



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:05 AM EDT

PDB ID : 4FE1 / pdb_00004fe1
Title : Improving the Accuracy of Macromolecular Structure Refinement at 7 Å Resolution
Authors : Fromme, R.; Adams, P.D.; Fromme, P.; Levitt, M.; Schroeder, G.F.; Brunger, A.T.
Deposited on : 2012-05-29
Resolution : 4.92 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

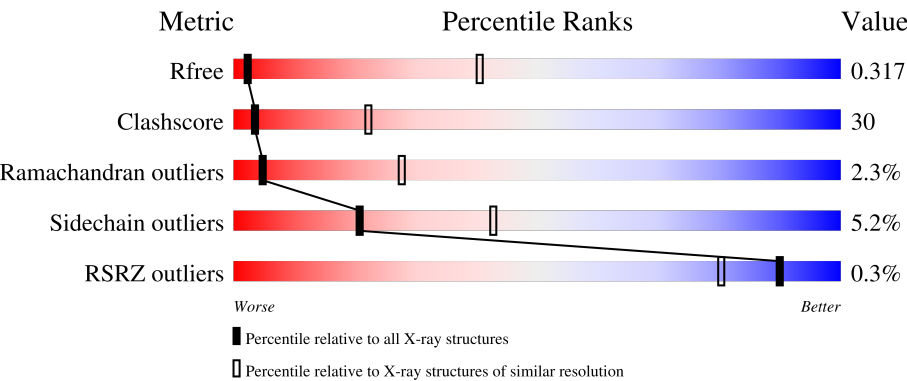
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.92 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1008 (5.88-3.96)
Clashscore	190562	1020 (5.82-3.98)
Ramachandran outliers	187476	1125 (5.94-3.90)
Sidechain outliers	187428	1105 (5.94-3.90)
RSRZ outliers	180081	1003 (5.88-3.96)

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

Mol	Chain	Length	Quality of chain
1	A	755	56% 37% •••
2	B	740	59% 36% •
3	C	80	71% 24% 5%
4	D	138	67% 28% 6%

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Mol	Chain	Length	Quality of chain
5	E	75	
6	F	164	
7	I	38	
8	J	41	
9	K	83	
10	L	154	
11	M	31	
12	X	35	

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
13	CLA	A	803	-	-	X	-
13	CLA	B	830	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 23997 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			539	342	93	104			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	46	Total	C	N	O	0	0	0
			222	130	46	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			

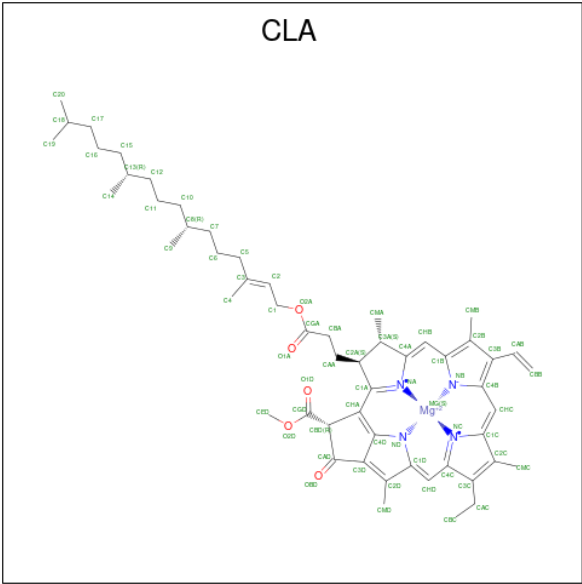
- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X	29	Total	C	N	O	0	0	0
			233	164	34	35			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	32	ALA	-	expression tag	UNP Q8DKP6
X	33	ALA	-	expression tag	UNP Q8DKP6
X	34	ALA	-	expression tag	UNP Q8DKP6
X	35	ALA	-	expression tag	UNP Q8DKP6

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
13	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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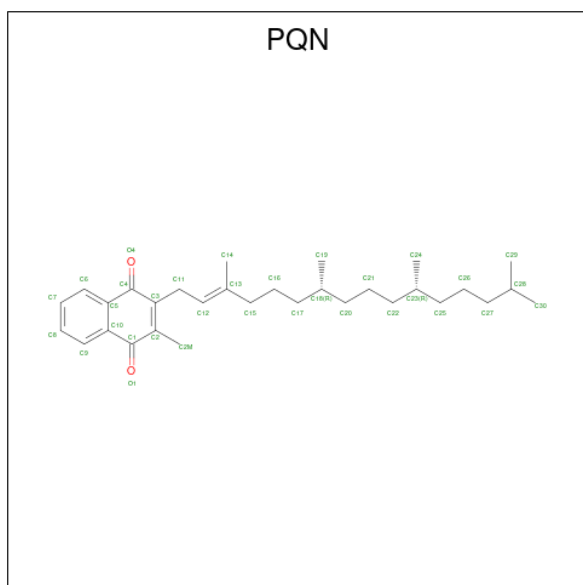
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	M	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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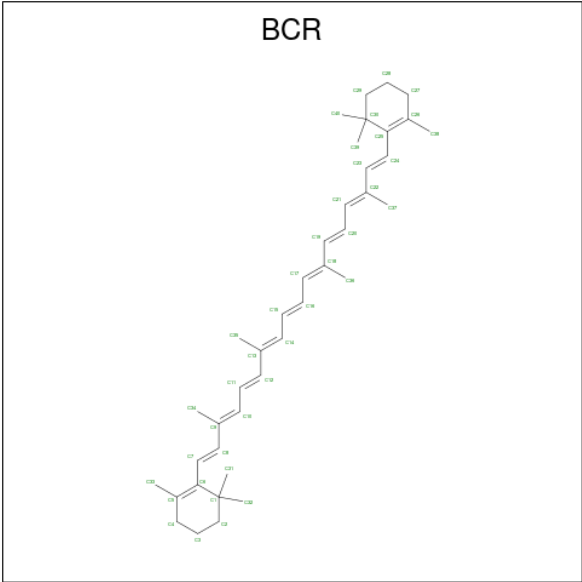
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



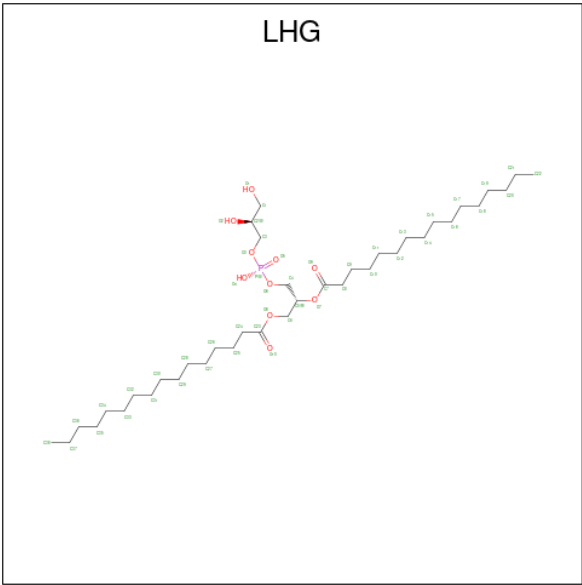
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 25 25	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0

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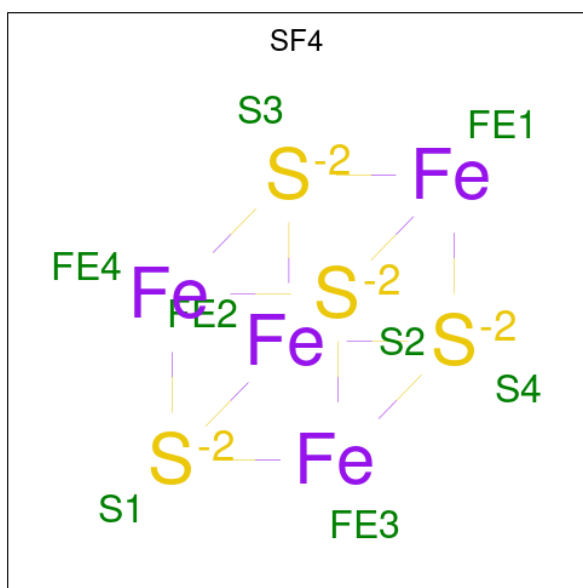
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C 40 40	0	0
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	M	1	Total C 40 40	0	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



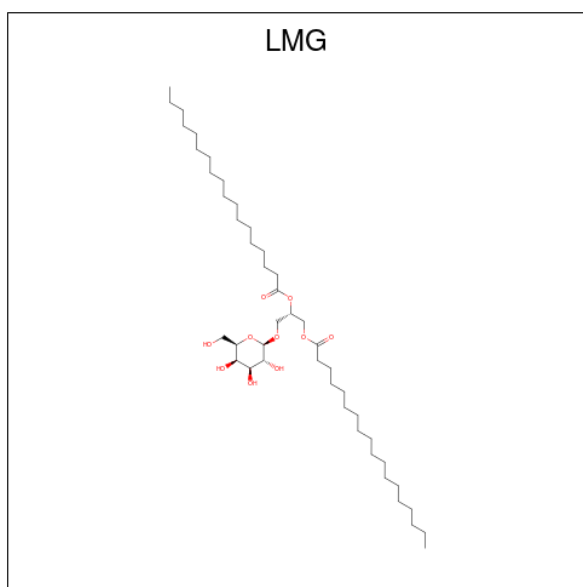
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C O P 49 38 10 1	0	0
16	A	1	Total C O P 27 16 10 1	0	0
16	X	1	Total C O P 23 12 10 1	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	B	1	Total	C	O	0	0
			55	45	10		

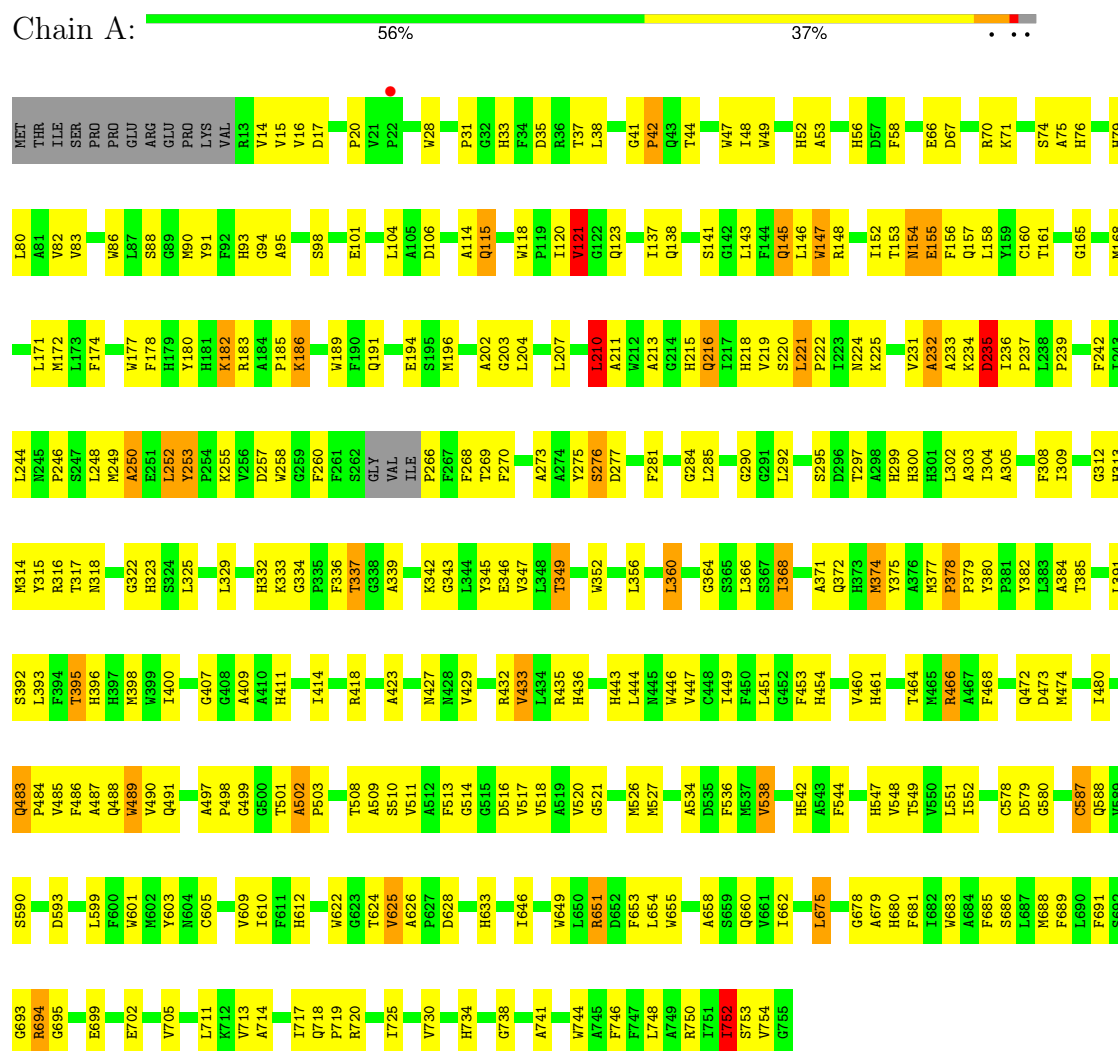
- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	1	Total	Ca	0	0
			1	1		

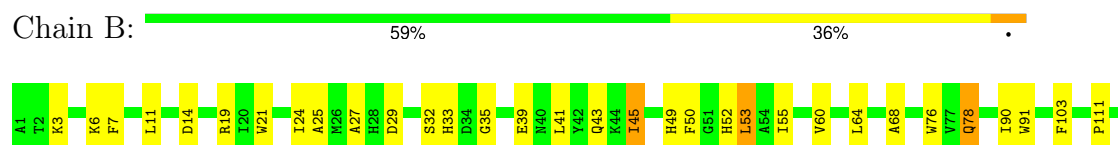
3 Residue-property plots

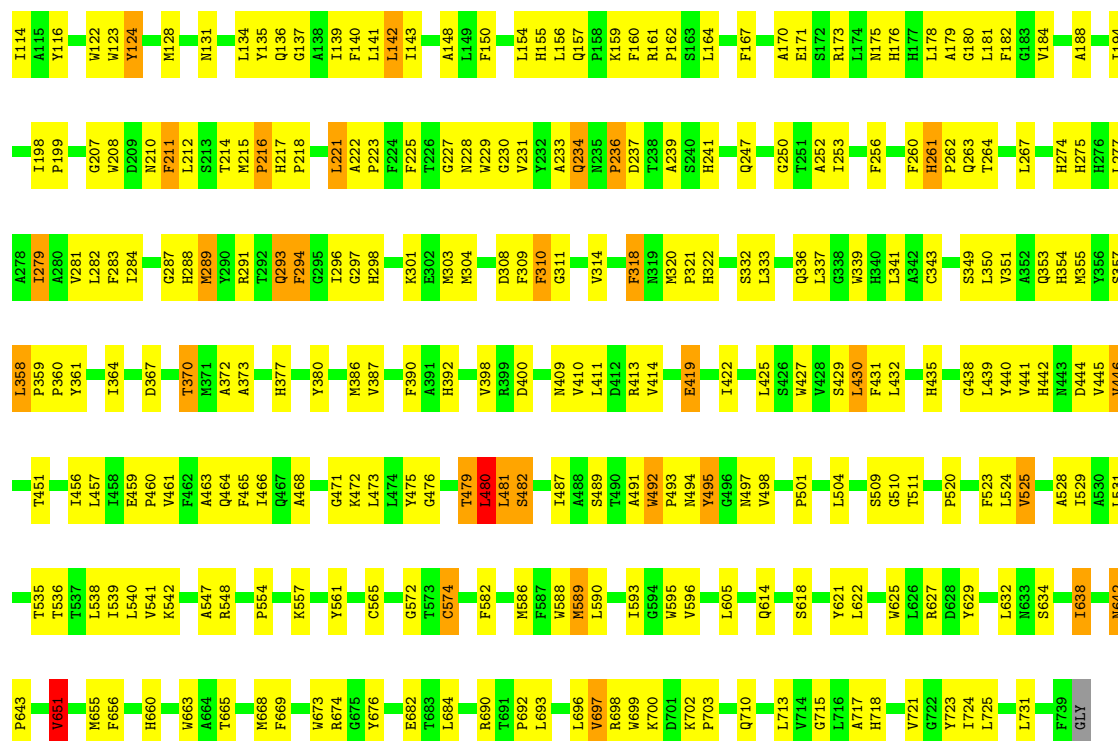
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





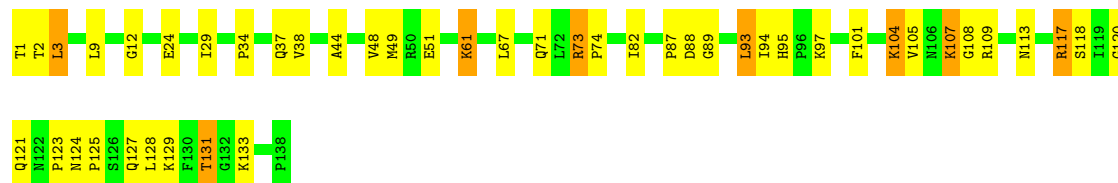
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 71% 24% 5%



• Molecule 4: Photosystem I reaction center subunit II

Chain D: 67% 28% 6%



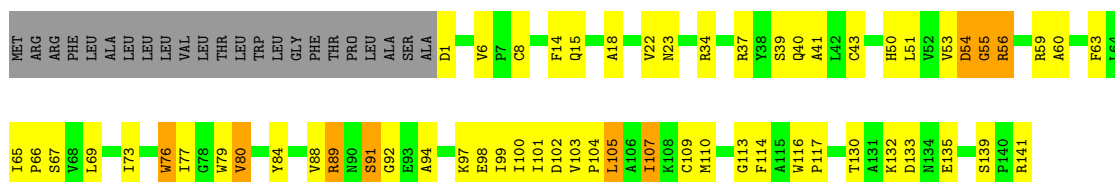
• Molecule 5: Photosystem I reaction center subunit IV

Chain E: 55% 33% 8%



• Molecule 6: Photosystem I reaction center subunit III

Chain F: 49% 31% 5% 14%



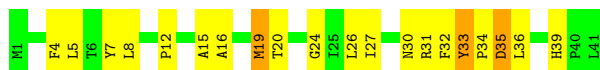
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 50% 42% 8%



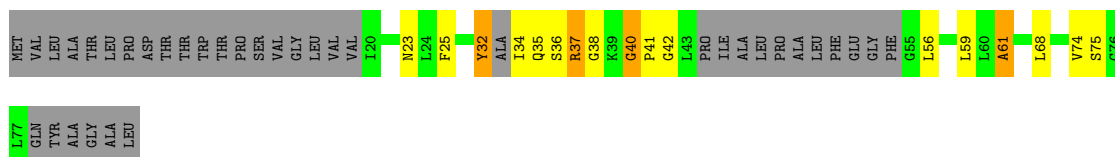
• Molecule 8: Photosystem I reaction center subunit IX

Chain J: 51% 41% 7%



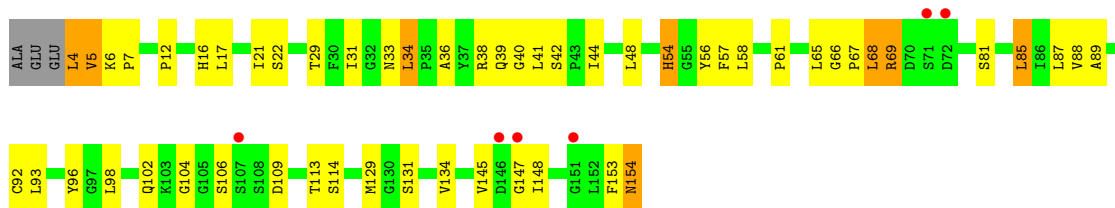
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K: 35% 16% 5% 45%



• Molecule 10: Photosystem I reaction center subunit XI

Chain L: 4% 63% 30% 5%



• Molecule 11: Photosystem I reaction center subunit XII

Chain M: 55% 39% 6%



• Molecule 12: Photosystem I 4.8K protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.97 – 4.92 97.97 – 4.92	Depositor EDS
% Data completeness (in resolution range)	96.4 (97.97-4.92) 96.3 (97.97-4.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.35 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1058)	Depositor
R, R_{free}	0.274 , 0.315 0.276 , 0.317	Depositor DCC
R_{free} test set	1534 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 259.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.175 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LHG, CA, LMG, SF4, PQN, BCR

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	0.51	0/5983	1.11	34/8158 (0.4%)
2	B	0.52	0/6096	1.08	31/8332 (0.4%)
3	C	0.50	0/608	1.25	7/824 (0.8%)
4	D	0.47	0/1101	1.06	3/1492 (0.2%)
5	E	0.52	0/551	1.16	2/750 (0.3%)
6	F	0.59	0/1087	1.15	6/1476 (0.4%)
7	I	0.51	0/312	1.10	2/425 (0.5%)
8	J	0.52	0/350	1.26	6/477 (1.3%)
9	K	0.61	0/220	1.71	10/300 (3.3%)
10	L	0.50	0/1148	1.16	12/1558 (0.8%)
11	M	0.73	0/244	1.37	2/332 (0.6%)
12	X	0.50	0/242	1.02	1/332 (0.3%)
All	All	0.52	0/17942	1.12	116/24456 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
4	D	0	1
All	All	0	3

There are no bond length outliers.

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	PRO	CA-C-N	11.32	131.07	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	PRO	C-N-CA	11.32	131.07	119.64
2	B	217	HIS	CA-C-N	11.03	133.62	119.84
2	B	217	HIS	C-N-CA	11.03	133.62	119.84
1	A	580	GLY	CA-C-N	10.30	129.91	119.82
1	A	580	GLY	C-N-CA	10.30	129.91	119.82
1	A	502	ALA	CA-C-N	9.91	129.55	119.24
1	A	502	ALA	C-N-CA	9.91	129.55	119.24
3	C	63	SER	N-CA-C	-9.18	102.21	113.50
6	F	54	ASP	N-CA-C	9.13	123.38	110.68
2	B	294	PHE	N-CA-C	-8.29	104.03	114.56
8	J	39	HIS	CA-C-N	8.02	129.87	119.84
8	J	39	HIS	C-N-CA	8.02	129.87	119.84
1	A	483	GLN	CA-C-N	7.56	129.29	119.84
1	A	483	GLN	C-N-CA	7.56	129.29	119.84
2	B	482	SER	N-CA-C	-7.45	104.21	113.38
2	B	651	VAL	CB-CA-C	-7.44	102.50	111.81
4	D	89	GLY	N-CA-C	-7.43	105.00	114.37
2	B	216	PRO	N-CA-C	-7.41	104.60	113.86
11	M	15	ALA	CA-C-N	7.28	129.91	120.44
11	M	15	ALA	C-N-CA	7.28	129.91	120.44
2	B	674	ARG	N-CA-C	7.28	123.31	111.37
1	A	651	ARG	N-CA-C	7.24	120.58	111.24
1	A	694	ARG	N-CA-C	7.22	120.02	111.71
1	A	41	GLY	CA-C-N	7.18	128.81	119.84
1	A	41	GLY	C-N-CA	7.18	128.81	119.84
9	K	40	GLY	CA-C-N	7.08	128.69	119.84
9	K	40	GLY	C-N-CA	7.08	128.69	119.84
9	K	34	ILE	CA-C-N	7.05	132.73	122.16
9	K	34	ILE	C-N-CA	7.05	132.73	122.16
1	A	284	GLY	N-CA-C	-7.00	102.84	111.45
2	B	358	LEU	CA-C-N	6.90	127.48	120.38
2	B	358	LEU	C-N-CA	6.90	127.48	120.38
10	L	66	GLY	CA-C-N	6.88	126.58	119.56
10	L	66	GLY	C-N-CA	6.88	126.58	119.56
1	A	521	GLY	N-CA-C	-6.84	99.29	112.02
9	K	25	PHE	N-CA-C	6.74	120.76	112.54
9	K	68	LEU	N-CA-C	-6.73	103.87	111.07
10	L	109	ASP	CA-C-N	6.53	126.22	119.56
10	L	109	ASP	C-N-CA	6.53	126.22	119.56
8	J	33	TYR	CA-C-N	6.52	127.41	120.11
8	J	33	TYR	C-N-CA	6.52	127.41	120.11
2	B	528	ALA	N-CA-C	-6.45	104.33	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	57	CYS	CA-C-N	6.43	127.88	119.84
3	C	57	CYS	C-N-CA	6.43	127.88	119.84
1	A	485	VAL	N-CA-C	6.42	117.94	110.62
3	C	51	LYS	N-CA-C	6.36	120.99	113.23
3	C	33	CYS	N-CA-C	6.32	118.68	109.07
2	B	215	MET	CA-C-N	6.29	125.92	119.56
2	B	215	MET	C-N-CA	6.29	125.92	119.56
6	F	107	ILE	N-CA-C	6.29	117.04	110.62
2	B	124	TYR	N-CA-C	-6.24	104.17	110.97
1	A	210	LEU	N-CA-C	-6.20	104.44	111.07
9	K	61	ALA	N-CA-C	-6.19	105.71	113.20
10	L	39	GLN	N-CA-C	6.11	119.20	110.10
1	A	106	ASP	CA-C-N	6.10	125.82	119.05
1	A	106	ASP	C-N-CA	6.10	125.82	119.05
9	K	32	TYR	CA-C-N	6.07	132.62	121.70
9	K	32	TYR	C-N-CA	6.07	132.62	121.70
10	L	5	VAL	N-CA-C	-6.01	101.78	109.30
1	A	516	ASP	N-CA-C	5.97	120.00	109.96
2	B	410	VAL	N-CA-C	5.96	117.41	110.62
1	A	253	TYR	CA-C-N	5.95	125.50	119.19
1	A	253	TYR	C-N-CA	5.95	125.50	119.19
6	F	133	ASP	N-CA-C	5.95	117.44	111.07
1	A	218	HIS	N-CA-C	5.92	120.58	113.23
2	B	170	ALA	N-CA-C	5.88	117.38	110.97
1	A	236	ILE	CA-C-N	5.84	126.18	119.93
1	A	236	ILE	C-N-CA	5.84	126.18	119.93
2	B	461	VAL	N-CA-C	5.84	116.57	110.62
2	B	33	HIS	N-CA-C	5.83	119.41	110.20
2	B	261	HIS	N-CA-C	-5.79	101.14	109.48
2	B	45	ILE	CB-CA-C	-5.72	104.66	111.81
1	A	154	ASN	N-CA-C	5.71	117.75	109.07
2	B	561	TYR	N-CA-C	5.69	117.16	111.07
6	F	76	TRP	N-CA-C	-5.69	104.77	110.97
2	B	289	MET	N-CA-C	5.69	120.23	113.12
2	B	525	VAL	CB-CA-C	-5.66	104.50	112.14
8	J	7	TYR	N-CA-C	-5.65	105.04	111.14
10	L	54	HIS	N-CA-C	5.64	118.63	111.69
2	B	642	ASN	CA-C-N	-5.62	114.31	119.82
2	B	642	ASN	C-N-CA	-5.62	114.31	119.82
3	C	79	ALA	N-CA-C	-5.62	106.32	112.72
1	A	213	ALA	N-CA-C	-5.61	105.25	111.71
4	D	3	LEU	N-CA-C	5.61	122.75	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	42	SER	CA-C-N	5.57	125.93	119.47
10	L	42	SER	C-N-CA	5.57	125.93	119.47
4	D	131	THR	N-CA-C	-5.54	100.67	109.59
3	C	56	ALA	N-CA-C	5.43	119.62	112.89
2	B	135	TYR	N-CA-C	5.42	117.19	111.28
10	L	113	THR	N-CA-C	-5.37	101.13	109.24
10	L	147	GLY	N-CA-C	5.36	119.16	112.73
5	E	3	ARG	CA-C-N	-5.34	115.06	122.86
5	E	3	ARG	C-N-CA	-5.34	115.06	122.86
7	I	14	PHE	N-CA-C	5.33	117.84	111.71
6	F	54	ASP	CB-CA-C	-5.32	104.38	111.88
8	J	35	ASP	N-CA-C	5.31	118.76	111.54
1	A	752	ILE	N-CA-C	-5.31	104.45	111.09
9	K	23	ASN	N-CA-C	-5.28	105.52	111.28
2	B	370	THR	OG1-CB-CG2	-5.22	98.86	109.30
12	X	28	ALA	N-CA-C	-5.22	105.28	110.97
1	A	337	THR	N-CA-C	5.20	119.12	112.26
2	B	78	GLN	CA-CB-CG	5.19	124.48	114.10
1	A	418	ARG	N-CA-C	5.17	119.64	112.45
1	A	316	ARG	CA-C-N	-5.16	115.39	121.90
1	A	316	ARG	C-N-CA	-5.16	115.39	121.90
10	L	154	ASN	N-CA-CB	-5.16	101.74	110.50
1	A	514	GLY	N-CA-C	-5.14	104.85	110.96
2	B	32	SER	N-CA-C	5.14	119.18	113.02
1	A	374	MET	N-CA-C	5.13	117.77	111.82
1	A	489	TRP	N-CA-C	5.13	116.56	111.07
2	B	460	PRO	N-CA-C	-5.13	105.56	112.48
2	B	495	TYR	N-CA-C	-5.07	104.90	111.74
2	B	293	GLN	N-CA-C	5.06	116.93	110.61
7	I	26	VAL	CG1-CB-CG2	5.04	121.90	110.80
6	F	23	ASN	N-CA-C	5.03	116.95	109.25

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	THR	Mainchain
2	B	35	GLY	Mainchain
4	D	88	ASP	Mainchain

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	5784	0	5639	340	0
2	B	5879	0	5632	344	0
3	C	598	0	580	16	0
4	D	1075	0	1077	31	0
5	E	539	0	528	14	0
6	F	1065	0	1077	53	0
7	I	301	0	306	24	0
8	J	338	0	347	24	0
9	K	222	0	111	9	0
10	L	1119	0	1125	49	1
11	M	241	0	264	23	0
12	X	233	0	231	11	0
13	A	2667	0	2635	435	0
13	B	2230	0	2182	406	0
13	F	45	0	33	4	0
13	I	65	0	72	15	0
13	J	147	0	129	15	0
13	L	195	0	216	26	0
13	M	99	0	81	16	0
13	X	45	0	33	4	0
14	A	33	0	46	7	0
14	B	33	0	46	6	0
15	A	240	0	336	38	0
15	B	345	0	481	82	0
15	F	40	0	56	12	0
15	I	40	0	56	9	0
15	J	80	0	112	9	0
15	L	80	0	112	16	0
15	M	40	0	56	11	0
16	A	76	0	98	11	0
16	X	23	0	16	1	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
18	B	55	0	86	18	0
19	L	1	0	0	0	0
All	All	23997	0	23799	1418	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (1418) 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)
13:B:806:CLA:H12	7:I:18:VAL:HG21	1.35	1.08
13:A:803:CLA:H151	13:A:842:CLA:HAB	1.36	1.08
13:B:831:CLA:HED1	8:J:36:LEU:H	1.06	1.07
13:B:817:CLA:HBD	13:B:821:CLA:HED2	1.37	1.06
13:A:828:CLA:H51	15:A:852:BCR:H312	1.33	1.05
15:A:852:BCR:H362	13:B:802:CLA:H42	1.37	1.05
14:A:846:PQN:H172	15:B:846:BCR:H382	1.40	1.01
2:B:425:LEU:HG	13:B:837:CLA:HBB1	1.44	0.99
1:A:487:ALA:HB2	13:A:838:CLA:HED3	1.43	0.99
13:B:807:CLA:H2	13:B:807:CLA:H13	1.46	0.97
10:L:153:PHE:O	10:L:154:ASN:HB2	1.65	0.96
13:B:806:CLA:H2	15:I:102:BCR:HC42	1.48	0.93
13:B:831:CLA:HED1	8:J:36:LEU:N	1.83	0.93
1:A:356:LEU:HD11	13:A:830:CLA:HBB1	1.49	0.93
8:J:31:ARG:HD3	15:J:1105:BCR:H312	1.47	0.93
2:B:318:PHE:HB2	13:B:821:CLA:HMA3	1.50	0.93
15:L:1005:BCR:H403	15:L:1005:BCR:H23C	1.51	0.93
13:A:818:CLA:O1D	13:A:818:CLA:HAA2	1.67	0.92
1:A:318:ASN:H	13:A:820:CLA:HED1	1.33	0.92
13:A:821:CLA:H2	13:A:825:CLA:HBB1	1.49	0.92
9:K:32:TYR:HA	9:K:35:GLN:H	1.35	0.91
2:B:60:VAL:HG21	13:B:826:CLA:H43	1.53	0.91
1:A:52:HIS:HB2	16:A:853:LHG:H112	1.52	0.90
13:F:1301:CLA:O1D	13:F:1301:CLA:HAA2	1.71	0.90
10:L:61:PRO:HB3	13:L:1004:CLA:HBB1	1.54	0.89
13:B:805:CLA:H71	13:B:827:CLA:H92	1.56	0.88
13:A:803:CLA:H18	13:A:842:CLA:H52	1.54	0.88
13:A:833:CLA:HMA3	15:I:102:BCR:H292	1.55	0.87
13:B:829:CLA:HAA2	13:B:829:CLA:CGD	2.04	0.87
13:A:832:CLA:H12	2:B:692:PRO:HG2	1.58	0.86
2:B:529:ILE:HG21	13:B:835:CLA:HAB	1.59	0.85
1:A:333:LYS:H	13:A:845:CLA:HBC2	1.39	0.85
2:B:136:GLN:NE2	13:B:812:CLA:O1D	2.09	0.85
10:L:33:ASN:HB3	13:L:1002:CLA:HAC1	1.57	0.85
1:A:508:THR:HG22	1:A:510:SER:H	1.41	0.85
13:L:1003:CLA:O1D	13:L:1003:CLA:HAA2	1.76	0.84
13:A:840:CLA:H11	13:B:830:CLA:HED3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:HIS:HB3	13:A:813:CLA:HED3	1.60	0.83
4:D:117:ARG:HG3	4:D:121:GLN:HB2	1.60	0.83
13:A:842:CLA:H72	13:J:1101:CLA:H12	1.60	0.83
13:L:1002:CLA:CGD	13:L:1002:CLA:HAA2	2.08	0.83
13:A:804:CLA:HAA2	13:A:804:CLA:O1D	1.80	0.82
13:I:101:CLA:HAA2	13:I:101:CLA:CGD	2.09	0.82
13:A:803:CLA:HED1	2:B:429:SER:HB2	1.61	0.82
8:J:12:PRO:HB2	15:J:1105:BCR:H391	1.59	0.82
1:A:118:TRP:CE3	13:A:809:CLA:H2A	2.15	0.82
13:B:804:CLA:HED2	13:B:804:CLA:H2	1.59	0.82
2:B:337:LEU:HD11	13:B:827:CLA:HBB1	1.62	0.82
13:B:806:CLA:HED3	7:I:11:PRO:HB3	1.59	0.81
13:A:832:CLA:O1D	13:A:832:CLA:HAA2	1.79	0.81
10:L:98:LEU:O	10:L:102:GLN:NE2	2.13	0.81
13:B:821:CLA:HAA2	13:B:821:CLA:CGD	2.10	0.81
13:B:831:CLA:H122	6:F:69:LEU:HD11	1.62	0.81
1:A:202:ALA:HB2	1:A:312:GLY:HA3	1.62	0.80
13:A:814:CLA:HAA2	13:A:814:CLA:CGD	2.10	0.80
1:A:308:PHE:HE2	13:A:821:CLA:HAB	1.47	0.80
13:B:807:CLA:H162	13:B:825:CLA:H203	1.64	0.80
2:B:353:GLN:HG3	13:B:823:CLA:HED3	1.64	0.80
1:A:141:SER:OG	13:A:808:CLA:HED3	1.82	0.79
13:L:1003:CLA:HAA2	13:L:1003:CLA:CGD	2.12	0.79
2:B:181:LEU:HD11	13:B:811:CLA:H12	1.64	0.78
13:B:803:CLA:HAA2	13:B:803:CLA:CGD	2.13	0.78
1:A:35:ASP:OD2	1:A:37:THR:OG1	2.02	0.78
1:A:444:LEU:HB2	13:A:839:CLA:HBB1	1.65	0.78
2:B:181:LEU:HG	13:B:811:CLA:H43	1.63	0.78
13:B:824:CLA:HAA2	13:B:824:CLA:CGD	2.13	0.78
13:A:805:CLA:HED3	13:A:825:CLA:H12	1.65	0.78
13:A:817:CLA:CGD	13:A:817:CLA:HAA2	2.13	0.78
13:B:814:CLA:HAA2	13:B:814:CLA:CGD	2.13	0.78
13:B:830:CLA:H152	15:F:1302:BCR:H353	1.65	0.78
13:A:806:CLA:H42	13:A:830:CLA:H52	1.65	0.78
13:A:813:CLA:HBD	13:A:825:CLA:C6	2.13	0.77
13:A:815:CLA:CGD	13:A:815:CLA:HAA2	2.14	0.77
13:A:819:CLA:HAB	13:A:819:CLA:H8	1.65	0.77
13:A:837:CLA:HAA2	13:A:837:CLA:O2D	1.85	0.77
13:B:809:CLA:CGD	13:B:809:CLA:HAA2	2.14	0.77
13:B:817:CLA:CBP	13:B:821:CLA:HED2	2.12	0.77
15:L:1006:BCR:HC8	15:L:1006:BCR:H331	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TRP:CZ3	13:A:809:CLA:H2A	2.20	0.77
13:A:813:CLA:HBD	13:A:825:CLA:H61	1.64	0.77
13:B:801:CLA:HAA2	13:B:801:CLA:CGD	2.14	0.77
1:A:549:THR:HG21	13:A:826:CLA:HAC2	1.65	0.77
1:A:675:LEU:HD11	13:A:828:CLA:H143	1.65	0.76
15:A:852:BCR:H362	13:B:802:CLA:C4	2.15	0.76
13:A:829:CLA:HAA2	13:A:829:CLA:CGD	2.15	0.76
2:B:173:ARG:HB3	13:B:822:CLA:HMD1	1.67	0.76
6:F:88:VAL:HG12	6:F:94:ALA:HA	1.68	0.76
13:B:805:CLA:H151	13:B:826:CLA:HBB2	1.67	0.76
13:A:832:CLA:H72	13:L:1003:CLA:H61	1.68	0.76
13:L:1004:CLA:HED3	13:L:1004:CLA:H62	1.68	0.76
1:A:90:MET:HE2	13:A:808:CLA:HED2	1.68	0.76
13:A:826:CLA:O1D	13:A:826:CLA:HAA2	1.86	0.76
13:B:808:CLA:CMA	13:I:101:CLA:HAB	2.16	0.76
13:B:823:CLA:HBA1	13:B:824:CLA:HED3	1.68	0.75
13:B:826:CLA:O2D	13:B:826:CLA:HAA2	1.87	0.75
13:A:827:CLA:HAA2	13:A:827:CLA:CGD	2.15	0.75
2:B:343:CYS:HB3	13:B:822:CLA:H42	1.68	0.75
13:B:811:CLA:H202	13:B:826:CLA:HBD	1.68	0.75
2:B:122:TRP:HH2	15:B:843:BCR:H391	1.51	0.75
13:A:841:CLA:HAA2	13:A:841:CLA:CGD	2.16	0.74
13:B:835:CLA:CGD	13:B:835:CLA:HAA2	2.16	0.74
13:A:813:CLA:H121	15:A:849:BCR:H353	1.68	0.74
11:M:29:LEU:HD13	13:M:1201:CLA:HMA2	1.68	0.74
1:A:118:TRP:CZ2	13:A:807:CLA:HED3	2.23	0.74
1:A:501:THR:O	13:A:836:CLA:ND	2.20	0.74
2:B:64:LEU:HD11	15:B:843:BCR:H271	1.67	0.74
1:A:366:LEU:HD11	13:A:819:CLA:H72	1.70	0.74
2:B:321:PRO:HB2	2:B:409:ASN:HA	1.68	0.74
4:D:123:PRO:HB2	4:D:128:LEU:HD11	1.69	0.74
13:J:1101:CLA:HAA2	13:J:1101:CLA:CGD	2.16	0.74
1:A:56:HIS:CE1	13:A:806:CLA:HED1	2.23	0.74
13:B:832:CLA:HAA2	13:B:832:CLA:CGD	2.17	0.74
13:B:835:CLA:HAA2	13:B:835:CLA:O1D	1.87	0.74
13:L:1002:CLA:H202	13:L:1002:CLA:H2	1.69	0.73
2:B:221:LEU:HD22	13:B:813:CLA:HBD	1.69	0.73
2:B:439:LEU:HD11	15:B:850:BCR:H342	1.70	0.73
2:B:128:MET:HE3	2:B:134:LEU:HD23	1.70	0.73
13:A:830:CLA:HAA2	13:A:830:CLA:CGD	2.19	0.73
2:B:49:HIS:HB3	13:B:811:CLA:HED1	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:GLY:O	13:B:814:CLA:H43	1.88	0.73
13:A:855:CLA:HAA2	13:A:855:CLA:CGD	2.18	0.73
2:B:281:VAL:HG22	15:B:841:BCR:H352	1.70	0.73
2:B:414:VAL:HG11	15:B:844:BCR:H401	1.69	0.73
13:A:824:CLA:CGD	13:A:824:CLA:HAA2	2.19	0.73
15:B:849:BCR:C21	13:L:1003:CLA:HAB	2.19	0.72
2:B:339:TRP:HE1	13:B:822:CLA:HMB3	1.54	0.72
13:B:808:CLA:HMA1	13:I:101:CLA:HAB	1.71	0.72
1:A:503:PRO:HG2	13:A:836:CLA:HMD1	1.71	0.72
1:A:49:TRP:HE3	16:A:853:LHG:H111	1.53	0.72
13:A:805:CLA:HAA2	13:A:805:CLA:CGD	2.19	0.72
13:B:819:CLA:CGD	13:B:819:CLA:HAA2	2.20	0.72
13:A:801:CLA:CHB	13:B:801:CLA:HMB2	2.19	0.72
13:A:842:CLA:HED1	16:A:853:LHG:H102	1.71	0.72
1:A:203:GLY:HA2	13:A:820:CLA:HBC1	1.72	0.72
1:A:453:PHE:O	13:A:834:CLA:HBB2	1.89	0.71
13:A:810:CLA:HAA2	13:A:810:CLA:CGD	2.20	0.71
13:A:816:CLA:CGD	13:A:816:CLA:HAA2	2.20	0.71
13:A:818:CLA:HBD	13:A:827:CLA:HAB	1.72	0.71
13:B:821:CLA:HAA2	13:B:821:CLA:O2D	1.90	0.71
13:B:837:CLA:CGD	13:B:837:CLA:HAA2	2.20	0.71
1:A:255:LYS:HB2	1:A:277:ASP:OD2	1.90	0.71
13:A:831:CLA:HED2	10:L:5:VAL:HG11	1.71	0.71
13:B:823:CLA:HED2	13:B:824:CLA:CAD	2.21	0.71
13:B:839:CLA:CGD	13:B:839:CLA:HAA2	2.20	0.71
13:A:845:CLA:CGD	13:A:845:CLA:HAA2	2.21	0.71
2:B:55:ILE:HD11	15:M:1203:BCR:HC7	1.72	0.71
4:D:29:ILE:HD13	4:D:67:LEU:HD23	1.72	0.71
1:A:90:MET:HE2	13:A:808:CLA:CED	2.21	0.71
2:B:179:ALA:HB2	2:B:287:GLY:HA3	1.71	0.71
2:B:445:VAL:HG21	13:B:831:CLA:HAC2	1.73	0.71
13:A:832:CLA:O1D	10:L:22:SER:HB3	1.91	0.70
13:A:823:CLA:HAA2	13:A:823:CLA:CGD	2.21	0.70
2:B:294:PHE:HB2	13:B:818:CLA:HED3	1.73	0.70
13:B:830:CLA:HHC	13:B:830:CLA:HBB1	1.72	0.70
13:A:822:CLA:HED3	9:K:37:ARG:N	2.07	0.70
13:J:1102:CLA:HAA2	13:J:1102:CLA:CGD	2.21	0.70
2:B:589:MET:HE3	2:B:593:ILE:HG13	1.74	0.70
2:B:622:LEU:HD12	13:B:802:CLA:H11	1.72	0.70
1:A:542:HIS:ND1	13:A:837:CLA:HAB	2.06	0.70
13:B:811:CLA:HAA2	13:B:811:CLA:CGD	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:818:CLA:H41	13:A:835:CLA:HED3	1.72	0.70
13:B:829:CLA:CGA	6:F:130:THR:HG21	2.22	0.70
2:B:318:PHE:HB2	13:B:821:CLA:CMA	2.21	0.69
1:A:204:LEU:HD11	13:A:829:CLA:H141	1.74	0.69
1:A:486:PHE:HB3	13:A:837:CLA:H11	1.75	0.69
13:B:812:CLA:HAA2	13:B:812:CLA:CGD	2.22	0.69
13:B:816:CLA:H62	13:B:816:CLA:HMB3	1.75	0.69
13:A:819:CLA:H3A	13:A:819:CLA:O2A	1.91	0.69
1:A:646:ILE:HG21	13:A:802:CLA:HBA2	1.75	0.69
13:B:817:CLA:HBD	13:B:821:CLA:CED	2.19	0.69
1:A:177:TRP:HB2	13:A:811:CLA:HMC2	1.74	0.69
13:B:838:CLA:HAA2	13:B:838:CLA:CGD	2.23	0.69
1:A:216:GLN:HA	1:A:220:SER:HB3	1.75	0.68
1:A:432:ARG:NH2	13:A:831:CLA:HED3	2.09	0.68
13:B:817:CLA:CGD	13:B:821:CLA:HED2	2.23	0.68
2:B:665:THR:HA	13:B:803:CLA:HAB	1.75	0.68
13:A:822:CLA:HAA2	13:A:822:CLA:CGD	2.23	0.68
13:A:825:CLA:HED2	13:A:829:CLA:H193	1.76	0.68
13:A:802:CLA:H152	15:B:847:BCR:H12C	1.75	0.68
13:B:804:CLA:O1D	13:B:804:CLA:H101	1.94	0.68
13:A:808:CLA:HAB	13:A:828:CLA:H13	1.76	0.67
13:A:803:CLA:HED1	2:B:429:SER:CB	2.25	0.67
2:B:651:VAL:HG11	13:B:807:CLA:HAC1	1.76	0.67
13:A:840:CLA:H162	13:A:841:CLA:HED1	1.76	0.67
2:B:529:ILE:HD13	13:B:835:CLA:HAB	1.77	0.67
2:B:354:HIS:HB3	13:B:815:CLA:HED1	1.77	0.67
2:B:663:TRP:CD2	13:B:801:CLA:HMA2	2.30	0.67
2:B:90:ILE:HB	2:B:111:PRO:HB2	1.75	0.67
2:B:427:TRP:HD1	13:B:830:CLA:HED1	1.58	0.67
10:L:145:VAL:HG11	13:L:1004:CLA:H51	1.75	0.67
13:B:831:CLA:HBA1	8:J:36:LEU:O	1.94	0.67
13:B:837:CLA:HAA2	13:B:837:CLA:O1D	1.95	0.67
2:B:529:ILE:HG21	13:B:835:CLA:CAB	2.25	0.66
2:B:60:VAL:HG21	13:B:826:CLA:C4	2.25	0.66
13:B:830:CLA:CBB	15:B:846:BCR:H323	2.24	0.66
13:A:823:CLA:CMA	13:A:845:CLA:HAC2	2.25	0.66
2:B:339:TRP:HE1	13:B:822:CLA:CMB	2.08	0.66
3:C:6:ILE:HG13	3:C:64:ILE:HD12	1.78	0.66
13:X:102:CLA:HAA2	13:X:102:CLA:CGD	2.26	0.66
1:A:680:HIS:HB3	13:B:802:CLA:O1D	1.95	0.66
13:A:813:CLA:HAA2	13:A:813:CLA:CGD	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:850:BCR:H331	15:B:850:BCR:C8	2.26	0.66
13:A:831:CLA:CGD	13:A:831:CLA:HAA2	2.25	0.66
13:A:808:CLA:HED2	13:A:828:CLA:HED2	1.78	0.66
13:A:826:CLA:H143	15:A:851:BCR:H391	1.78	0.66
13:B:834:CLA:HAA2	13:B:834:CLA:CGD	2.25	0.66
15:A:852:BCR:H321	15:A:852:BCR:HC8	1.76	0.66
11:M:26:SER:HB2	13:M:1201:CLA:H2	1.77	0.66
13:A:823:CLA:HMA3	13:A:845:CLA:HAC2	1.77	0.65
2:B:52:HIS:CD2	13:B:804:CLA:HMA3	2.31	0.65
8:J:26:LEU:HD23	15:J:1104:BCR:HC7	1.77	0.65
13:A:832:CLA:HBC2	13:A:839:CLA:HMC3	1.78	0.65
1:A:489:TRP:HZ3	13:A:837:CLA:H42	1.61	0.65
13:A:803:CLA:HAA2	13:A:803:CLA:CGD	2.26	0.65
10:L:34:LEU:HD12	13:L:1003:CLA:HED3	1.79	0.65
1:A:453:PHE:C	13:A:834:CLA:HBB2	2.21	0.65
2:B:548:ARG:NH2	4:D:124:ASN:OD1	2.30	0.65
13:B:804:CLA:HAA2	13:B:804:CLA:CGD	2.26	0.65
13:B:829:CLA:HAB	13:B:830:CLA:H171	1.79	0.64
13:A:806:CLA:CGD	13:A:806:CLA:HAA2	2.27	0.64
13:B:812:CLA:HAB	13:B:826:CLA:H161	1.79	0.64
1:A:449:ILE:HD13	13:B:803:CLA:HBA2	1.78	0.64
13:A:809:CLA:HMC2	2:B:445:VAL:HG13	1.80	0.64
13:A:821:CLA:HBC3	13:A:827:CLA:H18	1.78	0.64
1:A:372:GLN:HG3	13:A:826:CLA:HED1	1.80	0.64
1:A:542:HIS:CG	13:A:837:CLA:HAB	2.31	0.64
1:A:683:TRP:CD2	13:A:801:CLA:HMA2	2.33	0.64
1:A:685:PHE:HA	13:A:803:CLA:HAB	1.79	0.64
2:B:309:PHE:CE1	13:B:820:CLA:H2	2.33	0.64
2:B:90:ILE:HD13	13:B:808:CLA:HMD2	1.79	0.64
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.80	0.64
13:A:825:CLA:HBA1	13:A:829:CLA:H18	1.80	0.64
13:A:831:CLA:HBB2	13:A:839:CLA:HMC1	1.79	0.64
1:A:118:TRP:CZ2	13:A:809:CLA:HED2	2.33	0.64
2:B:267:LEU:HD22	13:B:815:CLA:HBA1	1.80	0.64
1:A:83:VAL:HG11	13:A:805:CLA:H71	1.80	0.64
2:B:492:TRP:HZ3	13:B:834:CLA:HMD3	1.62	0.64
2:B:509:SER:O	2:B:511:THR:N	2.27	0.64
13:B:805:CLA:H51	18:B:848:LMG:H331	1.79	0.64
13:B:828:CLA:CGD	13:B:828:CLA:HAA2	2.28	0.64
13:B:831:CLA:HAA2	13:B:831:CLA:O2D	1.97	0.64
13:A:802:CLA:H143	13:I:101:CLA:HBC3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:827:CLA:CGD	13:B:827:CLA:HAA2	2.28	0.63
1:A:378:PRO:HG2	1:A:384:ALA:HB2	1.79	0.63
13:A:812:CLA:HAA2	13:A:812:CLA:CGD	2.27	0.63
13:A:821:CLA:HBD	13:A:824:CLA:CED	2.28	0.63
13:B:807:CLA:H121	13:B:825:CLA:H171	1.81	0.63
6:F:91:SER:OG	6:F:92:GLY:N	2.24	0.63
1:A:120:ILE:HG12	1:A:121:VAL:HG13	1.80	0.63
13:B:808:CLA:O2D	13:B:808:CLA:HAA2	1.99	0.63
1:A:194:GLU:HG2	1:A:315:TYR:HB3	1.81	0.63
1:A:352:TRP:HB3	13:A:805:CLA:HAC1	1.81	0.63
13:A:818:CLA:H52	13:A:835:CLA:HBA1	1.81	0.63
13:B:816:CLA:HAA2	13:B:816:CLA:CGD	2.29	0.63
13:B:818:CLA:CGD	13:B:818:CLA:HAA2	2.29	0.62
1:A:345:TYR:O	1:A:349:THR:HB	1.99	0.62
13:A:837:CLA:HAA1	13:A:838:CLA:HED2	1.81	0.62
2:B:261:HIS:HD2	2:B:263:GLN:H	1.47	0.62
2:B:304:MET:HG3	2:B:322:HIS:O	2.00	0.62
8:J:16:ALA:HA	13:J:1101:CLA:H8	1.80	0.62
2:B:111:PRO:HG2	7:I:1:MET:HE2	1.81	0.62
2:B:466:ILE:HD13	13:B:832:CLA:HHC	1.81	0.62
13:B:806:CLA:H62	15:I:102:BCR:HC41	1.82	0.62
1:A:322:GLY:HA2	13:A:822:CLA:HMD2	1.82	0.62
13:A:801:CLA:HAA2	13:A:801:CLA:O2D	2.00	0.62
13:A:821:CLA:HBD	13:A:824:CLA:HED1	1.81	0.62
2:B:308:ASP:O	13:B:820:CLA:HBA2	1.99	0.62
13:B:838:CLA:H193	15:I:102:BCR:H362	1.81	0.62
1:A:302:LEU:HD11	13:A:817:CLA:HBB1	1.82	0.62
2:B:557:LYS:HD2	4:D:124:ASN:OD1	2.00	0.62
2:B:122:TRP:CH2	15:B:843:BCR:H391	2.35	0.61
2:B:358:LEU:HB2	13:B:815:CLA:HED3	1.82	0.61
13:B:803:CLA:HAA2	13:B:803:CLA:O1D	2.00	0.61
13:A:825:CLA:HAA2	13:A:825:CLA:O1D	1.99	0.61
13:A:843:CLA:CGD	13:A:843:CLA:HAA2	2.30	0.61
13:B:822:CLA:H61	13:B:824:CLA:H42	1.83	0.61
1:A:83:VAL:HG23	13:A:806:CLA:HMC2	1.82	0.61
1:A:487:ALA:HA	13:A:837:CLA:HED2	1.82	0.61
2:B:188:ALA:HA	13:B:813:CLA:CBB	2.30	0.61
14:B:840:PQN:H242	15:B:847:BCR:H17C	1.81	0.61
1:A:153:THR:N	1:A:157:GLN:OE1	2.33	0.61
13:A:804:CLA:HED2	13:A:811:CLA:CGD	2.30	0.61
13:A:801:CLA:HAA2	13:A:801:CLA:CGD	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:PHE:CZ	13:B:811:CLA:H71	2.36	0.61
2:B:725:LEU:HD11	13:B:827:CLA:H203	1.83	0.61
13:B:804:CLA:H8	13:B:822:CLA:HED2	1.81	0.61
1:A:300:HIS:O	1:A:304:ILE:HG12	2.01	0.61
13:A:833:CLA:C1A	15:B:849:BCR:H363	2.31	0.61
13:A:823:CLA:CBB	13:A:845:CLA:HAB	2.31	0.61
2:B:122:TRP:CE3	13:B:826:CLA:HED1	2.36	0.61
13:B:813:CLA:HAA2	13:B:813:CLA:CGD	2.30	0.61
13:B:825:CLA:H3A	13:B:825:CLA:CGA	2.30	0.61
13:A:829:CLA:H61	15:A:849:BCR:H373	1.82	0.61
2:B:53:LEU:HD21	13:B:811:CLA:HBA2	1.82	0.61
13:B:808:CLA:H201	7:I:26:VAL:CG2	2.31	0.61
13:B:831:CLA:HAA2	13:B:831:CLA:CGD	2.31	0.61
13:A:825:CLA:HBB2	15:A:850:BCR:H11C	1.83	0.60
2:B:60:VAL:HG11	15:B:843:BCR:H393	1.83	0.60
3:C:41:SER:OG	4:D:113:ASN:ND2	2.30	0.60
1:A:76:HIS:HB3	13:A:813:CLA:CED	2.31	0.60
2:B:41:LEU:O	2:B:45:ILE:HG12	2.01	0.60
1:A:66:GLU:OE2	1:A:186:LYS:HG3	2.01	0.60
1:A:490:VAL:HB	13:A:837:CLA:HED3	1.82	0.60
2:B:188:ALA:HA	13:B:813:CLA:HBB1	1.82	0.60
9:K:36:SER:O	9:K:38:GLY:N	2.27	0.60
1:A:688:MET:HB2	13:A:803:CLA:C1C	2.31	0.60
13:A:833:CLA:HAA2	13:A:833:CLA:CGD	2.30	0.60
2:B:29:ASP:CG	13:B:827:CLA:HED1	2.26	0.60
1:A:281:PHE:HE2	13:A:818:CLA:H43	1.66	0.60
1:A:681:PHE:CD2	15:A:852:BCR:H363	2.37	0.60
2:B:339:TRP:CH2	15:B:844:BCR:H372	2.36	0.60
13:B:808:CLA:HAA2	13:B:808:CLA:CGD	2.31	0.60
13:B:823:CLA:HBA1	13:B:824:CLA:CED	2.31	0.60
1:A:143:LEU:HD12	13:A:808:CLA:HED1	1.82	0.60
11:M:29:LEU:CB	13:M:1201:CLA:HBA2	2.31	0.60
13:M:1201:CLA:HAA2	13:M:1201:CLA:CGD	2.31	0.60
1:A:118:TRP:HZ3	13:A:809:CLA:HBA1	1.65	0.60
1:A:435:ARG:NH1	4:D:12:GLY:O	2.34	0.60
13:A:835:CLA:CED	13:A:836:CLA:HMA3	2.32	0.60
2:B:261:HIS:CD2	2:B:263:GLN:H	2.20	0.60
13:B:804:CLA:H112	13:B:822:CLA:O1D	2.02	0.60
1:A:427:ASN:OD1	1:A:432:ARG:NH1	2.34	0.60
1:A:694:ARG:HD3	2:B:572:GLY:HA3	1.82	0.60
13:A:840:CLA:HED2	2:B:427:TRP:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ASN:O	2:B:212:LEU:N	2.35	0.60
2:B:459:GLU:OE2	6:F:50:HIS:ND1	2.35	0.60
1:A:250:ALA:HA	1:A:258:TRP:CD1	2.36	0.60
15:A:852:BCR:H393	15:J:1104:BCR:H313	1.83	0.60
15:L:1006:BCR:H331	15:L:1006:BCR:C8	2.25	0.60
1:A:379:PRO:CB	13:A:819:CLA:HBA1	2.31	0.60
2:B:380:TYR:CD1	13:B:825:CLA:HAB	2.37	0.60
1:A:660:GLN:HE22	1:A:750:ARG:HD2	1.67	0.59
13:A:825:CLA:HAA2	13:A:825:CLA:CGD	2.32	0.59
2:B:207:GLY:HA2	13:B:812:CLA:OBD	2.02	0.59
2:B:440:TYR:CZ	2:B:524:LEU:HB3	2.38	0.59
13:B:810:CLA:HBC3	13:B:811:CLA:CAB	2.32	0.59
13:B:825:CLA:O1D	13:B:825:CLA:HAA2	2.01	0.59
13:A:836:CLA:CGD	13:A:836:CLA:HAA2	2.33	0.59
13:A:842:CLA:H72	13:J:1101:CLA:C1	2.32	0.59
2:B:480:LEU:C	2:B:482:SER:H	2.11	0.59
11:M:29:LEU:HD13	13:M:1201:CLA:CMA	2.31	0.59
1:A:250:ALA:HA	1:A:258:TRP:HD1	1.65	0.59
13:A:806:CLA:HAA2	13:A:806:CLA:O2D	2.02	0.59
2:B:713:LEU:HD11	18:B:848:LMG:H342	1.82	0.59
15:B:849:BCR:H23C	15:B:849:BCR:H392	1.83	0.59
1:A:14:VAL:HG21	13:A:810:CLA:HBA1	1.84	0.59
13:A:803:CLA:HBB1	13:B:802:CLA:C4B	2.33	0.59
1:A:432:ARG:HH21	13:A:831:CLA:HED3	1.68	0.59
2:B:222:ALA:HB3	2:B:223:PRO:HD3	1.84	0.59
2:B:693:LEU:HD21	10:L:34:LEU:HD23	1.83	0.59
13:L:1004:CLA:HAA2	13:L:1004:CLA:CGD	2.32	0.59
13:A:804:CLA:C3C	13:J:1101:CLA:HAB	2.33	0.59
13:B:817:CLA:O1A	13:B:821:CLA:HBD	2.01	0.59
13:A:836:CLA:HBD	13:A:855:CLA:O1D	2.02	0.59
1:A:392:SER:HB3	13:A:828:CLA:HMA1	1.85	0.59
13:B:826:CLA:H203	15:B:843:BCR:H362	1.85	0.59
15:A:847:BCR:H383	15:A:847:BCR:H23C	1.85	0.59
13:B:817:CLA:HMB3	13:B:822:CLA:H52	1.84	0.59
2:B:289:MET:HE1	13:B:817:CLA:OBD	2.02	0.58
13:B:806:CLA:H111	15:I:102:BCR:HC31	1.85	0.58
13:B:833:CLA:HAA2	13:B:833:CLA:CGD	2.33	0.58
1:A:52:HIS:CG	16:A:853:LHG:H131	2.38	0.58
2:B:360:PRO:CB	13:B:816:CLA:HBA1	2.33	0.58
8:J:15:ALA:O	8:J:19:MET:HB2	2.03	0.58
1:A:460:VAL:HG12	13:A:802:CLA:H12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:818:CLA:H3A	13:B:818:CLA:O2A	2.02	0.58
1:A:90:MET:SD	13:A:808:CLA:HBA1	2.44	0.58
13:A:803:CLA:C9	15:A:852:BCR:H19C	2.32	0.58
13:A:808:CLA:O1D	13:A:828:CLA:HED2	2.04	0.58
1:A:379:PRO:HB2	13:A:819:CLA:HBA1	1.84	0.58
1:A:391:LEU:O	1:A:395:THR:HG23	2.04	0.58
1:A:503:PRO:HD2	13:A:836:CLA:C3D	2.33	0.58
2:B:293:GLN:OE1	13:B:810:CLA:HBA2	2.04	0.58
13:B:803:CLA:H122	15:I:102:BCR:H281	1.84	0.58
1:A:446:TRP:HB2	13:A:843:CLA:HED3	1.85	0.58
13:A:803:CLA:H143	13:A:842:CLA:H111	1.86	0.58
2:B:361:TYR:CE2	13:B:816:CLA:HED3	2.38	0.58
13:I:101:CLA:HMA1	13:I:101:CLA:O2A	2.04	0.58
13:X:102:CLA:HAA2	13:X:102:CLA:O2D	2.03	0.58
1:A:196:MET:HB2	13:A:813:CLA:HBC2	1.84	0.58
1:A:366:LEU:HD21	13:A:819:CLA:H72	1.84	0.58
2:B:343:CYS:SG	13:B:824:CLA:H71	2.44	0.58
2:B:431:PHE:CZ	15:B:850:BCR:HC41	2.38	0.58
13:B:829:CLA:HAA2	13:B:829:CLA:O2D	2.04	0.58
15:B:842:BCR:C8	15:B:842:BCR:H321	2.33	0.58
10:L:7:PRO:HB3	10:L:12:PRO:HA	1.86	0.58
2:B:320:MET:SD	16:X:101:LHG:HC41	2.43	0.58
1:A:429:VAL:O	1:A:433:VAL:HG13	2.04	0.58
6:F:139:SER:O	6:F:141:ARG:NH1	2.37	0.58
13:A:803:CLA:HED2	2:B:538:LEU:CD2	2.34	0.57
2:B:419:GLU:OE1	6:F:141:ARG:NH2	2.37	0.57
4:D:61:LYS:HE2	4:D:94:ILE:HD12	1.86	0.57
6:F:54:ASP:O	6:F:56:ARG:N	2.33	0.57
6:F:97:LYS:HE2	6:F:102:ASP:HB2	1.85	0.57
13:A:835:CLA:CGD	13:A:835:CLA:HAA2	2.34	0.57
2:B:497:ASN:O	2:B:498:VAL:HB	2.04	0.57
13:B:824:CLA:H13	15:B:845:BCR:H15C	1.86	0.57
13:M:1201:CLA:HAA2	13:M:1201:CLA:CBD	2.34	0.57
1:A:95:ALA:HB2	1:A:158:LEU:HB2	1.84	0.57
13:A:804:CLA:HED2	13:A:811:CLA:O1D	2.05	0.57
2:B:427:TRP:CD1	13:B:830:CLA:HED1	2.39	0.57
1:A:300:HIS:HE2	13:A:819:CLA:C1B	2.16	0.57
13:B:803:CLA:H102	15:B:847:BCR:C36	2.34	0.57
5:E:24:ALA:O	5:E:25:SER:HB3	2.05	0.57
1:A:300:HIS:HB2	13:A:818:CLA:CHB	2.34	0.57
15:A:852:BCR:C8	15:A:852:BCR:H311	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:ILE:HD12	11:M:14:ILE:HD12	1.85	0.57
13:B:816:CLA:H62	13:B:816:CLA:CMB	2.33	0.57
2:B:140:PHE:CG	13:B:812:CLA:H12	2.40	0.57
11:M:29:LEU:HB2	13:M:1201:CLA:HBA2	1.87	0.57
1:A:156:PHE:CZ	13:A:816:CLA:HBA1	2.39	0.57
1:A:70:ARG:NE	1:A:185:PRO:O	2.31	0.57
13:A:831:CLA:HAA2	13:A:831:CLA:O1D	2.04	0.57
6:F:6:VAL:O	6:F:43:CYS:N	2.30	0.57
2:B:668:MET:HB2	13:B:803:CLA:C1C	2.33	0.57
6:F:132:LYS:HB2	6:F:135:GLU:HG3	1.86	0.57
13:A:822:CLA:HED3	9:K:37:ARG:H	1.70	0.57
2:B:211:PHE:CE1	15:B:843:BCR:H352	2.40	0.57
2:B:354:HIS:HB3	13:B:815:CLA:CED	2.35	0.57
13:B:811:CLA:H203	13:B:826:CLA:H2	1.87	0.57
13:B:825:CLA:H161	18:B:848:LMG:H273	1.87	0.57
13:B:802:CLA:HAA2	13:B:802:CLA:CGD	2.35	0.56
13:B:838:CLA:HED3	10:L:96:TYR:HD1	1.69	0.56
10:L:89:ALA:HB1	15:L:1005:BCR:H401	1.87	0.56
1:A:473:ASP:OD1	10:L:69:ARG:NH2	2.38	0.56
13:A:829:CLA:H61	15:A:849:BCR:C37	2.33	0.56
5:E:68:VAL:HG23	5:E:69:ALA:H	1.68	0.56
1:A:660:GLN:HG2	1:A:753:SER:CB	2.35	0.56
2:B:150:PHE:HD2	13:B:809:CLA:CBC	2.19	0.56
2:B:236:PRO:HA	2:B:252:ALA:HB3	1.86	0.56
2:B:343:CYS:HB3	13:B:822:CLA:C4	2.35	0.56
10:L:6:LYS:HB2	10:L:7:PRO:HD2	1.87	0.56
1:A:660:GLN:NE2	1:A:750:ARG:HD2	2.20	0.56
13:B:815:CLA:O1D	13:B:815:CLA:HAA2	2.05	0.56
7:I:20:TRP:HZ2	13:I:101:CLA:HBB	1.71	0.56
1:A:599:LEU:HD21	13:A:830:CLA:HBC1	1.88	0.56
15:A:852:BCR:HC8	15:A:852:BCR:H311	1.87	0.56
13:B:817:CLA:CGD	13:B:817:CLA:HAA2	2.36	0.56
9:K:59:LEU:C	9:K:61:ALA:H	2.13	0.56
13:A:840:CLA:HAA2	13:A:840:CLA:O2D	2.06	0.56
2:B:309:PHE:C	2:B:311:GLY:H	2.13	0.56
13:B:805:CLA:HAA2	13:B:805:CLA:CGD	2.34	0.56
12:X:20:LEU:HD21	13:X:102:CLA:HBB1	1.88	0.56
13:A:803:CLA:H91	13:A:803:CLA:C12	2.36	0.56
13:A:822:CLA:O1D	9:K:36:SER:HA	2.06	0.56
2:B:277:LEU:HD13	13:B:813:CLA:CMC	2.35	0.56
8:J:19:MET:HE3	8:J:19:MET:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:31:ILE:HA	10:L:34:LEU:HD22	1.87	0.56
11:M:26:SER:HB2	15:M:1203:BCR:HC31	1.88	0.56
1:A:246:PRO:HG3	13:A:815:CLA:HED1	1.87	0.56
13:A:820:CLA:HAA2	13:A:820:CLA:CGD	2.36	0.56
13:A:833:CLA:CMA	15:I:102:BCR:H292	2.33	0.56
2:B:274:HIS:HE1	13:B:814:CLA:C4D	2.19	0.56
2:B:425:LEU:HD13	2:B:538:LEU:HA	1.88	0.56
1:A:305:ALA:O	1:A:309:ILE:HG12	2.06	0.56
13:A:803:CLA:HAA2	13:A:803:CLA:O2D	2.05	0.56
2:B:184:VAL:HG11	15:B:842:BCR:C34	2.36	0.56
2:B:466:ILE:HB	13:B:835:CLA:CED	2.36	0.56
13:B:830:CLA:HHD	13:B:830:CLA:HBC2	1.87	0.56
1:A:313:HIS:CE1	15:A:847:BCR:H363	2.41	0.55
1:A:744:TRP:CD1	15:A:852:BCR:HC22	2.40	0.55
13:A:803:CLA:H92	15:A:852:BCR:H19C	1.87	0.55
2:B:131:ASN:HB2	11:M:1:MET:O	2.06	0.55
3:C:28:VAL:HG12	4:D:109:ARG:HB3	1.88	0.55
3:C:62:LEU:HB3	3:C:64:ILE:O	2.06	0.55
11:M:30:TYR:O	13:M:1201:CLA:HED2	2.06	0.55
2:B:373:ALA:HB1	13:B:825:CLA:CMA	2.36	0.55
1:A:490:VAL:HB	13:A:837:CLA:CED	2.37	0.55
13:A:803:CLA:HBB1	13:B:802:CLA:NB	2.21	0.55
13:I:101:CLA:HAA2	13:I:101:CLA:O1D	2.06	0.55
2:B:50:PHE:CZ	13:B:809:CLA:HBB1	2.42	0.55
13:A:819:CLA:H121	13:A:821:CLA:CBB	2.36	0.55
13:A:832:CLA:HAA2	13:A:832:CLA:CGD	2.36	0.55
2:B:229:TRP:HB2	13:B:814:CLA:O2A	2.06	0.55
2:B:360:PRO:HB2	13:B:816:CLA:HED2	1.87	0.55
13:B:810:CLA:HAA2	13:B:810:CLA:HBD	1.89	0.55
8:J:4:PHE:O	8:J:8:LEU:HG	2.06	0.55
1:A:17:ASP:HB3	1:A:20:PRO:HG3	1.88	0.55
13:A:823:CLA:HAA2	13:A:823:CLA:O2D	2.06	0.55
2:B:367:ASP:OD1	2:B:370:THR:HG23	2.06	0.55
13:B:802:CLA:HAA2	13:B:802:CLA:O2D	2.07	0.55
13:B:806:CLA:C1	7:I:18:VAL:HG21	2.23	0.55
13:B:815:CLA:C5	13:B:832:CLA:HED2	2.36	0.55
6:F:88:VAL:HG11	6:F:97:LYS:HB3	1.89	0.55
1:A:145:GLN:NE2	1:A:382:TYR:O	2.37	0.55
13:A:826:CLA:HBA2	13:A:827:CLA:HED3	1.89	0.55
13:A:832:CLA:H2	10:L:31:ILE:HG13	1.87	0.55
2:B:39:GLU:HA	2:B:164:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:MET:HE3	13:B:820:CLA:C3D	2.37	0.55
13:I:101:CLA:O1D	10:L:67:PRO:HG3	2.06	0.55
1:A:120:ILE:HD12	15:J:1105:BCR:H311	1.89	0.55
1:A:339:ALA:HB1	1:A:342:LYS:HD3	1.87	0.55
1:A:374:MET:HG2	13:A:819:CLA:O1A	2.07	0.55
13:A:832:CLA:HBD	10:L:21:ILE:CG2	2.37	0.55
13:B:813:CLA:HAA2	13:B:813:CLA:O2D	2.07	0.55
13:B:822:CLA:C6	13:B:824:CLA:H42	2.36	0.55
13:B:823:CLA:HED2	13:B:824:CLA:OBD	2.06	0.55
13:A:834:CLA:H52	10:L:61:PRO:HG3	1.89	0.54
2:B:466:ILE:HD11	13:B:835:CLA:H43	1.88	0.54
13:B:830:CLA:HAA2	13:B:830:CLA:O1D	2.07	0.54
5:E:26:VAL:HG13	5:E:35:PRO:HB2	1.88	0.54
8:J:5:LEU:HD23	8:J:8:LEU:HD12	1.89	0.54
13:A:826:CLA:HAA1	13:A:839:CLA:HED2	1.89	0.54
13:A:842:CLA:CED	16:A:853:LHG:H102	2.36	0.54
2:B:210:ASN:C	2:B:212:LEU:H	2.15	0.54
2:B:372:ALA:HB1	2:B:731:LEU:HD11	1.88	0.54
5:E:6:LYS:HD3	5:E:22:THR:HG22	1.88	0.54
6:F:73:ILE:O	6:F:77:ILE:HG13	2.07	0.54
11:M:29:LEU:O	11:M:30:TYR:HB2	2.06	0.54
1:A:42:PRO:HG3	1:A:47:TRP:CE3	2.41	0.54
1:A:662:ILE:HD12	2:B:627:ARG:HG3	1.89	0.54
12:X:23:ASN:HD21	13:X:102:CLA:CHA	2.21	0.54
13:B:827:CLA:HAA2	13:B:827:CLA:O2D	2.07	0.54
1:A:375:TYR:CZ	13:A:837:CLA:HBC3	2.42	0.54
2:B:39:GLU:O	2:B:43:GLN:HG3	2.07	0.54
2:B:194:ILE:HA	2:B:198:ILE:HD12	1.90	0.54
2:B:367:ASP:CG	2:B:370:THR:HG23	2.32	0.54
13:B:831:CLA:CED	8:J:36:LEU:H	1.98	0.54
4:D:120:GLY:HA3	5:E:13:GLU:CD	2.32	0.54
2:B:103:PHE:CZ	2:B:651:VAL:HG22	2.43	0.54
2:B:446:VAL:HG13	2:B:451:THR:O	2.07	0.54
15:L:1006:BCR:HC8	15:L:1006:BCR:C33	2.35	0.54
1:A:138:GLN:O	13:A:808:CLA:HMD2	2.08	0.54
13:A:804:CLA:O1D	13:A:811:CLA:H2	2.08	0.54
13:A:826:CLA:H112	13:A:826:CLA:H162	1.88	0.54
15:B:849:BCR:C33	15:B:849:BCR:H343	2.38	0.54
1:A:302:LEU:HD13	13:A:815:CLA:CMC	2.39	0.53
2:B:216:PRO:HD2	13:B:813:CLA:CAD	2.38	0.53
2:B:236:PRO:O	2:B:250:GLY:HA3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:VAL:HG12	3:C:64:ILE:HD11	1.88	0.53
1:A:28:TRP:CD2	13:A:811:CLA:H12	2.43	0.53
13:A:802:CLA:H162	13:I:101:CLA:HMC2	1.90	0.53
13:A:830:CLA:HAA2	13:A:830:CLA:O1D	2.08	0.53
2:B:392:HIS:CE1	13:B:827:CLA:NA	2.76	0.53
13:B:815:CLA:HAA2	13:B:815:CLA:CGD	2.39	0.53
8:J:31:ARG:CD	15:J:1105:BCR:H312	2.30	0.53
1:A:253:TYR:O	1:A:258:TRP:NE1	2.36	0.53
1:A:711:LEU:HD23	6:F:130:THR:HG22	1.90	0.53
2:B:614:GLN:O	2:B:618:SER:HB2	2.09	0.53
14:B:840:PQN:H291	18:B:848:LMG:H181	1.90	0.53
1:A:67:ASP:O	1:A:71:LYS:HG3	2.07	0.53
1:A:646:ILE:HG21	13:A:802:CLA:CBA	2.39	0.53
2:B:24:ILE:HG21	18:B:848:LMG:H182	1.90	0.53
13:B:805:CLA:H51	18:B:848:LMG:C33	2.38	0.53
6:F:79:TRP:HE3	15:F:1302:BCR:HC41	1.72	0.53
1:A:336:PHE:CD1	16:A:854:LHG:HC42	2.44	0.53
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.44	0.53
13:A:815:CLA:HAA2	13:A:815:CLA:O1D	2.07	0.53
13:A:819:CLA:HAA2	13:A:819:CLA:CGD	2.38	0.53
13:A:834:CLA:H101	15:B:849:BCR:H362	1.91	0.53
2:B:310:PHE:HE1	13:B:820:CLA:H71	1.74	0.53
6:F:76:TRP:CH2	6:F:114:PHE:HB3	2.44	0.53
15:L:1005:BCR:H331	15:L:1005:BCR:C8	2.38	0.53
1:A:356:LEU:O	1:A:360:LEU:HB2	2.08	0.53
1:A:651:ARG:HB2	2:B:638:ILE:HG23	1.90	0.53
13:A:842:CLA:H101	13:J:1101:CLA:H43	1.91	0.53
2:B:351:VAL:HA	13:B:816:CLA:H42	1.90	0.53
13:B:832:CLA:HAA2	13:B:832:CLA:O1D	2.08	0.53
4:D:9:LEU:HB2	4:D:48:VAL:HB	1.90	0.53
1:A:74:SER:OG	1:A:180:TYR:HB2	2.09	0.53
13:B:822:CLA:O2D	13:B:822:CLA:HAA2	2.09	0.53
1:A:466:ARG:HB2	1:A:474:MET:SD	2.49	0.53
13:B:803:CLA:H143	15:B:847:BCR:H362	1.90	0.53
13:B:806:CLA:HED3	7:I:11:PRO:CB	2.34	0.53
13:B:810:CLA:HAA2	13:B:810:CLA:CBD	2.39	0.53
13:B:830:CLA:CBB	13:B:831:CLA:HMB1	2.38	0.53
1:A:141:SER:CB	13:A:808:CLA:HED3	2.37	0.53
1:A:323:HIS:CE1	13:A:822:CLA:NA	2.77	0.53
1:A:730:VAL:HG22	13:A:842:CLA:CAD	2.38	0.53
13:A:810:CLA:HAA2	13:A:810:CLA:O2D	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:ILE:HD13	13:B:832:CLA:CHC	2.39	0.53
1:A:203:GLY:HA3	13:A:813:CLA:CBB	2.39	0.53
13:A:840:CLA:C1	13:B:830:CLA:HED3	2.33	0.53
13:B:824:CLA:H101	15:B:845:BCR:H17C	1.91	0.53
13:B:826:CLA:H192	15:B:843:BCR:H362	1.89	0.53
1:A:80:LEU:O	1:A:83:VAL:HG12	2.09	0.52
2:B:625:TRP:O	2:B:629:TYR:HB3	2.09	0.52
13:A:828:CLA:HAA2	13:A:828:CLA:CGD	2.40	0.52
13:A:832:CLA:HBC2	13:A:839:CLA:CMC	2.39	0.52
2:B:466:ILE:HB	13:B:835:CLA:HED1	1.90	0.52
2:B:693:LEU:HB2	15:B:849:BCR:H282	1.91	0.52
13:B:825:CLA:H3A	13:B:825:CLA:O2A	2.09	0.52
13:B:825:CLA:HAA2	13:B:825:CLA:CGD	2.40	0.52
15:B:849:BCR:H333	13:I:101:CLA:H41	1.91	0.52
10:L:54:HIS:HA	10:L:57:PHE:CE2	2.44	0.52
1:A:154:ASN:OD1	1:A:156:PHE:HB3	2.10	0.52
1:A:302:LEU:HD13	13:A:815:CLA:HMC1	1.91	0.52
13:A:803:CLA:CGA	13:A:803:CLA:H3A	2.40	0.52
13:A:808:CLA:H201	13:A:842:CLA:H12	1.90	0.52
2:B:29:ASP:OD2	13:B:827:CLA:HED1	2.09	0.52
2:B:122:TRP:HB2	13:B:826:CLA:HED2	1.92	0.52
2:B:277:LEU:HG	13:B:814:CLA:HBB1	1.91	0.52
1:A:93:HIS:CE1	13:A:807:CLA:NA	2.78	0.52
1:A:374:MET:HE1	1:A:393:LEU:HD13	1.92	0.52
13:A:832:CLA:HED2	10:L:16:HIS:NE2	2.23	0.52
15:A:852:BCR:H381	13:B:830:CLA:HMA3	1.90	0.52
13:B:816:CLA:H3A	13:B:816:CLA:O2A	2.10	0.52
11:M:13:VAL:O	11:M:16:LEU:HB2	2.10	0.52
1:A:534:ALA:O	1:A:538:VAL:HG22	2.10	0.52
13:B:838:CLA:H142	10:L:85:LEU:HD23	1.92	0.52
15:B:843:BCR:H383	15:B:843:BCR:H23C	1.91	0.52
1:A:587:CYS:HB2	2:B:673:TRP:HB3	1.90	0.52
2:B:282:LEU:HD12	13:B:817:CLA:CMC	2.40	0.52
2:B:669:PHE:CZ	13:B:839:CLA:HBC3	2.45	0.52
18:B:848:LMG:H202	13:M:1201:CLA:HBC1	1.91	0.52
5:E:29:THR:HB	5:E:32:VAL:HG23	1.92	0.52
1:A:332:HIS:CE1	13:A:823:CLA:C1A	2.93	0.52
2:B:184:VAL:HG11	15:B:842:BCR:H341	1.92	0.52
2:B:665:THR:CA	13:B:803:CLA:HAB	2.38	0.52
13:B:803:CLA:C12	15:I:102:BCR:H281	2.40	0.52
5:E:24:ALA:N	5:E:37:ILE:O	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:54:ASP:C	6:F:56:ARG:H	2.18	0.52
13:A:823:CLA:CHB	13:A:845:CLA:HMC3	2.39	0.52
13:A:834:CLA:CMC	13:B:803:CLA:H91	2.40	0.52
13:B:804:CLA:HMB1	13:B:804:CLA:HBB1	1.92	0.52
13:A:833:CLA:HAA2	13:A:833:CLA:O1D	2.11	0.51
2:B:7:PHE:CZ	2:B:27:ALA:HA	2.45	0.51
2:B:298:HIS:ND1	13:B:820:CLA:OBD	2.42	0.51
1:A:56:HIS:ND1	13:A:806:CLA:HED1	2.24	0.51
13:A:802:CLA:H152	15:B:847:BCR:C12	2.39	0.51
10:L:129:MET:SD	15:L:1006:BCR:H24C	2.50	0.51
1:A:215:HIS:CE1	13:A:814:CLA:C1A	2.92	0.51
13:A:834:CLA:HED2	10:L:65:LEU:O	2.10	0.51
2:B:150:PHE:HD2	13:B:809:CLA:HBC3	1.76	0.51
2:B:703:PRO:HB3	13:B:838:CLA:C2C	2.40	0.51
1:A:104:LEU:HD23	1:A:148:ARG:HH11	1.75	0.51
1:A:143:LEU:HD22	1:A:147:TRP:CH2	2.45	0.51
13:A:819:CLA:H3A	13:A:819:CLA:CGA	2.39	0.51
13:A:823:CLA:HMA3	13:A:845:CLA:CAC	2.40	0.51
2:B:156:LEU:O	2:B:161:ARG:NH1	2.37	0.51
13:B:817:CLA:HMB3	13:B:822:CLA:H71	1.92	0.51
5:E:27:ASP:O	5:E:35:PRO:HB3	2.11	0.51
2:B:435:HIS:HE1	13:B:830:CLA:C4D	2.24	0.51
2:B:554:PRO:HD2	3:C:61:PHE:CE1	2.46	0.51
1:A:454:HIS:HE1	13:A:833:CLA:C4D	2.24	0.51
13:A:803:CLA:HED2	2:B:538:LEU:HD23	1.91	0.51
2:B:180:GLY:HA3	13:B:811:CLA:CBB	2.41	0.51
7:I:17:VAL:HA	7:I:21:LEU:HB3	1.91	0.51
1:A:210:LEU:HD21	15:A:847:BCR:H342	1.93	0.51
1:A:436:HIS:CE1	13:A:831:CLA:C4D	2.93	0.51
15:A:852:BCR:C23	15:A:852:BCR:H403	2.40	0.51
2:B:157:GLN:O	2:B:161:ARG:HG3	2.11	0.51
2:B:309:PHE:HB2	2:B:314:VAL:HG11	1.92	0.51
13:B:807:CLA:H102	13:B:807:CLA:C5	2.41	0.51
10:L:56:TYR:HB2	10:L:131:SER:HB2	1.93	0.51
1:A:231:VAL:HG12	1:A:235:ASP:HB3	1.93	0.51
1:A:717:ILE:HG13	6:F:98:GLU:OE1	2.11	0.51
13:A:830:CLA:H121	13:A:842:CLA:HBA1	1.93	0.51
13:B:824:CLA:H101	15:B:845:BCR:C17	2.40	0.51
15:L:1005:BCR:H403	15:L:1005:BCR:C23	2.34	0.51
1:A:118:TRP:CZ2	13:A:807:CLA:HAA2	2.46	0.51
1:A:221:LEU:HB2	1:A:222:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:803:CLA:HBA2	2:B:430:LEU:HD13	1.93	0.51
2:B:318:PHE:CD1	13:B:820:CLA:HAB	2.45	0.51
13:B:808:CLA:H13	18:B:848:LMG:H221	1.93	0.51
3:C:6:ILE:HG13	3:C:64:ILE:CD1	2.40	0.51
1:A:104:LEU:HD11	1:A:153:THR:HA	1.93	0.50
1:A:548:VAL:O	1:A:552:ILE:HD13	2.11	0.50
4:D:101:PHE:HB2	4:D:104:LYS:HE3	1.94	0.50
6:F:80:VAL:HG22	6:F:109:CYS:O	2.11	0.50
1:A:308:PHE:CE2	13:A:821:CLA:HAB	2.36	0.50
1:A:660:GLN:HG2	1:A:753:SER:HB3	1.93	0.50
13:A:825:CLA:HAB	15:A:850:BCR:C34	2.41	0.50
2:B:123:TRP:HB3	2:B:128:MET:HB2	1.93	0.50
2:B:463:ALA:HB2	13:B:836:CLA:HED3	1.93	0.50
15:F:1302:BCR:H342	15:F:1302:BCR:C33	2.41	0.50
1:A:237:PRO:HB3	1:A:248:LEU:HD21	1.93	0.50
1:A:626:ALA:C	1:A:628:ASP:H	2.19	0.50
1:A:691:PHE:HB2	13:A:803:CLA:HBC2	1.93	0.50
13:A:807:CLA:HAA1	13:A:807:CLA:HBD	1.94	0.50
2:B:114:ILE:O	13:B:807:CLA:HMD1	2.11	0.50
2:B:651:VAL:HG13	13:B:808:CLA:HAC1	1.93	0.50
2:B:231:VAL:O	2:B:234:GLN:HG2	2.11	0.50
2:B:696:LEU:HD11	10:L:36:ALA:HB1	1.94	0.50
4:D:24:GLU:O	4:D:87:PRO:HD3	2.12	0.50
8:J:33:TYR:N	8:J:34:PRO:HD3	2.26	0.50
1:A:392:SER:HB3	13:A:828:CLA:CMA	2.41	0.50
13:A:813:CLA:O1D	13:A:825:CLA:H62	2.12	0.50
2:B:713:LEU:CD1	18:B:848:LMG:H342	2.42	0.50
4:D:34:PRO:O	4:D:51:GLU:HG3	2.12	0.50
10:L:67:PRO:HG2	10:L:68:LEU:HD23	1.94	0.50
1:A:191:GLN:HG2	13:A:825:CLA:H201	1.94	0.50
1:A:472:GLN:OE1	1:A:472:GLN:N	2.38	0.50
13:A:839:CLA:HAA2	13:A:839:CLA:CGD	2.42	0.50
3:C:65:ARG:HG2	3:C:67:TYR:CZ	2.47	0.50
1:A:118:TRP:HE3	13:A:809:CLA:H2A	1.70	0.50
13:A:802:CLA:HED1	2:B:660:HIS:CD2	2.46	0.50
13:A:840:CLA:H43	13:B:830:CLA:O1D	2.11	0.50
2:B:693:LEU:CB	15:B:849:BCR:H282	2.42	0.50
7:I:7:ALA:HB1	7:I:10:LEU:HD22	1.94	0.50
2:B:360:PRO:HG3	13:B:816:CLA:HBA1	1.94	0.50
13:B:806:CLA:CGD	13:B:806:CLA:CAA	2.89	0.50
1:A:161:THR:HG22	15:A:848:BCR:HC32	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD22	15:A:848:BCR:H361	1.93	0.50
13:A:826:CLA:HMA1	13:A:827:CLA:HED3	1.93	0.50
2:B:468:ALA:HA	2:B:472:LYS:O	2.12	0.50
6:F:73:ILE:O	6:F:76:TRP:HB3	2.12	0.50
1:A:542:HIS:HE1	1:A:612:HIS:ND1	2.10	0.49
2:B:155:HIS:HE1	13:B:809:CLA:C1A	2.25	0.49
2:B:288:HIS:CE1	15:B:841:BCR:H363	2.47	0.49
13:B:828:CLA:HAA2	13:B:828:CLA:O1D	2.12	0.49
13:I:101:CLA:H42	10:L:81:SER:HA	1.94	0.49
13:A:826:CLA:HAA1	13:A:839:CLA:CED	2.42	0.49
2:B:289:MET:HE1	13:B:817:CLA:CAD	2.42	0.49
2:B:339:TRP:HE1	13:B:822:CLA:C2B	2.25	0.49
2:B:718:HIS:HE1	13:B:839:CLA:C4D	2.25	0.49
13:B:838:CLA:H2	13:B:839:CLA:H142	1.94	0.49
13:A:813:CLA:HAA1	13:A:825:CLA:C4	2.42	0.49
2:B:194:ILE:HG12	2:B:253:ILE:HB	1.95	0.49
6:F:53:VAL:O	15:F:1302:BCR:H291	2.11	0.49
1:A:364:GLY:O	1:A:368:ILE:HD12	2.13	0.49
2:B:634:SER:O	2:B:638:ILE:HB	2.11	0.49
4:D:67:LEU:HD12	4:D:71:GLN:HG3	1.93	0.49
10:L:38:ARG:HE	13:L:1002:CLA:HAC2	1.76	0.49
2:B:275:HIS:HB2	13:B:815:CLA:CHB	2.42	0.49
13:B:838:CLA:C19	15:I:102:BCR:H362	2.42	0.49
13:M:1201:CLA:HAA2	13:M:1201:CLA:HBD	1.94	0.49
1:A:233:ALA:O	1:A:235:ASP:N	2.43	0.49
1:A:588:GLN:HA	1:A:593:ASP:CG	2.38	0.49
13:A:805:CLA:O1A	13:A:813:CLA:HED2	2.12	0.49
13:A:826:CLA:HBA1	13:A:827:CLA:CGD	2.42	0.49
15:A:852:BCR:H321	15:A:852:BCR:C8	2.43	0.49
2:B:651:VAL:HG13	13:B:808:CLA:HHB	1.94	0.49
15:B:841:BCR:H383	15:B:841:BCR:H23C	1.95	0.49
13:B:807:CLA:O1D	13:B:825:CLA:HED2	2.13	0.49
13:B:807:CLA:HMC2	15:B:847:BCR:HC32	1.94	0.49
1:A:215:HIS:CE1	13:A:814:CLA:NA	2.79	0.49
1:A:215:HIS:HE1	13:A:814:CLA:C1A	2.25	0.49
1:A:292:LEU:HD22	13:A:818:CLA:HBA1	1.95	0.49
13:A:820:CLA:HAA2	13:A:820:CLA:O1D	2.12	0.49
13:A:834:CLA:H3A	13:A:834:CLA:HBA2	1.56	0.49
13:A:840:CLA:H11	13:B:830:CLA:CED	2.37	0.49
2:B:291:ARG:HB2	2:B:297:GLY:O	2.12	0.49
1:A:91:TYR:CE2	1:A:161:THR:HG21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:MET:HE3	13:A:818:CLA:HED3	1.93	0.49
1:A:601:TRP:CH2	13:A:802:CLA:HAB	2.48	0.49
2:B:529:ILE:CG2	13:B:835:CLA:HAB	2.38	0.49
13:B:822:CLA:HMB3	13:B:822:CLA:HBB1	1.95	0.49
13:I:101:CLA:H143	10:L:87:LEU:HD11	1.95	0.49
11:M:16:LEU:HD21	15:M:1203:BCR:H19C	1.95	0.49
1:A:220:SER:O	1:A:224:ASN:HB2	2.13	0.49
13:A:801:CLA:H192	13:A:802:CLA:HMB2	1.94	0.49
13:A:808:CLA:HED2	13:A:828:CLA:CED	2.43	0.49
13:A:842:CLA:H91	13:A:842:CLA:H112	1.62	0.49
2:B:291:ARG:HB2	2:B:297:GLY:C	2.38	0.49
2:B:464:GLN:HG2	2:B:475:TYR:CE2	2.48	0.49
1:A:28:TRP:CZ3	13:A:811:CLA:H43	2.47	0.48
1:A:332:HIS:CE1	13:A:823:CLA:NA	2.81	0.48
13:B:804:CLA:C10	13:B:804:CLA:HED3	2.43	0.48
13:B:838:CLA:H143	10:L:88:VAL:HG11	1.95	0.48
1:A:273:ALA:O	1:A:276:SER:OG	2.24	0.48
1:A:473:ASP:HA	10:L:69:ARG:HH22	1.77	0.48
13:A:801:CLA:HAB	13:B:801:CLA:NA	2.28	0.48
13:A:822:CLA:HAA2	13:A:822:CLA:O2D	2.13	0.48
13:B:811:CLA:H143	13:B:811:CLA:H112	1.66	0.48
13:A:843:CLA:HBC1	14:B:840:PQN:H192	1.95	0.48
2:B:154:LEU:O	2:B:160:PHE:HB2	2.13	0.48
13:B:806:CLA:CGD	13:B:806:CLA:HAA2	2.43	0.48
1:A:146:LEU:HA	1:A:380:TYR:CD2	2.47	0.48
1:A:725:ILE:HG22	16:A:853:LHG:HC41	1.94	0.48
2:B:116:TYR:HB2	13:B:825:CLA:O1A	2.13	0.48
2:B:361:TYR:O	2:B:364:ILE:HG22	2.13	0.48
3:C:51:LYS:HD3	3:C:54:GLU:OE1	2.13	0.48
1:A:82:VAL:HG12	13:A:809:CLA:H193	1.96	0.48
1:A:658:ALA:O	1:A:662:ILE:HG12	2.13	0.48
1:A:686:SER:HB3	1:A:734:HIS:HB2	1.96	0.48
13:A:817:CLA:HMD3	13:A:836:CLA:O1D	2.14	0.48
2:B:491:ALA:HB3	2:B:495:TYR:HA	1.95	0.48
5:E:2:GLN:HG2	5:E:5:SER:OG	2.13	0.48
1:A:266:PRO:HB2	1:A:275:TYR:CZ	2.48	0.48
1:A:395:THR:OG1	13:A:828:CLA:HBB1	2.14	0.48
13:A:813:CLA:HBD	13:A:825:CLA:H62	1.92	0.48
2:B:498:VAL:O	2:B:501:PRO:HD2	2.13	0.48
13:B:804:CLA:O1D	13:B:804:CLA:HAA2	2.14	0.48
13:B:825:CLA:HBC3	18:B:848:LMG:H421	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:10:VAL:O	11:M:14:ILE:HG13	2.14	0.48
1:A:509:ALA:HA	13:A:818:CLA:H11	1.95	0.48
2:B:589:MET:HE2	2:B:590:LEU:HA	1.94	0.48
10:L:92:CYS:HB3	15:L:1005:BCR:C21	2.44	0.48
1:A:15:VAL:HG12	1:A:186:LYS:HD3	1.95	0.48
1:A:678:GLY:HA2	13:B:802:CLA:H41	1.95	0.48
2:B:76:TRP:HZ3	2:B:124:TYR:HB2	1.78	0.48
13:B:817:CLA:CMB	13:B:822:CLA:H71	2.44	0.48
13:B:836:CLA:C9	15:F:1302:BCR:H20C	2.44	0.48
6:F:107:ILE:HA	6:F:110:MET:HE3	1.95	0.48
12:X:25:LEU:O	12:X:29:TYR:HD1	1.96	0.48
1:A:511:VAL:HB	1:A:526:MET:HG3	1.96	0.48
13:A:808:CLA:HMD3	13:A:828:CLA:O1A	2.13	0.48
13:A:827:CLA:HMA2	13:A:835:CLA:H51	1.96	0.48
2:B:386:MET:HE1	15:B:845:BCR:H361	1.94	0.48
13:B:838:CLA:H151	13:B:839:CLA:H13	1.95	0.48
1:A:683:TRP:CG	13:A:801:CLA:HMA2	2.49	0.48
13:A:821:CLA:OBD	13:A:823:CLA:HMD3	2.14	0.48
13:A:834:CLA:H152	13:L:1003:CLA:HMB2	1.96	0.48
2:B:14:ASP:HB3	2:B:19:ARG:HB2	1.96	0.48
2:B:373:ALA:HB1	13:B:825:CLA:HMA2	1.94	0.48
2:B:655:MET:HE2	15:B:847:BCR:H333	1.96	0.48
13:B:806:CLA:HED2	7:I:15:ILE:CD1	2.43	0.48
13:B:828:CLA:HMB1	13:B:829:CLA:C3D	2.43	0.48
7:I:27:MET:HB3	15:L:1005:BCR:H352	1.96	0.48
12:X:18:LEU:O	12:X:21:ALA:HB3	2.14	0.48
1:A:714:ALA:O	6:F:89:ARG:NH2	2.42	0.47
13:A:802:CLA:H152	15:B:847:BCR:C10	2.44	0.47
13:A:813:CLA:HAA1	13:A:825:CLA:H41	1.96	0.47
13:A:813:CLA:H61	13:A:813:CLA:H102	1.68	0.47
13:A:842:CLA:H161	13:J:1101:CLA:H203	1.95	0.47
15:A:850:BCR:H331	15:A:850:BCR:C8	2.43	0.47
2:B:68:ALA:HB2	2:B:134:LEU:HB2	1.96	0.47
3:C:57:CYS:HA	3:C:58:PRO:HD3	1.63	0.47
1:A:120:ILE:O	1:A:123:GLN:HG2	2.14	0.47
1:A:143:LEU:CD1	13:A:808:CLA:HED1	2.44	0.47
13:A:832:CLA:HBD	10:L:21:ILE:HG21	1.96	0.47
2:B:339:TRP:HH2	13:B:821:CLA:HBC2	1.79	0.47
2:B:398:VAL:HG23	2:B:547:ALA:HB1	1.94	0.47
6:F:79:TRP:CZ3	15:F:1302:BCR:H332	2.49	0.47
1:A:346:GLU:OE1	1:A:346:GLU:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HD12	13:B:817:CLA:HMC1	1.97	0.47
2:B:358:LEU:CB	13:B:815:CLA:HED3	2.44	0.47
13:B:807:CLA:HAB	13:B:808:CLA:HAA1	1.95	0.47
4:D:117:ARG:HG2	4:D:118:SER:N	2.29	0.47
6:F:22:VAL:O	6:F:34:ARG:NH2	2.29	0.47
6:F:34:ARG:HD3	8:J:35:ASP:CG	2.40	0.47
1:A:118:TRP:CH2	13:A:807:CLA:HAA2	2.50	0.47
15:A:852:BCR:HC7	15:A:852:BCR:H331	1.67	0.47
1:A:31:PRO:HB2	1:A:47:TRP:HH2	1.80	0.47
2:B:463:ALA:HA	13:B:835:CLA:HED3	1.96	0.47
2:B:717:ALA:HA	18:B:848:LMG:H371	1.95	0.47
13:B:801:CLA:H2	13:B:802:CLA:C2D	2.45	0.47
13:B:812:CLA:HMB1	15:B:843:BCR:C21	2.44	0.47
1:A:290:GLY:HA3	1:A:520:VAL:HG21	1.96	0.47
13:A:831:CLA:HMB2	13:A:832:CLA:C2D	2.45	0.47
2:B:481:LEU:HD11	13:B:832:CLA:CAD	2.45	0.47
13:B:821:CLA:HAA2	13:B:821:CLA:CED	2.44	0.47
13:B:827:CLA:HBD	18:B:848:LMG:H302	1.97	0.47
13:B:836:CLA:H203	6:F:67:SER:OG	2.14	0.47
5:E:6:LYS:HA	5:E:21:GLY:O	2.14	0.47
7:I:3:GLY:HA3	7:I:5:TYR:CE2	2.49	0.47
8:J:20:THR:HG23	15:J:1105:BCR:H351	1.97	0.47
1:A:396:HIS:HE1	13:A:828:CLA:ND	2.08	0.47
13:A:807:CLA:HAA1	13:A:807:CLA:CBD	2.44	0.47
13:A:826:CLA:OBD	13:A:837:CLA:HBB1	2.15	0.47
13:A:838:CLA:H3A	13:A:838:CLA:HBA2	1.56	0.47
13:A:843:CLA:CGD	13:A:843:CLA:CAA	2.93	0.47
2:B:178:LEU:O	2:B:283:PHE:HB3	2.15	0.47
13:B:807:CLA:CMC	15:B:847:BCR:HC32	2.44	0.47
10:L:29:THR:O	10:L:33:ASN:ND2	2.44	0.47
1:A:35:ASP:HB3	1:A:38:LEU:HD12	1.97	0.47
1:A:94:GLY:O	1:A:98:SER:OG	2.16	0.47
1:A:702:GLU:OE2	5:E:45:TYR:OH	2.33	0.47
13:A:811:CLA:H3A	13:A:811:CLA:HBA2	1.55	0.47
2:B:466:ILE:HG21	13:B:835:CLA:HED1	1.97	0.47
13:B:808:CLA:HMA2	13:I:101:CLA:HAB	1.96	0.47
6:F:84:TYR:CZ	6:F:101:ILE:HG23	2.50	0.47
11:M:26:SER:CB	13:M:1201:CLA:H2	2.45	0.47
1:A:33:HIS:NE2	13:A:811:CLA:HED2	2.30	0.47
1:A:86:TRP:HA	13:A:807:CLA:HBB2	1.96	0.47
1:A:203:GLY:O	1:A:207:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:814:CLA:O1D	13:A:816:CLA:HMA1	2.14	0.47
13:A:832:CLA:H61	13:L:1003:CLA:H72	1.97	0.47
2:B:531:LEU:HD21	13:B:802:CLA:CBB	2.45	0.47
1:A:449:ILE:HD11	15:B:847:BCR:H403	1.97	0.47
13:A:802:CLA:H111	13:A:802:CLA:H142	1.57	0.47
13:A:827:CLA:H2	13:A:827:CLA:H61	1.66	0.47
15:A:852:BCR:H403	15:A:852:BCR:H23C	1.97	0.47
2:B:25:ALA:HB2	18:B:848:LMG:H121	1.97	0.47
2:B:221:LEU:O	2:B:225:PHE:HD1	1.98	0.47
2:B:466:ILE:CG2	13:B:835:CLA:HED1	2.45	0.47
2:B:595:TRP:CZ2	13:B:801:CLA:H172	2.50	0.47
8:J:24:GLY:HA3	13:J:1102:CLA:HBB1	1.96	0.47
11:M:14:ILE:O	11:M:18:PRO:HD2	2.15	0.47
1:A:407:GLY:HA3	13:A:830:CLA:HMC2	1.95	0.46
2:B:261:HIS:HD2	2:B:263:GLN:N	2.13	0.46
2:B:520:PRO:O	2:B:523:PHE:HB3	2.15	0.46
13:B:814:CLA:HAA2	13:B:814:CLA:O2D	2.15	0.46
13:B:816:CLA:H122	13:B:824:CLA:O1A	2.14	0.46
6:F:84:TYR:O	6:F:88:VAL:HG23	2.15	0.46
1:A:679:ALA:HB1	1:A:738:GLY:O	2.15	0.46
13:A:806:CLA:H42	13:A:830:CLA:C5	2.39	0.46
13:A:808:CLA:O1D	13:A:828:CLA:HAA2	2.16	0.46
13:A:832:CLA:H61	13:L:1003:CLA:H101	1.97	0.46
13:A:832:CLA:H102	13:L:1003:CLA:H122	1.96	0.46
2:B:188:ALA:CB	13:B:826:CLA:H202	2.45	0.46
13:B:806:CLA:H3A	13:B:806:CLA:HBA2	1.74	0.46
13:B:816:CLA:H3A	13:B:816:CLA:CGA	2.45	0.46
13:B:826:CLA:HAA2	13:B:826:CLA:CGD	2.45	0.46
13:B:830:CLA:HBC1	6:F:67:SER:OG	2.15	0.46
13:B:833:CLA:HAA2	13:B:833:CLA:O2D	2.15	0.46
4:D:117:ARG:CG	4:D:121:GLN:HB2	2.38	0.46
9:K:32:TYR:HA	9:K:35:GLN:N	2.16	0.46
1:A:28:TRP:CE3	13:A:811:CLA:H43	2.50	0.46
1:A:215:HIS:C	1:A:215:HIS:CD2	2.93	0.46
1:A:297:THR:O	1:A:300:HIS:HB3	2.15	0.46
1:A:603:TYR:OH	13:A:801:CLA:HED1	2.15	0.46
1:A:626:ALA:C	1:A:628:ASP:N	2.73	0.46
13:A:833:CLA:H51	15:B:847:BCR:C20	2.46	0.46
2:B:49:HIS:HB3	13:B:811:CLA:CED	2.40	0.46
2:B:422:ILE:HG23	2:B:538:LEU:HD11	1.97	0.46
2:B:289:MET:HE1	13:B:817:CLA:C3D	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:VAL:O	2:B:445:VAL:HG23	2.15	0.46
13:B:804:CLA:HBB1	13:B:804:CLA:CMB	2.45	0.46
1:A:101:GLU:HG3	1:A:155:GLU:HG2	1.97	0.46
2:B:198:ILE:HB	2:B:199:PRO:HD3	1.98	0.46
2:B:358:LEU:HB2	13:B:815:CLA:CED	2.45	0.46
4:D:117:ARG:HG2	4:D:118:SER:O	2.15	0.46
6:F:88:VAL:CG1	6:F:94:ALA:HA	2.43	0.46
10:L:34:LEU:HG	13:L:1003:CLA:O1D	2.16	0.46
11:M:19:ALA:HB2	15:M:1203:BCR:C13	2.45	0.46
1:A:160:CYS:SG	13:A:816:CLA:HBA2	2.56	0.46
1:A:371:ALA:HB3	1:A:398:MET:HE2	1.96	0.46
2:B:337:LEU:HD13	13:B:804:CLA:C3D	2.46	0.46
2:B:435:HIS:CE1	13:B:830:CLA:C4D	2.99	0.46
13:B:806:CLA:H121	15:M:1203:BCR:H12C	1.97	0.46
13:B:815:CLA:H72	13:B:832:CLA:O1A	2.15	0.46
1:A:231:VAL:O	1:A:232:ALA:HB3	2.16	0.46
1:A:497:ALA:O	1:A:502:ALA:HB3	2.15	0.46
1:A:660:GLN:NE2	1:A:754:VAL:HG13	2.29	0.46
13:A:803:CLA:HBD	2:B:535:THR:CG2	2.46	0.46
13:A:828:CLA:H8	15:A:852:BCR:H343	1.98	0.46
13:A:833:CLA:CBB	13:A:834:CLA:H2	2.46	0.46
2:B:304:MET:HG3	2:B:322:HIS:HB3	1.97	0.46
13:B:824:CLA:H142	13:B:824:CLA:H111	1.63	0.46
13:B:825:CLA:H111	18:B:848:LMG:H442	1.97	0.46
13:B:826:CLA:H51	15:B:842:BCR:H23C	1.97	0.46
13:B:836:CLA:H93	13:B:837:CLA:HBC1	1.97	0.46
15:F:1302:BCR:C8	15:F:1302:BCR:H311	2.46	0.46
11:M:13:VAL:HG23	15:M:1203:BCR:H402	1.98	0.46
13:A:823:CLA:HMA2	13:A:845:CLA:HAC2	1.97	0.46
13:B:827:CLA:C14	18:B:848:LMG:H231	2.46	0.46
6:F:103:VAL:HB	6:F:104:PRO:HD3	1.98	0.46
10:L:16:HIS:CD2	10:L:17:LEU:H	2.34	0.46
11:M:18:PRO:HB2	15:M:1203:BCR:H352	1.97	0.46
1:A:454:HIS:CE1	13:A:833:CLA:C4D	2.98	0.46
2:B:697:VAL:HA	10:L:96:TYR:OH	2.16	0.46
13:F:1301:CLA:CMB	8:J:26:LEU:HD11	2.46	0.46
1:A:378:PRO:HA	1:A:379:PRO:HD3	1.56	0.46
1:A:547:HIS:CE1	13:A:839:CLA:C1A	2.99	0.46
13:A:825:CLA:HBB1	13:A:825:CLA:HMB1	1.98	0.46
14:A:846:PQN:C17	15:B:846:BCR:H382	2.28	0.46
2:B:466:ILE:CB	13:B:835:CLA:HED1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:823:CLA:H3A	13:B:823:CLA:HBA2	1.66	0.46
15:B:846:BCR:C8	15:B:846:BCR:H331	2.45	0.46
3:C:57:CYS:HB3	3:C:62:LEU:CD2	2.46	0.46
12:X:23:ASN:C	12:X:23:ASN:HD22	2.23	0.46
1:A:118:TRP:CE2	13:A:809:CLA:HED2	2.50	0.45
1:A:303:ALA:HB1	13:A:817:CLA:HBC2	1.98	0.45
1:A:356:LEU:HD13	13:A:805:CLA:C3D	2.45	0.45
1:A:409:ALA:HA	15:A:851:BCR:HC41	1.98	0.45
1:A:444:LEU:HG	1:A:551:LEU:HB2	1.98	0.45
13:A:821:CLA:HMB1	13:A:825:CLA:HMA2	1.98	0.45
2:B:122:TRP:CZ2	15:B:843:BCR:H401	2.51	0.45
2:B:309:PHE:O	2:B:311:GLY:N	2.49	0.45
2:B:432:LEU:HD11	13:B:836:CLA:HMB2	1.98	0.45
2:B:531:LEU:HD21	13:B:802:CLA:HBB1	1.98	0.45
6:F:8:CYS:HB3	6:F:14:PHE:CD2	2.51	0.45
2:B:207:GLY:H	2:B:210:ASN:ND2	2.13	0.45
2:B:277:LEU:HD13	13:B:813:CLA:HMC2	1.98	0.45
13:B:815:CLA:H112	13:B:815:CLA:H91	1.72	0.45
6:F:63:PHE:C	6:F:66:PRO:HD2	2.41	0.45
6:F:116:TRP:CG	6:F:117:PRO:HD3	2.51	0.45
1:A:464:THR:HG22	1:A:468:PHE:CE1	2.52	0.45
1:A:579:ASP:OD1	3:C:52:ARG:NH2	2.48	0.45
13:A:808:CLA:H142	13:A:808:CLA:H111	1.77	0.45
13:A:820:CLA:H142	13:A:820:CLA:H111	1.53	0.45
1:A:454:HIS:HE1	13:A:833:CLA:C1A	2.30	0.45
1:A:685:PHE:CA	13:A:803:CLA:HAB	2.43	0.45
1:A:693:GLY:HA3	2:B:574:CYS:HB2	1.97	0.45
13:A:801:CLA:NA	13:B:801:CLA:HAB	2.31	0.45
13:A:830:CLA:H121	13:A:830:CLA:H161	1.86	0.45
13:A:840:CLA:H11	13:B:830:CLA:O1D	2.17	0.45
13:A:841:CLA:HAB	14:A:846:PQN:H202	1.98	0.45
2:B:284:ILE:O	2:B:288:HIS:ND1	2.42	0.45
4:D:124:ASN:HB2	4:D:127:GLN:CD	2.41	0.45
8:J:24:GLY:C	13:J:1102:CLA:HBB1	2.42	0.45
13:A:830:CLA:HBD	16:A:853:LHG:H262	1.98	0.45
2:B:441:VAL:HB	13:B:831:CLA:HMC2	1.99	0.45
13:B:807:CLA:H102	13:B:807:CLA:H51	1.98	0.45
13:B:824:CLA:H143	15:B:844:BCR:C19	2.47	0.45
6:F:37:ARG:O	6:F:40:GLN:HG2	2.17	0.45
13:A:804:CLA:HAA1	13:A:811:CLA:H51	1.98	0.45
13:A:840:CLA:H202	13:A:841:CLA:HED1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:ARG:HG2	13:B:822:CLA:OBD	2.16	0.45
2:B:236:PRO:HB2	2:B:237:ASP:H	1.53	0.45
2:B:702:LYS:HA	2:B:703:PRO:HD3	1.84	0.45
2:B:724:ILE:HG23	13:B:825:CLA:CBB	2.46	0.45
11:M:26:SER:CB	15:M:1203:BCR:HC41	2.47	0.45
15:M:1203:BCR:H322	15:M:1203:BCR:HC8	1.98	0.45
1:A:42:PRO:HG2	6:F:99:ILE:HD13	1.98	0.45
1:A:58:PHE:CD1	13:A:805:CLA:HMC2	2.52	0.45
13:A:820:CLA:H102	13:A:820:CLA:H62	1.79	0.45
14:A:846:PQN:H172	15:B:846:BCR:C38	2.30	0.45
2:B:350:LEU:HD23	13:B:816:CLA:H61	1.99	0.45
15:B:846:BCR:H383	15:B:846:BCR:H23C	1.99	0.45
1:A:189:TRP:CD1	13:A:812:CLA:HED3	2.52	0.45
1:A:436:HIS:CD2	13:A:831:CLA:NA	2.85	0.45
1:A:517:VAL:HG13	1:A:527:MET:HB3	1.98	0.45
13:A:819:CLA:HBC3	13:A:819:CLA:HMC3	1.99	0.45
13:A:842:CLA:H202	13:J:1101:CLA:H203	1.99	0.45
14:A:846:PQN:H161	14:A:846:PQN:H141	1.75	0.45
2:B:143:ILE:HD12	2:B:143:ILE:HG23	1.76	0.45
2:B:176:HIS:CE1	13:B:810:CLA:NA	2.84	0.45
13:B:804:CLA:HED3	13:B:804:CLA:H102	1.99	0.45
3:C:62:LEU:H	3:C:62:LEU:HG	1.54	0.45
6:F:8:CYS:HB2	6:F:39:SER:HA	1.99	0.45
15:F:1302:BCR:H15C	15:F:1302:BCR:H351	1.85	0.45
1:A:174:PHE:HD2	13:A:810:CLA:CBC	2.29	0.45
13:A:818:CLA:H91	13:A:836:CLA:O1A	2.17	0.45
13:A:834:CLA:H91	13:A:834:CLA:H112	1.57	0.45
13:A:834:CLA:H151	15:B:849:BCR:H372	1.99	0.45
2:B:207:GLY:H	2:B:210:ASN:HD21	1.65	0.45
2:B:438:GLY:HA3	13:B:831:CLA:CBB	2.47	0.45
2:B:509:SER:O	2:B:509:SER:OG	2.32	0.45
13:B:811:CLA:CGA	13:B:811:CLA:H3A	2.47	0.45
6:F:54:ASP:OD1	12:X:30:TYR:CE2	2.69	0.45
1:A:304:ILE:HD12	13:A:819:CLA:HBB1	1.99	0.45
1:A:717:ILE:HD11	6:F:99:ILE:HG23	1.99	0.45
13:A:826:CLA:HAA2	13:A:826:CLA:CGD	2.47	0.45
2:B:208:TRP:NE1	13:B:812:CLA:O1D	2.50	0.45
2:B:256:PHE:CD1	13:B:815:CLA:HMB3	2.52	0.45
13:B:808:CLA:H201	7:I:26:VAL:HG21	1.99	0.45
13:B:809:CLA:HAA2	13:B:809:CLA:O1D	2.17	0.45
13:B:836:CLA:C4	13:B:836:CLA:H71	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:838:CLA:HAB	14:B:840:PQN:H172	1.99	0.45
4:D:38:VAL:HG22	4:D:48:VAL:HG22	1.98	0.45
6:F:15:GLN:O	6:F:18:ALA:HB3	2.17	0.45
1:A:269:THR:O	1:A:270:PHE:HB2	2.16	0.44
1:A:649:TRP:O	1:A:653:PHE:HB3	2.17	0.44
13:A:801:CLA:H102	13:A:801:CLA:H62	1.79	0.44
13:A:804:CLA:H91	13:A:804:CLA:H112	1.77	0.44
13:A:809:CLA:H91	13:A:809:CLA:H111	1.63	0.44
13:A:840:CLA:H61	13:B:830:CLA:H42	1.99	0.44
15:A:847:BCR:HC8	15:A:848:BCR:H383	1.99	0.44
2:B:111:PRO:HG2	7:I:1:MET:CE	2.46	0.44
2:B:487:ILE:HG23	13:B:833:CLA:HMD3	1.99	0.44
13:B:801:CLA:HAA2	13:B:801:CLA:O1D	2.15	0.44
13:B:812:CLA:H8	15:B:843:BCR:H363	1.99	0.44
13:B:820:CLA:CGD	13:B:820:CLA:CAA	2.95	0.44
13:B:838:CLA:HED2	7:I:31:PHE:CZ	2.52	0.44
1:A:219:VAL:HG13	1:A:239:PRO:HB3	1.99	0.44
1:A:451:LEU:HD13	1:A:544:PHE:HA	1.98	0.44
1:A:487:ALA:O	1:A:491:GLN:HG3	2.17	0.44
1:A:748:LEU:O	1:A:752:ILE:HB	2.17	0.44
2:B:481:LEU:HA	2:B:489:SER:OG	2.17	0.44
13:B:808:CLA:H111	13:B:808:CLA:H151	1.77	0.44
10:L:93:LEU:HD21	15:L:1005:BCR:H383	1.99	0.44
13:L:1003:CLA:H91	13:L:1003:CLA:H112	1.59	0.44
1:A:104:LEU:HD23	1:A:148:ARG:NH1	2.33	0.44
1:A:118:TRP:HH2	13:A:807:CLA:CGA	2.30	0.44
1:A:168:MET:HG3	15:A:848:BCR:H322	1.99	0.44
13:A:804:CLA:HAA2	13:A:804:CLA:CGD	2.46	0.44
13:A:830:CLA:H143	16:A:853:LHG:H351	1.98	0.44
2:B:230:GLY:HA2	13:B:814:CLA:CBA	2.48	0.44
13:B:816:CLA:H111	13:B:816:CLA:H143	1.77	0.44
6:F:76:TRP:CZ2	13:F:1301:CLA:HED3	2.53	0.44
13:L:1004:CLA:H112	13:L:1004:CLA:H91	1.73	0.44
1:A:329:LEU:HD12	1:A:345:TYR:HB2	1.98	0.44
1:A:334:GLY:N	16:A:854:LHG:HC32	2.32	0.44
13:A:840:CLA:H2	13:B:830:CLA:H42	1.98	0.44
13:A:842:CLA:H41	13:A:842:CLA:H62	1.71	0.44
15:A:852:BCR:H351	15:A:852:BCR:H15C	1.65	0.44
13:B:805:CLA:HHB	13:B:827:CLA:HAB	2.00	0.44
13:B:807:CLA:H51	13:B:807:CLA:C10	2.44	0.44
13:A:839:CLA:HAA2	13:A:839:CLA:O2D	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:849:BCR:C8	15:A:849:BCR:H331	2.48	0.44
2:B:400:ASP:OD1	4:D:129:LYS:NZ	2.43	0.44
13:B:803:CLA:H151	13:B:803:CLA:H111	1.80	0.44
13:B:822:CLA:HBA1	13:B:822:CLA:H3A	1.66	0.44
8:J:12:PRO:HD3	13:J:1101:CLA:C3D	2.48	0.44
1:A:44:THR:HB	1:A:720:ARG:HG2	1.99	0.44
1:A:48:ILE:CG2	13:J:1101:CLA:HBD	2.48	0.44
1:A:237:PRO:HB2	1:A:242:PHE:CE1	2.52	0.44
1:A:360:LEU:HD21	13:A:830:CLA:CHC	2.48	0.44
1:A:552:ILE:HG13	2:B:676:TYR:OH	2.18	0.44
13:A:803:CLA:HBA2	2:B:430:LEU:CD1	2.48	0.44
13:A:843:CLA:H192	10:L:58:LEU:HD21	1.99	0.44
2:B:60:VAL:HB	2:B:141:LEU:HD13	1.99	0.44
2:B:136:GLN:HE21	13:B:812:CLA:CGA	2.31	0.44
2:B:439:LEU:CD1	15:B:850:BCR:H342	2.45	0.44
2:B:718:HIS:CE1	13:B:839:CLA:C4D	3.00	0.44
13:B:803:CLA:CGA	13:B:803:CLA:H3A	2.48	0.44
4:D:107:LYS:HE3	4:D:107:LYS:HB3	1.80	0.44
1:A:215:HIS:HB2	13:A:814:CLA:C1C	2.48	0.44
1:A:483:GLN:HA	1:A:484:PRO:HD3	1.63	0.44
13:B:826:CLA:H192	15:B:843:BCR:C36	2.48	0.44
13:B:828:CLA:HMB1	13:B:829:CLA:C2D	2.47	0.44
14:B:840:PQN:H202	14:B:840:PQN:H161	1.77	0.44
13:M:1202:CLA:H3A	13:M:1202:CLA:HBA2	1.72	0.44
1:A:120:ILE:HD13	8:J:27:ILE:HG23	2.00	0.44
1:A:449:ILE:HD13	13:B:803:CLA:CBA	2.47	0.44
13:A:811:CLA:H91	13:A:811:CLA:H112	1.67	0.44
13:A:833:CLA:C3B	13:A:834:CLA:HMB1	2.48	0.44
2:B:21:TRP:CG	2:B:710:GLN:HE22	2.36	0.44
2:B:332:SER:O	2:B:336:GLN:HG3	2.17	0.44
2:B:390:PHE:CE1	15:B:845:BCR:H373	2.53	0.44
4:D:82:ILE:O	4:D:93:LEU:HD23	2.17	0.44
5:E:5:SER:O	5:E:22:THR:HA	2.17	0.44
6:F:41:ALA:HA	6:F:59:ARG:HH22	1.82	0.44
1:A:79:HIS:O	1:A:82:VAL:HG22	2.17	0.44
13:A:803:CLA:C15	13:A:842:CLA:HAB	2.26	0.44
2:B:669:PHE:HB2	2:B:715:GLY:CA	2.48	0.44
13:B:805:CLA:H152	13:B:805:CLA:H112	1.58	0.44
1:A:285:LEU:HD21	1:A:378:PRO:HD2	1.99	0.43
1:A:299:HIS:HE1	13:A:817:CLA:CHA	2.31	0.43
1:A:317:THR:OG1	1:A:318:ASN:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:CYS:HB3	2:B:673:TRP:HE3	1.83	0.43
13:A:832:CLA:HBA2	2:B:690:ARG:O	2.18	0.43
2:B:90:ILE:HG12	13:B:808:CLA:OBD	2.17	0.43
2:B:373:ALA:HB1	13:B:825:CLA:HMA1	2.00	0.43
2:B:523:PHE:HE1	13:B:836:CLA:C2D	2.31	0.43
13:B:827:CLA:H142	18:B:848:LMG:H231	2.00	0.43
8:J:32:PHE:C	8:J:34:PRO:HD3	2.43	0.43
9:K:59:LEU:C	9:K:61:ALA:N	2.76	0.43
1:A:356:LEU:HD13	13:A:805:CLA:C2D	2.48	0.43
1:A:699:GLU:HB2	2:B:542:LYS:NZ	2.34	0.43
13:A:819:CLA:H93	13:A:829:CLA:H203	2.00	0.43
13:A:834:CLA:CGD	13:A:834:CLA:HAA2	2.48	0.43
13:A:840:CLA:HAB	13:A:840:CLA:H122	2.00	0.43
2:B:208:TRP:CE2	13:B:812:CLA:HBD	2.54	0.43
13:B:819:CLA:HMD2	15:B:841:BCR:H24C	2.00	0.43
15:L:1005:BCR:H331	15:L:1005:BCR:HC8	2.00	0.43
13:A:803:CLA:H18	13:A:842:CLA:C5	2.37	0.43
13:A:805:CLA:CED	13:A:825:CLA:H12	2.43	0.43
13:A:826:CLA:HMA1	13:A:827:CLA:CED	2.48	0.43
2:B:261:HIS:CD2	2:B:264:THR:H	2.36	0.43
2:B:293:GLN:CD	13:B:810:CLA:HBA2	2.43	0.43
2:B:622:LEU:HD13	13:B:802:CLA:HMA3	2.00	0.43
4:D:131:THR:C	4:D:133:LYS:H	2.26	0.43
1:A:88:SER:HB3	1:A:165:GLY:HA3	2.00	0.43
1:A:211:ALA:HA	13:A:815:CLA:CBB	2.48	0.43
13:A:806:CLA:H152	13:A:806:CLA:H112	1.68	0.43
13:A:834:CLA:O1D	10:L:67:PRO:HD3	2.17	0.43
2:B:50:PHE:HB3	2:B:148:ALA:O	2.17	0.43
2:B:337:LEU:HD13	13:B:804:CLA:C2D	2.48	0.43
3:C:57:CYS:HB3	3:C:62:LEU:HD23	1.99	0.43
13:A:827:CLA:H91	13:A:827:CLA:H112	1.77	0.43
13:A:833:CLA:C2B	13:A:834:CLA:HMB1	2.48	0.43
13:A:843:CLA:H111	13:A:843:CLA:H91	1.77	0.43
2:B:91:TRP:HA	7:I:1:MET:SD	2.59	0.43
2:B:308:ASP:O	13:B:820:CLA:CBA	2.66	0.43
2:B:398:VAL:CG2	2:B:547:ALA:HB1	2.47	0.43
2:B:471:GLY:HA3	2:B:504:LEU:CD2	2.48	0.43
2:B:480:LEU:HD21	12:X:29:TYR:CE2	2.53	0.43
13:B:806:CLA:H121	15:M:1203:BCR:C12	2.49	0.43
13:B:813:CLA:HAB	15:B:841:BCR:H333	2.00	0.43
6:F:76:TRP:NE1	6:F:113:GLY:HA3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:1002:CLA:HAA2	13:L:1002:CLA:O1D	2.18	0.43
1:A:75:ALA:HB1	13:A:805:CLA:HBB1	2.00	0.43
1:A:587:CYS:HB2	2:B:673:TRP:CB	2.49	0.43
13:A:840:CLA:C16	13:A:841:CLA:HED1	2.47	0.43
2:B:337:LEU:O	2:B:341:LEU:HG	2.19	0.43
2:B:355:MET:HE1	13:B:826:CLA:OBD	2.17	0.43
2:B:390:PHE:HB3	2:B:540:LEU:HB3	2.00	0.43
2:B:548:ARG:HH22	4:D:124:ASN:CG	2.26	0.43
2:B:693:LEU:O	2:B:696:LEU:HB2	2.17	0.43
6:F:76:TRP:HZ2	13:F:1301:CLA:HED3	1.84	0.43
10:L:92:CYS:HB3	15:L:1005:BCR:C19	2.49	0.43
1:A:177:TRP:HB2	13:A:811:CLA:CMC	2.45	0.43
1:A:689:PHE:HA	14:A:846:PQN:H9	2.00	0.43
13:B:823:CLA:HMA2	13:B:824:CLA:HED3	2.00	0.43
4:D:95:HIS:HA	4:D:97:LYS:N	2.34	0.43
1:A:461:HIS:HE1	13:A:834:CLA:CHA	2.31	0.43
1:A:510:SER:HB2	13:A:827:CLA:CMC	2.48	0.43
1:A:536:PHE:HE1	13:A:838:CLA:C2D	2.31	0.43
1:A:547:HIS:CE1	13:A:839:CLA:NA	2.87	0.43
13:A:826:CLA:H71	13:A:835:CLA:HAB	2.01	0.43
2:B:260:PHE:CZ	2:B:358:LEU:HD23	2.53	0.43
2:B:682:GLU:CD	3:C:80:TYR:HE2	2.26	0.43
13:B:808:CLA:H201	7:I:26:VAL:HG23	1.99	0.43
10:L:41:LEU:HD23	10:L:41:LEU:HA	1.69	0.43
1:A:395:THR:HB	1:A:610:ILE:HG21	2.01	0.43
1:A:451:LEU:HD21	13:A:838:CLA:HMB2	2.01	0.43
13:B:801:CLA:O1A	13:B:802:CLA:HMD3	2.19	0.43
13:B:815:CLA:H42	13:B:824:CLA:CBB	2.49	0.43
10:L:89:ALA:O	10:L:92:CYS:HB2	2.18	0.43
1:A:152:ILE:HG23	1:A:157:GLN:HB2	2.00	0.43
1:A:202:ALA:HB1	13:A:820:CLA:HBC3	2.01	0.43
13:A:834:CLA:HAA2	13:A:834:CLA:O1D	2.19	0.43
13:A:840:CLA:H3A	13:A:840:CLA:HBA2	1.58	0.43
2:B:442:HIS:CD2	2:B:456:ILE:HG13	2.54	0.43
2:B:588:TRP:HH2	13:B:802:CLA:CBB	2.32	0.43
6:F:99:ILE:HG13	6:F:100:ILE:N	2.33	0.43
1:A:14:VAL:HG22	13:A:812:CLA:O1D	2.19	0.42
2:B:279:ILE:HD13	2:B:279:ILE:HA	1.89	0.42
2:B:535:THR:O	2:B:539:ILE:HG13	2.19	0.42
1:A:28:TRP:CZ2	13:A:804:CLA:H11	2.54	0.42
1:A:547:HIS:HE1	13:A:839:CLA:CHA	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:803:CLA:H162	13:A:842:CLA:H102	2.01	0.42
2:B:536:THR:HG21	13:B:823:CLA:HBC3	2.01	0.42
13:B:803:CLA:H201	13:B:839:CLA:H71	2.00	0.42
13:B:811:CLA:HAA2	13:B:811:CLA:O1D	2.18	0.42
13:B:815:CLA:H51	13:B:832:CLA:HED2	2.01	0.42
15:B:845:BCR:C8	15:B:845:BCR:H331	2.48	0.42
1:A:86:TRP:O	1:A:90:MET:HG2	2.19	0.42
1:A:242:PHE:HB3	1:A:249:MET:SD	2.59	0.42
1:A:325:LEU:HB2	1:A:345:TYR:HE1	1.84	0.42
1:A:443:HIS:CE1	13:A:832:CLA:NA	2.86	0.42
13:A:808:CLA:H112	13:A:808:CLA:H91	1.82	0.42
2:B:3:LYS:HG3	7:I:38:ALA:OXT	2.19	0.42
2:B:210:ASN:C	2:B:212:LEU:N	2.77	0.42
2:B:233:ALA:O	2:B:234:GLN:O	2.37	0.42
2:B:360:PRO:CG	13:B:816:CLA:HBA1	2.49	0.42
2:B:493:PRO:HG2	2:B:494:ASN:H	1.84	0.42
13:B:805:CLA:H191	18:B:848:LMG:H272	2.02	0.42
13:B:820:CLA:CGD	13:B:820:CLA:HAA1	2.49	0.42
7:I:7:ALA:CB	7:I:10:LEU:HD22	2.50	0.42
13:L:1003:CLA:C4C	15:L:1005:BCR:H281	2.49	0.42
1:A:33:HIS:CE1	13:A:804:CLA:HED3	2.54	0.42
1:A:461:HIS:HE1	13:A:834:CLA:C1A	2.32	0.42
13:A:840:CLA:H101	13:B:830:CLA:H11	2.02	0.42
14:B:840:PQN:H301	18:B:848:LMG:H201	2.01	0.42
15:B:849:BCR:H15C	15:B:849:BCR:H351	1.68	0.42
6:F:102:ASP:OD2	6:F:105:LEU:HB2	2.20	0.42
10:L:34:LEU:HG	13:L:1003:CLA:CGD	2.49	0.42
13:M:1201:CLA:HMB1	15:M:1203:BCR:HC42	2.02	0.42
1:A:83:VAL:CG2	13:A:806:CLA:HMC2	2.47	0.42
1:A:268:PHE:HA	13:A:844:CLA:HAC1	2.02	0.42
1:A:380:TYR:OH	13:A:829:CLA:O1D	2.34	0.42
1:A:429:VAL:HG23	13:A:824:CLA:HBC3	2.01	0.42
13:A:842:CLA:CGD	13:A:842:CLA:CAA	2.98	0.42
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.49	0.42
1:A:210:LEU:HD21	15:A:847:BCR:C34	2.50	0.42
13:A:823:CLA:HBB1	13:A:845:CLA:HAB	1.99	0.42
13:A:830:CLA:H41	13:A:830:CLA:H61	1.63	0.42
13:A:838:CLA:HBB1	13:A:839:CLA:HMD2	2.02	0.42
2:B:360:PRO:HB3	13:B:816:CLA:HBA1	2.01	0.42
2:B:481:LEU:HD11	13:B:832:CLA:OBD	2.20	0.42
13:B:834:CLA:HED2	13:B:834:CLA:O1A	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:1302:BCR:H11C	15:F:1302:BCR:H341	1.87	0.42
1:A:146:LEU:HA	1:A:380:TYR:HD2	1.84	0.42
1:A:655:TRP:CD1	13:B:801:CLA:HBC1	2.55	0.42
13:A:825:CLA:H2	13:A:825:CLA:C7	2.50	0.42
13:A:833:CLA:H51	15:B:847:BCR:C21	2.50	0.42
13:A:835:CLA:HBA2	13:A:835:CLA:H3A	1.75	0.42
13:A:843:CLA:H72	13:A:843:CLA:HBB1	2.00	0.42
2:B:333:LEU:HB3	13:B:804:CLA:HAC1	2.01	0.42
15:B:844:BCR:H351	15:B:844:BCR:H15C	1.74	0.42
6:F:55:GLY:H	15:F:1302:BCR:H282	1.84	0.42
6:F:132:LYS:HD2	6:F:135:GLU:CD	2.44	0.42
7:I:18:VAL:O	7:I:23:PRO:HD3	2.19	0.42
1:A:215:HIS:HB2	13:A:814:CLA:NC	2.34	0.42
1:A:624:THR:OG1	1:A:625:VAL:N	2.52	0.42
13:A:807:CLA:H3A	13:A:807:CLA:HBA2	1.80	0.42
2:B:103:PHE:HZ	2:B:651:VAL:HG22	1.82	0.42
2:B:480:LEU:C	2:B:482:SER:N	2.77	0.42
2:B:668:MET:HB2	13:B:803:CLA:CHC	2.50	0.42
2:B:699:TRP:CZ3	13:B:838:CLA:HBC3	2.54	0.42
2:B:703:PRO:HG2	13:B:838:CLA:CBC	2.49	0.42
13:B:820:CLA:HBB1	13:B:820:CLA:H93	2.00	0.42
13:B:831:CLA:H61	13:B:831:CLA:H41	1.47	0.42
13:B:836:CLA:H91	15:F:1302:BCR:H20C	2.02	0.42
1:A:314:MET:HE1	13:A:821:CLA:OBD	2.20	0.42
1:A:429:VAL:HG23	13:A:824:CLA:CBC	2.50	0.42
1:A:502:ALA:N	1:A:503:PRO:HD3	2.35	0.42
1:A:513:PHE:CE2	13:A:827:CLA:HBC2	2.55	0.42
13:A:806:CLA:CHC	13:A:829:CLA:HAB	2.49	0.42
13:A:809:CLA:H111	13:A:809:CLA:H142	1.85	0.42
13:A:832:CLA:C4	13:L:1003:CLA:H93	2.50	0.42
2:B:52:HIS:CG	13:B:804:CLA:HMA3	2.54	0.42
2:B:64:LEU:HD21	15:B:843:BCR:H271	2.01	0.42
2:B:182:PHE:HB3	2:B:283:PHE:CD2	2.54	0.42
2:B:724:ILE:HG23	13:B:825:CLA:CAB	2.50	0.42
3:C:16:CYS:SG	3:C:17:VAL:N	2.93	0.42
1:A:118:TRP:HZ3	13:A:809:CLA:CBA	2.33	0.42
1:A:590:SER:OG	1:A:593:ASP:OD2	2.29	0.42
2:B:162:PRO:HB2	2:B:167:PHE:CE1	2.55	0.42
13:B:807:CLA:CGD	13:B:807:CLA:HAA2	2.50	0.42
13:B:812:CLA:CAC	15:B:843:BCR:H353	2.50	0.42
13:B:811:CLA:H91	13:B:811:CLA:H111	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:826:CLA:H42	15:B:843:BCR:C39	2.49	0.41
13:B:830:CLA:H102	13:B:830:CLA:H62	1.76	0.41
13:B:836:CLA:H3A	13:B:837:CLA:OBD	2.20	0.41
13:B:838:CLA:HAA2	13:B:838:CLA:O1D	2.20	0.41
15:B:849:BCR:H21C	13:L:1003:CLA:HAB	2.01	0.41
6:F:103:VAL:O	6:F:107:ILE:HG13	2.20	0.41
7:I:17:VAL:HG22	7:I:21:LEU:HD23	2.02	0.41
1:A:53:ALA:HB2	16:A:853:LHG:HC82	2.02	0.41
1:A:118:TRP:HZ2	13:A:807:CLA:HED3	1.78	0.41
1:A:270:PHE:CE1	13:A:844:CLA:HMD1	2.55	0.41
11:M:29:LEU:HB3	13:M:1201:CLA:HBA2	2.01	0.41
1:A:225:LYS:HD3	1:A:252:LEU:HB3	2.02	0.41
1:A:244:LEU:C	1:A:246:PRO:HD3	2.46	0.41
1:A:511:VAL:HB	1:A:526:MET:CG	2.49	0.41
1:A:746:PHE:CD1	13:A:801:CLA:HMD2	2.55	0.41
13:A:838:CLA:HMB1	13:A:839:CLA:CAD	2.50	0.41
2:B:11:LEU:HD23	2:B:11:LEU:HA	1.90	0.41
2:B:140:PHE:CE1	13:B:812:CLA:H61	2.56	0.41
2:B:239:ALA:HA	2:B:262:PRO:HG3	2.01	0.41
2:B:700:LYS:NZ	7:I:35:GLU:O	2.47	0.41
11:M:26:SER:O	13:M:1201:CLA:CGA	2.68	0.41
1:A:16:VAL:HG11	1:A:183:ARG:HB3	2.03	0.41
1:A:660:GLN:HE21	1:A:754:VAL:HG13	1.85	0.41
13:A:817:CLA:CGD	13:A:817:CLA:CAA	2.94	0.41
13:A:838:CLA:CGD	13:A:838:CLA:CAA	2.98	0.41
2:B:241:HIS:HD2	2:B:247:GLN:O	2.03	0.41
2:B:274:HIS:HE1	13:B:814:CLA:CHA	2.33	0.41
2:B:309:PHE:CE1	13:B:820:CLA:H72	2.55	0.41
13:B:822:CLA:HAA2	13:B:822:CLA:CGD	2.50	0.41
1:A:86:TRP:HA	13:A:807:CLA:CBB	2.50	0.41
1:A:157:GLN:HG2	13:A:814:CLA:CED	2.50	0.41
5:E:6:LYS:HB3	5:E:20:VAL:CG1	2.50	0.41
1:A:118:TRP:CZ3	13:A:809:CLA:HBA1	2.51	0.41
2:B:377:HIS:HB2	13:B:825:CLA:CHB	2.51	0.41
2:B:479:THR:HG21	12:X:29:TYR:O	2.21	0.41
15:B:850:BCR:H21C	8:J:36:LEU:HD22	2.03	0.41
4:D:73:ARG:HB2	4:D:74:PRO:HD3	2.01	0.41
10:L:4:LEU:HD22	10:L:5:VAL:N	2.36	0.41
1:A:161:THR:CG2	15:A:848:BCR:HC32	2.51	0.41
1:A:178:PHE:O	1:A:182:LYS:HB2	2.21	0.41
1:A:356:LEU:HD23	1:A:411:HIS:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:HIS:O	1:A:400:ILE:HG12	2.20	0.41
13:A:832:CLA:H91	13:A:832:CLA:H112	1.68	0.41
13:A:842:CLA:H202	13:J:1101:CLA:H171	2.03	0.41
2:B:64:LEU:HD21	15:B:843:BCR:H281	2.01	0.41
2:B:228:ASN:O	2:B:231:VAL:HG23	2.20	0.41
2:B:457:LEU:O	6:F:51:LEU:N	2.53	0.41
2:B:723:TYR:CE1	13:B:801:CLA:CGA	3.04	0.41
13:B:836:CLA:H102	13:B:836:CLA:H62	1.88	0.41
15:B:849:BCR:C8	15:B:849:BCR:H321	2.50	0.41
15:B:850:BCR:H15C	15:B:850:BCR:H351	1.85	0.41
13:J:1101:CLA:H41	13:J:1101:CLA:H61	1.94	0.41
1:A:120:ILE:HD12	15:J:1105:BCR:C31	2.51	0.41
1:A:221:LEU:HD11	1:A:295:SER:HB3	2.02	0.41
1:A:299:HIS:HE1	13:A:817:CLA:C4D	2.34	0.41
1:A:343:GLY:O	1:A:347:VAL:HG23	2.21	0.41
13:A:843:CLA:H191	13:L:1003:CLA:CBB	2.51	0.41
14:A:846:PQN:H191	14:A:846:PQN:H212	1.77	0.41
2:B:444:ASP:OD1	2:B:621:TYR:HB2	2.21	0.41
15:B:849:BCR:H11C	15:B:849:BCR:H341	1.77	0.41
4:D:124:ASN:HB2	4:D:127:GLN:NE2	2.36	0.41
1:A:292:LEU:CD2	13:A:818:CLA:HBA1	2.51	0.41
1:A:411:HIS:HA	1:A:414:ILE:HD12	2.03	0.41
1:A:423:ALA:HA	4:D:38:VAL:HG11	2.02	0.41
1:A:484:PRO:HD2	1:A:488:GLN:NE2	2.35	0.41
1:A:605:CYS:O	1:A:609:VAL:HG23	2.20	0.41
1:A:624:THR:C	1:A:625:VAL:HG23	2.46	0.41
1:A:718:GLN:HA	1:A:719:PRO:HD3	1.97	0.41
13:A:802:CLA:C15	15:B:847:BCR:H12C	2.47	0.41
13:A:821:CLA:H3A	13:A:821:CLA:HBA2	1.31	0.41
13:A:821:CLA:H143	13:A:824:CLA:H93	2.02	0.41
13:A:826:CLA:H51	13:A:837:CLA:C2	2.51	0.41
13:A:833:CLA:HAA1	15:B:849:BCR:H363	2.03	0.41
13:A:840:CLA:O1D	2:B:427:TRP:HB2	2.21	0.41
2:B:157:GLN:HE22	11:M:28:GLU:CD	2.28	0.41
2:B:413:ARG:HD3	13:B:828:CLA:OBD	2.20	0.41
13:B:822:CLA:H61	13:B:822:CLA:H41	1.55	0.41
15:B:849:BCR:H392	15:B:849:BCR:C23	2.50	0.41
4:D:37:GLN:O	4:D:49:MET:HG2	2.21	0.41
1:A:252:LEU:H	1:A:252:LEU:HG	1.50	0.41
1:A:654:LEU:HD22	13:A:801:CLA:HMD3	2.03	0.41
1:A:695:GLY:O	1:A:699:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:808:CLA:H62	13:A:828:CLA:H92	2.03	0.41
13:A:817:CLA:OBD	13:A:836:CLA:HED3	2.21	0.41
2:B:6:LYS:NZ	11:M:30:TYR:HB3	2.36	0.41
2:B:175:ASN:HB3	13:B:818:CLA:HMD2	2.03	0.41
2:B:425:LEU:CG	13:B:837:CLA:HBB1	2.31	0.41
13:B:804:CLA:H111	13:B:804:CLA:H142	1.83	0.41
4:D:12:GLY:HA2	10:L:12:PRO:O	2.21	0.41
13:I:101:CLA:H111	13:I:101:CLA:H91	1.74	0.41
1:A:28:TRP:CG	13:A:811:CLA:H12	2.55	0.40
1:A:143:LEU:O	1:A:146:LEU:HB3	2.21	0.40
1:A:257:ASP:O	1:A:258:TRP:HB2	2.20	0.40
1:A:332:HIS:HE1	13:A:823:CLA:CHA	2.33	0.40
13:A:826:CLA:HED3	13:A:827:CLA:HMD2	2.02	0.40
15:A:852:BCR:C36	13:B:802:CLA:H42	2.27	0.40
2:B:140:PHE:CZ	13:B:812:CLA:H61	2.55	0.40
2:B:387:VAL:HG11	2:B:586:MET:SD	2.61	0.40
2:B:465:PHE:HB2	12:X:30:TYR:CE1	2.55	0.40
2:B:473:LEU:O	2:B:476:GLY:N	2.46	0.40
13:B:822:CLA:CMB	13:B:822:CLA:HBB1	2.50	0.40
13:B:834:CLA:HBB1	13:B:834:CLA:HHC	2.03	0.40
6:F:99:ILE:HG13	6:F:100:ILE:HG13	2.04	0.40
13:A:843:CLA:HMD2	2:B:684:LEU:HD13	2.02	0.40
2:B:260:PHE:HZ	2:B:358:LEU:HD23	1.86	0.40
2:B:357:SER:C	2:B:359:PRO:HD3	2.46	0.40
2:B:638:ILE:HD11	2:B:656:PHE:CE2	2.57	0.40
2:B:703:PRO:HG2	13:B:838:CLA:HBC3	2.04	0.40
15:L:1005:BCR:HC41	13:M:1201:CLA:HMD2	2.03	0.40
1:A:114:ALA:O	1:A:115:GLN:C	2.64	0.40
1:A:333:LYS:O	13:A:845:CLA:HBC3	2.21	0.40
1:A:480:ILE:HD11	10:L:69:ARG:NH1	2.37	0.40
1:A:622:TRP:O	1:A:633:HIS:HD2	2.05	0.40
13:A:825:CLA:HAB	15:A:850:BCR:H341	2.03	0.40
13:A:833:CLA:CED	13:A:843:CLA:H11	2.51	0.40
13:A:845:CLA:HAA2	13:A:845:CLA:CBD	2.50	0.40
2:B:122:TRP:HZ2	15:B:843:BCR:H401	1.86	0.40
2:B:279:ILE:CD1	13:B:815:CLA:HBC2	2.51	0.40
13:B:806:CLA:H12	7:I:18:VAL:CG2	2.27	0.40
13:B:824:CLA:H122	15:B:845:BCR:H17C	2.02	0.40
15:B:849:BCR:H23C	15:B:849:BCR:C39	2.49	0.40
15:F:1302:BCR:H342	15:F:1302:BCR:H331	2.04	0.40
10:L:92:CYS:HB3	15:L:1005:BCR:C20	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:20:LEU:O	12:X:23:ASN:HB3	2.22	0.40
1:A:137:ILE:HG21	13:A:808:CLA:CHD	2.52	0.40
1:A:182:LYS:HA	1:A:182:LYS:HD3	1.87	0.40
1:A:257:ASP:CG	1:A:258:TRP:N	2.79	0.40
1:A:688:MET:HB2	13:A:803:CLA:CHC	2.51	0.40
2:B:137:GLY:HA2	13:B:812:CLA:O1A	2.22	0.40
2:B:142:LEU:HD12	2:B:142:LEU:HA	1.89	0.40
2:B:466:ILE:HD12	13:B:835:CLA:CED	2.51	0.40
2:B:642:ASN:HB2	2:B:643:PRO:HD2	2.03	0.40
2:B:721:VAL:CG2	13:B:827:CLA:H152	2.52	0.40
13:B:824:CLA:H121	15:B:844:BCR:C20	2.52	0.40
9:K:36:SER:C	9:K:38:GLY:H	2.24	0.40
1:A:171:LEU:HD12	13:A:810:CLA:HBC1	2.02	0.40
1:A:325:LEU:HB2	1:A:345:TYR:CE1	2.57	0.40
1:A:741:ALA:O	1:A:744:TRP:HB3	2.22	0.40
13:A:814:CLA:CGD	13:A:814:CLA:CAA	2.93	0.40
13:A:819:CLA:H8	13:A:819:CLA:CAB	2.46	0.40
13:A:819:CLA:CMA	13:A:819:CLA:HBA2	2.50	0.40
2:B:43:GLN:NE2	2:B:161:ARG:HB3	2.36	0.40
2:B:288:HIS:NE2	15:B:841:BCR:H363	2.37	0.40
2:B:541:VAL:HG22	15:B:844:BCR:H281	2.04	0.40
13:B:801:CLA:H2	13:B:802:CLA:C3D	2.51	0.40
13:B:830:CLA:HBB2	15:B:846:BCR:HC41	2.04	0.40
13:B:835:CLA:H112	13:B:835:CLA:H91	1.71	0.40
5:E:15:TYR:CE2	5:E:44:ASN:HA	2.57	0.40
7:I:19:CYS:HB3	13:I:101:CLA:CBB	2.51	0.40
8:J:30:ASN:ND2	15:J:1104:BCR:H332	2.36	0.40
12:X:9:TYR:O	12:X:10:ALA:HB2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:40:GLY:O	10:L:114:SER:OG[3_665]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/755 (98%)	685 (93%)	39 (5%)	12 (2%)	7	37
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	10	42
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	9	41
4	D	136/138 (99%)	123 (90%)	8 (6%)	5 (4%)	2	19
5	E	67/75 (89%)	53 (79%)	6 (9%)	8 (12%)	0	5
6	F	139/164 (85%)	127 (91%)	8 (6%)	4 (3%)	3	23
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	42/83 (51%)	30 (71%)	5 (12%)	7 (17%)	0	3
10	L	149/154 (97%)	138 (93%)	9 (6%)	2 (1%)	9	41
11	M	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3	20
12	X	27/35 (77%)	21 (78%)	5 (18%)	1 (4%)	2	19
All	All	2215/2334 (95%)	2039 (92%)	126 (6%)	50 (2%)	5	28

