



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:22 AM UTC

PDB ID : 5V8K / pdb_00005v8k
Title : Homodimeric reaction center of *H. modesticaldum*
Authors : Gisriel, C.; Sarrou, I.; Ferlez, B.; Golbeck, J.; Redding, K.E.; Fromme, R.
Deposited on : 2017-03-22
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

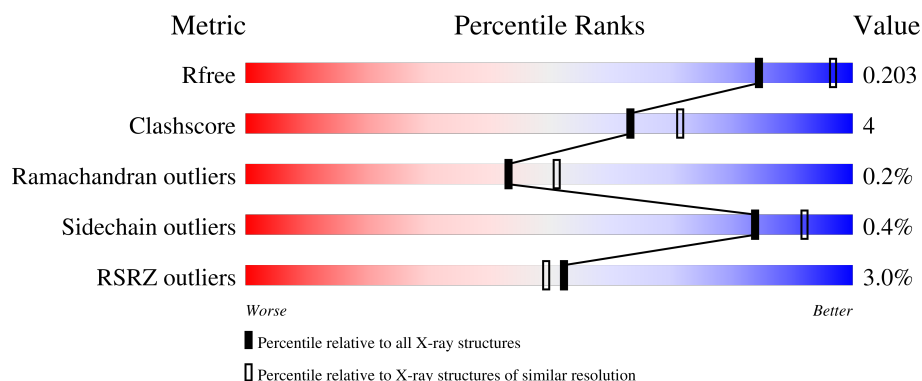
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	600	2% 93% 6%
2	B	25	24% 80% 20%

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
3	GB0	A	1001	X	-	-	-
4	GBF	A	1002	X	-	-	-
4	GBF	A	1004	X	-	-	-
4	GBF	A	1006	X	-	-	-
4	GBF	A	1007	X	-	-	-
4	GBF	A	1008	X	-	-	-
4	GBF	A	1009	X	-	-	-
4	GBF	A	1010	X	-	-	-
4	GBF	A	1011	X	-	-	-
4	GBF	A	1012	X	-	-	-
4	GBF	A	1013	X	-	-	-
4	GBF	A	1014	X	-	-	-
4	GBF	A	1015	X	-	-	-
4	GBF	A	1016	X	-	-	-
4	GBF	A	1017	X	-	-	-
4	GBF	A	1018	X	-	-	-
4	GBF	A	1019	X	-	-	-
4	GBF	A	1020	X	-	-	-
4	GBF	A	1021	X	-	-	-
4	GBF	A	1022	X	-	-	-
4	GBF	A	1023	X	-	-	-
4	GBF	A	1024	X	-	-	-
4	GBF	A	1025	X	-	-	-
4	GBF	A	1026	X	-	-	-
4	GBF	A	1027	X	-	-	-
4	GBF	A	1028	X	-	-	-
4	GBF	B	102	X	-	-	-
4	GBF	B	103	X	-	-	-
5	AOH	A	1003	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 13193 atoms, of which 6235 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 p800 reaction center core protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	600	9267	3111	4589	768	762	37	0	0	0

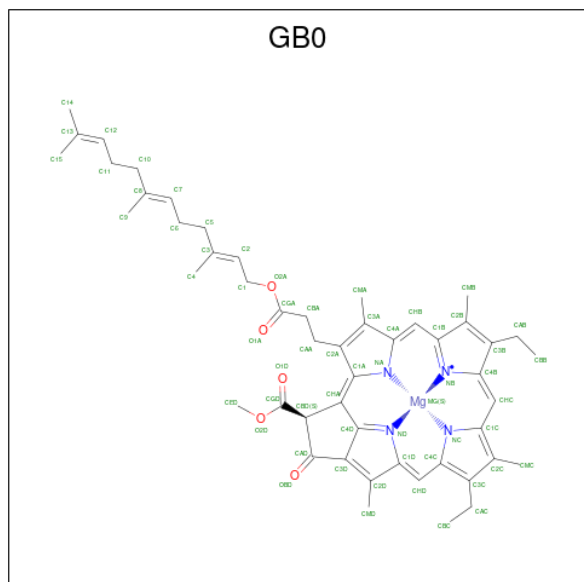
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	LEU	ASP	conflict	UNP Q1MX24
A	81	VAL	THR	conflict	UNP Q1MX24
A	566	GLN	GLU	conflict	UNP Q1MX24

- Molecule 2 is a protein called proteinsubunit pshX.

