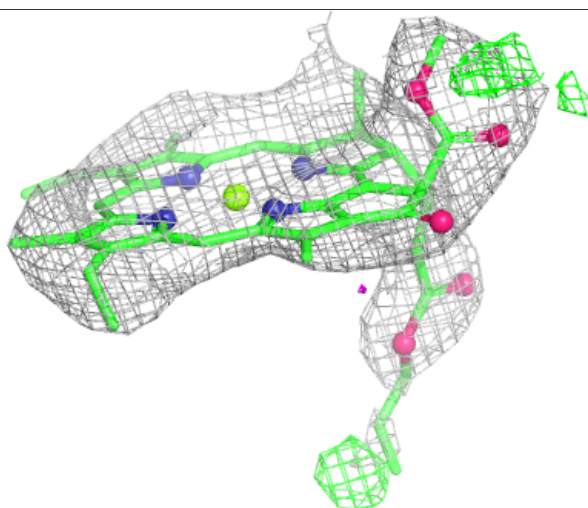
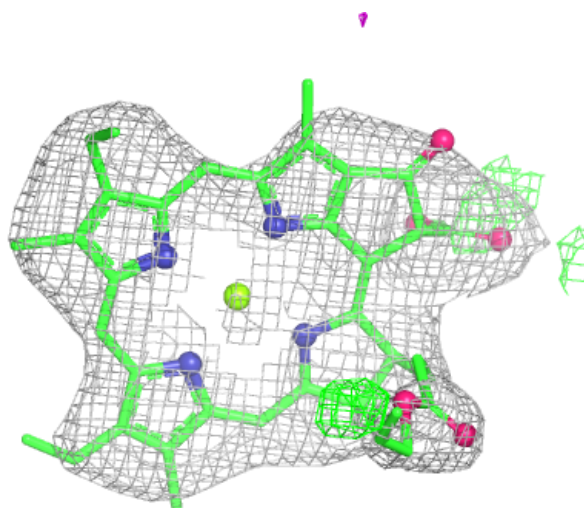
Electron density around LHG A 801:

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



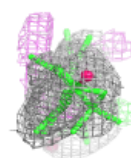
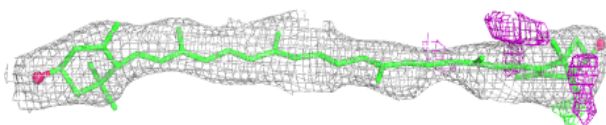
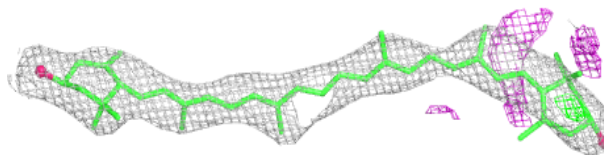
Electron density around CLA A 608:

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

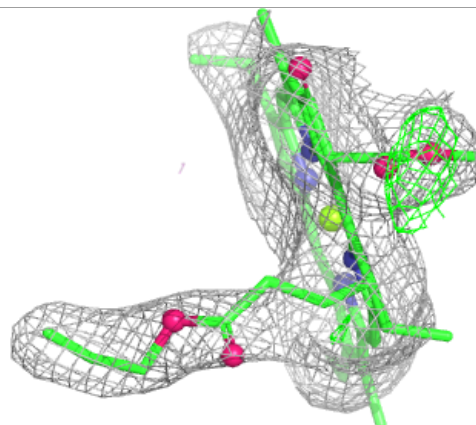
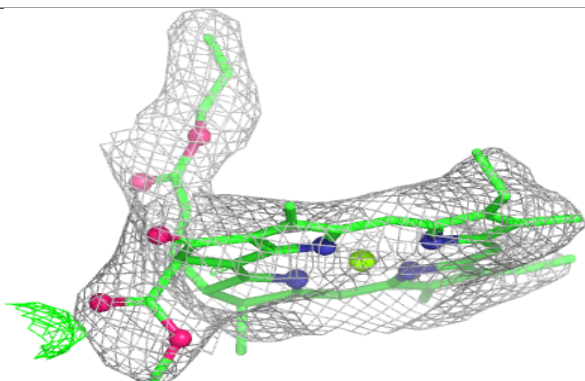
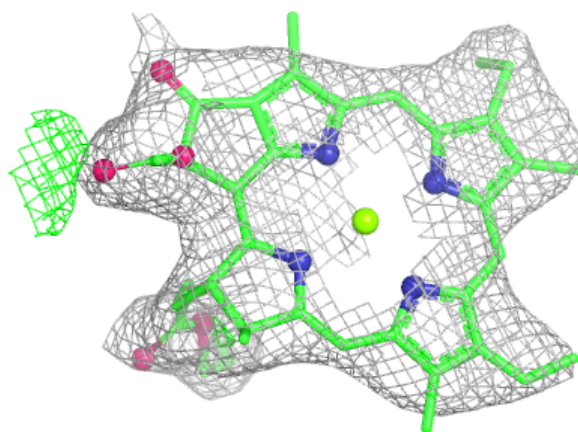


Electron density around LUX C 502:

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

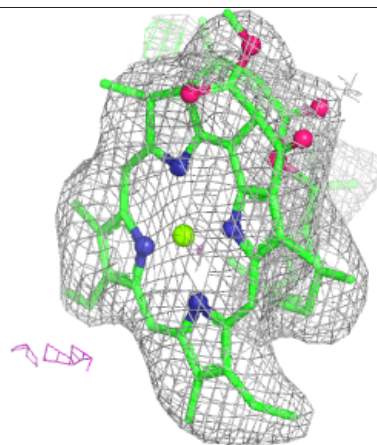
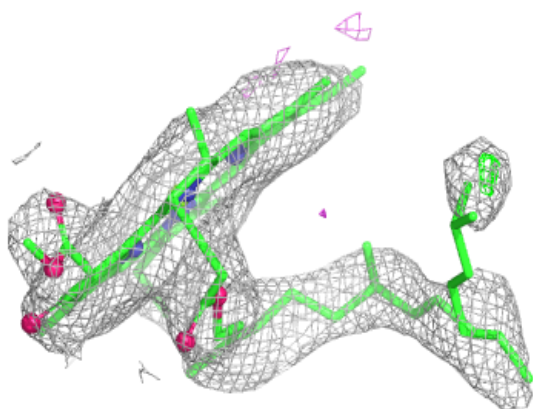
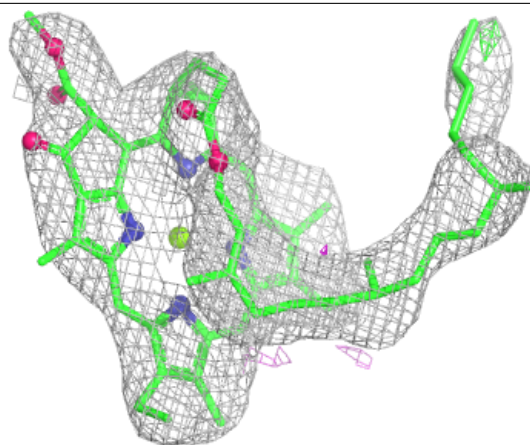
**Electron density around CLA C 608:**

