Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 05:20 am BST

PDB ID	:	2BHW
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

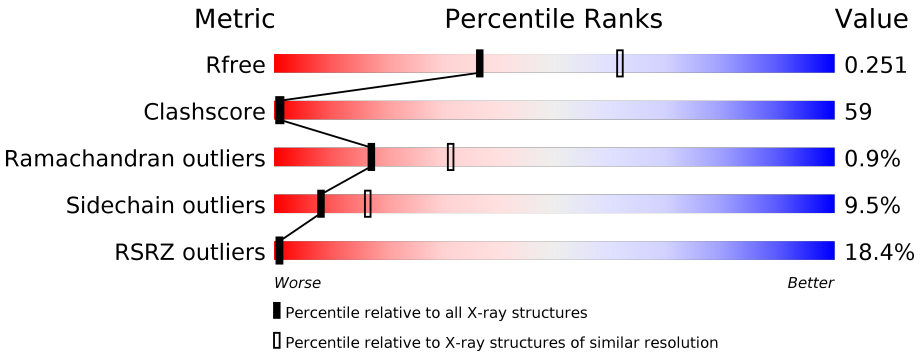
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	21% 55% 38%
1	B	232	16% 52% 40% 5%
1	C	232	16% 54% 38%

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	-	X	-
2	LUX	B	501	X	-	X	-
2	LUX	B	502	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	-	X	-
5	CLA	A	602	X	-	-	-
5	CLA	A	603	X	-	-	-
5	CLA	A	604	X	-	X	-
5	CLA	A	605	X	-	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	-	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	-	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	-
6	CHL	B	611	X	-	X	-
6	CHL	B	612	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	X
8	DGD	B	802	X	-	-	X
8	DGD	C	802	X	-	-	X

2 Entry composition

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.

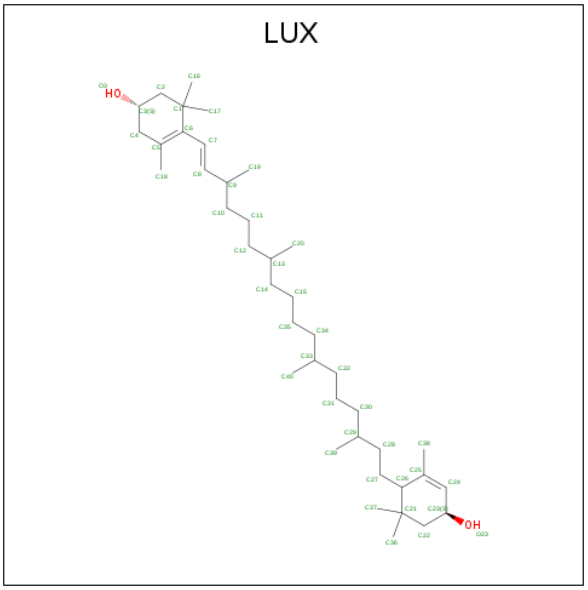
- Molecule 1 is a protein called CHLOROPHYLL A-B BINDING PROTEIN AB80.

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:

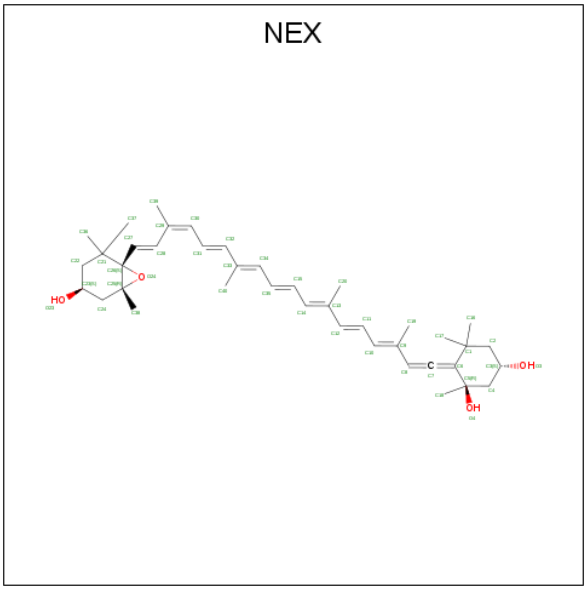
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	SER	CYS	conflict	UNP P07371
B	79	SER	CYS	conflict	UNP P07371
C	79	SER	CYS	conflict	UNP P07371

- 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'-OCTADECAHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUX) (formula: $C_{40}H_{72}O_2$).



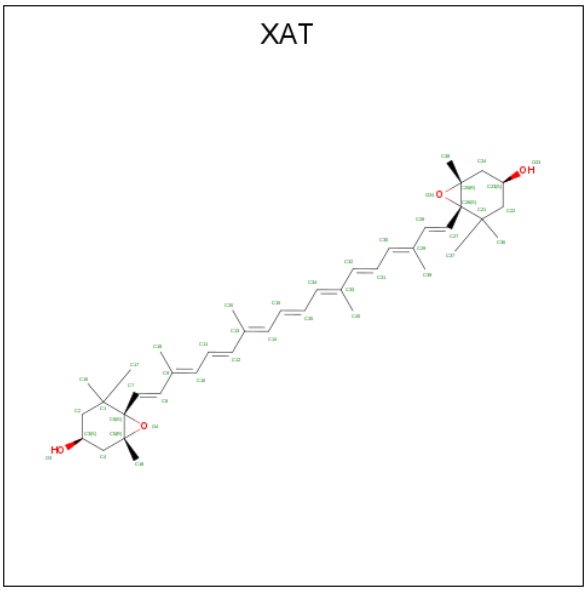
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 42 40 2	0	0
2	A	1	Total C O 42 40 2	0	0
2	B	1	Total C O 42 40 2	0	0
2	B	1	Total C O 42 40 2	0	0
2	C	1	Total C O 42 40 2	0	0
2	C	1	Total C O 42 40 2	0	0

- 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-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



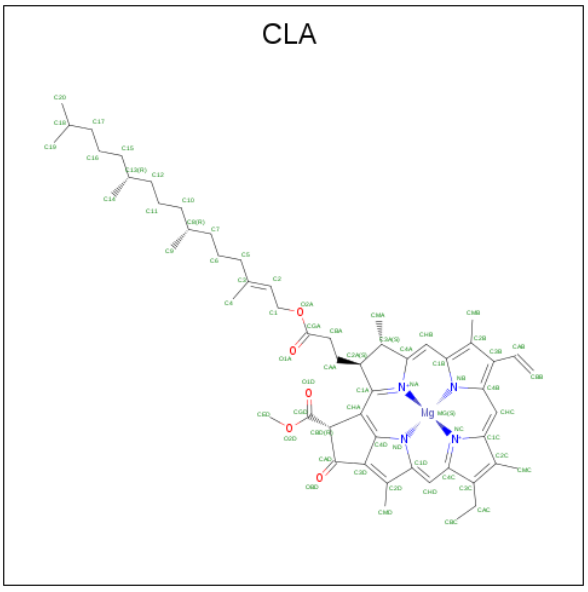
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 44 40 4	0	0
3	B	1	Total C O 44 40 4	0	0
3	C	1	Total C O 44 40 4	0	0

- 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 (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



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

- Molecule 5 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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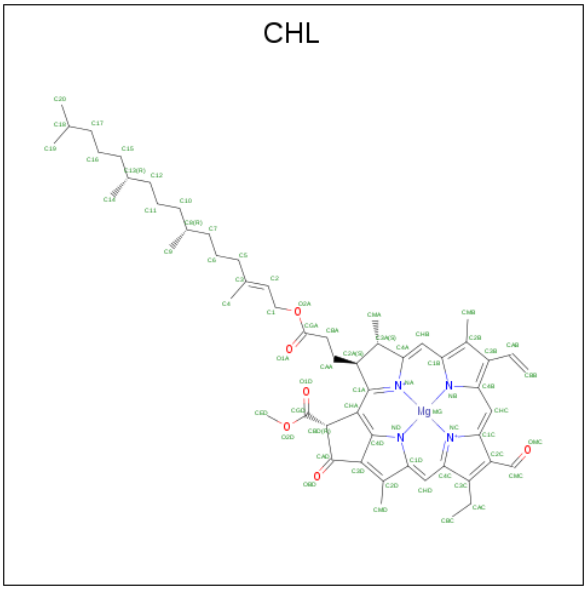
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		

- Molecule 6 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



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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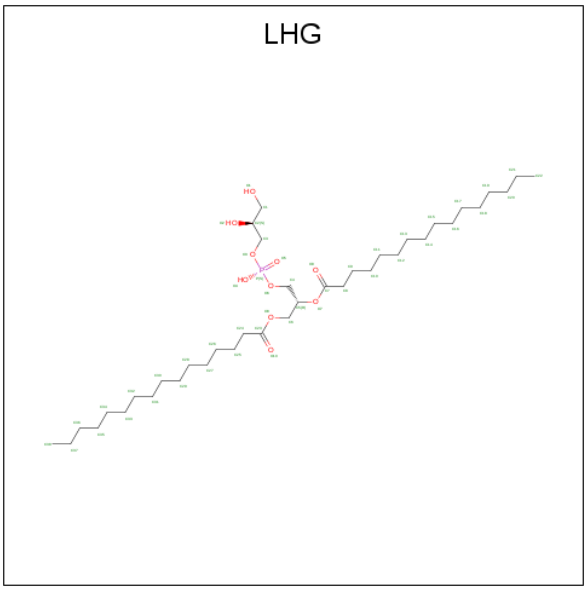
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	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 (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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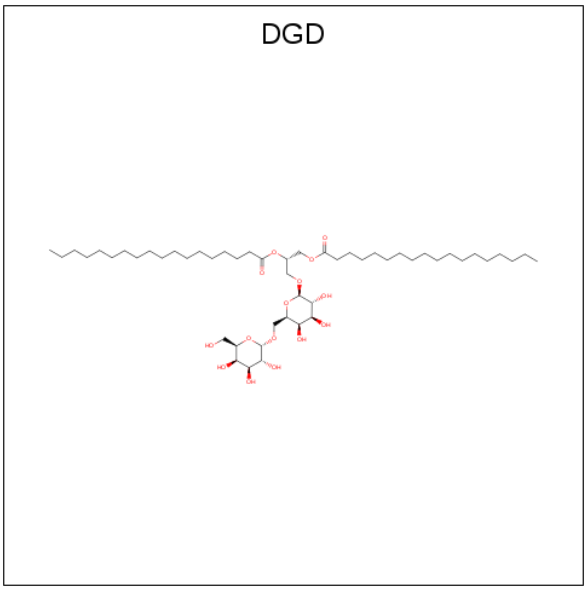
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 8 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: 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.

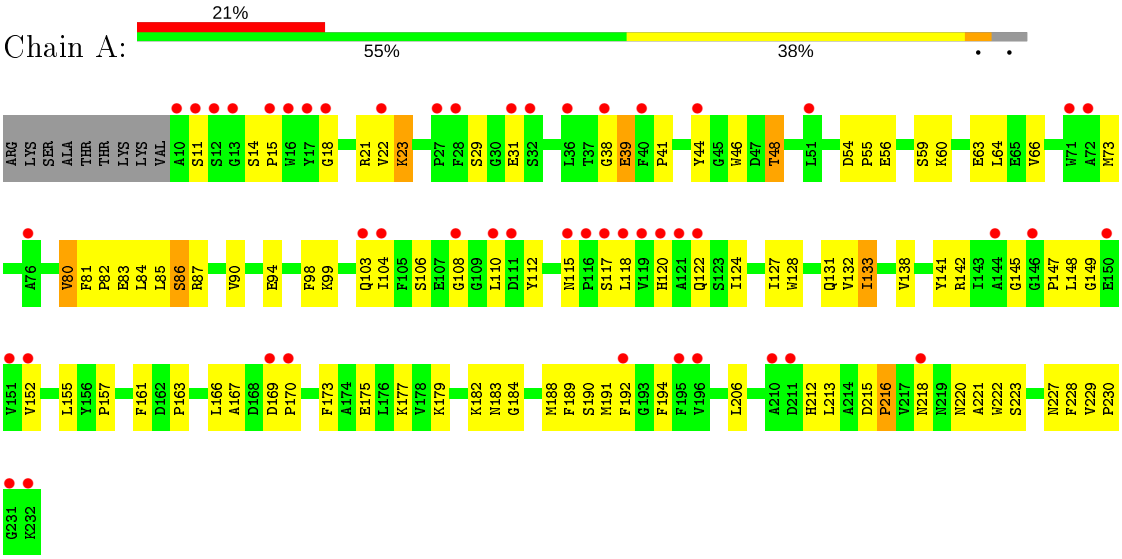
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	9	Total	O	0	0
			9	9		
9	B	7	Total	O	0	0
			7	7		
9	C	5	Total	O	0	0
			5	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

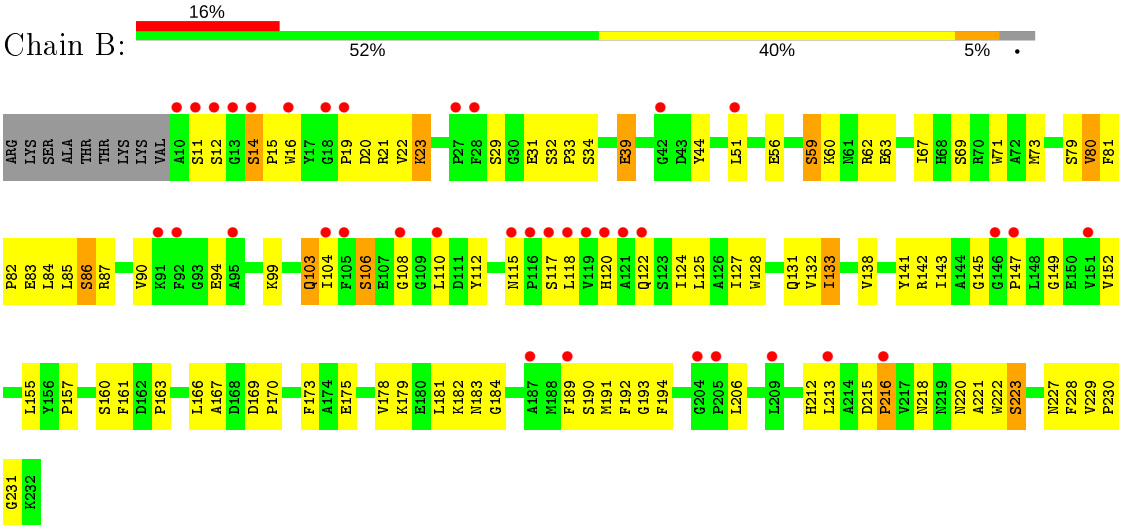
- Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80

Chain A:



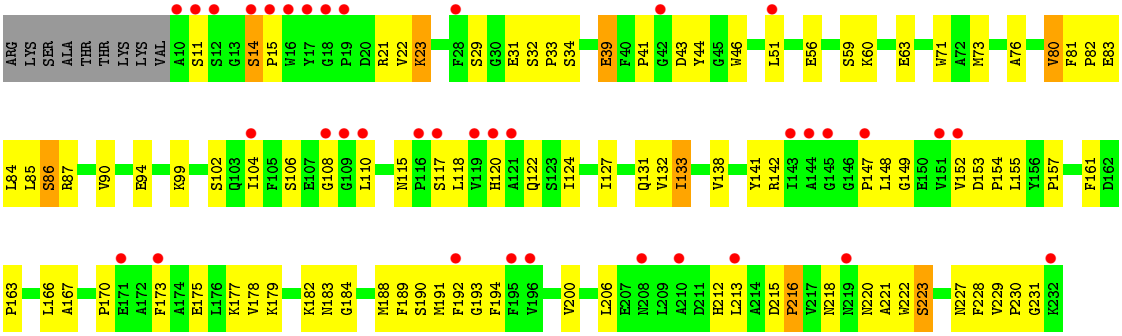
- Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80

Chain B:



- Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80

Chain C:


ARG LYS SER ALA THR THR LYS LYS VAL A10 S11 S12 G13 S14 P15 W16 Y17 G18 P19 D20 R21 V22 K23 F28 S29 G30 E31 S32 P33 S34 E39 F40 P41 G42 D43 Y44 G45 W46 L51 E56 S59 K60 E63 W71 A72 M73 A76 V80 F81 P82 E83
L84 L85 S86 R87 V90 E94 K99 S102 Q103 I104 F105 S106 E107 G108 G109 L110 N115 P116 S117 L118 V119 H120 A121 Q122 S123 I124 I127 Q131 V132 I133 V138 Y141 R142 I143 A144 G145 G146 P147 L148 G149 E150 V151 V152 D153 P154 L155 Y156 P157 F161 D162
P163 L166 A167 P170 E171 A172 F173 A174 E175 L176 K177 V178 K179 K182 N183 G184 M188 F189 S190 M191 F192 G193 F194 F195 V196 V200 L206 E207 N208 L209 A210 D211 H212 L213 A214 D215 P216 V217 N218 N219 N220 A221 W222 S223 N227 F228 V229 P230 G231 K232

4 Data and refinement statistics (i)

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 48.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 85.7 (48.22-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.51Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.220 , 0.241 0.232 , 0.251	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)	0.39 , 103.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, DGD, LUX, XAT, CHL, CLA, NEX

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	0.50	0/1735	0.66	0/2363
1	B	0.53	0/1735	0.69	0/2363
1	C	0.52	0/1735	0.66	0/2363
All	All	0.51	0/5205	0.67	0/7089

There are no bond length outliers.

There are no bond angle outliers.

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	127	0
1	B	1683	0	1601	138	0
1	C	1683	0	1601	135	0
2	A	84	0	134	50	0
2	B	84	0	134	49	0
2	C	84	0	134	50	0
3	A	44	0	56	4	0
3	B	44	0	56	4	0
3	C	44	0	56	4	0
4	A	44	0	56	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	44	0	56	16	0
4	C	44	0	56	16	0
5	A	490	0	508	133	0
5	B	490	0	508	141	0
5	C	490	0	508	131	0
6	A	352	0	338	114	0
6	B	352	0	338	112	0
6	C	352	0	338	114	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	982	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 59.

All (982) 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)
5:A:604:CLA:HMB1	5:A:604:CLA:HBB1	1.22	1.18
5:B:601:CLA:HMB1	5:B:601:CLA:HBB1	1.21	1.18
5:B:604:CLA:HMB1	5:B:604:CLA:HBB1	1.22	1.16
6:B:613:CHL:HBB1	6:B:613:CHL:HMB1	1.27	1.16
6:C:613:CHL:HBB1	6:C:613:CHL:HMB1	1.28	1.16
5:C:604:CLA:HBB1	5:C:604:CLA:HMB1	1.22	1.15
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
5:B:606:CLA:HBB1	5:B:606:CLA:HMB1	1.23	1.12
5:A:601:CLA:HMB1	5:A:601:CLA:HBB1	1.29	1.12
6:A:610:CHL:H92	6:A:612:CHL:H162	1.31	1.12
5:C:602:CLA:H91	5:C:602:CLA:H121	1.21	1.11
6:A:613:CHL:HMB1	6:A:613:CHL:HBB1	1.27	1.11
5:C:607:CLA:H121	5:C:607:CLA:H91	1.26	1.11
5:A:606:CLA:HMB1	5:A:606:CLA:HBB1	1.25	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:603:CLA:HMB1	5:A:603:CLA:HBB1	1.26	1.10
5:C:603:CLA:HMB1	5:C:603:CLA:HBB1	1.28	1.09
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:H121	5:A:602:CLA:H91	1.22	1.08
5:B:607:CLA:H91	5:B:607:CLA:H121	1.30	1.08
5:C:606:CLA:HMB1	5:C:606:CLA:HBB1	1.20	1.08
5:B:603:CLA:HMB1	5:B:603:CLA:HBB1	1.33	1.07
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:C:601:CLA:HBB1	5:C:601:CLA:HMB1	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:H152	6:B:612:CHL:H192	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: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
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
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:H152	6:C:612:CHL:H192	1.42	0.97
1:B:83:GLU:HB3	1:B:206:LEU:HD12	1.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:602:CLA:H121	5:B:602:CLA:C9	1.95	0.94
5:C:602:CLA:C9	5:C:602:CLA:H121	1.97	0.94
6:C:611:CHL:H192	6:C:611:CHL:H151	1.50	0.94
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
6:C:610:CHL:H142	6:C:612:CHL:H72	1.50	0.91
6:A:609:CHL:H62	6:C:610:CHL:H201	1.52	0.91
2:C:502:LUX:C36	5:C:606:CLA:HMB3	2.02	0.90
2:A:502:LUX:C36	5:A:606:CLA:HMB3	2.00	0.90
5:A:602:CLA:H121	5:A:602:CLA:C9	2.00	0.90
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
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
2:B:501:LUX:H373	5:B:603:CLA:C2B	2.02	0.89
2:B:502:LUX:C36	5:B:606:CLA:HMB3	2.02	0.89
6:C:611:CHL:H192	6:C:611:CHL:HAA2	1.54	0.89
1:A:14:SER:HB2	1:A:15:PRO:HD2	1.55	0.88
8:B:802:DGD:O2E	8:B:802:DGD:HD61	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
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:C12	5:A:607:CLA:H91	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
6:B:610:CHL:H201	6:C:609:CHL:H62	1.59	0.85
5:A:602:CLA:HBB1	5:A:602:CLA:HHC	1.59	0.84
1:A:118:LEU:HA	6:A:614:CHL:HED1	1.59	0.84
1:B:163:PRO:HD2	2:B:501:LUX:H3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:606:CLA:CBB	5:C:606:CLA:HMB1	2.07	0.84
1:B:118:LEU:HA	6:B:614:CHL:HED2	1.59	0.84
5:B:602:CLA:HBB1	5:B:602:CLA:HHC	1.59	0.84
6:A:611:CHL:H192	6:A:611:CHL:H151	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:C12	5:C:607:CLA:H91	2.08	0.84
1:C:104:ILE:HD12	1:C:127:ILE:HD12	1.60	0.84
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:118:LEU:HD13	5:C:606:CLA:C12	2.10	0.82
5:B:603:CLA:H92	5:B:608:CLA:HMD1	1.63	0.81
5:A:605:CLA:H191	6:A:612:CHL:H71	1.63	0.81
5:B:605:CLA:C19	6:B:612:CHL:H71	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
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
1:A:118:LEU:HA	6:A:614:CHL:HED2	1.62	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:A:607:CLA:C9	5:A:607:CLA:H121	2.09	0.79
1:A:117:SER:O	6:A:614:CHL:HED2	1.83	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
2:B:502:LUX:H362	5:B:606:CLA:HMB3	1.65	0.78
1:A:192:PHE:CD2	5:A:604:CLA:H18	2.18	0.78
1:A:85:LEU:HB3	1:A:90:VAL:HG21	1.66	0.78
6:A:609:CHL:H172	6:A:609:CHL:H141	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:601:CLA:H122	5:B:601:CLA:C9	2.14	0.78
6:B:611:CHL:HAA2	6:B:611:CHL:H192	1.65	0.78
1:A:213:LEU:HD11	5:A:608:CLA:HMC3	1.65	0.78
5:C:603:CLA:H92	5:C:608:CLA:HMD1	1.64	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
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
6:B:613:CHL:CBB	6:B:613:CHL:HMB1	2.13	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:C:502:LUX:H362	5:C:606:CLA:HMB3	1.66	0.76
2:B:502:LUX:H321	5:B:605:CLA:HMC2	1.66	0.76
4:C:504:XAT:O4	6:C:609:CHL:H192	1.86	0.76
2:C:502:LUX:H111	5:C:604:CLA:HMC2	1.68	0.76
5:C:604:CLA:HBB1	5:C:604:CLA:CMB	2.11	0.76
2:A:502:LUX:H362	5:A:606:CLA:HMB3	1.67	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:A:604:CLA:HBB1	5:A:604:CLA:CMB	2.12	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:HBB1	5:B:608:CLA:HHC	1.69	0.75
1:C:132:VAL:HG12	1:C:133:ILE:CD1	2.16	0.75
5:B:601:CLA:C12	5:B:601:CLA:H92	2.17	0.74
5:A:603:CLA:CHB	5:A:608:CLA:HMD3	2.15	0.74
5:B:601:CLA:CBB	5:B:601:CLA:HMB1	2.06	0.74
5:B:605:CLA:H121	5:B:605:CLA:H92	1.70	0.74
6:B:610:CHL:CBA	1:C:229:VAL:HG22	2.17	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:HBB1	6:C:611:CHL:HHC	1.67	0.74
2:A:502:LUX:H321	5:A:605:CLA:HMC2	1.70	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
2:B:501:LUX:H381	2:B:501:LUX:C28	2.17	0.74
1:B:192:PHE:CD2	5:B:604:CLA:H18	2.22	0.74
6:A:609:CHL:HHD	6:A:609:CHL:HBC2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HBB1	6:B:609:CHL:HHC	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
5:C:603:CLA:CHB	5:C:608:CLA:HMD3	2.19	0.73
4:C:504:XAT:H242	6:C:609:CHL:CMC	2.18	0.73
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
2:A:501:LUX:H122	5:A:601:CLA:HHC	1.72	0.72
1:A:73:MET:HG2	2:A:501:LUX:C35	2.18	0.72
5:A:604:CLA:CBB	5:A:604:CLA:HMB1	2.08	0.72
5:A:606:CLA:HMB1	5:A:606:CLA:CBB	2.11	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
2:A:501:LUX:H381	2:A:501:LUX:C28	2.19	0.71
1:A:122:GLN:HB2	6:A:614:CHL:CBB	2.20	0.71
6:C:609:CHL:H101	6:C:609:CHL:H142	1.72	0.71
6:B:611:CHL:HHC	6:B:611:CHL:HBB1	1.72	0.71
5:A:605:CLA:H92	5:A:605:CLA:H121	1.71	0.71
5:B:603:CLA:H172	5:B:608:CLA:HBA1	1.71	0.71
5:B:602:CLA:C14	5:B:607:CLA:H112	2.19	0.71
5:C:605:CLA:H191	6:C:612:CHL:H71	1.72	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:H142	6:A:609:CHL:H101	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:C9	5:A:607:CLA:C12	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: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:H381	2:C:501:LUX:C28	2.21	0.70
5:C:607:CLA:HBB1	5:C:607:CLA:HHC	1.73	0.70
6:A:609:CHL:C6	6:C:610:CHL:H201	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:605:CLA:HBB1	5:B:605:CLA:HHC	1.74	0.70
6:A:612:CHL:HHC	6:A:612:CHL:HBB1	1.73	0.70
5:B:603:CLA:C9	5:B:608:CLA:HMD1	2.20	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:H122	5:C:601:CLA:C9	2.22	0.69
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:C:142:ARG:NH2	6:C:612:CHL:O1D	2.24	0.69
5:B:607:CLA:C9	5:B:607:CLA:C12	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
5:A:602:CLA:C12	5:A:602:CLA:H91	2.12	0.69
1:A:142:ARG:NH2	6:A:612:CHL:O1D	2.19	0.69
1:C:131:GLN:HE22	6:C:610:CHL:HMC	1.58	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
5:B:606:CLA:HMB1	5:B:606:CLA:CBB	2.09	0.69
3:A:503:NEX:H403	6:A:613:CHL:O1A	1.93	0.68
1:A:86:SER:HA	1:A:90:VAL:O	1.93	0.68
5:B:604:CLA:HMB1	5:B:604:CLA:CBB	2.09	0.68
6:C:609:CHL:HHC	6:C:609:CHL:HBB1	1.75	0.68
5:B:601:CLA:C12	5:B:601:CLA:C9	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:H92	5:C:601:CLA:C12	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:C24	2:B:501:LUX:H363	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
2:C:502:LUX:H321	5:C:605:CLA:HMC2	1.77	0.67
5:B:607:CLA:HHC	5:B:607:CLA:HBB1	1.76	0.67
5:C:607:CLA:C5	5:C:607:CLA:H92	2.24	0.67
1:B:131:GLN:HE22	6:B:610:CHL:HMC	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:C:609:CHL:HHD	6:C:609:CHL:HBC2	1.77	0.67
5:A:601:CLA:H92	5:A:601:CLA:H122	1.77	0.66
5:A:603:CLA:H92	5:A:608:CLA:HMD1	1.77	0.66
6:A:610:CHL:HBB1	6:A:610:CHL:HHC	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
5:B:603:CLA:CHB	5:B:608:CLA:HMD3	2.25	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:HBB1	6:C:612:CHL:HHC	1.77	0.66
1:B:22:VAL:CG2	6:B:609:CHL:HBC3	2.26	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
1:B:142:ARG:NH2	6:B:612:CHL:O1D	2.22	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
6:A:613:CHL:CMB	6:A:613:CHL:HBB1	2.15	0.65
1:B:80:VAL:HG12	1:B:81:PHE:N	2.11	0.65
6:A:609:CHL:HBB1	6:A:609:CHL:HHC	1.78	0.65
5:B:604:CLA:CMB	5:B:604:CLA:HBB1	2.10	0.65
6:B:610:CHL:HBC2	1:C:222:TRP:CH2	2.31	0.65
5:C:608:CLA:HBB1	5:C:608:CLA:HHC	1.77	0.65
6:A:610:CHL:HBA1	1:B:229:VAL:CG2	2.23	0.65
6:B:612:CHL:HBC1	6:B:613:CHL:HBB2	1.78	0.65
3:B:503:NEX:H403	6:B:613:CHL:O1A	1.96	0.65
5:A:607:CLA:H92	5:A:607:CLA:C5	2.25	0.65
1:A:80:VAL:HG12	1:A:81:PHE:N	2.11	0.65
5:B:605:CLA:C9	5:B:605:CLA:C12	2.75	0.65
6:C:612:CHL:C15	6:C:612:CHL:H192	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:610:CHL:C14	6:C:612:CHL:H72	2.26	0.65
2:B:502:LUX:H111	5:B:604:CLA:HMC2	1.79	0.64
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
5:A:602:CLA:HMD2	5:A:607:CLA:C1D	2.27	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
5:A:608:CLA:HHC	5:A:608:CLA:HBB1	1.79	0.64
5:C:603:CLA:C9	5:C:608:CLA:HMD1	2.26	0.64
2:A:502:LUX:H111	5:A:604:CLA:HMC2	1.80	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
5:C:606:CLA:CMB	5:C:606:CLA:HBB1	2.10	0.64
6:C:610:CHL:HBB2	6:C:612:CHL:HBC1	1.78	0.64
5:C:601:CLA:H92	5:C:601:CLA:H122	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
5:C:604:CLA:CBB	5:C:604:CLA:HMB1	2.09	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:HBB1	6:B:610:CHL:HHC	1.80	0.63
4:C:504:XAT:H3	6:C:609:CHL:C19	2.29	0.63
2:A:502:LUX:H361	5:A:606:CLA:HMB3	1.79	0.63
4:B:504:XAT:H371	7:B:801:LHG:H362	1.81	0.63
6:C:610:CHL:HBB1	6:C:610:CHL:HHC	1.80	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
2:B:502:LUX:C24	2:B:502:LUX:H363	2.29	0.62
1:B:94:GLU:HG2	1:B:99:LYS:HB3	1.80	0.62
5:B:605:CLA:C12	5:B:605:CLA:H92	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:N	1:C:133:ILE:HD13	2.15	0.62
5:C:605:CLA:H192	5:C:605:CLA:H152	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:502:LUX:H381	2:C:502:LUX:C28	2.30	0.62
1:C:84:LEU:CD2	5:C:607:CLA:H191	2.30	0.62
1:C:21:ARG:HH11	1:C:21:ARG:HG2	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
1:A:81:PHE:HB3	1:A:82:PRO:CD	2.28	0.61
1:B:94:GLU:HG2	1:B:99:LYS:CB	2.30	0.61
5:C:602:CLA:C12	5:C:602:CLA:C9	2.78	0.61
5:C:605:CLA:C12	5:C:605:CLA:C9	2.78	0.61
5:B:601:CLA:H111	5:B:601:CLA:H162	1.82	0.61
5:C:607:CLA:C12	5:C:607:CLA:C9	2.70	0.61
6:A:611:CHL:C19	6:A:611:CHL:H151	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:603:CLA:HMB1	5:A:603:CLA:CBB	2.13	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:HHD	5:B:608:CLA:HBC2	1.83	0.61
2:A:501:LUX:H281	2:A:501:LUX:H381	1.82	0.61
1:A:222:TRP:HH2	6:C:610:CHL:HBC2	1.63	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
2:C:502:LUX:H361	5:C:606:CLA:HMB3	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
5:A:605:CLA:H192	5:A:605:CLA:H152	1.83	0.60
4:A:504:XAT:H371	7:A:801:LHG:H362	1.84	0.60
5:B:607:CLA:C5	5:B:607:CLA:H92	2.25	0.60
1:B:133:ILE:N	1:B:133:ILE:HD13	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:C:603:CLA:CMB	5:C:603:CLA:HBB1	2.15	0.60
1:C:63:GLU:HA	1:C:155:LEU:HD11	1.81	0.60
1:C:80:VAL:HG12	1:C:81:PHE:N	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ILE:HD12	1:B:127:ILE:CD1	2.28	0.59
1:B:73:MET:CG	2:B:501:LUX:H352	2.23	0.59
2:B:502:LUX:H361	5:B:606:CLA:HMB3	1.82	0.59
5:B:602:CLA:C9	5:B:602:CLA:C12	2.76	0.59
1:B:86:SER:HA	1:B:90:VAL:O	2.03	0.59
5:C:606:CLA:H91	6:C:614:CHL:O2D	2.02	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: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:H142	5:A:604:CLA:H101	1.86	0.58
5:A:603:CLA:H172	5:A:608:CLA:HBA1	1.84	0.58
1:A:22:VAL:CG2	6:A:609:CHL:HBC3	2.33	0.58
6:C:611:CHL:C19	6:C:611:CHL:HAA2	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: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
1:A:84:LEU:CD2	5:A:607:CLA:H191	2.34	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
6:C:610:CHL:H72	6:C:612:CHL:H172	1.86	0.58
5:A:605:CLA:C12	5:A:605:CLA:H92	2.32	0.58
2:B:501:LUX:H281	2:B:501:LUX:H381	1.84	0.58
6:B:609:CHL:HHD	6:B:609:CHL:HBC2	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:C19	6:A:611:CHL:HAA2	2.33	0.57
1:A:133:ILE:N	1:A:133:ILE:HD13	2.18	0.57
1:B:21:ARG:HG2	1:B:21:ARG:HH11	1.68	0.57
5:A:602:CLA:C12	5:A:602:CLA:C9	2.78	0.57
5:B:601:CLA:HBC1	6:B:611:CHL:H201	1.86	0.57
5:B:603:CLA:H172	5:B:608:CLA:CBA	2.35	0.57
2:A:501:LUX:H373	5:A:603:CLA:HMB3	1.85	0.57
5:B:606:CLA:H102	6:B:614:CHL:HED1	1.85	0.57
5:B:601:CLA:CMB	5:B:601:CLA:HBB1	2.12	0.57
1:B:73:MET:HG2	2:B:501:LUX:C15	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:607:CLA:C4C	7:C:801:LHG:HC61	2.35	0.57
1:A:149:GLY:O	6:A:611:CHL:HMC	2.04	0.57
1:A:85:LEU:HB3	1:A:90:VAL:CG2	2.34	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
2:B:502:LUX:C28	2:B:502:LUX:H381	2.35	0.56
2:B:501:LUX:C37	5:B:603:CLA:HMB3	2.34	0.56
2:B:502:LUX:H193	5:B:604:CLA:H141	1.86	0.56
6:A:610:CHL:H201	6:B:609:CHL:H8	1.87	0.56
6:B:610:CHL:H201	6:C:609:CHL:C8	2.34	0.56
5:A:605:CLA:H51	5:B:605:CLA:C4	2.26	0.56
2:B:501:LUX:H101	5:B:601:CLA:H52	1.87	0.56
5:B:602:CLA:HMD2	5:B:607:CLA:C1D	2.35	0.56
2:A:502:LUX:H122	5:A:604:CLA:HHC	1.88	0.56
2:B:501:LUX:H101	5:B:601:CLA:H72	1.86	0.56
1:B:213:LEU:HD11	5:B:608:CLA:HMC3	1.86	0.56
1:B:147:PRO:HG2	6:B:611:CHL:HBB2	1.88	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
2:C:501:LUX:H381	2:C:501:LUX:H281	1.86	0.56
1:C:73:MET:HG2	2:C:501:LUX:C15	2.35	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
5:C:603:CLA:HMB1	5:C:603:CLA:CBB	2.16	0.56
1:C:85:LEU:HB3	1:C:90:VAL:CG2	2.33	0.56
6:A:613:CHL:CBB	6:A:613:CHL:HMB1	2.13	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
5:C:603:CLA:C1B	5:C:608:CLA:HMD3	2.36	0.56
1:A:73:MET:HE2	1:A:183:ASN:C	2.26	0.55
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
2:C:501:LUX:H373	5:C:603:CLA:HMB3	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
1:C:213:LEU:HD11	5:C:608:CLA:HMC3	1.87	0.55
5:A:606:CLA:H91	6:A:614:CHL:O2D	2.06	0.55
1:C:83:GLU:CD	1:C:206:LEU:HB2	2.26	0.55
5:A:603:CLA:C1B	5:A:608:CLA:HMD3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:LUX:H373	5:B:603:CLA:HMB3	1.88	0.55
6:C:613:CHL:CMB	6:C:613:CHL:HBB1	2.16	0.55
6:C:613:CHL:CBB	6:C:613:CHL:HMB1	2.14	0.55
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
6:B:614:CHL:HHC	6:B:614:CHL:HBB1	1.88	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
2:A:501:LUX:C37	5:A:603:CLA:HMB3	2.36	0.54
4:C:504:XAT:H3	6:C:609:CHL:H191	1.89	0.54
6:B:610:CHL:C20	6:C:609:CHL:H8	2.37	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
2:C:501:LUX:C37	5:C:603:CLA:HMB3	2.38	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
1:A:83:GLU:CD	1:A:206:LEU:HB2	2.27	0.53
5:B:606:CLA:H91	6:B:614:CHL:CED	2.38	0.53
5:A:606:CLA:CMB	5:A:606:CLA:HBB1	2.14	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:73:MET:HE1	1:C:184:GLY:N	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:VAL:CG2	6:B:609:CHL:CBC	2.87	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
1:C:220:ASN:CG	5:C:608:CLA:HED1	2.29	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:118:LEU:HD23	6:C:614:CHL:CED	2.40	0.52
1:C:22:VAL:CG2	6:C:609:CHL:CBC	2.87	0.52
6:C:611:CHL:H192	6:C:611:CHL:CAA	2.34	0.52
5:A:604:CLA:HBC3	5:A:604:CLA:HMC1	1.92	0.52
6:B:609:CHL:C14	6:B:609:CHL:H172	2.35	0.52
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:C14	6:A:609:CHL:H172	2.38	0.52
1:B:81:PHE:HB3	1:B:82:PRO:CD	2.37	0.52
6:B:610:CHL:H203	6:C:609:CHL:H101	1.91	0.52
6:C:609:CHL:H142	6:C:609:CHL:C10	2.38	0.52
5:C:606:CLA:H91	6:C:614:CHL:CED	2.40	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:HHD	5:C:608:CLA:HBC2	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:C:73:MET:HE3	1:C:183:ASN:C	2.30	0.52
5:A:606:CLA:H102	6:A:614:CHL:HED1	1.92	0.51
2:A:501:LUX:H282	2:A:501:LUX:H381	1.91	0.51
6:A:609:CHL:H142	6:A:609:CHL:C10	2.39	0.51
6:A:614:CHL:HBB1	6:A:614:CHL:HHC	1.92	0.51
4:A:504:XAT:H403	7:A:801:LHG:H121	1.92	0.51
2:A:502:LUX:C20	5:A:604:CLA:H202	2.41	0.51
1:A:118:LEU:HD23	6:A:614:CHL:CED	2.40	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
1:B:73:MET:HE3	1:B:183:ASN:C	2.30	0.51
5:C:604:CLA:HBC3	5:C:604:CLA:HMC1	1.92	0.51
6:B:610:CHL:H201	6:C:609:CHL:C7	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:501:LUX:H111	5:B:601:CLA:HMC2	1.91	0.51
1:C:73:MET:CE	1:C:183:ASN:CB	2.89	0.51
1:A:118:LEU:O	1:A:120:HIS:N	2.38	0.51
1:A:56:GLU:O	1:A:60:LYS:HG2	2.10	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:C15	6:C:611:CHL:C19	2.84	0.51
5:B:603:CLA:C1B	5:B:608:CLA:HMD3	2.40	0.51
5:B:608:CLA:CHD	5:B:608:CLA:HBC2	2.41	0.51
6:A:610:CHL:H201	6:B:609:CHL:C8	2.40	0.51
6:A:609:CHL:CHD	6:A:609:CHL:HBC2	2.40	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:73:MET:HE3	1:A:184:GLY:N	2.26	0.50
1:A:189:PHE:HE1	6:A:609:CHL:HED2	1.75	0.50
1:A:215:ASP:CG	1:A:218:ASN:HD22	2.15	0.50
1:A:212:HIS:O	1:A:216:PRO:N	2.44	0.50
1:A:182:LYS:HE2	5:A:607:CLA:O1D	2.12	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
1:A:120:HIS:HD2	6:A:614:CHL:HMB3	1.77	0.50
6:A:609:CHL:C7	6:C:610:CHL:H201	2.41	0.50
1:B:115:ASN:HB3	1:B:118:LEU:CD1	2.41	0.50
1:B:22:VAL:HG21	6:B:609:CHL:HBC1	1.94	0.50
5:B:603:CLA:CMB	5:B:603:CLA:HBB1	2.21	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:A:179:LYS:HD3	5:A:602:CLA:HAA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:610:CHL:H203	6:B:609:CHL:H101	1.93	0.50
1:B:83:GLU:CD	1:B:206:LEU:HB2	2.33	0.50
1:C:220:ASN:O	1:C:223:SER:OG	2.29	0.50
1:C:192:PHE:CZ	5:C:604:CLA:H171	2.47	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: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:H122	5:C:605:CLA:C9	2.42	0.49
1:A:133:ILE:N	1:A:133:ILE:CD1	2.75	0.49
1:C:147:PRO:CG	6:C:611:CHL:HBB2	2.42	0.49
1:C:21:ARG:HD2	1:C:43:ASP:O	2.11	0.49
1:A:148:LEU:HD12	1:A:161:PHE:CZ	2.47	0.49
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: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:120:HIS:HD2	6:C:614:CHL:HMB3	1.76	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:HG3	1:B:39:GLU:O	2.12	0.49
6:B:610:CHL:H172	6:B:610:CHL:H141	1.93	0.49
1:C:229:VAL:HG12	1:C:230:PRO:O	2.12	0.49
2:C:501:LUX:H111	5:C:601:CLA:HMC2	1.94	0.49
1:C:194:PHE:CE1	2:C:501:LUX:H383	2.46	0.49
1:C:191:MET:HG2	2:C:502:LUX:H322	1.93	0.49
5:C:601:CLA:H92	5:C:601:CLA:H121	1.94	0.49
5:A:601:CLA:H121	5:A:601:CLA:H92	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:N	1:C:133:ILE:CD1	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
5:A:603:CLA:C9	5:A:608:CLA:HMD1	2.41	0.49
6:A:611:CHL:CAA	6:A:611:CHL:C19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:B:604:CLA:C14	5:B:604:CLA:H101	2.42	0.48
3:C:503:NEX:H35	3:C:503:NEX:H401	1.58	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
1:B:147:PRO:HB2	6:B:611:CHL:HBB2	1.94	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:HBA1	5:B:606:CLA:CHA	2.38	0.48
6:C:610:CHL:H142	6:C:612:CHL:C7	2.35	0.48
1:C:83:GLU:O	1:C:87:ARG:HG3	2.13	0.48
1:A:73:MET:CE	1:A:184:GLY:N	2.76	0.48
1:C:104:ILE:HD12	1:C:127:ILE:CD1	2.39	0.48
6:C:611:CHL:OMC	6:C:611:CHL:HHC	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
2:B:501:LUX:C37	5:B:603:CLA:CMB	2.89	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
5:B:607:CLA:H121	5:B:607:CLA:C9	2.09	0.48
1:B:182:LYS:NZ	7:B:801:LHG:O4	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
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
6:C:611:CHL:H162	6:C:611:CHL:H141	1.64	0.47
5:A:601:CLA:H91	5:A:601:CLA:H122	1.94	0.47
2:B:501:LUX:H372	2:B:501:LUX:H27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:44:TYR:HB2	5:B:604:CLA:HMD1	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
1:A:227:ASN:O	1:A:228:PHE:HB2	2.15	0.47
6:A:611:CHL:OMC	6:A:611:CHL:HHC	2.15	0.47
1:B:192:PHE:CD2	5:B:604:CLA:H171	2.50	0.47
1:C:73:MET:CE	1:C:184:GLY:N	2.78	0.47
2:C:502:LUX:H381	2:C:502:LUX:H281	1.95	0.47
2:A:501:LUX:H102	5:A:601:CLA:CHC	2.45	0.47
1:C:39:GLU:O	1:C:39:GLU:HG3	2.14	0.47
1:C:46:TRP:CZ2	6:C:609:CHL:HBA2	2.49	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
1:B:215:ASP:CG	1:B:218:ASN:HD22	2.18	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
6:A:609:CHL:H101	6:C:610:CHL:H203	1.97	0.47
1:B:161:PHE:O	2:B:501:LUX:H4C2	2.15	0.47
5:A:603:CLA:CMB	5:A:603:CLA:HBB1	2.14	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:H281	2:A:502:LUX:H381	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:H61	6:C:611:CHL:H2	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
5:A:601:CLA:HMB1	5:A:601:CLA:CBB	2.16	0.46
5:B:603:CLA:HMB1	5:B:603:CLA:CBB	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:613:CHL:HBB1	6:B:613:CHL:CMB	2.16	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
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:HBA1	5:C:606:CLA:CHA	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
1:A:73:MET:CE	1:A:183:ASN:CB	2.94	0.46
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
4:B:504:XAT:H34	5:B:603:CLA:H122	1.98	0.46
1:B:84:LEU:HD23	5:B:607:CLA:H191	1.98	0.46
1:B:63:GLU:O	1:B:67:ILE:HG12	2.16	0.46
1:B:73:MET:HE1	1:B:184:GLY:N	2.31	0.46
5:A:607:CLA:C4C	7:A:801:LHG:HC61	2.46	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
5:B:605:CLA:H12	1:C:51:LEU:HD21	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:73:MET:HE2	1:C:183:ASN:HB2	1.99	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
6:C:609:CHL:CHD	6:C:609:CHL:HBC2	2.46	0.45
1:A:190:SER:OG	2:A:501:LUX:H392	2.15	0.45
3:A:503:NEX:H35	3:A:503:NEX:H401	1.70	0.45
5:A:603:CLA:C1A	5:A:603:CLA:CGA	2.94	0.45
1:B:128:TRP:NE1	4:C:504:XAT:C20	2.78	0.45
2:C:502:LUX:H282	2:C:502:LUX:H381	1.99	0.45
5:C:607:CLA:C9	5:C:607:CLA:H52	2.36	0.45
6:A:609:CHL:HED3	7:A:801:LHG:H142	1.99	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
1:C:215:ASP:CG	1:C:218:ASN:HD22	2.19	0.45
5:C:605:CLA:H191	6:C:612:CHL:H51	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:120:HIS:HD2	6:B:614:CHL:HMB3	1.81	0.45
3:B:503:NEX:H401	3:B:503:NEX:H35	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
5:C:608:CLA:CHD	5:C:608:CLA:HBC2	2.47	0.45
1:B:132:VAL:HG12	1:B:133:ILE:N	2.32	0.45
6:A:610:CHL:C20	6:B:609:CHL:H62	2.33	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:H282	2:C:501:LUX:H381	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
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
4:C:504:XAT:H11	4:C:504:XAT:H191	1.81	0.45
3:C:503:NEX:H371	6:C:611:CHL:H171	1.98	0.45
5:A:601:CLA:O1A	5:A:601:CLA:H3A	2.17	0.45
4:B:504:XAT:C37	7:B:801:LHG:H362	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:603:CLA:H18	5:B:608:CLA:ND	2.33	0.44
5:C:605:CLA:HMD3	6:C:610:CHL:H192	1.98	0.44
1:A:21:ARG:HD3	1:A:38:GLY:HA3	1.99	0.44
1:B:141:TYR:HA	1:B:145:GLY:O	2.17	0.44
4:A:504:XAT:H201	4:A:504:XAT:H15	1.75	0.44
4:A:504:XAT:H35	4:A:504:XAT:H401	1.63	0.44
1:A:192:PHE:CZ	5:A:604:CLA:H171	2.50	0.44
1:B:138:VAL:HA	1:B:141:TYR:CD1	2.52	0.44
1:B:73:MET:CE	1:B:184:GLY:N	2.80	0.44
1:B:73:MET:HG2	2:B:501:LUX:C14	2.47	0.44
2:C:502:LUX:H27	2:C:502:LUX:H372	1.34	0.44
1:A:21:ARG:HH11	1:A:21:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C19	6:A:612:CHL:H152	2.27	0.44
1:B:192:PHE:CD2	5:B:604:CLA:C18	2.96	0.44
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.82	0.44
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: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:C:166:LEU:CD1	2:C:501:LUX:H173	2.48	0.44
1:A:191:MET:O	1:A:194:PHE:HB2	2.18	0.44
1:B:169:ASP:HA	1:B:170:PRO:HD3	1.82	0.44
5:A:605:CLA:H12	1:B:51:LEU:HD21	1.99	0.44
1:C:44:TYR:HB2	5:C:604:CLA:HMD1	1.99	0.44
6:C:610:CHL:H141	6:C:610:CHL:H172	2.00	0.44
1:A:44:TYR:HB2	5:A:604:CLA:HMD1	1.98	0.44
6:A:609:CHL:C10	6:C:610:CHL:H203	2.48	0.44
2:B:502:LUX:H281	2:B:502:LUX:H381	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
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:501:LUX:H111	5:A:601:CLA:HMC2	1.99	0.43
2:A:502:LUX:H282	2:A:502:LUX:H381	2.00	0.43
5:A:601:CLA:CMB	5:A:601:CLA:HBB1	2.17	0.43
2:B:502:LUX:H122	5:B:604:CLA:HAB	1.99	0.43
1:C:161:PHE:C	1:C:163:PRO:HD3	2.38	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:A:98:PHE:HB2	6:A:610:CHL:HMA2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:612:CHL:C15	6:C:612:CHL:C19	2.91	0.43
5:A:606:CLA:H112	5:A:606:CLA:H61	2.00	0.43
1:A:147:PRO:CG	6:A:611:CHL:HBB2	2.48	0.43
7:A:801:LHG:H242	7:A:801:LHG:HC62	1.77	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
1:B:128:TRP:HE1	4:C:504:XAT:C20	2.31	0.43
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
1:C:71:TRP:CD1	6:C:612:CHL:HMD3	2.54	0.43
1:A:161:PHE:C	1:A:163:PRO:HD3	2.39	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
1:B:220:ASN:CG	5:B:608:CLA:HED1	2.38	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
3:C:503:NEX:C35	6:C:611:CHL:HMB3	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
6:A:610:CHL:HMB1	6:A:610:CHL:HAB	1.85	0.43
4:B:504:XAT:H15	4:B:504:XAT:H201	1.62	0.43
1:B:94:GLU:HG2	1:B:99:LYS:HB2	2.01	0.43
5:C:601:CLA:CBB	5:C:601:CLA:HMB1	2.21	0.43
5:C:607:CLA:C9	5:C:607:CLA:C5	2.93	0.43
1:A:166:LEU:CD1	2:A:501:LUX:H173	2.49	0.43
1:A:66:VAL:HB	1:A:155:LEU:HD13	2.00	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
2:A:502:LUX:H162	2:A:502:LUX:H3	1.69	0.42
1:A:142:ARG:HG3	6:A:611:CHL:C1D	2.50	0.42
6:A:611:CHL:H52	6:A:611:CHL:H8	1.41	0.42
6:A:610:CHL:C20	6:B:609:CHL:C8	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PRO:HD2	5:C:601:CLA:OBD	2.18	0.42
8:B:802:DGD:C1E	1:C:231:GLY:H	2.32	0.42
1:C:76:ALA:N	1:C:191:MET:HE1	2.34	0.42
1:A:138:VAL:HG23	9:A:2003:HOH:O	2.20	0.42
3:A:503:NEX:C35	6:A:611:CHL:HMB3	2.49	0.42
5:B:606:CLA:C10	6:B:614:CHL:HED1	2.47	0.42
1:B:71:TRP:CD1	6:B:611:CHL:HED2	2.54	0.42
1:C:213:LEU:HD21	5:C:608:CLA:HHC	2.02	0.42
5:C:602:CLA:HMD2	5:C:607:CLA:C1D	2.48	0.42
6:C:609:CHL:H172	6:C:609:CHL:C14	2.43	0.42
4:C:504:XAT:H15	4:C:504:XAT:H201	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
6:A:612:CHL:HAB	6:A:612:CHL:HMB1	1.89	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
5:B:605:CLA:H91	5:B:605:CLA:H122	2.01	0.42
1:C:115:ASN:HB3	1:C:118:LEU:CG	2.50	0.42
1:C:15:PRO:O	1:C:22:VAL:HG12	2.19	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
1:A:192:PHE:HD2	5:A:603:CLA:HMC1	1.84	0.42
5:A:603:CLA:H161	5:A:608:CLA:C3D	2.49	0.42
5:A:605:CLA:C9	5:A:605:CLA:H121	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
5:A:605:CLA:HMB1	5:A:605:CLA:HAB	1.88	0.42
5:A:606:CLA:HMC1	5:A:606:CLA:HBC3	2.01	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:73:MET:HE1	1:A:183:ASN:HB2	2.02	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: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
1:B:19:PRO:CD	1:B:20:ASP:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TRP:NE1	4:B:504:XAT:C20	2.83	0.41
5:B:601:CLA:H122	5:B:601:CLA:H161	1.88	0.41
6:B:611:CHL:CAA	6:B:611:CHL:H192	2.43	0.41
5:C:604:CLA:CGA	5:C:604:CLA:H3A	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
6:B:614:CHL:HAB	6:B:614:CHL:HMB1	1.89	0.41
2:C:501:LUX:H312	5:C:602:CLA:HMC2	2.01	0.41
5:C:601:CLA:C3A	5:C:601:CLA:CGA	2.98	0.41
1:B:192:PHE:HD2	5:B:603:CLA:HMC1	1.86	0.41
5:B:603:CLA:H61	5:B:603:CLA:H2	1.85	0.41
8:C:802:DGD:HB52	8:C:802:DGD:HB21	1.91	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
6:A:609:CHL:C8	6:C:610:CHL:C20	2.98	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
2:B:501:LUX:H371	2:B:501:LUX:H271	1.68	0.41
5:B:603:CLA:C9	5:B:608:CLA:CMD	2.96	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:O	1:C:104:ILE:HG12	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
5:A:606:CLA:H93	6:A:614:CHL:OBD	2.21	0.41
3:B:503:NEX:C35	6:B:611:CHL:HMB3	2.51	0.41
6:B:611:CHL:C19	6:B:611:CHL:CAA	2.99	0.41
6:B:611:CHL:CHA	6:B:611:CHL:HBA2	2.51	0.41
6:B:612:CHL:HAB	6:B:612:CHL:HMB1	1.92	0.41
5:C:606:CLA:H61	5:C:606:CLA:H112	2.03	0.41
1:A:115:ASN:HB3	1:A:118:LEU:HG	2.01	0.41
5:A:608:CLA:HBC2	5:A:608:CLA:HHD	2.02	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
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:A:64:LEU:HD13	5:A:605:CLA:CAA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:501:LUX:H312	5:A:602:CLA:HMC2	2.04	0.40
5:A:608:CLA:HMB1	5:A:608:CLA:HAB	1.92	0.40
1:C:192:PHE:HD2	5:C:603:CLA:HMC1	1.85	0.40
6:C:611:CHL:HBA2	6:C:611:CHL:CHA	2.51	0.40
1:A:141:TYR:HA	1:A:145:GLY:O	2.21	0.40
1:A:15:PRO:O	1:A:22:VAL:HG12	2.21	0.40
4:A:504:XAT:C5	6:A:609:CHL:H192	2.51	0.40
5:C:605:CLA:H91	5:C:605:CLA:H122	2.03	0.40
1:A:157:PRO:HD3	6:A:611:CHL:HMD2	2.03	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:C1A	5:B:603:CLA:CGA	2.99	0.40
1:C:132:VAL:HG12	1:C:133:ILE:N	2.35	0.40
5:C:601:CLA:O1D	5:C:601:CLA:H2A	2.21	0.40
1:C:118:LEU:CD2	6:C:614:CHL:CED	3.00	0.40
5:A:607:CLA:HMB1	5:A:607:CLA:HAB	1.92	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
7:C:801:LHG:H312	7:C:801:LHG:H282	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	221/232 (95%)	210 (95%)	10 (4%)	1 (0%)	29 48
1	B	221/232 (95%)	210 (95%)	9 (4%)	2 (1%)	17 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	221/232 (95%)	208 (94%)	10 (4%)	3 (1%)	11 20
All	All	663/696 (95%)	628 (95%)	29 (4%)	6 (1%)	17 31

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%)	154 (91%)	15 (9%)	9 19
1	B	169/181 (93%)	150 (89%)	19 (11%)	6 11
1	C	169/181 (93%)	155 (92%)	14 (8%)	11 22
All	All	507/543 (93%)	459 (90%)	48 (10%)	8 17

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	23	LYS
1	A	31	GLU
1	A	39	GLU
1	A	48	THR
1	A	59	SER
1	A	80	VAL
1	A	86	SER
1	A	103	GLN

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Mol	Chain	Res	Type
1	A	106	SER
1	A	110	LEU
1	A	133	ILE
1	A	152	VAL
1	A	175	GLU
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	79	SER
1	B	80	VAL
1	B	86	SER
1	B	103	GLN
1	B	106	SER
1	B	110	LEU
1	B	133	ILE
1	B	143	ILE
1	B	152	VAL
1	B	175	GLU
1	B	223	SER
1	C	11	SER
1	C	23	LYS
1	C	31	GLU
1	C	34	SER
1	C	39	GLU
1	C	59	SER
1	C	80	VAL
1	C	86	SER
1	C	106	SER
1	C	110	LEU
1	C	133	ILE
1	C	152	VAL
1	C	175	GLU
1	C	223	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
8	DGD	C	802	-	39,39,67	1.41	5 (12%)	51,51,81	1.97	9 (17%)
2	LUX	A	502	-	43,43,43	4.59	26 (60%)	53,60,60	3.70	32 (60%)

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	1.71	6 (12%)	51,54,54	1.35	4 (7%)
7	LHG	C	801	5	48,48,48	1.68	6 (12%)	51,54,54	1.33	4 (7%)
5	CLA	B	604	1	59,73,73	1.48	10 (16%)	67,113,113	1.80	16 (23%)
5	CLA	A	608	1	42,56,73	1.75	9 (21%)	46,92,113	2.24	14 (30%)
6	CHL	C	613	-	37,54,74	1.70	7 (18%)	36,90,114	2.22	10 (27%)
5	CLA	C	604	1	59,73,73	1.27	9 (15%)	67,113,113	1.88	13 (19%)
3	NEX	C	503	-	38,46,46	2.25	8 (21%)	50,70,70	2.54	14 (28%)
5	CLA	B	601	1	59,73,73	1.35	12 (20%)	67,113,113	1.89	18 (26%)
2	LUX	B	502	-	43,43,43	4.65	25 (58%)	53,60,60	3.78	31 (58%)
5	CLA	B	606	-	51,65,73	1.35	10 (19%)	57,103,113	1.98	15 (26%)
5	CLA	B	608	1	42,56,73	1.61	9 (21%)	46,92,113	2.00	13 (28%)
5	CLA	B	607	7	59,73,73	1.60	10 (16%)	67,113,113	1.98	12 (17%)
5	CLA	A	601	1	59,73,73	1.30	8 (13%)	67,113,113	1.97	15 (22%)
6	CHL	C	614	1	36,50,74	2.01	9 (25%)	35,85,114	2.49	10 (28%)
6	CHL	A	610	9	60,74,74	1.59	12 (20%)	64,114,114	1.64	12 (18%)
6	CHL	B	614	1	36,50,74	1.98	9 (25%)	35,85,114	2.57	11 (31%)
6	CHL	C	609	1	60,74,74	1.56	9 (15%)	64,114,114	1.77	12 (18%)
5	CLA	C	603	1	59,73,73	1.25	8 (13%)	67,113,113	1.84	12 (17%)
5	CLA	A	607	7	59,73,73	1.54	10 (16%)	67,113,113	1.94	11 (16%)
6	CHL	C	612	1	60,74,74	1.65	12 (20%)	64,114,114	1.97	14 (21%)
5	CLA	C	607	7	59,73,73	1.47	11 (18%)	67,113,113	1.91	12 (17%)
4	XAT	C	504	-	39,47,47	2.20	13 (33%)	54,74,74	2.64	21 (38%)
5	CLA	C	606	-	51,65,73	1.39	8 (15%)	57,103,113	2.00	15 (26%)
6	CHL	A	614	1	36,50,74	1.89	8 (22%)	35,85,114	2.41	11 (31%)
3	NEX	A	503	-	38,46,46	2.32	11 (28%)	50,70,70	2.39	11 (22%)
4	XAT	B	504	-	39,47,47	2.20	14 (35%)	54,74,74	2.85	21 (38%)
5	CLA	B	605	1	59,73,73	1.42	11 (18%)	67,113,113	1.88	12 (17%)
8	DGD	A	802	-	39,39,67	1.32	4 (10%)	51,51,81	1.95	9 (17%)
3	NEX	B	503	-	38,46,46	2.40	10 (26%)	50,70,70	2.53	12 (24%)
5	CLA	C	605	1	59,73,73	1.37	10 (16%)	67,113,113	1.91	12 (17%)
6	CHL	C	610	9	60,74,74	1.62	12 (20%)	64,114,114	1.72	12 (18%)
2	LUX	A	501	-	43,43,43	4.65	26 (60%)	53,60,60	3.53	30 (56%)
2	LUX	B	501	-	43,43,43	4.71	25 (58%)	53,60,60	3.60	31 (58%)
6	CHL	A	609	1	60,74,74	1.48	10 (16%)	64,114,114	1.76	13 (20%)
5	CLA	C	602	1	54,68,73	1.53	10 (18%)	61,107,113	1.84	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CHL	B	610	9	60,74,74	1.62	10 (16%)	64,114,114	1.70	14 (21%)
5	CLA	B	602	1	54,68,73	1.57	11 (20%)	61,107,113	1.94	11 (18%)
4	XAT	A	504	-	39,47,47	2.21	15 (38%)	54,74,74	2.85	20 (37%)
5	CLA	B	603	1	59,73,73	1.33	8 (13%)	67,113,113	1.88	13 (19%)
6	CHL	B	611	9	60,74,74	1.52	10 (16%)	64,114,114	1.98	12 (18%)
5	CLA	A	603	1	59,73,73	1.27	9 (15%)	67,113,113	1.86	13 (19%)
6	CHL	B	609	1	60,74,74	1.56	9 (15%)	64,114,114	1.75	13 (20%)
2	LUX	C	502	-	43,43,43	4.52	26 (60%)	53,60,60	3.75	32 (60%)
5	CLA	A	605	1	59,73,73	1.37	9 (15%)	67,113,113	1.91	14 (20%)
6	CHL	A	613	-	37,54,74	1.82	8 (21%)	36,90,114	2.08	10 (27%)
5	CLA	A	604	1	59,73,73	1.36	7 (11%)	67,113,113	1.76	13 (19%)
6	CHL	A	611	9	60,74,74	1.48	11 (18%)	64,114,114	2.03	15 (23%)
5	CLA	C	601	1	59,73,73	1.34	7 (11%)	67,113,113	2.03	13 (19%)
6	CHL	B	613	-	37,54,74	1.68	8 (21%)	36,90,114	2.09	10 (27%)
6	CHL	A	612	1	60,74,74	1.55	11 (18%)	64,114,114	1.99	13 (20%)
6	CHL	B	612	1	60,74,74	1.53	12 (20%)	64,114,114	1.88	12 (18%)
5	CLA	C	608	1	42,56,73	1.53	8 (19%)	46,92,113	2.27	13 (28%)
7	LHG	B	801	5	48,48,48	1.66	6 (12%)	51,54,54	1.37	4 (7%)
6	CHL	C	611	9	60,74,74	1.51	11 (18%)	64,114,114	1.98	15 (23%)
5	CLA	A	602	1	54,68,73	1.42	8 (14%)	61,107,113	1.82	11 (18%)
5	CLA	A	606	-	51,65,73	1.32	7 (13%)	57,103,113	2.01	14 (24%)
2	LUX	C	501	-	43,43,43	4.65	25 (58%)	53,60,60	3.60	31 (58%)
8	DGD	B	802	-	39,39,67	1.32	4 (10%)	51,51,81	1.93	10 (19%)

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
8	DGD	C	802	-	1/1/11/13	16/24/64/95	0/2/2/2
2	LUX	A	502	-	5/5/12/15	10/29/67/67	0/2/2/2
7	LHG	A	801	5	-	22/53/53/53	-
7	LHG	C	801	5	-	22/53/53/53	-
5	CLA	B	604	1	4/4/20/25	12/37/135/135	-
5	CLA	A	608	1	3/3/16/25	6/17/115/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CHL	C	613	-	3/3/16/26	0/13/113/137	-
5	CLA	C	604	1	4/4/20/25	15/37/135/135	-
6	CHL	B	610	9	4/4/20/26	14/39/137/137	-
5	CLA	B	601	1	4/4/20/25	12/37/135/135	-
2	LUX	B	502	-	5/5/12/15	11/29/67/67	0/2/2/2
5	CLA	B	606	-	4/4/18/25	10/28/126/135	-
5	CLA	B	608	1	3/3/16/25	7/17/115/135	-
5	CLA	B	607	7	3/3/20/25	16/37/135/135	-
5	CLA	A	601	1	4/4/20/25	12/37/135/135	-
6	CHL	C	614	1	3/3/15/26	1/10/108/137	-
6	CHL	A	610	9	4/4/20/26	14/39/137/137	-
6	CHL	B	614	1	3/3/15/26	0/10/108/137	-
6	CHL	C	609	1	4/4/20/26	15/39/137/137	-
5	CLA	C	603	1	4/4/20/25	12/37/135/135	-
5	CLA	A	607	7	3/3/20/25	16/37/135/135	-
6	CHL	C	612	1	3/3/20/26	16/39/137/137	-
5	CLA	C	607	7	3/3/20/25	15/37/135/135	-
4	XAT	C	504	-	2/2/12/26	2/31/93/93	0/4/4/4
5	CLA	C	606	-	4/4/18/25	10/28/126/135	-
3	NEX	C	503	-	-	2/27/83/83	0/3/3/3
6	CHL	A	614	1	3/3/15/26	0/10/108/137	-
6	CHL	A	611	9	4/4/20/26	16/39/137/137	-
4	XAT	B	504	-	2/2/12/26	2/31/93/93	0/4/4/4
5	CLA	B	605	1	4/4/20/25	11/37/135/135	-
8	DGD	A	802	-	1/1/11/13	16/24/64/95	0/2/2/2
3	NEX	B	503	-	-	2/27/83/83	0/3/3/3
5	CLA	C	605	1	4/4/20/25	11/37/135/135	-
6	CHL	C	610	9	4/4/20/26	14/39/137/137	-
2	LUX	A	501	-	5/5/12/15	11/29/67/67	0/2/2/2
2	LUX	B	501	-	5/5/12/15	11/29/67/67	0/2/2/2
6	CHL	A	609	1	4/4/20/26	18/39/137/137	-
5	CLA	C	602	1	3/3/19/25	13/31/129/135	-
5	CLA	A	603	1	4/4/20/25	13/37/135/135	-
5	CLA	B	602	1	3/3/19/25	13/31/129/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XAT	A	504	-	2/2/12/26	0/31/93/93	0/4/4/4
5	CLA	B	603	1	4/4/20/25	12/37/135/135	-
6	CHL	B	611	9	4/4/20/26	17/39/137/137	-
6	CHL	B	609	1	4/4/20/26	16/39/137/137	-
2	LUX	C	502	-	5/5/12/15	10/29/67/67	0/2/2/2
5	CLA	A	605	1	4/4/20/25	11/37/135/135	-
6	CHL	A	613	-	3/3/16/26	0/13/113/137	-
5	CLA	A	604	1	4/4/20/25	12/37/135/135	-
3	NEX	A	503	-	-	2/27/83/83	0/3/3/3
5	CLA	C	601	1	4/4/20/25	13/37/135/135	-
6	CHL	B	613	-	3/3/16/26	0/13/113/137	-
6	CHL	A	612	1	3/3/20/26	16/39/137/137	-
6	CHL	B	612	1	3/3/20/26	14/39/137/137	-
5	CLA	C	608	1	3/3/16/25	6/17/115/135	-
7	LHG	B	801	5	-	22/53/53/53	-
6	CHL	C	611	9	4/4/20/26	16/39/137/137	-
5	CLA	A	602	1	3/3/19/25	13/31/129/135	-
5	CLA	A	606	-	4/4/18/25	9/28/126/135	-
2	LUX	C	501	-	5/5/12/15	11/29/67/67	0/2/2/2
8	DGD	B	802	-	1/1/11/13	17/24/64/95	0/2/2/2