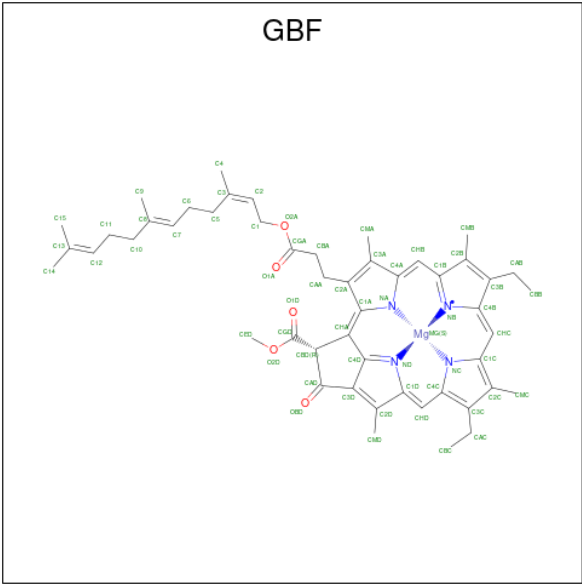
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	B	25	429	160	209	30	30	0	0	0

- Molecule 3 is Bacteriochlorophyll g' (CCD ID: GB0) (formula: $C_{50}H_{58}MgN_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	Mg	N	O	0	0
			110	50	50	1	4	5		
3	A	1	Total	C	H	Mg	N	O	0	0
			110	50	50	1	4	5		

- Molecule 4 is Bacteriochlorophyll g (CCD ID: GBF) (formula: C₅₀H₅₈MgN₄O₅).



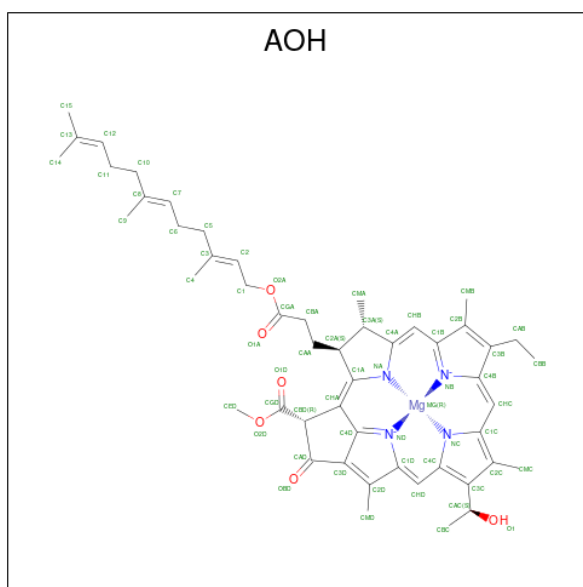
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 113	C 50	H 53	Mg 1	N 4	O 5	0	0
4	A	1	Total 87	C 40	H 37	Mg 1	N 4	O 5	0	0
4	A	1	Total 75	C 35	H 30	Mg 1	N 4	O 5	0	0
4	A	1	Total 114	C 50	H 54	Mg 1	N 4	O 5	0	0
4	A	1	Total 100	C 45	H 45	Mg 1	N 4	O 5	0	0
4	A	1	Total 73	C 35	H 28	Mg 1	N 4	O 5	0	0
4	A	1	Total 73	C 35	H 28	Mg 1	N 4	O 5	0	0
4	A	1	Total 113	C 50	H 53	Mg 1	N 4	O 5	0	0
4	A	1	Total 98	C 45	H 43	Mg 1	N 4	O 5	0	0
4	A	1	Total 100	C 45	H 45	Mg 1	N 4	O 5	0	0

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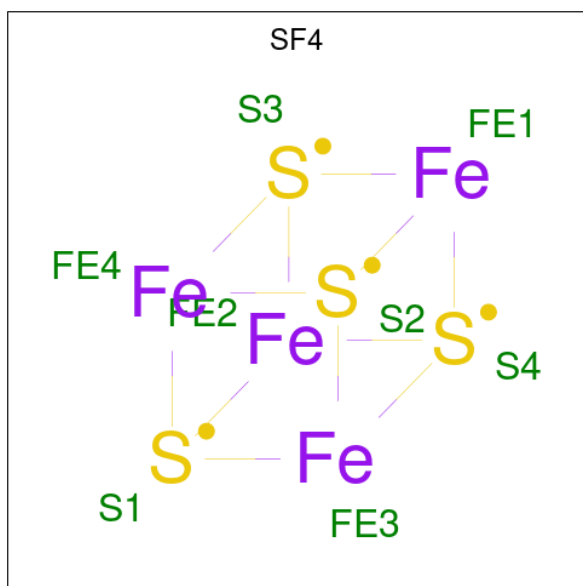
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	Mg	N	O	0	0
			75	35	30	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			112	50	52	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			73	35	28	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			112	50	52	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			87	40	37	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			113	50	53	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			113	50	53	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			113	50	53	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			75	35	30	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			113	50	53	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			87	40	37	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			75	35	30	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			113	50	53	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			86	40	36	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			113	50	53	1	4	5		
4	B	1	Total	C	H	Mg	N	O	0	0
			73	35	28	1	4	5		
4	B	1	Total	C	H	Mg	N	O	0	0
			113	50	53	1	4	5		

- Molecule 5 is 8(1)-OH-Chlorophyll aF (CCD ID: AOH) (formula: C₅₀H₆₀MgN₄O₆).