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	235	ASP
2	B	211	PHE
2	B	234	GLN
2	B	480	LEU
2	B	492	TRP
2	B	510	GLY
3	C	62	LEU
4	D	2	THR
6	F	55	GLY
6	F	91	SER
9	K	37	ARG

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Mol	Chain	Res	Type
9	K	41	PRO
9	K	42	GLY
12	X	10	ALA
1	A	578	CYS
2	B	236	PRO
2	B	565	CYS
4	D	3	LEU
5	E	36	VAL
5	E	55	VAL
6	F	60	ALA
9	K	74	VAL
10	L	104	GLY
10	L	106	SER
1	A	115	GLN
1	A	234	LYS
1	A	499	GLY
2	B	310	PHE
4	D	44	ALA
5	E	53	SER
6	F	89	ARG
9	K	75	SER
1	A	232	ALA
1	A	250	ALA
1	A	625	VAL
4	D	107	LYS
5	E	25	SER
5	E	35	PRO
5	E	68	VAL
1	A	42	PRO
1	A	182	LYS
1	A	498	PRO
2	B	481	LEU
4	D	108	GLY
11	M	30	TYR
5	E	30	PRO
9	K	40	GLY
9	K	56	LEU
5	E	54	GLY

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	589/603 (98%)	561 (95%)	28 (5%)	23	45
2	B	595/597 (100%)	565 (95%)	30 (5%)	22	43
3	C	67/67 (100%)	64 (96%)	3 (4%)	24	46
4	D	115/115 (100%)	107 (93%)	8 (7%)	14	36
5	E	59/64 (92%)	57 (97%)	2 (3%)	32	54
6	F	109/128 (85%)	105 (96%)	4 (4%)	30	51
7	I	32/32 (100%)	30 (94%)	2 (6%)	16	38
8	J	36/36 (100%)	35 (97%)	1 (3%)	38	59
10	L	117/119 (98%)	108 (92%)	9 (8%)	12	32
11	M	26/26 (100%)	23 (88%)	3 (12%)	5	19
12	X	20/24 (83%)	19 (95%)	1 (5%)	22	43
All	All	1765/1811 (98%)	1674 (95%)	91 (5%)	21	43

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	145	GLN
1	A	147	TRP
1	A	155	GLU
1	A	172	MET
1	A	186	LYS
1	A	210	LEU
1	A	216	GLN
1	A	221	LEU
1	A	235	ASP
1	A	252	LEU
1	A	260	PHE
1	A	276	SER
1	A	349	THR
1	A	360	LEU

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Mol	Chain	Res	Type
1	A	368	ILE
1	A	385	THR
1	A	395	THR
1	A	433	VAL
1	A	447	VAL
1	A	466	ARG
1	A	518	VAL
1	A	538	VAL
1	A	587	CYS
1	A	675	LEU
1	A	705	VAL
1	A	713	VAL
1	A	752	ILE
2	B	53	LEU
2	B	78	GLN
2	B	142	LEU
2	B	159	LYS
2	B	171	GLU
2	B	214	THR
2	B	218	PRO
2	B	221	LEU
2	B	279	ILE
2	B	296	ILE
2	B	301	LYS
2	B	318	PHE
2	B	349	SER
2	B	411	LEU
2	B	419	GLU
2	B	430	LEU
2	B	446	VAL
2	B	479	THR
2	B	480	LEU
2	B	525	VAL
2	B	574	CYS
2	B	582	PHE
2	B	589	MET
2	B	596	VAL
2	B	605	LEU
2	B	632	LEU
2	B	638	ILE
2	B	651	VAL
2	B	697	VAL

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Mol	Chain	Res	Type
2	B	698	ARG
3	C	15	GLN
3	C	65	ARG
3	C	75	SER
4	D	1	THR
4	D	61	LYS
4	D	73	ARG
4	D	93	LEU
4	D	104	LYS
4	D	105	VAL
4	D	117	ARG
4	D	125	PRO
5	E	1	VAL
5	E	63	HIS
6	F	1	ASP
6	F	56	ARG
6	F	80	VAL
6	F	105	LEU
7	I	10	LEU
7	I	15	ILE
8	J	19	MET
10	L	4	LEU
10	L	34	LEU
10	L	44	ILE
10	L	48	LEU
10	L	68	LEU
10	L	69	ARG
10	L	85	LEU
10	L	134	VAL
10	L	148	ILE
11	M	3	LEU
11	M	16	LEU
11	M	17	LEU
12	X	8	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	218	HIS
1	A	542	HIS
1	A	618	GLN

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Mol	Chain	Res	Type
2	B	52	HIS
2	B	136	GLN
2	B	210	ASN
2	B	228	ASN
2	B	261	HIS
3	C	37	GLN
4	D	71	GLN
4	D	127	GLN
5	E	18	ASN
10	L	119	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	SF4	A	856	2,1	0,12,12	-	-	-		
13	CLA	A	836	1	49,53,73	1.79	13 (26%)	58,89,113	1.94	6 (10%)
13	CLA	A	818	1	58,62,73	1.75	16 (27%)	68,99,113	2.06	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	824	1	63,67,73	1.70	18 (28%)	74,105,113	1.99	13 (17%)
14	PQN	B	840	-	34,34,34	0.92	1 (2%)	43,45,45	1.40	5 (11%)
13	CLA	B	822	-	58,62,73	1.80	18 (31%)	68,99,113	2.03	10 (14%)
13	CLA	A	807	1	55,59,73	1.80	15 (27%)	64,96,113	2.12	11 (17%)
13	CLA	A	837	-	55,59,73	1.84	15 (27%)	64,96,113	2.08	14 (21%)
15	BCR	J	1104	-	41,41,41	2.14	20 (48%)	56,56,56	2.27	23 (41%)
15	BCR	B	841	-	41,41,41	2.12	20 (48%)	56,56,56	2.13	22 (39%)
16	LHG	X	101	-	22,22,48	1.35	2 (9%)	25,28,54	1.03	1 (4%)
13	CLA	B	808	2	69,73,73	1.63	15 (21%)	82,113,113	1.88	10 (12%)
13	CLA	B	815	2	63,67,73	1.70	17 (26%)	74,105,113	1.75	10 (13%)
15	BCR	B	849	-	41,41,41	2.04	18 (43%)	56,56,56	2.36	20 (35%)
13	CLA	B	802	-	69,73,73	1.65	18 (26%)	82,113,113	2.08	13 (15%)
13	CLA	A	833	1	69,73,73	1.62	17 (24%)	82,113,113	1.71	8 (9%)
13	CLA	A	855	-	49,53,73	1.79	13 (26%)	58,89,113	2.03	9 (15%)
15	BCR	A	847	-	41,41,41	2.14	21 (51%)	56,56,56	2.07	21 (37%)
15	BCR	B	844	-	25,25,41	2.19	13 (52%)	33,33,56	2.12	12 (36%)
13	CLA	B	805	-	69,73,73	1.59	16 (23%)	82,113,113	1.77	10 (12%)
13	CLA	A	813	1	64,68,73	1.66	15 (23%)	76,107,113	1.91	11 (14%)
15	BCR	A	851	-	41,41,41	2.12	20 (48%)	56,56,56	2.18	19 (33%)
13	CLA	B	833	-	49,53,73	1.78	13 (26%)	58,89,113	2.10	5 (8%)
13	CLA	A	835	1	58,62,73	1.76	18 (31%)	68,99,113	1.81	7 (10%)
13	CLA	A	822	1	53,57,73	1.78	13 (24%)	61,93,113	2.21	9 (14%)
13	CLA	A	830	1	69,73,73	1.57	16 (23%)	82,113,113	1.90	12 (14%)
15	BCR	B	845	-	41,41,41	2.10	18 (43%)	56,56,56	2.39	22 (39%)
13	CLA	B	803	-	69,73,73	1.63	18 (26%)	82,113,113	1.78	10 (12%)
13	CLA	M	1202	-	49,53,73	1.77	13 (26%)	58,89,113	2.12	9 (15%)
15	BCR	L	1005	-	41,41,41	2.10	20 (48%)	56,56,56	2.28	24 (42%)
13	CLA	A	803	-	69,73,73	1.62	16 (23%)	82,113,113	1.74	12 (14%)
13	CLA	A	816	-	53,57,73	1.74	13 (24%)	61,93,113	1.89	8 (13%)
13	CLA	A	829	1	69,73,73	1.60	18 (26%)	82,113,113	1.93	12 (14%)
18	LMG	B	848	-	55,55,55	1.06	8 (14%)	63,63,63	1.22	3 (4%)
15	BCR	B	843	-	41,41,41	2.09	21 (51%)	56,56,56	2.42	26 (46%)
13	CLA	A	809	1	69,73,73	1.64	17 (24%)	82,113,113	2.01	16 (19%)
15	BCR	M	1203	-	41,41,41	2.09	18 (43%)	56,56,56	2.30	21 (37%)
15	BCR	L	1006	-	41,41,41	2.13	21 (51%)	56,56,56	2.04	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	X	102	12	49,53,73	1.81	15 (30%)	58,89,113	2.21	8 (13%)
15	BCR	A	850	-	41,41,41	2.18	21 (51%)	56,56,56	2.20	20 (35%)
13	CLA	A	806	-	69,73,73	1.60	15 (21%)	82,113,113	1.76	12 (14%)
13	CLA	B	809	2	49,53,73	1.78	14 (28%)	58,89,113	2.05	9 (15%)
13	CLA	A	804	13,1	63,67,73	1.71	16 (25%)	74,105,113	1.82	10 (13%)
13	CLA	A	812	1	58,62,73	1.74	16 (27%)	68,99,113	2.09	12 (17%)
13	CLA	A	805	-	69,73,73	1.61	17 (24%)	82,113,113	1.77	9 (10%)
14	PQN	A	846	-	34,34,34	0.99	1 (2%)	43,45,45	1.21	4 (9%)
17	SF4	C	102	3	0,12,12	-	-	-	-	-
13	CLA	J	1103	8	41,45,73	1.96	13 (31%)	50,78,113	1.68	4 (8%)
13	CLA	A	842	1	69,73,73	1.66	18 (26%)	82,113,113	1.63	9 (10%)
13	CLA	B	806	2	69,73,73	1.63	17 (24%)	82,113,113	1.88	12 (14%)
15	BCR	B	850	-	41,41,41	2.13	21 (51%)	56,56,56	2.38	23 (41%)
13	CLA	B	807	2	69,73,73	1.64	18 (26%)	82,113,113	1.92	11 (13%)
13	CLA	B	818	2	51,55,73	1.80	15 (29%)	60,91,113	1.84	5 (8%)
13	CLA	B	810	2	49,53,73	1.80	15 (30%)	58,89,113	1.87	7 (12%)
13	CLA	A	845	16	56,60,73	1.74	16 (28%)	65,97,113	2.12	14 (21%)
13	CLA	A	810	1	49,53,73	1.76	13 (26%)	58,89,113	2.12	8 (13%)
13	CLA	B	821	2	49,53,73	1.81	13 (26%)	58,89,113	1.85	9 (15%)
13	CLA	B	804	-	69,73,73	1.61	16 (23%)	82,113,113	1.80	11 (13%)
13	CLA	A	819	1	69,73,73	1.59	17 (24%)	82,113,113	2.03	13 (15%)
13	CLA	A	821	-	69,73,73	1.61	17 (24%)	82,113,113	1.93	11 (13%)
13	CLA	A	801	1	69,73,73	1.65	18 (26%)	82,113,113	1.83	13 (15%)
13	CLA	A	826	-	69,73,73	1.65	15 (21%)	82,113,113	1.83	13 (15%)
15	BCR	B	847	-	41,41,41	2.12	20 (48%)	56,56,56	2.29	21 (37%)
13	CLA	L	1003	10	69,73,73	1.62	17 (24%)	82,113,113	1.95	14 (17%)
13	CLA	A	841	-	55,59,73	1.79	13 (23%)	64,96,113	1.86	8 (12%)
13	CLA	B	834	-	49,53,73	1.78	13 (26%)	58,89,113	2.04	8 (13%)
13	CLA	A	840	1	69,73,73	1.61	17 (24%)	82,113,113	1.89	12 (14%)
13	CLA	A	839	1	51,55,73	1.73	11 (21%)	60,91,113	2.10	8 (13%)
13	CLA	M	1201	2	58,62,73	1.76	17 (29%)	68,99,113	2.09	13 (19%)
15	BCR	I	102	-	41,41,41	2.02	17 (41%)	56,56,56	2.35	24 (42%)
13	CLA	B	813	2	49,53,73	1.81	14 (28%)	58,89,113	2.05	9 (15%)
15	BCR	F	1302	-	41,41,41	2.10	21 (51%)	56,56,56	2.22	21 (37%)
13	CLA	A	834	1	69,73,73	1.66	19 (27%)	82,113,113	1.75	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	835	-	64,68,73	1.72	15 (23%)	76,107,113	1.89	15 (19%)
13	CLA	B	816	2	64,68,73	1.69	17 (26%)	76,107,113	1.84	13 (17%)
13	CLA	A	844	-	45,49,73	1.82	13 (28%)	54,83,113	1.67	8 (14%)
13	CLA	J	1102	8	49,53,73	1.77	12 (24%)	58,89,113	2.04	7 (12%)
13	CLA	B	824	2	69,73,73	1.62	15 (21%)	82,113,113	1.84	11 (13%)
13	CLA	B	826	2	69,73,73	1.62	17 (24%)	82,113,113	1.66	7 (8%)
13	CLA	B	823	-	50,54,73	1.81	13 (26%)	59,90,113	1.99	11 (18%)
13	CLA	A	802	-	69,73,73	1.65	18 (26%)	82,113,113	1.71	7 (8%)
13	CLA	J	1101	-	69,73,73	1.61	14 (20%)	82,113,113	1.88	14 (17%)
16	LHG	A	853	-	48,48,48	0.94	2 (4%)	51,54,54	1.07	2 (3%)
13	CLA	B	838	-	69,73,73	1.63	15 (21%)	82,113,113	1.92	13 (15%)
13	CLA	A	831	1	54,58,73	1.80	16 (29%)	64,95,113	1.92	9 (14%)
13	CLA	A	828	1	69,73,73	1.60	15 (21%)	82,113,113	1.84	11 (13%)
13	CLA	B	828	2	49,53,73	1.80	16 (32%)	58,89,113	1.96	7 (12%)
13	CLA	A	843	-	69,73,73	1.60	16 (23%)	82,113,113	1.87	12 (14%)
13	CLA	B	820	-	59,63,73	1.74	16 (27%)	70,101,113	1.83	10 (14%)
13	CLA	I	101	-	69,73,73	1.65	18 (26%)	82,113,113	1.91	14 (17%)
15	BCR	B	846	-	41,41,41	2.13	20 (48%)	56,56,56	2.09	19 (33%)
13	CLA	A	811	13,1	69,73,73	1.62	16 (23%)	82,113,113	1.90	11 (13%)
13	CLA	B	832	2	49,53,73	1.79	14 (28%)	58,89,113	2.01	9 (15%)
13	CLA	A	832	1	69,73,73	1.62	17 (24%)	82,113,113	1.93	11 (13%)
13	CLA	A	820	1	65,69,73	1.70	18 (27%)	77,108,113	1.82	13 (16%)
13	CLA	B	819	2	49,53,73	1.79	15 (30%)	58,89,113	2.03	8 (13%)
13	CLA	B	830	2	69,73,73	1.61	16 (23%)	82,113,113	1.87	9 (10%)
16	LHG	A	854	13	26,26,48	1.27	2 (7%)	29,32,54	1.17	2 (6%)
13	CLA	A	808	1	69,73,73	1.66	15 (21%)	82,113,113	2.06	12 (14%)
15	BCR	A	849	-	41,41,41	2.03	18 (43%)	56,56,56	2.25	23 (41%)
13	CLA	B	839	2	69,73,73	1.61	17 (24%)	82,113,113	1.78	11 (13%)
17	SF4	C	101	3	0,12,12	-	-	-	-	-
13	CLA	L	1004	-	69,73,73	1.61	16 (23%)	82,113,113	1.86	10 (12%)
13	CLA	A	827	-	69,73,73	1.61	16 (23%)	82,113,113	1.84	11 (13%)
15	BCR	A	848	-	41,41,41	2.14	20 (48%)	56,56,56	2.15	21 (37%)
13	CLA	B	837	2	51,55,73	1.75	15 (29%)	60,91,113	1.98	8 (13%)
15	BCR	A	852	-	41,41,41	2.15	21 (51%)	56,56,56	2.29	19 (33%)
13	CLA	A	825	-	69,73,73	1.62	16 (23%)	82,113,113	1.86	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	817	1	58,62,73	1.75	15 (25%)	68,99,113	1.83	11 (16%)
13	CLA	L	1002	10	69,73,73	1.62	18 (26%)	82,113,113	1.86	11 (13%)
13	CLA	B	817	-	69,73,73	1.62	17 (24%)	82,113,113	1.88	9 (10%)
13	CLA	B	825	2	69,73,73	1.64	15 (21%)	82,113,113	1.73	8 (9%)
13	CLA	B	814	2	59,63,73	1.70	15 (25%)	70,101,113	2.02	12 (17%)
13	CLA	B	812	2	69,73,73	1.63	18 (26%)	82,113,113	1.90	10 (12%)
13	CLA	A	823	1	55,59,73	1.79	16 (29%)	64,96,113	1.84	9 (14%)
13	CLA	F	1301	-	49,53,73	1.84	13 (26%)	58,89,113	2.11	11 (18%)
13	CLA	B	801	2	69,73,73	1.63	18 (26%)	82,113,113	1.80	11 (13%)
13	CLA	B	831	2	62,66,73	1.71	16 (25%)	73,104,113	2.10	12 (16%)
13	CLA	A	838	1	69,73,73	1.64	19 (27%)	82,113,113	1.89	12 (14%)
13	CLA	A	814	1	49,53,73	1.80	15 (30%)	58,89,113	1.92	9 (15%)
13	CLA	B	829	2	53,57,73	1.73	14 (26%)	61,93,113	1.84	11 (18%)
15	BCR	J	1105	-	41,41,41	2.14	20 (48%)	56,56,56	2.16	22 (39%)
15	BCR	B	842	-	41,41,41	2.16	21 (51%)	56,56,56	2.29	19 (33%)
13	CLA	B	827	2	69,73,73	1.60	16 (23%)	82,113,113	1.95	13 (15%)
13	CLA	A	815	1	49,53,73	1.77	14 (28%)	58,89,113	2.06	11 (18%)
13	CLA	B	836	2	69,73,73	1.63	18 (26%)	82,113,113	1.81	11 (13%)
13	CLA	B	811	-	69,73,73	1.65	16 (23%)	82,113,113	1.85	9 (10%)

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
17	SF4	A	856	2,1	-	-	0/6/5/5
13	CLA	A	836	1	-	6/15/91/115	-
13	CLA	A	818	1	-	7/26/102/115	-
13	CLA	A	824	1	-	9/32/108/115	-
14	PQN	B	840	-	-	5/23/43/43	0/2/2/2
13	CLA	B	822	-	-	9/26/102/115	-
13	CLA	A	807	1	-	6/23/99/115	-
13	CLA	A	837	-	-	4/23/99/115	-
15	BCR	J	1104	-	-	11/29/63/63	0/2/2/2
15	BCR	B	841	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LHG	X	101	-	-	8/26/26/53	-
13	CLA	B	808	2	-	9/39/115/115	-
13	CLA	B	815	2	-	9/32/108/115	-
15	BCR	B	849	-	-	14/29/63/63	0/2/2/2
13	CLA	B	802	-	-	12/39/115/115	-
13	CLA	A	833	1	-	8/39/115/115	-
13	CLA	A	855	-	-	2/15/91/115	-
15	BCR	A	847	-	-	8/29/63/63	0/2/2/2
15	BCR	B	844	-	-	6/18/35/63	0/1/1/2
13	CLA	B	805	-	-	7/39/115/115	-
13	CLA	A	813	1	-	9/33/109/115	-
15	BCR	A	851	-	-	8/29/63/63	0/2/2/2
13	CLA	B	833	-	-	6/15/91/115	-
13	CLA	A	835	1	-	7/26/102/115	-
13	CLA	A	822	1	-	7/20/96/115	-
13	CLA	A	830	1	-	10/39/115/115	-
15	BCR	B	845	-	-	10/29/63/63	0/2/2/2
13	CLA	B	803	-	-	13/39/115/115	-
13	CLA	M	1202	-	-	4/15/91/115	-
15	BCR	L	1005	-	-	9/29/63/63	0/2/2/2
13	CLA	A	803	-	-	8/39/115/115	-
13	CLA	A	816	-	-	5/20/96/115	-
13	CLA	A	829	1	-	10/39/115/115	-
18	LMG	B	848	-	-	11/50/70/70	0/1/1/1
15	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	A	809	1	-	10/39/115/115	-
15	BCR	M	1203	-	-	15/29/63/63	0/2/2/2
15	BCR	L	1006	-	-	8/29/63/63	0/2/2/2
13	CLA	X	102	12	-	7/15/91/115	-
15	BCR	A	850	-	-	6/29/63/63	0/2/2/2
13	CLA	A	806	-	-	8/39/115/115	-
13	CLA	B	809	2	-	4/15/91/115	-
13	CLA	A	804	13,1	-	8/32/108/115	-
13	CLA	A	812	1	-	9/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	805	-	-	9/39/115/115	-
14	PQN	A	846	-	-	6/23/43/43	0/2/2/2
17	SF4	C	102	3	-	-	0/6/5/5
13	CLA	J	1103	8	-	2/4/76/115	-
13	CLA	A	842	1	-	16/39/115/115	-
13	CLA	B	806	2	-	12/39/115/115	-
15	BCR	B	850	-	-	7/29/63/63	0/2/2/2
13	CLA	B	807	2	-	16/39/115/115	-
13	CLA	B	818	2	-	4/18/94/115	-
13	CLA	B	810	2	-	5/15/91/115	-
13	CLA	A	845	16	-	5/24/100/115	-
13	CLA	A	810	1	-	7/15/91/115	-
13	CLA	B	821	2	-	3/15/91/115	-
13	CLA	B	804	-	-	6/39/115/115	-
13	CLA	A	819	1	-	13/39/115/115	-
13	CLA	A	821	-	-	15/39/115/115	-
13	CLA	A	801	1	-	8/39/115/115	-
13	CLA	A	826	-	-	8/39/115/115	-
15	BCR	B	847	-	-	12/29/63/63	0/2/2/2
13	CLA	L	1003	10	-	15/39/115/115	-
13	CLA	A	841	-	-	5/23/99/115	-
13	CLA	B	834	-	-	3/15/91/115	-
13	CLA	A	840	1	-	12/39/115/115	-
13	CLA	A	839	1	-	5/18/94/115	-
13	CLA	M	1201	2	-	7/26/102/115	-
15	BCR	I	102	-	-	15/29/63/63	0/2/2/2
13	CLA	B	813	2	-	5/15/91/115	-
15	BCR	F	1302	-	-	10/29/63/63	0/2/2/2
13	CLA	A	834	1	-	12/39/115/115	-
13	CLA	B	835	-	-	9/33/109/115	-
13	CLA	B	816	2	-	6/33/109/115	-
13	CLA	A	844	-	-	4/9/81/115	-
13	CLA	J	1102	8	-	5/15/91/115	-
13	CLA	B	824	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	826	2	-	13/39/115/115	-
13	CLA	B	823	-	-	3/17/93/115	-
13	CLA	A	802	-	-	5/39/115/115	-
13	CLA	J	1101	-	-	7/39/115/115	-
16	LHG	A	853	-	-	20/53/53/53	-
13	CLA	B	838	-	-	14/39/115/115	-
13	CLA	A	831	1	-	3/21/97/115	-
13	CLA	A	828	1	-	16/39/115/115	-
13	CLA	B	828	2	-	5/15/91/115	-
13	CLA	A	843	-	-	8/39/115/115	-
13	CLA	B	820	-	-	8/27/103/115	-
13	CLA	I	101	-	-	11/39/115/115	-
15	BCR	B	846	-	-	8/29/63/63	0/2/2/2
13	CLA	A	811	13,1	-	15/39/115/115	-
13	CLA	B	832	2	-	3/15/91/115	-
13	CLA	A	832	1	-	17/39/115/115	-
13	CLA	A	820	1	-	10/35/111/115	-
13	CLA	B	819	2	-	2/15/91/115	-
13	CLA	B	830	2	-	11/39/115/115	-
16	LHG	A	854	13	-	8/31/31/53	-
13	CLA	A	808	1	-	12/39/115/115	-
15	BCR	A	849	-	-	5/29/63/63	0/2/2/2
13	CLA	B	839	2	-	8/39/115/115	-
17	SF4	C	101	3	-	-	0/6/5/5
13	CLA	L	1004	-	-	11/39/115/115	-
13	CLA	A	827	-	-	10/39/115/115	-
15	BCR	A	848	-	-	11/29/63/63	0/2/2/2
13	CLA	B	837	2	-	5/18/94/115	-
15	BCR	A	852	-	-	12/29/63/63	0/2/2/2
13	CLA	A	825	-	-	6/39/115/115	-
13	CLA	A	817	1	-	4/26/102/115	-
13	CLA	L	1002	10	-	10/39/115/115	-
13	CLA	B	817	-	-	10/39/115/115	-
13	CLA	B	825	2	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	814	2	-	6/27/103/115	-
13	CLA	B	812	2	-	12/39/115/115	-
13	CLA	A	823	1	-	4/23/99/115	-
13	CLA	F	1301	-	-	5/15/91/115	-
13	CLA	B	801	2	-	11/39/115/115	-
13	CLA	B	831	2	-	8/31/107/115	-
13	CLA	A	838	1	-	16/39/115/115	-
13	CLA	A	814	1	-	4/15/91/115	-
13	CLA	B	829	2	-	3/20/96/115	-
15	BCR	J	1105	-	-	14/29/63/63	0/2/2/2
15	BCR	B	842	-	-	12/29/63/63	0/2/2/2
13	CLA	B	827	2	-	8/39/115/115	-
13	CLA	A	815	1	-	2/15/91/115	-
13	CLA	B	836	2	-	11/39/115/115	-
13	CLA	B	811	-	-	12/39/115/115	-

All (1952) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1103	CLA	C3A-C2A	-4.48	1.50	1.54
13	A	808	CLA	MG-ND	-4.34	1.97	2.05
13	B	802	CLA	MG-ND	-4.27	1.97	2.05
13	A	824	CLA	CHB-C1B	-4.25	1.29	1.39
13	B	822	CLA	MG-ND	-4.23	1.97	2.05
13	B	835	CLA	MG-ND	-4.23	1.97	2.05
13	X	102	CLA	MG-ND	-4.23	1.97	2.05
13	F	1301	CLA	MG-ND	-4.21	1.97	2.05
13	A	834	CLA	CHB-C1B	-4.20	1.30	1.39
13	A	837	CLA	MG-ND	-4.19	1.97	2.05
13	B	813	CLA	MG-ND	-4.16	1.97	2.05
13	B	816	CLA	CHB-C1B	-4.16	1.30	1.39
13	A	836	CLA	MG-ND	-4.15	1.97	2.05
13	B	808	CLA	MG-ND	-4.14	1.97	2.05
13	L	1002	CLA	CHB-C1B	-4.14	1.30	1.39
13	A	842	CLA	MG-ND	-4.13	1.97	2.05
13	A	822	CLA	MG-ND	-4.11	1.97	2.05
13	A	801	CLA	CHB-C1B	-4.11	1.30	1.39
13	B	823	CLA	MG-ND	-4.11	1.97	2.05
13	B	801	CLA	CHB-C1B	-4.10	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	822	CLA	CHB-C1B	-4.09	1.30	1.39
13	B	812	CLA	MG-ND	-4.09	1.97	2.05
13	A	802	CLA	CHB-C1B	-4.09	1.30	1.39
13	B	803	CLA	CHB-C1B	-4.08	1.30	1.39
13	B	828	CLA	CHB-C1B	-4.08	1.30	1.39
13	A	838	CLA	MG-ND	-4.08	1.97	2.05
13	A	835	CLA	CHB-C1B	-4.08	1.30	1.39
13	B	833	CLA	MG-ND	-4.08	1.97	2.05
13	B	807	CLA	MG-ND	-4.08	1.97	2.05
13	B	811	CLA	MG-ND	-4.07	1.97	2.05
13	B	818	CLA	MG-ND	-4.06	1.97	2.05
13	A	824	CLA	MG-ND	-4.06	1.97	2.05
13	A	826	CLA	MG-ND	-4.05	1.97	2.05
13	B	828	CLA	MG-ND	-4.05	1.97	2.05
13	J	1101	CLA	MG-ND	-4.05	1.97	2.05
13	A	834	CLA	MG-ND	-4.05	1.97	2.05
13	B	804	CLA	CHB-C1B	-4.05	1.30	1.39
13	L	1003	CLA	CHB-C1B	-4.04	1.30	1.39
13	A	802	CLA	MG-ND	-4.04	1.97	2.05
13	B	825	CLA	MG-ND	-4.04	1.97	2.05
13	A	827	CLA	MG-ND	-4.04	1.97	2.05
13	A	855	CLA	MG-ND	-4.04	1.97	2.05
13	B	818	CLA	CHB-C1B	-4.03	1.30	1.39
13	A	841	CLA	MG-ND	-4.03	1.97	2.05
13	B	824	CLA	MG-ND	-4.03	1.97	2.05
13	A	831	CLA	CHB-C1B	-4.03	1.30	1.39
13	B	821	CLA	CHB-C1B	-4.03	1.30	1.39
13	B	825	CLA	CHB-C1B	-4.03	1.30	1.39
13	B	826	CLA	CHB-C1B	-4.02	1.30	1.39
13	B	819	CLA	CHB-C1B	-4.02	1.30	1.39
13	B	836	CLA	MG-ND	-4.02	1.97	2.05
13	A	804	CLA	CHB-C1B	-4.01	1.30	1.39
13	A	825	CLA	MG-ND	-4.01	1.97	2.05
13	I	101	CLA	MG-ND	-4.01	1.97	2.05
13	B	809	CLA	CHB-C1B	-4.01	1.30	1.39
13	J	1103	CLA	CHB-C1B	-4.01	1.30	1.39
13	A	814	CLA	MG-ND	-4.01	1.97	2.05
13	F	1301	CLA	CHB-C1B	-4.00	1.30	1.39
13	A	813	CLA	MG-ND	-4.00	1.97	2.05
13	B	838	CLA	MG-ND	-4.00	1.97	2.05
13	A	803	CLA	CHB-C1B	-4.00	1.30	1.39
13	A	809	CLA	CHB-C1B	-4.00	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	828	CLA	CHB-C1B	-4.00	1.30	1.39
13	B	834	CLA	MG-ND	-4.00	1.97	2.05
13	A	820	CLA	CHB-C1B	-4.00	1.30	1.39
13	B	831	CLA	MG-ND	-4.00	1.97	2.05
13	A	818	CLA	CHB-C1B	-3.99	1.30	1.39
13	A	815	CLA	CHB-C1B	-3.98	1.30	1.39
13	A	812	CLA	MG-ND	-3.98	1.97	2.05
13	A	833	CLA	MG-ND	-3.98	1.97	2.05
13	B	806	CLA	MG-ND	-3.98	1.97	2.05
13	J	1102	CLA	MG-ND	-3.98	1.97	2.05
13	A	826	CLA	CHB-C1B	-3.98	1.30	1.39
13	B	816	CLA	MG-ND	-3.97	1.97	2.05
13	B	817	CLA	MG-ND	-3.97	1.97	2.05
13	A	810	CLA	CHB-C1B	-3.97	1.30	1.39
13	B	810	CLA	CHB-C1B	-3.97	1.30	1.39
13	L	1002	CLA	MG-ND	-3.97	1.97	2.05
13	M	1202	CLA	MG-ND	-3.97	1.97	2.05
13	B	829	CLA	CHB-C1B	-3.97	1.30	1.39
13	A	837	CLA	CHB-C1B	-3.96	1.30	1.39
13	A	809	CLA	MG-ND	-3.96	1.97	2.05
13	B	820	CLA	MG-ND	-3.96	1.97	2.05
13	L	1004	CLA	MG-ND	-3.96	1.97	2.05
13	A	836	CLA	CHB-C1B	-3.95	1.30	1.39
13	X	102	CLA	CHB-C1B	-3.95	1.30	1.39
13	A	803	CLA	MG-ND	-3.95	1.98	2.05
13	A	815	CLA	MG-ND	-3.94	1.98	2.05
13	B	821	CLA	MG-ND	-3.94	1.98	2.05
13	B	803	CLA	MG-ND	-3.94	1.98	2.05
13	L	1003	CLA	MG-ND	-3.94	1.98	2.05
13	A	843	CLA	MG-ND	-3.94	1.98	2.05
13	A	811	CLA	CHB-C1B	-3.94	1.30	1.39
13	A	820	CLA	MG-ND	-3.94	1.98	2.05
13	B	802	CLA	CHB-C1B	-3.93	1.30	1.39
13	B	837	CLA	CHB-C1B	-3.92	1.30	1.39
13	A	816	CLA	MG-ND	-3.92	1.98	2.05
13	A	817	CLA	CHB-C1B	-3.92	1.30	1.39
13	B	813	CLA	CHB-C1B	-3.92	1.30	1.39
13	B	830	CLA	CHB-C1B	-3.92	1.30	1.39
13	A	814	CLA	CHB-C1B	-3.92	1.30	1.39
13	A	838	CLA	CHB-C1B	-3.91	1.30	1.39
13	B	807	CLA	CHB-C1B	-3.91	1.30	1.39
13	B	832	CLA	CHB-C1B	-3.91	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	831	CLA	MG-ND	-3.90	1.98	2.05
13	B	839	CLA	CHB-C1B	-3.90	1.30	1.39
13	B	819	CLA	MG-ND	-3.90	1.98	2.05
13	A	839	CLA	CHB-C1B	-3.90	1.30	1.39
13	A	811	CLA	MG-ND	-3.90	1.98	2.05
13	A	806	CLA	MG-ND	-3.89	1.98	2.05
13	A	805	CLA	CHB-C1B	-3.89	1.30	1.39
13	B	827	CLA	CHB-C1B	-3.89	1.30	1.39
13	A	833	CLA	CHB-C1B	-3.89	1.30	1.39
13	A	821	CLA	MG-ND	-3.89	1.98	2.05
13	B	823	CLA	CHB-C1B	-3.88	1.30	1.39
13	A	818	CLA	MG-ND	-3.88	1.98	2.05
13	A	832	CLA	MG-ND	-3.88	1.98	2.05
13	B	822	CLA	CHB-C1B	-3.88	1.30	1.39
13	B	815	CLA	MG-ND	-3.88	1.98	2.05
13	A	845	CLA	CHB-C1B	-3.88	1.30	1.39
13	A	813	CLA	CHB-C1B	-3.87	1.30	1.39
13	A	819	CLA	CHB-C1B	-3.87	1.30	1.39
13	I	101	CLA	CHB-C1B	-3.87	1.30	1.39
13	A	808	CLA	CHB-C1B	-3.87	1.30	1.39
13	B	832	CLA	MG-ND	-3.87	1.98	2.05
13	B	837	CLA	MG-ND	-3.86	1.98	2.05
13	A	835	CLA	MG-ND	-3.86	1.98	2.05
13	B	806	CLA	CHB-C1B	-3.86	1.30	1.39
13	B	810	CLA	MG-ND	-3.86	1.98	2.05
13	A	816	CLA	CHB-C1B	-3.85	1.30	1.39
14	A	846	PQN	C12-C13	3.85	1.41	1.33
13	A	855	CLA	CHB-C1B	-3.85	1.30	1.39
13	B	833	CLA	CHB-C1B	-3.85	1.30	1.39
13	A	842	CLA	CHB-C1B	-3.85	1.30	1.39
13	B	811	CLA	CHB-C1B	-3.85	1.30	1.39
13	A	825	CLA	CHB-C1B	-3.84	1.30	1.39
13	J	1102	CLA	CHB-C1B	-3.84	1.30	1.39
13	B	817	CLA	CHB-C1B	-3.83	1.30	1.39
13	A	801	CLA	MG-ND	-3.83	1.98	2.05
13	A	844	CLA	CHB-C1B	-3.83	1.30	1.39
13	B	815	CLA	CHB-C1B	-3.83	1.30	1.39
13	M	1201	CLA	CHB-C1B	-3.83	1.30	1.39
13	A	804	CLA	MG-ND	-3.83	1.98	2.05
13	B	834	CLA	CHB-C1B	-3.83	1.30	1.39
13	B	824	CLA	CHB-C1B	-3.82	1.30	1.39
13	B	831	CLA	CHB-C1B	-3.82	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	809	CLA	MG-ND	-3.82	1.98	2.05
13	L	1004	CLA	CHB-C1B	-3.81	1.30	1.39
13	B	808	CLA	CHB-C1B	-3.81	1.30	1.39
13	A	829	CLA	CHB-C1B	-3.81	1.30	1.39
13	M	1202	CLA	CHB-C1B	-3.81	1.30	1.39
13	A	819	CLA	MG-ND	-3.80	1.98	2.05
13	B	838	CLA	CHB-C1B	-3.80	1.30	1.39
13	A	844	CLA	MG-ND	-3.80	1.98	2.05
13	B	836	CLA	CHB-C1B	-3.79	1.30	1.39
13	A	807	CLA	CHB-C1B	-3.79	1.30	1.39
13	A	806	CLA	CHB-C1B	-3.79	1.30	1.39
13	B	814	CLA	CHB-C1B	-3.79	1.30	1.39
13	A	823	CLA	CHB-C1B	-3.79	1.30	1.39
13	A	841	CLA	CHB-C1B	-3.78	1.30	1.39
13	J	1101	CLA	CHB-C1B	-3.78	1.31	1.39
13	A	829	CLA	MG-ND	-3.77	1.98	2.05
13	B	812	CLA	CHB-C1B	-3.77	1.31	1.39
13	B	820	CLA	CHB-C1B	-3.77	1.31	1.39
13	B	805	CLA	MG-ND	-3.77	1.98	2.05
13	A	821	CLA	CHB-C1B	-3.77	1.31	1.39
13	A	843	CLA	CHB-C1B	-3.76	1.31	1.39
13	A	807	CLA	MG-ND	-3.76	1.98	2.05
13	A	830	CLA	CHB-C1B	-3.75	1.31	1.39
13	A	827	CLA	CHB-C1B	-3.75	1.31	1.39
13	B	805	CLA	CHB-C1B	-3.75	1.31	1.39
13	M	1201	CLA	MG-ND	-3.74	1.98	2.05
13	B	801	CLA	MG-ND	-3.74	1.98	2.05
13	B	807	CLA	C1D-C2D	-3.74	1.37	1.45
13	B	835	CLA	CHB-C1B	-3.73	1.31	1.39
13	B	839	CLA	MG-ND	-3.73	1.98	2.05
15	A	852	BCR	C20-C21	3.72	1.54	1.43
13	A	828	CLA	MG-ND	-3.72	1.98	2.05
13	A	823	CLA	MG-ND	-3.72	1.98	2.05
13	A	845	CLA	MG-ND	-3.72	1.98	2.05
13	B	826	CLA	MG-ND	-3.72	1.98	2.05
13	A	817	CLA	MG-ND	-3.71	1.98	2.05
13	B	827	CLA	MG-ND	-3.71	1.98	2.05
13	A	840	CLA	MG-ND	-3.70	1.98	2.05
13	A	812	CLA	CHB-C1B	-3.70	1.31	1.39
16	A	854	LHG	O7-C5	-3.70	1.37	1.46
16	X	101	LHG	O7-C5	-3.70	1.37	1.46
13	B	829	CLA	MG-ND	-3.70	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	811	CLA	C2-C3	3.70	1.41	1.33
13	A	840	CLA	CHB-C1B	-3.68	1.31	1.39
13	B	835	CLA	O2D-CED	-3.68	1.37	1.45
13	A	839	CLA	MG-ND	-3.66	1.98	2.05
13	A	808	CLA	C1D-C2D	-3.66	1.38	1.45
13	A	810	CLA	MG-ND	-3.66	1.98	2.05
13	A	832	CLA	CHB-C1B	-3.65	1.31	1.39
14	B	840	PQN	C12-C13	3.65	1.41	1.33
15	A	850	BCR	C20-C21	3.64	1.54	1.43
15	B	842	BCR	C20-C21	3.64	1.54	1.43
13	B	804	CLA	MG-ND	-3.64	1.98	2.05
15	B	844	BCR	C20-C21	3.63	1.54	1.43
15	A	848	BCR	C20-C21	3.62	1.54	1.43
15	A	851	BCR	C20-C21	3.61	1.54	1.43
13	J	1103	CLA	MG-ND	-3.61	1.98	2.05
15	J	1105	BCR	C20-C21	3.61	1.54	1.43
13	B	814	CLA	MG-ND	-3.60	1.98	2.05
15	L	1005	BCR	C20-C21	3.59	1.54	1.43
15	B	850	BCR	C20-C21	3.58	1.54	1.43
15	B	845	BCR	C20-C21	3.58	1.54	1.43
13	A	805	CLA	MG-ND	-3.57	1.98	2.05
15	L	1006	BCR	C20-C21	3.57	1.54	1.43
15	A	850	BCR	C23-C22	3.56	1.53	1.46
15	J	1104	BCR	C20-C21	3.54	1.54	1.43
13	B	830	CLA	MG-ND	-3.54	1.98	2.05
15	M	1203	BCR	C20-C21	3.53	1.54	1.43
13	A	837	CLA	O2D-CED	-3.53	1.37	1.45
15	A	852	BCR	C23-C22	3.52	1.53	1.46
13	F	1301	CLA	C1D-C2D	-3.52	1.38	1.45
15	B	847	BCR	C20-C21	3.51	1.54	1.43
13	A	807	CLA	C1D-C2D	-3.51	1.38	1.45
15	B	842	BCR	C23-C22	3.51	1.53	1.46
15	B	846	BCR	C20-C21	3.50	1.54	1.43
13	A	825	CLA	C2-C3	3.50	1.41	1.33
13	A	805	CLA	C2-C3	3.49	1.41	1.33
15	A	847	BCR	C20-C21	3.49	1.54	1.43
13	A	826	CLA	C2-C3	3.49	1.41	1.33
15	J	1105	BCR	C23-C22	3.48	1.53	1.46
15	B	849	BCR	C20-C21	3.47	1.54	1.43
16	A	853	LHG	O7-C5	-3.47	1.38	1.46
13	A	830	CLA	MG-ND	-3.46	1.98	2.05
13	A	814	CLA	O2D-CED	-3.46	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	845	BCR	C23-C22	3.45	1.53	1.46
13	A	832	CLA	C2-C3	3.45	1.41	1.33
15	J	1104	BCR	C23-C22	3.44	1.53	1.46
13	A	804	CLA	C1D-C2D	-3.44	1.38	1.45
15	A	848	BCR	C23-C22	3.44	1.53	1.46
13	A	842	CLA	C2-C3	3.44	1.41	1.33
13	B	826	CLA	C2-C3	3.44	1.41	1.33
15	F	1302	BCR	C20-C21	3.43	1.53	1.43
13	A	808	CLA	C2-C3	3.43	1.41	1.33
13	B	827	CLA	C2-C3	3.43	1.41	1.33
13	B	802	CLA	C1D-C2D	-3.43	1.38	1.45
15	B	847	BCR	C23-C22	3.42	1.53	1.46
15	B	843	BCR	C20-C21	3.42	1.53	1.43
15	B	841	BCR	C20-C21	3.42	1.53	1.43
13	A	823	CLA	C1D-C2D	-3.42	1.38	1.45
13	B	826	CLA	O2D-CED	-3.41	1.37	1.45
13	B	835	CLA	C2-C3	3.41	1.40	1.33
13	A	837	CLA	C2-C3	3.39	1.40	1.33
15	B	846	BCR	C23-C22	3.39	1.53	1.46
13	A	809	CLA	C1D-C2D	-3.39	1.38	1.45
13	A	809	CLA	C2-C3	3.39	1.40	1.33
13	A	818	CLA	C1D-C2D	-3.39	1.38	1.45
13	A	811	CLA	C2-C3	3.38	1.40	1.33
13	A	835	CLA	C2-C3	3.38	1.40	1.33
13	B	808	CLA	C1D-C2D	-3.38	1.38	1.45
13	M	1201	CLA	C2-C3	3.37	1.40	1.33
13	A	801	CLA	C2-C3	3.37	1.40	1.33
13	A	839	CLA	C1D-C2D	-3.37	1.38	1.45
13	B	830	CLA	C2-C3	3.36	1.40	1.33
15	M	1203	BCR	C23-C22	3.36	1.53	1.46
15	B	844	BCR	C23-C22	3.35	1.53	1.46
13	B	831	CLA	C1D-C2D	-3.35	1.38	1.45
13	B	838	CLA	C1D-C2D	-3.35	1.38	1.45
15	A	847	BCR	C23-C22	3.35	1.53	1.46
13	A	804	CLA	C2-C3	3.35	1.40	1.33
13	A	834	CLA	C2-C3	3.35	1.40	1.33
13	B	815	CLA	C2-C3	3.35	1.40	1.33
13	B	815	CLA	C1D-C2D	-3.35	1.38	1.45
13	B	822	CLA	C2-C3	3.34	1.40	1.33
13	A	830	CLA	C2-C3	3.34	1.40	1.33
13	B	831	CLA	C2-C3	3.34	1.40	1.33
15	L	1006	BCR	C23-C22	3.34	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	824	CLA	C2-C3	3.34	1.40	1.33
15	I	102	BCR	C20-C21	3.34	1.53	1.43
13	X	102	CLA	O2A-CGA	3.34	1.41	1.30
13	B	828	CLA	O2A-CGA	3.33	1.41	1.30
13	B	805	CLA	C4C-C3C	3.33	1.50	1.45
13	J	1102	CLA	O2A-CGA	3.33	1.41	1.30
13	A	855	CLA	O2A-CGA	3.32	1.41	1.30
13	B	836	CLA	C2-C3	3.32	1.40	1.33
13	F	1301	CLA	O2A-CGA	3.32	1.41	1.30
13	B	813	CLA	O2A-CGA	3.32	1.41	1.30
15	A	849	BCR	C20-C21	3.32	1.53	1.43
13	B	833	CLA	O2A-CGA	3.32	1.41	1.30
13	A	817	CLA	C2-C3	3.32	1.40	1.33
13	B	839	CLA	C2-C3	3.32	1.40	1.33
13	B	817	CLA	C1D-C2D	-3.32	1.38	1.45
13	B	814	CLA	C2-C3	3.32	1.40	1.33
13	A	828	CLA	C1D-C2D	-3.31	1.38	1.45
13	A	821	CLA	C2-C3	3.31	1.40	1.33
13	A	840	CLA	C1D-C2D	-3.31	1.38	1.45
13	A	815	CLA	O2A-CGA	3.31	1.41	1.30
15	A	851	BCR	C23-C22	3.31	1.53	1.46
13	B	821	CLA	O2A-CGA	3.31	1.41	1.30
13	I	101	CLA	C1D-C2D	-3.31	1.38	1.45
13	B	838	CLA	C2-C3	3.31	1.40	1.33
15	A	850	BCR	C11-C10	3.31	1.53	1.43
13	B	819	CLA	O2A-CGA	3.31	1.41	1.30
13	B	834	CLA	O2A-CGA	3.31	1.41	1.30
13	A	805	CLA	C1D-C2D	-3.31	1.38	1.45
13	A	840	CLA	C2-C3	3.30	1.40	1.33
13	A	811	CLA	C1D-C2D	-3.30	1.38	1.45
13	A	836	CLA	C1D-C2D	-3.30	1.38	1.45
13	B	814	CLA	C1D-C2D	-3.30	1.38	1.45
13	B	827	CLA	C1D-C2D	-3.30	1.38	1.45
15	B	841	BCR	C23-C22	3.30	1.53	1.46
15	B	844	BCR	C15-C14	3.30	1.53	1.43
13	A	833	CLA	C2-C3	3.30	1.40	1.33
15	B	842	BCR	C15-C14	3.30	1.53	1.43
13	A	844	CLA	O2A-CGA	3.29	1.41	1.30
15	A	852	BCR	C19-C18	3.29	1.53	1.46
13	B	809	CLA	O2A-CGA	3.29	1.41	1.30
13	A	842	CLA	C1D-C2D	-3.29	1.38	1.45
13	A	836	CLA	O2A-CGA	3.29	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	850	BCR	C23-C22	3.28	1.53	1.46
13	A	824	CLA	C2-C3	3.28	1.40	1.33
13	A	827	CLA	C1D-C2D	-3.28	1.38	1.45
13	A	827	CLA	C2-C3	3.28	1.40	1.33
15	L	1006	BCR	C15-C14	3.28	1.53	1.43
13	A	844	CLA	C4D-CHA	-3.28	1.33	1.43
15	A	852	BCR	C16-C17	3.28	1.53	1.43
13	A	810	CLA	O2A-CGA	3.28	1.41	1.30
13	A	845	CLA	C2-C3	3.28	1.40	1.33
13	A	838	CLA	C2-C3	3.27	1.40	1.33
13	A	802	CLA	C2-C3	3.27	1.40	1.33
15	A	847	BCR	C15-C14	3.27	1.53	1.43
13	A	829	CLA	C2-C3	3.27	1.40	1.33
13	A	834	CLA	C1D-C2D	-3.27	1.38	1.45
13	J	1101	CLA	C2-C3	3.27	1.40	1.33
13	B	805	CLA	C2-C3	3.27	1.40	1.33
13	L	1003	CLA	C2-C3	3.26	1.40	1.33
13	B	825	CLA	C2-C3	3.26	1.40	1.33
15	F	1302	BCR	C15-C14	3.26	1.53	1.43
13	M	1202	CLA	O2A-CGA	3.26	1.41	1.30
13	B	810	CLA	O2A-CGA	3.26	1.41	1.30
15	B	847	BCR	C15-C14	3.26	1.53	1.43
13	A	817	CLA	C1D-C2D	-3.26	1.38	1.45
13	A	831	CLA	O2D-CED	-3.26	1.38	1.45
13	B	803	CLA	C2-C3	3.26	1.40	1.33
15	A	848	BCR	C15-C14	3.26	1.53	1.43
13	B	825	CLA	C1D-C2D	-3.26	1.38	1.45
13	A	807	CLA	O2D-CGD	3.26	1.41	1.33
15	A	850	BCR	C15-C14	3.26	1.53	1.43
13	A	826	CLA	C1D-C2D	-3.25	1.38	1.45
13	B	833	CLA	C1D-C2D	-3.25	1.38	1.45
13	L	1002	CLA	C2-C3	3.25	1.40	1.33
13	A	814	CLA	O2A-CGA	3.25	1.41	1.30
15	L	1005	BCR	C23-C22	3.25	1.52	1.46
13	A	837	CLA	C1D-C2D	-3.25	1.38	1.45
15	B	842	BCR	C16-C17	3.25	1.53	1.43
15	B	850	BCR	C11-C10	3.25	1.53	1.43
13	B	822	CLA	C1D-C2D	-3.25	1.38	1.45
13	B	806	CLA	C1D-C2D	-3.24	1.38	1.45
13	A	820	CLA	C1D-C2D	-3.24	1.38	1.45
16	A	854	LHG	O8-C6	-3.24	1.37	1.45
13	B	820	CLA	C1D-C2D	-3.24	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	830	CLA	C1D-C2D	-3.24	1.38	1.45
15	J	1104	BCR	C11-C10	3.24	1.53	1.43
13	B	808	CLA	C2-C3	3.24	1.40	1.33
15	B	842	BCR	C8-C9	3.23	1.52	1.46
13	A	812	CLA	C2-C3	3.23	1.40	1.33
13	A	841	CLA	C2-C3	3.23	1.40	1.33
15	B	849	BCR	C23-C22	3.23	1.52	1.46
15	J	1104	BCR	C8-C9	3.23	1.52	1.46
13	M	1201	CLA	C1D-C2D	-3.23	1.38	1.45
13	A	820	CLA	C2-C3	3.23	1.40	1.33
15	J	1104	BCR	C15-C14	3.23	1.53	1.43
13	I	101	CLA	C2-C3	3.23	1.40	1.33
15	B	844	BCR	C16-C17	3.23	1.53	1.43
13	A	813	CLA	C2-C3	3.23	1.40	1.33
15	J	1105	BCR	C15-C14	3.23	1.53	1.43
13	A	838	CLA	C1D-C2D	-3.22	1.39	1.45
13	B	812	CLA	C1D-C2D	-3.22	1.39	1.45
15	B	846	BCR	C15-C14	3.22	1.53	1.43
13	A	823	CLA	C2-C3	3.22	1.40	1.33
13	A	844	CLA	C4C-C3C	3.22	1.50	1.45
13	B	817	CLA	C2-C3	3.22	1.40	1.33
13	B	832	CLA	O2A-CGA	3.22	1.41	1.30
13	B	823	CLA	C1D-C2D	-3.21	1.39	1.45
13	A	843	CLA	C1D-C2D	-3.21	1.39	1.45
13	A	845	CLA	C4C-C3C	3.21	1.50	1.45
13	A	814	CLA	C1D-C2D	-3.21	1.39	1.45
15	A	850	BCR	C16-C17	3.20	1.53	1.43
13	A	832	CLA	O2A-CGA	3.20	1.42	1.33
15	B	843	BCR	C15-C14	3.20	1.53	1.43
13	A	837	CLA	O2A-CGA	3.20	1.42	1.33
13	X	102	CLA	C1D-C2D	-3.20	1.39	1.45
13	M	1202	CLA	C1D-C2D	-3.20	1.39	1.45
13	B	801	CLA	C2-C3	3.19	1.40	1.33
13	A	840	CLA	C1C-C2C	3.19	1.51	1.44
15	L	1005	BCR	C11-C10	3.19	1.53	1.43
15	F	1302	BCR	C16-C17	3.19	1.53	1.43
15	A	849	BCR	C23-C22	3.19	1.52	1.46
15	A	847	BCR	C8-C9	3.19	1.52	1.46
13	B	811	CLA	O2A-CGA	3.19	1.42	1.33
15	B	849	BCR	C15-C14	3.19	1.53	1.43
16	X	101	LHG	O8-C6	-3.18	1.38	1.45
15	B	841	BCR	C15-C14	3.18	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	822	CLA	C1D-C2D	-3.18	1.39	1.45
13	A	829	CLA	C4C-C3C	3.18	1.50	1.45
13	A	831	CLA	C1D-C2D	-3.18	1.39	1.45
13	A	833	CLA	C1D-C2D	-3.18	1.39	1.45
13	A	828	CLA	C2-C3	3.18	1.40	1.33
15	A	848	BCR	C11-C10	3.18	1.53	1.43
13	B	801	CLA	C1D-C2D	-3.18	1.39	1.45
15	J	1104	BCR	C16-C17	3.18	1.53	1.43
13	B	839	CLA	C4C-C3C	3.18	1.50	1.45
15	L	1006	BCR	C11-C10	3.18	1.53	1.43
13	B	835	CLA	O2A-CGA	3.18	1.42	1.33
13	B	827	CLA	C1C-C2C	3.18	1.51	1.44
13	L	1004	CLA	C2-C3	3.18	1.40	1.33
13	A	808	CLA	O2D-CED	-3.17	1.38	1.45
13	B	802	CLA	C2-C3	3.17	1.40	1.33
15	F	1302	BCR	C23-C22	3.17	1.52	1.46
15	B	843	BCR	C11-C10	3.17	1.53	1.43
15	A	852	BCR	C15-C14	3.17	1.53	1.43
13	B	804	CLA	C1D-C2D	-3.17	1.39	1.45
15	A	847	BCR	C16-C17	3.17	1.53	1.43
15	A	851	BCR	C15-C14	3.17	1.53	1.43
13	A	812	CLA	C1D-C2D	-3.17	1.39	1.45
15	B	842	BCR	C11-C10	3.16	1.53	1.43
13	A	806	CLA	C4C-C3C	3.16	1.50	1.45
15	A	850	BCR	C12-C13	3.16	1.52	1.46
13	B	816	CLA	C2-C3	3.16	1.40	1.33
15	A	850	BCR	C19-C18	3.16	1.52	1.46
15	B	841	BCR	C11-C10	3.16	1.53	1.43
13	A	813	CLA	C1D-C2D	-3.16	1.39	1.45
13	J	1103	CLA	C4C-C3C	3.16	1.50	1.45
15	A	847	BCR	C11-C10	3.16	1.53	1.43
15	B	841	BCR	C8-C9	3.16	1.52	1.46
13	B	818	CLA	O2D-CED	-3.16	1.38	1.45
15	M	1203	BCR	C15-C14	3.16	1.53	1.43
13	B	831	CLA	O2D-CED	-3.16	1.38	1.45
13	B	815	CLA	O2D-CED	-3.16	1.38	1.45
15	B	850	BCR	C8-C9	3.15	1.52	1.46
15	B	850	BCR	C15-C14	3.15	1.53	1.43
15	B	847	BCR	C16-C17	3.15	1.53	1.43
13	B	837	CLA	C1D-C2D	-3.15	1.39	1.45
13	A	803	CLA	C2-C3	3.15	1.40	1.33
13	A	810	CLA	C1D-C2D	-3.15	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	832	CLA	C1D-C2D	-3.15	1.39	1.45
13	B	834	CLA	C1D-C2D	-3.15	1.39	1.45
13	L	1004	CLA	C1D-C2D	-3.15	1.39	1.45
13	L	1004	CLA	C4C-C3C	3.14	1.50	1.45
13	B	816	CLA	C1D-C2D	-3.14	1.39	1.45
13	B	807	CLA	C2-C3	3.14	1.40	1.33
13	B	811	CLA	C4C-C3C	3.14	1.50	1.45
15	A	848	BCR	C16-C17	3.14	1.52	1.43
13	B	812	CLA	C2-C3	3.14	1.40	1.33
13	B	824	CLA	C1D-C2D	-3.14	1.39	1.45
15	L	1005	BCR	C15-C14	3.14	1.52	1.43
13	B	806	CLA	C2-C3	3.14	1.40	1.33
13	A	801	CLA	C1D-C2D	-3.14	1.39	1.45
13	A	806	CLA	C1D-C2D	-3.14	1.39	1.45
13	B	835	CLA	C1D-C2D	-3.14	1.39	1.45
13	B	809	CLA	C1D-C2D	-3.14	1.39	1.45
13	B	828	CLA	C1D-C2D	-3.14	1.39	1.45
13	B	838	CLA	C1C-C2C	3.14	1.50	1.44
13	A	821	CLA	C1D-C2D	-3.13	1.39	1.45
13	A	826	CLA	O2A-CGA	3.13	1.42	1.33
13	A	813	CLA	C4C-C3C	3.13	1.50	1.45
13	A	841	CLA	C4C-C3C	3.13	1.50	1.45
13	A	819	CLA	C2-C3	3.13	1.40	1.33
13	A	802	CLA	C4C-C3C	3.13	1.50	1.45
13	B	826	CLA	C1D-C2D	-3.13	1.39	1.45
15	J	1105	BCR	C16-C17	3.13	1.52	1.43
15	A	851	BCR	C8-C9	3.13	1.52	1.46
15	B	844	BCR	C19-C18	3.13	1.52	1.46
13	B	819	CLA	C1D-C2D	-3.13	1.39	1.45
13	A	824	CLA	C4C-C3C	3.12	1.50	1.45
13	J	1103	CLA	C4D-CHA	-3.12	1.34	1.43
15	B	841	BCR	C16-C17	3.12	1.52	1.43
13	J	1101	CLA	C1D-C2D	-3.12	1.39	1.45
13	A	814	CLA	C1C-C2C	3.12	1.50	1.44
13	A	825	CLA	C1D-C2D	-3.12	1.39	1.45
15	B	847	BCR	C11-C10	3.12	1.52	1.43
15	L	1006	BCR	C16-C17	3.12	1.52	1.43
13	A	807	CLA	C1C-C2C	3.12	1.50	1.44
15	B	842	BCR	C19-C18	3.12	1.52	1.46
13	B	811	CLA	C1D-C2D	-3.12	1.39	1.45
15	J	1105	BCR	C11-C10	3.12	1.52	1.43
13	B	818	CLA	C1D-C2D	-3.11	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	849	BCR	C16-C17	3.11	1.52	1.43
15	I	102	BCR	C15-C14	3.11	1.52	1.43
15	B	850	BCR	C16-C17	3.11	1.52	1.43
13	B	821	CLA	O2D-CED	-3.11	1.38	1.45
15	M	1203	BCR	C16-C17	3.11	1.52	1.43
13	B	804	CLA	C2-C3	3.11	1.40	1.33
15	A	848	BCR	C19-C18	3.11	1.52	1.46
15	A	851	BCR	C11-C10	3.11	1.52	1.43
13	B	819	CLA	C4C-C3C	3.11	1.50	1.45
13	B	815	CLA	C4C-C3C	3.11	1.50	1.45
13	M	1201	CLA	O2A-CGA	3.11	1.42	1.33
13	A	803	CLA	O2D-CED	-3.10	1.38	1.45
13	A	835	CLA	C1D-C2D	-3.10	1.39	1.45
13	B	823	CLA	C4C-C3C	3.10	1.50	1.45
13	A	802	CLA	C1D-C2D	-3.10	1.39	1.45
15	J	1104	BCR	C19-C18	3.10	1.52	1.46
13	A	806	CLA	C2-C3	3.10	1.40	1.33
15	B	845	BCR	C15-C14	3.10	1.52	1.43
13	A	808	CLA	O2A-CGA	3.10	1.42	1.33
13	B	813	CLA	C1D-C2D	-3.10	1.39	1.45
13	B	832	CLA	C1C-C2C	3.10	1.50	1.44
15	B	846	BCR	C11-C10	3.10	1.52	1.43
13	A	819	CLA	C1D-C2D	-3.09	1.39	1.45
13	B	836	CLA	C1D-C2D	-3.09	1.39	1.45
15	B	843	BCR	C16-C17	3.09	1.52	1.43
15	A	848	BCR	C8-C9	3.09	1.52	1.46
15	F	1302	BCR	C11-C10	3.09	1.52	1.43
13	B	807	CLA	C1C-C2C	3.09	1.50	1.44
15	B	846	BCR	C16-C17	3.09	1.52	1.43
15	B	845	BCR	C16-C17	3.09	1.52	1.43
13	B	824	CLA	C4C-C3C	3.09	1.50	1.45
15	A	851	BCR	C16-C17	3.09	1.52	1.43
13	M	1202	CLA	C4C-C3C	3.09	1.50	1.45
13	B	829	CLA	C1D-C2D	-3.08	1.39	1.45
15	B	846	BCR	C8-C9	3.08	1.52	1.46
13	B	802	CLA	C1C-C2C	3.08	1.50	1.44
15	I	102	BCR	C23-C22	3.08	1.52	1.46
13	L	1003	CLA	O2A-CGA	3.08	1.42	1.33
13	A	818	CLA	C2-C3	3.08	1.40	1.33
13	A	815	CLA	C4C-C3C	3.08	1.50	1.45
13	B	810	CLA	C1D-C2D	-3.07	1.39	1.45
15	A	852	BCR	C11-C10	3.07	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	845	BCR	C8-C9	3.07	1.52	1.46
13	B	808	CLA	C1C-C2C	3.07	1.50	1.44
13	B	801	CLA	C4C-C3C	3.07	1.50	1.45
15	A	850	BCR	C8-C9	3.07	1.52	1.46
13	A	804	CLA	O2D-CED	-3.07	1.38	1.45
13	A	808	CLA	C1C-C2C	3.07	1.50	1.44
15	B	843	BCR	C19-C18	3.06	1.52	1.46
13	A	803	CLA	C1D-C2D	-3.06	1.39	1.45
13	A	830	CLA	C1D-C2D	-3.06	1.39	1.45
13	A	802	CLA	O2A-CGA	3.06	1.42	1.33
13	B	824	CLA	O2A-CGA	3.06	1.42	1.33
13	L	1002	CLA	C1C-C2C	3.06	1.50	1.44
15	F	1302	BCR	C8-C9	3.06	1.52	1.46
16	A	853	LHG	O8-C6	-3.06	1.38	1.45
13	B	811	CLA	C1C-C2C	3.06	1.50	1.44
13	B	834	CLA	C4C-C3C	3.06	1.50	1.45
15	M	1203	BCR	C19-C18	3.06	1.52	1.46
15	M	1203	BCR	C11-C10	3.06	1.52	1.43
13	A	855	CLA	C4C-C3C	3.06	1.50	1.45
13	A	809	CLA	C1C-C2C	3.06	1.50	1.44
13	A	839	CLA	C1C-C2C	3.06	1.50	1.44
13	B	812	CLA	C4C-C3C	3.05	1.50	1.45
13	A	844	CLA	C1C-C2C	3.05	1.50	1.44
13	A	835	CLA	C4C-C3C	3.05	1.50	1.45
13	A	825	CLA	O2A-CGA	3.05	1.42	1.33
13	B	801	CLA	O2A-CGA	3.05	1.42	1.33
13	B	825	CLA	C1C-C2C	3.05	1.50	1.44
13	J	1102	CLA	C1D-C2D	-3.05	1.39	1.45
15	B	850	BCR	C19-C18	3.05	1.52	1.46
13	L	1003	CLA	C1D-C2D	-3.05	1.39	1.45
13	A	826	CLA	C1C-C2C	3.05	1.50	1.44
13	B	803	CLA	C1D-C2D	-3.05	1.39	1.45
13	A	839	CLA	C4C-C3C	3.05	1.50	1.45
13	B	820	CLA	C2-C3	3.05	1.40	1.33
13	B	822	CLA	C4C-C3C	3.05	1.50	1.45
15	I	102	BCR	C16-C17	3.05	1.52	1.43
15	A	849	BCR	C15-C14	3.05	1.52	1.43
13	A	813	CLA	C1C-C2C	3.05	1.50	1.44
13	A	843	CLA	C2-C3	3.05	1.40	1.33
13	A	804	CLA	C1C-C2C	3.04	1.50	1.44
13	A	828	CLA	C1C-C2C	3.04	1.50	1.44
13	F	1301	CLA	C1C-C2C	3.04	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	839	CLA	C1D-C2D	-3.04	1.39	1.45
15	J	1105	BCR	C19-C18	3.04	1.52	1.46
15	B	847	BCR	C8-C9	3.04	1.52	1.46
13	B	818	CLA	C4C-C3C	3.04	1.50	1.45
13	M	1202	CLA	C1C-C2C	3.04	1.50	1.44
13	B	808	CLA	C4C-C3C	3.04	1.50	1.45
15	J	1105	BCR	C8-C9	3.04	1.52	1.46
13	A	841	CLA	C1D-C2D	-3.04	1.39	1.45
15	B	843	BCR	C23-C22	3.04	1.52	1.46
15	L	1006	BCR	C19-C18	3.03	1.52	1.46
15	B	850	BCR	C12-C13	3.03	1.52	1.46
13	A	833	CLA	C4C-C3C	3.03	1.50	1.45
13	B	817	CLA	C4C-C3C	3.03	1.50	1.45
13	B	804	CLA	O2A-CGA	3.03	1.42	1.33
13	B	818	CLA	C1C-C2C	3.03	1.50	1.44
15	B	843	BCR	C12-C13	3.03	1.52	1.46
13	A	827	CLA	O2A-CGA	3.03	1.42	1.33
13	A	816	CLA	C4C-C3C	3.03	1.50	1.45
13	B	837	CLA	C4C-C3C	3.03	1.50	1.45
15	B	845	BCR	C11-C10	3.03	1.52	1.43
15	L	1005	BCR	C19-C18	3.03	1.52	1.46
15	B	846	BCR	C19-C18	3.03	1.52	1.46
15	A	851	BCR	C19-C18	3.03	1.52	1.46
13	B	802	CLA	O2A-CGA	3.03	1.42	1.33
13	B	824	CLA	C1C-C2C	3.02	1.50	1.44
15	A	849	BCR	C11-C10	3.02	1.52	1.43
13	A	832	CLA	C4C-C3C	3.02	1.50	1.45
15	B	843	BCR	C8-C9	3.02	1.52	1.46
13	A	823	CLA	C1C-C2C	3.02	1.50	1.44
13	B	822	CLA	C1B-NB	-3.02	1.33	1.37
13	A	855	CLA	C1D-C2D	-3.02	1.39	1.45
13	A	805	CLA	C4C-C3C	3.01	1.50	1.45
13	A	838	CLA	C1C-C2C	3.01	1.50	1.44
13	B	821	CLA	C1D-C2D	-3.01	1.39	1.45
13	A	821	CLA	C4C-C3C	3.01	1.50	1.45
13	A	826	CLA	O2D-CED	-3.01	1.38	1.45
15	B	845	BCR	C19-C18	3.01	1.52	1.46
13	A	843	CLA	C1C-C2C	3.01	1.50	1.44
15	L	1005	BCR	C12-C13	3.01	1.52	1.46
13	A	803	CLA	C4C-C3C	3.01	1.50	1.45
13	A	820	CLA	C4C-C3C	3.01	1.50	1.45
13	L	1002	CLA	C4C-C3C	3.01	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	841	CLA	O2A-CGA	3.01	1.42	1.33
13	B	809	CLA	C4C-C3C	3.01	1.50	1.45
13	A	806	CLA	O2D-CED	-3.00	1.38	1.45
13	A	836	CLA	C4C-C3C	3.00	1.50	1.45
13	A	832	CLA	C1C-C2C	3.00	1.50	1.44
13	B	813	CLA	C4C-C3C	3.00	1.50	1.45
13	B	837	CLA	C1C-C2C	3.00	1.50	1.44
13	B	836	CLA	C1C-C2C	3.00	1.50	1.44
13	A	822	CLA	O2A-CGA	3.00	1.42	1.33
13	B	820	CLA	C4C-C3C	3.00	1.50	1.45
13	B	826	CLA	C4C-C3C	3.00	1.50	1.45
13	A	817	CLA	C1C-C2C	2.99	1.50	1.44
13	A	817	CLA	C4C-C3C	2.99	1.50	1.45
13	B	831	CLA	O2A-CGA	2.99	1.42	1.33
13	B	823	CLA	O2D-CED	-2.99	1.38	1.45
13	J	1102	CLA	C4C-C3C	2.99	1.50	1.45
13	A	840	CLA	C4C-C3C	2.99	1.50	1.45
13	B	806	CLA	C1C-C2C	2.99	1.50	1.44
13	J	1103	CLA	C1D-C2D	-2.99	1.39	1.45
13	A	818	CLA	C4C-C3C	2.98	1.50	1.45
13	B	822	CLA	O2A-CGA	2.98	1.42	1.33
13	B	827	CLA	O2D-CED	-2.98	1.38	1.45
15	L	1005	BCR	C16-C17	2.98	1.52	1.43
13	B	808	CLA	O2A-CGA	2.98	1.42	1.33
13	B	810	CLA	C4C-C3C	2.98	1.50	1.45
13	A	830	CLA	O2A-CGA	2.98	1.42	1.33
13	M	1201	CLA	C1C-C2C	2.98	1.50	1.44
13	A	811	CLA	O2A-CGA	2.98	1.42	1.33
13	A	801	CLA	O2A-CGA	2.97	1.42	1.33
13	A	816	CLA	C1D-C2D	-2.97	1.39	1.45
13	B	831	CLA	C4C-C3C	2.97	1.50	1.45
13	A	842	CLA	C4C-C3C	2.97	1.50	1.45
13	A	814	CLA	C4C-C3C	2.97	1.50	1.45
13	A	826	CLA	C4C-C3C	2.97	1.50	1.45
13	I	101	CLA	C1C-C2C	2.97	1.50	1.44
15	A	849	BCR	C16-C17	2.97	1.52	1.43
13	B	825	CLA	C4C-C3C	2.97	1.50	1.45
13	A	811	CLA	C1C-C2C	2.97	1.50	1.44
13	A	830	CLA	C1C-C2C	2.97	1.50	1.44
13	J	1101	CLA	C1C-C2C	2.97	1.50	1.44
15	I	102	BCR	C11-C10	2.97	1.52	1.43
15	A	848	BCR	C12-C13	2.97	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	804	CLA	O2A-CGA	2.97	1.42	1.33
13	A	821	CLA	C1C-C2C	2.97	1.50	1.44
13	A	806	CLA	C1C-C2C	2.97	1.50	1.44
15	A	847	BCR	C12-C13	2.97	1.52	1.46
13	B	801	CLA	C1C-C2C	2.96	1.50	1.44
13	L	1003	CLA	C4C-C3C	2.96	1.50	1.45
15	B	847	BCR	C19-C18	2.96	1.52	1.46
15	B	849	BCR	C11-C10	2.96	1.52	1.43
13	B	806	CLA	O2D-CED	-2.96	1.38	1.45
15	J	1105	BCR	C12-C13	2.96	1.52	1.46
13	A	812	CLA	C4C-C3C	2.96	1.50	1.45
13	B	838	CLA	C4C-C3C	2.96	1.50	1.45
13	J	1101	CLA	C4C-C3C	2.96	1.50	1.45
13	A	831	CLA	C1C-C2C	2.96	1.50	1.44
15	B	841	BCR	C12-C13	2.96	1.52	1.46
15	L	1005	BCR	C8-C9	2.96	1.52	1.46
13	A	842	CLA	O2D-CED	-2.96	1.38	1.45
13	B	825	CLA	O2D-CED	-2.96	1.38	1.45
15	F	1302	BCR	C19-C18	2.96	1.52	1.46
15	L	1006	BCR	C8-C9	2.95	1.52	1.46
13	A	825	CLA	C1C-C2C	2.95	1.50	1.44
13	A	804	CLA	C4C-C3C	2.95	1.50	1.45
13	A	801	CLA	C4C-C3C	2.95	1.50	1.45
15	B	841	BCR	C19-C18	2.95	1.52	1.46
13	B	833	CLA	C1C-C2C	2.95	1.50	1.44
13	J	1101	CLA	O2A-CGA	2.95	1.42	1.33
13	A	831	CLA	C4C-C3C	2.95	1.50	1.45
13	A	829	CLA	O2A-CGA	2.95	1.41	1.33
13	A	834	CLA	O2A-CGA	2.95	1.41	1.33
13	B	803	CLA	C4C-C3C	2.95	1.50	1.45
13	A	836	CLA	C1C-C2C	2.95	1.50	1.44
13	A	824	CLA	C1D-C2D	-2.95	1.39	1.45
13	J	1103	CLA	C1C-C2C	2.95	1.50	1.44
15	B	845	BCR	C40-C30	-2.95	1.48	1.53
13	B	818	CLA	O2A-CGA	2.94	1.41	1.33
13	A	837	CLA	C1C-C2C	2.94	1.50	1.44
13	A	837	CLA	C4C-C3C	2.94	1.50	1.45
15	I	102	BCR	C8-C9	2.94	1.52	1.46
13	B	805	CLA	O2D-CED	-2.94	1.38	1.45
13	M	1201	CLA	C4C-C3C	2.94	1.50	1.45
15	A	852	BCR	C8-C9	2.94	1.52	1.46
13	A	821	CLA	O2A-CGA	2.94	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1102	CLA	C1C-C2C	2.94	1.50	1.44
13	L	1004	CLA	O2A-CGA	2.94	1.41	1.33
13	A	803	CLA	C1C-C2C	2.94	1.50	1.44
15	B	849	BCR	C8-C9	2.94	1.52	1.46
13	B	838	CLA	O2D-CED	-2.94	1.38	1.45
15	B	841	BCR	C26-C25	2.94	1.39	1.34
13	A	816	CLA	O2A-CGA	2.94	1.41	1.33
15	A	847	BCR	C19-C18	2.94	1.52	1.46
13	B	830	CLA	C1C-C2C	2.93	1.50	1.44
15	B	842	BCR	C12-C13	2.93	1.52	1.46
13	B	835	CLA	C4C-C3C	2.93	1.50	1.45
13	A	805	CLA	C1C-C2C	2.93	1.50	1.44
13	F	1301	CLA	C4C-C3C	2.93	1.50	1.45
15	A	849	BCR	C8-C9	2.93	1.52	1.46
13	A	828	CLA	C4C-C3C	2.93	1.50	1.45
13	A	810	CLA	C4C-C3C	2.93	1.50	1.45
13	L	1002	CLA	C1D-C2D	-2.93	1.39	1.45
13	B	834	CLA	C1C-C2C	2.93	1.50	1.44
13	A	825	CLA	C4C-C3C	2.93	1.50	1.45
13	A	802	CLA	C1C-C2C	2.93	1.50	1.44
13	B	828	CLA	C4C-C3C	2.93	1.50	1.45
13	B	832	CLA	O2D-CED	-2.93	1.38	1.45
13	A	845	CLA	C1D-C2D	-2.93	1.39	1.45
13	A	834	CLA	O2D-CED	-2.92	1.38	1.45
13	A	805	CLA	O2A-CGA	2.92	1.41	1.33
13	B	839	CLA	O2A-CGA	2.92	1.41	1.33
13	A	801	CLA	C1C-C2C	2.92	1.50	1.44
13	A	816	CLA	C1C-C2C	2.92	1.50	1.44
15	I	102	BCR	C32-C1	-2.92	1.48	1.53
13	A	817	CLA	O2A-CGA	2.92	1.41	1.33
13	A	842	CLA	C1C-C2C	2.92	1.50	1.44
13	A	820	CLA	O2A-CGA	2.92	1.41	1.33
13	A	829	CLA	C1C-C2C	2.92	1.50	1.44
13	B	836	CLA	C4C-C3C	2.92	1.50	1.45
13	B	820	CLA	C1C-C2C	2.92	1.50	1.44
13	A	839	CLA	O2A-CGA	2.92	1.41	1.33
15	F	1302	BCR	C12-C13	2.92	1.52	1.46
13	A	815	CLA	C1D-C2D	-2.92	1.39	1.45
15	B	843	BCR	C32-C1	-2.92	1.48	1.53
13	B	823	CLA	C1C-C2C	2.92	1.50	1.44
13	A	803	CLA	O2A-CGA	2.91	1.41	1.33
13	B	833	CLA	C4C-C3C	2.91	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	816	CLA	C1C-C2C	2.91	1.50	1.44
13	A	816	CLA	O2D-CED	-2.91	1.38	1.45
13	A	827	CLA	O2D-CED	-2.91	1.38	1.45
13	B	827	CLA	O2A-CGA	2.91	1.41	1.33
15	B	846	BCR	C12-C13	2.91	1.52	1.46
13	B	829	CLA	C4C-C3C	2.91	1.50	1.45
13	A	823	CLA	O2D-CED	-2.91	1.38	1.45
13	A	832	CLA	C1D-C2D	-2.91	1.39	1.45
13	A	811	CLA	C4C-C3C	2.91	1.50	1.45
13	A	822	CLA	O2D-CED	-2.91	1.38	1.45
15	B	846	BCR	C32-C1	-2.91	1.48	1.53
13	A	824	CLA	O2A-CGA	2.90	1.41	1.33
13	B	812	CLA	C1C-C2C	2.90	1.50	1.44
13	A	835	CLA	C1C-C2C	2.90	1.50	1.44
13	B	829	CLA	O2D-CED	-2.90	1.38	1.45
13	B	820	CLA	O2D-CED	-2.89	1.38	1.45
13	A	801	CLA	C1B-NB	-2.89	1.34	1.37
15	B	849	BCR	C19-C18	2.89	1.52	1.46
13	B	805	CLA	C1D-C2D	-2.89	1.39	1.45
13	A	829	CLA	C1D-C2D	-2.89	1.39	1.45
13	B	826	CLA	O2A-CGA	2.89	1.41	1.33
13	A	813	CLA	O2A-CGA	2.89	1.41	1.33
13	B	809	CLA	C1C-C2C	2.89	1.50	1.44
13	B	832	CLA	C4C-C3C	2.89	1.49	1.45
13	A	807	CLA	C2-C3	2.89	1.39	1.33
13	I	101	CLA	O2A-CGA	2.89	1.41	1.33
18	B	848	LMG	O8-C28	2.89	1.41	1.33
15	L	1005	BCR	C32-C1	-2.89	1.48	1.53
13	B	803	CLA	O2A-CGA	2.89	1.41	1.33
13	A	838	CLA	C4C-C3C	2.89	1.49	1.45
13	A	833	CLA	O2A-CGA	2.89	1.41	1.33
13	A	842	CLA	O2A-CGA	2.89	1.41	1.33
15	J	1105	BCR	C32-C1	-2.88	1.48	1.53
13	B	830	CLA	C4C-C3C	2.88	1.49	1.45
13	B	830	CLA	O2A-CGA	2.88	1.41	1.33
13	B	838	CLA	O2A-CGA	2.88	1.41	1.33
15	A	847	BCR	C26-C25	2.88	1.39	1.34
13	B	810	CLA	O2D-CED	-2.88	1.38	1.45
13	A	812	CLA	C1C-C2C	2.88	1.50	1.44
13	B	837	CLA	O2A-CGA	2.88	1.41	1.33
15	J	1104	BCR	C12-C13	2.88	1.52	1.46
13	A	843	CLA	C4C-C3C	2.88	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	847	BCR	C12-C13	2.88	1.52	1.46
13	L	1004	CLA	O2D-CED	-2.88	1.38	1.45
13	A	824	CLA	C1C-C2C	2.88	1.50	1.44
13	B	829	CLA	C1C-C2C	2.88	1.50	1.44
15	B	847	BCR	C32-C1	-2.88	1.48	1.53
13	A	830	CLA	C4C-C3C	2.88	1.49	1.45
13	B	836	CLA	O2A-CGA	2.88	1.41	1.33
13	A	833	CLA	O2D-CED	-2.88	1.38	1.45
13	A	809	CLA	O2A-CGA	2.88	1.41	1.33
13	A	835	CLA	O2A-CGA	2.88	1.41	1.33
13	B	816	CLA	O2D-CED	-2.88	1.38	1.45
13	A	855	CLA	C1C-C2C	2.88	1.50	1.44
13	L	1002	CLA	O2D-CED	-2.88	1.38	1.45
15	L	1006	BCR	C5-C6	2.87	1.39	1.34
13	I	101	CLA	O2D-CED	-2.87	1.38	1.45
13	B	807	CLA	C4C-C3C	2.87	1.49	1.45
13	X	102	CLA	C4C-C3C	2.87	1.49	1.45
13	L	1004	CLA	C1C-C2C	2.87	1.50	1.44
13	A	844	CLA	C1D-ND	-2.87	1.34	1.37
13	B	839	CLA	C1C-C2C	2.87	1.50	1.44
13	A	837	CLA	C1B-NB	-2.87	1.34	1.37
13	B	836	CLA	O2D-CED	-2.87	1.38	1.45
13	B	815	CLA	C1C-C2C	2.87	1.50	1.44
13	B	829	CLA	O2A-CGA	2.87	1.41	1.33
15	B	850	BCR	C32-C1	-2.87	1.48	1.53
13	A	838	CLA	O2D-CED	-2.87	1.38	1.45
13	B	804	CLA	C1C-C2C	2.87	1.50	1.44
13	A	836	CLA	O2D-CED	-2.87	1.38	1.45
13	A	817	CLA	O2D-CED	-2.87	1.38	1.45
15	A	849	BCR	C32-C1	-2.86	1.48	1.53
13	A	835	CLA	O2D-CED	-2.86	1.38	1.45
13	A	841	CLA	O2D-CED	-2.86	1.38	1.45
13	X	102	CLA	C1D-ND	-2.86	1.34	1.37
13	A	812	CLA	O2A-CGA	2.86	1.41	1.33
13	A	822	CLA	C1C-C2C	2.86	1.50	1.44
13	A	830	CLA	O2D-CED	-2.86	1.38	1.45
13	A	843	CLA	O2D-CED	-2.86	1.38	1.45
13	B	802	CLA	O2D-CED	-2.86	1.38	1.45
13	B	801	CLA	C1B-NB	-2.86	1.34	1.37
13	B	816	CLA	C4C-C3C	2.86	1.49	1.45
13	L	1003	CLA	O2D-CED	-2.86	1.38	1.45
13	A	841	CLA	C1C-C2C	2.85	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	809	CLA	O2D-CED	-2.85	1.38	1.45
13	B	805	CLA	C1C-C2C	2.85	1.50	1.44
13	A	823	CLA	C1B-NB	-2.85	1.34	1.37
13	B	830	CLA	O2D-CED	-2.85	1.38	1.45
13	B	804	CLA	C4C-C3C	2.85	1.49	1.45
13	A	828	CLA	O2A-CGA	2.85	1.41	1.33
13	A	836	CLA	C1D-ND	-2.85	1.34	1.37
13	A	825	CLA	O2D-CED	-2.85	1.38	1.45
15	A	851	BCR	C32-C1	-2.85	1.48	1.53
13	L	1002	CLA	O2A-CGA	2.85	1.41	1.33
13	A	844	CLA	C1D-C2D	-2.84	1.39	1.45
15	A	851	BCR	C12-C13	2.84	1.52	1.46
13	B	803	CLA	O2D-CED	-2.84	1.39	1.45
13	B	808	CLA	C1D-ND	-2.84	1.34	1.37
13	B	821	CLA	C4C-C3C	2.84	1.49	1.45
13	B	803	CLA	C1C-C2C	2.84	1.50	1.44
13	B	802	CLA	C4C-C3C	2.84	1.49	1.45
13	I	101	CLA	C1D-ND	-2.84	1.34	1.37
15	B	842	BCR	C32-C1	-2.84	1.48	1.53
13	B	804	CLA	O2D-CED	-2.84	1.39	1.45
13	X	102	CLA	C1C-C2C	2.84	1.50	1.44
13	B	817	CLA	C1D-ND	-2.84	1.34	1.37
13	B	806	CLA	C4C-C3C	2.83	1.49	1.45
13	A	801	CLA	O2D-CED	-2.83	1.39	1.45
13	F	1301	CLA	O2D-CED	-2.83	1.39	1.45
13	B	822	CLA	C1C-C2C	2.83	1.50	1.44
13	B	807	CLA	C1D-ND	-2.83	1.34	1.37
13	B	822	CLA	C1D-ND	-2.83	1.34	1.37
15	A	850	BCR	C26-C25	2.83	1.39	1.34
13	B	812	CLA	O2A-CGA	2.83	1.41	1.33
13	J	1101	CLA	O2D-CED	-2.83	1.39	1.45
13	A	845	CLA	O2D-CED	-2.83	1.39	1.45
13	B	816	CLA	C1B-NB	-2.83	1.34	1.37
13	A	815	CLA	O2D-CED	-2.83	1.39	1.45
15	B	849	BCR	C32-C1	-2.83	1.48	1.53
13	B	821	CLA	C1C-C2C	2.83	1.50	1.44
13	A	829	CLA	O2D-CED	-2.83	1.39	1.45
13	A	805	CLA	O2D-CED	-2.83	1.39	1.45
13	A	855	CLA	O2D-CED	-2.83	1.39	1.45
13	A	802	CLA	O2D-CED	-2.82	1.39	1.45
13	B	811	CLA	O2D-CED	-2.82	1.39	1.45
13	A	820	CLA	O2D-CED	-2.82	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	837	CLA	O2D-CED	-2.82	1.39	1.45
15	M	1203	BCR	C12-C13	2.82	1.52	1.46
13	A	840	CLA	O2A-CGA	2.82	1.41	1.33
15	M	1203	BCR	C8-C9	2.82	1.52	1.46
13	B	814	CLA	C1C-C2C	2.82	1.50	1.44
13	B	814	CLA	C4C-C3C	2.82	1.49	1.45
15	J	1104	BCR	C32-C1	-2.82	1.48	1.53
13	A	824	CLA	O2D-CED	-2.82	1.39	1.45
13	A	834	CLA	C4C-C3C	2.82	1.49	1.45
13	B	813	CLA	C1B-NB	-2.82	1.34	1.37
13	A	810	CLA	C1C-C2C	2.81	1.50	1.44
15	B	846	BCR	C26-C25	2.81	1.39	1.34
13	B	813	CLA	C1C-C2C	2.81	1.50	1.44
15	A	850	BCR	C32-C1	-2.81	1.48	1.53
13	A	806	CLA	O2A-CGA	2.81	1.41	1.33
13	B	808	CLA	C1B-NB	-2.81	1.34	1.37
13	A	811	CLA	O2D-CED	-2.81	1.39	1.45
15	A	852	BCR	C12-C13	2.81	1.52	1.46
13	A	821	CLA	O2D-CED	-2.81	1.39	1.45
13	L	1003	CLA	C1C-C2C	2.81	1.50	1.44
13	A	820	CLA	C1D-ND	-2.81	1.34	1.37
13	B	822	CLA	O2D-CED	-2.81	1.39	1.45
13	A	841	CLA	C1D-ND	-2.81	1.34	1.37
13	A	813	CLA	O2D-CED	-2.81	1.39	1.45
13	A	822	CLA	C4C-C3C	2.81	1.49	1.45
13	B	814	CLA	O2D-CED	-2.81	1.39	1.45
13	A	809	CLA	C4C-C3C	2.81	1.49	1.45
13	B	825	CLA	O2A-CGA	2.80	1.41	1.33
13	B	839	CLA	O2D-CED	-2.80	1.39	1.45
15	B	842	BCR	C26-C25	2.80	1.39	1.34
13	M	1201	CLA	O2D-CED	-2.80	1.39	1.45
15	M	1203	BCR	C32-C1	-2.80	1.48	1.53
13	B	828	CLA	C1C-C2C	2.80	1.50	1.44
13	A	810	CLA	O2D-CED	-2.80	1.39	1.45
13	A	840	CLA	O2D-CED	-2.80	1.39	1.45
13	A	819	CLA	C4C-C3C	2.80	1.49	1.45
13	A	833	CLA	C1C-C2C	2.80	1.50	1.44
15	L	1006	BCR	C32-C1	-2.80	1.48	1.53
13	B	838	CLA	C1D-ND	-2.80	1.34	1.37
13	A	834	CLA	C1D-ND	-2.80	1.34	1.37
13	B	810	CLA	C1C-C2C	2.80	1.50	1.44
13	B	819	CLA	C1C-C2C	2.80	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	848	BCR	C32-C1	-2.80	1.48	1.53
13	A	842	CLA	C1D-ND	-2.79	1.34	1.37
13	B	808	CLA	O2D-CED	-2.79	1.39	1.45
13	A	855	CLA	C1B-NB	-2.79	1.34	1.37
13	A	832	CLA	O2D-CED	-2.79	1.39	1.45
13	B	806	CLA	C1D-ND	-2.79	1.34	1.37
13	B	834	CLA	O2D-CED	-2.79	1.39	1.45
13	A	819	CLA	C1D-ND	-2.79	1.34	1.37
13	A	822	CLA	C1D-ND	-2.79	1.34	1.37
13	A	845	CLA	O2A-CGA	2.79	1.41	1.33
13	B	823	CLA	C1B-NB	-2.79	1.34	1.37
13	B	805	CLA	O2A-CGA	2.79	1.41	1.33
15	I	102	BCR	C19-C18	2.79	1.51	1.46
13	B	831	CLA	C1C-C2C	2.79	1.50	1.44
13	A	826	CLA	C1B-NB	-2.79	1.34	1.37
15	A	849	BCR	C19-C18	2.79	1.51	1.46
13	A	823	CLA	C4C-C3C	2.79	1.49	1.45
13	B	801	CLA	O2D-CED	-2.79	1.39	1.45
15	B	849	BCR	C26-C25	2.79	1.39	1.34
15	F	1302	BCR	C26-C25	2.79	1.39	1.34
13	I	101	CLA	C4C-C3C	2.79	1.49	1.45
13	A	820	CLA	C1B-NB	-2.79	1.34	1.37
15	A	852	BCR	C32-C1	-2.79	1.48	1.53
13	B	804	CLA	C1B-NB	-2.79	1.34	1.37
15	A	847	BCR	C32-C1	-2.79	1.48	1.53
13	J	1103	CLA	C1D-ND	-2.78	1.34	1.37
13	B	812	CLA	O2D-CED	-2.78	1.39	1.45
13	B	819	CLA	O2D-CED	-2.78	1.39	1.45
13	A	808	CLA	C4C-C3C	2.78	1.49	1.45
13	A	818	CLA	C1B-NB	-2.78	1.34	1.37
13	B	818	CLA	C1D-ND	-2.78	1.34	1.37
13	X	102	CLA	O2D-CED	-2.78	1.39	1.45
13	B	823	CLA	C1D-ND	-2.78	1.34	1.37
13	B	823	CLA	O2A-CGA	2.78	1.41	1.33
13	A	839	CLA	O2D-CED	-2.78	1.39	1.45
15	L	1006	BCR	C12-C13	2.78	1.51	1.46
13	B	807	CLA	O2D-CED	-2.78	1.39	1.45
15	B	847	BCR	C40-C30	-2.77	1.48	1.53
13	A	820	CLA	C1C-C2C	2.77	1.50	1.44
13	A	855	CLA	C1D-ND	-2.77	1.34	1.37
13	A	815	CLA	C1C-C2C	2.77	1.50	1.44
13	B	828	CLA	O2D-CED	-2.77	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	823	CLA	O2A-CGA	2.77	1.41	1.33
13	A	803	CLA	C1D-ND	-2.77	1.34	1.37
13	B	819	CLA	C1B-NB	-2.77	1.34	1.37
13	B	817	CLA	O2A-CGA	2.77	1.41	1.33
13	A	834	CLA	C1C-C2C	2.77	1.50	1.44
13	A	808	CLA	C1B-NB	-2.77	1.34	1.37
13	A	818	CLA	O2D-CED	-2.77	1.39	1.45
15	B	845	BCR	C32-C1	-2.77	1.48	1.53
13	A	812	CLA	C1D-ND	-2.77	1.34	1.37
13	B	809	CLA	O2D-CED	-2.77	1.39	1.45
13	A	802	CLA	C1D-ND	-2.77	1.34	1.37
13	A	809	CLA	C1D-ND	-2.77	1.34	1.37
13	A	812	CLA	O2D-CED	-2.77	1.39	1.45
13	A	826	CLA	C1D-ND	-2.77	1.34	1.37
13	B	833	CLA	O2D-CED	-2.76	1.39	1.45
13	A	827	CLA	C1C-C2C	2.76	1.50	1.44
13	B	803	CLA	C1B-NB	-2.76	1.34	1.37
13	B	824	CLA	O2D-CED	-2.76	1.39	1.45
13	A	823	CLA	C1D-ND	-2.75	1.34	1.37
13	B	816	CLA	O2A-CGA	2.75	1.41	1.33
15	B	841	BCR	C32-C1	-2.75	1.48	1.53
13	A	831	CLA	O2A-CGA	2.75	1.41	1.33
13	A	827	CLA	C1D-ND	-2.75	1.34	1.37
13	A	828	CLA	O2D-CED	-2.75	1.39	1.45
13	A	819	CLA	O2D-CED	-2.75	1.39	1.45
13	L	1002	CLA	C1D-ND	-2.75	1.34	1.37
13	F	1301	CLA	C1B-NB	-2.75	1.34	1.37
13	A	807	CLA	C4C-C3C	2.75	1.49	1.45
15	F	1302	BCR	C32-C1	-2.75	1.48	1.53
13	B	832	CLA	C1B-NB	-2.75	1.34	1.37
13	B	806	CLA	O2A-CGA	2.75	1.41	1.33
13	B	836	CLA	C1D-ND	-2.74	1.34	1.37
13	A	821	CLA	C1D-ND	-2.74	1.34	1.37
13	B	835	CLA	C1C-C2C	2.74	1.50	1.44
13	L	1004	CLA	C1B-NB	-2.74	1.34	1.37
13	B	810	CLA	C1D-ND	-2.74	1.34	1.37
13	A	820	CLA	C3D-C4D	-2.74	1.38	1.44
13	B	818	CLA	C1B-NB	-2.74	1.34	1.37
13	B	834	CLA	C1B-NB	-2.74	1.34	1.37
13	A	808	CLA	C1D-ND	-2.74	1.34	1.37
13	B	836	CLA	C1B-NB	-2.74	1.34	1.37
13	A	841	CLA	C1B-NB	-2.74	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	807	CLA	O2A-CGA	2.73	1.41	1.33
13	M	1202	CLA	O2D-CED	-2.73	1.39	1.45
13	A	845	CLA	C1C-C2C	2.73	1.50	1.44
13	A	838	CLA	C1D-ND	-2.73	1.34	1.37
13	A	843	CLA	C1D-ND	-2.73	1.34	1.37
13	A	838	CLA	O2A-CGA	2.73	1.41	1.33
13	B	830	CLA	C1D-ND	-2.73	1.34	1.37
13	F	1301	CLA	C1D-ND	-2.73	1.34	1.37
13	A	819	CLA	O2A-CGA	2.73	1.41	1.33
13	B	826	CLA	C1C-C2C	2.73	1.50	1.44
13	L	1004	CLA	C1D-ND	-2.73	1.34	1.37
13	B	820	CLA	C1B-NB	-2.73	1.34	1.37
13	B	833	CLA	C1D-ND	-2.73	1.34	1.37
13	A	835	CLA	C1D-ND	-2.73	1.34	1.37
13	A	817	CLA	O2D-CGD	2.72	1.39	1.33
13	A	819	CLA	C1B-NB	-2.72	1.34	1.37
13	B	807	CLA	C1B-NB	-2.72	1.34	1.37
13	B	809	CLA	C1B-NB	-2.72	1.34	1.37
13	B	814	CLA	O2A-CGA	2.72	1.41	1.33
13	B	817	CLA	C1C-C2C	2.72	1.50	1.44
15	B	845	BCR	C12-C13	2.72	1.51	1.46
13	A	816	CLA	C1D-ND	-2.72	1.34	1.37
13	L	1003	CLA	C1B-NB	-2.72	1.34	1.37
13	B	835	CLA	C1D-ND	-2.72	1.34	1.37
13	A	819	CLA	C1C-C2C	2.71	1.50	1.44
13	J	1102	CLA	O2D-CED	-2.71	1.39	1.45
13	B	815	CLA	O2A-CGA	2.71	1.41	1.33
13	L	1003	CLA	C1D-ND	-2.71	1.34	1.37
13	A	807	CLA	O2A-CGA	2.71	1.41	1.33
15	B	842	BCR	C40-C30	-2.71	1.48	1.53
15	M	1203	BCR	C40-C30	-2.71	1.48	1.53
13	B	813	CLA	O2D-CED	-2.71	1.39	1.45
13	A	809	CLA	C1B-NB	-2.71	1.34	1.37
13	A	844	CLA	C3D-C4D	-2.71	1.38	1.44
15	B	847	BCR	C26-C25	2.71	1.39	1.34
13	A	807	CLA	O2D-CED	-2.70	1.39	1.45
13	B	813	CLA	MG-NB	-2.70	2.00	2.05
13	B	828	CLA	C1B-NB	-2.70	1.34	1.37
13	A	832	CLA	C5-C3	2.70	1.56	1.51
13	B	821	CLA	C1D-ND	-2.70	1.34	1.37
13	A	805	CLA	C1B-NB	-2.70	1.34	1.37
13	J	1102	CLA	C1B-NB	-2.70	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	821	CLA	O2D-CGD	2.70	1.39	1.33
13	B	802	CLA	C1B-NB	-2.70	1.34	1.37
13	B	806	CLA	C1B-NB	-2.69	1.34	1.37
13	B	817	CLA	C1B-NB	-2.69	1.34	1.37
13	A	802	CLA	C1B-NB	-2.69	1.34	1.37
13	B	820	CLA	C1D-ND	-2.69	1.34	1.37
15	B	843	BCR	C40-C30	-2.69	1.48	1.53
13	A	818	CLA	C1C-C2C	2.69	1.50	1.44
13	B	810	CLA	O2D-CGD	2.69	1.39	1.33
13	A	843	CLA	O2A-CGA	2.68	1.41	1.33
13	B	824	CLA	C1D-ND	-2.68	1.34	1.37
13	J	1102	CLA	C1D-ND	-2.68	1.34	1.37
13	A	824	CLA	C1B-NB	-2.68	1.34	1.37
13	B	817	CLA	O2D-CED	-2.68	1.39	1.45
13	B	811	CLA	C5-C3	2.68	1.56	1.51
15	B	844	BCR	C40-C30	-2.68	1.48	1.53
13	A	825	CLA	C5-C3	2.68	1.56	1.51
15	B	849	BCR	C12-C13	2.68	1.51	1.46
13	A	833	CLA	O2D-CGD	2.68	1.39	1.33
13	A	804	CLA	C1B-NB	-2.67	1.34	1.37
13	B	811	CLA	C1B-NB	-2.67	1.34	1.37
15	L	1005	BCR	C26-C25	2.67	1.39	1.34
13	J	1101	CLA	C1B-NB	-2.67	1.34	1.37
18	B	848	LMG	C4-C5	2.67	1.58	1.53
13	A	834	CLA	C5-C3	2.67	1.56	1.51
13	A	828	CLA	C1B-NB	-2.67	1.34	1.37
13	A	838	CLA	C1B-NB	-2.67	1.34	1.37
13	A	806	CLA	C1D-ND	-2.67	1.34	1.37
13	B	829	CLA	C1B-NB	-2.67	1.34	1.37
15	I	102	BCR	C40-C30	-2.67	1.48	1.53
13	A	831	CLA	C1D-ND	-2.66	1.34	1.37
15	A	848	BCR	C26-C25	2.66	1.39	1.34
13	B	830	CLA	C1B-NB	-2.66	1.34	1.37
13	B	832	CLA	C1D-ND	-2.66	1.34	1.37
13	B	837	CLA	C1D-ND	-2.66	1.34	1.37
15	A	849	BCR	C26-C25	2.66	1.39	1.34
13	A	813	CLA	C1D-ND	-2.66	1.34	1.37
13	A	831	CLA	C2-C3	2.66	1.40	1.32
13	A	815	CLA	C1B-NB	-2.66	1.34	1.37
15	J	1105	BCR	C40-C30	-2.66	1.48	1.53
13	A	807	CLA	C1B-NB	-2.66	1.34	1.37
13	B	815	CLA	C1D-ND	-2.66	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	818	CLA	O2A-CGA	2.65	1.41	1.33
13	B	803	CLA	C1D-ND	-2.65	1.34	1.37
13	B	805	CLA	C1D-ND	-2.65	1.34	1.37
13	B	836	CLA	C3D-C4D	-2.65	1.38	1.44
13	B	828	CLA	C1D-ND	-2.65	1.34	1.37
13	M	1201	CLA	C1B-NB	-2.65	1.34	1.37
13	M	1201	CLA	C1D-ND	-2.65	1.34	1.37
15	L	1005	BCR	C40-C30	-2.65	1.48	1.53
15	M	1203	BCR	C26-C25	2.65	1.39	1.34
13	A	817	CLA	C1D-ND	-2.65	1.34	1.37
13	A	832	CLA	C1D-ND	-2.65	1.34	1.37
13	B	801	CLA	C1D-ND	-2.65	1.34	1.37
13	B	822	CLA	C3D-C4D	-2.65	1.38	1.44
13	J	1101	CLA	C1D-ND	-2.64	1.34	1.37
13	A	833	CLA	C1B-NB	-2.64	1.34	1.37
13	A	829	CLA	C1B-NB	-2.64	1.34	1.37
13	B	834	CLA	C1D-ND	-2.64	1.34	1.37
13	A	802	CLA	C3D-C4D	-2.64	1.38	1.44
15	A	849	BCR	C12-C13	2.64	1.51	1.46
13	B	812	CLA	C3D-C4D	-2.64	1.38	1.44
15	L	1006	BCR	C26-C25	2.64	1.38	1.34
13	B	829	CLA	O2D-CGD	2.64	1.39	1.33
15	A	852	BCR	C26-C25	2.64	1.38	1.34
13	A	813	CLA	C1B-NB	-2.64	1.34	1.37
13	A	824	CLA	C1D-ND	-2.64	1.34	1.37
13	B	838	CLA	C1B-NB	-2.64	1.34	1.37
13	A	839	CLA	C3D-C4D	-2.64	1.38	1.44
13	A	825	CLA	C1B-NB	-2.64	1.34	1.37
13	B	816	CLA	C1D-ND	-2.64	1.34	1.37
13	B	826	CLA	C1B-NB	-2.64	1.34	1.37
13	A	815	CLA	C1D-ND	-2.63	1.34	1.37
13	B	833	CLA	C1B-NB	-2.63	1.34	1.37
13	B	813	CLA	C1D-ND	-2.63	1.34	1.37
13	B	825	CLA	C1B-NB	-2.63	1.34	1.37
13	A	843	CLA	C1B-NB	-2.63	1.34	1.37
13	A	827	CLA	C1B-NB	-2.63	1.34	1.37
13	M	1202	CLA	C1B-NB	-2.63	1.34	1.37
13	A	842	CLA	C5-C3	2.63	1.56	1.51
13	A	841	CLA	O2D-CGD	2.63	1.39	1.33
13	X	102	CLA	C1B-NB	-2.62	1.34	1.37
13	A	833	CLA	C1D-ND	-2.62	1.34	1.37
15	J	1104	BCR	C40-C30	-2.62	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	816	CLA	O2D-CGD	2.62	1.39	1.33
13	A	811	CLA	C1B-NB	-2.62	1.34	1.37
13	B	812	CLA	C1D-ND	-2.62	1.34	1.37
13	I	101	CLA	O2D-CGD	2.62	1.39	1.33
13	B	830	CLA	C3D-C4D	-2.62	1.38	1.44
15	B	844	BCR	C26-C25	2.62	1.38	1.34
15	A	848	BCR	C40-C30	-2.62	1.48	1.53
13	B	810	CLA	C1B-NB	-2.62	1.34	1.37
13	B	831	CLA	C1B-NB	-2.62	1.34	1.37
13	A	829	CLA	C5-C3	2.62	1.56	1.51
13	A	842	CLA	C1B-NB	-2.62	1.34	1.37
15	A	851	BCR	C40-C30	-2.61	1.48	1.53
13	A	828	CLA	O2D-CGD	2.61	1.39	1.33
13	B	839	CLA	C1D-ND	-2.61	1.34	1.37
15	A	850	BCR	C40-C30	-2.61	1.48	1.53
13	A	842	CLA	O2D-CGD	2.61	1.39	1.33
13	A	831	CLA	C3D-C4D	-2.61	1.38	1.44
15	B	846	BCR	C40-C30	-2.61	1.48	1.53
13	A	835	CLA	C1B-NB	-2.61	1.34	1.37
13	A	812	CLA	C1B-NB	-2.61	1.34	1.37
13	B	819	CLA	C1D-ND	-2.61	1.34	1.37
13	A	831	CLA	C1B-NB	-2.60	1.34	1.37
13	A	837	CLA	C1D-ND	-2.60	1.34	1.37
15	B	850	BCR	C40-C30	-2.60	1.48	1.53
13	A	838	CLA	C3D-C4D	-2.60	1.38	1.44
13	B	820	CLA	O2D-CGD	2.60	1.39	1.33
13	A	838	CLA	C5-C3	2.60	1.56	1.51
13	B	813	CLA	C3D-C4D	-2.60	1.38	1.44
13	B	802	CLA	C1D-ND	-2.60	1.34	1.37
15	A	851	BCR	C26-C25	2.60	1.38	1.34
13	B	823	CLA	C3D-C4D	-2.60	1.38	1.44
13	J	1103	CLA	C3D-C4D	-2.60	1.38	1.44
13	A	806	CLA	C1B-NB	-2.60	1.34	1.37
13	B	812	CLA	C1B-NB	-2.60	1.34	1.37
13	A	819	CLA	C3D-C4D	-2.60	1.38	1.44
13	B	817	CLA	C3D-C4D	-2.60	1.38	1.44
13	B	835	CLA	C1B-NB	-2.60	1.34	1.37
15	I	102	BCR	C26-C25	2.60	1.38	1.34
13	B	815	CLA	C3D-C4D	-2.60	1.38	1.44
13	A	830	CLA	C5-C3	2.60	1.56	1.51
13	A	825	CLA	C1D-ND	-2.60	1.34	1.37
15	B	849	BCR	C40-C30	-2.60	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	821	CLA	C3D-C4D	-2.60	1.38	1.44
13	L	1002	CLA	C1B-NB	-2.60	1.34	1.37
13	B	826	CLA	C1D-ND	-2.59	1.34	1.37
13	B	837	CLA	C1B-NB	-2.59	1.34	1.37
13	A	810	CLA	C1B-NB	-2.59	1.34	1.37
13	B	830	CLA	O2D-CGD	2.59	1.39	1.33
13	A	823	CLA	O2D-CGD	2.59	1.39	1.33
13	A	814	CLA	C1D-ND	-2.59	1.34	1.37
13	B	821	CLA	C1B-NB	-2.59	1.34	1.37
13	B	839	CLA	C1B-NB	-2.59	1.34	1.37
13	A	816	CLA	C1B-NB	-2.58	1.34	1.37
13	B	824	CLA	C1B-NB	-2.58	1.34	1.37
13	A	809	CLA	O2D-CGD	2.58	1.39	1.33
13	B	830	CLA	C5-C3	2.58	1.56	1.51
13	M	1201	CLA	C3D-C4D	-2.58	1.38	1.44
13	I	101	CLA	C1B-NB	-2.58	1.34	1.37
13	A	845	CLA	C1B-NB	-2.58	1.34	1.37
15	B	850	BCR	C26-C25	2.58	1.38	1.34
13	B	816	CLA	C3D-C4D	-2.58	1.38	1.44
13	A	835	CLA	O2D-CGD	2.57	1.39	1.33
13	B	835	CLA	C5-C3	2.57	1.56	1.51
13	A	803	CLA	C1B-NB	-2.57	1.34	1.37
13	A	844	CLA	C1B-NB	-2.57	1.34	1.37
13	B	804	CLA	C1D-ND	-2.57	1.34	1.37
13	A	821	CLA	C5-C3	2.57	1.56	1.51
13	B	839	CLA	C3D-C4D	-2.57	1.38	1.44
15	A	849	BCR	C40-C30	-2.57	1.48	1.53
15	A	847	BCR	C40-C30	-2.57	1.48	1.53
13	A	805	CLA	C5-C3	2.57	1.56	1.51
13	B	831	CLA	C1D-ND	-2.57	1.34	1.37
15	A	849	BCR	C5-C6	2.57	1.38	1.34
13	B	827	CLA	C1D-ND	-2.57	1.34	1.37
13	B	822	CLA	MG-NB	-2.57	2.00	2.05
15	B	843	BCR	C26-C25	2.57	1.38	1.34
13	B	814	CLA	C1B-NB	-2.56	1.34	1.37
15	I	102	BCR	C12-C13	2.56	1.51	1.46
13	A	820	CLA	O2D-CGD	2.56	1.39	1.33
13	B	806	CLA	C3D-C4D	-2.56	1.38	1.44
13	J	1103	CLA	C1B-NB	-2.56	1.34	1.37
15	J	1104	BCR	C26-C25	2.56	1.38	1.34
13	A	834	CLA	C3D-C4D	-2.56	1.38	1.44
15	B	841	BCR	C40-C30	-2.56	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	809	CLA	C1D-ND	-2.56	1.34	1.37
13	B	825	CLA	C3D-C4D	-2.56	1.38	1.44
15	J	1105	BCR	C26-C25	2.55	1.38	1.34
13	A	817	CLA	C1B-NB	-2.55	1.34	1.37
13	A	827	CLA	C4C-C3C	2.55	1.49	1.45
13	A	809	CLA	C5-C3	2.55	1.56	1.51
13	A	811	CLA	C5-C3	2.55	1.56	1.51
13	A	826	CLA	C3D-C4D	-2.55	1.38	1.44
13	M	1201	CLA	C5-C3	2.55	1.56	1.51
13	B	805	CLA	C3D-C4D	-2.55	1.38	1.44
13	A	808	CLA	C5-C3	2.55	1.56	1.51
15	L	1006	BCR	C40-C30	-2.55	1.48	1.53
13	B	827	CLA	C5-C3	2.54	1.56	1.51
13	A	836	CLA	C1B-NB	-2.54	1.34	1.37
13	M	1202	CLA	O2D-CGD	2.54	1.39	1.33
15	F	1302	BCR	C40-C30	-2.54	1.48	1.53
13	A	845	CLA	C1D-ND	-2.54	1.34	1.37
13	A	822	CLA	C1B-NB	-2.54	1.34	1.37
13	A	839	CLA	C1D-ND	-2.54	1.34	1.37
13	A	804	CLA	C5-C3	2.53	1.56	1.51
13	A	814	CLA	C1B-NB	-2.53	1.34	1.37
13	B	805	CLA	C1B-NB	-2.53	1.34	1.37
13	A	811	CLA	C1D-ND	-2.53	1.34	1.37
13	B	825	CLA	C1D-ND	-2.53	1.34	1.37
13	B	838	CLA	C5-C3	2.53	1.56	1.51
15	A	852	BCR	C40-C30	-2.53	1.49	1.53
13	A	842	CLA	C3D-C4D	-2.53	1.38	1.44
13	B	803	CLA	C5-C3	2.53	1.56	1.51
13	A	817	CLA	C3D-C4D	-2.53	1.38	1.44
13	A	841	CLA	C3D-C4D	-2.53	1.38	1.44
13	B	833	CLA	C3D-C4D	-2.53	1.38	1.44
13	M	1202	CLA	C1D-ND	-2.53	1.34	1.37
13	A	832	CLA	C1B-NB	-2.53	1.34	1.37
15	B	849	BCR	C5-C6	2.52	1.38	1.34
13	A	840	CLA	C1B-NB	-2.52	1.34	1.37
13	B	810	CLA	C3D-C4D	-2.52	1.38	1.44
13	A	801	CLA	C5-C3	2.52	1.56	1.51
13	A	818	CLA	C1D-ND	-2.52	1.34	1.37
13	A	835	CLA	C3D-C4D	-2.52	1.38	1.44
13	B	811	CLA	C1D-ND	-2.52	1.34	1.37
13	A	840	CLA	C1D-ND	-2.52	1.34	1.37
15	J	1104	BCR	C5-C6	2.52	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	839	CLA	C1B-NB	-2.52	1.34	1.37
13	B	838	CLA	C3D-C4D	-2.51	1.38	1.44
13	B	815	CLA	C1B-NB	-2.51	1.34	1.37
13	A	806	CLA	C3D-C4D	-2.51	1.38	1.44
13	A	855	CLA	C3D-C4D	-2.51	1.38	1.44
13	B	822	CLA	C5-C3	2.51	1.56	1.51
13	B	828	CLA	O2D-CGD	2.51	1.39	1.33
13	A	840	CLA	C3D-C4D	-2.51	1.38	1.44
13	A	818	CLA	C3D-C4D	-2.51	1.38	1.44
13	A	821	CLA	C1B-NB	-2.51	1.34	1.37
13	B	825	CLA	C5-C3	2.51	1.56	1.51
13	A	807	CLA	C3D-C4D	-2.51	1.38	1.44
15	B	846	BCR	C5-C6	2.51	1.38	1.34
13	F	1301	CLA	O2D-CGD	2.50	1.39	1.33
13	F	1301	CLA	C3D-C4D	-2.50	1.38	1.44
13	A	804	CLA	C3D-C4D	-2.50	1.38	1.44
13	A	826	CLA	C5-C3	2.50	1.56	1.51
13	B	814	CLA	C1D-ND	-2.50	1.34	1.37
13	B	820	CLA	C3D-C4D	-2.50	1.38	1.44
13	B	813	CLA	O2D-CGD	2.50	1.39	1.33
13	A	833	CLA	C3D-C4D	-2.50	1.38	1.44
13	B	825	CLA	O2D-CGD	2.50	1.39	1.33
13	A	835	CLA	C5-C3	2.50	1.56	1.51
13	A	818	CLA	O2D-CGD	2.50	1.39	1.33
13	A	823	CLA	C3D-C4D	-2.50	1.38	1.44
13	J	1102	CLA	O2D-CGD	2.50	1.39	1.33
13	B	816	CLA	O2D-CGD	2.50	1.39	1.33
13	B	837	CLA	C3D-C4D	-2.49	1.38	1.44
13	A	804	CLA	C1D-ND	-2.49	1.34	1.37
15	B	846	BCR	C39-C30	-2.49	1.49	1.53
13	B	801	CLA	O2D-CGD	2.49	1.39	1.33
13	B	805	CLA	O2D-CGD	2.49	1.39	1.33
15	A	847	BCR	C5-C6	2.49	1.38	1.34
13	B	824	CLA	C5-C3	2.49	1.56	1.51
13	B	812	CLA	O2D-CGD	2.49	1.39	1.33
13	A	840	CLA	O2D-CGD	2.48	1.39	1.33
13	A	810	CLA	C1D-ND	-2.48	1.34	1.37
13	J	1102	CLA	C3D-C4D	-2.48	1.38	1.44
13	B	839	CLA	C5-C3	2.48	1.56	1.51
13	A	827	CLA	C5-C3	2.48	1.56	1.51
13	A	806	CLA	O2D-CGD	2.48	1.39	1.33
13	B	817	CLA	C5-C3	2.48	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	815	CLA	O2D-CGD	2.48	1.39	1.33
13	A	811	CLA	C3D-C4D	-2.48	1.38	1.44
13	B	827	CLA	C4C-C3C	2.48	1.49	1.45
13	B	824	CLA	C3D-C4D	-2.48	1.38	1.44
15	J	1105	BCR	C39-C30	-2.48	1.49	1.53
13	B	819	CLA	O2D-CGD	2.47	1.39	1.33
13	L	1002	CLA	C3D-C4D	-2.47	1.38	1.44
15	B	842	BCR	C24-C23	2.47	1.40	1.33
13	A	824	CLA	C5-C3	2.47	1.56	1.51
13	A	802	CLA	O2D-CGD	2.47	1.39	1.33
13	I	101	CLA	C5-C3	2.47	1.56	1.51
13	I	101	CLA	C3D-C4D	-2.47	1.38	1.44
13	M	1202	CLA	C3D-C4D	-2.47	1.38	1.44
13	A	807	CLA	C1D-ND	-2.47	1.34	1.37
13	B	820	CLA	O2A-CGA	2.47	1.40	1.33
13	A	801	CLA	C1D-ND	-2.47	1.34	1.37
13	B	809	CLA	C3D-C4D	-2.47	1.38	1.44
13	A	834	CLA	O2D-CGD	2.47	1.39	1.33
13	A	845	CLA	C3D-C4D	-2.47	1.38	1.44
13	B	815	CLA	O2D-CGD	2.46	1.39	1.33
13	A	819	CLA	O2D-CGD	2.46	1.39	1.33
13	B	815	CLA	C5-C3	2.46	1.56	1.51
13	B	835	CLA	MG-NB	-2.46	2.00	2.05
13	A	829	CLA	C1D-ND	-2.46	1.34	1.37
13	B	834	CLA	C3D-C4D	-2.46	1.38	1.44
13	B	802	CLA	C3D-C4D	-2.46	1.38	1.44
13	A	838	CLA	MG-NB	-2.46	2.00	2.05
13	B	808	CLA	C3D-C4D	-2.46	1.38	1.44
13	B	806	CLA	C5-C3	2.46	1.56	1.51
13	A	836	CLA	O2D-CGD	2.46	1.39	1.33
13	A	805	CLA	C1D-ND	-2.46	1.34	1.37
13	B	829	CLA	C1D-ND	-2.46	1.34	1.37
15	A	850	BCR	C24-C25	2.46	1.53	1.45
13	B	823	CLA	O2D-CGD	2.46	1.39	1.33
13	B	820	CLA	C5-C3	2.45	1.56	1.51
13	B	836	CLA	C5-C3	2.45	1.56	1.51
15	B	844	BCR	C39-C30	-2.45	1.49	1.53
13	B	837	CLA	O2D-CGD	2.45	1.39	1.33
15	A	851	BCR	C39-C30	-2.45	1.49	1.53
13	X	102	CLA	C3D-C4D	-2.45	1.38	1.44
13	A	838	CLA	O2D-CGD	2.45	1.39	1.33
18	B	848	LMG	O7-C8	-2.45	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	855	CLA	O2D-CGD	2.45	1.39	1.33
13	A	816	CLA	C3D-C4D	-2.45	1.38	1.44
15	A	852	BCR	C20-C19	2.45	1.41	1.34
13	B	839	CLA	O2D-CGD	2.45	1.39	1.33
13	L	1004	CLA	C5-C3	2.45	1.56	1.51
13	L	1004	CLA	C3D-C4D	-2.44	1.38	1.44
13	A	814	CLA	C3D-C4D	-2.44	1.38	1.44
13	B	814	CLA	C3D-C4D	-2.44	1.38	1.44
13	B	832	CLA	C3D-C4D	-2.44	1.38	1.44
13	A	808	CLA	MG-NB	-2.44	2.00	2.05
13	A	843	CLA	O2D-CGD	2.44	1.39	1.33
13	B	812	CLA	MG-NB	-2.44	2.00	2.05
13	B	831	CLA	C5-C3	2.44	1.56	1.51
15	B	845	BCR	C5-C6	2.44	1.38	1.34
13	B	804	CLA	O2D-CGD	2.44	1.39	1.33
15	A	850	BCR	C24-C23	2.44	1.40	1.33
13	A	803	CLA	C3D-C4D	-2.44	1.38	1.44
13	B	818	CLA	C3D-C4D	-2.44	1.38	1.44
13	A	826	CLA	O2D-CGD	2.43	1.39	1.33
13	A	837	CLA	MG-NB	-2.43	2.01	2.05
13	J	1101	CLA	C5-C3	2.43	1.56	1.51
13	A	845	CLA	O2D-CGD	2.43	1.39	1.33
13	B	806	CLA	O2D-CGD	2.43	1.39	1.33
13	B	832	CLA	O2D-CGD	2.43	1.39	1.33
18	B	848	LMG	O6-C1	2.43	1.48	1.41
15	A	847	BCR	C24-C25	2.43	1.53	1.45
13	A	825	CLA	O2D-CGD	2.43	1.39	1.33
15	A	852	BCR	C24-C23	2.43	1.40	1.33
13	A	828	CLA	C3D-C4D	-2.43	1.38	1.44
13	A	829	CLA	C3D-C4D	-2.43	1.38	1.44
13	A	832	CLA	O2D-CGD	2.43	1.39	1.33
15	B	847	BCR	C39-C30	-2.43	1.49	1.53
13	B	803	CLA	C3D-C4D	-2.43	1.38	1.44
13	B	807	CLA	C5-C3	2.43	1.56	1.51
13	A	808	CLA	C3D-C4D	-2.43	1.38	1.44
15	J	1104	BCR	C24-C25	2.43	1.53	1.45
13	A	828	CLA	C5-C3	2.42	1.56	1.51
13	A	834	CLA	CHB-C4A	-2.42	1.31	1.37
15	A	848	BCR	C5-C6	2.42	1.38	1.34
15	L	1005	BCR	C39-C30	-2.42	1.49	1.53
15	M	1203	BCR	C39-C30	-2.42	1.49	1.53
13	B	818	CLA	O2D-CGD	2.42	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	833	CLA	C5-C3	2.42	1.56	1.51
13	A	834	CLA	C1B-NB	-2.42	1.34	1.37
13	A	819	CLA	C5-C3	2.42	1.56	1.51
13	A	804	CLA	O2D-CGD	2.42	1.39	1.33
13	A	836	CLA	C3D-C4D	-2.42	1.38	1.44
15	B	845	BCR	C24-C23	2.42	1.40	1.33
15	B	842	BCR	C24-C25	2.42	1.53	1.45
13	B	827	CLA	C3D-C4D	-2.42	1.38	1.44
13	A	810	CLA	O2D-CGD	2.41	1.39	1.33
13	B	802	CLA	O2D-CGD	2.41	1.39	1.33
13	A	812	CLA	O2D-CGD	2.41	1.39	1.33
13	L	1003	CLA	C3D-C4D	-2.41	1.38	1.44
13	A	813	CLA	C3D-C4D	-2.41	1.38	1.44
15	B	841	BCR	C24-C25	2.41	1.53	1.45
13	B	824	CLA	O2D-CGD	2.41	1.39	1.33
15	B	841	BCR	C39-C30	-2.41	1.49	1.53
13	A	818	CLA	C5-C3	2.41	1.56	1.51
13	M	1201	CLA	O2D-CGD	2.41	1.39	1.33
13	B	820	CLA	O2A-C1	-2.41	1.39	1.46
13	B	834	CLA	O2D-CGD	2.41	1.39	1.33
15	B	850	BCR	C5-C6	2.41	1.38	1.34
13	A	805	CLA	O2D-CGD	2.41	1.39	1.33
13	J	1101	CLA	C3D-C4D	-2.41	1.38	1.44
13	B	828	CLA	C3D-C4D	-2.41	1.38	1.44
13	B	811	CLA	C3D-C4D	-2.40	1.38	1.44
13	A	839	CLA	O2D-CGD	2.40	1.39	1.33
13	A	812	CLA	C3D-C4D	-2.40	1.38	1.44
13	A	809	CLA	C3D-C4D	-2.40	1.38	1.44
13	A	810	CLA	C3D-C4D	-2.40	1.38	1.44
13	A	815	CLA	C3D-C4D	-2.40	1.38	1.44
13	B	802	CLA	MG-NB	-2.40	2.01	2.05
13	B	835	CLA	C3D-C4D	-2.40	1.38	1.44
15	A	847	BCR	C39-C30	-2.40	1.49	1.53
15	A	852	BCR	C24-C25	2.40	1.53	1.45
13	B	802	CLA	C5-C3	2.40	1.56	1.51
13	A	832	CLA	MG-NB	-2.40	2.01	2.05
13	B	809	CLA	O2D-CGD	2.39	1.39	1.33
13	A	840	CLA	C5-C3	2.39	1.56	1.51
13	A	827	CLA	C3D-C4D	-2.39	1.38	1.44
13	A	832	CLA	C3D-C4D	-2.39	1.38	1.44
15	A	851	BCR	C5-C6	2.39	1.38	1.34
13	A	825	CLA	C3D-C4D	-2.39	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1101	CLA	O2D-CGD	2.39	1.39	1.33
13	B	821	CLA	C3D-C4D	-2.39	1.38	1.44
13	A	828	CLA	C1D-ND	-2.39	1.34	1.37
13	A	824	CLA	C3D-C4D	-2.39	1.38	1.44
13	B	804	CLA	C5-C3	2.39	1.56	1.51
15	F	1302	BCR	C39-C30	-2.39	1.49	1.53
13	B	817	CLA	O2D-CGD	2.39	1.39	1.33
15	F	1302	BCR	C5-C6	2.39	1.38	1.34
15	L	1005	BCR	C24-C25	2.39	1.53	1.45
13	A	807	CLA	CBD-CAD	-2.39	1.45	1.56
13	A	829	CLA	O2D-CGD	2.39	1.39	1.33
13	B	807	CLA	O2D-CGD	2.39	1.39	1.33
13	A	822	CLA	O2D-CGD	2.38	1.39	1.33
15	A	848	BCR	C39-C30	-2.38	1.49	1.53
13	B	801	CLA	C3D-C4D	-2.38	1.38	1.44
13	J	1101	CLA	MG-NB	-2.38	2.01	2.05
13	B	811	CLA	O2D-CGD	2.38	1.39	1.33
13	A	827	CLA	O2D-CGD	2.38	1.39	1.33
13	A	813	CLA	O2D-CGD	2.38	1.39	1.33
13	A	820	CLA	C5-C3	2.38	1.56	1.51
13	A	803	CLA	O2D-CGD	2.38	1.39	1.33
13	B	836	CLA	O2D-CGD	2.37	1.39	1.33
13	B	819	CLA	C3D-C4D	-2.37	1.38	1.44
13	X	102	CLA	O2D-CGD	2.37	1.39	1.33
13	A	812	CLA	C5-C3	2.37	1.56	1.51
15	J	1104	BCR	C24-C23	2.37	1.40	1.33
13	B	818	CLA	MG-NB	-2.37	2.01	2.05
15	A	849	BCR	C39-C30	-2.37	1.49	1.53
13	A	821	CLA	O2D-CGD	2.37	1.39	1.33
15	B	845	BCR	C24-C25	2.36	1.53	1.45
13	A	843	CLA	MG-NB	-2.36	2.01	2.05
13	A	841	CLA	MG-NB	-2.36	2.01	2.05
13	L	1004	CLA	O2D-CGD	2.36	1.39	1.33
13	A	830	CLA	O2D-CGD	2.36	1.39	1.33
13	B	811	CLA	MG-NB	-2.36	2.01	2.05
18	B	848	LMG	C4-C3	2.36	1.58	1.52
15	B	842	BCR	C39-C30	-2.36	1.49	1.53
18	B	848	LMG	C3-C2	2.36	1.58	1.52
13	B	804	CLA	C3D-C4D	-2.36	1.38	1.44
13	B	833	CLA	O2D-CGD	2.35	1.39	1.33
13	A	801	CLA	C3D-C4D	-2.35	1.38	1.44
13	A	824	CLA	CHB-C4A	-2.35	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	852	BCR	C39-C30	-2.35	1.49	1.53
13	A	802	CLA	C5-C3	2.35	1.56	1.51
15	J	1105	BCR	C24-C25	2.35	1.53	1.45
13	A	803	CLA	C5-C3	2.35	1.56	1.51
13	B	805	CLA	C5-C3	2.35	1.56	1.51
13	B	812	CLA	CBD-CAD	-2.35	1.46	1.56
13	B	808	CLA	C5-C3	2.35	1.56	1.51
13	B	826	CLA	C3D-C4D	-2.35	1.38	1.44
15	L	1006	BCR	C39-C30	-2.35	1.49	1.53
13	B	814	CLA	O2D-CGD	2.35	1.39	1.33
15	B	845	BCR	C39-C30	-2.35	1.49	1.53
13	L	1002	CLA	O2D-CGD	2.35	1.39	1.33
15	B	842	BCR	C5-C6	2.35	1.38	1.34
13	B	822	CLA	O2D-CGD	2.35	1.39	1.33
15	I	102	BCR	C39-C30	-2.35	1.49	1.53
15	A	850	BCR	C5-C6	2.35	1.38	1.34
13	A	813	CLA	C5-C3	2.34	1.56	1.51
13	L	1003	CLA	C5-C3	2.34	1.56	1.51
15	B	847	BCR	C24-C23	2.34	1.40	1.33
15	B	846	BCR	C24-C25	2.34	1.53	1.45
13	A	845	CLA	C5-C3	2.34	1.56	1.51
15	J	1105	BCR	C5-C6	2.34	1.38	1.34
13	B	831	CLA	C3D-C4D	-2.34	1.38	1.44
15	B	850	BCR	C39-C30	-2.34	1.49	1.53
15	J	1105	BCR	C31-C1	-2.34	1.49	1.53
15	A	847	BCR	C24-C23	2.34	1.40	1.33
13	B	808	CLA	MG-NB	-2.34	2.01	2.05
13	L	1003	CLA	O2D-CGD	2.34	1.39	1.33
13	B	838	CLA	O2D-CGD	2.33	1.39	1.33
13	A	837	CLA	C3D-C4D	-2.33	1.38	1.44
13	A	855	CLA	MG-NB	-2.33	2.01	2.05
15	B	844	BCR	C24-C23	2.33	1.40	1.33
13	A	817	CLA	C5-C3	2.33	1.56	1.51
13	B	829	CLA	C3D-C4D	-2.33	1.38	1.44
15	B	843	BCR	C39-C30	-2.33	1.49	1.53
13	A	806	CLA	C5-C3	2.33	1.56	1.51
13	B	808	CLA	O2D-CGD	2.33	1.39	1.33
15	B	847	BCR	C24-C25	2.33	1.53	1.45
15	B	841	BCR	C5-C6	2.33	1.38	1.34
13	L	1003	CLA	MG-NB	-2.33	2.01	2.05
13	B	803	CLA	O2D-CGD	2.33	1.38	1.33
13	B	812	CLA	C5-C3	2.32	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	843	CLA	C3D-C4D	-2.32	1.39	1.44
15	L	1006	BCR	C24-C25	2.32	1.53	1.45
13	A	802	CLA	MG-NB	-2.32	2.01	2.05
13	A	812	CLA	MG-NB	-2.32	2.01	2.05
13	B	811	CLA	C1-C2	2.32	1.55	1.49
15	B	846	BCR	C24-C23	2.32	1.40	1.33
13	A	832	CLA	C1-C2	2.31	1.55	1.49
15	J	1104	BCR	C39-C30	-2.31	1.49	1.53
13	A	801	CLA	O2D-CGD	2.31	1.38	1.33
13	B	802	CLA	CBD-CAD	-2.31	1.46	1.56
15	B	842	BCR	C7-C6	2.31	1.53	1.45
15	B	849	BCR	C39-C30	-2.30	1.49	1.53
15	J	1105	BCR	C24-C23	2.30	1.40	1.33
13	L	1002	CLA	C5-C3	2.30	1.56	1.51
13	B	824	CLA	MG-NB	-2.30	2.01	2.05
15	B	844	BCR	C29-C28	-2.30	1.47	1.52
13	B	814	CLA	C5-C3	2.30	1.56	1.51
13	A	811	CLA	O2D-CGD	2.30	1.38	1.33
15	A	852	BCR	C5-C6	2.30	1.38	1.34
13	A	844	CLA	C1A-CHA	-2.30	1.33	1.43
15	B	844	BCR	C20-C19	2.30	1.40	1.34
13	B	807	CLA	C3D-C4D	-2.29	1.39	1.44
13	A	844	CLA	MG-NB	-2.29	2.01	2.05
13	A	820	CLA	MG-NB	-2.29	2.01	2.05
13	A	829	CLA	MG-NB	-2.29	2.01	2.05
15	L	1005	BCR	C5-C6	2.29	1.38	1.34
13	F	1301	CLA	MG-NB	-2.29	2.01	2.05
13	A	831	CLA	O2D-CGD	2.29	1.38	1.33
15	B	844	BCR	C24-C25	2.29	1.52	1.45
13	B	801	CLA	C5-C3	2.29	1.56	1.51
15	B	841	BCR	C24-C23	2.29	1.39	1.33
13	B	807	CLA	CBD-CAD	-2.29	1.46	1.56
15	L	1006	BCR	C24-C23	2.29	1.39	1.33
13	B	832	CLA	MG-NB	-2.29	2.01	2.05
13	A	830	CLA	C3D-C4D	-2.28	1.39	1.44
15	A	850	BCR	C39-C30	-2.28	1.49	1.53
15	A	848	BCR	C24-C25	2.28	1.52	1.45
15	A	848	BCR	C24-C23	2.28	1.39	1.33
13	A	822	CLA	C3D-C4D	-2.28	1.39	1.44
13	B	838	CLA	MG-NB	-2.28	2.01	2.05
15	L	1005	BCR	C24-C23	2.28	1.39	1.33
13	A	843	CLA	C5-C3	2.27	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	825	CLA	MG-NB	-2.27	2.01	2.05
13	A	830	CLA	C1B-NB	-2.27	1.34	1.37
13	B	836	CLA	MG-NB	-2.27	2.01	2.05
15	A	849	BCR	C24-C25	2.27	1.52	1.45
13	A	835	CLA	CHB-C4A	-2.27	1.32	1.37
15	A	850	BCR	C20-C19	2.27	1.40	1.34
13	A	814	CLA	MG-NB	-2.27	2.01	2.05
15	B	850	BCR	C24-C23	2.27	1.39	1.33
13	B	820	CLA	MG-NB	-2.27	2.01	2.05
13	A	830	CLA	C1D-ND	-2.27	1.34	1.37
13	A	834	CLA	C1B-C2B	-2.26	1.37	1.43
15	B	845	BCR	C31-C1	-2.26	1.49	1.53
13	B	834	CLA	MG-NB	-2.26	2.01	2.05
15	J	1105	BCR	C20-C19	2.26	1.40	1.34
15	B	843	BCR	C5-C6	2.26	1.38	1.34
13	B	806	CLA	MG-NB	-2.26	2.01	2.05
13	A	805	CLA	C1-C2	2.26	1.55	1.49
13	L	1002	CLA	CHB-C4A	-2.25	1.32	1.37
15	L	1005	BCR	C31-C1	-2.25	1.49	1.53
15	A	851	BCR	C24-C25	2.25	1.52	1.45
15	B	842	BCR	C29-C28	-2.25	1.47	1.52
15	B	846	BCR	C29-C28	-2.25	1.47	1.52
13	B	816	CLA	CHB-C4A	-2.25	1.32	1.37
13	B	816	CLA	C5-C3	2.25	1.55	1.51
15	M	1203	BCR	C29-C28	-2.25	1.47	1.52
15	A	851	BCR	C24-C23	2.25	1.39	1.33
13	A	824	CLA	O2D-CGD	2.25	1.38	1.33
13	A	815	CLA	MG-NB	-2.25	2.01	2.05
13	L	1002	CLA	MG-NB	-2.25	2.01	2.05
15	B	846	BCR	C31-C1	-2.25	1.49	1.53
15	M	1203	BCR	C24-C25	2.25	1.52	1.45
15	M	1203	BCR	C24-C23	2.24	1.39	1.33
13	A	816	CLA	MG-NB	-2.24	2.01	2.05
15	B	850	BCR	C7-C6	2.24	1.52	1.45
15	A	849	BCR	C24-C23	2.24	1.39	1.33
13	I	101	CLA	CBD-CAD	-2.24	1.46	1.56
15	B	841	BCR	C29-C28	-2.24	1.47	1.52
15	B	847	BCR	C29-C28	-2.24	1.47	1.52
15	B	849	BCR	C24-C25	2.23	1.52	1.45
13	A	802	CLA	CHB-C4A	-2.23	1.32	1.37
15	B	843	BCR	C24-C25	2.23	1.52	1.45
15	B	845	BCR	C26-C25	2.23	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	847	BCR	C7-C6	2.23	1.52	1.45
15	B	849	BCR	C24-C23	2.23	1.39	1.33
15	A	848	BCR	C31-C1	-2.23	1.49	1.53
13	B	806	CLA	O2A-C1	-2.23	1.40	1.46
15	J	1104	BCR	C7-C6	2.23	1.52	1.45
13	A	834	CLA	MG-NB	-2.23	2.01	2.05
13	B	805	CLA	MG-NB	-2.23	2.01	2.05
13	B	833	CLA	MG-NB	-2.23	2.01	2.05
13	J	1103	CLA	C1A-CHA	-2.23	1.33	1.43
15	L	1006	BCR	C20-C19	2.22	1.40	1.34
15	J	1104	BCR	C31-C1	-2.22	1.49	1.53
15	B	841	BCR	C31-C1	-2.22	1.49	1.53
15	A	851	BCR	C29-C28	-2.22	1.47	1.52
13	B	821	CLA	CHB-C4A	-2.22	1.32	1.37
13	B	801	CLA	MG-NB	-2.22	2.01	2.05
13	X	102	CLA	MG-NB	-2.22	2.01	2.05
15	A	847	BCR	C29-C28	-2.22	1.47	1.52
15	B	849	BCR	C29-C28	-2.22	1.47	1.52
13	B	823	CLA	MG-NB	-2.22	2.01	2.05
15	L	1006	BCR	C31-C1	-2.21	1.49	1.53
15	F	1302	BCR	C31-C1	-2.21	1.49	1.53
18	B	848	LMG	O1-C7	-2.21	1.39	1.43
13	B	810	CLA	MG-NB	-2.21	2.01	2.05
15	F	1302	BCR	C24-C25	2.21	1.52	1.45
13	A	818	CLA	MG-NB	-2.21	2.01	2.05
15	B	850	BCR	C20-C19	2.21	1.40	1.34
13	B	826	CLA	C5-C3	2.21	1.55	1.51
15	B	843	BCR	C20-C19	2.21	1.40	1.34
15	B	843	BCR	C7-C6	2.21	1.52	1.45
13	A	805	CLA	C3D-C4D	-2.20	1.39	1.44
13	L	1003	CLA	CHB-C4A	-2.20	1.32	1.37
13	A	842	CLA	CBD-CAD	-2.20	1.46	1.56
13	A	806	CLA	MG-NB	-2.20	2.01	2.05
15	B	850	BCR	C24-C25	2.20	1.52	1.45
15	L	1005	BCR	C29-C28	-2.20	1.47	1.52
15	A	849	BCR	C29-C28	-2.20	1.47	1.52
13	B	815	CLA	MG-NB	-2.20	2.01	2.05
13	B	816	CLA	MG-NB	-2.20	2.01	2.05
15	A	847	BCR	C31-C1	-2.20	1.49	1.53
13	I	101	CLA	MG-NB	-2.20	2.01	2.05
15	F	1302	BCR	C7-C6	2.20	1.52	1.45
13	A	835	CLA	MG-NB	-2.20	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	835	CLA	C1-C2	2.20	1.55	1.49
15	A	848	BCR	C20-C19	2.20	1.40	1.34
13	L	1004	CLA	MG-NB	-2.19	2.01	2.05
13	A	823	CLA	MG-NB	-2.19	2.01	2.05
15	F	1302	BCR	C24-C23	2.19	1.39	1.33
15	A	851	BCR	C20-C19	2.19	1.40	1.34
15	B	847	BCR	C5-C6	2.19	1.38	1.34
13	B	836	CLA	CBD-CAD	-2.19	1.46	1.56
13	B	826	CLA	CHB-C4A	-2.19	1.32	1.37
15	J	1105	BCR	C29-C28	-2.19	1.47	1.52
15	J	1104	BCR	C20-C19	2.19	1.40	1.34
13	A	813	CLA	MG-NB	-2.19	2.01	2.05
13	A	808	CLA	CBD-CAD	-2.19	1.46	1.56
13	B	801	CLA	CHB-C4A	-2.19	1.32	1.37
13	A	801	CLA	MG-NB	-2.19	2.01	2.05
15	A	848	BCR	C29-C28	-2.19	1.47	1.52
15	L	1006	BCR	C7-C6	2.19	1.52	1.45
13	B	826	CLA	CBD-CAD	-2.18	1.46	1.56
15	A	852	BCR	C29-C28	-2.18	1.47	1.52
13	A	826	CLA	MG-NB	-2.18	2.01	2.05
15	M	1203	BCR	C31-C1	-2.18	1.49	1.53
13	A	801	CLA	CHB-C4A	-2.18	1.32	1.37
15	A	850	BCR	C29-C28	-2.18	1.47	1.52
13	B	802	CLA	C1B-C2B	-2.18	1.38	1.43
13	A	822	CLA	CHB-C4A	-2.18	1.32	1.37
13	B	803	CLA	MG-NB	-2.18	2.01	2.05
13	A	824	CLA	C1B-C2B	-2.18	1.38	1.43
13	B	806	CLA	CBD-CAD	-2.18	1.46	1.56
15	I	102	BCR	C24-C23	2.17	1.39	1.33
15	A	852	BCR	C7-C6	2.17	1.52	1.45
13	J	1103	CLA	CHB-C4A	-2.17	1.32	1.37
15	A	851	BCR	C31-C1	-2.17	1.49	1.53
15	B	846	BCR	C7-C6	2.17	1.52	1.45
13	A	803	CLA	CHB-C4A	-2.17	1.32	1.37
13	B	829	CLA	CHB-C4A	-2.17	1.32	1.37
15	A	852	BCR	C31-C1	-2.17	1.49	1.53
13	L	1002	CLA	C1B-C2B	-2.17	1.38	1.43
15	F	1302	BCR	C29-C28	-2.17	1.47	1.52
15	M	1203	BCR	C20-C19	2.17	1.40	1.34
13	A	807	CLA	MG-NB	-2.17	2.01	2.05
13	A	827	CLA	MG-NB	-2.17	2.01	2.05
13	A	815	CLA	CHB-C4A	-2.17	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	850	BCR	C31-C1	-2.17	1.49	1.53
15	B	850	BCR	C29-C28	-2.16	1.47	1.52
13	A	809	CLA	CHB-C4A	-2.16	1.32	1.37
13	B	838	CLA	CBD-CAD	-2.16	1.46	1.56
13	M	1202	CLA	MG-NB	-2.16	2.01	2.05
13	B	803	CLA	CHB-C4A	-2.16	1.32	1.37
15	B	842	BCR	C8-C7	2.16	1.39	1.33
15	A	850	BCR	C11-C12	2.16	1.40	1.34
13	M	1201	CLA	CBD-CAD	-2.16	1.46	1.56
15	B	843	BCR	C24-C23	2.16	1.39	1.33
15	L	1005	BCR	C20-C19	2.16	1.40	1.34
15	B	847	BCR	C7-C6	2.16	1.52	1.45
15	B	845	BCR	C20-C19	2.16	1.40	1.34
13	B	837	CLA	MG-NB	-2.15	2.01	2.05
13	B	818	CLA	CHB-C4A	-2.15	1.32	1.37
15	B	842	BCR	C20-C19	2.15	1.40	1.34
13	A	831	CLA	C5-C3	2.15	1.56	1.50
13	B	831	CLA	CBD-CAD	-2.15	1.46	1.56
15	B	841	BCR	C7-C6	2.15	1.52	1.45
13	B	802	CLA	CHB-C4A	-2.15	1.32	1.37
13	B	827	CLA	C1B-NB	-2.15	1.35	1.37
13	B	828	CLA	MG-NB	-2.15	2.01	2.05
13	A	821	CLA	MG-NB	-2.14	2.01	2.05
13	A	831	CLA	CHB-C4A	-2.14	1.32	1.37
15	B	850	BCR	C8-C7	2.14	1.39	1.33
13	A	803	CLA	MG-NB	-2.14	2.01	2.05
13	A	809	CLA	MG-NB	-2.14	2.01	2.05
15	I	102	BCR	C29-C28	-2.14	1.47	1.52
13	B	836	CLA	C1A-CHA	-2.14	1.34	1.43
13	B	817	CLA	MG-NB	-2.14	2.01	2.05
15	I	102	BCR	C31-C1	-2.14	1.49	1.53
15	B	849	BCR	C20-C19	2.14	1.40	1.34
13	A	811	CLA	CBD-CAD	-2.14	1.46	1.56
13	A	814	CLA	CBD-CAD	-2.14	1.46	1.56
13	B	817	CLA	CBD-CAD	-2.13	1.46	1.56
15	B	847	BCR	C20-C19	2.13	1.40	1.34
13	J	1102	CLA	MG-NB	-2.13	2.01	2.05
15	I	102	BCR	C24-C25	2.13	1.52	1.45
13	A	822	CLA	CBD-CAD	-2.13	1.46	1.56
13	B	804	CLA	CHB-C4A	-2.13	1.32	1.37
13	B	827	CLA	O2D-CGD	2.13	1.38	1.33
13	B	827	CLA	CMB-C2B	2.13	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	819	CLA	C1A-CHA	-2.13	1.34	1.43
13	A	845	CLA	O2A-C1	-2.13	1.40	1.46
13	B	829	CLA	CBD-CAD	-2.12	1.47	1.56
13	A	829	CLA	C1-C2	2.12	1.55	1.49
15	A	847	BCR	C20-C19	2.12	1.40	1.34
13	A	808	CLA	C1-C2	2.12	1.55	1.49
15	J	1105	BCR	C7-C6	2.12	1.52	1.45
15	L	1006	BCR	C29-C28	-2.12	1.47	1.52
13	A	804	CLA	CHB-C4A	-2.12	1.32	1.37
18	B	848	LMG	O7-C10	2.12	1.40	1.34
13	B	810	CLA	CHB-C4A	-2.12	1.32	1.37
13	A	838	CLA	CHB-C4A	-2.12	1.32	1.37
13	B	825	CLA	CHB-C4A	-2.12	1.32	1.37
13	A	802	CLA	C1B-C2B	-2.12	1.38	1.43
15	A	849	BCR	C31-C1	-2.11	1.49	1.53
13	A	830	CLA	CBD-CAD	-2.11	1.47	1.56
13	A	842	CLA	C1A-CHA	-2.11	1.34	1.43
13	B	819	CLA	CHB-C4A	-2.11	1.32	1.37
13	B	826	CLA	O2D-CGD	2.11	1.38	1.33
13	L	1002	CLA	CBD-CAD	-2.11	1.47	1.56
13	B	804	CLA	MG-NB	-2.11	2.01	2.05
13	A	826	CLA	C1-C2	2.11	1.55	1.49
15	B	843	BCR	C31-C1	-2.11	1.49	1.53
13	A	820	CLA	CBD-CAD	-2.11	1.47	1.56
13	B	839	CLA	MG-NB	-2.11	2.01	2.05
15	B	850	BCR	C31-C1	-2.11	1.49	1.53
13	B	828	CLA	CHB-C4A	-2.11	1.32	1.37
13	B	820	CLA	CBD-CAD	-2.10	1.47	1.56
13	A	801	CLA	C1-C2	2.10	1.55	1.49
13	A	833	CLA	CHC-C4B	-2.10	1.34	1.39
13	A	801	CLA	C1B-C2B	-2.10	1.38	1.43
13	A	802	CLA	C1A-CHA	-2.10	1.34	1.43
15	B	845	BCR	C7-C6	2.10	1.52	1.45
13	B	809	CLA	CHB-C4A	-2.10	1.32	1.37
15	B	846	BCR	C20-C19	2.10	1.40	1.34
13	B	830	CLA	C1-C2	2.10	1.55	1.49
13	M	1201	CLA	MG-NB	-2.10	2.01	2.05
15	B	841	BCR	C20-C19	2.10	1.40	1.34
13	M	1201	CLA	C1-C2	2.10	1.55	1.49
13	B	830	CLA	CHB-C4A	-2.10	1.32	1.37
15	A	851	BCR	C7-C6	2.10	1.52	1.45
13	B	817	CLA	C1A-CHA	-2.10	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	816	CLA	C1B-C2B	-2.10	1.38	1.43
13	A	825	CLA	CBD-CAD	-2.10	1.47	1.56
13	X	102	CLA	CHB-C4A	-2.10	1.32	1.37
15	B	843	BCR	C8-C7	2.10	1.39	1.33
13	B	827	CLA	C1-C2	2.09	1.55	1.49
13	A	837	CLA	CHB-C4A	-2.09	1.32	1.37
13	B	814	CLA	CBD-CAD	-2.09	1.47	1.56
13	A	818	CLA	O2A-C1	-2.09	1.40	1.46
13	B	832	CLA	CHB-C4A	-2.09	1.32	1.37
13	A	845	CLA	MG-NB	-2.09	2.01	2.05
13	A	837	CLA	CBD-CAD	-2.09	1.47	1.56
13	B	813	CLA	CHB-C4A	-2.09	1.32	1.37
13	F	1301	CLA	CHB-C4A	-2.09	1.32	1.37
15	B	847	BCR	C31-C1	-2.09	1.49	1.53
13	A	843	CLA	CBD-CAD	-2.09	1.47	1.56
13	B	827	CLA	CBD-CAD	-2.09	1.47	1.56
13	A	802	CLA	CBD-CAD	-2.09	1.47	1.56
13	B	807	CLA	CHB-C4A	-2.09	1.32	1.37
13	B	813	CLA	C1B-C2B	-2.09	1.38	1.43
13	B	818	CLA	C1B-C2B	-2.09	1.38	1.43
13	A	818	CLA	CHB-C4A	-2.09	1.32	1.37
13	B	807	CLA	MG-NB	-2.09	2.01	2.05
13	B	839	CLA	CHB-C4A	-2.08	1.32	1.37
13	A	834	CLA	CBD-CAD	-2.08	1.47	1.56
13	B	836	CLA	C1-C2	2.08	1.55	1.49
13	J	1103	CLA	MG-NB	-2.08	2.01	2.05
13	A	810	CLA	CBD-CAD	-2.08	1.47	1.56
13	A	807	CLA	O2A-C1	-2.08	1.40	1.46
13	A	824	CLA	MG-NB	-2.08	2.01	2.05
13	A	820	CLA	C1A-CHA	-2.08	1.34	1.43
13	B	804	CLA	CBD-CAD	-2.08	1.47	1.56
13	B	831	CLA	C1-C2	2.08	1.55	1.49
13	B	822	CLA	CHB-C4A	-2.08	1.32	1.37
13	A	832	CLA	CBD-CAD	-2.08	1.47	1.56
13	B	822	CLA	CBD-CAD	-2.08	1.47	1.56
13	A	825	CLA	C1-C2	2.08	1.55	1.49
13	A	812	CLA	CBD-CAD	-2.07	1.47	1.56
13	B	822	CLA	C1-C2	2.07	1.55	1.49
13	A	817	CLA	CBD-CAD	-2.07	1.47	1.56
15	A	852	BCR	C11-C12	2.07	1.40	1.34
13	A	819	CLA	MG-NB	-2.07	2.01	2.05
13	M	1201	CLA	C1A-CHA	-2.07	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	847	BCR	C11-C12	2.07	1.40	1.34
13	B	822	CLA	C1B-C2B	-2.07	1.38	1.43
13	B	837	CLA	CBD-CAD	-2.07	1.47	1.56
15	B	849	BCR	C7-C6	2.07	1.52	1.45
13	A	833	CLA	CBD-CAD	-2.07	1.47	1.56
13	B	837	CLA	C1A-CHA	-2.07	1.34	1.43
13	A	840	CLA	CBD-CAD	-2.07	1.47	1.56
13	A	819	CLA	CBD-CAD	-2.07	1.47	1.56
13	A	835	CLA	C1-C2	2.07	1.55	1.49
15	B	842	BCR	C11-C12	2.07	1.40	1.34
13	B	823	CLA	CBD-CAD	-2.07	1.47	1.56
13	A	820	CLA	CHB-C4A	-2.07	1.32	1.37
15	F	1302	BCR	C20-C19	2.07	1.40	1.34
13	A	836	CLA	CHB-C4A	-2.07	1.32	1.37
13	A	830	CLA	C1-C2	2.07	1.55	1.49
13	A	842	CLA	C1-C2	2.07	1.55	1.49
13	B	801	CLA	C1A-CHA	-2.07	1.34	1.43
13	A	804	CLA	MG-NB	-2.07	2.01	2.05
15	L	1005	BCR	C7-C6	2.07	1.52	1.45
13	B	810	CLA	C1A-CHA	-2.06	1.34	1.43
13	A	855	CLA	CHB-C4A	-2.06	1.32	1.37
13	A	834	CLA	C1-C2	2.06	1.55	1.49
13	A	829	CLA	CBD-CAD	-2.06	1.47	1.56
13	A	837	CLA	C1-C2	2.06	1.55	1.49
13	B	832	CLA	CBD-CAD	-2.06	1.47	1.56
13	A	821	CLA	CBD-CAD	-2.06	1.47	1.56
13	B	839	CLA	C1-C2	2.06	1.55	1.49
13	A	821	CLA	C1-C2	2.06	1.55	1.49
13	A	821	CLA	C1A-CHA	-2.06	1.34	1.43
15	J	1104	BCR	C8-C7	2.06	1.39	1.33
13	A	830	CLA	CMB-C2B	2.06	1.55	1.50
13	B	803	CLA	CBD-CAD	-2.06	1.47	1.56
13	B	826	CLA	MG-NB	-2.06	2.01	2.05
13	B	810	CLA	CBD-CAD	-2.06	1.47	1.56
13	B	807	CLA	C1A-CHA	-2.05	1.34	1.43
15	B	841	BCR	C11-C12	2.05	1.40	1.34
13	B	836	CLA	CHB-C4A	-2.05	1.32	1.37
13	A	840	CLA	C1-C2	2.05	1.55	1.49
13	A	843	CLA	O2A-C1	-2.05	1.40	1.46
13	B	826	CLA	C1-C2	2.05	1.55	1.49
15	B	842	BCR	C31-C1	-2.05	1.49	1.53
13	B	824	CLA	C1-C2	2.05	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	821	CLA	CBD-CAD	-2.05	1.47	1.56
15	F	1302	BCR	C8-C7	2.05	1.39	1.33
13	B	819	CLA	MG-NB	-2.05	2.01	2.05
13	B	818	CLA	CBD-CAD	-2.05	1.47	1.56
13	B	833	CLA	CBD-CAD	-2.05	1.47	1.56
13	B	808	CLA	CBD-CAD	-2.05	1.47	1.56
13	B	835	CLA	CBD-CAD	-2.05	1.47	1.56
13	B	801	CLA	C1B-C2B	-2.05	1.38	1.43
13	B	809	CLA	CBD-CAD	-2.05	1.47	1.56
13	B	811	CLA	CHB-C4A	-2.05	1.32	1.37
13	A	810	CLA	CHB-C4A	-2.05	1.32	1.37
13	A	838	CLA	CBD-CAD	-2.05	1.47	1.56
13	B	828	CLA	CHC-C4B	-2.04	1.34	1.39
13	A	831	CLA	CBD-CAD	-2.04	1.47	1.56
13	A	828	CLA	CBD-CAD	-2.04	1.47	1.56
13	B	837	CLA	CHB-C4A	-2.04	1.32	1.37
13	X	102	CLA	CBD-CAD	-2.04	1.47	1.56
13	B	816	CLA	C1A-CHA	-2.04	1.34	1.43
13	A	831	CLA	MG-NB	-2.04	2.01	2.05
15	B	847	BCR	C11-C12	2.04	1.40	1.34
13	A	813	CLA	CHB-C4A	-2.04	1.32	1.37
15	J	1105	BCR	C11-C12	2.04	1.40	1.34
15	B	846	BCR	C11-C12	2.04	1.40	1.34
13	A	805	CLA	MG-NB	-2.04	2.01	2.05
13	A	844	CLA	CHB-C4A	-2.04	1.32	1.37
13	B	831	CLA	CHC-C4B	-2.04	1.34	1.39
13	A	840	CLA	C1A-CHA	-2.04	1.34	1.43
15	A	848	BCR	C7-C6	2.04	1.52	1.45
13	I	101	CLA	CHB-C4A	-2.04	1.32	1.37
13	A	804	CLA	C1-C2	2.04	1.55	1.49
13	A	842	CLA	CHB-C4A	-2.04	1.32	1.37
13	B	829	CLA	MG-NB	-2.04	2.01	2.05
15	A	848	BCR	C11-C12	2.04	1.40	1.34
15	B	850	BCR	C11-C12	2.04	1.40	1.34
13	L	1002	CLA	C1A-CHA	-2.04	1.34	1.43
15	B	843	BCR	C29-C28	-2.04	1.47	1.52
13	A	815	CLA	C1B-C2B	-2.04	1.38	1.43
13	B	812	CLA	C1A-CHA	-2.04	1.34	1.43
13	B	825	CLA	MG-NB	-2.04	2.01	2.05
13	A	827	CLA	C1-C2	2.04	1.55	1.49
13	A	835	CLA	C1B-C2B	-2.04	1.38	1.43
13	I	101	CLA	C1-C2	2.04	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	852	BCR	C21-C22	2.04	1.40	1.35
13	L	1003	CLA	C1A-CHA	-2.03	1.34	1.43
13	A	801	CLA	CHC-C4B	-2.03	1.34	1.39
13	L	1003	CLA	CBD-CAD	-2.03	1.47	1.56
13	A	817	CLA	C1-C2	2.03	1.54	1.49
13	B	834	CLA	CBD-CAD	-2.03	1.47	1.56
15	J	1104	BCR	C11-C12	2.03	1.40	1.34
13	A	805	CLA	CBD-CAD	-2.03	1.47	1.56
13	B	831	CLA	MG-NB	-2.03	2.01	2.05
13	B	805	CLA	CBD-CAD	-2.03	1.47	1.56
13	M	1202	CLA	CBD-CAD	-2.03	1.47	1.56
13	B	807	CLA	O2A-C1	-2.03	1.40	1.46
15	B	843	BCR	C11-C12	2.03	1.40	1.34
13	A	816	CLA	C1A-CHA	-2.03	1.34	1.43
13	B	828	CLA	CBD-CAD	-2.03	1.47	1.56
13	A	819	CLA	CHB-C4A	-2.03	1.32	1.37
13	A	820	CLA	C1-C2	2.03	1.54	1.49
13	A	805	CLA	CHB-C4A	-2.03	1.32	1.37
15	A	850	BCR	C7-C6	2.03	1.52	1.45
13	L	1004	CLA	CBD-CAD	-2.03	1.47	1.56
13	A	823	CLA	O2A-C1	-2.03	1.40	1.46
13	A	814	CLA	CHB-C4A	-2.03	1.32	1.37
13	A	838	CLA	C1A-CHA	-2.03	1.34	1.43
13	I	101	CLA	C1A-CHA	-2.03	1.34	1.43
13	A	811	CLA	CHB-C4A	-2.03	1.32	1.37
13	A	838	CLA	C1B-C2B	-2.03	1.38	1.43
13	A	834	CLA	C1A-CHA	-2.03	1.34	1.43
13	A	809	CLA	C1-C2	2.03	1.54	1.49
13	B	805	CLA	C1A-CHA	-2.03	1.34	1.43
13	A	833	CLA	CHB-C4A	-2.02	1.32	1.37
13	B	830	CLA	C1B-C2B	-2.02	1.38	1.43
15	L	1006	BCR	C11-C12	2.02	1.40	1.34
15	A	849	BCR	C7-C6	2.02	1.52	1.45
13	A	809	CLA	CBD-CAD	-2.02	1.47	1.56
13	B	812	CLA	CHB-C4A	-2.02	1.32	1.37
13	A	832	CLA	C1A-CHA	-2.02	1.34	1.43
13	A	829	CLA	C1B-C2B	-2.02	1.38	1.43
13	A	814	CLA	O2D-CGD	2.02	1.38	1.33
13	A	838	CLA	C1-C2	2.02	1.54	1.49
13	A	829	CLA	CHB-C4A	-2.02	1.32	1.37
13	B	814	CLA	MG-NB	-2.02	2.01	2.05
15	M	1203	BCR	C7-C6	2.02	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	806	CLA	CBD-CAD	-2.02	1.47	1.56
13	B	809	CLA	MG-NB	-2.02	2.01	2.05
15	A	850	BCR	C17-C18	2.02	1.40	1.35
13	A	823	CLA	CBD-CAD	-2.02	1.47	1.56
13	B	806	CLA	C1A-CHA	-2.02	1.34	1.43
13	B	817	CLA	CHB-C4A	-2.02	1.32	1.37
13	X	102	CLA	C1B-C2B	-2.02	1.38	1.43
13	B	815	CLA	CBD-CAD	-2.02	1.47	1.56
13	A	842	CLA	CHC-C4B	-2.01	1.34	1.39
13	A	814	CLA	C1B-C2B	-2.01	1.38	1.43
13	B	819	CLA	CBD-CAD	-2.01	1.47	1.56
13	B	803	CLA	C1B-C2B	-2.01	1.38	1.43
13	A	824	CLA	C1A-CHA	-2.01	1.34	1.43
15	L	1006	BCR	C8-C7	2.01	1.39	1.33
13	B	815	CLA	O2A-C1	-2.01	1.40	1.46
13	B	815	CLA	CHB-C4A	-2.01	1.32	1.37
13	A	811	CLA	C1-C2	2.01	1.54	1.49
15	A	851	BCR	C11-C12	2.01	1.39	1.34
13	A	833	CLA	C1-C2	2.01	1.54	1.49
13	A	835	CLA	C1A-CHA	-2.01	1.34	1.43
13	L	1004	CLA	CHB-C4A	-2.01	1.32	1.37
15	I	102	BCR	C5-C6	2.01	1.37	1.34
13	A	803	CLA	CBD-CAD	-2.01	1.47	1.56
13	B	801	CLA	CBD-CAD	-2.01	1.47	1.56
13	A	840	CLA	MG-NB	-2.01	2.01	2.05
15	L	1005	BCR	C11-C12	2.01	1.39	1.34
13	B	803	CLA	C1A-CHA	-2.01	1.34	1.43
13	A	836	CLA	C1A-CHA	-2.01	1.34	1.43
13	B	819	CLA	CHC-C4B	-2.01	1.34	1.39
13	B	839	CLA	CBD-CAD	-2.01	1.47	1.56
13	A	845	CLA	CHB-C4A	-2.00	1.32	1.37
15	A	847	BCR	C8-C7	2.00	1.39	1.33
13	A	828	CLA	CHB-C4A	-2.00	1.32	1.37
15	B	844	BCR	C17-C18	2.00	1.40	1.35
13	A	824	CLA	C1-C2	2.00	1.54	1.49
13	B	828	CLA	C1B-C2B	-2.00	1.38	1.43
13	B	802	CLA	C1-C2	2.00	1.54	1.49
13	B	812	CLA	C1B-C2B	-2.00	1.38	1.43
15	F	1302	BCR	C11-C12	2.00	1.39	1.34
13	A	823	CLA	C1A-CHA	-2.00	1.34	1.43
13	A	827	CLA	C3C-C2C	-2.00	1.32	1.36
13	A	812	CLA	C1A-CHA	-2.00	1.34	1.43