All (652) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	LUX	C24-C25	19.56	1.57	1.33
2	B	502	LUX	C24-C25	18.51	1.56	1.33
2	A	501	LUX	C24-C25	18.34	1.56	1.33
2	B	501	LUX	C24-C25	18.20	1.55	1.33
2	A	502	LUX	C24-C25	18.19	1.55	1.33
2	C	502	LUX	C24-C25	17.42	1.54	1.33
2	B	501	LUX	C21-C26	-14.54	1.41	1.55
2	A	501	LUX	C21-C26	-13.75	1.42	1.55
2	C	501	LUX	C21-C26	-13.14	1.42	1.55
2	A	502	LUX	C21-C26	-13.04	1.42	1.55
2	B	502	LUX	C21-C26	-12.80	1.42	1.55
2	C	502	LUX	C21-C26	-12.01	1.43	1.55
3	B	503	NEX	O24-C25	-8.29	1.34	1.46
3	C	503	NEX	O24-C25	-7.79	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	NEX	O24-C25	-7.67	1.35	1.46
7	A	801	LHG	P-O5	7.51	1.77	1.50
7	C	801	LHG	P-O5	7.31	1.76	1.50
7	B	801	LHG	P-O5	7.24	1.76	1.50
2	B	501	LUX	C27-C26	-7.04	1.38	1.54
2	B	502	LUX	C5-C6	6.93	1.46	1.34
2	B	502	LUX	C28-C27	-6.89	1.33	1.53
2	C	502	LUX	C27-C26	-6.83	1.38	1.54
4	C	504	XAT	O24-C25	-6.68	1.36	1.46
2	A	502	LUX	C27-C26	-6.58	1.39	1.54
4	A	504	XAT	O24-C25	-6.57	1.36	1.46
4	B	504	XAT	O24-C25	-6.54	1.36	1.46
2	A	502	LUX	C5-C6	6.50	1.45	1.34
2	A	501	LUX	C28-C27	-6.38	1.34	1.53
2	B	501	LUX	C5-C6	6.37	1.45	1.34
2	B	502	LUX	C10-C9	-6.31	1.35	1.54
3	B	503	NEX	C12-C13	-6.25	1.32	1.45
2	A	502	LUX	C10-C9	-6.20	1.35	1.54
2	C	502	LUX	C5-C6	6.19	1.45	1.34
2	C	501	LUX	C5-C6	6.16	1.45	1.34
5	B	607	CLA	MG-NA	6.15	2.20	2.06
2	A	502	LUX	C28-C27	-6.08	1.35	1.53
2	C	502	LUX	C28-C27	-6.07	1.35	1.53
2	B	502	LUX	C27-C26	-6.06	1.40	1.54
2	C	502	LUX	C10-C9	-6.03	1.35	1.54
3	A	503	NEX	C12-C13	-6.02	1.33	1.45
2	A	501	LUX	C10-C9	-6.01	1.35	1.54
5	A	607	CLA	MG-NA	5.95	2.20	2.06
6	C	612	CHL	CMC-C2C	5.92	1.57	1.45
2	B	501	LUX	C10-C9	-5.90	1.36	1.54
6	C	614	CHL	CMC-C2C	5.81	1.57	1.45
6	C	609	CHL	CMC-C2C	5.76	1.57	1.45
2	B	501	LUX	C26-C25	-5.73	1.34	1.52
2	A	501	LUX	C27-C26	-5.73	1.41	1.54
2	C	501	LUX	C10-C9	-5.72	1.36	1.54
2	B	501	LUX	C28-C27	-5.70	1.36	1.53
6	A	613	CHL	CMC-C2C	5.67	1.57	1.45
6	B	609	CHL	CMC-C2C	5.65	1.57	1.45
6	B	612	CHL	CMC-C2C	5.60	1.57	1.45
2	B	502	LUX	C26-C25	-5.55	1.34	1.52
2	C	502	LUX	C26-C25	-5.53	1.34	1.52
6	B	613	CHL	CMC-C2C	5.50	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LUX	C5-C6	5.49	1.43	1.34
6	A	610	CHL	CMC-C2C	5.47	1.56	1.45
3	C	503	NEX	C12-C13	-5.46	1.34	1.45
2	A	501	LUX	C26-C25	-5.40	1.35	1.52
6	A	612	CHL	CMC-C2C	5.39	1.56	1.45
6	C	613	CHL	CMC-C2C	5.36	1.56	1.45
2	A	502	LUX	C9-C8	-5.35	1.34	1.51
6	C	614	CHL	C4B-NB	5.29	1.39	1.35
2	C	502	LUX	C9-C8	-5.25	1.35	1.51
2	C	501	LUX	C28-C27	-5.24	1.38	1.53
2	A	502	LUX	C26-C25	-5.21	1.35	1.52
3	A	503	NEX	C32-C33	-5.20	1.34	1.45
2	C	501	LUX	C26-C25	-5.19	1.35	1.52
6	A	611	CHL	CMC-C2C	5.17	1.56	1.45
6	B	614	CHL	CMC-C2C	5.16	1.56	1.45
3	B	503	NEX	C32-C33	-5.10	1.35	1.45
6	A	614	CHL	CMC-C2C	5.06	1.55	1.45
4	A	504	XAT	C32-C33	-5.02	1.35	1.45
6	B	610	CHL	CMC-C2C	5.00	1.55	1.45
7	A	801	LHG	P-O3	4.98	1.79	1.59
5	B	604	CLA	O2D-CGD	4.98	1.45	1.33
5	A	604	CLA	C4B-NB	4.98	1.39	1.35
2	C	502	LUX	C18-C5	-4.95	1.42	1.50
6	B	614	CHL	C4B-NB	4.95	1.39	1.35
2	C	501	LUX	C9-C8	-4.90	1.36	1.51
4	C	504	XAT	C32-C33	-4.87	1.35	1.45
7	C	801	LHG	P-O3	4.87	1.79	1.59
2	B	502	LUX	C9-C8	-4.82	1.36	1.51
6	B	611	CHL	CMC-C2C	4.79	1.55	1.45
2	C	501	LUX	C27-C26	-4.78	1.43	1.54
7	B	801	LHG	P-O3	4.78	1.78	1.59
5	A	608	CLA	O2D-CGD	4.76	1.44	1.33
6	C	610	CHL	CMC-C2C	4.74	1.55	1.45
4	A	504	XAT	C12-C13	-4.72	1.35	1.45
6	C	611	CHL	CMC-C2C	4.72	1.55	1.45
5	B	603	CLA	C4B-NB	4.70	1.39	1.35
4	B	504	XAT	C32-C33	-4.67	1.35	1.45
2	A	501	LUX	C9-C8	-4.66	1.36	1.51
5	C	607	CLA	MG-NA	4.65	2.17	2.06
6	A	609	CHL	CMC-C2C	4.65	1.55	1.45
5	A	608	CLA	C3B-C2B	-4.64	1.33	1.40
6	B	610	CHL	C4B-NB	4.59	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	610	CHL	C3B-C2B	-4.53	1.34	1.40
4	A	504	XAT	C28-C29	-4.53	1.36	1.45
3	C	503	NEX	C28-C29	-4.51	1.36	1.45
5	B	605	CLA	O2D-CGD	4.51	1.44	1.33
5	A	601	CLA	O2D-CGD	4.51	1.44	1.33
2	B	501	LUX	C9-C8	-4.50	1.37	1.51
6	A	614	CHL	C4B-NB	4.48	1.39	1.35
6	A	610	CHL	O2D-CGD	4.46	1.44	1.33
6	C	611	CHL	O2D-CGD	4.40	1.43	1.33
4	C	504	XAT	C28-C29	-4.39	1.36	1.45
4	B	504	XAT	C12-C13	-4.38	1.36	1.45
6	C	610	CHL	O2D-CGD	4.37	1.43	1.33
5	C	605	CLA	O2D-CGD	4.37	1.43	1.33
6	B	610	CHL	O2D-CGD	4.36	1.43	1.33
5	C	603	CLA	O2D-CGD	4.35	1.43	1.33
5	A	605	CLA	O2D-CGD	4.33	1.43	1.33
5	A	602	CLA	O2D-CGD	4.32	1.43	1.33
6	C	610	CHL	C4B-NB	4.29	1.39	1.35
2	C	501	LUX	C15-C14	-4.27	1.33	1.52
6	B	611	CHL	O2D-CGD	4.26	1.43	1.33
5	C	602	CLA	O2D-CGD	4.26	1.43	1.33
3	C	503	NEX	C32-C33	-4.26	1.36	1.45
5	B	602	CLA	O2D-CGD	4.25	1.43	1.33
2	A	502	LUX	C31-C30	-4.23	1.34	1.52
5	B	601	CLA	C4B-NB	4.23	1.39	1.35
2	B	501	LUX	C31-C30	-4.23	1.34	1.52
5	B	603	CLA	O2D-CGD	4.23	1.43	1.33
5	B	608	CLA	C3B-C2B	-4.20	1.34	1.40
2	A	502	LUX	C11-C12	-4.19	1.34	1.52
4	B	504	XAT	C28-C29	-4.17	1.37	1.45
2	A	502	LUX	C31-C32	-4.13	1.34	1.52
6	B	611	CHL	MG-NA	4.12	2.16	2.06
5	B	604	CLA	C4B-NB	4.11	1.38	1.35
2	B	502	LUX	C11-C12	-4.11	1.34	1.52
6	C	614	CHL	O2D-CGD	4.10	1.43	1.33
5	A	603	CLA	O2D-CGD	4.10	1.43	1.33
2	B	502	LUX	C31-C32	-4.09	1.34	1.52
2	A	501	LUX	C4-C5	-4.08	1.44	1.51
6	C	612	CHL	C4B-NB	4.07	1.38	1.35
2	C	502	LUX	C15-C14	-4.06	1.34	1.52
6	B	614	CHL	O2D-CGD	4.05	1.43	1.33
8	C	802	DGD	O5D-C1E	4.05	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	NEX	C28-C29	-4.04	1.37	1.45
6	A	614	CHL	O2D-CGD	4.02	1.43	1.33
6	A	609	CHL	C4B-NB	4.02	1.38	1.35
2	A	501	LUX	C15-C14	-3.99	1.35	1.52
7	A	801	LHG	P-O6	3.99	1.75	1.59
2	C	502	LUX	C11-C12	-3.97	1.35	1.52
5	C	601	CLA	C3B-C2B	-3.96	1.34	1.40
2	B	502	LUX	C31-C30	-3.95	1.35	1.52
5	B	602	CLA	C4B-NB	3.94	1.38	1.35
2	C	502	LUX	C31-C30	-3.93	1.35	1.52
6	A	612	CHL	C4B-NB	3.92	1.38	1.35
7	B	801	LHG	O8-C23	3.92	1.44	1.33
5	B	605	CLA	C3B-C2B	-3.91	1.34	1.40
6	B	612	CHL	O2D-CGD	3.91	1.42	1.33
7	A	801	LHG	O8-C23	3.90	1.44	1.33
5	B	602	CLA	MG-NA	3.90	2.15	2.06
5	C	608	CLA	O2D-CGD	3.88	1.42	1.33
6	A	613	CHL	O2D-CGD	3.88	1.42	1.33
5	A	608	CLA	C4B-NB	3.88	1.38	1.35
2	A	501	LUX	C31-C30	-3.88	1.35	1.52
4	C	504	XAT	C12-C13	-3.87	1.37	1.45
6	B	610	CHL	C3B-C2B	-3.85	1.35	1.40
6	C	612	CHL	MG-NA	3.85	2.15	2.06
2	A	501	LUX	C35-C34	-3.82	1.35	1.52
6	B	609	CHL	MG-NC	3.81	2.15	2.06
5	B	607	CLA	C4B-NB	3.81	1.38	1.35
5	C	601	CLA	O2D-CGD	3.80	1.42	1.33
2	B	501	LUX	C11-C12	-3.79	1.35	1.52
2	B	501	LUX	C35-C34	-3.79	1.35	1.52
2	C	501	LUX	C35-C34	-3.78	1.36	1.52
5	A	607	CLA	O2D-CGD	3.78	1.42	1.33
2	C	502	LUX	C11-C10	-3.77	1.36	1.52
6	C	614	CHL	C1B-NB	3.77	1.38	1.35
5	C	606	CLA	O2D-CGD	3.76	1.42	1.33
3	A	503	NEX	C11-C10	-3.75	1.31	1.43
3	A	503	NEX	C28-C29	-3.74	1.37	1.45
5	C	607	CLA	C4B-NB	3.73	1.38	1.35
2	C	502	LUX	C31-C32	-3.73	1.36	1.52
2	B	501	LUX	C15-C14	-3.73	1.36	1.52
5	B	608	CLA	O2D-CGD	3.71	1.42	1.33
6	A	609	CHL	O2D-CGD	3.70	1.42	1.33
7	C	801	LHG	O8-C23	3.70	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	604	CLA	O2D-CGD	3.70	1.42	1.33
5	C	604	CLA	C4B-NB	3.69	1.38	1.35
2	C	501	LUX	C4-C5	-3.69	1.45	1.51
6	B	614	CHL	C1B-NB	3.68	1.38	1.35
6	B	609	CHL	C4B-NB	3.68	1.38	1.35
5	A	602	CLA	C3B-C2B	-3.68	1.35	1.40
2	A	502	LUX	C15-C14	-3.68	1.36	1.52
2	A	501	LUX	C11-C12	-3.67	1.36	1.52
5	C	602	CLA	MG-NA	3.67	2.15	2.06
6	C	609	CHL	O2D-CGD	3.66	1.42	1.33
7	C	801	LHG	P-O6	3.66	1.74	1.59
6	C	610	CHL	C3B-C2B	-3.64	1.35	1.40
5	C	607	CLA	O2D-CGD	3.64	1.42	1.33
5	A	606	CLA	O2D-CGD	3.63	1.42	1.33
6	C	613	CHL	O2D-CGD	3.61	1.42	1.33
8	A	802	DGD	O5D-C1E	3.60	1.46	1.40
6	B	609	CHL	O2D-CGD	3.60	1.42	1.33
2	B	502	LUX	C32-C33	-3.59	1.33	1.52
2	A	501	LUX	C31-C32	-3.59	1.36	1.52
5	B	606	CLA	O2D-CGD	3.58	1.41	1.33
6	A	611	CHL	O2D-CGD	3.58	1.41	1.33
2	B	502	LUX	C11-C10	-3.58	1.36	1.52
2	B	501	LUX	C11-C10	-3.57	1.36	1.52
5	B	608	CLA	C4B-NB	3.56	1.38	1.35
2	B	501	LUX	C31-C32	-3.56	1.36	1.52
6	C	612	CHL	O2D-CGD	3.55	1.41	1.33
5	C	608	CLA	C3B-C2B	-3.54	1.35	1.40
5	B	607	CLA	O2D-CGD	3.52	1.41	1.33
4	B	504	XAT	C8-C9	-3.51	1.38	1.45
5	C	605	CLA	C4B-NB	3.51	1.38	1.35
5	C	602	CLA	C4B-NB	3.51	1.38	1.35
6	A	612	CHL	O2D-CGD	3.51	1.41	1.33
2	B	502	LUX	C35-C34	-3.51	1.37	1.52
6	B	613	CHL	O2D-CGD	3.50	1.41	1.33
2	C	502	LUX	C35-C34	-3.50	1.37	1.52
5	A	608	CLA	CMC-C2C	3.49	1.58	1.50
2	C	502	LUX	C32-C33	-3.49	1.34	1.52
8	B	802	DGD	O5D-C1E	3.48	1.46	1.40
2	A	502	LUX	C11-C10	-3.47	1.37	1.52
3	C	503	NEX	C15-C14	-3.47	1.32	1.43
2	C	501	LUX	C18-C5	-3.46	1.45	1.50
7	B	801	LHG	P-O6	3.45	1.73	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	LUX	C31-C30	-3.45	1.37	1.52
5	A	604	CLA	O2D-CGD	3.43	1.41	1.33
6	A	609	CHL	MG-NC	3.42	2.14	2.06
2	C	501	LUX	C11-C12	-3.41	1.37	1.52
2	B	501	LUX	C30-C29	-3.40	1.34	1.52
2	C	501	LUX	C32-C33	-3.40	1.34	1.52
2	C	501	LUX	C31-C32	-3.39	1.37	1.52
5	A	605	CLA	C3B-C2B	-3.38	1.35	1.40
6	B	610	CHL	CHC-C1C	3.38	1.43	1.35
5	C	601	CLA	CMC-C2C	3.37	1.57	1.50
2	B	502	LUX	C12-C13	-3.35	1.34	1.52
2	A	501	LUX	C11-C10	-3.32	1.37	1.52
2	A	502	LUX	C12-C13	-3.31	1.35	1.52
6	B	612	CHL	C3B-C2B	-3.30	1.35	1.40
6	B	609	CHL	C3B-C2B	-3.30	1.35	1.40
6	C	610	CHL	O1D-CGD	3.30	1.29	1.21
6	A	612	CHL	C3B-C2B	-3.30	1.35	1.40
2	A	502	LUX	C32-C33	-3.30	1.35	1.52
6	C	609	CHL	C3B-C2B	-3.29	1.35	1.40
2	B	502	LUX	C18-C5	-3.29	1.45	1.50
3	B	503	NEX	C15-C14	-3.29	1.33	1.43
6	C	613	CHL	C1B-NB	3.28	1.38	1.35
2	B	501	LUX	C14-C13	-3.28	1.35	1.52
2	B	502	LUX	C15-C14	-3.27	1.38	1.52
2	C	502	LUX	C14-C13	-3.26	1.35	1.52
2	A	501	LUX	C14-C13	-3.25	1.35	1.52
5	A	607	CLA	C4B-NB	3.25	1.38	1.35
5	B	601	CLA	O1D-CGD	3.24	1.29	1.21
2	C	502	LUX	C34-C33	-3.23	1.35	1.52
2	C	501	LUX	C30-C29	-3.22	1.35	1.52
2	A	502	LUX	C35-C34	-3.21	1.38	1.52
5	A	602	CLA	O1D-CGD	3.21	1.29	1.21
5	B	604	CLA	O1D-CGD	3.21	1.29	1.21
5	C	605	CLA	C3B-C2B	-3.21	1.35	1.40
5	B	607	CLA	CHC-C1C	3.20	1.43	1.35
5	C	606	CLA	C4B-NB	3.19	1.38	1.35
6	A	613	CHL	C4B-NB	3.19	1.38	1.35
5	A	601	CLA	CMC-C2C	3.18	1.57	1.50
2	C	501	LUX	C28-C29	-3.18	1.35	1.52
6	C	610	CHL	CHC-C1C	3.18	1.43	1.35
2	B	502	LUX	C14-C13	-3.17	1.35	1.52
5	B	601	CLA	C3B-C2B	-3.17	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	NEX	C11-C10	-3.17	1.33	1.43
6	B	614	CHL	MG-NA	3.17	2.13	2.06
2	B	501	LUX	C18-C5	-3.16	1.45	1.50
5	B	602	CLA	C1B-NB	3.15	1.38	1.35
6	A	614	CHL	MG-NC	3.15	2.13	2.06
2	B	502	LUX	C28-C29	-3.15	1.36	1.52
6	B	612	CHL	O2A-CGA	3.15	1.42	1.33
2	A	501	LUX	C30-C29	-3.13	1.36	1.52
5	B	607	CLA	O2A-CGA	3.12	1.42	1.33
6	C	611	CHL	O1D-CGD	3.12	1.29	1.21
6	A	614	CHL	CHC-C1C	3.11	1.43	1.35
2	A	501	LUX	C18-C5	-3.11	1.45	1.50
2	C	501	LUX	C14-C13	-3.11	1.36	1.52
6	A	612	CHL	MG-NA	3.10	2.13	2.06
5	C	602	CLA	O1D-CGD	3.10	1.29	1.21
5	B	605	CLA	C4B-NB	3.09	1.38	1.35
2	C	501	LUX	C11-C10	-3.08	1.38	1.52
3	C	503	NEX	C11-C10	-3.08	1.33	1.43
5	A	603	CLA	C4B-NB	3.08	1.38	1.35
5	A	603	CLA	O1D-CGD	3.07	1.28	1.21
5	B	604	CLA	MG-NC	3.07	2.13	2.06
6	B	614	CHL	O1D-CGD	3.07	1.28	1.21
2	B	501	LUX	C32-C33	-3.07	1.36	1.52
5	B	604	CLA	C1B-NB	3.06	1.37	1.35
2	A	501	LUX	C28-C29	-3.06	1.36	1.52
6	A	614	CHL	C3B-C2B	-3.05	1.36	1.40
6	A	611	CHL	C1B-NB	3.05	1.37	1.35
2	B	502	LUX	C34-C33	-3.05	1.36	1.52
2	C	502	LUX	C30-C29	-3.05	1.36	1.52
2	B	501	LUX	C4-C5	-3.04	1.46	1.51
2	C	501	LUX	C12-C13	-3.04	1.36	1.52
5	B	608	CLA	O1D-CGD	3.04	1.28	1.21
5	B	606	CLA	C4B-NB	3.03	1.37	1.35
3	A	503	NEX	C15-C14	-3.02	1.34	1.43
5	A	605	CLA	C4B-NB	3.01	1.37	1.35
6	C	609	CHL	MG-NC	3.01	2.13	2.06
2	A	501	LUX	C12-C13	-3.00	1.36	1.52
2	C	502	LUX	C12-C13	-2.99	1.36	1.52
5	B	602	CLA	O1D-CGD	2.99	1.28	1.21
5	A	604	CLA	MG-NC	2.99	2.13	2.06
6	A	612	CHL	O2A-CGA	2.98	1.42	1.33
6	C	611	CHL	C4B-NB	2.98	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	LUX	C30-C29	-2.98	1.36	1.52
6	A	610	CHL	O1D-CGD	2.97	1.28	1.21
3	C	503	NEX	C35-C34	-2.97	1.34	1.43
6	A	611	CHL	C3B-C2B	-2.97	1.36	1.40
5	A	602	CLA	CMC-C2C	2.97	1.57	1.50
5	C	608	CLA	MG-NC	2.96	2.13	2.06
6	C	611	CHL	C3B-C2B	-2.96	1.36	1.40
5	A	607	CLA	C3B-C2B	-2.96	1.36	1.40
2	A	502	LUX	C7-C6	-2.95	1.34	1.45
2	B	501	LUX	C12-C13	-2.95	1.37	1.52
4	C	504	XAT	C4-C3	2.94	1.56	1.52
5	B	607	CLA	C1B-NB	2.94	1.37	1.35
6	A	613	CHL	MG-NC	2.91	2.13	2.06
5	C	608	CLA	CHC-C1C	2.91	1.42	1.35
2	A	501	LUX	C34-C33	-2.91	1.37	1.52
5	C	607	CLA	O2A-CGA	2.91	1.41	1.33
5	C	601	CLA	O1D-CGD	2.90	1.28	1.21
6	C	612	CHL	O2A-CGA	2.90	1.41	1.33
5	C	602	CLA	C3B-C2B	-2.89	1.36	1.40
6	B	612	CHL	C4B-NB	2.89	1.37	1.35
7	C	801	LHG	O7-C7	2.88	1.42	1.34
6	A	614	CHL	O1D-CGD	2.88	1.28	1.21
5	A	604	CLA	O1D-CGD	2.87	1.28	1.21
5	C	603	CLA	C4B-NB	2.87	1.37	1.35
6	C	612	CHL	C3B-C2B	-2.87	1.36	1.40
2	A	502	LUX	C14-C13	-2.87	1.37	1.52
5	A	607	CLA	O2A-CGA	2.87	1.41	1.33
2	C	502	LUX	C28-C29	-2.86	1.37	1.52
4	C	504	XAT	C8-C9	-2.86	1.39	1.45
2	A	501	LUX	C32-C33	-2.84	1.37	1.52
5	B	604	CLA	CMC-C2C	2.84	1.56	1.50
2	B	502	LUX	C4-C5	-2.84	1.46	1.51
4	C	504	XAT	C15-C14	-2.84	1.34	1.43
6	C	612	CHL	CHC-C1C	2.84	1.42	1.35
2	A	502	LUX	C28-C29	-2.83	1.37	1.52
6	A	611	CHL	MG-NA	2.83	2.13	2.06
6	C	614	CHL	O1D-CGD	2.82	1.28	1.21
5	C	601	CLA	MG-NC	2.82	2.13	2.06
2	B	501	LUX	C34-C33	-2.81	1.37	1.52
5	A	607	CLA	CHC-C1C	2.81	1.42	1.35
5	C	605	CLA	O1D-CGD	2.81	1.28	1.21
6	A	610	CHL	C3D-C2D	-2.81	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	CLA	O1D-CGD	2.80	1.28	1.21
2	B	501	LUX	C28-C29	-2.80	1.37	1.52
2	B	502	LUX	C16-C1	-2.80	1.48	1.53
5	B	602	CLA	C3B-C2B	-2.80	1.36	1.40
6	B	610	CHL	C2-C3	2.80	1.39	1.33
6	B	614	CHL	CHC-C1C	2.79	1.42	1.35
6	C	609	CHL	CHC-C1C	2.79	1.42	1.35
6	A	613	CHL	O1D-CGD	2.79	1.28	1.21
5	C	607	CLA	C3B-C2B	-2.79	1.36	1.40
5	B	604	CLA	C1D-C2D	2.78	1.48	1.42
2	A	501	LUX	C17-C1	-2.78	1.48	1.53
2	C	501	LUX	C34-C33	-2.77	1.38	1.52
5	C	605	CLA	CMC-C2C	2.77	1.56	1.50
5	A	601	CLA	O2A-CGA	2.77	1.41	1.33
5	B	607	CLA	C3B-C2B	-2.77	1.36	1.40
6	B	611	CHL	C3B-C2B	-2.77	1.36	1.40
2	A	501	LUX	C7-C6	-2.77	1.35	1.45
6	C	613	CHL	CHC-C1C	2.76	1.42	1.35
5	B	601	CLA	C2-C3	2.76	1.39	1.33
5	B	605	CLA	CMC-C2C	2.75	1.56	1.50
5	C	608	CLA	O2A-CGA	2.75	1.41	1.33
6	B	613	CHL	CHC-C1C	2.74	1.42	1.35
5	A	605	CLA	CMC-C2C	2.74	1.56	1.50
5	A	606	CLA	CMC-C2C	2.74	1.56	1.50
2	C	501	LUX	C35-C15	-2.74	1.36	1.51
5	C	604	CLA	CMC-C2C	2.74	1.56	1.50
2	A	502	LUX	C34-C33	-2.73	1.38	1.52
6	B	611	CHL	C1B-NB	2.73	1.37	1.35
8	A	802	DGD	O3G-C1D	2.73	1.44	1.40
5	C	606	CLA	CMC-C2C	2.73	1.56	1.50
5	C	607	CLA	CHC-C1C	2.72	1.41	1.35
5	A	608	CLA	MG-NC	2.72	2.12	2.06
6	C	609	CHL	C4B-NB	2.72	1.37	1.35
4	A	504	XAT	C15-C14	-2.72	1.35	1.43
5	B	602	CLA	CMC-C2C	2.72	1.56	1.50
6	B	609	CHL	O1D-CGD	2.71	1.28	1.21
5	A	608	CLA	CHC-C1C	2.71	1.41	1.35
2	C	501	LUX	C7-C6	-2.71	1.35	1.45
6	C	614	CHL	CHC-C1C	2.71	1.41	1.35
5	B	601	CLA	O2D-CGD	2.71	1.39	1.33
4	C	504	XAT	C11-C10	-2.71	1.35	1.43
5	C	602	CLA	CMC-C2C	2.71	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	613	CHL	O1D-CGD	2.70	1.28	1.21
6	C	610	CHL	O2A-CGA	2.70	1.41	1.33
6	B	610	CHL	O2A-CGA	2.69	1.41	1.33
2	B	502	LUX	C30-C29	-2.69	1.38	1.52
6	C	611	CHL	C1B-NB	2.68	1.37	1.35
2	A	502	LUX	C18-C5	-2.68	1.46	1.50
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	604	CLA	O1D-CGD	2.68	1.27	1.21
5	C	604	CLA	C1B-NB	2.68	1.37	1.35
6	A	609	CHL	CHC-C1C	2.67	1.41	1.35
3	B	503	NEX	C31-C30	-2.67	1.35	1.43
2	B	502	LUX	C7-C6	-2.66	1.35	1.45
6	A	611	CHL	C4B-NB	2.66	1.37	1.35
6	A	610	CHL	CHC-C1C	2.66	1.41	1.35
5	B	608	CLA	O2A-CGA	2.66	1.41	1.33
4	B	504	XAT	C4-C3	2.65	1.56	1.52
2	C	502	LUX	O23-C23	-2.65	1.38	1.43
4	A	504	XAT	C4-C5	2.65	1.55	1.52
5	A	606	CLA	C3B-C2B	-2.65	1.36	1.40
2	B	501	LUX	C35-C15	-2.65	1.36	1.51
2	B	501	LUX	C7-C6	-2.65	1.35	1.45
6	C	610	CHL	C2-C3	2.65	1.39	1.33
5	C	601	CLA	CHC-C1C	2.64	1.41	1.35
6	A	611	CHL	O1D-CGD	2.63	1.27	1.21
2	A	501	LUX	C35-C15	-2.63	1.36	1.51
5	A	608	CLA	O2A-CGA	2.63	1.41	1.33
6	A	610	CHL	C2-C3	2.63	1.39	1.33
5	C	603	CLA	O1D-CGD	2.62	1.27	1.21
5	A	601	CLA	C4B-NB	2.62	1.37	1.35
5	C	602	CLA	C1B-NB	2.62	1.37	1.35
6	A	613	CHL	CHC-C1C	2.61	1.41	1.35
6	C	609	CHL	OMC-CMC	2.61	1.28	1.22
6	B	610	CHL	O1D-CGD	2.61	1.27	1.21
5	C	606	CLA	O1D-CGD	2.61	1.27	1.21
5	C	608	CLA	O1D-CGD	2.61	1.27	1.21
4	B	504	XAT	C4-C5	2.60	1.55	1.52
5	B	606	CLA	MG-NC	2.60	2.12	2.06
8	C	802	DGD	O6D-C1D	2.60	1.48	1.41
5	A	604	CLA	CMC-C2C	2.60	1.56	1.50
5	B	606	CLA	CMC-C2C	2.60	1.56	1.50
5	A	608	CLA	O1D-CGD	2.59	1.27	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	603	CLA	C3D-C2D	-2.59	1.34	1.39
6	C	612	CHL	C2-C3	2.58	1.39	1.33
3	A	503	NEX	C31-C30	-2.58	1.35	1.43
5	A	603	CLA	MG-NA	2.57	2.12	2.06
7	A	801	LHG	O7-C7	2.57	1.41	1.34
5	B	603	CLA	CMC-C2C	2.56	1.56	1.50
5	B	605	CLA	C3B-CAB	-2.56	1.42	1.47
5	A	601	CLA	C3B-C2B	-2.56	1.36	1.40
8	B	802	DGD	C4E-C3E	2.55	1.58	1.52
6	C	609	CHL	O1D-CGD	2.54	1.27	1.21
5	B	605	CLA	CHC-C1C	2.54	1.41	1.35
5	B	606	CLA	C3B-C2B	-2.54	1.36	1.40
5	B	607	CLA	CMC-C2C	2.54	1.56	1.50
6	A	612	CHL	C2-C3	2.53	1.39	1.33
6	C	611	CHL	CHC-C1C	2.53	1.41	1.35
2	C	502	LUX	C7-C6	-2.53	1.36	1.45
8	C	802	DGD	O3G-C1D	2.52	1.44	1.40
6	B	614	CHL	MG-NC	2.52	2.12	2.06
2	C	502	LUX	C35-C15	-2.51	1.37	1.51
3	B	503	NEX	C35-C34	-2.50	1.35	1.43
6	B	611	CHL	O1D-CGD	2.50	1.27	1.21
5	A	608	CLA	C1D-C2D	2.50	1.48	1.42
5	C	606	CLA	CHC-C1C	2.50	1.41	1.35
5	C	603	CLA	CMC-C2C	2.50	1.56	1.50
6	C	609	CHL	O2A-CGA	2.49	1.40	1.33
5	C	602	CLA	O2A-CGA	2.49	1.40	1.33
5	A	605	CLA	CHC-C1C	2.48	1.41	1.35
7	B	801	LHG	O7-C5	-2.48	1.40	1.46
4	C	504	XAT	C4-C5	2.48	1.55	1.52
5	B	608	CLA	CHC-C1C	2.48	1.41	1.35
5	C	604	CLA	MG-NC	2.48	2.12	2.06
6	C	611	CHL	MG-NC	2.47	2.12	2.06
5	B	602	CLA	O2A-CGA	2.47	1.40	1.33
5	A	606	CLA	C4B-NB	2.47	1.37	1.35
6	B	611	CHL	CHC-C1C	2.46	1.41	1.35
6	B	613	CHL	O1D-CGD	2.45	1.27	1.21
3	A	503	NEX	C37-C21	-2.45	1.49	1.53
5	A	604	CLA	CHC-C1C	2.45	1.41	1.35
4	C	504	XAT	C16-C1	-2.45	1.49	1.53
5	B	607	CLA	C2-C3	2.45	1.38	1.33
5	C	607	CLA	CMC-C2C	2.45	1.56	1.50
5	B	608	CLA	C1D-C2D	2.44	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	NEX	C37-C21	-2.44	1.49	1.53
6	A	610	CHL	C4B-NB	2.44	1.37	1.35
5	A	607	CLA	CMC-C2C	2.44	1.56	1.50
5	B	608	CLA	CMC-C2C	2.44	1.56	1.50
6	B	613	CHL	C4B-NB	2.44	1.37	1.35
8	A	802	DGD	O6D-C1D	2.44	1.48	1.41
3	A	503	NEX	C35-C34	-2.42	1.35	1.43
5	A	606	CLA	C3D-C2D	-2.42	1.35	1.39
6	B	612	CHL	MG-NA	2.42	2.12	2.06
2	C	502	LUX	C4-C5	-2.42	1.47	1.51
6	B	612	CHL	C2-C3	2.42	1.38	1.33
5	B	603	CLA	MG-NC	2.41	2.12	2.06
6	B	610	CHL	MG-NC	2.41	2.12	2.06
6	A	612	CHL	CHC-C1C	2.41	1.41	1.35
4	A	504	XAT	C8-C9	-2.40	1.40	1.45
4	B	504	XAT	C31-C30	-2.40	1.36	1.43
5	A	607	CLA	C2-C3	2.40	1.38	1.33
6	B	609	CHL	CHC-C1C	2.39	1.41	1.35
5	C	602	CLA	CHC-C1C	2.39	1.41	1.35
2	C	502	LUX	C16-C1	-2.39	1.49	1.53
4	B	504	XAT	C15-C14	-2.38	1.36	1.43
5	B	602	CLA	C2-C3	2.38	1.38	1.33
5	A	605	CLA	O1D-CGD	2.38	1.27	1.21
5	C	608	CLA	C1D-C2D	2.37	1.47	1.42
6	A	614	CHL	C1B-NB	2.37	1.37	1.35
5	A	602	CLA	O2A-CGA	2.37	1.40	1.33
5	C	604	CLA	C1D-C2D	2.36	1.47	1.42
6	C	614	CHL	MG-NC	2.36	2.11	2.06
2	A	502	LUX	C16-C1	-2.36	1.49	1.53
5	B	603	CLA	O2A-CGA	2.35	1.40	1.33
5	A	603	CLA	O2A-CGA	2.35	1.40	1.33
5	A	602	CLA	C2-C3	2.35	1.38	1.33
5	A	607	CLA	C1B-NB	2.35	1.37	1.35
6	A	609	CHL	C1B-NB	2.34	1.37	1.35
6	C	613	CHL	MG-NC	2.34	2.11	2.06
6	A	611	CHL	C1-C2	-2.34	1.42	1.49
5	A	603	CLA	CMC-C2C	2.34	1.55	1.50
2	A	501	LUX	C16-C1	-2.34	1.49	1.53
2	A	502	LUX	C35-C15	-2.34	1.38	1.51
5	A	607	CLA	O1D-CGD	2.34	1.27	1.21
5	A	601	CLA	O1D-CGD	2.33	1.27	1.21
5	B	605	CLA	C2-C3	2.33	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	XAT	C20-C13	-2.33	1.46	1.50
2	B	502	LUX	C35-C15	-2.33	1.38	1.51
4	A	504	XAT	C2-C1	-2.33	1.50	1.54
5	C	607	CLA	C2-C3	2.33	1.38	1.33
6	A	610	CHL	C3B-CAB	-2.31	1.43	1.47
4	C	504	XAT	C31-C30	-2.31	1.36	1.43
5	C	608	CLA	C3B-CAB	-2.31	1.43	1.47
5	C	604	CLA	CHC-C1C	2.31	1.40	1.35
5	A	602	CLA	MG-NC	2.30	2.11	2.06
6	A	611	CHL	CHC-C1C	2.30	1.40	1.35
6	A	611	CHL	MG-NC	2.30	2.11	2.06
3	C	503	NEX	C31-C30	-2.29	1.36	1.43
6	B	613	CHL	C1B-NB	2.29	1.37	1.35
5	B	606	CLA	O1D-CGD	2.29	1.27	1.21
5	B	605	CLA	O2A-CGA	2.29	1.40	1.33
5	A	605	CLA	C2-C3	2.29	1.38	1.33
5	B	602	CLA	C3B-CAB	-2.29	1.43	1.47
5	B	604	CLA	CHC-C1C	2.28	1.40	1.35
5	B	606	CLA	O2A-CGA	2.28	1.40	1.33
6	B	611	CHL	C4B-NB	2.28	1.37	1.35
6	C	612	CHL	MG-NC	2.27	2.11	2.06
4	A	504	XAT	C35-C34	-2.27	1.36	1.43
6	B	612	CHL	CHC-C1C	2.27	1.40	1.35
5	C	606	CLA	C3B-C2B	-2.27	1.37	1.40
5	C	605	CLA	CHC-C1C	2.27	1.40	1.35
5	B	603	CLA	O1D-CGD	2.27	1.26	1.21
5	C	605	CLA	O2A-CGA	2.26	1.39	1.33
5	A	605	CLA	O2A-CGA	2.26	1.39	1.33
8	C	802	DGD	O6E-C1E	2.25	1.47	1.41
6	B	610	CHL	C3D-C2D	-2.25	1.35	1.39
6	B	611	CHL	C1-C2	-2.25	1.42	1.49
6	B	612	CHL	C3B-CAB	-2.25	1.43	1.47
6	A	610	CHL	MG-NC	2.25	2.11	2.06
6	A	612	CHL	MG-NC	2.25	2.11	2.06
3	A	503	NEX	C10-C9	-2.24	1.32	1.35
4	A	504	XAT	C31-C30	-2.24	1.36	1.43
5	A	605	CLA	C3B-CAB	-2.24	1.43	1.47
6	C	612	CHL	CBA-CGA	2.24	1.57	1.50
6	C	611	CHL	C3B-CAB	-2.24	1.43	1.47
5	B	605	CLA	MG-NA	2.24	2.11	2.06
5	C	607	CLA	C1B-NB	2.24	1.37	1.35
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	612	CHL	C1B-NB	2.22	1.37	1.35
2	C	501	LUX	C23-C24	2.22	1.53	1.50
6	A	610	CHL	CAC-C3C	2.22	1.56	1.51
8	B	802	DGD	O6E-C1E	2.22	1.47	1.41
5	B	601	CLA	MG-NA	2.22	2.11	2.06
6	A	609	CHL	C3B-C2B	-2.21	1.37	1.40
5	C	601	CLA	O2A-CGA	2.21	1.39	1.33
5	B	601	CLA	CMC-C2C	2.21	1.55	1.50
8	B	802	DGD	O6D-C1D	2.21	1.47	1.41
6	B	613	CHL	OBD-CAD	2.21	1.25	1.22
6	C	614	CHL	C3B-C2B	-2.20	1.37	1.40
4	B	504	XAT	C35-C34	-2.20	1.36	1.43
7	C	801	LHG	O7-C5	-2.20	1.41	1.46
6	B	614	CHL	C3B-C2B	-2.20	1.37	1.40
2	A	502	LUX	C4-C5	-2.19	1.47	1.51
7	B	801	LHG	O7-C7	2.19	1.40	1.34
6	A	609	CHL	O2A-CGA	2.19	1.39	1.33
5	C	605	CLA	C3D-C2D	-2.19	1.35	1.39
6	C	610	CHL	C3B-CAB	-2.19	1.43	1.47
4	B	504	XAT	C11-C10	-2.19	1.36	1.43
5	A	606	CLA	MG-NC	2.19	2.11	2.06
4	C	504	XAT	C35-C34	-2.19	1.36	1.43
6	C	610	CHL	C3D-C2D	-2.18	1.35	1.39
4	A	504	XAT	C24-C25	-2.18	1.49	1.52
5	B	605	CLA	MG-NC	2.17	2.11	2.06
6	B	613	CHL	MG-NC	2.17	2.11	2.06
6	A	611	CHL	C5-C3	2.17	1.55	1.51
5	B	603	CLA	CHC-C1C	2.16	1.40	1.35
5	A	602	CLA	C4B-NB	2.16	1.37	1.35
2	A	502	LUX	C17-C1	-2.16	1.49	1.53
6	A	613	CHL	OBD-CAD	2.16	1.25	1.22
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	C	605	CLA	C2-C3	2.15	1.38	1.33
8	C	802	DGD	C4E-C3E	2.14	1.57	1.52
5	A	606	CLA	O1D-CGD	2.14	1.26	1.21
5	B	606	CLA	CHC-C1C	2.14	1.40	1.35
6	A	613	CHL	MG-NA	-2.14	2.01	2.06
5	A	601	CLA	C2-C3	2.13	1.38	1.33
6	B	612	CHL	CBA-CGA	2.13	1.56	1.50
6	A	609	CHL	O1D-CGD	2.13	1.26	1.21
5	B	602	CLA	CHC-C1C	2.13	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	801	LHG	O7-C5	-2.12	1.41	1.46
6	A	609	CHL	OBD-CAD	2.12	1.25	1.22
5	B	608	CLA	MG-NC	2.12	2.11	2.06
5	B	604	CLA	OBD-CAD	2.12	1.25	1.22
5	A	603	CLA	C3D-C2D	-2.12	1.35	1.39
2	B	501	LUX	C17-C1	-2.12	1.49	1.53
3	B	503	NEX	C28-C27	2.12	1.37	1.32
5	C	602	CLA	C2-C3	2.12	1.38	1.33
5	A	604	CLA	O2A-CGA	2.11	1.39	1.33
5	B	606	CLA	C3D-C2D	-2.11	1.35	1.39
5	A	601	CLA	CHC-C1C	2.11	1.40	1.35
6	C	612	CHL	O1D-CGD	2.11	1.26	1.21
5	C	604	CLA	O2A-CGA	2.11	1.39	1.33
5	B	606	CLA	C2-C3	2.11	1.38	1.33
5	B	601	CLA	O2A-CGA	2.11	1.39	1.33
6	C	610	CHL	MG-NA	2.11	2.11	2.06
6	B	612	CHL	MG-NC	2.10	2.11	2.06
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	601	CLA	CHC-C1C	2.10	1.40	1.35
4	B	504	XAT	C16-C1	-2.10	1.49	1.53
6	B	609	CHL	CAC-C3C	2.09	1.56	1.51
5	B	601	CLA	C5-C3	2.09	1.55	1.51
4	A	504	XAT	C11-C10	-2.09	1.37	1.43
6	C	611	CHL	O2A-CGA	2.08	1.39	1.33
5	C	603	CLA	C2-C3	2.08	1.38	1.33
5	A	603	CLA	C2-C3	2.08	1.38	1.33
4	A	504	XAT	C8-C7	2.08	1.37	1.32
4	A	504	XAT	C16-C1	-2.07	1.49	1.53
4	B	504	XAT	C8-C7	2.07	1.37	1.32
4	A	504	XAT	C17-C1	-2.07	1.49	1.53
5	B	607	CLA	O1D-CGD	2.07	1.26	1.21
5	C	607	CLA	O1D-CGD	2.06	1.26	1.21
6	C	611	CHL	C4-C3	2.06	1.56	1.50
5	C	603	CLA	MG-NC	2.06	2.11	2.06
6	B	609	CHL	O2A-CGA	2.06	1.39	1.33
6	C	614	CHL	MG-NA	2.05	2.11	2.06
6	A	612	CHL	C1B-NB	2.05	1.37	1.35
5	B	603	CLA	C2-C3	2.05	1.37	1.33
6	C	610	CHL	MG-NC	2.04	2.11	2.06
5	C	603	CLA	O2A-CGA	2.04	1.39	1.33
3	A	503	NEX	C28-C27	2.04	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	611	CHL	C3B-CAB	-2.04	1.43	1.47
4	C	504	XAT	C8-C7	2.04	1.37	1.32
5	C	606	CLA	C3D-C2D	-2.04	1.35	1.39
6	A	612	CHL	O1D-CGD	2.03	1.26	1.21
5	B	601	CLA	C3C-C2C	2.03	1.41	1.36
6	B	612	CHL	C5-C3	2.02	1.55	1.51
6	C	613	CHL	C4B-NB	2.01	1.37	1.35
8	A	802	DGD	C4E-C3E	2.00	1.57	1.52