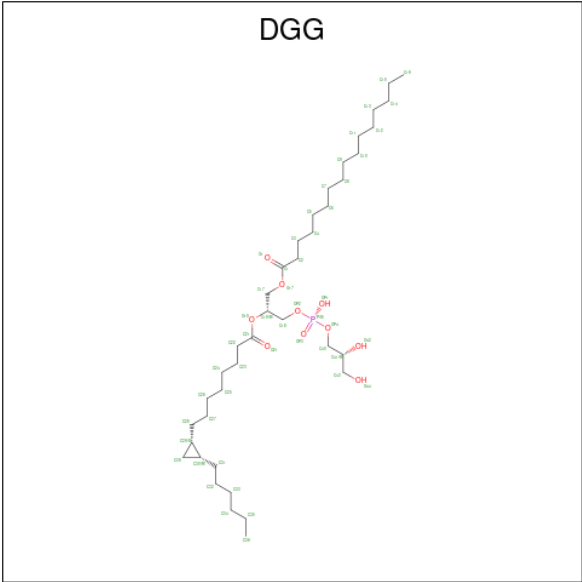
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	Mg	N	O	0	0
			113	50	52	1	4	6		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 7 is 1-[GLYCEROLYLPHOSPHONYL]-2-[8-(2-HEXYL-CYCLOPROPYL)-OCTANAL-1-YL]-3-[HEXADECANAL-1-YL]-GLYCEROL (CCD ID: DGG) (formula: $\text{C}_{39}\text{H}_{75}\text{O}_{10}\text{P}$).

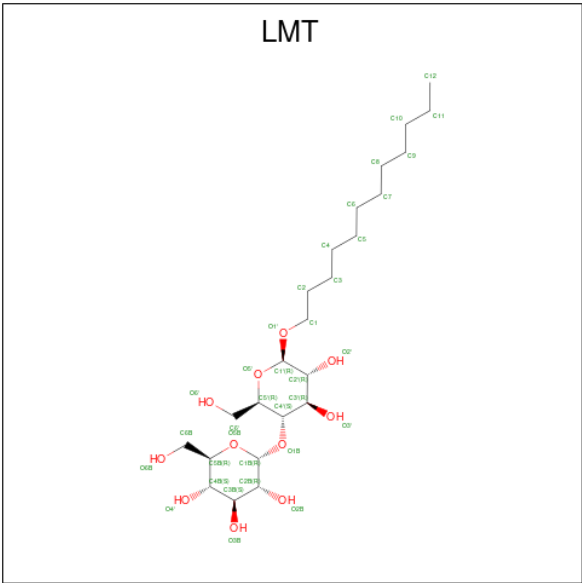


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	O	P	0	0
			88	30	47	10	1		
7	A	1	Total	C	H	O	P	0	0
			93	33	49	10	1		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

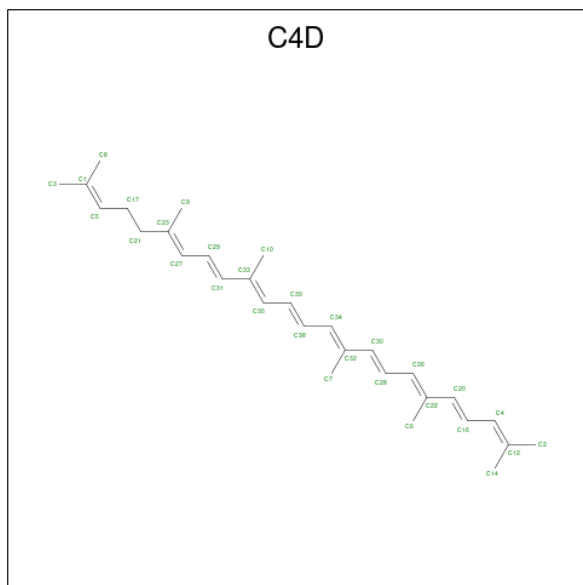
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Ca	0	0
			2	2		

- Molecule 9 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			35	24	11		
9	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 10 is 4,4'-Diaponeurosporene (CCD ID: C4D) (formula: C₃₀H₄₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	H	0	0
			72	30	42		