All (1470) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	809	CLA	C4A-NA-C1A	11.40	111.88	106.68
13	A	808	CLA	C4A-NA-C1A	11.29	111.83	106.68
13	A	830	CLA	C4A-NA-C1A	11.20	111.79	106.68
13	M	1202	CLA	C4A-NA-C1A	11.11	111.75	106.68
13	B	827	CLA	C4A-NA-C1A	11.09	111.74	106.68
13	A	839	CLA	C4A-NA-C1A	11.07	111.73	106.68
13	A	819	CLA	C4A-NA-C1A	11.06	111.73	106.68
13	A	807	CLA	C4A-NA-C1A	10.95	111.67	106.68
13	A	825	CLA	C4A-NA-C1A	10.90	111.65	106.68
13	B	814	CLA	C4A-NA-C1A	10.85	111.63	106.68
13	A	826	CLA	C4A-NA-C1A	10.77	111.59	106.68
13	F	1301	CLA	C4A-NA-C1A	10.76	111.59	106.68
13	A	845	CLA	C4A-NA-C1A	10.68	111.55	106.68
13	B	830	CLA	C4A-NA-C1A	10.65	111.54	106.68
13	B	806	CLA	C4A-NA-C1A	10.62	111.52	106.68
13	B	833	CLA	C4A-NA-C1A	10.60	111.52	106.68
13	B	822	CLA	C4A-NA-C1A	10.57	111.50	106.68
13	M	1201	CLA	C4A-NA-C1A	10.56	111.50	106.68
13	A	810	CLA	C4A-NA-C1A	10.52	111.48	106.68
13	A	812	CLA	C4A-NA-C1A	10.49	111.47	106.68
13	A	816	CLA	C4A-NA-C1A	10.49	111.46	106.68
13	A	843	CLA	C4A-NA-C1A	10.49	111.46	106.68
13	A	838	CLA	C4A-NA-C1A	10.48	111.46	106.68
13	B	810	CLA	C4A-NA-C1A	10.47	111.46	106.68
13	A	831	CLA	C4A-NA-C1A	10.45	111.45	106.68
13	A	827	CLA	C4A-NA-C1A	10.42	111.43	106.68
13	B	807	CLA	C4A-NA-C1A	10.42	111.43	106.68
13	B	817	CLA	C4A-NA-C1A	10.42	111.43	106.68
13	A	832	CLA	C4A-NA-C1A	10.39	111.42	106.68
13	A	818	CLA	C4A-NA-C1A	10.38	111.41	106.68
13	A	821	CLA	C4A-NA-C1A	10.34	111.40	106.68
13	A	811	CLA	C4A-NA-C1A	10.34	111.40	106.68
13	A	820	CLA	C4A-NA-C1A	10.34	111.39	106.68
13	B	831	CLA	C4A-NA-C1A	10.32	111.39	106.68
13	I	101	CLA	C4A-NA-C1A	10.26	111.36	106.68
13	A	837	CLA	C4A-NA-C1A	10.26	111.36	106.68
13	B	838	CLA	C4A-NA-C1A	10.25	111.35	106.68
13	B	832	CLA	C4A-NA-C1A	10.24	111.35	106.68
13	A	833	CLA	C4A-NA-C1A	10.19	111.33	106.68
13	B	805	CLA	C4A-NA-C1A	10.18	111.33	106.68
13	B	834	CLA	C4A-NA-C1A	10.18	111.32	106.68
13	L	1004	CLA	C4A-NA-C1A	10.17	111.32	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	820	CLA	C4A-NA-C1A	10.15	111.31	106.68
13	L	1003	CLA	C4A-NA-C1A	10.14	111.31	106.68
13	A	855	CLA	C4A-NA-C1A	10.14	111.31	106.68
13	A	836	CLA	C4A-NA-C1A	10.13	111.30	106.68
13	A	813	CLA	C4A-NA-C1A	10.13	111.30	106.68
13	A	804	CLA	C4A-NA-C1A	10.12	111.30	106.68
13	A	806	CLA	C4A-NA-C1A	10.11	111.29	106.68
13	B	826	CLA	C4A-NA-C1A	10.07	111.27	106.68
13	B	837	CLA	C4A-NA-C1A	10.06	111.27	106.68
13	A	805	CLA	C4A-NA-C1A	10.06	111.27	106.68
13	B	804	CLA	C4A-NA-C1A	10.03	111.26	106.68
13	B	839	CLA	C4A-NA-C1A	10.03	111.26	106.68
13	J	1102	CLA	C4A-NA-C1A	10.03	111.26	106.68
13	A	823	CLA	C4A-NA-C1A	10.02	111.25	106.68
13	L	1002	CLA	C4A-NA-C1A	10.01	111.25	106.68
13	B	819	CLA	C4A-NA-C1A	10.01	111.25	106.68
13	B	809	CLA	C4A-NA-C1A	10.01	111.25	106.68
13	A	803	CLA	C4A-NA-C1A	10.00	111.24	106.68
13	B	815	CLA	C4A-NA-C1A	9.97	111.23	106.68
13	A	829	CLA	C4A-NA-C1A	9.97	111.23	106.68
13	A	817	CLA	C4A-NA-C1A	9.96	111.22	106.68
13	A	835	CLA	C4A-NA-C1A	9.96	111.22	106.68
13	A	841	CLA	C4A-NA-C1A	9.96	111.22	106.68
13	B	835	CLA	C4A-NA-C1A	9.96	111.22	106.68
13	J	1101	CLA	C4A-NA-C1A	9.96	111.22	106.68
13	A	828	CLA	C4A-NA-C1A	9.92	111.21	106.68
13	B	818	CLA	C4A-NA-C1A	9.91	111.20	106.68
13	A	840	CLA	C4A-NA-C1A	9.91	111.20	106.68
13	B	821	CLA	C4A-NA-C1A	9.87	111.18	106.68
13	B	823	CLA	C4A-NA-C1A	9.87	111.18	106.68
13	B	825	CLA	C4A-NA-C1A	9.87	111.18	106.68
13	B	836	CLA	C4A-NA-C1A	9.87	111.18	106.68
13	A	815	CLA	C4A-NA-C1A	9.86	111.18	106.68
13	A	822	CLA	C4A-NA-C1A	9.84	111.17	106.68
13	A	842	CLA	C4A-NA-C1A	9.84	111.17	106.68
13	B	811	CLA	C4A-NA-C1A	9.83	111.17	106.68
13	B	808	CLA	C4A-NA-C1A	9.83	111.16	106.68
13	B	816	CLA	C4A-NA-C1A	9.78	111.14	106.68
13	B	812	CLA	C4A-NA-C1A	9.72	111.11	106.68
13	B	829	CLA	C4A-NA-C1A	9.72	111.11	106.68
13	A	814	CLA	C4A-NA-C1A	9.71	111.11	106.68
13	B	824	CLA	C4A-NA-C1A	9.69	111.10	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	102	CLA	C4A-NA-C1A	9.62	111.07	106.68
13	B	828	CLA	C4A-NA-C1A	9.49	111.01	106.68
13	A	834	CLA	C4A-NA-C1A	9.43	110.98	106.68
13	A	824	CLA	C4A-NA-C1A	9.04	110.81	106.68
13	B	813	CLA	C4A-NA-C1A	9.03	110.80	106.68
13	B	802	CLA	C4A-NA-C1A	8.95	110.76	106.68
13	B	803	CLA	C4A-NA-C1A	8.92	110.75	106.68
13	A	802	CLA	C4A-NA-C1A	8.85	110.72	106.68
13	J	1103	CLA	C4A-NA-C1A	8.76	110.68	106.68
13	X	102	CLA	O2D-CGD-CBD	8.65	126.35	111.23
13	A	801	CLA	C4A-NA-C1A	8.63	110.62	106.68
13	B	802	CLA	O2D-CGD-CBD	8.61	126.28	111.23
13	A	822	CLA	O2D-CGD-CBD	8.58	126.23	111.23
13	B	831	CLA	O2D-CGD-CBD	8.55	126.18	111.23
13	B	801	CLA	C4A-NA-C1A	8.54	110.58	106.68
13	A	844	CLA	C4A-NA-C1A	8.43	110.53	106.68
13	B	817	CLA	O2D-CGD-CBD	7.99	125.19	111.23
13	A	808	CLA	O2D-CGD-CBD	7.82	124.90	111.23
13	A	812	CLA	O2D-CGD-CBD	7.80	124.87	111.23
13	A	840	CLA	O2D-CGD-CBD	7.78	124.83	111.23
13	A	832	CLA	O2D-CGD-CBD	7.75	124.77	111.23
13	A	824	CLA	O2D-CGD-CBD	7.65	124.61	111.23
15	A	852	BCR	C15-C14-C13	-7.63	116.57	127.28
13	A	821	CLA	O2D-CGD-CBD	7.55	124.43	111.23
13	A	811	CLA	O2D-CGD-CBD	7.45	124.26	111.23
13	B	833	CLA	O2D-CGD-CBD	7.43	124.22	111.23
13	M	1201	CLA	O2D-CGD-CBD	7.42	124.21	111.23
13	A	819	CLA	O2D-CGD-CBD	7.40	124.16	111.23
13	B	807	CLA	O2D-CGD-CBD	7.37	124.12	111.23
13	B	813	CLA	O2D-CGD-CBD	7.36	124.10	111.23
13	B	808	CLA	O2D-CGD-CBD	7.27	123.95	111.23
15	B	849	BCR	C15-C14-C13	-7.27	117.08	127.28
13	B	812	CLA	O2D-CGD-CBD	7.24	123.89	111.23
13	B	822	CLA	O2D-CGD-CBD	7.21	123.83	111.23
13	B	827	CLA	O2D-CGD-CBD	7.18	123.78	111.23
13	A	810	CLA	O2D-CGD-CBD	7.17	123.77	111.23
13	A	801	CLA	O2D-CGD-CBD	7.17	123.76	111.23
13	A	839	CLA	O2D-CGD-CBD	7.07	123.59	111.23
13	B	814	CLA	O2D-CGD-CBD	7.01	123.48	111.23
13	B	809	CLA	O2D-CGD-CBD	6.98	123.43	111.23
13	B	824	CLA	O2D-CGD-CBD	6.88	123.25	111.23
13	L	1003	CLA	O2D-CGD-CBD	6.87	123.24	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	829	CLA	O2D-CGD-CBD	6.85	123.21	111.23
13	B	811	CLA	O2D-CGD-CBD	6.84	123.19	111.23
13	J	1102	CLA	O2D-CGD-CBD	6.84	123.19	111.23
13	B	801	CLA	O2D-CGD-CBD	6.77	123.07	111.23
13	A	845	CLA	O2D-CGD-CBD	6.77	123.06	111.23
13	A	815	CLA	O2D-CGD-CBD	6.75	123.04	111.23
13	A	813	CLA	O2D-CGD-CBD	6.74	123.02	111.23
13	B	837	CLA	O2D-CGD-CBD	6.73	123.00	111.23
13	B	819	CLA	O2D-CGD-CBD	6.73	123.00	111.23
13	L	1004	CLA	O2D-CGD-CBD	6.68	122.90	111.23
13	B	834	CLA	O2D-CGD-CBD	6.62	122.81	111.23
13	F	1301	CLA	O2D-CGD-CBD	6.59	122.75	111.23
13	J	1101	CLA	O2D-CGD-CBD	6.57	122.71	111.23
13	B	836	CLA	O2D-CGD-CBD	6.56	122.69	111.23
13	A	855	CLA	O2D-CGD-CBD	6.55	122.68	111.23
13	A	805	CLA	O2D-CGD-CBD	6.53	122.64	111.23
13	A	838	CLA	O2D-CGD-CBD	6.49	122.58	111.23
13	A	825	CLA	O2D-CGD-CBD	6.48	122.57	111.23
13	L	1002	CLA	O2D-CGD-CBD	6.47	122.54	111.23
13	B	830	CLA	O2D-CGD-CBD	6.43	122.48	111.23
13	M	1202	CLA	O2D-CGD-CBD	6.41	122.44	111.23
13	B	828	CLA	O2D-CGD-CBD	6.39	122.39	111.23
13	I	101	CLA	O2D-CGD-CBD	6.38	122.38	111.23
13	A	818	CLA	O2D-CGD-CBD	6.26	122.18	111.23
13	A	843	CLA	O2D-CGD-CBD	6.22	122.11	111.23
13	B	803	CLA	O2D-CGD-CBD	6.11	121.91	111.23
13	B	832	CLA	O2D-CGD-CBD	6.11	121.91	111.23
13	A	836	CLA	O2D-CGD-CBD	6.10	121.90	111.23
13	B	804	CLA	O2D-CGD-CBD	6.06	121.83	111.23
13	B	839	CLA	O2D-CGD-CBD	6.05	121.81	111.23
15	A	850	BCR	C7-C8-C9	-6.03	117.31	126.23
13	B	802	CLA	O1D-CGD-CBD	-5.96	112.77	124.52
13	A	828	CLA	O2D-CGD-CBD	5.94	121.61	111.23
13	A	822	CLA	O1D-CGD-CBD	-5.93	112.82	124.52
13	A	830	CLA	O2D-CGD-CBD	5.92	121.58	111.23
18	B	848	LMG	C30-C29-C28	5.90	135.30	113.69
13	B	838	CLA	O2D-CGD-CBD	5.89	121.53	111.23
15	B	849	BCR	C11-C10-C9	-5.88	119.03	127.28
13	B	835	CLA	O2D-CGD-CBD	5.81	121.38	111.23
13	A	809	CLA	O2D-CGD-CBD	5.76	121.30	111.23
13	B	816	CLA	O2D-CGD-CBD	5.65	121.10	111.23
15	F	1302	BCR	C15-C14-C13	-5.64	119.38	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	827	CLA	O2D-CGD-CBD	5.63	121.07	111.23
15	B	843	BCR	C2-C1-C6	5.56	118.51	110.44
15	B	844	BCR	C15-C14-C13	-5.55	119.01	127.48
13	B	823	CLA	O2D-CGD-CBD	5.53	120.90	111.23
15	J	1104	BCR	C29-C30-C25	5.53	118.47	110.44
13	A	837	CLA	O2D-CGD-CBD	5.53	120.89	111.23
13	A	834	CLA	O2D-CGD-CBD	5.49	120.83	111.23
15	B	845	BCR	C29-C30-C25	5.45	118.36	110.44
15	B	850	BCR	C2-C1-C6	5.43	118.33	110.44
15	B	845	BCR	C15-C14-C13	-5.43	119.66	127.28
13	X	102	CLA	O1D-CGD-CBD	-5.43	113.81	124.52
15	B	842	BCR	C2-C1-C6	5.40	118.28	110.44
13	A	814	CLA	O2D-CGD-CBD	5.39	120.66	111.23
15	M	1203	BCR	C33-C5-C6	-5.38	118.61	124.48
15	B	845	BCR	C38-C26-C25	-5.38	118.61	124.48
15	B	847	BCR	C2-C1-C6	5.35	118.21	110.44
13	B	806	CLA	O2D-CGD-CBD	5.28	120.47	111.23
13	A	802	CLA	O2D-CGD-CBD	5.28	120.47	111.23
13	A	807	CLA	CED-O2D-CGD	5.24	127.80	115.92
15	B	847	BCR	C33-C5-C6	-5.19	118.82	124.48
15	A	852	BCR	C15-C16-C17	-5.17	112.94	123.52
13	A	826	CLA	O2D-CGD-CBD	5.16	120.24	111.23
15	M	1203	BCR	C2-C1-C6	5.13	117.90	110.44
15	I	102	BCR	C2-C1-C6	5.13	117.89	110.44
13	I	101	CLA	O1D-CGD-CBD	-5.12	114.42	124.52
13	A	818	CLA	C1-O2A-CGA	5.12	129.04	116.65
13	A	804	CLA	O2D-CGD-CBD	5.07	120.10	111.23
15	B	850	BCR	C7-C8-C9	-5.07	118.73	126.23
15	L	1005	BCR	C16-C17-C18	-5.07	120.16	127.28
15	B	842	BCR	C15-C14-C13	-5.04	120.22	127.28
15	A	852	BCR	C33-C5-C6	-5.01	119.02	124.48
15	B	842	BCR	C33-C5-C6	-4.97	119.06	124.48
13	B	806	CLA	C1-C2-C3	-4.88	118.20	126.20
13	A	807	CLA	C4-C3-C5	4.84	121.82	116.13
15	B	850	BCR	C38-C26-C25	-4.83	119.21	124.48
13	A	829	CLA	C1-O2A-CGA	4.83	128.35	116.65
13	B	802	CLA	C1-C2-C3	-4.79	118.35	126.20
15	B	843	BCR	C29-C30-C25	4.75	117.34	110.44
13	A	835	CLA	O2D-CGD-CBD	4.69	119.44	111.23
13	B	825	CLA	O2D-CGD-CBD	4.67	119.39	111.23
13	A	806	CLA	C1-C2-C3	-4.65	118.57	126.20
15	I	102	BCR	C33-C5-C6	-4.65	119.42	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	840	CLA	O1D-CGD-CBD	-4.64	115.37	124.52
15	A	851	BCR	C15-C14-C13	-4.61	120.82	127.28
15	I	102	BCR	C38-C26-C25	-4.59	119.48	124.48
15	L	1006	BCR	C16-C17-C18	-4.59	120.84	127.28
15	L	1005	BCR	C38-C26-C25	-4.57	119.50	124.48
15	B	843	BCR	C16-C17-C18	-4.54	120.92	127.28
13	A	831	CLA	O2D-CGD-CBD	4.54	119.16	111.23
15	B	843	BCR	C33-C5-C6	-4.53	119.54	124.48
15	F	1302	BCR	C33-C5-C6	-4.52	119.55	124.48
15	A	849	BCR	C16-C17-C18	-4.52	120.94	127.28
13	A	832	CLA	O1D-CGD-CBD	-4.51	115.62	124.52
15	A	852	BCR	C38-C26-C25	-4.50	119.58	124.48
15	B	850	BCR	C15-C14-C13	-4.49	120.98	127.28
15	B	847	BCR	C16-C17-C18	-4.48	120.99	127.28
15	A	851	BCR	C38-C26-C25	-4.47	119.61	124.48
13	A	829	CLA	CAA-CBA-CGA	-4.45	100.57	113.21
15	J	1105	BCR	C38-C26-C25	-4.45	119.63	124.48
13	A	820	CLA	O2D-CGD-CBD	4.44	118.99	111.23
15	L	1006	BCR	C38-C26-C25	-4.38	119.70	124.48
13	B	805	CLA	C1-C2-C3	-4.35	119.06	126.20
13	A	803	CLA	O2D-CGD-CBD	4.35	118.84	111.23
15	A	851	BCR	C33-C5-C6	-4.35	119.74	124.48
15	F	1302	BCR	C11-C10-C9	-4.34	121.19	127.28
15	B	850	BCR	C16-C17-C18	-4.34	121.19	127.28
15	L	1006	BCR	C24-C23-C22	-4.33	119.82	126.23
13	B	838	CLA	CAA-CBA-CGA	-4.33	100.92	113.21
15	A	850	BCR	C24-C23-C22	-4.32	119.84	126.23
15	A	851	BCR	C24-C23-C22	-4.32	119.85	126.23
15	B	849	BCR	C38-C26-C25	-4.31	119.78	124.48
13	A	806	CLA	O2D-CGD-CBD	4.31	118.76	111.23
15	B	843	BCR	C23-C24-C25	-4.30	115.52	127.00
15	A	847	BCR	C2-C1-C6	4.30	116.68	110.44
15	B	841	BCR	C2-C1-C6	4.28	116.66	110.44
15	L	1005	BCR	C33-C5-C6	-4.27	119.83	124.48
15	B	843	BCR	C3-C4-C5	4.26	121.65	114.06
13	A	819	CLA	C4-C3-C5	4.26	122.62	115.23
15	J	1104	BCR	C2-C1-C6	4.23	116.58	110.44
15	A	848	BCR	C38-C26-C25	-4.23	119.87	124.48
15	B	847	BCR	C38-C26-C25	-4.21	119.89	124.48
15	B	842	BCR	C24-C23-C22	-4.21	120.00	126.23
15	J	1105	BCR	C33-C5-C6	-4.21	119.89	124.48
15	A	848	BCR	C33-C5-C6	-4.20	119.91	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	826	CLA	O2D-CGD-CBD	4.18	118.54	111.23
15	L	1005	BCR	C2-C1-C6	4.18	116.51	110.44
15	B	841	BCR	C16-C17-C18	-4.18	121.42	127.28
13	B	802	CLA	C4D-C3D-CAD	-4.17	103.57	108.11
15	J	1104	BCR	C38-C26-C25	-4.17	119.93	124.48
13	A	845	CLA	CAA-CBA-CGA	-4.17	101.36	113.21
15	B	850	BCR	C11-C10-C9	-4.17	121.43	127.28
13	B	805	CLA	O2D-CGD-CBD	4.17	118.52	111.23
15	A	849	BCR	C20-C21-C22	-4.17	121.43	127.28
15	A	850	BCR	C38-C26-C25	-4.17	119.94	124.48
14	B	840	PQN	C11-C12-C13	-4.17	119.66	126.83
15	B	841	BCR	C33-C5-C6	-4.16	119.94	124.48
15	J	1104	BCR	C33-C5-C6	-4.15	119.95	124.48
15	L	1005	BCR	C7-C8-C9	-4.15	120.10	126.23
15	B	846	BCR	C16-C17-C18	-4.13	121.48	127.28
15	M	1203	BCR	C8-C7-C6	-4.13	115.97	127.00
15	A	850	BCR	C2-C1-C6	4.12	116.43	110.44
13	B	831	CLA	O1D-CGD-CBD	-4.12	116.39	124.52
15	A	848	BCR	C24-C23-C22	-4.12	120.14	126.23
13	B	812	CLA	O1D-CGD-CBD	-4.11	116.42	124.52
15	A	848	BCR	C2-C1-C6	4.10	116.39	110.44
13	A	808	CLA	O2D-CGD-O1D	-4.09	115.89	123.85
15	B	845	BCR	C2-C1-C6	4.07	116.35	110.44
15	B	842	BCR	C11-C10-C9	-4.06	121.58	127.28
15	J	1104	BCR	C28-C27-C26	4.06	121.29	114.06
15	B	844	BCR	C38-C26-C25	-4.06	120.06	124.48
15	A	848	BCR	C16-C17-C18	-4.05	121.60	127.28
15	B	843	BCR	C38-C26-C25	-4.05	120.06	124.48
15	B	845	BCR	C24-C23-C22	-4.04	120.26	126.23
15	B	846	BCR	C2-C1-C6	4.03	116.30	110.44
15	A	849	BCR	C33-C5-C6	-4.03	120.09	124.48
15	A	848	BCR	C7-C8-C9	-4.02	120.28	126.23
15	A	851	BCR	C16-C17-C18	-4.00	121.67	127.28
15	A	847	BCR	C16-C17-C18	-3.99	121.69	127.28
13	B	829	CLA	O2D-CGD-CBD	3.98	118.19	111.23
15	B	842	BCR	C3-C4-C5	3.98	121.16	114.06
13	A	819	CLA	O1D-CGD-CBD	-3.98	116.67	124.52
15	L	1006	BCR	C2-C1-C6	3.98	116.21	110.44
15	J	1104	BCR	C7-C8-C9	-3.97	120.36	126.23
15	J	1105	BCR	C2-C1-C6	3.97	116.21	110.44
13	A	841	CLA	O2D-CGD-CBD	3.95	118.14	111.23
15	A	847	BCR	C29-C30-C25	3.95	116.18	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	823	CLA	C1-C2-C3	-3.95	119.72	126.20
13	B	804	CLA	C1-C2-C3	-3.95	119.73	126.20
13	A	812	CLA	O1D-CGD-CBD	-3.94	116.75	124.52
15	A	849	BCR	C7-C8-C9	-3.93	120.42	126.23
13	B	829	CLA	CAA-CBA-CGA	-3.93	102.06	113.21
15	B	846	BCR	C20-C21-C22	-3.92	121.78	127.28
15	A	847	BCR	C33-C5-C6	-3.91	120.21	124.48
13	A	821	CLA	C1-C2-C3	-3.90	119.81	126.20
15	I	102	BCR	C7-C8-C9	-3.90	120.47	126.23
15	B	850	BCR	C24-C23-C22	-3.89	120.47	126.23
15	A	849	BCR	C38-C26-C25	-3.89	120.24	124.48
15	L	1005	BCR	C16-C15-C14	-3.89	115.56	123.52
15	B	842	BCR	C38-C26-C25	-3.89	120.24	124.48
16	A	854	LHG	O7-C7-C8	3.88	119.88	111.48
15	B	846	BCR	C33-C5-C6	-3.88	120.25	124.48
15	B	842	BCR	C20-C21-C22	-3.88	121.84	127.28
13	A	809	CLA	O2A-CGA-CBA	3.87	123.64	111.83
15	M	1203	BCR	C3-C4-C5	3.87	120.95	114.06
16	A	853	LHG	O7-C7-C8	3.86	119.83	111.48
15	L	1005	BCR	C24-C23-C22	-3.85	120.54	126.23
15	I	102	BCR	C23-C24-C25	-3.85	116.73	127.00
15	B	849	BCR	C33-C5-C6	-3.84	120.29	124.48
15	B	845	BCR	C28-C27-C26	3.84	120.91	114.06
15	J	1104	BCR	C15-C14-C13	-3.84	121.90	127.28
15	F	1302	BCR	C2-C1-C6	3.83	116.01	110.44
15	A	849	BCR	C15-C14-C13	-3.83	121.91	127.28
13	B	807	CLA	O1D-CGD-CBD	-3.82	116.99	124.52
15	L	1006	BCR	C20-C21-C22	-3.81	121.94	127.28
15	B	846	BCR	C10-C11-C12	-3.79	112.22	123.20
15	B	849	BCR	C7-C8-C9	-3.79	120.63	126.23
15	M	1203	BCR	C10-C11-C12	-3.79	112.23	123.20
13	A	815	CLA	O1D-CGD-CBD	-3.79	117.05	124.52
15	B	841	BCR	C29-C30-C25	3.78	115.93	110.44
15	M	1203	BCR	C38-C26-C25	-3.78	120.36	124.48
13	A	833	CLA	O2D-CGD-CBD	3.77	117.83	111.23
13	A	823	CLA	O2D-CGD-CBD	3.77	117.82	111.23
13	A	818	CLA	O2D-CGD-O1D	-3.77	116.52	123.85
15	J	1105	BCR	C29-C30-C25	3.76	115.90	110.44
15	B	845	BCR	C33-C5-C6	-3.75	120.39	124.48
15	B	847	BCR	C20-C21-C22	-3.74	122.03	127.28
15	B	849	BCR	C16-C17-C18	-3.74	122.04	127.28
15	J	1105	BCR	C24-C23-C22	-3.73	120.71	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	852	BCR	C29-C30-C25	3.72	115.84	110.44
13	A	839	CLA	O2D-CGD-O1D	-3.71	116.62	123.85
15	A	851	BCR	C2-C1-C6	3.71	115.83	110.44
15	A	850	BCR	C20-C21-C22	-3.70	122.08	127.28
15	F	1302	BCR	C38-C26-C25	-3.70	120.45	124.48
13	B	838	CLA	O2A-CGA-CBA	3.69	123.10	111.83
15	B	846	BCR	C29-C30-C25	3.69	115.81	110.44
15	A	850	BCR	C16-C17-C18	-3.69	122.10	127.28
13	B	810	CLA	O2D-CGD-CBD	3.69	117.68	111.23
15	A	849	BCR	C2-C1-C6	3.68	115.79	110.44
13	A	843	CLA	O1D-CGD-CBD	-3.68	117.26	124.52
13	A	802	CLA	C1-C2-C3	-3.68	120.17	126.20
15	J	1105	BCR	C16-C17-C18	-3.67	122.13	127.28
13	B	830	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
15	B	850	BCR	C3-C4-C5	3.66	120.59	114.06
13	A	828	CLA	C1-C2-C3	-3.66	120.20	126.20
15	B	845	BCR	C15-C16-C17	-3.66	116.03	123.52
13	L	1003	CLA	O1D-CGD-CBD	-3.65	117.33	124.52
13	A	831	CLA	C1-C2-C3	-3.64	120.86	126.76
15	B	843	BCR	C10-C11-C12	-3.64	112.64	123.20
15	I	102	BCR	C3-C4-C5	3.64	120.55	114.06
13	M	1201	CLA	O1D-CGD-CBD	-3.63	117.35	124.52
15	B	849	BCR	C15-C16-C17	-3.63	116.09	123.52
15	A	850	BCR	C11-C10-C9	-3.63	122.19	127.28
15	F	1302	BCR	C15-C16-C17	-3.63	116.10	123.52
15	M	1203	BCR	C24-C23-C22	-3.63	120.87	126.23
13	A	812	CLA	C1-C2-C3	-3.62	120.26	126.20
13	B	817	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
13	B	803	CLA	C4D-C3D-CAD	-3.62	104.18	108.11
15	B	847	BCR	C3-C4-C5	3.61	120.49	114.06
13	A	825	CLA	O1D-CGD-CBD	-3.60	117.41	124.52
15	A	847	BCR	C20-C21-C22	-3.60	122.23	127.28
15	B	845	BCR	C20-C21-C22	-3.60	122.24	127.28
13	A	821	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
13	B	813	CLA	C3B-C4B-NB	-3.59	107.33	110.53
15	A	850	BCR	C29-C30-C25	3.58	115.64	110.44
13	A	834	CLA	C3B-C4B-NB	-3.58	107.33	110.53
15	B	844	BCR	C29-C30-C25	3.58	115.64	110.44
13	B	820	CLA	O2D-CGD-CBD	3.58	117.48	111.23
15	A	848	BCR	C29-C30-C25	3.58	115.63	110.44
15	J	1105	BCR	C15-C14-C13	-3.58	122.26	127.28
15	M	1203	BCR	C29-C30-C25	3.57	115.63	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	1005	BCR	C11-C10-C9	-3.57	122.27	127.28
15	B	841	BCR	C10-C11-C12	-3.57	112.87	123.20
13	B	801	CLA	C1-C2-C3	-3.56	120.36	126.20
13	A	816	CLA	O2D-CGD-CBD	3.56	117.46	111.23
15	I	102	BCR	C16-C17-C18	-3.56	122.28	127.28
15	A	849	BCR	C29-C30-C25	3.56	115.60	110.44
15	A	850	BCR	C33-C5-C6	-3.55	120.61	124.48
13	L	1003	CLA	C1-C2-C3	-3.55	120.38	126.20
13	B	825	CLA	C1-O2A-CGA	3.55	125.23	116.65
15	B	850	BCR	C20-C21-C22	-3.54	122.31	127.28
13	A	817	CLA	O2D-CGD-CBD	3.54	117.42	111.23
15	A	849	BCR	C10-C11-C12	-3.54	112.95	123.20
15	I	102	BCR	C10-C11-C12	-3.54	112.95	123.20
15	B	850	BCR	C33-C5-C6	-3.53	120.63	124.48
15	A	852	BCR	C2-C1-C6	3.52	115.56	110.44
13	B	806	CLA	C1-O2A-CGA	3.52	125.18	116.65
15	L	1006	BCR	C29-C30-C25	3.52	115.56	110.44
13	B	807	CLA	C1-C2-C3	-3.52	120.44	126.20
13	B	811	CLA	O2A-CGA-CBA	3.51	122.55	111.83
13	A	803	CLA	C1-C2-C3	-3.51	120.44	126.20
15	B	849	BCR	C2-C1-C6	3.51	115.53	110.44
13	A	824	CLA	O1D-CGD-CBD	-3.50	117.61	124.52
13	A	808	CLA	O2A-CGA-CBA	3.50	122.50	111.83
13	B	818	CLA	O2D-CGD-CBD	3.50	117.34	111.23
15	B	841	BCR	C20-C21-C22	-3.50	122.38	127.28
15	B	849	BCR	C23-C24-C25	-3.50	117.66	127.00
13	A	842	CLA	C4-C3-C5	3.49	121.29	115.23
13	A	820	CLA	C1-C2-C3	-3.49	120.48	126.20
15	F	1302	BCR	C20-C21-C22	-3.49	122.39	127.28
13	A	841	CLA	C4-C3-C5	3.48	120.23	116.13
15	L	1005	BCR	C29-C30-C25	3.47	115.48	110.44
13	A	824	CLA	C4D-C3D-CAD	-3.47	104.34	108.11
13	B	802	CLA	C3B-C4B-NB	-3.47	107.43	110.53
13	B	837	CLA	O1D-CGD-CBD	-3.47	117.68	124.52
15	A	847	BCR	C10-C11-C12	-3.46	113.16	123.20
16	X	101	LHG	O7-C7-C8	3.46	118.97	111.48
15	A	852	BCR	C38-C26-C27	3.46	120.97	113.60
15	M	1203	BCR	C16-C17-C18	-3.45	122.43	127.28
15	B	845	BCR	C10-C11-C12	-3.45	113.20	123.20
13	I	101	CLA	C1-C2-C3	-3.45	120.55	126.20
13	L	1002	CLA	C4D-C3D-CAD	-3.45	104.36	108.11
13	B	815	CLA	O2D-CGD-CBD	3.45	117.25	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	850	BCR	C23-C24-C25	-3.44	117.80	127.00
13	A	809	CLA	CAA-CBA-CGA	-3.44	103.43	113.21
15	B	846	BCR	C24-C23-C22	-3.43	121.17	126.23
13	A	838	CLA	C3B-C4B-NB	-3.42	107.47	110.53
13	A	817	CLA	CAA-CBA-CGA	-3.42	103.50	113.21
13	B	838	CLA	C1-C2-C3	-3.42	120.60	126.20
15	J	1105	BCR	C38-C26-C27	3.42	120.88	113.60
15	F	1302	BCR	C7-C8-C9	-3.41	121.18	126.23
13	A	811	CLA	O1D-CGD-CBD	-3.41	117.79	124.52
15	L	1005	BCR	C38-C26-C27	3.41	120.86	113.60
13	F	1301	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
13	A	832	CLA	C3B-C4B-NB	-3.40	107.49	110.53
15	I	102	BCR	C15-C14-C13	-3.39	122.53	127.28
13	B	820	CLA	C1-C2-C3	-3.38	120.66	126.20
15	A	847	BCR	C24-C23-C22	-3.38	121.24	126.23
15	B	850	BCR	C38-C26-C27	3.38	120.79	113.60
13	A	817	CLA	C1-C2-C3	-3.37	120.68	126.20
15	J	1104	BCR	C16-C17-C18	-3.36	122.57	127.28
13	B	801	CLA	O1D-CGD-CBD	-3.35	117.90	124.52
13	B	816	CLA	C4-C3-C5	3.35	121.05	115.23
13	A	802	CLA	C3B-C4B-NB	-3.35	107.54	110.53
13	B	813	CLA	O1D-CGD-CBD	-3.35	117.92	124.52
15	F	1302	BCR	C24-C23-C22	-3.34	121.29	126.23
15	F	1302	BCR	C29-C30-C25	3.34	115.30	110.44
15	B	842	BCR	C29-C30-C25	3.34	115.29	110.44
13	A	808	CLA	C3B-C4B-NB	-3.34	107.55	110.53
13	B	838	CLA	C4-C3-C5	3.34	121.02	115.23
15	B	843	BCR	C23-C22-C21	-3.33	113.77	119.01
15	A	848	BCR	C20-C21-C22	-3.33	122.61	127.28
15	B	841	BCR	C24-C23-C22	-3.33	121.31	126.23
15	A	848	BCR	C38-C26-C27	3.33	120.70	113.60
15	A	851	BCR	C20-C21-C22	-3.33	122.61	127.28
15	B	847	BCR	C8-C7-C6	-3.33	118.11	127.00
15	I	102	BCR	C8-C7-C6	-3.32	118.13	127.00
13	A	813	CLA	C1-O2A-CGA	3.32	124.68	116.65
13	A	830	CLA	C4-C3-C5	3.32	120.98	115.23
15	I	102	BCR	C38-C26-C27	3.31	120.66	113.60
13	A	819	CLA	CBA-CAA-C2A	-3.31	103.95	113.79
13	B	831	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
14	A	846	PQN	C11-C12-C13	-3.30	121.14	126.83
13	B	817	CLA	O1D-CGD-CBD	-3.30	118.00	124.52
13	A	829	CLA	O1D-CGD-CBD	-3.30	118.02	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	847	BCR	C29-C30-C25	3.29	115.22	110.44
13	B	812	CLA	C4D-C3D-CAD	-3.28	104.55	108.11
15	B	842	BCR	C15-C16-C17	-3.28	116.82	123.52
13	B	821	CLA	CED-O2D-CGD	3.27	123.34	115.92
15	A	852	BCR	C33-C5-C4	3.27	120.57	113.60
15	A	848	BCR	C33-C5-C4	3.27	120.56	113.60
13	A	832	CLA	O2A-CGA-CBA	3.27	121.80	111.83
15	I	102	BCR	C21-C20-C19	-3.27	113.73	123.20
15	B	841	BCR	C15-C14-C13	-3.26	122.70	127.28
15	B	846	BCR	C8-C7-C6	-3.26	118.28	127.00
13	A	810	CLA	O1D-CGD-CBD	-3.26	118.08	124.52
15	B	847	BCR	C24-C23-C22	-3.26	121.41	126.23
13	B	833	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
13	B	812	CLA	C3B-C4B-NB	-3.26	107.62	110.53
15	B	841	BCR	C33-C5-C4	3.26	120.54	113.60
13	A	809	CLA	C1-C2-C3	-3.26	120.86	126.20
13	B	814	CLA	C1-O2A-CGA	3.25	124.53	116.65
13	B	808	CLA	O1D-CGD-CBD	-3.25	118.11	124.52
15	J	1105	BCR	C8-C7-C6	-3.25	118.31	127.00
15	A	849	BCR	C23-C24-C25	-3.25	118.32	127.00
15	A	851	BCR	C38-C26-C27	3.25	120.52	113.60
13	B	836	CLA	C1-O2A-CGA	3.25	124.51	116.65
13	B	831	CLA	C1-C2-C3	-3.24	120.88	126.20
15	J	1104	BCR	C33-C5-C4	3.24	120.51	113.60
15	J	1105	BCR	C33-C5-C4	3.24	120.50	113.60
15	B	847	BCR	C12-C13-C14	-3.23	113.92	119.01
15	M	1203	BCR	C38-C26-C27	3.23	120.49	113.60
13	A	843	CLA	C1-O2A-CGA	3.23	124.47	116.65
13	A	814	CLA	C3B-C4B-NB	-3.23	107.65	110.53
15	M	1203	BCR	C15-C14-C13	-3.23	122.75	127.28
13	B	811	CLA	O1D-CGD-CBD	-3.23	118.15	124.52
13	A	818	CLA	C4-C3-C5	3.23	120.83	115.23
15	A	850	BCR	C38-C26-C27	3.22	120.47	113.60
13	B	804	CLA	C4-C3-C5	3.22	120.82	115.23
13	B	836	CLA	C3B-C4B-NB	-3.22	107.66	110.53
13	B	822	CLA	O1D-CGD-CBD	-3.22	118.17	124.52
13	B	808	CLA	C4D-C3D-CAD	-3.22	104.61	108.11
13	B	820	CLA	C4-C3-C5	3.20	120.79	115.23
13	B	824	CLA	O1D-CGD-CBD	-3.20	118.20	124.52
15	B	843	BCR	C7-C8-C9	-3.20	121.50	126.23
15	L	1006	BCR	C38-C26-C27	3.20	120.41	113.60
13	B	830	CLA	O2A-CGA-CBA	3.20	121.58	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	1302	BCR	C33-C5-C4	3.19	120.41	113.60
15	M	1203	BCR	C20-C21-C22	-3.19	122.80	127.28
13	L	1002	CLA	C3B-C4B-NB	-3.19	107.68	110.53
13	A	843	CLA	C4-C3-C5	3.19	120.77	115.23
13	L	1003	CLA	CAA-CBA-CGA	-3.19	104.15	113.21
15	I	102	BCR	C24-C23-C22	-3.19	121.52	126.23
13	A	823	CLA	C4-C3-C5	3.19	119.88	116.13
13	A	824	CLA	C1-C2-C3	-3.19	120.98	126.20
13	L	1002	CLA	C1-C2-C3	-3.19	120.98	126.20
15	L	1005	BCR	C33-C5-C4	3.19	120.39	113.60
13	B	836	CLA	O1D-CGD-CBD	-3.18	118.24	124.52
15	J	1105	BCR	C20-C21-C22	-3.18	122.81	127.28
13	A	808	CLA	CGD-CBD-CAD	-3.18	100.54	110.85
13	A	828	CLA	O1D-CGD-CBD	-3.18	118.24	124.52
13	J	1101	CLA	C3B-C4B-NB	-3.18	107.69	110.53
15	B	844	BCR	C15-C16-C17	-3.18	117.02	123.52
15	B	843	BCR	C28-C27-C26	3.18	119.72	114.06
13	B	818	CLA	C3B-C4B-NB	-3.18	107.69	110.53
13	A	845	CLA	C1-C2-C3	-3.17	121.00	126.20
13	B	827	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
14	B	840	PQN	C11-C3-C2	-3.17	119.46	124.89
13	B	833	CLA	O1D-CGD-CBD	-3.17	118.27	124.52
13	B	831	CLA	C4D-C3D-CAD	-3.17	104.67	108.11
15	B	844	BCR	C38-C26-C27	3.16	120.34	113.60
13	A	807	CLA	O2A-CGA-CBA	3.16	121.48	111.83
15	B	847	BCR	C10-C11-C12	-3.16	114.04	123.20
13	A	801	CLA	O1D-CGD-CBD	-3.16	118.29	124.52
15	F	1302	BCR	C23-C24-C25	-3.16	118.56	127.00
13	A	807	CLA	C1-C2-C3	-3.15	121.03	126.20
15	B	849	BCR	C33-C5-C4	3.15	120.32	113.60
13	B	815	CLA	C1-O2A-CGA	3.15	124.27	116.65
15	A	851	BCR	C7-C8-C9	-3.15	121.58	126.23
13	B	827	CLA	C3B-C4B-NB	-3.14	107.72	110.53
15	B	847	BCR	C38-C26-C27	3.14	120.30	113.60
13	B	804	CLA	O2A-CGA-CBA	3.14	121.42	111.83
15	A	849	BCR	C38-C26-C27	3.14	120.30	113.60
13	A	855	CLA	O1D-CGD-CBD	-3.14	118.32	124.52
13	J	1102	CLA	O1D-CGD-CBD	-3.14	118.33	124.52
13	B	834	CLA	O1D-CGD-CBD	-3.14	118.33	124.52
15	B	846	BCR	C38-C26-C25	-3.14	121.06	124.48
13	B	826	CLA	C1-O2A-CGA	3.13	124.24	116.65
15	A	851	BCR	C29-C30-C25	3.13	114.99	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	819	CLA	O1D-CGD-CBD	-3.13	118.34	124.52
13	A	815	CLA	C3B-C4B-NB	-3.13	107.74	110.53
13	B	809	CLA	C4D-C3D-CAD	-3.13	104.71	108.11
13	M	1202	CLA	O1D-CGD-CBD	-3.13	118.35	124.52
13	B	832	CLA	O1D-CGD-CBD	-3.13	118.35	124.52
13	A	808	CLA	C1-C2-C3	-3.13	121.08	126.20
15	L	1006	BCR	C8-C7-C6	-3.13	118.65	127.00
13	A	842	CLA	O2D-CGD-CBD	3.12	116.69	111.23
15	L	1006	BCR	C10-C11-C12	-3.12	114.15	123.20
13	L	1004	CLA	O2A-CGA-CBA	3.12	121.36	111.83
13	A	830	CLA	C4D-C3D-CAD	-3.12	104.71	108.11
13	B	835	CLA	C4D-C3D-CAD	-3.12	104.72	108.11
15	A	852	BCR	C7-C8-C9	-3.12	121.62	126.23
13	B	819	CLA	C4D-C3D-CAD	-3.12	104.72	108.11
13	A	824	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
13	A	816	CLA	O2A-CGA-CBA	3.11	121.33	111.83
15	B	849	BCR	C38-C26-C27	3.11	120.23	113.60
13	B	809	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
13	A	835	CLA	C3B-C4B-NB	-3.10	107.76	110.53
13	B	835	CLA	O2A-CGA-CBA	3.10	121.29	111.83
13	A	837	CLA	C4-C3-C5	3.10	119.78	116.13
13	L	1002	CLA	O1D-CGD-CBD	-3.10	118.41	124.52
13	A	844	CLA	C3B-C4B-NB	-3.10	107.77	110.53
13	B	803	CLA	C3B-C4B-NB	-3.10	107.77	110.53
13	A	801	CLA	C4D-C3D-CAD	-3.10	104.74	108.11
15	A	850	BCR	C33-C5-C4	3.09	120.19	113.60
15	J	1105	BCR	C7-C8-C9	-3.09	121.66	126.23
13	B	825	CLA	C4-C3-C5	3.09	120.59	115.23
13	J	1102	CLA	C4D-C3D-CAD	-3.09	104.75	108.11
15	A	850	BCR	C15-C14-C13	-3.09	122.94	127.28
13	A	813	CLA	O1D-CGD-CBD	-3.09	118.43	124.52
15	A	847	BCR	C33-C5-C4	3.08	120.17	113.60
15	B	844	BCR	C24-C23-C22	-3.08	121.67	126.23
13	A	829	CLA	C3B-C4B-NB	-3.08	107.78	110.53
13	B	822	CLA	C1-C2-C3	-3.08	121.16	126.20
13	B	802	CLA	O2A-CGA-CBA	3.08	121.21	111.83
15	A	851	BCR	C33-C5-C4	3.07	120.15	113.60
15	B	845	BCR	C8-C7-C6	-3.07	118.80	127.00
15	B	850	BCR	C29-C30-C25	3.07	114.90	110.44
13	A	828	CLA	C4-C3-C5	3.07	120.55	115.23
13	J	1101	CLA	O2A-CGA-CBA	3.07	121.19	111.83
13	B	814	CLA	O1D-CGD-CBD	-3.06	118.48	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	821	CLA	C3B-C4B-NB	-3.05	107.81	110.53
13	A	812	CLA	C4-C3-C5	3.05	120.52	115.23
15	J	1104	BCR	C10-C11-C12	-3.05	114.36	123.20
13	B	811	CLA	C1-C2-C3	-3.05	121.20	126.20
13	A	837	CLA	O1D-CGD-CBD	-3.05	118.51	124.52
15	B	843	BCR	C15-C14-C13	-3.05	123.01	127.28
13	A	804	CLA	C4-C3-C5	3.05	120.51	115.23
15	L	1005	BCR	C20-C21-C22	-3.04	123.01	127.28
13	B	806	CLA	CAA-CBA-CGA	-3.04	104.57	113.21
15	B	845	BCR	C33-C5-C4	3.04	120.08	113.60
13	A	838	CLA	O1D-CGD-CBD	-3.04	118.52	124.52
13	A	826	CLA	C3B-C4B-NB	-3.04	107.82	110.53
13	B	808	CLA	C4-C3-C5	3.04	120.50	115.23
18	B	848	LMG	O8-C28-C29	3.04	121.10	111.83
13	A	837	CLA	C2A-C1A-CHA	3.04	129.14	123.87
13	B	808	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
13	B	820	CLA	C3B-C4B-NB	-3.03	107.82	110.53
13	A	801	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
13	B	803	CLA	C4-C3-C5	3.03	120.49	115.23
13	B	812	CLA	C4-C3-C5	3.03	120.49	115.23
13	A	811	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
13	B	801	CLA	C4D-C3D-CAD	-3.03	104.81	108.11
13	A	801	CLA	C1-C2-C3	-3.03	121.23	126.20
13	B	827	CLA	O1D-CGD-CBD	-3.03	118.54	124.52
13	B	824	CLA	C4-C3-C5	3.03	120.49	115.23
13	B	817	CLA	C4-C3-C5	3.03	120.48	115.23
13	B	833	CLA	C3B-C4B-NB	-3.02	107.83	110.53
13	L	1004	CLA	C3B-C4B-NB	-3.02	107.83	110.53
13	B	838	CLA	C3B-C4B-NB	-3.02	107.83	110.53
13	B	813	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
13	B	815	CLA	C3B-C4B-NB	-3.02	107.83	110.53
13	A	834	CLA	C4-C3-C5	3.02	120.46	115.23
13	A	827	CLA	O2A-CGA-CBA	3.01	121.02	111.83
15	B	846	BCR	C12-C13-C14	-3.01	114.27	119.01
15	B	847	BCR	C33-C5-C4	3.01	120.02	113.60
13	B	822	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
15	B	846	BCR	C33-C5-C4	3.01	120.01	113.60
15	F	1302	BCR	C38-C26-C27	3.01	120.01	113.60
15	B	847	BCR	C7-C8-C9	-3.01	121.79	126.23
13	A	838	CLA	C1-O2A-CGA	3.00	123.92	116.65
13	I	101	CLA	C4-C3-C5	3.00	120.44	115.23
13	A	825	CLA	C3B-C4B-NB	-3.00	107.85	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	1101	CLA	C1-C2-C3	-3.00	121.28	126.20
15	B	847	BCR	C16-C15-C14	-3.00	117.38	123.52
15	J	1104	BCR	C20-C21-C22	-3.00	123.08	127.28
15	B	849	BCR	C11-C12-C13	-3.00	118.15	126.36
15	M	1203	BCR	C33-C5-C4	2.99	119.98	113.60
13	B	818	CLA	O2A-CGA-CBA	2.99	120.96	111.83
15	I	102	BCR	C12-C13-C14	-2.99	114.30	119.01
13	A	832	CLA	C4-C3-C5	2.99	120.41	115.23
13	B	814	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
15	A	849	BCR	C8-C7-C6	-2.99	119.02	127.00
15	B	844	BCR	C23-C24-C25	-2.98	119.03	127.00
15	A	847	BCR	C7-C8-C9	-2.98	121.82	126.23
13	L	1003	CLA	C4D-C3D-CAD	-2.98	104.87	108.11
15	L	1005	BCR	C21-C20-C19	-2.98	114.58	123.20
13	A	813	CLA	C3B-C4B-NB	-2.97	107.88	110.53
13	A	855	CLA	C3B-C4B-NB	-2.97	107.88	110.53
13	B	812	CLA	CAA-CBA-CGA	-2.96	104.79	113.21
13	A	803	CLA	C4-C3-C5	2.96	120.37	115.23
13	B	839	CLA	C4-C3-C5	2.96	120.37	115.23
13	A	809	CLA	C4-C3-C5	2.96	120.37	115.23
13	L	1004	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	A	845	CLA	C1-O2A-CGA	2.96	123.81	116.65
15	B	841	BCR	C7-C8-C9	-2.96	121.86	126.23
13	B	827	CLA	C4-C3-C5	2.96	120.36	115.23
13	A	803	CLA	C3B-C4B-NB	-2.96	107.89	110.53
13	L	1003	CLA	C3B-C4B-NB	-2.95	107.89	110.53
13	A	811	CLA	C4-C3-C5	2.95	120.36	115.23
13	A	821	CLA	O1D-CGD-CBD	-2.95	118.70	124.52
13	A	834	CLA	O1D-CGD-CBD	-2.95	118.70	124.52
13	B	814	CLA	C4D-C3D-CAD	-2.95	104.90	108.11
13	A	845	CLA	O1D-CGD-CBD	-2.95	118.70	124.52
13	L	1004	CLA	C4-C3-C5	2.95	120.34	115.23
13	A	834	CLA	CBB-CAB-C3B	-2.95	112.81	127.53
13	A	824	CLA	C4-C3-C5	2.95	120.34	115.23
16	A	854	LHG	O8-C23-C24	2.94	120.08	111.15
15	I	102	BCR	C29-C30-C25	2.94	114.71	110.44
13	B	824	CLA	C3B-C4B-NB	-2.94	107.91	110.53
15	A	849	BCR	C33-C5-C4	2.94	119.86	113.60
13	B	803	CLA	O1D-CGD-CBD	-2.93	118.73	124.52
13	A	810	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	B	823	CLA	C3B-C4B-NB	-2.93	107.91	110.53
13	X	102	CLA	C3B-C4B-NB	-2.93	107.91	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	808	CLA	O2A-CGA-CBA	2.93	120.77	111.83
13	A	837	CLA	O2A-CGA-CBA	2.93	120.77	111.83
15	B	841	BCR	C38-C26-C25	-2.93	121.29	124.48
13	B	809	CLA	O1D-CGD-CBD	-2.93	118.74	124.52
15	A	847	BCR	C38-C26-C25	-2.93	121.29	124.48
13	A	816	CLA	C3B-C4B-NB	-2.93	107.92	110.53
15	L	1005	BCR	C35-C13-C12	2.93	122.56	118.09
15	J	1105	BCR	C10-C11-C12	-2.92	114.73	123.20
15	A	851	BCR	C15-C16-C17	-2.92	117.54	123.52
13	A	806	CLA	C3B-C4B-NB	-2.92	107.92	110.53
15	B	845	BCR	C38-C26-C27	2.92	119.82	113.60
13	A	807	CLA	CGD-CBD-CAD	-2.92	101.39	110.85
13	A	812	CLA	C3B-C4B-NB	-2.92	107.92	110.53
13	A	843	CLA	C3B-C4B-NB	-2.92	107.92	110.53
13	A	827	CLA	C4-C3-C5	2.92	120.29	115.23
15	A	851	BCR	C8-C7-C6	-2.92	119.21	127.00
13	A	829	CLA	C4-C3-C5	2.91	120.28	115.23
13	A	819	CLA	C1-O2A-CGA	2.91	123.70	116.65
13	B	804	CLA	O1D-CGD-CBD	-2.91	118.78	124.52
15	I	102	BCR	C33-C5-C4	2.91	119.80	113.60
13	B	813	CLA	C4D-C3D-CAD	-2.91	104.95	108.11
13	I	101	CLA	C1-O2A-CGA	2.91	123.69	116.65
13	A	835	CLA	C4-C3-C5	2.90	120.27	115.23
13	A	805	CLA	O1D-CGD-CBD	-2.90	118.80	124.52
13	B	830	CLA	C3B-C4B-NB	-2.90	107.94	110.53
15	B	841	BCR	C8-C7-C6	-2.90	119.25	127.00
13	A	805	CLA	O2A-CGA-CBA	2.90	120.67	111.83
15	I	102	BCR	C20-C21-C22	-2.90	123.21	127.28
13	A	830	CLA	C1-O2A-CGA	2.90	123.67	116.65
13	B	806	CLA	C4-C3-C5	2.90	120.26	115.23
15	A	851	BCR	C10-C11-C12	-2.90	114.80	123.20
15	B	842	BCR	C7-C8-C9	-2.90	121.95	126.23
13	A	838	CLA	C4-C3-C5	2.89	120.25	115.23
13	A	841	CLA	O2A-CGA-CBA	2.89	120.66	111.83
15	J	1105	BCR	C11-C10-C9	-2.89	123.22	127.28
13	B	839	CLA	O1D-CGD-CBD	-2.89	118.81	124.52
15	B	846	BCR	C38-C26-C27	2.89	119.76	113.60
13	B	828	CLA	O1D-CGD-CBD	-2.89	118.82	124.52
13	A	837	CLA	C3B-C4B-NB	-2.89	107.95	110.53
13	A	810	CLA	C4D-C3D-CAD	-2.89	104.97	108.11
15	B	843	BCR	C8-C7-C6	-2.89	119.29	127.00
13	A	845	CLA	O2D-CGD-O1D	-2.88	118.23	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	1005	BCR	C8-C7-C6	-2.88	119.29	127.00
13	B	807	CLA	C2D-C1D-ND	2.87	112.97	110.13
13	B	807	CLA	C3B-C4B-NB	-2.87	107.97	110.53
15	B	841	BCR	C38-C26-C27	2.87	119.71	113.60
13	A	806	CLA	C4-C3-C5	2.86	120.20	115.23
13	B	824	CLA	O2A-CGA-CBA	2.86	120.57	111.83
13	M	1202	CLA	C3B-C4B-NB	-2.86	107.97	110.53
15	A	848	BCR	C10-C11-C12	-2.86	114.91	123.20
13	A	813	CLA	C4-C3-C5	2.86	120.19	115.23
13	B	808	CLA	C3B-C4B-NB	-2.86	107.98	110.53
13	A	839	CLA	O2A-CGA-CBA	2.86	120.55	111.83
13	J	1101	CLA	O1D-CGD-CBD	-2.86	118.89	124.52
13	A	821	CLA	O2A-CGA-CBA	2.85	120.54	111.83
13	B	830	CLA	C4-C3-C5	2.85	120.18	115.23
13	B	811	CLA	C3B-C4B-NB	-2.85	107.98	110.53
15	B	842	BCR	C38-C26-C27	2.85	119.67	113.60
13	A	831	CLA	C4D-C3D-CAD	-2.85	105.01	108.11
13	B	830	CLA	C1-C2-C3	-2.85	121.53	126.20
15	I	102	BCR	C11-C10-C9	-2.85	123.28	127.28
13	B	834	CLA	C3B-C4B-NB	-2.85	107.99	110.53
15	A	849	BCR	C15-C16-C17	-2.85	117.70	123.52
13	B	825	CLA	C3B-C4B-NB	-2.85	107.99	110.53
13	A	840	CLA	C1-O2A-CGA	2.84	123.52	116.65
13	A	834	CLA	O2A-CGA-CBA	2.84	120.49	111.83
13	B	827	CLA	C2D-C1D-ND	2.84	112.93	110.13
13	B	807	CLA	C4-C3-C5	2.84	120.15	115.23
13	B	802	CLA	C4-C3-C5	2.84	120.15	115.23
13	B	815	CLA	C4-C3-C5	2.83	120.15	115.23
13	A	818	CLA	C3B-C4B-NB	-2.83	108.00	110.53
16	A	853	LHG	O8-C23-C24	2.83	120.46	111.83
13	B	834	CLA	C4D-C3D-CAD	-2.83	105.03	108.11
15	A	847	BCR	C38-C26-C27	2.83	119.62	113.60
13	B	801	CLA	C4-C3-C5	2.83	120.13	115.23
13	A	808	CLA	O1D-CGD-CBD	-2.82	118.96	124.52
13	B	822	CLA	C4-C3-C5	2.82	120.12	115.23
13	L	1002	CLA	C4-C3-C5	2.82	120.12	115.23
13	A	812	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
13	B	832	CLA	C3B-C4B-NB	-2.81	108.02	110.53
15	L	1005	BCR	C10-C11-C12	-2.81	115.07	123.20
13	L	1004	CLA	O1D-CGD-CBD	-2.81	118.98	124.52
13	J	1101	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
13	A	833	CLA	C4D-C3D-CAD	-2.80	105.06	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	807	CLA	C3B-C4B-NB	-2.80	108.03	110.53
15	I	102	BCR	C15-C16-C17	-2.80	117.78	123.52
13	A	827	CLA	C4D-C3D-CAD	-2.80	105.06	108.11
13	A	801	CLA	C4-C3-C5	2.80	120.09	115.23
15	B	845	BCR	C29-C28-C27	2.80	117.43	111.28
13	B	812	CLA	C1-O2A-CGA	2.80	123.42	116.65
13	A	802	CLA	C4-C3-C5	2.79	120.08	115.23
13	A	830	CLA	O1D-CGD-CBD	-2.79	119.01	124.52
15	B	849	BCR	C8-C7-C6	-2.79	119.55	127.00
13	A	844	CLA	CAD-CBD-CHA	-2.79	102.11	105.12
13	B	805	CLA	C4-C3-C5	2.79	120.07	115.23
13	B	803	CLA	O2A-CGA-CBA	2.79	120.34	111.83
13	B	816	CLA	O1D-CGD-CBD	-2.79	119.02	124.52
13	A	828	CLA	C1-O2A-CGA	2.78	123.39	116.65
13	J	1102	CLA	C3B-C4B-NB	-2.78	108.05	110.53
13	A	833	CLA	C4-C3-C5	2.78	120.06	115.23
15	M	1203	BCR	C15-C16-C17	-2.78	117.83	123.52
13	B	803	CLA	C1-C2-C3	-2.78	121.64	126.20
13	A	816	CLA	C4D-C3D-CAD	-2.78	105.09	108.11
15	B	845	BCR	C7-C8-C9	-2.78	122.13	126.23
13	M	1201	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
13	J	1102	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
13	A	809	CLA	C3B-C4B-NB	-2.77	108.06	110.53
13	A	809	CLA	C2D-C1D-ND	2.77	112.87	110.13
13	A	818	CLA	CAA-CBA-CGA	-2.77	105.34	113.21
13	L	1003	CLA	CAA-C2A-C3A	-2.77	105.52	113.00
13	A	836	CLA	C3B-C4B-NB	-2.76	108.06	110.53
13	M	1201	CLA	C4-C3-C5	2.76	120.02	115.23
13	L	1004	CLA	C1-C2-C3	-2.76	121.67	126.20
13	A	807	CLA	C2D-C1D-ND	2.76	112.86	110.13
13	A	827	CLA	C1-C2-C3	-2.76	121.67	126.20
13	J	1101	CLA	C4-C3-C5	2.76	120.02	115.23
15	L	1006	BCR	C15-C14-C13	-2.76	123.41	127.28
15	A	849	BCR	C24-C23-C22	-2.76	122.15	126.23
15	B	846	BCR	C16-C15-C14	-2.76	117.88	123.52
13	A	830	CLA	C2D-C1D-ND	2.75	112.85	110.13
13	A	845	CLA	C4-C3-C5	2.75	120.01	115.23
15	A	851	BCR	C11-C10-C9	-2.75	123.42	127.28
13	A	817	CLA	C1-O2A-CGA	2.75	123.30	116.65
15	A	847	BCR	C8-C7-C6	-2.75	119.66	127.00
13	B	801	CLA	O2A-CGA-CBA	2.75	120.21	111.83
13	B	823	CLA	O1D-CGD-CBD	-2.75	119.10	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	811	CLA	C4D-C3D-CAD	-2.75	105.12	108.11
13	B	821	CLA	O2D-CGD-CBD	2.74	116.03	111.23
13	A	841	CLA	C3B-C4B-NB	-2.74	108.08	110.53
15	B	841	BCR	C27-C26-C25	-2.74	119.00	122.70
13	L	1003	CLA	C4-C3-C5	2.74	119.98	115.23
13	F	1301	CLA	C3B-C4B-NB	-2.74	108.09	110.53
13	A	829	CLA	C4D-C3D-CAD	-2.73	105.14	108.11
13	A	811	CLA	O2A-CGA-CBA	2.73	120.16	111.83
13	A	855	CLA	C4D-C3D-CAD	-2.73	105.14	108.11
15	A	849	BCR	C16-C15-C14	-2.73	117.94	123.52
15	A	852	BCR	C10-C11-C12	-2.73	115.30	123.20
15	M	1203	BCR	C23-C24-C25	-2.73	119.71	127.00
13	B	828	CLA	C3B-C4B-NB	-2.73	108.10	110.53
13	M	1201	CLA	C3B-C4B-NB	-2.73	108.10	110.53
13	B	824	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
13	A	820	CLA	C4-C3-C5	2.72	119.96	115.23
13	A	817	CLA	C4-C3-C5	2.72	119.95	115.23
13	A	802	CLA	O2A-CGA-CBA	2.72	120.14	111.83
13	A	824	CLA	C3B-C4B-NB	-2.72	108.10	110.53
13	A	813	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	A	802	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	A	805	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	A	814	CLA	CAA-CBA-CGA	-2.72	105.24	112.49
13	X	102	CLA	C4D-C3D-CAD	-2.72	105.15	108.11
13	A	823	CLA	C3B-C4B-NB	-2.72	108.11	110.53
15	A	848	BCR	C8-C7-C6	-2.71	119.75	127.00
13	A	837	CLA	C4D-C3D-CAD	-2.71	105.16	108.11
13	A	826	CLA	O2A-CGA-CBA	2.71	120.10	111.83
15	M	1203	BCR	C12-C13-C14	-2.71	114.75	119.01
13	B	816	CLA	C3B-C4B-NB	-2.71	108.11	110.53
13	A	840	CLA	C2D-C1D-ND	2.71	112.81	110.13
14	B	840	PQN	C2M-C2-C3	-2.71	120.00	124.45
15	J	1104	BCR	C11-C10-C9	-2.70	123.48	127.28
13	M	1201	CLA	C1-C2-C3	-2.70	121.77	126.20
15	B	845	BCR	C16-C17-C18	-2.70	123.49	127.28
13	A	836	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
13	B	831	CLA	O2A-CGA-CBA	2.70	120.08	111.83
13	B	838	CLA	C4D-C3D-CAD	-2.70	105.17	108.11
13	B	836	CLA	C4-C3-C5	2.70	119.91	115.23
13	A	830	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	B	847	BCR	C23-C24-C25	-2.70	119.80	127.00
13	B	835	CLA	C3B-C4B-NB	-2.70	108.12	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	819	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
13	A	813	CLA	C4D-C3D-CAD	-2.69	105.18	108.11
13	B	820	CLA	C1-O2A-CGA	2.69	123.16	116.65
13	A	828	CLA	C4D-C3D-CAD	-2.69	105.19	108.11
13	A	827	CLA	C3B-C4B-NB	-2.68	108.13	110.53
15	M	1203	BCR	C2-C3-C4	2.68	117.17	111.28
15	B	843	BCR	C2-C3-C4	2.68	117.17	111.28
13	B	805	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	J	1104	BCR	C15-C16-C17	-2.68	118.04	123.52
15	A	847	BCR	C27-C26-C25	-2.68	119.09	122.70
13	B	806	CLA	C3B-C4B-NB	-2.68	108.14	110.53
13	B	811	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
13	A	809	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
15	J	1104	BCR	C23-C24-C25	-2.67	119.86	127.00
13	A	804	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
13	A	822	CLA	O2A-CGA-CBA	2.67	119.97	111.83
13	B	814	CLA	C2D-C1D-ND	2.67	112.77	110.13
15	J	1104	BCR	C29-C28-C27	2.67	117.14	111.28
13	A	827	CLA	O1D-CGD-CBD	-2.66	119.27	124.52
13	A	833	CLA	O2A-CGA-CBA	2.66	119.94	111.83
15	A	852	BCR	C23-C24-C25	-2.65	119.91	127.00
13	B	838	CLA	O1D-CGD-CBD	-2.65	119.29	124.52
13	B	801	CLA	C3B-C4B-NB	-2.65	108.16	110.53
13	B	820	CLA	CAA-C2A-C3A	2.65	120.16	113.00
15	B	843	BCR	C39-C30-C25	-2.65	106.09	110.24
13	A	839	CLA	C3B-C4B-NB	-2.65	108.16	110.53
13	A	845	CLA	C3B-C4B-NB	-2.65	108.16	110.53
15	B	845	BCR	C23-C24-C25	-2.65	119.92	127.00
15	B	843	BCR	C21-C20-C19	-2.65	115.53	123.20
13	B	827	CLA	C1-O2A-CGA	2.65	123.06	116.65
15	A	849	BCR	C11-C10-C9	-2.65	123.57	127.28
15	B	842	BCR	C33-C5-C4	2.64	119.23	113.60
15	A	851	BCR	C23-C24-C25	-2.64	119.94	127.00
15	A	848	BCR	C23-C24-C25	-2.64	119.94	127.00
13	B	806	CLA	O1D-CGD-CBD	-2.64	119.31	124.52
15	A	852	BCR	C11-C10-C9	-2.64	123.58	127.28
15	A	848	BCR	C15-C14-C13	-2.64	123.58	127.28
13	B	828	CLA	C4D-C3D-CAD	-2.64	105.24	108.11
13	A	837	CLA	C2D-C1D-ND	2.64	112.74	110.13
13	A	843	CLA	C4D-C3D-CAD	-2.64	105.24	108.11
13	A	819	CLA	C3B-C4B-NB	-2.64	108.18	110.53
13	A	831	CLA	O2A-CGA-CBA	2.64	119.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	849	BCR	C29-C30-C25	2.64	114.27	110.44
13	B	828	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
13	I	101	CLA	C2D-C1D-ND	2.63	112.73	110.13
15	B	850	BCR	C10-C11-C12	-2.63	115.57	123.20
13	A	822	CLA	C3B-C4B-NB	-2.63	108.18	110.53
15	M	1203	BCR	C27-C26-C25	-2.63	119.15	122.70
13	A	826	CLA	C4-C3-C5	2.62	119.78	115.23
13	B	837	CLA	C3B-C4B-NB	-2.62	108.19	110.53
13	M	1201	CLA	C2D-C1D-ND	2.62	112.72	110.13
13	B	824	CLA	C4D-C3D-CAD	-2.62	105.26	108.11
13	B	814	CLA	C7-C6-C5	-2.62	106.28	113.26
13	A	807	CLA	C4D-C3D-CAD	-2.62	105.26	108.11
13	A	841	CLA	C1-C2-C3	-2.62	121.91	126.20
13	A	804	CLA	C1-O2A-CGA	2.62	122.98	116.65
13	A	837	CLA	CAA-C2A-C3A	-2.61	105.93	113.00
13	A	845	CLA	C4D-C3D-CAD	-2.61	105.27	108.11
13	A	804	CLA	C3B-C4B-NB	-2.61	108.20	110.53
13	A	832	CLA	O2A-C1-C2	2.61	118.15	108.11
15	B	846	BCR	C27-C26-C25	-2.61	119.18	122.70
13	F	1301	CLA	C2A-C1A-CHA	2.61	128.39	123.87
15	B	850	BCR	C35-C13-C12	2.61	122.07	118.09
13	A	829	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
13	B	816	CLA	C7-C6-C5	-2.60	106.34	113.26
15	B	843	BCR	C33-C5-C4	2.60	119.13	113.60
13	B	830	CLA	CAA-CBA-CGA	-2.60	105.84	113.21
15	A	849	BCR	C12-C13-C14	-2.59	114.93	119.01
13	A	811	CLA	C4D-C3D-CAD	-2.59	105.29	108.11
13	B	816	CLA	C4D-C3D-CAD	-2.59	105.29	108.11
13	A	803	CLA	O2A-CGA-CBA	2.59	119.74	111.83
15	A	850	BCR	C4-C5-C6	-2.59	119.20	122.70
13	A	819	CLA	C5-C3-C2	-2.59	115.35	121.17
13	B	826	CLA	C3B-C4B-NB	-2.59	108.22	110.53
13	A	827	CLA	C2D-C1D-ND	2.58	112.68	110.13
13	B	818	CLA	C4D-C3D-CAD	-2.58	105.30	108.11
13	A	842	CLA	C1-O2A-CGA	2.58	122.89	116.65
13	A	825	CLA	C1-O2A-CGA	2.58	122.89	116.65
13	J	1103	CLA	C3B-C4B-NB	-2.57	108.23	110.53
15	B	849	BCR	C24-C23-C22	-2.57	122.43	126.23
13	A	826	CLA	C1-C2-C3	-2.57	121.98	126.20
13	B	835	CLA	C4-C3-C5	2.57	119.69	115.23
13	A	811	CLA	C3B-C4B-NB	-2.57	108.24	110.53
13	A	814	CLA	O1D-CGD-CBD	-2.57	119.45	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	834	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
13	A	831	CLA	C3B-C4B-NB	-2.56	108.24	110.53
13	B	839	CLA	C4D-C3D-CAD	-2.56	105.33	108.11
15	B	847	BCR	C31-C1-C6	-2.56	106.23	110.24
15	J	1105	BCR	C23-C24-C25	-2.56	120.17	127.00
13	B	831	CLA	C4-C3-C5	2.56	119.67	115.23
13	B	807	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
13	B	822	CLA	C4D-C3D-CAD	-2.56	105.33	108.11
13	M	1201	CLA	O2A-CGA-CBA	2.55	119.62	111.83
15	A	848	BCR	C11-C10-C9	-2.55	123.70	127.28
15	A	852	BCR	C24-C23-C22	-2.55	122.46	126.23
15	B	841	BCR	C12-C13-C14	-2.55	115.00	119.01
13	M	1202	CLA	C4D-C3D-CAD	-2.54	105.34	108.11
15	J	1104	BCR	C24-C23-C22	-2.54	122.47	126.23
13	B	812	CLA	CMD-C2D-C1D	2.54	129.20	124.73
13	A	838	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
13	A	838	CLA	C11-C10-C8	-2.54	107.52	115.97
13	A	809	CLA	C3A-C2A-C1A	2.54	105.14	101.34
13	A	836	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
13	A	842	CLA	C1-C2-C3	-2.54	122.04	126.20
13	B	835	CLA	O1D-CGD-CBD	-2.54	119.52	124.52
15	A	850	BCR	C16-C15-C14	-2.53	118.33	123.52
15	B	844	BCR	C16-C17-C18	-2.53	123.72	127.28
13	A	820	CLA	C3B-C4B-NB	-2.53	108.27	110.53
13	B	822	CLA	C3B-C4B-NB	-2.53	108.27	110.53
13	A	840	CLA	CAA-CBA-CGA	-2.53	106.02	113.21
13	M	1201	CLA	CMD-C2D-C1D	2.53	129.18	124.73
13	B	829	CLA	C3B-C4B-NB	-2.53	108.28	110.53
13	B	810	CLA	C3B-C4B-NB	-2.52	108.28	110.53
13	A	817	CLA	C3B-C4B-NB	-2.52	108.28	110.53
13	A	805	CLA	C2D-C1D-ND	2.52	112.62	110.13
13	B	817	CLA	O2A-CGA-CBA	2.52	119.52	111.83
15	B	842	BCR	C2-C3-C4	2.52	116.81	111.28
15	A	848	BCR	C12-C13-C14	-2.51	115.05	119.01
13	A	812	CLA	C1-O2A-CGA	2.51	122.74	116.65
13	A	810	CLA	C2D-C1D-ND	2.51	112.61	110.13
15	L	1006	BCR	C16-C15-C14	-2.51	118.39	123.52
13	A	840	CLA	C1-C2-C3	-2.51	122.09	126.20
13	A	843	CLA	CAA-CBA-CGA	-2.51	106.09	113.21
13	I	101	CLA	C3B-C4B-NB	-2.51	108.29	110.53
13	B	822	CLA	O2A-CGA-CBA	2.51	119.47	111.83
13	B	832	CLA	C4D-C3D-CAD	-2.50	105.39	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	823	CLA	CAA-C2A-C1A	2.50	120.17	111.97
13	B	823	CLA	O2A-CGA-CBA	2.50	121.59	112.14
13	A	840	CLA	C3B-C4B-NB	-2.50	108.30	110.53
13	A	819	CLA	O2A-CGA-CBA	2.50	119.46	111.83
15	A	848	BCR	C16-C15-C14	-2.50	118.40	123.52
13	B	837	CLA	O2A-CGA-CBA	2.50	119.45	111.83
13	A	817	CLA	C4D-C3D-CAD	-2.50	105.39	108.11
15	B	844	BCR	C21-C20-C19	-2.50	115.97	123.20
13	B	831	CLA	C2D-C1D-ND	2.49	112.59	110.13
13	A	820	CLA	C4D-C3D-CAD	-2.49	105.40	108.11
15	A	852	BCR	C1-C6-C7	2.49	122.41	115.65
13	A	838	CLA	OBD-CAD-C3D	-2.49	122.59	128.42
13	A	837	CLA	CAA-C2A-C1A	2.49	120.14	111.97
13	A	822	CLA	C4D-C3D-CAD	-2.49	105.40	108.11
13	A	855	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
15	I	102	BCR	C2-C3-C4	2.49	116.75	111.28
13	B	814	CLA	CAA-CBA-CGA	-2.49	106.14	113.21
13	B	805	CLA	O2A-CGA-CBA	2.49	119.42	111.83
13	A	825	CLA	C4-C3-C5	2.48	119.53	115.23
13	A	801	CLA	C3B-C4B-NB	-2.48	108.32	110.53
13	B	817	CLA	C3B-C4B-NB	-2.48	108.32	110.53
13	B	801	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
13	A	822	CLA	C2D-C1D-ND	2.48	112.58	110.13
13	B	839	CLA	CAA-CBA-CGA	-2.48	106.18	113.21
13	A	820	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
13	L	1002	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
15	M	1203	BCR	C7-C8-C9	-2.46	122.59	126.23
15	A	847	BCR	C15-C14-C13	-2.46	123.82	127.28
13	A	828	CLA	C2D-C1D-ND	2.46	112.56	110.13
13	B	839	CLA	C3B-C4B-NB	-2.46	108.33	110.53
13	B	836	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
13	A	835	CLA	O2A-CGA-CBA	2.46	119.34	111.83
13	J	1101	CLA	CBA-CAA-C2A	2.46	121.11	113.79
13	B	821	CLA	C3B-C4B-NB	-2.46	108.33	110.53
13	J	1101	CLA	CAA-CBA-CGA	2.46	120.19	113.21
13	A	828	CLA	C3B-C4B-NB	-2.46	108.34	110.53
13	A	808	CLA	C4-C3-C5	2.46	119.49	115.23
13	A	809	CLA	C4D-CHA-C1A	-2.45	118.32	121.24
15	B	849	BCR	C4-C5-C6	-2.45	119.39	122.70
13	M	1202	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
15	B	843	BCR	C16-C15-C14	-2.45	118.51	123.52
13	B	837	CLA	C4D-C3D-CAD	-2.45	105.45	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	816	CLA	O2A-CGA-CBA	2.45	119.30	111.83
13	A	807	CLA	CMD-C2D-C1D	2.45	129.03	124.73
15	B	841	BCR	C16-C15-C14	-2.44	118.52	123.52
13	B	809	CLA	CAA-CBA-CGA	-2.44	105.97	112.49
13	B	827	CLA	C2C-C1C-NC	-2.44	107.42	109.98
13	B	835	CLA	C1-C2-C3	-2.44	122.20	126.20
13	A	838	CLA	CAA-CBA-CGA	-2.44	106.28	113.21
13	A	839	CLA	CAA-CBA-CGA	-2.44	106.28	113.21
13	B	835	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
13	A	817	CLA	C2D-C1D-ND	2.44	112.54	110.13
13	B	809	CLA	C3B-C4B-NB	-2.44	108.35	110.53
13	A	821	CLA	C4-C3-C5	2.44	119.46	115.23
13	B	835	CLA	C2A-C1A-CHA	2.44	128.09	123.87
15	I	102	BCR	C16-C15-C14	-2.43	118.54	123.52
13	B	827	CLA	C4D-C3D-CAD	-2.43	105.47	108.11
13	B	819	CLA	C3B-C4B-NB	-2.43	108.36	110.53
13	B	817	CLA	C1-C2-C3	-2.43	122.22	126.20
13	A	831	CLA	C5-C3-C4	2.43	120.17	114.59
13	B	802	CLA	C2D-C1D-ND	2.42	112.53	110.13
15	B	850	BCR	C15-C16-C17	-2.42	118.56	123.52
15	B	845	BCR	C40-C30-C25	-2.42	106.44	110.24
15	A	848	BCR	C27-C26-C25	-2.42	119.43	122.70
13	B	821	CLA	C4D-C3D-CAD	-2.42	105.48	108.11
13	B	838	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
13	M	1201	CLA	CAA-CBA-CGA	-2.42	106.35	113.21
15	B	849	BCR	C21-C20-C19	-2.42	116.20	123.20
13	A	801	CLA	C2D-C1D-ND	2.41	112.52	110.13
13	A	801	CLA	O2A-CGA-CBA	2.41	119.19	111.83
13	B	814	CLA	C3B-C4B-NB	-2.41	108.38	110.53
13	A	811	CLA	C1-C2-C3	-2.41	122.25	126.20
13	A	825	CLA	O2A-CGA-CBA	2.41	119.18	111.83
13	A	819	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
13	A	826	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
15	A	852	BCR	C27-C26-C25	-2.41	119.45	122.70
15	B	843	BCR	C12-C13-C14	-2.41	115.22	119.01
15	B	846	BCR	C23-C24-C25	-2.40	120.58	127.00
13	A	839	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
13	B	820	CLA	CAA-CBA-CGA	-2.40	106.39	113.21
15	L	1006	BCR	C36-C18-C17	-2.40	118.93	122.82
13	B	809	CLA	C2D-C1D-ND	2.40	112.50	110.13
15	A	849	BCR	C21-C20-C19	-2.40	116.25	123.20
15	A	849	BCR	C27-C26-C25	-2.40	119.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	810	CLA	CED-O2D-CGD	2.39	121.35	115.92
15	J	1105	BCR	C15-C16-C17	-2.39	118.62	123.52
13	A	817	CLA	CED-O2D-CGD	2.39	121.34	115.92
14	B	840	PQN	C14-C13-C15	2.39	119.38	115.23
13	L	1004	CLA	C4D-C3D-CAD	-2.39	105.51	108.11
13	A	840	CLA	CMD-C2D-C1D	2.38	128.93	124.73
13	A	842	CLA	CED-O2D-CGD	2.38	121.32	115.92
13	B	823	CLA	CMD-C2D-C1D	2.38	128.91	124.73
15	J	1105	BCR	C27-C26-C25	-2.38	119.49	122.70
14	A	846	PQN	C11-C3-C2	-2.37	120.82	124.89
13	B	804	CLA	C2D-C1D-ND	2.37	112.47	110.13
13	A	823	CLA	CAA-CBA-CGA	-2.37	106.47	113.21
13	B	839	CLA	C1-O2A-CGA	2.37	122.39	116.65
13	B	806	CLA	C2D-C1D-ND	2.37	112.47	110.13
13	A	811	CLA	C2D-C1D-ND	2.37	112.47	110.13
15	F	1302	BCR	C21-C20-C19	-2.37	116.34	123.20
14	A	846	PQN	C2M-C2-C3	-2.37	120.56	124.45
15	B	843	BCR	C38-C26-C27	2.37	118.64	113.60
13	L	1003	CLA	C1-O2A-CGA	2.36	122.37	116.65
13	A	809	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
15	J	1104	BCR	C38-C26-C27	2.36	118.62	113.60
15	B	847	BCR	C21-C20-C19	-2.36	116.37	123.20
15	B	841	BCR	C4-C5-C6	-2.36	119.52	122.70
13	A	832	CLA	CMD-C2D-C1D	2.36	128.88	124.73
13	B	823	CLA	C4D-C3D-CAD	-2.35	105.55	108.11
13	A	831	CLA	C2D-C1D-ND	2.35	112.45	110.13
15	B	845	BCR	C4-C5-C6	-2.35	119.53	122.70
13	F	1301	CLA	OBD-CAD-C3D	-2.35	122.93	128.42
15	A	848	BCR	C4-C5-C6	-2.35	119.53	122.70
13	J	1101	CLA	C4D-C3D-CAD	-2.34	105.56	108.11
13	B	837	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
15	J	1104	BCR	C4-C5-C6	-2.34	119.54	122.70
13	A	818	CLA	O2A-C1-C2	-2.34	99.10	108.11
15	F	1302	BCR	C27-C26-C25	-2.34	119.54	122.70
13	A	840	CLA	C4-C3-C5	2.34	119.29	115.23
15	F	1302	BCR	C34-C9-C10	-2.34	119.03	122.82
13	B	801	CLA	C2D-C1D-ND	2.34	112.44	110.13
13	A	808	CLA	C2D-C1D-ND	2.34	112.44	110.13
13	B	832	CLA	C2D-C1D-ND	2.34	112.44	110.13
15	L	1005	BCR	C30-C25-C24	2.34	121.98	115.65
13	A	819	CLA	C2D-C1D-ND	2.34	112.44	110.13
15	B	841	BCR	C15-C16-C17	-2.33	118.75	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	843	CLA	C2D-C1D-ND	2.33	112.43	110.13
13	A	818	CLA	CAA-C2A-C3A	-2.33	106.71	113.00
15	B	841	BCR	C23-C24-C25	-2.33	120.78	127.00
13	A	803	CLA	C11-C12-C13	-2.33	108.23	115.97
13	A	835	CLA	O2D-CGD-O1D	-2.32	119.32	123.85
15	B	843	BCR	C34-C9-C10	-2.32	119.05	122.82
15	B	843	BCR	C35-C13-C12	2.32	121.64	118.09
13	B	827	CLA	C7-C6-C5	-2.32	107.08	113.26
13	A	825	CLA	C4D-C3D-CAD	-2.32	105.59	108.11
15	B	844	BCR	C35-C13-C12	2.32	119.92	114.59
15	B	846	BCR	C15-C16-C17	-2.32	118.78	123.52
13	F	1301	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
13	A	837	CLA	C1-C2-C3	-2.32	122.40	126.20
15	L	1005	BCR	C15-C14-C13	-2.32	124.03	127.28
13	B	803	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
13	A	810	CLA	C3B-C4B-NB	-2.31	108.46	110.53
13	B	839	CLA	O2A-CGA-CBA	2.31	118.89	111.83
13	A	845	CLA	C2D-C1D-ND	2.31	112.42	110.13
13	B	807	CLA	C11-C10-C8	-2.31	108.28	115.97
13	A	814	CLA	C2D-C1D-ND	2.31	112.41	110.13
13	A	819	CLA	C7-C6-C5	-2.31	107.11	113.26
15	B	846	BCR	C39-C30-C25	-2.31	106.62	110.24
13	B	831	CLA	C3B-C4B-NB	-2.31	108.47	110.53
13	A	831	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
13	A	804	CLA	C2D-C1D-ND	2.31	112.41	110.13
15	L	1006	BCR	C4-C5-C6	-2.31	119.59	122.70
13	A	816	CLA	CED-O2D-CGD	2.31	121.15	115.92
15	L	1005	BCR	C36-C18-C19	2.30	121.61	118.09
15	A	850	BCR	C10-C11-C12	-2.30	116.52	123.20
15	A	847	BCR	C12-C13-C14	-2.30	115.39	119.01
13	A	830	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
15	B	842	BCR	C16-C17-C18	-2.30	124.05	127.28
13	B	832	CLA	CAA-CBA-CGA	-2.30	106.35	112.49
15	A	850	BCR	C27-C26-C25	-2.30	119.59	122.70
15	J	1104	BCR	C39-C30-C25	-2.30	106.64	110.24
13	A	824	CLA	O2A-CGA-CBA	2.30	118.84	111.83
15	B	844	BCR	C27-C26-C25	-2.30	119.60	122.70
15	A	852	BCR	C8-C7-C6	-2.30	120.86	127.00
13	B	838	CLA	CBA-CAA-C2A	2.30	120.63	113.79
13	A	829	CLA	CMD-C2D-C1D	2.30	128.77	124.73
13	B	839	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
13	A	824	CLA	CGD-CBD-CAD	2.30	118.28	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1201	CLA	C4D-C3D-CAD	-2.30	105.61	108.11
13	B	824	CLA	C1-C2-C3	-2.30	122.44	126.20
15	B	846	BCR	C8-C9-C10	-2.30	115.40	119.01
13	F	1301	CLA	C2D-C1D-ND	2.30	112.40	110.13
13	B	804	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
13	B	821	CLA	CAA-C2A-C3A	-2.30	106.80	113.00
15	J	1105	BCR	C4-C5-C6	-2.29	119.60	122.70
13	A	842	CLA	C3B-C4B-NB	-2.29	108.48	110.53
15	B	843	BCR	C29-C28-C27	2.29	116.31	111.28
15	B	841	BCR	C21-C20-C19	-2.29	116.56	123.20
15	A	847	BCR	C4-C5-C6	-2.29	119.61	122.70
13	B	821	CLA	C2D-C1D-ND	2.29	112.39	110.13
15	B	843	BCR	C15-C16-C17	-2.28	118.84	123.52
13	A	833	CLA	CED-O2D-CGD	2.28	121.10	115.92
18	B	848	LMG	C7-O1-C1	2.28	118.69	113.80
13	B	807	CLA	C4D-CHA-C1A	-2.28	118.53	121.24
13	A	825	CLA	CAA-CBA-CGA	-2.28	106.74	113.21
13	A	803	CLA	C2D-C1D-ND	2.28	112.38	110.13
13	B	830	CLA	C2D-C1D-ND	2.28	112.38	110.13
13	B	810	CLA	C4D-C3D-CAD	-2.27	105.64	108.11
15	A	849	BCR	C35-C13-C12	2.27	121.56	118.09
13	L	1003	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
15	L	1006	BCR	C12-C13-C14	-2.27	115.44	119.01
15	B	850	BCR	C32-C1-C6	-2.27	106.69	110.24
13	B	826	CLA	C2D-C1D-ND	2.27	112.37	110.13
13	J	1103	CLA	CAD-CBD-CHA	-2.27	102.67	105.12
13	A	844	CLA	CHD-C1D-ND	-2.26	121.61	124.80
13	A	837	CLA	CMD-C2D-C1D	2.26	128.72	124.73
13	B	808	CLA	C7-C6-C5	-2.26	107.23	113.26
13	B	837	CLA	C2D-C1D-ND	2.26	112.37	110.13
15	B	850	BCR	C33-C5-C4	2.26	118.42	113.60
15	M	1203	BCR	C21-C20-C19	-2.26	116.64	123.20
15	L	1005	BCR	C27-C26-C25	-2.26	119.65	122.70
15	B	843	BCR	C11-C10-C9	-2.26	124.11	127.28
13	A	842	CLA	C4D-C3D-CAD	-2.26	105.65	108.11
15	A	847	BCR	C16-C15-C14	-2.26	118.89	123.52
15	B	850	BCR	C16-C15-C14	-2.26	118.89	123.52
15	L	1006	BCR	C37-C22-C21	-2.26	119.15	122.82
13	A	805	CLA	C3B-C4B-NB	-2.26	108.52	110.53
15	A	850	BCR	C35-C13-C12	2.26	121.53	118.09
13	B	815	CLA	C2D-C1D-ND	2.25	112.36	110.13
13	F	1301	CLA	CAA-C2A-C3A	-2.25	106.91	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	804	CLA	O2A-CGA-CBA	2.25	118.70	111.83
13	A	808	CLA	C4D-C3D-CAD	-2.25	105.66	108.11
13	A	809	CLA	CGD-CBD-CAD	-2.25	103.56	110.85
13	A	803	CLA	C4D-C3D-CAD	-2.25	105.67	108.11
15	B	842	BCR	C31-C1-C6	-2.25	106.72	110.24
13	A	807	CLA	C4D-CHA-C1A	-2.24	118.57	121.24
13	A	806	CLA	O2A-CGA-CBA	2.24	118.67	111.83
13	I	101	CLA	CMD-C2D-C1D	2.24	128.68	124.73
13	B	834	CLA	CMD-C2D-C1D	2.24	128.67	124.73
13	A	806	CLA	C4D-C3D-CAD	-2.24	105.68	108.11
13	M	1201	CLA	C1-O2A-CGA	2.24	122.07	116.65
13	B	835	CLA	C2D-C1D-ND	2.24	112.34	110.13
13	A	820	CLA	C1-O2A-CGA	2.24	122.06	116.65
15	A	847	BCR	C30-C25-C26	-2.23	119.58	122.64
13	B	803	CLA	C2D-C1D-ND	2.23	112.33	110.13
13	B	808	CLA	C2D-C1D-ND	2.23	112.33	110.13
15	B	849	BCR	C32-C1-C6	-2.23	106.75	110.24
15	B	849	BCR	C34-C9-C10	-2.23	119.21	122.82
13	A	812	CLA	CAA-CBA-CGA	-2.22	106.90	113.21
13	B	821	CLA	CMD-C2D-C1D	2.22	128.64	124.73
13	B	829	CLA	C4D-C3D-CAD	-2.22	105.70	108.11
13	B	815	CLA	C4D-C3D-CAD	-2.22	105.70	108.11
13	B	804	CLA	C3B-C4B-NB	-2.21	108.55	110.53
13	B	829	CLA	C2D-C1D-ND	2.21	112.32	110.13
13	A	829	CLA	C7-C6-C5	-2.21	107.36	113.26
13	A	813	CLA	C11-C10-C8	-2.21	108.61	115.97
13	J	1103	CLA	C2A-C3A-C4A	2.21	104.18	101.59
13	B	836	CLA	CMD-C2D-C1D	2.20	128.61	124.73
13	A	838	CLA	C2D-C1D-ND	2.20	112.30	110.13
15	L	1006	BCR	C33-C5-C4	2.20	118.28	113.60
15	M	1203	BCR	C16-C15-C14	-2.20	119.02	123.52
13	A	845	CLA	C3C-C4C-NC	-2.20	107.62	110.43
13	A	832	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
13	B	816	CLA	C1-O2A-CGA	2.19	121.96	116.65
14	A	846	PQN	C14-C13-C15	2.19	119.04	115.23
15	B	846	BCR	C4-C5-C6	-2.19	119.74	122.70
13	B	824	CLA	C1-O2A-CGA	2.19	121.96	116.65
13	I	101	CLA	C4D-C3D-CAD	-2.19	105.72	108.11
13	B	836	CLA	C4D-C3D-CAD	-2.19	105.73	108.11
13	A	820	CLA	C2D-C1D-ND	2.19	112.29	110.13
13	A	815	CLA	O2A-CGA-CBA	2.19	120.91	114.00
13	A	827	CLA	C2C-C1C-NC	-2.19	107.69	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	820	CLA	CED-O2D-CGD	2.18	120.87	115.92
13	A	806	CLA	C11-C10-C8	-2.18	108.71	115.97
13	A	843	CLA	C6-C7-C8	-2.18	108.72	115.97
13	B	806	CLA	C4D-C3D-CAD	-2.18	105.74	108.11
13	A	826	CLA	C11-C10-C8	-2.18	108.72	115.97
13	B	802	CLA	CMD-C2D-C1D	2.18	128.57	124.73
15	J	1104	BCR	C21-C20-C19	-2.18	116.89	123.20
13	A	812	CLA	C2D-C1D-ND	2.18	112.28	110.13
13	B	819	CLA	C2D-C1D-ND	2.18	112.28	110.13
13	A	833	CLA	C2D-C1D-ND	2.18	112.28	110.13
13	A	834	CLA	C2D-C1D-ND	2.18	112.28	110.13
13	B	838	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
13	M	1202	CLA	C2D-C1D-ND	2.18	112.28	110.13
15	F	1302	BCR	C8-C7-C6	-2.17	121.19	127.00
13	A	824	CLA	C11-C10-C8	-2.17	108.74	115.97
13	A	816	CLA	C2D-C1D-ND	2.17	112.28	110.13
13	B	816	CLA	CAA-C2A-C3A	-2.17	107.12	113.00
15	J	1104	BCR	C12-C13-C14	-2.17	115.59	119.01
13	B	807	CLA	C4D-C3D-CAD	-2.17	105.75	108.11
13	B	816	CLA	C2D-C1D-ND	2.17	112.28	110.13
13	B	812	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
13	B	815	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
13	A	804	CLA	OBD-CAD-C3D	-2.17	123.34	128.42
13	A	821	CLA	C16-C15-C13	-2.17	108.75	115.97
15	A	852	BCR	C20-C21-C22	-2.17	124.23	127.28
15	F	1302	BCR	C10-C11-C12	-2.17	116.91	123.20
13	A	841	CLA	CMD-C2D-C1D	2.17	128.55	124.73
13	A	815	CLA	CHD-C1D-ND	-2.17	121.75	124.80
13	B	814	CLA	C4-C3-C5	2.17	118.99	115.23
13	A	823	CLA	C2D-C1D-ND	2.17	112.27	110.13
15	B	843	BCR	C36-C18-C17	-2.17	119.31	122.82
13	B	829	CLA	CMD-C2D-C1D	2.16	128.54	124.73
13	M	1202	CLA	CMD-C2D-C1D	2.16	128.54	124.73
13	A	835	CLA	C1-O2A-CGA	2.16	121.89	116.65
15	L	1005	BCR	C4-C5-C6	-2.16	119.78	122.70
13	A	815	CLA	C4D-C3D-CAD	-2.16	105.76	108.11
13	B	802	CLA	CGD-CBD-CAD	-2.16	103.85	110.85
13	B	832	CLA	CMD-C2D-C1D	2.16	128.53	124.73
15	B	842	BCR	C21-C20-C19	-2.16	116.94	123.20
15	L	1006	BCR	C33-C5-C6	-2.16	122.13	124.48
13	A	814	CLA	CMD-C2D-C1D	2.16	128.53	124.73
13	A	839	CLA	C2D-C1D-ND	2.16	112.26	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	848	BCR	C21-C20-C19	-2.16	116.95	123.20
15	A	851	BCR	C36-C18-C17	-2.16	119.32	122.82
13	A	809	CLA	C4D-C3D-CAD	-2.16	105.77	108.11
15	A	847	BCR	C1-C6-C5	-2.15	119.69	122.64
13	A	833	CLA	C3B-C4B-NB	-2.15	108.61	110.53
15	J	1104	BCR	C1-C6-C5	-2.15	119.69	122.64
13	B	831	CLA	CED-O2D-CGD	-2.15	111.03	115.92
13	A	845	CLA	CMD-C2D-C1D	2.15	128.52	124.73
13	A	825	CLA	C2D-C1D-ND	2.15	112.26	110.13
13	A	827	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
13	L	1002	CLA	C2D-C1D-ND	2.15	112.25	110.13
13	B	825	CLA	C4D-C3D-CAD	-2.15	105.77	108.11
13	B	820	CLA	C2D-C1D-ND	2.15	112.25	110.13
13	B	823	CLA	CBA-CAA-C2A	-2.15	107.40	113.79
13	B	835	CLA	C1-O2A-CGA	2.15	121.85	116.65
13	I	101	CLA	O2A-CGA-CBA	2.15	118.39	111.83
13	A	811	CLA	CMD-C2D-C1D	2.15	128.51	124.73
15	J	1105	BCR	C21-C20-C19	-2.15	116.98	123.20
13	A	840	CLA	C4D-C3D-CAD	-2.14	105.78	108.11
15	B	842	BCR	C30-C25-C26	-2.14	119.71	122.64
15	F	1302	BCR	C16-C17-C18	-2.14	124.27	127.28
13	A	830	CLA	O2A-CGA-CBA	2.14	118.37	111.83
13	L	1002	CLA	O2A-CGA-CBA	2.14	118.37	111.83
15	B	847	BCR	C15-C14-C13	-2.14	124.28	127.28
13	A	824	CLA	CHD-C1D-ND	-2.14	121.79	124.80
15	F	1302	BCR	C1-C6-C5	-2.14	119.71	122.64
15	B	847	BCR	C27-C26-C25	-2.14	119.82	122.70
13	L	1002	CLA	CHD-C1D-ND	-2.14	121.80	124.80
13	A	823	CLA	CED-O2D-CGD	2.14	120.76	115.92
13	B	827	CLA	O2A-CGA-CBA	2.14	118.35	111.83
13	J	1101	CLA	C11-C10-C8	-2.14	108.86	115.97
13	A	801	CLA	C11-C10-C8	-2.14	108.87	115.97
15	A	850	BCR	C30-C25-C26	-2.13	119.72	122.64
13	A	843	CLA	C11-C10-C8	-2.13	108.88	115.97
13	A	838	CLA	CMD-C2D-C1D	2.13	128.48	124.73
13	I	101	CLA	C11-C10-C8	-2.13	108.88	115.97
15	A	850	BCR	C31-C1-C6	-2.13	106.90	110.24
13	A	826	CLA	C1-O2A-CGA	2.13	121.80	116.65
13	A	826	CLA	C2D-C1D-ND	2.12	112.23	110.13
15	A	847	BCR	C21-C20-C19	-2.12	117.05	123.20
13	J	1102	CLA	C2D-C1D-ND	2.12	112.23	110.13
13	A	818	CLA	C2D-C1D-ND	2.12	112.23	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	842	CLA	C2D-C1D-ND	2.12	112.23	110.13
13	A	845	CLA	CHD-C1D-ND	-2.12	121.82	124.80
13	A	805	CLA	C4-C3-C5	2.12	118.91	115.23
15	L	1006	BCR	C23-C24-C25	-2.12	121.34	127.00
13	A	832	CLA	CHD-C1D-ND	-2.12	121.82	124.80
15	B	850	BCR	C2-C3-C4	2.12	115.93	111.28
13	A	844	CLA	O2A-CGA-CBA	2.12	120.69	114.00
13	B	832	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
13	B	829	CLA	C1-O2A-CGA	2.12	121.77	116.65
13	B	815	CLA	C11-C10-C8	-2.11	108.94	115.97
13	A	814	CLA	C4D-C3D-CAD	-2.11	105.81	108.11
13	A	809	CLA	C11-C10-C8	-2.11	108.94	115.97
15	I	102	BCR	C31-C1-C6	-2.11	106.93	110.24
13	A	819	CLA	C16-C15-C13	-2.11	108.94	115.97
13	A	844	CLA	OBD-CAD-C3D	-2.11	125.16	128.60
13	B	838	CLA	C2D-C1D-ND	2.11	112.22	110.13
15	B	845	BCR	C21-C20-C19	-2.11	117.09	123.20
15	A	849	BCR	C20-C19-C18	-2.11	120.58	126.36
13	B	839	CLA	C2D-C1D-ND	2.11	112.21	110.13
13	A	804	CLA	CMD-C2D-C1D	2.11	128.44	124.73
13	A	803	CLA	C7-C6-C5	-2.11	107.65	113.26
13	A	855	CLA	O2A-CGA-CBA	2.10	120.64	114.00
15	I	102	BCR	C27-C26-C25	-2.10	119.86	122.70
13	A	809	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
13	A	826	CLA	CMD-C2D-C1D	2.10	128.43	124.73
15	A	847	BCR	C15-C16-C17	-2.10	119.22	123.52
13	A	813	CLA	C2D-C1D-ND	2.10	112.20	110.13
13	L	1003	CLA	C2D-C1D-ND	2.10	112.20	110.13
15	B	850	BCR	C1-C6-C5	-2.10	119.77	122.64
13	A	825	CLA	CMD-C2D-C1D	2.10	128.43	124.73
15	J	1105	BCR	C39-C30-C25	-2.10	106.95	110.24
13	A	823	CLA	O2A-CGA-CBA	2.10	118.23	111.83
13	B	825	CLA	CMD-C2D-C1D	2.10	128.42	124.73
13	A	812	CLA	C4D-C3D-CAD	-2.10	105.83	108.11
15	J	1105	BCR	C16-C15-C14	-2.09	119.23	123.52
15	A	851	BCR	C27-C26-C25	-2.09	119.87	122.70
15	L	1006	BCR	C1-C6-C5	-2.09	119.77	122.64
13	B	835	CLA	CMD-C2D-C1D	2.09	128.41	124.73
13	X	102	CLA	O2A-CGA-CBA	2.09	120.61	114.00
15	A	852	BCR	C30-C25-C26	-2.09	119.78	122.64
13	A	837	CLA	C1-O2A-CGA	2.09	121.71	116.65
15	L	1006	BCR	C27-C26-C25	-2.09	119.88	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	805	CLA	C11-C10-C8	-2.09	109.03	115.97
13	A	821	CLA	CMD-C2D-C1D	2.09	128.40	124.73
15	B	845	BCR	C11-C10-C9	-2.09	124.35	127.28
15	B	841	BCR	C1-C6-C5	-2.09	119.79	122.64
15	L	1005	BCR	C12-C13-C14	-2.09	115.73	119.01
15	A	851	BCR	C21-C20-C19	-2.08	117.16	123.20
13	A	832	CLA	C2D-C1D-ND	2.08	112.19	110.13
13	A	841	CLA	CED-O2D-CGD	2.08	120.64	115.92
13	A	844	CLA	CMD-C2D-C1D	2.08	128.40	124.73
13	B	801	CLA	C11-C10-C8	-2.08	109.04	115.97
13	A	817	CLA	CMD-C2D-C1D	2.08	128.40	124.73
13	B	805	CLA	CMD-C2D-C1D	2.08	128.40	124.73
13	B	821	CLA	CHD-C1D-ND	-2.08	121.87	124.80
13	B	813	CLA	C2D-C1D-ND	2.08	112.19	110.13
13	B	836	CLA	C11-C10-C8	-2.08	109.05	115.97
13	A	840	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
13	A	810	CLA	CMD-C2D-C1D	2.08	128.39	124.73
13	B	806	CLA	CMD-C2D-C1D	2.08	128.39	124.73
15	F	1302	BCR	C1-C6-C7	2.08	121.29	115.65
13	B	805	CLA	CHD-C1D-ND	-2.08	121.88	124.80
13	A	812	CLA	CMD-C2D-C1D	2.08	128.38	124.73
13	B	834	CLA	C2D-C1D-ND	2.08	112.18	110.13
15	B	850	BCR	C40-C30-C25	-2.07	106.99	110.24
13	A	844	CLA	C3C-C4C-NC	-2.07	107.78	110.43
15	B	844	BCR	C20-C21-C22	-2.07	124.37	127.28
13	A	806	CLA	C11-C12-C13	-2.07	109.09	115.97
13	M	1202	CLA	O2A-CGA-CBA	2.07	120.54	114.00
13	B	804	CLA	CMD-C2D-C1D	2.07	128.37	124.73
13	A	829	CLA	CHD-C1D-ND	-2.07	121.89	124.80
13	A	830	CLA	CMD-C2D-C1D	2.07	128.37	124.73
13	A	822	CLA	C2A-C1A-CHA	2.07	127.46	123.87
13	A	826	CLA	C2A-C1A-CHA	2.07	127.45	123.87
15	I	102	BCR	C19-C18-C17	-2.07	115.76	119.01
13	B	817	CLA	C2D-C1D-ND	2.07	112.17	110.13
13	A	805	CLA	O2A-C1-C2	2.06	116.05	108.11
13	B	811	CLA	C2A-C1A-CHA	2.06	127.45	123.87
13	B	835	CLA	CAA-C2A-C1A	2.06	118.74	111.97
13	A	816	CLA	CHD-C1D-ND	-2.06	121.90	124.80
13	B	824	CLA	C2D-C1D-ND	2.06	112.17	110.13
13	A	824	CLA	C3C-C4C-NC	-2.06	107.79	110.43
13	A	843	CLA	C11-C12-C13	-2.06	109.11	115.97
15	A	848	BCR	C36-C18-C17	-2.06	119.48	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	102	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
15	L	1005	BCR	C1-C6-C5	-2.06	119.82	122.64
13	A	828	CLA	C11-C10-C8	-2.06	109.12	115.97
13	A	828	CLA	CMD-C2D-C1D	2.06	128.35	124.73
13	L	1003	CLA	CHD-C1D-ND	-2.06	121.91	124.80
15	B	845	BCR	C19-C18-C17	-2.06	115.77	119.01
13	B	828	CLA	C2D-C1D-ND	2.06	112.16	110.13
13	X	102	CLA	C2D-C1D-ND	2.05	112.16	110.13
13	A	822	CLA	CHD-C1D-ND	-2.05	121.92	124.80
13	B	805	CLA	C4D-C3D-CAD	-2.05	105.88	108.11
13	I	101	CLA	C11-C12-C13	-2.05	109.15	115.97
13	B	815	CLA	C1-C2-C3	-2.05	122.84	126.20
13	A	820	CLA	O2A-CGA-CBA	2.05	118.08	111.83
13	A	815	CLA	CMD-C2D-C1D	2.05	128.33	124.73
13	B	816	CLA	O2D-CGD-O1D	-2.05	119.87	123.85
13	A	821	CLA	C2D-C1D-ND	2.05	112.15	110.13
15	A	852	BCR	C1-C6-C5	-2.04	119.84	122.64
13	A	813	CLA	C6-C7-C8	-2.04	109.17	115.97
13	L	1003	CLA	C3C-C4C-NC	-2.04	107.81	110.43
13	B	831	CLA	CMD-C2D-C1D	2.04	128.32	124.73
15	B	841	BCR	C30-C25-C26	-2.04	119.84	122.64
13	B	829	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
13	B	810	CLA	C2D-C1D-ND	2.04	112.15	110.13
14	B	840	PQN	C2M-C2-C1	2.04	120.44	116.68
15	J	1105	BCR	C12-C13-C14	-2.04	115.80	119.01
13	A	830	CLA	C11-C10-C8	-2.04	109.19	115.97
13	A	820	CLA	C2A-C3A-C4A	2.04	105.16	101.87
15	L	1006	BCR	C30-C25-C26	-2.04	119.85	122.64
13	A	855	CLA	C2D-C1D-ND	2.04	112.14	110.13
13	A	834	CLA	C11-C10-C8	-2.04	109.19	115.97
15	B	842	BCR	C10-C11-C12	-2.04	117.30	123.20
13	A	806	CLA	O2D-CGD-O1D	-2.04	119.89	123.85
13	A	806	CLA	C1-O2A-CGA	2.04	121.58	116.65
13	A	803	CLA	O2D-CGD-O1D	-2.04	119.89	123.85
13	A	814	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
15	A	850	BCR	C37-C22-C21	-2.03	119.52	122.82
13	B	822	CLA	CMD-C2D-C1D	2.03	128.31	124.73
13	B	804	CLA	C4D-C3D-CAD	-2.03	105.90	108.11
13	A	826	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
13	A	815	CLA	C2D-C1D-ND	2.03	112.14	110.13
13	A	836	CLA	C2D-C1D-ND	2.03	112.13	110.13
13	B	813	CLA	CHD-C1D-ND	-2.03	121.95	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	826	CLA	O2A-CGA-CBA	2.03	118.01	111.83
13	A	815	CLA	O2D-CGD-O1D	-2.03	119.91	123.85
13	F	1301	CLA	CMD-C2D-C1D	2.02	128.29	124.73
13	J	1101	CLA	C2D-C1D-ND	2.02	112.13	110.13
13	A	855	CLA	CHD-C1D-ND	-2.02	121.95	124.80
13	B	825	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
13	F	1301	CLA	O2A-CGA-CBA	2.02	120.39	114.00
15	J	1104	BCR	C8-C7-C6	-2.02	121.59	127.00
13	B	823	CLA	C2A-C1A-CHA	2.02	127.38	123.87
13	A	820	CLA	C11-C10-C8	-2.02	109.24	115.97
13	J	1101	CLA	C11-C12-C13	-2.02	109.24	115.97
13	A	820	CLA	CMD-C2D-C1D	2.02	128.29	124.73
13	B	829	CLA	O2A-CGA-CBA	2.02	118.00	111.83
15	A	849	BCR	C37-C22-C21	-2.02	119.54	122.82
13	B	835	CLA	CED-O2D-CGD	-2.02	111.33	115.92
13	B	810	CLA	CMD-C2D-C1D	2.02	128.28	124.73
13	B	802	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
13	I	101	CLA	C7-C6-C5	-2.02	107.89	113.26
13	B	829	CLA	CED-O2D-CGD	2.02	120.49	115.92
13	B	816	CLA	CMD-C2D-C1D	2.02	128.28	124.73
13	B	836	CLA	C2D-C1D-ND	2.02	112.12	110.13
13	A	801	CLA	CMD-C2D-C1D	2.01	128.28	124.73
13	A	803	CLA	CMD-C2D-C1D	2.01	128.28	124.73
13	A	815	CLA	C2C-C1C-NC	-2.01	107.87	109.98
13	B	826	CLA	C6-C7-C8	-2.01	109.27	115.97
13	B	823	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
13	A	808	CLA	CED-O2D-CGD	-2.01	111.35	115.92
15	L	1006	BCR	C7-C8-C9	-2.01	123.26	126.23
13	B	809	CLA	CMD-C2D-C1D	2.01	128.27	124.73
13	L	1004	CLA	C7-C6-C5	-2.01	107.91	113.26
13	B	814	CLA	CMD-C2D-C1D	2.01	128.27	124.73
13	B	802	CLA	C11-C10-C8	-2.01	109.29	115.97
15	B	849	BCR	C27-C26-C25	-2.01	119.99	122.70
15	L	1005	BCR	C30-C25-C26	-2.01	119.89	122.64
13	B	827	CLA	CMD-C2D-C1D	2.01	128.26	124.73
13	A	801	CLA	C1-O2A-CGA	2.01	121.51	116.65
13	B	813	CLA	CMD-C2D-C1D	2.01	128.26	124.73
15	B	847	BCR	C37-C22-C21	-2.01	119.57	122.82
15	B	850	BCR	C27-C26-C25	-2.00	120.00	122.70
13	B	806	CLA	C7-C6-C5	-2.00	107.93	113.26
13	A	806	CLA	C2D-C1D-ND	2.00	112.11	110.13
13	B	819	CLA	CMD-C2D-C1D	2.00	128.25	124.73