All (861) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	LUX	C27-C26-C25	12.98	136.38	111.96
2	C	501	LUX	C27-C26-C25	12.57	135.60	111.96
2	B	502	LUX	C27-C26-C25	12.25	135.00	111.96
2	B	501	LUX	C27-C26-C25	12.24	134.99	111.96
2	A	502	LUX	C27-C26-C25	12.02	134.56	111.96
2	C	502	LUX	C27-C26-C25	11.31	133.22	111.96
2	A	502	LUX	C37-C21-C36	10.78	123.78	107.89
6	B	614	CHL	C4A-NA-C1A	10.71	111.52	106.71
6	A	612	CHL	C4A-NA-C1A	10.37	111.37	106.71
4	B	504	XAT	C37-C21-C22	-10.37	90.97	108.98
4	A	504	XAT	C37-C21-C22	-10.34	91.02	108.98
6	C	612	CHL	C4A-NA-C1A	10.28	111.33	106.71
2	C	502	LUX	C37-C21-C36	10.26	123.03	107.89
5	C	608	CLA	C4A-NA-C1A	10.23	111.31	106.71
6	C	614	CHL	C4A-NA-C1A	10.16	111.27	106.71
3	B	503	NEX	O24-C25-C26	9.98	67.22	58.96
2	B	502	LUX	C37-C21-C36	9.97	122.59	107.89
5	B	607	CLA	C4A-NA-C1A	9.95	111.18	106.71
2	C	501	LUX	C37-C21-C36	9.60	122.05	107.89
5	A	607	CLA	C4A-NA-C1A	9.59	111.02	106.71
6	A	614	CHL	C4A-NA-C1A	9.56	111.00	106.71
5	B	602	CLA	C4A-NA-C1A	9.53	110.99	106.71
6	B	611	CHL	C4A-NA-C1A	9.48	110.97	106.71
6	A	611	CHL	C4A-NA-C1A	9.45	110.95	106.71
3	A	503	NEX	O24-C25-C26	9.44	66.77	58.96
5	C	607	CLA	C4A-NA-C1A	9.40	110.93	106.71
5	C	605	CLA	C4A-NA-C1A	9.38	110.92	106.71
2	B	501	LUX	C37-C21-C36	9.33	121.64	107.89
3	C	503	NEX	O24-C25-C26	9.29	66.64	58.96
5	A	608	CLA	C4A-NA-C1A	9.28	110.88	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	606	CLA	C4A-NA-C1A	9.16	110.83	106.71
4	C	504	XAT	O24-C25-C26	9.15	66.53	58.96
5	C	602	CLA	C4A-NA-C1A	9.14	110.81	106.71
6	C	611	CHL	C4A-NA-C1A	9.13	110.81	106.71
5	C	606	CLA	C4A-NA-C1A	9.11	110.80	106.71
5	B	605	CLA	C4A-NA-C1A	8.95	110.73	106.71
5	C	601	CLA	C4A-NA-C1A	8.87	110.69	106.71
2	A	501	LUX	C37-C21-C36	8.84	120.92	107.89
5	A	603	CLA	C4A-NA-C1A	8.83	110.68	106.71
6	B	612	CHL	C4A-NA-C1A	8.83	110.68	106.71
2	A	501	LUX	C37-C21-C26	-8.80	92.99	110.44
5	A	605	CLA	C4A-NA-C1A	8.78	110.66	106.71
5	B	606	CLA	C4A-NA-C1A	8.77	110.65	106.71
5	C	603	CLA	C4A-NA-C1A	8.69	110.61	106.71
4	A	504	XAT	O24-C25-C26	8.65	66.11	58.96
5	B	603	CLA	C4A-NA-C1A	8.65	110.59	106.71
5	A	602	CLA	C4A-NA-C1A	8.65	110.59	106.71
4	B	504	XAT	O24-C25-C26	8.57	66.05	58.96
8	A	802	DGD	O6E-C5E-C4E	8.53	125.18	109.69
8	C	802	DGD	O6E-C5E-C4E	8.41	124.97	109.69
8	B	802	DGD	O6E-C5E-C4E	8.39	124.94	109.69
2	C	501	LUX	C37-C21-C26	-8.34	93.91	110.44
4	C	504	XAT	C37-C21-C22	-8.31	94.55	108.98
6	C	613	CHL	C4A-NA-C1A	8.08	110.34	106.71
6	C	610	CHL	C4A-NA-C1A	8.04	110.32	106.71
6	C	609	CHL	C4A-NA-C1A	8.00	110.30	106.71
5	B	608	CLA	C4A-NA-C1A	7.93	110.27	106.71
2	B	502	LUX	C1-C6-C5	-7.87	111.53	122.61
5	B	601	CLA	C4A-NA-C1A	7.85	110.23	106.71
2	C	502	LUX	C18-C5-C6	-7.71	115.87	124.53
2	A	502	LUX	C37-C21-C26	-7.68	95.21	110.44
5	C	604	CLA	C4A-NA-C1A	7.54	110.10	106.71
6	A	609	CHL	C4A-NA-C1A	7.53	110.09	106.71
2	C	502	LUX	C28-C27-C26	7.47	128.35	114.23
5	A	601	CLA	C4A-NA-C1A	7.40	110.03	106.71
2	B	502	LUX	C28-C27-C26	7.35	128.14	114.23
6	B	609	CHL	C4A-NA-C1A	7.35	110.01	106.71
5	B	604	CLA	C4A-NA-C1A	7.32	110.00	106.71
2	B	501	LUX	C37-C21-C26	-7.29	95.97	110.44
6	B	613	CHL	C4A-NA-C1A	7.20	109.94	106.71
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	610	CHL	C4A-NA-C1A	7.10	109.90	106.71
5	A	604	CLA	C4A-NA-C1A	7.04	109.87	106.71
2	C	501	LUX	C28-C27-C26	7.03	127.52	114.23
2	C	502	LUX	C1-C6-C5	-6.95	112.83	122.61
6	A	610	CHL	C4A-NA-C1A	6.94	109.83	106.71
3	B	503	NEX	C1-C2-C3	6.94	129.31	113.64
6	A	613	CHL	C4A-NA-C1A	6.93	109.82	106.71
3	C	503	NEX	C1-C2-C3	6.86	129.14	113.64
3	A	503	NEX	C1-C2-C3	6.83	129.06	113.64
2	B	502	LUX	C37-C21-C26	-6.13	98.28	110.44
2	C	502	LUX	C37-C21-C26	-5.92	98.69	110.44
4	B	504	XAT	O4-C5-C18	-5.88	108.00	115.06
2	B	502	LUX	C36-C21-C22	5.71	120.25	109.44
2	C	502	LUX	C31-C30-C29	5.68	134.26	115.92
7	A	801	LHG	C25-C24-C23	5.65	134.18	113.62
2	C	501	LUX	C22-C23-C24	-5.65	105.31	111.74
2	A	501	LUX	C28-C27-C26	5.65	124.92	114.23
2	A	502	LUX	C1-C6-C5	-5.52	114.84	122.61
4	A	504	XAT	C19-C9-C10	-5.46	115.27	122.92
2	B	501	LUX	C36-C21-C26	-5.43	99.67	110.44
7	C	801	LHG	C25-C24-C23	5.33	133.00	113.62
2	B	502	LUX	C31-C30-C29	5.28	132.97	115.92
7	B	801	LHG	C25-C24-C23	5.27	132.77	113.62
2	B	501	LUX	C36-C21-C22	5.24	119.36	109.44
2	B	502	LUX	C18-C5-C6	-5.19	118.70	124.53
2	A	501	LUX	C36-C21-C26	-5.18	100.17	110.44
8	C	802	DGD	O6D-C5D-C6D	5.16	117.09	106.67
5	C	601	CLA	CAA-C2A-C3A	-5.14	98.69	112.78
8	A	802	DGD	O6D-C5D-C6D	5.14	117.04	106.67
2	B	501	LUX	C22-C23-C24	-5.07	105.97	111.74
5	A	601	CLA	CMB-C2B-C1B	-5.05	120.71	128.46
3	B	503	NEX	C39-C29-C30	-5.04	115.86	122.92
2	C	502	LUX	C36-C21-C22	4.94	118.78	109.44
8	B	802	DGD	O6D-C5D-C6D	4.90	116.56	106.67
5	C	601	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
2	C	501	LUX	C36-C21-C26	-4.88	100.76	110.44
3	C	503	NEX	C40-C33-C34	-4.88	116.09	122.92
2	A	502	LUX	C36-C21-C22	4.81	118.55	109.44
4	C	504	XAT	C18-C5-C4	4.77	119.65	114.28
2	A	502	LUX	C31-C30-C29	4.72	131.18	115.92
4	C	504	XAT	C25-C24-C23	-4.70	103.45	112.75
2	B	502	LUX	C2-C3-C4	-4.70	103.88	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	NEX	C39-C29-C30	-4.69	116.35	122.92
4	A	504	XAT	C25-C24-C23	-4.68	103.49	112.75
6	A	611	CHL	C4D-C3D-CAD	-4.64	105.88	108.47
2	B	502	LUX	C19-C9-C8	4.62	121.06	110.86
5	B	601	CLA	CAA-C2A-C3A	-4.54	100.34	112.78
2	A	502	LUX	C18-C5-C6	-4.54	119.43	124.53
5	A	605	CLA	O2D-CGD-CBD	4.52	119.30	111.27
4	C	504	XAT	O4-C5-C18	-4.50	109.66	115.06
3	C	503	NEX	C39-C29-C30	-4.50	116.62	122.92
5	A	601	CLA	C4D-C3D-CAD	-4.48	105.97	108.47
3	A	503	NEX	O24-C25-C38	-4.48	109.69	115.06
8	C	802	DGD	C3G-O3G-C1D	-4.43	106.49	113.84
3	B	503	NEX	C28-C29-C30	4.40	125.70	118.94
6	C	614	CHL	O2D-CGD-CBD	4.39	119.07	111.27
5	B	604	CLA	CAA-C2A-C3A	-4.37	100.81	112.78
6	B	609	CHL	O2D-CGD-CBD	4.35	119.00	111.27
2	A	501	LUX	C36-C21-C22	4.34	117.66	109.44
4	B	504	XAT	C15-C14-C13	-4.34	121.11	127.31
5	C	607	CLA	O2D-CGD-CBD	4.31	118.93	111.27
2	A	501	LUX	C31-C30-C29	4.31	129.84	115.92
8	A	802	DGD	O5D-C1E-C2E	4.29	115.01	108.30
5	C	603	CLA	CMB-C2B-C1B	-4.29	121.86	128.46
5	A	607	CLA	O2D-CGD-CBD	4.28	118.88	111.27
6	A	609	CHL	O2D-CGD-CBD	4.28	118.87	111.27
2	C	502	LUX	C15-C14-C13	4.27	129.72	115.92
4	A	504	XAT	C40-C33-C34	-4.26	116.95	122.92
4	B	504	XAT	C25-C24-C23	-4.26	104.31	112.75
5	C	601	CLA	C4D-C3D-CAD	-4.23	106.11	108.47
6	A	614	CHL	O2D-CGD-CBD	4.22	118.77	111.27
2	C	501	LUX	C36-C21-C22	4.22	117.42	109.44
5	A	604	CLA	CAA-C2A-C3A	-4.22	101.24	112.78
5	B	607	CLA	O2D-CGD-CBD	4.22	118.76	111.27
6	B	614	CHL	O2D-CGD-CBD	4.20	118.74	111.27
2	B	501	LUX	C31-C30-C29	4.20	129.50	115.92
2	C	501	LUX	C31-C30-C29	4.20	129.50	115.92
5	B	603	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
2	A	501	LUX	C22-C23-C24	-4.17	106.99	111.74
2	B	501	LUX	C19-C9-C8	4.17	120.07	110.86
7	C	801	LHG	O8-C23-C24	4.16	124.95	111.91
5	A	606	CLA	CMB-C2B-C1B	-4.12	122.12	128.46
5	A	603	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
8	B	802	DGD	C3G-O3G-C1D	-4.09	107.06	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	604	CLA	CAA-C2A-C3A	-4.07	101.62	112.78
4	A	504	XAT	O4-C5-C18	-4.07	110.18	115.06
2	C	502	LUX	C19-C9-C8	4.06	119.83	110.86
5	B	605	CLA	OBD-CAD-CBD	-4.05	120.10	125.89
4	B	504	XAT	C19-C9-C10	-4.03	117.28	122.92
5	C	605	CLA	OBD-CAD-CBD	-4.03	120.14	125.89
6	B	611	CHL	C1-C2-C3	4.01	132.99	126.04
6	C	613	CHL	CMB-C2B-C1B	-4.01	122.30	128.46
2	A	502	LUX	C15-C14-C13	4.01	128.88	115.92
5	C	604	CLA	C4D-C3D-CAD	-4.00	106.24	108.47
7	B	801	LHG	O8-C23-C24	4.00	124.47	111.91
3	A	503	NEX	C28-C29-C30	3.99	125.06	118.94
2	B	502	LUX	C31-C32-C33	3.99	128.81	115.92
2	A	501	LUX	C3-C4-C5	3.99	119.80	111.85
6	A	612	CHL	O2D-CGD-CBD	3.98	118.34	111.27
5	C	604	CLA	OBD-CAD-CBD	-3.98	120.21	125.89
2	A	502	LUX	C3-C4-C5	3.98	119.78	111.85
5	B	606	CLA	O2D-CGD-CBD	3.94	118.28	111.27
5	C	606	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
2	C	501	LUX	C11-C12-C13	3.92	128.60	115.92
5	C	604	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
5	B	602	CLA	C4D-C3D-CAD	-3.90	106.30	108.47
4	B	504	XAT	C12-C13-C14	3.89	124.91	118.94
2	B	502	LUX	C37-C21-C22	-3.89	102.07	109.44
3	B	503	NEX	C40-C33-C34	-3.88	117.48	122.92
2	A	501	LUX	C19-C9-C8	3.88	119.43	110.86
8	C	802	DGD	O5D-C1E-C2E	3.88	114.36	108.30
6	B	613	CHL	CMB-C2B-C1B	-3.87	122.51	128.46
2	B	501	LUX	C1-C6-C5	-3.87	117.16	122.61
6	B	612	CHL	O2D-CGD-CBD	3.86	118.14	111.27
2	B	502	LUX	C15-C14-C13	3.86	128.40	115.92
2	C	501	LUX	C10-C9-C8	3.86	121.44	110.59
5	B	605	CLA	O2D-CGD-CBD	3.85	118.12	111.27
2	C	501	LUX	C3-C4-C5	3.84	119.50	111.85
6	C	609	CHL	O2D-CGD-CBD	3.83	118.08	111.27
7	A	801	LHG	O8-C23-C24	3.83	123.93	111.91
5	A	601	CLA	O2A-CGA-CBA	3.83	123.92	111.91
2	C	502	LUX	C18-C5-C4	3.82	121.44	114.36
5	C	604	CLA	O2D-CGD-CBD	3.81	118.05	111.27
5	A	604	CLA	O2D-CGD-CBD	3.81	118.04	111.27
4	A	504	XAT	C19-C9-C8	3.81	124.08	118.08
5	A	608	CLA	O2D-CGD-CBD	3.81	118.04	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	CLA	CAA-C2A-C3A	-3.81	102.36	112.78
2	B	502	LUX	C3-C4-C5	3.80	119.43	111.85
5	B	605	CLA	C4D-C3D-CAD	-3.79	106.36	108.47
2	B	501	LUX	C11-C12-C13	3.79	128.18	115.92
2	B	501	LUX	O23-C23-C22	3.79	120.33	110.74
3	A	503	NEX	C38-C25-C24	3.79	118.55	114.28
8	C	802	DGD	O6E-C5E-C6E	3.78	115.83	106.44
2	A	502	LUX	C11-C12-C13	3.78	128.13	115.92
5	A	606	CLA	O2D-CGD-CBD	3.77	117.97	111.27
5	B	608	CLA	C4D-C3D-CAD	-3.77	106.37	108.47
2	A	502	LUX	C2-C3-C4	-3.76	105.16	110.30
6	A	613	CHL	CMB-C2B-C1B	-3.75	122.70	128.46
5	C	605	CLA	O2D-CGD-CBD	3.75	117.93	111.27
8	B	802	DGD	O5D-C1E-C2E	3.75	114.15	108.30
6	C	611	CHL	C4D-C3D-CAD	-3.74	106.38	108.47
8	B	802	DGD	O6E-C5E-C6E	3.73	115.71	106.44
5	C	605	CLA	C11-C10-C8	3.72	127.95	115.92
2	B	501	LUX	C3-C4-C5	3.72	119.25	111.85
5	A	605	CLA	C11-C10-C8	3.71	127.92	115.92
6	B	612	CHL	OBD-CAD-CBD	-3.71	120.59	125.89
3	B	503	NEX	C35-C34-C33	-3.71	122.02	127.31
5	B	606	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
5	B	603	CLA	O2D-CGD-CBD	3.70	117.84	111.27
2	A	502	LUX	C19-C9-C8	3.69	119.00	110.86
2	C	502	LUX	C1-C2-C3	-3.68	105.33	113.64
5	C	606	CLA	O2D-CGD-CBD	3.68	117.80	111.27
5	C	601	CLA	O2A-CGA-CBA	3.67	123.43	111.91
5	A	605	CLA	OBD-CAD-CBD	-3.67	120.65	125.89
5	A	608	CLA	C4D-C3D-CAD	-3.66	106.43	108.47
2	A	502	LUX	C31-C32-C33	3.66	127.75	115.92
2	A	501	LUX	C10-C9-C8	3.65	120.86	110.59
8	A	802	DGD	O6E-C5E-C6E	3.65	115.52	106.44
2	B	501	LUX	C10-C9-C8	3.64	120.82	110.59
2	A	501	LUX	C11-C12-C13	3.63	127.66	115.92
3	B	503	NEX	O24-C25-C38	-3.63	110.71	115.06
6	C	612	CHL	O2D-CGD-CBD	3.63	117.71	111.27
8	A	802	DGD	C3G-O3G-C1D	-3.61	107.85	113.84
4	C	504	XAT	O3-C3-C4	3.60	116.95	109.80
5	A	601	CLA	CMB-C2B-C3B	3.60	131.41	124.68
5	B	601	CLA	O2A-CGA-CBA	3.58	123.14	111.91
4	B	504	XAT	C40-C33-C34	-3.58	117.91	122.92
6	B	610	CHL	O2D-CGD-CBD	3.58	117.62	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	XAT	C35-C34-C33	-3.57	122.22	127.31
2	B	502	LUX	C22-C23-C24	-3.57	107.68	111.74
2	C	502	LUX	C37-C21-C22	-3.56	102.69	109.44
6	A	613	CHL	O2D-CGD-CBD	3.56	117.60	111.27
3	C	503	NEX	C28-C29-C30	3.56	124.40	118.94
6	A	611	CHL	OBD-CAD-CBD	-3.56	120.81	125.89
6	B	610	CHL	O2A-CGA-CBA	3.55	123.06	111.91
6	A	610	CHL	O2A-CGA-CBA	3.55	123.06	111.91
8	C	802	DGD	O5D-C6D-C5D	3.54	115.59	109.05
4	A	504	XAT	C27-C28-C29	-3.53	120.06	125.53
6	C	611	CHL	C1-C2-C3	3.52	132.14	126.04
4	A	504	XAT	C35-C34-C33	-3.52	122.28	127.31
5	C	602	CLA	C11-C10-C8	3.52	127.30	115.92
2	C	502	LUX	C36-C21-C26	-3.52	103.47	110.44
6	C	611	CHL	OBD-CAD-CBD	-3.51	120.88	125.89
5	A	601	CLA	O2D-CGD-CBD	3.51	117.50	111.27
5	A	607	CLA	CAA-C2A-C3A	-3.50	103.18	112.78
3	C	503	NEX	C35-C34-C33	-3.50	122.31	127.31
5	B	608	CLA	O2D-CGD-CBD	3.50	117.49	111.27
5	B	607	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
6	C	610	CHL	O2A-CGA-CBA	3.50	122.89	111.91
5	B	608	CLA	O2A-CGA-CBA	3.50	122.89	111.91
3	A	503	NEX	C35-C34-C33	-3.50	122.32	127.31
2	A	501	LUX	C35-C34-C33	3.49	127.22	115.92
5	B	602	CLA	C11-C10-C8	3.49	127.21	115.92
5	B	607	CLA	OBD-CAD-CBD	-3.49	120.91	125.89
5	A	607	CLA	OBD-CAD-CBD	-3.48	120.92	125.89
5	A	602	CLA	C4D-C3D-CAD	-3.48	106.53	108.47
5	B	603	CLA	CBA-CAA-C2A	3.47	124.11	113.86
6	C	614	CHL	C4D-C3D-CAD	-3.47	106.54	108.47
5	B	604	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
6	A	610	CHL	O2D-CGD-CBD	3.46	117.42	111.27
5	B	605	CLA	C11-C10-C8	3.46	127.10	115.92
2	C	501	LUX	C19-C9-C10	3.46	121.12	110.99
5	C	608	CLA	O2A-CGA-CBA	3.45	122.75	111.91
5	C	607	CLA	CAA-C2A-C3A	-3.45	103.32	112.78
5	A	602	CLA	OBD-CAD-CBD	-3.45	120.96	125.89
5	B	606	CLA	O2A-CGA-CBA	3.45	122.74	111.91
5	C	608	CLA	CBC-CAC-C3C	-3.45	102.92	112.43
5	A	608	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
5	A	602	CLA	C11-C10-C8	3.44	127.04	115.92
2	A	502	LUX	C10-C9-C8	3.43	120.23	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	603	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
6	A	611	CHL	CAA-C2A-C3A	-3.43	103.39	112.78
5	B	604	CLA	OBD-CAD-CBD	-3.42	121.00	125.89
2	C	502	LUX	C10-C9-C8	3.42	120.21	110.59
6	B	612	CHL	C4D-C3D-CAD	-3.41	106.57	108.47
5	A	604	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
5	C	606	CLA	C4D-C3D-CAD	-3.40	106.57	108.47
5	C	604	CLA	O2A-CGA-CBA	3.40	122.57	111.91
6	C	611	CHL	OMC-CMC-C2C	-3.39	118.03	125.69
5	B	602	CLA	OBD-CAD-CBD	-3.38	121.06	125.89
5	B	607	CLA	C4D-C3D-CAD	-3.38	106.58	108.47
6	B	611	CHL	OMC-CMC-C2C	-3.38	118.05	125.69
5	B	603	CLA	CAA-C2A-C3A	-3.37	103.55	112.78
4	C	504	XAT	C19-C9-C10	-3.37	118.20	122.92
4	B	504	XAT	C17-C1-C2	-3.37	103.13	108.98
5	C	606	CLA	O2A-CGA-CBA	3.37	122.47	111.91
6	B	613	CHL	O2D-CGD-CBD	3.36	117.24	111.27
6	A	611	CHL	C1-C2-C3	3.36	131.85	126.04
4	A	504	XAT	C12-C13-C14	3.36	124.10	118.94
2	A	501	LUX	C18-C5-C4	3.35	120.56	114.36
3	C	503	NEX	C37-C21-C36	-3.35	102.43	107.37
5	A	606	CLA	O2A-CGA-CBA	3.34	122.40	111.91
5	C	608	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
5	C	603	CLA	O2A-CGA-CBA	3.34	122.39	111.91
3	C	503	NEX	C16-C1-C6	3.34	113.46	110.47
3	B	503	NEX	C38-C25-C24	3.34	118.04	114.28
2	A	502	LUX	C19-C9-C10	3.34	120.76	110.99
6	B	611	CHL	CMB-C2B-C1B	-3.34	123.34	128.46
6	C	613	CHL	O2D-CGD-CBD	3.33	117.19	111.27
4	C	504	XAT	C27-C28-C29	-3.33	120.36	125.53
2	A	502	LUX	C35-C34-C33	3.33	126.68	115.92
5	B	603	CLA	O2A-CGA-CBA	3.33	122.35	111.91
3	C	503	NEX	C37-C21-C22	3.33	114.76	108.98
6	B	611	CHL	CAA-C2A-C3A	-3.32	103.67	112.78
5	C	607	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
5	C	603	CLA	O2D-CGD-CBD	3.31	117.16	111.27
4	C	504	XAT	C15-C14-C13	-3.31	122.59	127.31
2	C	501	LUX	C35-C34-C33	3.30	126.58	115.92
4	A	504	XAT	C37-C21-C36	3.30	112.23	107.37
5	C	601	CLA	C11-C10-C8	3.29	126.56	115.92
2	B	501	LUX	C18-C5-C6	-3.29	120.83	124.53
5	A	608	CLA	CAA-C2A-C3A	-3.29	103.78	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	608	CLA	O2A-CGA-CBA	3.28	122.21	111.91
5	B	604	CLA	O2D-CGD-CBD	3.28	117.10	111.27
5	B	601	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
5	C	607	CLA	C11-C10-C8	3.28	126.51	115.92
6	C	612	CHL	CAA-C2A-C3A	-3.27	103.81	112.78
5	A	605	CLA	C4D-C3D-CAD	-3.26	106.65	108.47
5	B	607	CLA	C11-C10-C8	3.26	126.47	115.92
2	C	501	LUX	C1-C2-C3	3.26	121.01	113.64
5	A	604	CLA	O2A-CGA-CBA	3.26	122.14	111.91
5	C	605	CLA	C4D-C3D-CAD	-3.26	106.65	108.47
5	C	603	CLA	CBA-CAA-C2A	3.25	123.46	113.86
5	A	605	CLA	O2A-CGA-CBA	3.25	122.11	111.91
5	C	605	CLA	O2A-CGA-CBA	3.25	122.11	111.91
2	C	501	LUX	O23-C23-C24	3.24	117.85	110.53
2	C	502	LUX	C35-C34-C33	3.23	126.37	115.92
2	A	501	LUX	C39-C29-C30	3.23	122.98	111.29
6	B	612	CHL	CAA-C2A-C3A	-3.23	103.94	112.78
5	C	608	CLA	O2D-CGD-CBD	3.22	117.00	111.27
5	C	603	CLA	CMB-C2B-C3B	3.22	130.70	124.68
2	C	501	LUX	C18-C5-C6	-3.21	120.93	124.53
2	A	502	LUX	C18-C5-C4	3.21	120.29	114.36
6	C	610	CHL	OMC-CMC-C2C	-3.20	118.44	125.69
4	C	504	XAT	C40-C33-C34	-3.20	118.44	122.92
5	A	603	CLA	O2A-CGA-CBA	3.20	121.94	111.91
4	C	504	XAT	C38-C25-C24	3.19	117.87	114.28
5	A	607	CLA	C11-C10-C8	3.19	126.23	115.92
5	C	603	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
2	C	502	LUX	C11-C12-C13	3.18	126.19	115.92
6	A	612	CHL	CAA-C2A-C3A	-3.18	104.08	112.78
3	B	503	NEX	C16-C1-C6	3.17	113.31	110.47
2	B	502	LUX	C10-C9-C8	3.16	119.49	110.59
2	A	502	LUX	C40-C33-C34	3.16	122.74	111.29
5	C	602	CLA	OBD-CAD-CBD	-3.16	121.38	125.89
6	C	613	CHL	CMB-C2B-C3B	3.16	130.59	124.68
5	B	602	CLA	O2A-CGA-CBA	3.15	121.80	111.91
2	B	502	LUX	C39-C29-C30	3.15	122.70	111.29
5	B	601	CLA	C11-C10-C8	3.15	126.10	115.92
6	C	613	CHL	C4D-C3D-CAD	-3.15	106.72	108.47
6	A	612	CHL	C1-C2-C3	3.14	131.48	126.04
2	C	502	LUX	C31-C32-C33	3.14	126.07	115.92
2	C	502	LUX	C20-C13-C12	3.14	122.66	111.29
5	A	603	CLA	CBA-CAA-C2A	3.14	123.12	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	611	CHL	C4D-C3D-CAD	-3.13	106.72	108.47
2	B	501	LUX	C15-C14-C13	3.13	126.04	115.92
5	B	607	CLA	C1-C2-C3	3.13	131.45	126.04
2	B	501	LUX	C35-C34-C33	3.13	126.02	115.92
6	B	613	CHL	OBD-CAD-CBD	-3.12	121.43	125.89
6	C	611	CHL	CMB-C2B-C1B	-3.12	123.67	128.46
2	C	501	LUX	O23-C23-C22	3.11	118.62	110.74
2	B	502	LUX	C36-C21-C26	-3.11	104.26	110.44
5	A	602	CLA	O2A-CGA-CBA	3.11	121.67	111.91
4	B	504	XAT	C20-C13-C14	-3.11	118.57	122.92
6	B	614	CHL	C4D-C3D-CAD	-3.10	106.74	108.47
5	A	607	CLA	C4D-C3D-CAD	-3.10	106.74	108.47
6	B	609	CHL	O2A-CGA-CBA	3.10	121.63	111.91
6	C	610	CHL	O2D-CGD-CBD	3.09	116.77	111.27
6	B	612	CHL	C1-C2-C3	3.09	131.39	126.04
7	B	801	LHG	O7-C7-C8	3.09	118.16	111.50
2	B	501	LUX	C20-C13-C12	3.09	122.47	111.29
5	A	603	CLA	CMB-C2B-C3B	3.08	130.44	124.68
5	A	603	CLA	C4D-C3D-CAD	-3.08	106.75	108.47
6	A	612	CHL	C4D-C3D-CAD	-3.08	106.75	108.47
5	B	601	CLA	C4D-C3D-CAD	-3.07	106.76	108.47
2	C	502	LUX	C19-C9-C10	3.07	119.97	110.99
4	B	504	XAT	C31-C30-C29	-3.06	122.94	127.31
6	A	614	CHL	C4D-C3D-CAD	-3.06	106.77	108.47
5	A	608	CLA	OBD-CAD-CBD	-3.05	121.53	125.89
5	C	601	CLA	CMB-C2B-C3B	3.05	130.39	124.68
4	C	504	XAT	C18-C5-C6	-3.05	117.15	122.26
6	B	611	CHL	OBD-CAD-CBD	-3.05	121.54	125.89
3	C	503	NEX	C38-C25-C24	3.04	117.70	114.28
2	C	502	LUX	C7-C6-C5	-3.04	114.10	121.46
6	C	609	CHL	OMC-CMC-C2C	-3.04	118.82	125.69
5	A	601	CLA	OBD-CAD-CBD	-3.04	121.56	125.89
6	B	613	CHL	C4D-C3D-CAD	-3.04	106.78	108.47
5	A	601	CLA	C11-C10-C8	3.03	125.72	115.92
5	C	602	CLA	O2A-CGA-CBA	3.03	121.42	111.91
6	B	609	CHL	OBD-CAD-CBD	-3.03	121.57	125.89
5	B	606	CLA	C4D-C3D-CAD	-3.03	106.78	108.47
2	A	501	LUX	C15-C14-C13	3.02	125.70	115.92
2	A	502	LUX	C20-C13-C12	3.02	122.24	111.29
5	A	608	CLA	C3A-C2A-C1A	3.02	105.86	101.34
2	A	501	LUX	C2-C3-C4	3.01	114.43	110.30
6	A	611	CHL	CMB-C2B-C1B	-3.01	123.83	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	604	CLA	C4D-C3D-CAD	-3.01	106.79	108.47
5	C	602	CLA	C4D-C3D-CAD	-3.01	106.79	108.47
5	A	604	CLA	C4D-C3D-CAD	-3.01	106.79	108.47
2	A	502	LUX	C37-C21-C22	-3.01	103.73	109.44
6	A	613	CHL	CMB-C2B-C3B	3.01	130.31	124.68
6	A	611	CHL	O2D-CGD-CBD	3.01	116.61	111.27
6	C	612	CHL	C1-C2-C3	3.00	131.24	126.04
6	B	612	CHL	O2A-CGA-CBA	3.00	121.33	111.91
5	A	604	CLA	C2A-C3A-C4A	2.99	106.70	101.87
6	A	611	CHL	OMC-CMC-C2C	-2.99	118.92	125.69
6	B	611	CHL	O2A-CGA-CBA	2.99	121.30	111.91
2	A	502	LUX	C8-C7-C6	-2.99	119.99	125.96
5	B	605	CLA	O2A-CGA-CBA	2.99	121.29	111.91
2	C	502	LUX	C39-C29-C30	2.99	122.11	111.29
2	B	501	LUX	C40-C33-C34	2.98	122.08	111.29
2	C	501	LUX	C19-C9-C8	2.98	117.44	110.86
5	C	608	CLA	CAA-C2A-C3A	-2.98	104.63	112.78
2	A	501	LUX	C19-C9-C10	2.98	119.70	110.99
5	B	604	CLA	O2A-CGA-CBA	2.97	121.24	111.91
6	B	614	CHL	CMB-C2B-C1B	-2.97	123.90	128.46
6	C	613	CHL	OBD-CAD-CBD	-2.97	121.65	125.89
3	C	503	NEX	C38-C25-C26	-2.97	117.29	122.26
4	A	504	XAT	C15-C14-C13	-2.96	123.08	127.31
2	B	501	LUX	C18-C5-C4	2.96	119.84	114.36
6	A	612	CHL	O2A-CGA-CBA	2.96	121.20	111.91
5	B	608	CLA	OBD-CAD-CBD	-2.96	121.67	125.89
2	A	502	LUX	C1-C2-C3	-2.95	106.97	113.64
6	A	613	CHL	OBD-CAD-CBD	-2.95	121.68	125.89
4	B	504	XAT	C38-C25-C24	2.95	117.60	114.28
5	A	603	CLA	O2D-CGD-CBD	2.95	116.50	111.27
6	C	612	CHL	CMB-C2B-C1B	-2.95	123.94	128.46
6	A	609	CHL	O2A-CGA-CBA	2.94	121.15	111.91
6	B	613	CHL	CMB-C2B-C3B	2.94	130.18	124.68
5	B	602	CLA	O2D-CGD-CBD	2.94	116.49	111.27
5	C	607	CLA	C4D-C3D-CAD	-2.94	106.83	108.47
5	B	603	CLA	CMB-C2B-C3B	2.93	130.17	124.68
4	A	504	XAT	O3-C3-C4	2.93	115.63	109.80
2	B	502	LUX	C20-C13-C14	2.93	121.90	111.29
5	B	604	CLA	C2A-C3A-C4A	2.93	106.60	101.87
6	C	609	CHL	CMA-C3A-C4A	-2.93	103.90	111.77
2	B	501	LUX	C39-C29-C28	2.93	121.89	111.29
5	A	607	CLA	CMB-C2B-C1B	-2.92	123.97	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	503	NEX	C27-C28-C29	-2.92	121.00	125.53
5	A	606	CLA	CMB-C2B-C3B	2.92	130.13	124.68
6	A	611	CHL	O2A-CGA-CBA	2.90	121.02	111.91
6	C	611	CHL	CAA-C2A-C3A	-2.90	104.83	112.78
2	C	501	LUX	C40-C33-C34	2.90	121.81	111.29
2	C	501	LUX	C39-C29-C30	2.90	121.81	111.29
5	B	605	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
2	C	502	LUX	C8-C7-C6	-2.89	120.19	125.96
6	C	611	CHL	O2A-CGA-CBA	2.89	120.97	111.91
6	A	609	CHL	CMA-C3A-C4A	-2.88	104.02	111.77
2	B	502	LUX	C19-C9-C10	2.88	119.42	110.99
6	B	611	CHL	O2D-CGD-CBD	2.88	116.38	111.27
5	A	604	CLA	OBD-CAD-CBD	-2.87	121.79	125.89
6	C	609	CHL	O2A-CGA-CBA	2.87	120.92	111.91
6	C	612	CHL	OBD-CAD-CBD	-2.87	121.80	125.89
2	B	502	LUX	C35-C34-C33	2.87	125.19	115.92
5	C	604	CLA	CMB-C2B-C3B	2.87	130.04	124.68
2	B	502	LUX	C40-C33-C34	2.87	121.67	111.29
2	C	502	LUX	C40-C33-C34	2.86	121.66	111.29
5	C	601	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
6	C	613	CHL	OMC-CMC-C2C	-2.86	119.22	125.69
6	B	614	CHL	OBD-CAD-CBD	-2.86	121.81	125.89
5	A	605	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
5	A	602	CLA	O2D-CGD-CBD	2.86	116.35	111.27
5	C	607	CLA	OBD-CAD-CBD	-2.85	121.83	125.89
6	B	609	CHL	CMA-C3A-C4A	-2.84	104.13	111.77
2	A	502	LUX	C36-C21-C26	-2.84	104.80	110.44
5	B	603	CLA	C2A-C3A-C4A	2.84	106.46	101.87
4	A	504	XAT	C17-C1-C2	-2.84	104.05	108.98
5	B	601	CLA	OBD-CAD-CBD	-2.84	121.84	125.89
4	B	504	XAT	C36-C21-C22	2.84	113.91	108.98
5	B	607	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
5	A	607	CLA	O2A-CGA-CBA	2.82	120.77	111.91
5	B	608	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
5	C	606	CLA	OBD-CAD-CBD	-2.82	121.87	125.89
6	B	610	CHL	C1-C2-C3	2.82	130.92	126.04
6	B	609	CHL	C4D-C3D-CAD	-2.81	106.90	108.47
6	C	609	CHL	OBD-CAD-CBD	-2.81	121.88	125.89
5	C	607	CLA	C1-C2-C3	2.81	130.91	126.04
6	C	610	CHL	OBD-CAD-CBD	-2.81	121.88	125.89
5	C	601	CLA	CBC-CAC-C3C	-2.81	104.69	112.43
5	A	601	CLA	CAA-CBA-CGA	-2.80	105.06	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	LUX	C39-C29-C30	2.80	121.45	111.29
2	B	502	LUX	C11-C12-C13	2.80	124.97	115.92
4	A	504	XAT	C32-C33-C34	2.79	123.23	118.94
2	C	501	LUX	C31-C32-C33	2.79	124.94	115.92
2	A	501	LUX	C20-C13-C12	2.79	121.40	111.29
4	C	504	XAT	C12-C13-C14	2.79	123.22	118.94
6	C	612	CHL	O2A-CGA-CBA	2.79	120.66	111.91
5	B	602	CLA	C1-C2-C3	2.79	130.86	126.04
6	A	610	CHL	OBD-CAD-CBD	-2.79	121.91	125.89
6	B	614	CHL	OMC-CMC-C2C	-2.78	119.39	125.69
6	A	614	CHL	OBD-CAD-CBD	-2.78	121.92	125.89
6	A	613	CHL	C4D-C3D-CAD	-2.78	106.92	108.47
8	A	802	DGD	O5D-C6D-C5D	2.78	114.19	109.05
5	C	608	CLA	OBD-CAD-CBD	-2.77	121.93	125.89
2	B	501	LUX	C19-C9-C10	2.77	119.11	110.99
6	A	609	CHL	CMB-C2B-C1B	-2.77	124.20	128.46
4	B	504	XAT	C18-C5-C4	2.77	117.40	114.28
5	A	607	CLA	C1-C2-C3	2.77	130.83	126.04
5	C	608	CLA	C4D-C3D-CAD	-2.77	106.93	108.47
5	A	603	CLA	OBD-CAD-CBD	-2.76	121.95	125.89
4	B	504	XAT	O3-C3-C4	2.76	115.29	109.80
5	A	606	CLA	C1-C2-C3	2.75	130.80	126.04
4	A	504	XAT	C18-C5-C4	2.75	117.37	114.28
5	C	607	CLA	O2A-CGA-CBA	2.75	120.53	111.91
6	C	613	CHL	CAA-CBA-CGA	-2.75	107.69	113.59
6	C	614	CHL	CMB-C2B-C1B	-2.74	124.25	128.46
3	A	503	NEX	C40-C33-C34	-2.73	119.09	122.92
6	B	610	CHL	OMC-CMC-C2C	-2.73	119.51	125.69
2	A	501	LUX	C40-C33-C32	2.72	121.16	111.29
2	C	502	LUX	C39-C29-C28	2.72	121.15	111.29
5	B	606	CLA	OBD-CAD-CBD	-2.72	122.01	125.89
2	C	502	LUX	C3-C4-C5	2.72	117.27	111.85
3	B	503	NEX	C38-C25-C26	-2.71	117.71	122.26
5	C	601	CLA	O2D-CGD-CBD	2.71	116.09	111.27
6	A	611	CHL	C17-C16-C15	2.71	125.70	113.24
5	C	601	CLA	CED-O2D-CGD	2.71	122.07	115.94
5	B	601	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
2	B	502	LUX	C8-C7-C6	-2.71	120.55	125.96
6	A	614	CHL	CAA-C2A-C3A	-2.71	109.78	116.10
5	C	606	CLA	CMB-C2B-C3B	2.70	129.74	124.68
6	A	612	CHL	OBD-CAD-CBD	-2.70	122.03	125.89
2	A	501	LUX	C40-C33-C34	2.70	121.06	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	609	CHL	C2C-C3C-C4C	2.69	108.41	106.49
8	C	802	DGD	O6D-C1D-C2D	2.69	116.05	110.35
6	C	611	CHL	O2D-CGD-CBD	2.69	116.05	111.27
6	C	612	CHL	C4D-C3D-CAD	-2.68	106.97	108.47
5	B	607	CLA	O2A-CGA-CBA	2.68	120.32	111.91
6	B	610	CHL	C4D-C3D-CAD	-2.67	106.98	108.47
5	A	601	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
5	C	602	CLA	O2D-CGD-CBD	2.67	116.02	111.27
5	A	606	CLA	OBD-CAD-CBD	-2.66	122.09	125.89
6	B	612	CHL	CMB-C2B-C1B	-2.66	124.37	128.46
6	A	614	CHL	CMB-C2B-C1B	-2.66	124.37	128.46
5	C	605	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
5	A	606	CLA	C4D-C3D-CAD	-2.66	106.99	108.47
5	B	604	CLA	CMB-C2B-C3B	2.66	129.66	124.68
2	B	502	LUX	C18-C5-C4	2.66	119.28	114.36
5	A	602	CLA	C1-C2-C3	2.66	130.64	126.04
6	A	614	CHL	OMC-CMC-C2C	-2.66	119.68	125.69
5	B	606	CLA	CMB-C2B-C3B	2.65	129.64	124.68
2	B	501	LUX	C31-C32-C33	2.64	124.46	115.92
2	A	502	LUX	C35-C15-C14	2.64	122.97	113.62
6	A	609	CHL	OBD-CAD-CBD	-2.64	122.12	125.89
5	C	604	CLA	C2A-C3A-C4A	2.64	106.13	101.87
6	B	609	CHL	CMB-C2B-C1B	-2.64	124.41	128.46
2	C	502	LUX	C2-C3-C4	-2.63	106.70	110.30
2	C	501	LUX	C15-C14-C13	2.63	124.42	115.92
6	C	614	CHL	OBD-CAD-CBD	-2.63	122.14	125.89
5	B	603	CLA	C4D-C3D-CAD	-2.63	107.00	108.47
2	B	502	LUX	C20-C13-C12	2.63	120.80	111.29
6	C	610	CHL	CED-O2D-CGD	2.63	121.88	115.94
6	C	612	CHL	C1D-CHD-C4C	2.62	126.01	122.56
5	C	603	CLA	C2A-C3A-C4A	2.62	106.09	101.87
7	A	801	LHG	O7-C7-C8	2.62	117.14	111.50
6	A	613	CHL	OMC-CMC-C2C	-2.62	119.77	125.69
6	A	610	CHL	CED-O2D-CGD	2.62	121.85	115.94
6	A	610	CHL	CMB-C2B-C1B	-2.61	124.46	128.46
5	B	603	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
5	C	606	CLA	C1-C2-C3	2.60	130.55	126.04
6	B	612	CHL	C1D-CHD-C4C	2.60	125.99	122.56
7	C	801	LHG	O7-C7-C8	2.60	117.11	111.50
2	B	502	LUX	C15-C35-C34	2.60	122.83	113.62
6	C	613	CHL	C3A-C2A-C1A	2.60	105.23	101.34
5	B	602	CLA	CMB-C2B-C1B	-2.59	124.48	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	602	CLA	C1-C2-C3	2.59	130.52	126.04
2	A	502	LUX	C27-C28-C29	2.59	125.89	115.27
5	A	601	CLA	CED-O2D-CGD	2.59	121.78	115.94
4	B	504	XAT	C32-C33-C34	2.58	122.90	118.94
5	C	608	CLA	CMB-C2B-C3B	2.58	129.50	124.68
5	C	607	CLA	C1D-CHD-C4C	2.55	125.93	122.56
6	B	613	CHL	OMC-CMC-C2C	-2.55	119.92	125.69
2	A	501	LUX	C31-C32-C33	2.55	124.15	115.92
4	A	504	XAT	C38-C25-C24	2.54	117.14	114.28
6	C	609	CHL	CMB-C2B-C1B	-2.54	124.56	128.46
3	C	503	NEX	C40-C33-C32	2.54	122.08	118.08
5	A	603	CLA	C2A-C3A-C4A	2.53	105.96	101.87
6	A	613	CHL	CAA-CBA-CGA	-2.53	108.15	113.59
5	B	601	CLA	CMA-C3A-C4A	-2.53	104.97	111.77
6	B	610	CHL	CED-O2D-CGD	2.52	121.64	115.94
5	A	604	CLA	C1D-CHD-C4C	2.51	125.88	122.56
6	C	610	CHL	CMB-C2B-C1B	-2.51	124.60	128.46
6	A	612	CHL	CMB-C2B-C1B	-2.51	124.61	128.46
4	C	504	XAT	C32-C33-C34	2.51	122.79	118.94
2	B	501	LUX	O3-C3-C2	2.50	114.78	109.80
5	B	608	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
6	A	612	CHL	C1D-CHD-C4C	2.50	125.86	122.56
6	A	614	CHL	C2A-C3A-C4A	2.50	104.97	101.78
8	B	802	DGD	O6D-C5D-C4D	2.49	114.22	109.69
5	C	606	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
5	B	605	CLA	C3A-C2A-C1A	2.49	105.06	101.34
2	B	501	LUX	C1-C2-C3	2.49	119.26	113.64
5	B	601	CLA	O2D-CGD-CBD	2.48	115.68	111.27
3	A	503	NEX	C38-C25-C26	-2.48	118.11	122.26
5	C	603	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
6	C	610	CHL	C4D-C3D-CAD	-2.47	107.09	108.47
6	B	614	CHL	C2A-C3A-C4A	2.47	104.94	101.78
8	B	802	DGD	O5D-C6D-C5D	2.47	113.62	109.05
6	C	611	CHL	C17-C16-C15	2.47	124.59	113.24
2	B	501	LUX	C35-C15-C14	2.47	122.36	113.62
6	B	611	CHL	C17-C16-C15	2.47	124.58	113.24
6	B	614	CHL	CAA-C2A-C3A	-2.46	110.35	116.10
2	A	502	LUX	C20-C13-C14	2.46	120.19	111.29
5	A	606	CLA	O2A-CGA-O1A	-2.46	117.40	123.59
4	B	504	XAT	C27-C28-C29	-2.45	121.72	125.53
5	B	604	CLA	C1D-CHD-C4C	2.45	125.79	122.56
6	C	614	CHL	OMC-CMC-C2C	-2.45	120.16	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	603	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
2	A	502	LUX	C15-C35-C34	2.44	122.26	113.62
8	B	802	DGD	O6D-C1D-C2D	2.44	115.51	110.35
6	A	610	CHL	C1-C2-C3	2.44	130.26	126.04
4	B	504	XAT	O4-C5-C4	2.44	115.21	113.38
6	A	612	CHL	C2A-C3A-C4A	2.44	105.81	101.87
2	C	501	LUX	C1-C6-C5	-2.44	119.18	122.61
5	B	607	CLA	C1D-CHD-C4C	2.44	125.77	122.56
2	B	501	LUX	C27-C28-C29	2.44	125.28	115.27
6	B	609	CHL	O2D-CGD-O1D	-2.43	119.09	123.84
5	C	606	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
6	B	610	CHL	CMB-C2B-C1B	-2.43	124.74	128.46
2	A	502	LUX	C39-C29-C28	2.42	120.04	111.29
5	A	603	CLA	C1D-CHD-C4C	2.41	125.74	122.56
5	A	608	CLA	C1D-CHD-C4C	2.41	125.74	122.56
6	A	613	CHL	C3A-C2A-C1A	2.41	104.94	101.34
6	B	610	CHL	OBD-CAD-CBD	-2.41	122.46	125.89
7	B	801	LHG	O10-C23-C24	-2.41	114.34	123.73
5	B	601	CLA	C2A-C3A-C4A	2.41	105.75	101.87
5	B	602	CLA	CMA-C3A-C4A	-2.40	105.31	111.77
6	C	609	CHL	C2A-C3A-C4A	2.40	105.75	101.87
6	C	609	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
6	C	610	CHL	C1-C2-C3	2.40	130.19	126.04
5	B	606	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
6	C	609	CHL	CBA-CAA-C2A	2.40	120.93	113.86
6	A	610	CHL	O2A-CGA-O1A	-2.40	117.55	123.59
5	C	606	CLA	C1D-CHD-C4C	2.40	125.72	122.56
6	B	611	CHL	CMB-C2B-C3B	2.39	129.16	124.68
5	B	601	CLA	CGD-CBD-CAD	2.39	118.47	110.73
5	C	602	CLA	CMA-C3A-C4A	-2.39	105.36	111.77
2	C	501	LUX	C20-C13-C14	2.39	119.93	111.29
7	C	801	LHG	O10-C23-C24	-2.38	114.44	123.73
6	A	610	CHL	OMC-CMC-C2C	-2.38	120.30	125.69
2	C	501	LUX	C18-C5-C4	2.38	118.76	114.36
8	B	802	DGD	C1E-O6E-C5E	2.38	118.35	113.69
2	C	501	LUX	C20-C13-C12	2.37	119.89	111.29
5	A	604	CLA	CMB-C2B-C3B	2.37	129.11	124.68
5	A	607	CLA	C3C-C4C-NC	-2.37	107.92	110.57
5	A	606	CLA	CAA-C2A-C3A	-2.36	106.30	112.78
2	C	501	LUX	C40-C33-C32	2.35	119.81	111.29
5	B	605	CLA	C2A-C1A-CHA	2.35	127.97	123.86
5	A	602	CLA	C3A-C2A-C1A	2.35	104.86	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	613	CHL	C3A-C2A-C1A	2.35	104.85	101.34
6	A	609	CHL	C4D-C3D-CAD	-2.34	107.16	108.47
5	A	602	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
5	C	605	CLA	C3A-C2A-C1A	2.34	104.84	101.34
5	B	606	CLA	C2A-C3A-C4A	2.34	105.65	101.87
5	B	603	CLA	OBD-CAD-CBD	-2.34	122.56	125.89
6	B	614	CHL	C1D-CHD-C4C	2.34	125.64	122.56
2	C	502	LUX	C35-C15-C14	2.33	121.88	113.62
4	A	504	XAT	C37-C21-C26	2.33	116.34	110.05
5	A	605	CLA	C3A-C2A-C1A	2.33	104.83	101.34
2	A	501	LUX	O23-C23-C24	2.33	115.80	110.53
6	B	609	CHL	C2C-C3C-C4C	2.33	108.15	106.49
5	C	605	CLA	OBD-CAD-C3D	2.33	131.84	127.98
8	A	802	DGD	O2G-C1B-C2B	2.32	119.19	111.91
5	C	606	CLA	C3C-C4C-NC	-2.32	107.97	110.57
5	A	606	CLA	C1D-CHD-C4C	2.32	125.62	122.56
5	C	602	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
6	A	612	CHL	OMC-CMC-C2C	-2.32	120.45	125.69
5	A	602	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
8	A	802	DGD	O6D-C1D-C2D	2.31	115.25	110.35
5	B	601	CLA	C5-C3-C2	2.31	125.80	121.12
5	B	606	CLA	C1-C2-C3	2.31	130.04	126.04
6	B	612	CHL	C2A-C3A-C4A	2.31	105.60	101.87
5	B	605	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
6	A	609	CHL	CBA-CAA-C2A	2.30	120.66	113.86
6	A	609	CHL	O2D-CGD-O1D	-2.30	119.33	123.84
2	A	501	LUX	C18-C5-C6	-2.30	121.94	124.53
6	C	614	CHL	CAA-C2A-C3A	-2.30	110.73	116.10
5	B	606	CLA	CMA-C3A-C4A	-2.30	105.60	111.77
3	B	503	NEX	C10-C11-C12	-2.30	116.05	123.22
4	A	504	XAT	C15-C35-C34	-2.30	118.77	123.47
5	B	604	CLA	CAA-CBA-CGA	-2.29	106.55	113.25
5	B	603	CLA	C1D-CHD-C4C	2.29	125.58	122.56
2	A	501	LUX	O23-C23-C22	2.29	116.53	110.74
2	C	502	LUX	C27-C28-C29	2.28	124.62	115.27
5	C	603	CLA	C1D-CHD-C4C	2.27	125.56	122.56
5	A	605	CLA	C1D-CHD-C4C	2.27	125.56	122.56
2	B	502	LUX	C39-C29-C28	2.27	119.50	111.29
5	C	605	CLA	C1D-CHD-C4C	2.26	125.54	122.56
6	B	610	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
2	C	501	LUX	C8-C7-C6	-2.26	121.45	125.96
2	B	501	LUX	C39-C29-C30	2.26	119.46	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	608	CLA	O1D-CGD-CBD	-2.26	119.87	124.48
5	B	602	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
6	C	612	CHL	C2A-C3A-C4A	2.25	105.50	101.87
6	C	610	CHL	O2A-CGA-O1A	-2.25	117.92	123.59
6	C	609	CHL	C4D-C3D-CAD	-2.25	107.22	108.47
5	B	606	CLA	C3C-C4C-NC	-2.24	108.06	110.57
5	A	601	CLA	CMD-C2D-C3D	2.24	128.88	124.68
6	C	611	CHL	OBD-CAD-C3D	2.24	131.70	127.98
5	B	604	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
5	C	604	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
5	B	601	CLA	OBD-CAD-C3D	2.23	131.69	127.98
6	B	614	CHL	C2C-C3C-C4C	2.23	108.08	106.49
5	A	605	CLA	C2A-C1A-CHA	2.23	127.76	123.86
5	A	607	CLA	C1D-CHD-C4C	2.23	125.50	122.56
4	C	504	XAT	C35-C34-C33	-2.23	124.13	127.31
5	C	601	CLA	OBD-CAD-CBD	-2.23	122.71	125.89
6	B	612	CHL	OMC-CMC-C2C	-2.23	120.65	125.69
2	B	502	LUX	C40-C33-C32	2.23	119.35	111.29
8	C	802	DGD	O2G-C1B-C2B	2.22	118.89	111.91
2	A	501	LUX	C27-C28-C29	2.22	124.40	115.27
6	C	611	CHL	CMB-C2B-C3B	2.22	128.84	124.68
4	B	504	XAT	C37-C21-C26	2.22	116.04	110.05
8	B	802	DGD	O2G-C1B-C2B	2.22	118.87	111.91
8	A	802	DGD	C1E-O6E-C5E	2.22	118.04	113.69
5	B	604	CLA	OBD-CAD-C3D	2.22	131.66	127.98
5	C	605	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
6	A	614	CHL	CMA-C3A-C2A	-2.22	110.93	116.10
5	C	604	CLA	OBD-CAD-C3D	2.21	131.65	127.98
4	C	504	XAT	C36-C21-C22	2.21	112.82	108.98
5	A	601	CLA	C1-C2-C3	2.21	129.86	126.04
6	C	612	CHL	O2A-CGA-O1A	-2.20	118.04	123.59
5	C	604	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
2	C	502	LUX	C20-C13-C14	2.20	119.25	111.29
3	A	503	NEX	C15-C14-C13	-2.20	124.17	127.31
6	C	613	CHL	CMD-C2D-C3D	2.20	128.79	124.68
6	B	613	CHL	OBD-CAD-C3D	2.20	131.63	127.98
2	A	501	LUX	C35-C15-C14	2.20	121.40	113.62
6	C	614	CHL	C2A-C3A-C4A	2.19	104.58	101.78
5	C	608	CLA	C2A-C1A-CHA	2.19	127.68	123.86
3	C	503	NEX	C10-C11-C12	-2.19	116.39	123.22
5	A	601	CLA	CGD-CBD-CAD	2.18	117.81	110.73
2	B	502	LUX	C7-C6-C5	-2.18	116.17	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	802	DGD	C1E-O6E-C5E	2.18	117.96	113.69
5	B	602	CLA	C3A-C2A-C1A	2.18	104.60	101.34
5	A	606	CLA	C2A-C3A-C4A	2.17	105.38	101.87
2	C	502	LUX	C38-C25-C24	-2.17	118.91	123.56
4	C	504	XAT	C15-C35-C34	-2.17	119.03	123.47
5	C	605	CLA	C2A-C1A-CHA	2.17	127.64	123.86
6	A	611	CHL	CMD-C2D-C3D	2.16	128.72	124.68
5	A	604	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
6	A	609	CHL	C2A-C3A-C4A	2.16	105.36	101.87
5	B	605	CLA	C1D-CHD-C4C	2.16	125.40	122.56
4	A	504	XAT	C20-C13-C14	-2.15	119.91	122.92
2	C	502	LUX	C40-C33-C32	2.15	119.08	111.29
3	A	503	NEX	C10-C11-C12	-2.15	116.51	123.22
6	B	610	CHL	O2A-CGA-O1A	-2.15	118.17	123.59
5	C	608	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
2	A	502	LUX	C7-C6-C5	-2.15	116.26	121.46
6	A	610	CHL	C4D-C3D-CAD	-2.14	107.27	108.47
6	C	612	CHL	C2C-C3C-C4C	2.14	108.02	106.49
6	A	614	CHL	O1D-CGD-CBD	-2.14	120.10	124.48
6	B	614	CHL	CMA-C3A-C2A	-2.14	111.11	116.10
6	A	613	CHL	OBD-CAD-C3D	2.14	131.53	127.98
5	C	607	CLA	CMB-C2B-C3B	2.14	128.67	124.68
5	C	606	CLA	C2A-C3A-C4A	2.14	105.32	101.87
5	B	606	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
5	A	604	CLA	CAA-C2A-C1A	2.13	118.97	111.97
6	A	610	CHL	C1D-CHD-C4C	2.13	125.37	122.56
2	B	501	LUX	C15-C35-C34	2.13	121.16	113.62
5	C	602	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
6	C	611	CHL	C2A-C3A-C4A	2.12	105.29	101.87
2	B	501	LUX	C38-C25-C24	-2.12	119.03	123.56
4	C	504	XAT	C17-C1-C2	-2.12	105.31	108.98
6	A	612	CHL	C2C-C3C-C4C	2.12	108.00	106.49
2	C	501	LUX	C39-C29-C28	2.11	118.95	111.29
5	A	606	CLA	C2A-C1A-CHA	2.11	127.55	123.86
5	A	602	CLA	CED-O2D-CGD	2.11	120.71	115.94
6	A	614	CHL	C2C-C3C-C4C	2.11	107.99	106.49
6	B	609	CHL	CBA-CAA-C2A	2.11	120.09	113.86
5	C	601	CLA	CGD-CBD-CAD	2.11	117.56	110.73
2	C	501	LUX	C15-C35-C34	2.11	121.08	113.62
4	B	504	XAT	C19-C9-C8	2.11	121.39	118.08
6	B	612	CHL	O2A-CGA-O1A	-2.11	118.28	123.59
5	B	604	CLA	O2A-CGA-O1A	-2.10	118.29	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	LUX	C27-C28-C29	2.10	123.90	115.27
5	A	608	CLA	C2C-C1C-NC	-2.10	108.00	109.97
3	B	503	NEX	C11-C12-C13	-2.10	120.52	126.42
2	A	501	LUX	C20-C13-C14	2.10	118.89	111.29
6	B	610	CHL	C2A-C3A-C4A	2.10	105.25	101.87
6	B	609	CHL	OMC-CMC-C2C	-2.10	120.95	125.69
2	A	501	LUX	C38-C25-C24	-2.09	119.08	123.56
6	C	614	CHL	CMA-C3A-C2A	-2.09	111.21	116.10
7	A	801	LHG	O10-C23-C24	-2.09	115.57	123.73
5	C	603	CLA	OBD-CAD-CBD	-2.09	122.91	125.89
5	A	604	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
5	A	605	CLA	OBD-CAD-C3D	2.09	131.46	127.98
5	B	607	CLA	C2C-C1C-NC	-2.09	108.01	109.97
6	C	611	CHL	C11-C10-C8	-2.09	109.16	115.92
5	C	604	CLA	C1D-CHD-C4C	2.09	125.32	122.56
6	C	612	CHL	OMC-CMC-C2C	-2.09	120.96	125.69
5	A	608	CLA	C2A-C1A-CHA	2.09	127.51	123.86
4	C	504	XAT	C8-C9-C10	2.08	122.14	118.94
5	A	608	CLA	CED-O2D-CGD	2.08	120.65	115.94
5	B	606	CLA	C1D-CHD-C4C	2.08	125.31	122.56
6	A	611	CHL	O2A-C1-C2	-2.08	103.16	108.64
6	B	609	CHL	C2A-C3A-C4A	2.08	105.23	101.87
6	B	611	CHL	O2A-CGA-O1A	-2.08	118.34	123.59
5	A	606	CLA	C3A-C2A-C1A	2.08	104.45	101.34
5	B	608	CLA	CED-O2D-CGD	2.07	120.63	115.94
5	B	604	CLA	CED-O2D-CGD	2.07	120.63	115.94
5	B	601	CLA	CMA-C3A-C2A	-2.07	105.47	113.83
5	A	605	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
5	C	606	CLA	C3A-C2A-C1A	2.07	104.44	101.34
5	B	608	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
6	C	612	CHL	C2A-C1A-CHA	2.06	127.47	123.86
6	B	613	CHL	CAA-CBA-CGA	-2.06	109.16	113.59
5	B	601	CLA	CMB-C2B-C3B	2.06	128.53	124.68
5	C	608	CLA	C3A-C2A-C1A	2.06	104.42	101.34
6	C	609	CHL	CAA-C2A-C1A	-2.06	105.22	111.97
5	B	608	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
5	A	603	CLA	C12-C11-C10	-2.06	103.78	113.24
6	B	609	CHL	O2A-CGA-O1A	-2.06	118.40	123.59
5	B	608	CLA	C1D-CHD-C4C	2.05	125.27	122.56
5	B	601	CLA	CMD-C2D-C3D	2.05	128.52	124.68
6	B	610	CHL	C12-C11-C10	-2.05	103.80	113.24
6	C	610	CHL	C2A-C3A-C4A	2.05	105.18	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	606	CLA	C2A-C1A-CHA	2.05	127.45	123.86
4	C	504	XAT	C20-C13-C14	-2.05	120.05	122.92
2	A	501	LUX	C39-C29-C28	2.05	118.71	111.29
6	C	614	CHL	CBC-CAC-C3C	-2.05	106.79	112.43
4	C	504	XAT	C37-C21-C26	2.05	115.57	110.05
5	C	606	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
5	A	608	CLA	CMB-C2B-C3B	2.04	128.50	124.68
2	B	501	LUX	C40-C33-C32	2.04	118.68	111.29
5	C	602	CLA	CED-O2D-CGD	2.04	120.55	115.94
5	C	608	CLA	CHD-C4C-NC	2.04	127.41	124.20
6	A	611	CHL	CMB-C2B-C3B	2.04	128.49	124.68
6	B	610	CHL	C7-C6-C5	-2.03	107.83	113.36
5	B	604	CLA	C12-C11-C10	-2.03	103.90	113.24
6	C	611	CHL	CMD-C2D-C3D	2.03	128.48	124.68
5	C	607	CLA	C2A-C3A-C4A	2.03	105.15	101.87
6	A	611	CHL	C2A-C3A-C4A	2.03	105.15	101.87
6	A	611	CHL	O2A-CGA-O1A	-2.03	118.47	123.59
6	A	609	CHL	C1D-CHD-C4C	2.03	125.23	122.56
5	A	605	CLA	C1-C2-C3	2.03	129.55	126.04
6	C	610	CHL	C12-C11-C10	-2.02	103.94	113.24
5	B	605	CLA	OBD-CAD-C3D	2.02	131.34	127.98
6	A	612	CHL	C2A-C1A-CHA	2.02	127.39	123.86
6	A	610	CHL	C2A-C3A-C4A	2.02	105.13	101.87
2	A	502	LUX	C40-C33-C32	2.02	118.61	111.29
5	B	608	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
5	B	603	CLA	CED-O2D-CGD	2.02	120.50	115.94
6	A	609	CHL	C7-C6-C5	-2.02	107.88	113.36
5	A	605	CLA	CED-O2D-CGD	2.02	120.50	115.94
5	C	603	CLA	C12-C11-C10	-2.02	103.97	113.24
2	C	501	LUX	C26-C25-C24	2.01	124.79	116.65
5	B	608	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
5	B	607	CLA	C3C-C4C-NC	-2.01	108.32	110.57
5	B	601	CLA	CHD-C4C-NC	2.00	127.36	124.20

All (189) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	802	DGD	C5E
6	C	612	CHL	NC
6	C	612	CHL	ND
6	C	612	CHL	NA
2	A	502	LUX	C13

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Mol	Chain	Res	Type	Atom
2	A	502	LUX	C33
2	A	502	LUX	C29
2	A	502	LUX	C26
2	A	502	LUX	C9
5	B	604	CLA	C8
5	B	604	CLA	NC
5	B	604	CLA	ND
5	B	604	CLA	NA
5	A	608	CLA	NC
5	A	608	CLA	ND
5	A	608	CLA	NA
6	C	613	CHL	NC
6	C	613	CHL	ND
6	C	613	CHL	NA
5	C	604	CLA	C8
5	C	604	CLA	NC
5	C	604	CLA	ND
5	C	604	CLA	NA
5	B	601	CLA	C8
5	B	601	CLA	NC
5	B	601	CLA	ND
5	B	601	CLA	NA
2	B	502	LUX	C13
2	B	502	LUX	C33
2	B	502	LUX	C29
2	B	502	LUX	C26
2	B	502	LUX	C9
5	B	606	CLA	C8
5	B	606	CLA	NC
5	B	606	CLA	ND
5	B	606	CLA	NA
5	B	608	CLA	NC
5	B	608	CLA	ND
5	B	608	CLA	NA
5	B	607	CLA	NC
5	B	607	CLA	ND
5	B	607	CLA	NA
5	A	601	CLA	C8
5	A	601	CLA	NC
5	A	601	CLA	ND
5	A	601	CLA	NA
6	C	614	CHL	NC

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Mol	Chain	Res	Type	Atom
6	C	614	CHL	ND
6	C	614	CHL	NA
6	A	610	CHL	C8
6	A	610	CHL	NC
6	A	610	CHL	ND
6	A	610	CHL	NA
6	B	614	CHL	NC
6	B	614	CHL	ND
6	B	614	CHL	NA
6	C	609	CHL	C8
6	C	609	CHL	NC
6	C	609	CHL	ND
6	C	609	CHL	NA
5	C	603	CLA	C8
5	C	603	CLA	NC
5	C	603	CLA	ND
5	C	603	CLA	NA
5	A	607	CLA	NC
5	A	607	CLA	ND
5	A	607	CLA	NA
4	A	504	XAT	C6
4	A	504	XAT	C26
5	C	607	CLA	NC
5	C	607	CLA	ND
5	C	607	CLA	NA
4	C	504	XAT	C6
4	C	504	XAT	C26
6	B	610	CHL	C8
6	B	610	CHL	NC
6	B	610	CHL	ND
6	B	610	CHL	NA
5	C	606	CLA	C8
5	C	606	CLA	NC
5	C	606	CLA	ND
5	C	606	CLA	NA
6	A	614	CHL	NC
6	A	614	CHL	ND
6	A	614	CHL	NA
4	B	504	XAT	C6
4	B	504	XAT	C26
5	B	605	CLA	C8
5	B	605	CLA	NC

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Mol	Chain	Res	Type	Atom
5	B	605	CLA	ND
5	B	605	CLA	NA
8	A	802	DGD	C5E
5	C	605	CLA	C8
5	C	605	CLA	NC
5	C	605	CLA	ND
5	C	605	CLA	NA
6	C	610	CHL	C8
6	C	610	CHL	NC
6	C	610	CHL	ND
6	C	610	CHL	NA
2	A	501	LUX	C13
2	A	501	LUX	C33
2	A	501	LUX	C29
2	A	501	LUX	C26
2	A	501	LUX	C9
2	B	501	LUX	C13
2	B	501	LUX	C33
2	B	501	LUX	C29
2	B	501	LUX	C26
2	B	501	LUX	C9
6	A	609	CHL	C8
6	A	609	CHL	NC
6	A	609	CHL	ND
6	A	609	CHL	NA
5	C	602	CLA	NC
5	C	602	CLA	ND
5	C	602	CLA	NA
5	A	603	CLA	C8
5	A	603	CLA	NC
5	A	603	CLA	ND
5	A	603	CLA	NA
5	B	602	CLA	NC
5	B	602	CLA	ND
5	B	602	CLA	NA
6	B	612	CHL	NC
6	B	612	CHL	ND
6	B	612	CHL	NA
5	B	603	CLA	C8
5	B	603	CLA	NC
5	B	603	CLA	ND
5	B	603	CLA	NA

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Mol	Chain	Res	Type	Atom
6	B	611	CHL	C8
6	B	611	CHL	NC
6	B	611	CHL	ND
6	B	611	CHL	NA
6	B	609	CHL	C8
6	B	609	CHL	NC
6	B	609	CHL	ND
6	B	609	CHL	NA
2	C	502	LUX	C13
2	C	502	LUX	C33
2	C	502	LUX	C29
2	C	502	LUX	C26
2	C	502	LUX	C9
5	A	605	CLA	C8
5	A	605	CLA	NC
5	A	605	CLA	ND
5	A	605	CLA	NA
6	A	613	CHL	NC
6	A	613	CHL	ND
6	A	613	CHL	NA
5	A	604	CLA	C8
5	A	604	CLA	NC
5	A	604	CLA	ND
5	A	604	CLA	NA
6	A	611	CHL	C8
6	A	611	CHL	NC
6	A	611	CHL	ND
6	A	611	CHL	NA
5	C	601	CLA	C8
5	C	601	CLA	NC
5	C	601	CLA	ND
5	C	601	CLA	NA
6	B	613	CHL	NC
6	B	613	CHL	ND
6	B	613	CHL	NA
6	A	612	CHL	NC
6	A	612	CHL	ND
6	A	612	CHL	NA
5	C	608	CLA	NC
5	C	608	CLA	ND
5	C	608	CLA	NA
6	C	611	CHL	C8

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Mol	Chain	Res	Type	Atom
6	C	611	CHL	NC
6	C	611	CHL	ND
6	C	611	CHL	NA
5	A	602	CLA	NC
5	A	602	CLA	ND
5	A	602	CLA	NA
5	A	606	CLA	C8
5	A	606	CLA	NC
5	A	606	CLA	ND
5	A	606	CLA	NA
2	C	501	LUX	C13
2	C	501	LUX	C33
2	C	501	LUX	C29
2	C	501	LUX	C26
2	C	501	LUX	C9
8	B	802	DGD	C5E

All (656) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	802	DGD	O6D-C1D-O3G-C3G
8	C	802	DGD	C2E-C1E-O5D-C6D
8	C	802	DGD	O6E-C1E-O5D-C6D
6	C	612	CHL	C1A-C2A-CAA-CBA
6	C	612	CHL	C3A-C2A-CAA-CBA
6	C	612	CHL	C11-C10-C8-C9
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
7	A	801	LHG	C3-O3-P-O4
7	A	801	LHG	C3-O3-P-O5
7	A	801	LHG	C3-O3-P-O6
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	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-O5
7	C	801	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
7	C	801	LHG	C24-C23-O8-C6
5	A	608	CLA	C1A-C2A-CAA-CBA
5	A	608	CLA	C3A-C2A-CAA-CBA
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
5	B	606	CLA	C1A-C2A-CAA-CBA
5	B	608	CLA	C1A-C2A-CAA-CBA
5	B	607	CLA	C1A-C2A-CAA-CBA
5	B	607	CLA	C3A-C2A-CAA-CBA
6	A	610	CHL	C11-C10-C8-C9
6	C	609	CHL	CHA-CBD-CGD-O1D
6	C	609	CHL	CHA-CBD-CGD-O2D
6	C	609	CHL	C11-C10-C8-C9
5	C	603	CLA	C11-C10-C8-C9
5	A	607	CLA	C1A-C2A-CAA-CBA
5	A	607	CLA	C3A-C2A-CAA-CBA
5	C	607	CLA	C1A-C2A-CAA-CBA
5	C	607	CLA	C3A-C2A-CAA-CBA
6	B	610	CHL	C11-C10-C8-C9
5	C	606	CLA	C1A-C2A-CAA-CBA
8	A	802	DGD	O6D-C1D-O3G-C3G
8	A	802	DGD	C2E-C1E-O5D-C6D
8	A	802	DGD	O6E-C1E-O5D-C6D
6	C	610	CHL	C11-C10-C8-C9
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	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
6	A	609	CHL	C11-C10-C8-C9
5	A	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
6	B	612	CHL	C1A-C2A-CAA-CBA
6	B	612	CHL	C11-C10-C8-C9
5	B	603	CLA	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	609	CHL	C11-C10-C8-C9
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
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
5	C	608	CLA	C1A-C2A-CAA-CBA
5	C	608	CLA	C3A-C2A-CAA-CBA
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-O5
7	B	801	LHG	O10-C23-O8-C6
7	B	801	LHG	C24-C23-O8-C6
6	C	611	CHL	C1A-C2A-CAA-CBA
5	A	606	CLA	C1A-C2A-CAA-CBA
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
8	B	802	DGD	O6D-C1D-O3G-C3G
8	B	802	DGD	C2E-C1E-O5D-C6D
8	B	802	DGD	O6E-C1E-O5D-C6D
6	C	612	CHL	C15-C16-C17-C18
5	B	607	CLA	C5-C6-C7-C8
5	B	607	CLA	C8-C10-C11-C12
5	A	607	CLA	C5-C6-C7-C8
5	A	607	CLA	C8-C10-C11-C12
5	C	607	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
5	C	607	CLA	C8-C10-C11-C12
6	B	610	CHL	C13-C15-C16-C17
5	B	605	CLA	C8-C10-C11-C12
5	B	605	CLA	C15-C16-C17-C18
5	C	605	CLA	C8-C10-C11-C12
5	C	605	CLA	C15-C16-C17-C18
5	C	602	CLA	C8-C10-C11-C12
5	B	602	CLA	C8-C10-C11-C12
6	B	612	CHL	C15-C16-C17-C18
6	B	611	CHL	C5-C6-C7-C8
6	B	611	CHL	C15-C16-C17-C18
5	A	605	CLA	C8-C10-C11-C12
5	A	605	CLA	C15-C16-C17-C18
6	A	611	CHL	C5-C6-C7-C8
6	A	611	CHL	C15-C16-C17-C18
5	C	601	CLA	C8-C10-C11-C12
6	A	612	CHL	C15-C16-C17-C18
6	C	611	CHL	C5-C6-C7-C8
5	A	602	CLA	C8-C10-C11-C12
5	B	601	CLA	C8-C10-C11-C12
5	A	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
8	C	802	DGD	O1B-C1B-O2G-C2G
8	B	802	DGD	O1B-C1B-O2G-C2G
5	B	601	CLA	C3-C5-C6-C7
5	B	606	CLA	C3-C5-C6-C7
5	A	601	CLA	C3-C5-C6-C7
6	B	609	CHL	C3-C5-C6-C7
5	A	605	CLA	C3-C5-C6-C7
5	C	601	CLA	C3-C5-C6-C7
5	A	606	CLA	C3-C5-C6-C7
8	C	802	DGD	O6D-C5D-C6D-O5D
8	A	802	DGD	O6D-C5D-C6D-O5D
8	B	802	DGD	O6D-C5D-C6D-O5D
5	C	601	CLA	C4-C3-C5-C6
5	C	601	CLA	C2-C3-C5-C6
6	C	609	CHL	C2A-CAA-CBA-CGA
6	A	609	CHL	C2A-CAA-CBA-CGA
6	B	609	CHL	C2A-CAA-CBA-CGA
8	A	802	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
8	C	802	DGD	C2B-C3B-C4B-C5B
7	A	801	LHG	C33-C34-C35-C36
7	C	801	LHG	C33-C34-C35-C36
8	A	802	DGD	C2B-C3B-C4B-C5B
7	B	801	LHG	C33-C34-C35-C36
8	B	802	DGD	C2B-C3B-C4B-C5B
6	C	609	CHL	C3-C5-C6-C7
5	C	606	CLA	C3-C5-C6-C7
5	C	605	CLA	C3-C5-C6-C7
6	A	609	CHL	C3-C5-C6-C7
8	C	802	DGD	C2B-C1B-O2G-C2G
6	A	610	CHL	CBA-CGA-O2A-C1
6	B	610	CHL	CBA-CGA-O2A-C1
8	A	802	DGD	C2B-C1B-O2G-C2G
6	C	610	CHL	CBA-CGA-O2A-C1
8	B	802	DGD	C2B-C1B-O2G-C2G
8	A	802	DGD	C4D-C5D-C6D-O5D
6	A	610	CHL	O1A-CGA-O2A-C1
6	B	610	CHL	O1A-CGA-O2A-C1
6	C	610	CHL	O1A-CGA-O2A-C1
5	B	605	CLA	C3-C5-C6-C7
8	C	802	DGD	C4D-C5D-C6D-O5D
8	B	802	DGD	C4D-C5D-C6D-O5D
8	B	802	DGD	C4E-C5E-C6E-O5E
6	C	611	CHL	C3-C5-C6-C7
8	C	802	DGD	C4E-C5E-C6E-O5E
8	A	802	DGD	C4E-C5E-C6E-O5E
5	B	605	CLA	CBA-CGA-O2A-C1
6	B	611	CHL	C3-C5-C6-C7
5	C	605	CLA	CBA-CGA-O2A-C1
5	A	605	CLA	CBA-CGA-O2A-C1
6	B	610	CHL	C10-C11-C12-C13
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
5	B	601	CLA	C11-C10-C8-C9
2	B	502	LUX	C11-C12-C13-C20
2	B	502	LUX	C39-C29-C30-C31
2	B	502	LUX	C31-C32-C33-C40
5	B	607	CLA	C11-C10-C8-C9
5	B	607	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
5	A	601	CLA	C11-C10-C8-C9
6	A	610	CHL	C11-C12-C13-C14
6	C	609	CHL	C14-C13-C15-C16
5	A	607	CLA	C11-C10-C8-C9
5	A	607	CLA	C14-C13-C15-C16
5	C	607	CLA	C11-C10-C8-C9
5	C	607	CLA	C14-C13-C15-C16
6	B	610	CHL	C11-C12-C13-C14
5	B	605	CLA	C11-C10-C8-C9
5	C	605	CLA	C11-C10-C8-C9
6	C	610	CHL	C11-C12-C13-C14
2	A	501	LUX	C39-C29-C30-C31
2	A	501	LUX	C31-C32-C33-C40
2	B	501	LUX	C27-C28-C29-C39
2	B	501	LUX	C39-C29-C30-C31
6	A	609	CHL	C14-C13-C15-C16
5	C	602	CLA	C11-C10-C8-C9
5	B	602	CLA	C11-C10-C8-C9
6	B	609	CHL	C14-C13-C15-C16
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	605	CLA	C11-C10-C8-C9
6	A	611	CHL	C14-C13-C15-C16
5	C	601	CLA	C11-C10-C8-C9
6	C	611	CHL	C11-C10-C8-C9
6	C	611	CHL	C14-C13-C15-C16
5	A	602	CLA	C11-C10-C8-C9
2	C	501	LUX	C39-C29-C30-C31
2	C	501	LUX	C31-C32-C33-C40
6	A	610	CHL	C10-C11-C12-C13
6	B	611	CHL	C10-C11-C12-C13
6	C	611	CHL	C10-C11-C12-C13
5	C	603	CLA	C13-C15-C16-C17
6	C	610	CHL	C10-C11-C12-C13
6	A	611	CHL	C10-C11-C12-C13
7	C	801	LHG	O1-C1-C2-O2
5	C	602	CLA	C10-C11-C12-C13
5	B	602	CLA	C10-C11-C12-C13
6	A	609	CHL	C2C-C3C-CAC-CBC
6	C	612	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
5	B	607	CLA	C11-C12-C13-C15
5	A	607	CLA	C11-C12-C13-C15
5	C	607	CLA	C11-C12-C13-C15
6	B	610	CHL	C11-C12-C13-C15
6	C	610	CHL	C11-C12-C13-C15
6	A	612	CHL	C12-C13-C15-C16
6	A	611	CHL	C3-C5-C6-C7
5	C	605	CLA	O1A-CGA-O2A-C1
5	A	605	CLA	O1A-CGA-O2A-C1
5	A	602	CLA	C10-C11-C12-C13
5	A	603	CLA	C3-C5-C6-C7
5	B	607	CLA	C13-C15-C16-C17
5	A	607	CLA	C13-C15-C16-C17
5	B	603	CLA	C13-C15-C16-C17
5	A	603	CLA	C13-C15-C16-C17
7	B	801	LHG	C4-O6-P-O3
5	C	607	CLA	C13-C15-C16-C17
5	B	608	CLA	O2A-C1-C2-C3
5	A	601	CLA	C4-C3-C5-C6
5	C	604	CLA	C16-C17-C18-C20
8	C	802	DGD	O2G-C2G-C3G-O3G
8	A	802	DGD	O2G-C2G-C3G-O3G
8	B	802	DGD	O2G-C2G-C3G-O3G
5	A	606	CLA	C2C-C3C-CAC-CBC
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
5	A	604	CLA	C16-C17-C18-C20
7	A	801	LHG	C13-C14-C15-C16
5	B	605	CLA	O1A-CGA-O2A-C1
7	C	801	LHG	C11-C10-C9-C8
5	C	604	CLA	C2C-C3C-CAC-CBC
7	B	801	LHG	C11-C10-C9-C8
4	C	504	XAT	C28-C29-C30-C31
4	B	504	XAT	C28-C29-C30-C31
5	C	602	CLA	C11-C12-C13-C15
6	C	612	CHL	C4-C3-C5-C6
5	C	602	CLA	C4-C3-C5-C6
5	B	602	CLA	C4-C3-C5-C6
6	B	612	CHL	C4-C3-C5-C6
6	A	612	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	A	801	LHG	C11-C10-C9-C8
7	A	801	LHG	C26-C27-C28-C29
7	B	801	LHG	C11-C12-C13-C14
5	B	603	CLA	C14-C13-C15-C16
7	C	801	LHG	C26-C27-C28-C29
7	B	801	LHG	C26-C27-C28-C29
5	B	606	CLA	C2A-CAA-CBA-CGA
5	C	603	CLA	C2A-CAA-CBA-CGA
5	B	603	CLA	C2A-CAA-CBA-CGA
5	A	606	CLA	C2A-CAA-CBA-CGA
7	A	801	LHG	O1-C1-C2-C3
7	C	801	LHG	O1-C1-C2-C3
7	B	801	LHG	O1-C1-C2-C3
7	A	801	LHG	C11-C12-C13-C14
7	C	801	LHG	C15-C16-C17-C18
5	B	607	CLA	C16-C17-C18-C19
6	B	611	CHL	C16-C17-C18-C20
5	A	602	CLA	C11-C12-C13-C15
7	C	801	LHG	C13-C14-C15-C16
7	C	801	LHG	C11-C12-C13-C14
5	C	602	CLA	C3-C5-C6-C7
5	B	602	CLA	C3-C5-C6-C7
7	A	801	LHG	C25-C26-C27-C28
7	B	801	LHG	C13-C14-C15-C16
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	B	612	CHL	C3A-C2A-CAA-CBA
6	B	611	CHL	C3A-C2A-CAA-CBA
6	A	611	CHL	C3A-C2A-CAA-CBA
6	C	611	CHL	C3A-C2A-CAA-CBA
5	A	606	CLA	C3A-C2A-CAA-CBA
5	B	604	CLA	C16-C17-C18-C19
5	A	607	CLA	C16-C17-C18-C19
5	C	607	CLA	C16-C17-C18-C19
6	C	611	CHL	C16-C17-C18-C20
7	B	801	LHG	C25-C26-C27-C28
5	C	608	CLA	O2A-C1-C2-C3
5	C	603	CLA	C3-C5-C6-C7
7	B	801	LHG	C15-C16-C17-C18
5	A	602	CLA	C4-C3-C5-C6
5	B	607	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
5	A	607	CLA	C2-C3-C5-C6
5	C	607	CLA	C2-C3-C5-C6
5	C	602	CLA	C2-C3-C5-C6
6	B	612	CHL	C2-C3-C5-C6
5	C	606	CLA	C2A-CAA-CBA-CGA
7	A	801	LHG	O1-C1-C2-O2
7	B	801	LHG	O1-C1-C2-O2
6	C	609	CHL	C2C-C3C-CAC-CBC
5	A	602	CLA	O1A-CGA-O2A-C1
5	B	602	CLA	C11-C12-C13-C15
6	A	611	CHL	C16-C17-C18-C20
7	C	801	LHG	C25-C26-C27-C28
5	A	604	CLA	C2C-C3C-CAC-CBC
6	C	611	CHL	C13-C15-C16-C17
7	B	801	LHG	C19-C20-C21-C22
5	C	604	CLA	C16-C17-C18-C19
5	B	607	CLA	C16-C17-C18-C20
5	A	607	CLA	C16-C17-C18-C20
5	A	604	CLA	C16-C17-C18-C19
2	A	501	LUX	C5-C6-C7-C8
2	B	501	LUX	C5-C6-C7-C8
5	A	602	CLA	C3-C5-C6-C7
2	C	501	LUX	C5-C6-C7-C8
8	C	802	DGD	C5B-C6B-C7B-C8B
6	B	609	CHL	CBA-CGA-O2A-C1
5	C	607	CLA	C4-C3-C5-C6
6	C	612	CHL	C2-C3-C5-C6
5	A	601	CLA	C11-C10-C8-C7
6	A	610	CHL	C11-C12-C13-C15
5	B	602	CLA	C2-C3-C5-C6
6	B	612	CHL	C12-C13-C15-C16
6	A	612	CHL	C2-C3-C5-C6
5	A	602	CLA	C2-C3-C5-C6
6	A	610	CHL	C16-C17-C18-C20
7	A	801	LHG	C19-C20-C21-C22
7	C	801	LHG	C19-C20-C21-C22
5	C	606	CLA	C2C-C3C-CAC-CBC
8	A	802	DGD	C5B-C6B-C7B-C8B
8	B	802	DGD	C1B-C2B-C3B-C4B
6	B	611	CHL	C13-C15-C16-C17
5	B	603	CLA	C3-C5-C6-C7
6	C	612	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	B	606	CLA	C2C-C3C-CAC-CBC
6	A	609	CHL	CBA-CGA-O2A-C1
8	C	802	DGD	C1B-C2B-C3B-C4B
8	B	802	DGD	C5B-C6B-C7B-C8B
5	A	608	CLA	O2A-C1-C2-C3
8	A	802	DGD	C2D-C1D-O3G-C3G
8	B	802	DGD	C2D-C1D-O3G-C3G
5	C	607	CLA	C16-C17-C18-C20
6	B	610	CHL	C16-C17-C18-C20
6	C	610	CHL	C16-C17-C18-C20
5	B	607	CLA	C4-C3-C5-C6
5	A	607	CLA	C4-C3-C5-C6
8	A	802	DGD	C1B-C2B-C3B-C4B
5	A	601	CLA	C2-C3-C5-C6
6	A	609	CHL	C4C-C3C-CAC-CBC
6	B	612	CHL	C10-C11-C12-C13
5	B	604	CLA	C1A-C2A-CAA-CBA
5	C	604	CLA	C1A-C2A-CAA-CBA
5	B	601	CLA	C1A-C2A-CAA-CBA
5	A	601	CLA	C1A-C2A-CAA-CBA
5	C	603	CLA	C1A-C2A-CAA-CBA
5	A	603	CLA	C1A-C2A-CAA-CBA
5	B	603	CLA	C1A-C2A-CAA-CBA
5	A	604	CLA	C1A-C2A-CAA-CBA
5	C	601	CLA	C1A-C2A-CAA-CBA
5	C	602	CLA	C11-C12-C13-C14
7	A	801	LHG	C15-C16-C17-C18
7	C	801	LHG	C4-O6-P-O3
5	C	602	CLA	O1A-CGA-O2A-C1
6	C	611	CHL	C16-C17-C18-C19
5	B	602	CLA	O1A-CGA-O2A-C1
6	B	611	CHL	C16-C17-C18-C19
6	A	611	CHL	C16-C17-C18-C19
5	A	604	CLA	C3-C5-C6-C7
6	B	609	CHL	C2C-C3C-CAC-CBC
6	A	612	CHL	CBA-CGA-O2A-C1
6	A	612	CHL	C10-C11-C12-C13
2	A	502	LUX	C7-C8-C9-C10
2	B	502	LUX	C7-C8-C9-C10
2	A	501	LUX	C7-C8-C9-C10
2	B	501	LUX	C7-C8-C9-C10
2	C	502	LUX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	C	501	LUX	C7-C8-C9-C10
5	C	604	CLA	C10-C11-C12-C13
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	607	CLA	C12-C13-C15-C16
5	A	601	CLA	C6-C7-C8-C10
5	A	601	CLA	C12-C13-C15-C16
6	A	610	CHL	C11-C10-C8-C7
6	C	609	CHL	C11-C10-C8-C7
6	C	609	CHL	C12-C13-C15-C16
6	B	610	CHL	C11-C10-C8-C7
5	B	605	CLA	C11-C10-C8-C7
5	C	605	CLA	C6-C7-C8-C10
5	C	605	CLA	C11-C10-C8-C7
6	C	610	CHL	C11-C10-C8-C7
6	A	609	CHL	C6-C7-C8-C10
6	A	609	CHL	C12-C13-C15-C16
6	B	611	CHL	C11-C10-C8-C7
6	B	609	CHL	C12-C13-C15-C16
5	A	605	CLA	C11-C10-C8-C7
5	C	601	CLA	C6-C7-C8-C10
5	C	601	CLA	C11-C10-C8-C7
5	B	601	CLA	C6-C7-C8-C9
5	A	601	CLA	C6-C7-C8-C9
5	C	603	CLA	C14-C13-C15-C16
5	A	603	CLA	C14-C13-C15-C16
5	C	601	CLA	C6-C7-C8-C9
8	B	802	DGD	C6B-C7B-C8B-C9B
5	A	604	CLA	C10-C11-C12-C13
6	C	609	CHL	CBA-CGA-O2A-C1
5	A	604	CLA	CBA-CGA-O2A-C1
5	B	604	CLA	C10-C11-C12-C13
6	C	612	CHL	CBA-CGA-O2A-C1
5	C	603	CLA	CBA-CGA-O2A-C1
5	B	602	CLA	C11-C12-C13-C14
5	A	602	CLA	C11-C12-C13-C14
5	A	603	CLA	CBA-CGA-O2A-C1
5	A	602	CLA	CBA-CGA-O2A-C1
5	C	604	CLA	C4C-C3C-CAC-CBC
7	A	801	LHG	C4-O6-P-O3
6	B	609	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
5	B	601	CLA	C13-C15-C16-C17
6	B	612	CHL	CBA-CGA-O2A-C1
6	B	611	CHL	C2-C1-O2A-CGA
5	C	605	CLA	C6-C7-C8-C9
5	A	605	CLA	C6-C7-C8-C9
8	C	802	DGD	C6B-C7B-C8B-C9B
5	A	606	CLA	C4C-C3C-CAC-CBC
5	A	604	CLA	C2A-CAA-CBA-CGA
6	C	612	CHL	C10-C11-C12-C13
5	C	607	CLA	C10-C11-C12-C13
5	C	601	CLA	C13-C15-C16-C17
6	C	612	CHL	C11-C10-C8-C7
5	C	603	CLA	C11-C10-C8-C7
5	C	607	CLA	C12-C13-C15-C16
5	B	605	CLA	C6-C7-C8-C10
6	A	609	CHL	C11-C10-C8-C7
6	B	612	CHL	C11-C10-C8-C7
5	B	603	CLA	C11-C10-C8-C7
5	B	603	CLA	C12-C13-C15-C16
6	B	611	CHL	C12-C13-C15-C16
6	B	609	CHL	C6-C7-C8-C10
6	B	609	CHL	C11-C10-C8-C7
5	A	605	CLA	C6-C7-C8-C10
6	A	611	CHL	C11-C10-C8-C7
6	A	611	CHL	C12-C13-C15-C16
6	C	611	CHL	C11-C10-C8-C7
4	B	504	XAT	C39-C29-C30-C31
6	A	611	CHL	C13-C15-C16-C17
5	B	603	CLA	CBA-CGA-O2A-C1
5	B	608	CLA	CAD-CBD-CGD-O2D
5	B	605	CLA	CAD-CBD-CGD-O2D
5	B	602	CLA	CAD-CBD-CGD-O2D
5	A	602	CLA	CAD-CBD-CGD-O2D
8	B	802	DGD	C7B-C8B-C9B-CAB
5	A	604	CLA	C4C-C3C-CAC-CBC
5	B	604	CLA	C3-C5-C6-C7
6	A	609	CHL	O1A-CGA-O2A-C1
8	C	802	DGD	C2D-C1D-O3G-C3G
5	C	602	CLA	CBA-CGA-O2A-C1
8	A	802	DGD	C6B-C7B-C8B-C9B
8	A	802	DGD	C8B-C9B-CAB-CBB
6	C	612	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
5	B	605	CLA	C6-C7-C8-C9
6	B	609	CHL	C6-C7-C8-C9
6	A	611	CHL	C6-C7-C8-C9
5	A	603	CLA	C2A-CAA-CBA-CGA
7	A	801	LHG	C4-O6-P-O4
7	C	801	LHG	C4-O6-P-O4
7	B	801	LHG	C4-O6-P-O4
6	A	612	CHL	O1A-CGA-O2A-C1
5	B	607	CLA	C11-C10-C8-C7
6	C	609	CHL	C6-C7-C8-C10
5	A	607	CLA	C11-C10-C8-C7
5	A	607	CLA	C12-C13-C15-C16
5	C	607	CLA	C11-C10-C8-C7
5	C	602	CLA	C11-C10-C8-C7
5	A	603	CLA	C11-C10-C8-C7
5	B	602	CLA	C11-C10-C8-C7
5	A	605	CLA	C12-C13-C15-C16
6	A	612	CHL	C11-C10-C8-C7
6	C	611	CHL	C12-C13-C15-C16
5	A	602	CLA	C11-C10-C8-C7
5	C	608	CLA	C2C-C3C-CAC-CBC
8	A	802	DGD	C7B-C8B-C9B-CAB
7	A	801	LHG	C4-C5-C6-O8
5	C	606	CLA	C4C-C3C-CAC-CBC
7	A	801	LHG	O7-C5-C6-O8
5	C	606	CLA	CBA-CGA-O2A-C1
6	C	612	CHL	C14-C13-C15-C16
5	C	604	CLA	C6-C7-C8-C9
6	A	609	CHL	C6-C7-C8-C9
6	A	612	CHL	C14-C13-C15-C16
6	C	609	CHL	O1A-CGA-O2A-C1
5	C	608	CLA	O1A-CGA-O2A-C1
5	C	604	CLA	C3-C5-C6-C7
5	B	606	CLA	C4C-C3C-CAC-CBC
5	B	601	CLA	C2-C3-C5-C6
6	C	612	CHL	C4C-C3C-CAC-CBC
5	C	604	CLA	C2A-CAA-CBA-CGA
6	A	610	CHL	C2A-CAA-CBA-CGA
6	B	610	CHL	C2A-CAA-CBA-CGA
6	B	612	CHL	C2-C1-O2A-CGA
6	A	611	CHL	C2-C1-O2A-CGA
5	A	606	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
5	B	601	CLA	C4-C3-C5-C6
6	C	609	CHL	C4C-C3C-CAC-CBC
5	C	603	CLA	C12-C13-C15-C16
5	B	605	CLA	C12-C13-C15-C16
5	A	603	CLA	C12-C13-C15-C16
6	B	611	CHL	C6-C7-C8-C10
5	A	606	CLA	C6-C7-C8-C10
5	B	601	CLA	C14-C13-C15-C16
6	C	609	CHL	C6-C7-C8-C9
6	B	612	CHL	C14-C13-C15-C16
5	C	604	CLA	CBA-CGA-O2A-C1
5	B	606	CLA	CBA-CGA-O2A-C1
8	C	802	DGD	C8B-C9B-CAB-CBB
5	B	608	CLA	C2C-C3C-CAC-CBC
5	A	604	CLA	O1A-CGA-O2A-C1
6	C	612	CHL	C2-C1-O2A-CGA
6	A	612	CHL	C2-C1-O2A-CGA
5	B	604	CLA	C2A-CAA-CBA-CGA
6	C	610	CHL	C2A-CAA-CBA-CGA
5	B	604	CLA	C2C-C3C-CAC-CBC
5	A	607	CLA	C10-C11-C12-C13
5	B	604	CLA	C6-C7-C8-C9
5	A	603	CLA	C6-C7-C8-C9
6	B	612	CHL	C11-C12-C13-C14
6	B	611	CHL	C6-C7-C8-C9
5	A	604	CLA	C6-C7-C8-C9
6	C	611	CHL	C11-C12-C13-C14
3	C	503	NEX	C39-C29-C30-C31
3	A	503	NEX	C39-C29-C30-C31
3	B	503	NEX	C39-C29-C30-C31
5	A	608	CLA	C2A-CAA-CBA-CGA
8	B	802	DGD	C8B-C9B-CAB-CBB
5	B	604	CLA	C12-C13-C15-C16
5	C	604	CLA	C12-C13-C15-C16
6	A	610	CHL	C6-C7-C8-C10
6	B	610	CHL	C6-C7-C8-C10
5	C	606	CLA	C6-C7-C8-C10
5	C	602	CLA	C6-C7-C8-C10
5	A	604	CLA	C12-C13-C15-C16
5	C	601	CLA	C12-C13-C15-C16
5	A	602	CLA	C6-C7-C8-C10
8	C	802	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
5	C	604	CLA	C13-C15-C16-C17
3	C	503	NEX	C28-C29-C30-C31
3	A	503	NEX	C28-C29-C30-C31
6	C	611	CHL	C2-C1-O2A-CGA
5	A	608	CLA	O1A-CGA-O2A-C1
6	C	611	CHL	C6-C7-C8-C9
5	A	601	CLA	C13-C15-C16-C17
6	A	612	CHL	C2C-C3C-CAC-CBC
5	B	608	CLA	C2A-CAA-CBA-CGA
5	C	608	CLA	C2A-CAA-CBA-CGA
7	C	801	LHG	C4-C5-C6-O8
7	B	801	LHG	C4-C5-C6-O8
6	B	609	CHL	C4C-C3C-CAC-CBC
5	B	602	CLA	CBA-CGA-O2A-C1
5	B	608	CLA	C4C-C3C-CAC-CBC
6	A	609	CHL	C4-C3-C5-C6
5	C	605	CLA	C12-C13-C15-C16
6	C	610	CHL	C6-C7-C8-C10
5	B	602	CLA	C6-C7-C8-C10
5	B	603	CLA	C11-C12-C13-C15
7	C	801	LHG	O7-C5-C6-O8
7	B	801	LHG	O7-C5-C6-O8
4	C	504	XAT	C39-C29-C30-C31
6	B	609	CHL	C4-C3-C5-C6
5	B	604	CLA	C13-C15-C16-C17
6	A	612	CHL	C11-C12-C13-C14
5	A	608	CLA	CAD-CBD-CGD-O2D
5	B	606	CLA	CAD-CBD-CGD-O2D
5	C	606	CLA	CAD-CBD-CGD-O2D
5	C	605	CLA	CAD-CBD-CGD-O2D
5	C	602	CLA	CAD-CBD-CGD-O2D
5	B	607	CLA	C10-C11-C12-C13
5	C	603	CLA	CAA-CBA-CGA-O2A
7	A	801	LHG	C27-C28-C29-C30
5	A	603	CLA	CAA-CBA-CGA-O2A
5	C	604	CLA	CHA-CBD-CGD-O1D
5	C	604	CLA	CHA-CBD-CGD-O2D
6	A	609	CHL	CHA-CBD-CGD-O1D
6	A	609	CHL	CHA-CBD-CGD-O2D
6	B	609	CHL	CHA-CBD-CGD-O1D
6	B	609	CHL	CHA-CBD-CGD-O2D
5	B	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	B	503	NEX	C28-C29-C30-C31
6	C	612	CHL	O1A-CGA-O2A-C1
6	C	609	CHL	C11-C12-C13-C15
6	C	610	CHL	C12-C13-C15-C16
6	B	609	CHL	C11-C12-C13-C15
6	A	611	CHL	C6-C7-C8-C10
5	B	607	CLA	C11-C12-C13-C14
6	A	610	CHL	C6-C7-C8-C9
5	A	606	CLA	CAA-CBA-CGA-O2A
5	B	604	CLA	CBA-CGA-O2A-C1
5	C	606	CLA	CAA-CBA-CGA-O2A
2	B	502	LUX	C11-C10-C9-C8
2	A	501	LUX	C11-C10-C9-C8
2	B	501	LUX	C11-C10-C9-C8
2	C	501	LUX	C11-C10-C9-C8
6	A	612	CHL	C4C-C3C-CAC-CBC
7	C	801	LHG	C27-C28-C29-C30
5	B	606	CLA	CAA-CBA-CGA-O2A
6	B	612	CHL	C2C-C3C-CAC-CBC
5	B	604	CLA	C4C-C3C-CAC-CBC
7	B	801	LHG	C9-C10-C11-C12
6	C	614	CHL	CAD-CBD-CGD-O1D
5	C	603	CLA	CAA-CBA-CGA-O1A
5	C	604	CLA	C14-C13-C15-C16
5	A	601	CLA	C14-C13-C15-C16
5	A	607	CLA	C11-C12-C13-C14
6	B	610	CHL	C6-C7-C8-C9
6	C	610	CHL	C6-C7-C8-C9
6	B	611	CHL	C11-C12-C13-C14
5	A	605	CLA	C14-C13-C15-C16
5	C	601	CLA	C14-C13-C15-C16
5	C	601	CLA	C2A-CAA-CBA-CGA
5	B	606	CLA	C6-C7-C8-C10
6	A	610	CHL	C12-C13-C15-C16
5	C	603	CLA	C11-C12-C13-C15
6	B	610	CHL	C12-C13-C15-C16
6	A	609	CHL	C11-C12-C13-C15
5	A	603	CLA	C11-C12-C13-C15
7	A	801	LHG	O8-C23-C24-C25
7	B	801	LHG	O8-C23-C24-C25
5	B	603	CLA	CAA-CBA-CGA-O1A
7	C	801	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
6	A	609	CHL	CAA-CBA-CGA-O1A
6	A	609	CHL	CAA-CBA-CGA-O2A
5	A	603	CLA	CAA-CBA-CGA-O1A
8	B	802	DGD	O2G-C1B-C2B-C3B