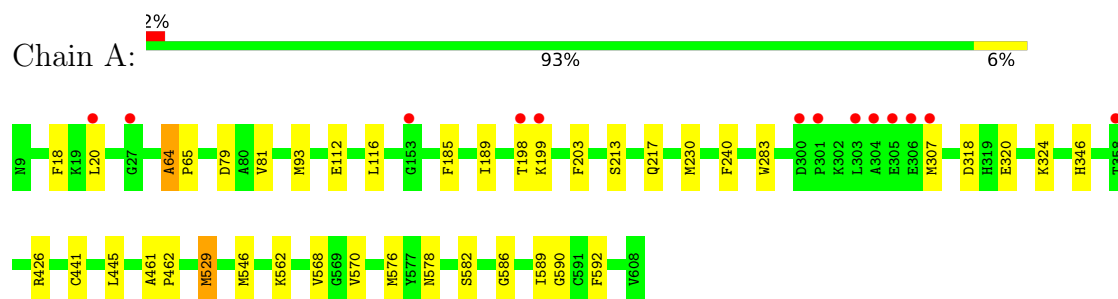
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	230	Total	O	0	0
			230	230		
11	B	9	Total	O	0	0
			9	9		

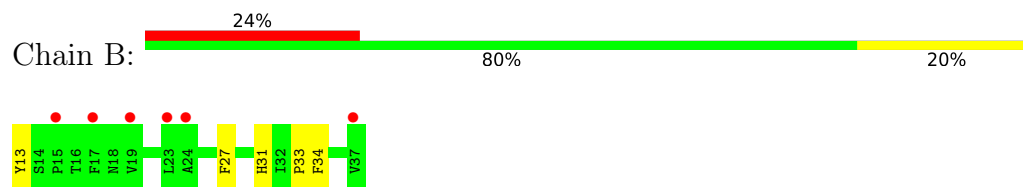
3 Residue-property plots [i](#)

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: p800 reaction center core protein



- Molecule 2: proteinsubunit pshX



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.36Å 89.71Å 111.64Å 90.00° 108.15° 90.00°	Depositor
Resolution (Å)	29.08 – 2.20 29.08 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.08-2.20) 98.2 (29.08-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.20Å)	Xtriage
Refinement program	PHENIX DEV_2450	Depositor
R, R_{free}	0.158 , 0.191 0.176 , 0.203	Depositor DCC
R_{free} test set	2941 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13193	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: DGG, GB0, AOH, CA, LMT, SF4, C4D, GBF

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	0.53	0/4835	0.71	4/6562 (0.1%)
2	B	0.54	0/232	0.46	0/317
All	All	0.53	0/5067	0.70	4/6879 (0.1%)

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	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	64	ALA	CA-C-N	19.54	144.26	119.84
1	A	64	ALA	C-N-CA	19.54	144.26	119.84
1	A	64	ALA	C-N-CD	-8.77	89.04	125.00
1	A	529	MET	CG-SD-CE	-5.40	89.02	100.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	ALA	Peptide,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	4678	4589	4589	36	0
2	B	220	209	209	4	0
3	A	120	100	0	0	0
4	A	1340	1066	0	2	0
4	B	105	81	0	0	0
5	A	61	52	0	0	0
6	A	8	0	0	0	0
7	A	85	96	105	13	0
8	A	2	0	0	0	0
9	A	70	0	92	7	0
10	B	30	42	0	0	0
11	A	230	0	0	1	0
11	B	9	0	0	1	0
All	All	6958	6235	4995	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 47 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)
9:A:1034:LMT:H61	9:A:1035:LMT:H61	1.42	0.98
1:A:592:PHE:CG	7:A:1030:DGG:HC71	2.21	0.76
9:A:1034:LMT:H52	9:A:1035:LMT:H42	1.66	0.75
1:A:18:PHE:CZ	7:A:1030:DGG:H252	2.24	0.73
1:A:582:SER:CB	7:A:1030:DGG:H402	2.22	0.69

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/600 (100%)	584 (98%)	13 (2%)	1 (0%)	43	51
2	B	23/25 (92%)	23 (100%)	0	0	100	100
All	All	621/625 (99%)	607 (98%)	13 (2%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	463/476 (97%)	461 (100%)	2 (0%)	84	92
2	B	23/23 (100%)	23 (100%)	0	100	100
All	All	486/499 (97%)	484 (100%)	2 (0%)	84	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	CYS
1	A	445	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	567	GLN
1	A	458	GLN
1	A	176	ASN
1	A	142	HIS