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



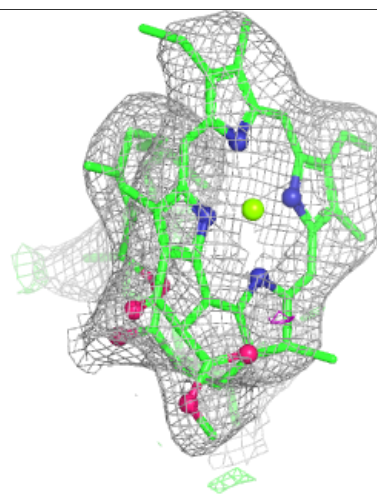
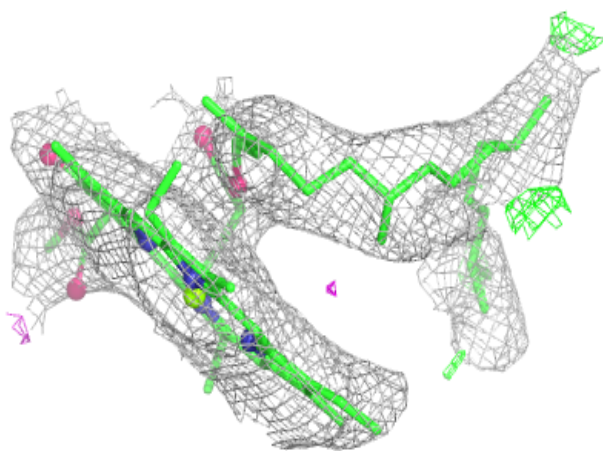
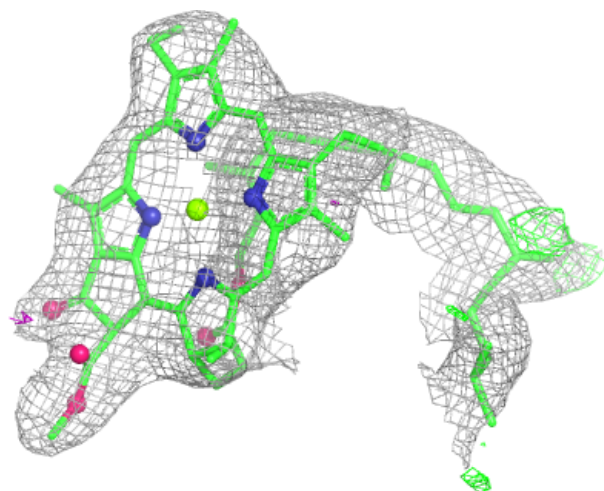
Electron density around CLA A 603:

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



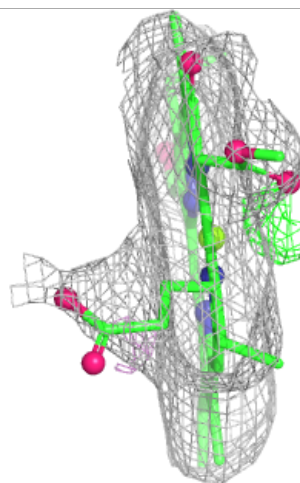
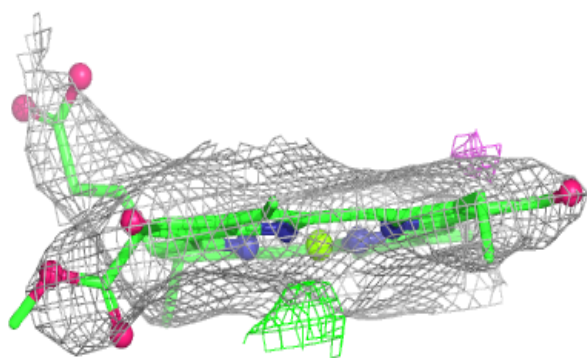
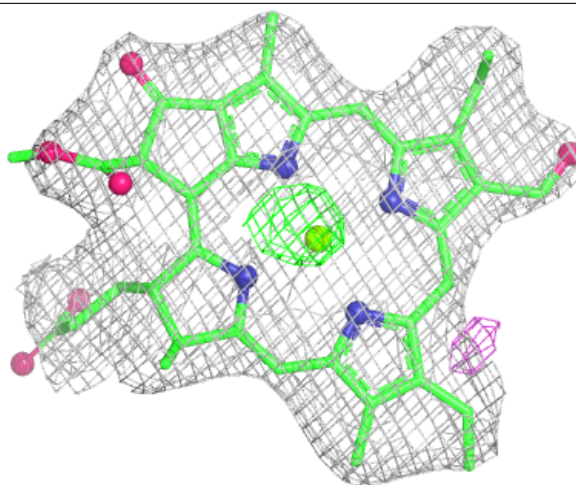
Electron density around CLA B 603:

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



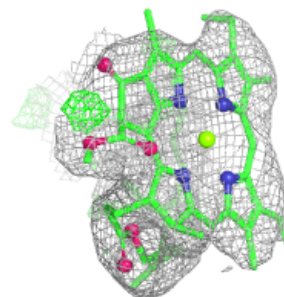
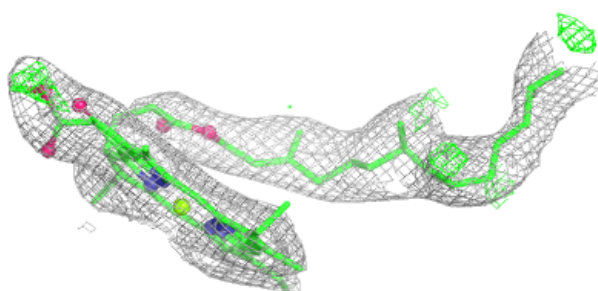
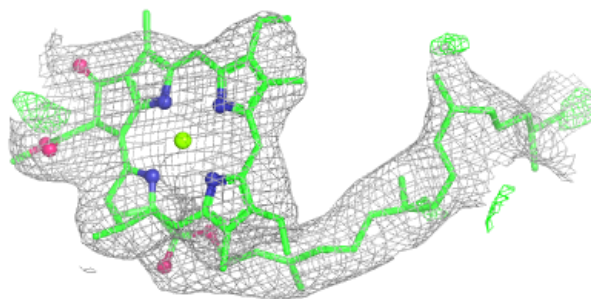
Electron density around CHL C 613:

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

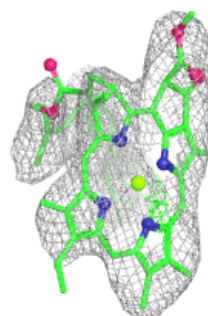
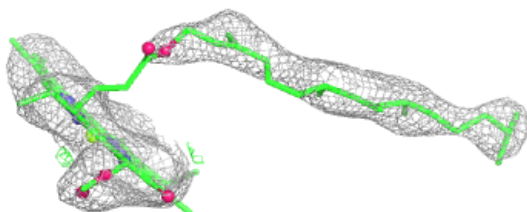
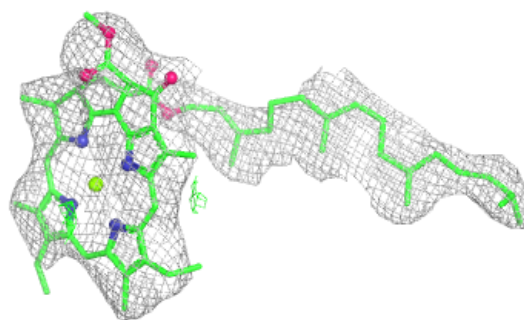


Electron density around CLA C 601:

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

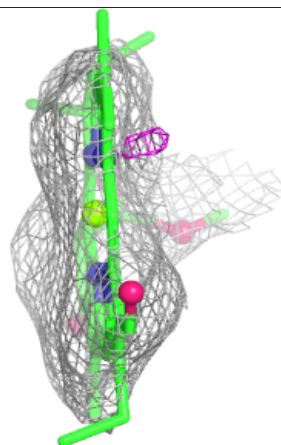
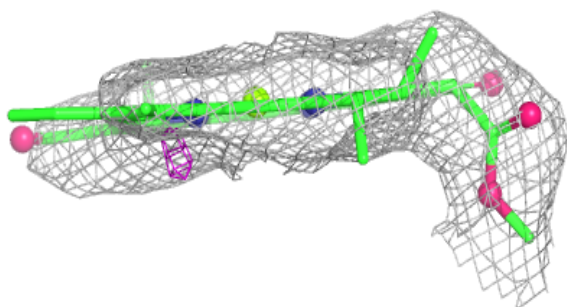
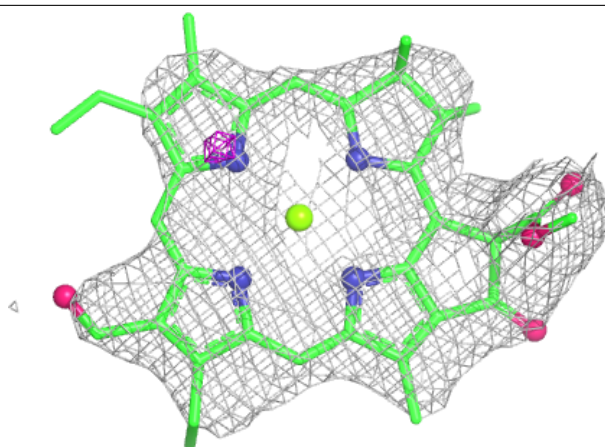
**Electron density around CLA A 607:**

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



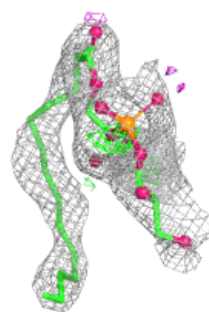
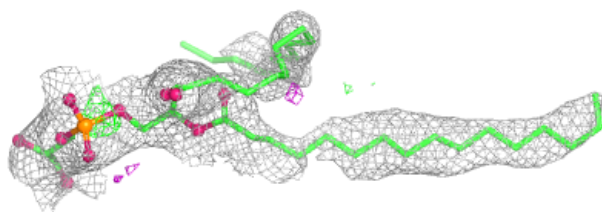
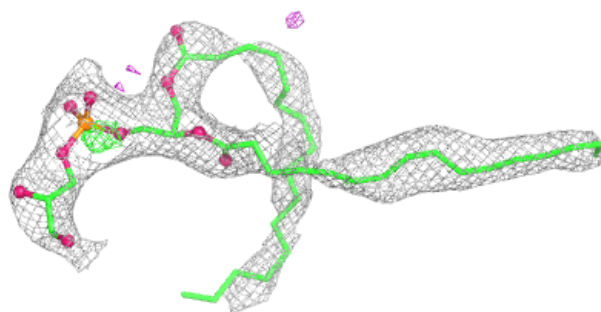
Electron density around CHL A 614:

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



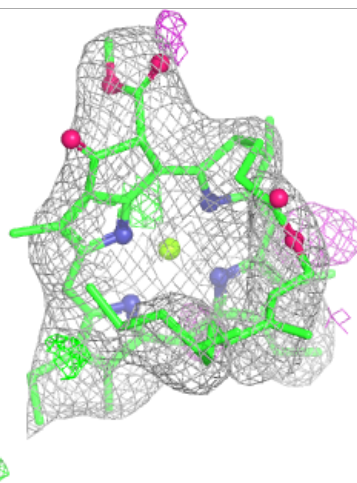
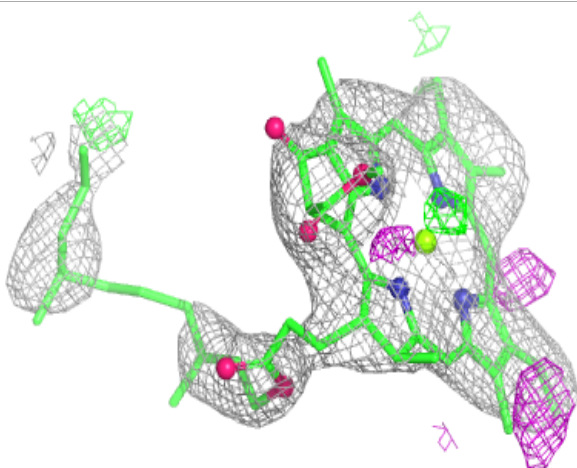
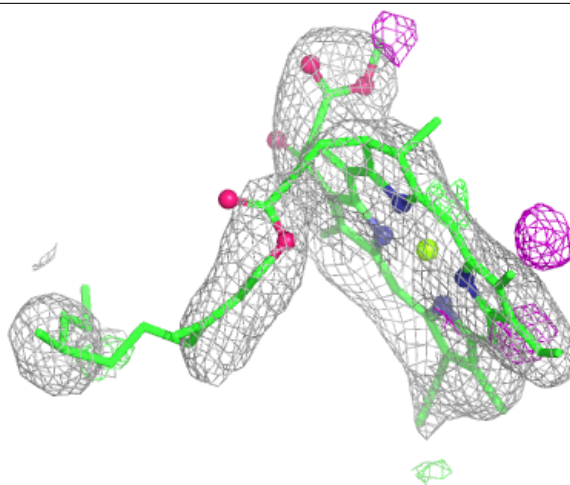
Electron density around LHG C 801:

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



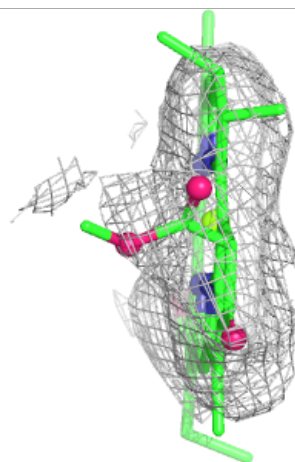
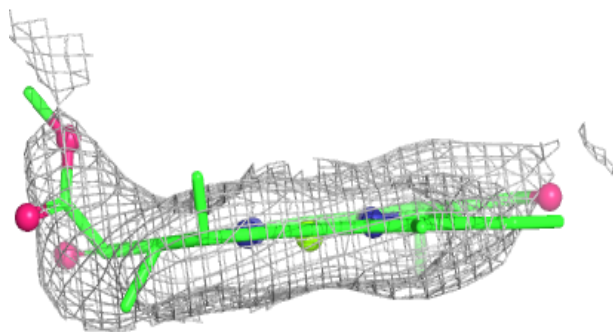
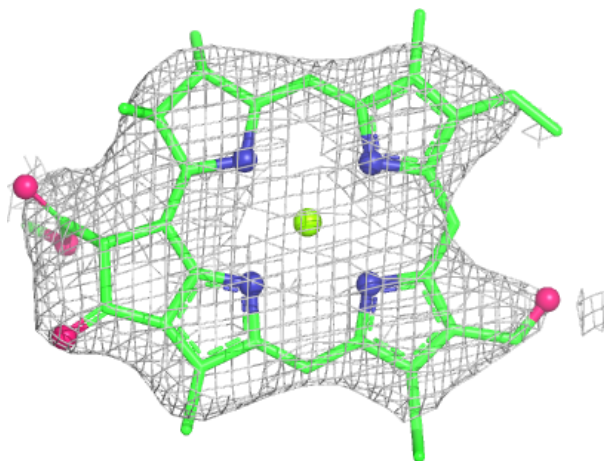
Electron density around CLA B 606:

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



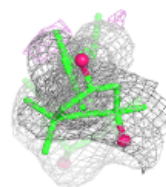
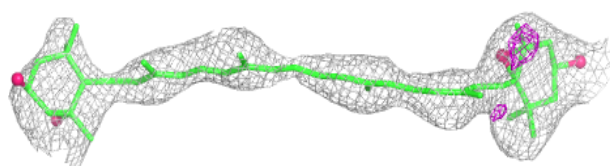
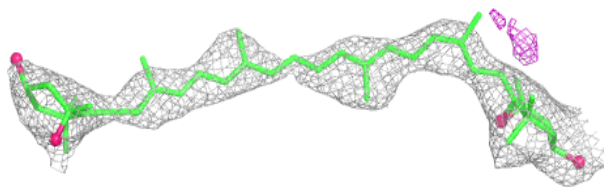
Electron density around CHL B 614:

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

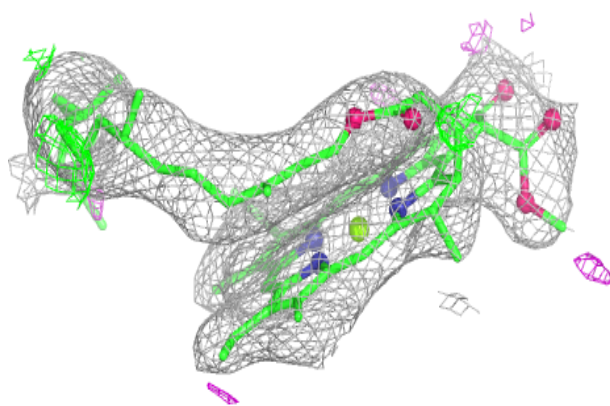
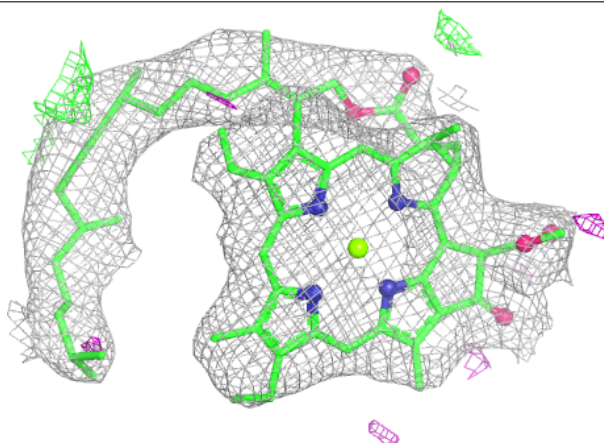