There are no ring outliers.

60 monomers are involved in 801 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	802	DGD	4	0
2	A	502	LUX	21	0
7	A	801	LHG	12	0
7	C	801	LHG	13	0
5	B	604	CLA	24	0
5	A	608	CLA	16	0
6	C	613	CHL	5	0
5	C	604	CLA	20	0
3	C	503	NEX	4	0
5	B	601	CLA	23	0
2	B	502	LUX	18	0
5	B	606	CLA	17	0
5	B	608	CLA	21	0
5	B	607	CLA	17	0
5	A	601	CLA	21	0
6	C	614	CHL	14	0
6	A	610	CHL	31	0
6	B	614	CHL	16	0
6	C	609	CHL	30	0
5	C	603	CLA	17	0
5	A	607	CLA	17	0
6	C	612	CHL	21	0
5	C	607	CLA	19	0
4	C	504	XAT	16	0
5	C	606	CLA	17	0
6	A	614	CHL	15	0
3	A	503	NEX	4	0
4	B	504	XAT	16	0
5	B	605	CLA	23	0
8	A	802	DGD	4	0
3	B	503	NEX	4	0
5	C	605	CLA	21	0
6	C	610	CHL	31	0

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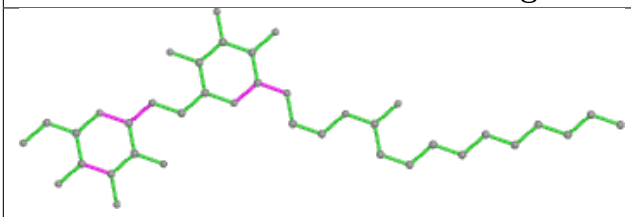
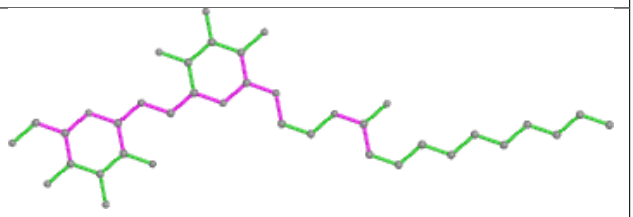
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	LUX	29	0
2	B	501	LUX	31	0
6	A	609	CHL	31	0
5	C	602	CLA	11	0
6	B	610	CHL	28	0
5	B	602	CLA	11	0
4	A	504	XAT	18	0
5	B	603	CLA	24	0
6	B	611	CHL	22	0
5	A	603	CLA	18	0
6	B	609	CHL	27	0
2	C	502	LUX	19	0
5	A	605	CLA	21	0
6	A	613	CHL	6	0
5	A	604	CLA	22	0
6	A	611	CHL	22	0
5	C	601	CLA	23	0
6	B	613	CHL	9	0
6	A	612	CHL	18	0
6	B	612	CHL	22	0
5	C	608	CLA	16	0
7	B	801	LHG	13	0
6	C	611	CHL	23	0
5	A	602	CLA	13	0
5	A	606	CLA	18	0
2	C	501	LUX	31	0
8	B	802	DGD	2	0

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

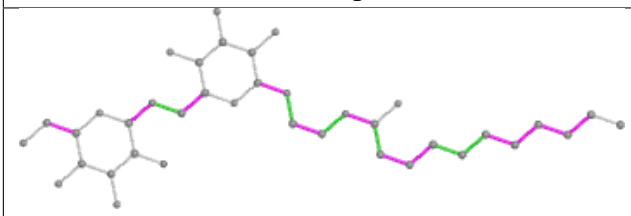
Ligand DGD C 802



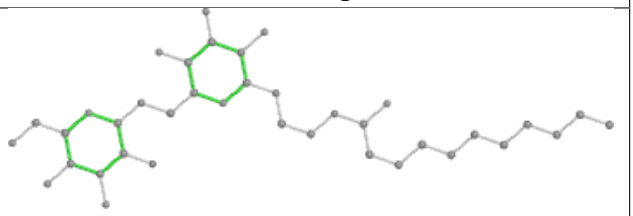
Bond lengths



Bond angles

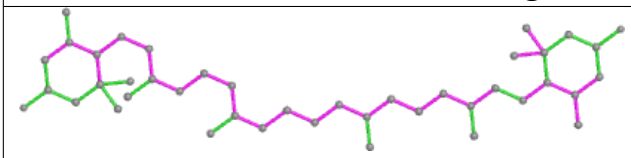


Torsions

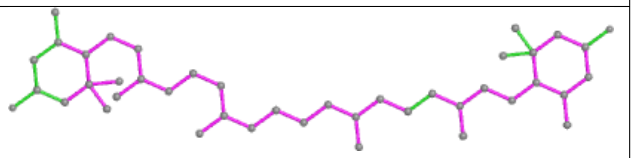


Rings

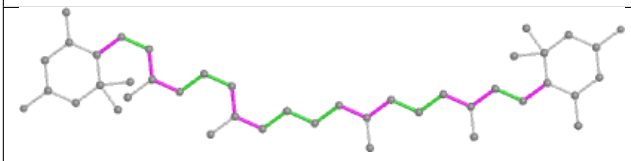
Ligand LUX A 502



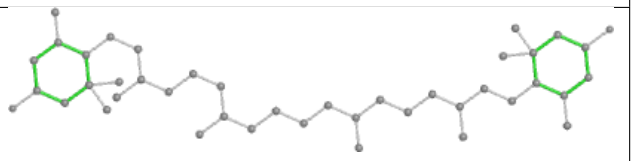
Bond lengths



Bond angles

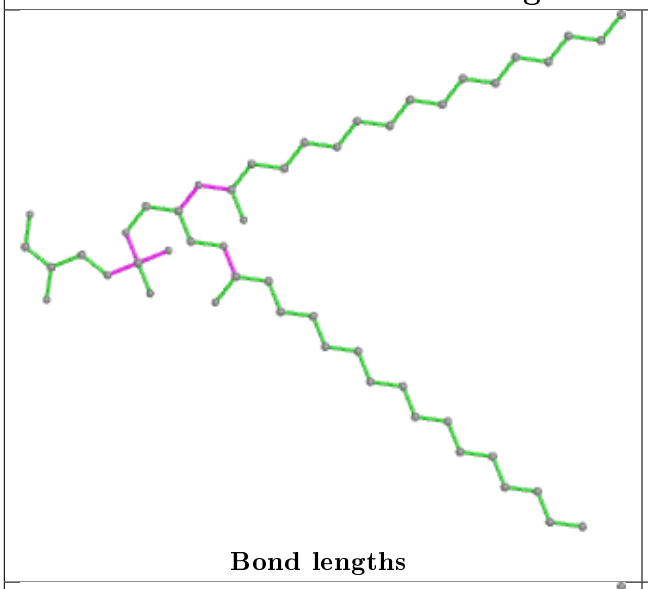


Torsions

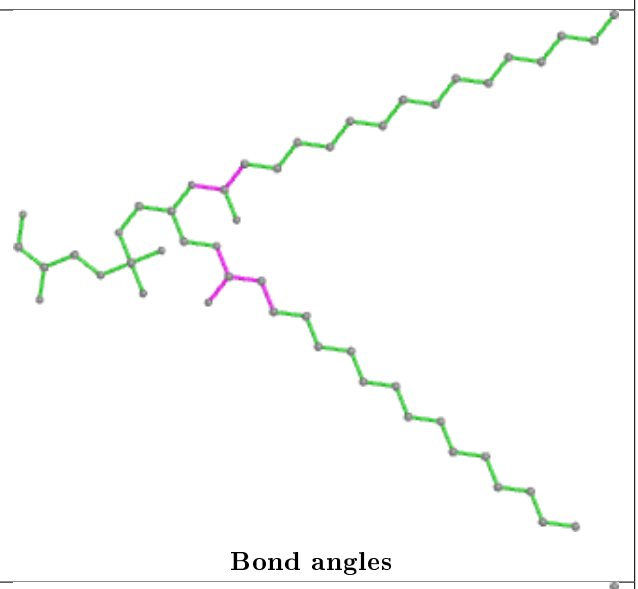


Rings

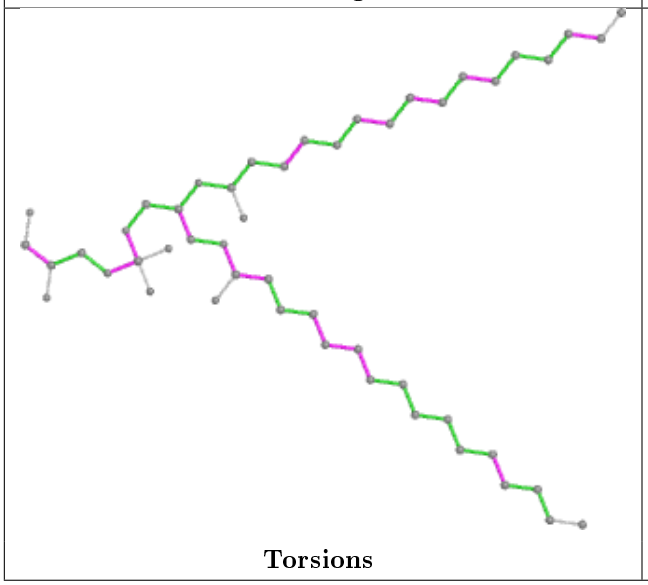
Ligand LHG A 801



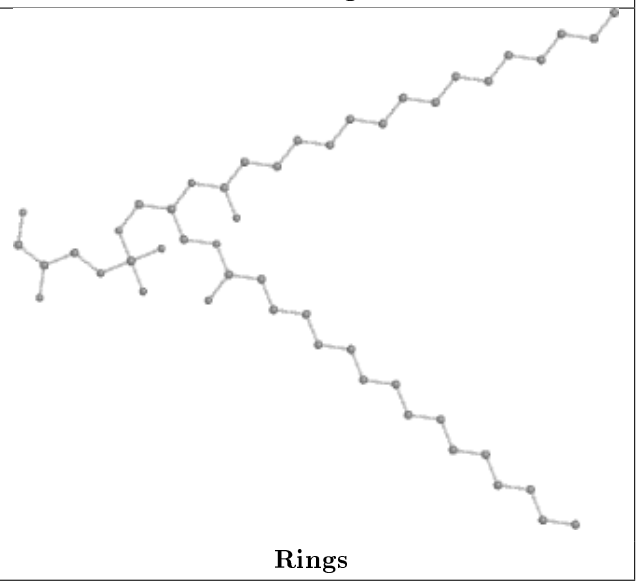
Bond lengths



Bond angles

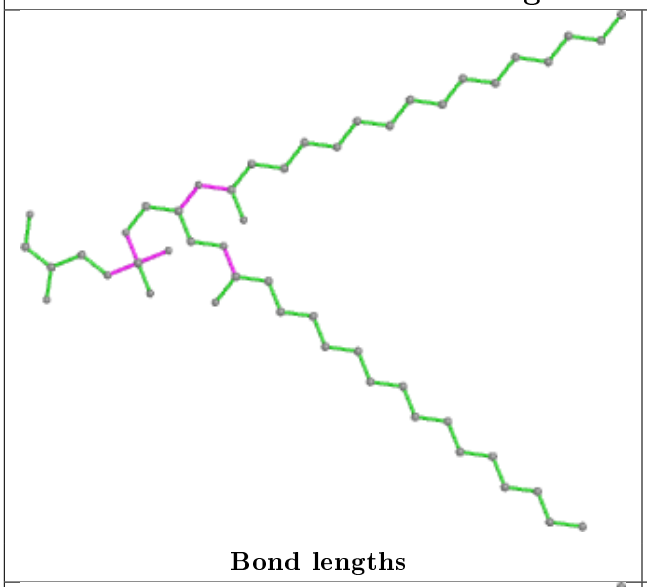


Torsions

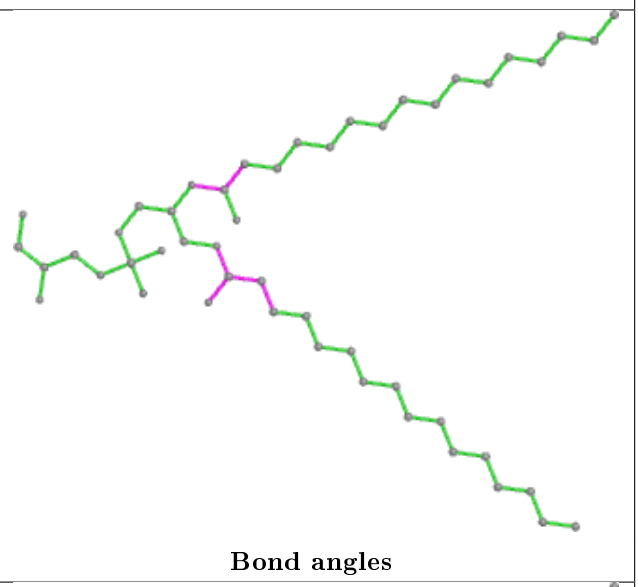


Rings

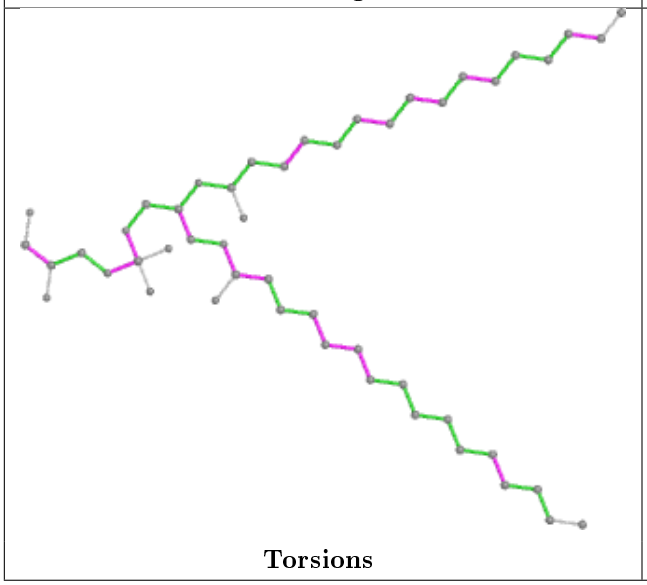
Ligand LHG C 801



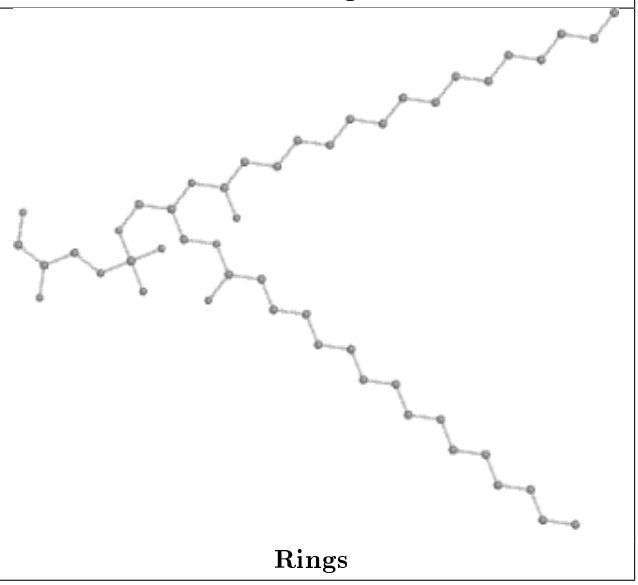
Bond lengths



Bond angles

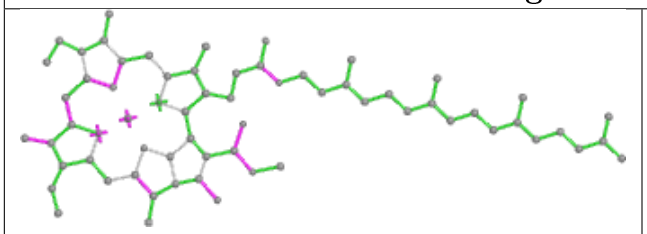


Torsions

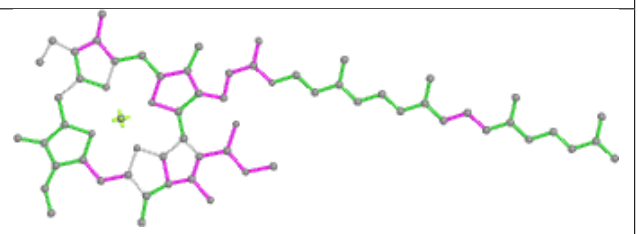


Rings

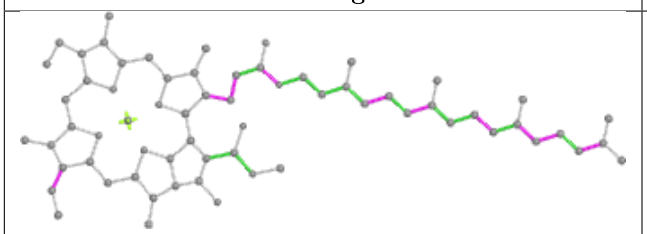
Ligand CLA B 604



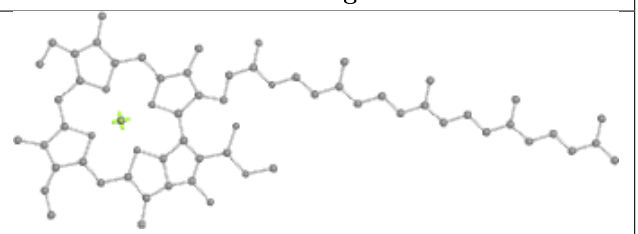
Bond lengths



Bond angles

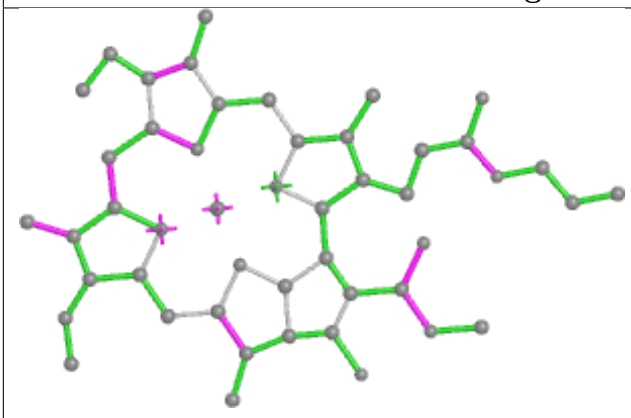


Torsions

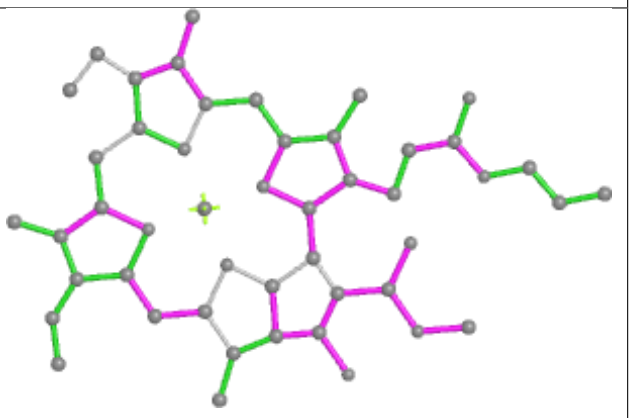


Rings

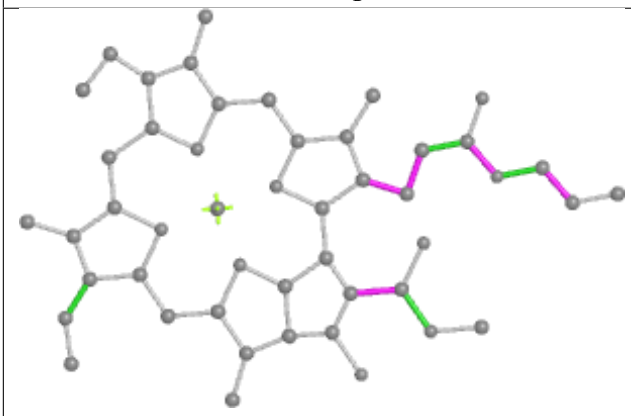
Ligand CLA A 608



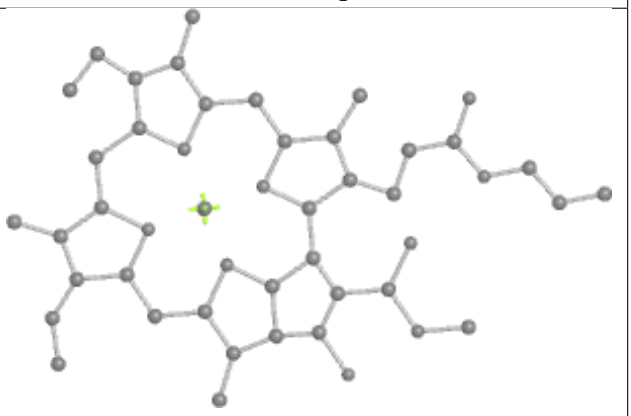
Bond lengths



Bond angles

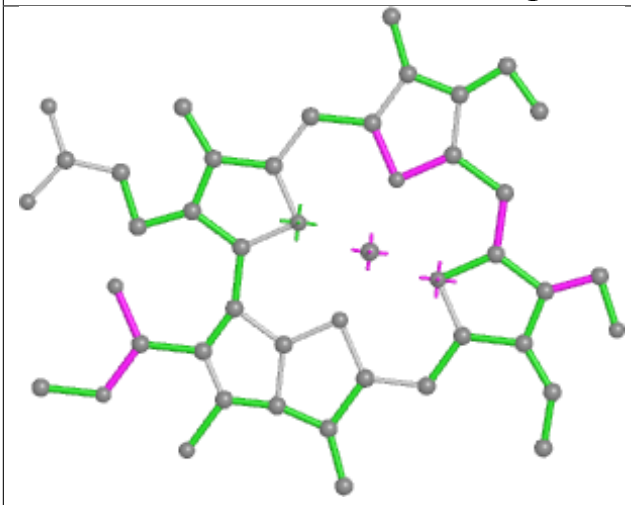


Torsions

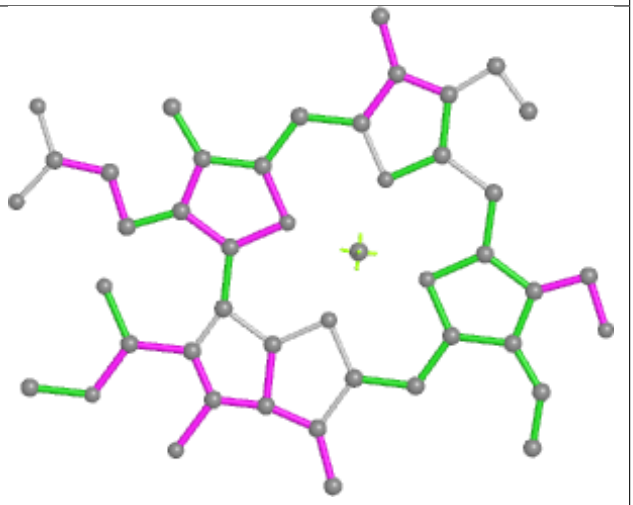


Rings

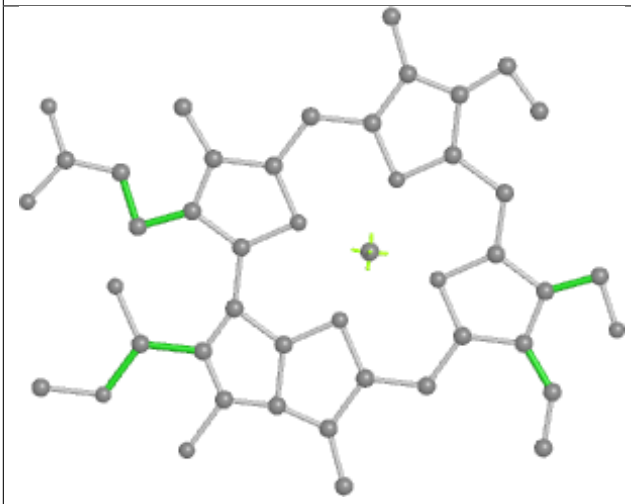
Ligand CHL C 613



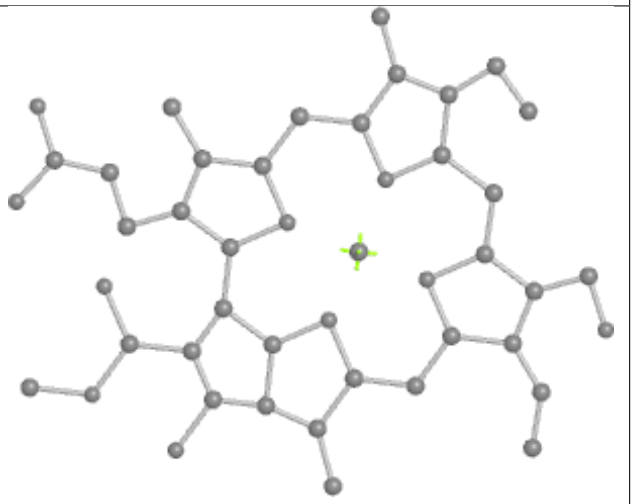
Bond lengths



Bond angles

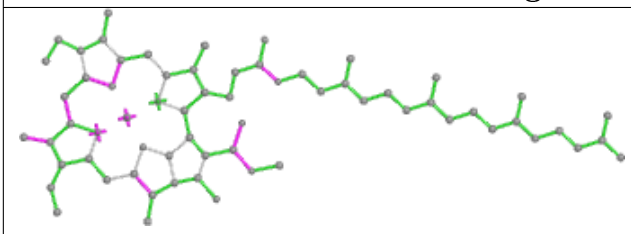


Torsions



Rings

Ligand CLA C 604



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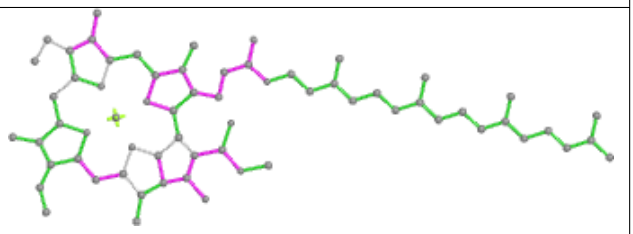
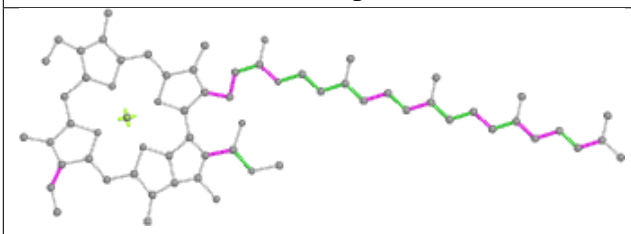
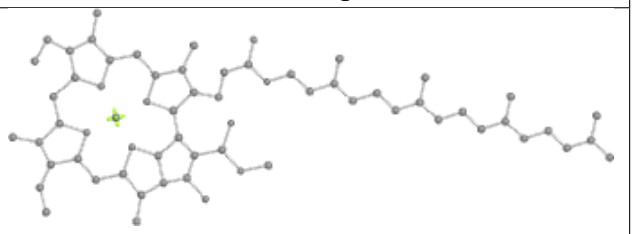