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Mol	Chain	Res	Type
1	A	261	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 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 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$
4	GBF	A	1020	-	66,68,68	2.73	24 (36%)	80,107,107	5.21	40 (50%)
4	GBF	A	1025	-	51,53,68	3.17	23 (45%)	62,89,107	5.73	36 (58%)
4	GBF	B	102	-	51,53,68	3.34	23 (45%)	62,89,107	5.67	38 (61%)
4	GBF	A	1024	-	56,58,68	2.97	24 (42%)	68,95,107	5.23	39 (57%)
4	GBF	A	1026	8	66,68,68	2.66	25 (37%)	80,107,107	4.96	40 (50%)
7	DGG	A	1031	-	43,43,50	1.02	2 (4%)	46,49,59	1.23	4 (8%)
4	GBF	A	1016	-	51,53,68	3.32	25 (49%)	62,89,107	5.64	36 (58%)
4	GBF	A	1022	-	51,53,68	3.08	26 (50%)	62,89,107	5.60	31 (50%)
4	GBF	A	1021	-	66,68,68	2.71	22 (33%)	80,107,107	5.05	39 (48%)
4	GBF	A	1008	-	61,63,68	2.84	22 (36%)	74,101,107	5.07	40 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GBF	A	1012	-	61,63,68	2.89	24 (39%)	74,101,107	5.32	43 (58%)
4	GBF	A	1023	-	66,68,68	2.69	21 (31%)	80,107,107	5.23	41 (51%)
4	GBF	A	1014	1	51,53,68	3.21	25 (49%)	62,89,107	5.61	38 (61%)
9	LMT	A	1035	-	36,36,36	0.85	1 (2%)	47,47,47	1.08	3 (6%)
6	SF4	A	1029	1	0,12,12	-	-	-	-	-
3	GB0	A	1005	-	66,68,68	2.87	24 (36%)	80,107,107	5.02	43 (53%)
4	GBF	A	1009	-	51,53,68	3.34	24 (47%)	62,89,107	5.71	35 (56%)
4	GBF	B	103	-	66,68,68	2.97	23 (34%)	80,107,107	4.78	45 (56%)
4	GBF	A	1011	11	66,68,68	2.80	26 (39%)	80,107,107	4.82	37 (46%)
4	GBF	A	1010	1	51,53,68	3.25	26 (50%)	62,89,107	5.72	36 (58%)
9	LMT	A	1034	-	36,36,36	0.70	0	47,47,47	1.22	7 (14%)
4	GBF	A	1006	-	51,53,68	3.13	25 (49%)	62,89,107	5.40	35 (56%)
10	C4D	B	101	-	29,29,29	0.72	0	34,34,34	1.77	11 (32%)
4	GBF	A	1027	-	56,58,68	3.09	25 (44%)	68,95,107	5.36	37 (54%)
4	GBF	A	1004	-	56,58,68	3.08	26 (46%)	68,95,107	5.37	39 (57%)
4	GBF	A	1015	-	66,68,68	2.73	24 (36%)	80,107,107	4.88	39 (48%)
7	DGG	A	1030	-	40,40,50	0.94	2 (5%)	43,46,59	1.23	4 (9%)
4	GBF	A	1019	11	66,68,68	2.74	23 (34%)	80,107,107	4.93	40 (50%)
5	AOH	A	1003	11	65,69,69	1.83	17 (26%)	75,109,109	2.41	26 (34%)
4	GBF	A	1007	-	66,68,68	2.68	24 (36%)	80,107,107	4.93	41 (51%)
4	GBF	A	1013	-	61,63,68	2.98	25 (40%)	74,101,107	5.06	39 (52%)
4	GBF	A	1017	11	66,68,68	2.77	24 (36%)	80,107,107	5.10	40 (50%)
4	GBF	A	1028	11	66,68,68	2.83	25 (37%)	80,107,107	4.83	39 (48%)
4	GBF	A	1018	1	56,58,68	3.05	23 (41%)	68,95,107	5.30	37 (54%)
4	GBF	A	1002	11	66,68,68	2.76	24 (36%)	80,107,107	4.67	39 (48%)
3	GB0	A	1001	-	66,68,68	2.72	26 (39%)	80,107,107	5.07	44 (55%)