Electron density around NEX B 503:

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

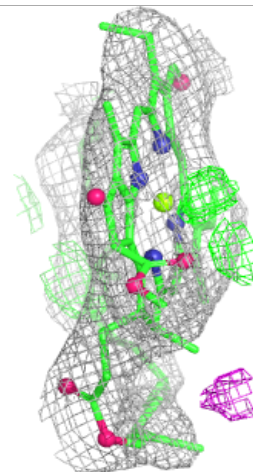
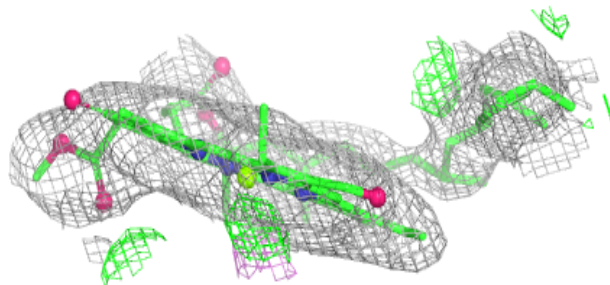
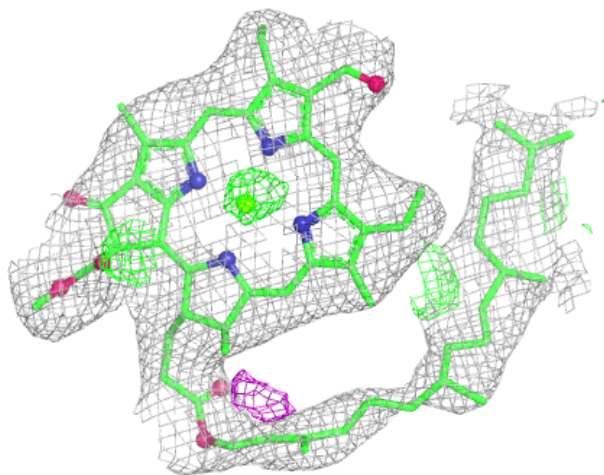
**Electron density around CLA B 604:**

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



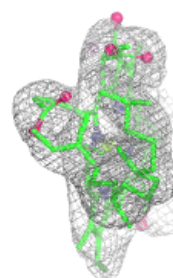
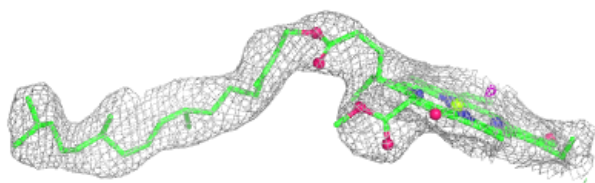
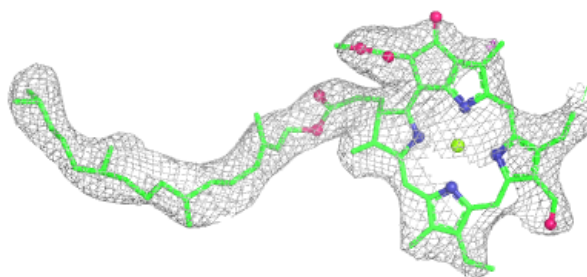
Electron density around CHL B 610:

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

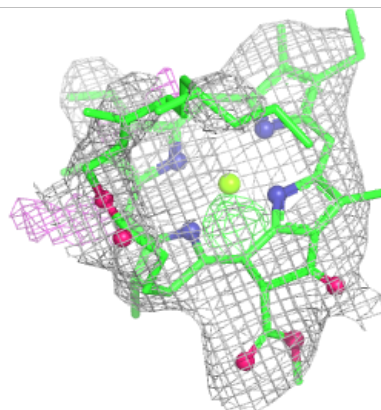
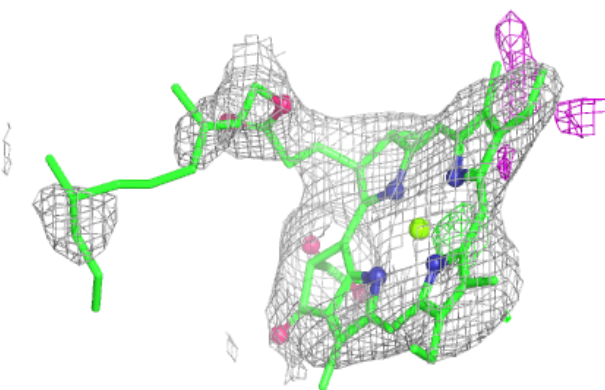
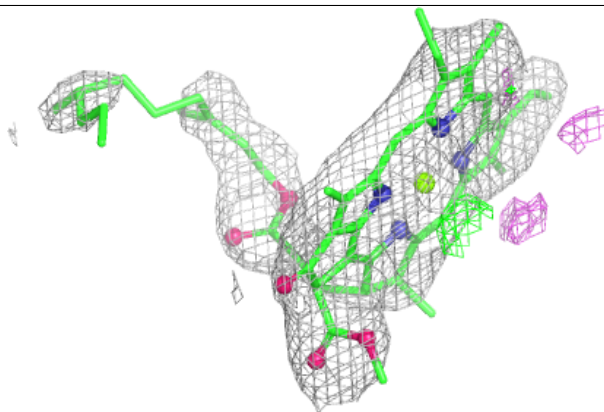


Electron density around CHL A 609:

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

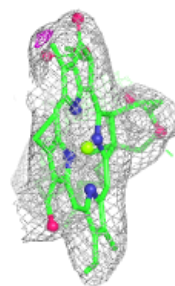
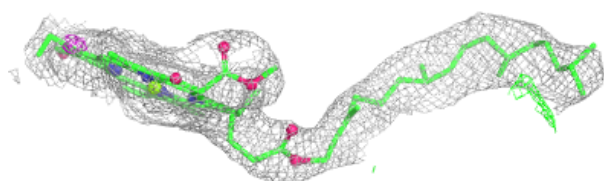
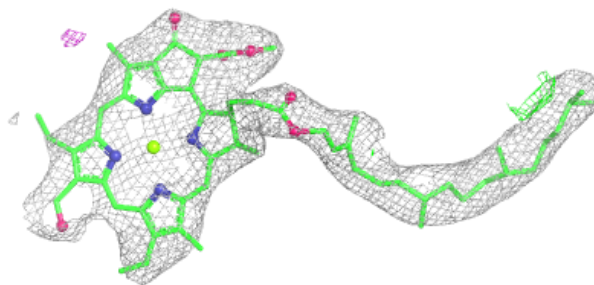
**Electron density around CLA C 606:**