There are no chirality outliers.

All (1055) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CLA	C2B-C3B-CAB-CBB
13	A	801	CLA	C4B-C3B-CAB-CBB
13	A	802	CLA	C4B-C3B-CAB-CBB
13	A	804	CLA	C2B-C3B-CAB-CBB
13	A	804	CLA	C4B-C3B-CAB-CBB
13	A	804	CLA	CAD-CBD-CGD-O2D
13	A	805	CLA	O2A-C1-C2-C3
13	A	806	CLA	C2B-C3B-CAB-CBB
13	A	806	CLA	C4B-C3B-CAB-CBB
13	A	807	CLA	C3A-C2A-CAA-CBA
13	A	807	CLA	C2B-C3B-CAB-CBB
13	A	807	CLA	C4B-C3B-CAB-CBB
13	A	807	CLA	C4-C3-C5-C6
13	A	808	CLA	C2B-C3B-CAB-CBB
13	A	808	CLA	C4B-C3B-CAB-CBB
13	A	808	CLA	C11-C12-C13-C14
13	A	810	CLA	C2B-C3B-CAB-CBB
13	A	810	CLA	C4B-C3B-CAB-CBB
13	A	810	CLA	CHA-CBD-CGD-O1D
13	A	810	CLA	CHA-CBD-CGD-O2D
13	A	811	CLA	C2B-C3B-CAB-CBB
13	A	811	CLA	C4B-C3B-CAB-CBB
13	A	811	CLA	CHA-CBD-CGD-O1D
13	A	811	CLA	CHA-CBD-CGD-O2D
13	A	812	CLA	C2B-C3B-CAB-CBB
13	A	812	CLA	C4B-C3B-CAB-CBB
13	A	813	CLA	CHA-CBD-CGD-O1D
13	A	813	CLA	CHA-CBD-CGD-O2D
13	A	814	CLA	C2B-C3B-CAB-CBB
13	A	814	CLA	C4B-C3B-CAB-CBB
13	A	816	CLA	C2B-C3B-CAB-CBB
13	A	816	CLA	C4B-C3B-CAB-CBB
13	A	817	CLA	C2B-C3B-CAB-CBB
13	A	817	CLA	C4B-C3B-CAB-CBB
13	A	818	CLA	C4B-C3B-CAB-CBB
13	A	818	CLA	CAD-CBD-CGD-O1D
13	A	818	CLA	CAD-CBD-CGD-O2D
13	A	819	CLA	CHA-CBD-CGD-O1D
13	A	819	CLA	CHA-CBD-CGD-O2D
13	A	820	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	A	821	CLA	C1A-C2A-CAA-CBA
13	A	821	CLA	C3A-C2A-CAA-CBA
13	A	821	CLA	CHA-CBD-CGD-O1D
13	A	821	CLA	CHA-CBD-CGD-O2D
13	A	822	CLA	C2B-C3B-CAB-CBB
13	A	822	CLA	C4B-C3B-CAB-CBB
13	A	822	CLA	CHA-CBD-CGD-O2D
13	A	824	CLA	C2B-C3B-CAB-CBB
13	A	824	CLA	C4B-C3B-CAB-CBB
13	A	824	CLA	C2-C3-C5-C6
13	A	824	CLA	C4-C3-C5-C6
13	A	826	CLA	C2B-C3B-CAB-CBB
13	A	826	CLA	C4B-C3B-CAB-CBB
13	A	826	CLA	CAD-CBD-CGD-O1D
13	A	826	CLA	CAD-CBD-CGD-O2D
13	A	827	CLA	C4B-C3B-CAB-CBB
13	A	830	CLA	C2B-C3B-CAB-CBB
13	A	830	CLA	C4B-C3B-CAB-CBB
13	A	831	CLA	C2B-C3B-CAB-CBB
13	A	831	CLA	C4B-C3B-CAB-CBB
13	A	832	CLA	C2B-C3B-CAB-CBB
13	A	832	CLA	C4B-C3B-CAB-CBB
13	A	832	CLA	O2A-C1-C2-C3
13	A	834	CLA	C2B-C3B-CAB-CBB
13	A	834	CLA	C4B-C3B-CAB-CBB
13	A	836	CLA	C2B-C3B-CAB-CBB
13	A	836	CLA	C4B-C3B-CAB-CBB
13	A	837	CLA	C4B-C3B-CAB-CBB
13	A	837	CLA	CHA-CBD-CGD-O1D
13	A	837	CLA	CHA-CBD-CGD-O2D
13	A	838	CLA	C3A-C2A-CAA-CBA
13	A	838	CLA	C2B-C3B-CAB-CBB
13	A	838	CLA	C4B-C3B-CAB-CBB
13	A	838	CLA	CHA-CBD-CGD-O2D
13	A	839	CLA	C2B-C3B-CAB-CBB
13	A	839	CLA	C4B-C3B-CAB-CBB
13	A	839	CLA	CHA-CBD-CGD-O1D
13	A	839	CLA	CHA-CBD-CGD-O2D
13	A	840	CLA	C3A-C2A-CAA-CBA
13	A	840	CLA	C2B-C3B-CAB-CBB
13	A	840	CLA	C4B-C3B-CAB-CBB
13	A	840	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	A	840	CLA	CHA-CBD-CGD-O2D
13	A	841	CLA	C2B-C3B-CAB-CBB
13	A	841	CLA	C4B-C3B-CAB-CBB
13	A	842	CLA	C3A-C2A-CAA-CBA
13	A	842	CLA	C2B-C3B-CAB-CBB
13	A	842	CLA	C4B-C3B-CAB-CBB
13	A	843	CLA	C1A-C2A-CAA-CBA
13	A	843	CLA	C3A-C2A-CAA-CBA
13	A	844	CLA	C4B-C3B-CAB-CBB
13	A	845	CLA	C2B-C3B-CAB-CBB
13	A	845	CLA	C4B-C3B-CAB-CBB
13	A	855	CLA	C2B-C3B-CAB-CBB
13	A	855	CLA	C4B-C3B-CAB-CBB
13	B	801	CLA	C2B-C3B-CAB-CBB
13	B	801	CLA	C4B-C3B-CAB-CBB
13	B	802	CLA	CHA-CBD-CGD-O1D
13	B	802	CLA	CHA-CBD-CGD-O2D
13	B	803	CLA	C2B-C3B-CAB-CBB
13	B	803	CLA	C4B-C3B-CAB-CBB
13	B	805	CLA	C4B-C3B-CAB-CBB
13	B	806	CLA	C1A-C2A-CAA-CBA
13	B	806	CLA	C3A-C2A-CAA-CBA
13	B	806	CLA	C2B-C3B-CAB-CBB
13	B	806	CLA	C4B-C3B-CAB-CBB
13	B	807	CLA	C1A-C2A-CAA-CBA
13	B	807	CLA	C3A-C2A-CAA-CBA
13	B	807	CLA	C2B-C3B-CAB-CBB
13	B	807	CLA	C4B-C3B-CAB-CBB
13	B	807	CLA	CHA-CBD-CGD-O1D
13	B	807	CLA	CHA-CBD-CGD-O2D
13	B	808	CLA	C2B-C3B-CAB-CBB
13	B	808	CLA	C4B-C3B-CAB-CBB
13	B	808	CLA	CHA-CBD-CGD-O1D
13	B	808	CLA	CHA-CBD-CGD-O2D
13	B	809	CLA	C2B-C3B-CAB-CBB
13	B	809	CLA	C4B-C3B-CAB-CBB
13	B	810	CLA	C2B-C3B-CAB-CBB
13	B	810	CLA	C4B-C3B-CAB-CBB
13	B	812	CLA	C4B-C3B-CAB-CBB
13	B	813	CLA	C2B-C3B-CAB-CBB
13	B	813	CLA	C4B-C3B-CAB-CBB
13	B	814	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	B	814	CLA	C4B-C3B-CAB-CBB
13	B	814	CLA	CHA-CBD-CGD-O1D
13	B	814	CLA	CHA-CBD-CGD-O2D
13	B	815	CLA	C2B-C3B-CAB-CBB
13	B	815	CLA	C4B-C3B-CAB-CBB
13	B	816	CLA	C2B-C3B-CAB-CBB
13	B	816	CLA	C4B-C3B-CAB-CBB
13	B	817	CLA	CHA-CBD-CGD-O1D
13	B	817	CLA	CHA-CBD-CGD-O2D
13	B	818	CLA	C2B-C3B-CAB-CBB
13	B	818	CLA	C4B-C3B-CAB-CBB
13	B	819	CLA	C2B-C3B-CAB-CBB
13	B	819	CLA	C4B-C3B-CAB-CBB
13	B	820	CLA	C1A-C2A-CAA-CBA
13	B	820	CLA	C3A-C2A-CAA-CBA
13	B	820	CLA	C2B-C3B-CAB-CBB
13	B	820	CLA	C4B-C3B-CAB-CBB
13	B	821	CLA	C4B-C3B-CAB-CBB
13	B	822	CLA	C3A-C2A-CAA-CBA
13	B	822	CLA	CHA-CBD-CGD-O1D
13	B	822	CLA	CHA-CBD-CGD-O2D
13	B	824	CLA	C2B-C3B-CAB-CBB
13	B	824	CLA	C4B-C3B-CAB-CBB
13	B	827	CLA	C2B-C3B-CAB-CBB
13	B	827	CLA	C4B-C3B-CAB-CBB
13	B	827	CLA	CHA-CBD-CGD-O1D
13	B	827	CLA	CHA-CBD-CGD-O2D
13	B	827	CLA	C11-C12-C13-C14
13	B	828	CLA	C2B-C3B-CAB-CBB
13	B	828	CLA	C4B-C3B-CAB-CBB
13	B	829	CLA	C2B-C3B-CAB-CBB
13	B	829	CLA	C4B-C3B-CAB-CBB
13	B	830	CLA	CAD-CBD-CGD-O1D
13	B	830	CLA	CAD-CBD-CGD-O2D
13	B	831	CLA	C2B-C3B-CAB-CBB
13	B	831	CLA	C4B-C3B-CAB-CBB
13	B	831	CLA	CHA-CBD-CGD-O1D
13	B	831	CLA	CHA-CBD-CGD-O2D
13	B	833	CLA	C2B-C3B-CAB-CBB
13	B	833	CLA	C4B-C3B-CAB-CBB
13	B	833	CLA	CHA-CBD-CGD-O1D
13	B	833	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	B	835	CLA	C2B-C3B-CAB-CBB
13	B	835	CLA	C4B-C3B-CAB-CBB
13	B	836	CLA	C3A-C2A-CAA-CBA
13	B	836	CLA	C4B-C3B-CAB-CBB
13	B	836	CLA	CHA-CBD-CGD-O1D
13	B	836	CLA	CHA-CBD-CGD-O2D
13	B	837	CLA	C2B-C3B-CAB-CBB
13	B	837	CLA	C4B-C3B-CAB-CBB
13	B	838	CLA	C2B-C3B-CAB-CBB
13	B	838	CLA	C4B-C3B-CAB-CBB
13	B	839	CLA	C2B-C3B-CAB-CBB
13	B	839	CLA	C4B-C3B-CAB-CBB
13	F	1301	CLA	CAD-CBD-CGD-O1D
13	F	1301	CLA	CAD-CBD-CGD-O2D
13	J	1101	CLA	C2B-C3B-CAB-CBB
13	J	1101	CLA	C4B-C3B-CAB-CBB
13	J	1102	CLA	C2B-C3B-CAB-CBB
13	J	1102	CLA	C4B-C3B-CAB-CBB
13	J	1103	CLA	C2B-C3B-CAB-CBB
13	J	1103	CLA	C4B-C3B-CAB-CBB
13	L	1003	CLA	C2B-C3B-CAB-CBB
13	L	1003	CLA	C4B-C3B-CAB-CBB
13	L	1004	CLA	C2B-C3B-CAB-CBB
13	L	1004	CLA	C4B-C3B-CAB-CBB
13	M	1201	CLA	C2B-C3B-CAB-CBB
13	M	1201	CLA	C4B-C3B-CAB-CBB
13	M	1201	CLA	CHA-CBD-CGD-O1D
13	M	1201	CLA	CHA-CBD-CGD-O2D
13	M	1202	CLA	C2B-C3B-CAB-CBB
13	M	1202	CLA	C4B-C3B-CAB-CBB
13	X	102	CLA	C2B-C3B-CAB-CBB
13	X	102	CLA	C4B-C3B-CAB-CBB
15	A	847	BCR	C36-C18-C19-C20
15	A	848	BCR	C36-C18-C19-C20
15	A	848	BCR	C37-C22-C23-C24
15	A	849	BCR	C36-C18-C19-C20
15	A	850	BCR	C36-C18-C19-C20
15	A	850	BCR	C37-C22-C23-C24
15	A	850	BCR	C23-C24-C25-C26
15	A	850	BCR	C23-C24-C25-C30
15	A	851	BCR	C36-C18-C19-C20
15	A	851	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	A	852	BCR	C7-C8-C9-C34
15	A	852	BCR	C16-C17-C18-C19
15	A	852	BCR	C18-C19-C20-C21
15	A	852	BCR	C21-C22-C23-C24
15	A	852	BCR	C23-C24-C25-C26
15	A	852	BCR	C23-C24-C25-C30
15	B	841	BCR	C6-C7-C8-C9
15	B	841	BCR	C36-C18-C19-C20
15	B	842	BCR	C1-C6-C7-C8
15	B	842	BCR	C5-C6-C7-C8
15	B	842	BCR	C6-C7-C8-C9
15	B	842	BCR	C11-C10-C9-C34
15	B	842	BCR	C36-C18-C19-C20
15	B	842	BCR	C21-C22-C23-C24
15	B	843	BCR	C7-C8-C9-C34
15	B	843	BCR	C17-C18-C19-C20
15	B	843	BCR	C18-C19-C20-C21
15	B	844	BCR	C36-C18-C19-C20
15	B	845	BCR	C17-C18-C19-C20
15	B	845	BCR	C21-C22-C23-C24
15	B	845	BCR	C37-C22-C23-C24
15	B	846	BCR	C36-C18-C19-C20
15	B	847	BCR	C11-C12-C13-C35
15	B	847	BCR	C36-C18-C19-C20
15	B	847	BCR	C37-C22-C23-C24
15	B	849	BCR	C1-C6-C7-C8
15	B	849	BCR	C5-C6-C7-C8
15	B	849	BCR	C6-C7-C8-C9
15	B	849	BCR	C7-C8-C9-C34
15	B	849	BCR	C18-C19-C20-C21
15	B	849	BCR	C37-C22-C23-C24
15	B	849	BCR	C23-C24-C25-C26
15	B	850	BCR	C7-C8-C9-C10
15	B	850	BCR	C7-C8-C9-C34
15	B	850	BCR	C36-C18-C19-C20
15	F	1302	BCR	C1-C6-C7-C8
15	F	1302	BCR	C5-C6-C7-C8
15	F	1302	BCR	C6-C7-C8-C9
15	F	1302	BCR	C17-C18-C19-C20
15	F	1302	BCR	C18-C19-C20-C21
15	I	102	BCR	C6-C7-C8-C9
15	I	102	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
15	I	102	BCR	C16-C17-C18-C19
15	I	102	BCR	C17-C18-C19-C20
15	I	102	BCR	C37-C22-C23-C24
15	J	1104	BCR	C5-C6-C7-C8
15	J	1104	BCR	C7-C8-C9-C10
15	J	1104	BCR	C17-C18-C19-C20
15	J	1104	BCR	C18-C19-C20-C21
15	J	1105	BCR	C7-C8-C9-C34
15	J	1105	BCR	C17-C18-C19-C20
15	J	1105	BCR	C37-C22-C23-C24
15	L	1005	BCR	C6-C7-C8-C9
15	L	1005	BCR	C7-C8-C9-C34
15	L	1006	BCR	C6-C7-C8-C9
15	L	1006	BCR	C7-C8-C9-C10
15	L	1006	BCR	C11-C10-C9-C8
15	L	1006	BCR	C36-C18-C19-C20
15	M	1203	BCR	C6-C7-C8-C9
15	M	1203	BCR	C7-C8-C9-C10
15	M	1203	BCR	C7-C8-C9-C34
15	M	1203	BCR	C11-C12-C13-C35
15	M	1203	BCR	C17-C18-C19-C20
16	A	854	LHG	C3-O3-P-O5
16	A	854	LHG	C4-O6-P-O3
16	A	854	LHG	C8-C7-O7-C5
16	X	101	LHG	C3-O3-P-O5
16	A	854	LHG	O9-C7-O7-C5
13	A	801	CLA	C3-C5-C6-C7
13	A	803	CLA	C3-C5-C6-C7
13	A	805	CLA	C3-C5-C6-C7
13	A	820	CLA	C3-C5-C6-C7
13	A	824	CLA	C3-C5-C6-C7
13	A	832	CLA	C3-C5-C6-C7
13	A	833	CLA	C3-C5-C6-C7
13	A	834	CLA	C3-C5-C6-C7
13	B	804	CLA	C3-C5-C6-C7
13	B	805	CLA	C3-C5-C6-C7
13	B	812	CLA	C3-C5-C6-C7
13	B	815	CLA	C3-C5-C6-C7
13	B	820	CLA	C3-C5-C6-C7
13	B	831	CLA	C3-C5-C6-C7
13	L	1004	CLA	C3-C5-C6-C7
14	B	840	PQN	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	A	812	CLA	C4-C3-C5-C6
13	A	812	CLA	C2-C3-C5-C6
14	A	846	PQN	C12-C13-C15-C16
13	A	816	CLA	C2A-CAA-CBA-CGA
13	J	1101	CLA	C2A-CAA-CBA-CGA
13	A	828	CLA	C3-C5-C6-C7
13	B	811	CLA	C3-C5-C6-C7
13	B	822	CLA	C3-C5-C6-C7
13	B	824	CLA	C3-C5-C6-C7
13	A	827	CLA	C3-C5-C6-C7
13	A	830	CLA	C3-C5-C6-C7
13	B	835	CLA	C3-C5-C6-C7
13	A	842	CLA	C3-C5-C6-C7
13	A	830	CLA	C4-C3-C5-C6
13	A	832	CLA	C4-C3-C5-C6
13	A	842	CLA	C4-C3-C5-C6
13	A	830	CLA	C2-C3-C5-C6
13	A	842	CLA	C2-C3-C5-C6
13	B	831	CLA	C2-C3-C5-C6
13	B	811	CLA	C5-C6-C7-C8
18	B	848	LMG	O6-C5-C6-O5
16	X	101	LHG	O9-C7-O7-C5
13	B	807	CLA	C5-C6-C7-C8
13	A	819	CLA	C4-C3-C5-C6
13	B	822	CLA	C4-C3-C5-C6
13	B	831	CLA	C4-C3-C5-C6
13	A	819	CLA	C2-C3-C5-C6
13	A	832	CLA	C2-C3-C5-C6
13	B	822	CLA	C2-C3-C5-C6
13	B	839	CLA	C3-C5-C6-C7
13	A	803	CLA	C11-C10-C8-C9
13	A	809	CLA	C11-C12-C13-C14
13	A	811	CLA	C14-C13-C15-C16
13	A	820	CLA	C11-C12-C13-C14
13	A	830	CLA	C11-C12-C13-C14
13	B	808	CLA	C14-C13-C15-C16
13	B	811	CLA	C11-C12-C13-C14
13	B	812	CLA	C11-C12-C13-C14
13	B	817	CLA	C14-C13-C15-C16
13	B	826	CLA	C11-C12-C13-C14
13	B	830	CLA	C14-C13-C15-C16
13	B	838	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	A	846	PQN	C21-C22-C23-C24
15	A	847	BCR	C7-C8-C9-C34
15	A	848	BCR	C11-C12-C13-C35
15	A	851	BCR	C11-C12-C13-C35
15	A	852	BCR	C36-C18-C19-C20
15	A	852	BCR	C37-C22-C23-C24
15	B	841	BCR	C11-C12-C13-C35
15	B	842	BCR	C37-C22-C23-C24
15	B	843	BCR	C36-C18-C19-C20
15	B	843	BCR	C37-C22-C23-C24
15	B	844	BCR	C37-C22-C23-C24
15	B	845	BCR	C36-C18-C19-C20
15	B	846	BCR	C11-C12-C13-C35
15	B	849	BCR	C36-C18-C19-C20
15	F	1302	BCR	C7-C8-C9-C34
15	F	1302	BCR	C36-C18-C19-C20
15	F	1302	BCR	C37-C22-C23-C24
15	I	102	BCR	C7-C8-C9-C34
15	J	1104	BCR	C7-C8-C9-C34
15	J	1104	BCR	C36-C18-C19-C20
15	J	1105	BCR	C11-C12-C13-C35
15	J	1105	BCR	C36-C18-C19-C20
15	L	1005	BCR	C37-C22-C23-C24
15	L	1006	BCR	C7-C8-C9-C34
15	L	1006	BCR	C11-C12-C13-C35
15	M	1203	BCR	C36-C18-C19-C20
15	M	1203	BCR	C37-C22-C23-C24
13	A	811	CLA	C2A-CAA-CBA-CGA
13	A	822	CLA	C2A-CAA-CBA-CGA
13	B	828	CLA	C2A-CAA-CBA-CGA
13	J	1102	CLA	C2A-CAA-CBA-CGA
13	X	102	CLA	C2A-CAA-CBA-CGA
16	A	853	LHG	O7-C5-C6-O8
13	B	803	CLA	C10-C11-C12-C13
13	B	825	CLA	C8-C10-C11-C12
13	B	836	CLA	C8-C10-C11-C12
16	A	853	LHG	C7-C8-C9-C10
13	A	819	CLA	C10-C11-C12-C13
13	B	803	CLA	C8-C10-C11-C12
13	B	824	CLA	C5-C6-C7-C8
13	B	839	CLA	C4-C3-C5-C6
15	A	852	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
13	B	807	CLA	C3-C5-C6-C7
13	B	815	CLA	C8-C10-C11-C12
13	L	1002	CLA	C5-C6-C7-C8
13	A	808	CLA	C2A-CAA-CBA-CGA
13	A	810	CLA	C2A-CAA-CBA-CGA
13	A	812	CLA	C2A-CAA-CBA-CGA
13	A	818	CLA	C2A-CAA-CBA-CGA
13	A	820	CLA	C2A-CAA-CBA-CGA
13	A	823	CLA	C2A-CAA-CBA-CGA
13	A	831	CLA	C2A-CAA-CBA-CGA
13	A	833	CLA	C2A-CAA-CBA-CGA
13	A	842	CLA	C2A-CAA-CBA-CGA
13	A	843	CLA	C2A-CAA-CBA-CGA
13	B	806	CLA	C2A-CAA-CBA-CGA
13	L	1002	CLA	C2A-CAA-CBA-CGA
13	L	1004	CLA	C2A-CAA-CBA-CGA
15	I	102	BCR	C18-C19-C20-C21
15	J	1105	BCR	C18-C19-C20-C21
15	M	1203	BCR	C18-C19-C20-C21
13	A	808	CLA	C8-C10-C11-C12
13	A	811	CLA	C8-C10-C11-C12
13	A	813	CLA	C8-C10-C11-C12
13	A	821	CLA	C8-C10-C11-C12
13	A	825	CLA	C5-C6-C7-C8
13	A	825	CLA	C8-C10-C11-C12
13	A	832	CLA	C8-C10-C11-C12
13	B	816	CLA	C10-C11-C12-C13
13	B	825	CLA	C10-C11-C12-C13
13	B	827	CLA	C8-C10-C11-C12
14	A	846	PQN	C23-C25-C26-C27
13	A	840	CLA	C3-C5-C6-C7
13	A	804	CLA	C5-C6-C7-C8
13	A	819	CLA	C5-C6-C7-C8
13	B	801	CLA	C8-C10-C11-C12
13	B	826	CLA	C5-C6-C7-C8
13	B	826	CLA	C8-C10-C11-C12
13	B	826	CLA	C10-C11-C12-C13
13	B	827	CLA	C10-C11-C12-C13
13	L	1004	CLA	C8-C10-C11-C12
13	A	804	CLA	C8-C10-C11-C12
13	A	824	CLA	C8-C10-C11-C12
13	A	842	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	B	824	CLA	C8-C10-C11-C12
13	A	832	CLA	C5-C6-C7-C8
13	B	825	CLA	C5-C6-C7-C8
13	B	838	CLA	C10-C11-C12-C13
13	L	1002	CLA	C10-C11-C12-C13
14	A	846	PQN	C15-C16-C17-C18
13	A	835	CLA	C3-C5-C6-C7
13	A	820	CLA	C10-C11-C12-C13
13	A	819	CLA	C2A-CAA-CBA-CGA
13	A	828	CLA	C2A-CAA-CBA-CGA
13	A	838	CLA	C2A-CAA-CBA-CGA
13	B	810	CLA	C2A-CAA-CBA-CGA
13	A	802	CLA	C10-C11-C12-C13
13	A	842	CLA	C5-C6-C7-C8
13	B	803	CLA	C5-C6-C7-C8
13	B	806	CLA	C5-C6-C7-C8
13	B	838	CLA	C8-C10-C11-C12
13	A	809	CLA	C8-C10-C11-C12
13	B	804	CLA	C8-C10-C11-C12
13	B	811	CLA	C8-C10-C11-C12
13	A	805	CLA	C10-C11-C12-C13
13	A	830	CLA	C5-C6-C7-C8
13	A	838	CLA	C5-C6-C7-C8
13	I	101	CLA	C8-C10-C11-C12
13	A	838	CLA	C10-C11-C12-C13
13	B	836	CLA	C5-C6-C7-C8
13	B	838	CLA	C5-C6-C7-C8
13	B	826	CLA	C3-C5-C6-C7
16	X	101	LHG	C8-C7-O7-C5
15	B	846	BCR	C11-C10-C9-C34
15	B	847	BCR	C11-C10-C9-C34
15	L	1005	BCR	C20-C21-C22-C37
13	A	827	CLA	C10-C11-C12-C13
15	A	849	BCR	C7-C8-C9-C34
15	B	841	BCR	C7-C8-C9-C34
15	B	850	BCR	C37-C22-C23-C24
15	I	102	BCR	C36-C18-C19-C20
15	A	851	BCR	C21-C22-C23-C24
15	A	852	BCR	C17-C18-C19-C20
15	B	849	BCR	C17-C18-C19-C20
15	L	1005	BCR	C7-C8-C9-C10
15	L	1005	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
13	A	802	CLA	C2A-CAA-CBA-CGA
13	B	815	CLA	C2A-CAA-CBA-CGA
13	F	1301	CLA	C2A-CAA-CBA-CGA
13	A	808	CLA	C16-C17-C18-C19
15	A	852	BCR	C20-C21-C22-C23
15	B	842	BCR	C16-C17-C18-C19
15	B	843	BCR	C16-C17-C18-C19
15	B	844	BCR	C16-C17-C18-C19
15	B	847	BCR	C16-C17-C18-C19
15	B	850	BCR	C16-C17-C18-C19
15	J	1104	BCR	C16-C17-C18-C19
15	J	1105	BCR	C11-C10-C9-C8
15	J	1105	BCR	C16-C17-C18-C19
15	L	1005	BCR	C20-C21-C22-C23
15	M	1203	BCR	C11-C10-C9-C8
15	M	1203	BCR	C16-C17-C18-C19
13	A	833	CLA	C10-C11-C12-C13
13	A	826	CLA	C16-C17-C18-C19
13	B	835	CLA	C11-C12-C13-C14
15	F	1302	BCR	C14-C15-C16-C17
13	B	807	CLA	C10-C11-C12-C13
18	B	848	LMG	C23-C24-C25-C26
13	A	803	CLA	C4B-C3B-CAB-CBB
13	A	809	CLA	C4B-C3B-CAB-CBB
13	A	813	CLA	C4B-C3B-CAB-CBB
13	A	819	CLA	C4B-C3B-CAB-CBB
13	A	833	CLA	C4B-C3B-CAB-CBB
13	A	843	CLA	C4B-C3B-CAB-CBB
13	B	817	CLA	C4B-C3B-CAB-CBB
13	B	826	CLA	C4B-C3B-CAB-CBB
13	A	808	CLA	C16-C17-C18-C20
13	A	826	CLA	C16-C17-C18-C20
13	B	807	CLA	C16-C17-C18-C19
13	B	807	CLA	C16-C17-C18-C20
13	B	835	CLA	C11-C12-C13-C15
13	B	836	CLA	C2A-CAA-CBA-CGA
13	A	833	CLA	C8-C10-C11-C12
13	A	843	CLA	C3-C5-C6-C7
13	L	1003	CLA	C3-C5-C6-C7
13	B	839	CLA	C2-C3-C5-C6
16	A	853	LHG	C9-C10-C11-C12
16	A	853	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
16	A	853	LHG	C11-C10-C9-C8
13	A	832	CLA	C16-C17-C18-C19
13	A	802	CLA	C2B-C3B-CAB-CBB
13	A	818	CLA	C2B-C3B-CAB-CBB
13	A	820	CLA	C2B-C3B-CAB-CBB
13	A	827	CLA	C2B-C3B-CAB-CBB
13	A	833	CLA	C2B-C3B-CAB-CBB
13	A	837	CLA	C2B-C3B-CAB-CBB
13	A	843	CLA	C2B-C3B-CAB-CBB
13	A	844	CLA	C2B-C3B-CAB-CBB
13	B	805	CLA	C2B-C3B-CAB-CBB
13	B	812	CLA	C2B-C3B-CAB-CBB
13	B	821	CLA	C2B-C3B-CAB-CBB
13	B	836	CLA	C2B-C3B-CAB-CBB
15	B	847	BCR	C1-C6-C7-C8
15	B	849	BCR	C23-C24-C25-C30
15	J	1104	BCR	C1-C6-C7-C8
15	J	1105	BCR	C23-C24-C25-C30
15	M	1203	BCR	C1-C6-C7-C8
15	M	1203	BCR	C5-C6-C7-C8
13	A	840	CLA	C2A-CAA-CBA-CGA
13	B	807	CLA	C2A-CAA-CBA-CGA
13	B	820	CLA	C2A-CAA-CBA-CGA
15	A	847	BCR	C18-C19-C20-C21
15	A	849	BCR	C18-C19-C20-C21
15	B	841	BCR	C18-C19-C20-C21
15	B	844	BCR	C18-C19-C20-C21
15	B	845	BCR	C18-C19-C20-C21
15	B	846	BCR	C10-C11-C12-C13
15	B	846	BCR	C18-C19-C20-C21
13	B	816	CLA	C8-C10-C11-C12
13	A	838	CLA	C16-C17-C18-C19
13	B	807	CLA	C14-C13-C15-C16
14	B	840	PQN	C21-C22-C23-C24
13	B	812	CLA	C8-C10-C11-C12
15	J	1105	BCR	C6-C7-C8-C9
13	B	817	CLA	C16-C17-C18-C20
13	B	826	CLA	C2A-CAA-CBA-CGA
13	B	832	CLA	C2A-CAA-CBA-CGA
13	A	832	CLA	C16-C17-C18-C20
13	A	813	CLA	C2C-C3C-CAC-CBC
13	B	830	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	A	806	CLA	C3-C5-C6-C7
13	A	808	CLA	C3-C5-C6-C7
13	A	830	CLA	C8-C10-C11-C12
13	B	830	CLA	C2C-C3C-CAC-CBC
13	I	101	CLA	C5-C6-C7-C8
13	A	812	CLA	C5-C6-C7-C8
13	B	820	CLA	C5-C6-C7-C8
13	B	817	CLA	C16-C17-C18-C19
13	A	811	CLA	C3-C5-C6-C7
13	B	804	CLA	C10-C11-C12-C13
13	B	816	CLA	C2A-CAA-CBA-CGA
13	B	818	CLA	C2A-CAA-CBA-CGA
13	A	807	CLA	C1A-C2A-CAA-CBA
13	A	838	CLA	C1A-C2A-CAA-CBA
13	A	840	CLA	C1A-C2A-CAA-CBA
13	A	842	CLA	C1A-C2A-CAA-CBA
13	B	836	CLA	C1A-C2A-CAA-CBA
13	A	809	CLA	C11-C12-C13-C15
13	A	821	CLA	C11-C12-C13-C15
13	A	834	CLA	C11-C12-C13-C15
13	B	802	CLA	C12-C13-C15-C16
13	B	811	CLA	C11-C12-C13-C15
13	B	826	CLA	C11-C12-C13-C15
13	B	827	CLA	C11-C12-C13-C15
13	B	830	CLA	C12-C13-C15-C16
13	I	101	CLA	C12-C13-C15-C16
13	L	1002	CLA	C12-C13-C15-C16
13	L	1004	CLA	C12-C13-C15-C16
13	B	812	CLA	C5-C6-C7-C8
13	L	1003	CLA	C8-C10-C11-C12
13	B	804	CLA	C2A-CAA-CBA-CGA
13	A	819	CLA	C11-C12-C13-C14
13	A	838	CLA	C11-C12-C13-C14
13	B	802	CLA	C14-C13-C15-C16
13	B	805	CLA	C14-C13-C15-C16
13	L	1002	CLA	C14-C13-C15-C16
13	A	804	CLA	C10-C11-C12-C13
16	A	853	LHG	C33-C34-C35-C36
18	B	848	LMG	C31-C32-C33-C34
16	A	853	LHG	C4-C5-C6-O8
16	A	854	LHG	C4-C5-C6-O8
16	A	853	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
13	A	809	CLA	C3-C5-C6-C7
13	A	808	CLA	C10-C11-C12-C13
13	B	806	CLA	C16-C17-C18-C20
13	A	811	CLA	C10-C11-C12-C13
13	A	820	CLA	C5-C6-C7-C8
16	A	853	LHG	C28-C29-C30-C31
13	B	817	CLA	C2A-CAA-CBA-CGA
13	B	834	CLA	C2A-CAA-CBA-CGA
13	B	822	CLA	O2A-C1-C2-C3
18	B	848	LMG	C29-C30-C31-C32
15	B	850	BCR	C18-C19-C20-C21
14	B	840	PQN	C15-C16-C17-C18
15	A	847	BCR	C16-C17-C18-C19
15	B	845	BCR	C16-C17-C18-C19
15	B	847	BCR	C20-C21-C22-C23
15	A	847	BCR	C6-C7-C8-C9
15	A	852	BCR	C6-C7-C8-C9
15	B	849	BCR	C22-C23-C24-C25
13	A	835	CLA	C5-C6-C7-C8
13	B	835	CLA	C2-C3-C5-C6
13	I	101	CLA	C16-C17-C18-C20
13	L	1003	CLA	C16-C17-C18-C20
13	A	804	CLA	C11-C12-C13-C14
18	B	848	LMG	C13-C14-C15-C16
13	A	805	CLA	C8-C10-C11-C12
13	A	840	CLA	C5-C6-C7-C8
16	A	854	LHG	C10-C11-C12-C13
13	A	829	CLA	CAA-CBA-CGA-O2A
16	A	853	LHG	C13-C14-C15-C16
16	A	853	LHG	C19-C20-C21-C22
13	A	834	CLA	C5-C6-C7-C8
13	B	806	CLA	C16-C17-C18-C19
13	A	805	CLA	C11-C12-C13-C14
13	A	806	CLA	C14-C13-C15-C16
13	A	828	CLA	C11-C12-C13-C14
13	A	832	CLA	C11-C12-C13-C14
13	A	834	CLA	C11-C12-C13-C14
13	B	801	CLA	C11-C12-C13-C14
13	B	802	CLA	C11-C12-C13-C14
13	I	101	CLA	C14-C13-C15-C16
13	L	1004	CLA	C14-C13-C15-C16
13	A	828	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	A	815	CLA	C4B-C3B-CAB-CBB
13	A	829	CLA	C4B-C3B-CAB-CBB
13	A	835	CLA	C4B-C3B-CAB-CBB
13	B	802	CLA	C4B-C3B-CAB-CBB
13	B	811	CLA	C4B-C3B-CAB-CBB
13	B	823	CLA	C4B-C3B-CAB-CBB
13	F	1301	CLA	C4B-C3B-CAB-CBB
13	M	1201	CLA	C5-C6-C7-C8
13	A	805	CLA	C11-C12-C13-C15
13	A	806	CLA	C12-C13-C15-C16
13	A	808	CLA	C11-C12-C13-C15
13	A	809	CLA	C12-C13-C15-C16
13	A	819	CLA	C11-C12-C13-C15
13	A	828	CLA	C11-C12-C13-C15
13	A	838	CLA	C11-C12-C13-C15
13	B	801	CLA	C11-C12-C13-C15
13	B	801	CLA	C12-C13-C15-C16
13	B	802	CLA	C11-C12-C13-C15
13	B	805	CLA	C12-C13-C15-C16
13	B	811	CLA	C12-C13-C15-C16
13	A	803	CLA	C4-C3-C5-C6
13	A	811	CLA	C3A-C2A-CAA-CBA
13	A	812	CLA	C3A-C2A-CAA-CBA
13	A	825	CLA	C4-C3-C5-C6
13	A	829	CLA	C3A-C2A-CAA-CBA
13	A	834	CLA	C3A-C2A-CAA-CBA
13	A	840	CLA	C4-C3-C5-C6
13	B	815	CLA	C4-C3-C5-C6
13	B	838	CLA	C3A-C2A-CAA-CBA
13	L	1004	CLA	C3A-C2A-CAA-CBA
13	B	811	CLA	C10-C11-C12-C13
15	B	841	BCR	C17-C18-C19-C20
15	J	1105	BCR	C7-C8-C9-C10
13	A	828	CLA	C5-C6-C7-C8
16	X	101	LHG	C4-C5-C6-O8
13	A	827	CLA	C4-C3-C5-C6
13	B	835	CLA	C4-C3-C5-C6
13	B	838	CLA	C4-C3-C5-C6
18	B	848	LMG	C21-C22-C23-C24
13	A	803	CLA	C2-C3-C5-C6
13	A	827	CLA	C2-C3-C5-C6
13	B	802	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	I	101	CLA	C16-C17-C18-C19
13	L	1003	CLA	C16-C17-C18-C19
13	F	1301	CLA	C2B-C3B-CAB-CBB
15	A	851	BCR	C1-C6-C7-C8
15	B	845	BCR	C23-C24-C25-C30
15	I	102	BCR	C1-C6-C7-C8
15	J	1105	BCR	C23-C24-C25-C26
13	B	830	CLA	C10-C11-C12-C13
18	B	848	LMG	C30-C31-C32-C33
13	A	834	CLA	C2A-CAA-CBA-CGA
13	B	813	CLA	C2A-CAA-CBA-CGA
13	B	815	CLA	C2-C3-C5-C6
13	A	809	CLA	C14-C13-C15-C16
13	B	811	CLA	C14-C13-C15-C16
13	B	836	CLA	C11-C12-C13-C14
13	L	1003	CLA	C14-C13-C15-C16
16	A	853	LHG	C35-C36-C37-C38
13	A	827	CLA	C16-C17-C18-C20
13	A	838	CLA	C16-C17-C18-C20
13	A	816	CLA	O2A-C1-C2-C3
18	B	848	LMG	C4-C5-C6-O5
13	B	825	CLA	CAA-CBA-CGA-O2A
13	A	840	CLA	C2-C3-C5-C6
13	B	824	CLA	C10-C11-C12-C13
15	A	848	BCR	C35-C13-C14-C15
15	B	841	BCR	C20-C21-C22-C37
15	B	843	BCR	C20-C21-C22-C37
15	B	846	BCR	C20-C21-C22-C37
15	B	847	BCR	C35-C13-C14-C15
15	I	102	BCR	C35-C13-C14-C15
15	J	1104	BCR	C11-C10-C9-C34
15	J	1104	BCR	C20-C21-C22-C37
15	L	1006	BCR	C20-C21-C22-C37
15	M	1203	BCR	C35-C13-C14-C15
13	A	801	CLA	C5-C6-C7-C8
13	A	811	CLA	C12-C13-C15-C16
13	B	812	CLA	C12-C13-C15-C16
13	B	826	CLA	C12-C13-C15-C16
13	B	836	CLA	C11-C12-C13-C15
13	L	1003	CLA	C12-C13-C15-C16
13	A	828	CLA	CAA-CBA-CGA-O2A
15	A	849	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
15	A	850	BCR	C21-C22-C23-C24
15	B	847	BCR	C21-C22-C23-C24
15	B	849	BCR	C7-C8-C9-C10
15	J	1105	BCR	C21-C22-C23-C24
13	B	822	CLA	C5-C6-C7-C8
13	A	813	CLA	C4C-C3C-CAC-CBC
13	B	826	CLA	CAA-CBA-CGA-O2A
13	A	825	CLA	C2-C3-C5-C6
13	B	815	CLA	C11-C12-C13-C14
15	B	842	BCR	C11-C10-C9-C8
15	I	102	BCR	C11-C10-C9-C8
15	M	1203	BCR	C20-C21-C22-C23
18	B	848	LMG	C40-C41-C42-C43
13	A	821	CLA	C4-C3-C5-C6
13	A	835	CLA	C2A-CAA-CBA-CGA
13	A	843	CLA	C8-C10-C11-C12
16	A	854	LHG	O7-C5-C6-O8
16	X	101	LHG	O7-C5-C6-O8
13	A	803	CLA	C14-C13-C15-C16
13	B	804	CLA	C11-C12-C13-C14
13	B	825	CLA	C14-C13-C15-C16
13	A	827	CLA	C16-C17-C18-C19
18	B	848	LMG	C34-C35-C36-C37
13	A	818	CLA	C5-C6-C7-C8
16	A	853	LHG	C31-C32-C33-C34
13	A	820	CLA	C8-C10-C11-C12
13	A	829	CLA	C10-C11-C12-C13
13	B	839	CLA	C8-C10-C11-C12
14	A	846	PQN	C13-C15-C16-C17
15	B	845	BCR	C7-C8-C9-C34
13	A	823	CLA	C4B-C3B-CAB-CBB
13	I	101	CLA	C4B-C3B-CAB-CBB
13	A	828	CLA	C4-C3-C5-C6
15	B	842	BCR	C17-C18-C19-C20
15	B	843	BCR	C7-C8-C9-C10
15	B	850	BCR	C17-C18-C19-C20
13	A	821	CLA	C2A-CAA-CBA-CGA
13	A	829	CLA	C12-C13-C15-C16
13	A	832	CLA	C12-C13-C15-C16
13	A	838	CLA	C12-C13-C15-C16
13	A	842	CLA	C12-C13-C15-C16
13	I	101	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
13	A	842	CLA	C16-C17-C18-C20
13	A	805	CLA	C4-C3-C5-C6
13	B	806	CLA	C4-C3-C5-C6
13	A	821	CLA	C2-C3-C5-C6
13	I	101	CLA	C3-C5-C6-C7
13	B	814	CLA	C2A-CAA-CBA-CGA
13	B	801	CLA	C14-C13-C15-C16
13	B	826	CLA	C14-C13-C15-C16
15	M	1203	BCR	C19-C20-C21-C22
13	A	805	CLA	C5-C6-C7-C8
13	A	816	CLA	C1-C2-C3-C4
13	A	822	CLA	C1-C2-C3-C4
13	B	829	CLA	C1-C2-C3-C4
13	L	1003	CLA	C5-C6-C7-C8
13	A	809	CLA	CAD-CBD-CGD-O2D
13	A	824	CLA	CAD-CBD-CGD-O2D
13	A	828	CLA	CAD-CBD-CGD-O2D
13	A	832	CLA	CAD-CBD-CGD-O2D
13	B	803	CLA	CAD-CBD-CGD-O2D
13	B	825	CLA	CAD-CBD-CGD-O2D
13	B	828	CLA	CAD-CBD-CGD-O2D
13	B	835	CLA	CAD-CBD-CGD-O2D
13	A	821	CLA	C10-C11-C12-C13
13	A	836	CLA	C2A-CAA-CBA-CGA
16	A	853	LHG	C15-C16-C17-C18
13	A	804	CLA	CAD-CBD-CGD-O1D
13	A	822	CLA	CHA-CBD-CGD-O1D
13	A	824	CLA	CAD-CBD-CGD-O1D
13	A	827	CLA	CHA-CBD-CGD-O1D
13	A	827	CLA	CHA-CBD-CGD-O2D
13	A	832	CLA	CAD-CBD-CGD-O1D
13	A	838	CLA	CHA-CBD-CGD-O1D
13	A	845	CLA	CHA-CBD-CGD-O1D
13	A	845	CLA	CHA-CBD-CGD-O2D
13	B	803	CLA	CAD-CBD-CGD-O1D
13	B	806	CLA	CHA-CBD-CGD-O1D
13	B	806	CLA	CHA-CBD-CGD-O2D
13	B	825	CLA	CAD-CBD-CGD-O1D
13	B	828	CLA	CAD-CBD-CGD-O1D
13	B	835	CLA	CAD-CBD-CGD-O1D
13	B	839	CLA	CHA-CBD-CGD-O1D
13	B	839	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	X	102	CLA	CHA-CBD-CGD-O1D
13	X	102	CLA	CHA-CBD-CGD-O2D
15	B	845	BCR	C19-C20-C21-C22
16	A	853	LHG	C3-O3-P-O5
16	A	853	LHG	C4-O6-P-O5
16	X	101	LHG	C3-O3-P-O6
13	J	1101	CLA	C3-C5-C6-C7
13	A	803	CLA	C2B-C3B-CAB-CBB
13	A	809	CLA	C2B-C3B-CAB-CBB
13	A	813	CLA	C2B-C3B-CAB-CBB
13	A	819	CLA	C2B-C3B-CAB-CBB
13	A	835	CLA	C2B-C3B-CAB-CBB
13	B	817	CLA	C2B-C3B-CAB-CBB
13	B	823	CLA	C2B-C3B-CAB-CBB
13	B	826	CLA	C2B-C3B-CAB-CBB
13	A	809	CLA	C5-C6-C7-C8
13	B	838	CLA	C2-C3-C5-C6
16	A	854	LHG	C9-C10-C11-C12
13	A	813	CLA	C11-C12-C13-C15
13	A	842	CLA	C16-C17-C18-C19
13	B	815	CLA	C5-C6-C7-C8
13	A	802	CLA	C11-C12-C13-C14
13	A	829	CLA	C14-C13-C15-C16
13	A	840	CLA	C11-C12-C13-C14
13	B	812	CLA	C14-C13-C15-C16
13	B	824	CLA	C11-C12-C13-C14
15	A	848	BCR	C16-C17-C18-C19
15	A	851	BCR	C16-C17-C18-C19
15	B	841	BCR	C16-C17-C18-C19
15	B	849	BCR	C16-C17-C18-C19
13	B	816	CLA	CAA-CBA-CGA-O2A
15	B	844	BCR	C19-C20-C21-C22
13	L	1003	CLA	CAA-CBA-CGA-O2A
13	A	801	CLA	C16-C17-C18-C20
13	M	1201	CLA	CAA-CBA-CGA-O2A
13	B	801	CLA	C3-C5-C6-C7
15	A	848	BCR	C21-C22-C23-C24
13	A	818	CLA	CAA-CBA-CGA-O2A
13	A	824	CLA	C2A-CAA-CBA-CGA
13	B	802	CLA	C2A-CAA-CBA-CGA
15	B	842	BCR	C19-C20-C21-C22
15	J	1105	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
13	A	832	CLA	C14-C13-C15-C16
13	A	838	CLA	C14-C13-C15-C16
13	A	842	CLA	C14-C13-C15-C16
13	A	803	CLA	C10-C11-C12-C13
13	L	1003	CLA	C2C-C3C-CAC-CBC
13	A	828	CLA	C10-C11-C12-C13
13	B	812	CLA	C2A-CAA-CBA-CGA
13	B	803	CLA	C11-C12-C13-C15
13	B	805	CLA	C11-C12-C13-C15
13	B	824	CLA	C12-C13-C15-C16
13	B	803	CLA	C16-C17-C18-C20
13	B	834	CLA	CAA-CBA-CGA-O2A
13	A	817	CLA	C3A-C2A-CAA-CBA
13	L	1002	CLA	C4-C3-C5-C6
13	A	845	CLA	CAA-CBA-CGA-O2A
15	A	848	BCR	C11-C10-C9-C34
15	B	849	BCR	C19-C20-C21-C22
13	B	801	CLA	C5-C6-C7-C8
13	B	805	CLA	C10-C11-C12-C13
13	B	811	CLA	C4-C3-C5-C6
13	B	818	CLA	CAA-CBA-CGA-O2A
13	A	805	CLA	C2-C3-C5-C6
13	B	806	CLA	C2-C3-C5-C6
13	A	829	CLA	CAA-CBA-CGA-O1A
13	J	1101	CLA	C10-C11-C12-C13
13	B	834	CLA	CAA-CBA-CGA-O1A
13	A	842	CLA	C11-C10-C8-C9
13	B	824	CLA	C14-C13-C15-C16
13	B	838	CLA	C11-C10-C8-C9
13	I	101	CLA	C11-C12-C13-C14
13	A	801	CLA	C16-C17-C18-C19
13	B	810	CLA	CAA-CBA-CGA-O1A
13	B	832	CLA	CAA-CBA-CGA-O1A
13	B	830	CLA	C4C-C3C-CAC-CBC
13	A	811	CLA	C1A-C2A-CAA-CBA
13	A	829	CLA	C1A-C2A-CAA-CBA
13	B	822	CLA	C1A-C2A-CAA-CBA
13	B	838	CLA	C1A-C2A-CAA-CBA
15	A	849	BCR	C16-C17-C18-C19
15	J	1104	BCR	C11-C10-C9-C8
13	A	815	CLA	C2B-C3B-CAB-CBB
13	A	821	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	A	823	CLA	C2B-C3B-CAB-CBB
13	A	829	CLA	C2B-C3B-CAB-CBB
13	B	811	CLA	C2B-C3B-CAB-CBB
13	I	101	CLA	C2B-C3B-CAB-CBB
15	A	847	BCR	C1-C6-C7-C8
15	A	848	BCR	C1-C6-C7-C8
15	A	851	BCR	C5-C6-C7-C8
15	B	845	BCR	C23-C24-C25-C26
15	B	847	BCR	C5-C6-C7-C8
15	I	102	BCR	C23-C24-C25-C30
15	L	1005	BCR	C23-C24-C25-C26
13	B	832	CLA	CAA-CBA-CGA-O2A
16	A	853	LHG	C16-C17-C18-C19
13	B	810	CLA	CAA-CBA-CGA-O2A
15	A	848	BCR	C19-C20-C21-C22
13	A	830	CLA	C11-C12-C13-C15
13	B	838	CLA	C12-C13-C15-C16
13	A	813	CLA	C11-C12-C13-C14
13	A	810	CLA	CAA-CBA-CGA-O1A
13	X	102	CLA	CAA-CBA-CGA-O2A
13	B	809	CLA	CAA-CBA-CGA-O1A
13	X	102	CLA	CAA-CBA-CGA-O1A
15	L	1006	BCR	C37-C22-C23-C24
14	B	840	PQN	C14-C13-C15-C16
13	L	1002	CLA	C2-C3-C5-C6
13	A	811	CLA	C11-C12-C13-C14
13	A	833	CLA	C14-C13-C15-C16
13	B	830	CLA	C8-C10-C11-C12
15	F	1302	BCR	C19-C20-C21-C22
15	I	102	BCR	C19-C20-C21-C22
16	A	853	LHG	C26-C27-C28-C29
15	B	843	BCR	C22-C23-C24-C25
15	B	847	BCR	C6-C7-C8-C9
13	B	812	CLA	C4-C3-C5-C6
13	L	1004	CLA	C4-C3-C5-C6
13	B	809	CLA	CAA-CBA-CGA-O2A
13	A	828	CLA	C2-C3-C5-C6
13	B	811	CLA	C2-C3-C5-C6
13	A	810	CLA	CAA-CBA-CGA-O2A
13	A	820	CLA	C4-C3-C5-C6
13	L	1003	CLA	C4-C3-C5-C6
13	A	814	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	A	844	CLA	CAA-CBA-CGA-O2A
13	A	822	CLA	CAA-CBA-CGA-O2A
13	B	837	CLA	CAA-CBA-CGA-O2A
13	A	814	CLA	CAA-CBA-CGA-O1A
13	B	833	CLA	CAA-CBA-CGA-O2A
13	B	801	CLA	C16-C17-C18-C20
13	A	826	CLA	C8-C10-C11-C12
15	B	846	BCR	C35-C13-C14-C15
13	A	812	CLA	CAA-CBA-CGA-O2A
13	B	812	CLA	CAA-CBA-CGA-O2A
13	L	1004	CLA	C2-C3-C5-C6
13	B	833	CLA	CAA-CBA-CGA-O1A
13	J	1102	CLA	CAA-CBA-CGA-O2A
15	B	846	BCR	C9-C10-C11-C12
13	A	821	CLA	C14-C13-C15-C16
13	A	826	CLA	C14-C13-C15-C16
13	A	832	CLA	C11-C10-C8-C9
13	B	838	CLA	C11-C12-C13-C14
13	L	1003	CLA	C11-C12-C13-C14
13	A	808	CLA	C2-C1-O2A-CGA
13	B	802	CLA	C2-C1-O2A-CGA
13	B	803	CLA	C2-C1-O2A-CGA
13	A	819	CLA	C3-C5-C6-C7
13	B	803	CLA	C16-C17-C18-C19
13	L	1004	CLA	C16-C17-C18-C20
13	A	828	CLA	C3A-C2A-CAA-CBA
13	B	817	CLA	C3A-C2A-CAA-CBA
13	B	823	CLA	C3A-C2A-CAA-CBA
13	B	807	CLA	CAA-CBA-CGA-O2A
13	A	844	CLA	CAA-CBA-CGA-O1A
13	B	830	CLA	O2A-C1-C2-C3
13	B	803	CLA	C3-C5-C6-C7
13	B	830	CLA	C2A-CAA-CBA-CGA
13	A	829	CLA	C8-C10-C11-C12
13	A	834	CLA	C8-C10-C11-C12
16	X	101	LHG	C1-C2-C3-O3
16	A	853	LHG	C14-C15-C16-C17
13	B	813	CLA	CAA-CBA-CGA-O1A
13	J	1102	CLA	CAA-CBA-CGA-O1A
14	A	846	PQN	C14-C13-C15-C16
13	A	828	CLA	C16-C17-C18-C19
13	B	802	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	L	1002	CLA	C11-C12-C13-C14
16	X	101	LHG	O6-C4-C5-C6
15	A	850	BCR	C17-C18-C19-C20
13	B	820	CLA	C2C-C3C-CAC-CBC
13	L	1002	CLA	C16-C17-C18-C20
13	A	817	CLA	C2A-CAA-CBA-CGA
13	B	837	CLA	C2A-CAA-CBA-CGA
13	A	811	CLA	C11-C12-C13-C15
13	A	828	CLA	C12-C13-C15-C16
13	A	833	CLA	C12-C13-C15-C16
13	B	808	CLA	C12-C13-C15-C16
13	B	812	CLA	C11-C12-C13-C15
13	B	831	CLA	C6-C7-C8-C10
13	L	1002	CLA	C11-C12-C13-C15
13	L	1003	CLA	C11-C12-C13-C15
13	B	802	CLA	C2B-C3B-CAB-CBB
13	B	825	CLA	C2B-C3B-CAB-CBB
15	A	847	BCR	C5-C6-C7-C8
15	A	848	BCR	C5-C6-C7-C8
15	A	848	BCR	C23-C24-C25-C30
15	I	102	BCR	C5-C6-C7-C8
15	I	102	BCR	C23-C24-C25-C26
15	L	1005	BCR	C23-C24-C25-C30
13	A	832	CLA	CAA-CBA-CGA-O2A
13	A	801	CLA	C2-C1-O2A-CGA
13	A	811	CLA	C2-C1-O2A-CGA
13	A	819	CLA	C2-C1-O2A-CGA
13	A	842	CLA	C2-C1-O2A-CGA
13	M	1201	CLA	C2-C1-O2A-CGA
13	A	825	CLA	CAA-CBA-CGA-O2A
13	A	839	CLA	C2A-CAA-CBA-CGA
13	A	834	CLA	C16-C17-C18-C20
13	A	821	CLA	C3-C5-C6-C7
15	B	842	BCR	C18-C19-C20-C21
15	B	847	BCR	C10-C11-C12-C13
18	B	848	LMG	C41-C42-C43-C44
13	J	1101	CLA	CAA-CBA-CGA-O2A
13	B	825	CLA	CAA-CBA-CGA-O1A
13	B	826	CLA	CAA-CBA-CGA-O1A
13	A	821	CLA	C11-C12-C13-C14
13	A	835	CLA	CAA-CBA-CGA-O2A
13	B	808	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	A	812	CLA	C1A-C2A-CAA-CBA
13	A	821	CLA	C4B-C3B-CAB-CBB
13	A	834	CLA	C1A-C2A-CAA-CBA
13	B	825	CLA	C4B-C3B-CAB-CBB
13	A	838	CLA	C4-C3-C5-C6
15	A	847	BCR	C17-C18-C19-C20
15	B	844	BCR	C17-C18-C19-C20
15	A	851	BCR	C19-C20-C21-C22
13	A	828	CLA	CAA-CBA-CGA-O1A
13	A	806	CLA	CAA-CBA-CGA-O2A
13	B	825	CLA	C2A-CAA-CBA-CGA
13	A	841	CLA	CAA-CBA-CGA-O2A
13	A	823	CLA	C2-C3-C5-C6
13	A	841	CLA	C2-C3-C5-C6
13	B	807	CLA	C2-C1-O2A-CGA
13	B	808	CLA	C2-C1-O2A-CGA
13	B	814	CLA	C2-C1-O2A-CGA
13	B	807	CLA	C12-C13-C15-C16
13	B	817	CLA	C12-C13-C15-C16
13	B	838	CLA	C11-C12-C13-C15
16	A	853	LHG	C10-C11-C12-C13
13	A	834	CLA	CAA-CBA-CGA-O2A
13	A	806	CLA	C2A-CAA-CBA-CGA
13	B	803	CLA	C2A-CAA-CBA-CGA
13	M	1202	CLA	CAA-CBA-CGA-O1A
13	A	825	CLA	CAA-CBA-CGA-O1A
13	B	813	CLA	CAA-CBA-CGA-O2A
13	A	828	CLA	C14-C13-C15-C16
14	B	840	PQN	C24-C23-C25-C26
13	J	1101	CLA	CAA-CBA-CGA-O1A
13	B	837	CLA	C2-C1-O2A-CGA
13	A	835	CLA	CAA-CBA-CGA-O1A
13	A	801	CLA	CAA-CBA-CGA-O2A
13	A	836	CLA	CAA-CBA-CGA-O2A
13	A	820	CLA	CAA-CBA-CGA-O2A
13	A	830	CLA	CAA-CBA-CGA-O2A
13	B	808	CLA	CAA-CBA-CGA-O1A
13	A	807	CLA	CAD-CBD-CGD-O2D
13	A	836	CLA	CAD-CBD-CGD-O2D
13	A	843	CLA	CAD-CBD-CGD-O2D
13	L	1003	CLA	CAD-CBD-CGD-O2D
13	B	804	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	A	806	CLA	CAA-CBA-CGA-O1A
13	B	821	CLA	CAA-CBA-CGA-O2A
13	M	1202	CLA	CAA-CBA-CGA-O2A
13	A	841	CLA	CAA-CBA-CGA-O1A
13	A	808	CLA	CAA-CBA-CGA-O2A
13	B	801	CLA	CAA-CBA-CGA-O2A
13	A	836	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

123 monomers are involved in 1016 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	836	CLA	9	0
13	A	818	CLA	11	0
13	A	824	CLA	6	0
14	B	840	PQN	6	0
13	B	822	CLA	20	0
13	A	807	CLA	11	0
13	A	837	CLA	12	0
15	J	1104	BCR	3	0
15	B	841	BCR	6	0
16	X	101	LHG	1	0
13	B	808	CLA	15	0
13	B	815	CLA	16	0
15	B	849	BCR	16	0
13	B	802	CLA	17	0
13	A	833	CLA	15	0
13	A	855	CLA	2	0
15	A	847	BCR	5	0
15	B	844	BCR	6	0
13	B	805	CLA	8	0
13	A	813	CLA	14	0
15	A	851	BCR	2	0
13	B	833	CLA	3	0
13	A	835	CLA	7	0
13	A	822	CLA	7	0
13	A	830	CLA	13	0
15	B	845	BCR	7	0
13	B	803	CLA	16	0
13	M	1202	CLA	1	0
15	L	1005	BCR	12	0
13	A	803	CLA	26	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	816	CLA	4	0
13	A	829	CLA	9	0
18	B	848	LMG	18	0
15	B	843	BCR	17	0
13	A	809	CLA	12	0
15	M	1203	BCR	11	0
15	L	1006	BCR	4	0
13	X	102	CLA	4	0
15	A	850	BCR	4	0
13	A	806	CLA	10	0
13	B	809	CLA	6	0
13	A	804	CLA	10	0
13	A	812	CLA	3	0
13	A	805	CLA	10	0
14	A	846	PQN	7	0
13	A	842	CLA	20	0
13	B	806	CLA	14	0
15	B	850	BCR	6	0
13	B	807	CLA	13	0
13	B	818	CLA	4	0
13	B	810	CLA	6	0
13	A	845	CLA	11	0
13	A	810	CLA	5	0
13	B	821	CLA	11	0
13	B	804	CLA	16	0
13	A	819	CLA	16	0
13	A	821	CLA	12	0
13	A	801	CLA	12	0
13	A	826	CLA	16	0
15	B	847	BCR	13	0
13	L	1003	CLA	16	0
13	A	841	CLA	5	0
13	B	834	CLA	4	0
13	A	840	CLA	16	0
13	A	839	CLA	13	0
13	M	1201	CLA	15	0
15	I	102	BCR	9	0
13	B	813	CLA	9	0
15	F	1302	BCR	12	0
13	A	834	CLA	18	0
13	B	835	CLA	15	0
13	B	816	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	844	CLA	2	0
13	J	1102	CLA	3	0
13	B	824	CLA	18	0
13	B	826	CLA	17	0
13	B	823	CLA	8	0
13	A	802	CLA	13	0
13	J	1101	CLA	12	0
16	A	853	LHG	9	0
13	B	838	CLA	15	0
13	A	831	CLA	9	0
13	A	828	CLA	15	0
13	B	828	CLA	5	0
13	A	843	CLA	10	0
13	B	820	CLA	11	0
13	I	101	CLA	15	0
15	B	846	BCR	7	0
13	A	811	CLA	13	0
13	B	832	CLA	9	0
13	A	832	CLA	19	0
13	A	820	CLA	7	0
13	B	819	CLA	2	0
13	B	830	CLA	23	0
16	A	854	LHG	2	0
13	A	808	CLA	19	0
15	A	849	BCR	4	0
13	B	839	CLA	7	0
13	L	1004	CLA	5	0
13	A	827	CLA	13	0
15	A	848	BCR	5	0
13	B	837	CLA	6	0
15	A	852	BCR	19	0
13	A	825	CLA	20	0
13	A	817	CLA	8	0
13	L	1002	CLA	5	0
13	B	817	CLA	14	0
13	B	825	CLA	18	0
13	B	814	CLA	8	0
13	B	812	CLA	14	0
13	A	823	CLA	13	0
13	F	1301	CLA	4	0
13	B	801	CLA	12	0
13	B	831	CLA	12	0

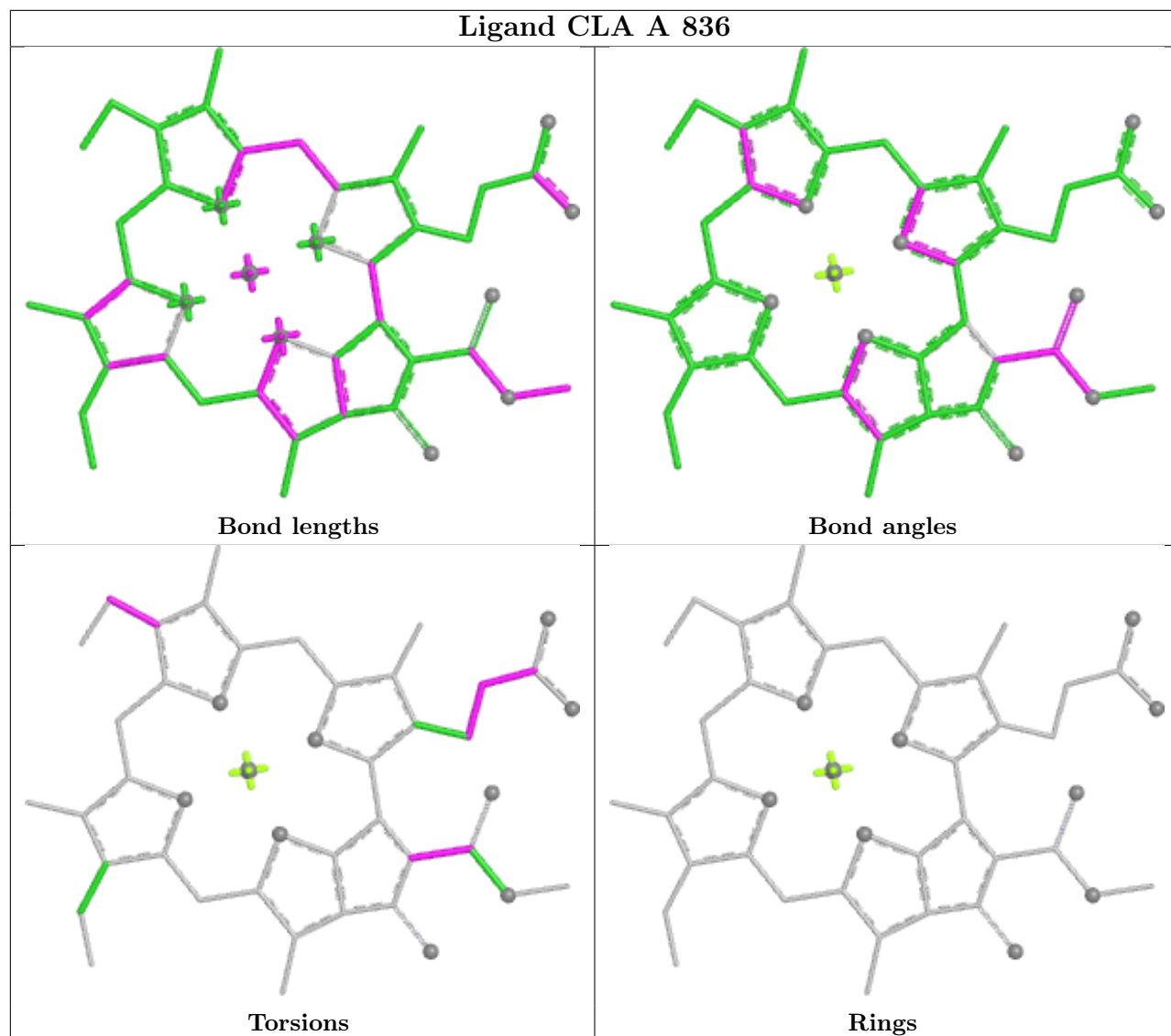
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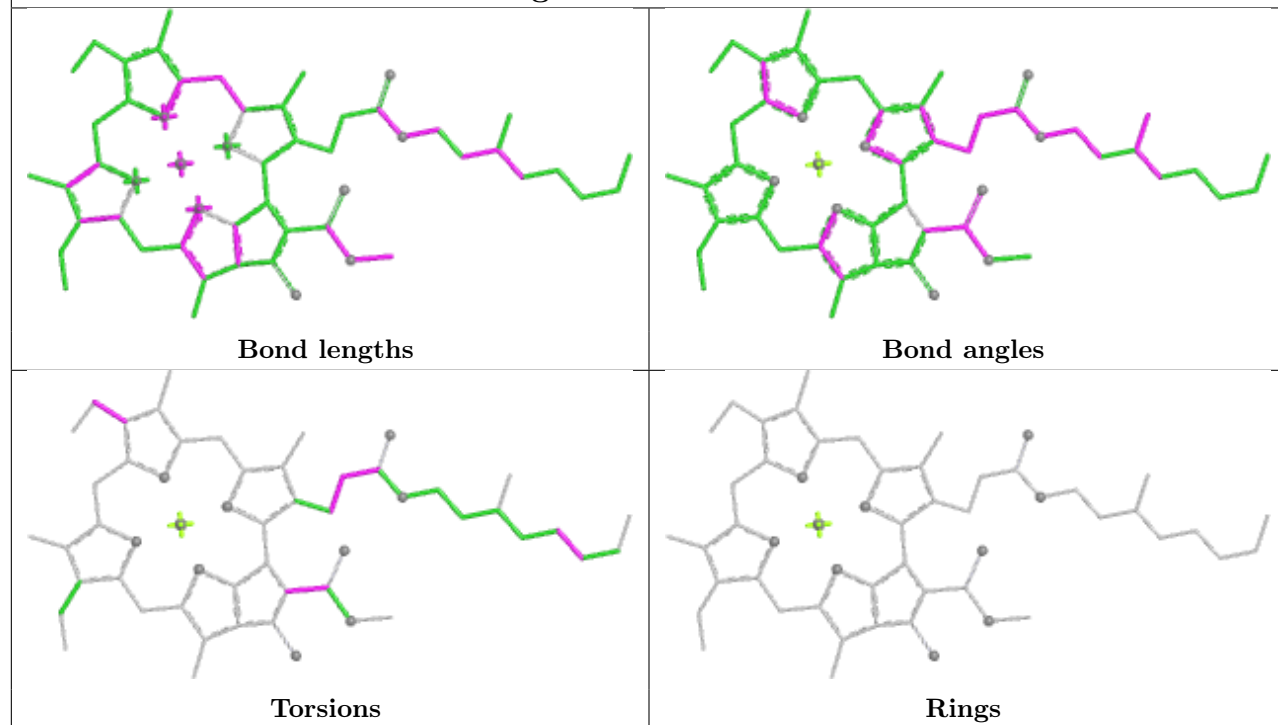
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	838	CLA	8	0
13	A	814	CLA	9	0
13	B	829	CLA	6	0
15	J	1105	BCR	6	0
15	B	842	BCR	4	0
13	B	827	CLA	13	0
13	A	815	CLA	6	0
13	B	836	CLA	10	0
13	B	811	CLA	15	0

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

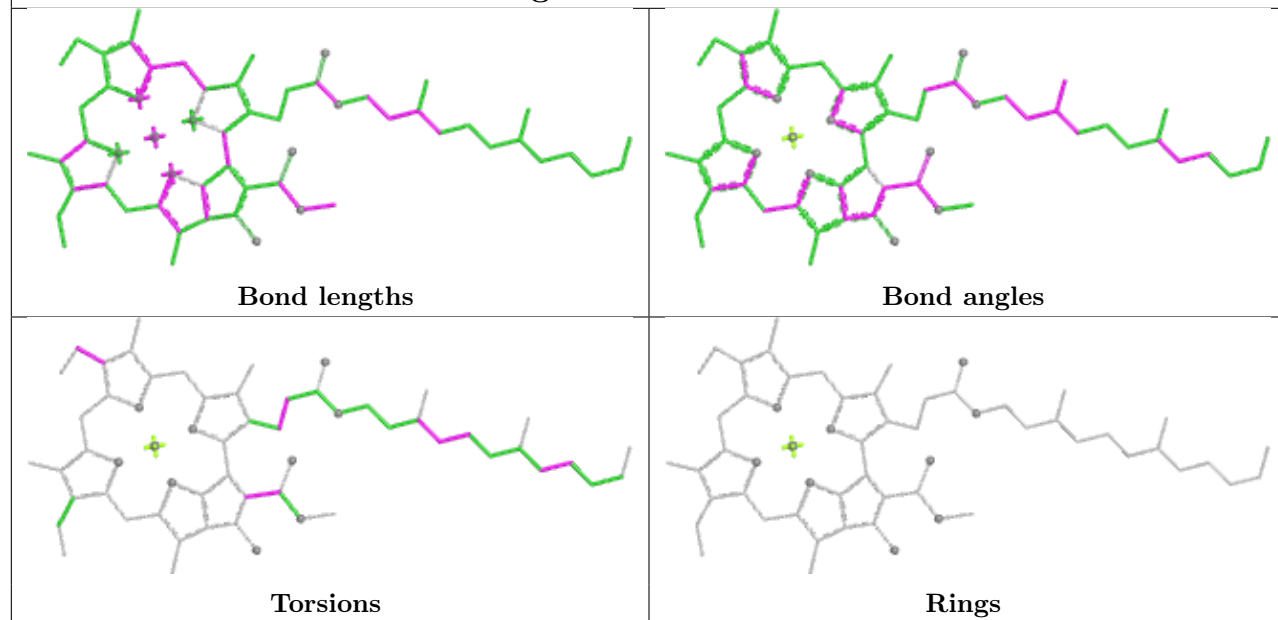
Ligand CLA A 836

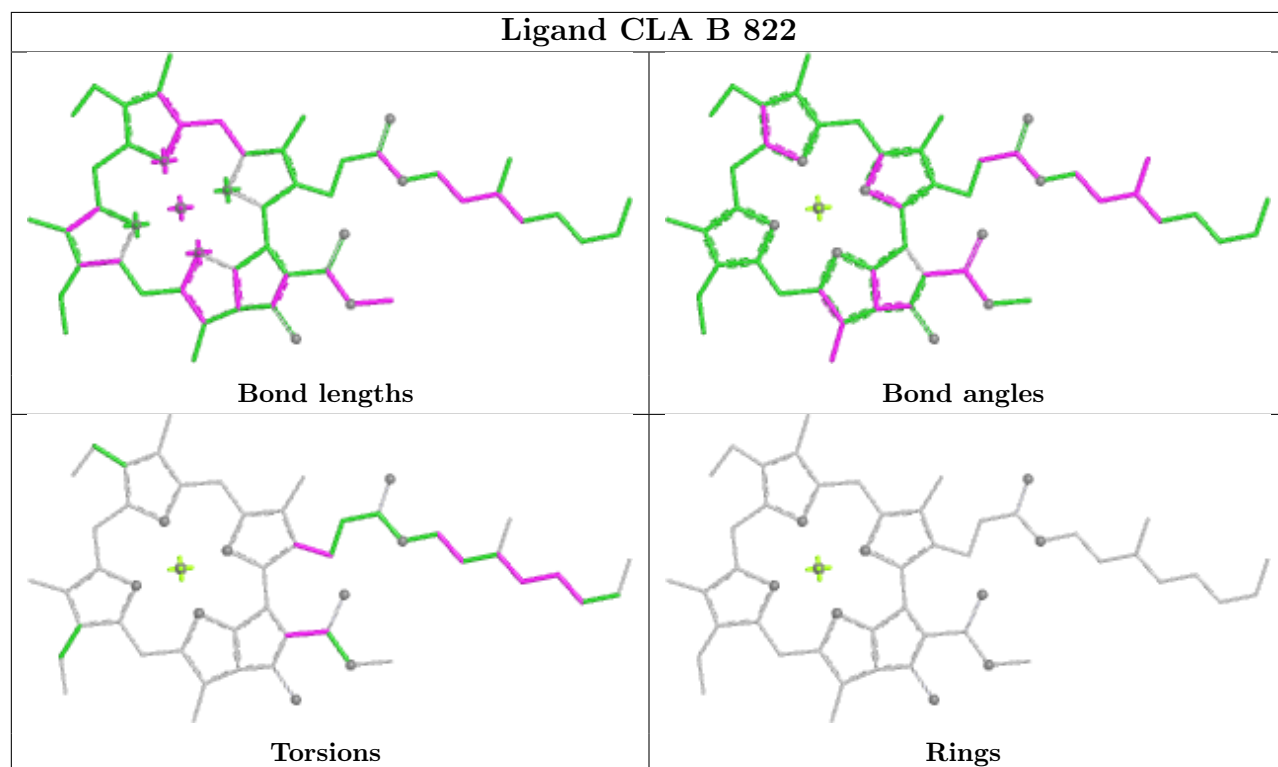
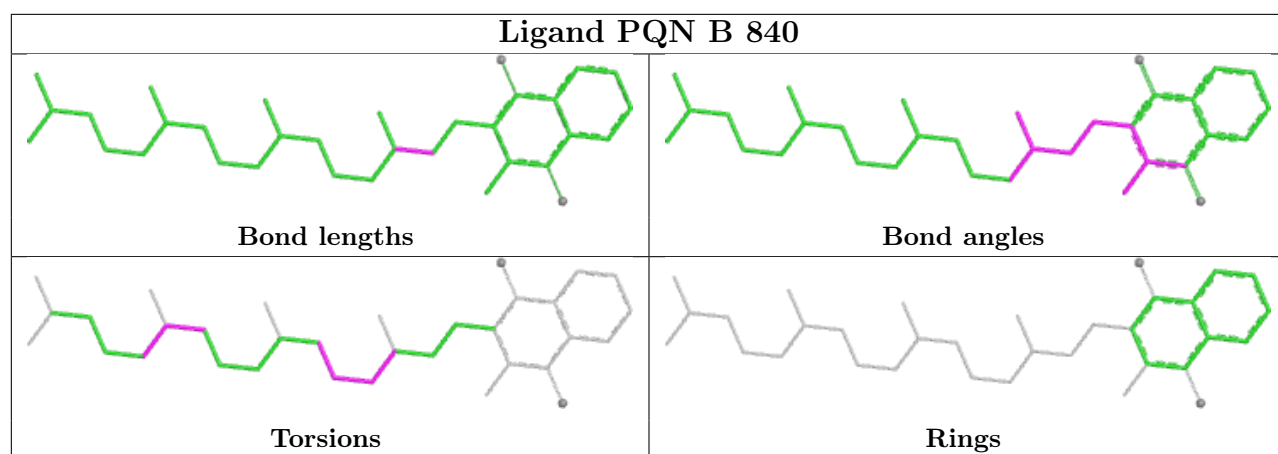