Bond angles

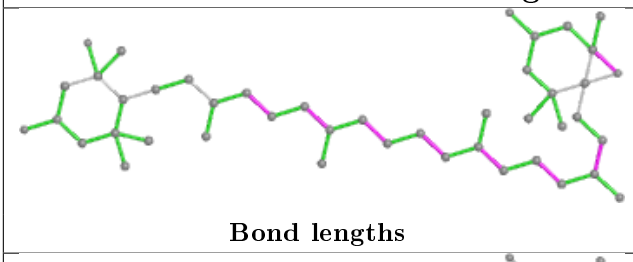


Torsions

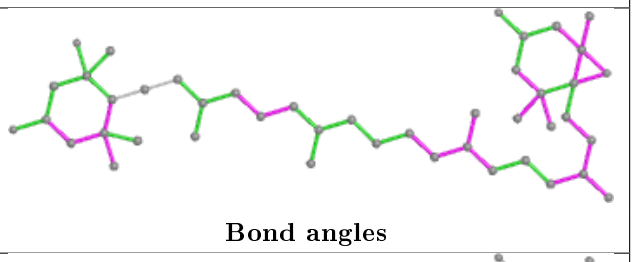


Rings

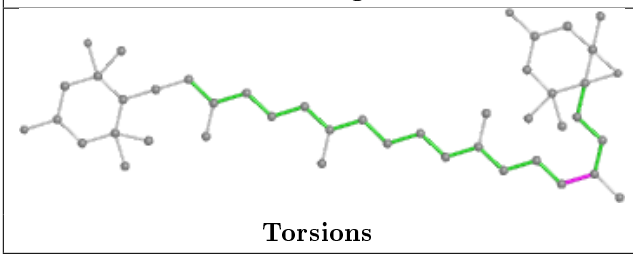
Ligand NEX C 503



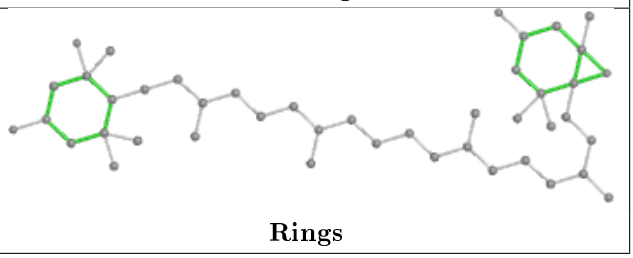
Bond lengths



Bond angles

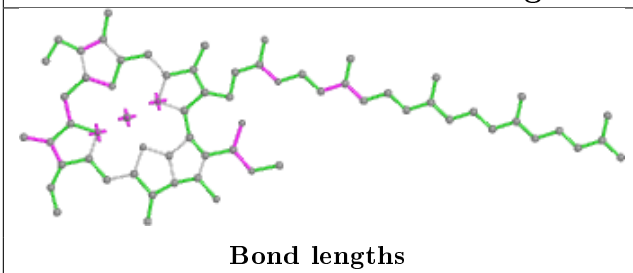


Torsions

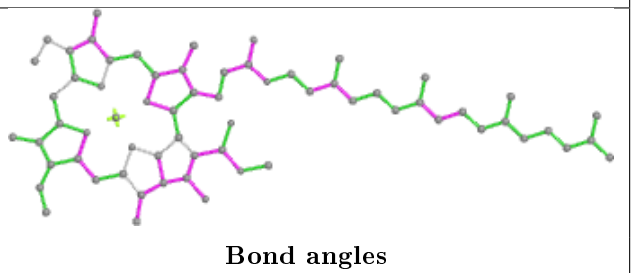


Rings

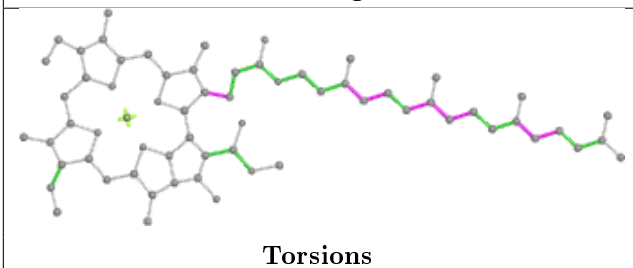
Ligand CLA B 601



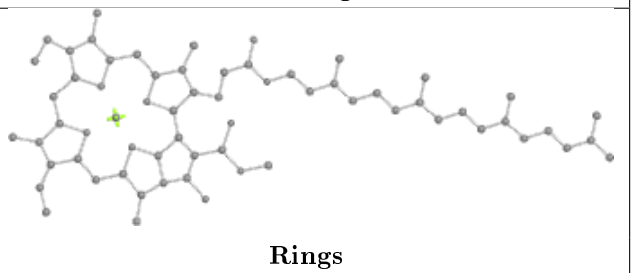
Bond lengths



Bond angles

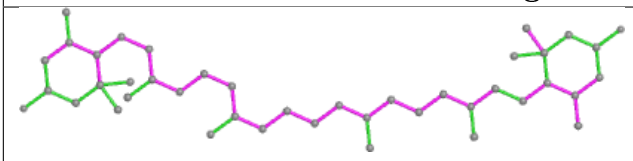


Torsions

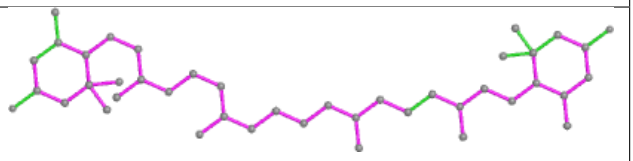


Rings

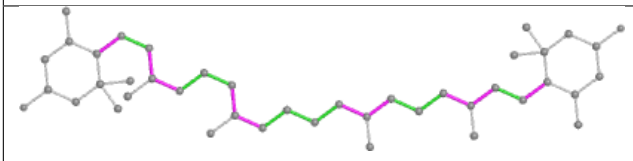
Ligand LUX B 502



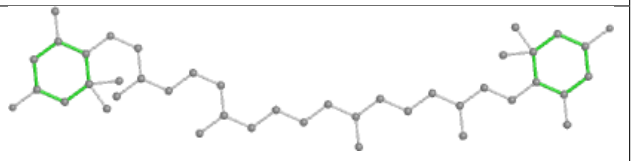
Bond lengths



Bond angles

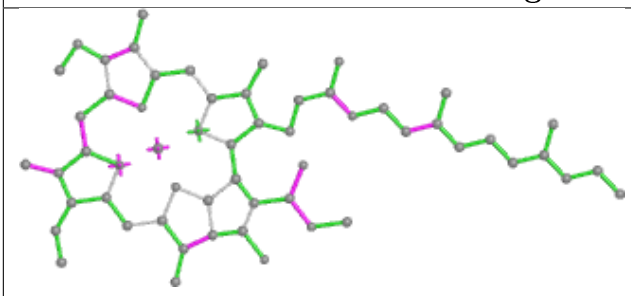


Torsions

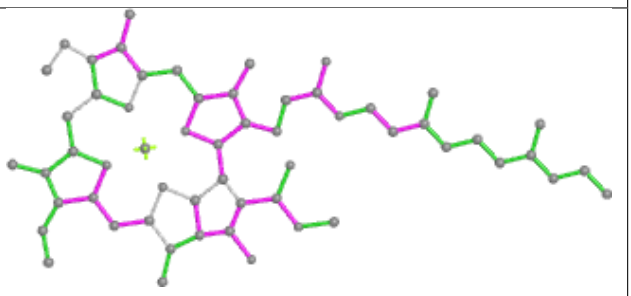


Rings

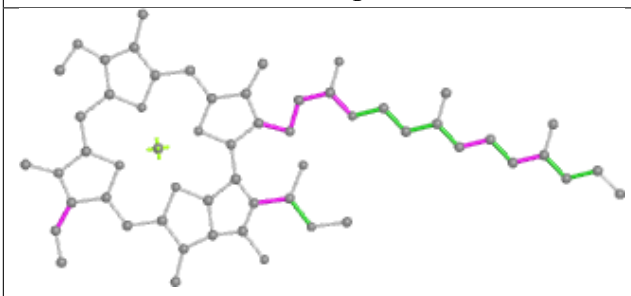
Ligand CLA B 606



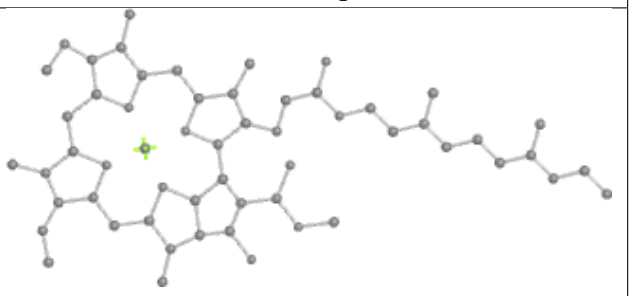
Bond lengths



Bond angles

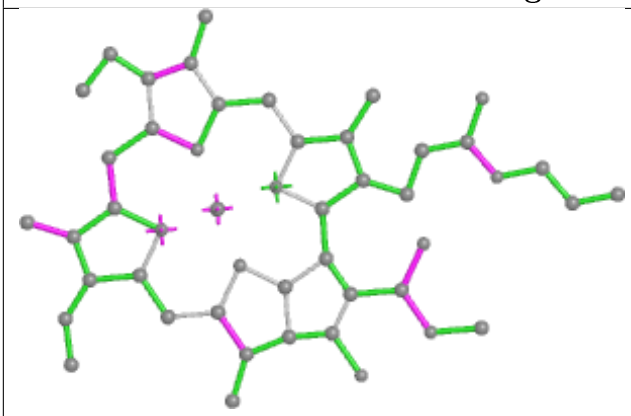


Torsions

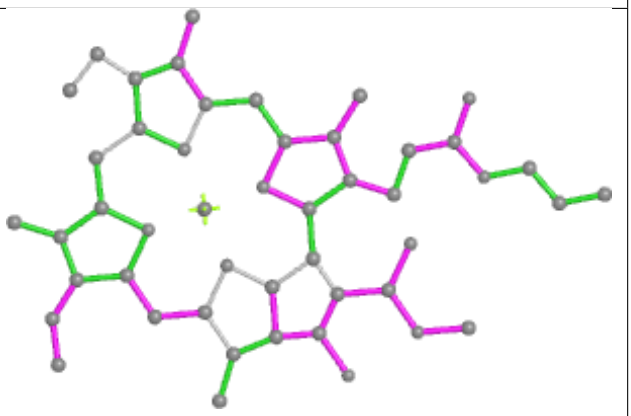


Rings

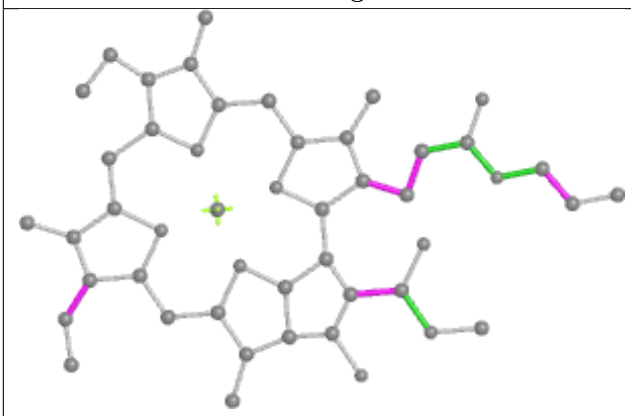
Ligand CLA B 608



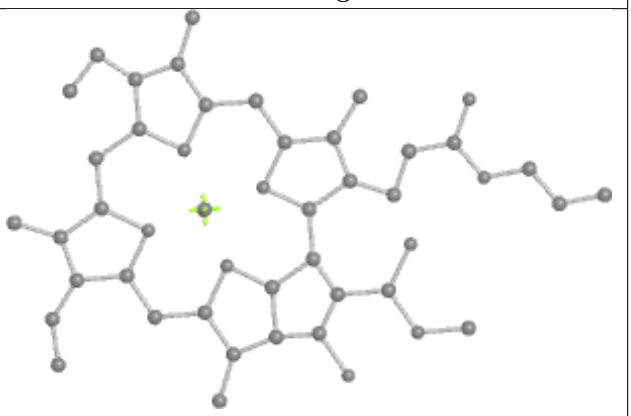
Bond lengths



Bond angles

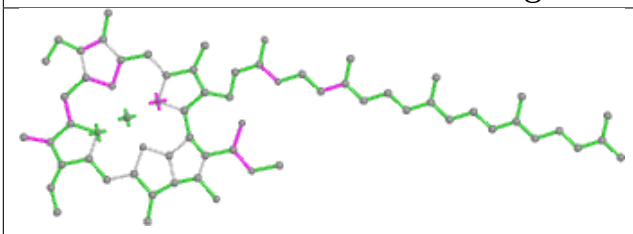


Torsions

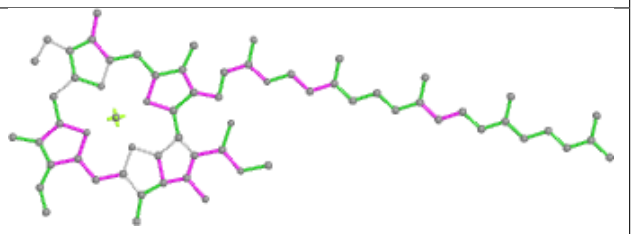


Rings

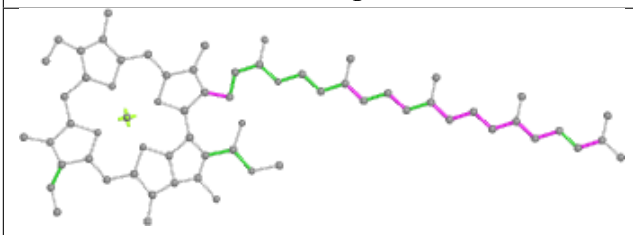
Ligand CLA B 607



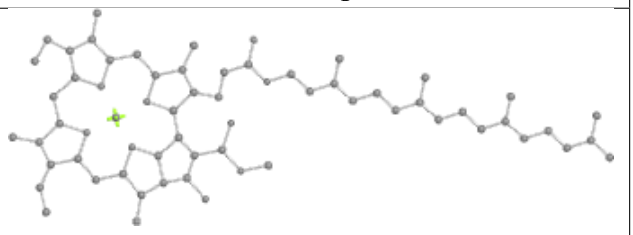
Bond lengths



Bond angles

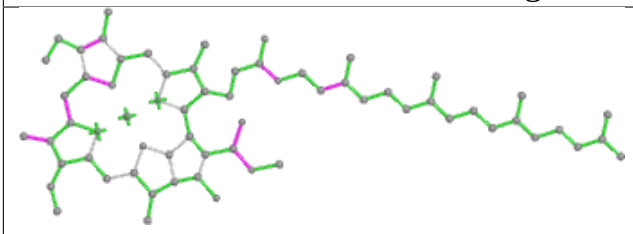


Torsions

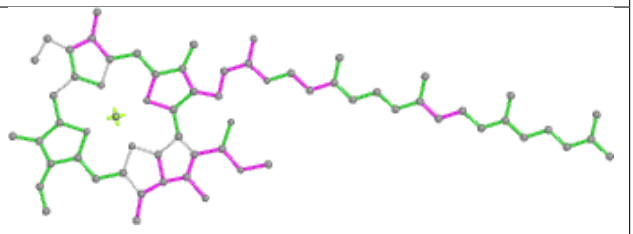


Rings

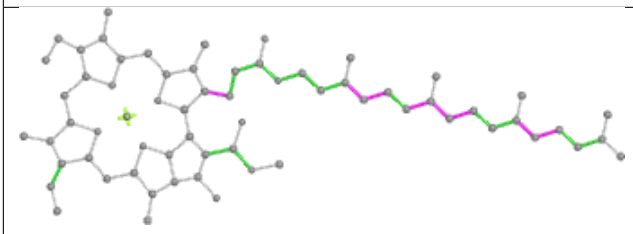
Ligand CLA A 601



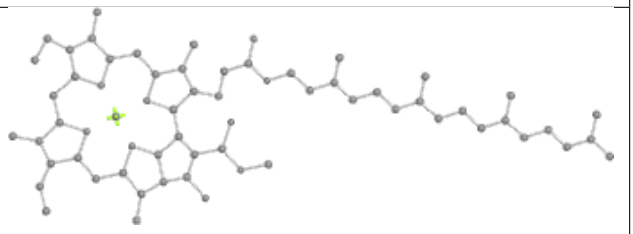
Bond lengths



Bond angles

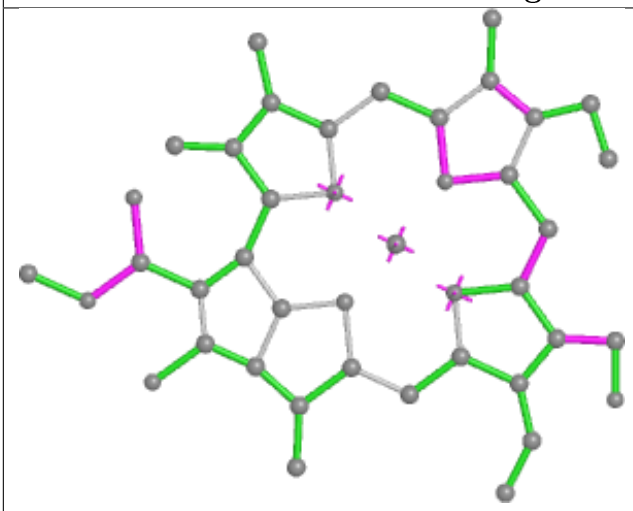


Torsions

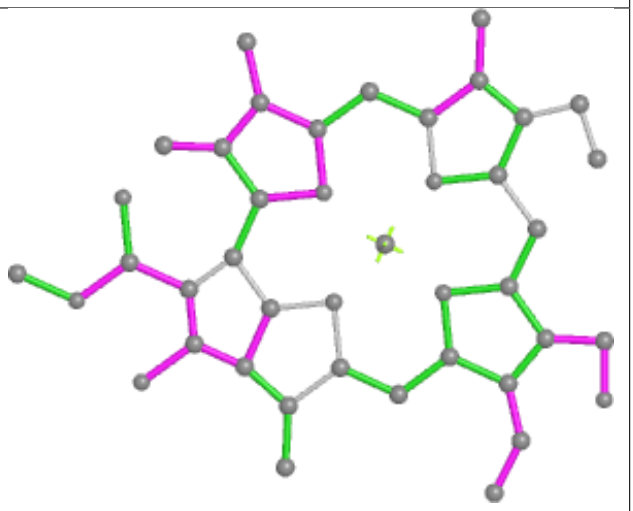


Rings

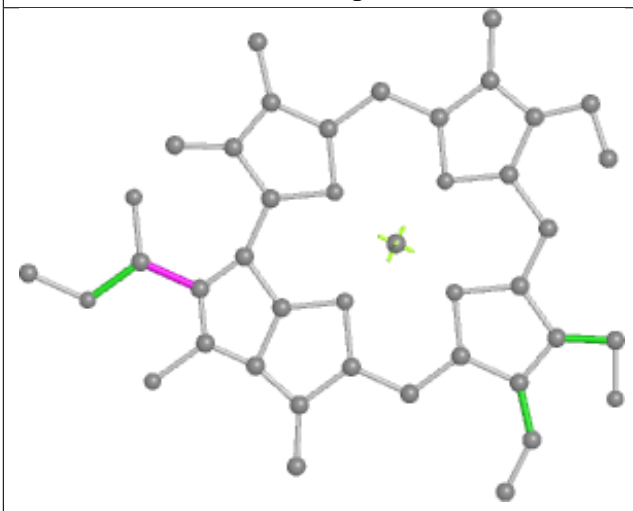
Ligand CHL C 614



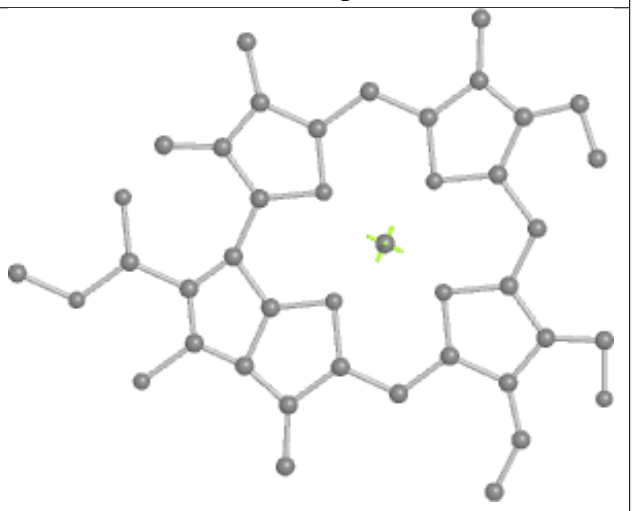
Bond lengths



Bond angles

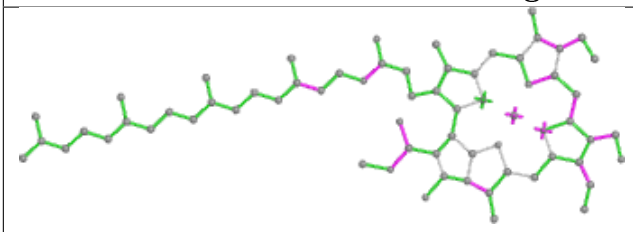


Torsions

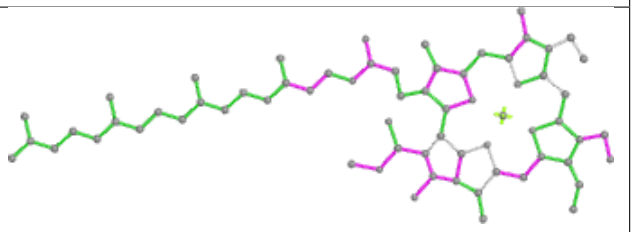


Rings

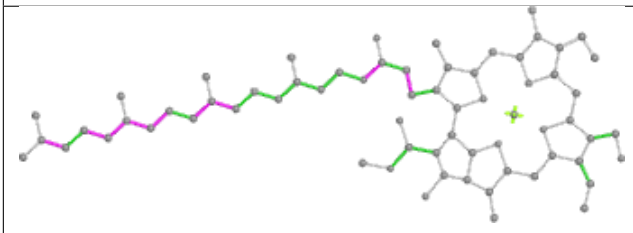
Ligand CHL A 610



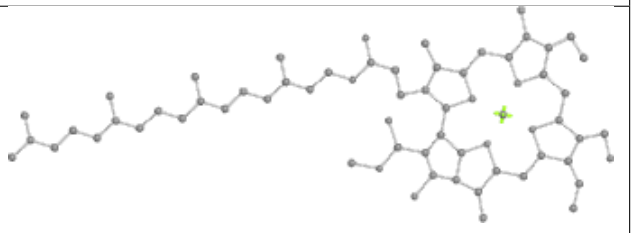
Bond lengths



Bond angles

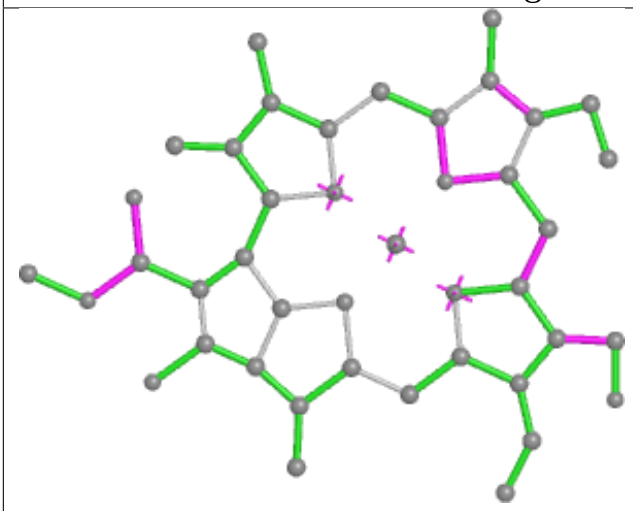


Torsions

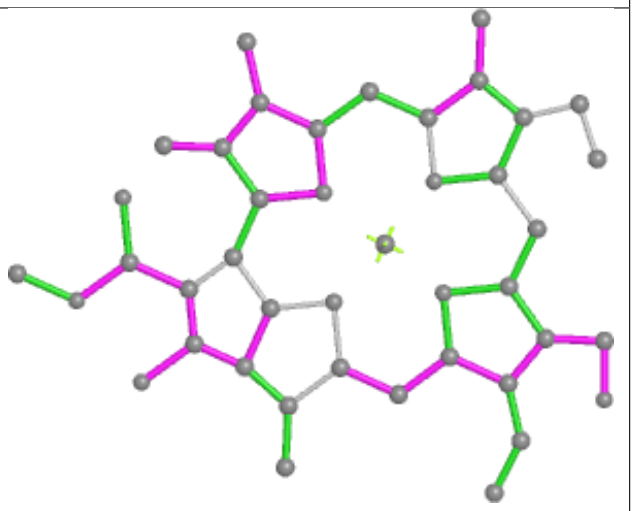


Rings

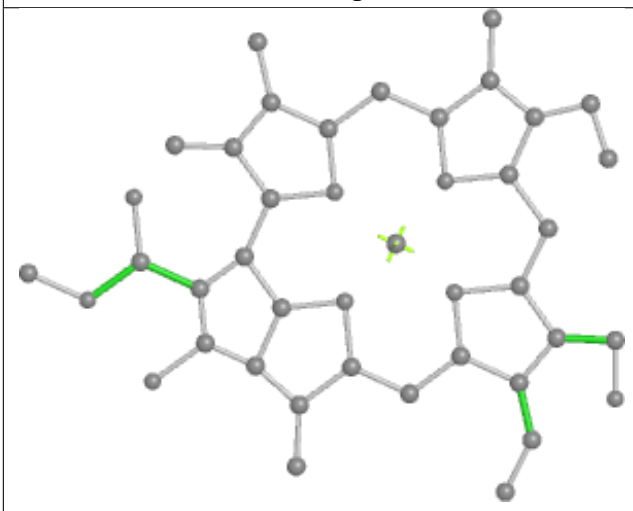
Ligand CHL B 614



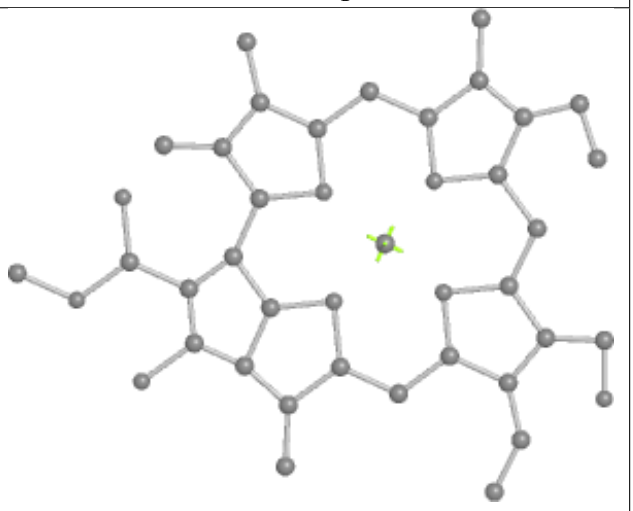
Bond lengths



Bond angles

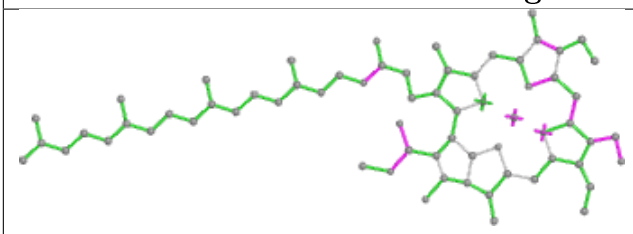


Torsions

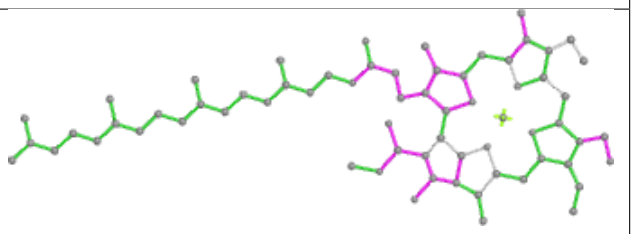


Rings

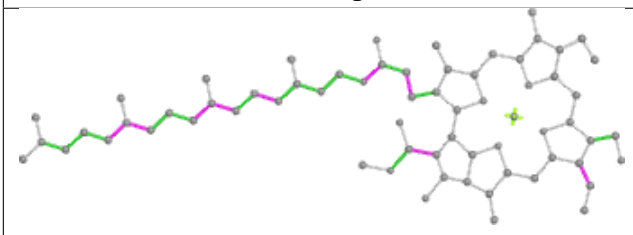
Ligand CHL C 609



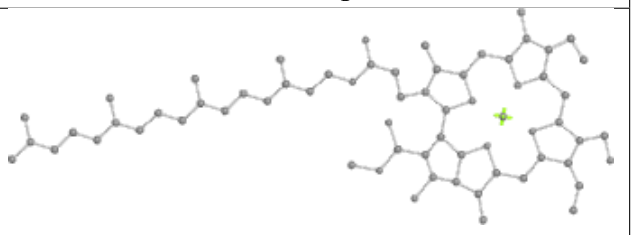
Bond lengths



Bond angles

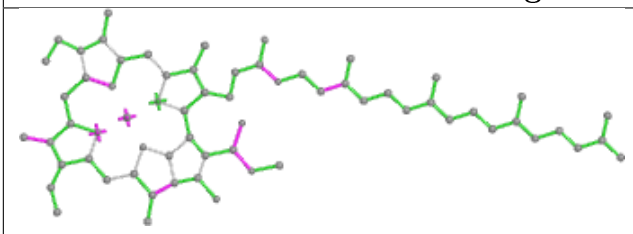


Torsions

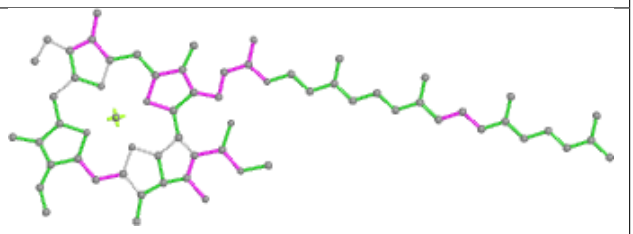


Rings

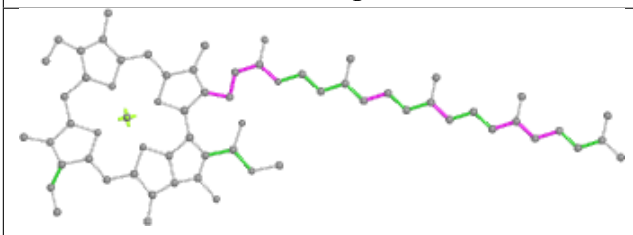
Ligand CLA C 603



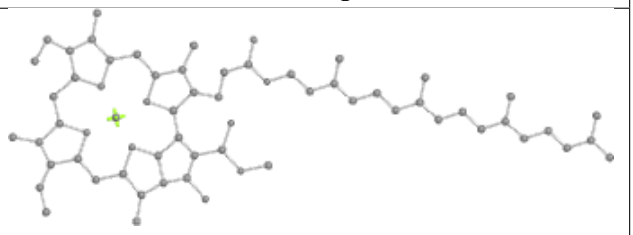
Bond lengths



Bond angles

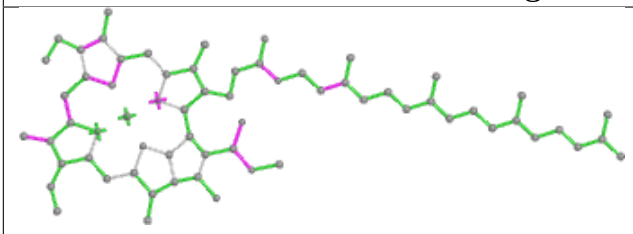


Torsions

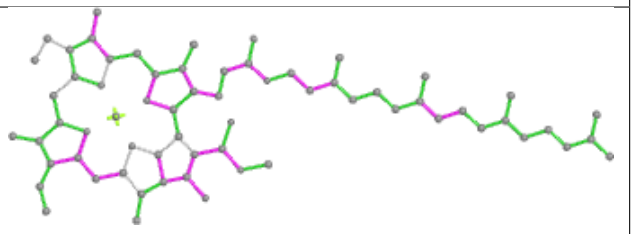


Rings

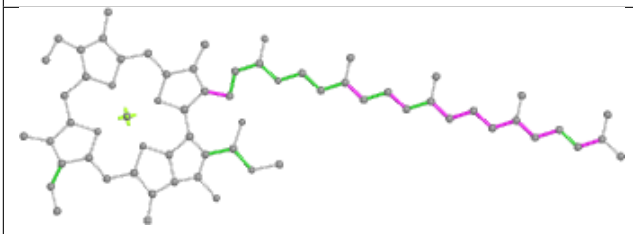
Ligand CLA A 607



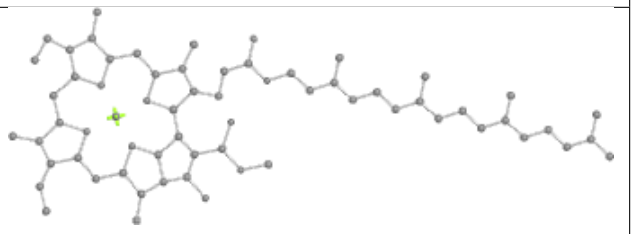
Bond lengths



Bond angles

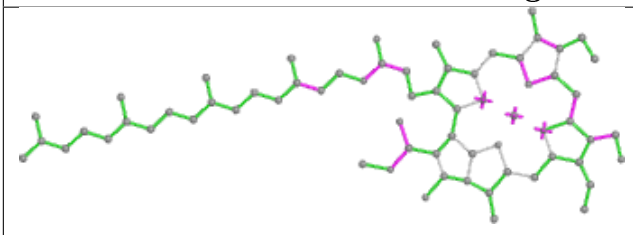


Torsions

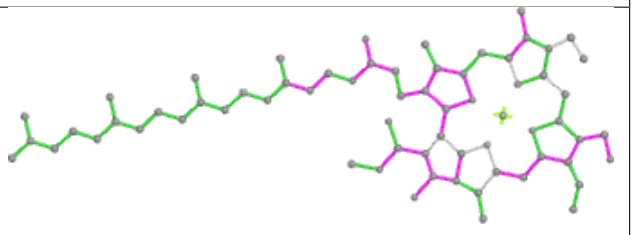


Rings

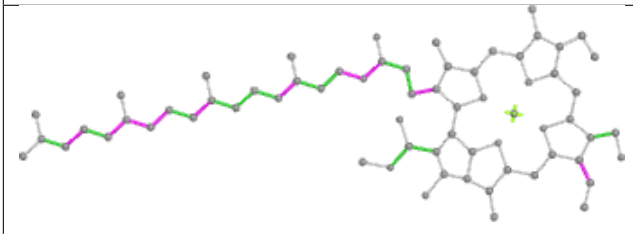
Ligand CHL C 612



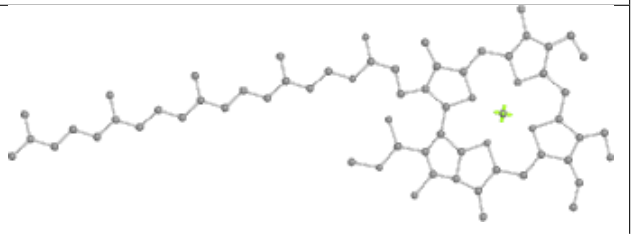
Bond lengths



Bond angles

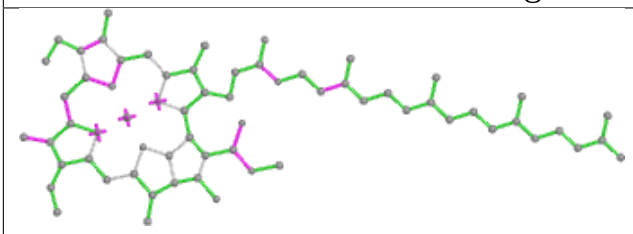


Torsions

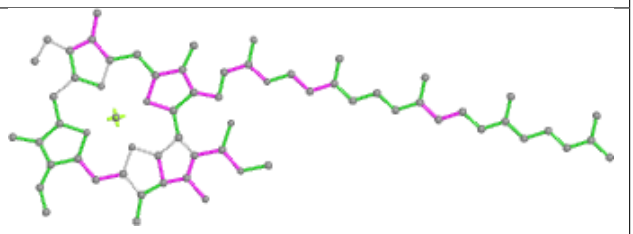


Rings

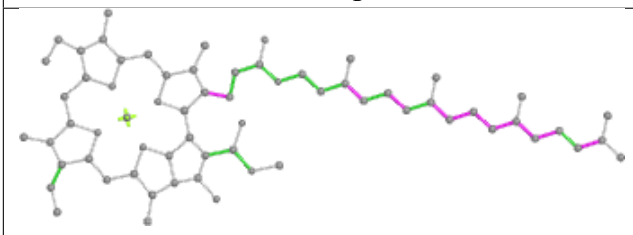
Ligand CLA C 607



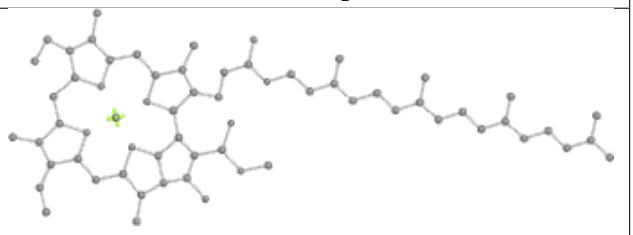
Bond lengths



Bond angles

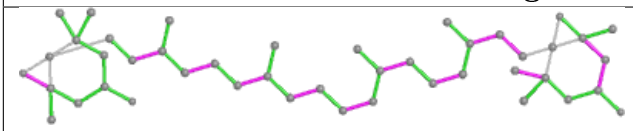


Torsions

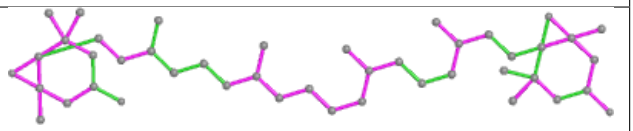


Rings

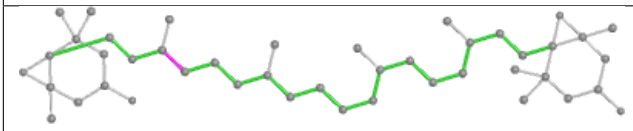
Ligand XAT C 504



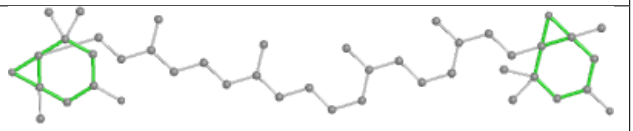
Bond lengths



Bond angles

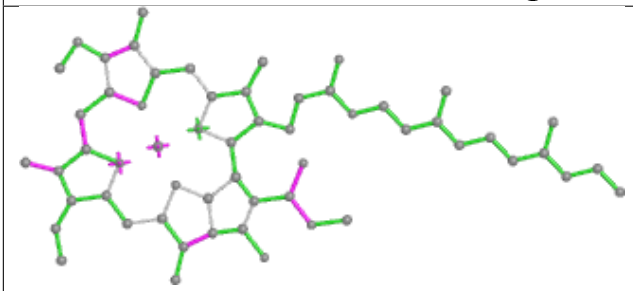


Torsions

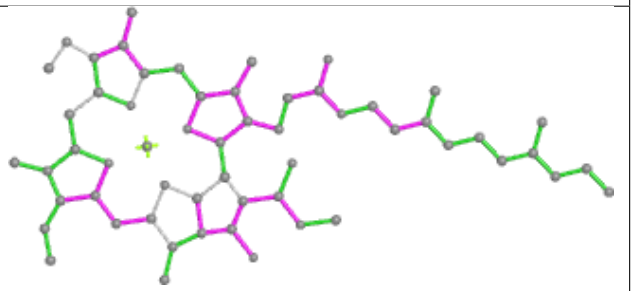


Rings

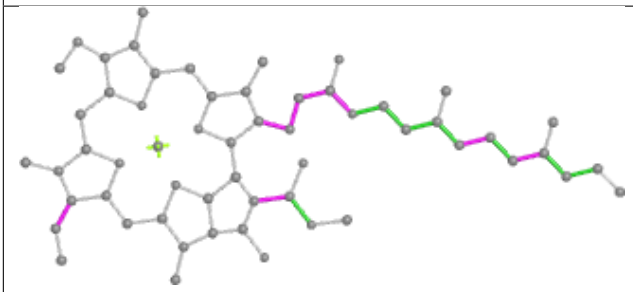
Ligand CLA C 606



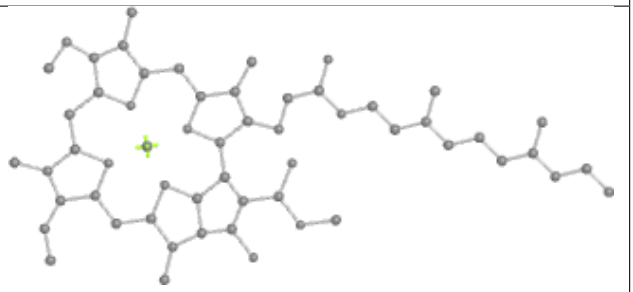
Bond lengths



Bond angles

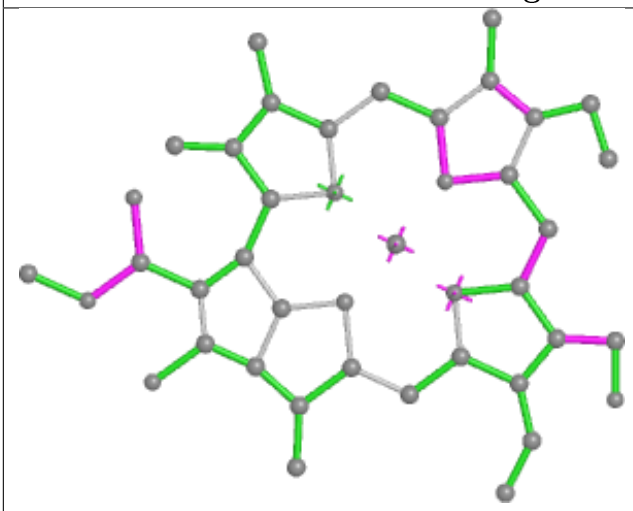


Torsions

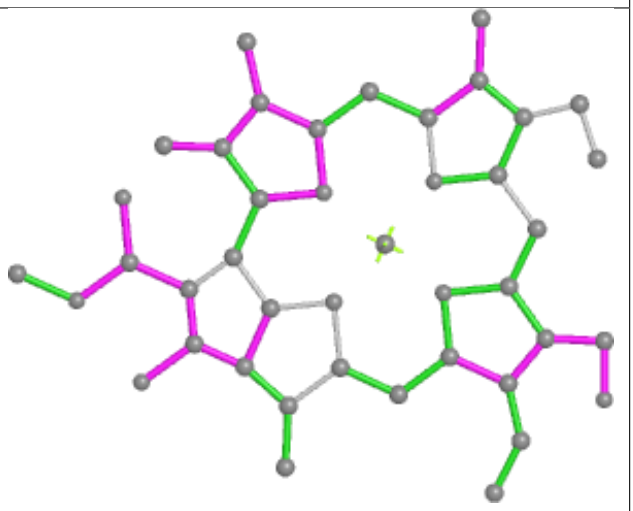


Rings

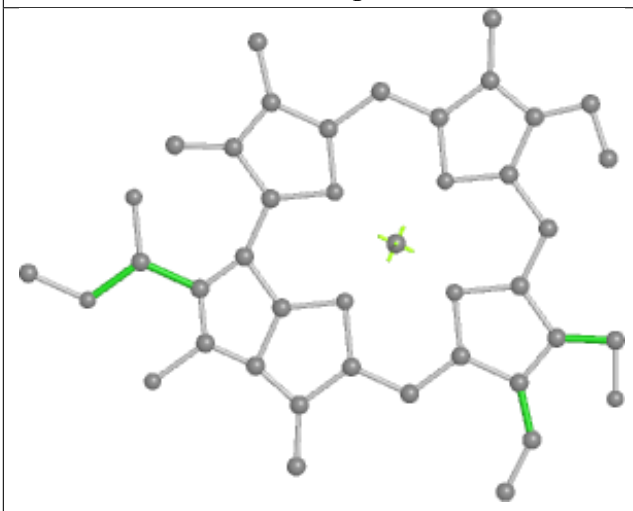
Ligand CHL A 614



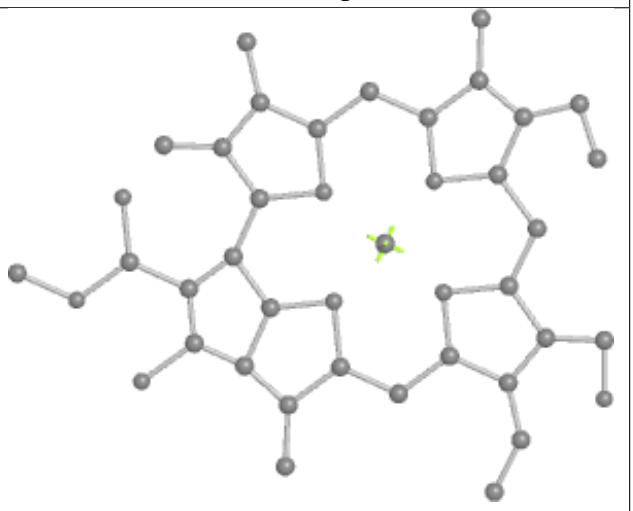
Bond lengths



Bond angles

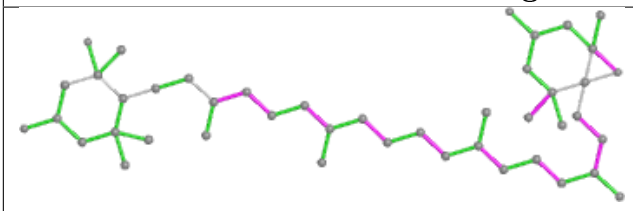


Torsions

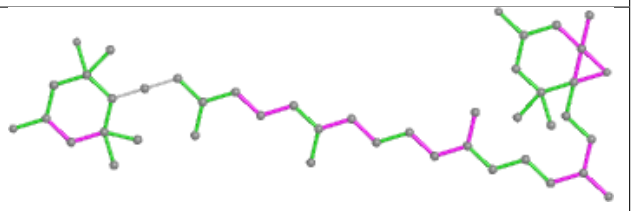


Rings

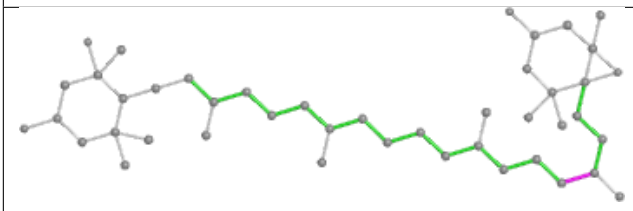
Ligand NEX A 503



Bond lengths



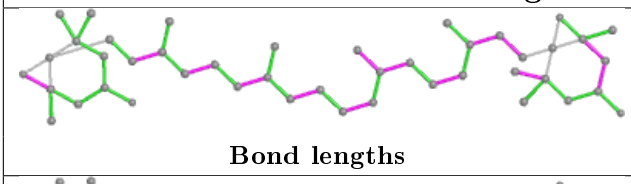
Bond angles



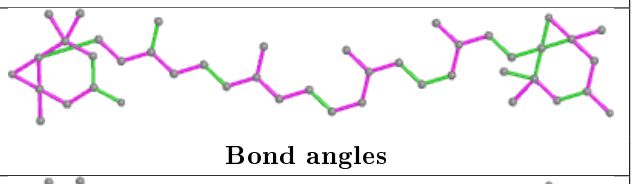
Torsions

Rings

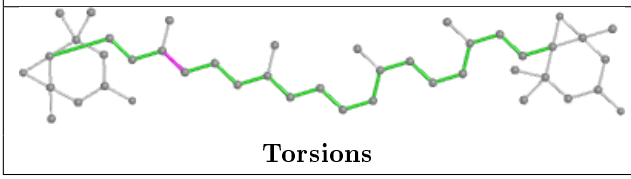
Ligand XAT B 504



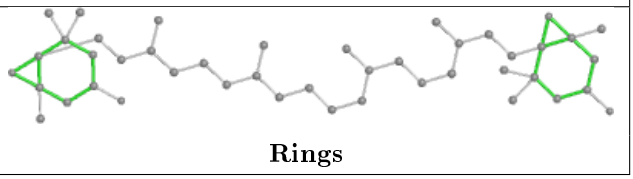
Bond lengths



Bond angles

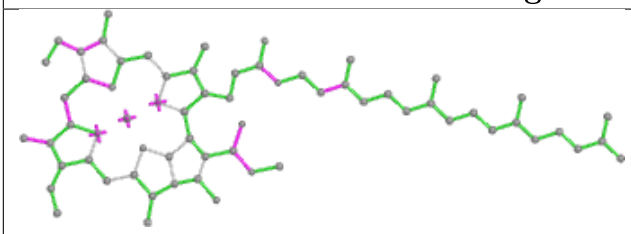


Torsions

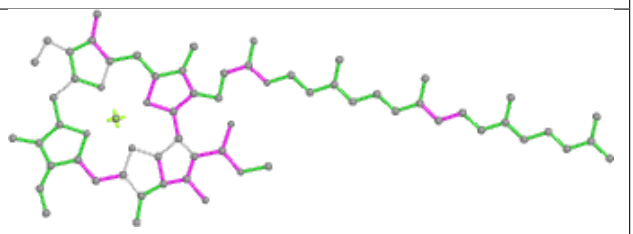


Rings

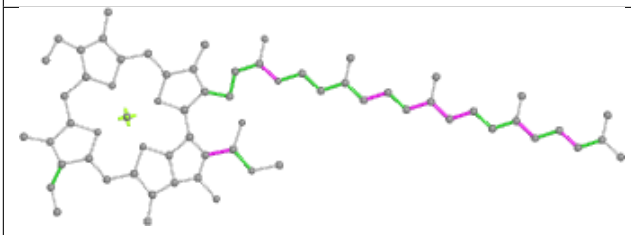
Ligand CLA B 605



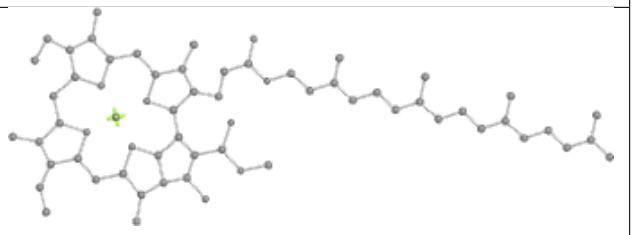
Bond lengths



Bond angles

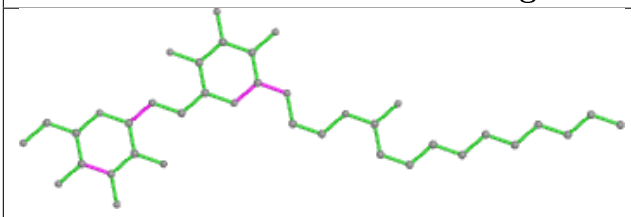


Torsions

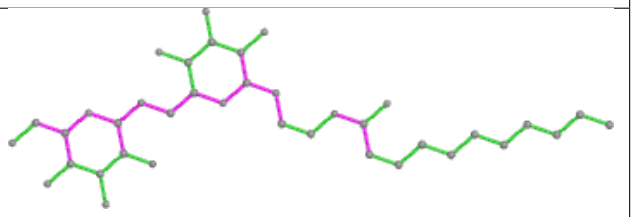


Rings

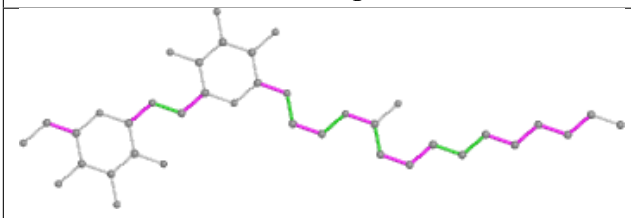
Ligand DGD A 802



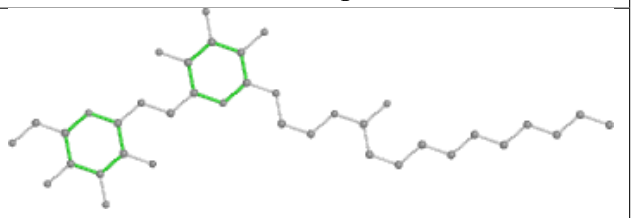
Bond lengths



Bond angles

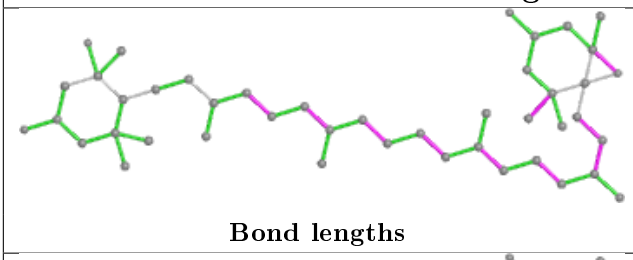


Torsions

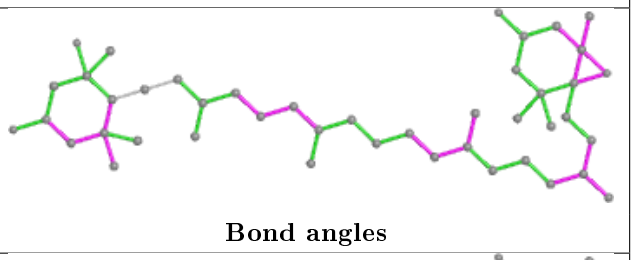


Rings

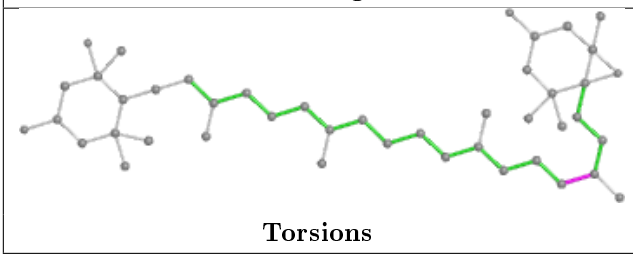
Ligand NEX B 503



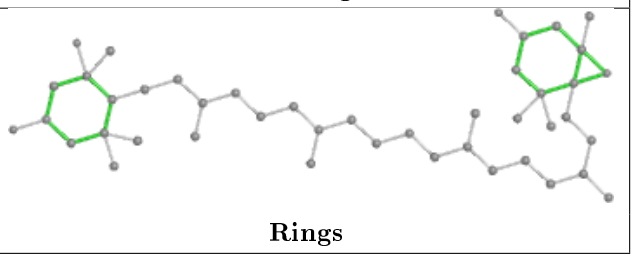
Bond lengths



Bond angles

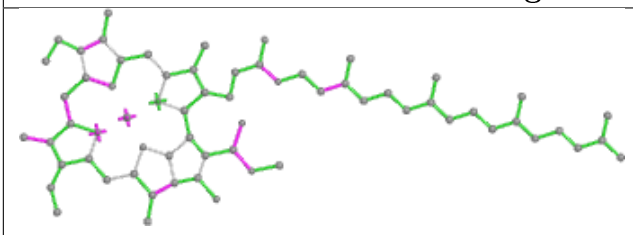


Torsions

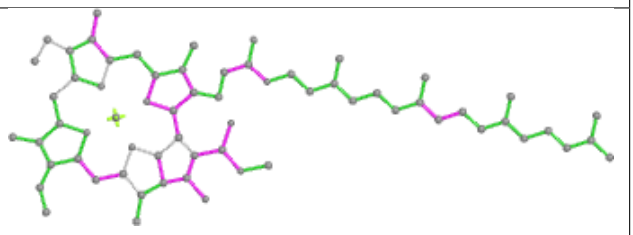


Rings

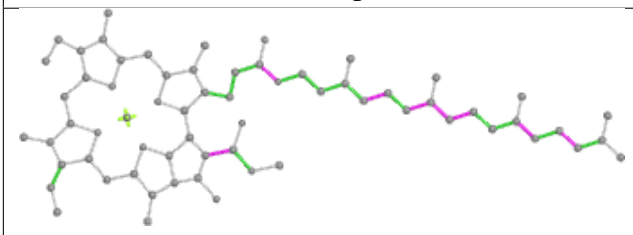
Ligand CLA C 605



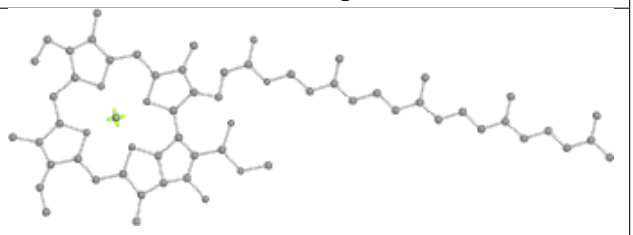
Bond lengths



Bond angles

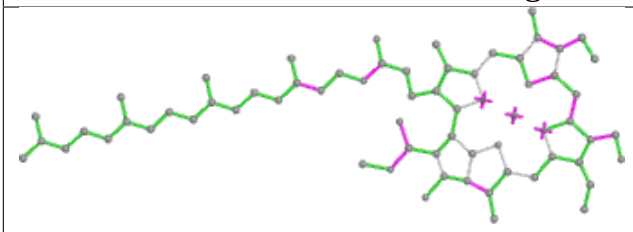


Torsions

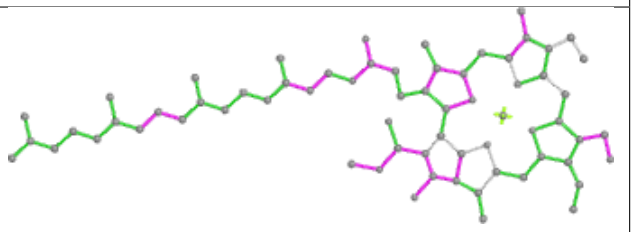


Rings

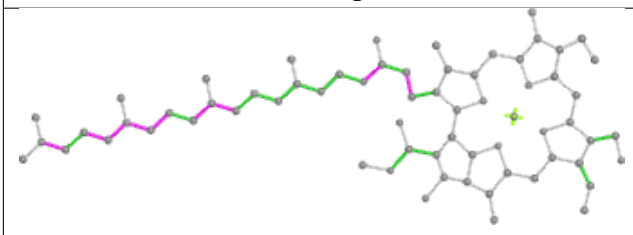
Ligand CHL C 610



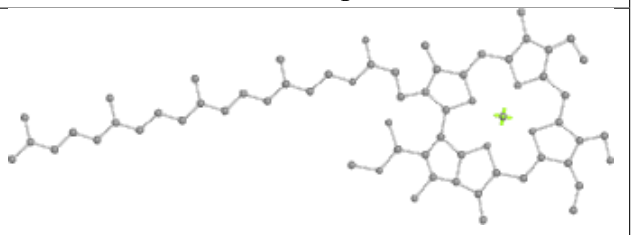
Bond lengths



Bond angles

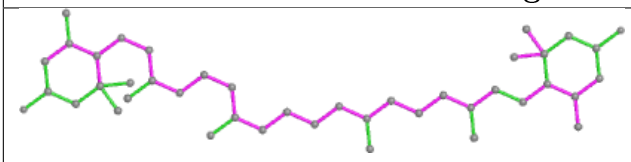


Torsions

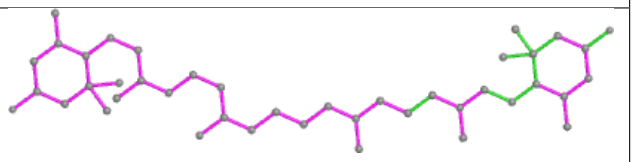


Rings

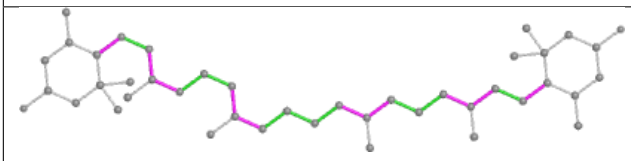
Ligand LUX A 501



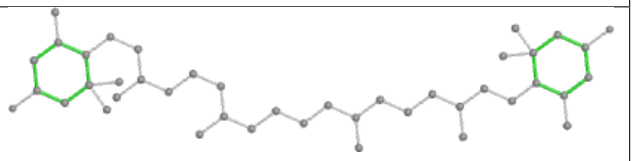
Bond lengths



Bond angles

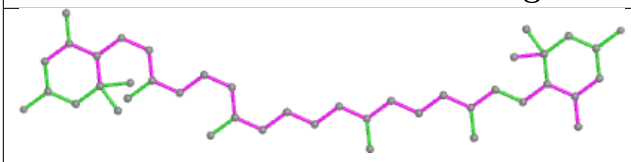


Torsions

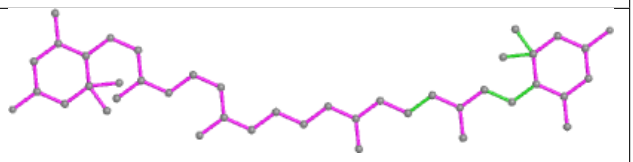


Rings

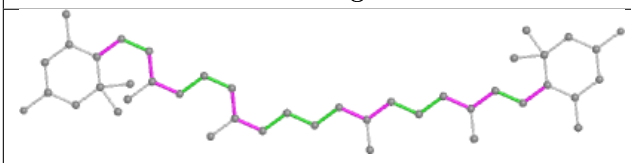
Ligand LUX B 501



Bond lengths



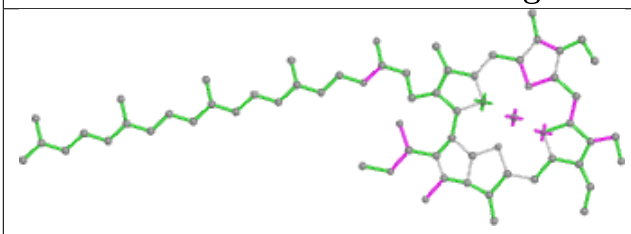
Bond angles



Torsions

Rings

Ligand CHL A 609



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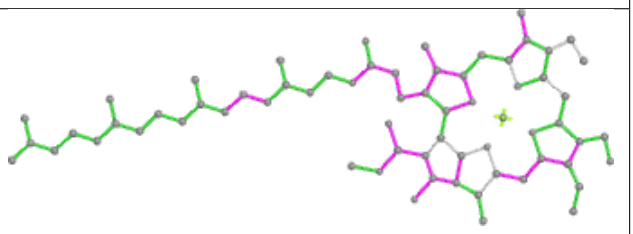
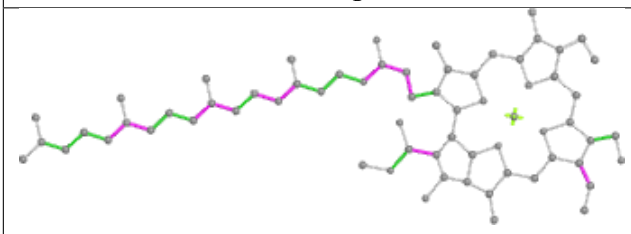
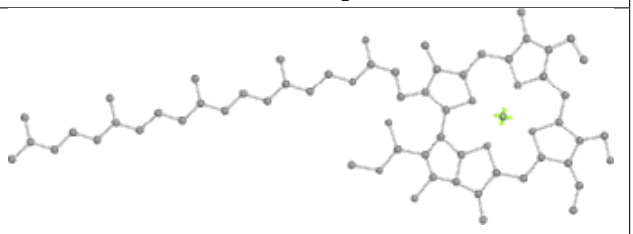


Bond angles

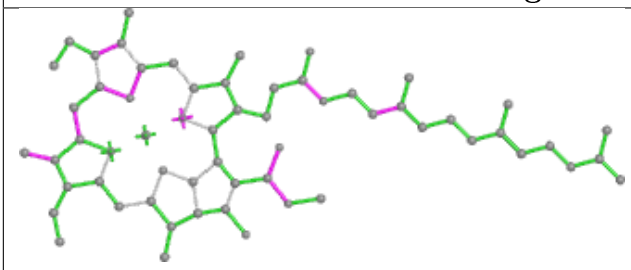


Torsions

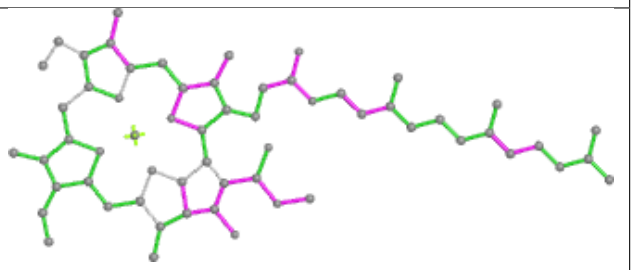


Rings

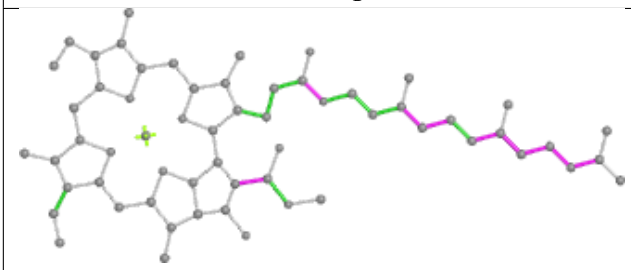
Ligand CLA C 602



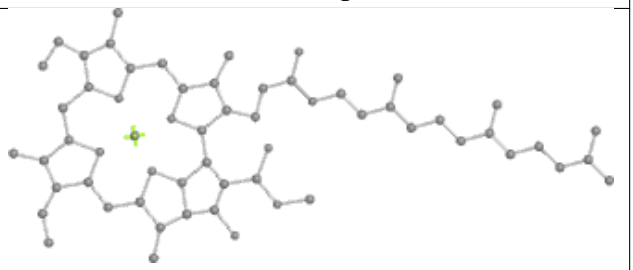
Bond lengths



Bond angles

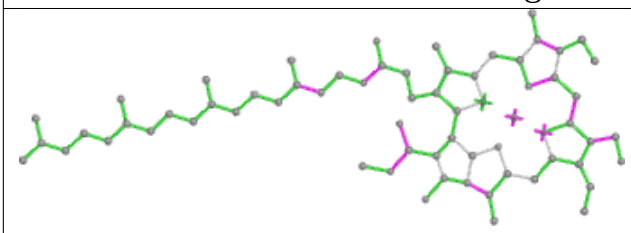


Torsions

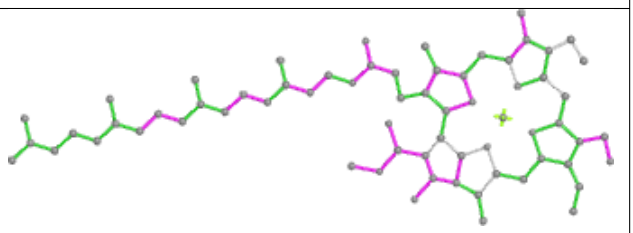


Rings

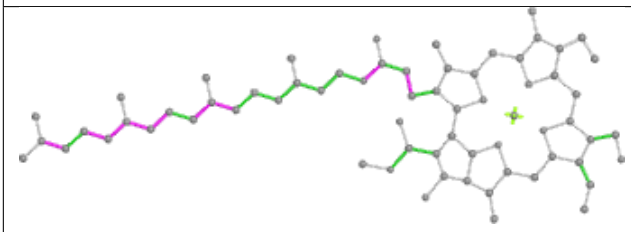
Ligand CHL B 610



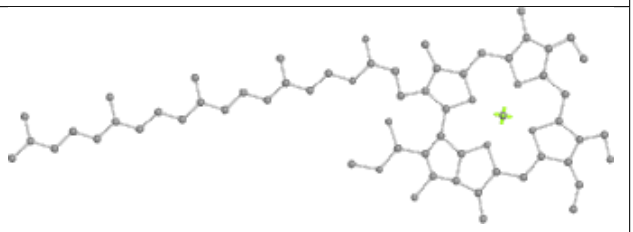
Bond lengths



Bond angles

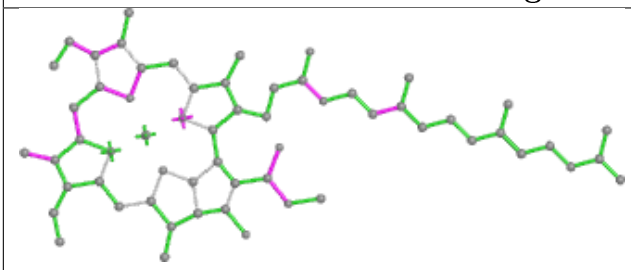


Torsions

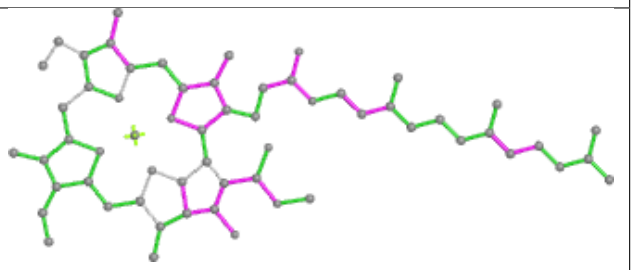


Rings

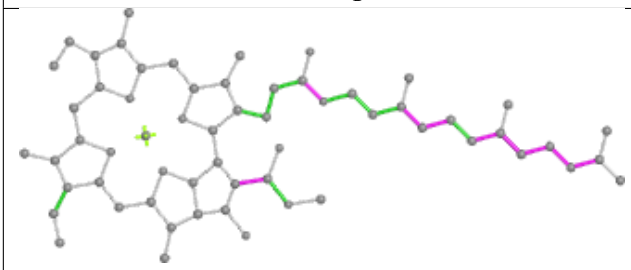
Ligand CLA B 602



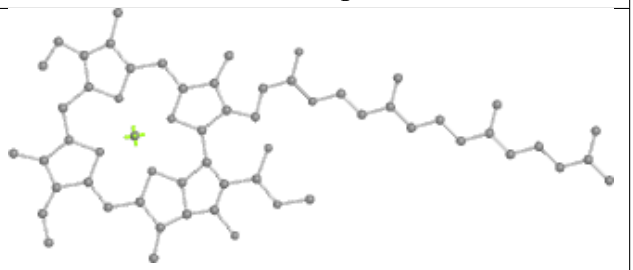
Bond lengths



Bond angles

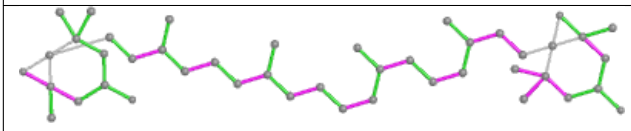


Torsions

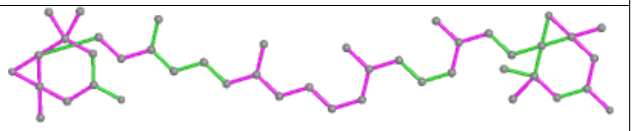


Rings

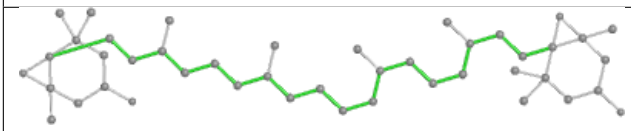
Ligand XAT A 504



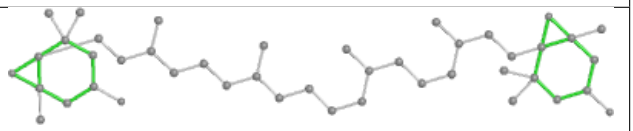
Bond lengths



Bond angles

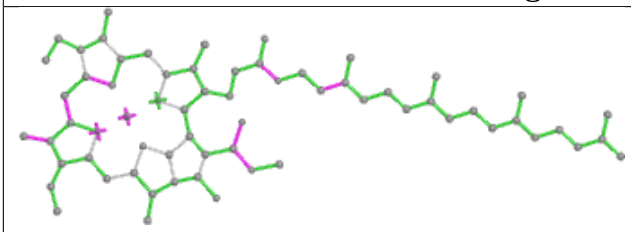


Torsions

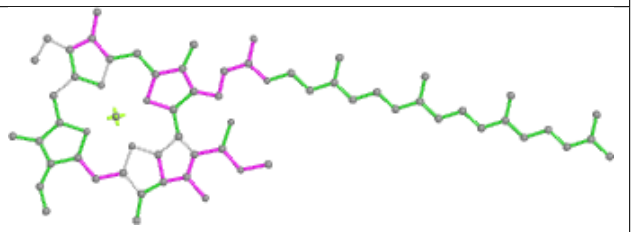


Rings

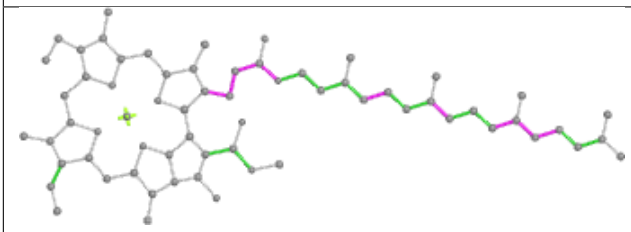
Ligand CLA B 603



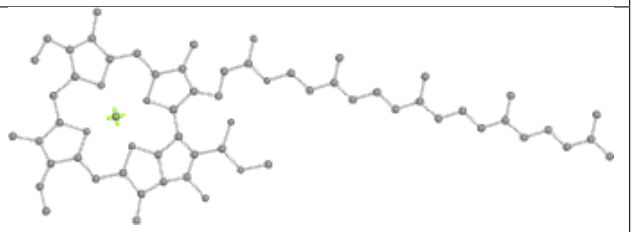
Bond lengths



Bond angles

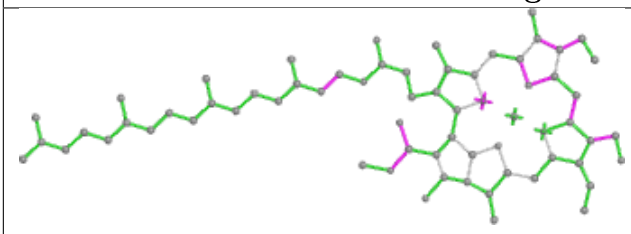


Torsions

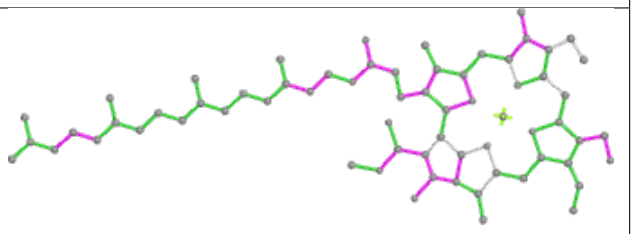


Rings

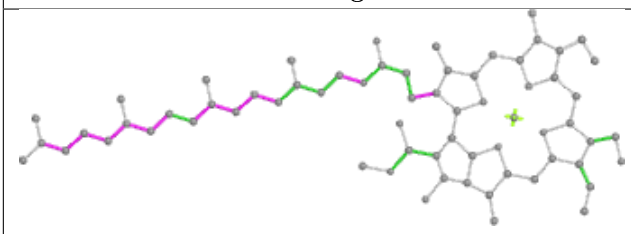
Ligand CHL B 611



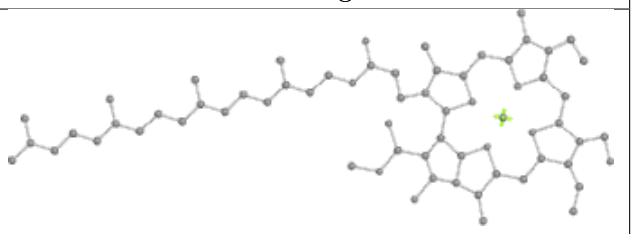
Bond lengths



Bond angles

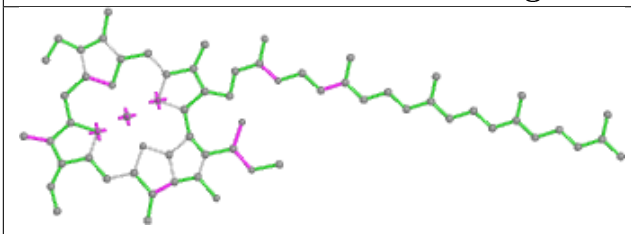


Torsions

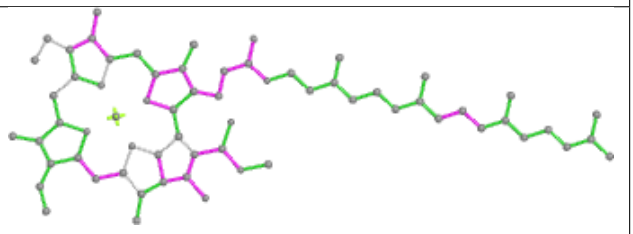


Rings

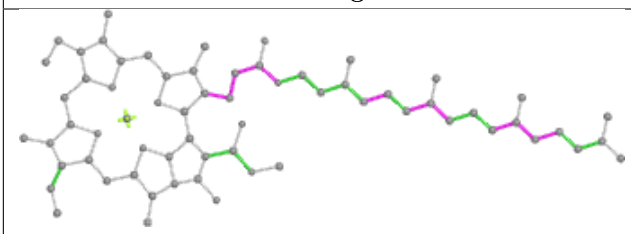
Ligand CLA A 603



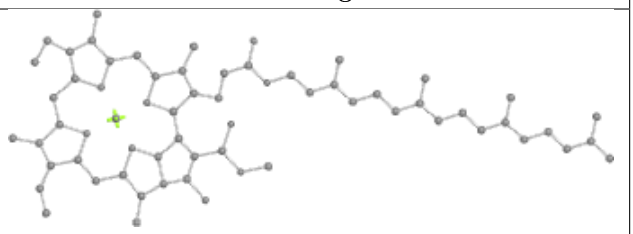
Bond lengths



Bond angles

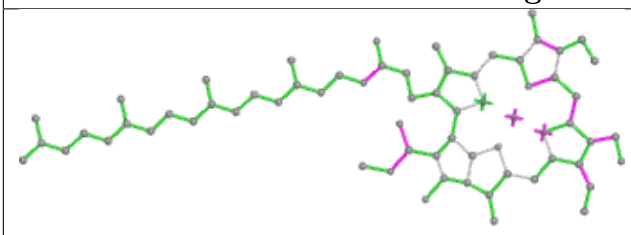


Torsions

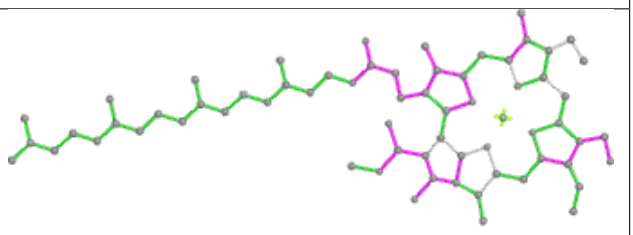


Rings

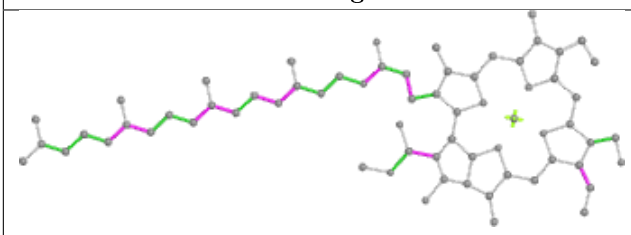
Ligand CHL B 609



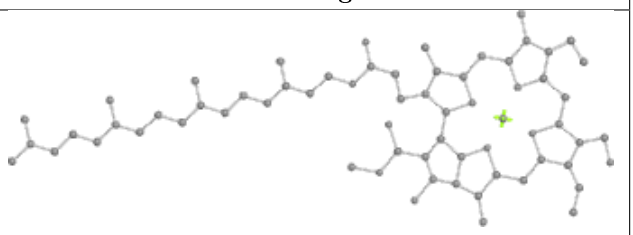
Bond lengths



Bond angles

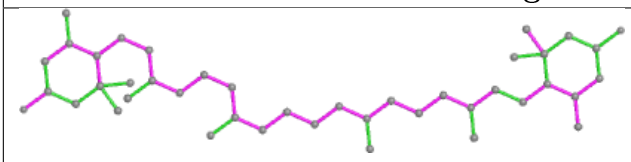


Torsions

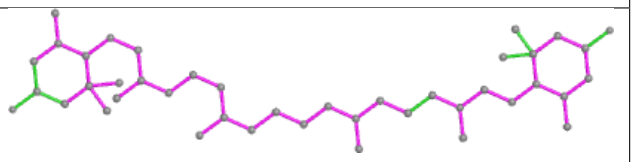


Rings

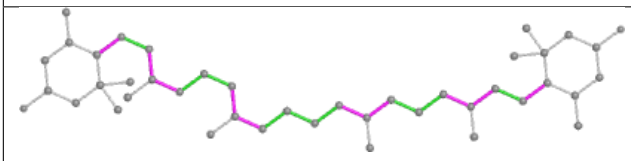
Ligand LUX C 502



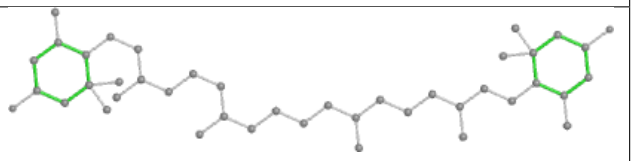
Bond lengths



Bond angles

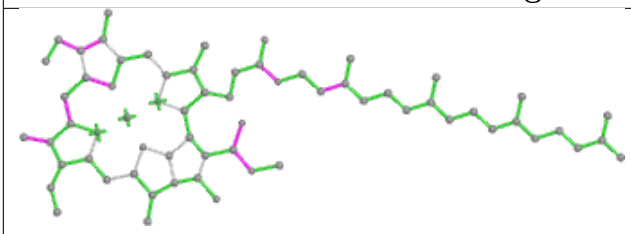


Torsions

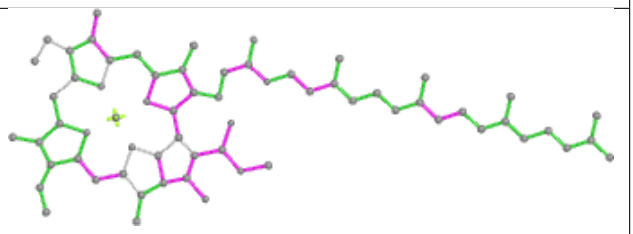


Rings

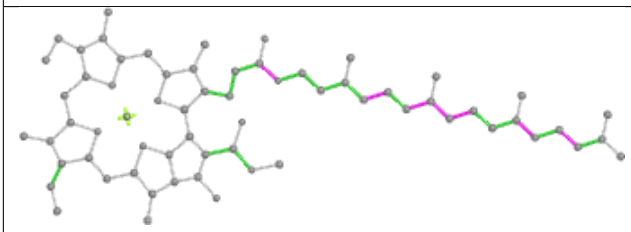
Ligand CLA A 605



Bond lengths



Bond angles



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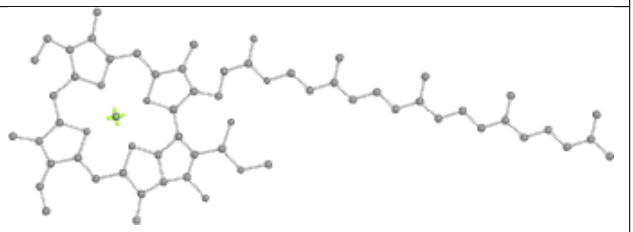
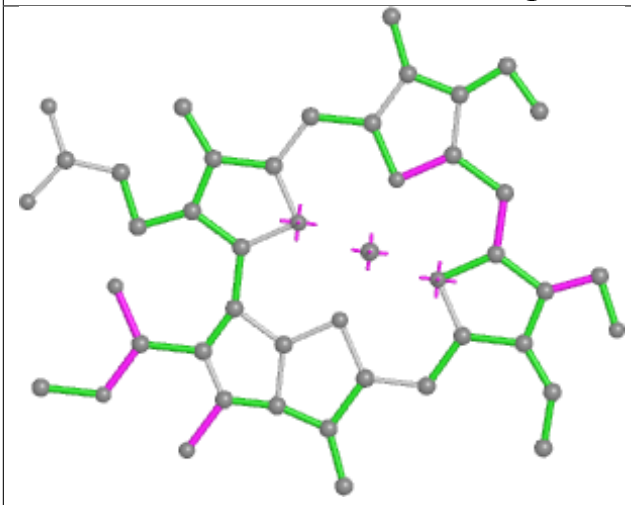
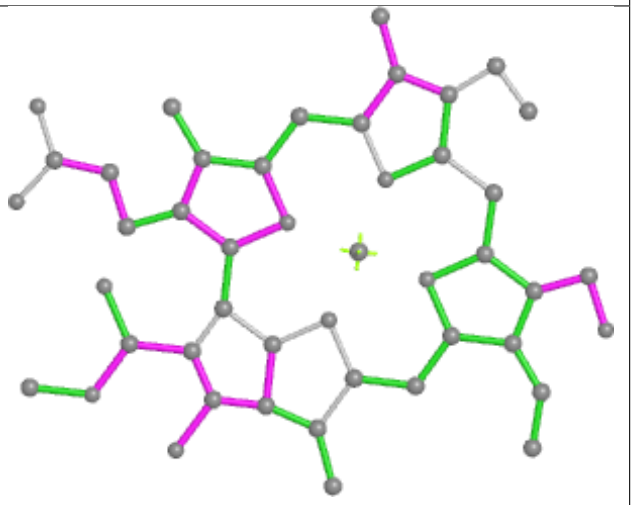