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
4	GBF	A	1020	-	1/1/15/15	11/33/89/89	-
4	GBF	A	1025	-	1/1/9/15	8/15/71/89	-
4	GBF	B	102	-	1/1/9/15	10/15/71/89	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GBF	A	1024	-	1/1/11/15	5/21/77/89	-
4	GBF	A	1026	8	1/1/15/15	13/33/89/89	-
7	DGG	A	1031	-	-	18/48/48/59	-
4	GBF	A	1016	-	1/1/9/15	7/15/71/89	-
4	GBF	A	1022	-	1/1/9/15	5/15/71/89	-
4	GBF	A	1021	-	1/1/15/15	16/33/89/89	-
4	GBF	A	1008	-	1/1/13/15	7/27/83/89	-
4	GBF	A	1012	-	1/1/13/15	12/27/83/89	-
4	GBF	A	1023	-	1/1/15/15	7/33/89/89	-
4	GBF	A	1014	1	1/1/9/15	5/15/71/89	-
9	LMT	A	1035	-	-	7/21/61/61	0/2/2/2
6	SF4	A	1029	1	-	-	0/6/5/5
3	GB0	A	1005	-	-	10/33/89/89	-
4	GBF	A	1009	-	1/1/9/15	7/15/71/89	-
4	GBF	B	103	-	1/1/15/15	14/33/89/89	-
4	GBF	A	1011	11	1/1/15/15	7/33/89/89	-
4	GBF	A	1010	1	1/1/9/15	8/15/71/89	-
9	LMT	A	1034	-	-	10/21/61/61	0/2/2/2
4	GBF	A	1006	-	1/1/9/15	8/15/71/89	-
10	C4D	B	101	-	-	0/31/31/31	-
4	GBF	A	1027	-	1/1/11/15	10/21/77/89	-
4	GBF	A	1004	-	1/1/11/15	10/21/77/89	-
4	GBF	A	1015	-	1/1/15/15	9/33/89/89	-
7	DGG	A	1030	-	-	14/45/45/59	-
4	GBF	A	1019	11	1/1/15/15	8/33/89/89	-
5	AOH	A	1003	11	3/3/21/21	8/35/111/111	-
4	GBF	A	1007	-	1/1/15/15	11/33/89/89	-
4	GBF	A	1013	-	1/1/13/15	12/27/83/89	-
4	GBF	A	1017	11	1/1/15/15	6/33/89/89	-
4	GBF	A	1028	11	1/1/15/15	10/33/89/89	-
4	GBF	A	1018	1	1/1/11/15	8/21/77/89	-
4	GBF	A	1002	11	1/1/15/15	8/33/89/89	-
3	GB0	A	1001	-	1/1/15/15	5/33/89/89	-

The worst 5 of 723 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1027	GBF	C1A-CHA	10.09	1.51	1.35
3	A	1005	GB0	C1A-CHA	10.06	1.51	1.35
4	A	1009	GBF	C1D-C2D	10.01	1.64	1.44
4	A	1016	GBF	C1D-C2D	9.81	1.64	1.44
4	A	1024	GBF	C1A-CHA	9.81	1.51	1.35

The worst 5 of 1181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1021	GBF	C1D-ND-C4D	-18.48	98.25	106.68
4	A	1020	GBF	C1D-ND-C4D	-18.43	98.27	106.68
4	A	1025	GBF	C1D-ND-C4D	-18.06	98.44	106.68
4	A	1010	GBF	C1D-ND-C4D	-17.76	98.58	106.68
4	A	1023	GBF	C1D-ND-C4D	-17.56	98.67	106.68

5 of 31 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1001	GB0	NA
4	A	1002	GBF	NA
4	A	1004	GBF	NA
4	A	1006	GBF	NA
4	A	1007	GBF	NA

5 of 314 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	GB0	C1A-C2A-CAA-CBA
3	A	1001	GB0	C2B-C3B-CAB-CBB
3	A	1001	GB0	C4B-C3B-CAB-CBB
3	A	1005	GB0	C1A-C2A-CAA-CBA
4	A	1002	GBF	C1A-C2A-CAA-CBA

There are no ring outliers.

6 monomers are involved in 21 short contacts:

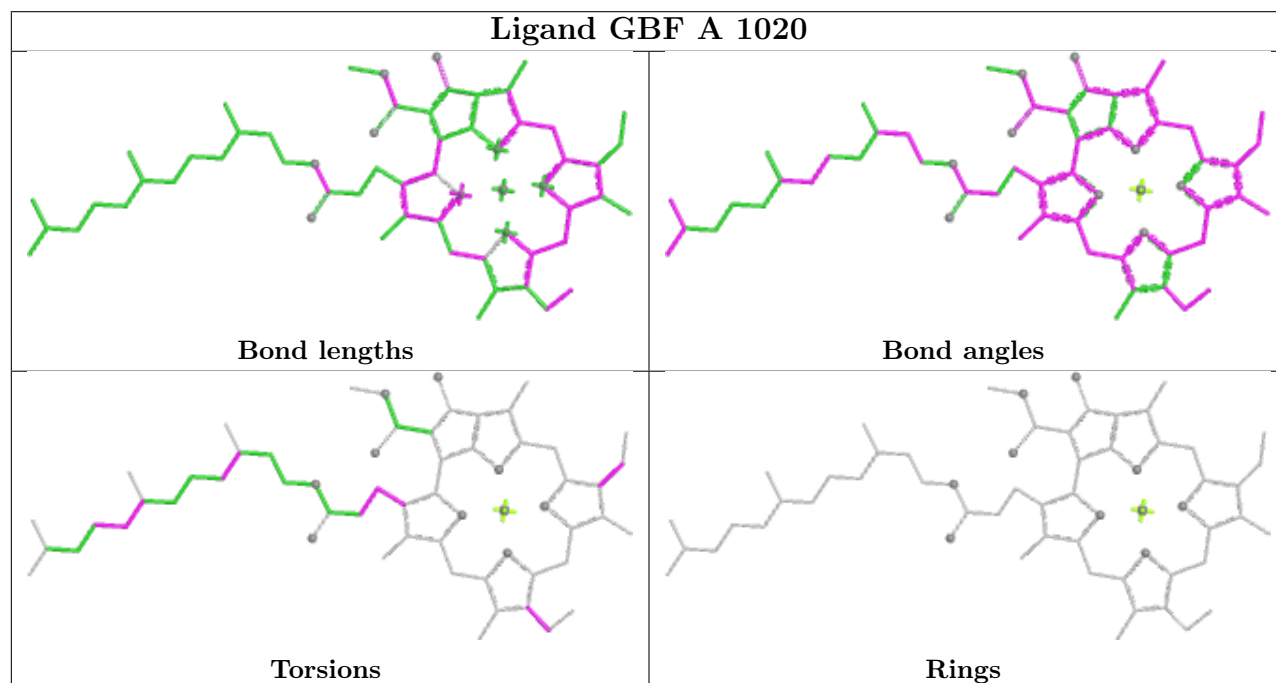
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1025	GBF	1	0
4	A	1026	GBF	1	0
7	A	1031	DGG	4	0
9	A	1035	LMT	6	0
9	A	1034	LMT	6	0