Ligand CLA A 818

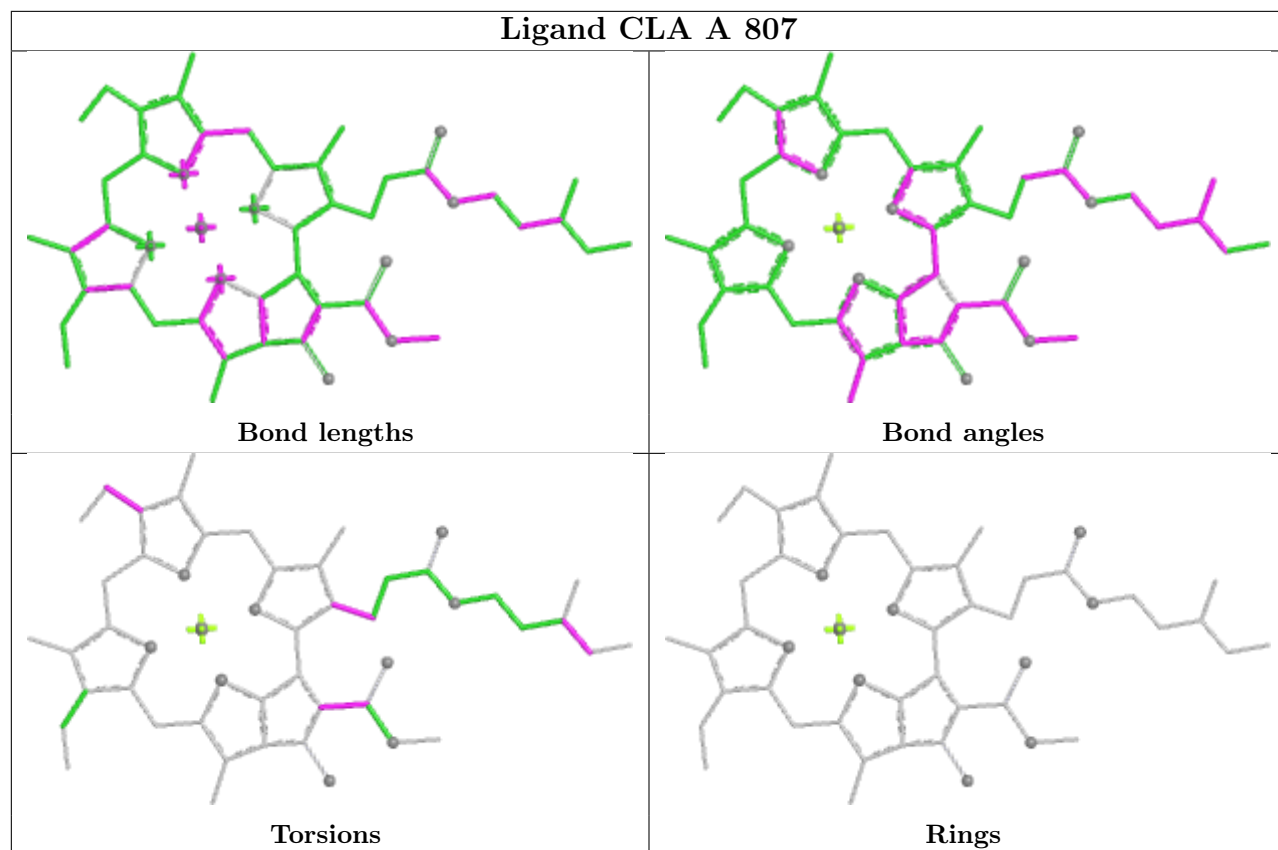


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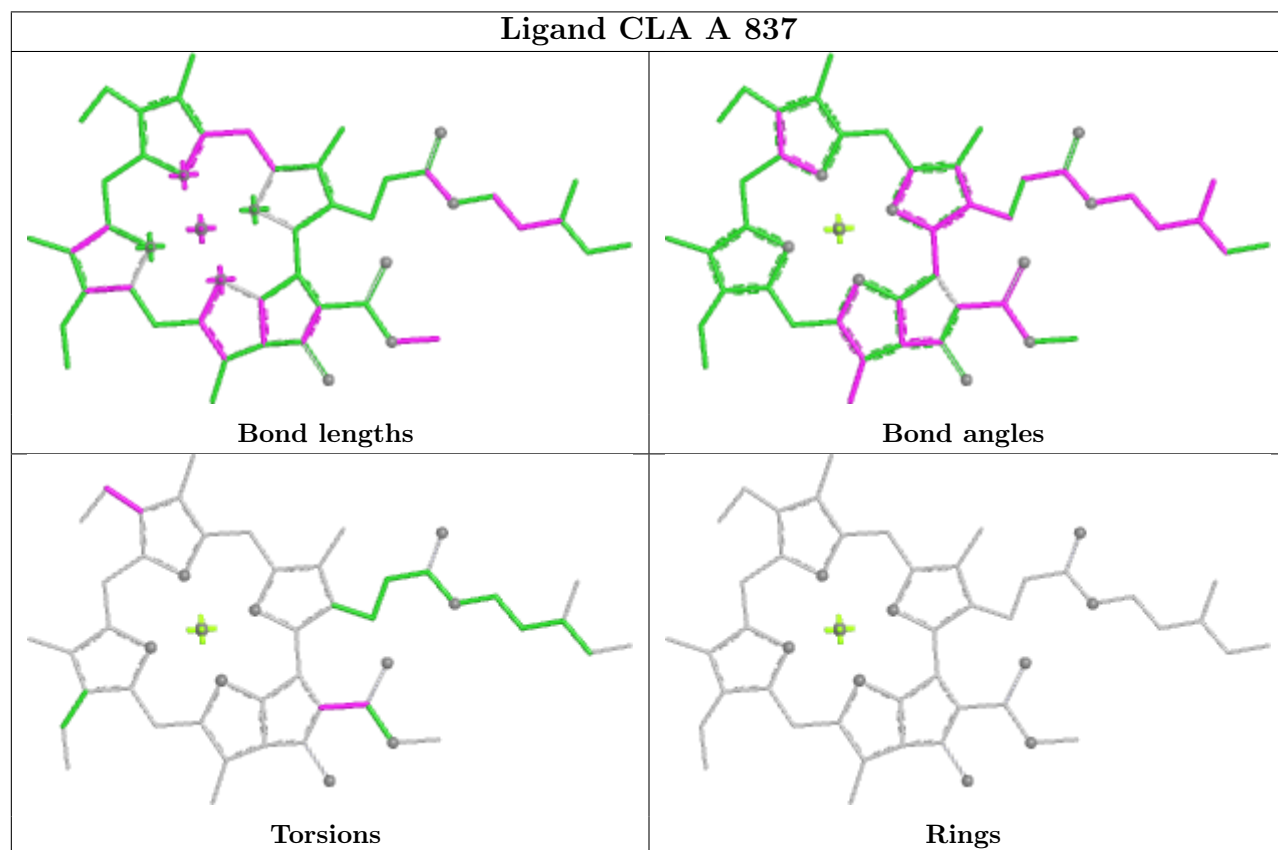


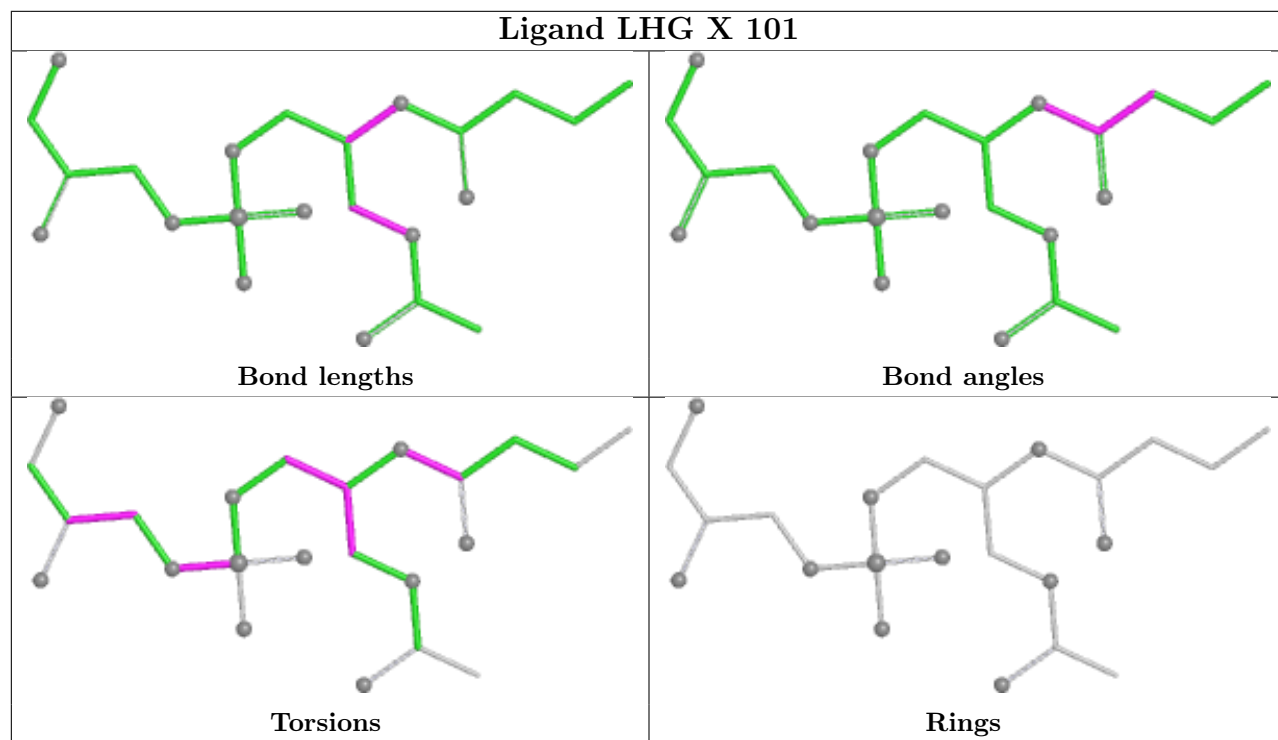
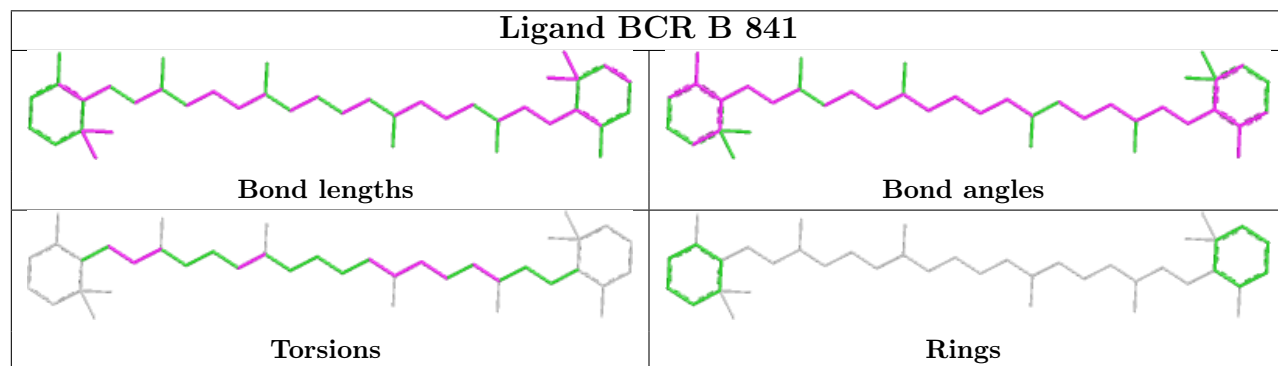
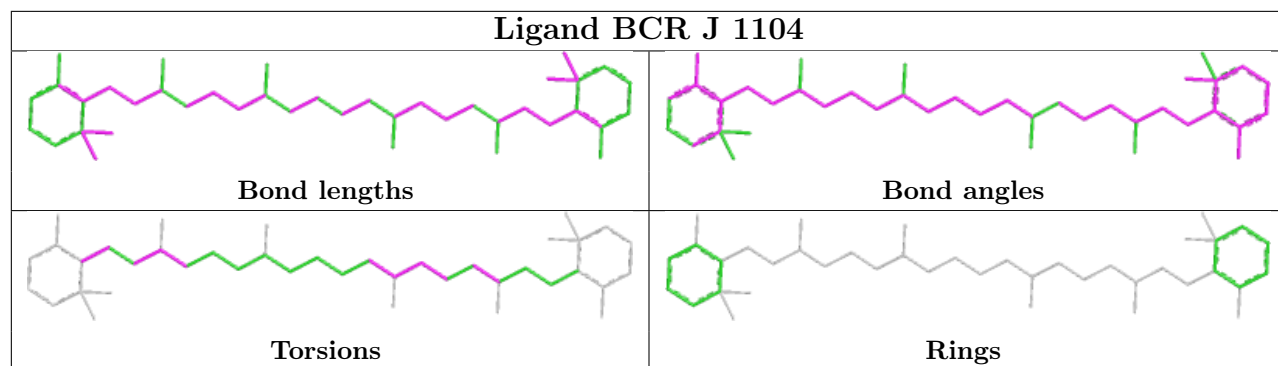


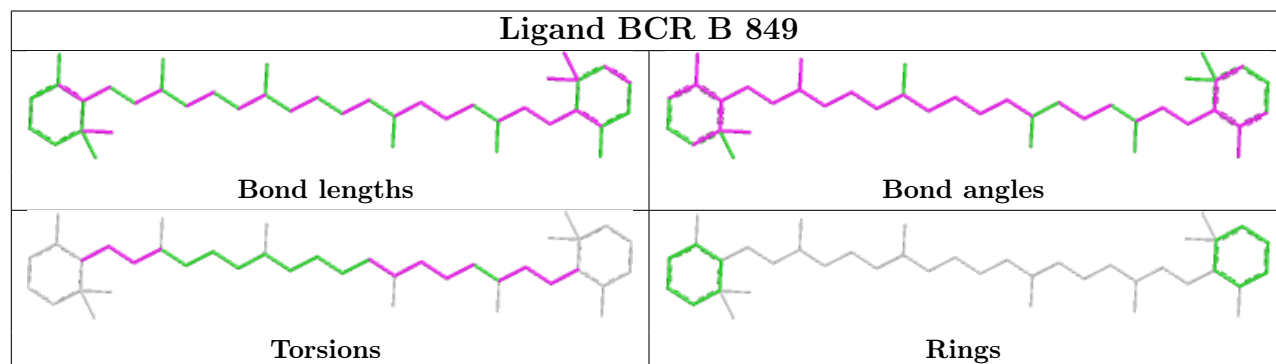
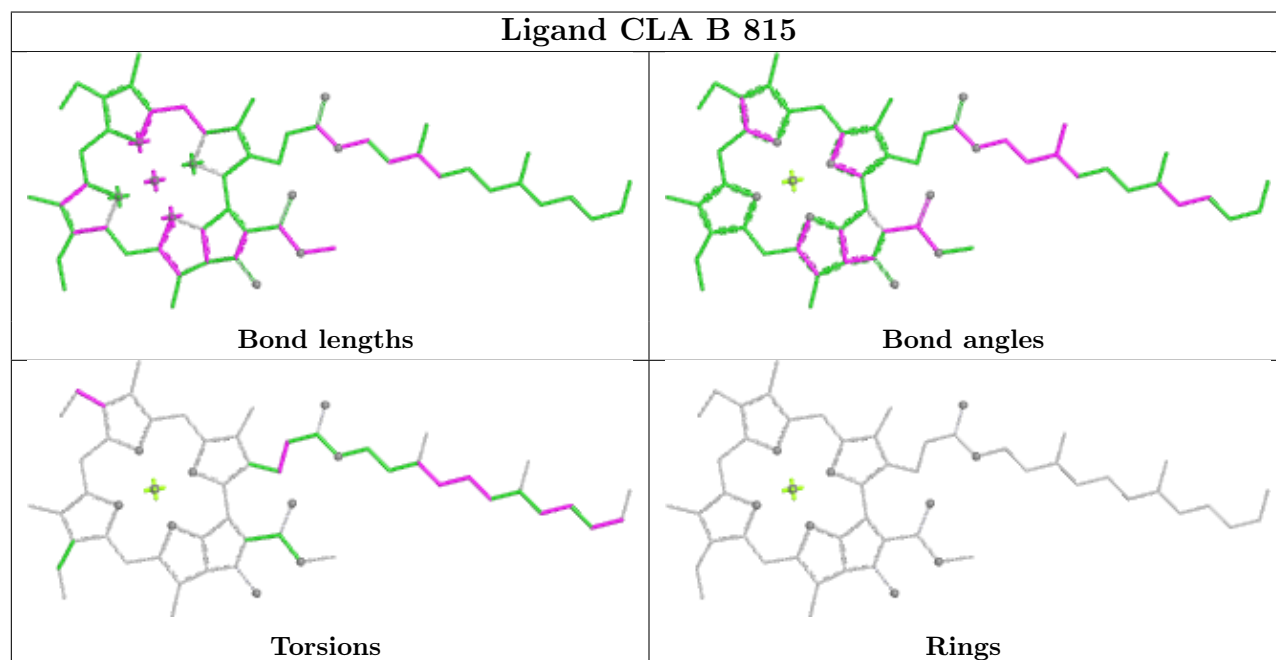
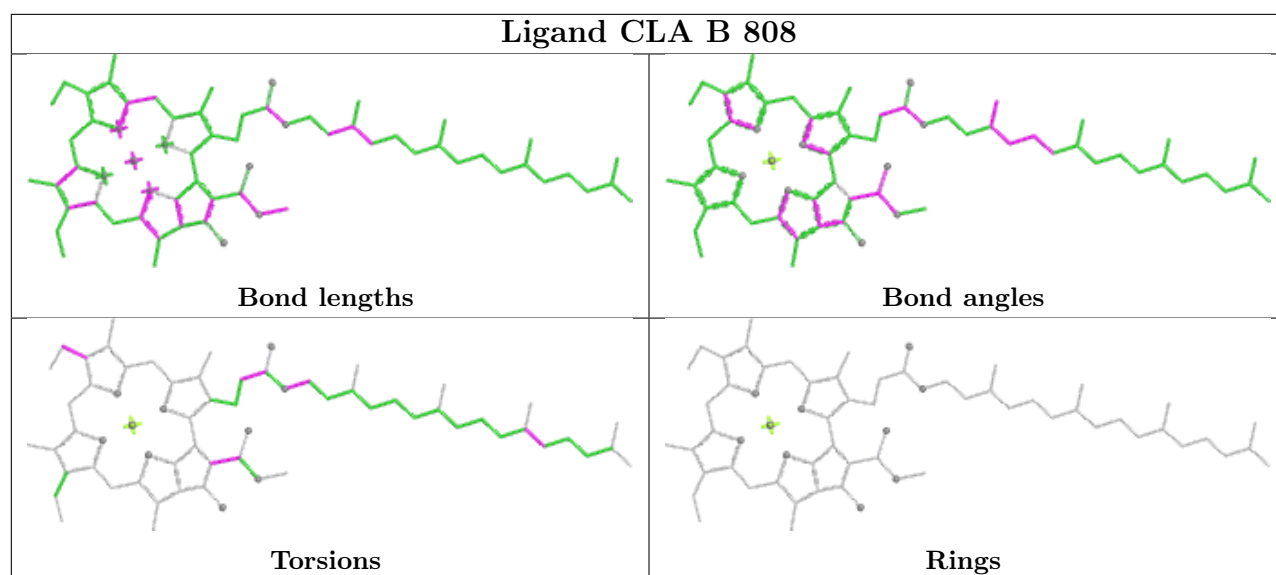
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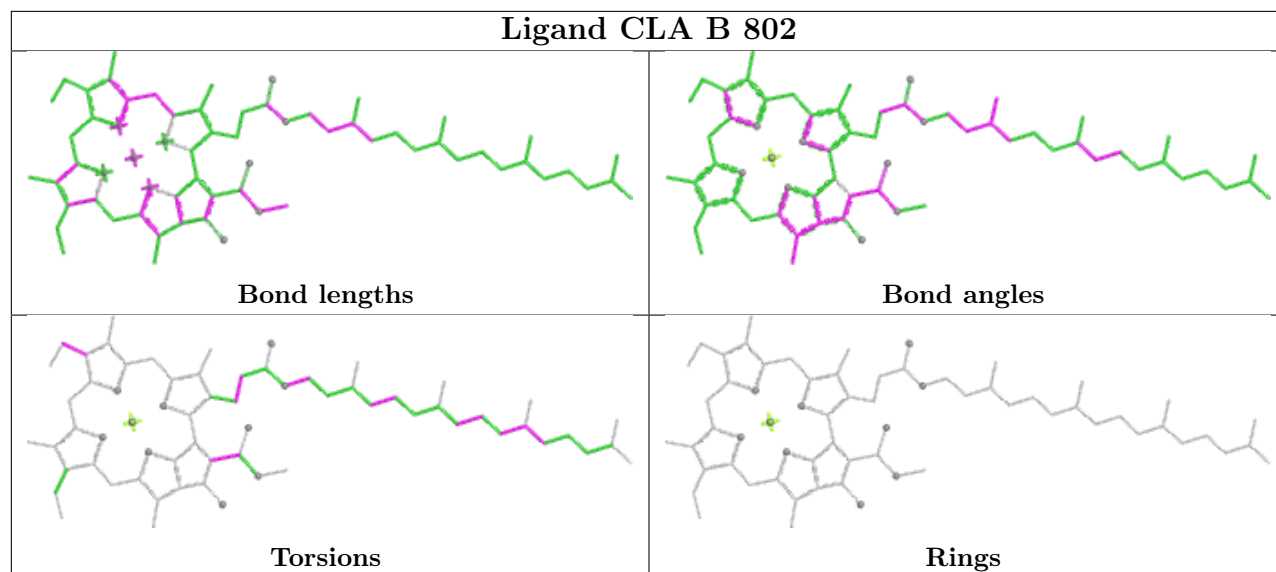
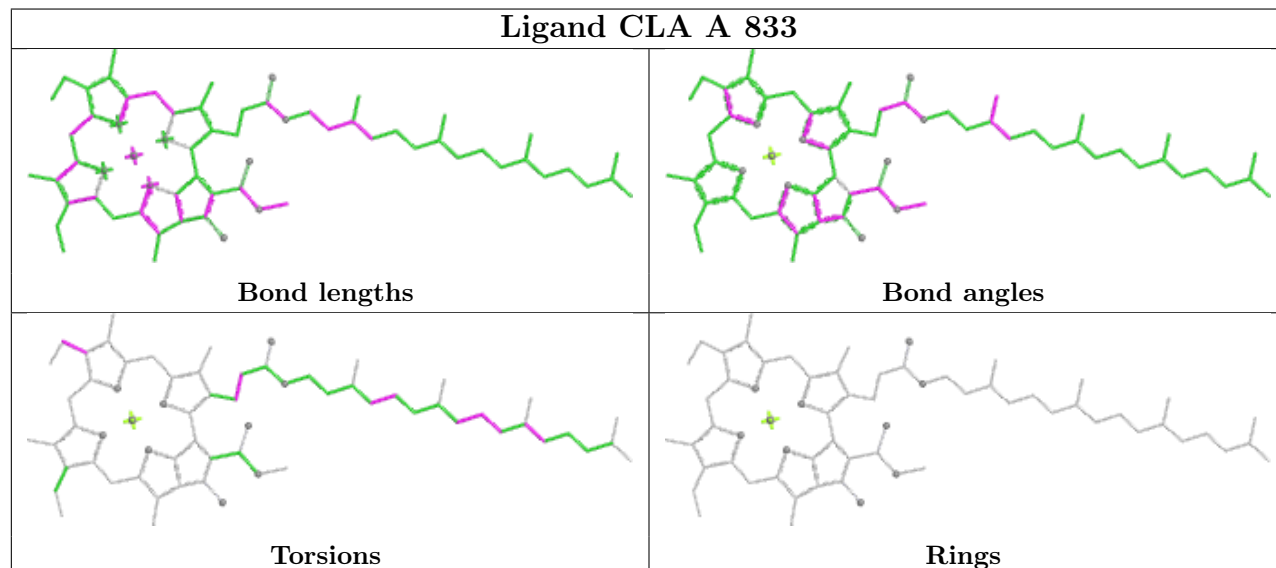


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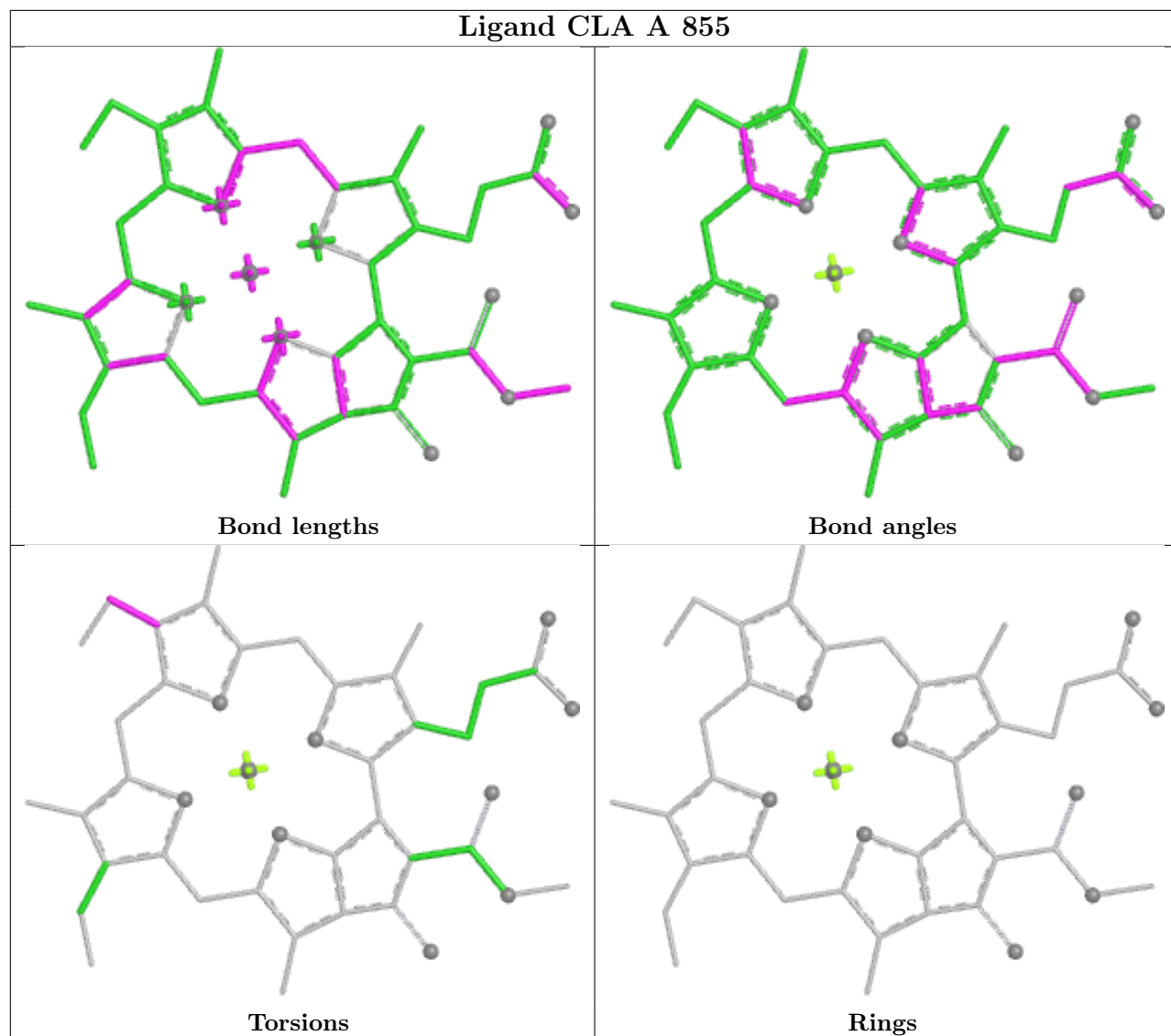




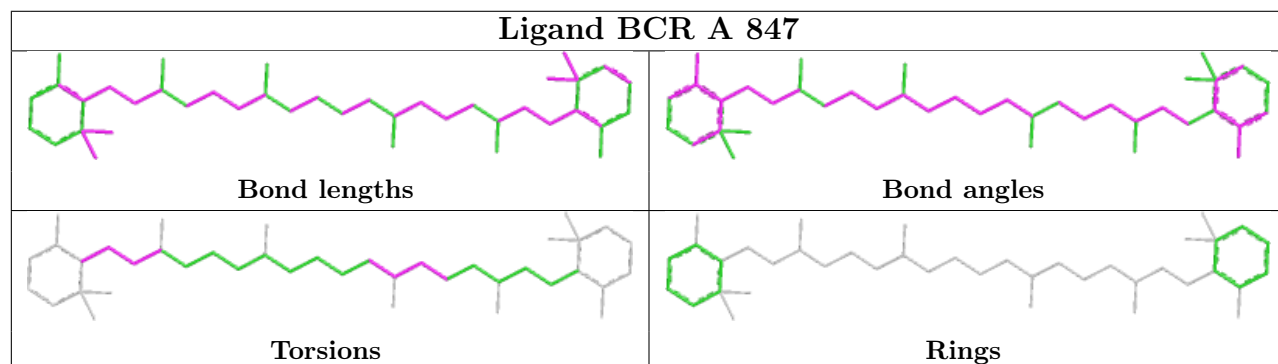


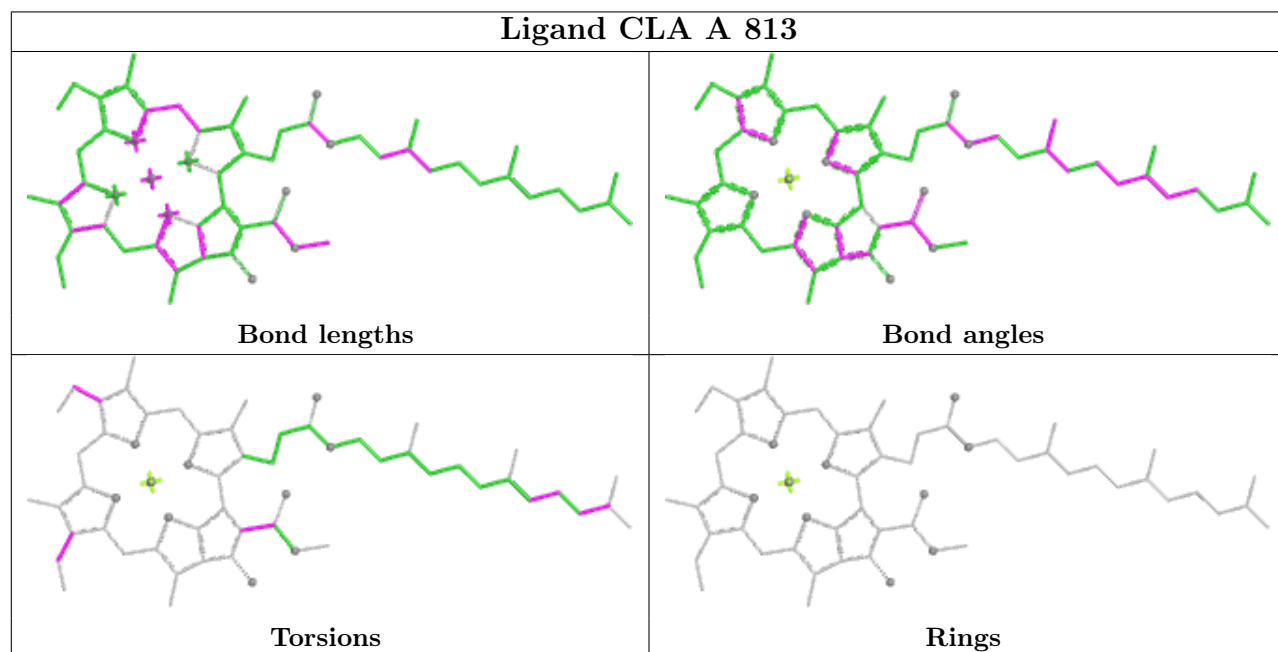
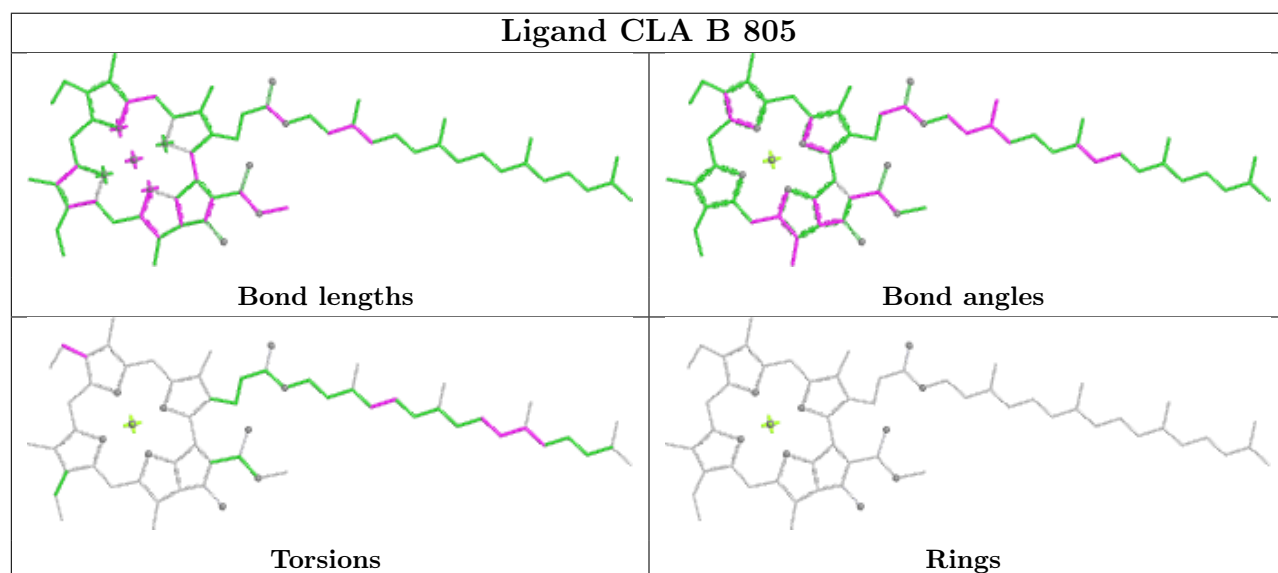
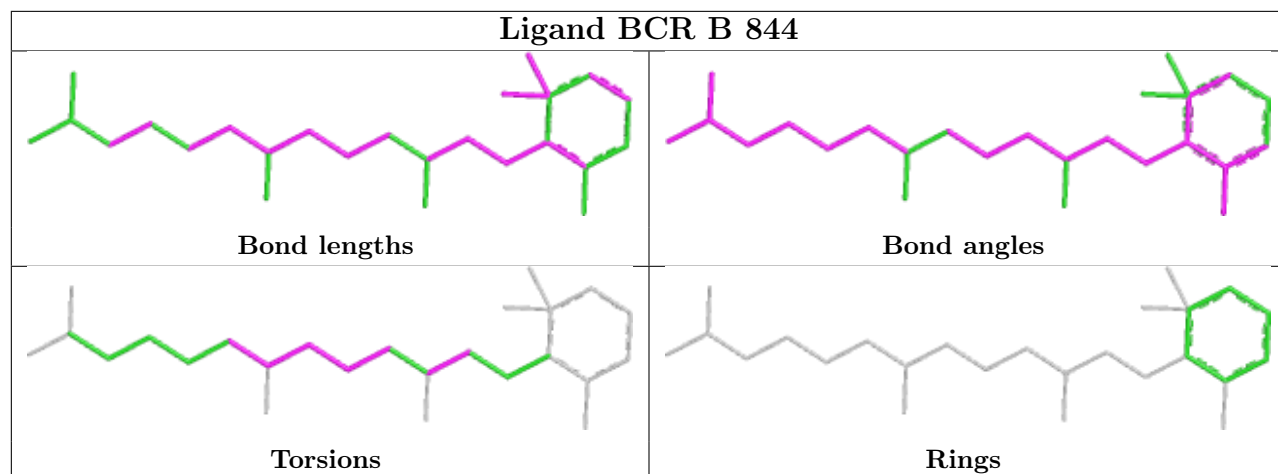
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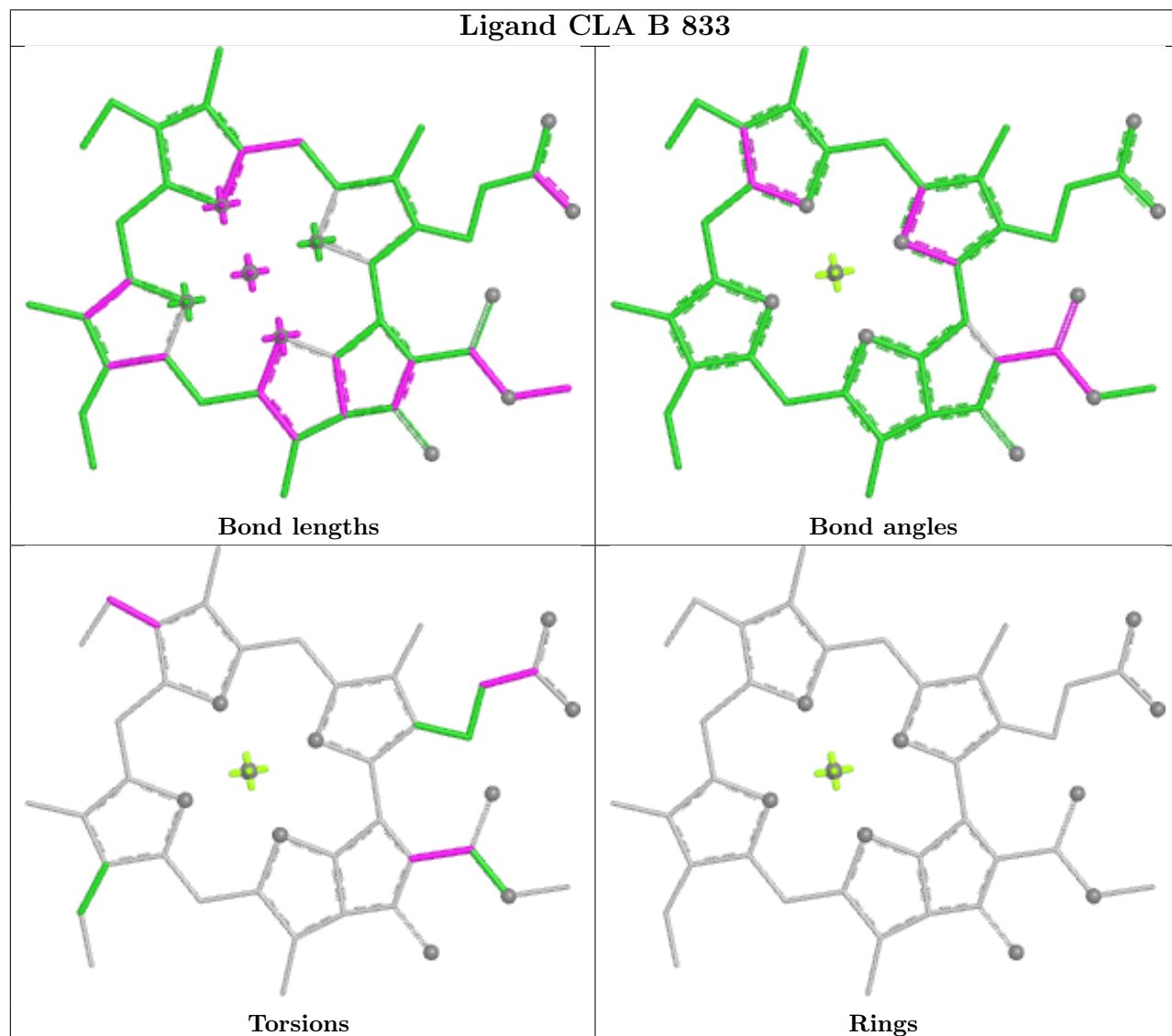
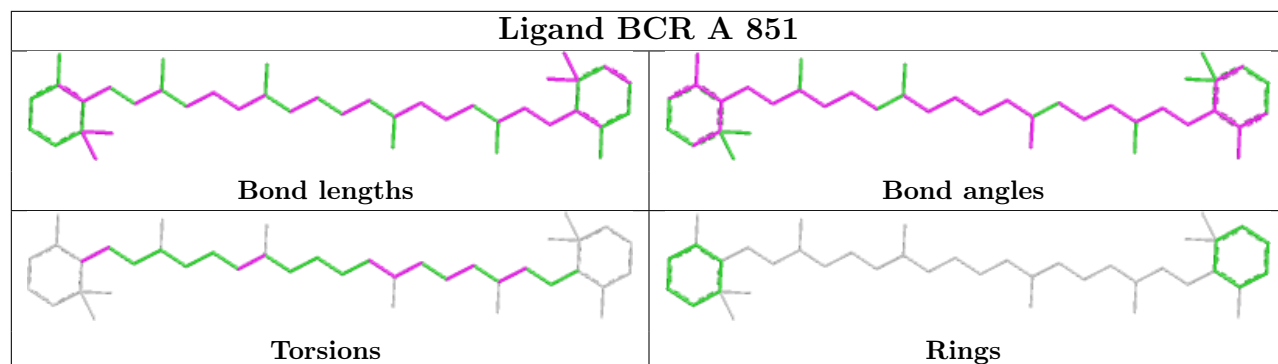
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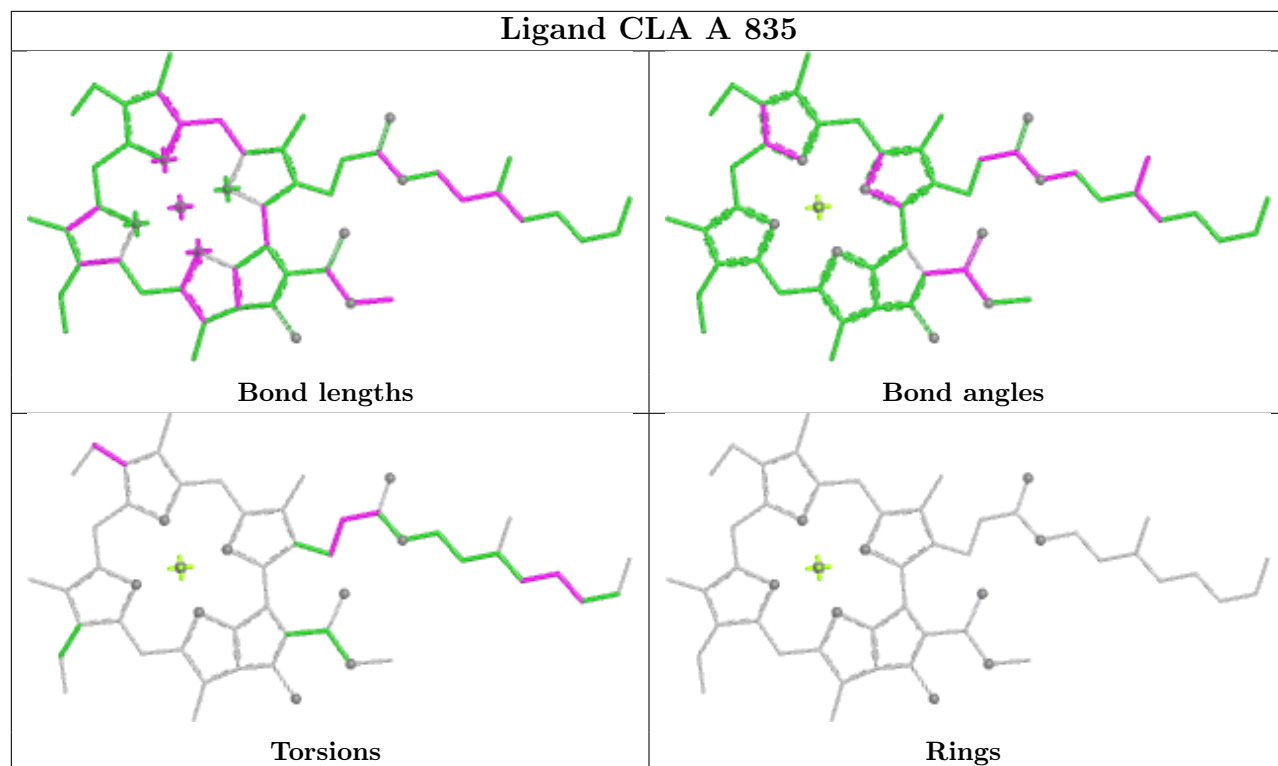
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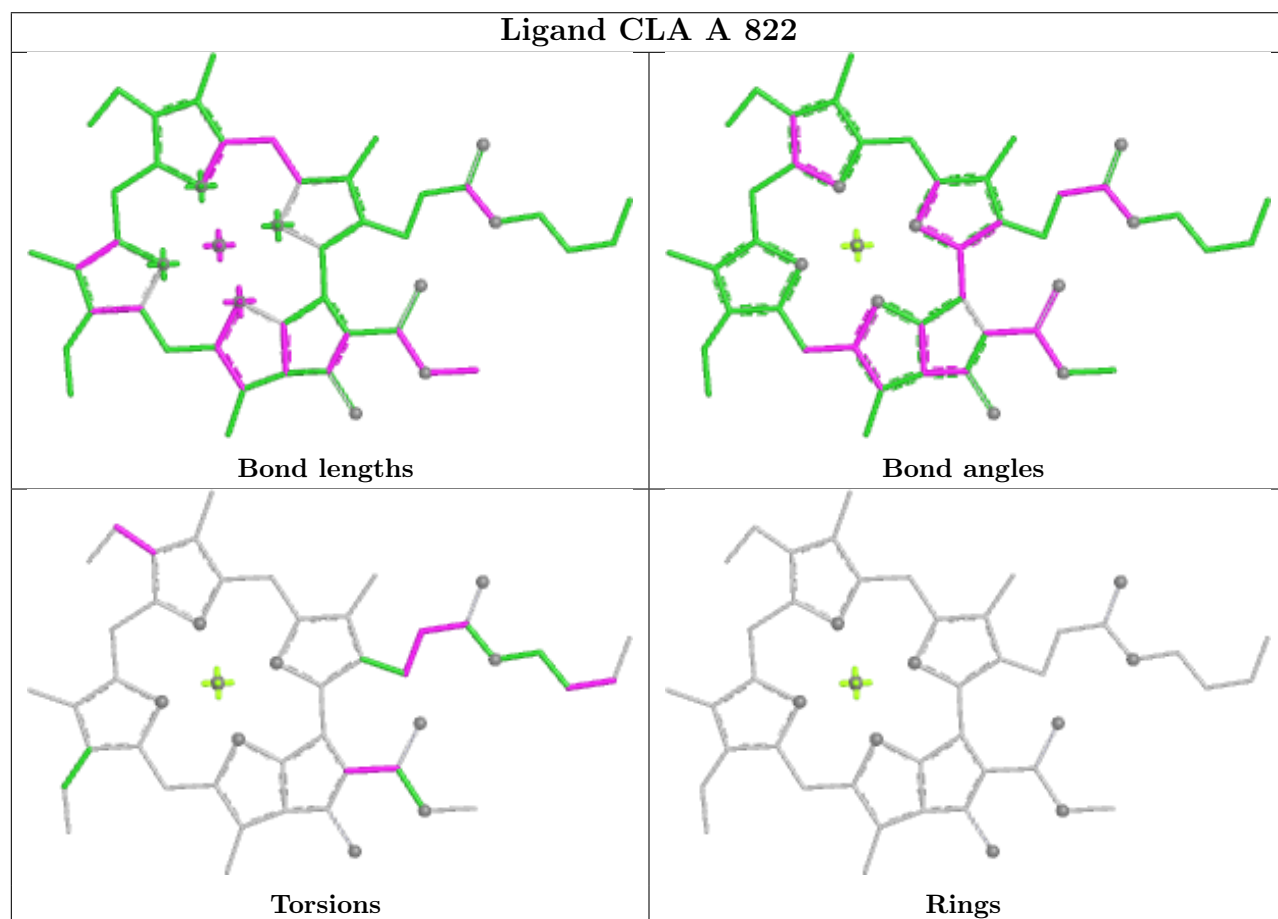


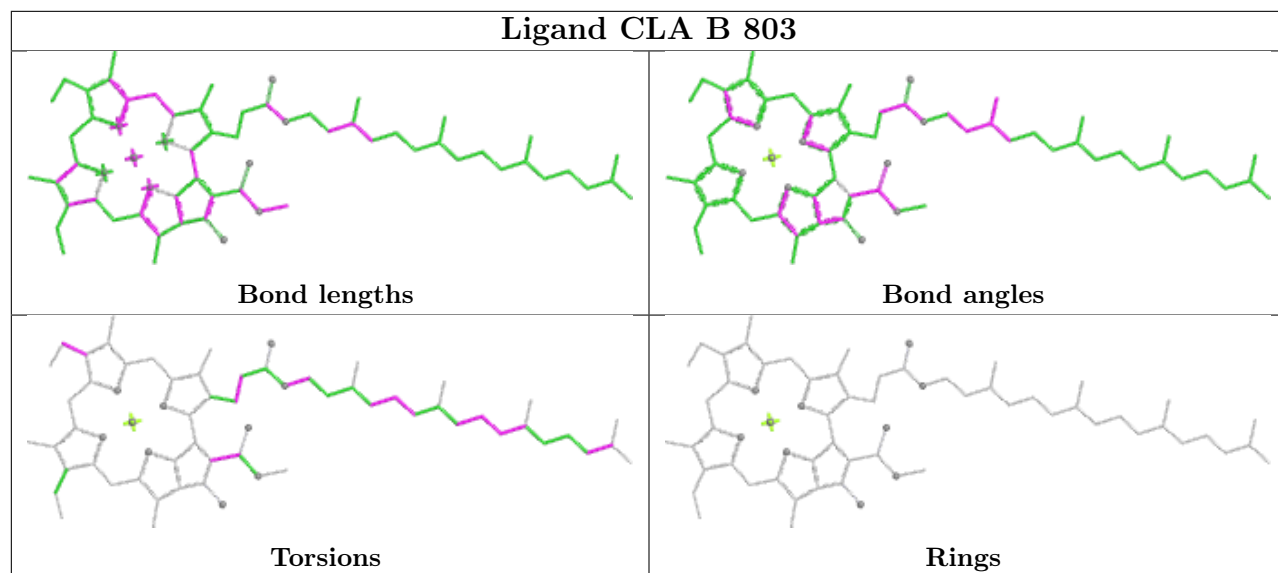
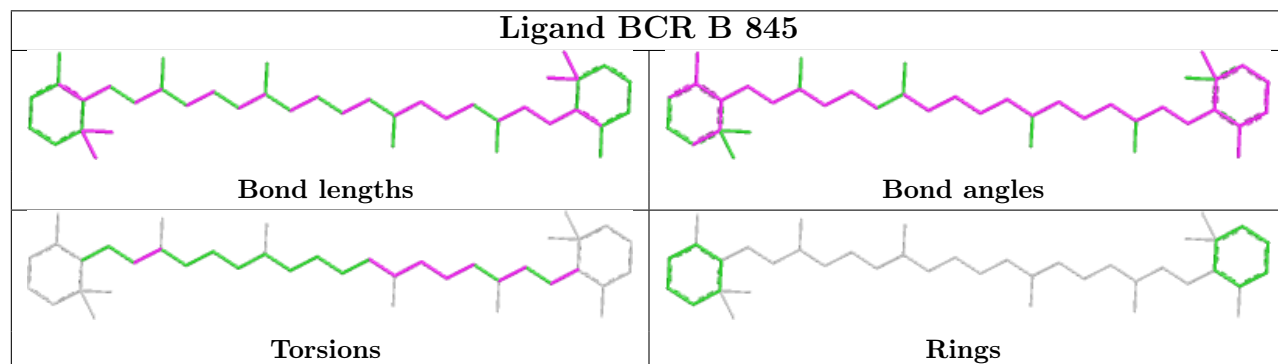
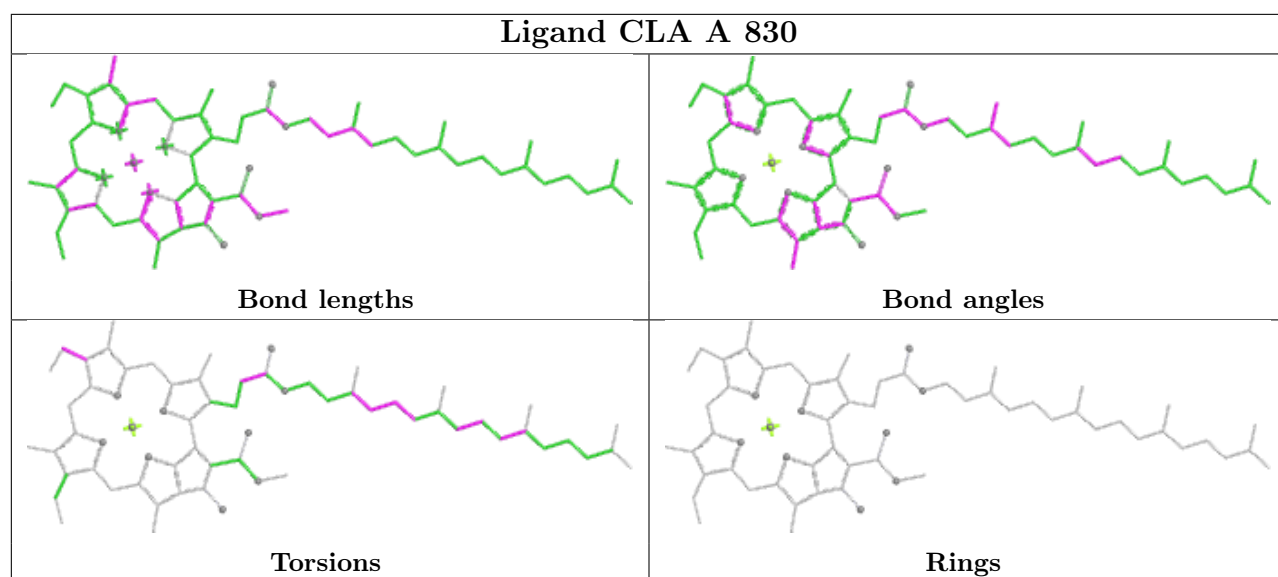


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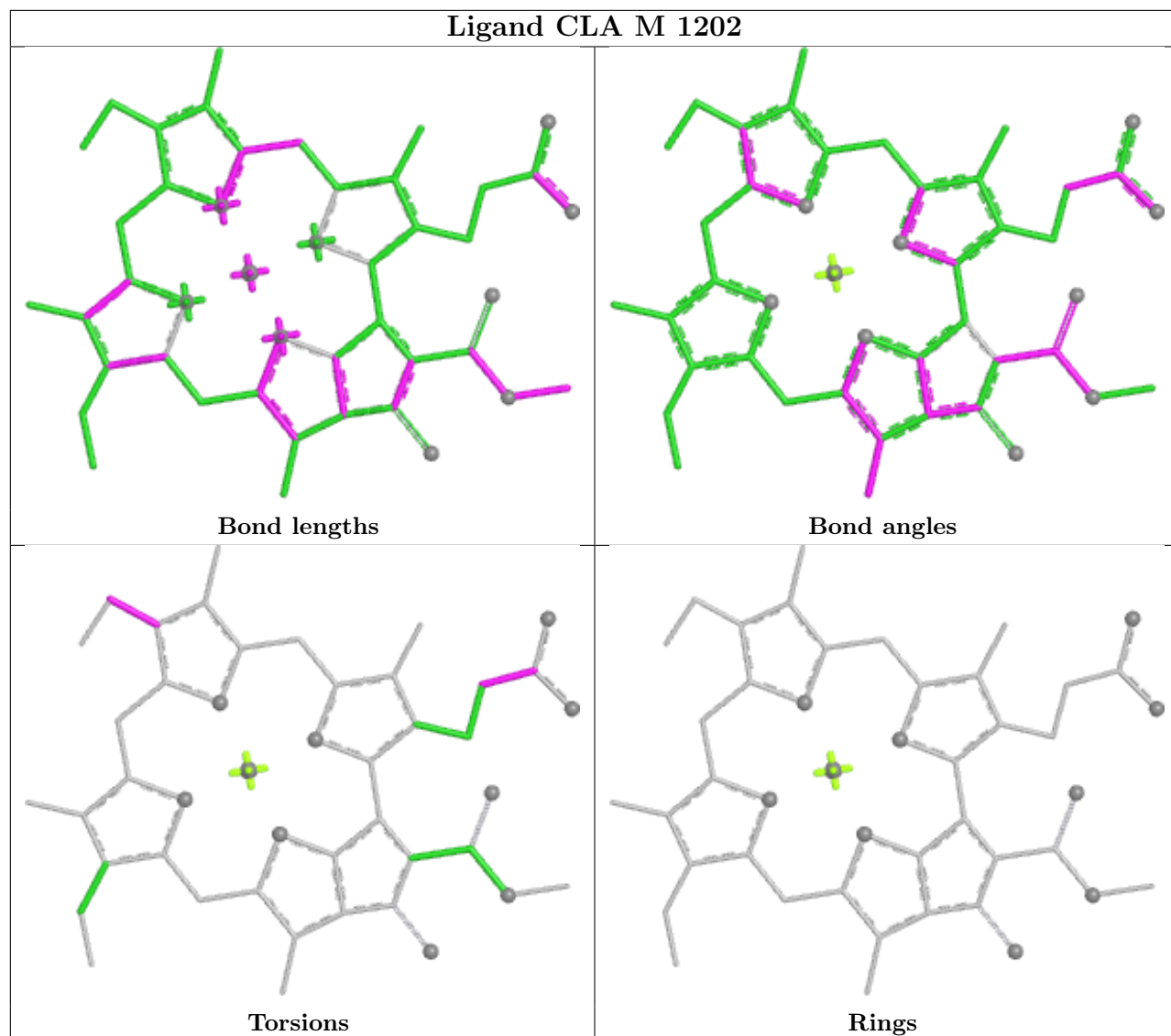


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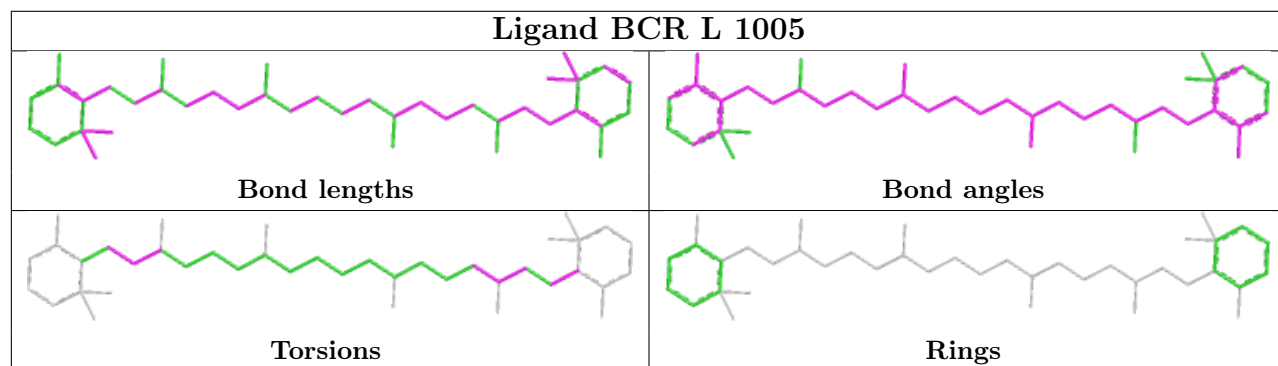




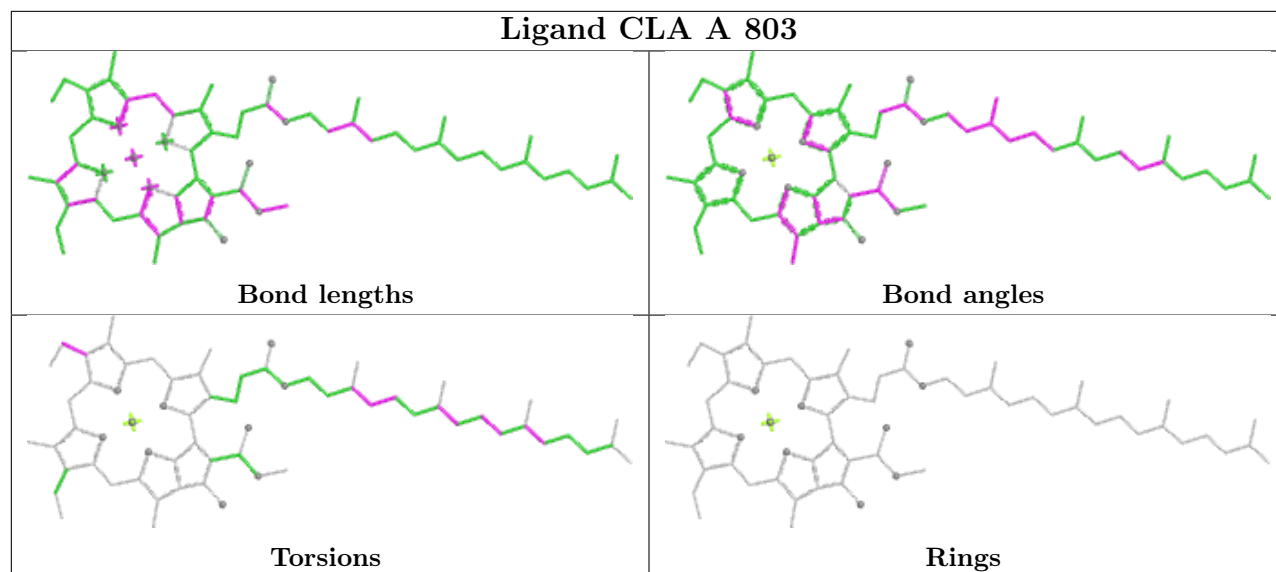
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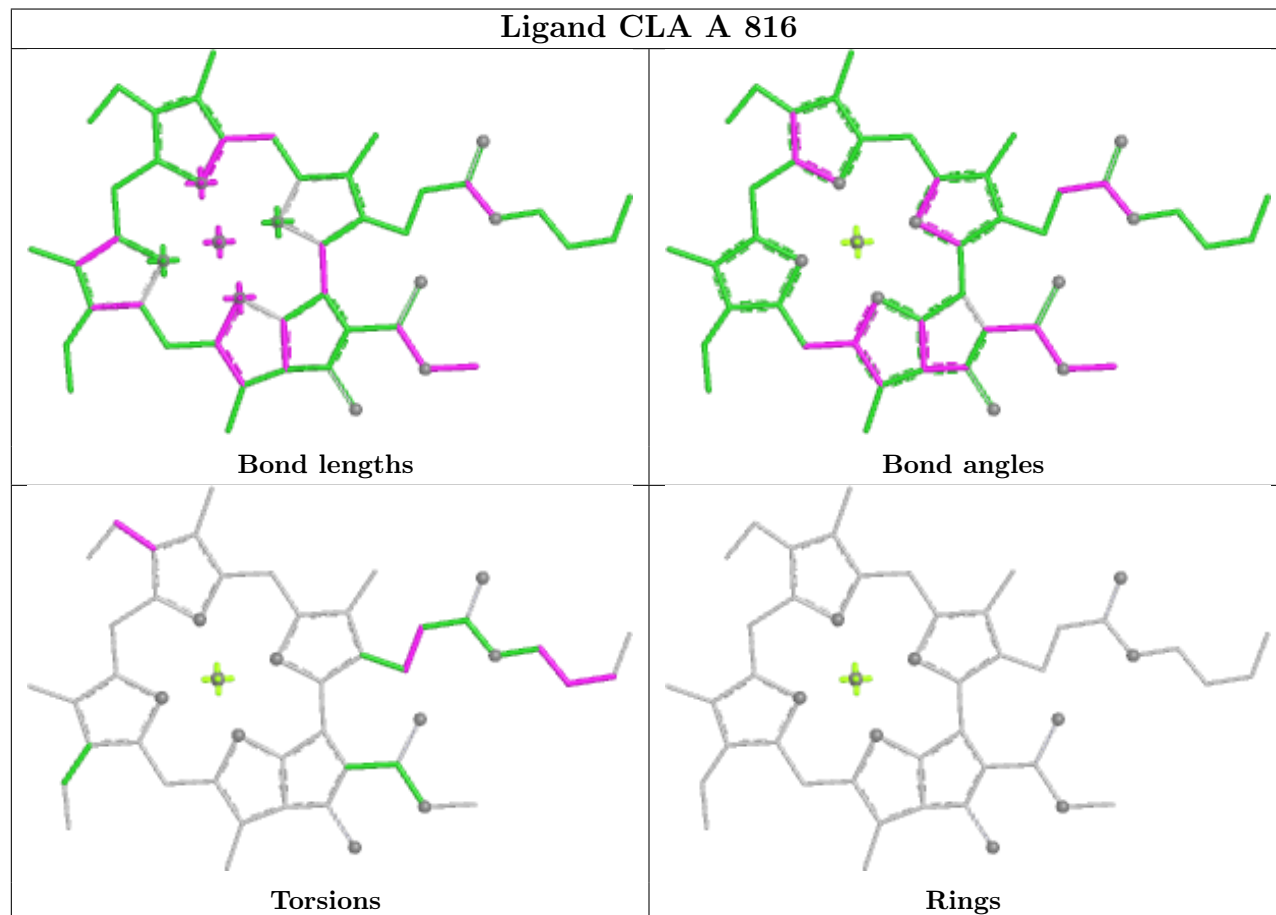
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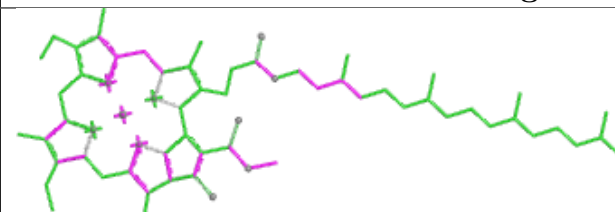
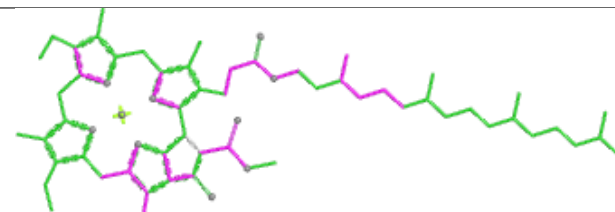
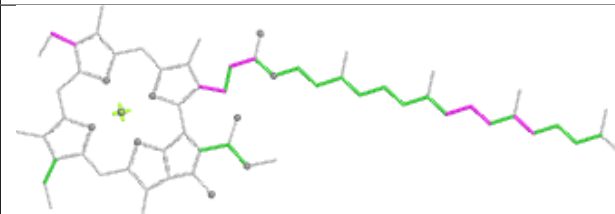
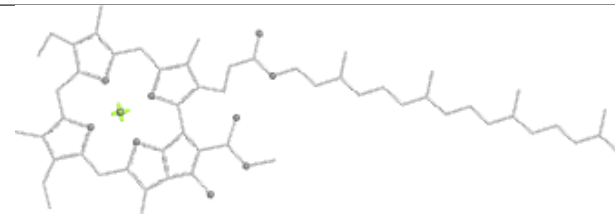


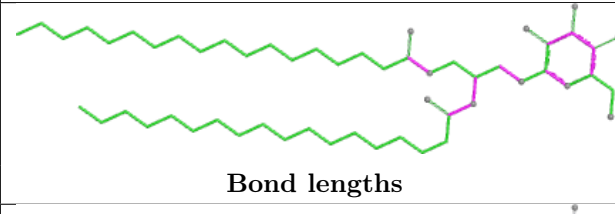
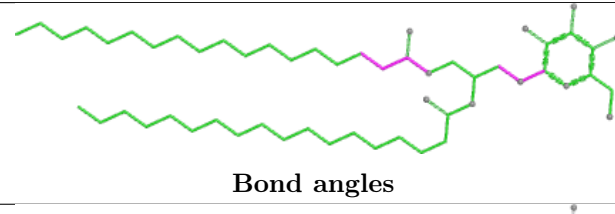
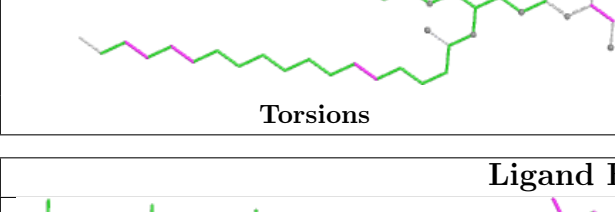
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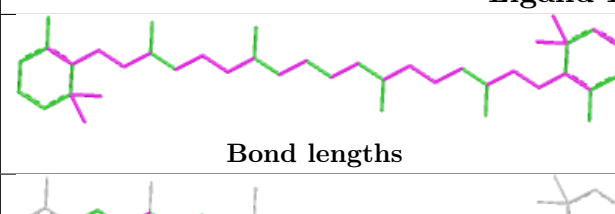
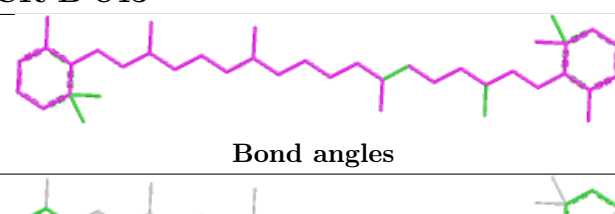
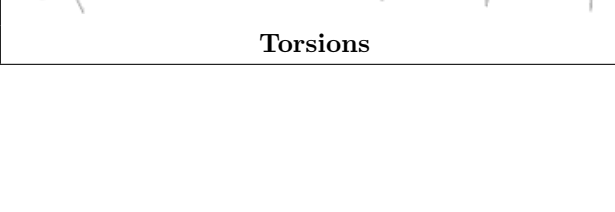
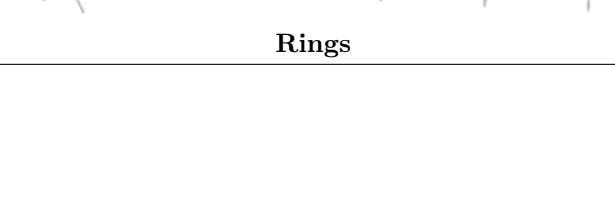


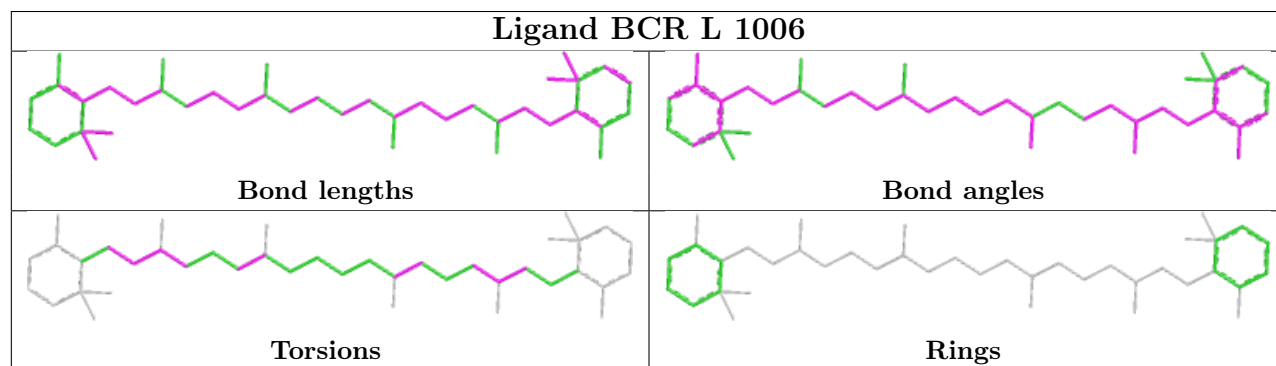
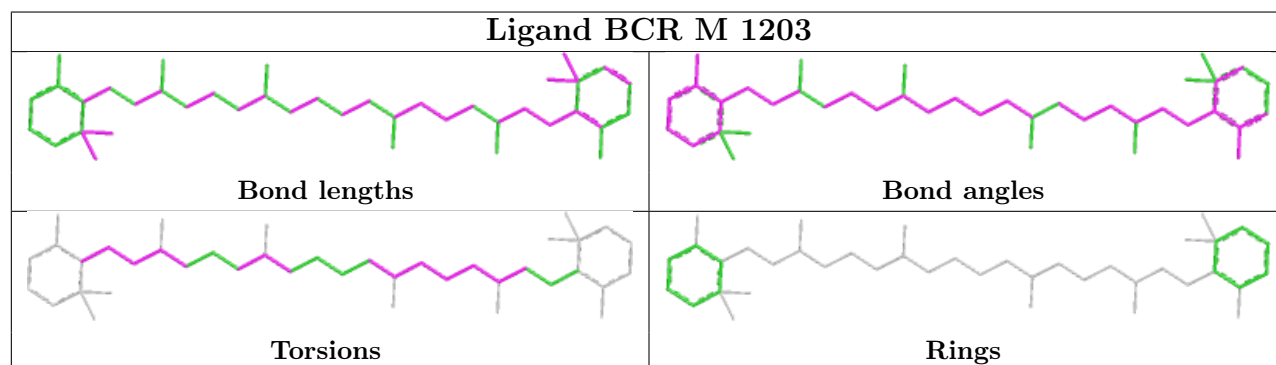
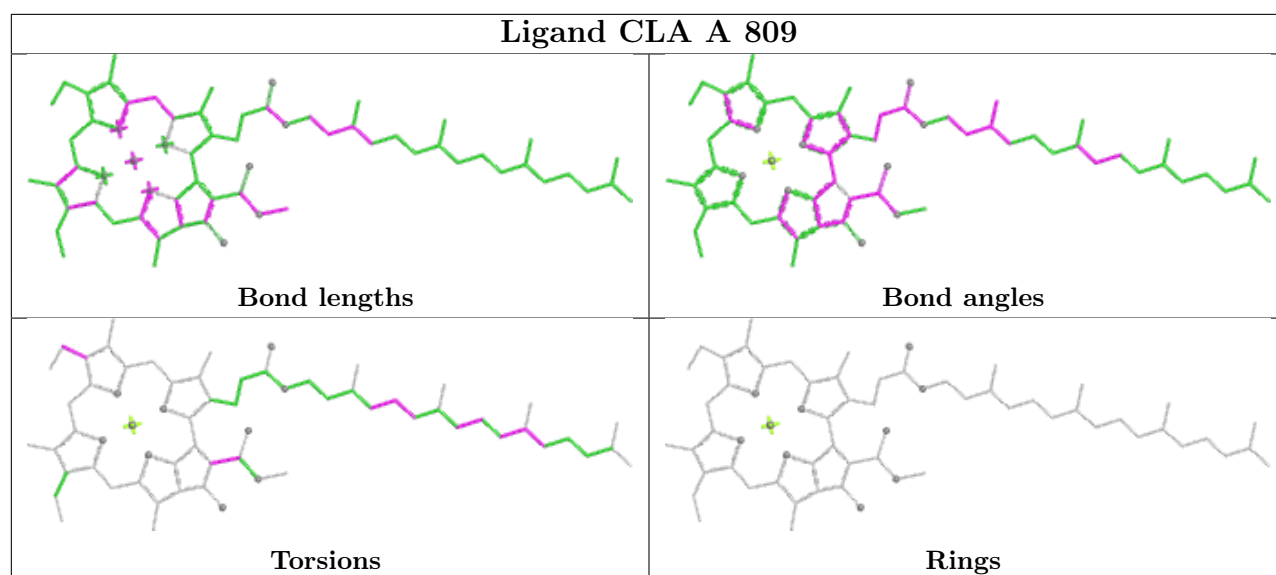
Ligand CLA A 816



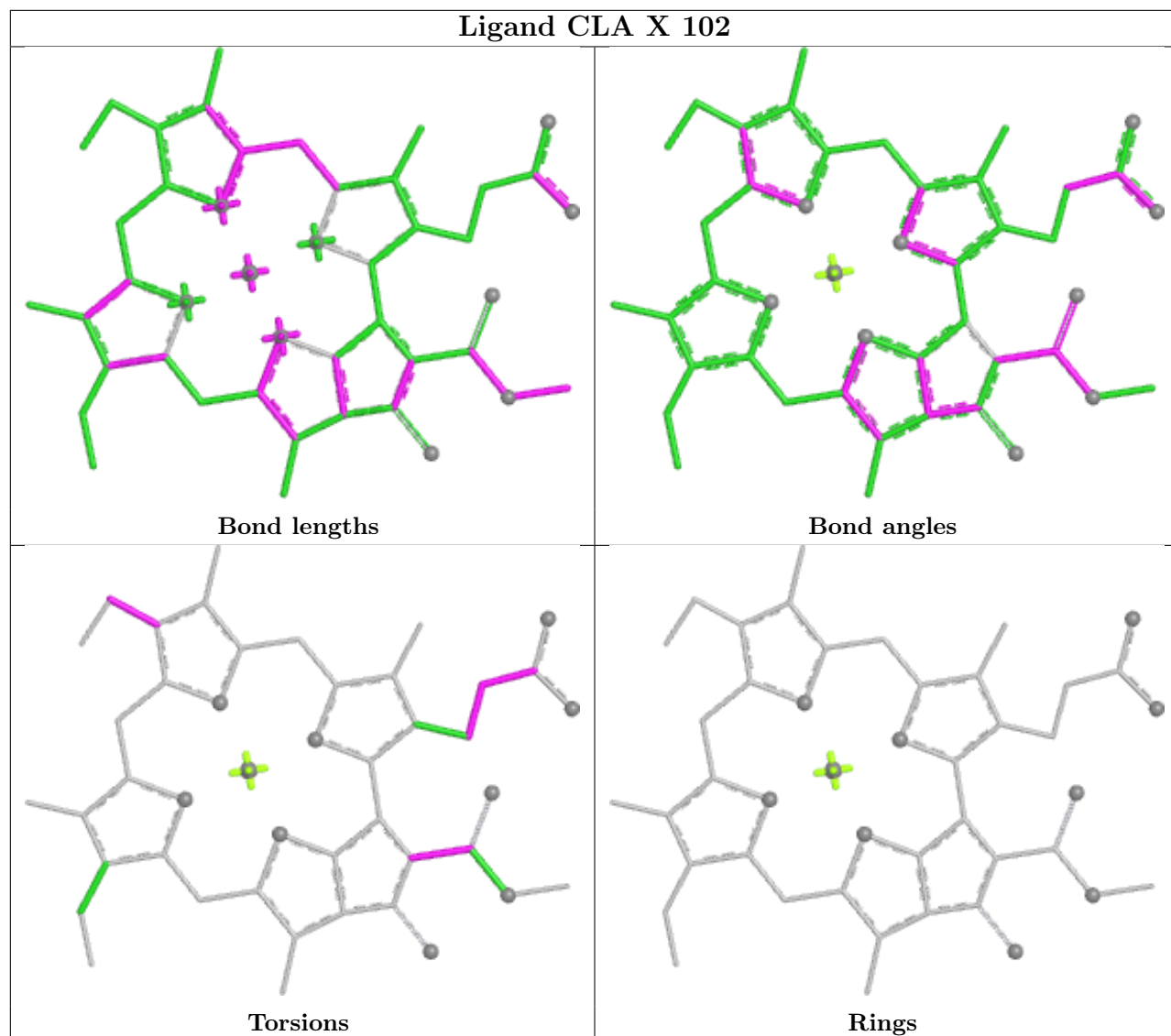
Ligand CLA A 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG B 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

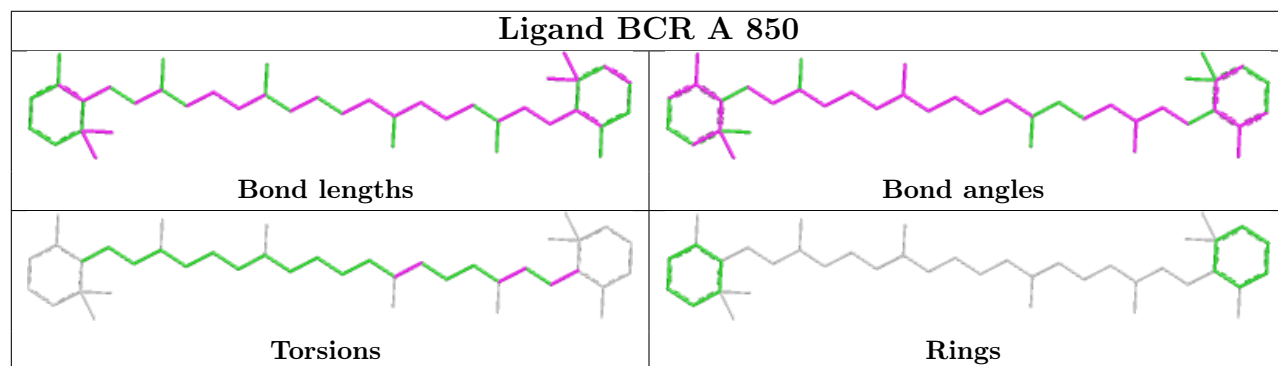
Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings



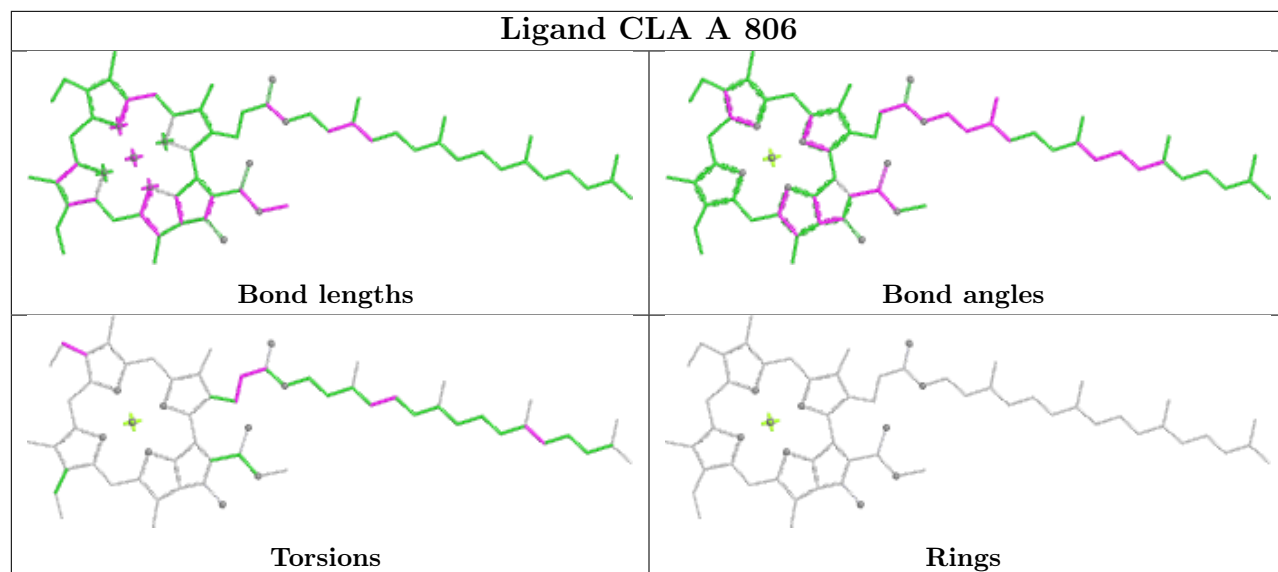
Ligand CLA X 102



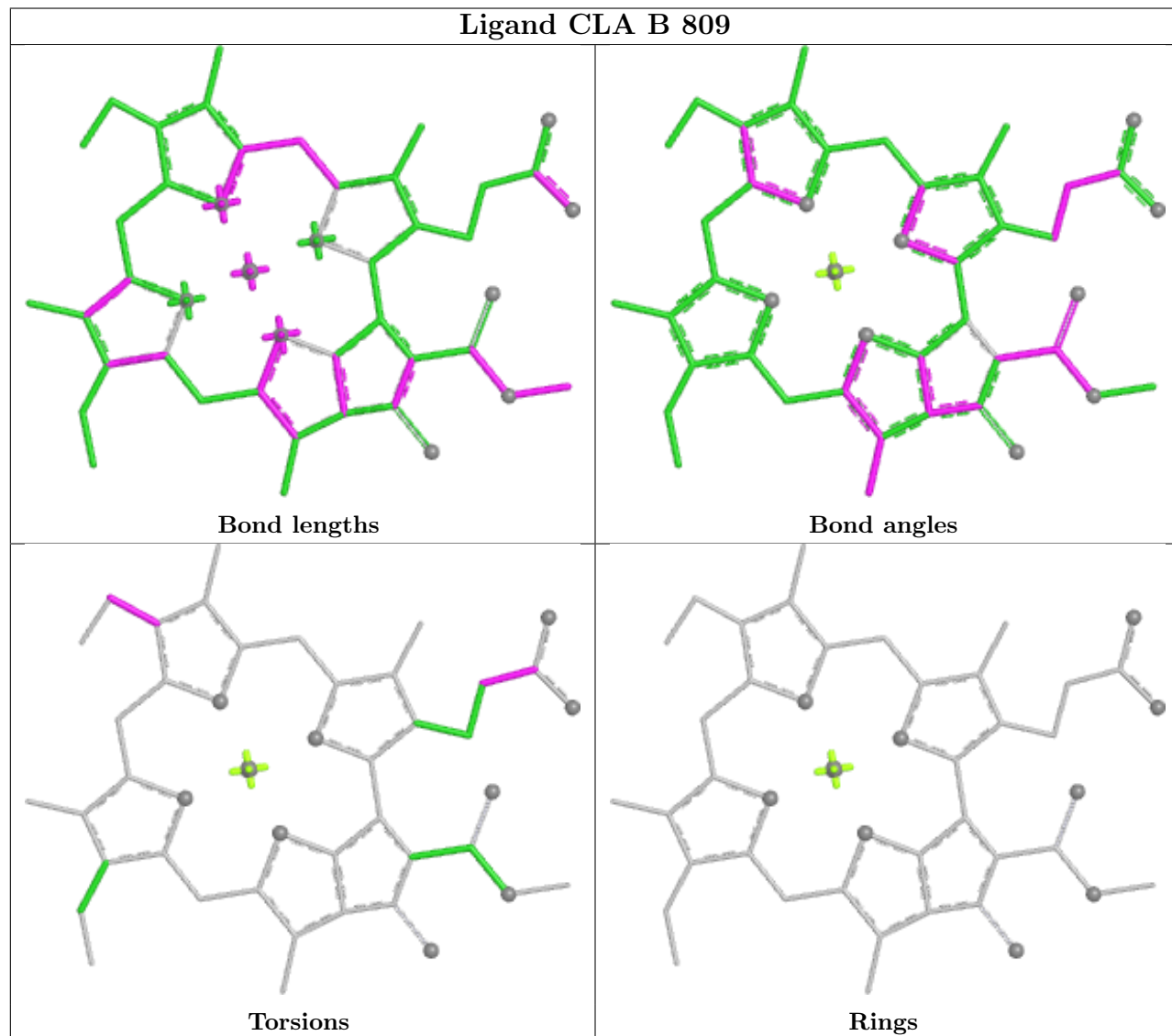
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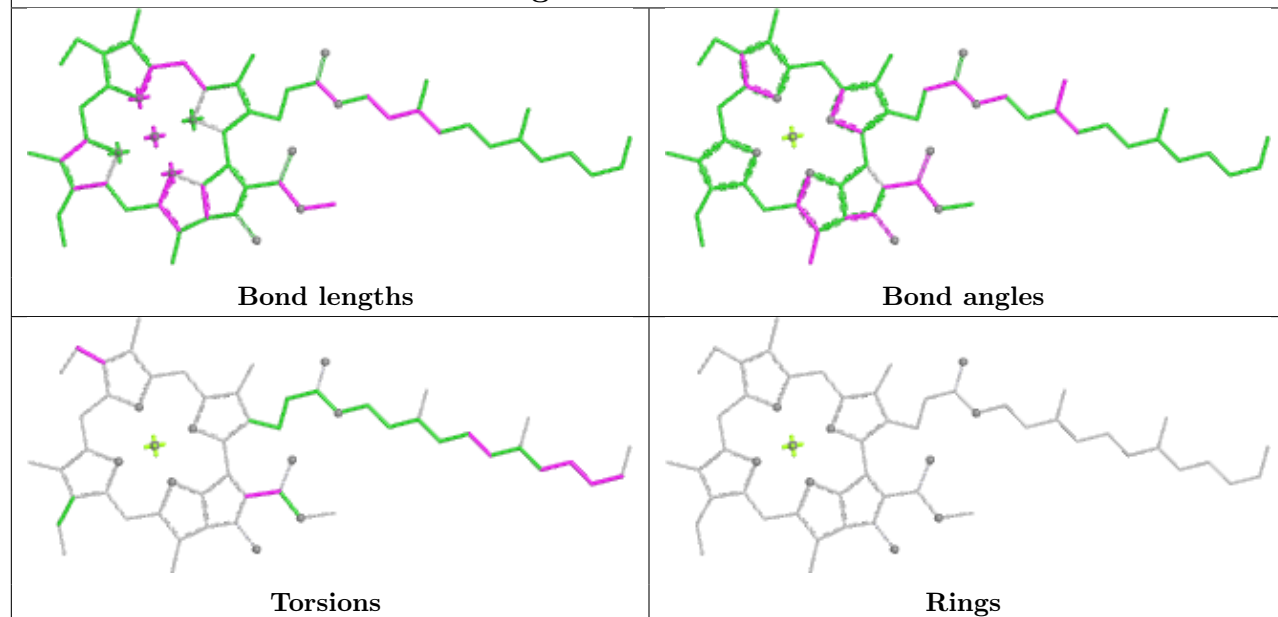
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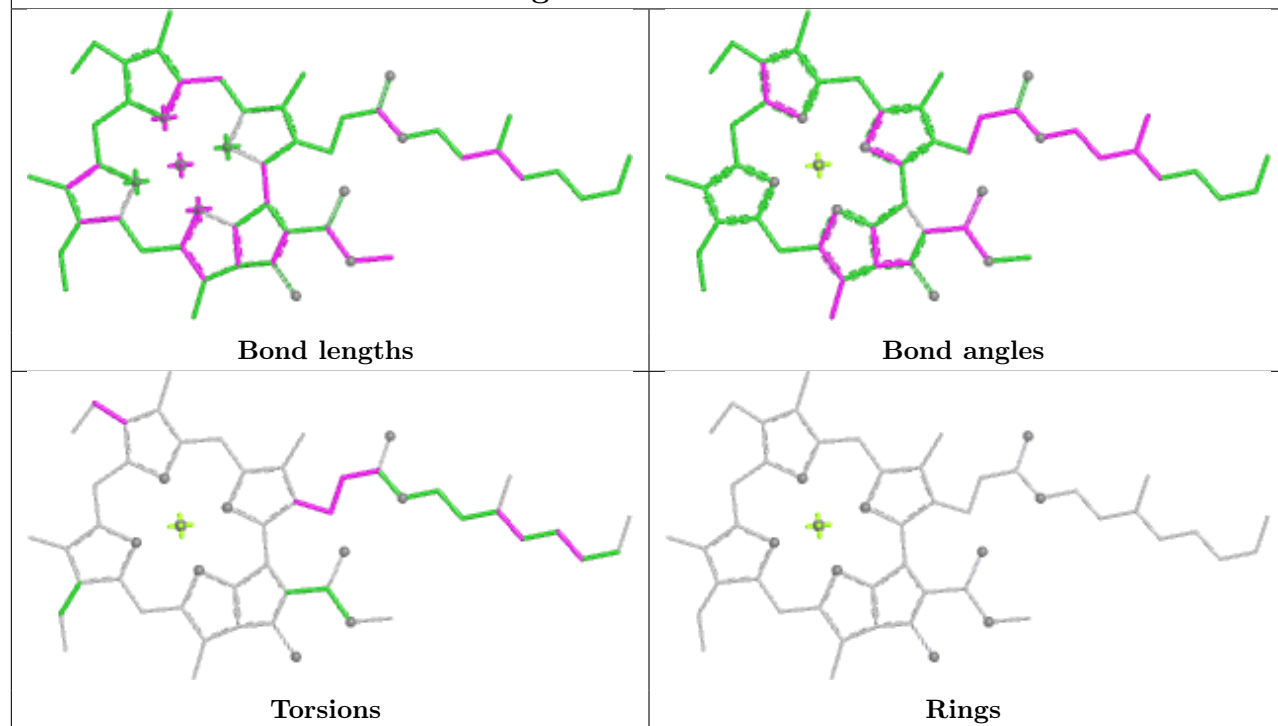
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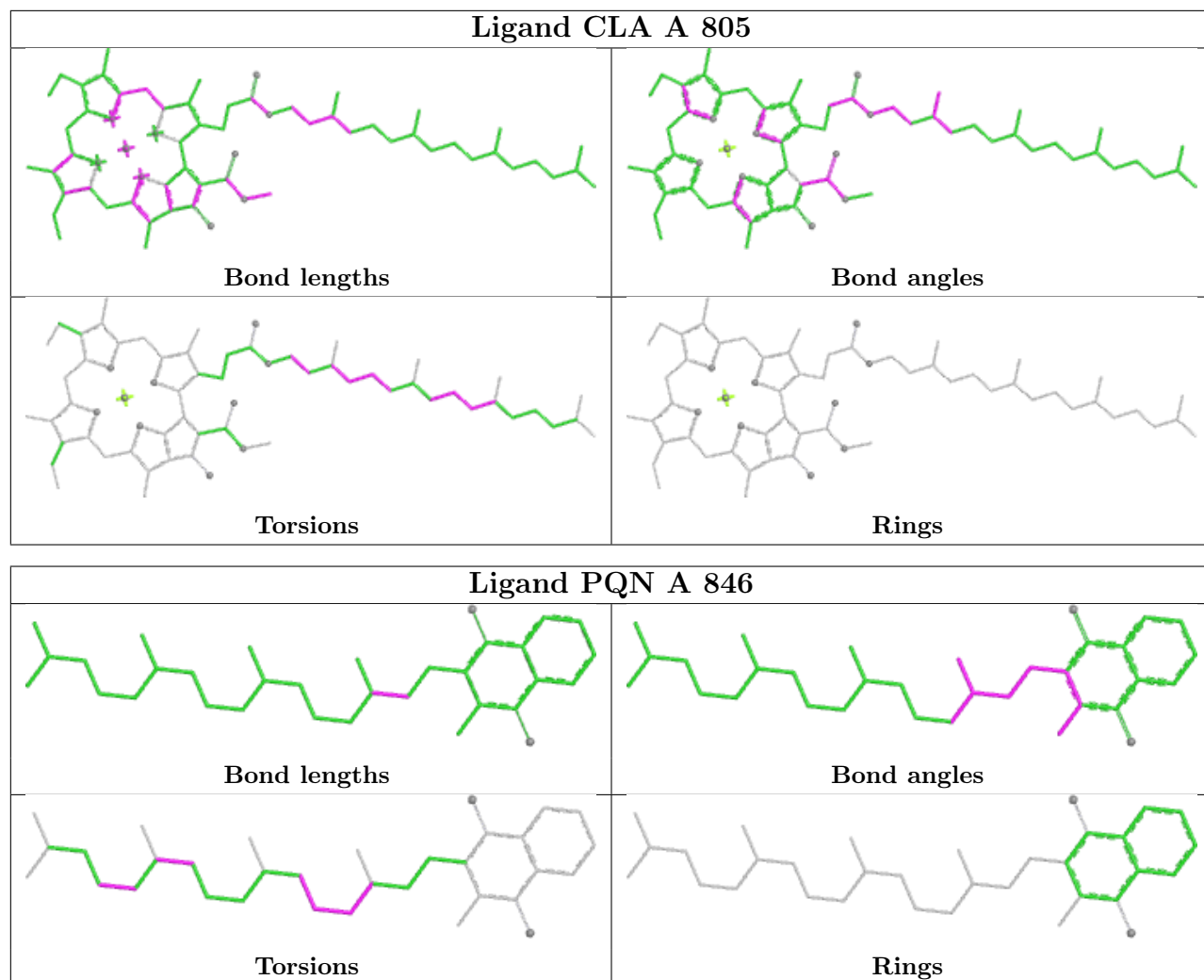


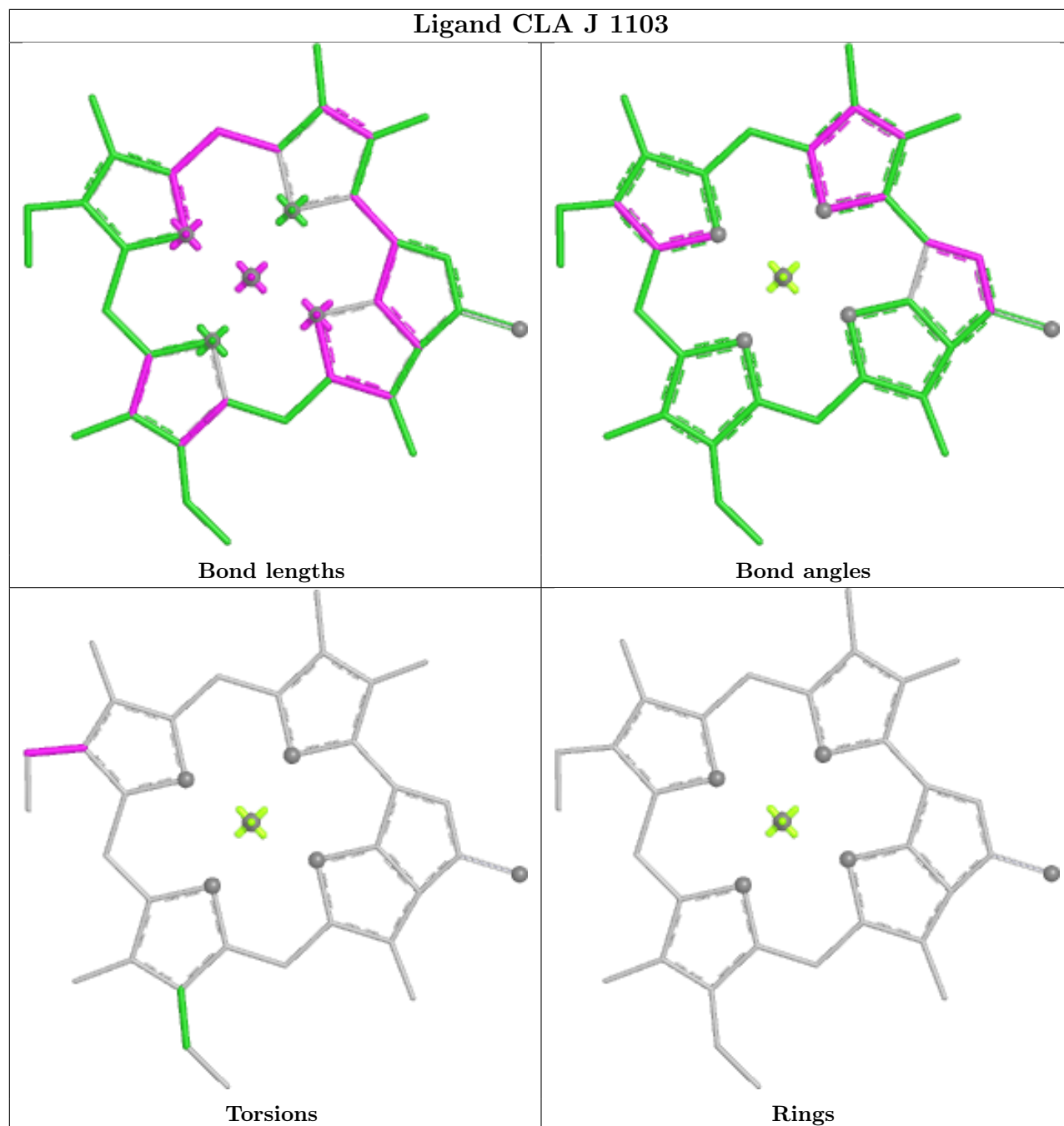
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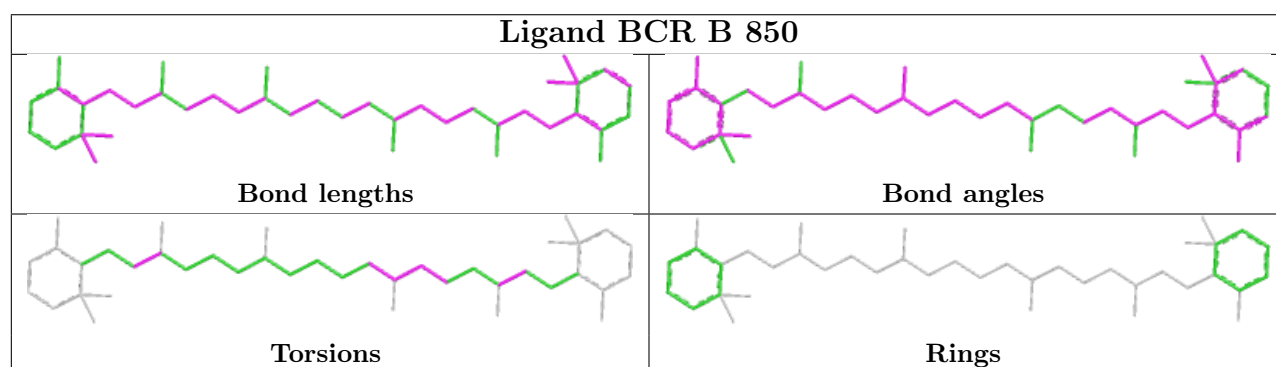
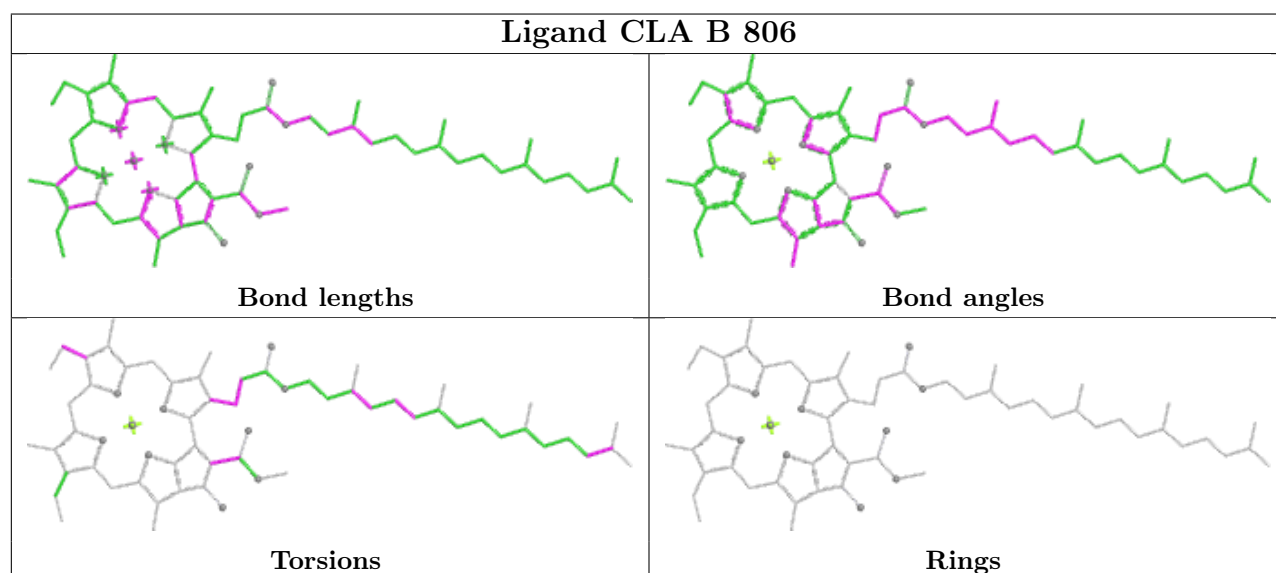
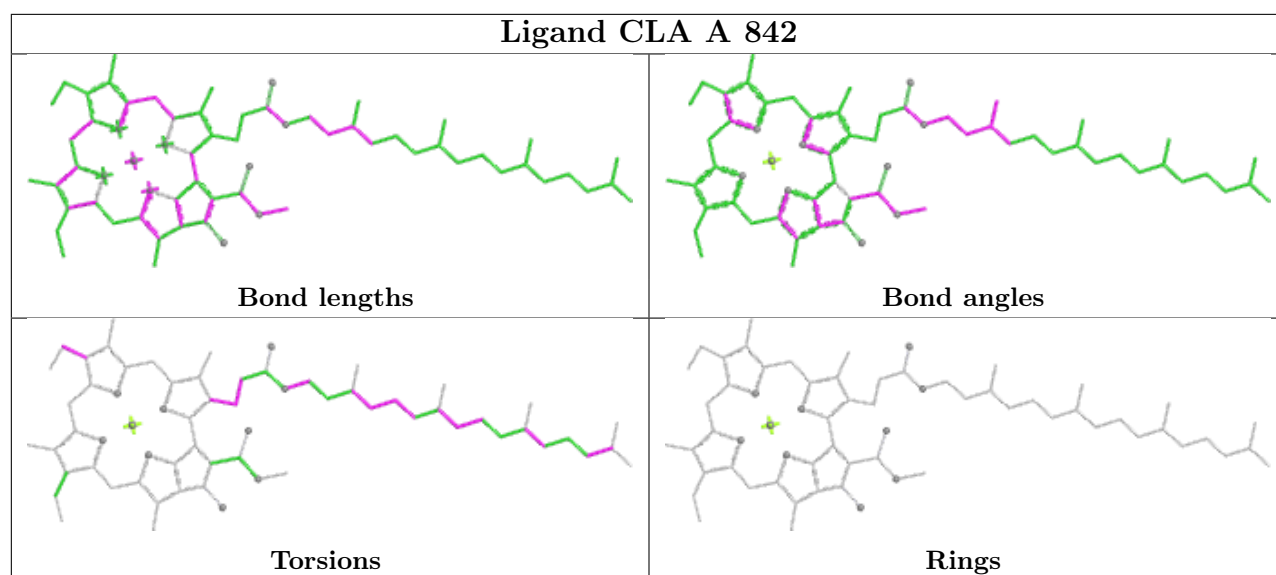


Ligand CLA A 812

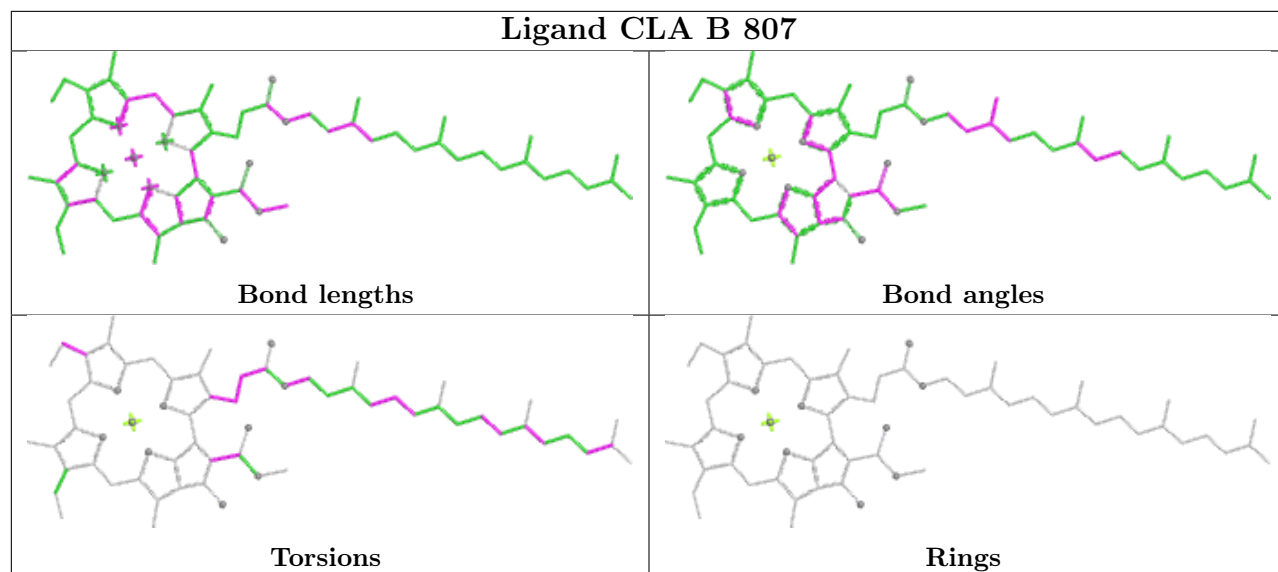




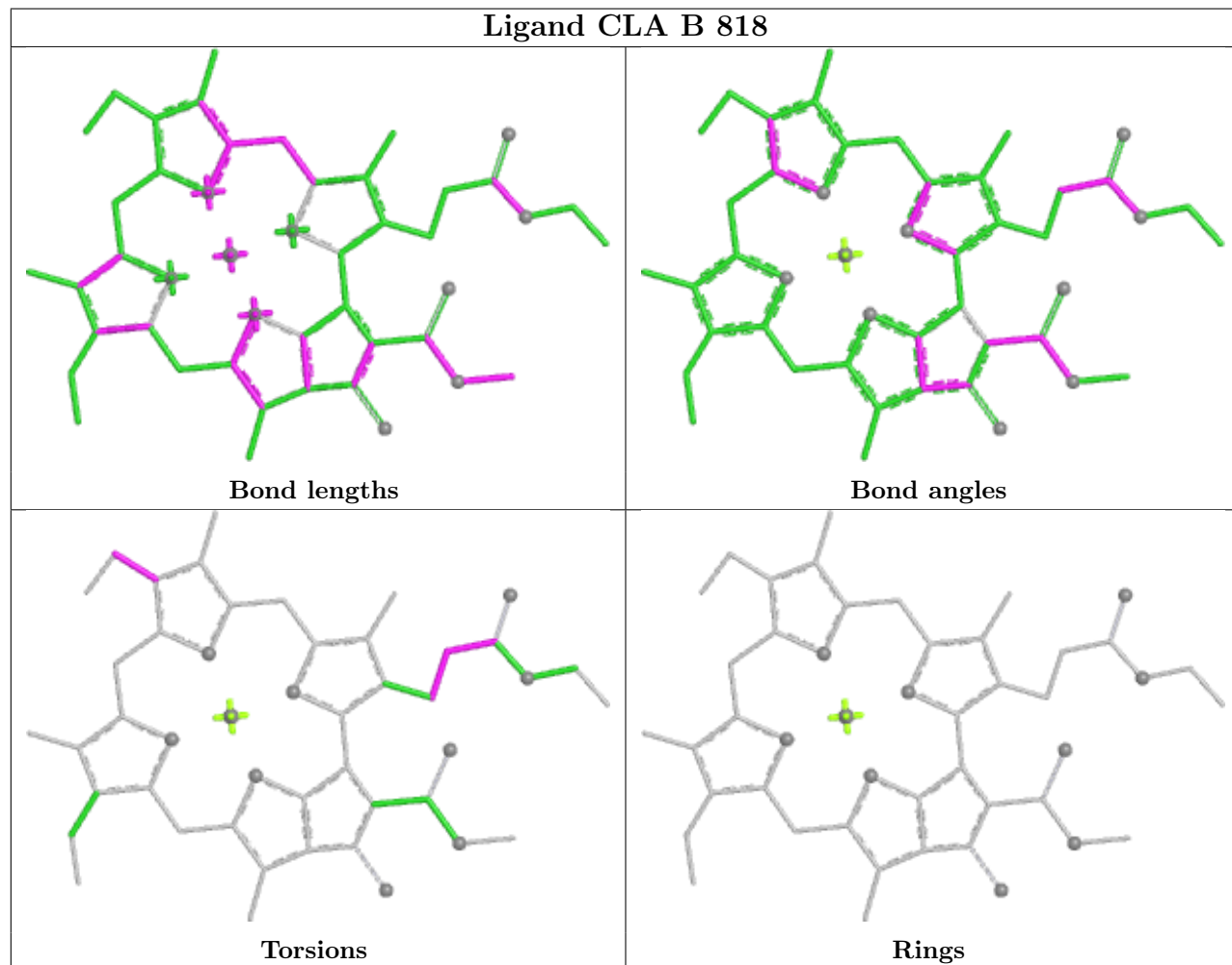




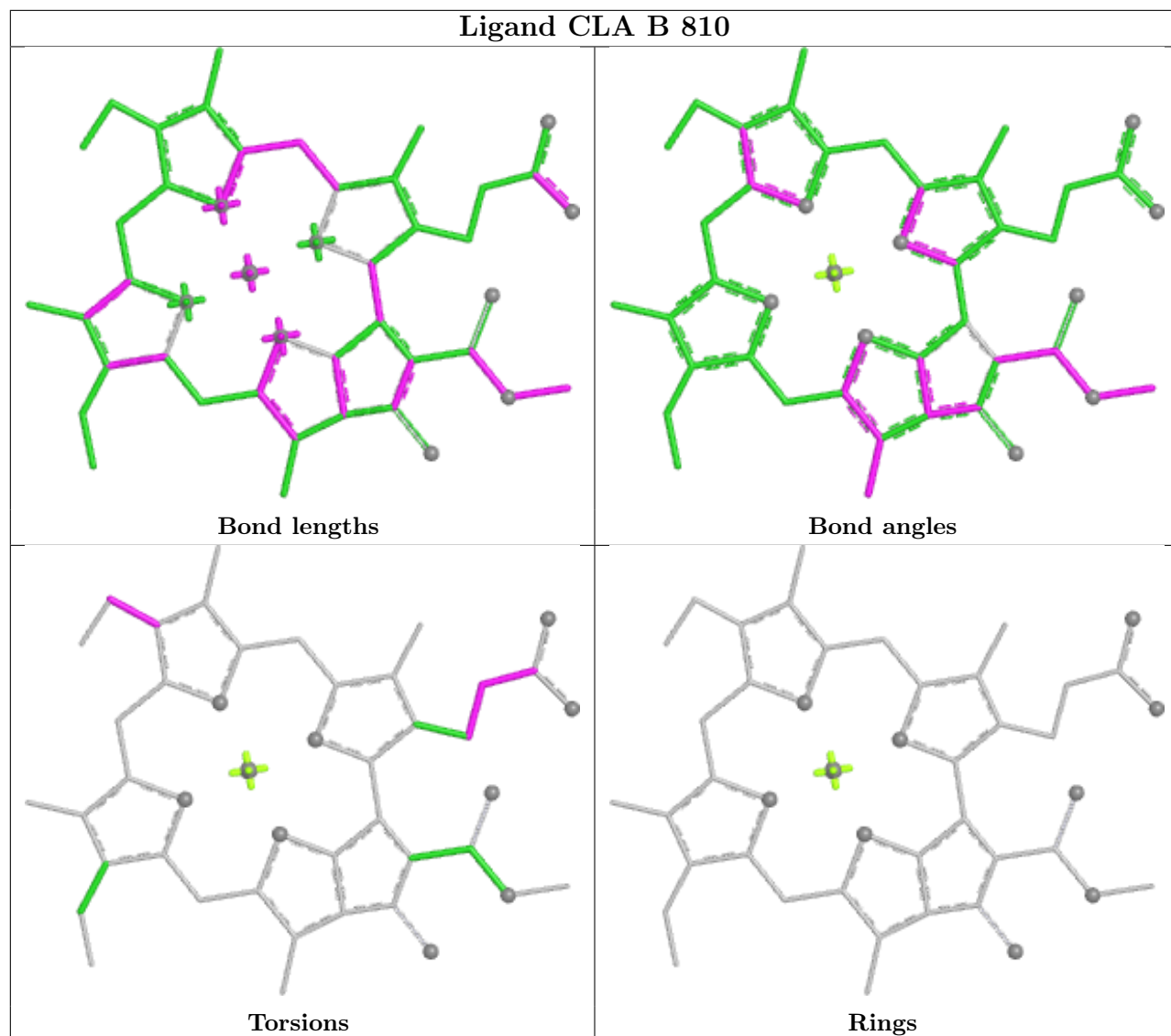
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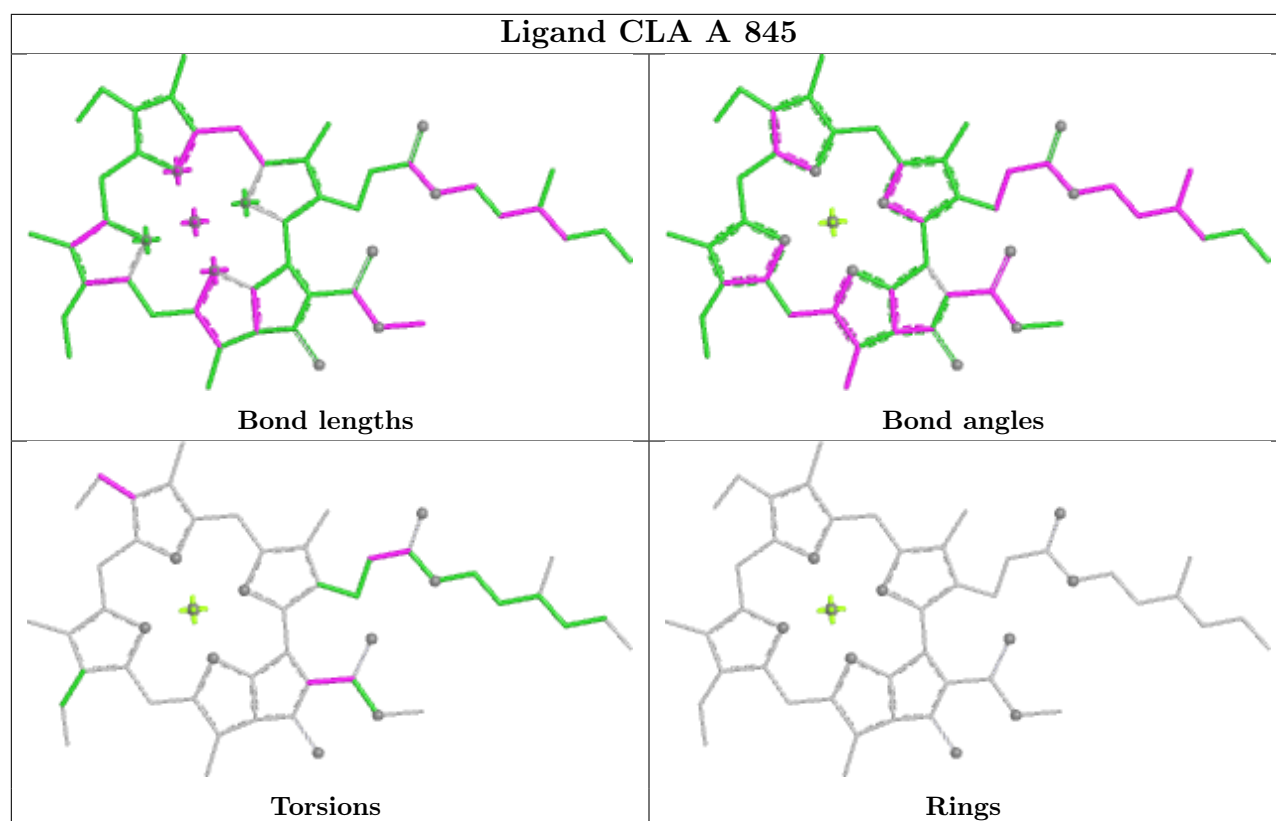


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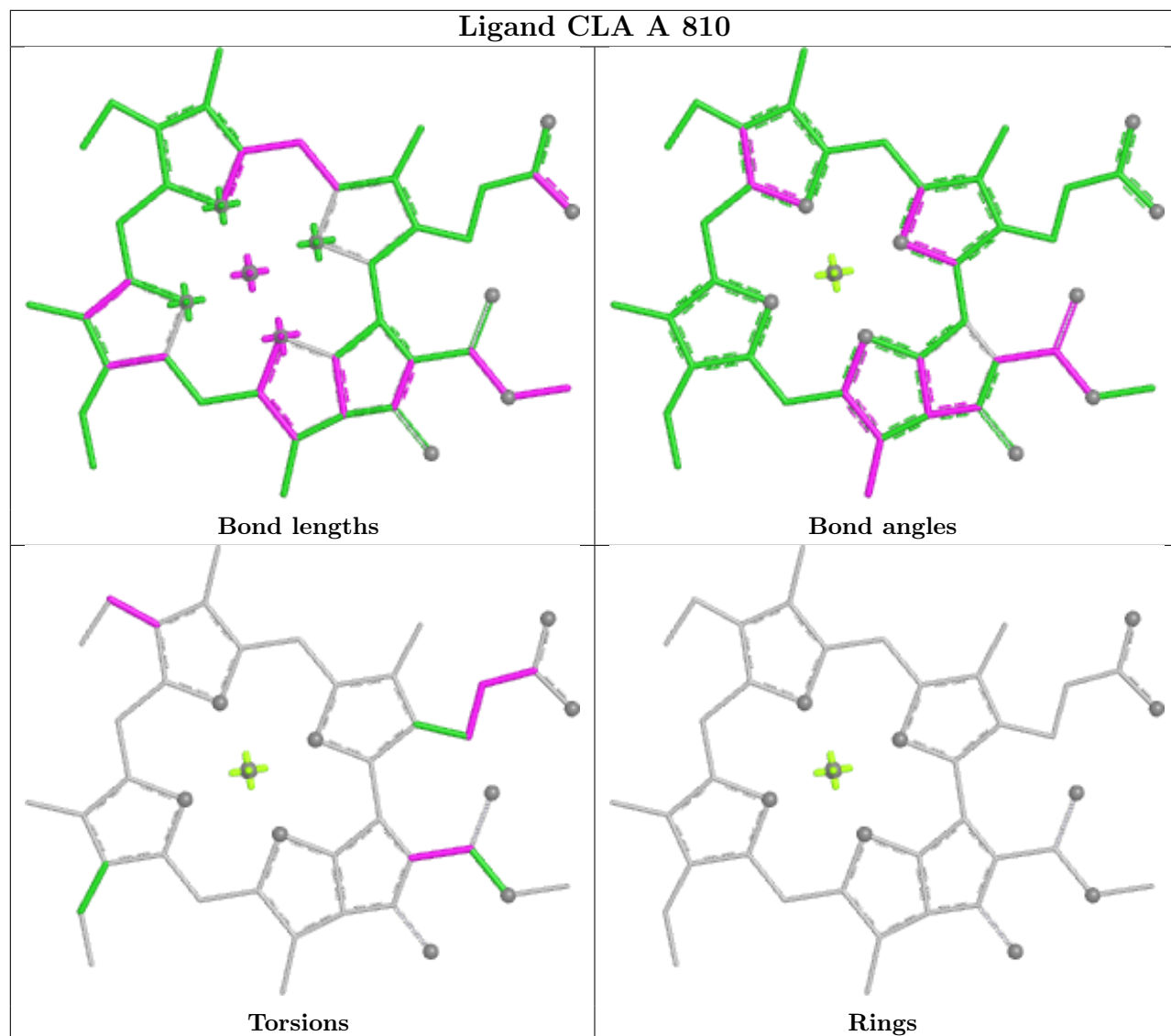