Rings

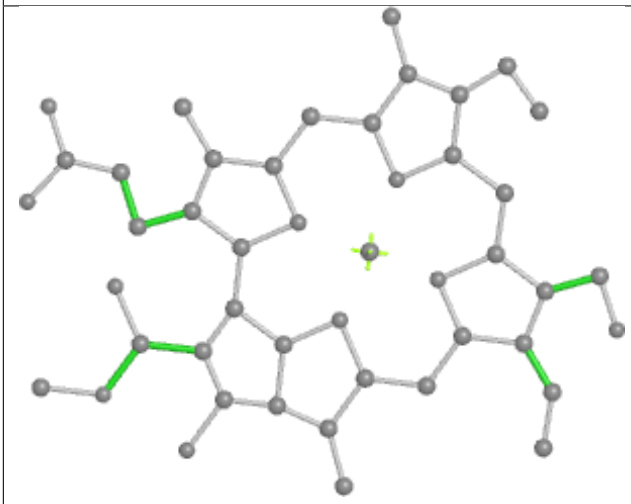
Ligand CHL A 613



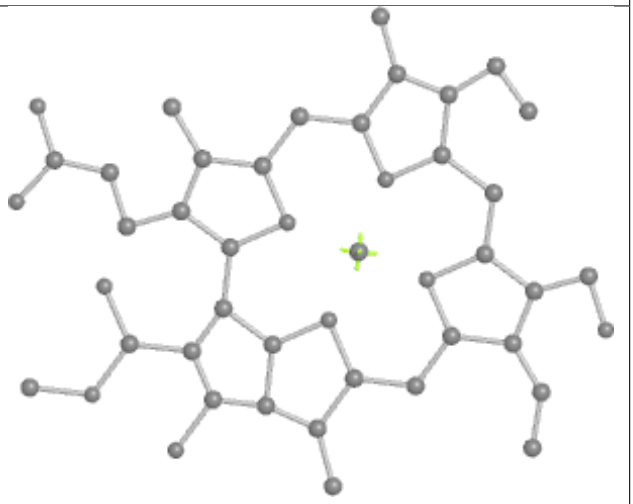
Bond lengths



Bond angles

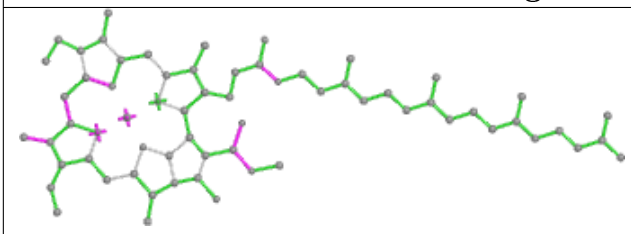


Torsions

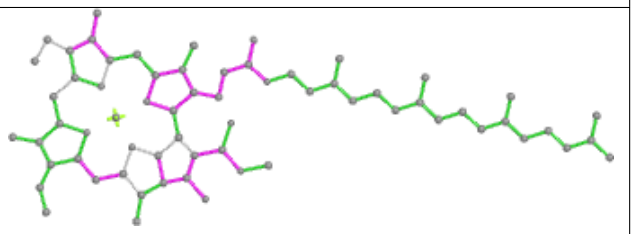


Rings

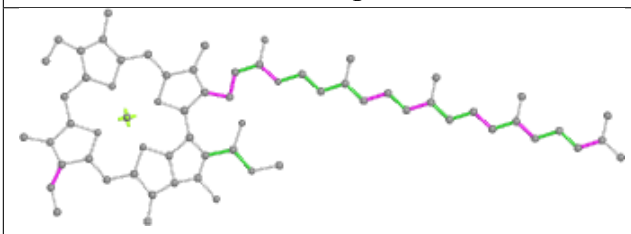
Ligand CLA A 604



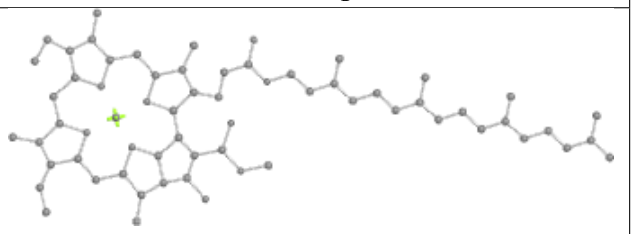
Bond lengths



Bond angles

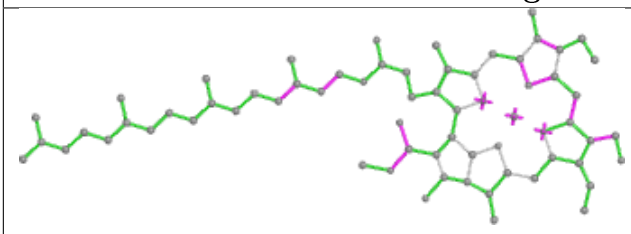


Torsions

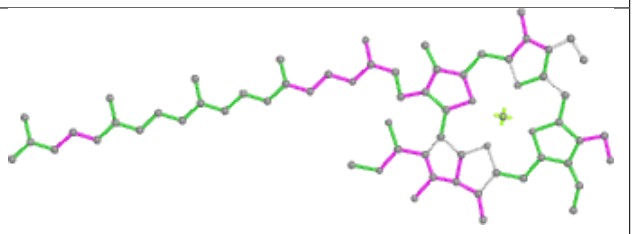


Rings

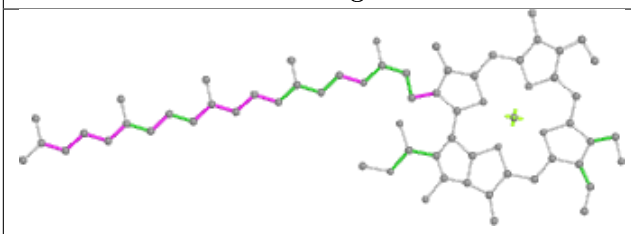
Ligand CHL A 611



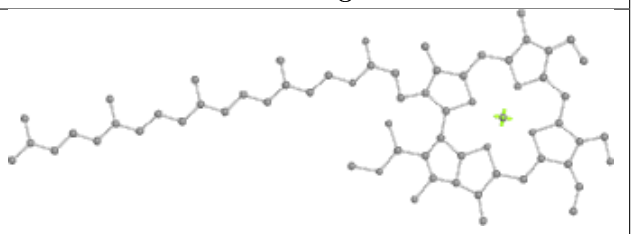
Bond lengths



Bond angles

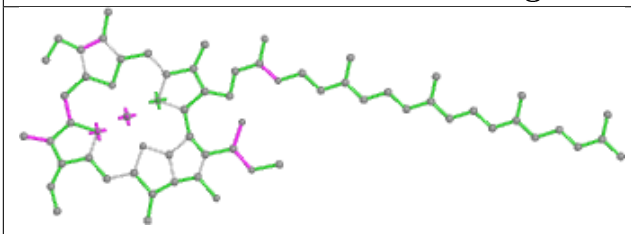


Torsions

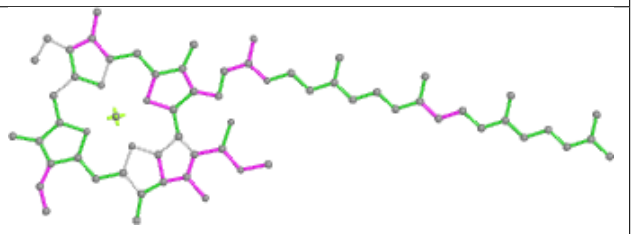


Rings

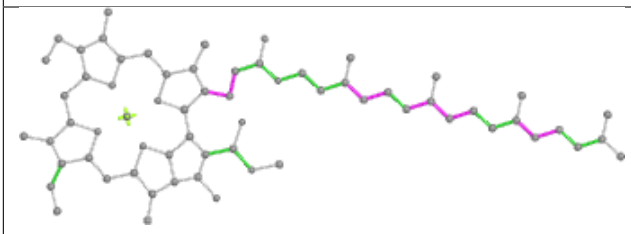
Ligand CLA C 601



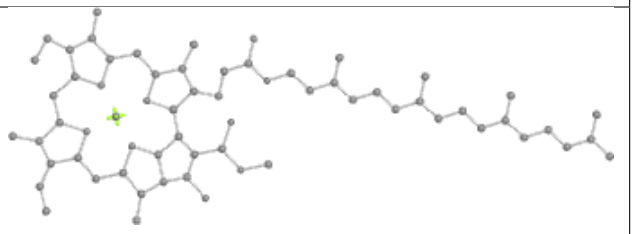
Bond lengths



Bond angles

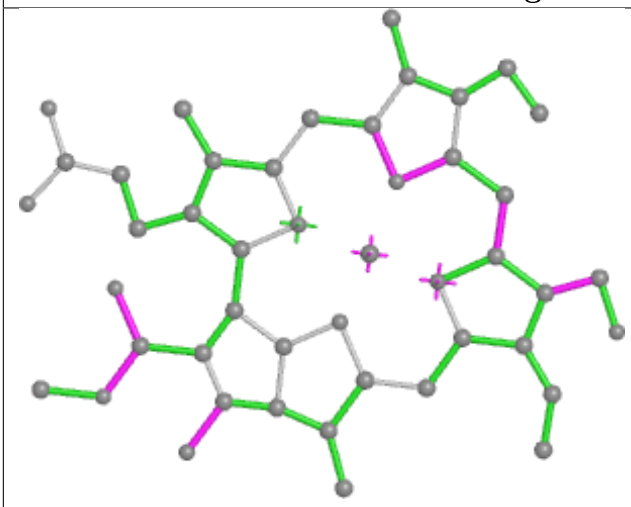


Torsions

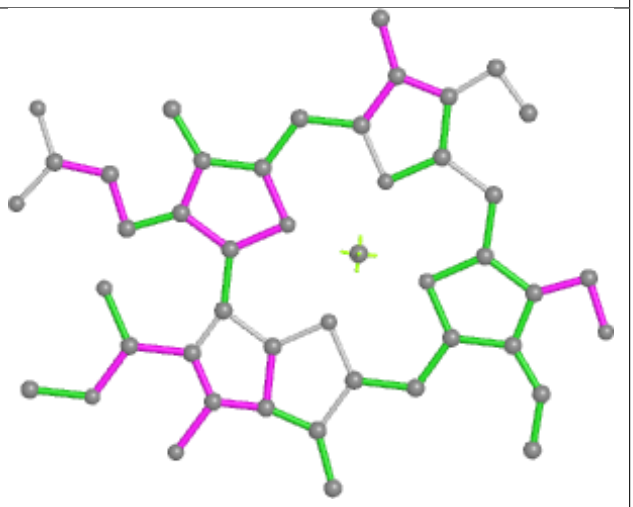


Rings

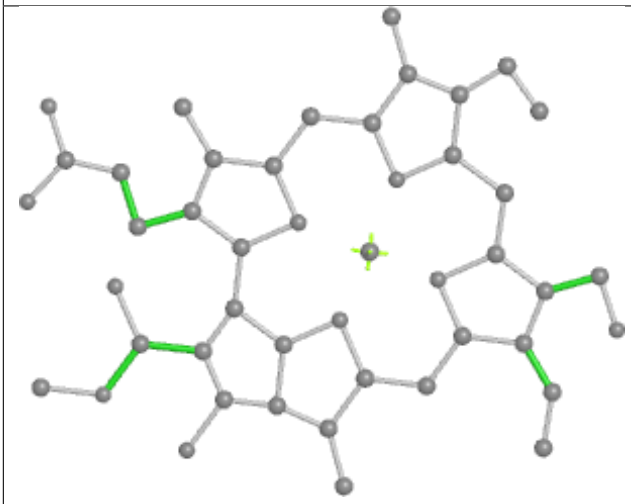
Ligand CHL B 613



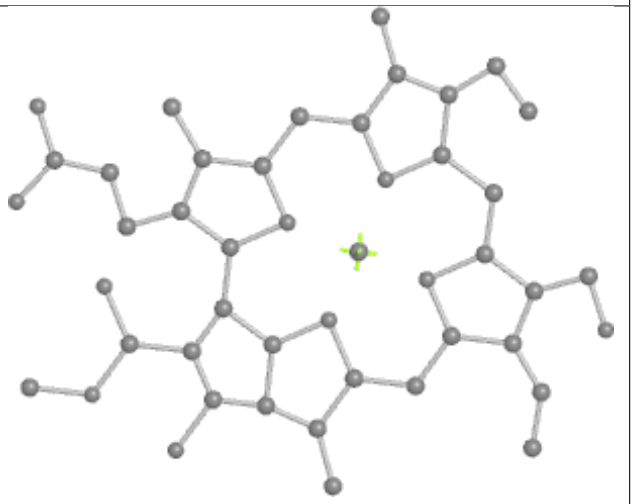
Bond lengths



Bond angles

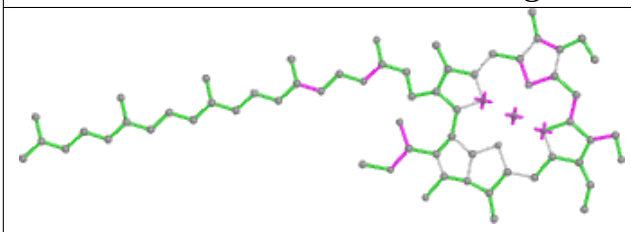


Torsions

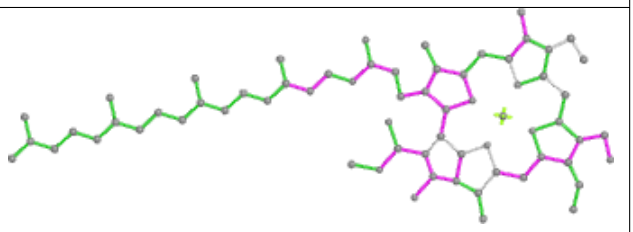


Rings

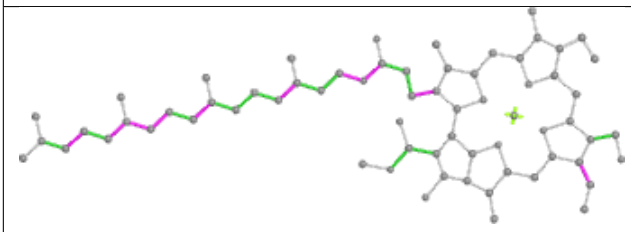
Ligand CHL A 612



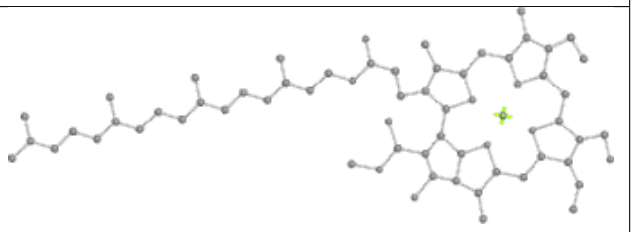
Bond lengths



Bond angles

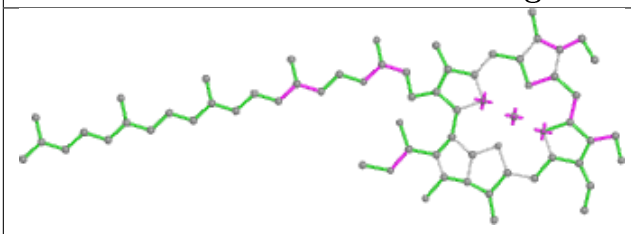


Torsions

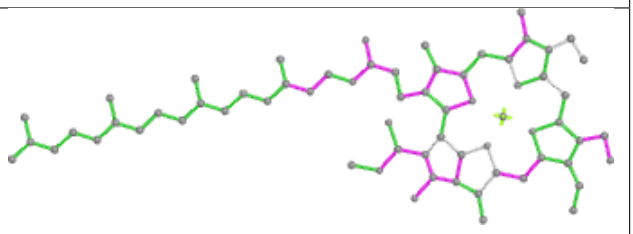


Rings

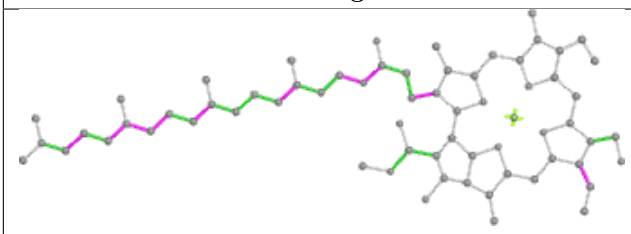
Ligand CHL B 612



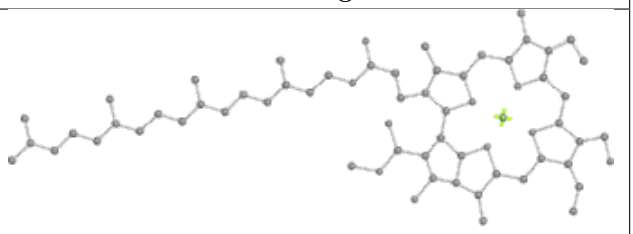
Bond lengths



Bond angles

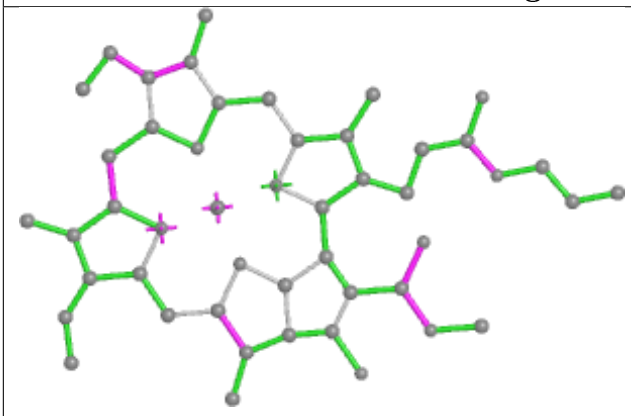


Torsions

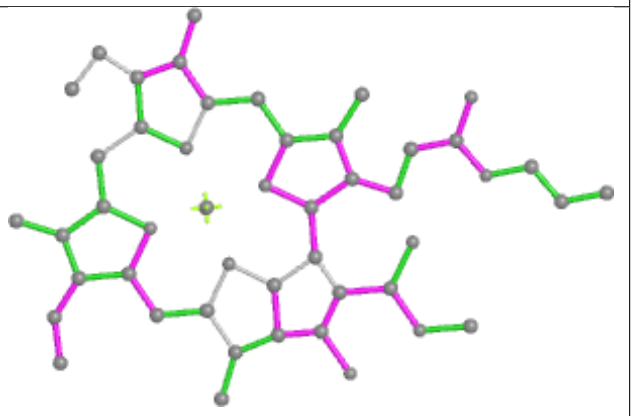


Rings

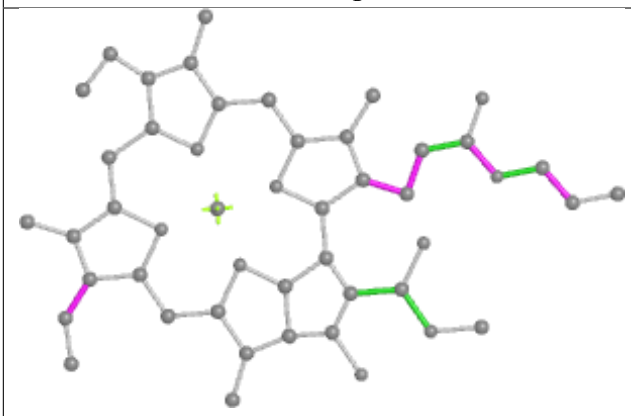
Ligand CLA C 608



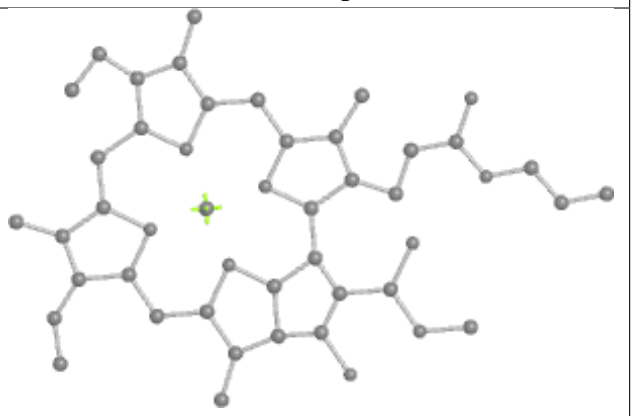
Bond lengths



Bond angles

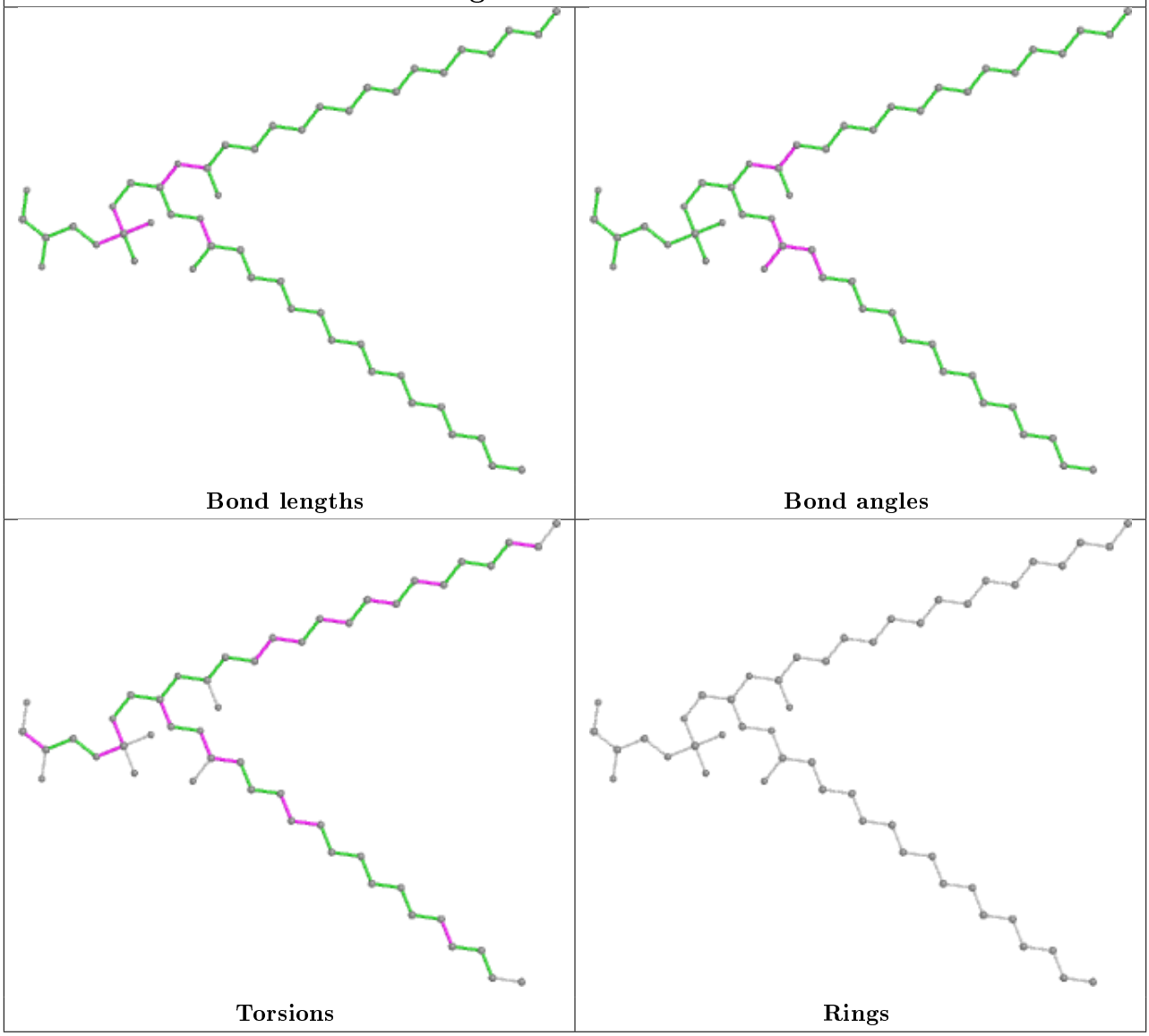


Torsions

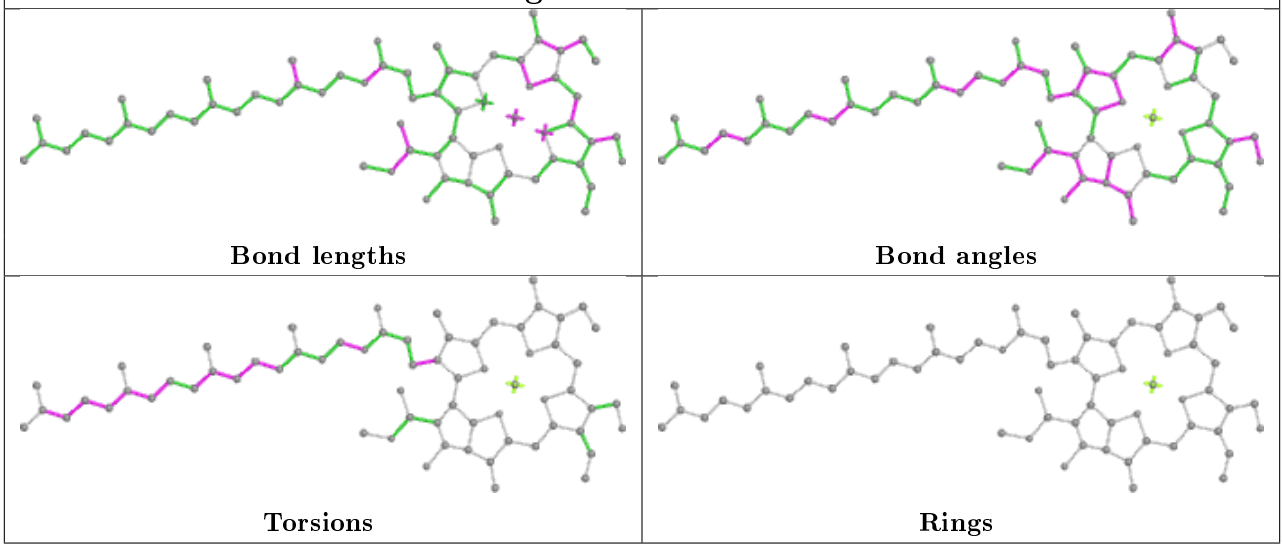


Rings

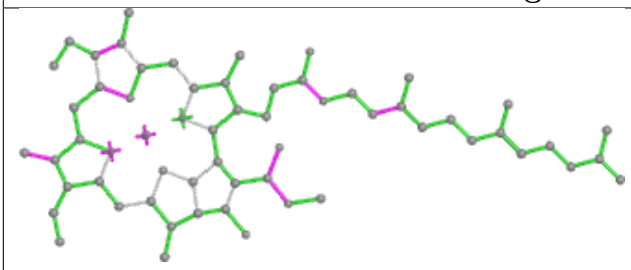
Ligand LHG B 801



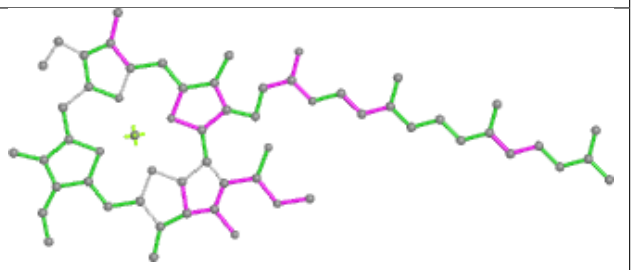
Ligand CHL C 611



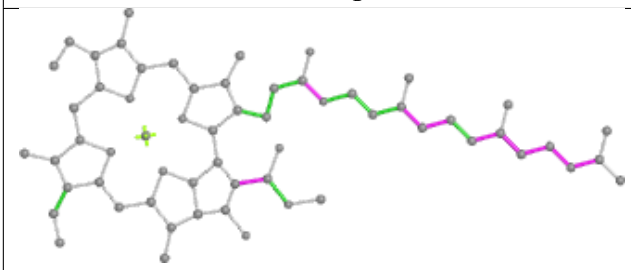
Ligand CLA A 602



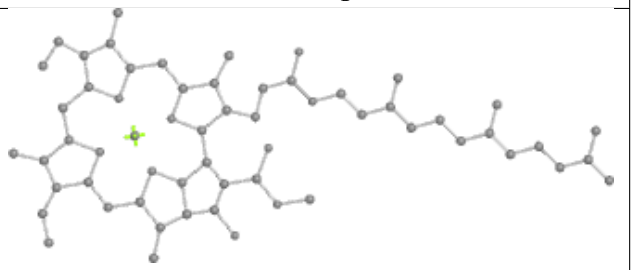
Bond lengths



Bond angles

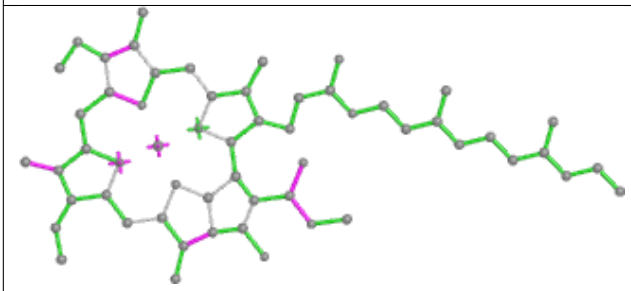


Torsions

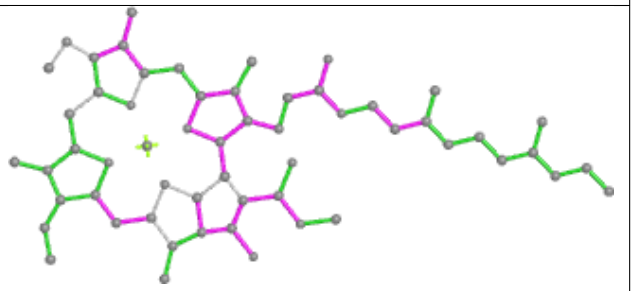


Rings

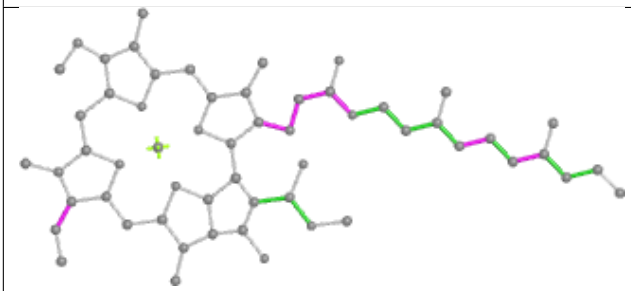
Ligand CLA A 606



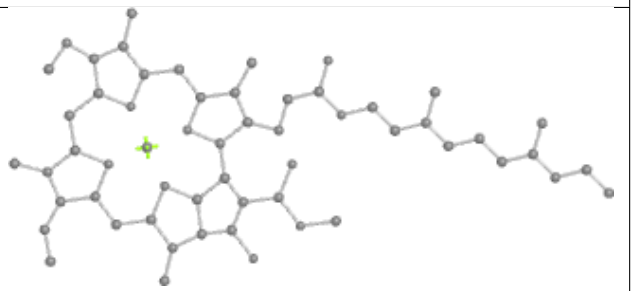
Bond lengths



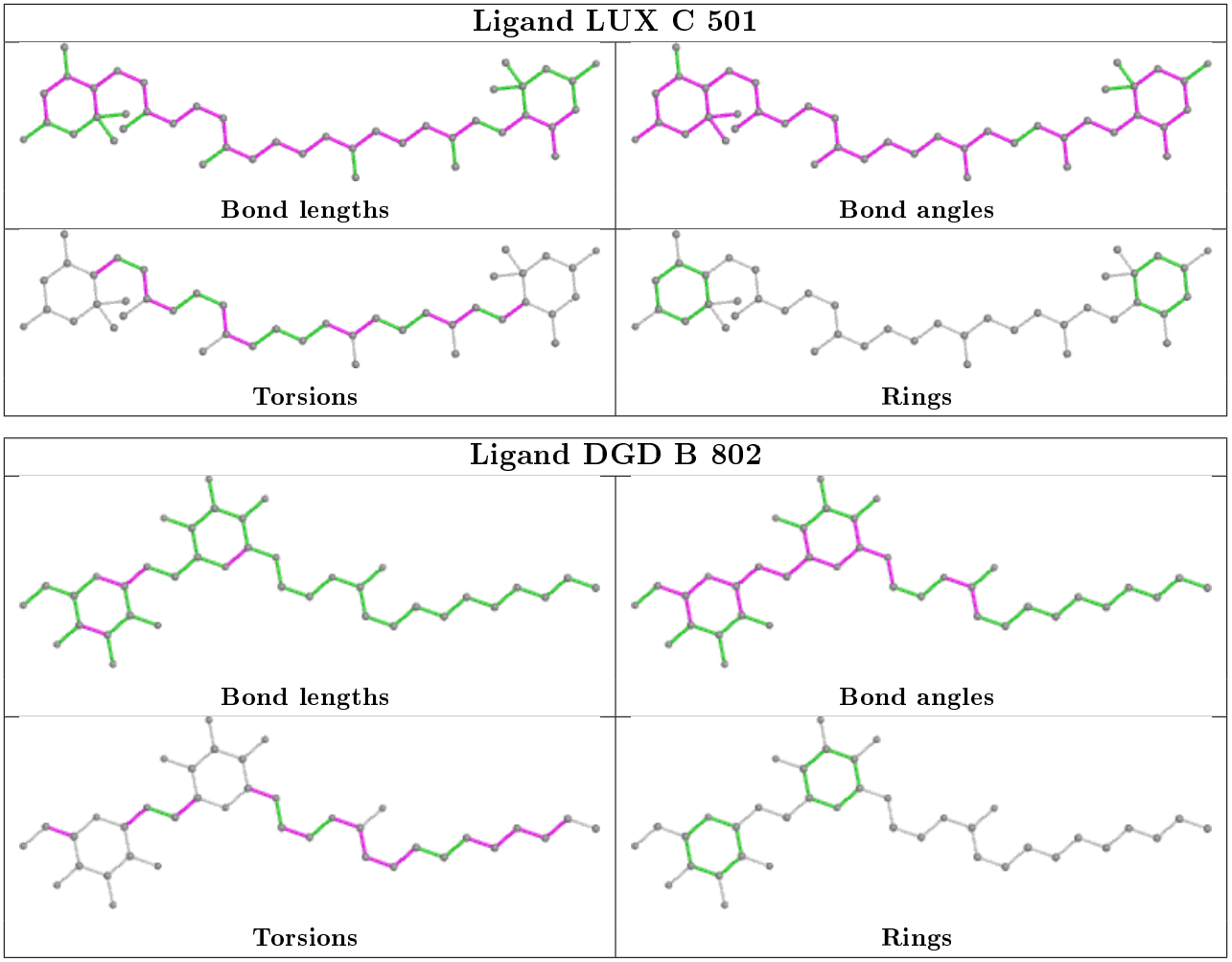
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	1.16	49 (21%)	0	0	72, 91, 109, 128	0
1	B	223/232 (96%)	1.01	37 (16%)	1	1	70, 89, 107, 126	0
1	C	223/232 (96%)	1.05	37 (16%)	1	1	73, 91, 109, 129	0
All	All	669/696 (96%)	1.07	123 (18%)	1	1	70, 90, 109, 129	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	SER	9.7
1	B	12	SER	9.3
1	B	10	ALA	7.8
1	C	10	ALA	7.3
1	B	11	SER	6.7
1	A	10	ALA	6.6
1	A	232	LYS	6.1
1	A	118	LEU	6.0
1	B	213	LEU	5.6
1	A	36	LEU	5.2
1	B	118	LEU	5.1
1	C	12	SER	4.9
1	A	121	ALA	4.8
1	C	151	VAL	4.5
1	A	11	SER	4.5
1	A	28	PHE	4.3
1	C	18	GLY	4.2
1	A	119	VAL	4.1
1	C	121	ALA	4.0
1	B	121	ALA	4.0
1	C	110	LEU	3.9
1	A	32	SER	3.8
1	B	151	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	143	ILE	3.8
1	A	12	SER	3.8
1	B	13	GLY	3.7
1	A	110	LEU	3.7
1	C	16	TRP	3.7
1	B	116	PRO	3.7
1	A	18	GLY	3.6
1	A	104	ILE	3.6
1	C	213	LEU	3.6
1	A	146	GLY	3.6
1	C	145	GLY	3.6
1	C	219	ASN	3.5
1	A	108	GLY	3.4
1	A	17	TYR	3.4
1	A	122	GLN	3.3
1	C	120	HIS	3.3
1	B	117	SER	3.3
1	C	117	SER	3.3
1	A	170	PRO	3.3
1	A	16	TRP	3.3
1	C	208	ASN	3.3
1	B	110	LEU	3.2
1	A	44	TYR	3.2
1	A	169	ASP	3.2
1	A	117	SER	3.1
1	B	115	ASN	3.1
1	A	120	HIS	3.1
1	B	119	VAL	3.1
1	C	152	VAL	3.1
1	B	18	GLY	3.0
1	B	122	GLN	3.0
1	A	210	ALA	3.0
1	C	19	PRO	2.9
1	A	31	GLU	2.9
1	C	232	LYS	2.9
1	B	104	ILE	2.9
1	C	147	PRO	2.8
1	C	196	VAL	2.8
1	A	144	ALA	2.8
1	C	108	GLY	2.8
1	B	216	PRO	2.7
1	A	151	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	108	GLY	2.7
1	B	95	ALA	2.7
1	C	116	PRO	2.7
1	C	119	VAL	2.7
1	A	115	ASN	2.7
1	C	28	PHE	2.6
1	A	72	ALA	2.6
1	C	173	PHE	2.6
1	C	144	ALA	2.6
1	A	231	GLY	2.6
1	B	92	PHE	2.5
1	A	27	PRO	2.5
1	A	22	VAL	2.5
1	B	51	LEU	2.5
1	A	51	LEU	2.5
1	A	111	ASP	2.5
1	C	14	SER	2.4
1	B	205	PRO	2.4
1	A	196	VAL	2.4
1	A	192	PHE	2.4
1	A	13	GLY	2.4
1	B	204	GLY	2.4
1	C	195	PHE	2.4
1	C	109	GLY	2.4
1	B	209	LEU	2.4
1	A	152	VAL	2.4
1	C	171	GLU	2.4
1	B	19	PRO	2.4
1	C	15	PRO	2.4
1	A	211	ASP	2.4
1	B	14	SER	2.4
1	C	210	ALA	2.3
1	A	40	PHE	2.3
1	B	16	TRP	2.3
1	B	120	HIS	2.3
1	C	192	PHE	2.3
1	C	42	GLY	2.2
1	A	150	GLU	2.2
1	A	218	ASN	2.2
1	A	38	GLY	2.2
1	B	42	GLY	2.2
1	B	91	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	104	ILE	2.2
1	B	28	PHE	2.2
1	B	146	GLY	2.2
1	B	189	PHE	2.2
1	B	147	PRO	2.2
1	C	51	LEU	2.2
1	A	76	ALA	2.1
1	A	116	PRO	2.1
1	A	195	PHE	2.1
1	B	187	ALA	2.1
1	B	27	PRO	2.1
1	A	103	GLN	2.0
1	B	105	PHE	2.0
1	C	17	TYR	2.0
1	A	15	PRO	2.0
1	A	71	TRP	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 carbohydrates 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, 95^{th} 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	0.41	0.50	104,118,139,140	0
8	DGD	A	802	38/66	0.49	0.46	106,119,140,140	0
8	DGD	C	802	38/66	0.58	0.43	106,119,141,141	0
3	NEX	C	503	44/44	0.65	0.40	67,98,128,133	0
3	NEX	A	503	44/44	0.80	0.30	66,97,128,132	0
3	NEX	B	503	44/44	0.81	0.35	64,96,126,131	0
6	CHL	C	612	66/66	0.83	0.31	77,85,102,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CHL	C	614	42/66	0.83	0.41	99,107,113,137	0
5	CLA	A	607	65/65	0.83	0.23	77,90,103,106	0
6	CHL	A	612	66/66	0.83	0.36	76,85,102,104	0
5	CLA	C	607	65/65	0.83	0.22	77,91,104,106	0
2	LUX	B	502	42/42	0.84	0.35	53,76,113,126	0
5	CLA	B	607	65/65	0.84	0.24	75,88,101,104	0
5	CLA	C	604	65/65	0.85	0.30	60,72,97,102	0
7	LHG	B	801	49/49	0.85	0.28	72,88,109,115	0
5	CLA	A	604	65/65	0.85	0.27	59,71,96,101	0
6	CHL	B	614	42/66	0.86	0.42	97,105,111,134	0
5	CLA	B	601	65/65	0.86	0.23	68,77,111,113	0
5	CLA	B	604	65/65	0.87	0.30	56,69,95,100	0
6	CHL	C	609	66/66	0.87	0.24	77,85,98,101	0
4	XAT	C	504	44/44	0.87	0.20	65,91,117,149	0
6	CHL	A	609	66/66	0.87	0.22	75,85,97,100	0
2	LUX	C	502	42/42	0.88	0.35	58,79,115,128	0
6	CHL	A	614	42/66	0.88	0.43	99,106,113,136	0
5	CLA	C	601	65/65	0.88	0.24	70,79,113,115	0
5	CLA	A	601	65/65	0.88	0.23	69,79,112,115	0
4	XAT	B	504	44/44	0.88	0.21	63,89,115,147	0
2	LUX	C	501	42/42	0.88	0.26	62,88,120,136	0
6	CHL	B	609	66/66	0.88	0.22	75,83,95,99	0
2	LUX	A	502	42/42	0.89	0.32	57,78,115,128	0
5	CLA	B	606	57/65	0.89	0.28	78,89,105,109	0
5	CLA	B	608	48/65	0.89	0.22	88,97,115,117	0
6	CHL	C	611	66/66	0.89	0.28	69,85,118,124	0
7	LHG	A	801	49/49	0.89	0.25	74,90,110,116	0
6	CHL	A	611	66/66	0.89	0.24	70,85,117,123	0
7	LHG	C	801	49/49	0.90	0.24	74,90,111,117	0
5	CLA	C	608	48/65	0.90	0.21	90,99,117,119	0
6	CHL	C	610	66/66	0.90	0.24	67,81,108,110	0
2	LUX	B	501	42/42	0.90	0.26	59,86,118,134	0
5	CLA	A	606	57/65	0.90	0.26	79,90,107,110	0
5	CLA	A	608	48/65	0.90	0.16	90,99,116,118	0
5	CLA	B	603	65/65	0.90	0.20	74,83,100,103	0
6	CHL	B	612	66/66	0.91	0.27	74,83,100,102	0
6	CHL	B	613	46/66	0.91	0.20	71,80,106,119	0
5	CLA	C	606	57/65	0.91	0.25	80,91,107,111	0
6	CHL	B	611	66/66	0.91	0.26	68,82,115,121	0
6	CHL	C	613	46/66	0.91	0.17	73,82,107,121	0
4	XAT	A	504	44/44	0.91	0.18	65,91,117,148	0
5	CLA	A	602	60/65	0.91	0.24	79,87,115,116	0

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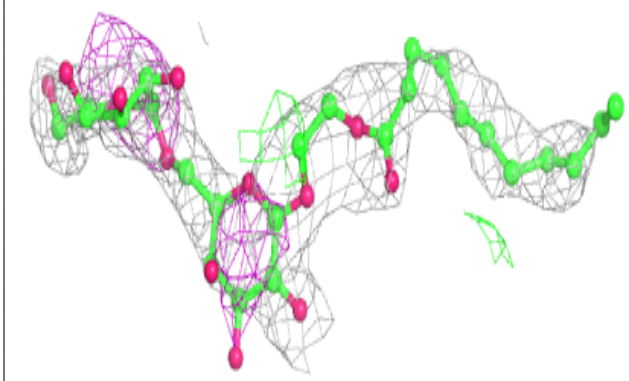
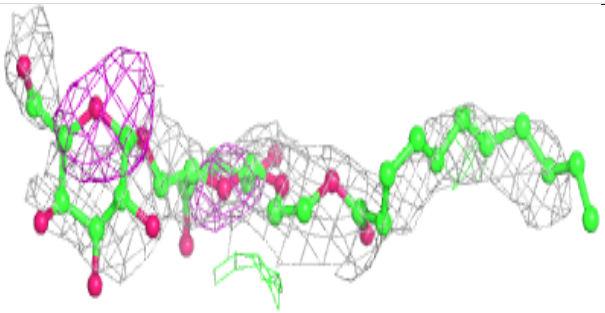
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CLA	A	605	65/65	0.91	0.49	77,86,107,110	0
5	CLA	C	602	60/65	0.91	0.21	80,87,116,117	0
5	CLA	A	603	65/65	0.91	0.21	75,85,102,105	0
5	CLA	B	602	60/65	0.92	0.19	77,85,114,114	0
6	CHL	A	613	46/66	0.92	0.20	73,81,107,120	0
2	LUX	A	501	42/42	0.92	0.27	61,87,120,136	0
5	CLA	C	603	65/65	0.92	0.22	75,85,102,105	0
6	CHL	B	610	66/66	0.92	0.23	65,79,106,108	0
5	CLA	C	605	65/65	0.92	0.41	77,86,108,110	0
6	CHL	A	610	66/66	0.92	0.29	65,80,108,110	0
5	CLA	B	605	65/65	0.93	0.45	75,84,105,108	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 B 802:

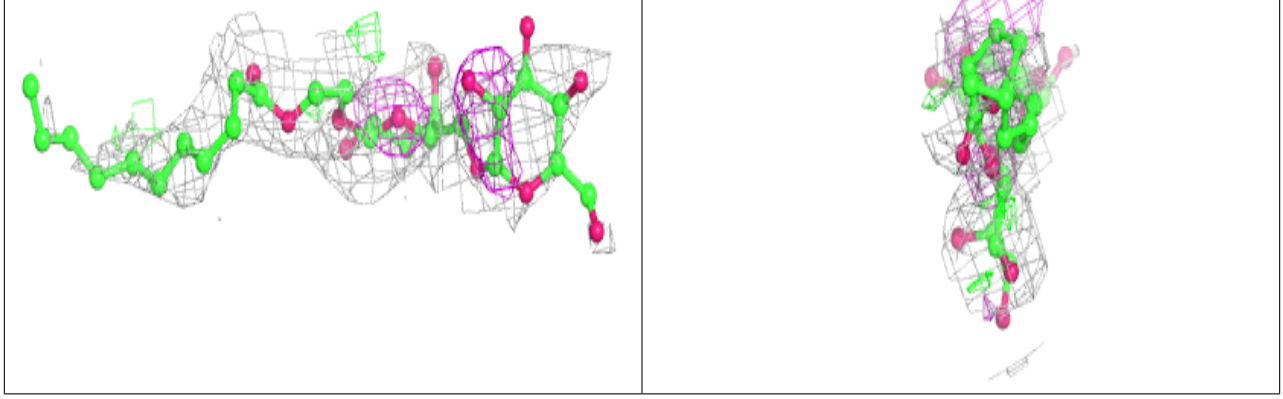
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





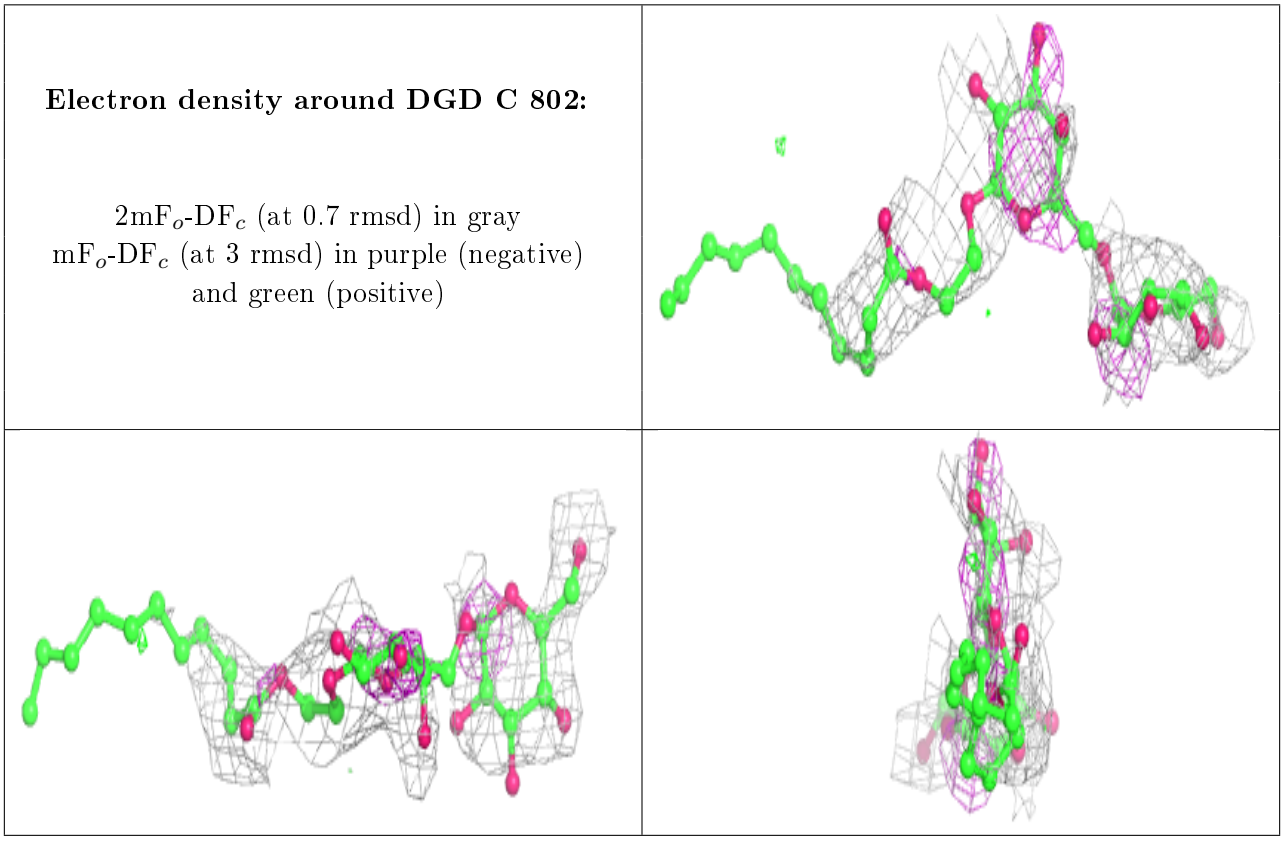
Electron density around DGD A 802:

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



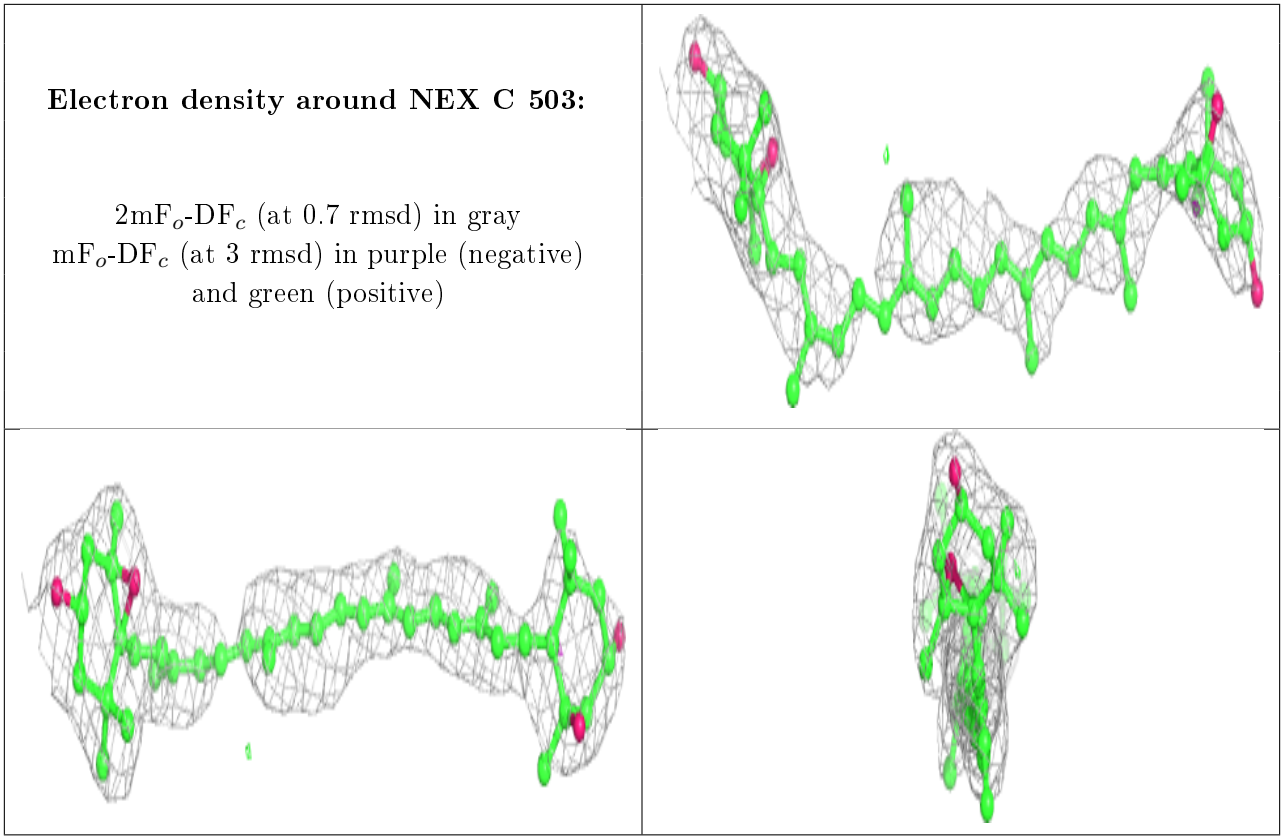
Electron density around DGD C 802:

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



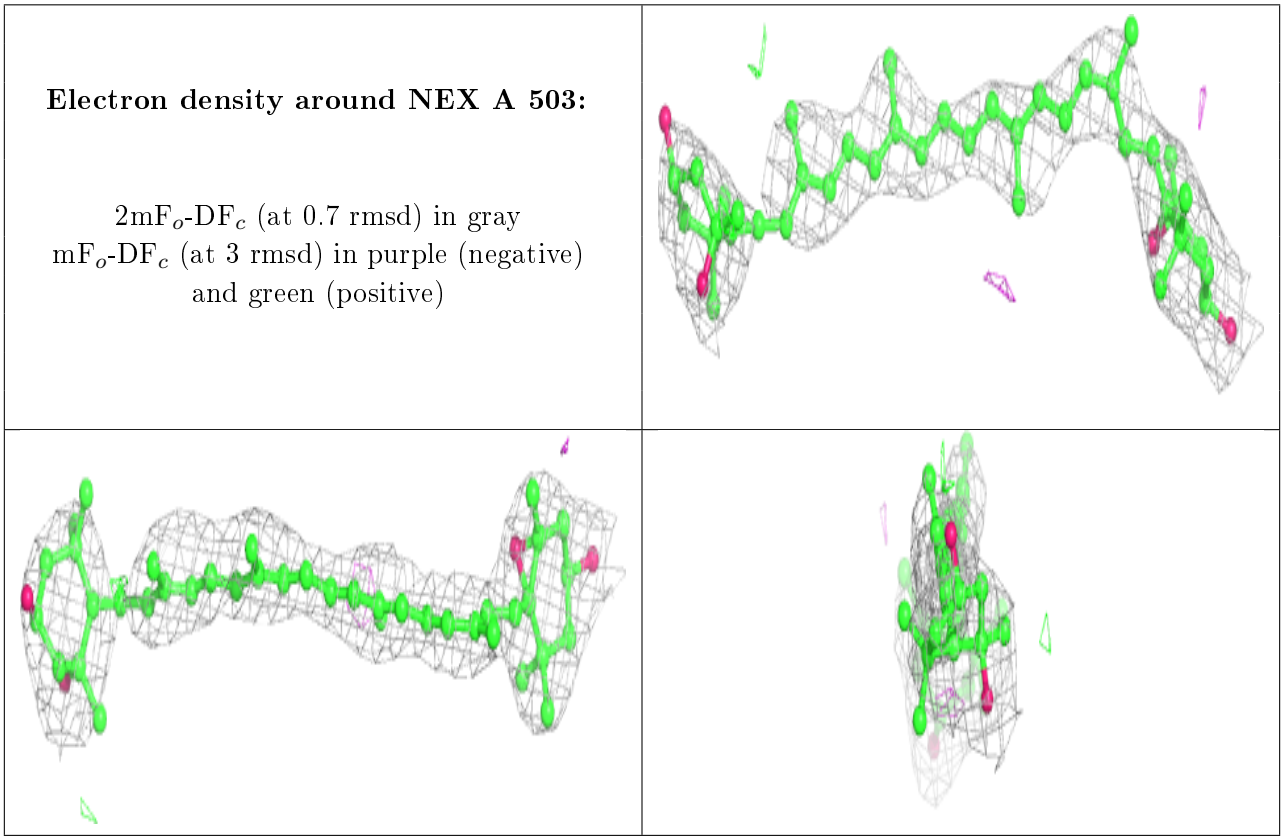
Electron density around NEX C 503:

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



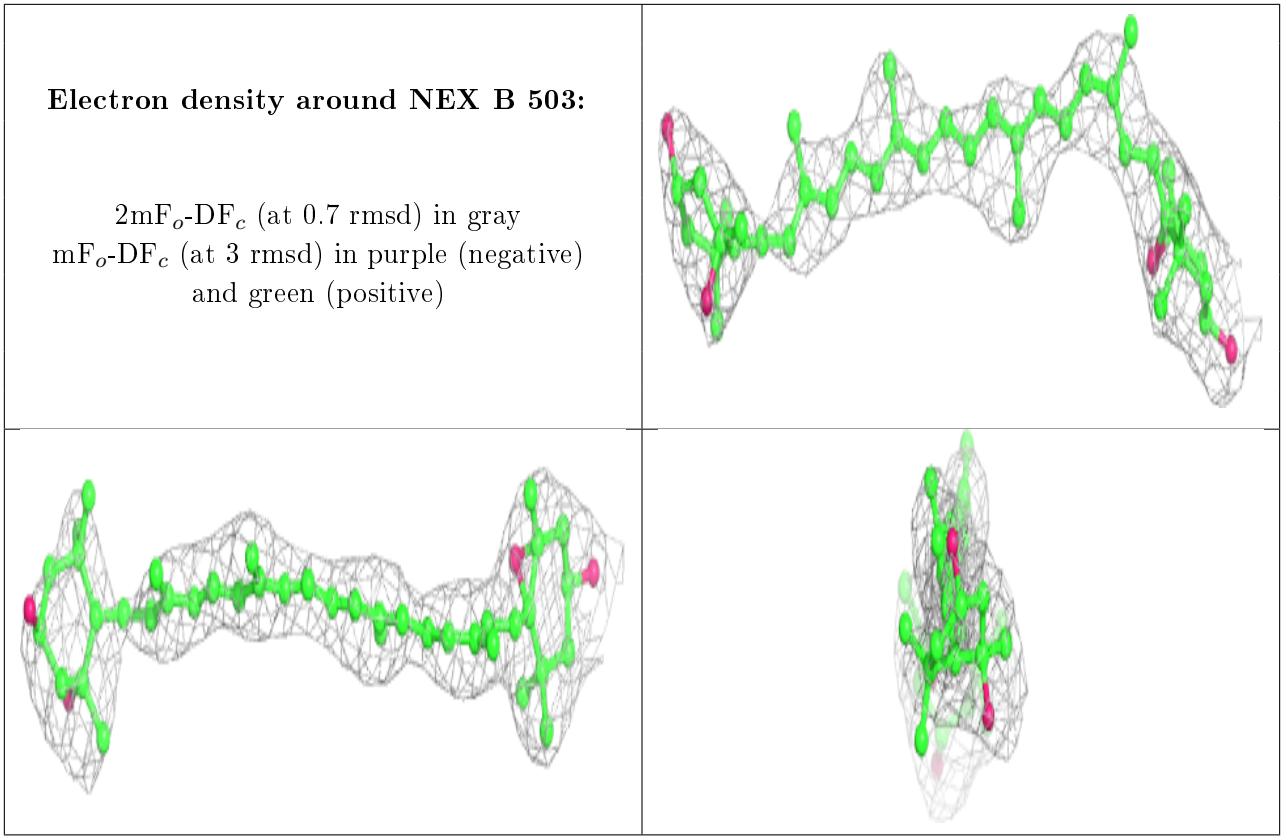
Electron density around NEX A 503:

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



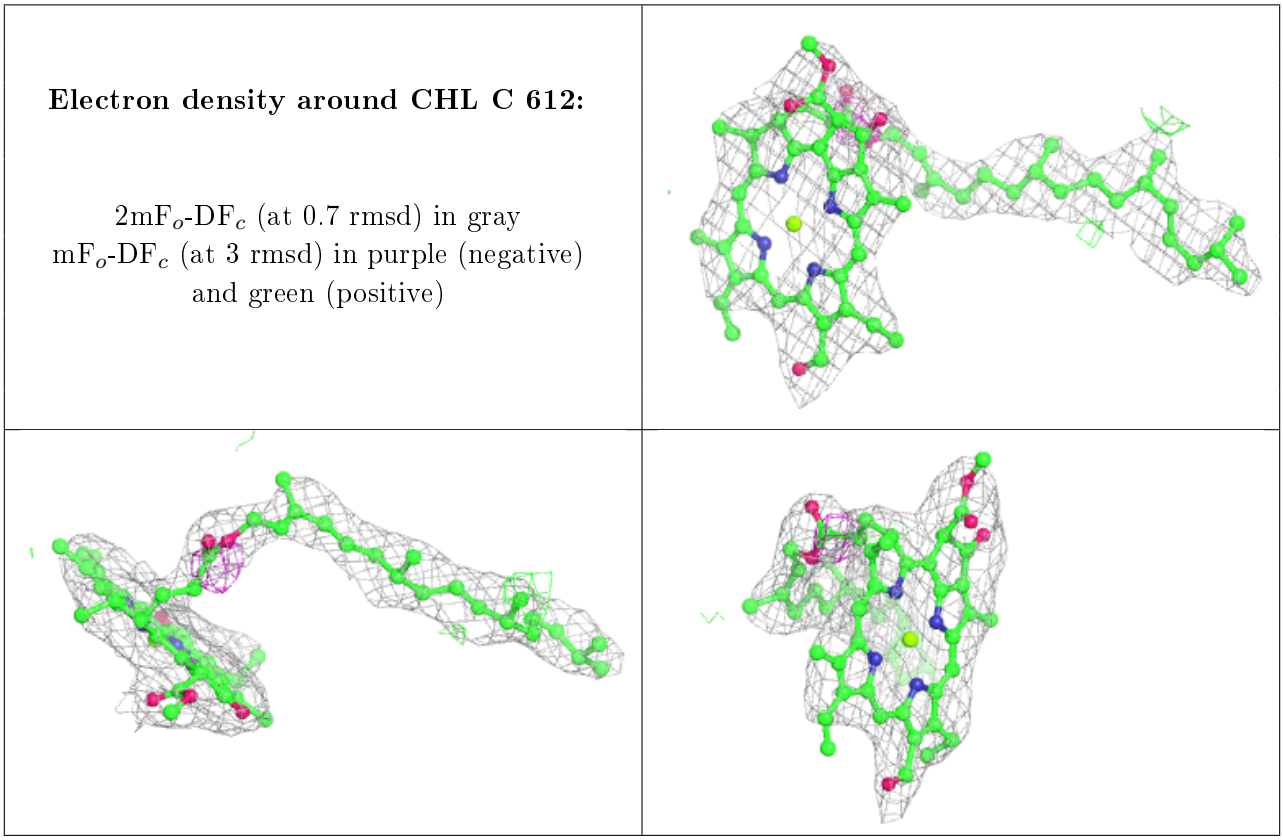
Electron density around NEX B 503:

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



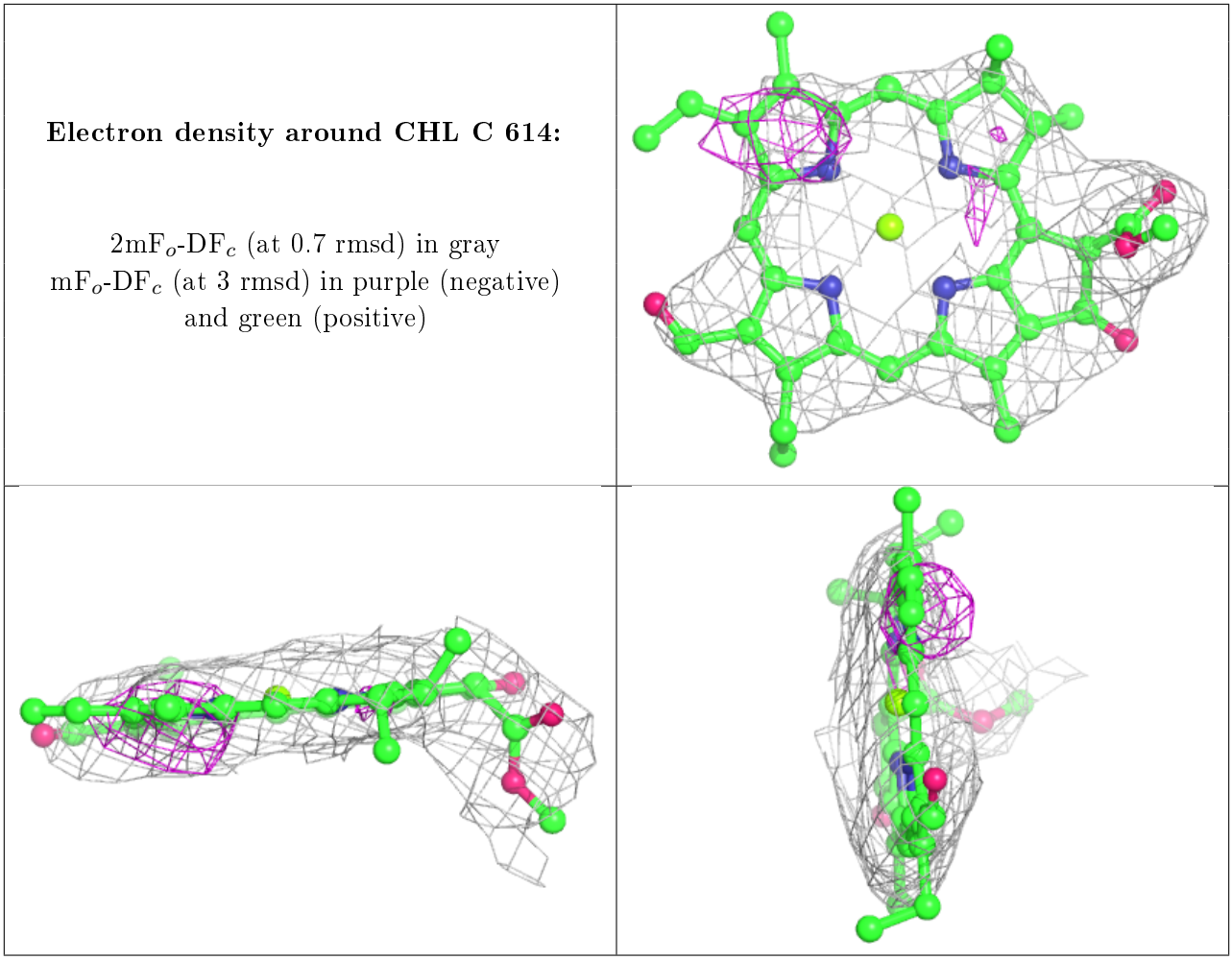
Electron density around CHL C 612:

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



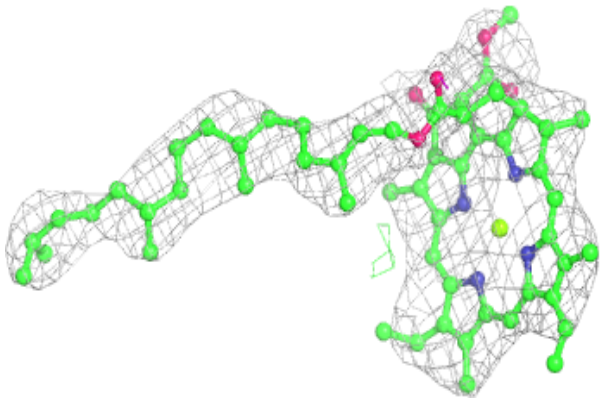
Electron density around CHL C 614:

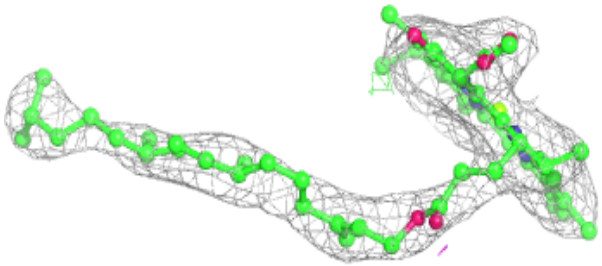
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

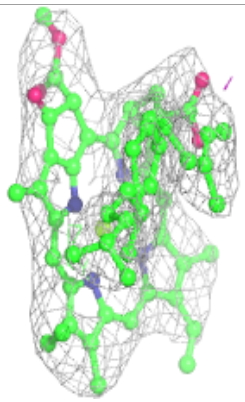


Electron density around CLA A 607:

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

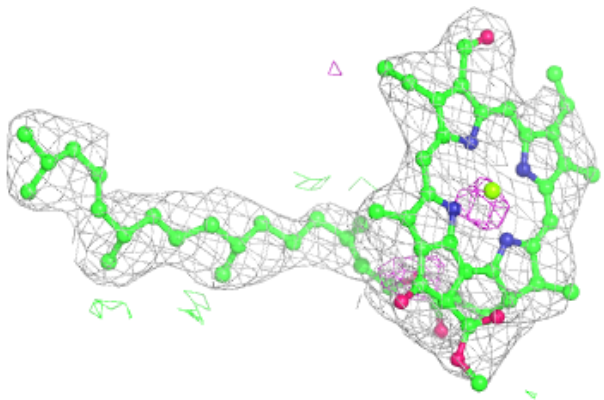


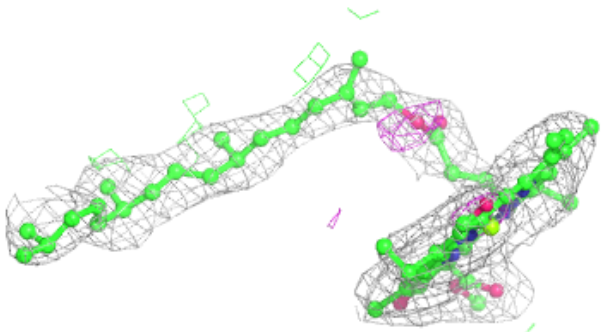


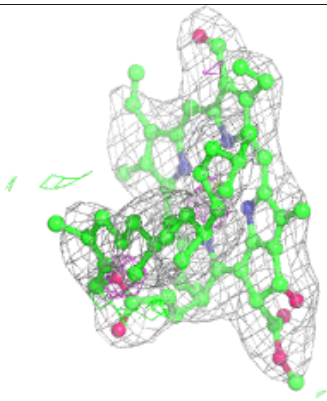


Electron density around CHL A 612:

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

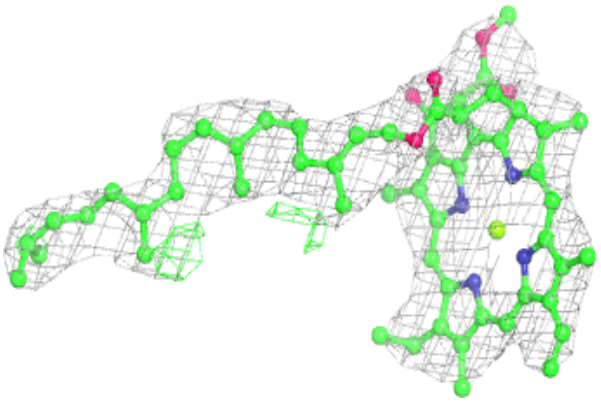


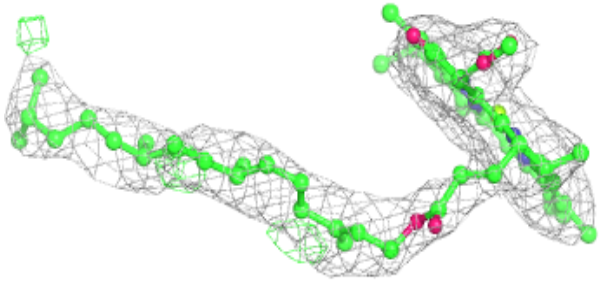


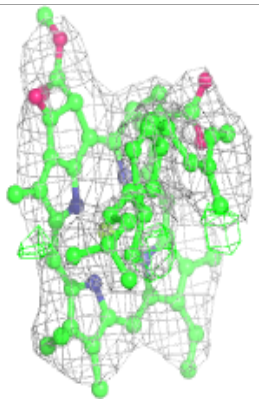


Electron density around CLA C 607:

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

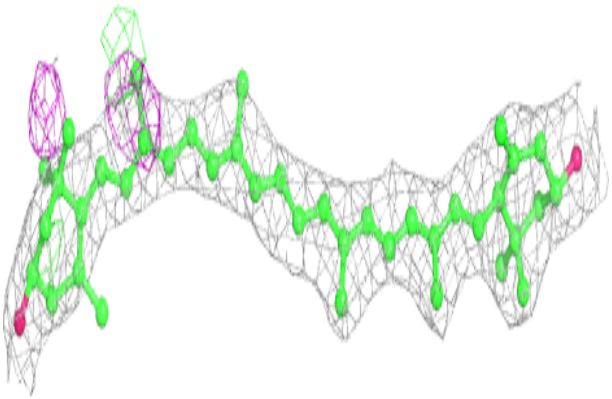


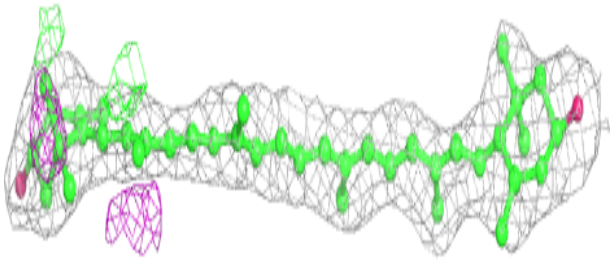


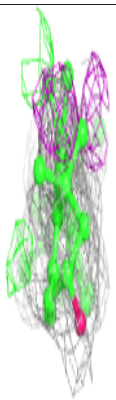


Electron density around LUX B 502:

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

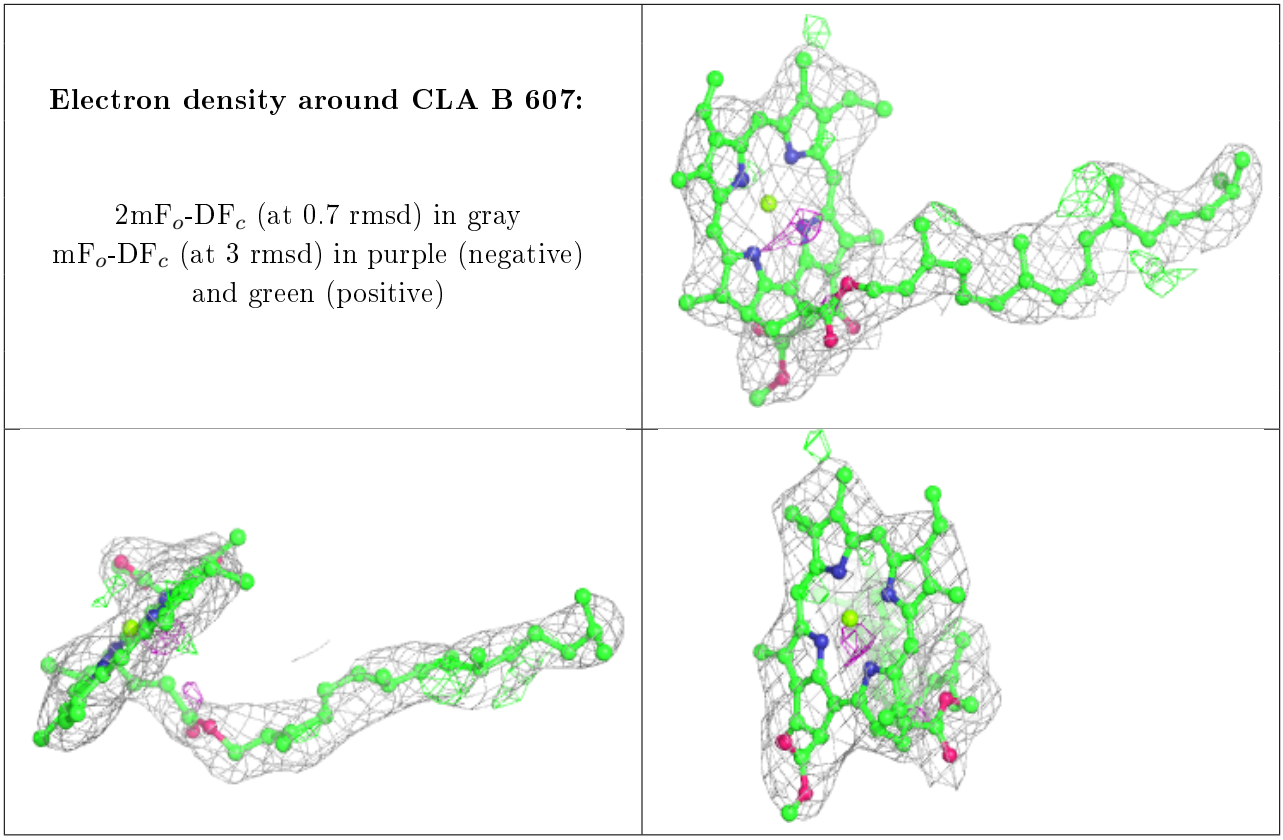






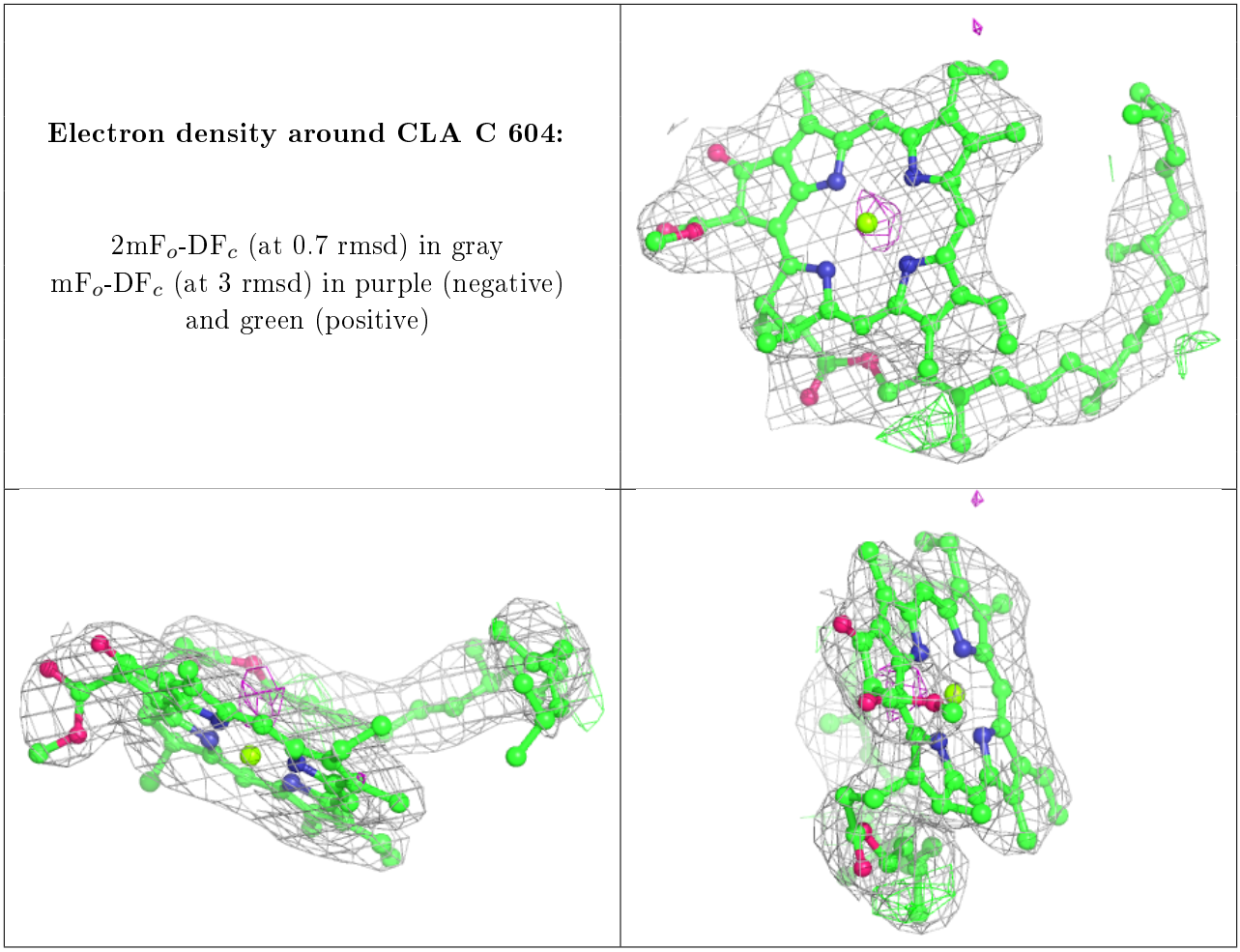
Electron density around CLA B 607:

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



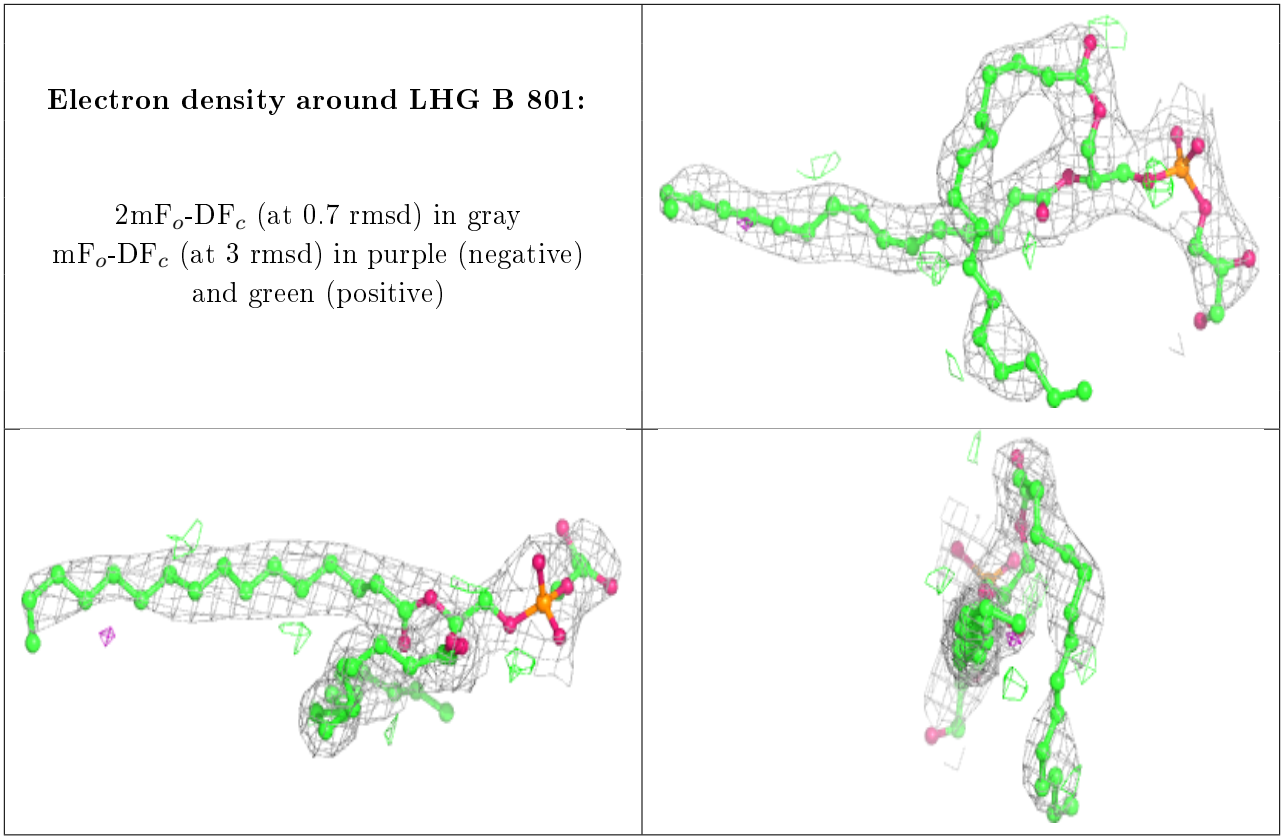
Electron density around CLA C 604:

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



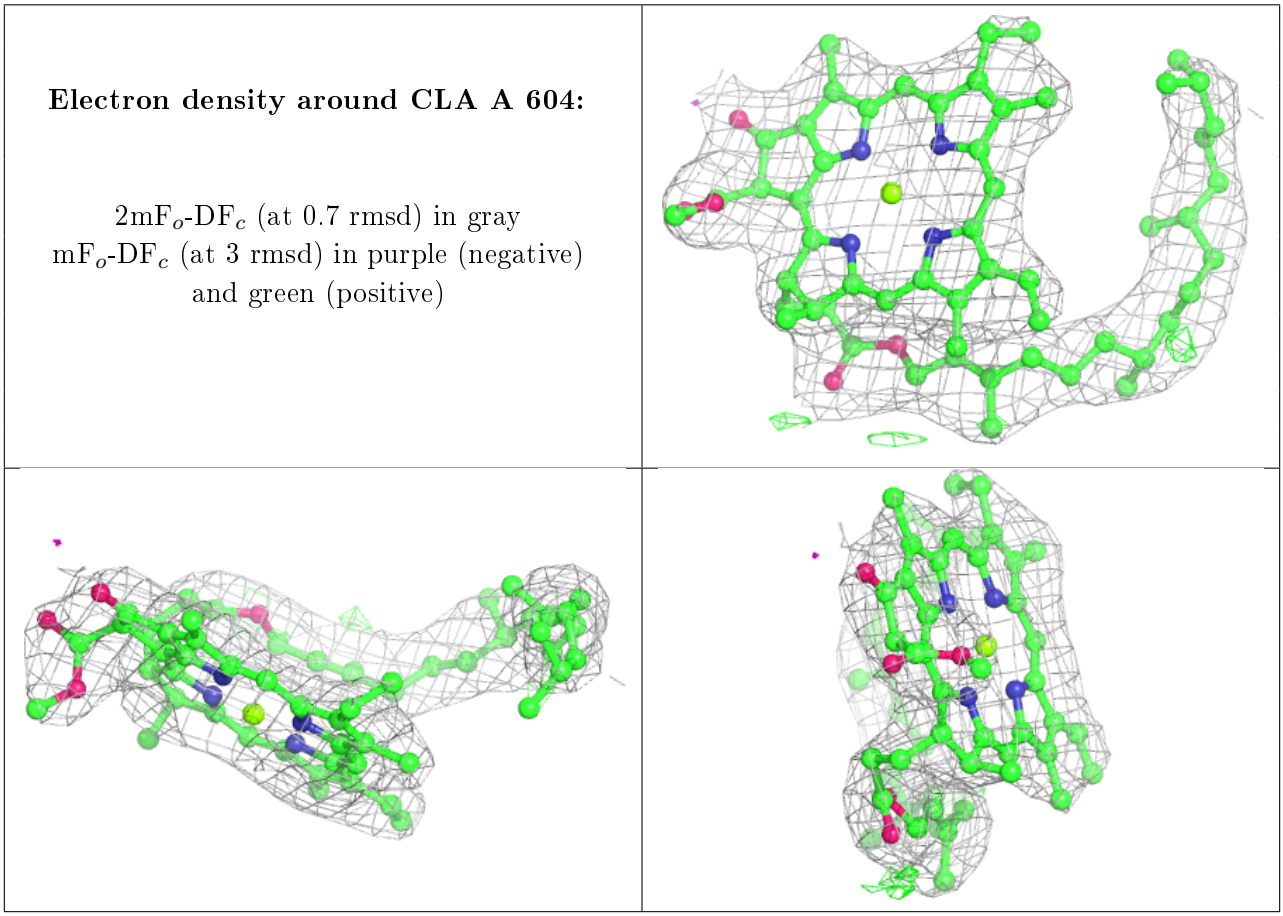
Electron density around LHG B 801:

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



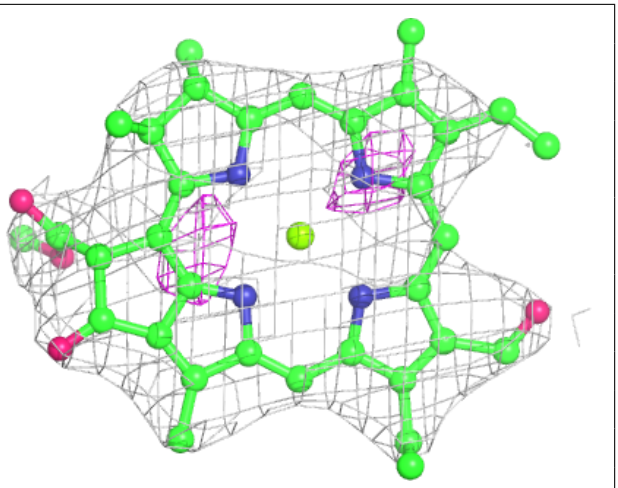
Electron density around CLA A 604:

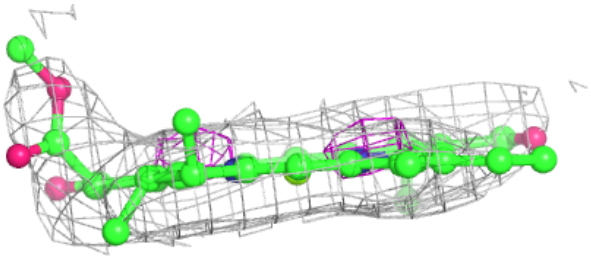
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

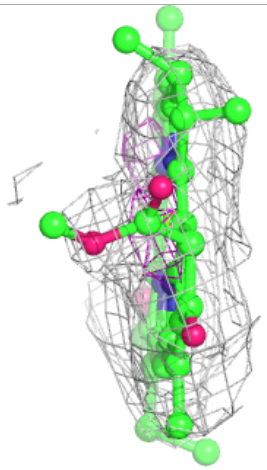


Electron density around CHL B 614:

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

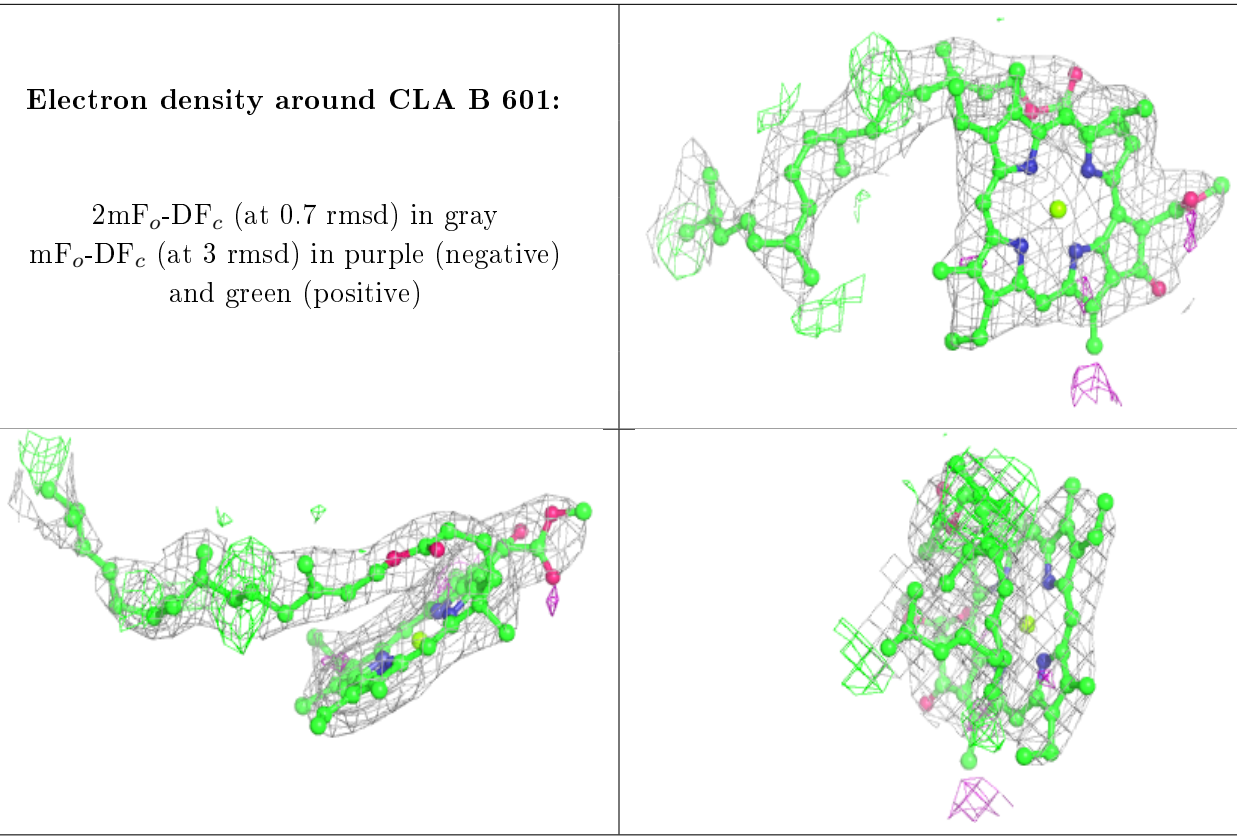






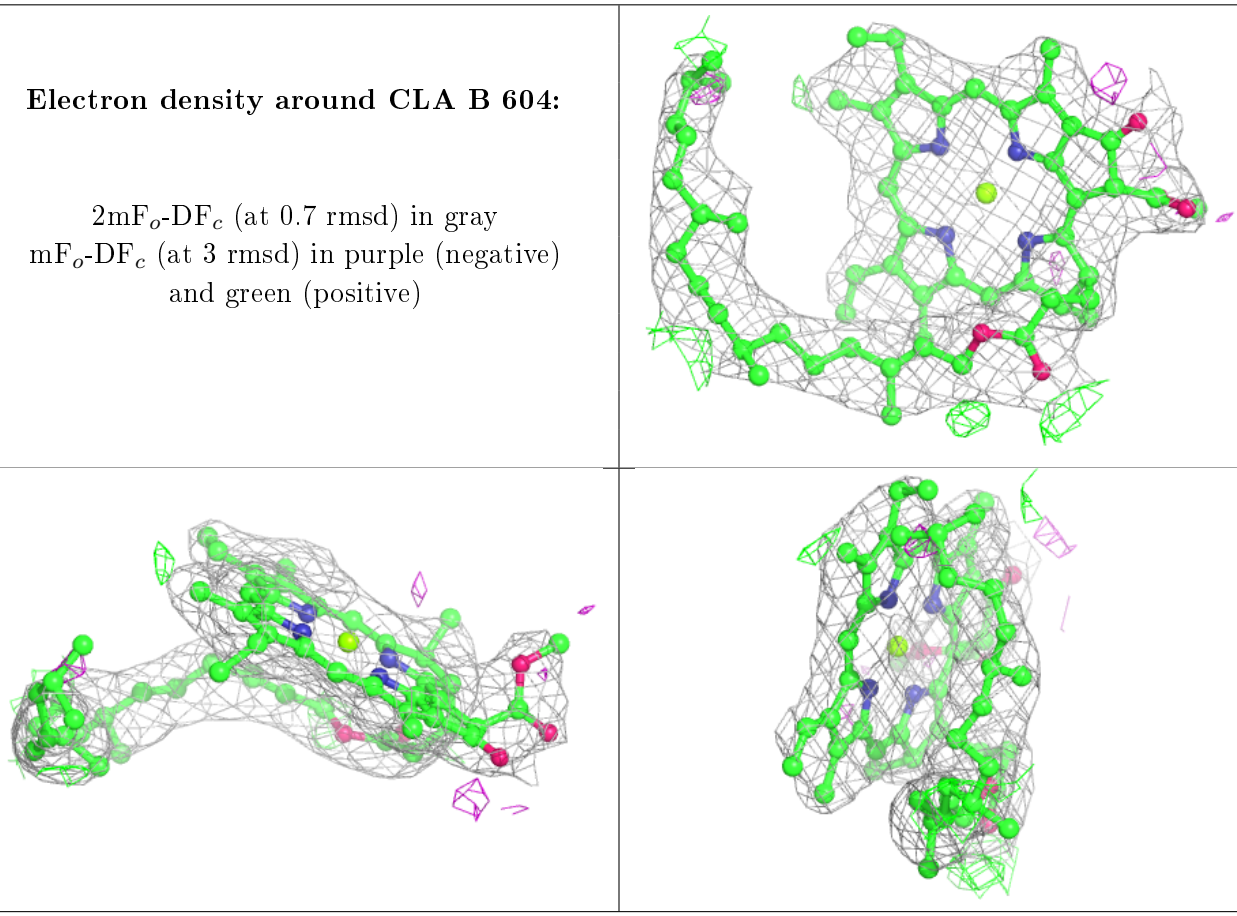
Electron density around CLA B 601:

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



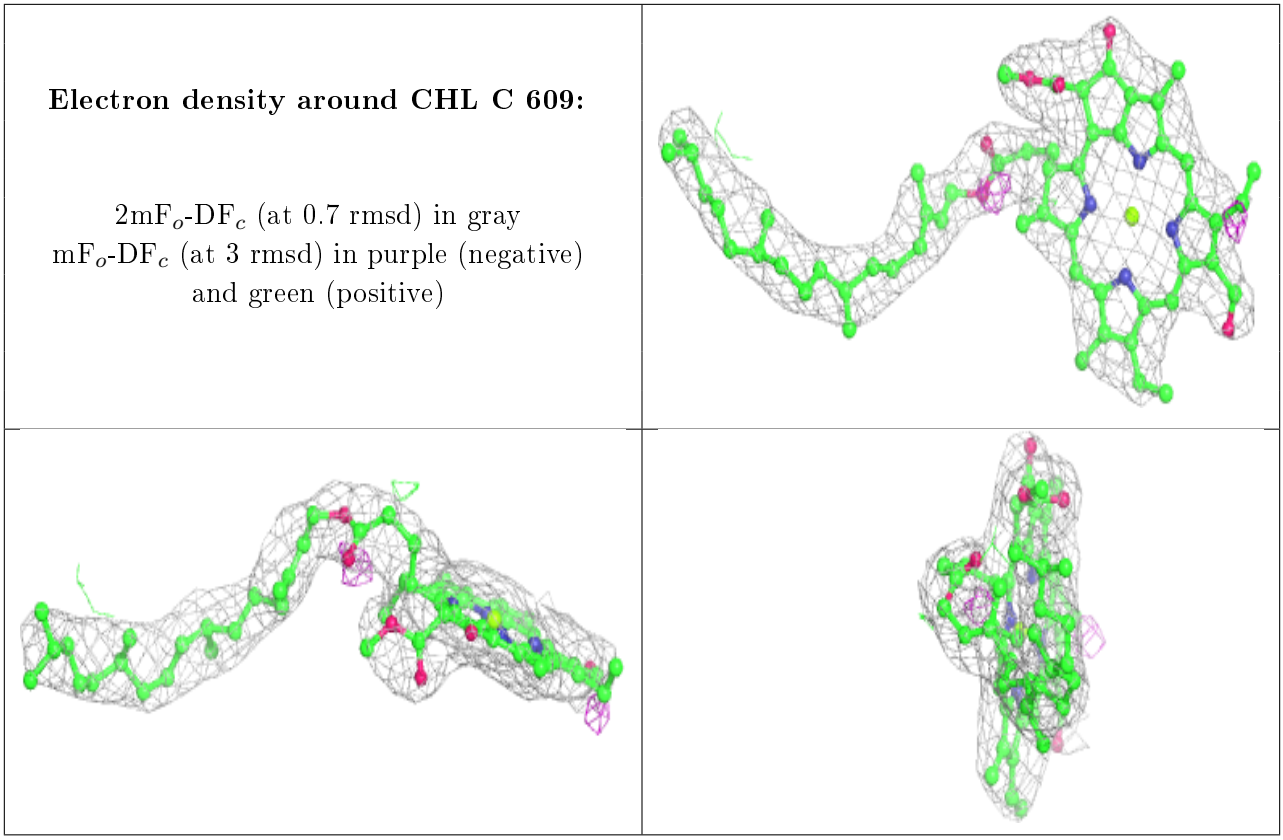
Electron density around CLA B 604:

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



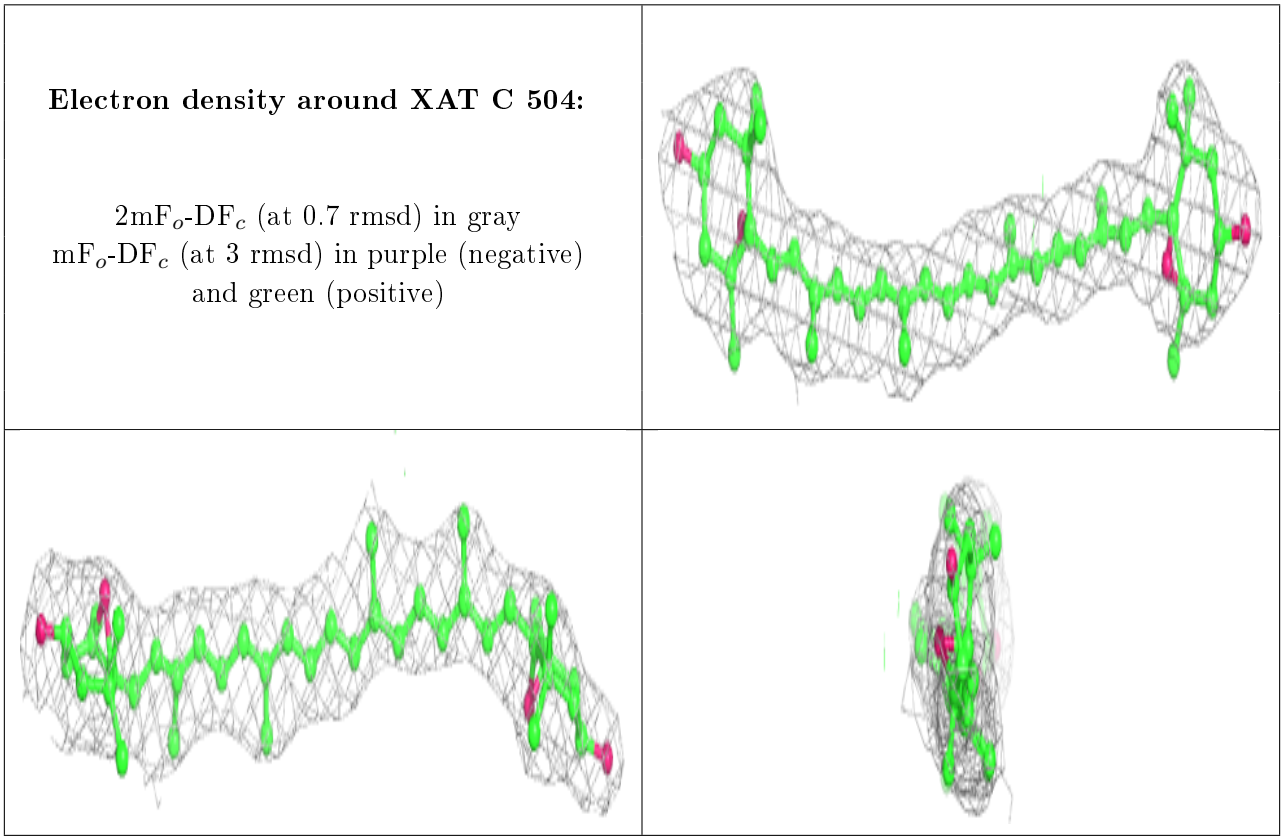
Electron density around CHL C 609:

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



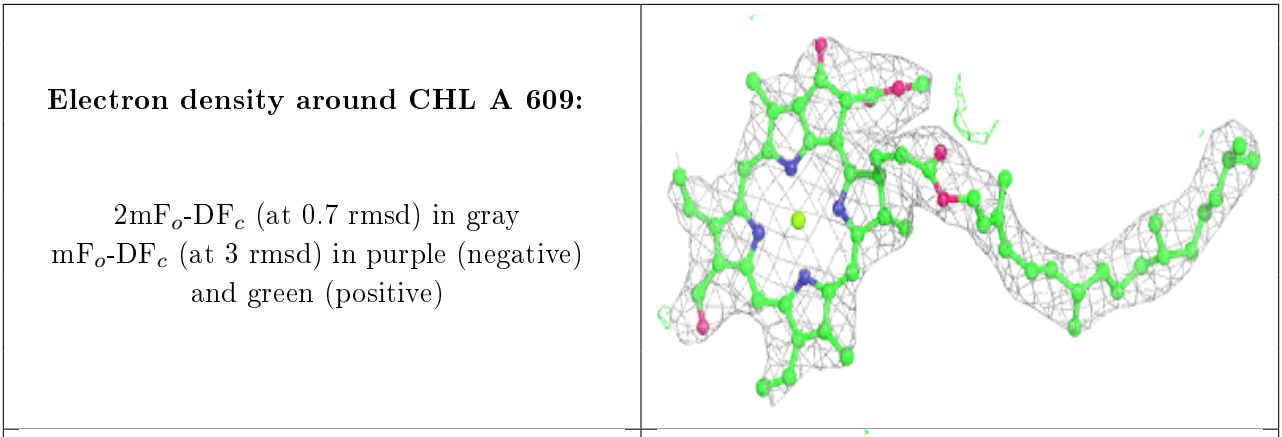
Electron density around XAT C 504:

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



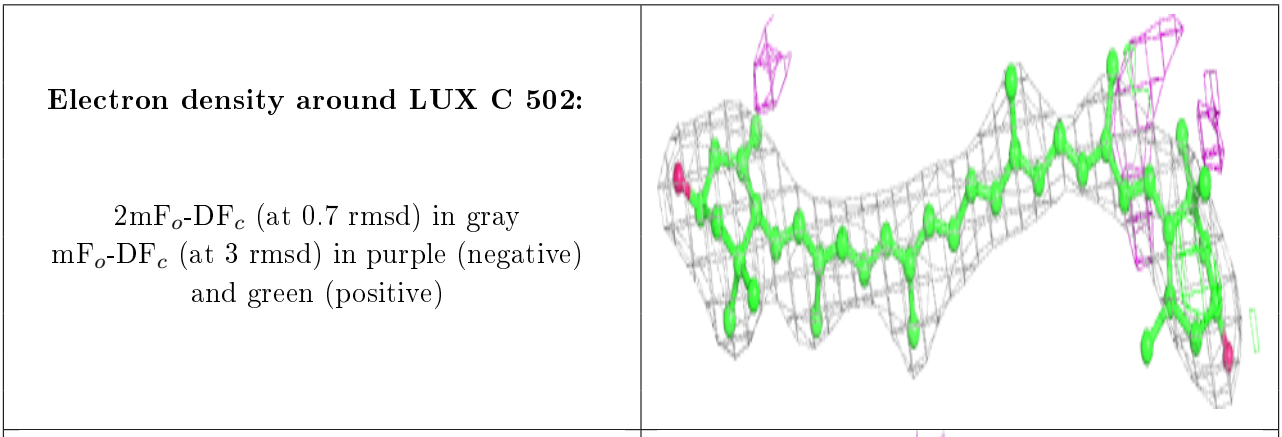
Electron density around CHL A 609:

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



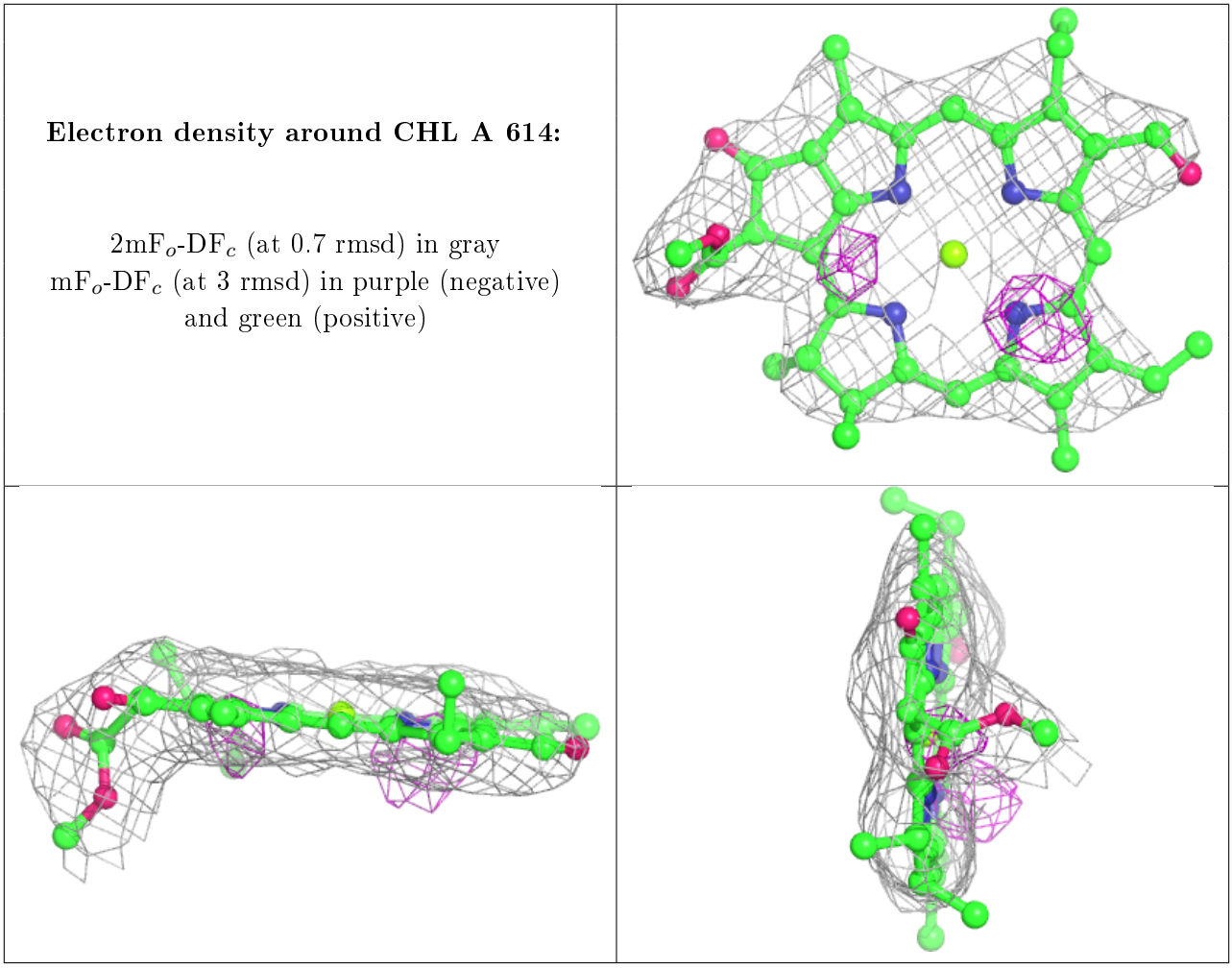
Electron density around LUX C 502:

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



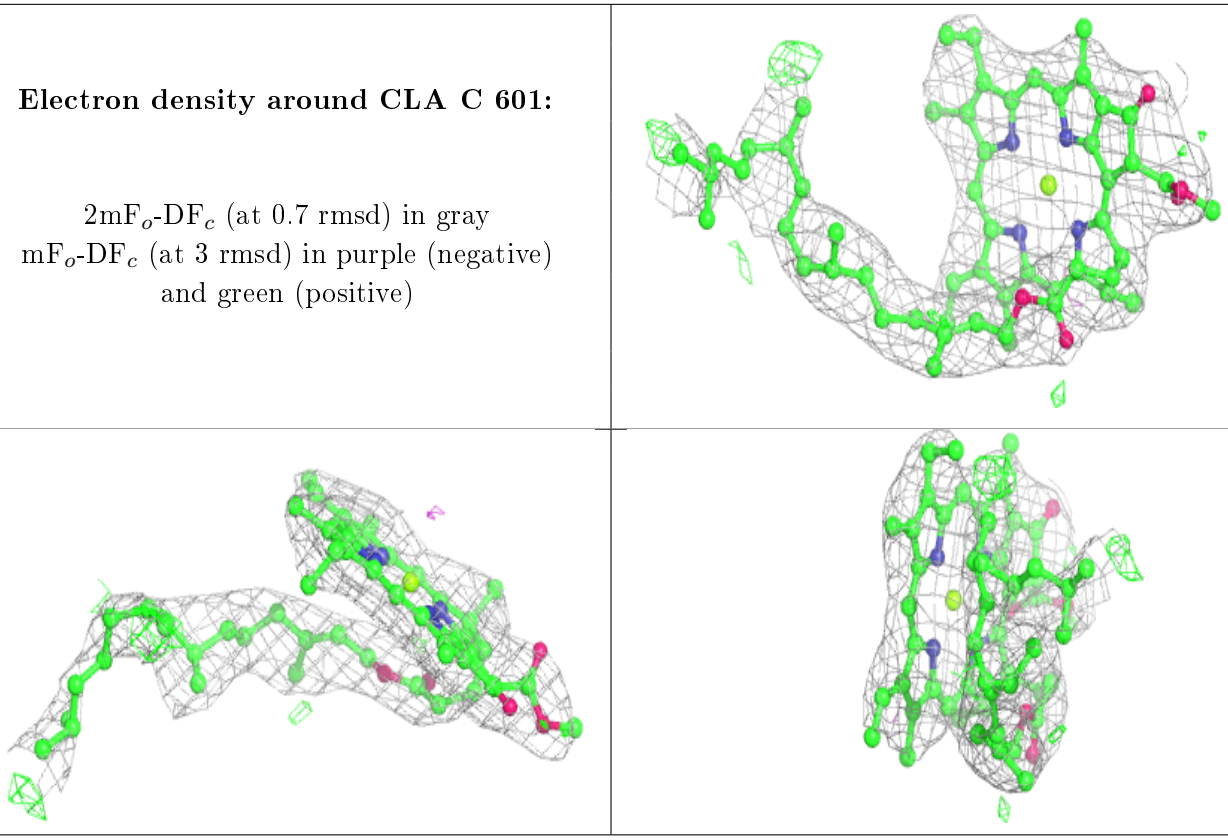
Electron density around CHL A 614:

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



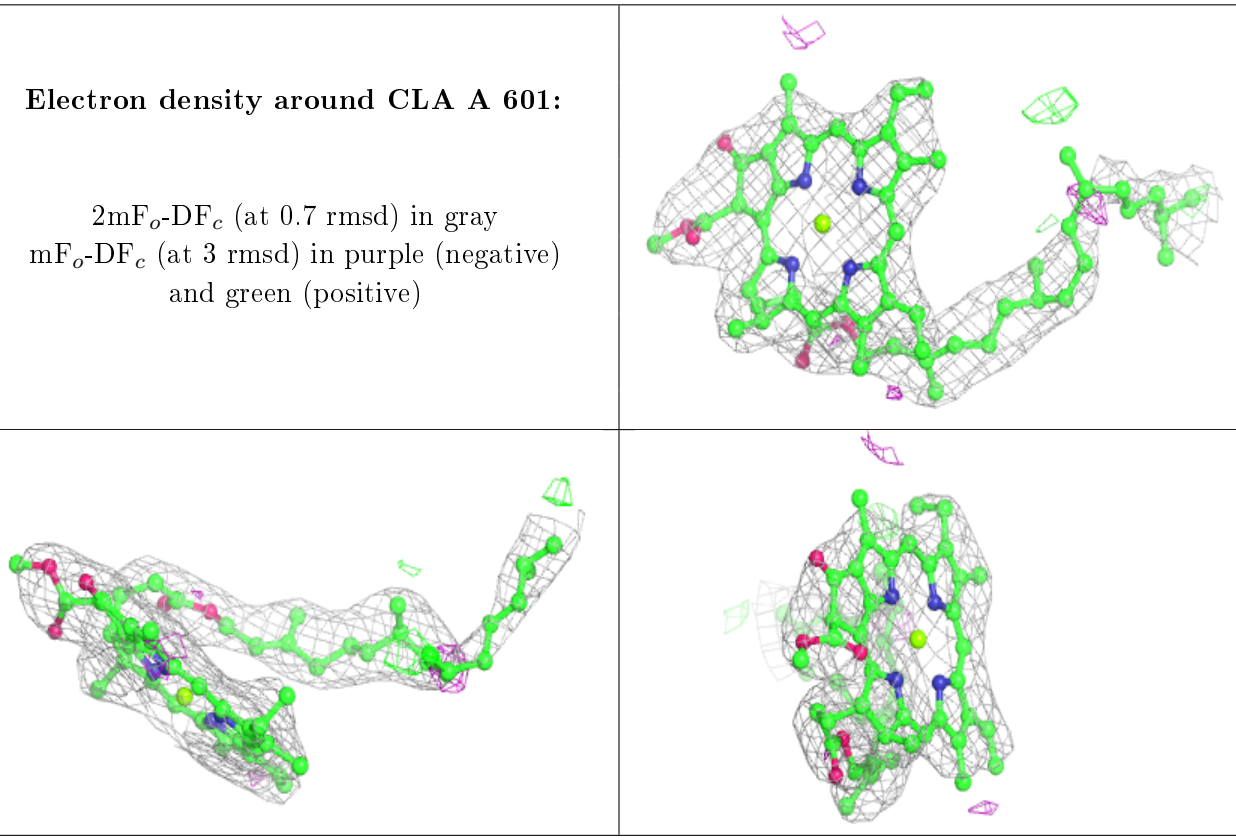
Electron density around CLA C 601:

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



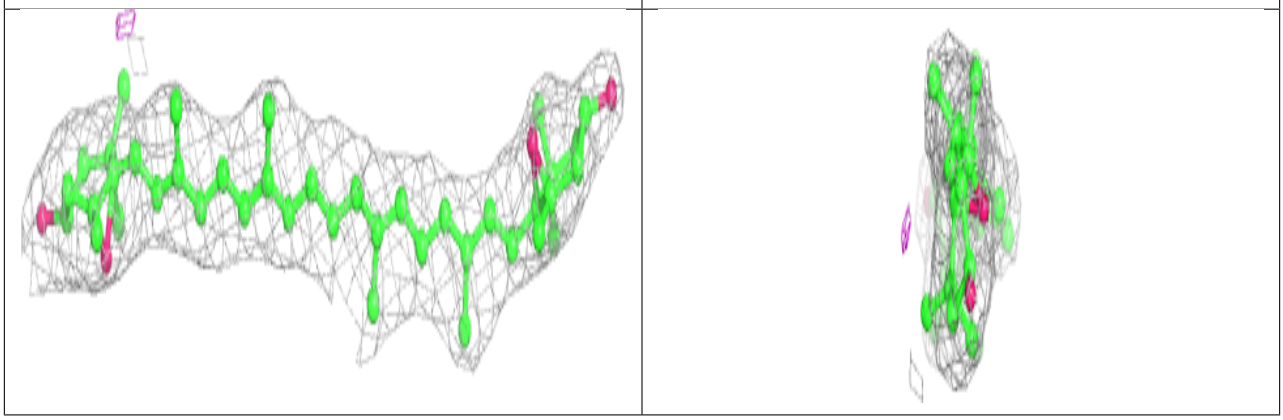
Electron density around CLA A 601:

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



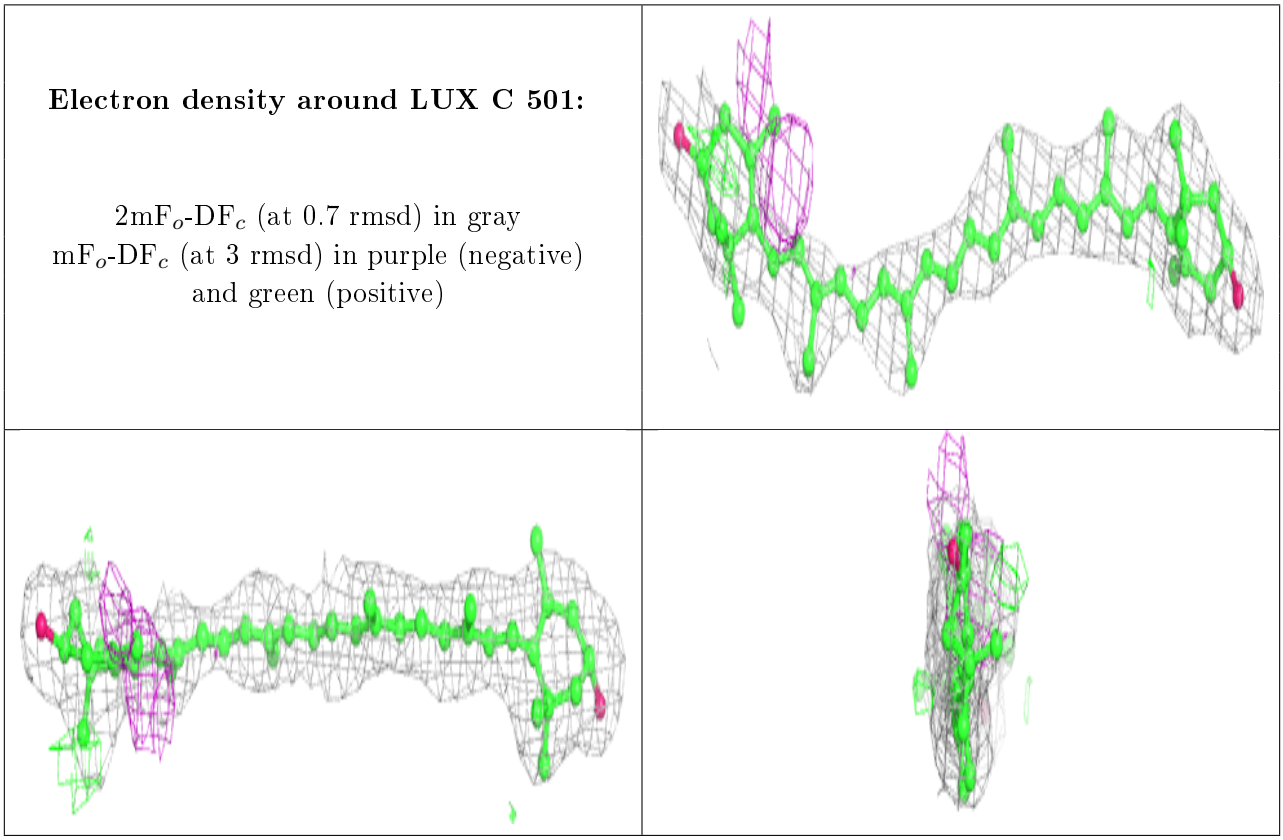
Electron density around XAT B 504:

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



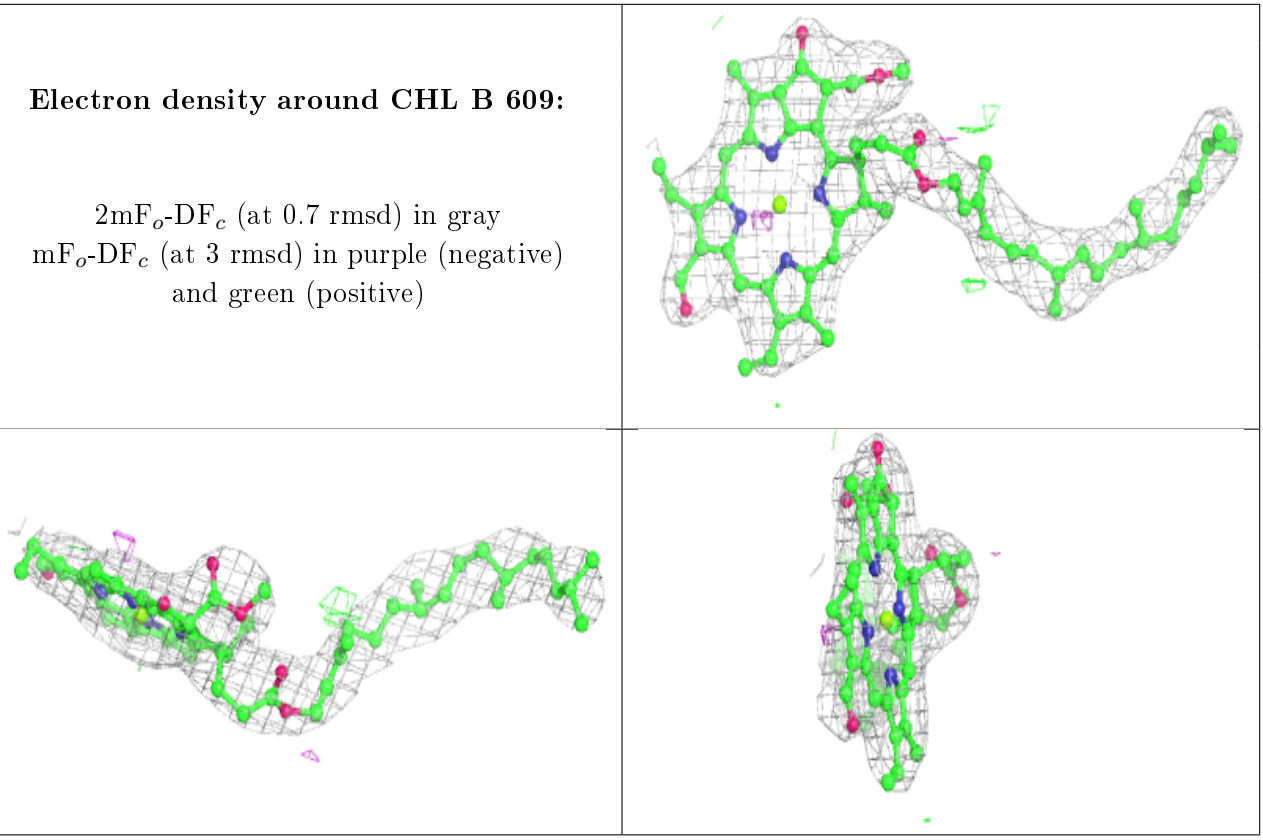
Electron density around LUX C 501:

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



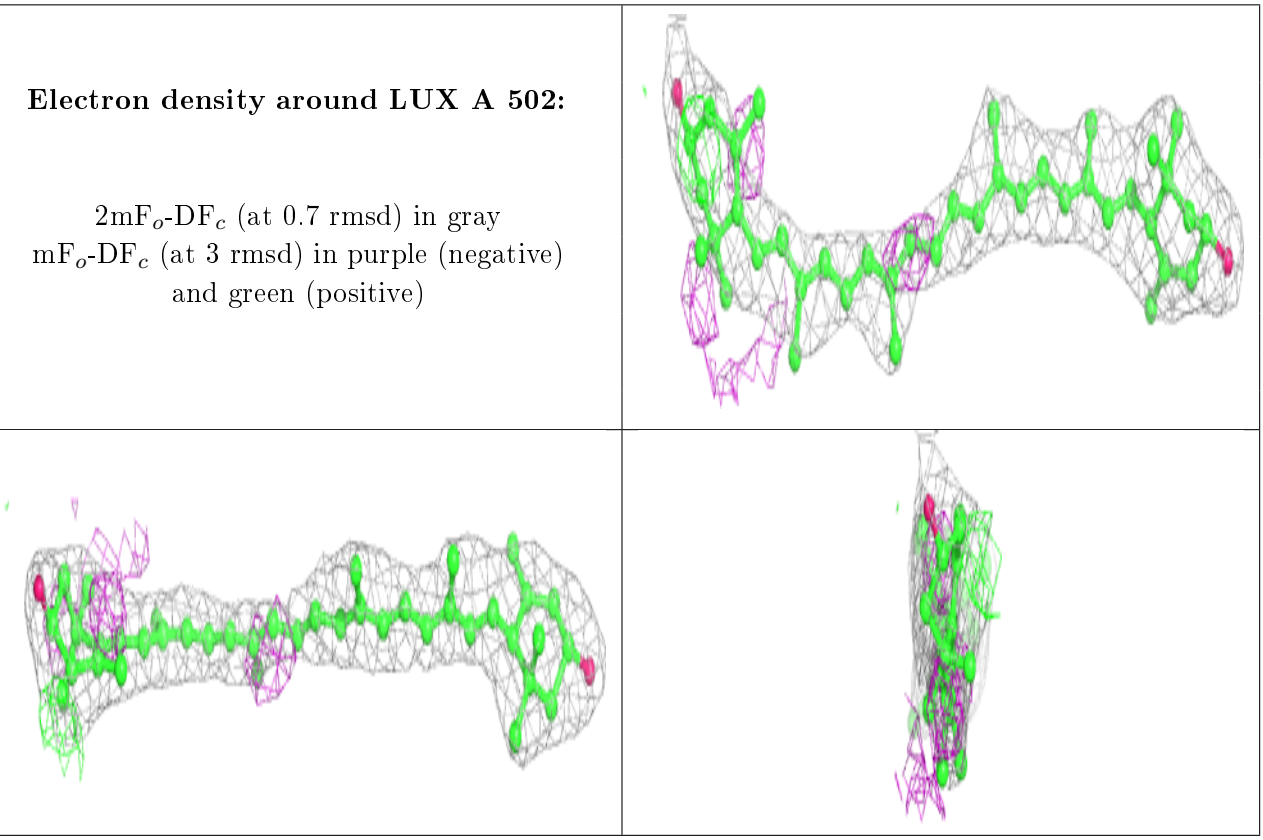
Electron density around CHL B 609:

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



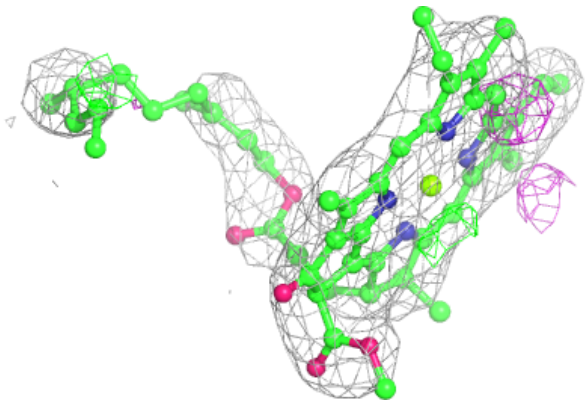
Electron density around LUX A 502:

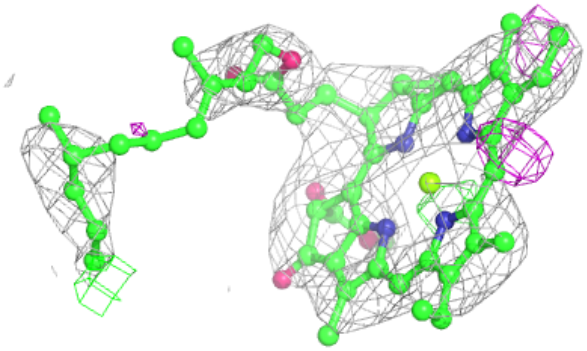
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

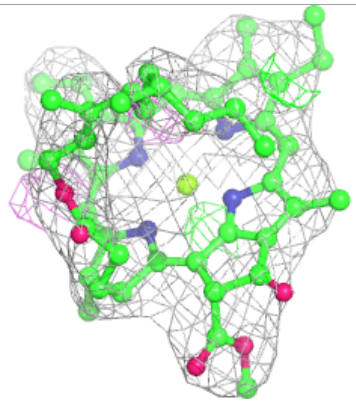


Electron density around CLA B 606:

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

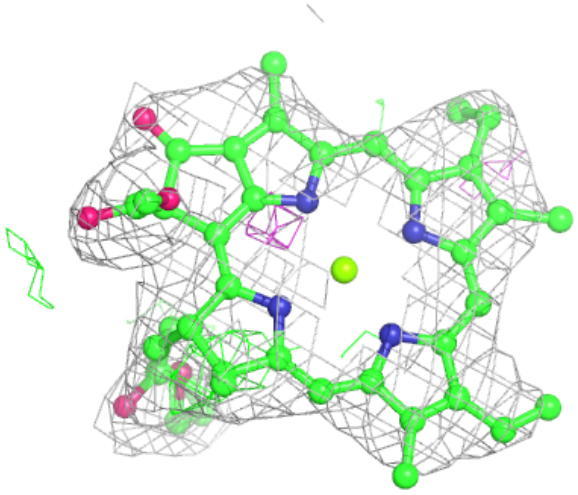


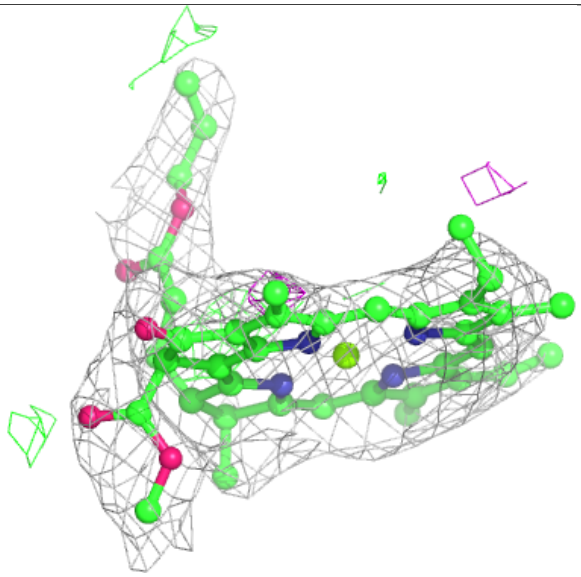


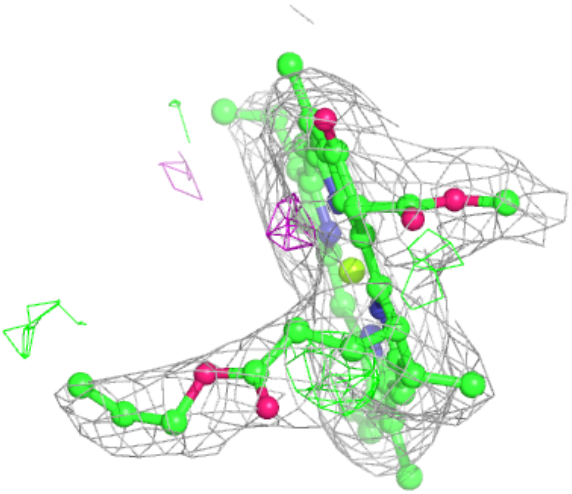


Electron density around CLA B 608:

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

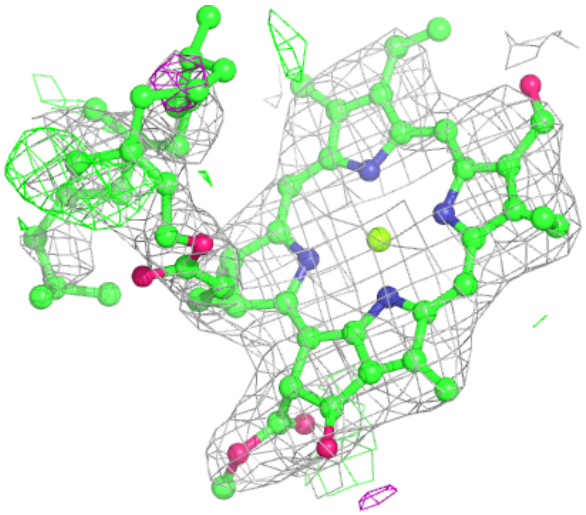


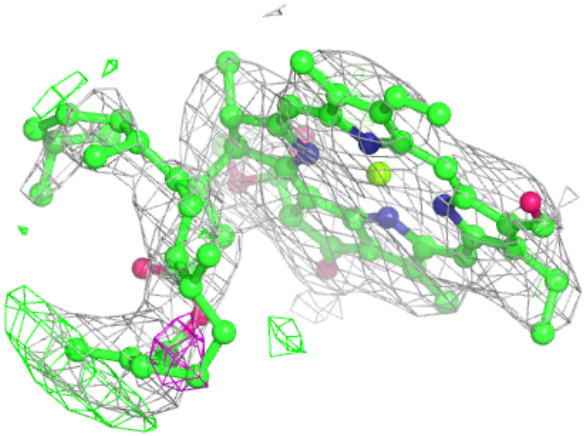


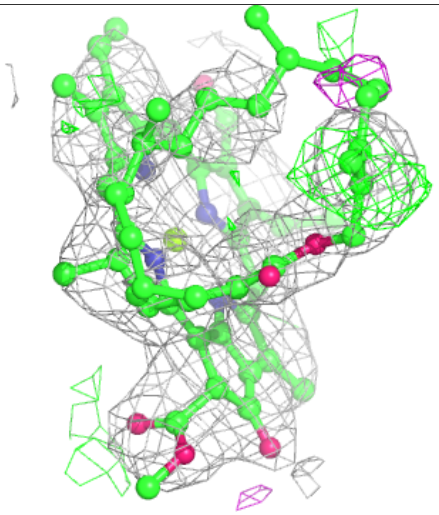


Electron density around CHL C 611:

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

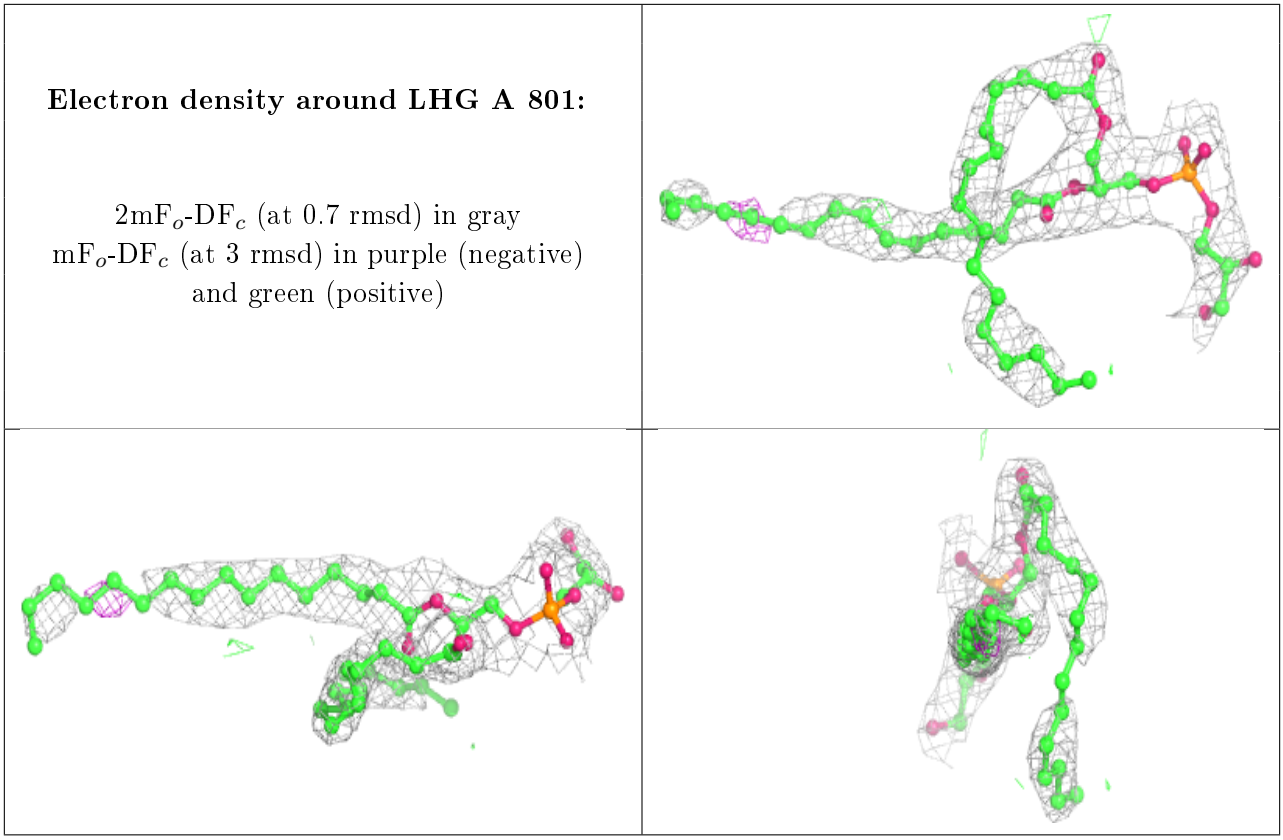






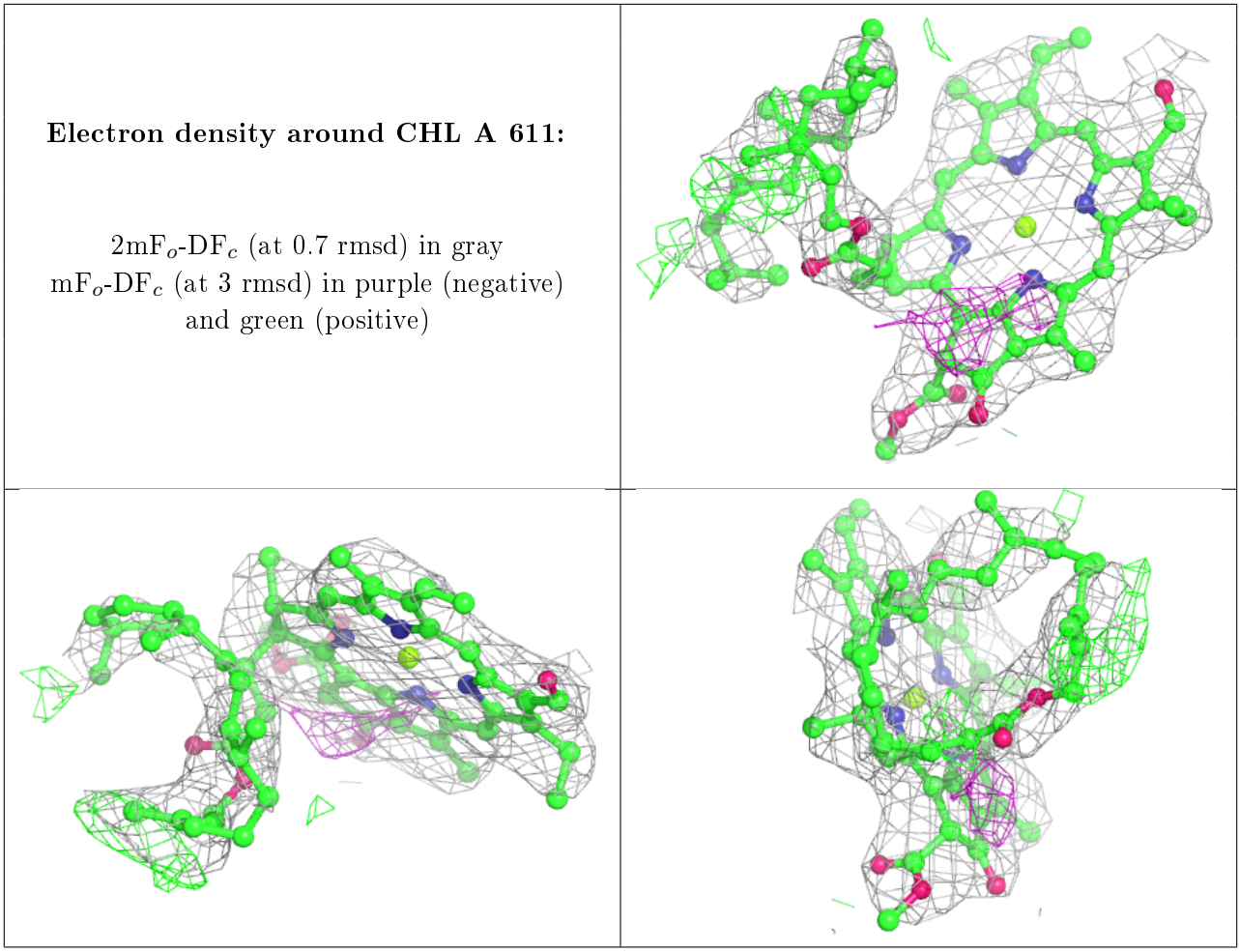
Electron density around LHG A 801:

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



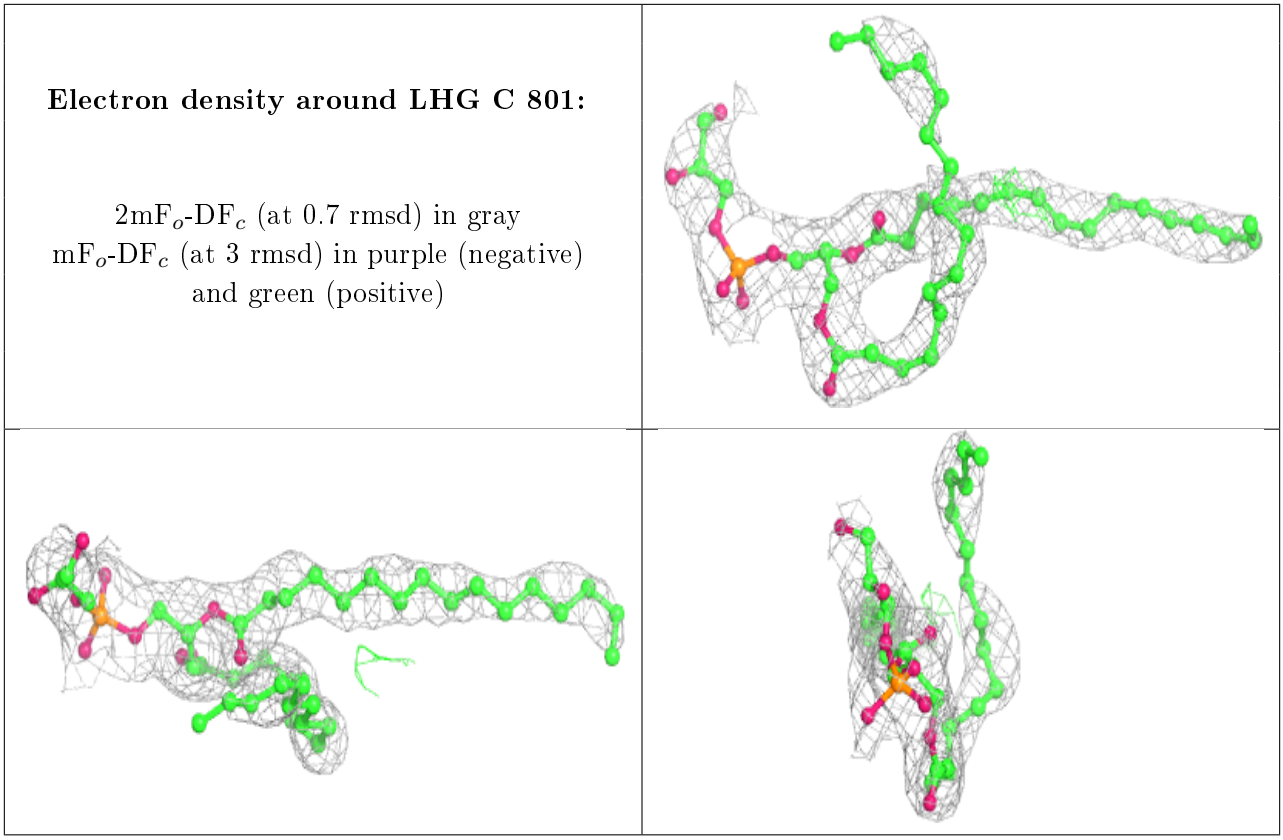
Electron density around CHL A 611:

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



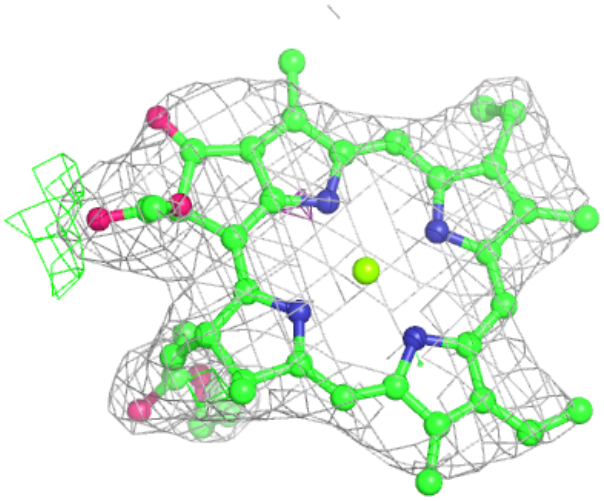
Electron density around LHG C 801:

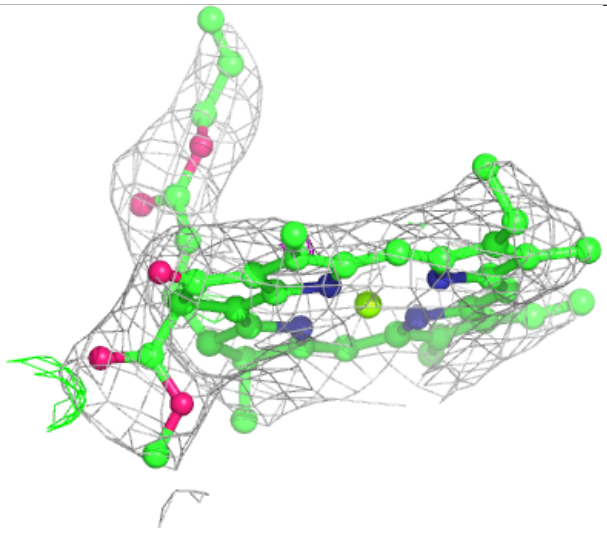
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

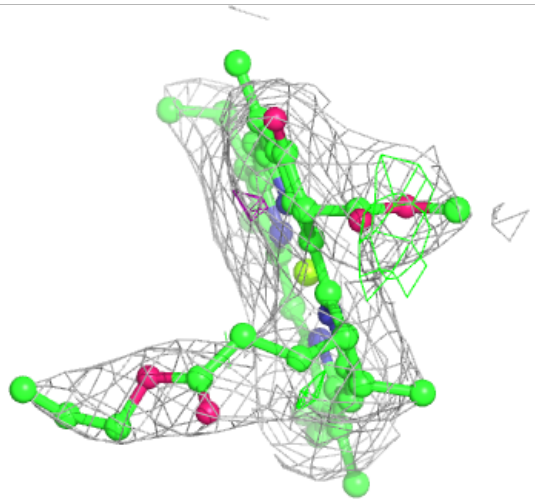


Electron density around CLA C 608:

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

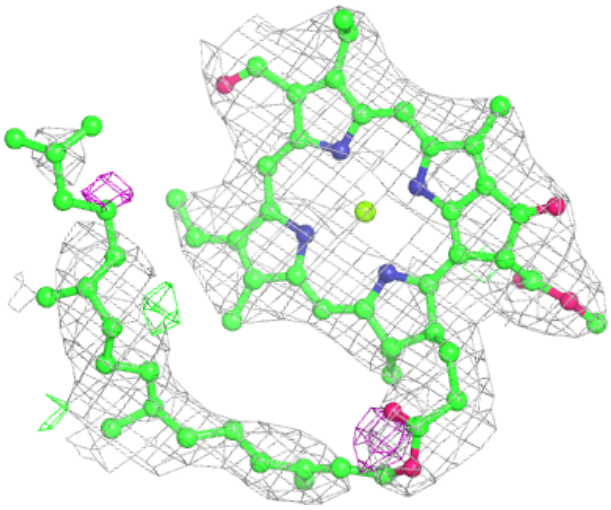


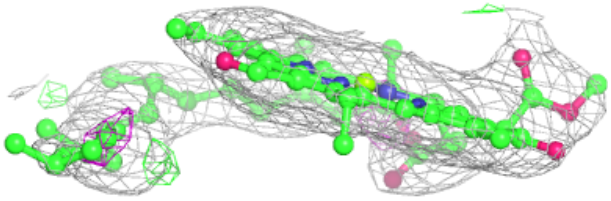


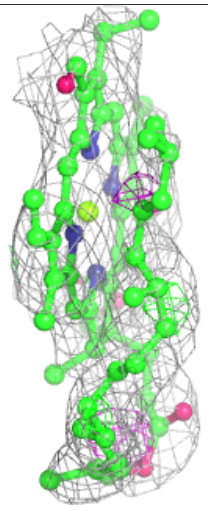


Electron density around CHL C 610:

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

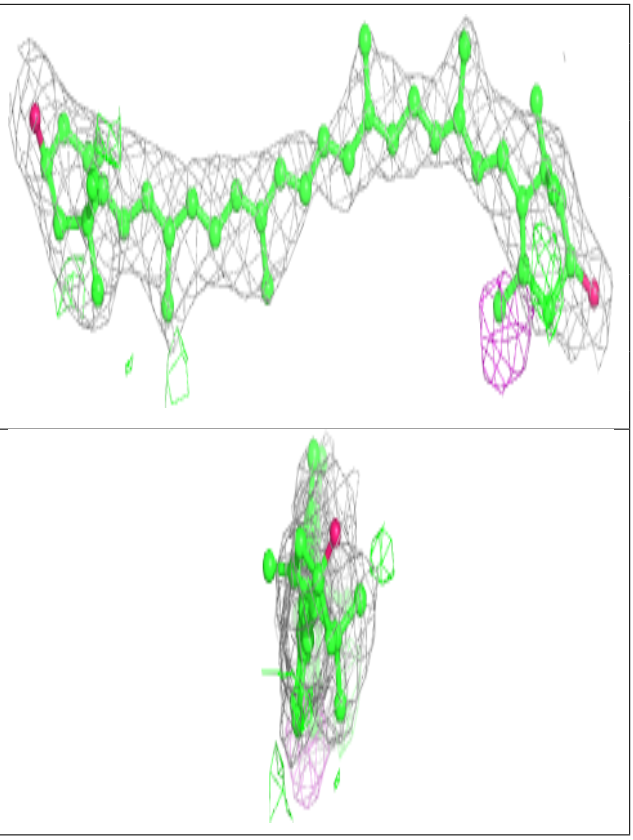






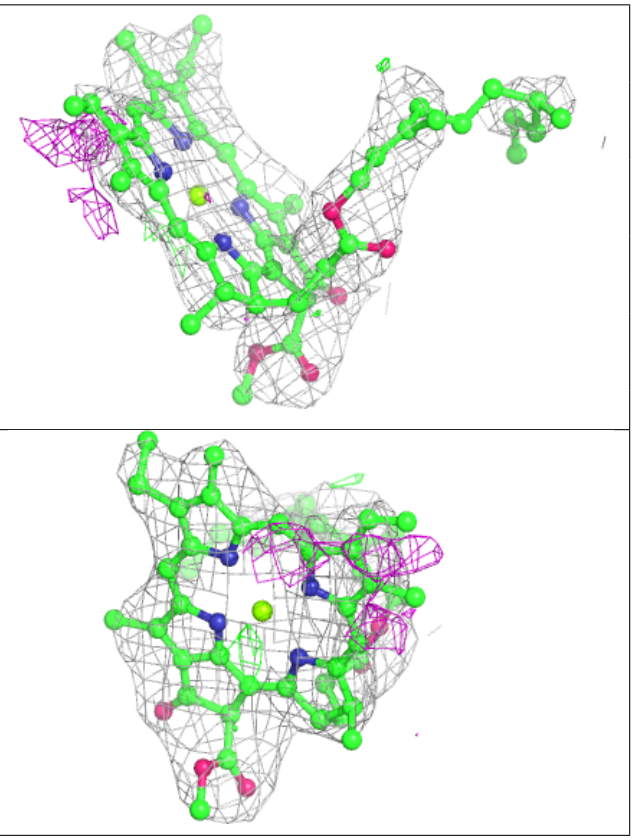
Electron density around LUX B 501:

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



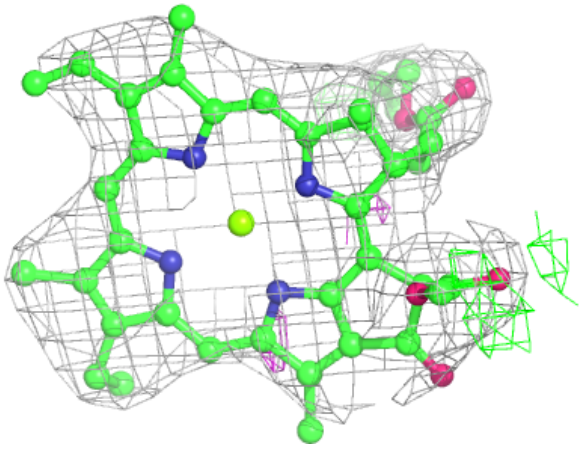
Electron density around CLA A 606:

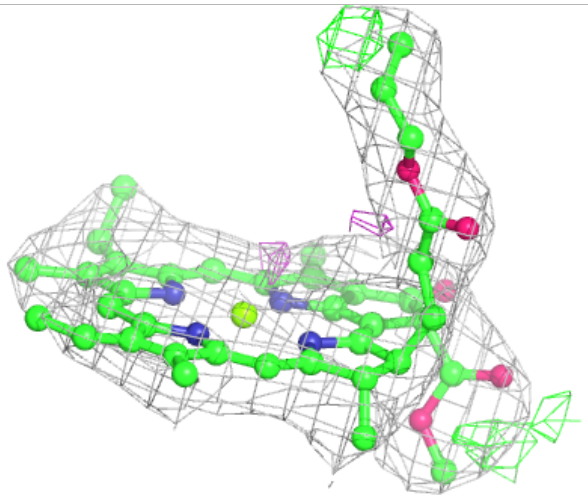
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

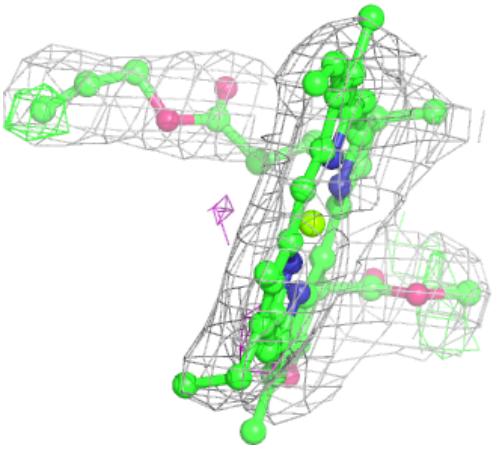


Electron density around CLA A 608:

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

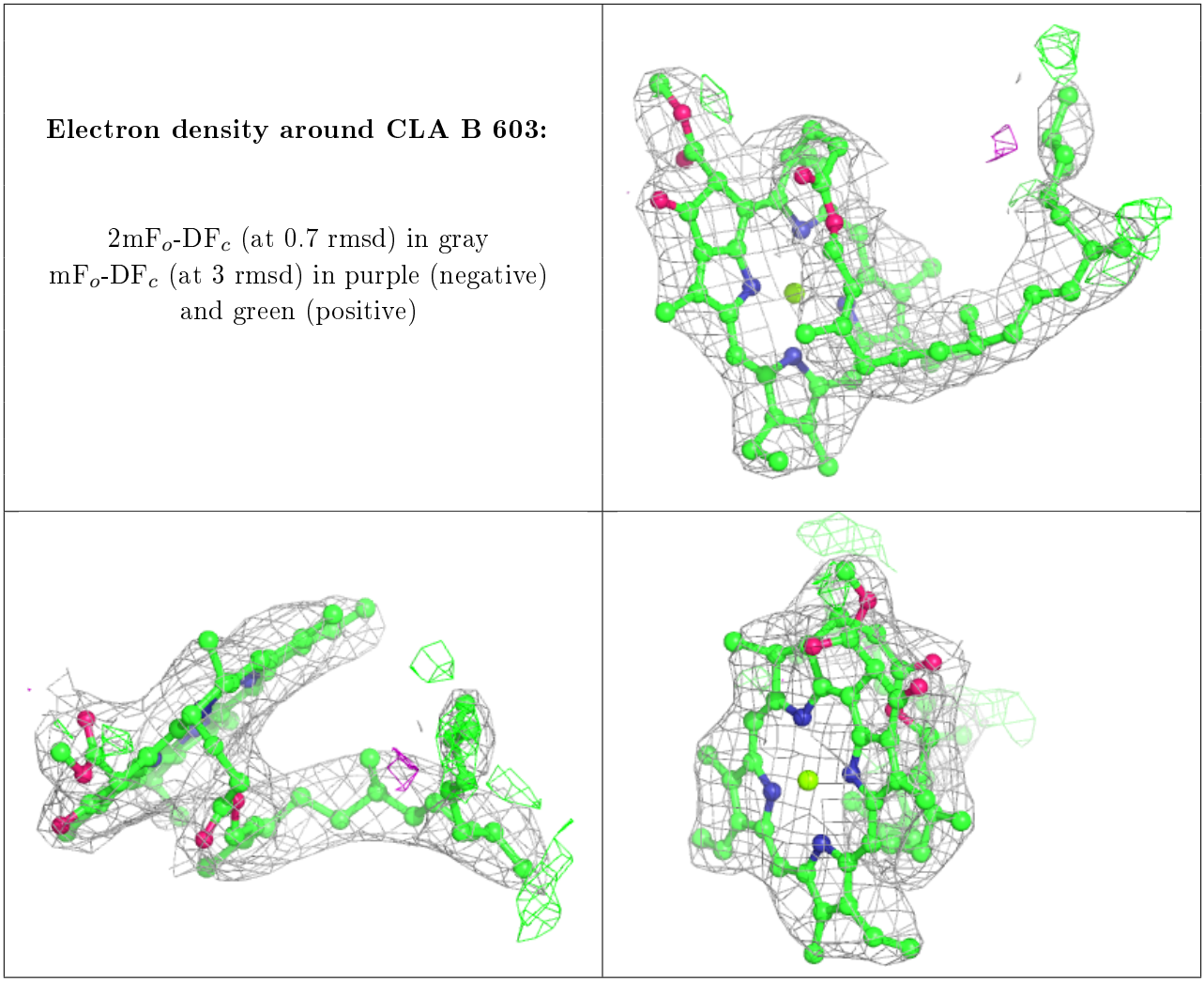






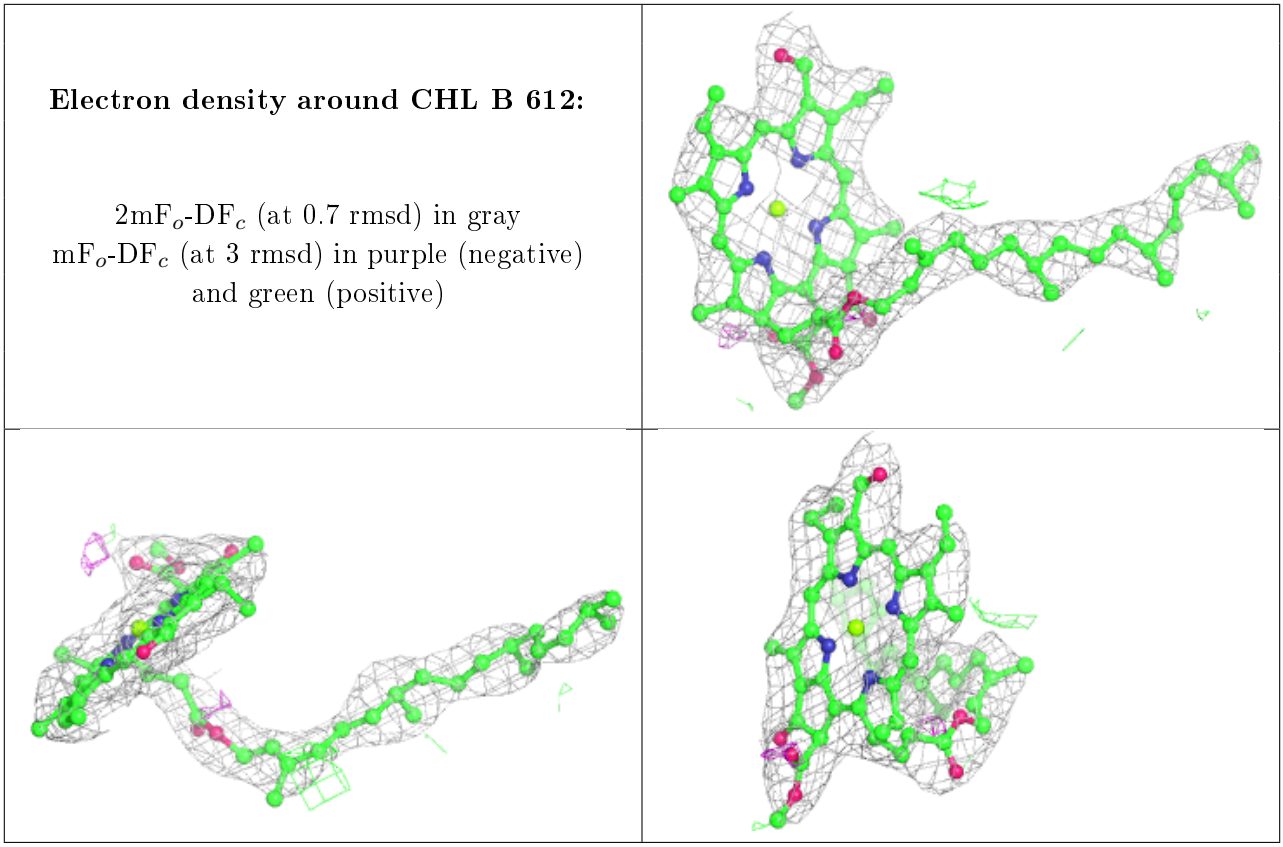
Electron density around CLA B 603:

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



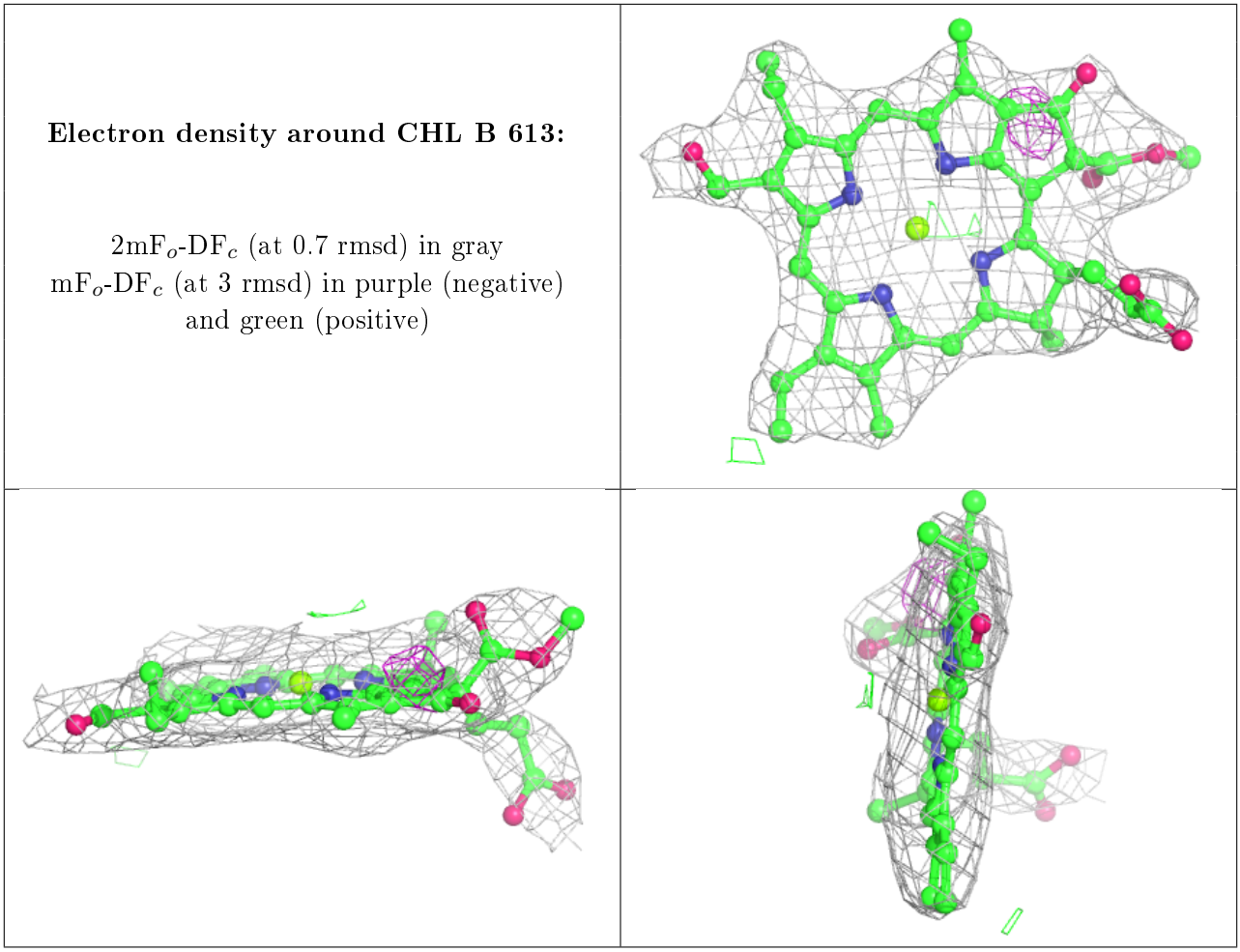
Electron density around CHL B 612:

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



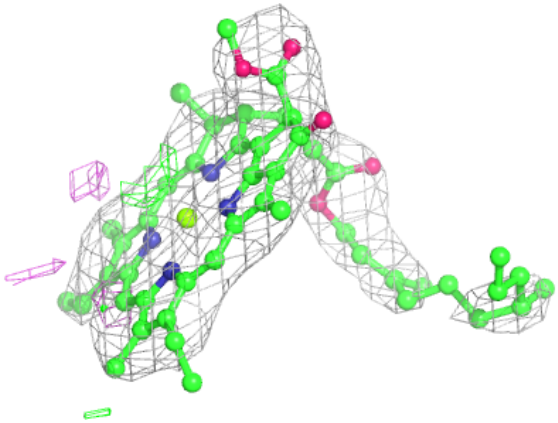
Electron density around CHL B 613:

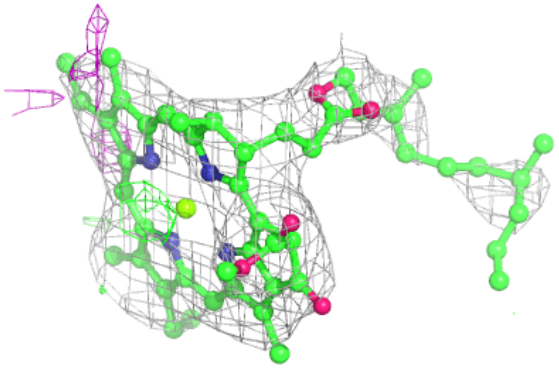
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

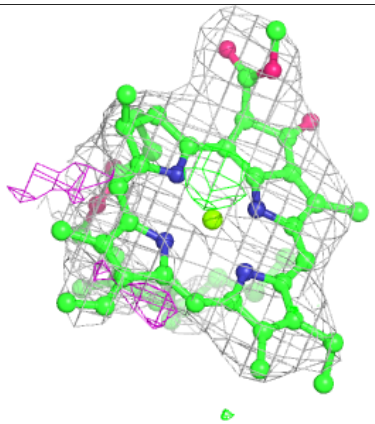


Electron density around CLA C 606:

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

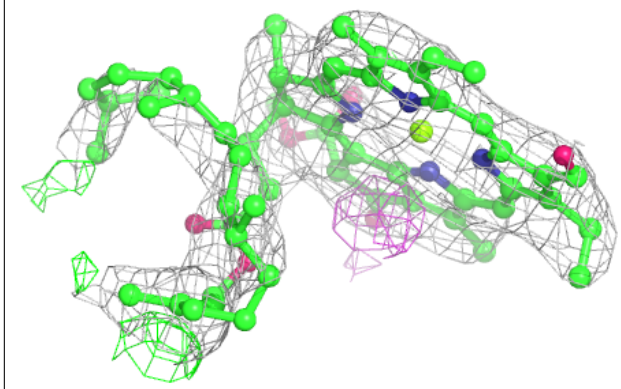


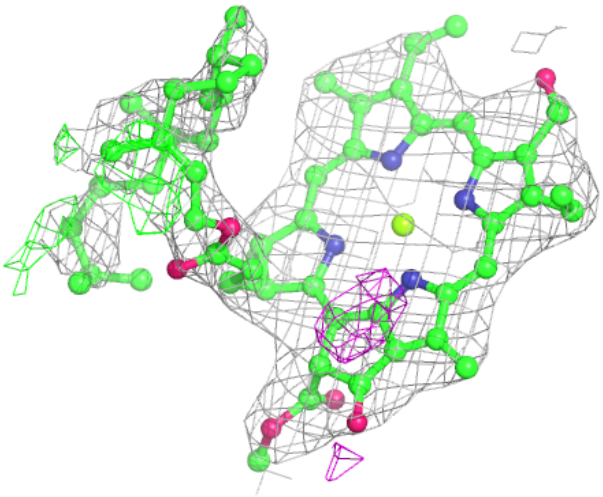


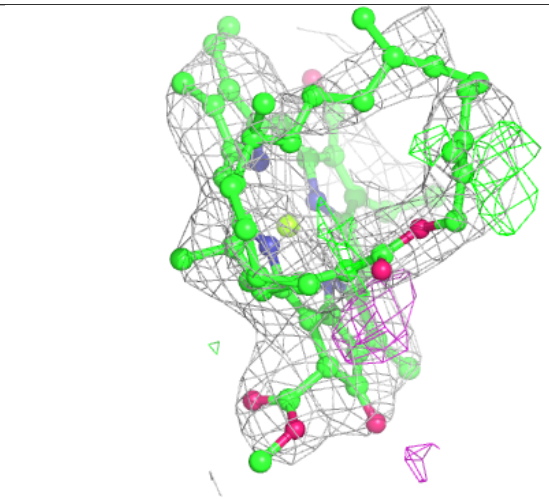


Electron density around CHL B 611:

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

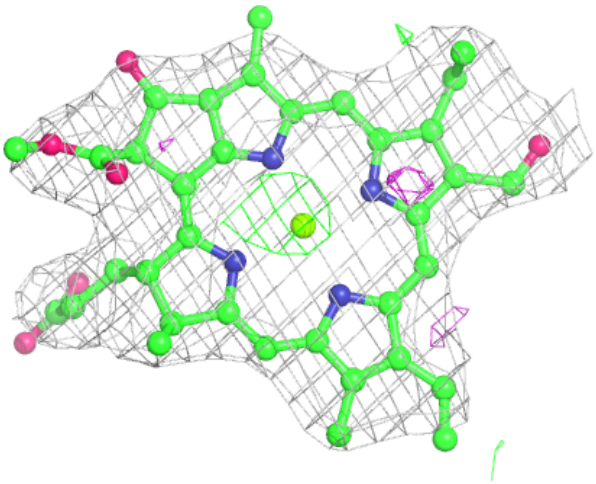


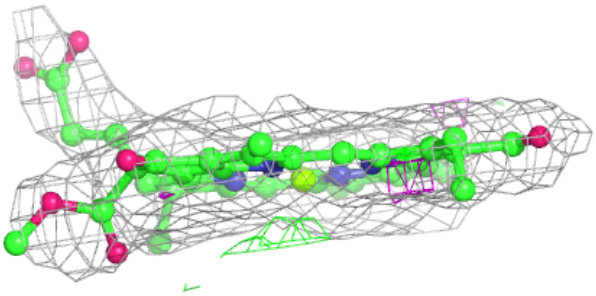




Electron density around CHL C 613:

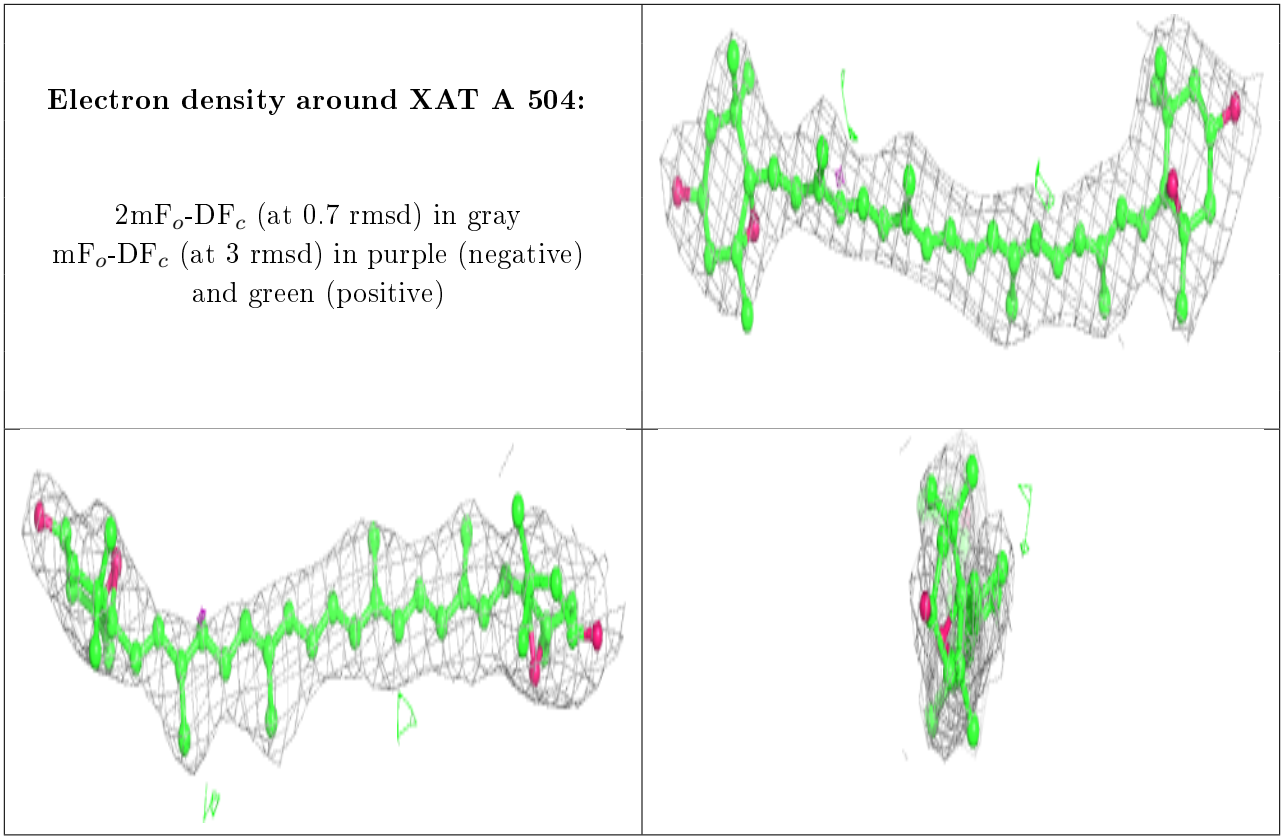
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





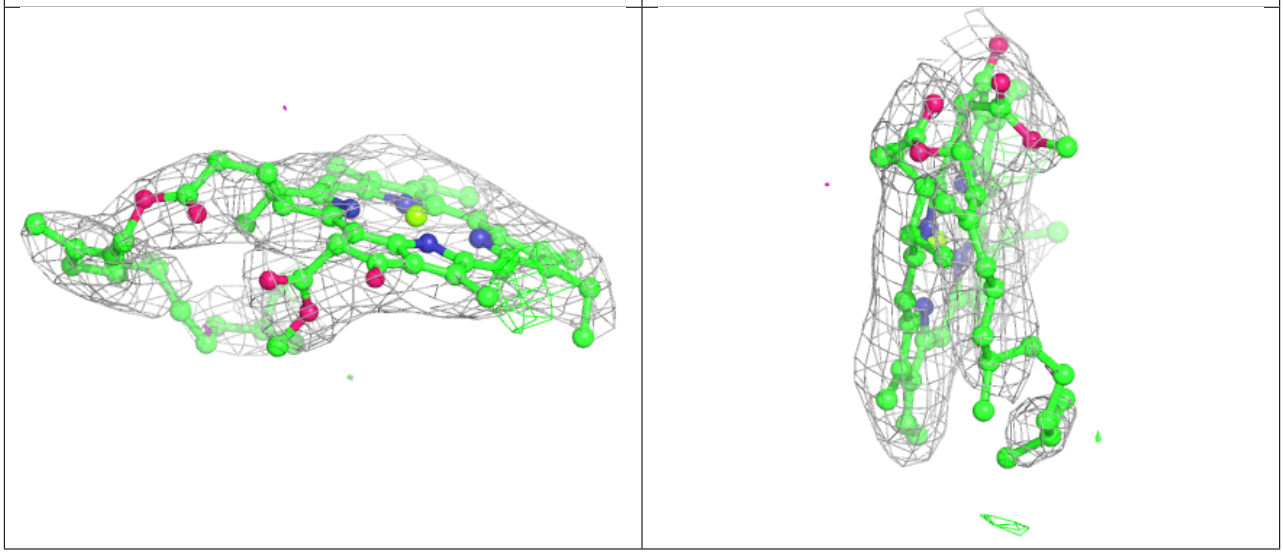
Electron density around XAT A 504:

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



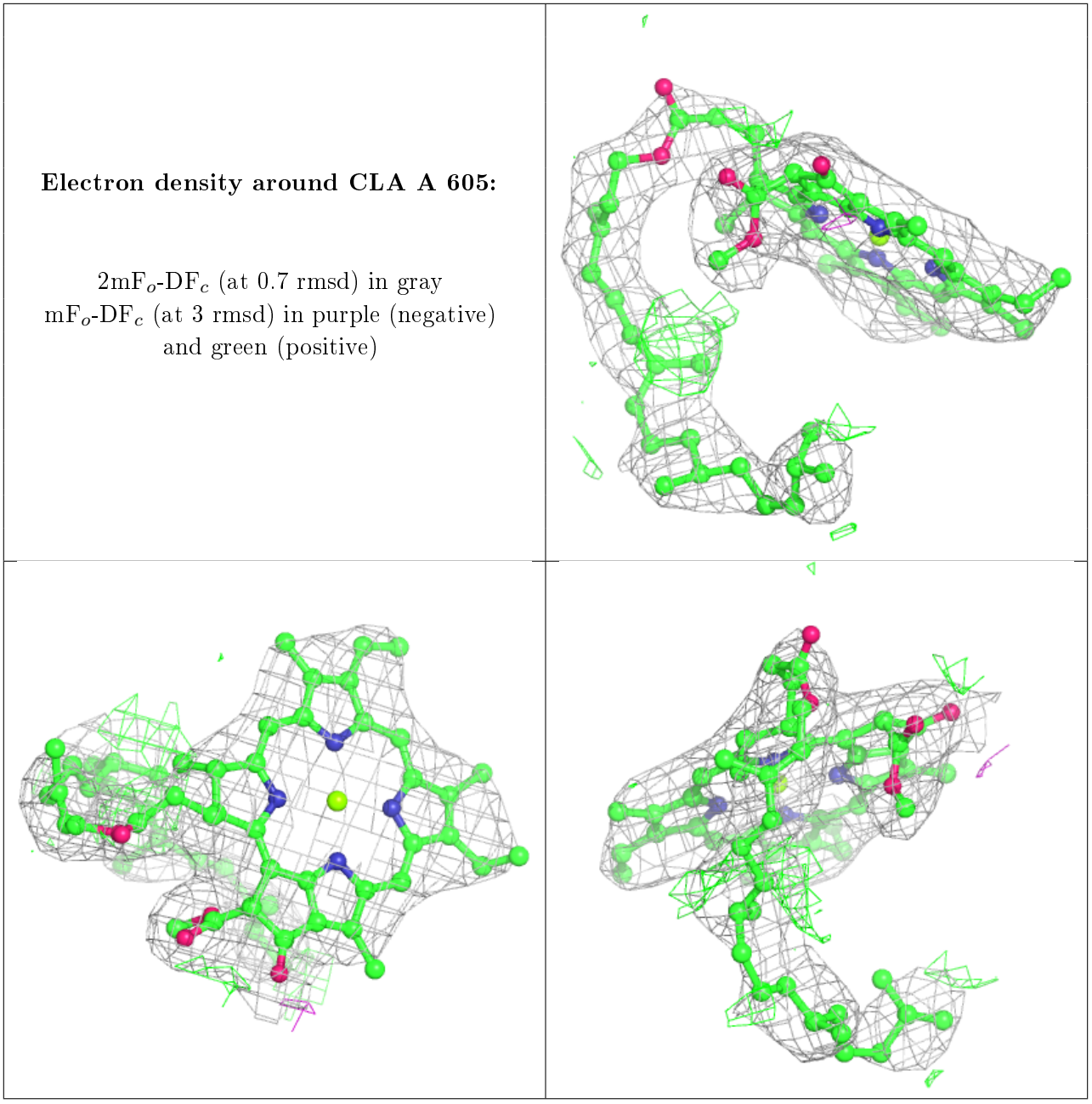
Electron density around CLA A 602:

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



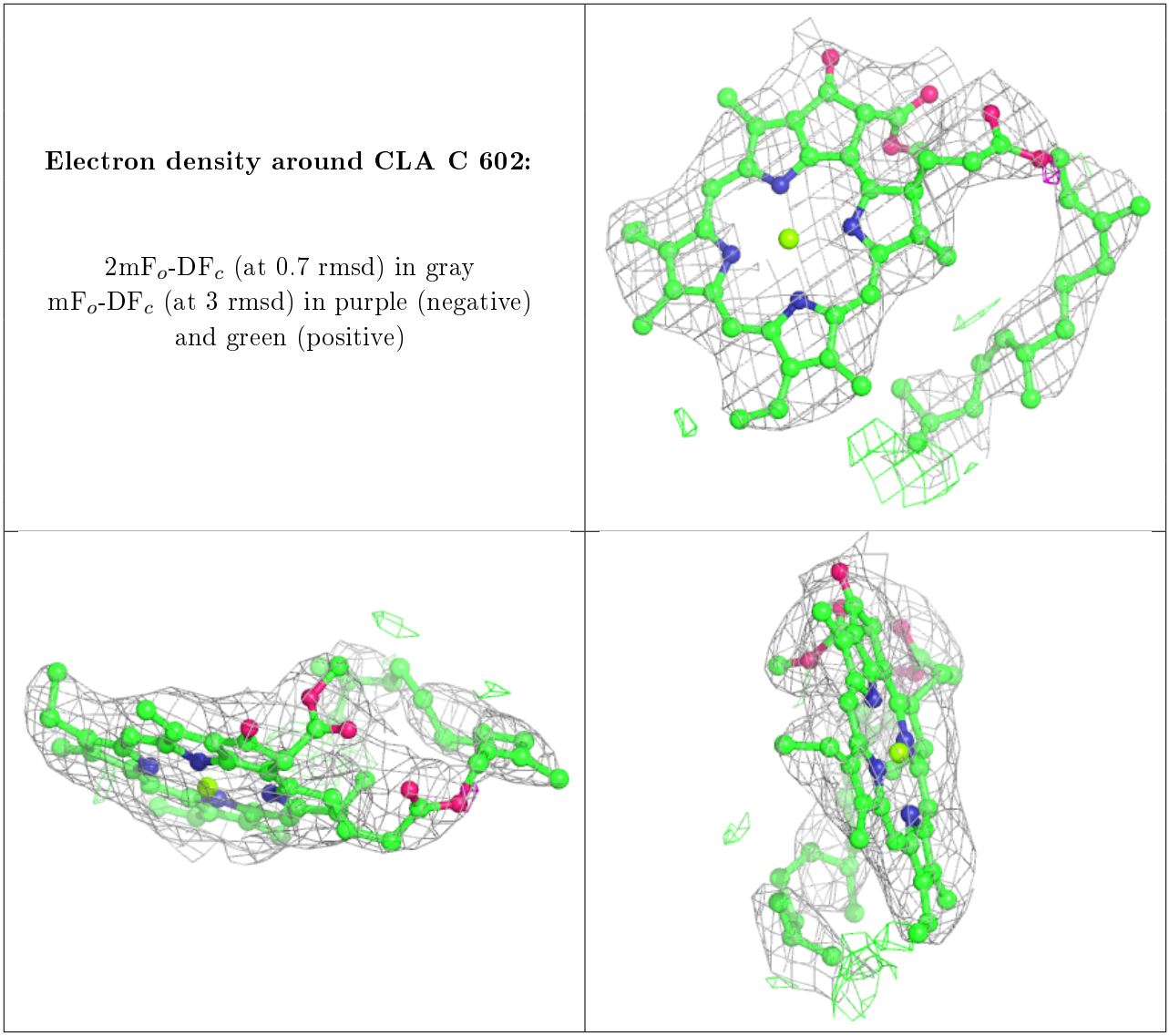
Electron density around CLA A 605:

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



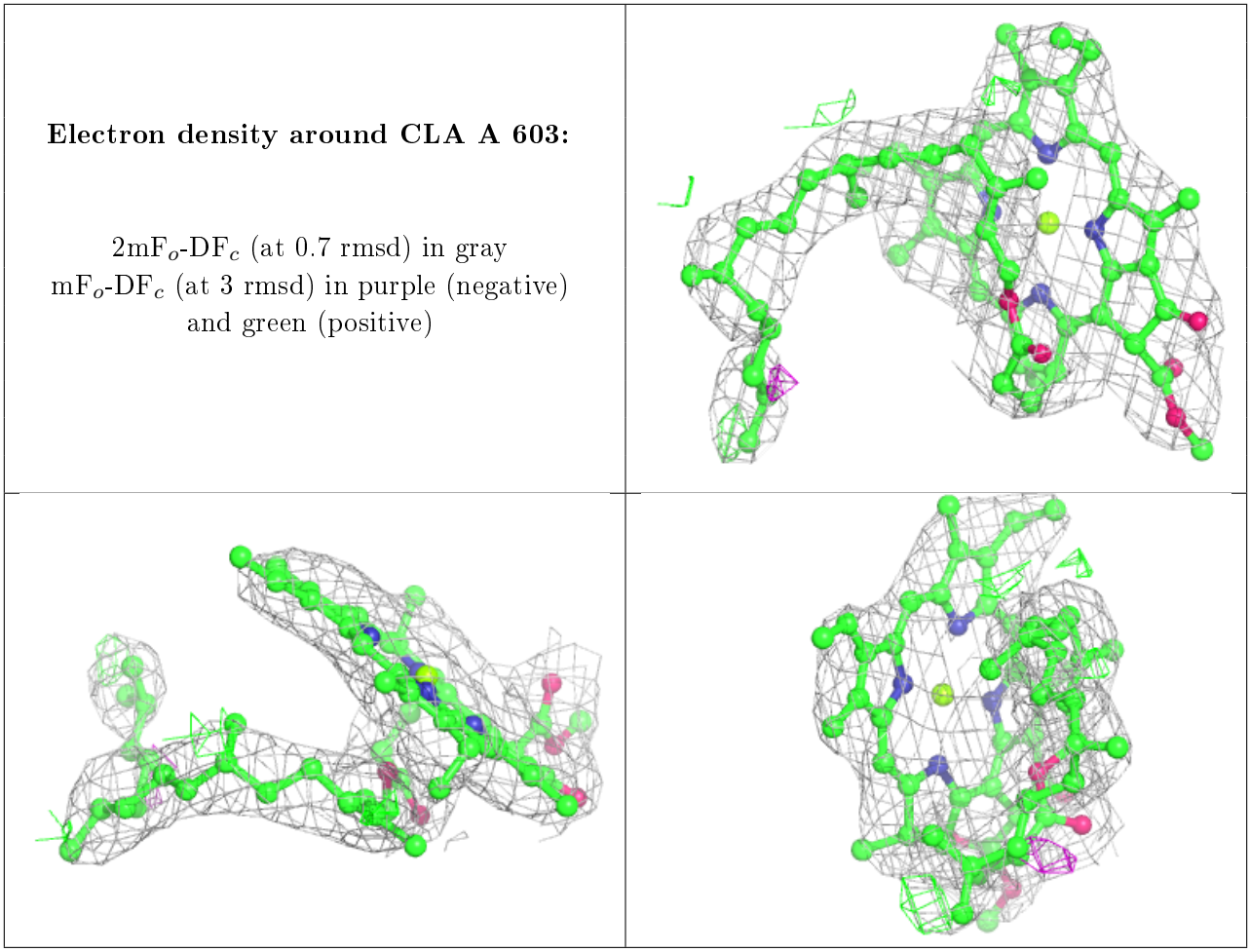
Electron density around CLA C 602:

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



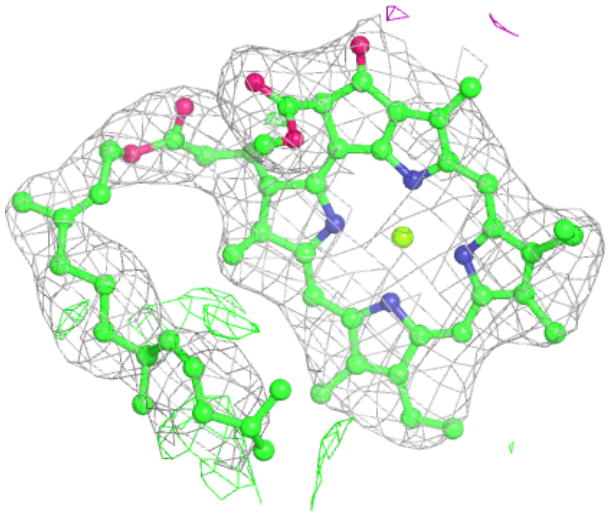
Electron density around CLA A 603:

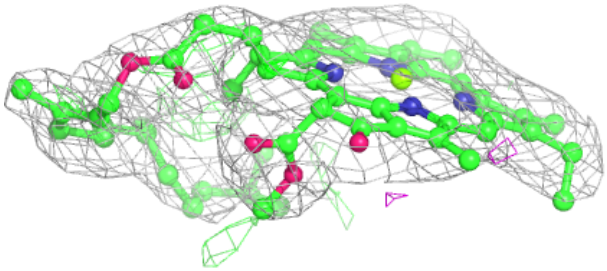
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

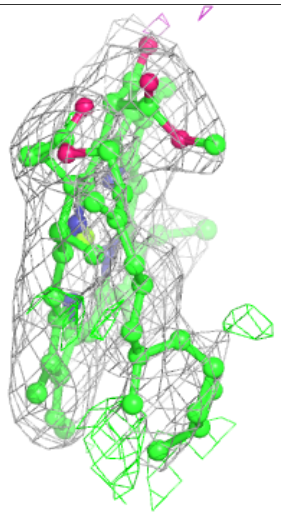


Electron density around CLA B 602:

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

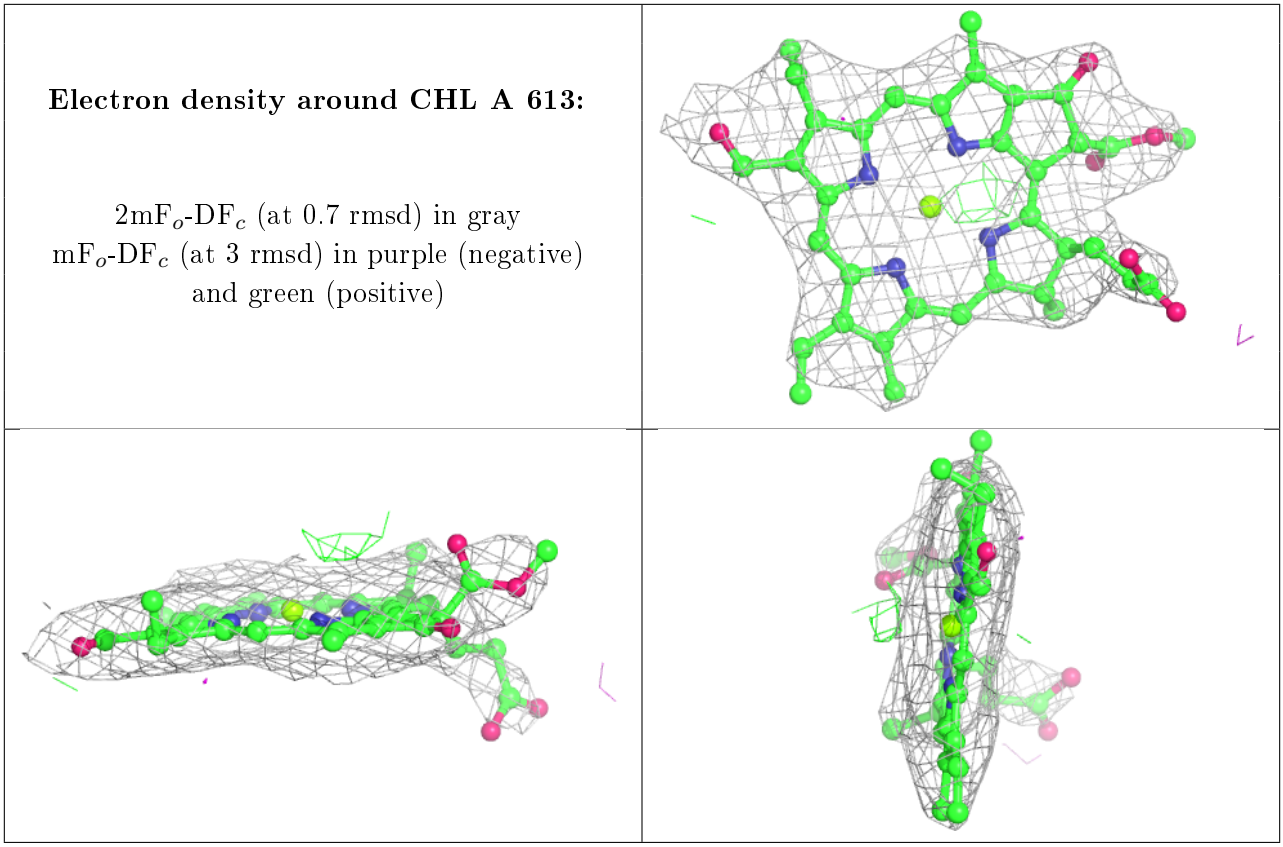






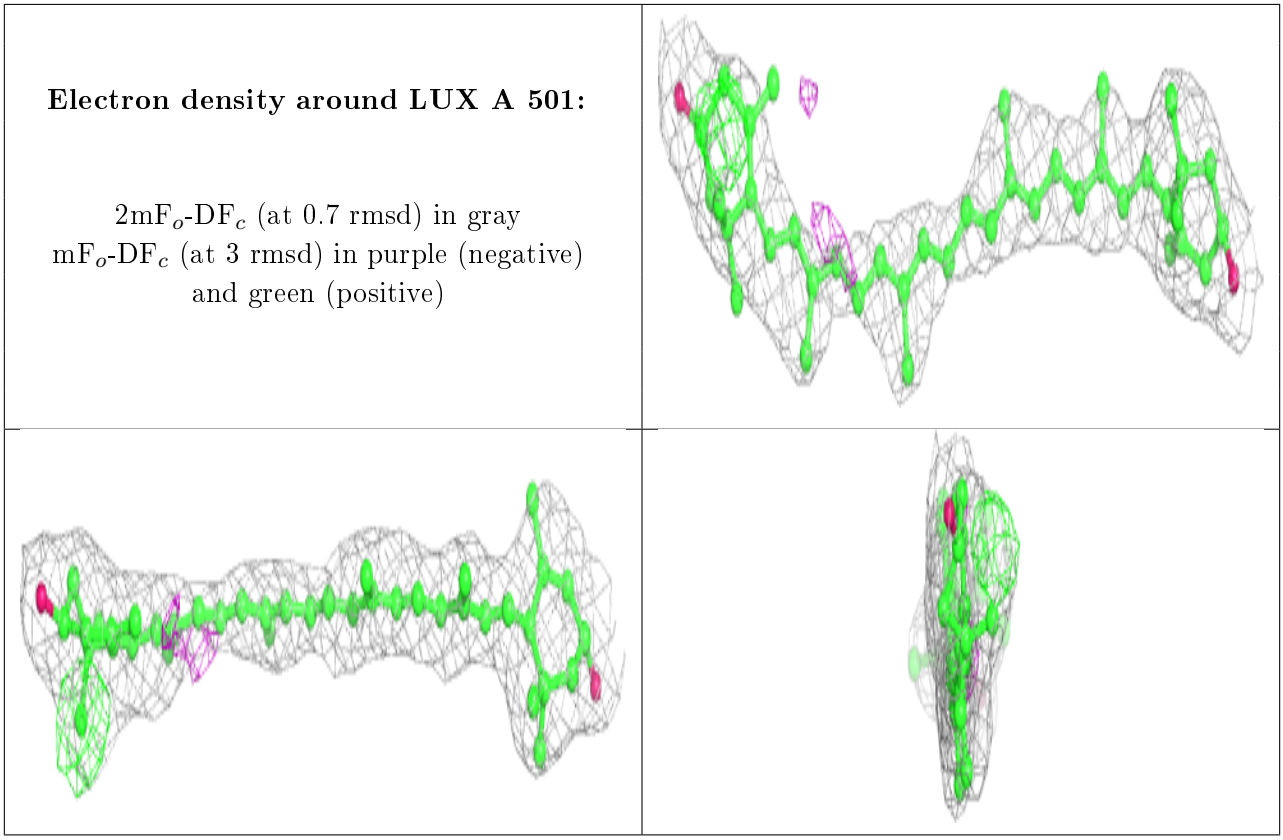
Electron density around CHL A 613:

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



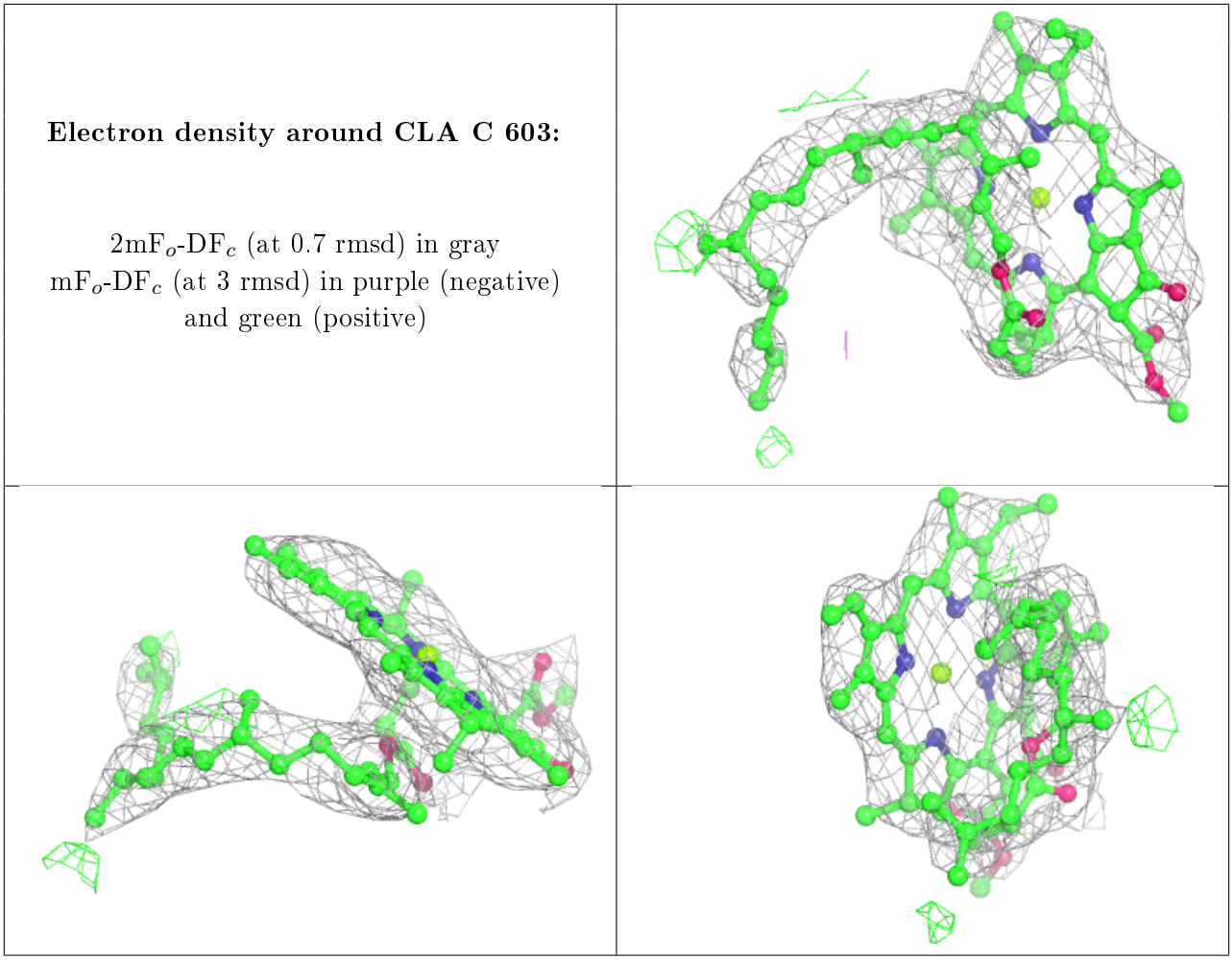
Electron density around LUX A 501:

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



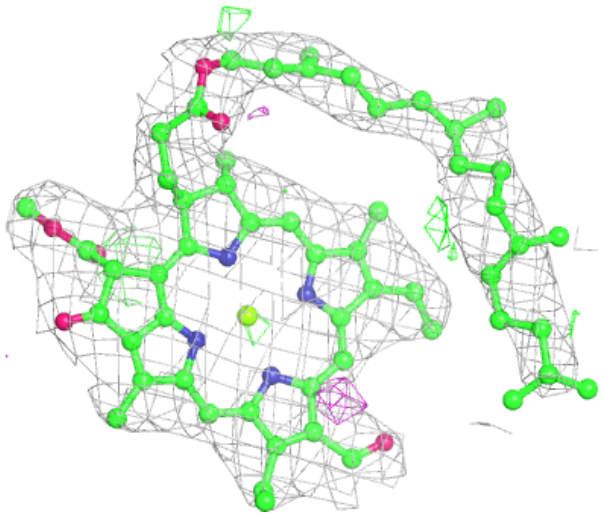
Electron density around CLA C 603:

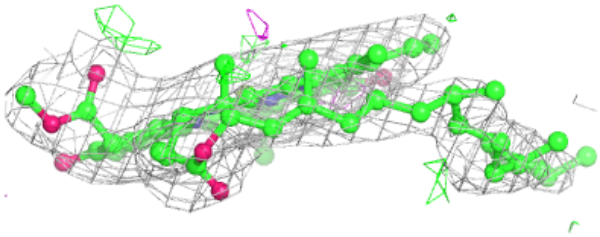
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

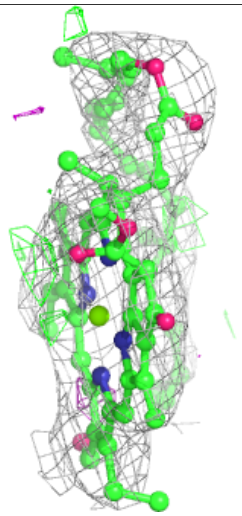


Electron density around CHL B 610:

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

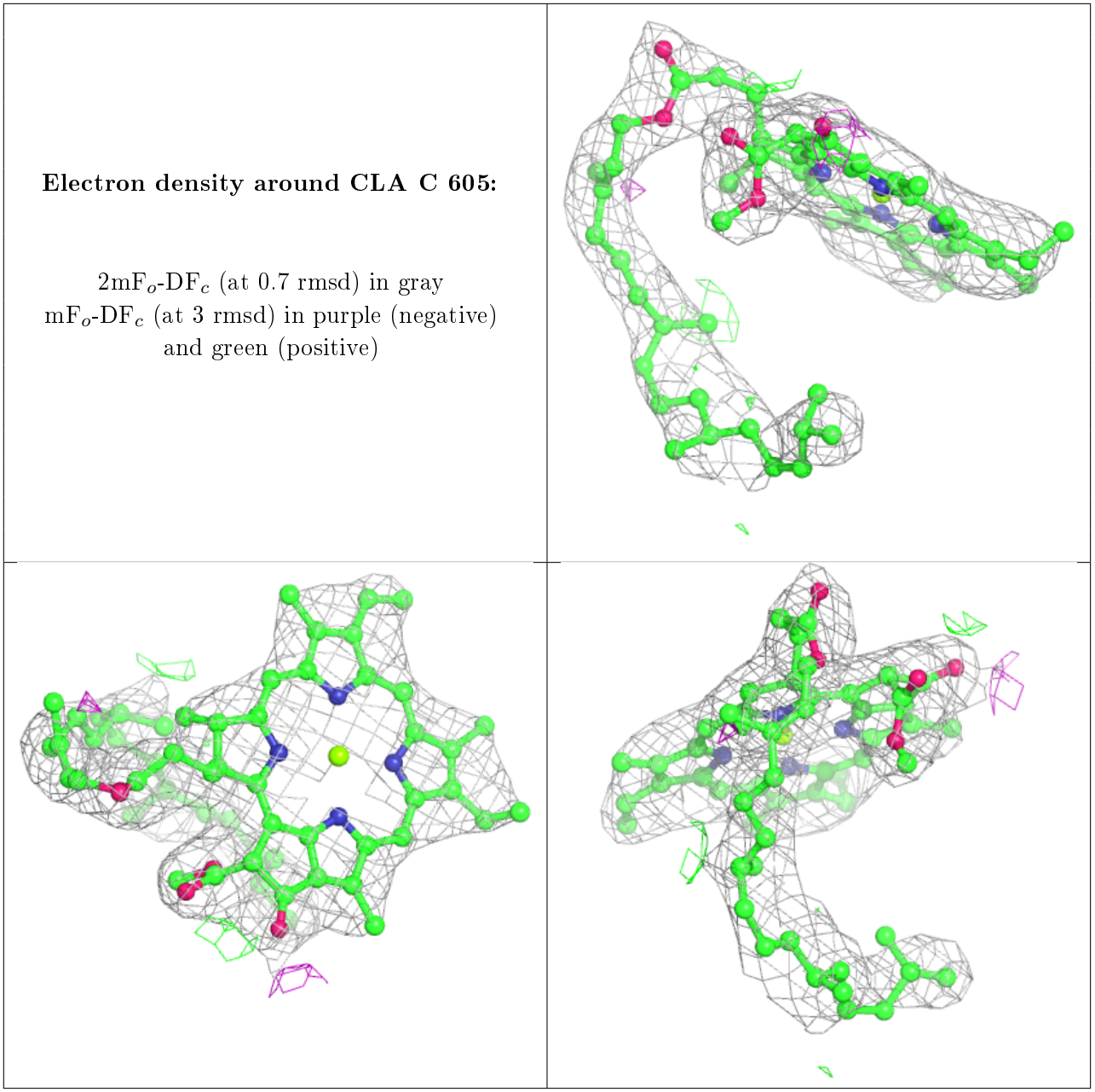






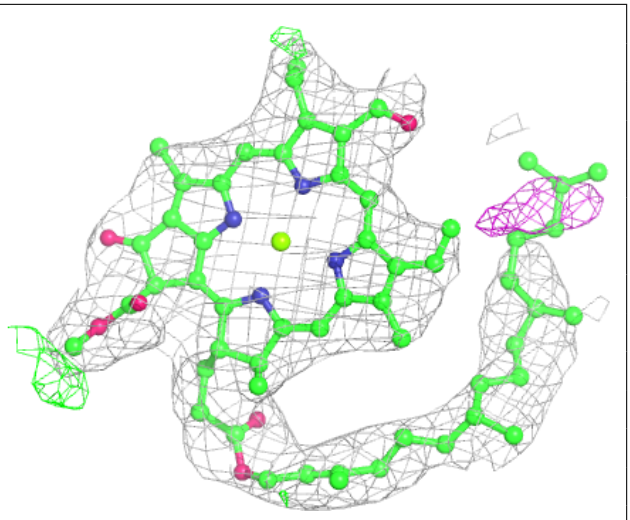
Electron density around CLA C 605:

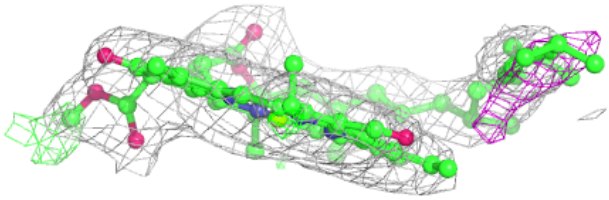
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

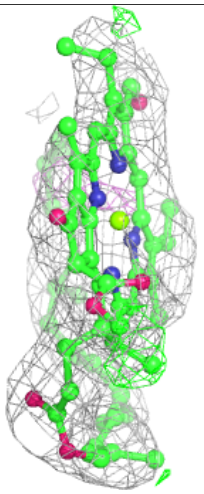


Electron density around CHL A 610:

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

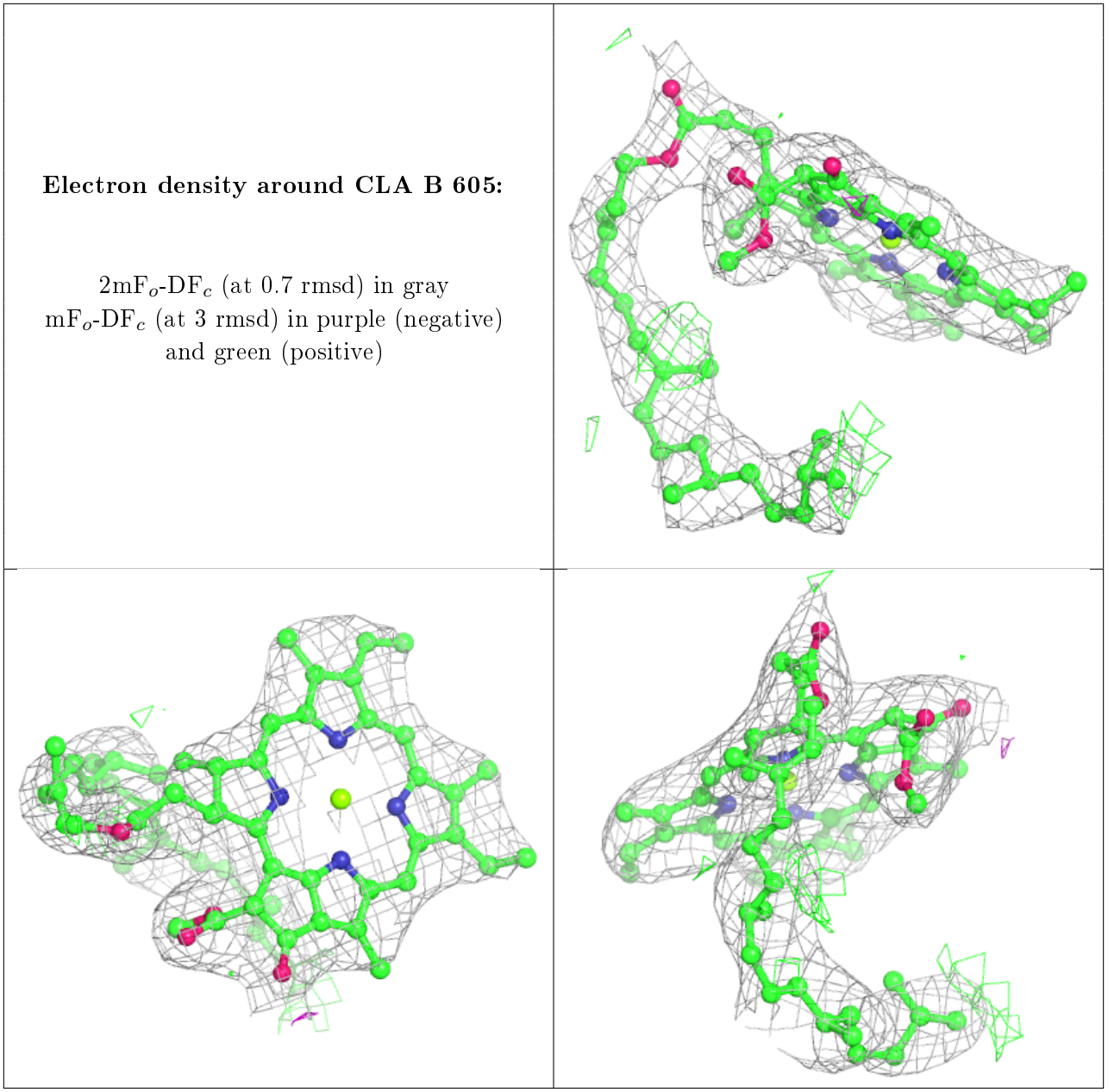






Electron density around CLA B 605:

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



6.5 Other polymers

There are no such residues in this entry.