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



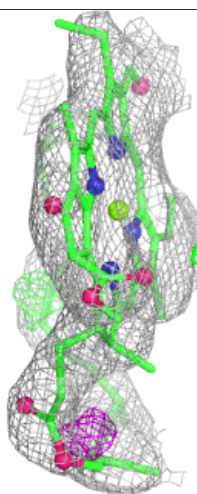
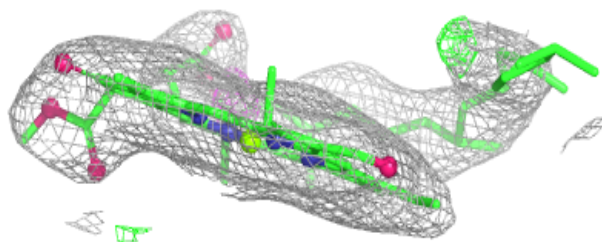
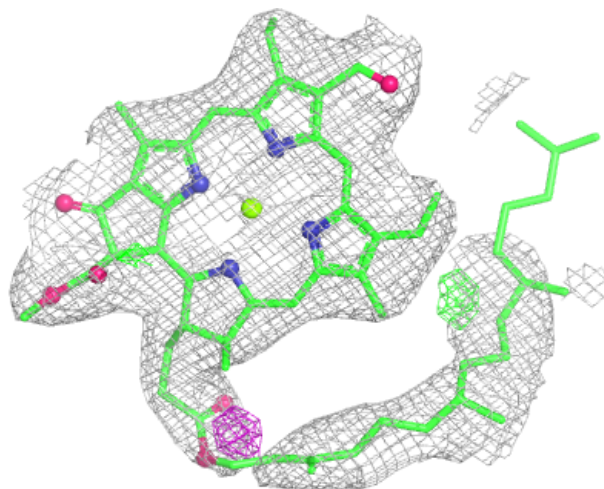
Electron density around CHL C 609:

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



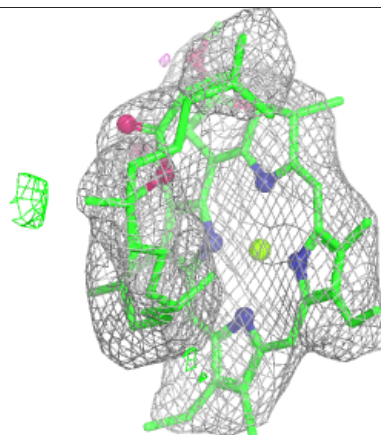
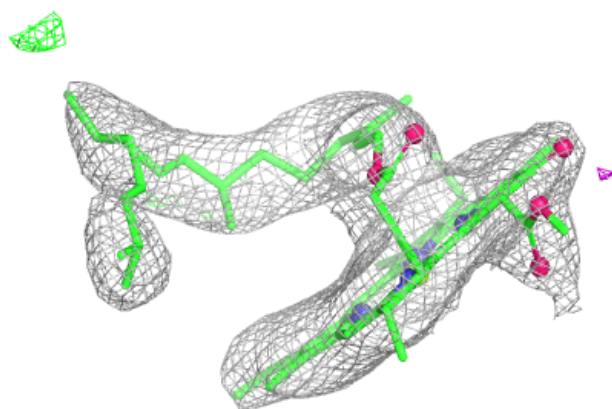
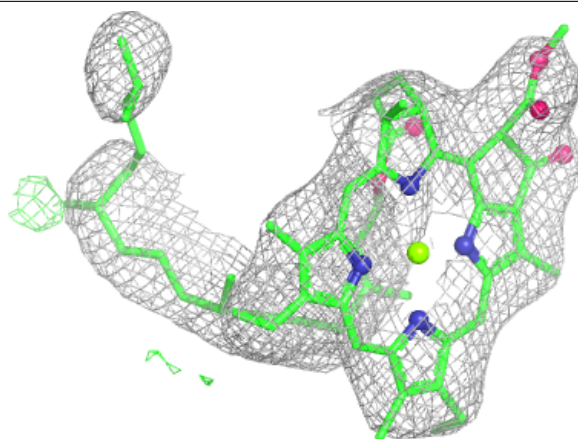
Electron density around CHL C 610:

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

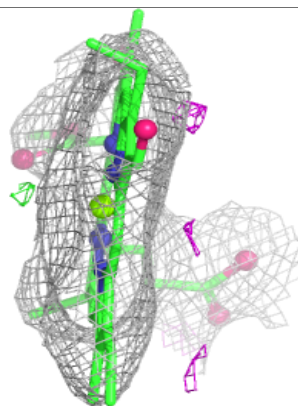
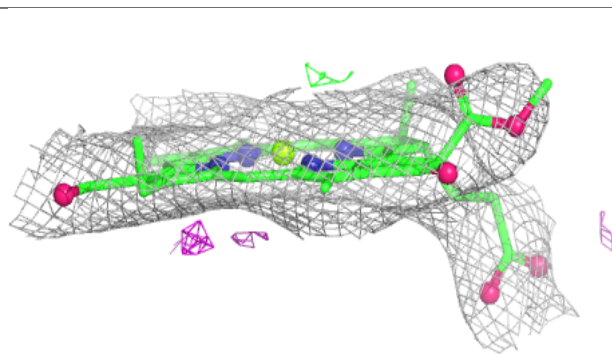
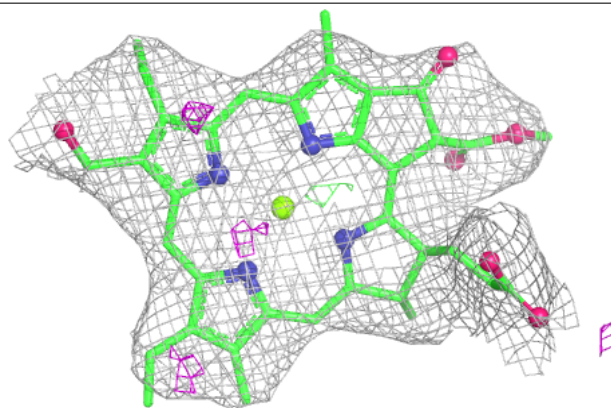