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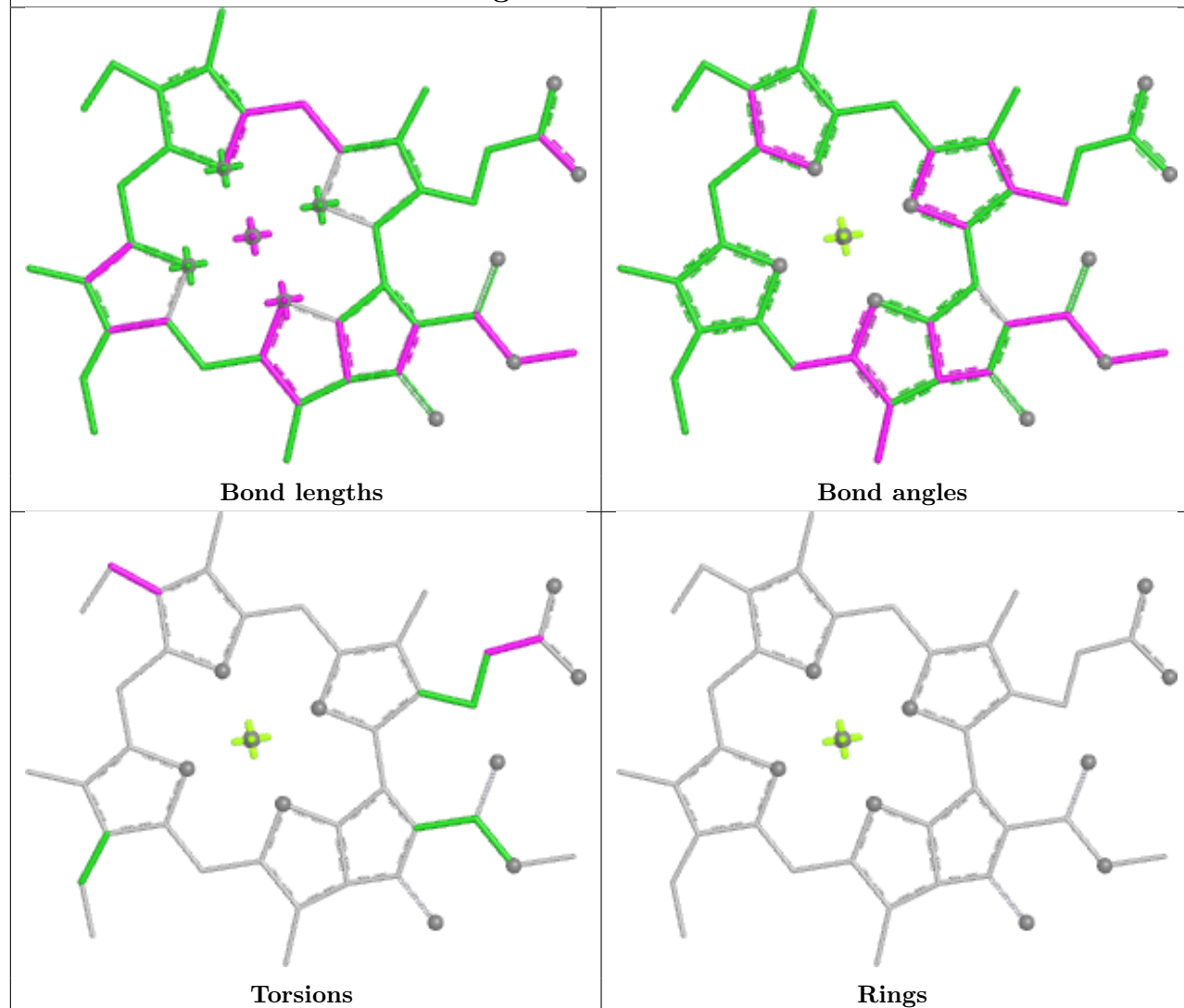




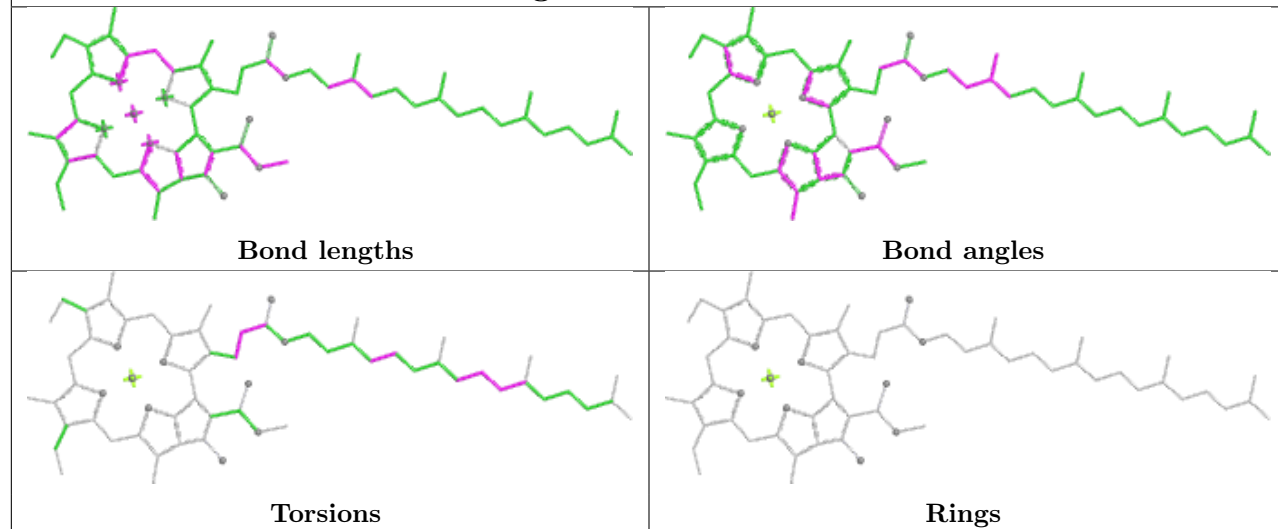
Ligand CLA A 810

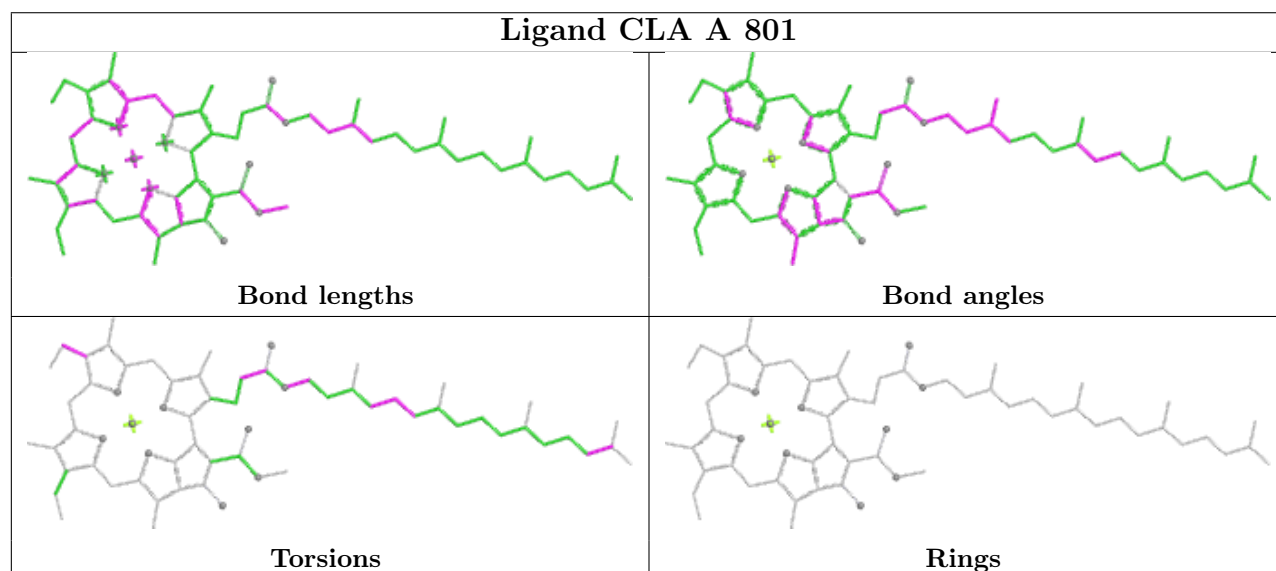
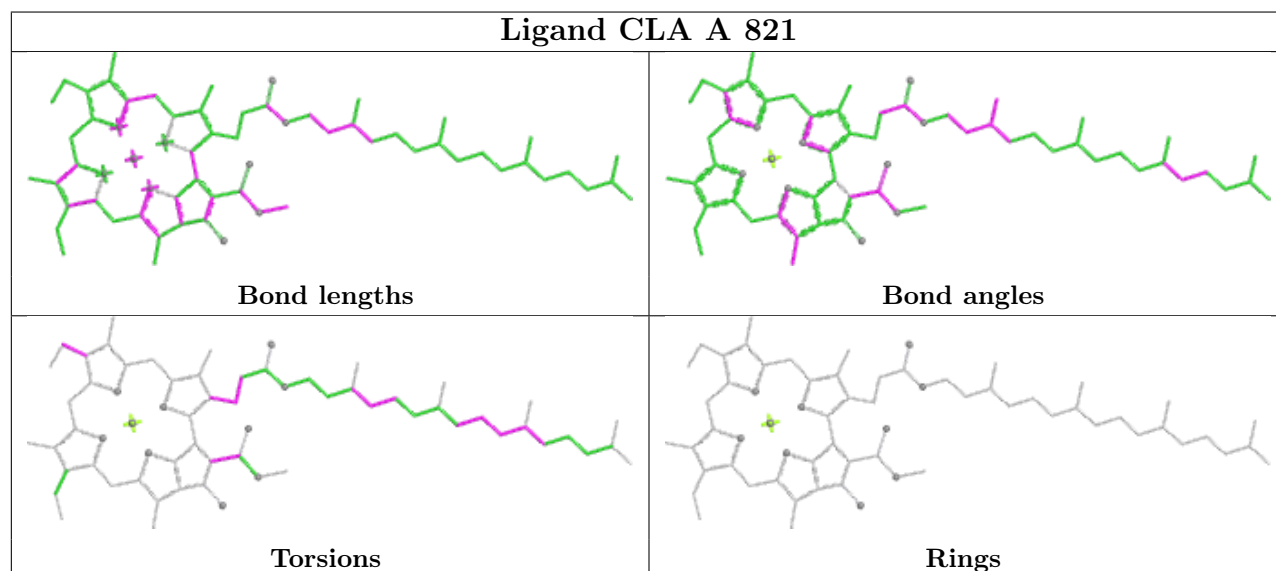
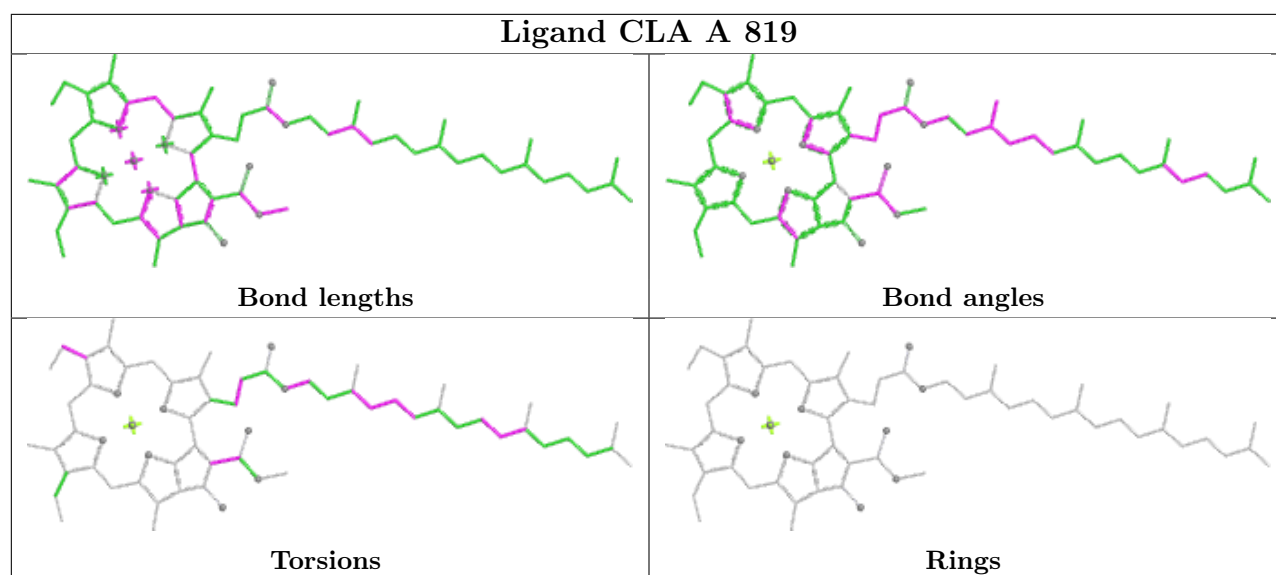


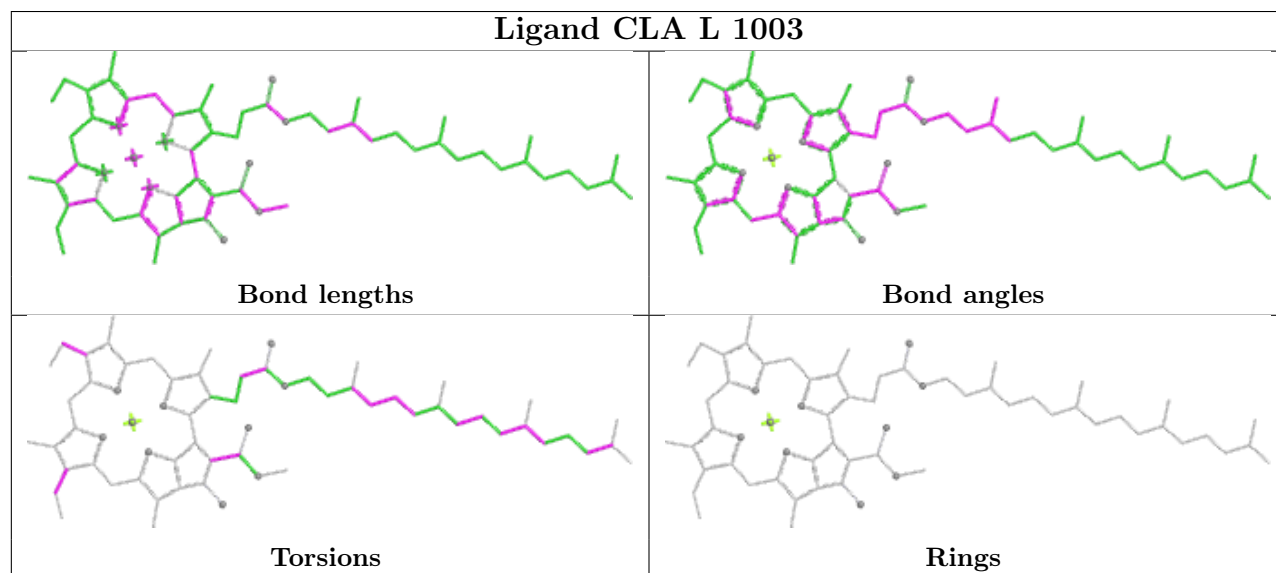
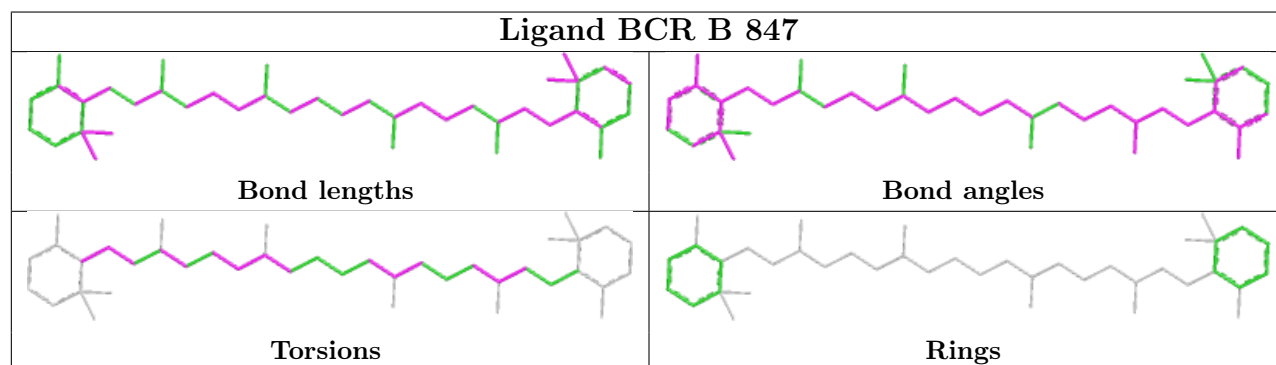
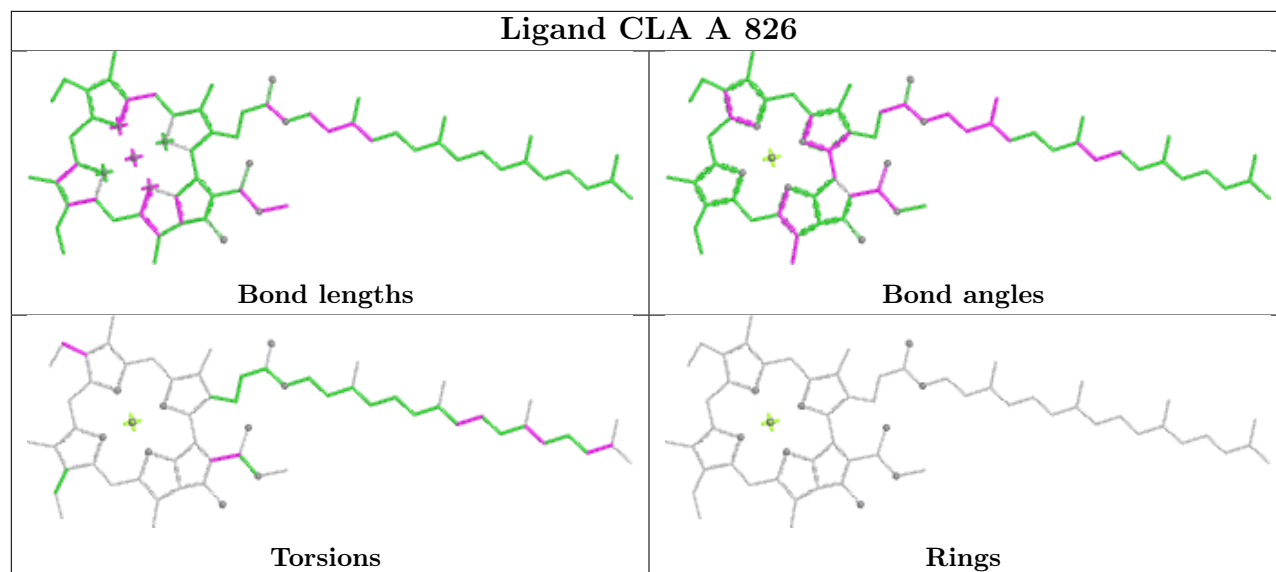
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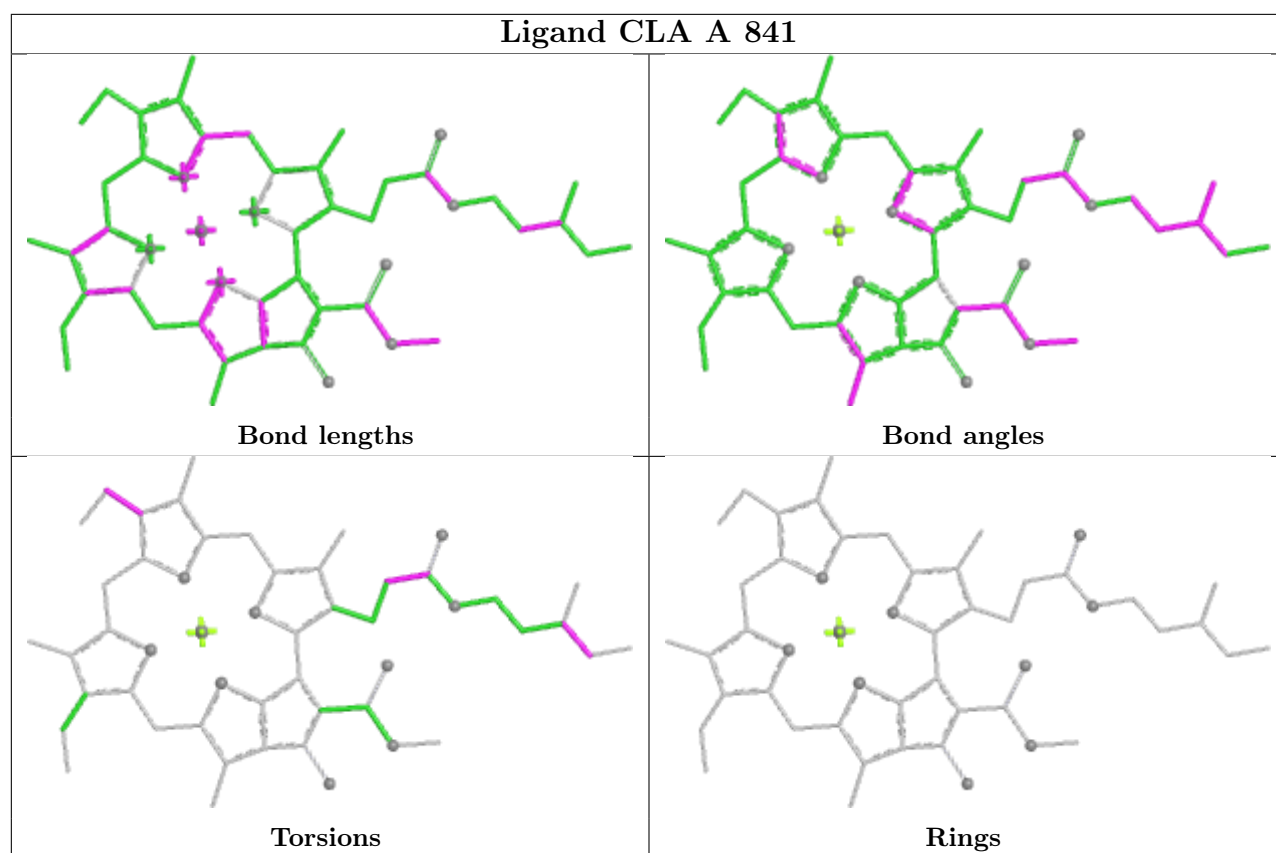


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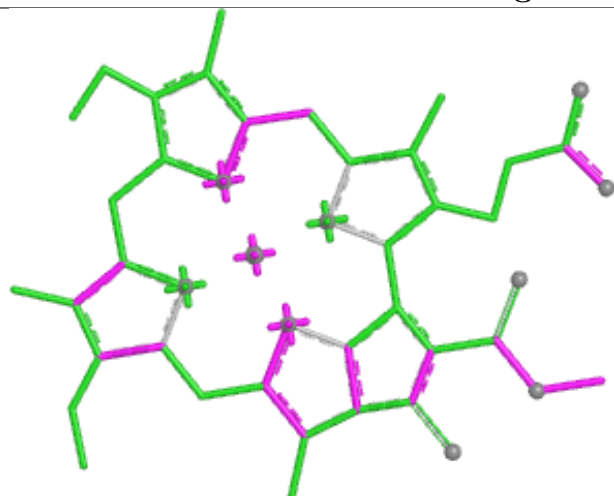




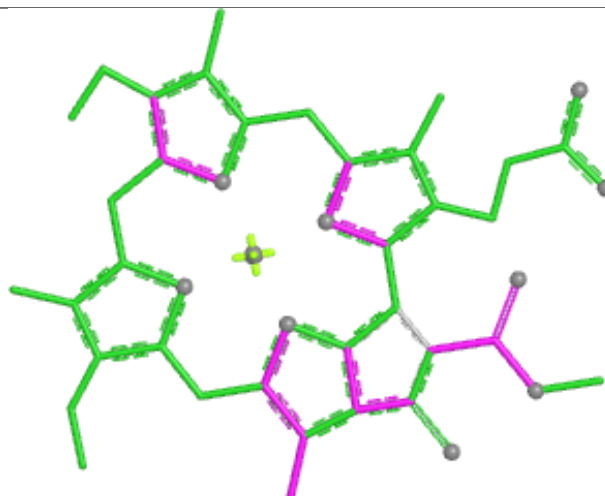




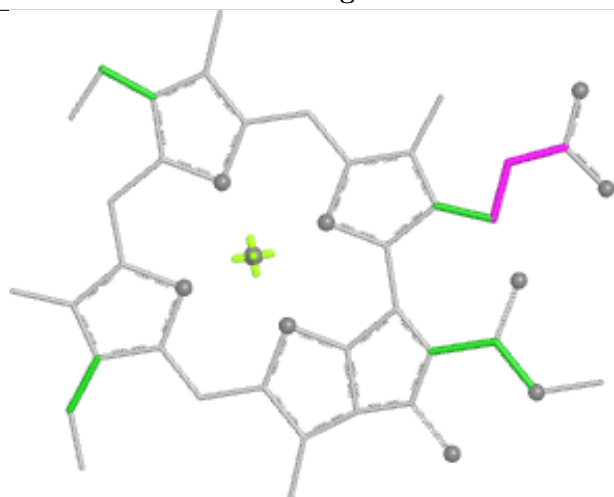
Ligand CLA B 834



Bond lengths



Bond angles

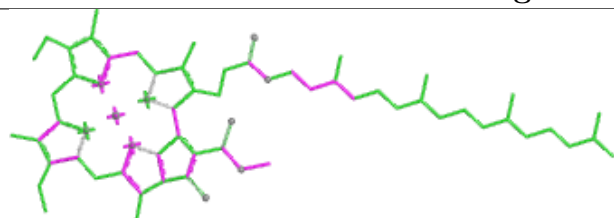


Torsions

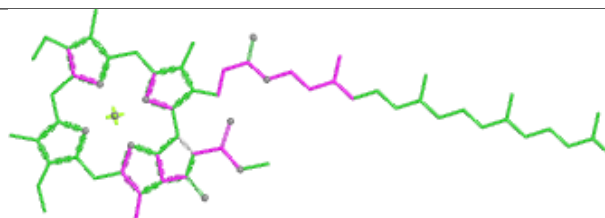


Rings

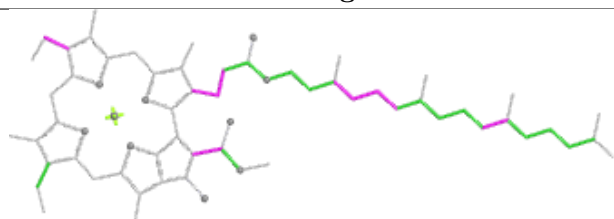
Ligand CLA A 840



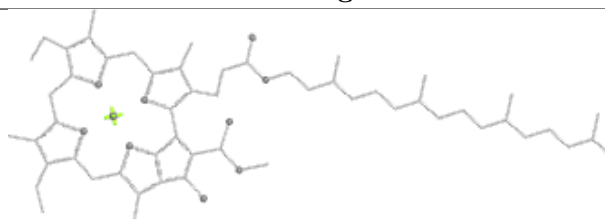
Bond lengths



Bond angles

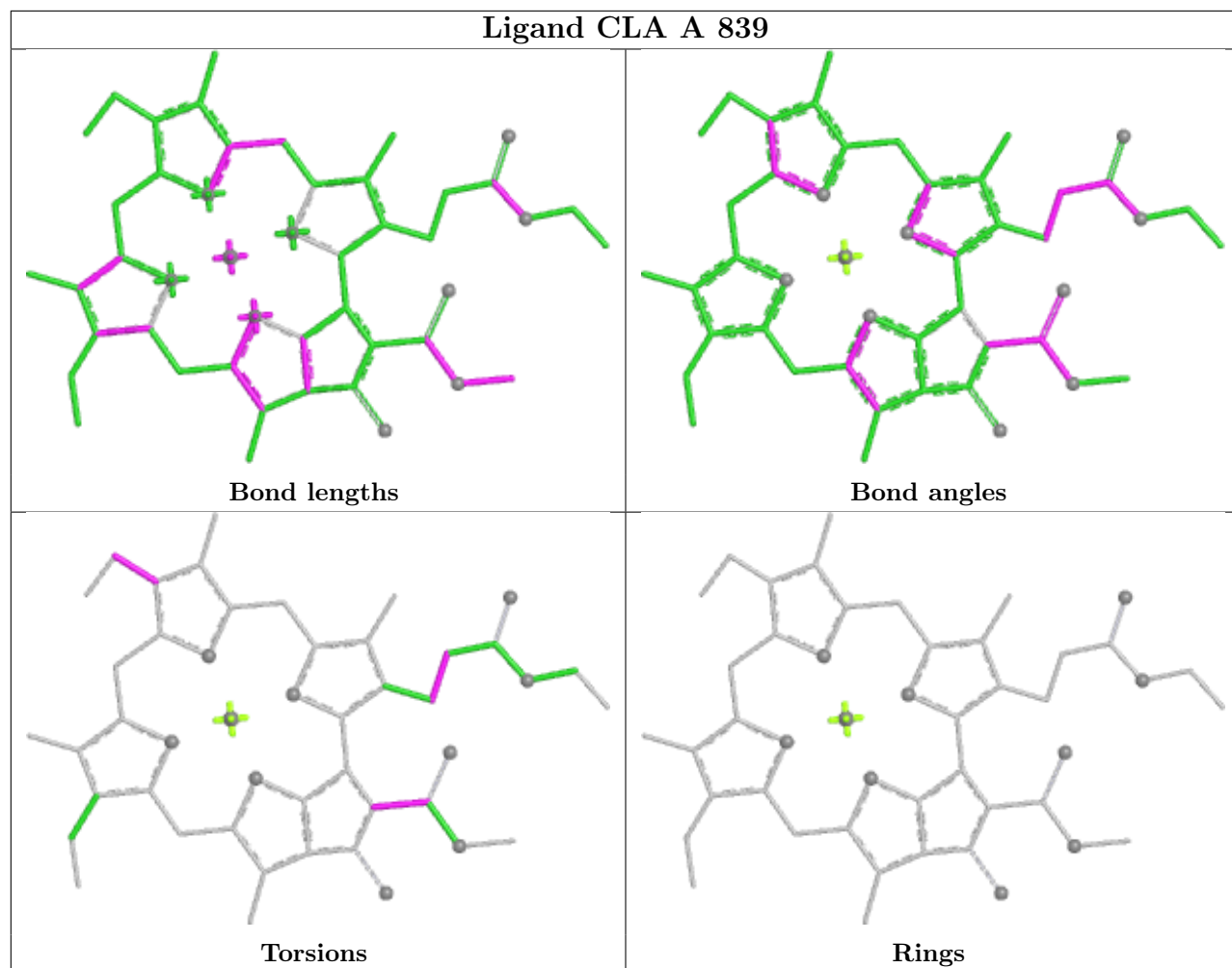


Torsions

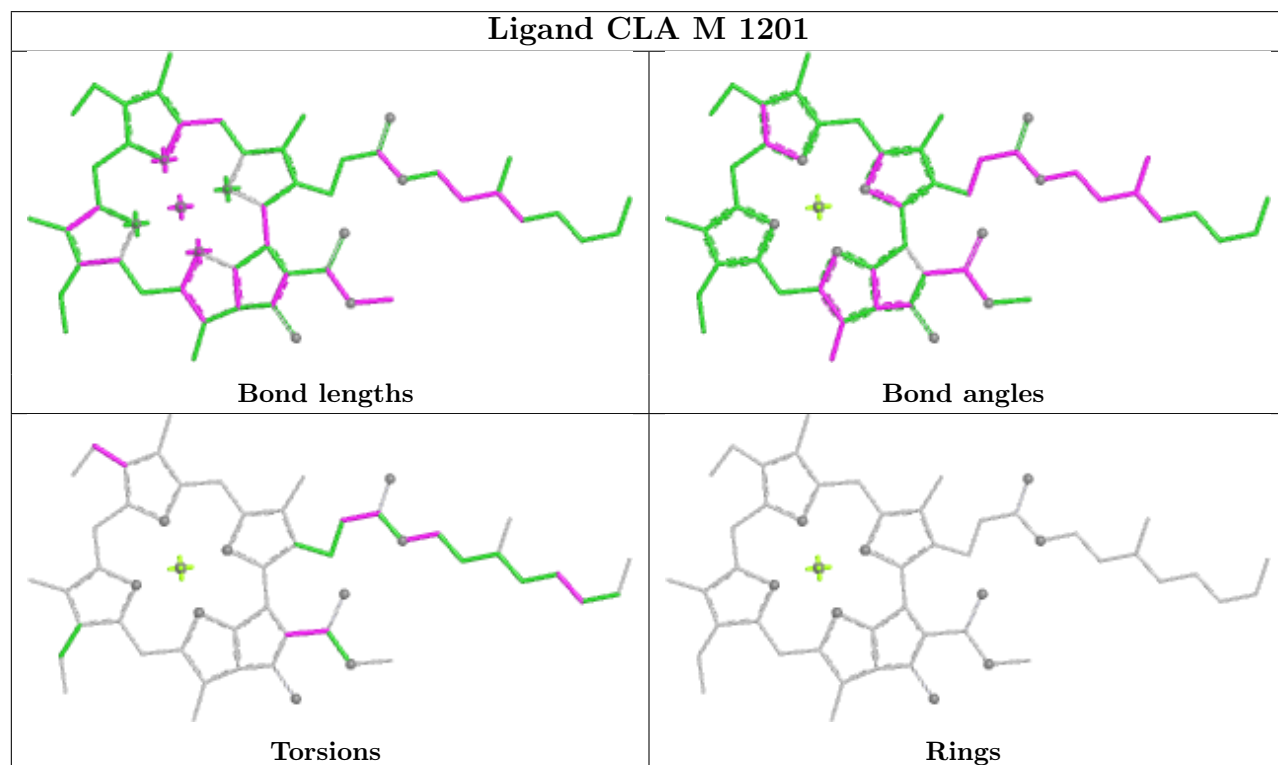


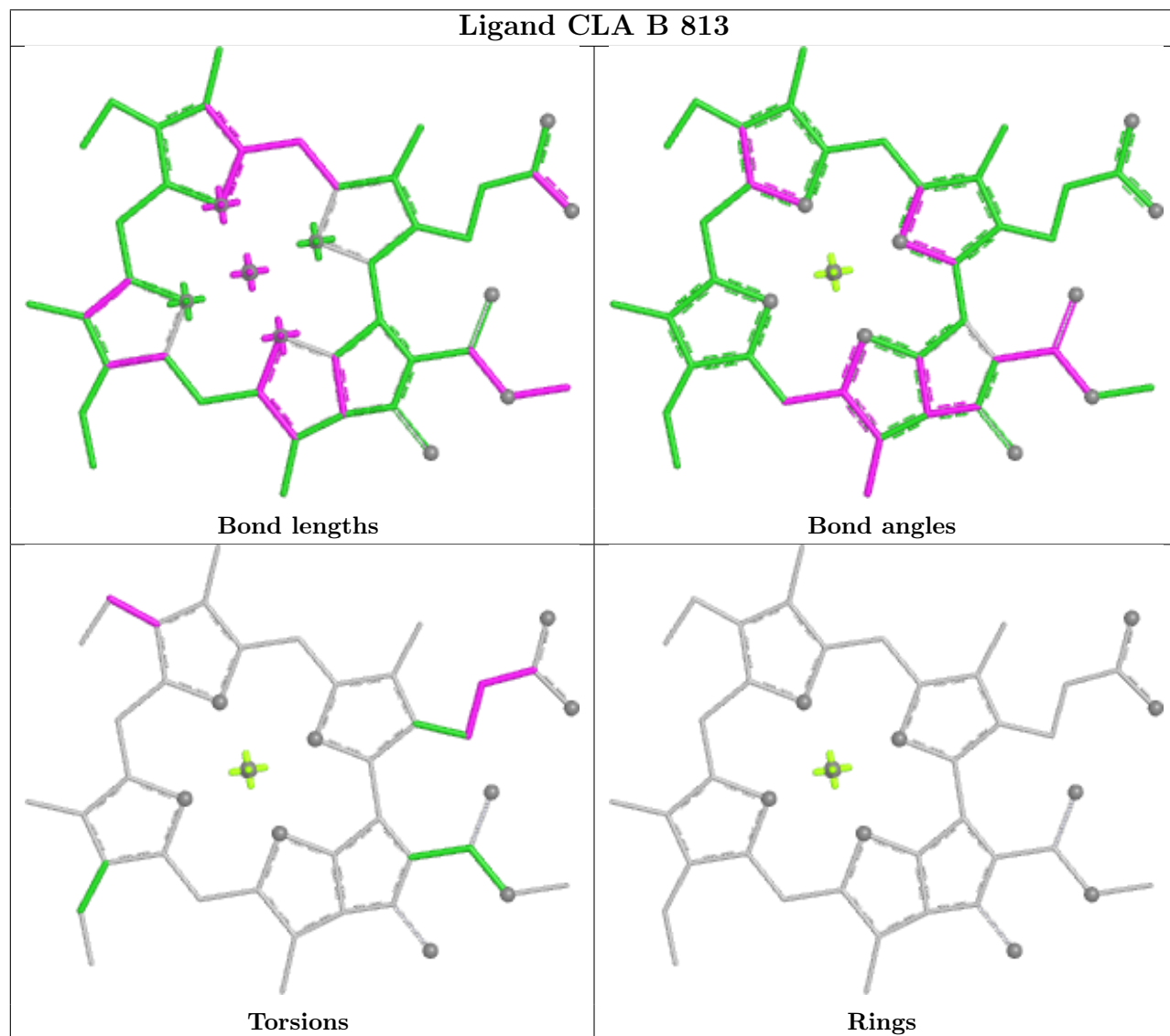
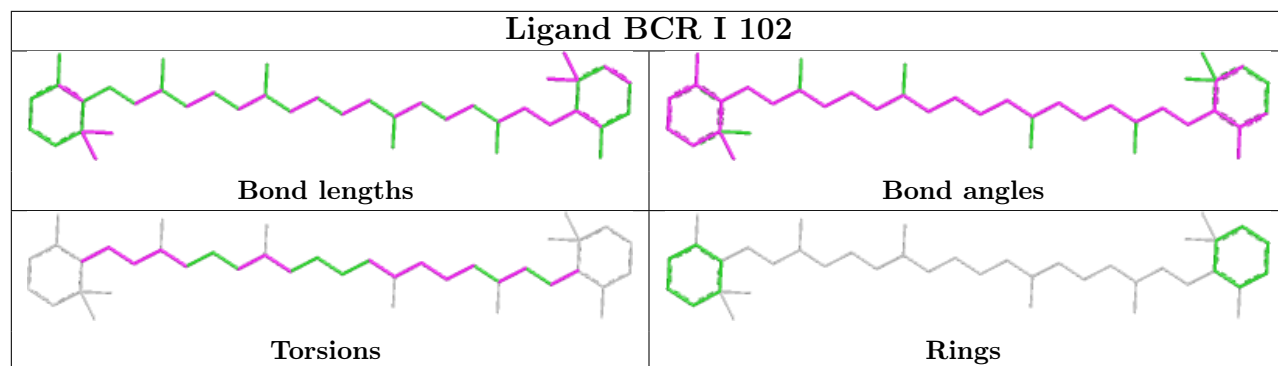
Rings

Ligand CLA A 839

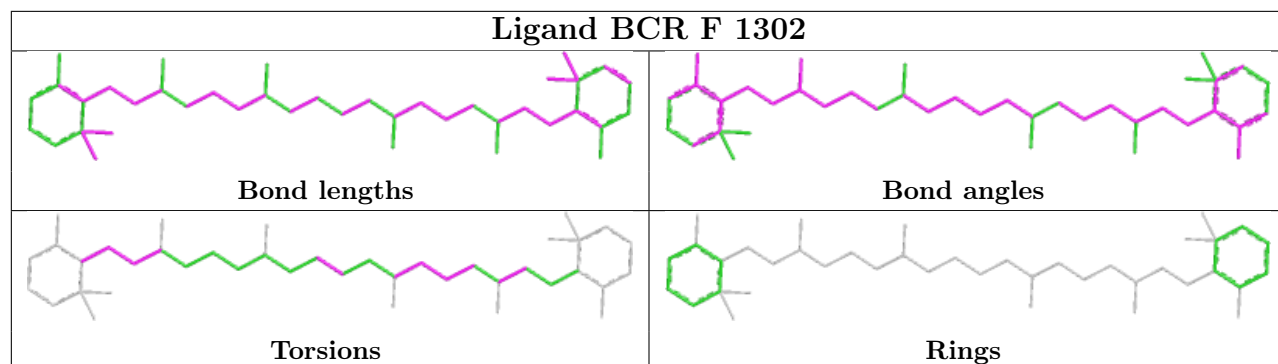


Ligand CLA M 1201

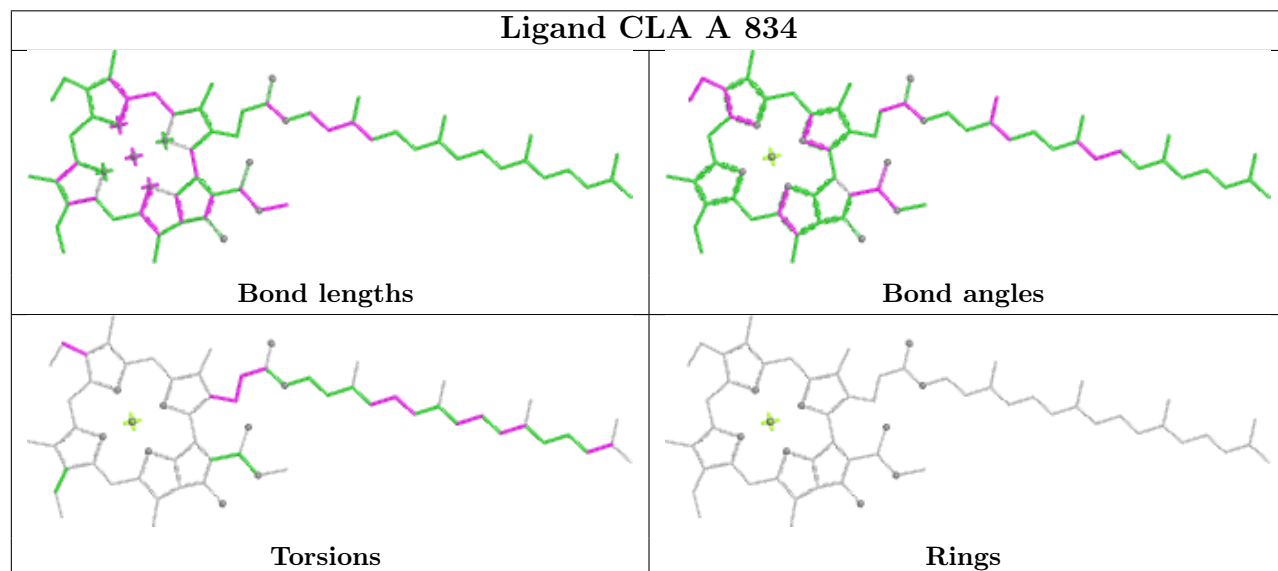




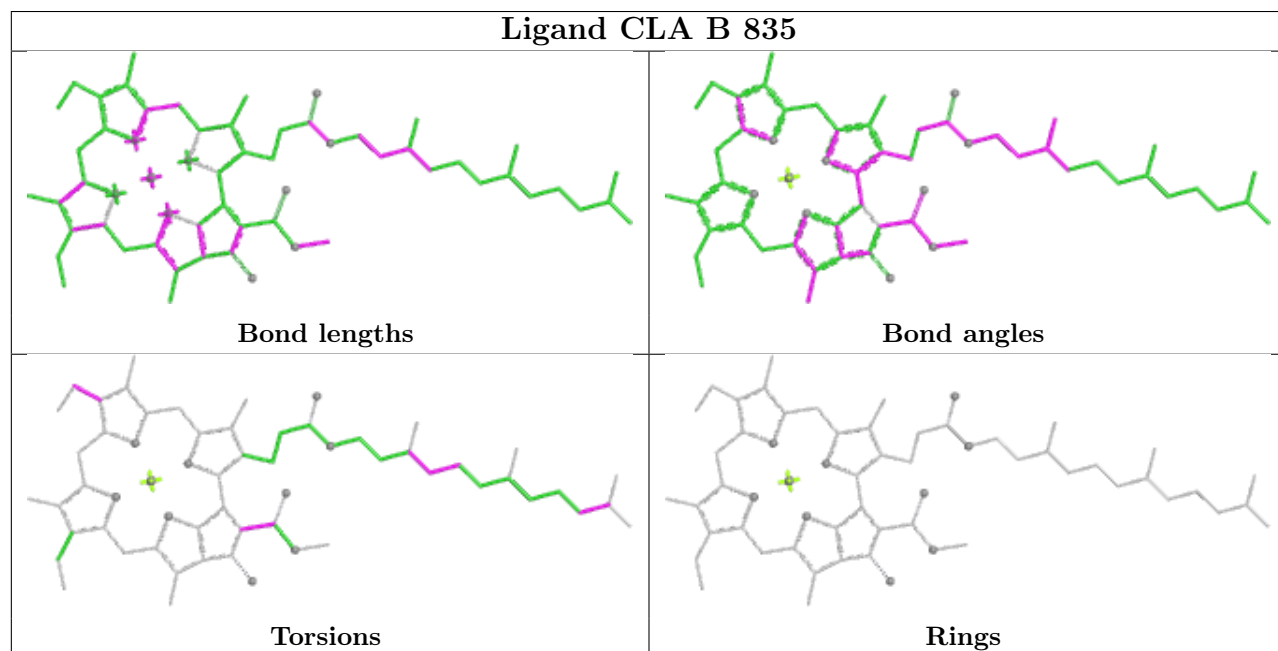
Ligand BCR F 1302



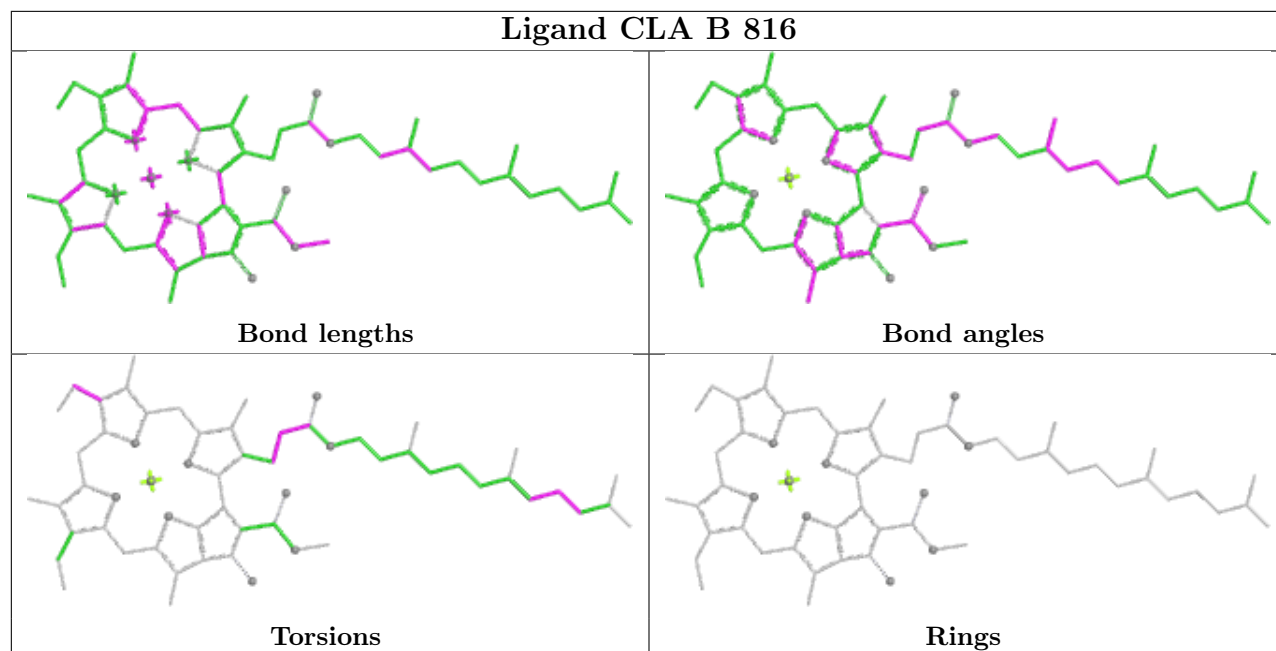
Ligand CLA A 834



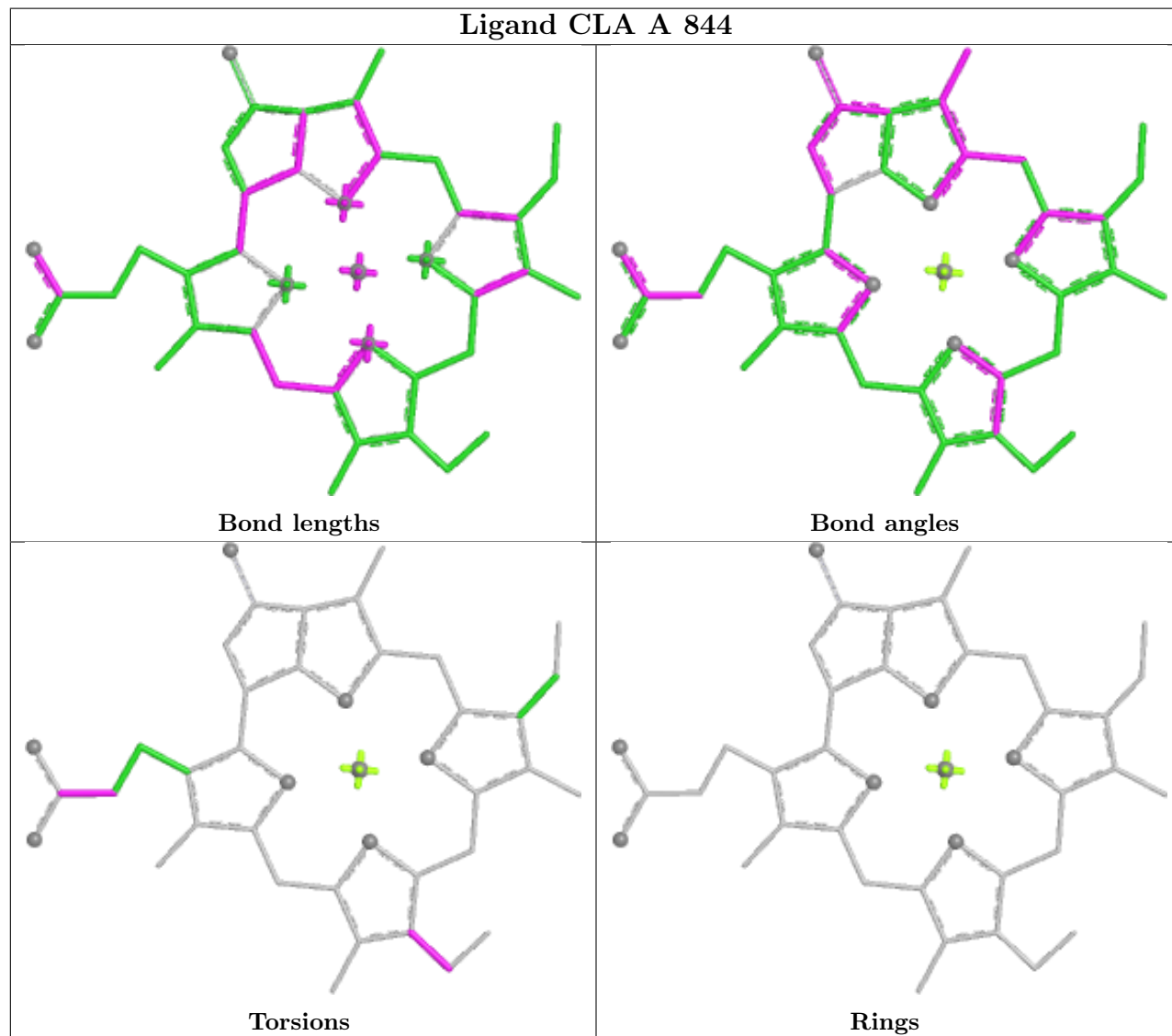
Ligand CLA B 835

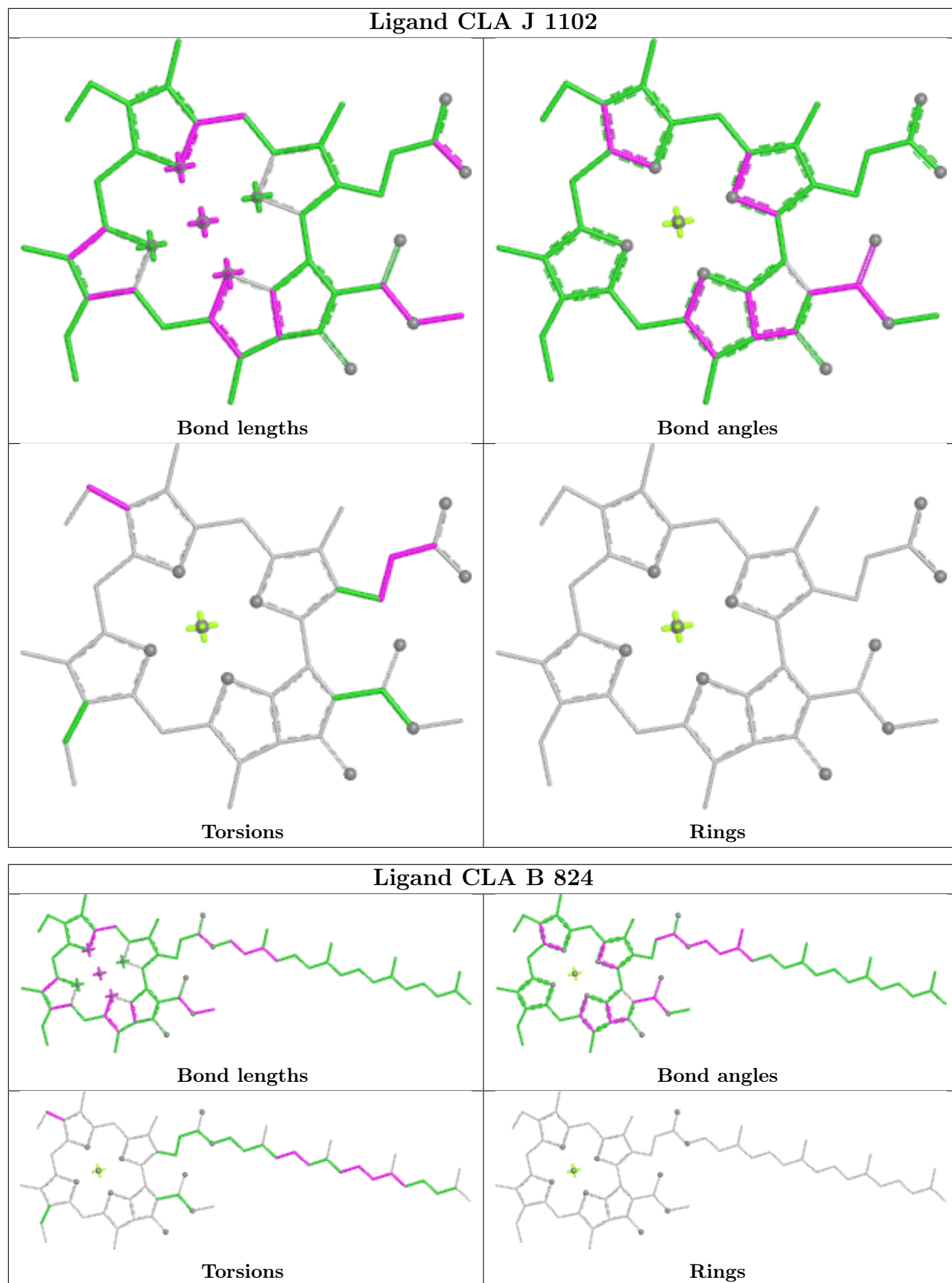


Ligand CLA B 816

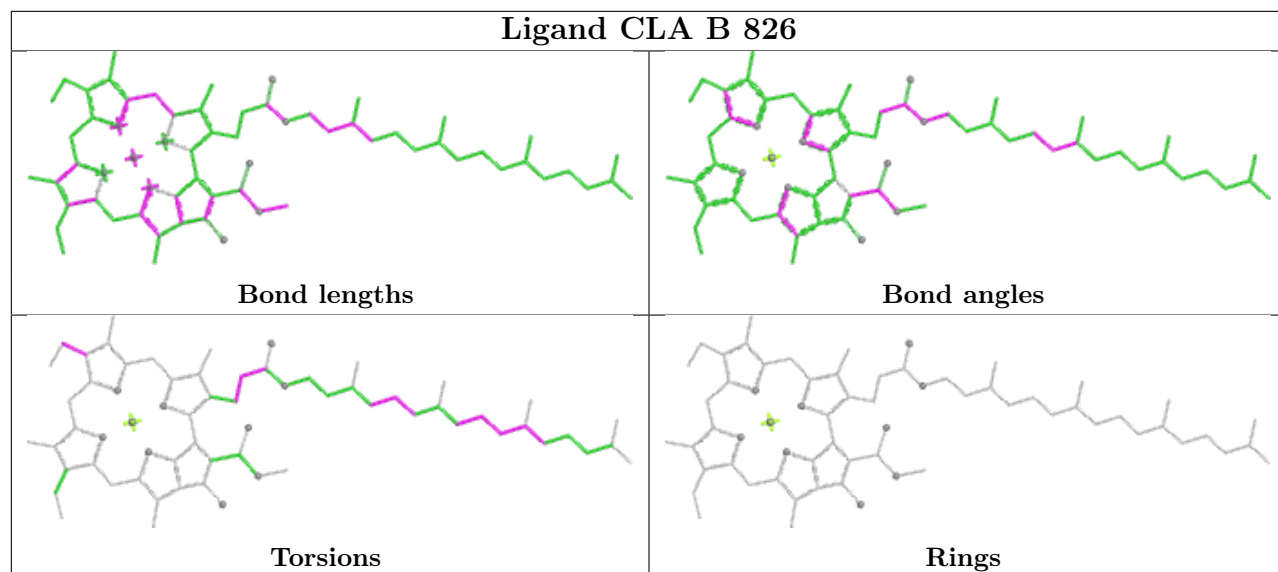


Ligand CLA A 844

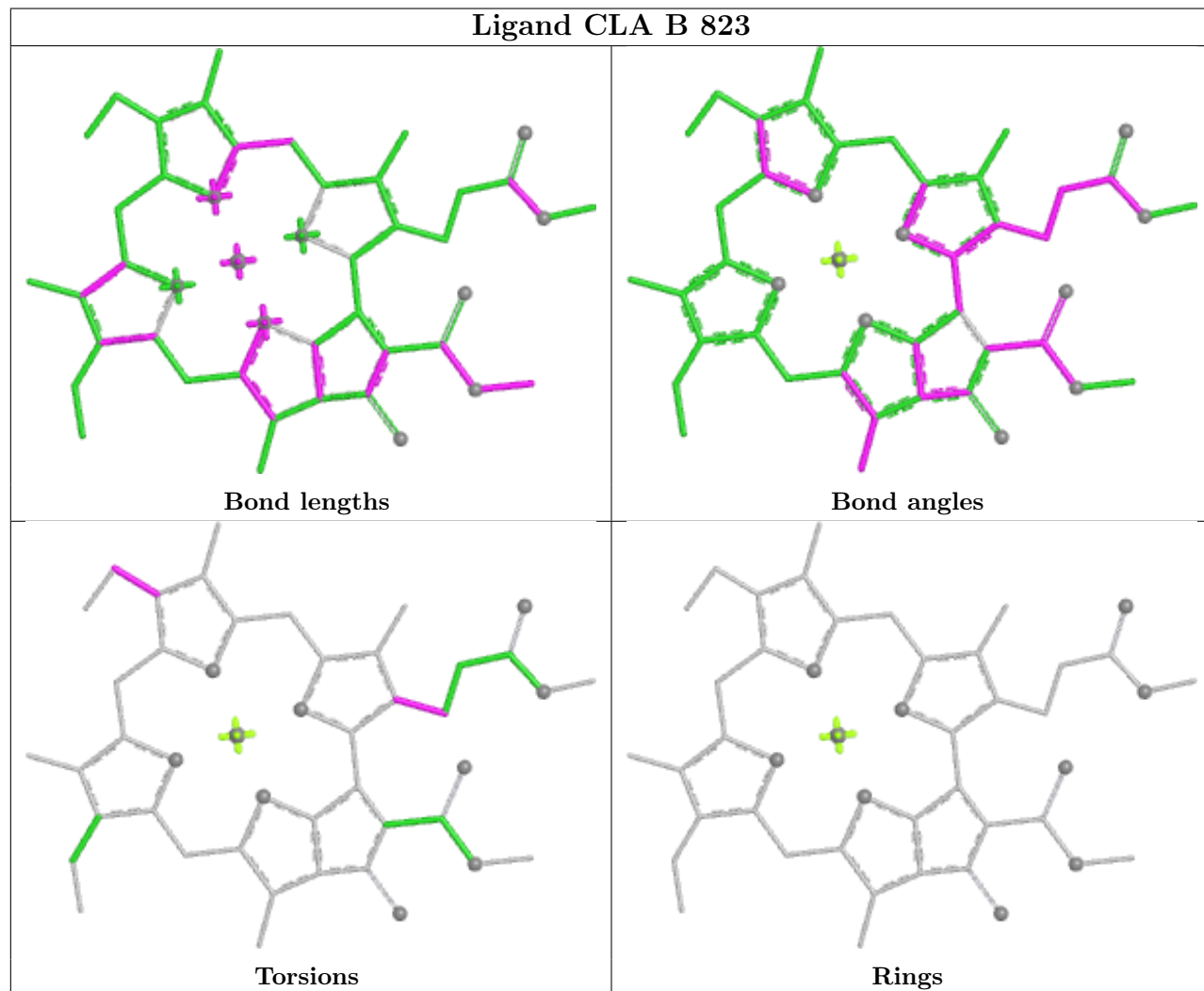




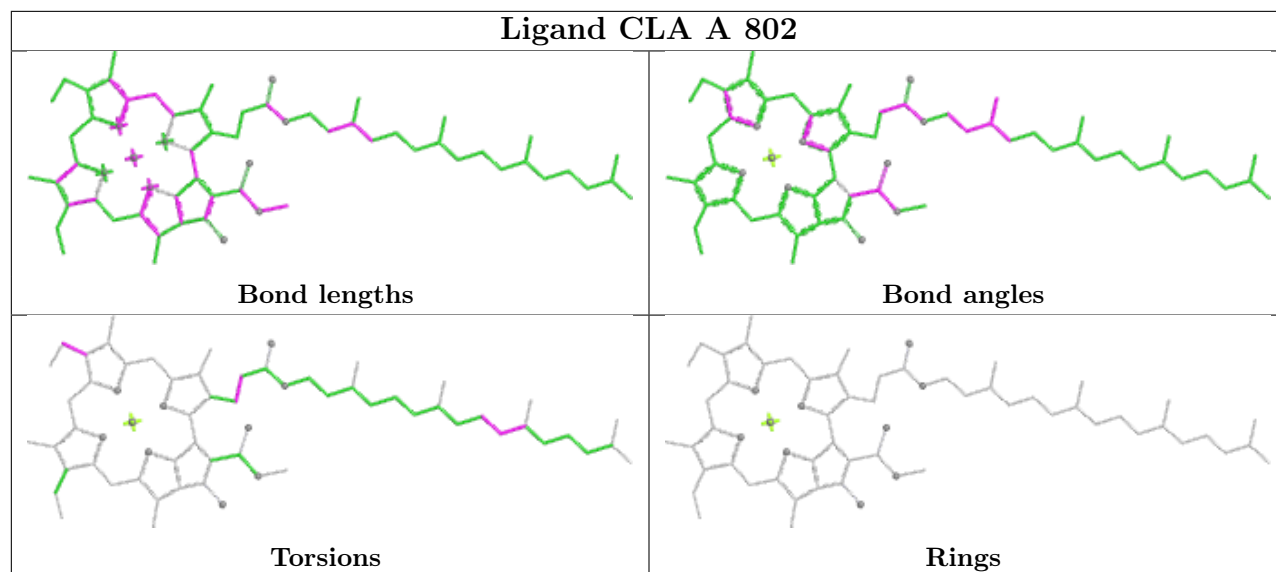
Ligand CLA B 826



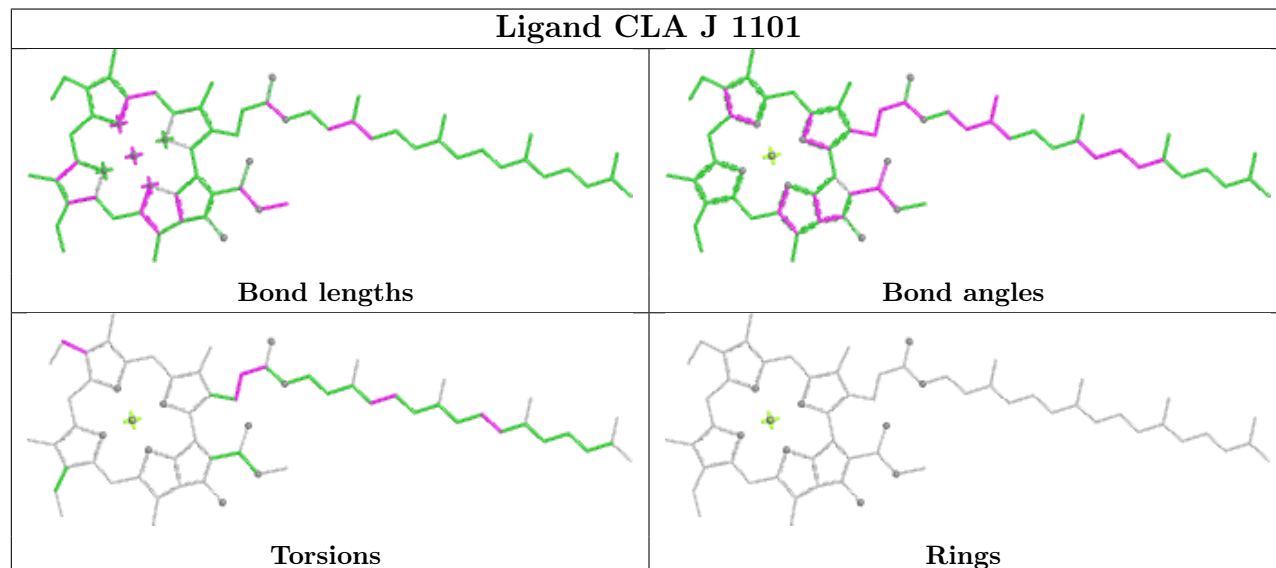
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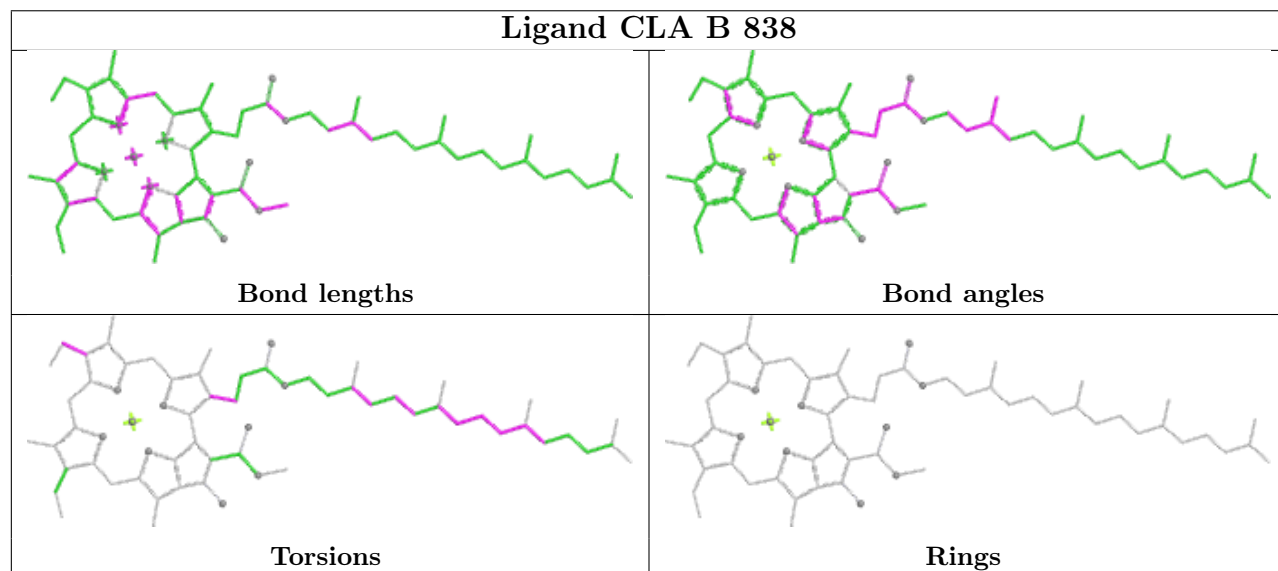
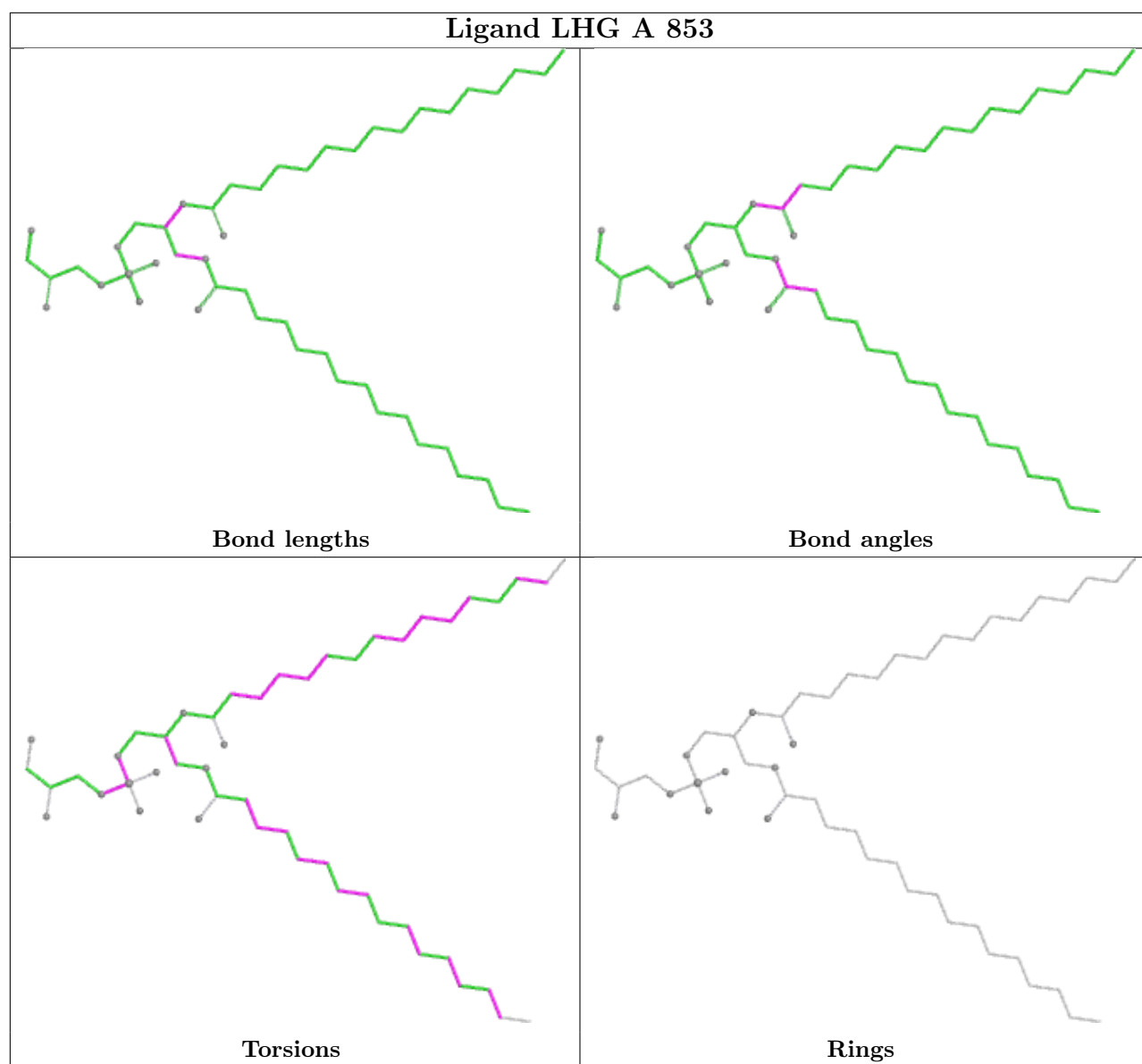


Ligand CLA A 802

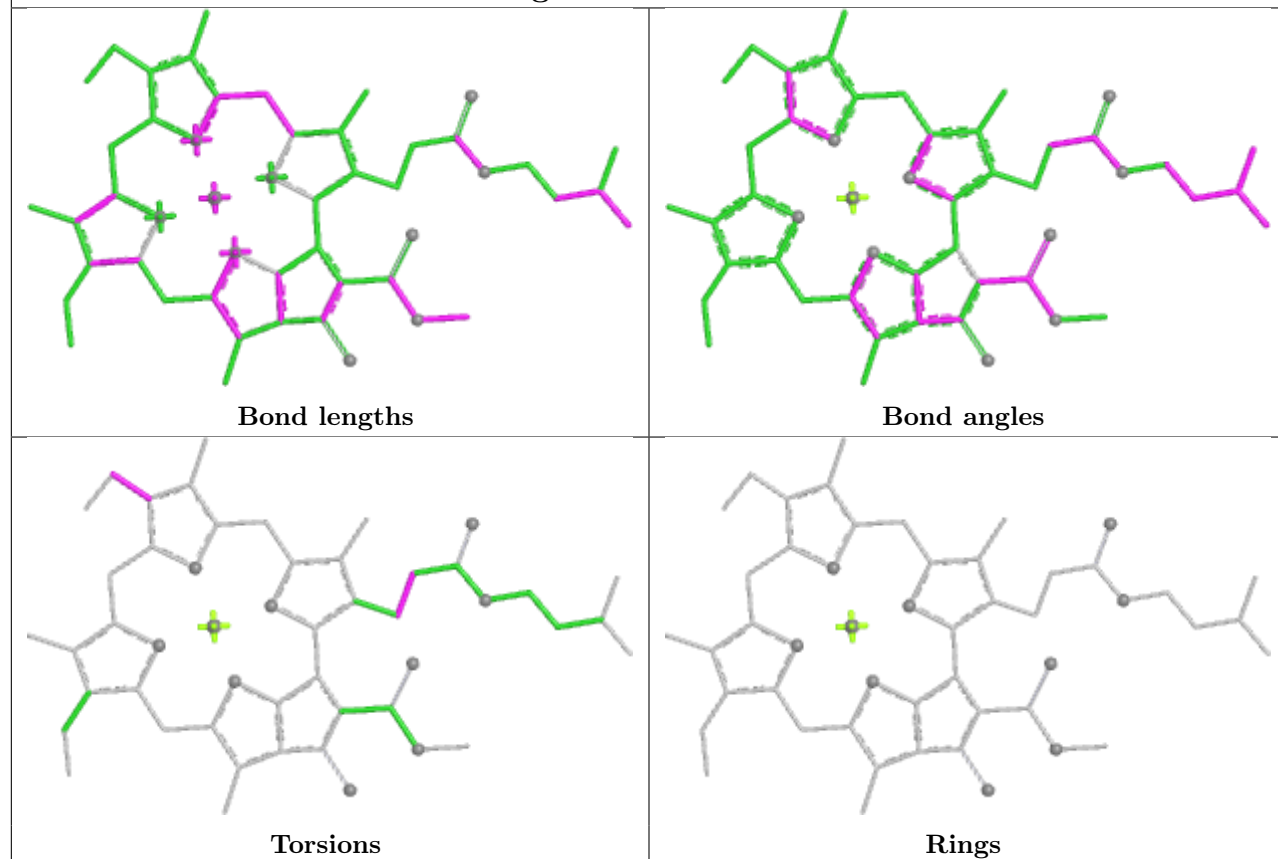


Ligand CLA J 1101

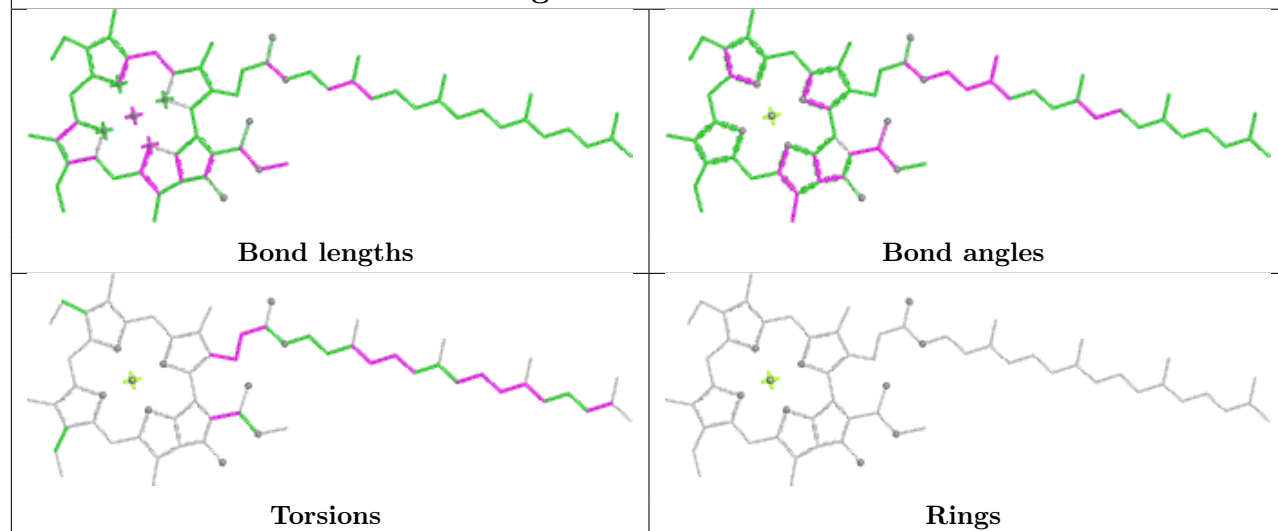




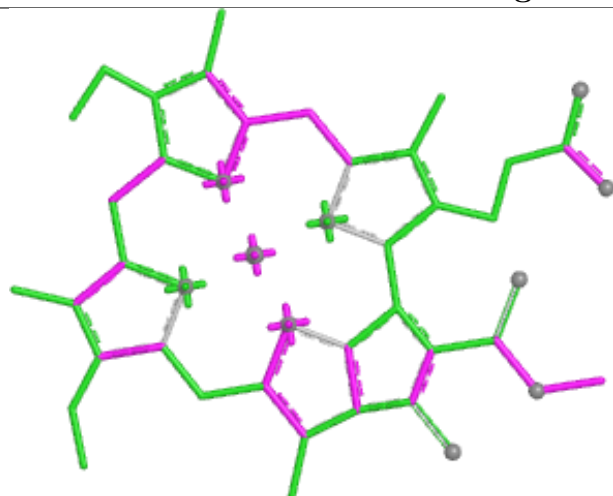
Ligand CLA A 831



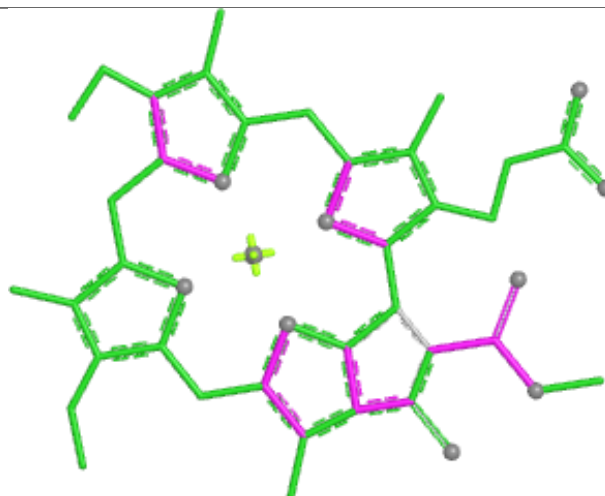
Ligand CLA A 828



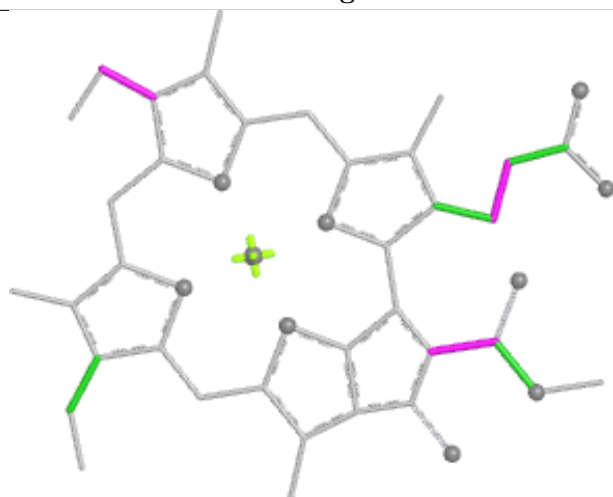
Ligand CLA B 828



Bond lengths



Bond angles

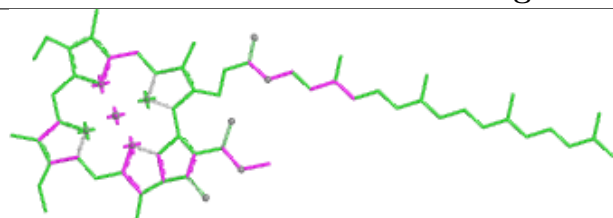


Torsions

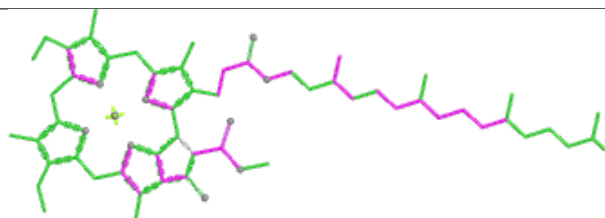


Rings

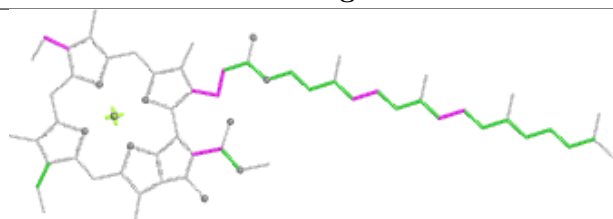
Ligand CLA A 843



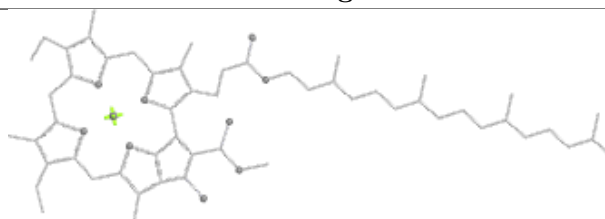
Bond lengths



Bond angles

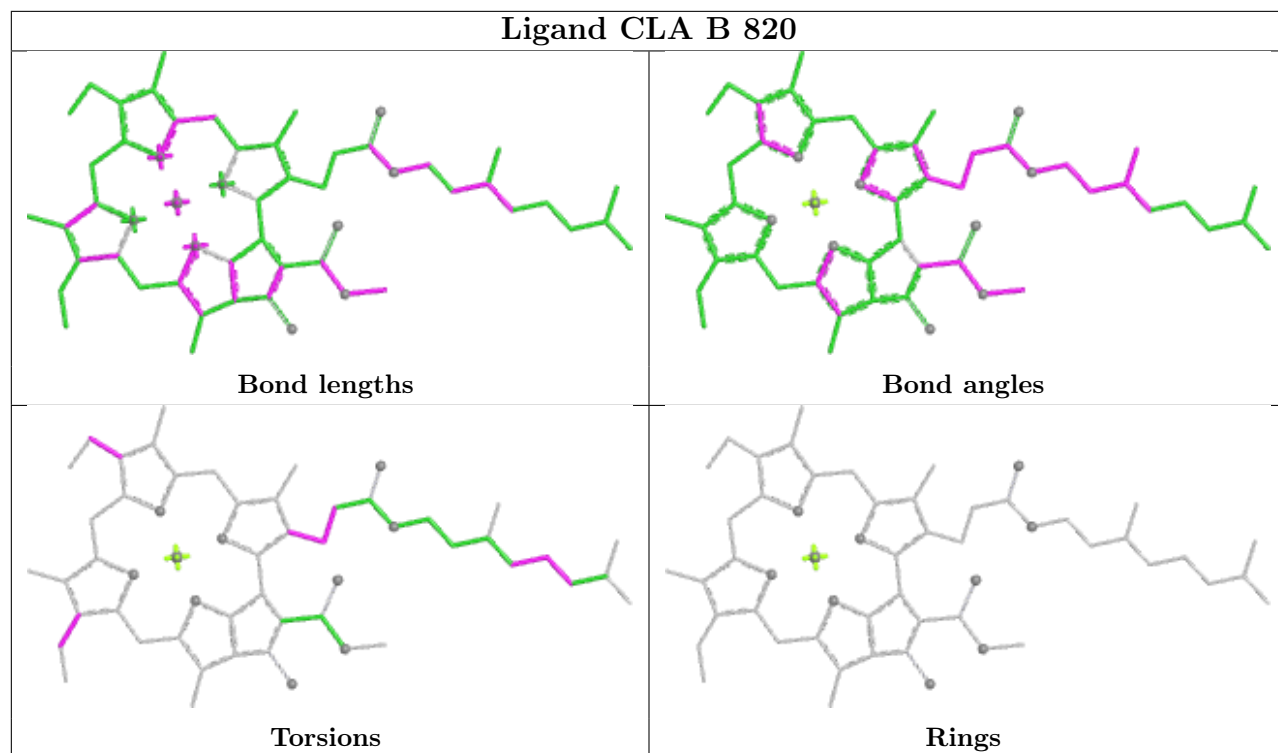


Torsions

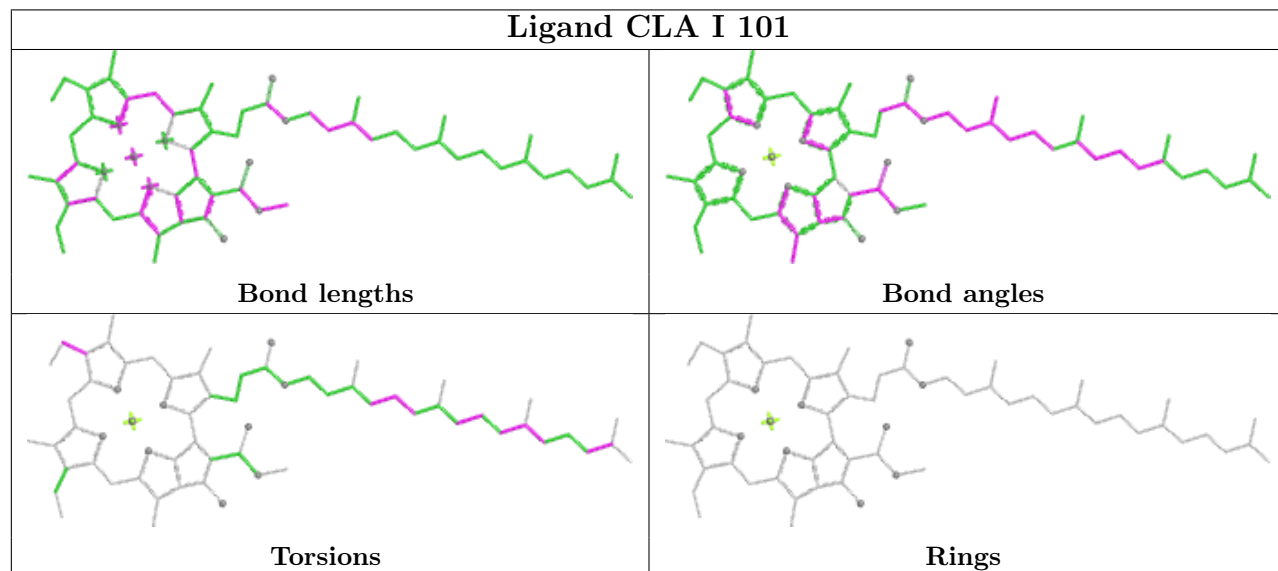


Rings

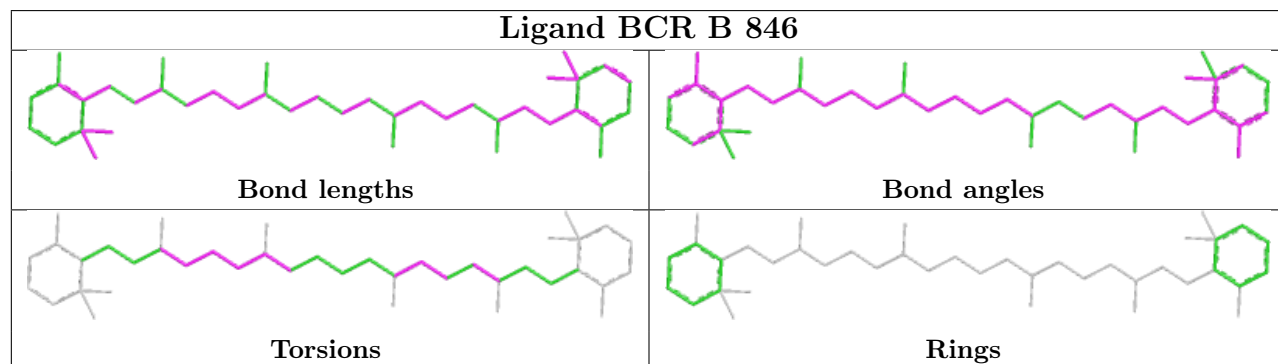
Ligand CLA B 820



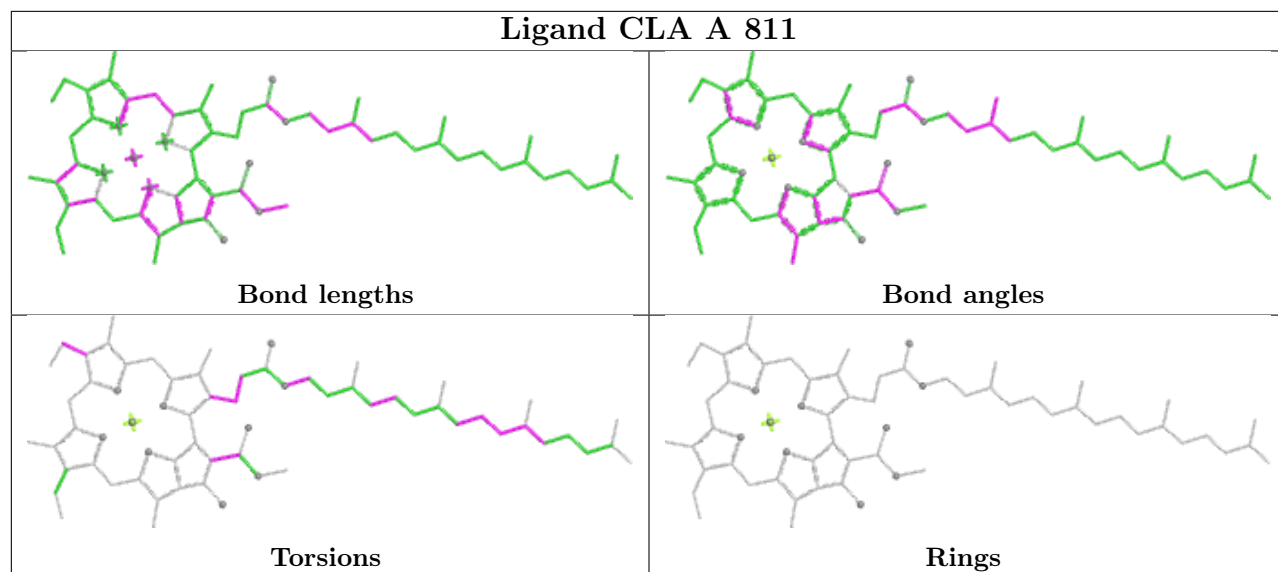
Ligand CLA I 101



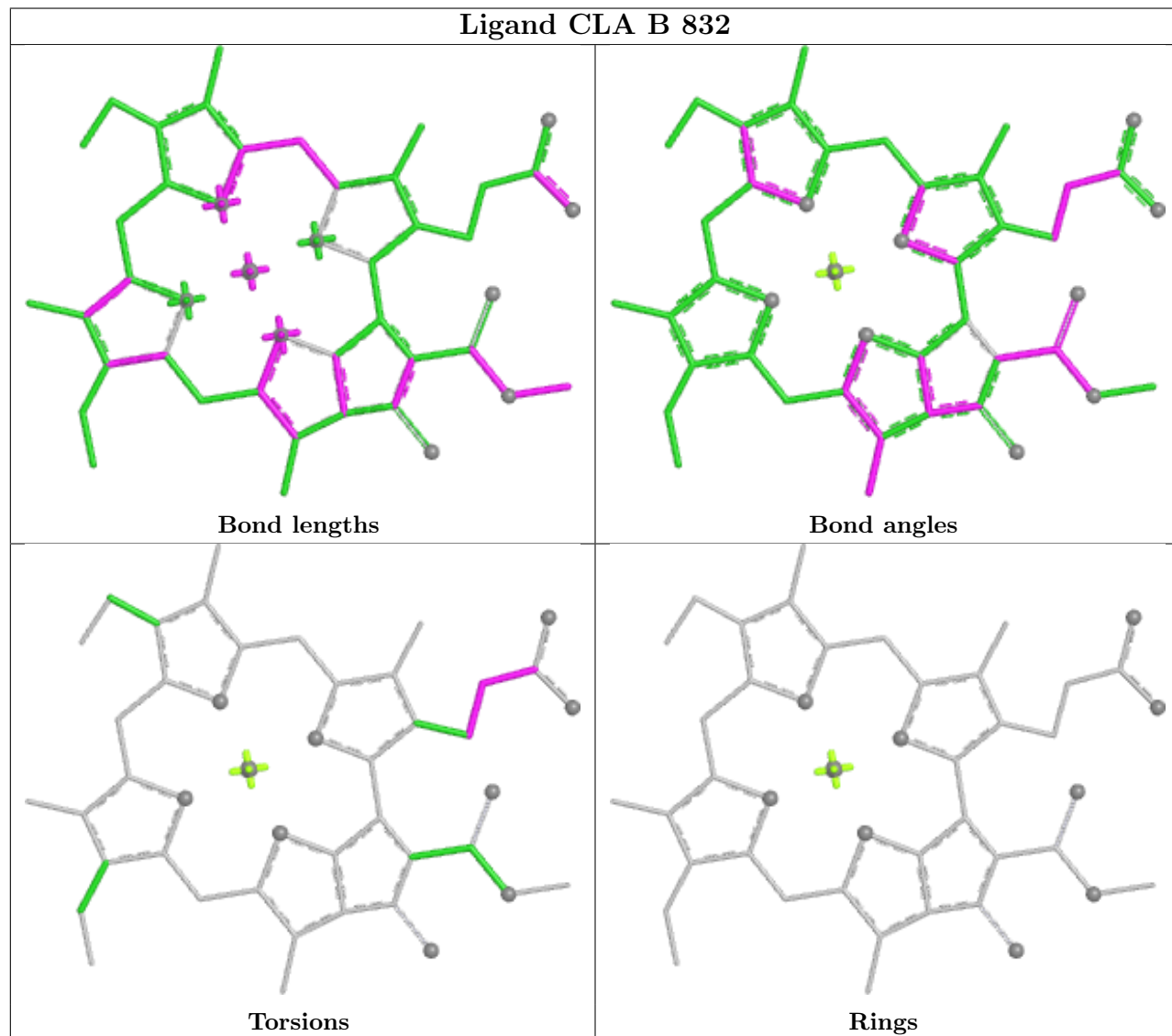
Ligand BCR B 846

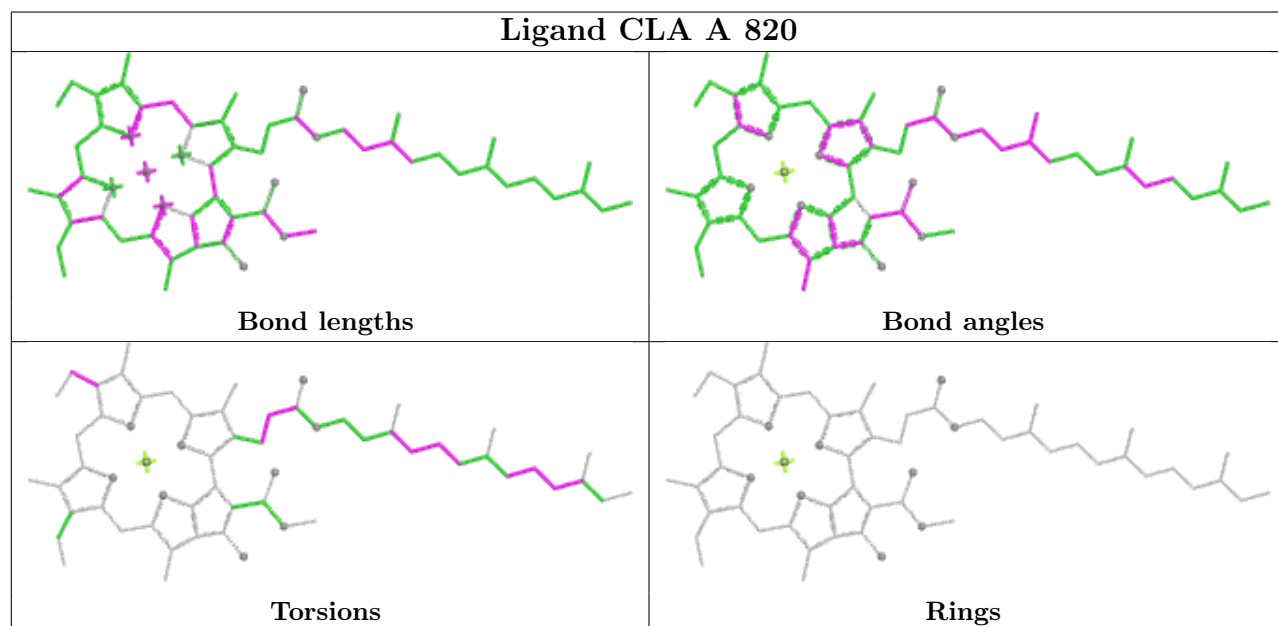
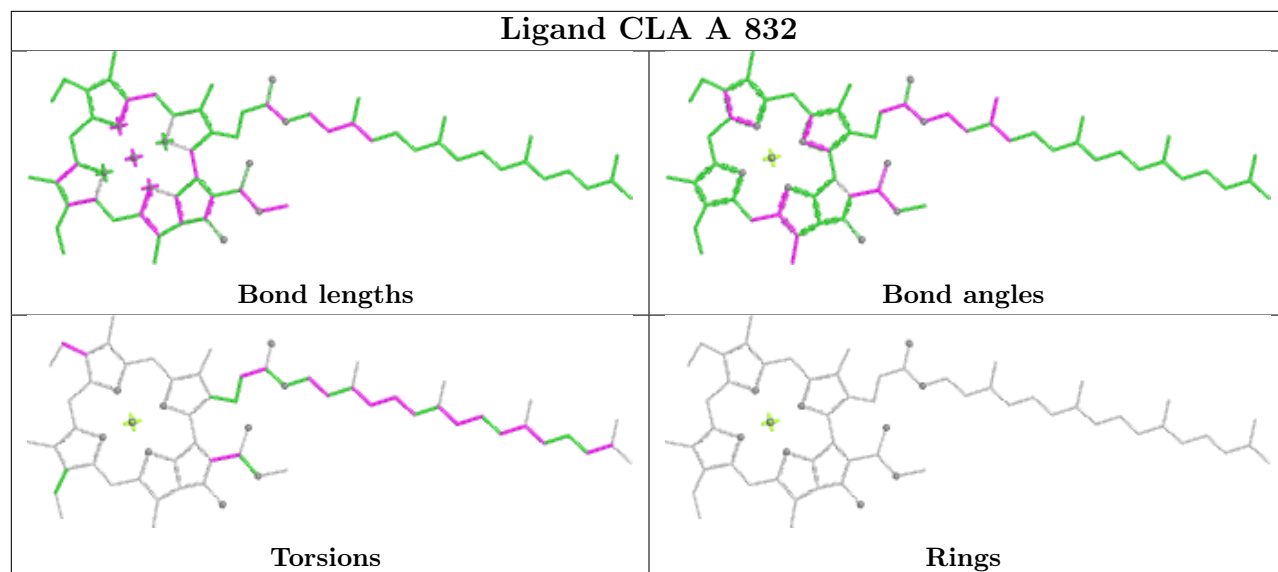


Ligand CLA A 811

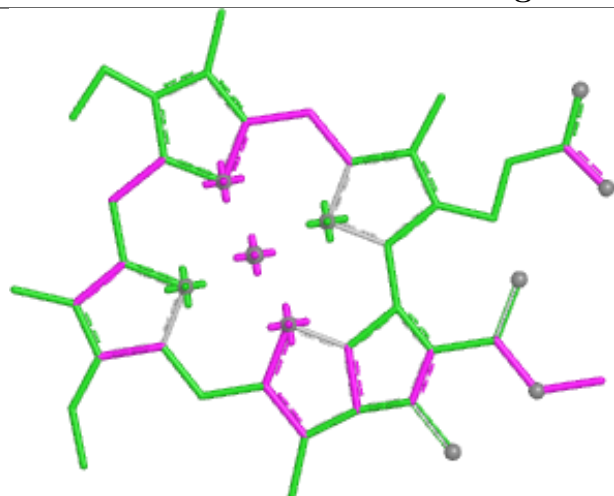


Ligand CLA B 832

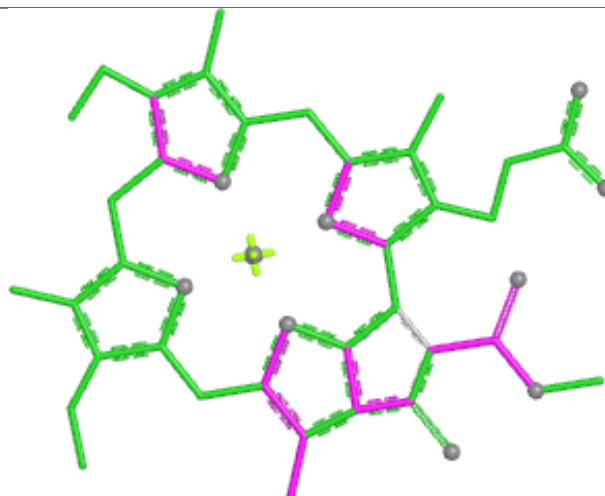




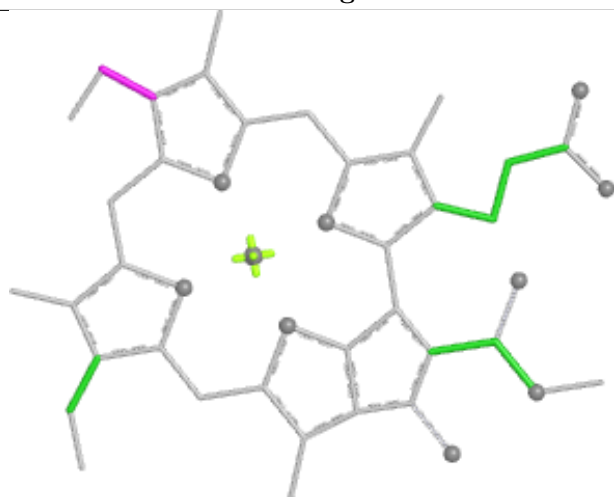
Ligand CLA B 819



Bond lengths



Bond angles

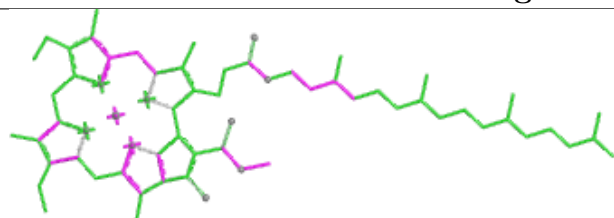


Torsions

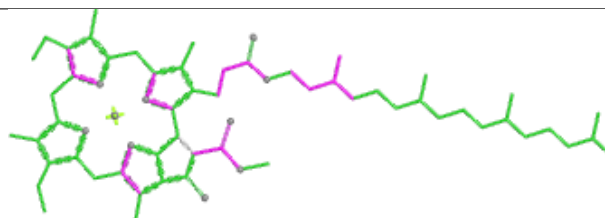


Rings

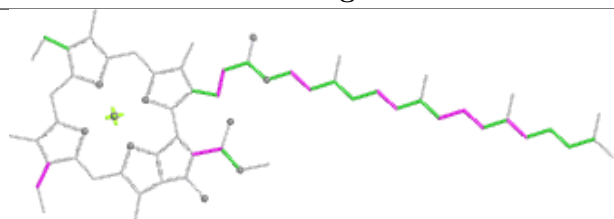
Ligand CLA B 830



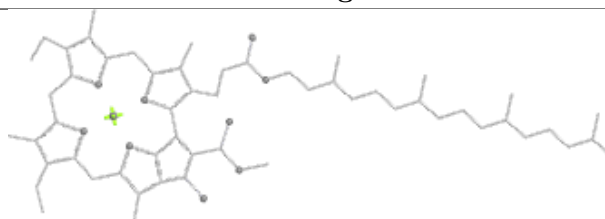
Bond lengths



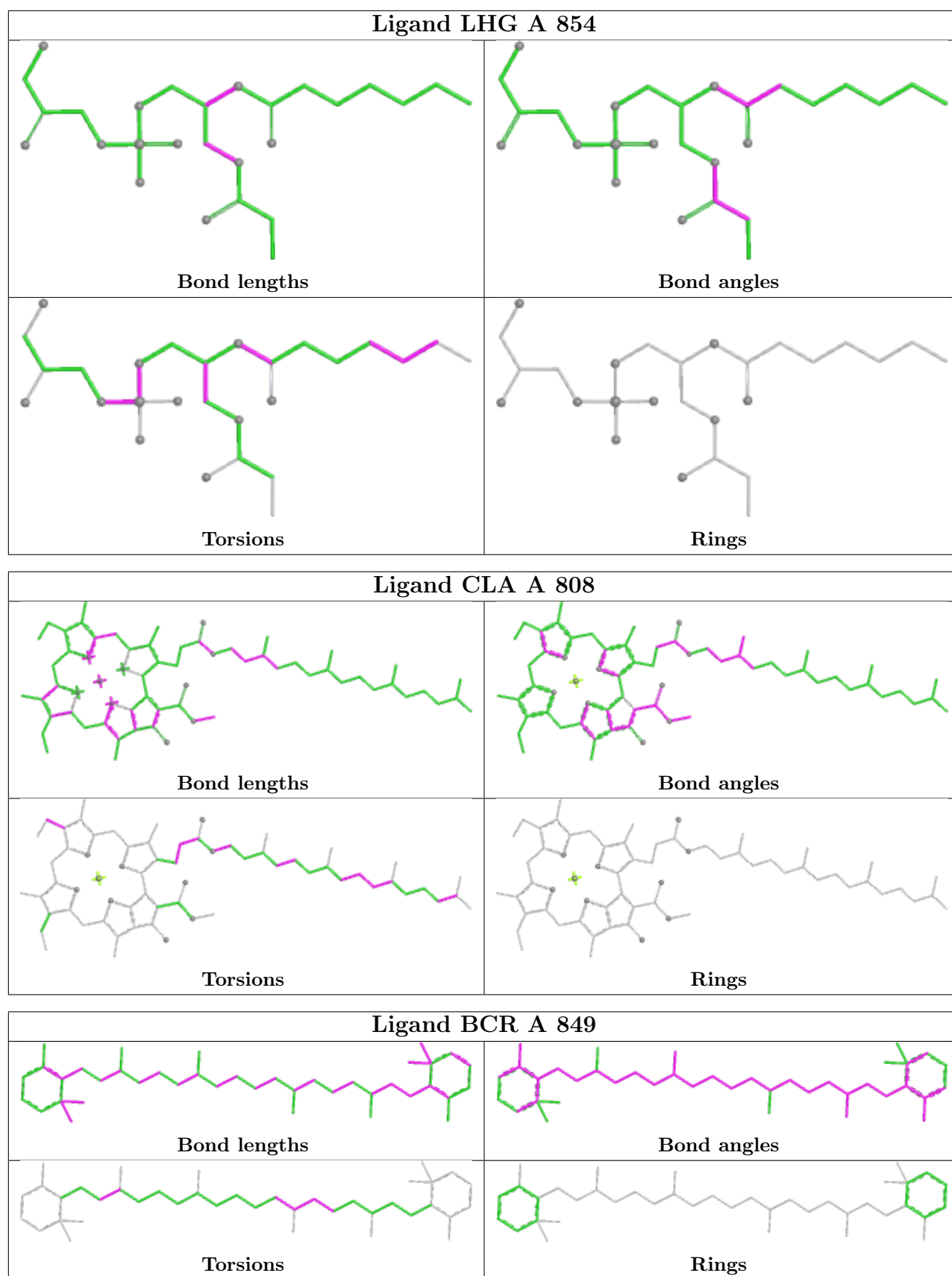
Bond angles



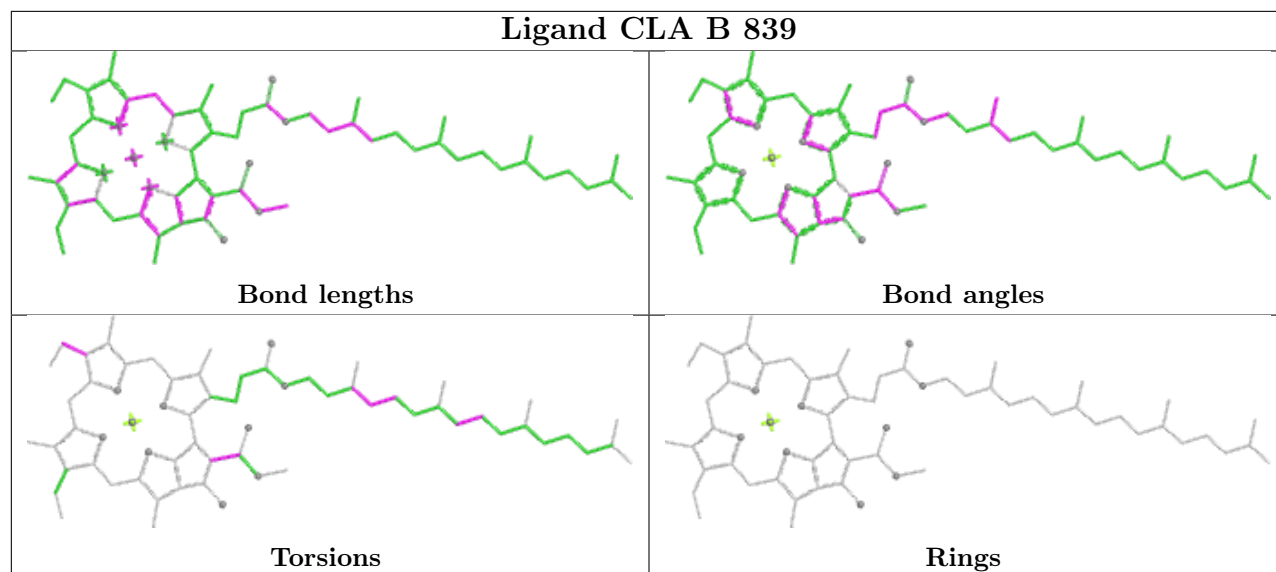
Torsions



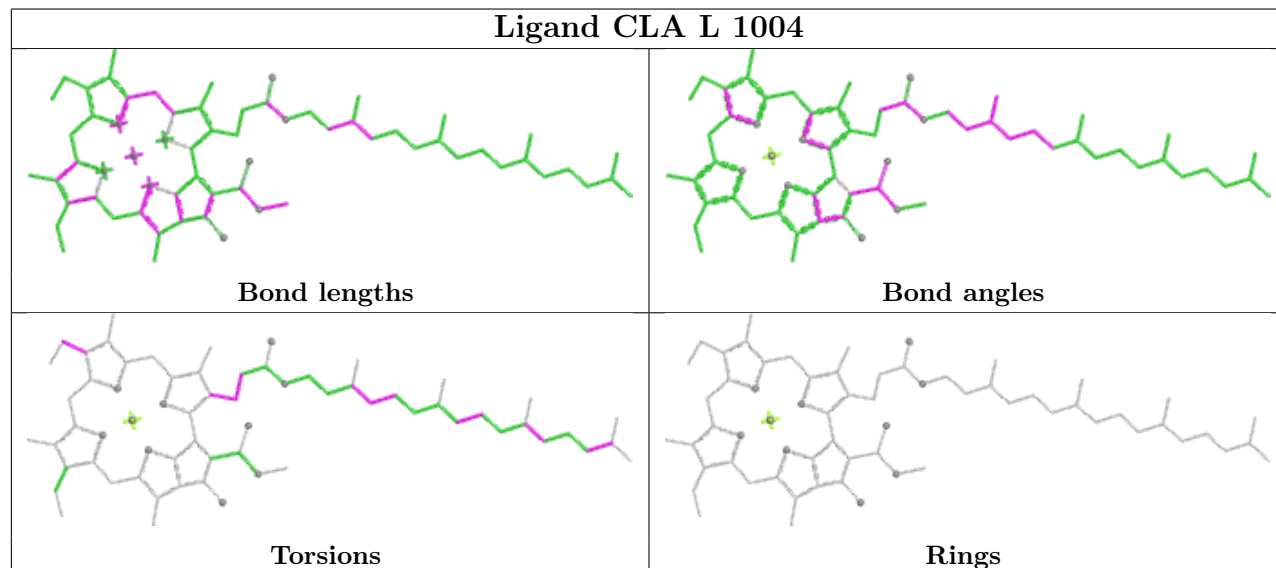
Rings



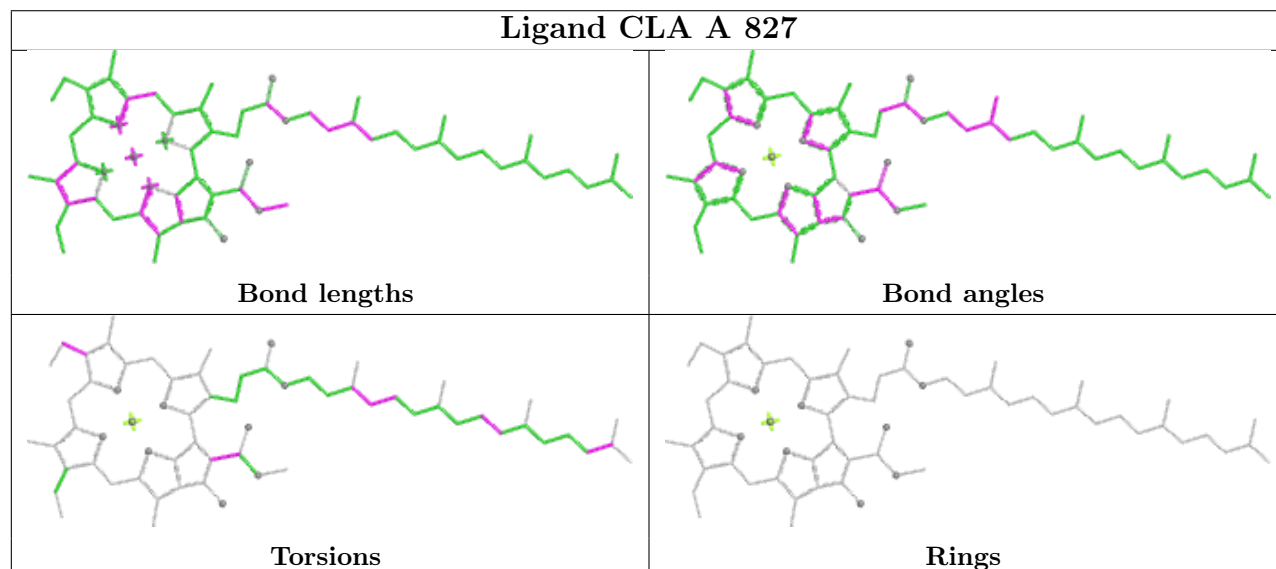
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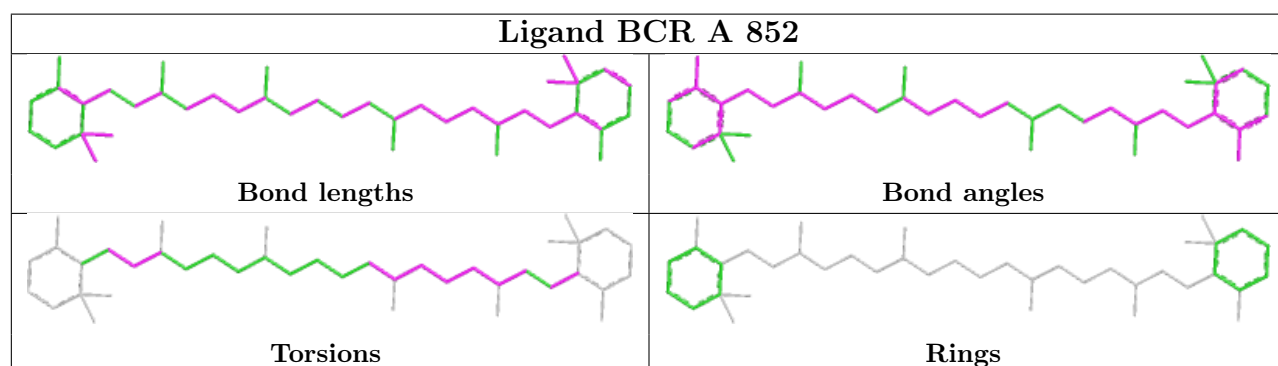
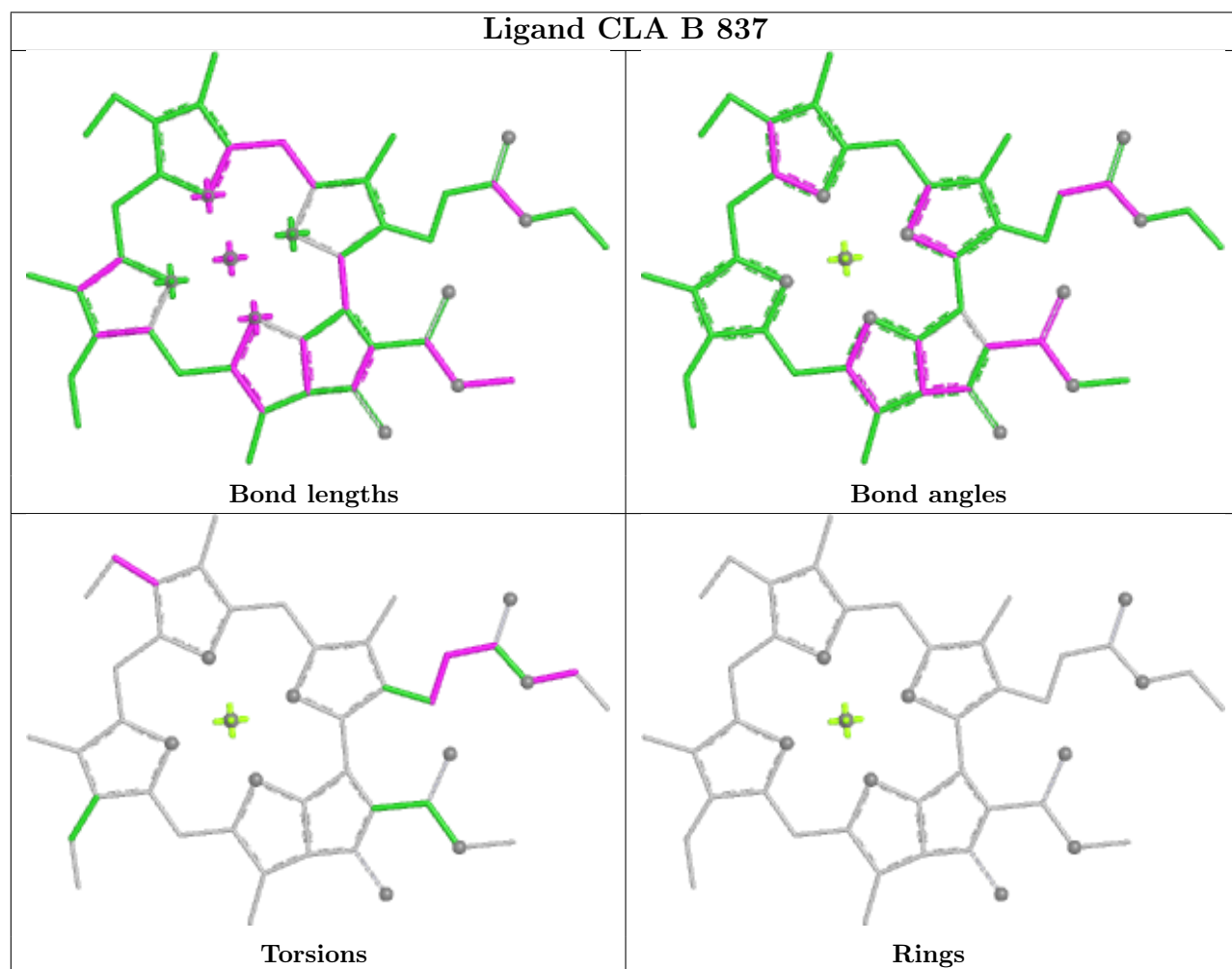
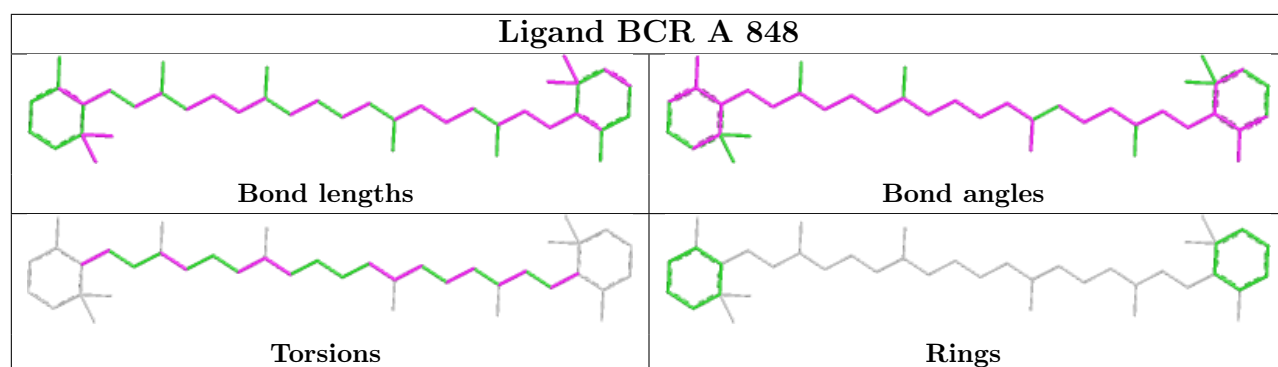