Electron density around CLA C 603:

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

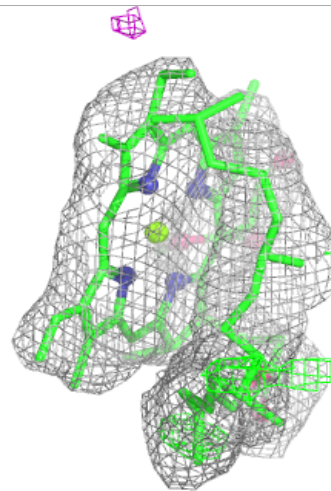
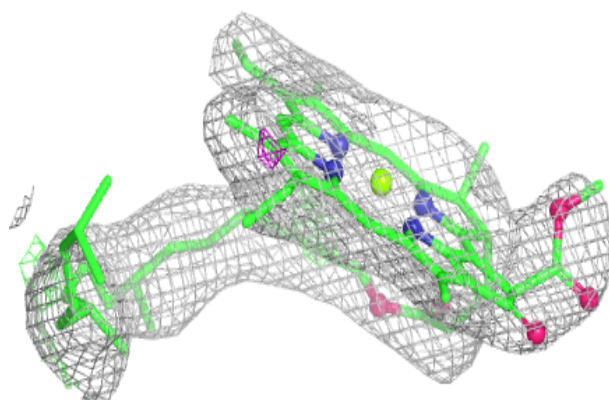
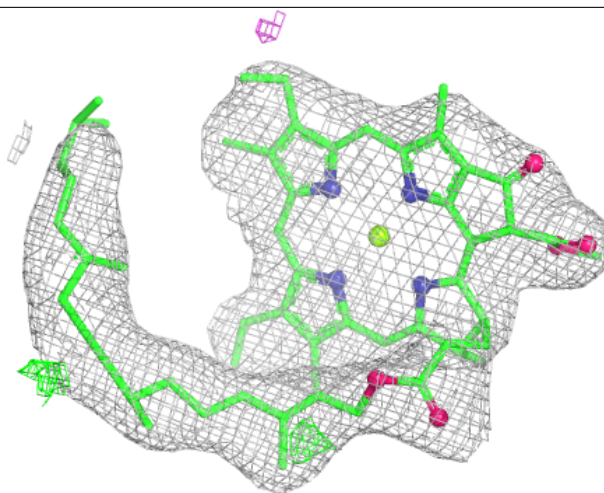
**Electron density around CHL A 613:**

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



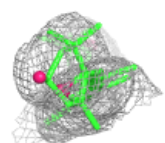
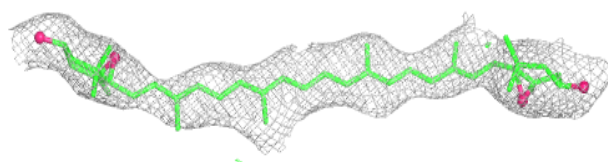
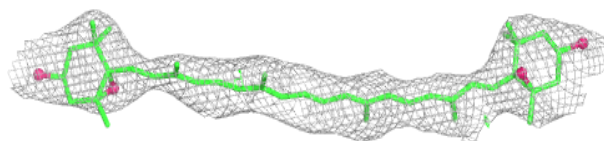
Electron density around CLA C 604:

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



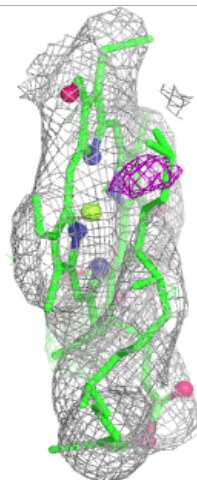
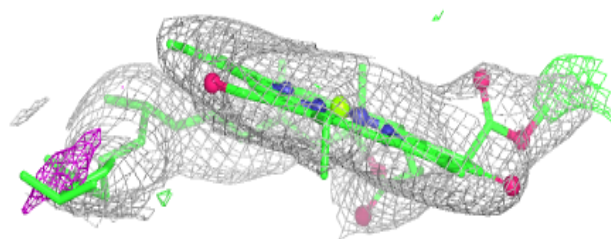
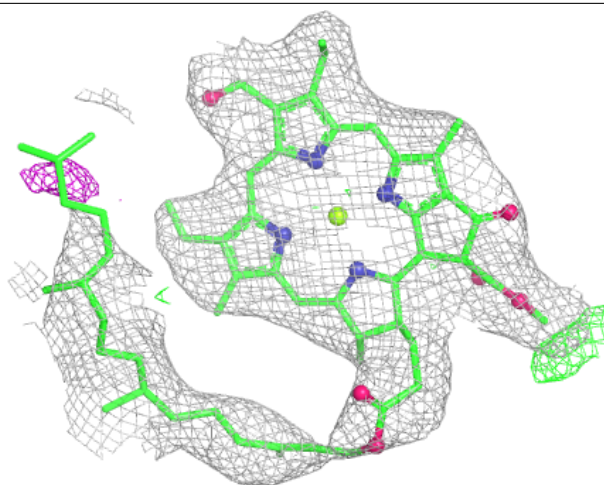
Electron density around XAT C 504:

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



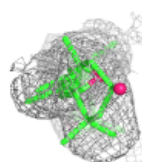
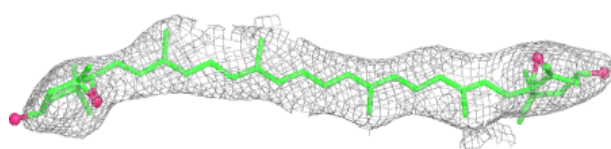
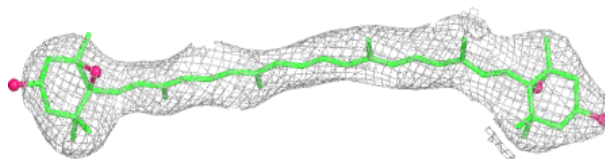
Electron density around CHL A 610:

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

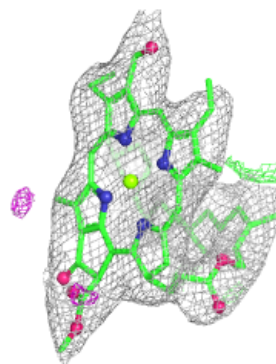
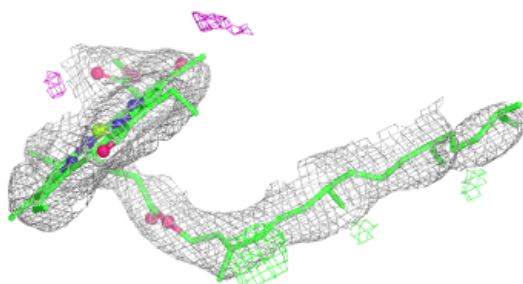
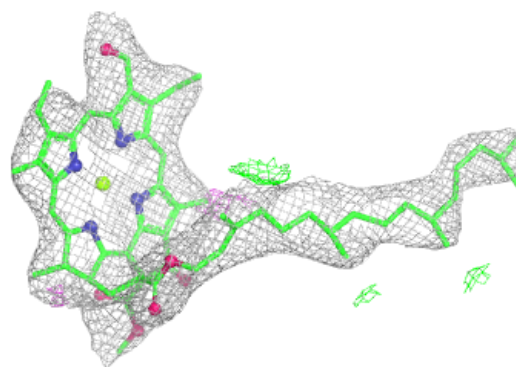


Electron density around XAT B 504:

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

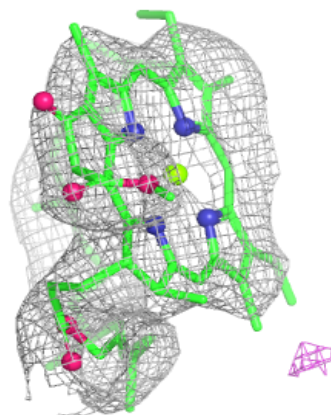
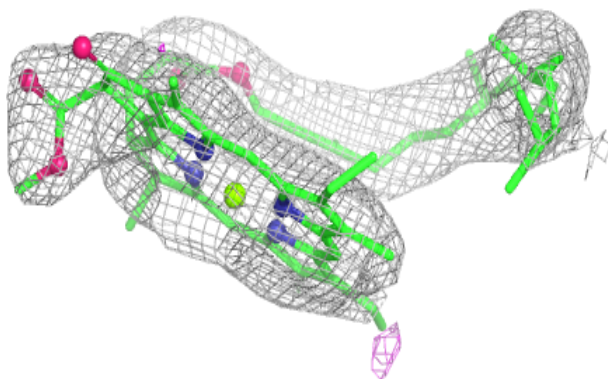
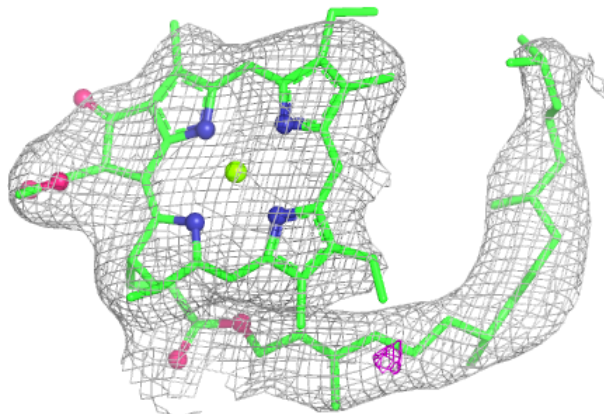
**Electron density around CHL B 612:**

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



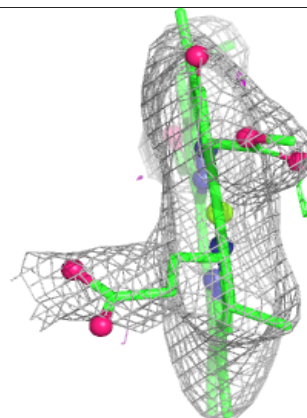
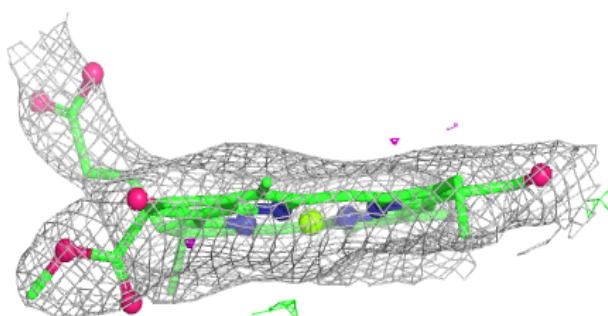
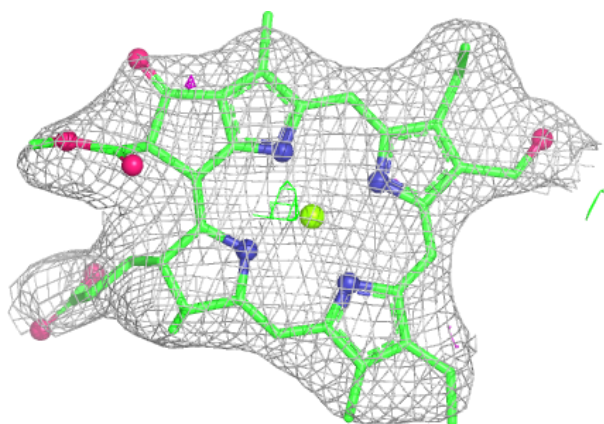
Electron density around CLA A 604:

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

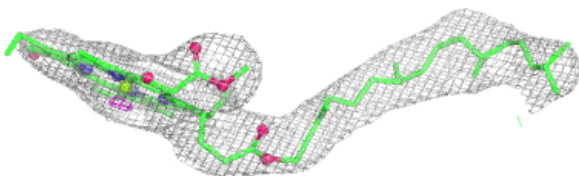
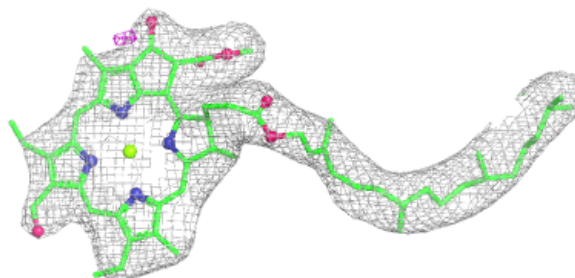


Electron density around CHL B 613:

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

**Electron density around CHL B 609:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.