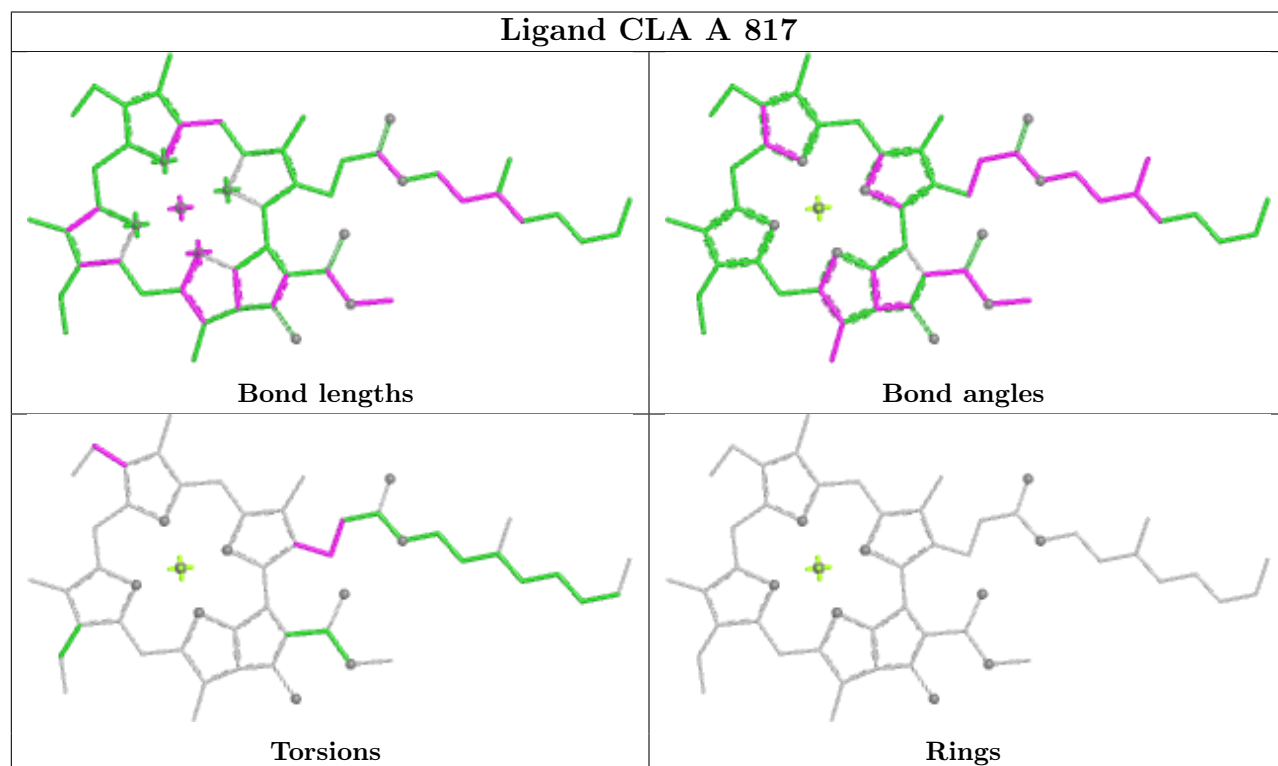
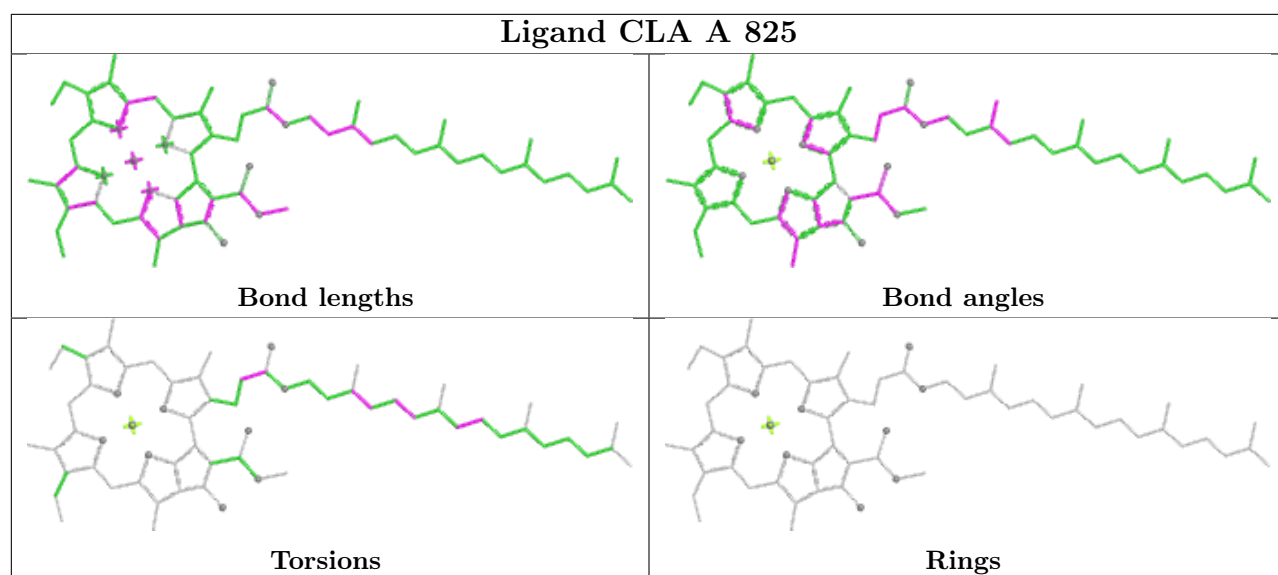
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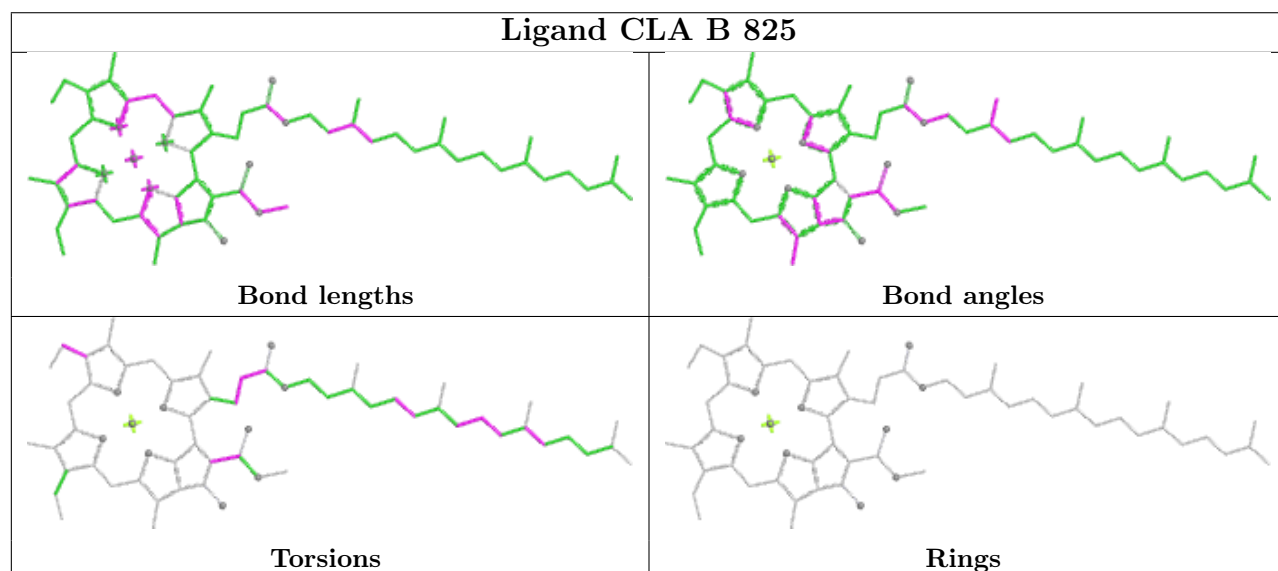
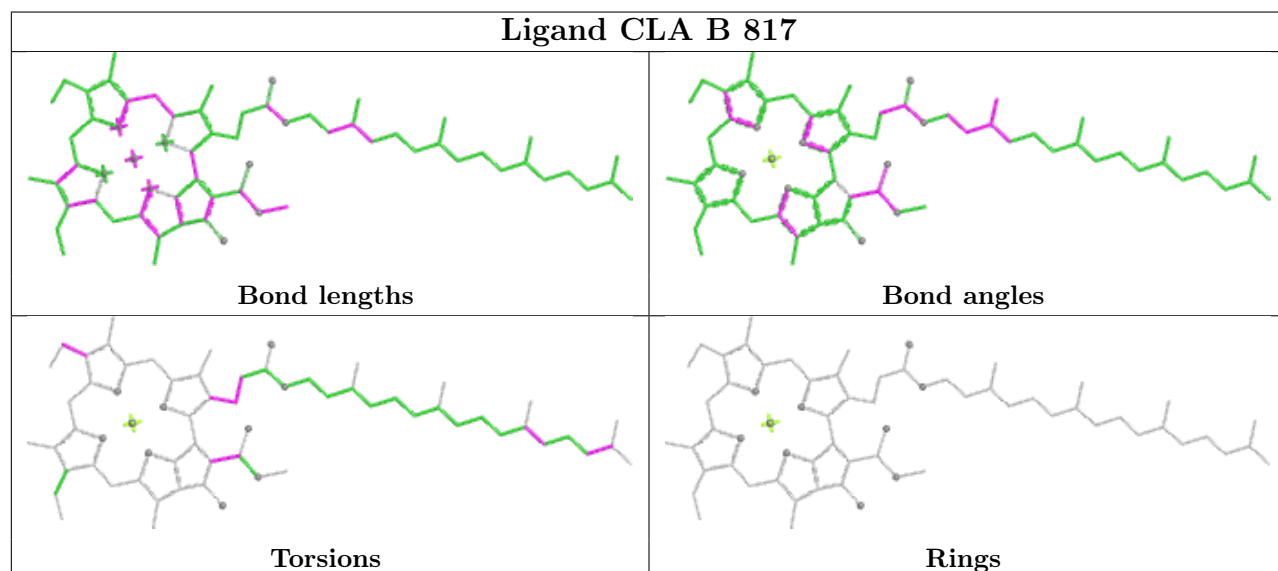
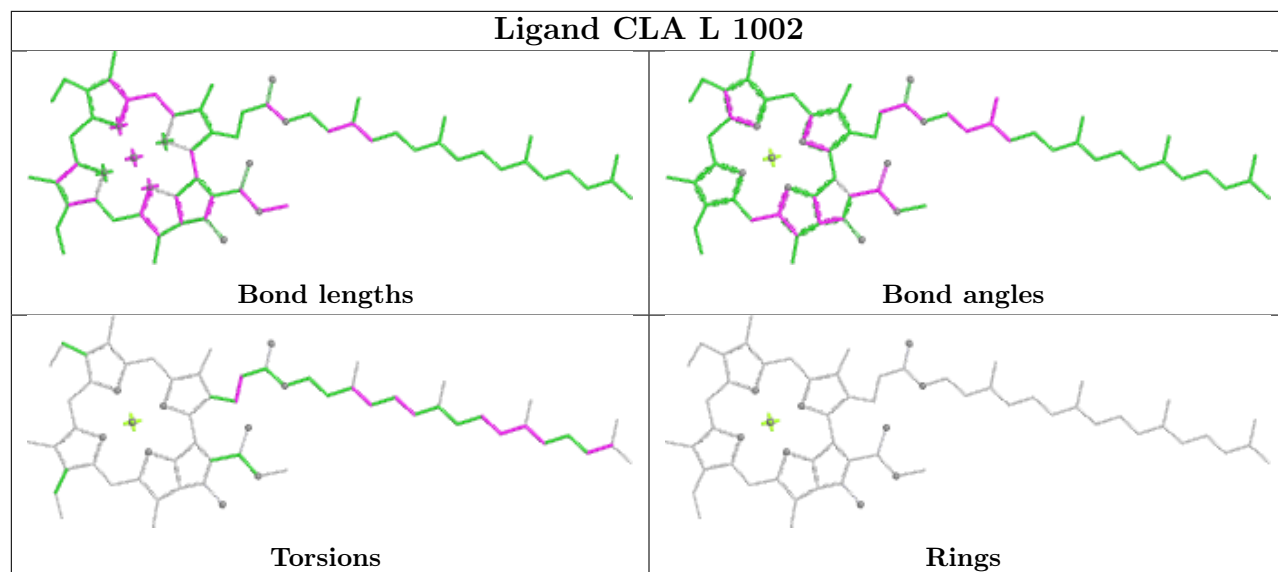


Ligand CLA A 827

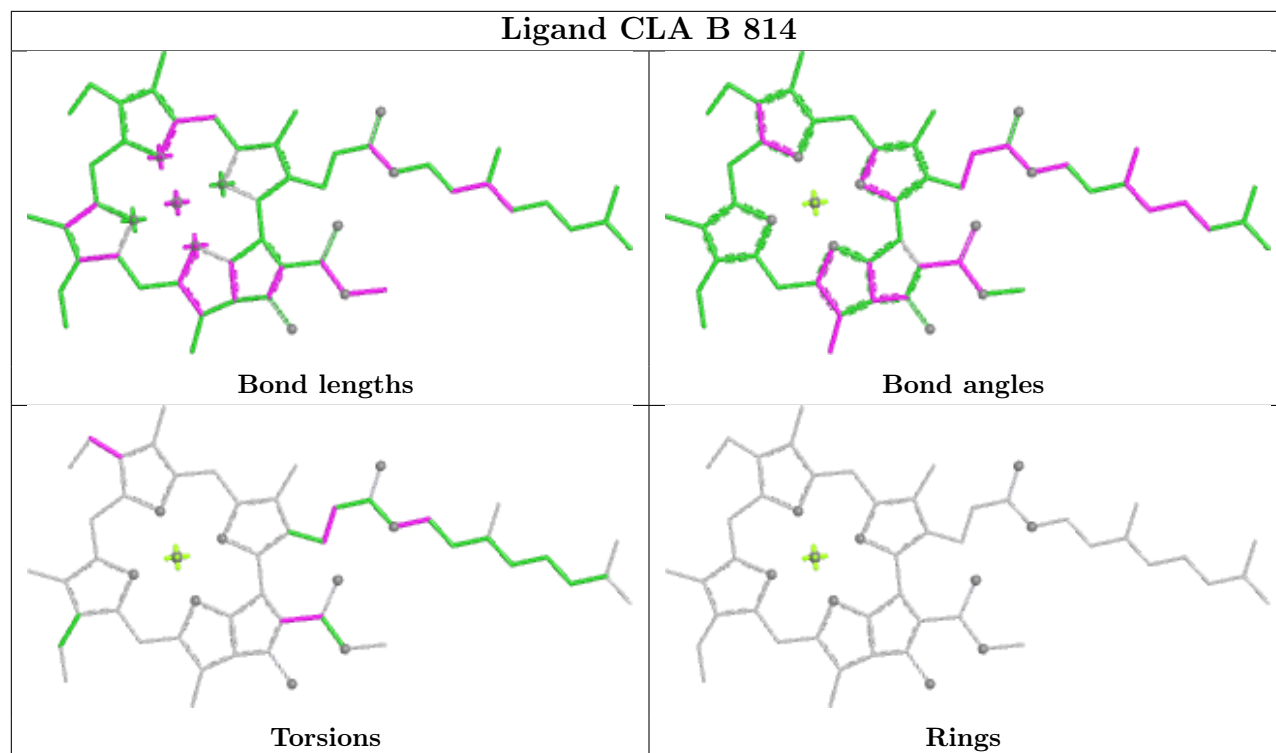




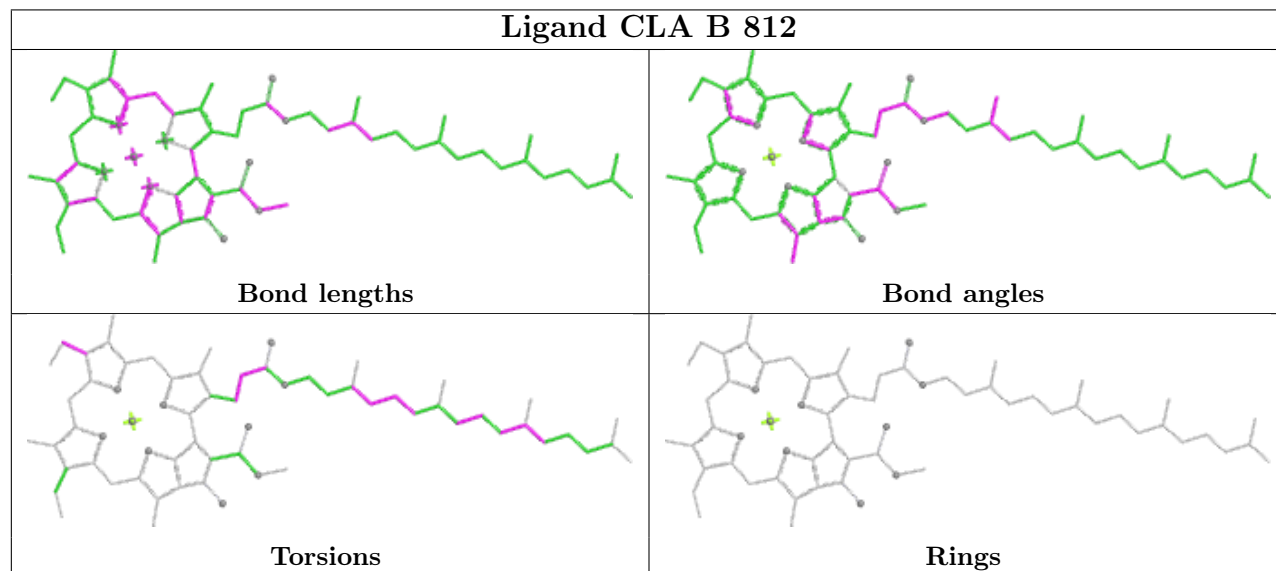




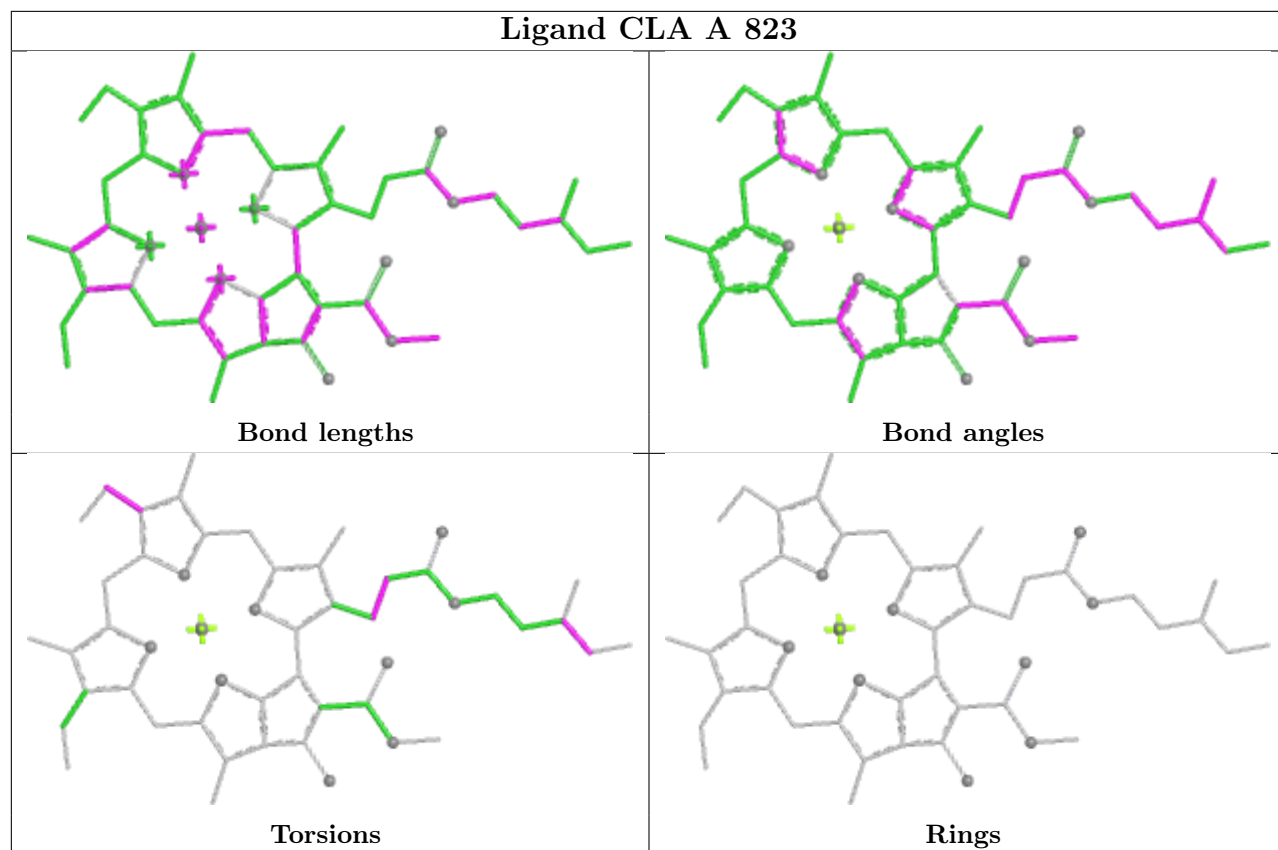
Ligand CLA B 814



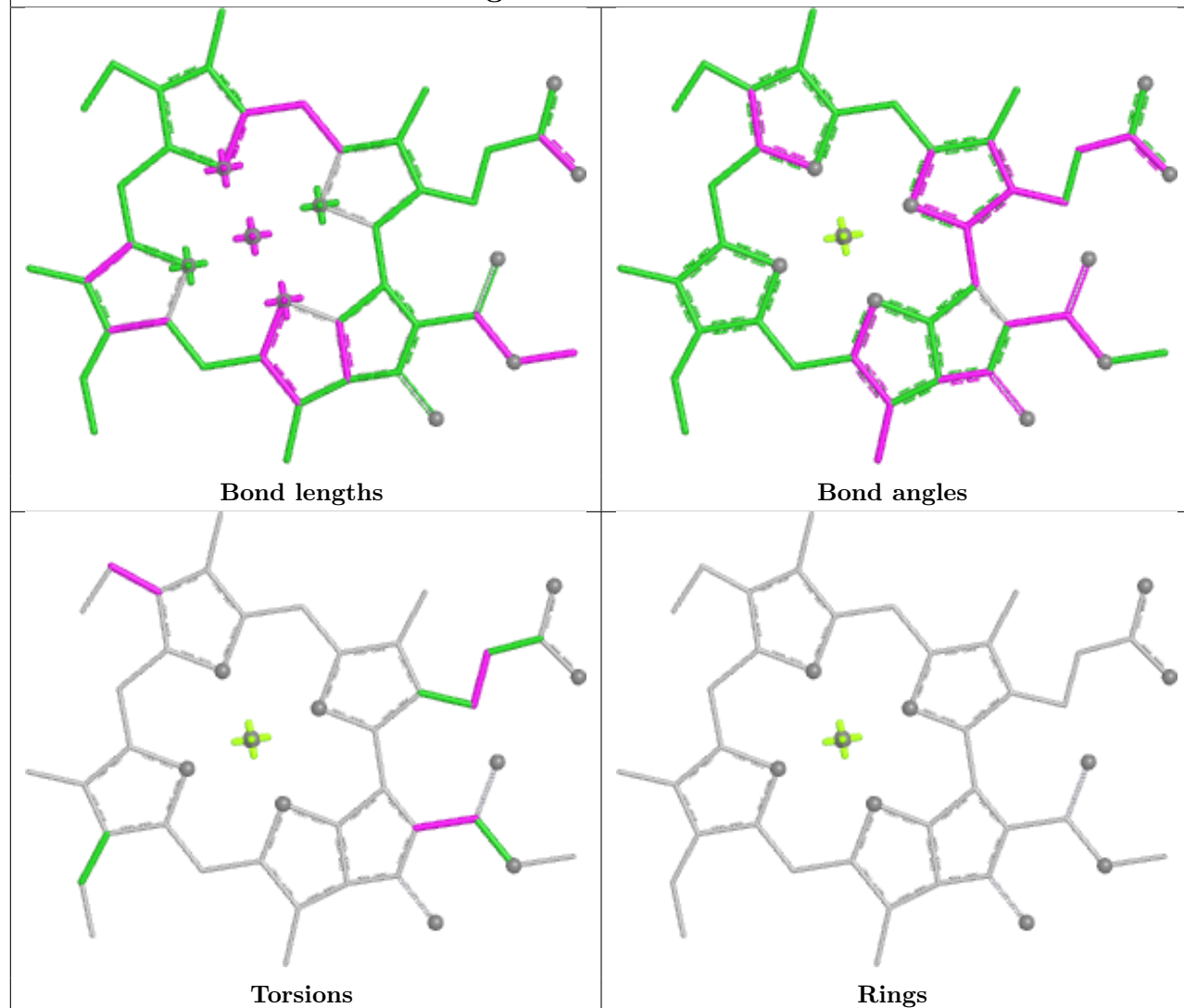
Ligand CLA B 812



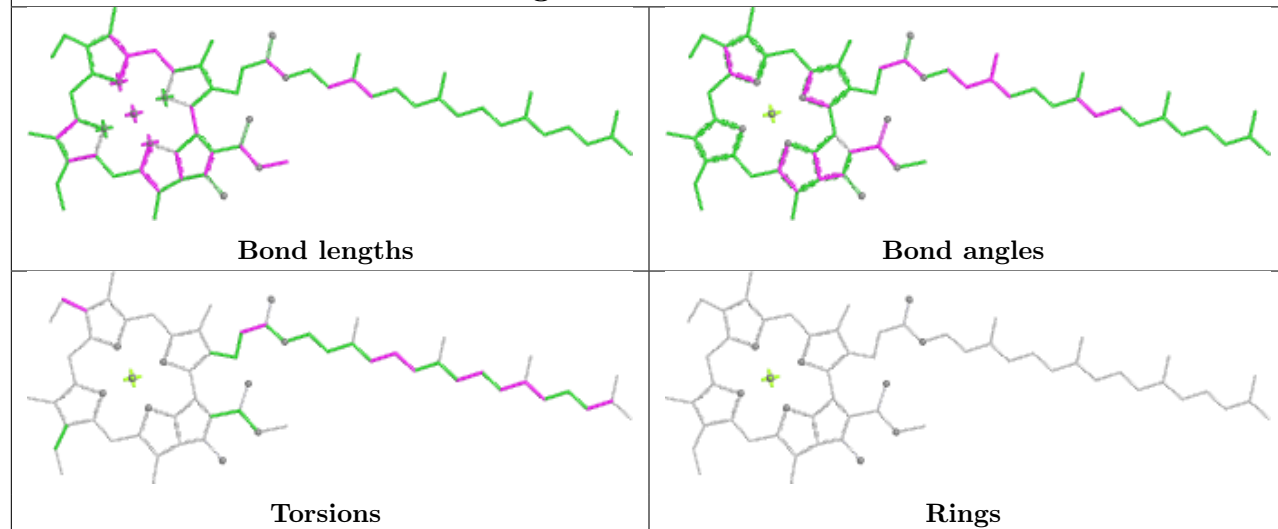
Ligand CLA A 823



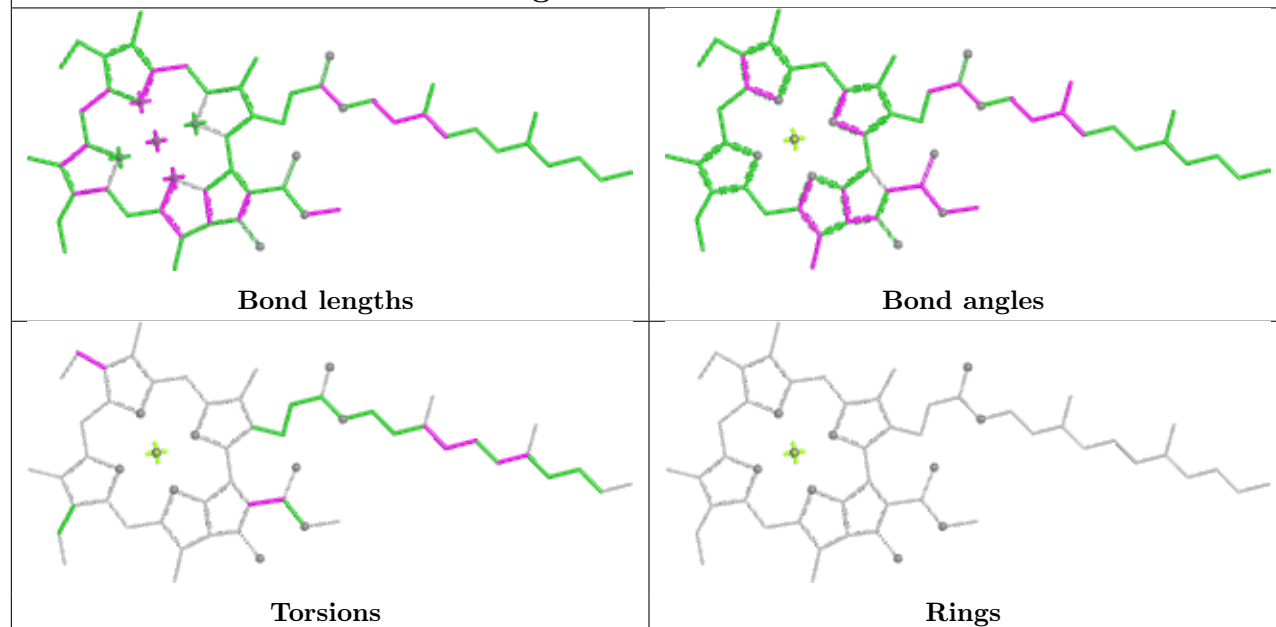
Ligand CLA F 1301



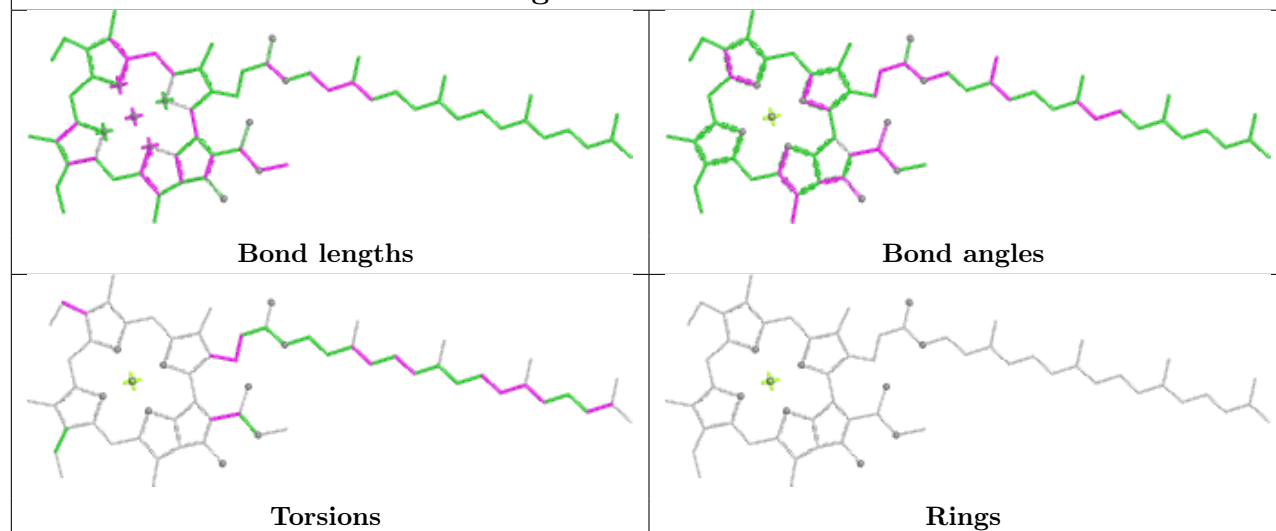
Ligand CLA B 801



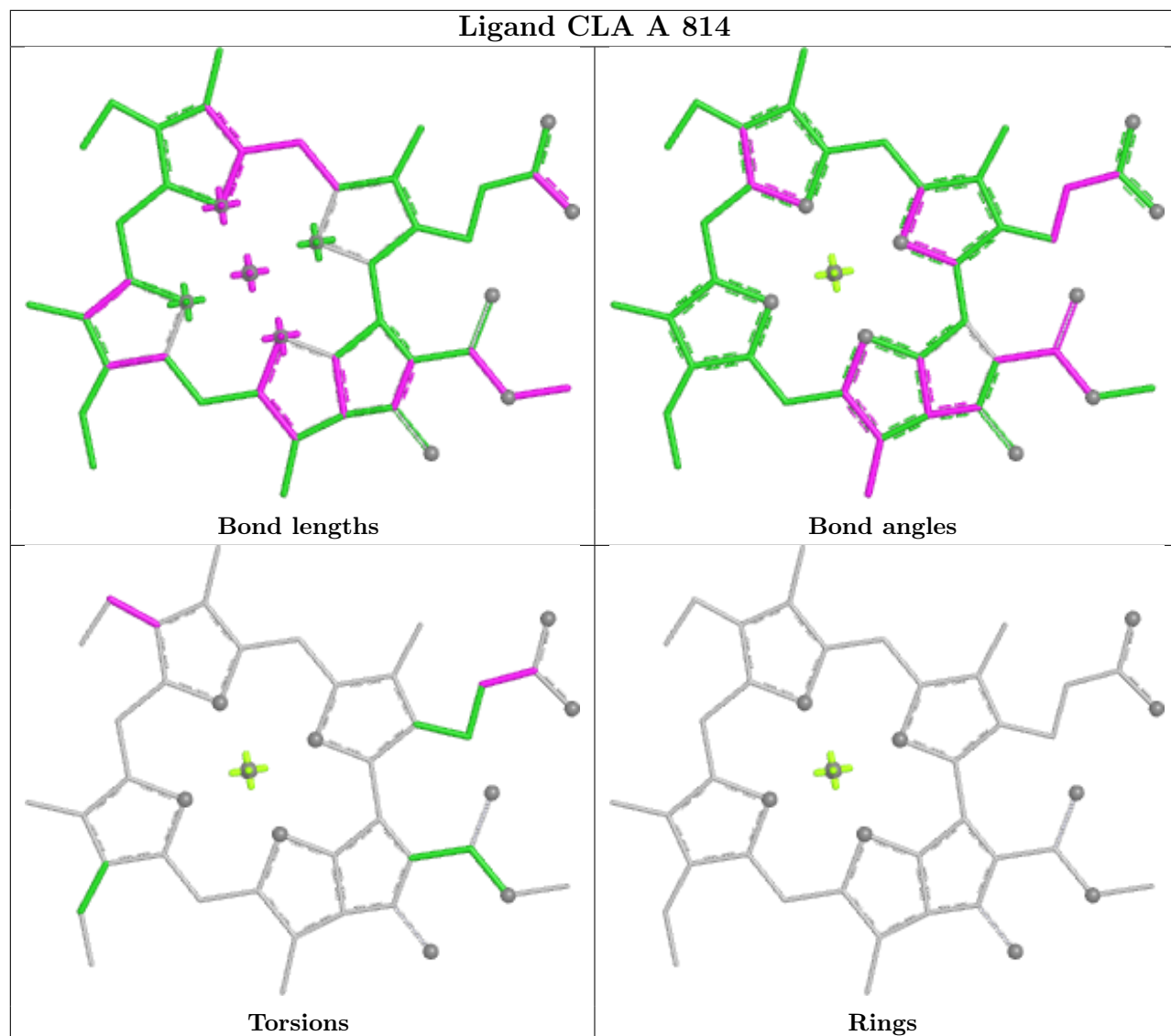
Ligand CLA B 831



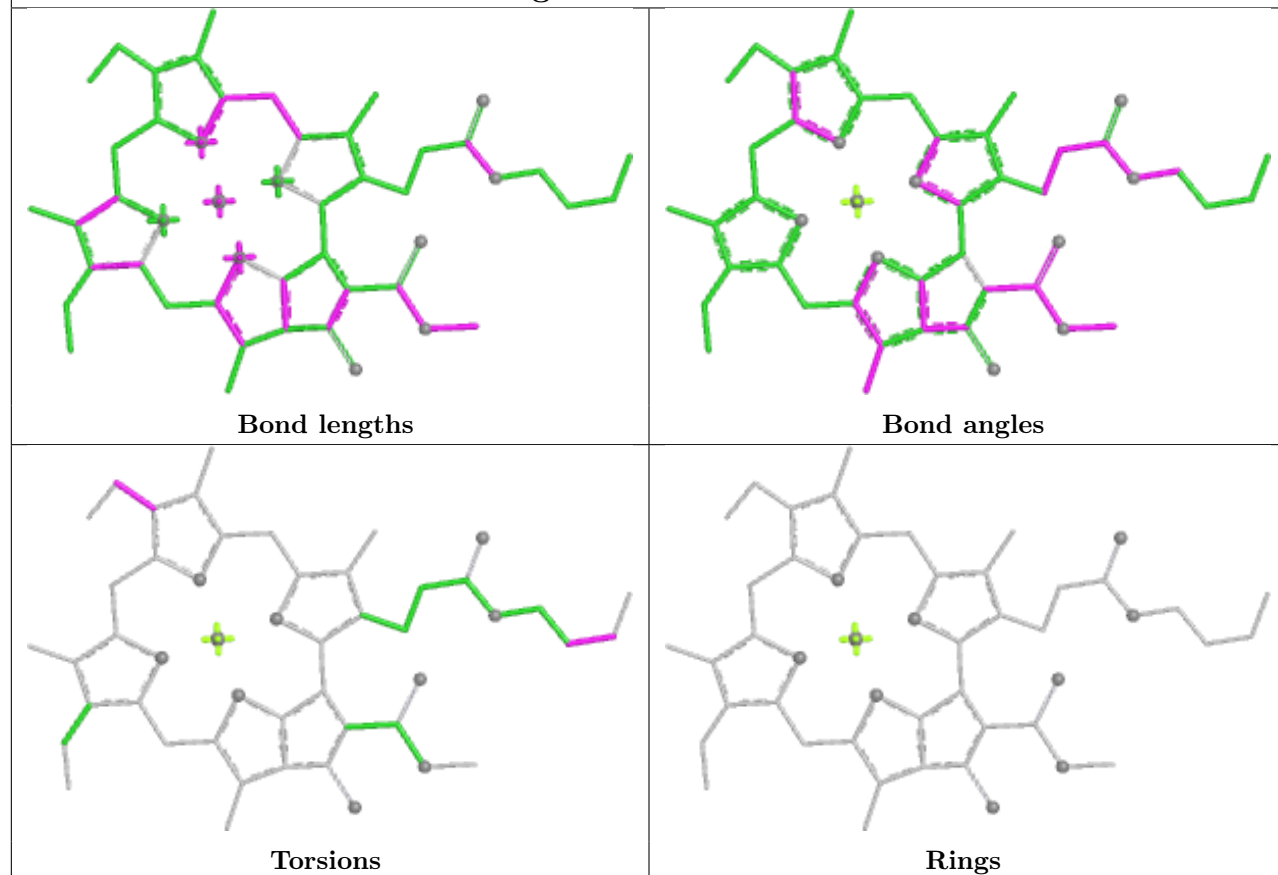
Ligand CLA A 838



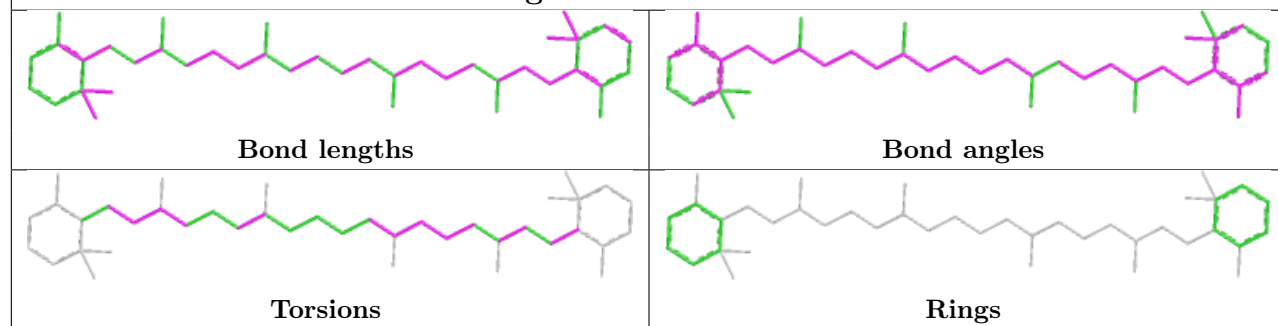
Ligand CLA A 814



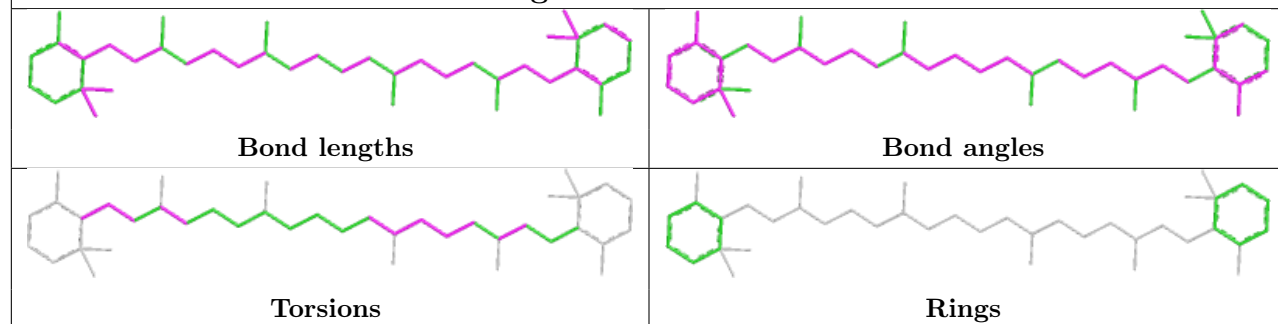
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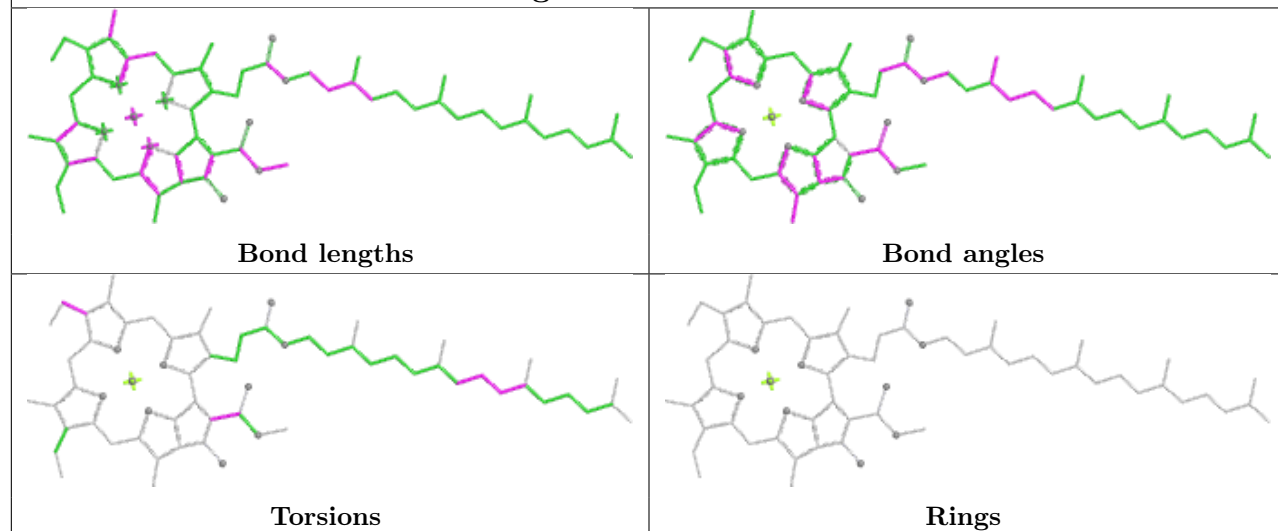
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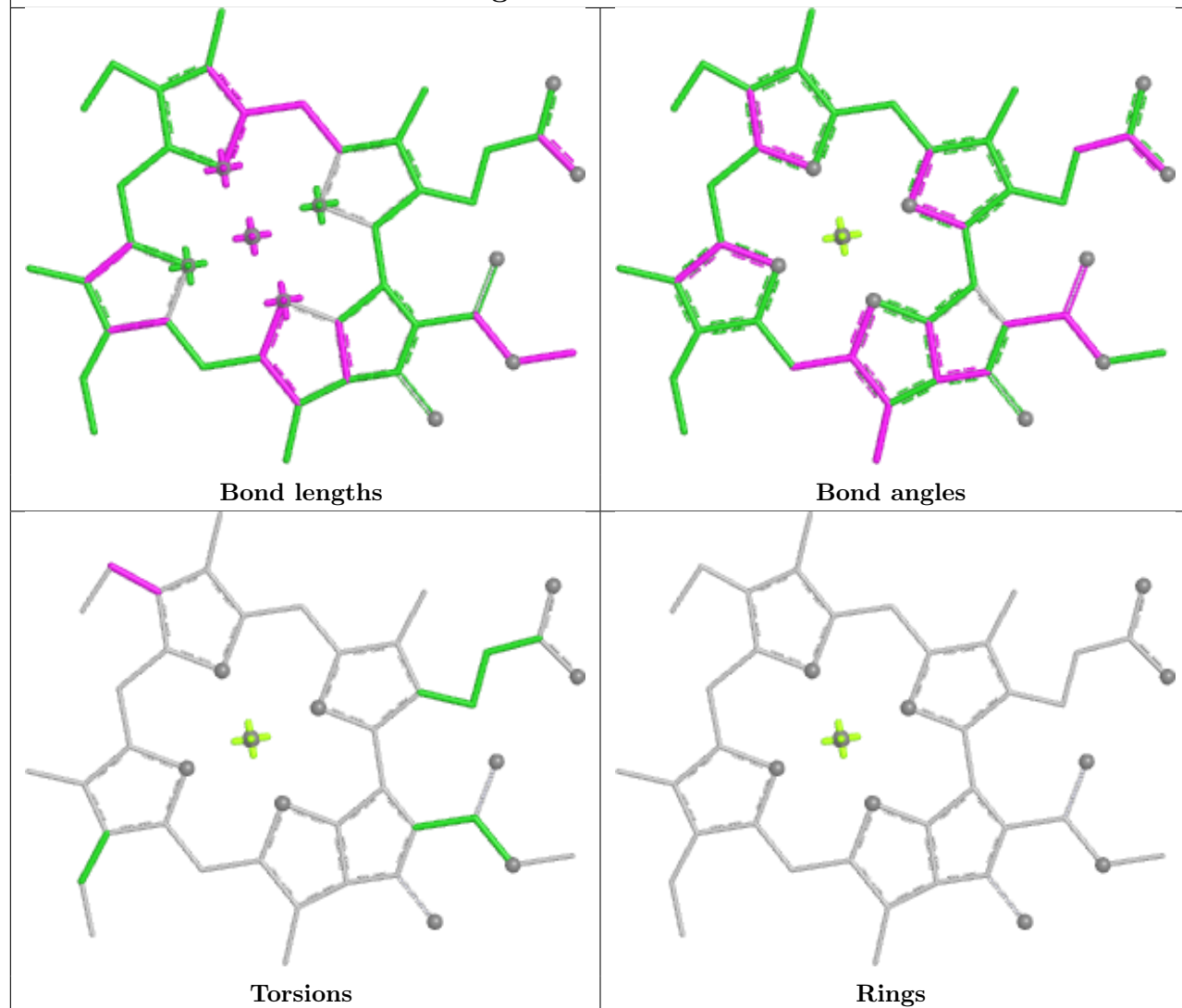
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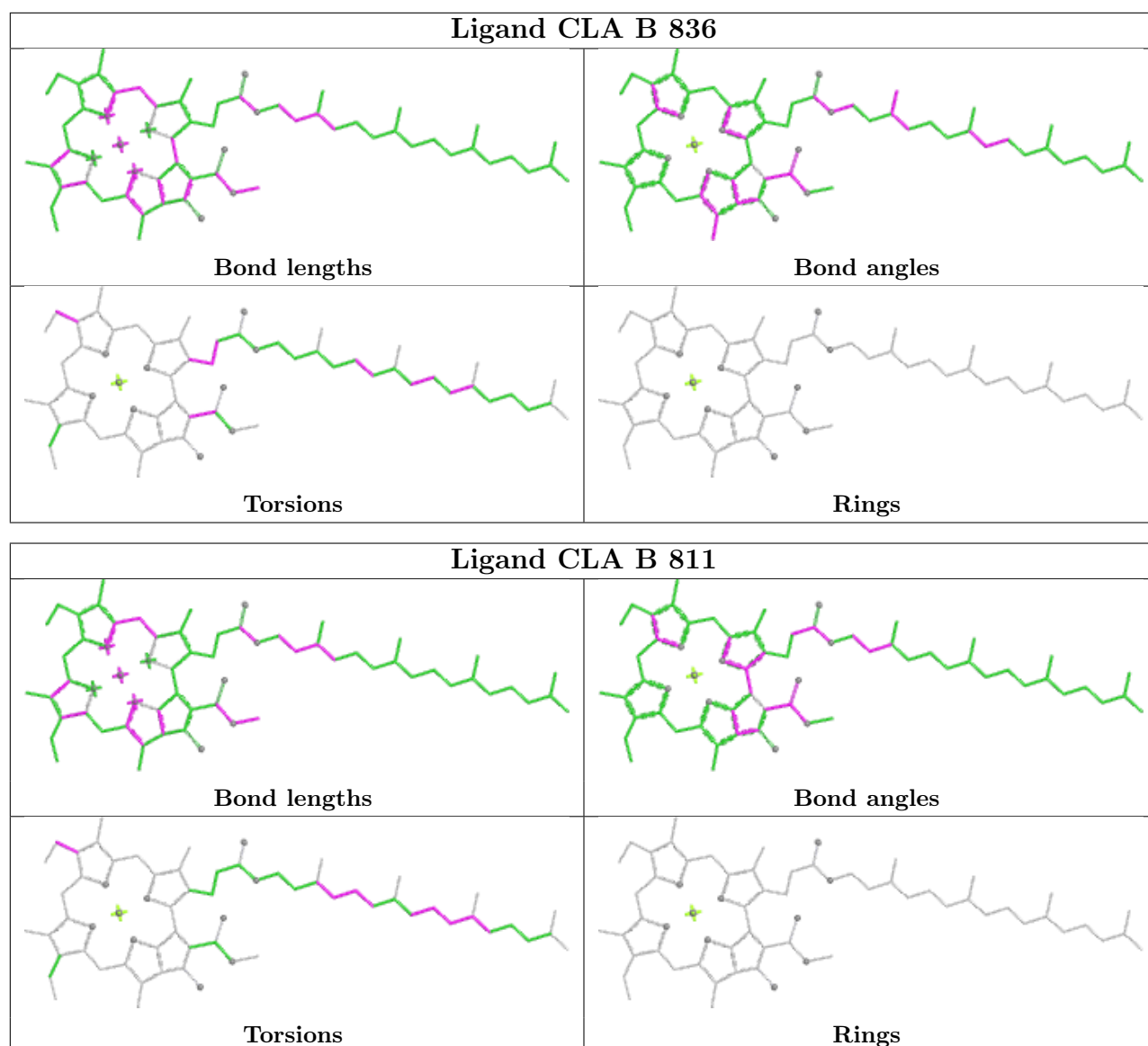


Ligand CLA B 827



Ligand CLA A 815





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	740/755 (98%)	-0.50	1 (0%) 92 87	42, 99, 157, 202	0
2	B	739/740 (99%)	-0.55	0 100 100	34, 76, 126, 215	0
3	C	80/80 (100%)	-0.70	0 100 100	46, 72, 126, 138	0
4	D	138/138 (100%)	-0.62	0 100 100	45, 72, 117, 137	0
5	E	69/75 (92%)	-0.58	0 100 100	77, 100, 148, 194	0
6	F	141/164 (85%)	-0.62	0 100 100	54, 83, 136, 158	0
7	I	38/38 (100%)	-0.65	0 100 100	10, 36, 74, 78	0
8	J	41/41 (100%)	-0.77	0 100 100	65, 89, 136, 165	0
9	K	46/83 (55%)	-0.67	0 100 100	55, 87, 141, 169	0
10	L	151/154 (98%)	-0.22	6 (3%) 42 37	14, 49, 104, 140	0
11	M	31/31 (100%)	-0.70	0 100 100	31, 51, 80, 92	0
12	X	29/35 (82%)	-0.56	0 100 100	59, 80, 120, 155	0
All	All	2243/2334 (96%)	-0.54	7 (0%) 90 80	10, 81, 141, 215	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	L	107	SER	3.8
10	L	146	ASP	3.8
1	A	22	PRO	3.3
10	L	147	GLY	3.1
10	L	72	ASP	2.6
10	L	151	GLY	2.3
10	L	71	SER	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	CLA	A	812	54/65	0.97	0.11	136,181,240,396	0
13	CLA	B	829	49/65	0.97	0.11	80,85,125,141	0
13	CLA	B	832	45/65	0.97	0.12	71,121,142,247	0
13	CLA	B	834	45/65	0.97	0.10	91,118,151,158	0
15	BCR	A	847	40/40	0.97	0.12	98,140,151,162	0
15	BCR	A	849	40/40	0.97	0.12	95,136,179,183	0
18	LMG	B	848	55/55	0.97	0.12	42,51,67,114	0
13	CLA	A	813	60/65	0.98	0.08	115,146,178,366	0
13	CLA	A	815	45/65	0.98	0.09	111,150,177,185	0
13	CLA	A	816	49/65	0.98	0.12	119,163,187,193	0
13	CLA	A	817	54/65	0.98	0.08	83,104,164,172	0
13	CLA	A	820	61/65	0.98	0.09	119,135,166,198	0
13	CLA	A	822	49/65	0.98	0.10	102,126,157,235	0
13	CLA	A	823	51/65	0.98	0.09	74,129,153,156	0
13	CLA	A	827	65/65	0.98	0.10	68,103,137,248	0
13	CLA	A	829	65/65	0.98	0.10	83,108,179,197	0
13	CLA	A	835	54/65	0.98	0.11	54,79,117,204	0
13	CLA	A	839	47/65	0.98	0.08	48,51,119,202	0
13	CLA	A	840	65/65	0.98	0.10	77,87,117,198	0
13	CLA	A	841	51/65	0.98	0.09	80,105,182,204	0
13	CLA	A	842	65/65	0.98	0.09	62,82,149,162	0
13	CLA	A	843	65/65	0.98	0.10	56,83,169,197	0
13	CLA	A	844	41/65	0.98	0.08	116,136,148,281	0
13	CLA	A	845	52/65	0.98	0.09	56,78,188,214	0
13	CLA	A	855	45/65	0.98	0.08	95,118,140,153	0
13	CLA	B	802	65/65	0.98	0.09	61,82,112,165	0
13	CLA	B	803	65/65	0.98	0.11	40,68,95,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	CLA	B	808	65/65	0.98	0.10	36,41,97,103	0
13	CLA	B	810	45/65	0.98	0.09	47,84,145,182	0
13	CLA	B	812	65/65	0.98	0.10	37,42,111,117	0
13	CLA	B	813	45/65	0.98	0.09	51,86,132,141	0
13	CLA	B	814	55/65	0.98	0.10	77,122,182,325	0
13	CLA	B	815	59/65	0.98	0.10	55,58,76,293	0
13	CLA	B	820	55/65	0.98	0.09	77,105,141,146	0
13	CLA	B	821	45/65	0.98	0.09	63,69,105,191	0
13	CLA	B	823	46/65	0.98	0.09	59,68,120,137	0
13	CLA	B	824	65/65	0.98	0.10	58,65,88,96	0
13	CLA	B	828	45/65	0.98	0.09	70,80,132,193	0
13	CLA	A	804	59/65	0.98	0.09	83,99,117,144	0
13	CLA	B	831	58/65	0.98	0.10	80,101,148,333	0
13	CLA	A	807	51/65	0.98	0.09	87,100,151,177	0
13	CLA	B	833	45/65	0.98	0.09	77,104,141,148	0
13	CLA	A	809	65/65	0.98	0.11	78,117,148,152	0
13	CLA	B	835	60/65	0.98	0.08	65,106,240,292	0
13	CLA	B	838	65/65	0.98	0.11	35,45,102,125	0
13	CLA	B	839	65/65	0.98	0.09	35,49,151,215	0
13	CLA	F	1301	45/65	0.98	0.09	94,137,167,175	0
13	CLA	J	1102	45/65	0.98	0.08	75,111,128,280	0
14	PQN	A	846	33/33	0.98	0.09	55,64,82,82	0
14	PQN	B	840	33/33	0.98	0.10	56,84,105,121	0
13	CLA	A	810	45/65	0.98	0.10	109,136,151,223	0
15	BCR	A	848	40/40	0.98	0.11	112,132,147,157	0
13	CLA	A	811	65/65	0.98	0.11	95,134,173,321	0
15	BCR	B	841	40/40	0.98	0.13	65,105,151,155	0
15	BCR	B	843	40/40	0.98	0.10	45,59,82,86	0
15	BCR	B	845	40/40	0.98	0.09	60,66,78,82	0
15	BCR	B	846	40/40	0.98	0.10	75,91,131,137	0
15	BCR	B	847	40/40	0.98	0.11	40,51,116,126	0
15	BCR	B	849	40/40	0.98	0.09	12,43,147,152	0
15	BCR	B	850	40/40	0.98	0.09	83,107,144,146	0
15	BCR	J	1104	40/40	0.98	0.10	64,78,113,120	0
15	BCR	L	1005	40/40	0.98	0.10	11,16,81,93	0
15	BCR	L	1006	40/40	0.98	0.10	16,24,64,78	0
15	BCR	M	1203	40/40	0.98	0.09	43,48,87,92	0
16	LHG	X	101	23/49	0.98	0.08	78,81,207,208	0
13	CLA	A	801	65/65	0.98	0.09	44,53,82,89	0
19	CA	L	1001	1/1	0.98	0.10	22,22,22,22	0
13	CLA	B	822	54/65	0.99	0.08	61,86,118,158	0
13	CLA	A	836	45/65	0.99	0.08	63,96,163,234	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	CLA	A	837	51/65	0.99	0.07	52,56,96,147	0
13	CLA	B	825	65/65	0.99	0.08	40,60,136,157	0
13	CLA	B	826	65/65	0.99	0.08	42,47,127,149	0
13	CLA	B	827	65/65	0.99	0.08	44,66,95,108	0
13	CLA	A	838	65/65	0.99	0.08	45,81,109,114	0
13	CLA	A	818	54/65	0.99	0.07	92,136,168,207	0
13	CLA	B	830	65/65	0.99	0.08	82,91,129,139	0
13	CLA	A	819	65/65	0.99	0.08	97,140,181,328	0
13	CLA	A	803	65/65	0.99	0.09	76,100,142,222	0
13	CLA	A	821	65/65	0.99	0.08	72,100,164,266	0
13	CLA	A	808	65/65	0.99	0.08	72,89,172,177	0
13	CLA	A	814	45/65	0.99	0.07	108,150,172,174	0
13	CLA	B	836	65/65	0.99	0.09	69,98,146,234	0
13	CLA	B	837	47/65	0.99	0.08	65,71,119,193	0
13	CLA	A	824	59/65	0.99	0.08	59,101,164,321	0
13	CLA	A	825	65/65	0.99	0.07	74,102,152,193	0
13	CLA	B	801	65/65	0.99	0.08	57,68,123,322	0
13	CLA	I	101	65/65	0.99	0.08	33,57,85,338	0
13	CLA	J	1101	65/65	0.99	0.09	77,129,178,357	0
13	CLA	A	826	65/65	0.99	0.08	53,80,112,127	0
13	CLA	J	1103	37/65	0.99	0.07	85,117,155,158	0
13	CLA	L	1002	65/65	0.99	0.09	29,65,103,148	0
13	CLA	L	1003	65/65	0.99	0.08	16,52,179,216	0
13	CLA	L	1004	65/65	0.99	0.08	21,31,64,72	0
13	CLA	M	1201	54/65	0.99	0.07	34,42,121,127	0
13	CLA	M	1202	45/65	0.99	0.09	51,149,183,198	0
13	CLA	X	102	45/65	0.99	0.08	67,104,127,283	0
13	CLA	A	802	65/65	0.99	0.08	40,77,110,230	0
13	CLA	B	804	65/65	0.99	0.08	45,51,117,199	0
13	CLA	B	805	65/65	0.99	0.07	41,48,97,150	0
13	CLA	B	806	65/65	0.99	0.09	33,63,107,170	0
13	CLA	B	807	65/65	0.99	0.08	38,65,106,122	0
15	BCR	A	850	40/40	0.99	0.09	56,96,126,139	0
15	BCR	A	851	40/40	0.99	0.07	50,58,118,132	0
15	BCR	A	852	40/40	0.99	0.10	78,107,149,162	0
13	CLA	A	828	65/65	0.99	0.08	59,74,127,289	0
15	BCR	B	842	40/40	0.99	0.07	48,76,129,134	0
13	CLA	B	809	45/65	0.99	0.08	39,95,125,308	0
15	BCR	B	844	25/40	0.99	0.08	65,68,113,118	0
13	CLA	A	805	65/65	0.99	0.08	85,98,117,126	0
13	CLA	B	811	65/65	0.99	0.08	48,71,108,145	0
13	CLA	A	830	65/65	0.99	0.06	59,71,105,119	0

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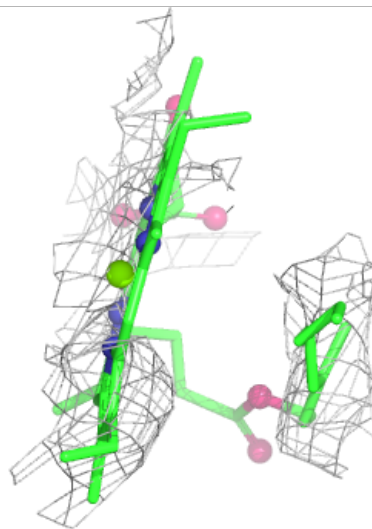
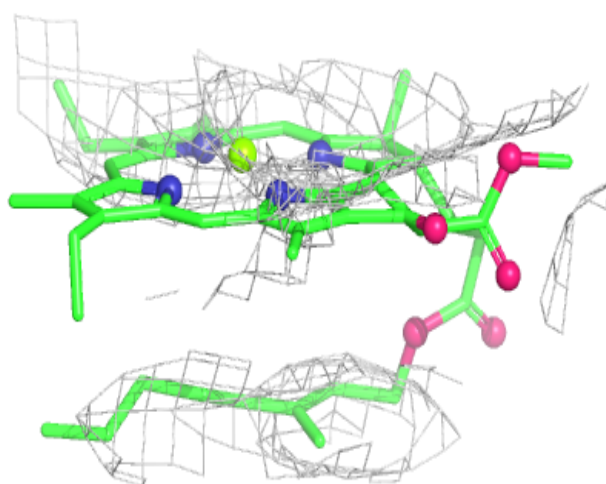
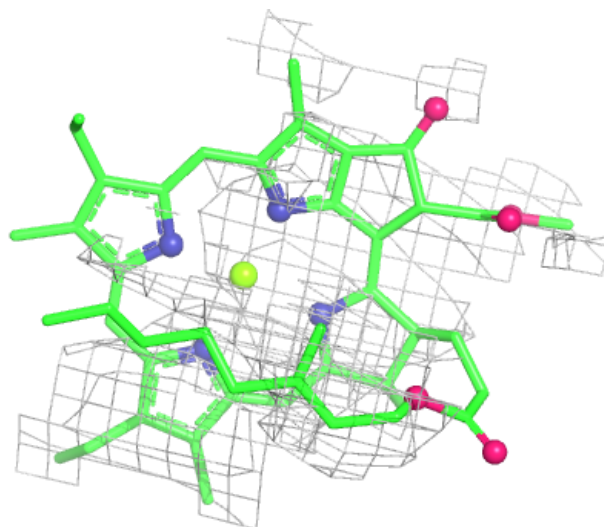
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	CLA	A	831	50/65	0.99	0.08	45,76,105,144	0
13	CLA	A	832	65/65	0.99	0.07	42,45,81,134	0
15	BCR	F	1302	40/40	0.99	0.11	70,94,125,128	0
15	BCR	I	102	40/40	0.99	0.08	19,20,48,52	0
13	CLA	A	833	65/65	0.99	0.09	39,45,110,121	0
15	BCR	J	1105	40/40	0.99	0.07	63,67,71,71	0
13	CLA	B	816	60/65	0.99	0.09	46,53,111,221	0
13	CLA	B	817	65/65	0.99	0.09	57,65,113,125	0
13	CLA	B	818	47/65	0.99	0.09	56,99,146,292	0
16	LHG	A	853	49/49	0.99	0.09	57,74,107,127	0
16	LHG	A	854	27/49	0.99	0.06	49,58,88,122	0
13	CLA	B	819	45/65	0.99	0.10	98,131,171,173	0
13	CLA	A	834	65/65	0.99	0.08	39,40,92,96	0
13	CLA	A	806	65/65	0.99	0.09	63,80,155,164	0
17	SF4	C	102	8/8	1.00	0.03	47,48,122,359	0
17	SF4	A	856	8/8	1.00	0.04	49,50,150,174	0
17	SF4	C	101	8/8	1.00	0.03	48,48,49,62	0

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

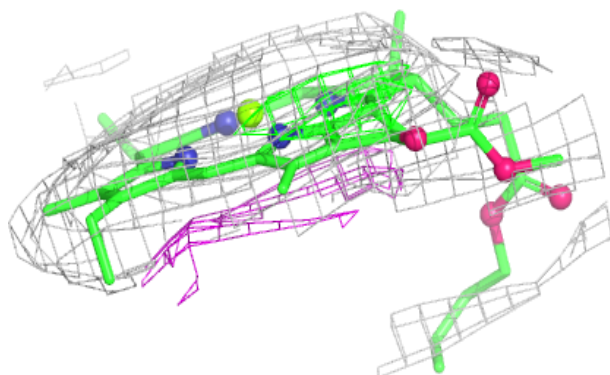
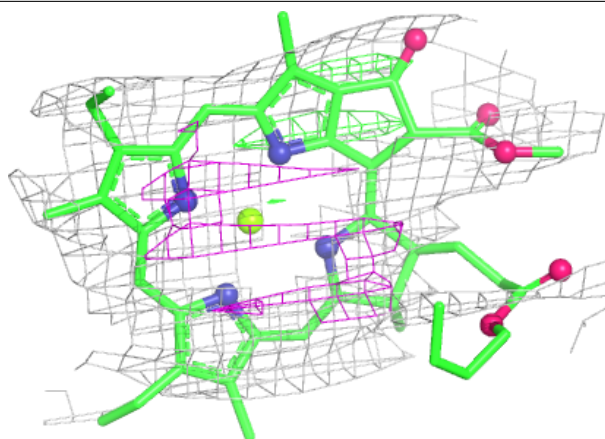
Electron density around CLA A 812:

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



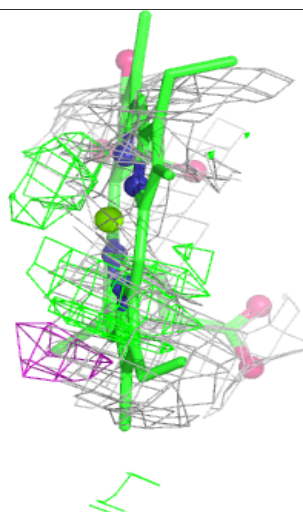
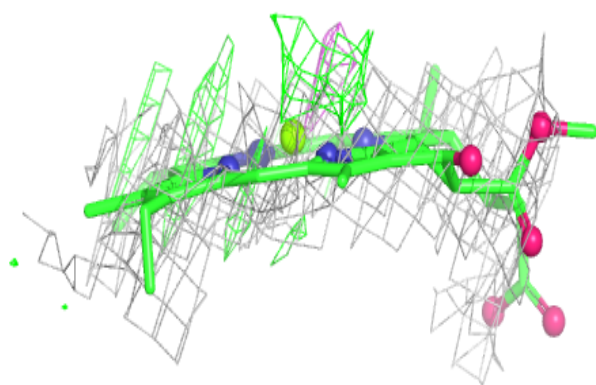
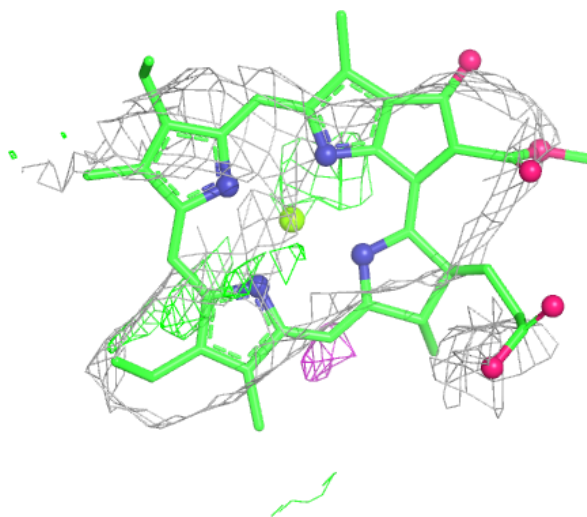
Electron density around CLA B 829:

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



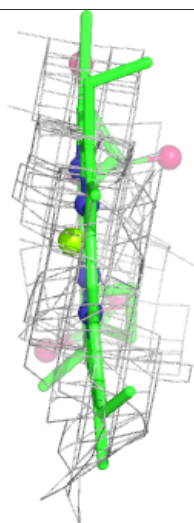
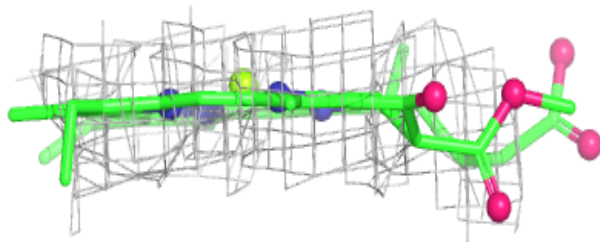
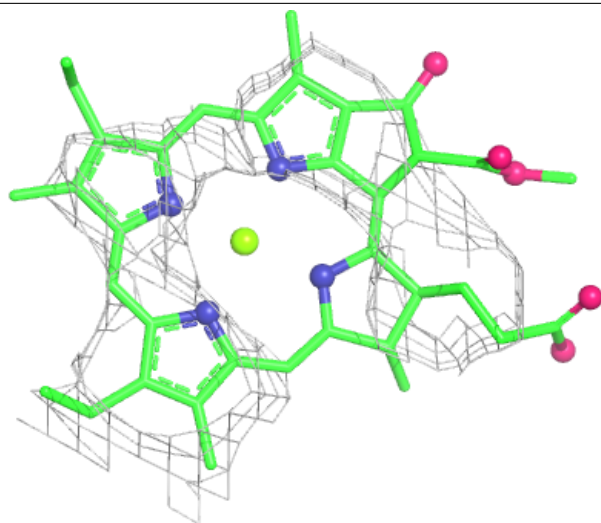
Electron density around CLA B 832:

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



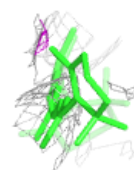
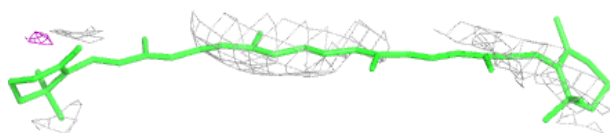
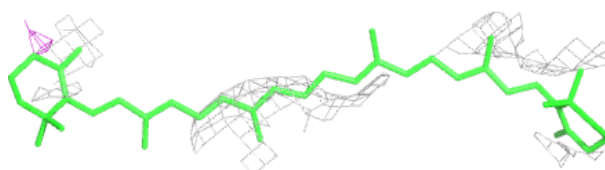
Electron density around CLA B 834:

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

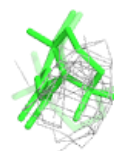
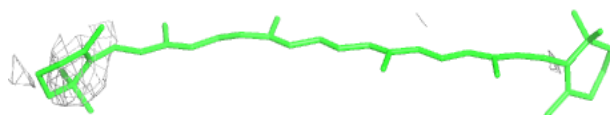


Electron density around BCR A 847:

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

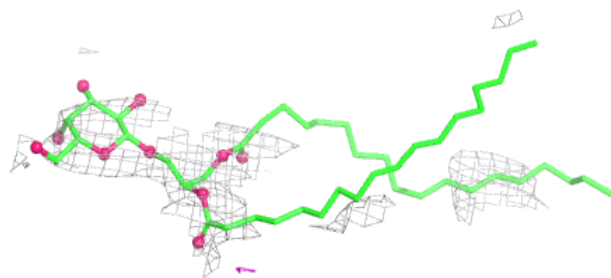
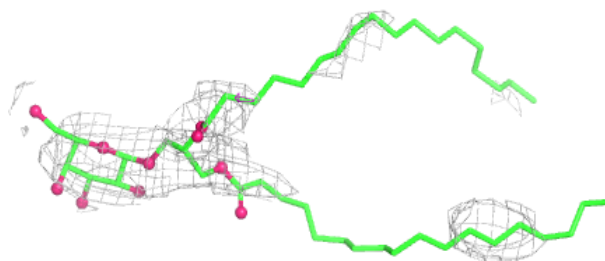
**Electron density around BCR A 849:**

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



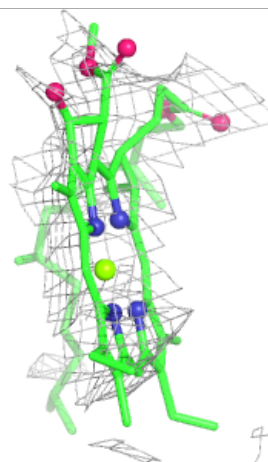
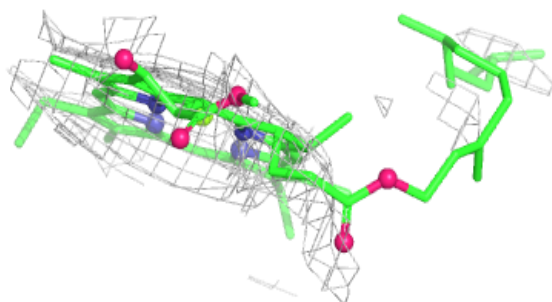
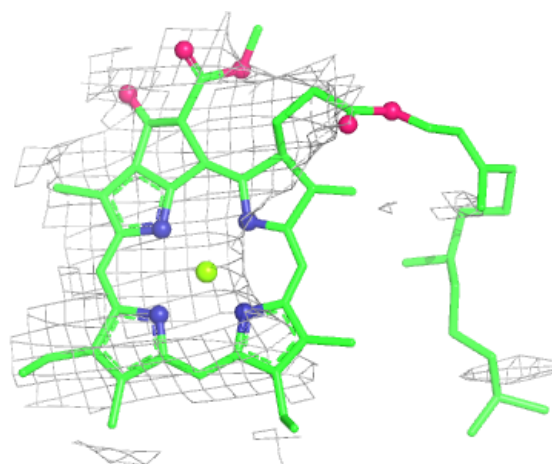
Electron density around LMG B 848:

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



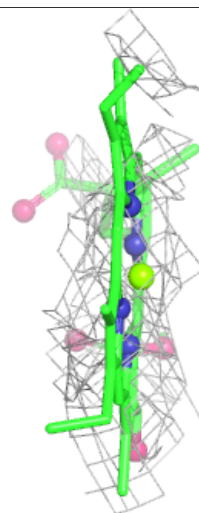
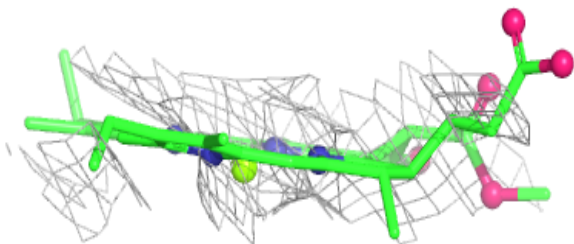
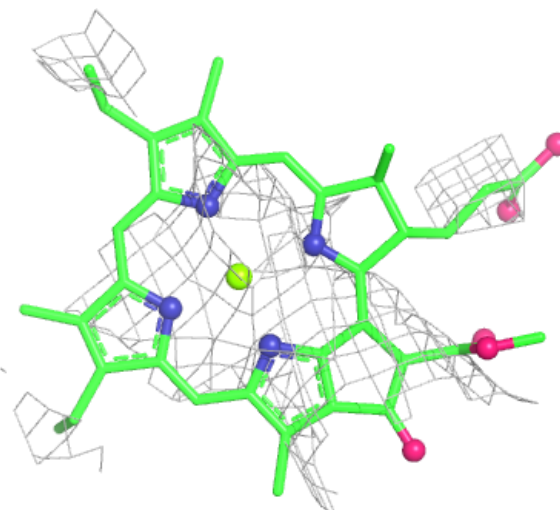
Electron density around CLA A 813:

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



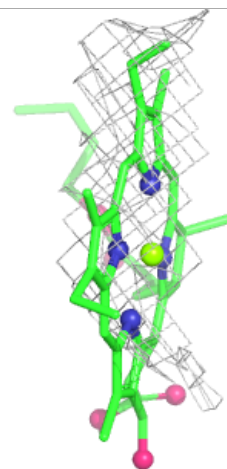
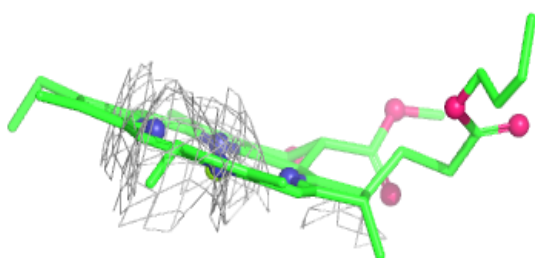
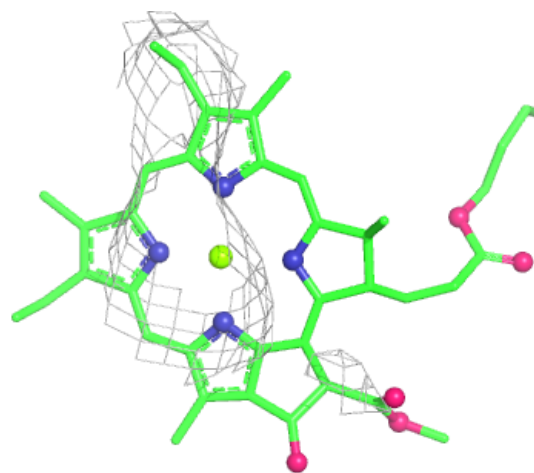
Electron density around CLA A 815:

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



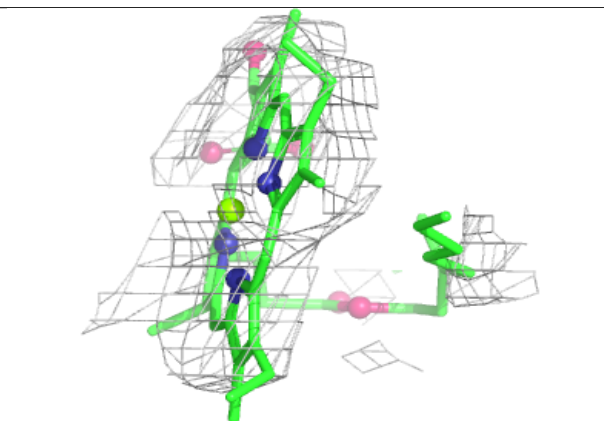
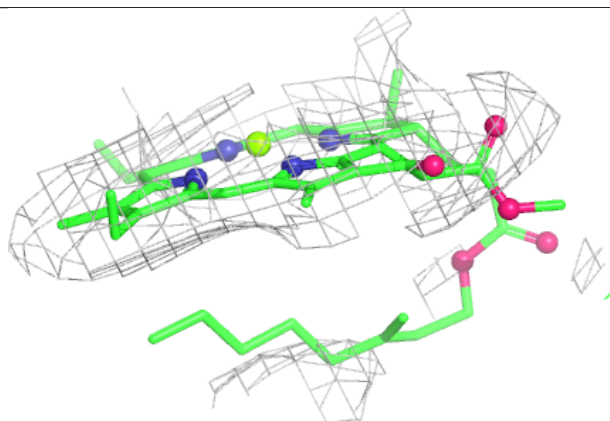
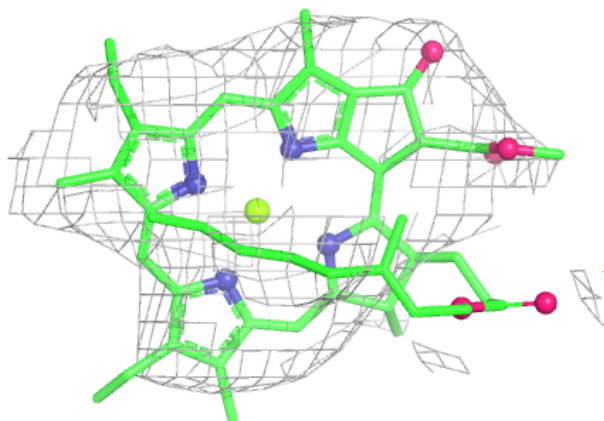
Electron density around CLA A 816:

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

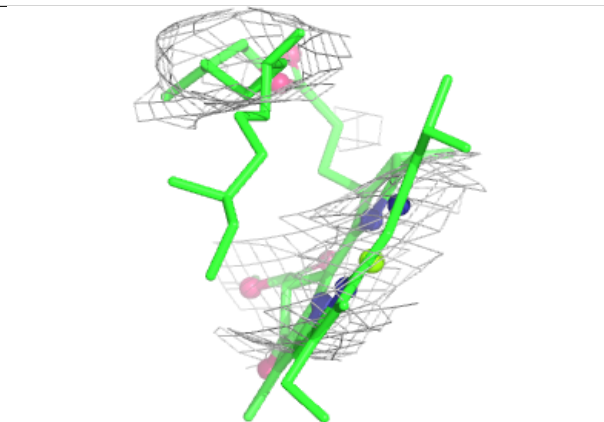
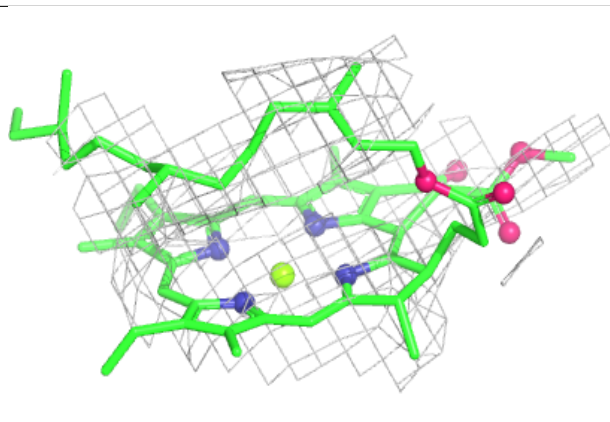
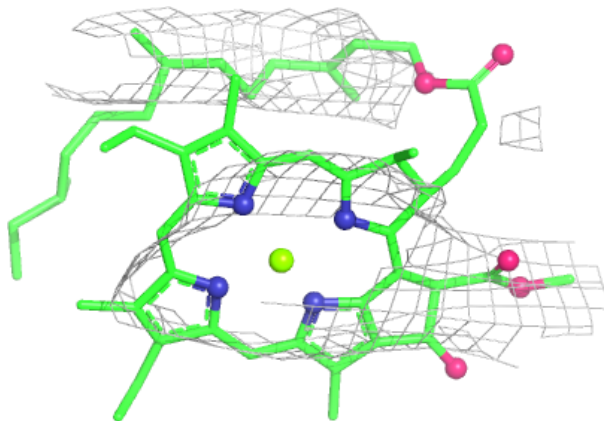


Electron density around CLA A 817:

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

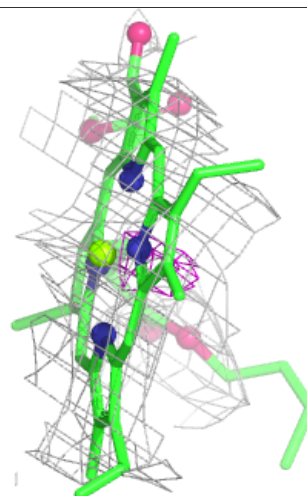
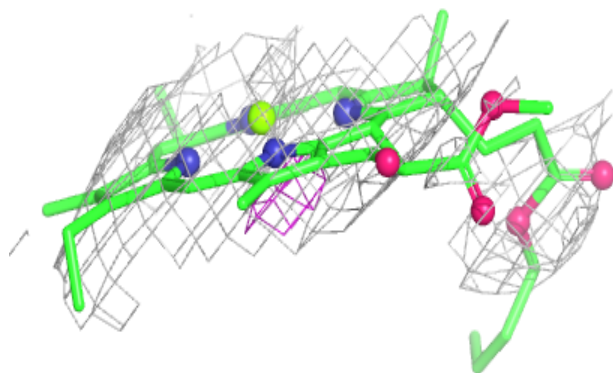
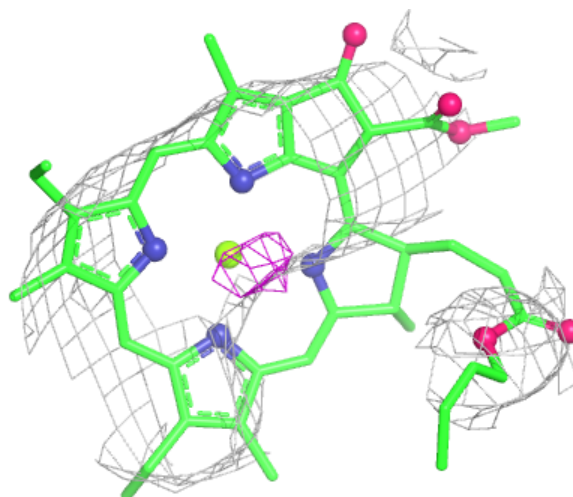
**Electron density around CLA A 820:**

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



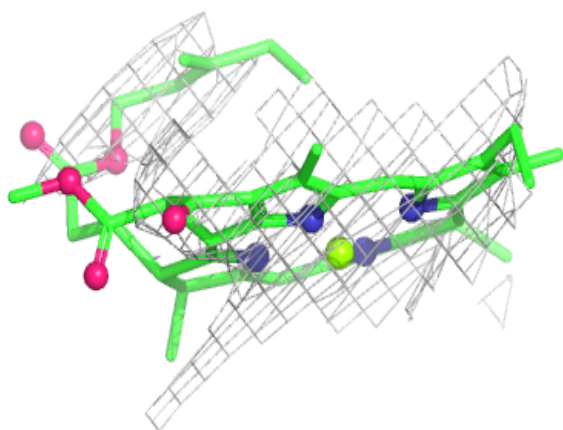
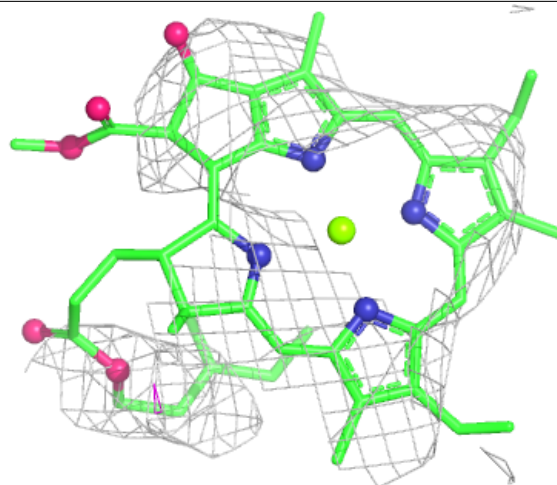
Electron density around CLA A 822:

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



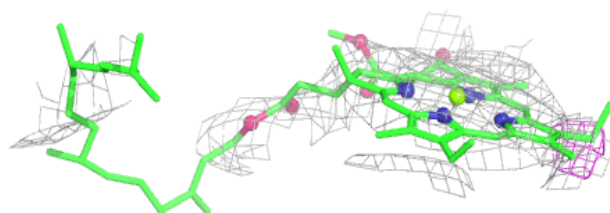
Electron density around CLA A 823:

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

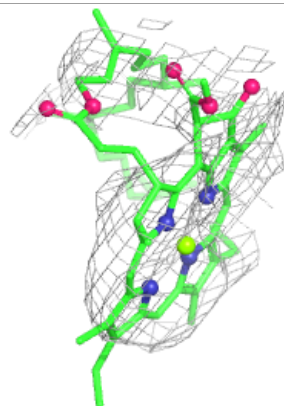
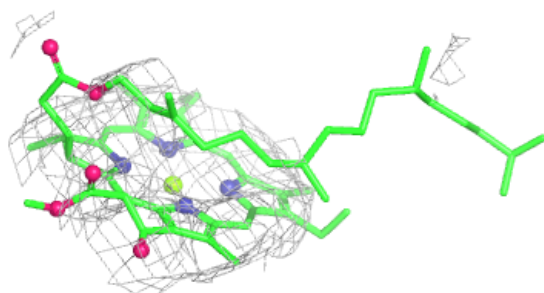
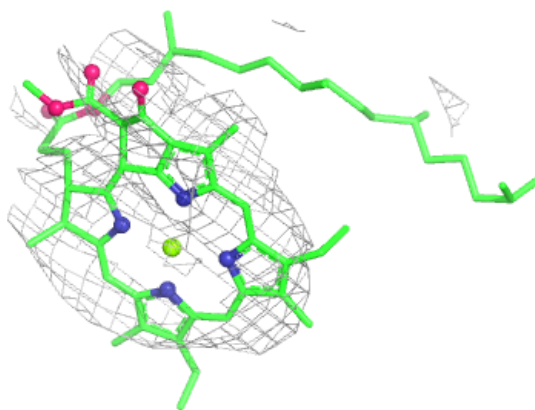


Electron density around CLA A 827:

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

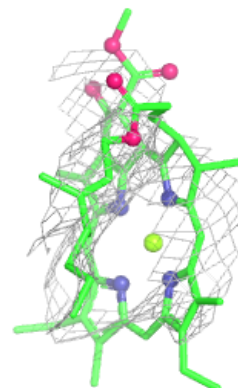
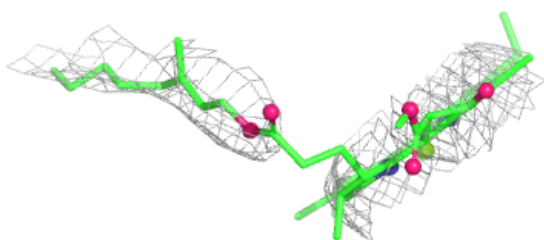
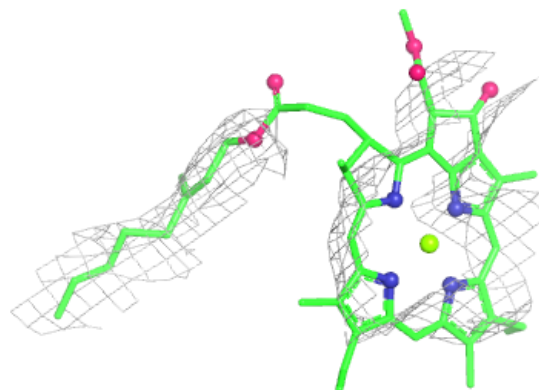
**Electron density around CLA A 829:**

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



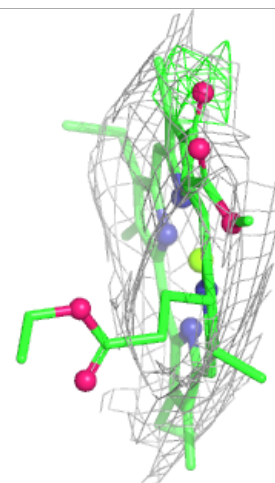
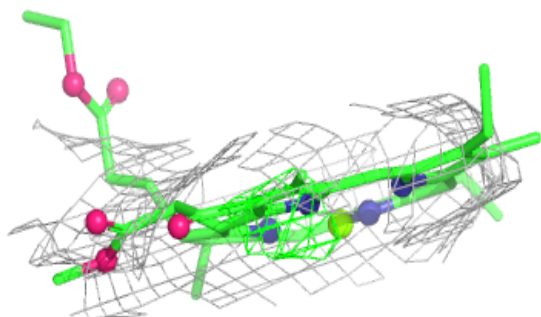
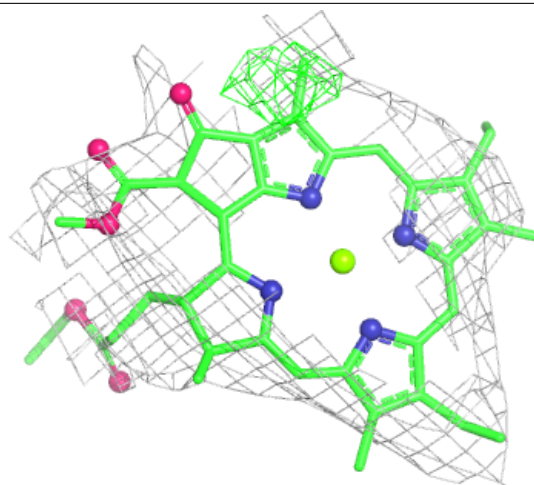
Electron density around CLA A 835:

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



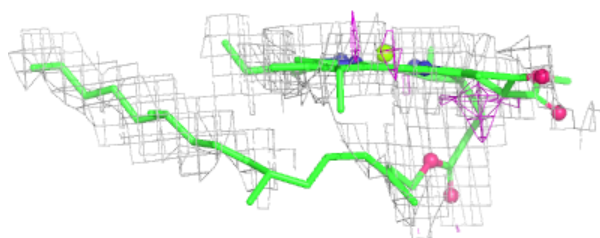
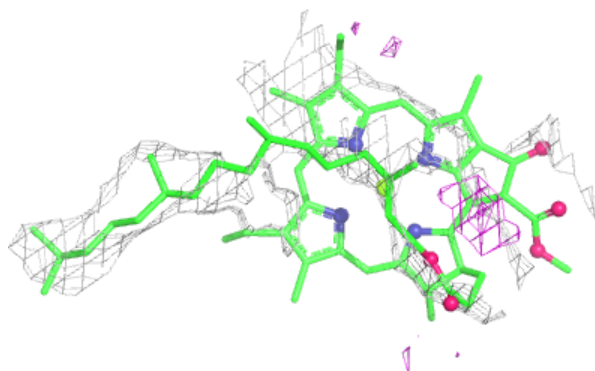
Electron density around CLA A 839:

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

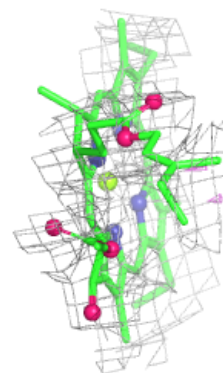
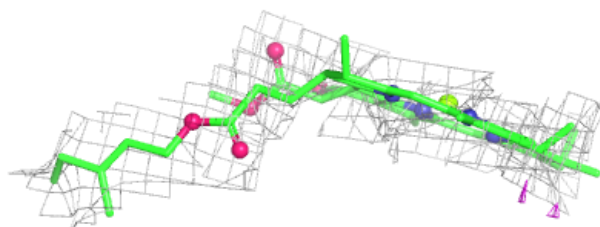
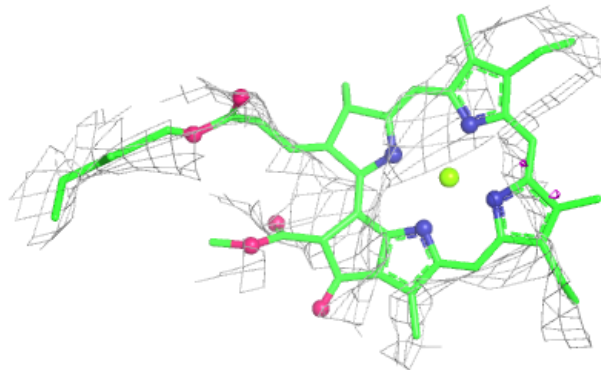


Electron density around CLA A 840:

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

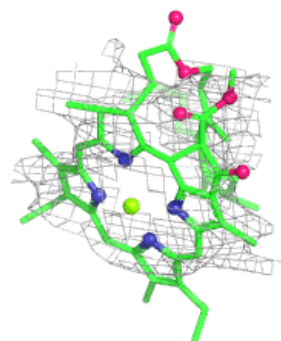
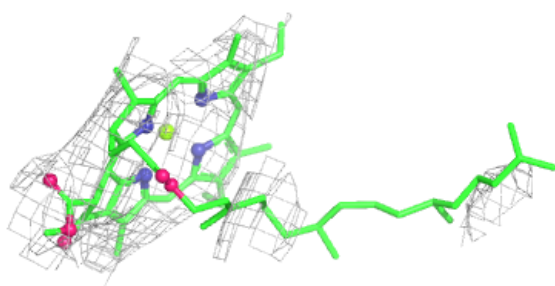
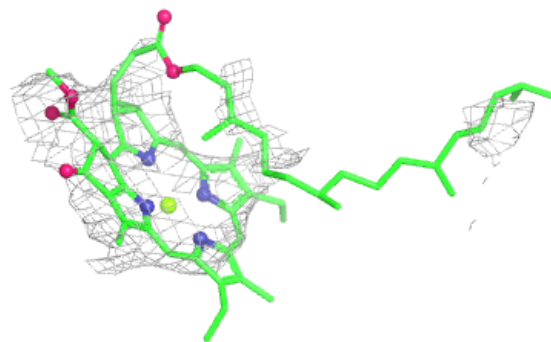
**Electron density around CLA A 841:**

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



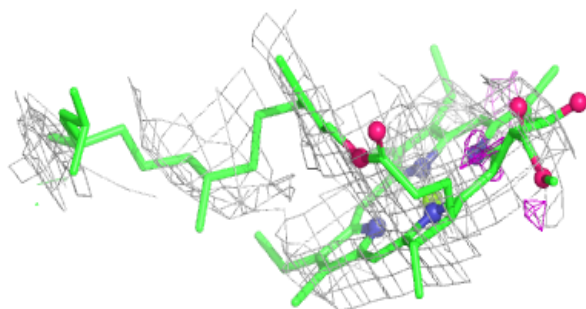
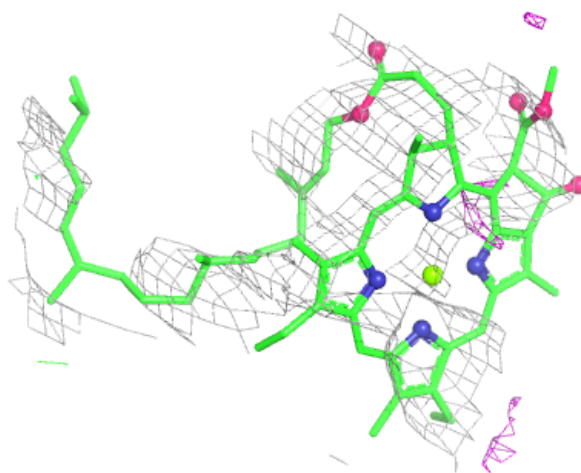
Electron density around CLA A 842:

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



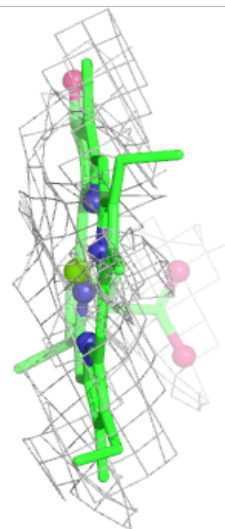
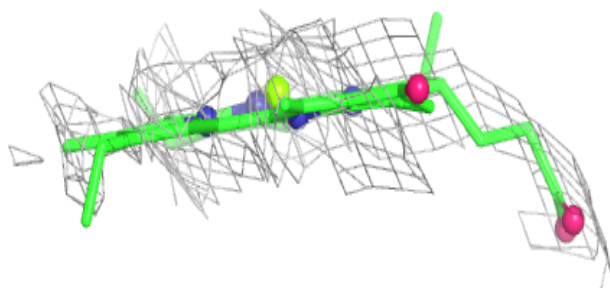
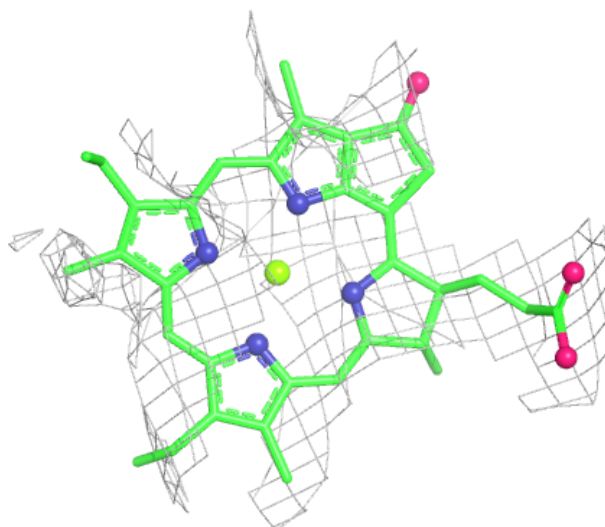
Electron density around CLA A 843:

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



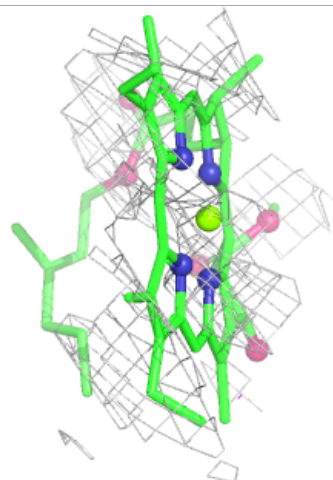
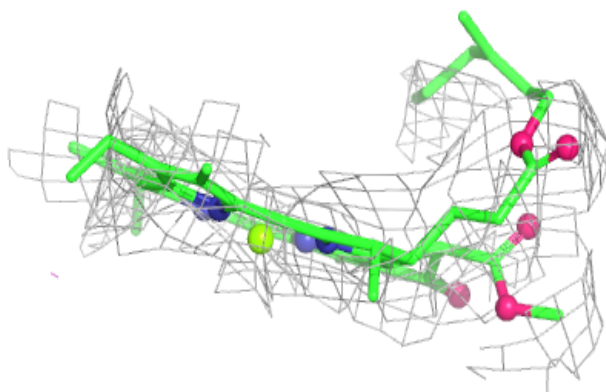
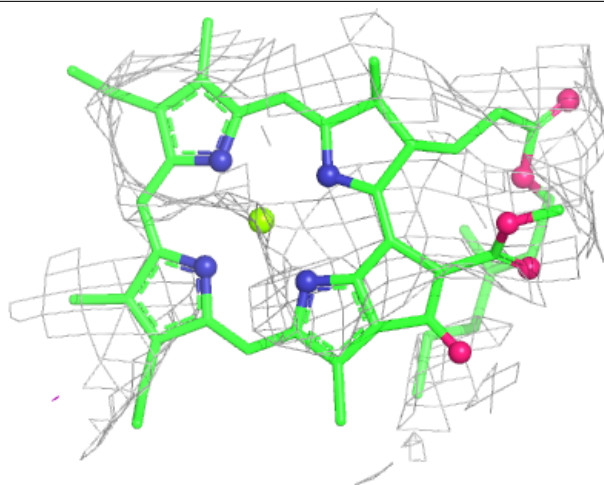
Electron density around CLA A 844:

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



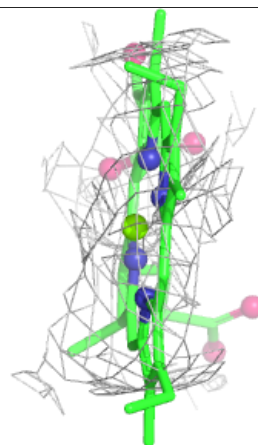
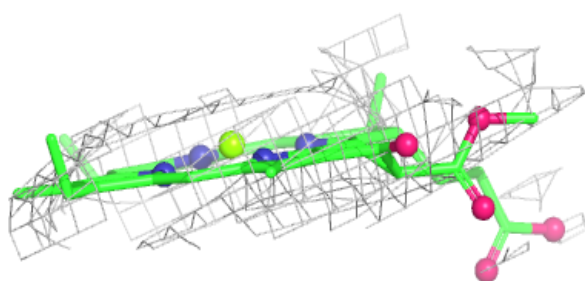
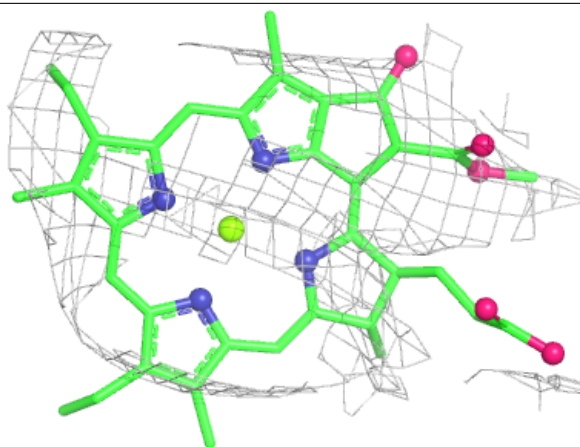
Electron density around CLA A 845:

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



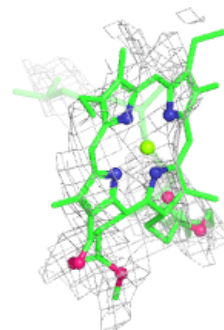
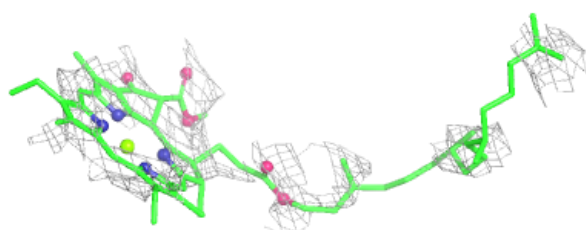
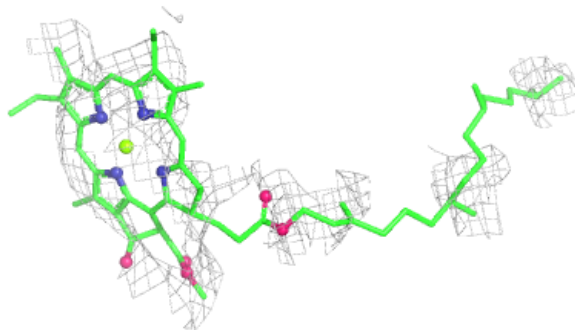
Electron density around CLA A 855:

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

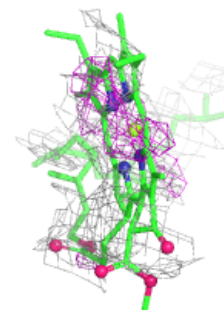
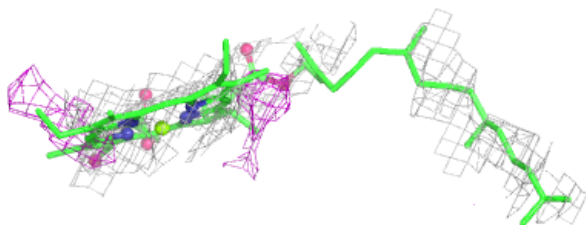
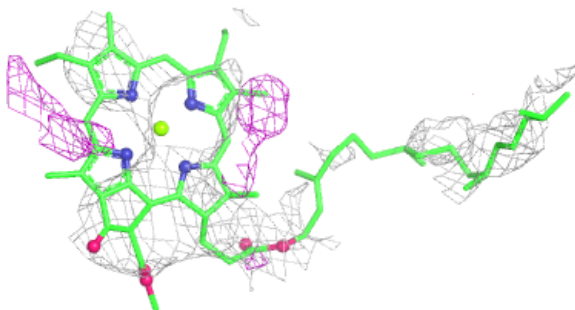


Electron density around CLA B 802:

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

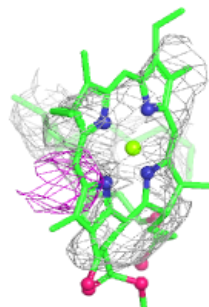
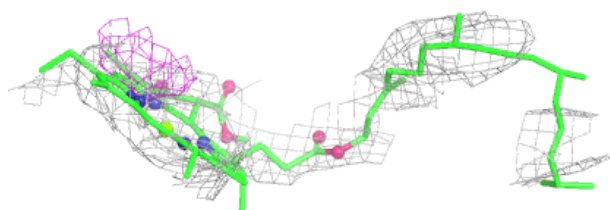
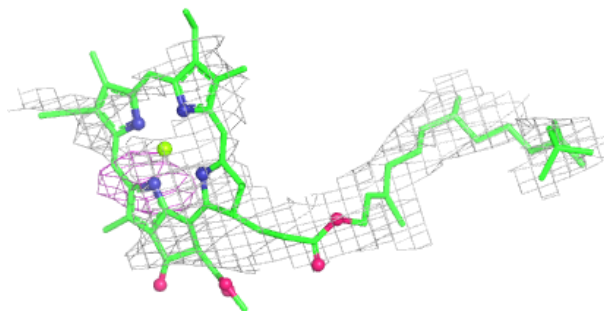
**Electron density around CLA B 803:**

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



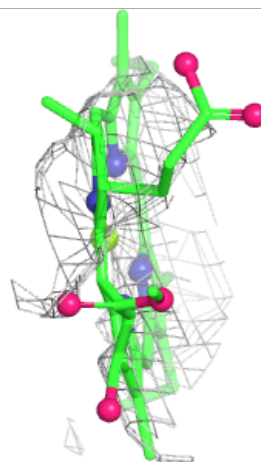
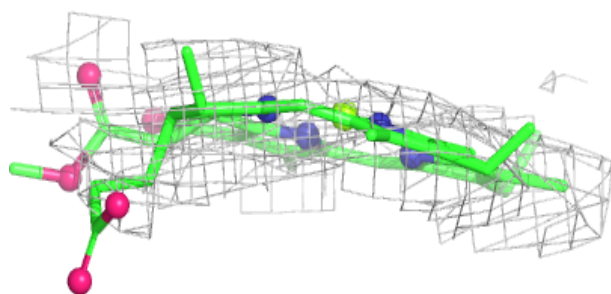
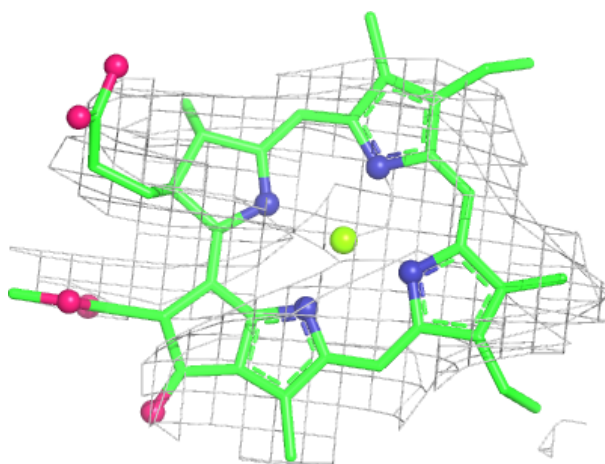
Electron density around CLA B 808:

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



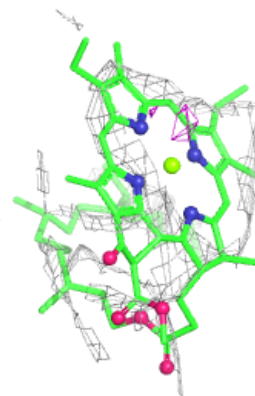
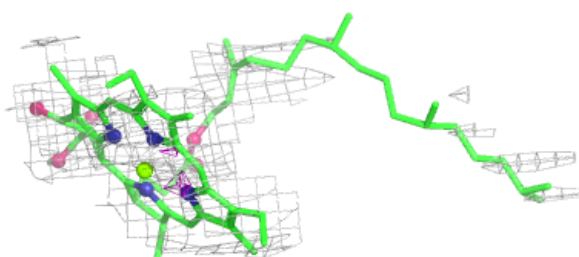
Electron density around CLA B 810:

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



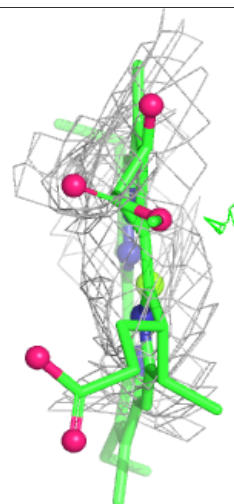
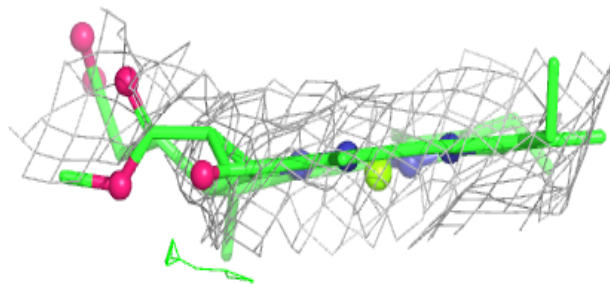
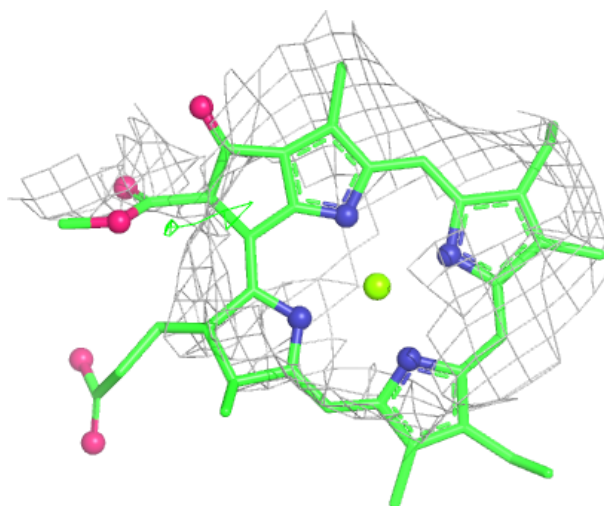
Electron density around CLA B 812:

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



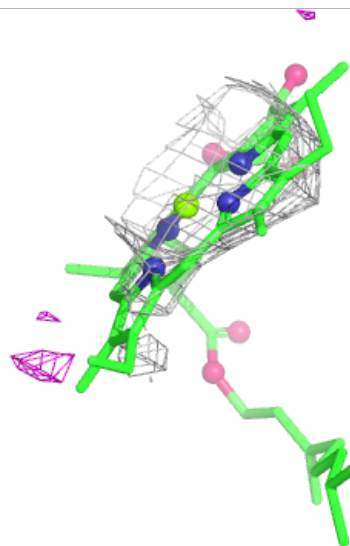
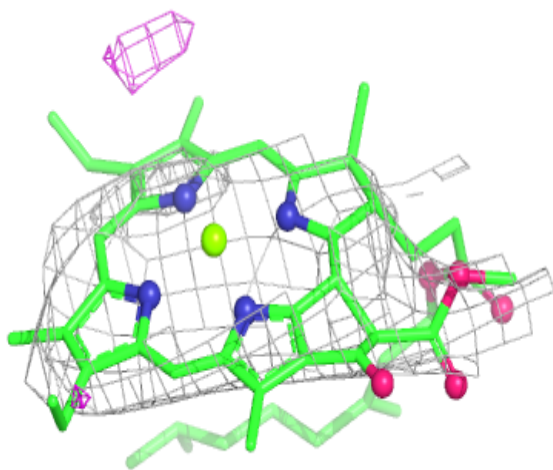
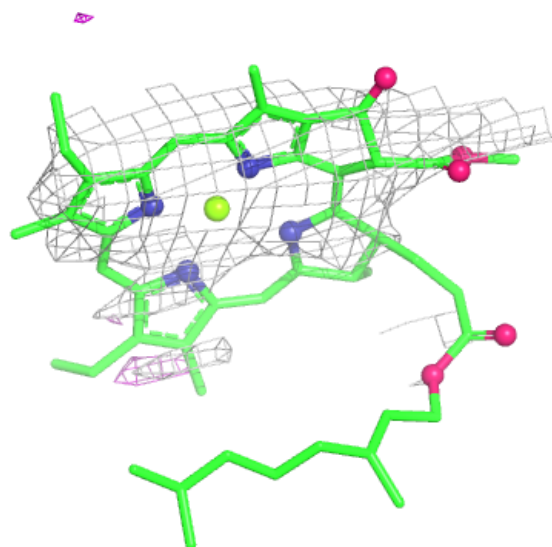
Electron density around CLA B 813:

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



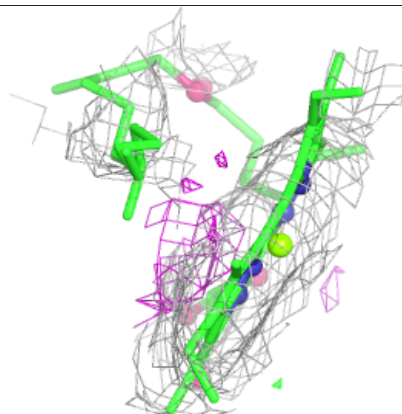
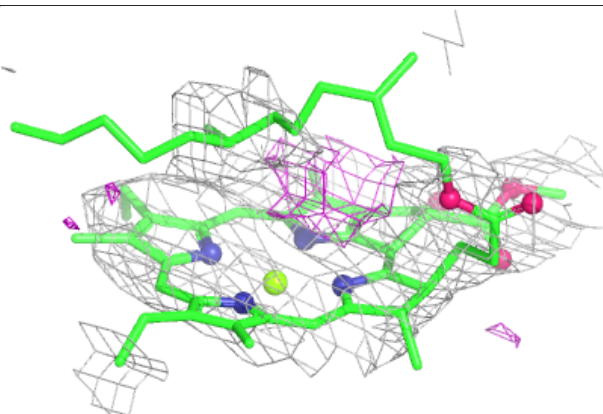
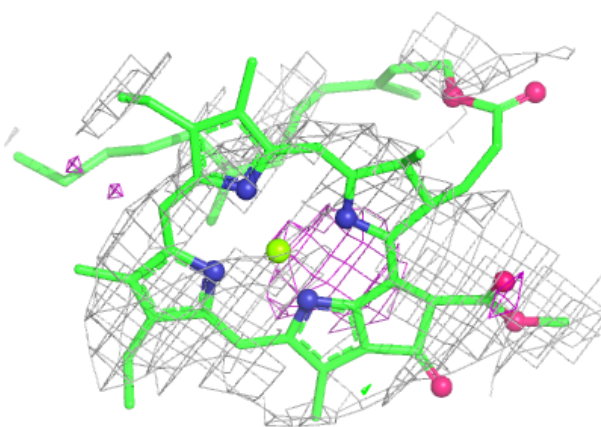
Electron density around CLA B 814:

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



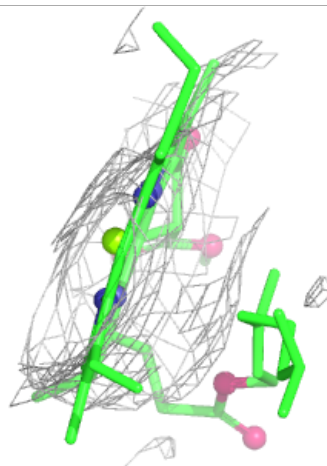
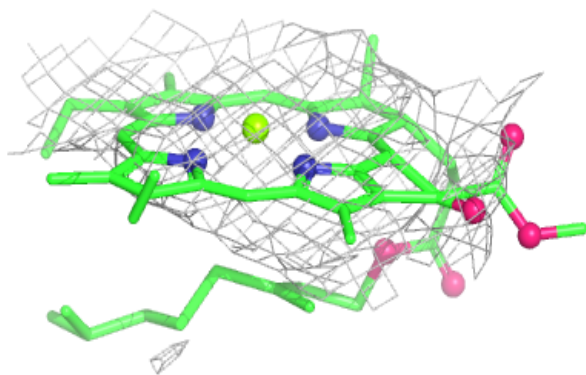
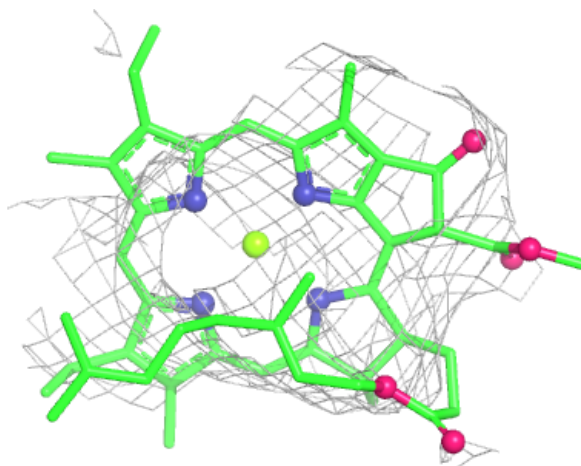
Electron density around CLA B 815:

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



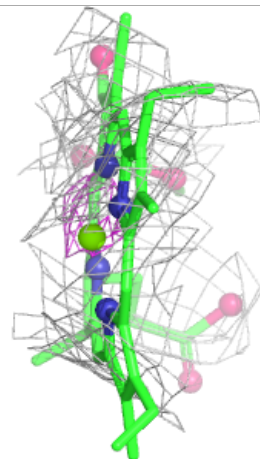
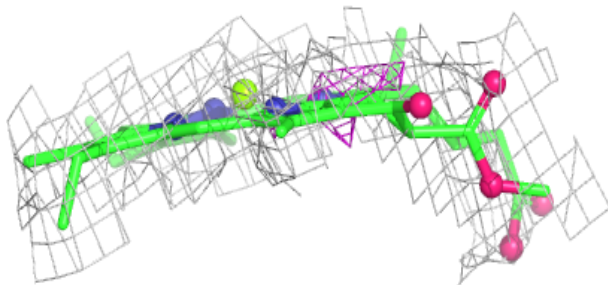
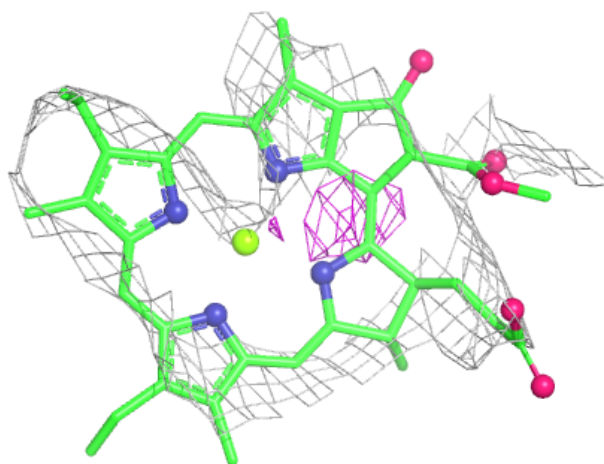
Electron density around CLA B 820:

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



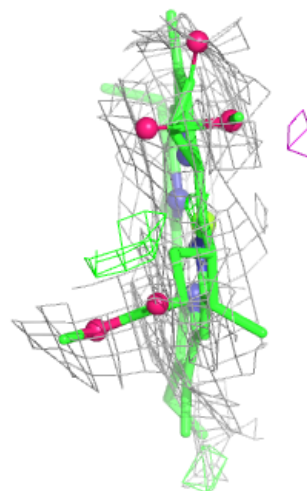
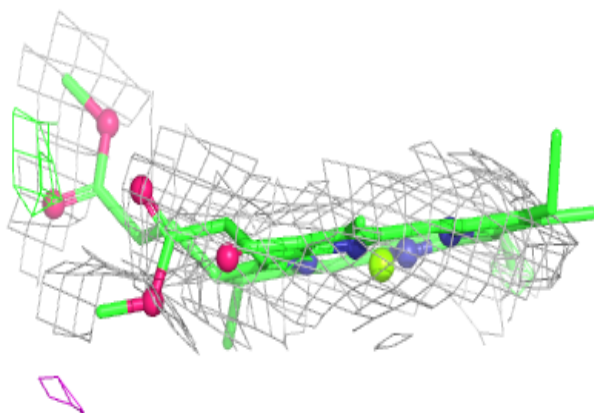
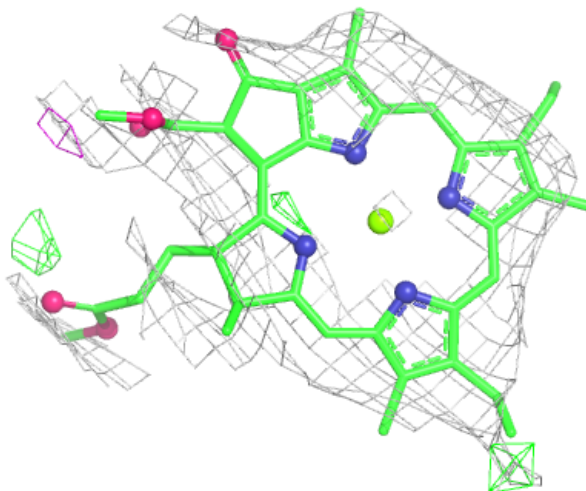
Electron density around CLA B 821:

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



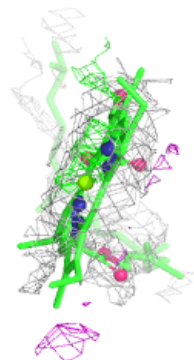
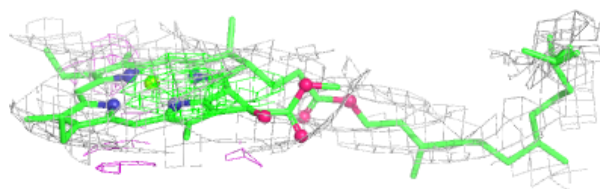
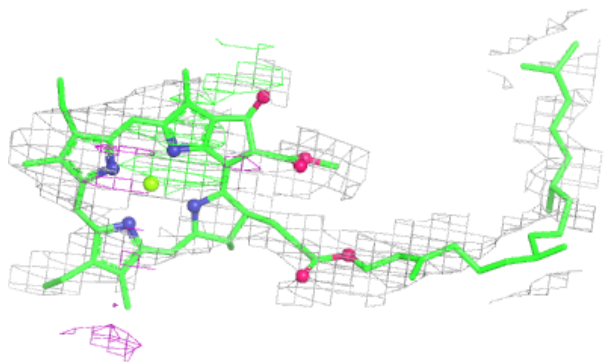
Electron density around CLA B 823:

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



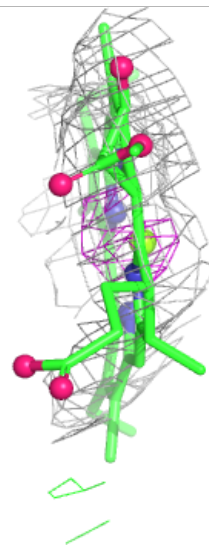
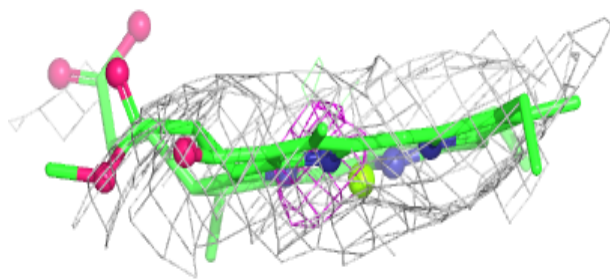
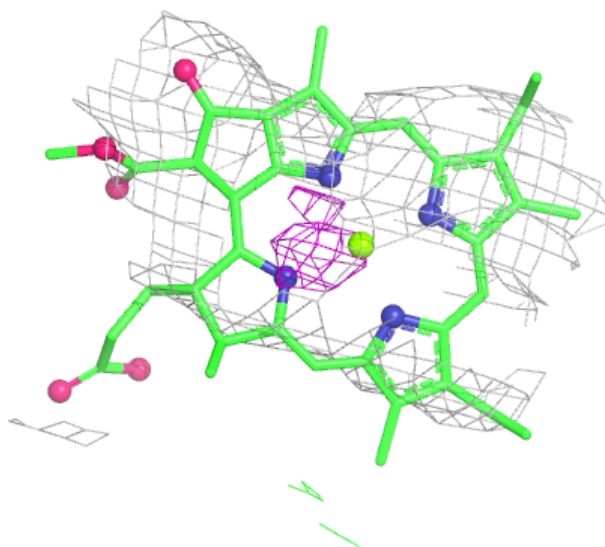
Electron density around CLA B 824:

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



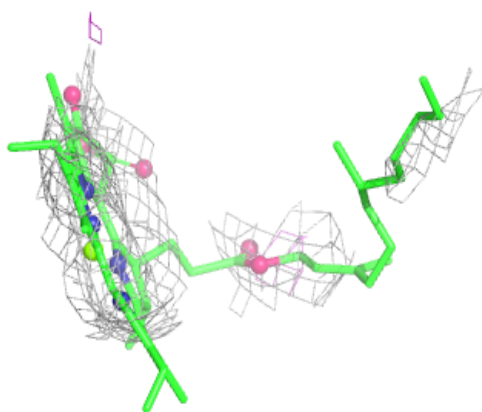
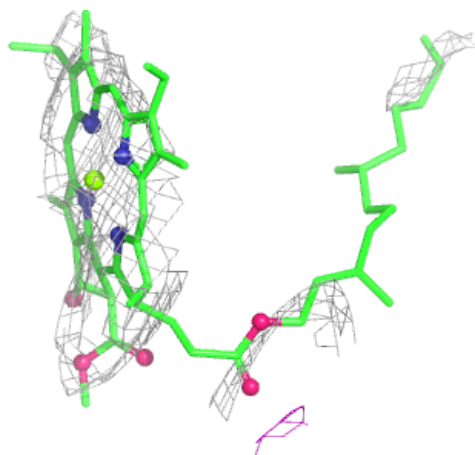
Electron density around CLA B 828:

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



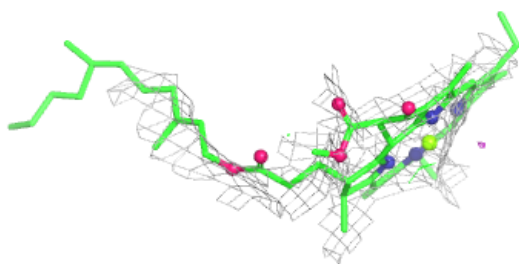
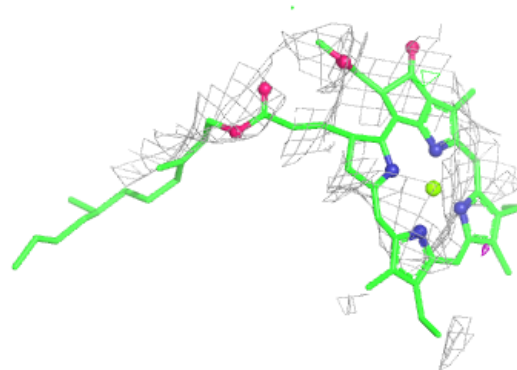
Electron density around CLA A 804:

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



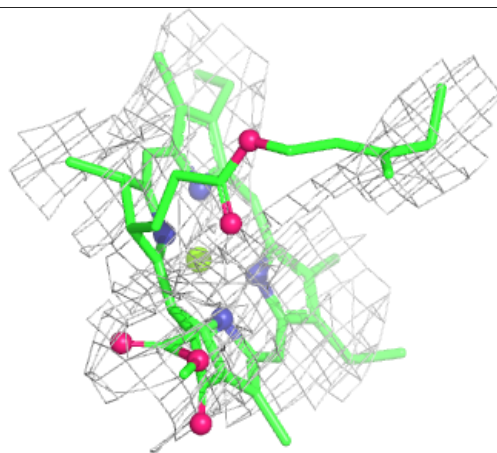
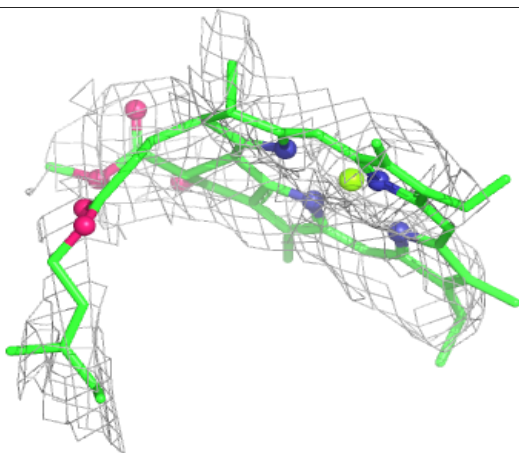
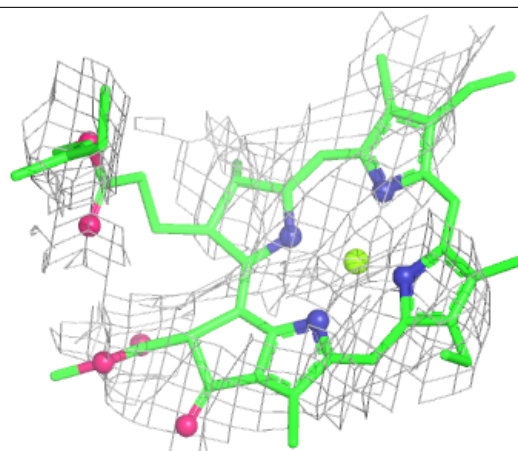
Electron density around CLA B 831:

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



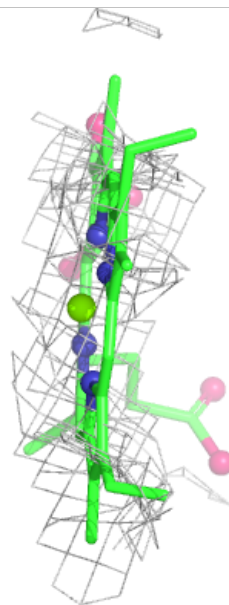
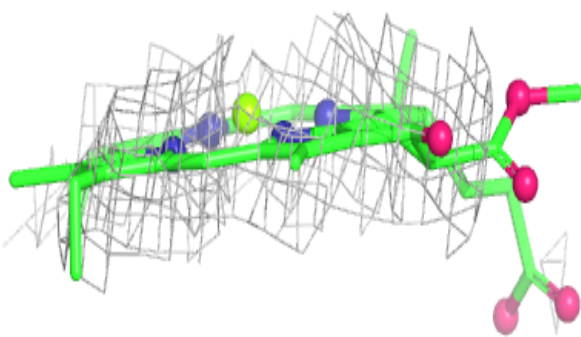
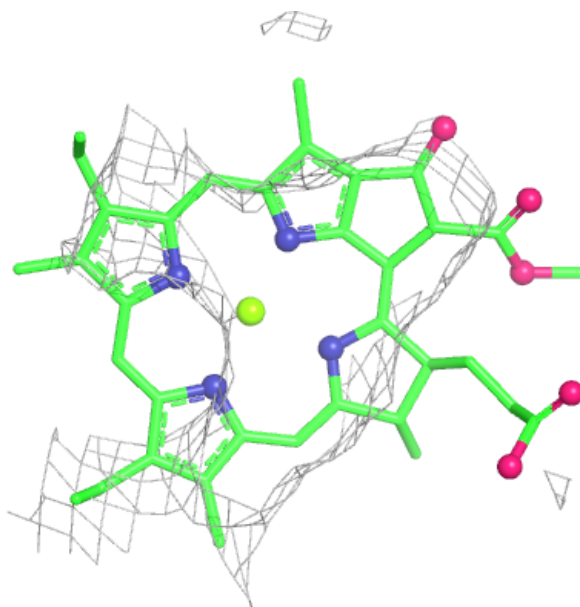
Electron density around CLA A 807:

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



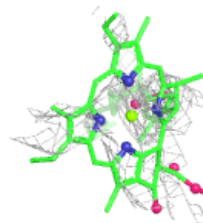
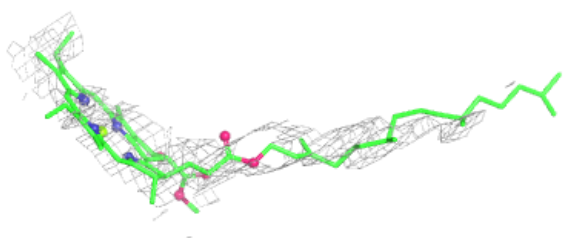
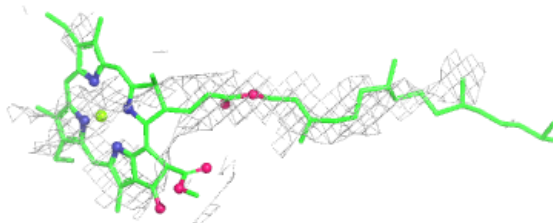
Electron density around CLA B 833:

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

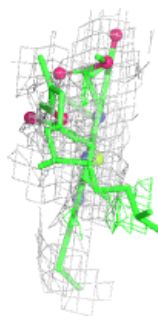
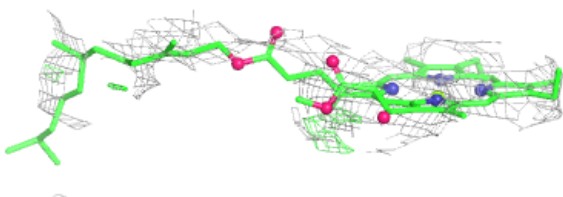


Electron density around CLA A 809:

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

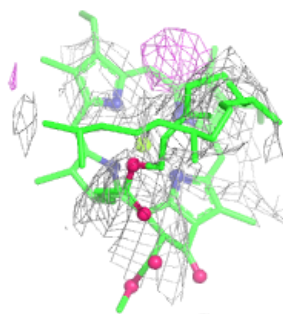
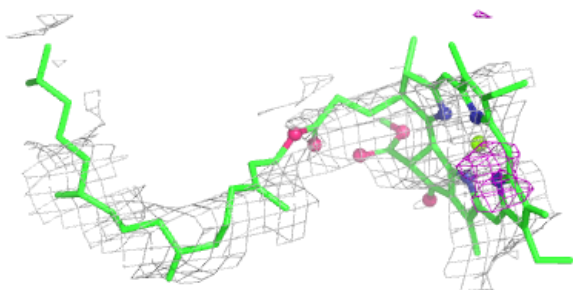
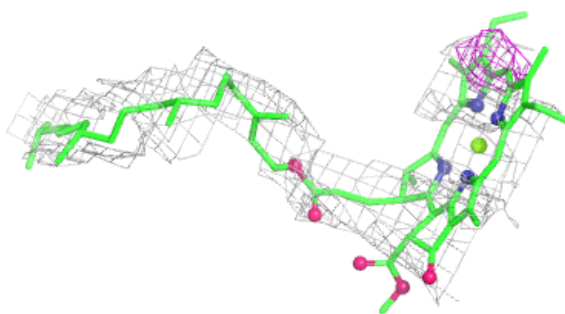
**Electron density around CLA B 835:**

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

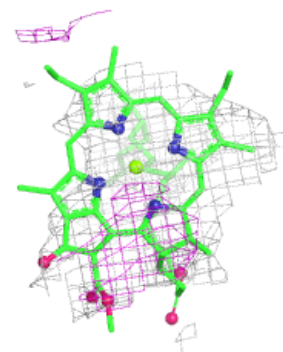
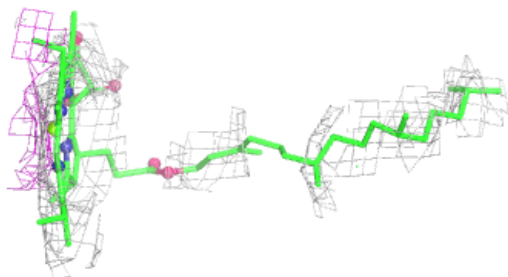
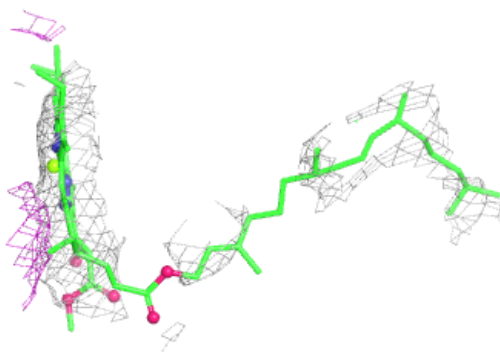


Electron density around CLA B 838:

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

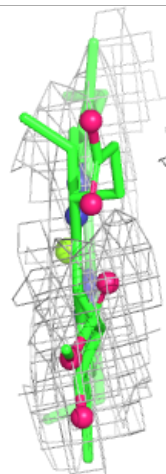
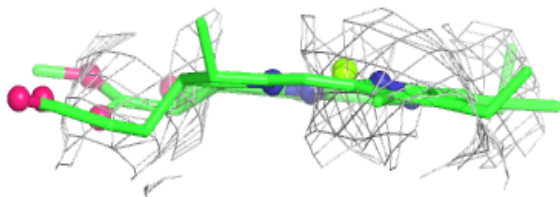
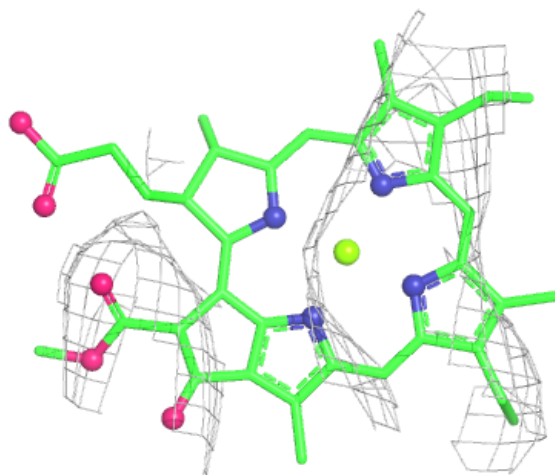
**Electron density around CLA B 839:**

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



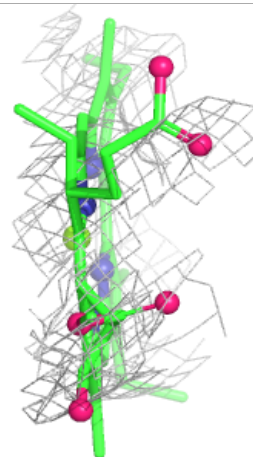
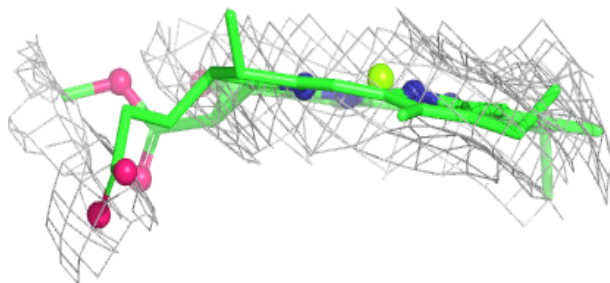
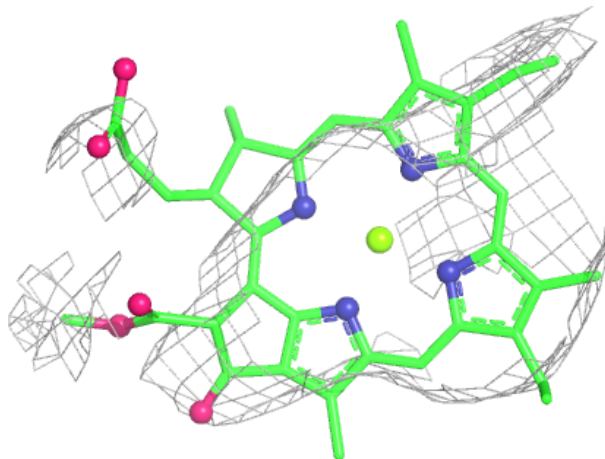
Electron density around CLA F 1301:

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



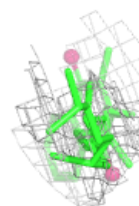
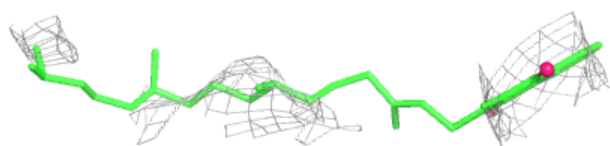
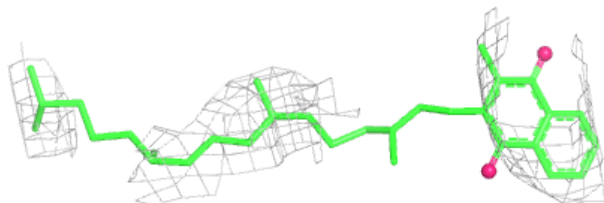
Electron density around CLA J 1102:

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

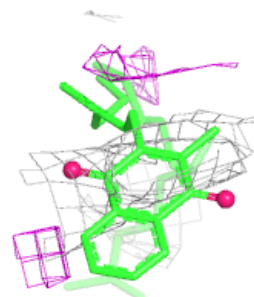
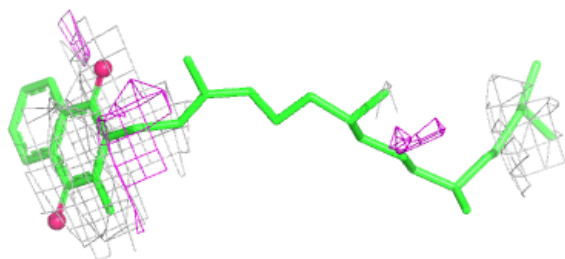
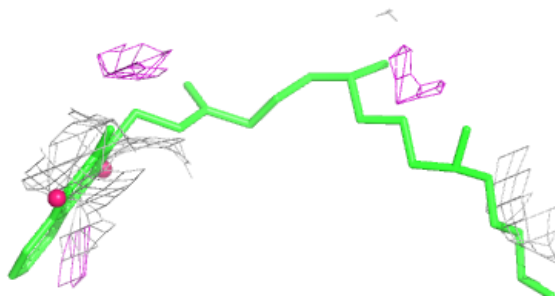


Electron density around PQN A 846:

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

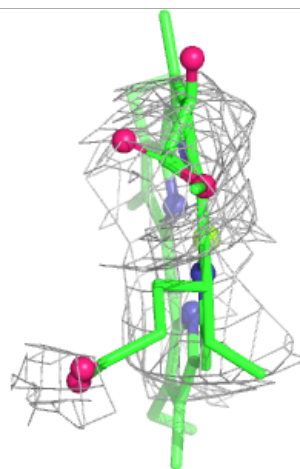
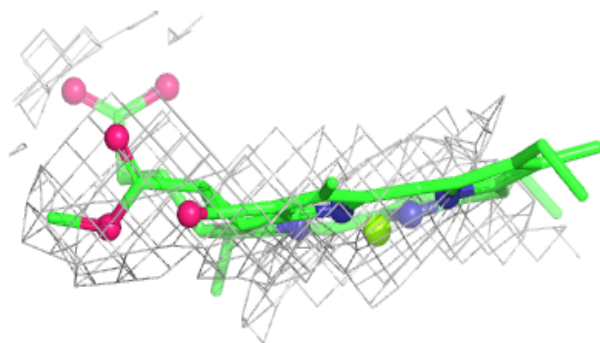
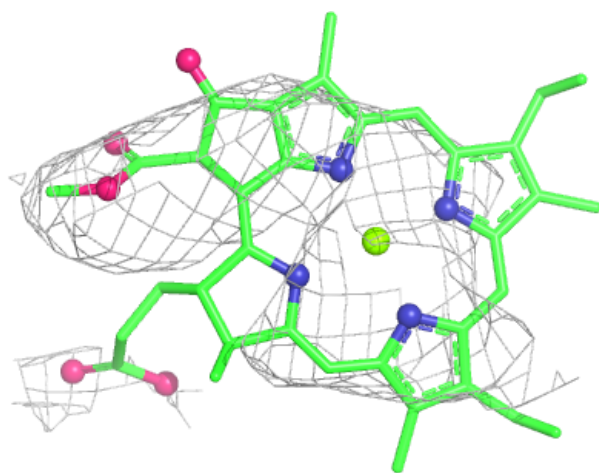
**Electron density around PQN B 840:**

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



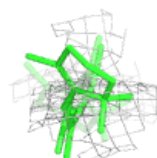
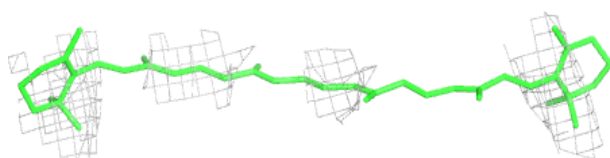
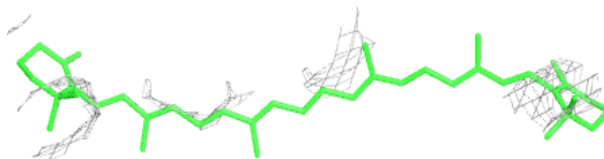
Electron density around CLA A 810:

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

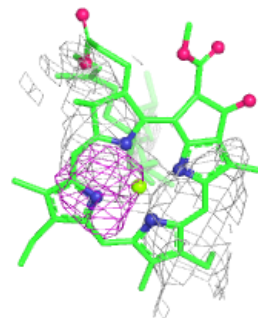
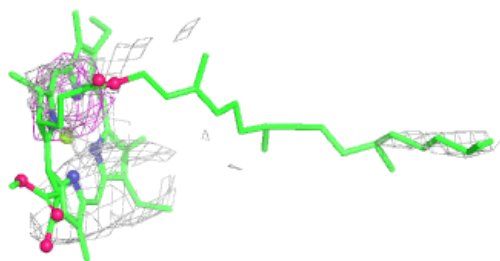
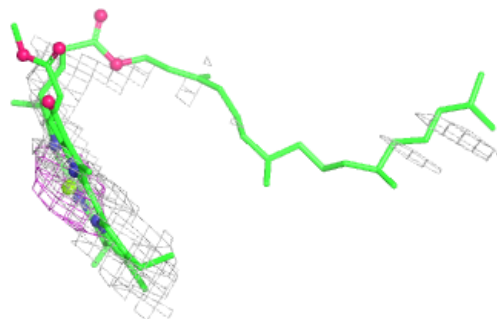


Electron density around BCR A 848:

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

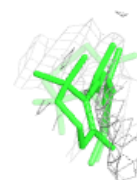
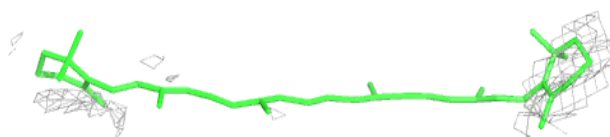
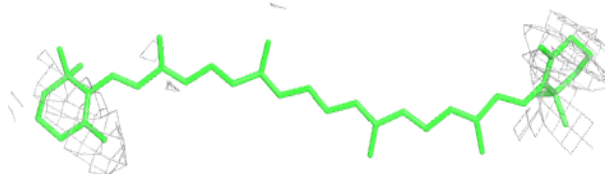
**Electron density around CLA A 811:**

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

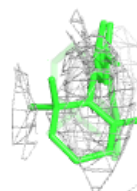
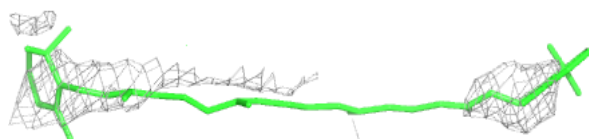


Electron density around BCR B 841:

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

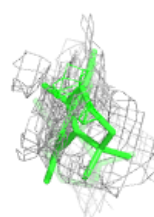
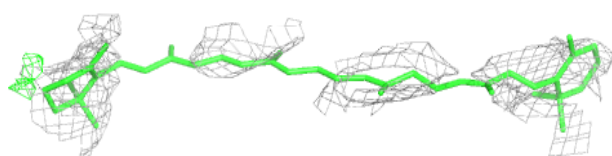
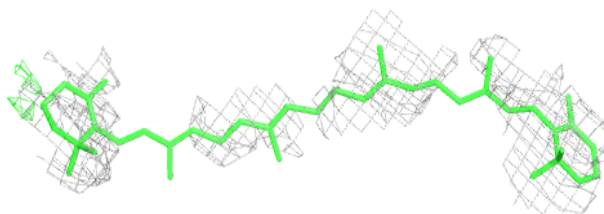
**Electron density around BCR B 843:**

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

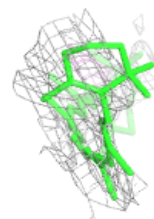
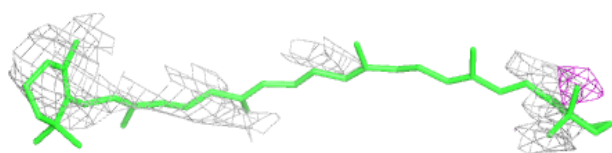
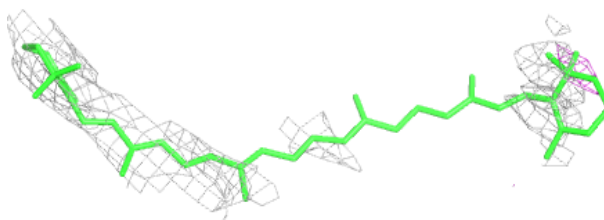


Electron density around BCR B 845:

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

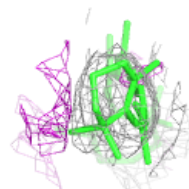
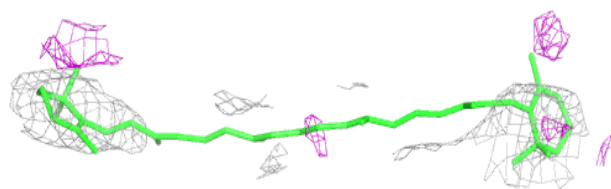
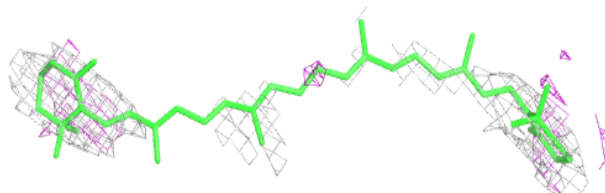
**Electron density around BCR B 846:**

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

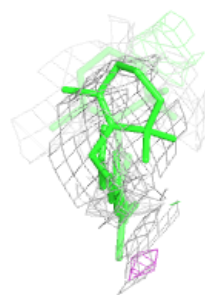
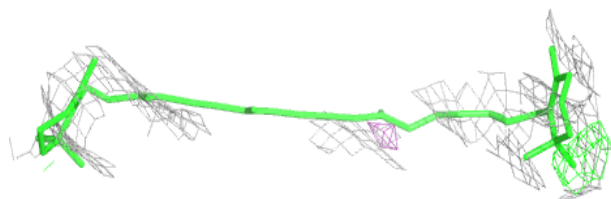
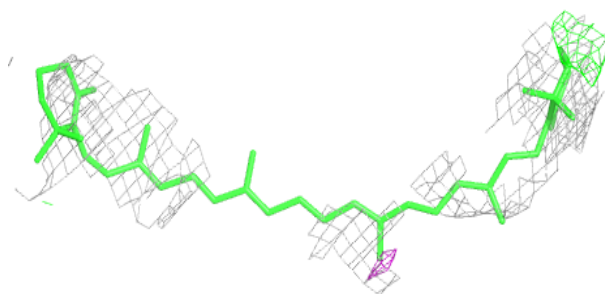


Electron density around BCR B 847:

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

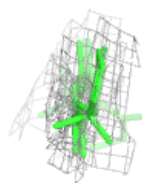
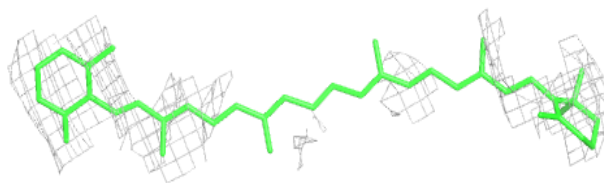
**Electron density around BCR B 849:**

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

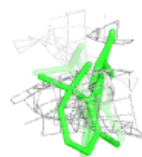
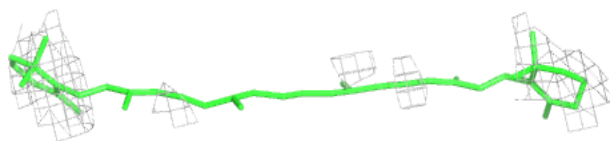
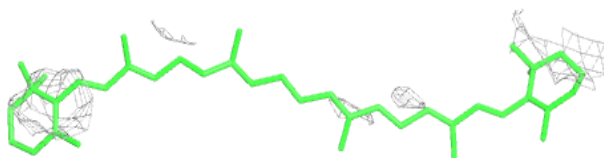


Electron density around BCR B 850:

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

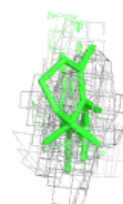
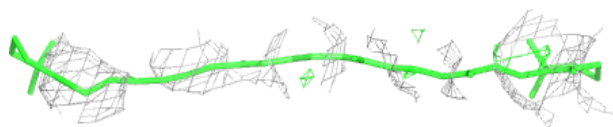
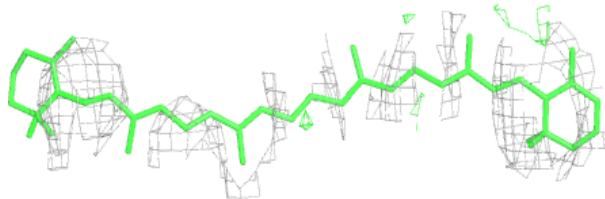
**Electron density around BCR J 1104:**

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

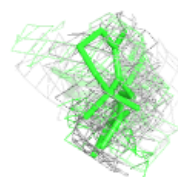
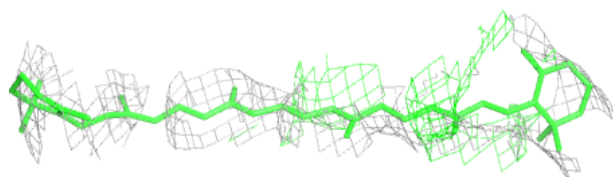
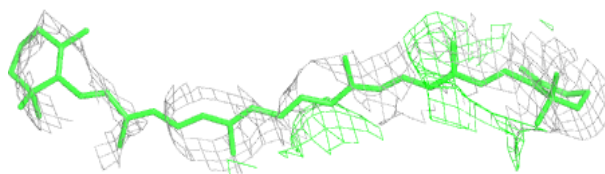


Electron density around BCR L 1005:

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

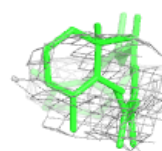
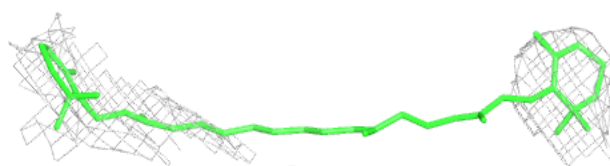
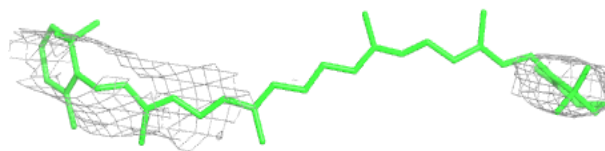
**Electron density around BCR L 1006:**

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



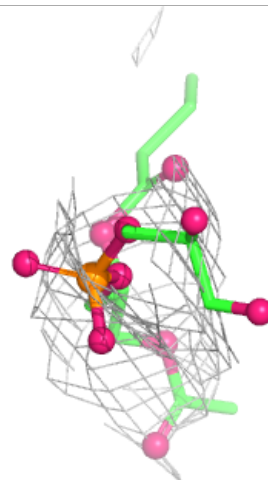
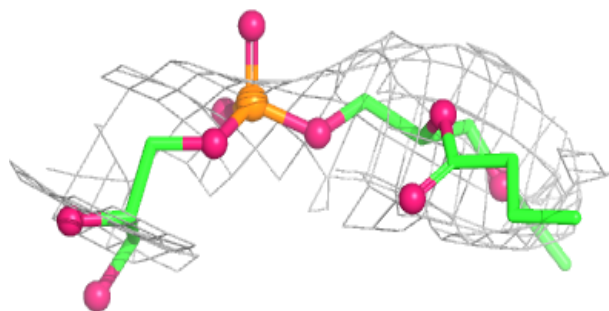
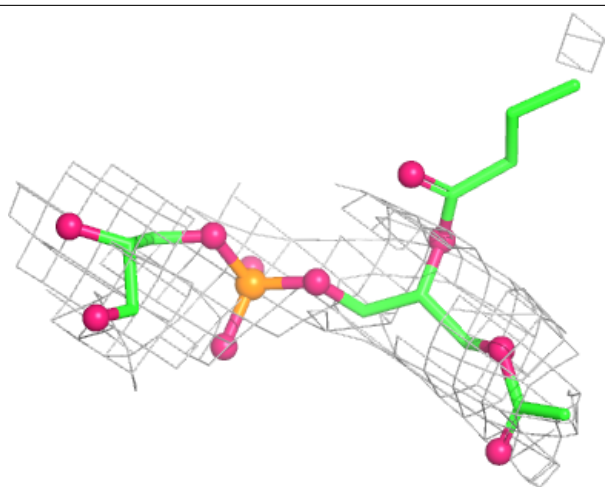
Electron density around BCR M 1203:

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



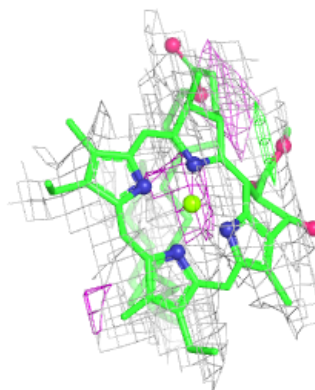
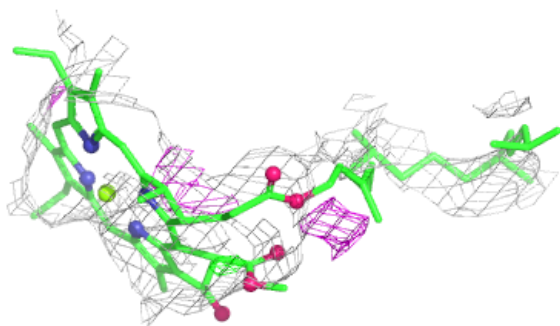
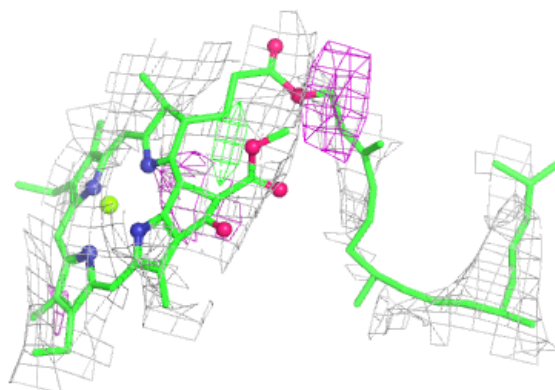
Electron density around LHG X 101:

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



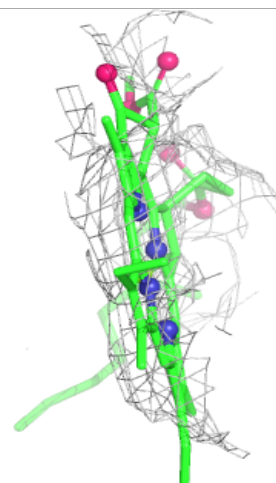
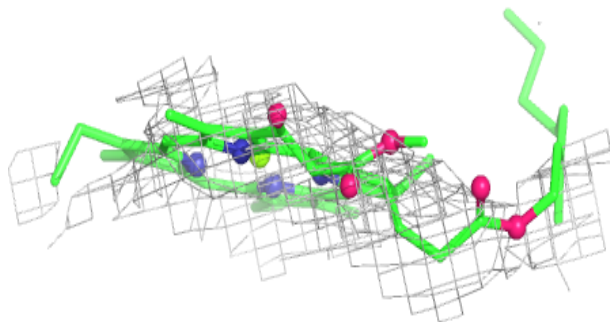
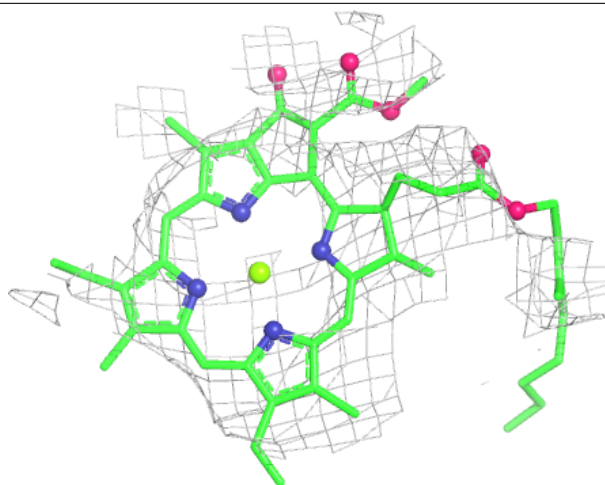
Electron density around CLA A 801:

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



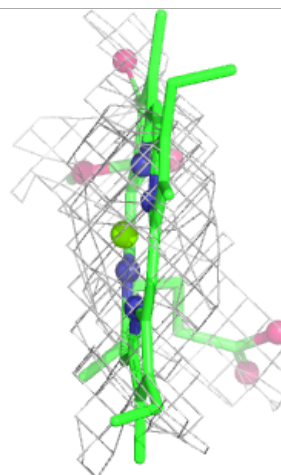
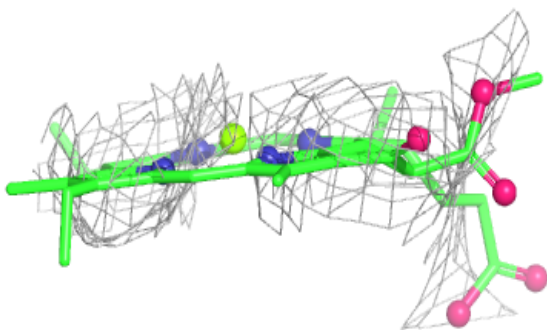
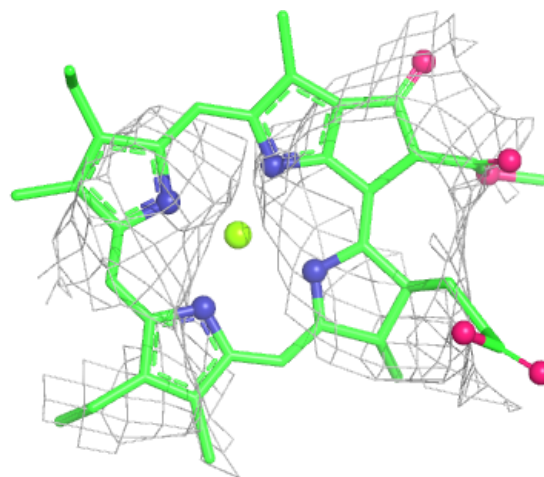
Electron density around CLA B 822:

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



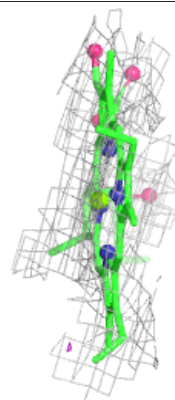
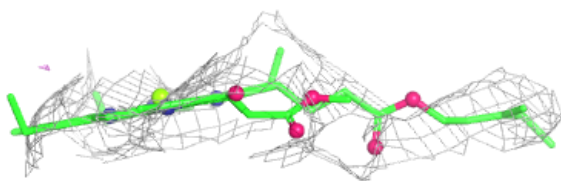
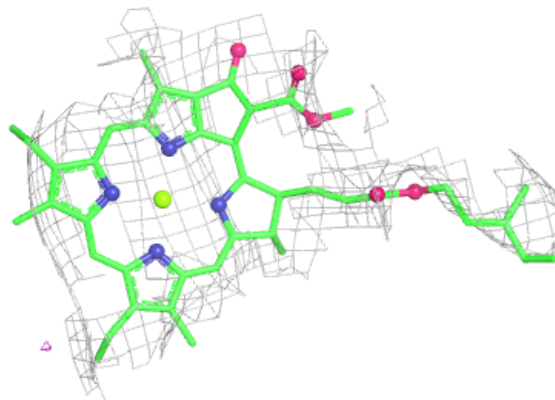
Electron density around CLA A 836:

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



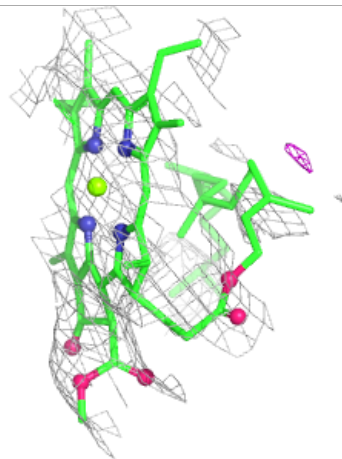
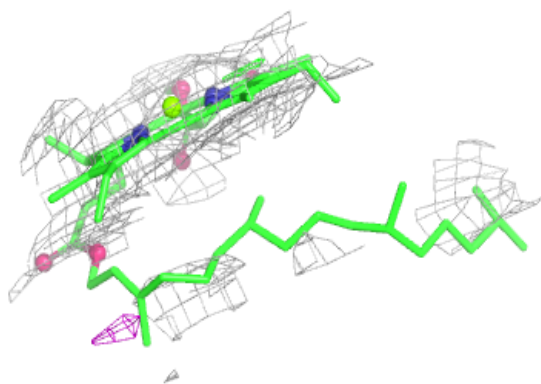
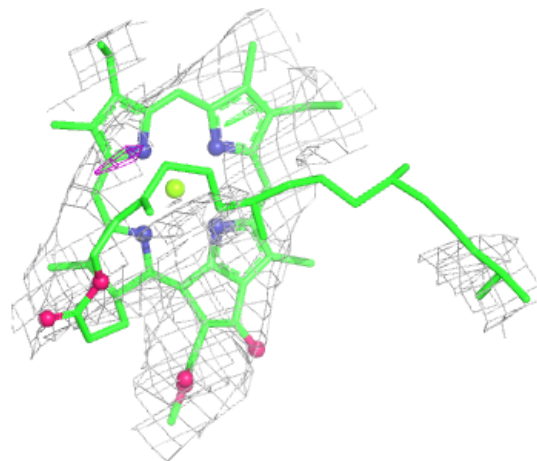
Electron density around CLA A 837:

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



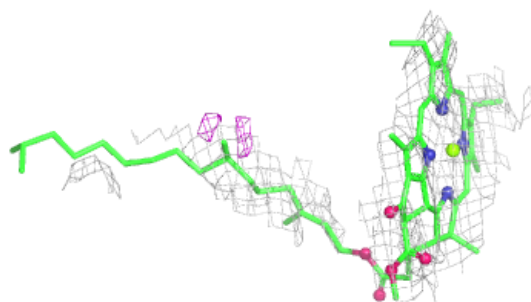
Electron density around CLA B 825:

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

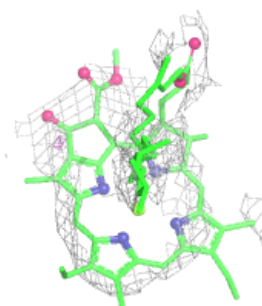
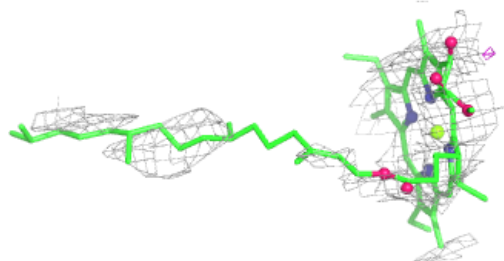
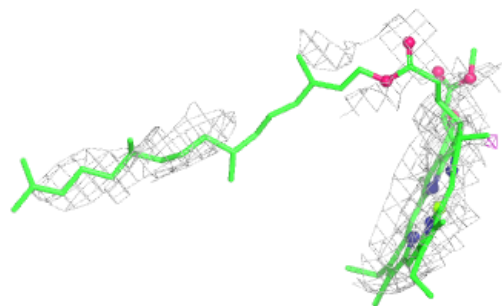


Electron density around CLA B 826:

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

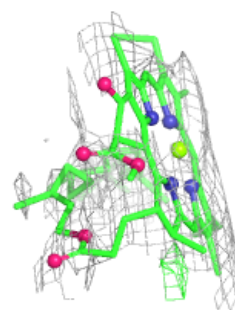
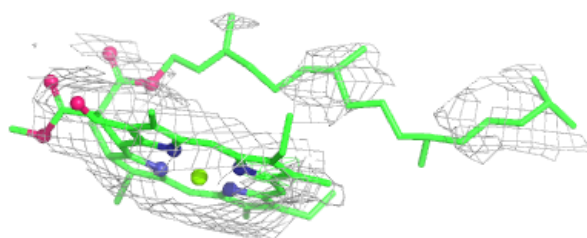
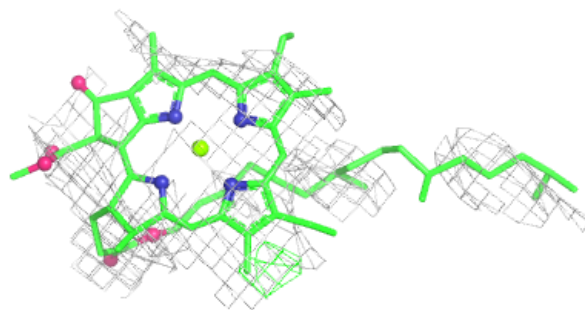
**Electron density around CLA B 827:**

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



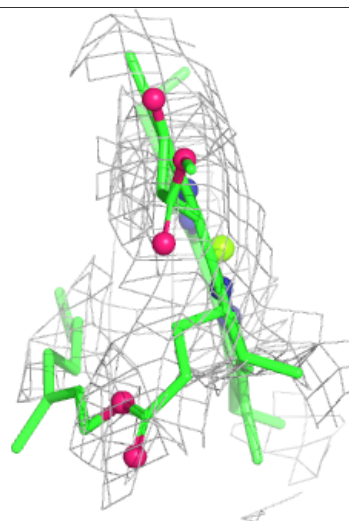
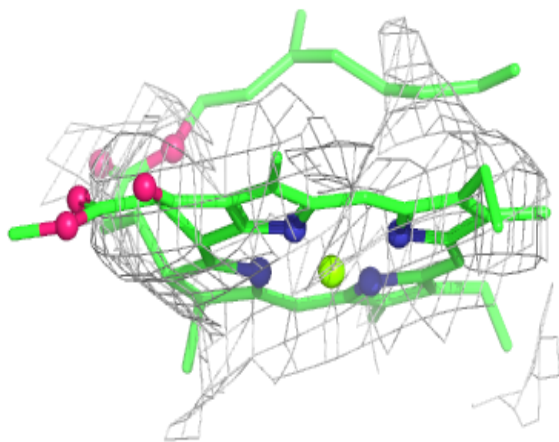
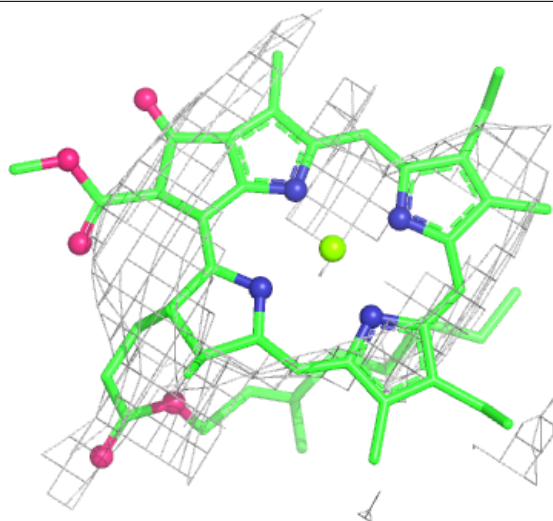
Electron density around CLA A 838:

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



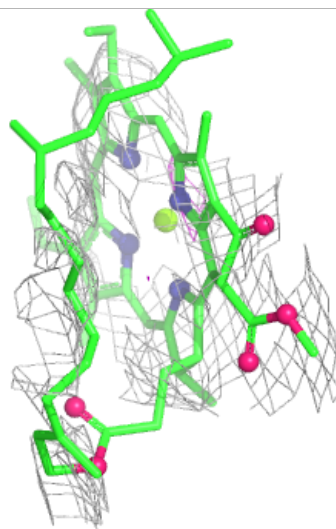
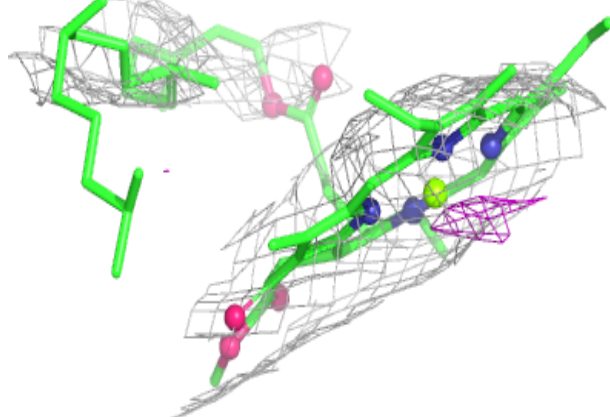
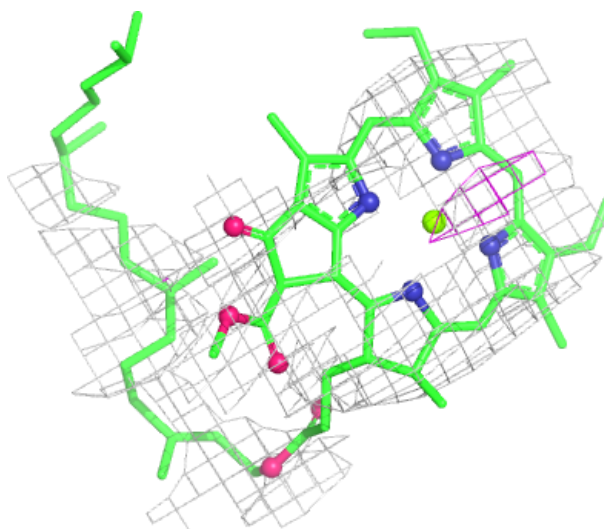
Electron density around CLA A 818:

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



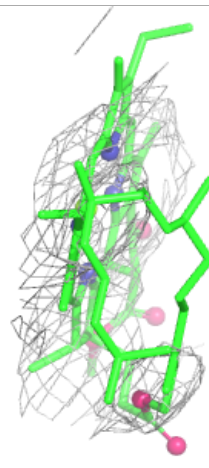
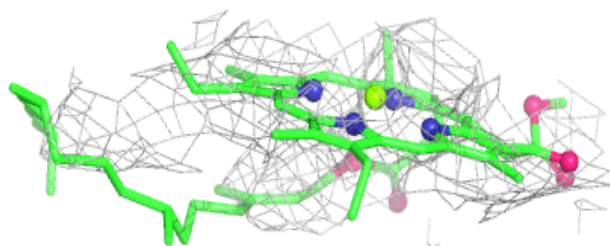
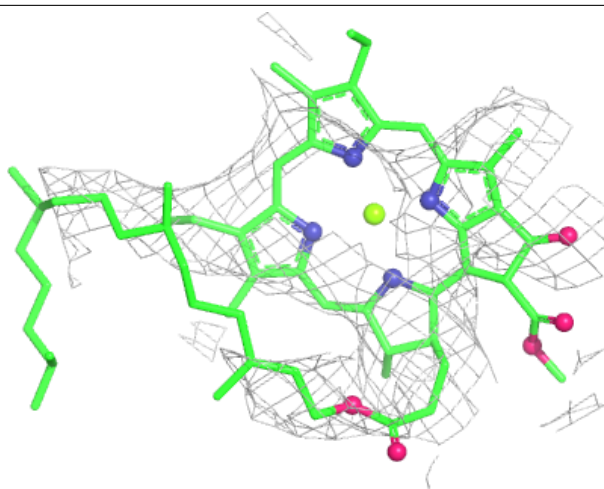
Electron density around CLA B 830:

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



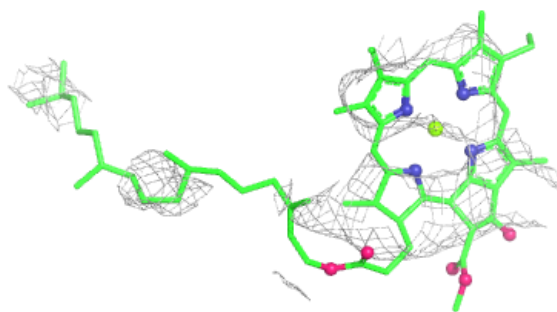
Electron density around CLA A 819:

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

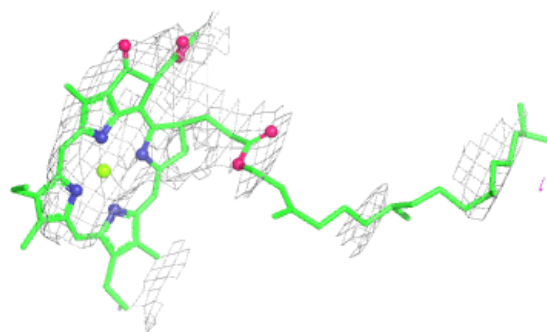


Electron density around CLA A 803:

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

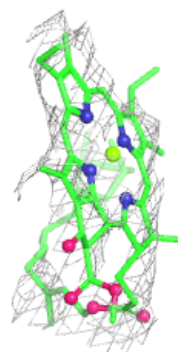
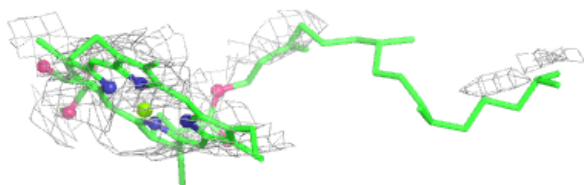
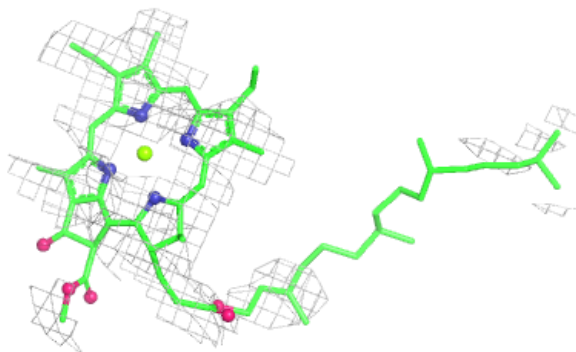
**Electron density around CLA A 821:**

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

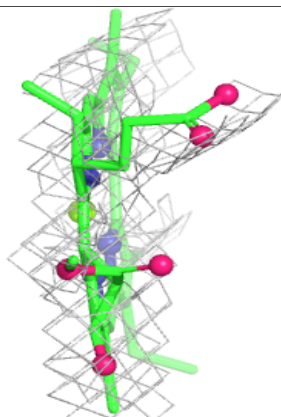
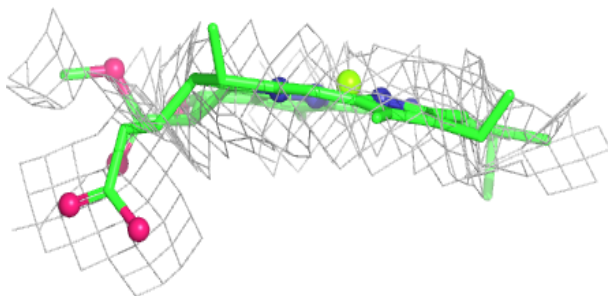
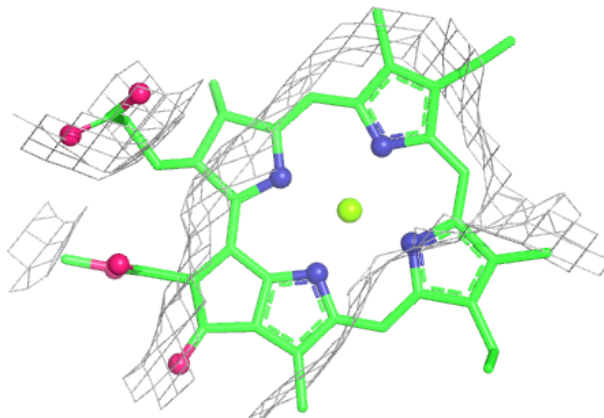


Electron density around CLA A 808:

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

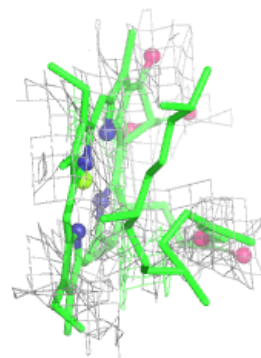
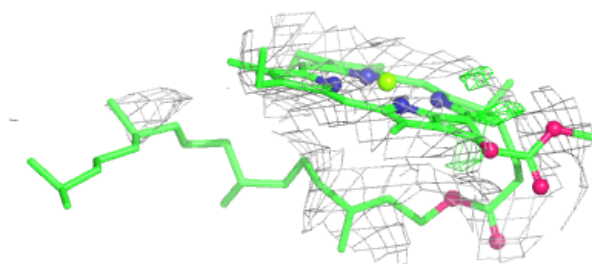
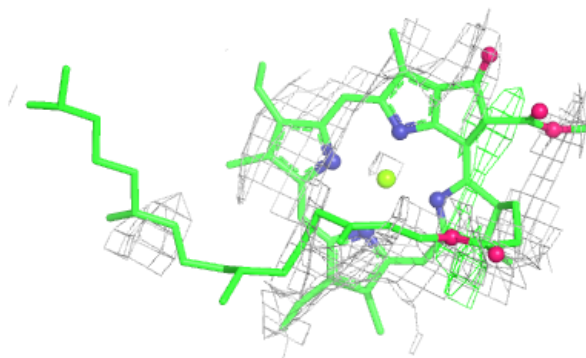
**Electron density around CLA A 814:**

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



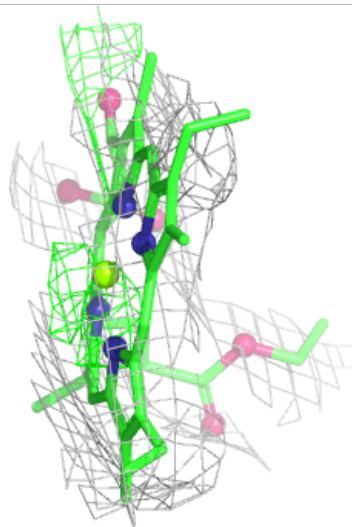
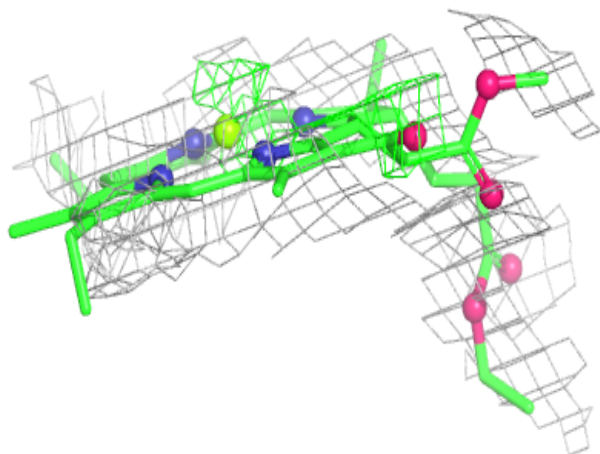
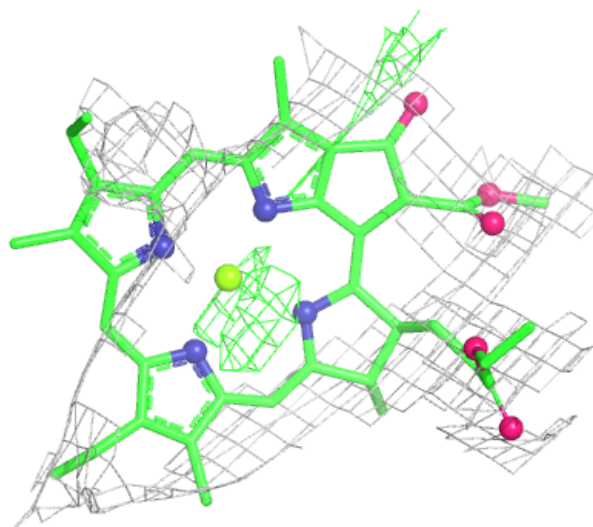
Electron density around CLA B 836:

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



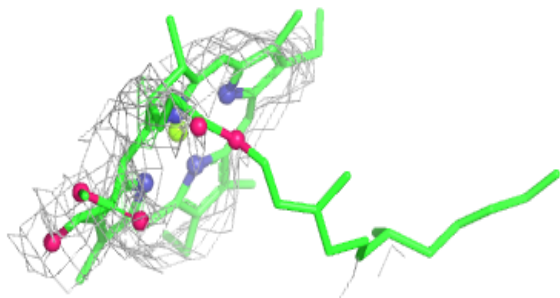
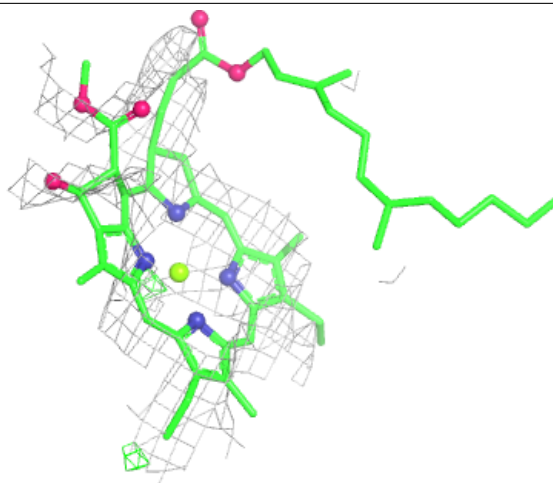
Electron density around CLA B 837:

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



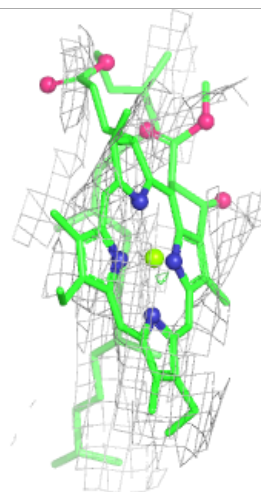
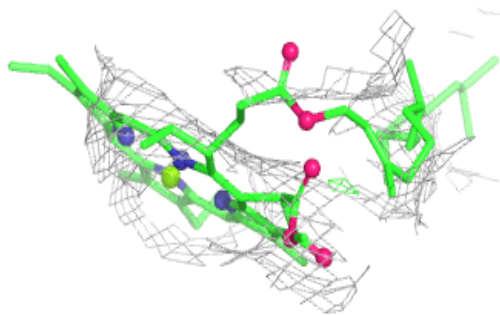
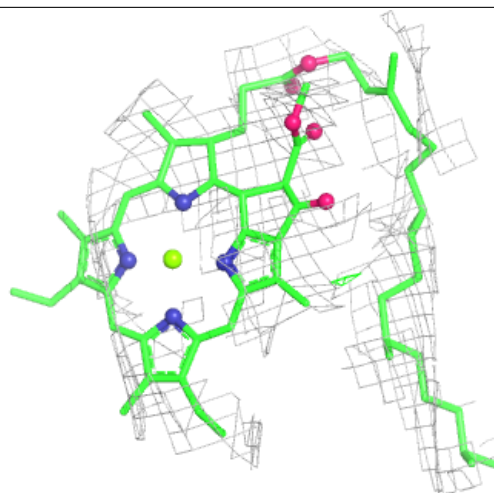
Electron density around CLA A 824:

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



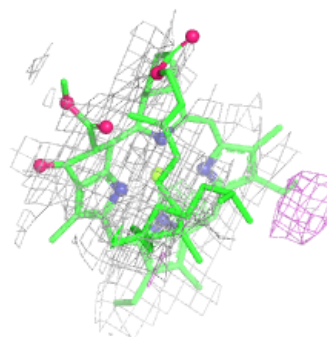
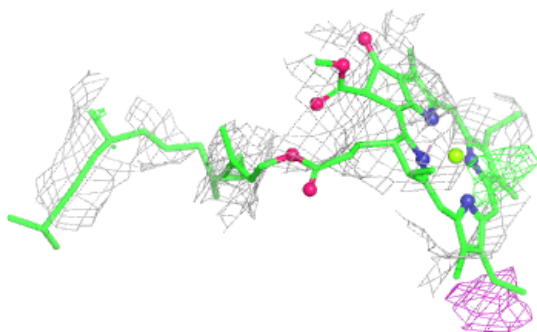
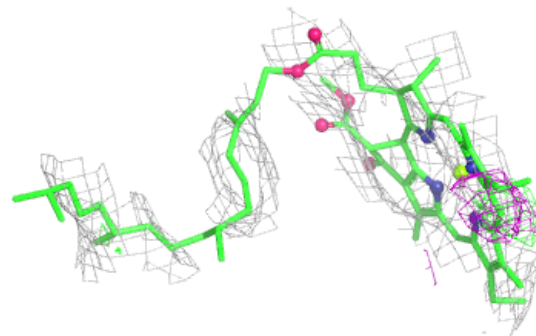
Electron density around CLA A 825:

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

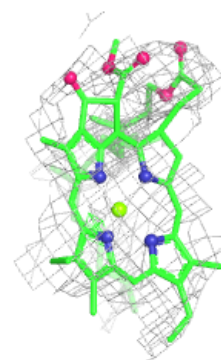
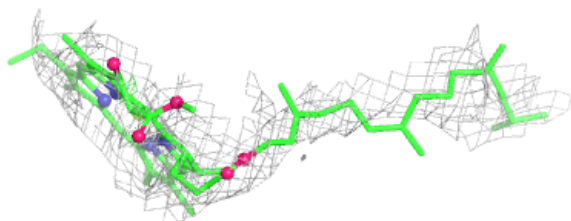
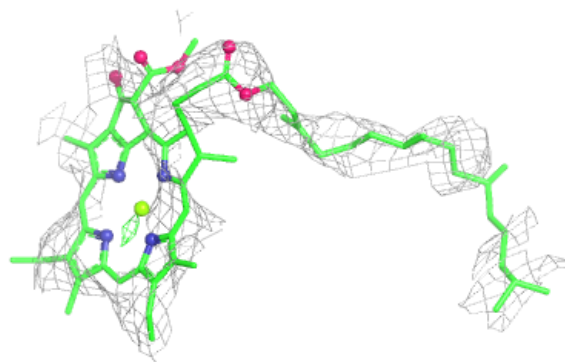


Electron density around CLA B 801:

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

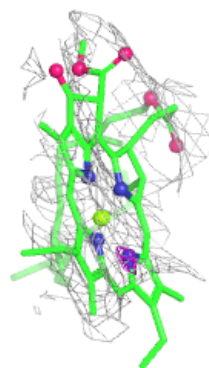
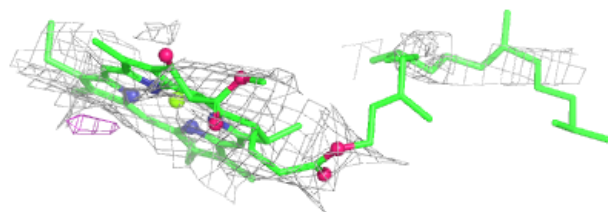
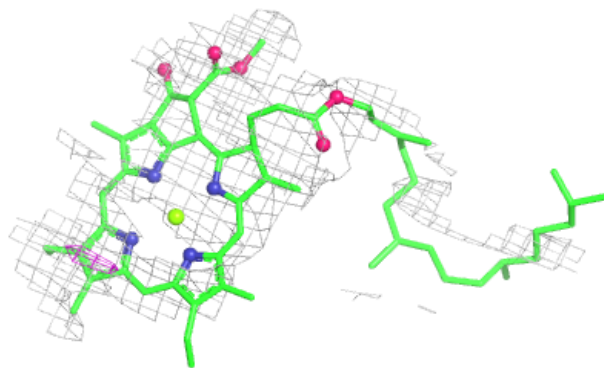
**Electron density around CLA I 101:**

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

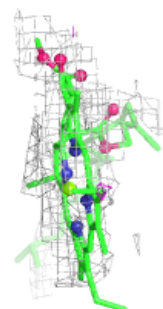
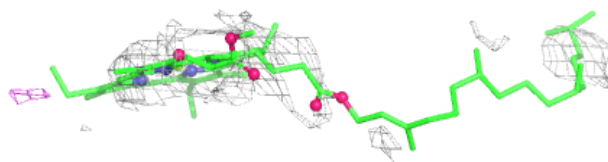
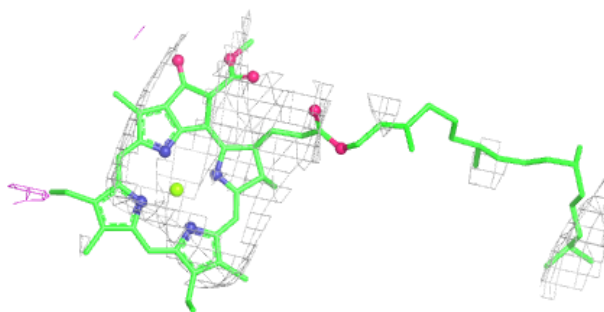


Electron density around CLA J 1101:

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

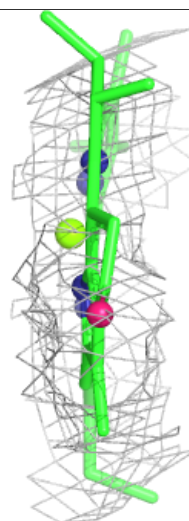
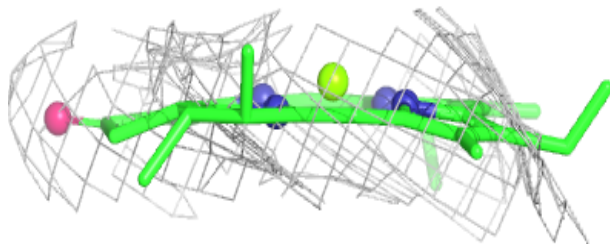
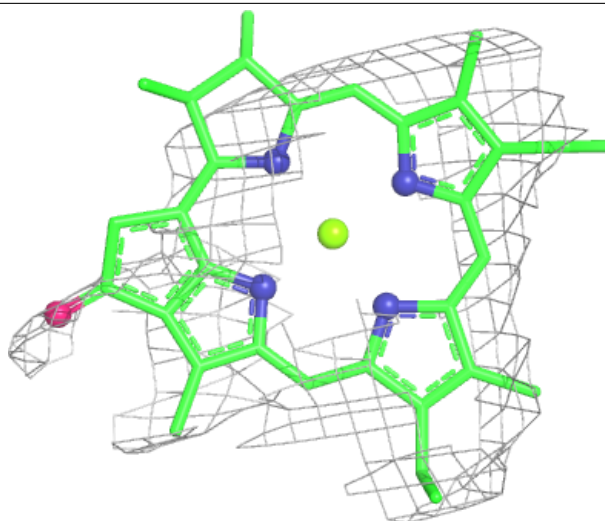
**Electron density around CLA A 826:**

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



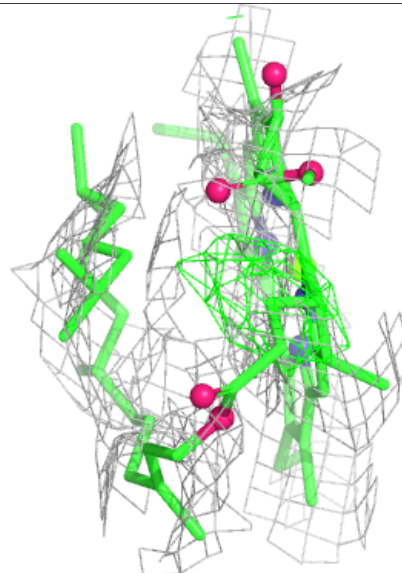
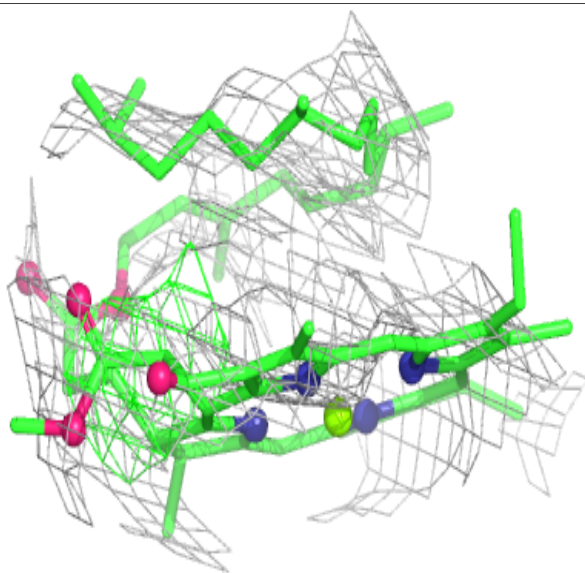
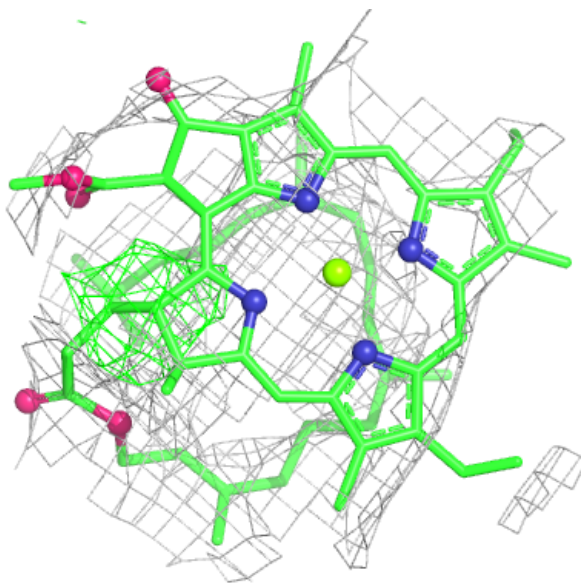
Electron density around CLA J 1103:

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



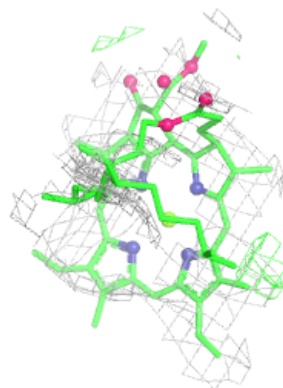
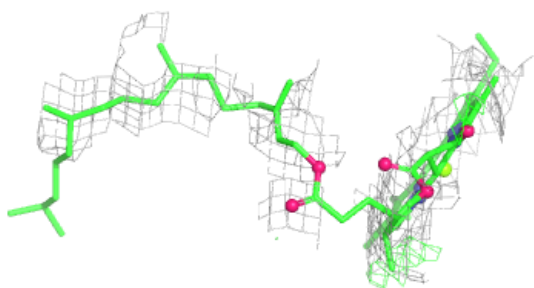
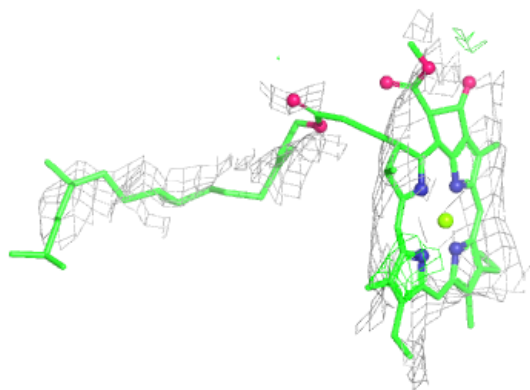
Electron density around CLA L 1002:

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

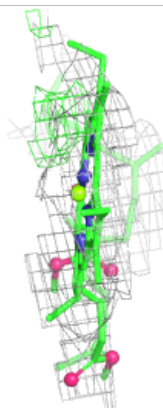
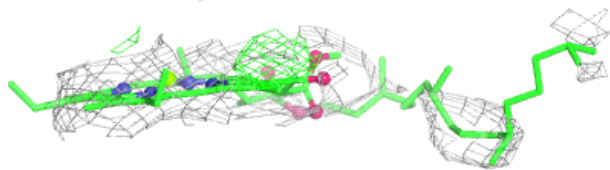
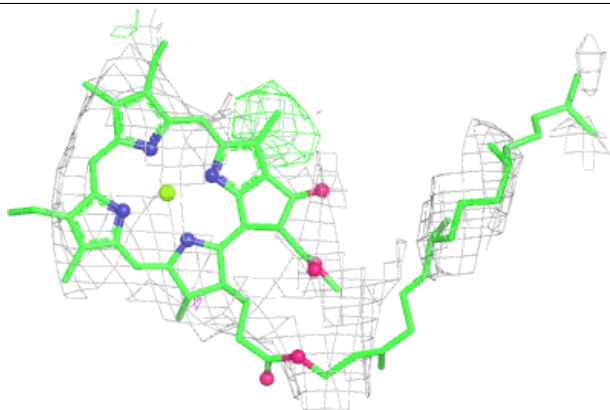


Electron density around CLA L 1003:

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

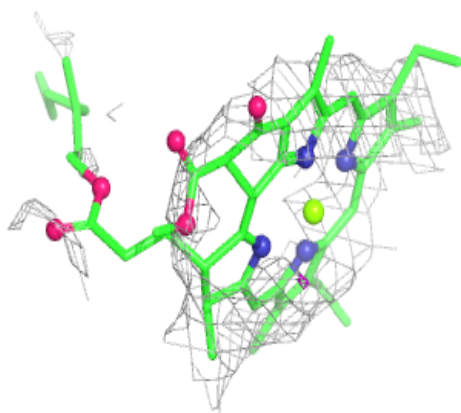
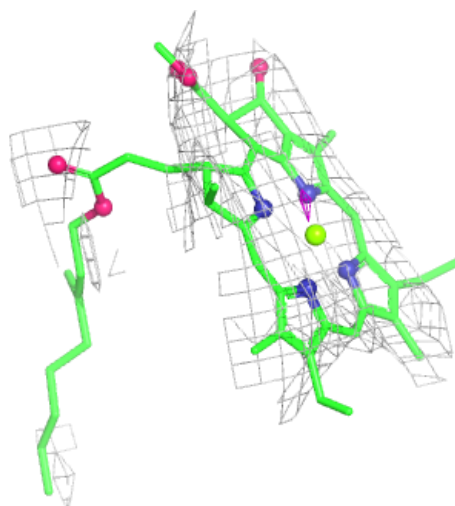
**Electron density around CLA L 1004:**

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



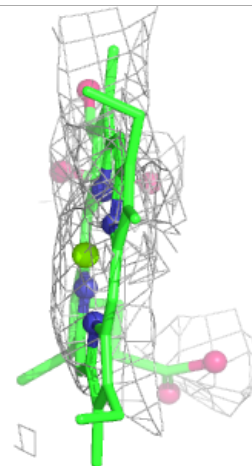
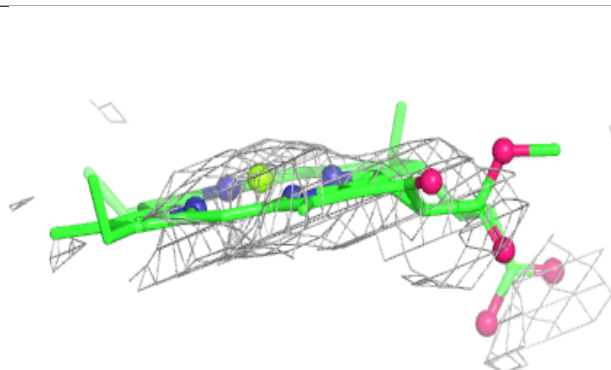
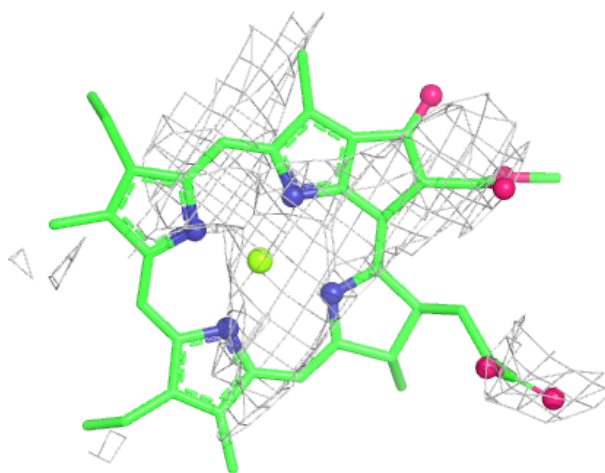
Electron density around CLA M 1201:

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



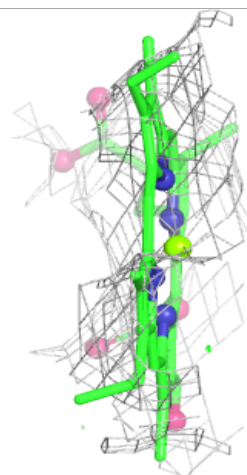
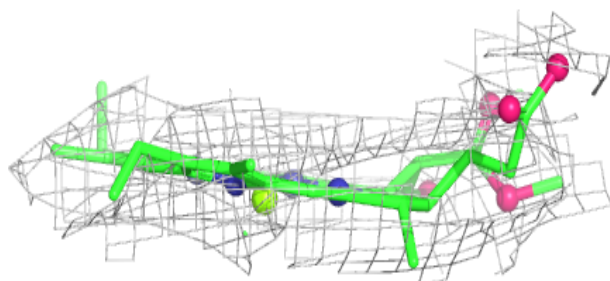
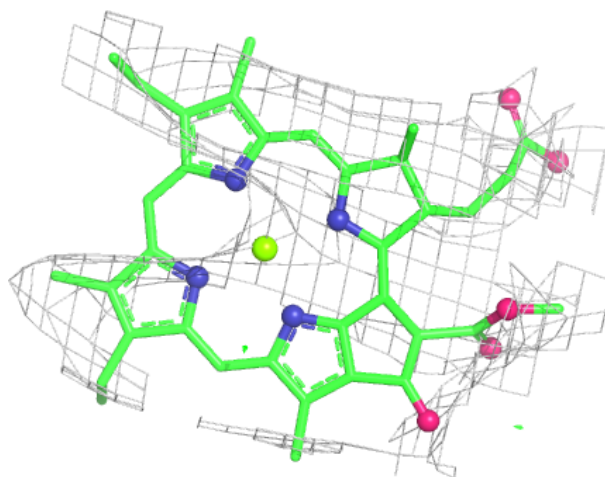
Electron density around CLA M 1202:

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



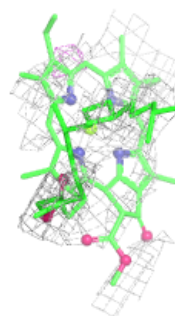
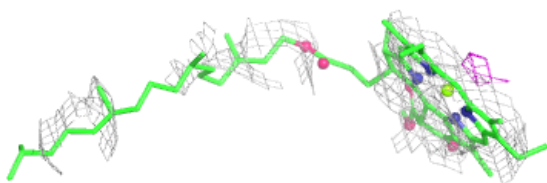
Electron density around CLA X 102:

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



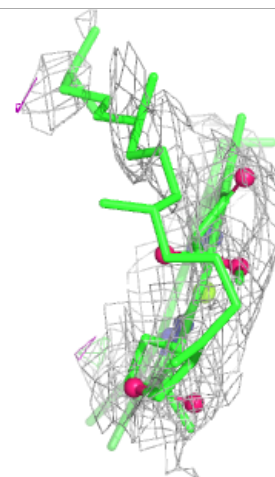
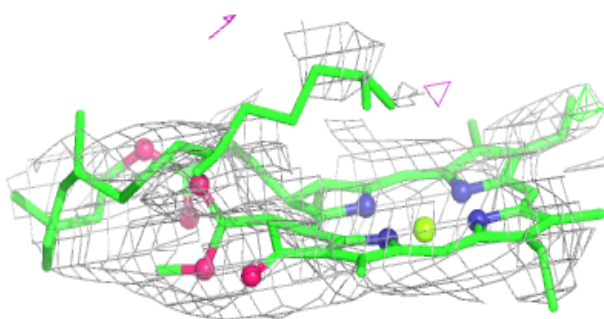
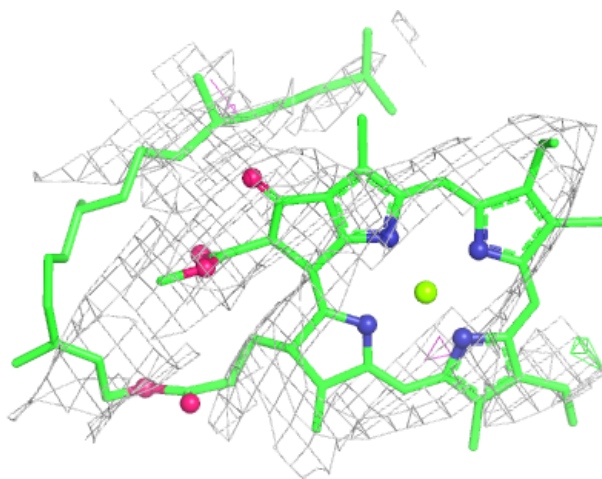
Electron density around CLA A 802:

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



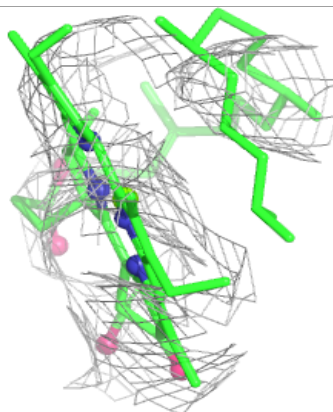
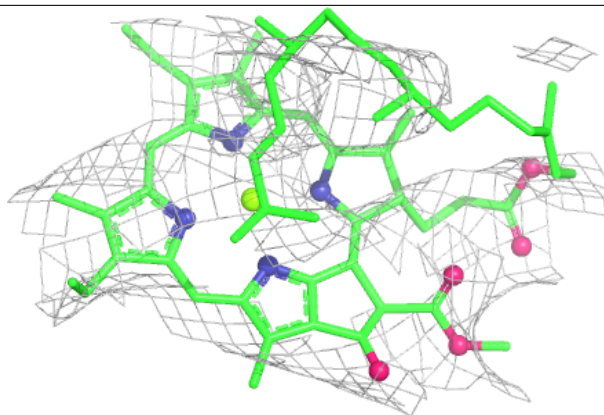
Electron density around CLA B 804:

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

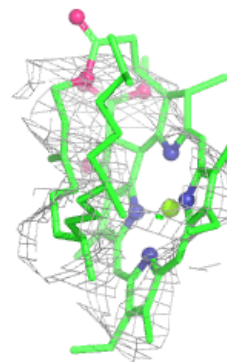
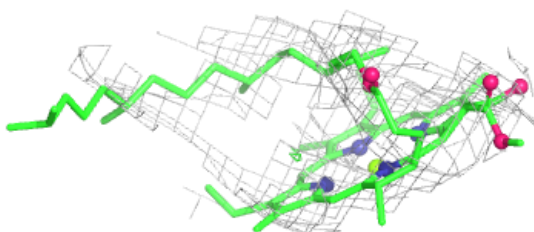
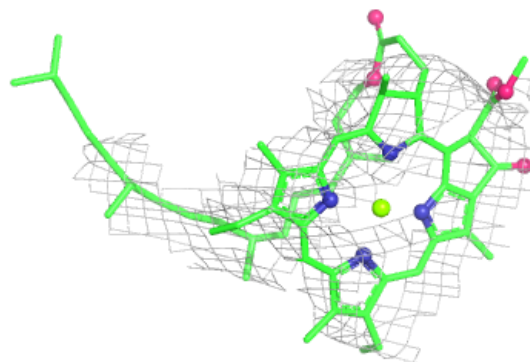


Electron density around CLA B 805:

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

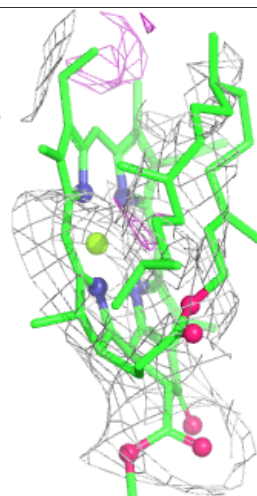
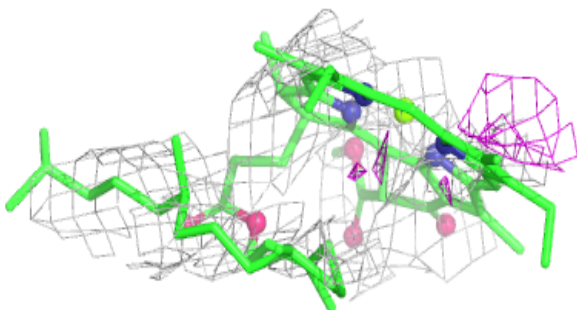
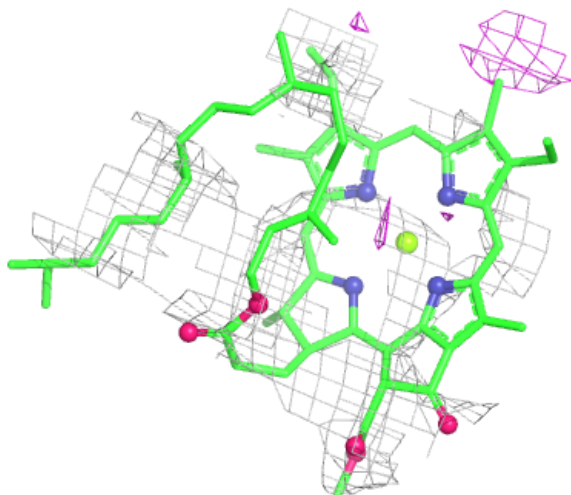
**Electron density around CLA B 806:**

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



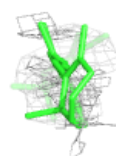
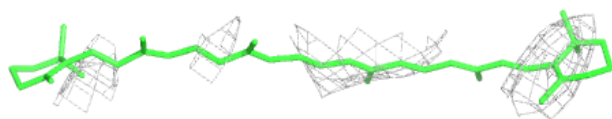
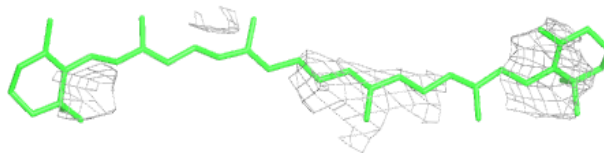
Electron density around CLA B 807:

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

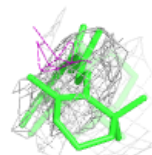
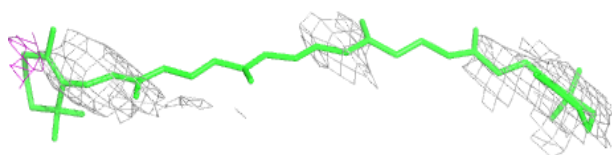
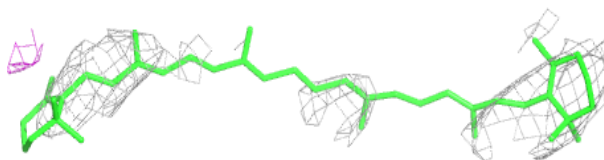


Electron density around BCR A 850:

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

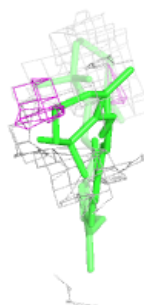
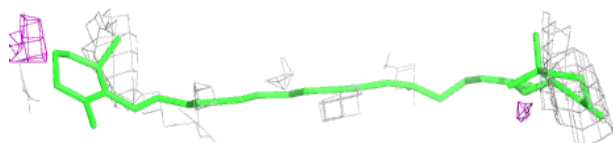
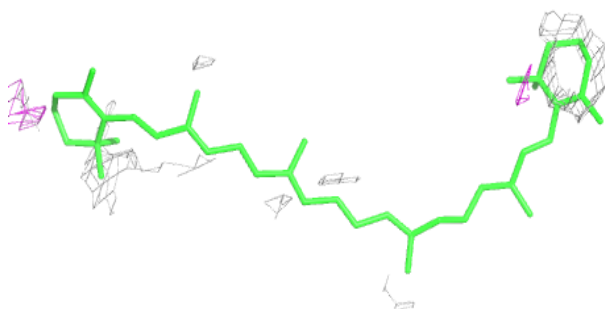
**Electron density around BCR A 851:**

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

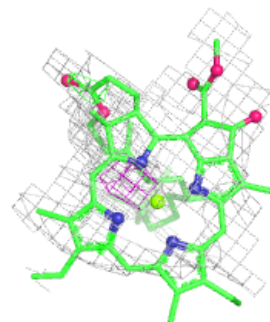
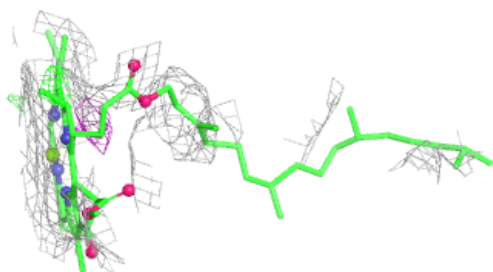
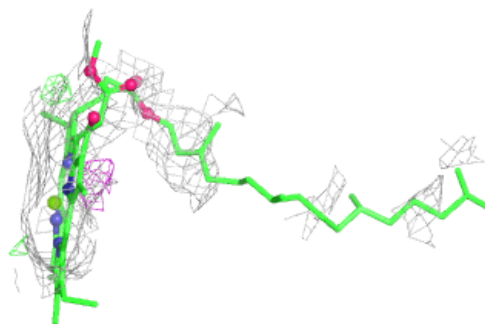


Electron density around BCR A 852:

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

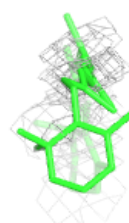
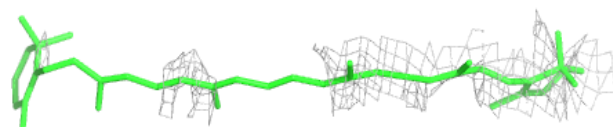
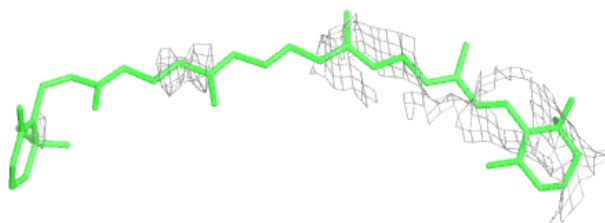
**Electron density around CLA A 828:**

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



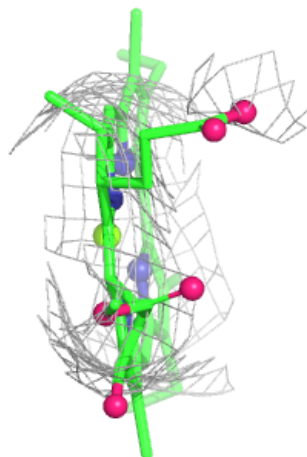
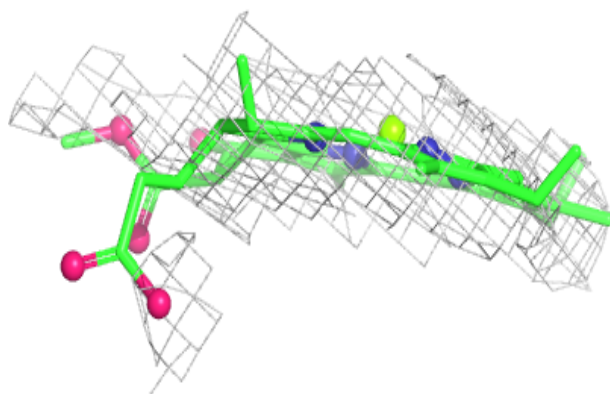
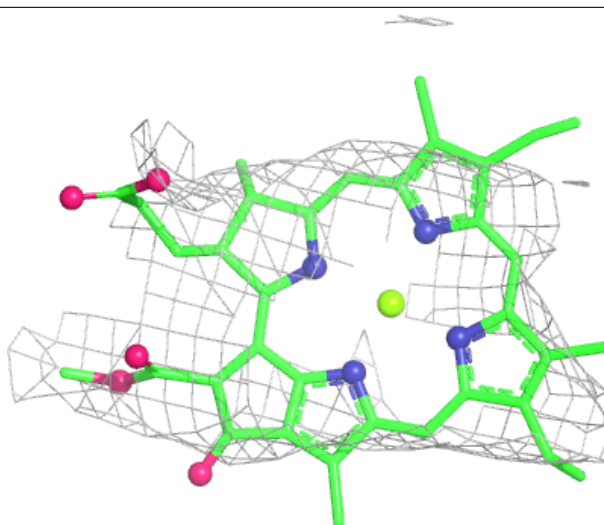
Electron density around BCR B 842:

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



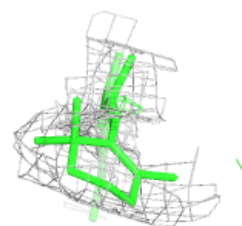
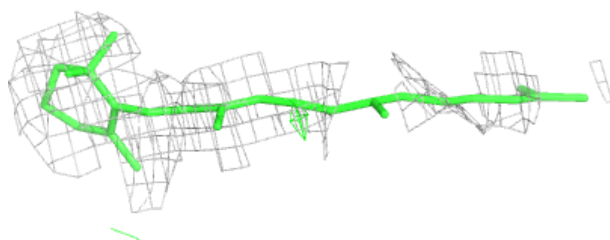
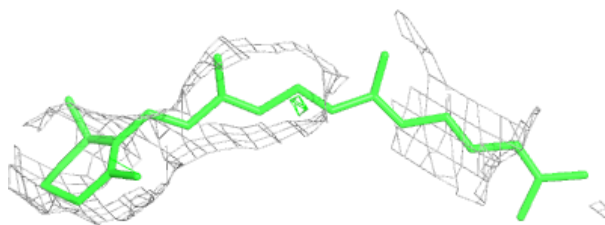
Electron density around CLA B 809:

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

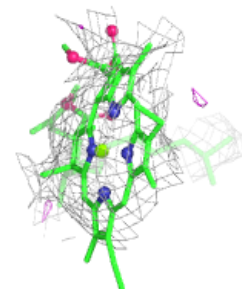
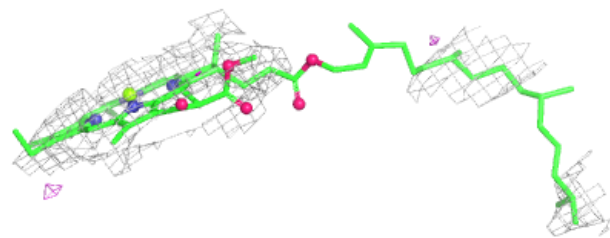
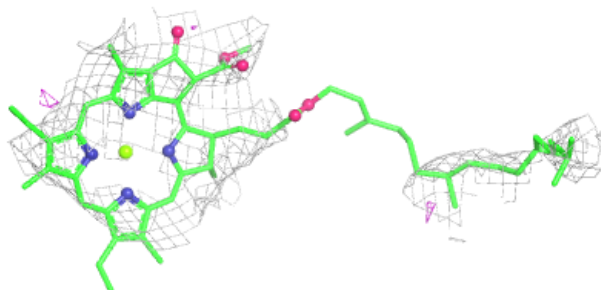


Electron density around BCR B 844:

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

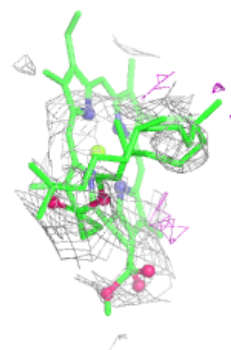
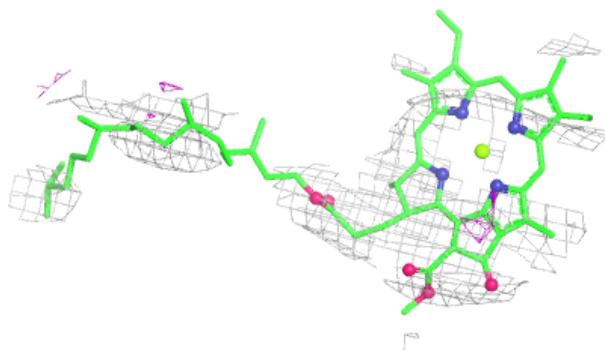
**Electron density around CLA A 805:**

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

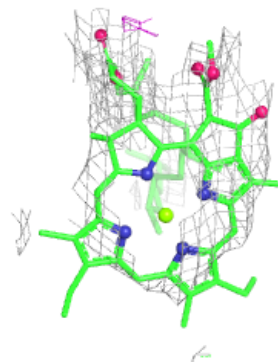
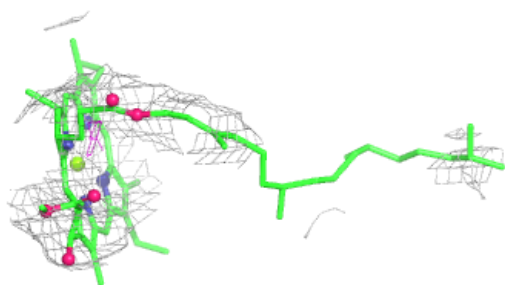
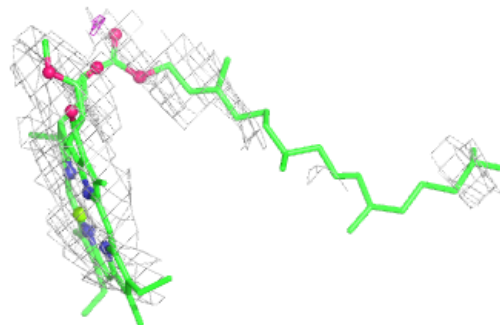


Electron density around CLA B 811:

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

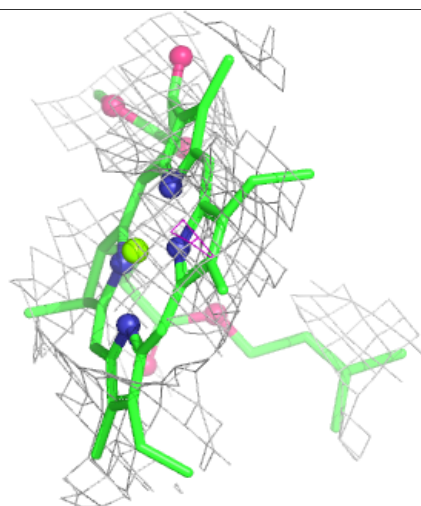
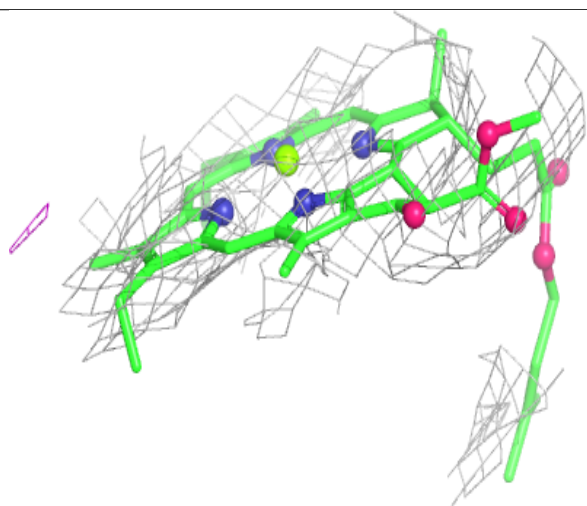
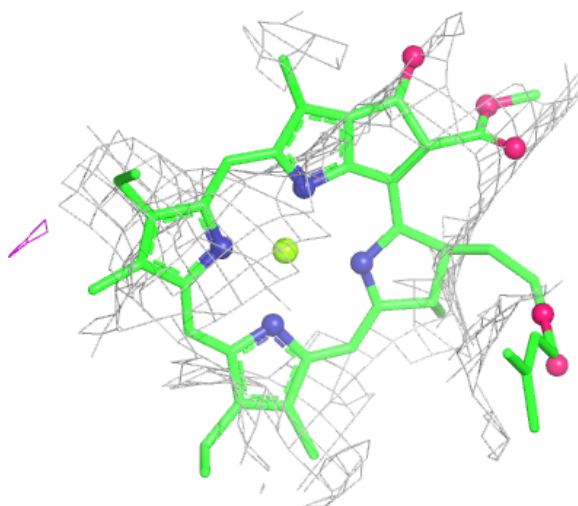
**Electron density around CLA A 830:**

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



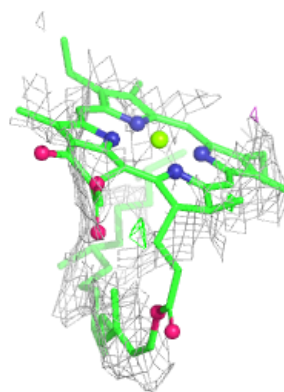
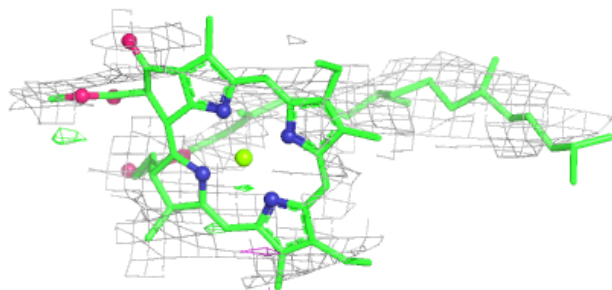
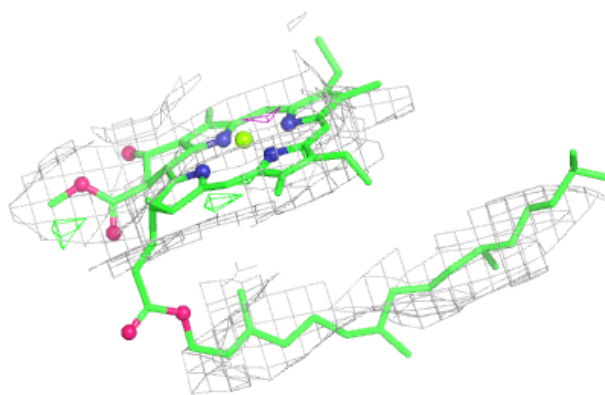
Electron density around CLA A 831:

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

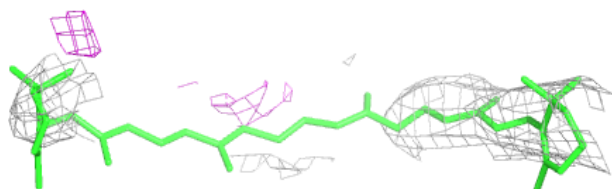
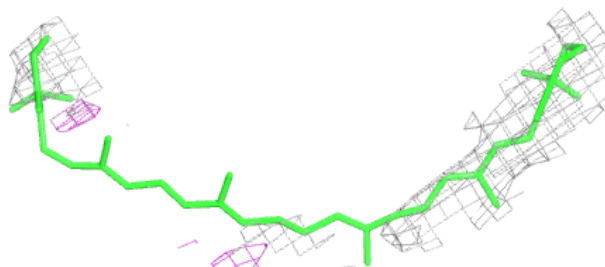


Electron density around CLA A 832:

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

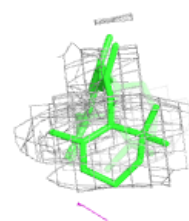
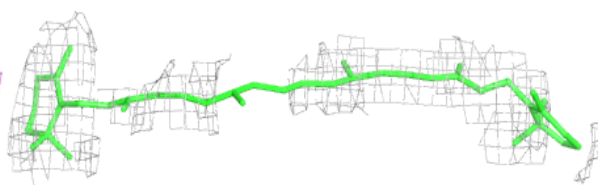
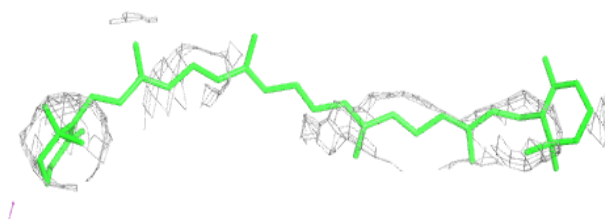
**Electron density around BCR F 1302:**

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

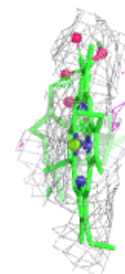
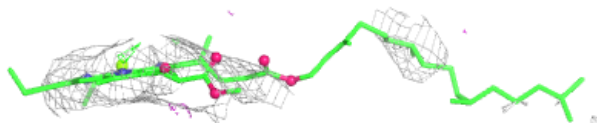


Electron density around BCR I 102:

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

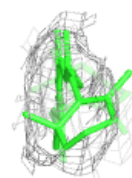
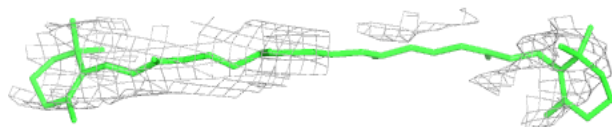
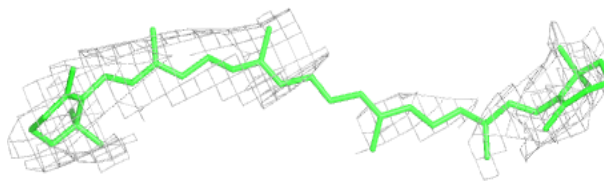
**Electron density around CLA A 833:**

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

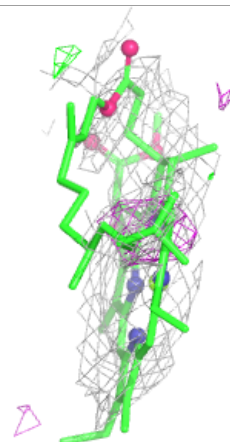
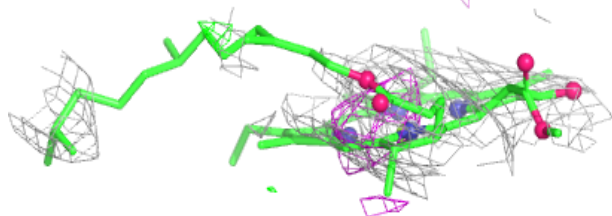
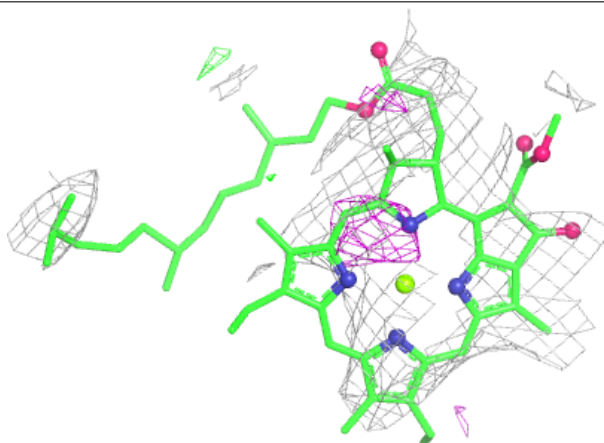


Electron density around BCR J 1105:

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

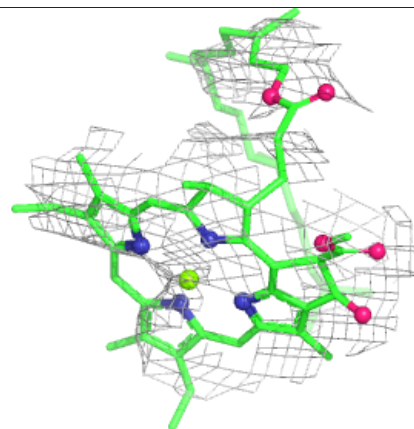
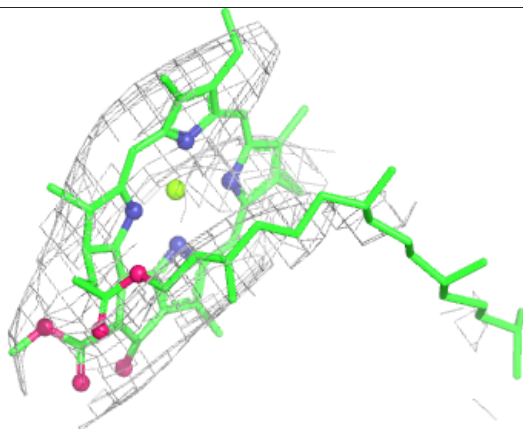
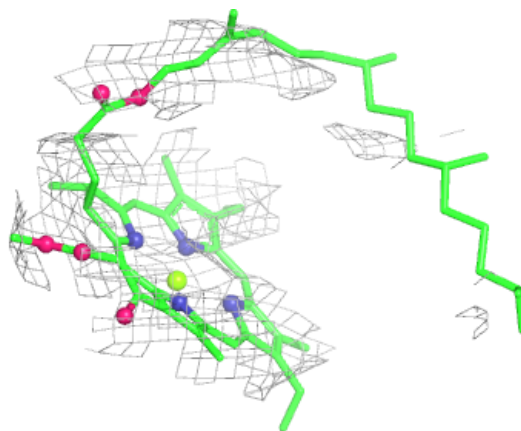
**Electron density around CLA B 816:**

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



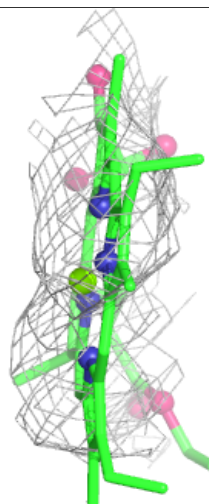
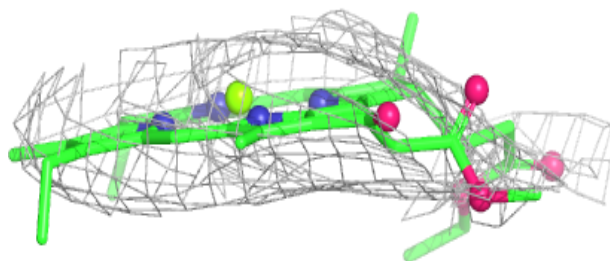
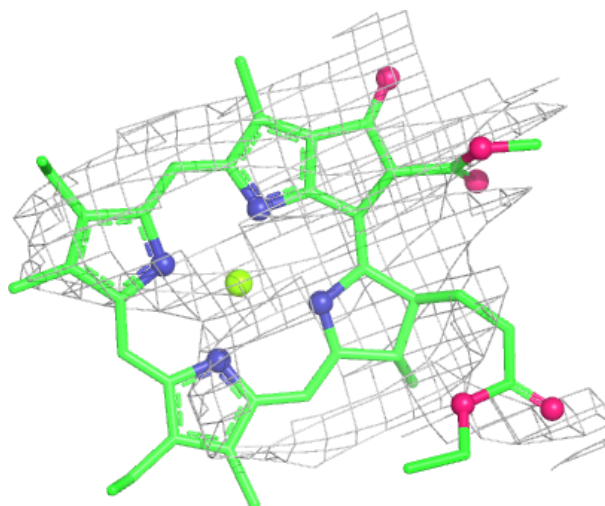
Electron density around CLA B 817:

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



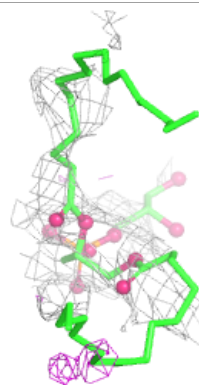
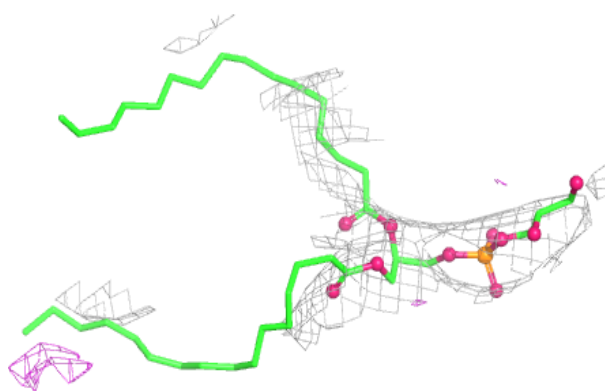
Electron density around CLA B 818:

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

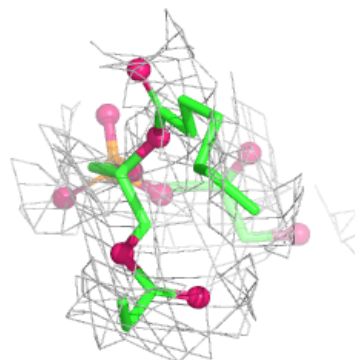
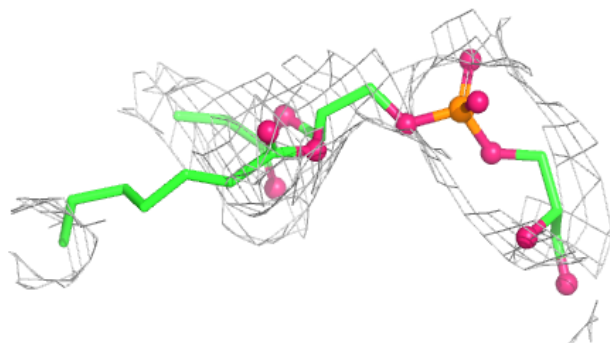
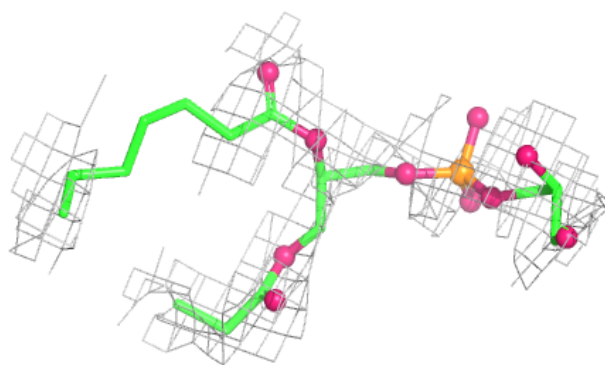


Electron density around LHG A 853:

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

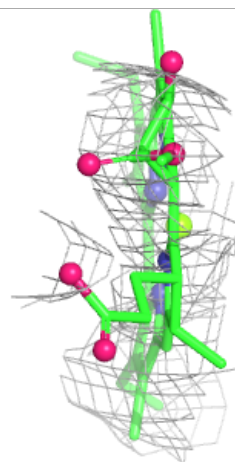
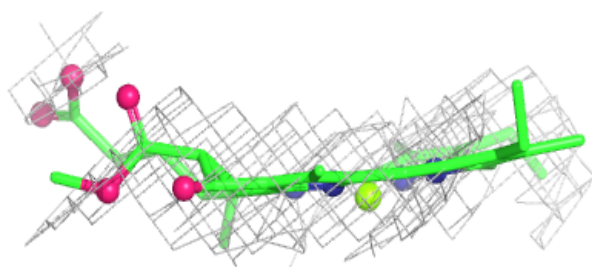
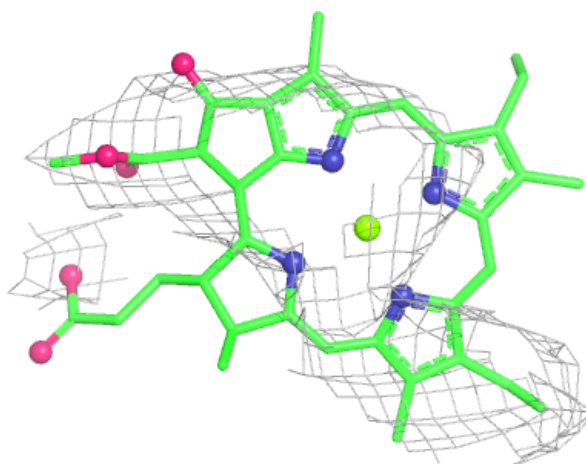
**Electron density around LHG A 854:**

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



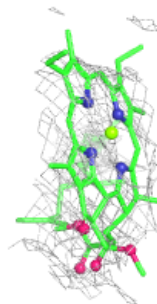
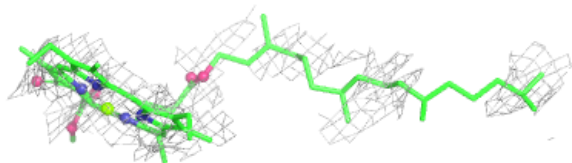
Electron density around CLA B 819:

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

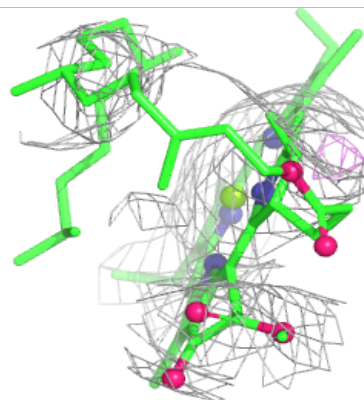
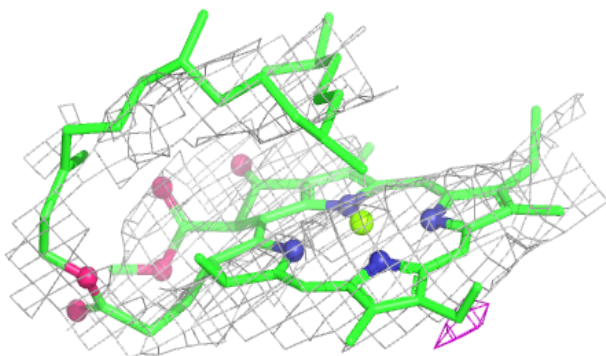
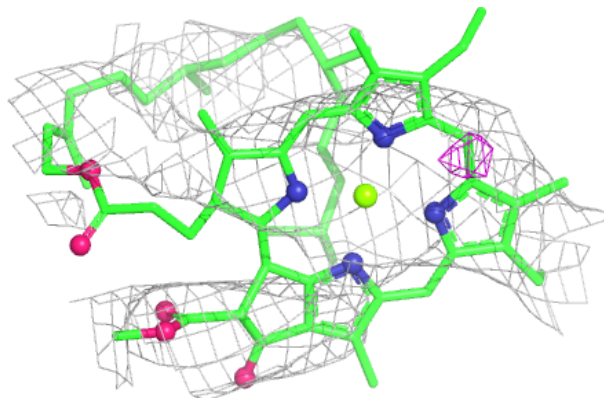


Electron density around CLA A 834:

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

**Electron density around CLA A 806:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.