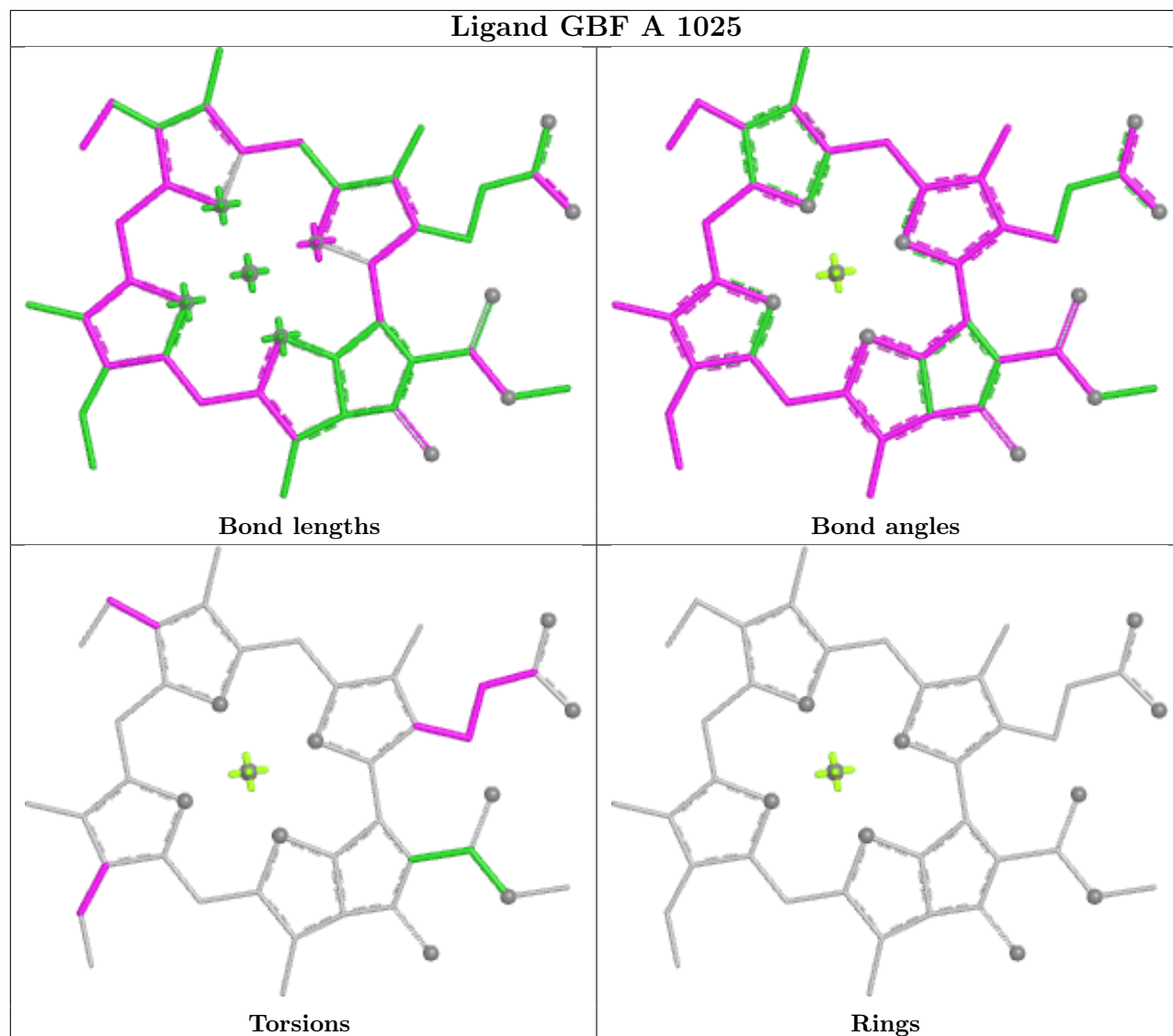
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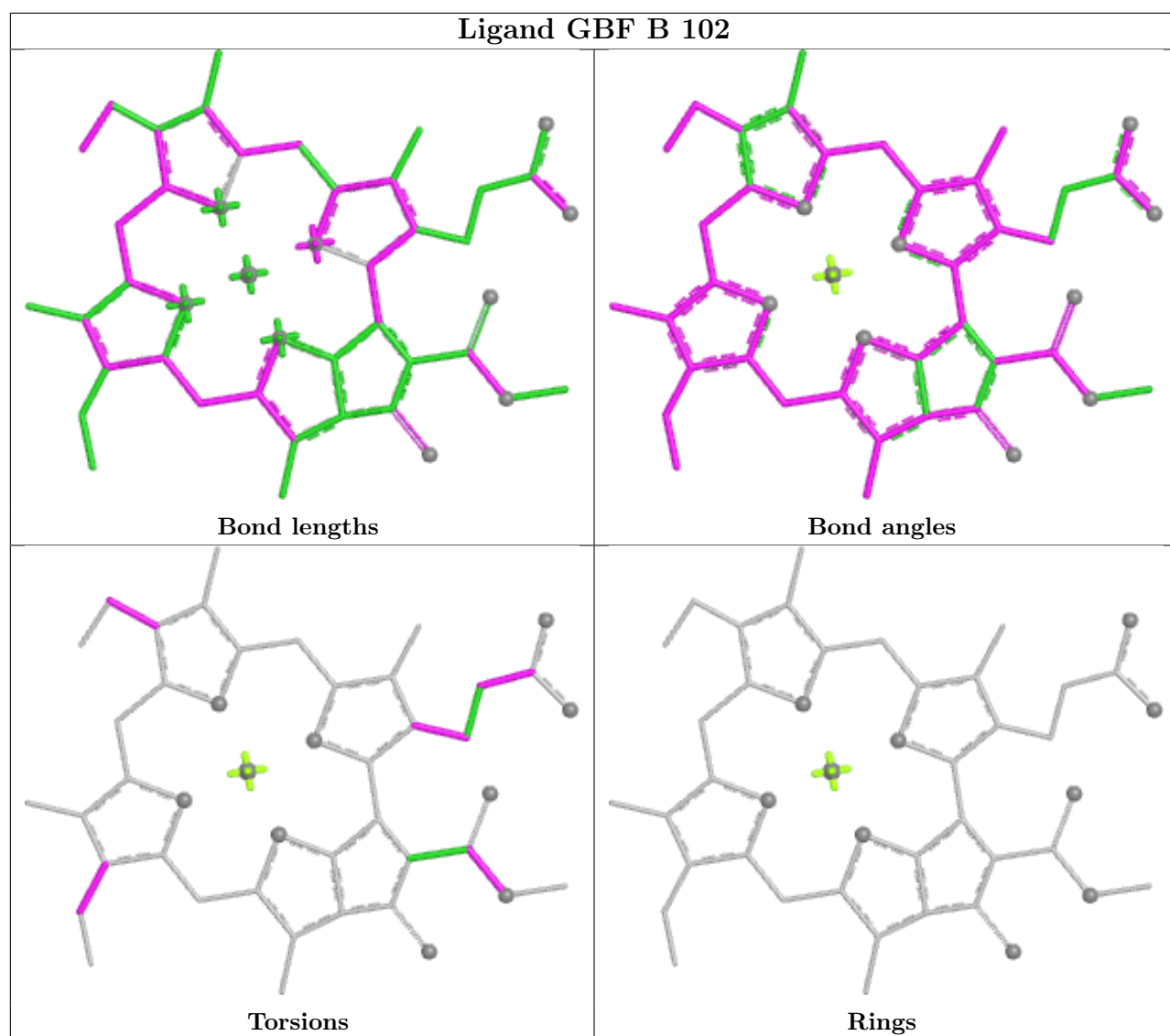
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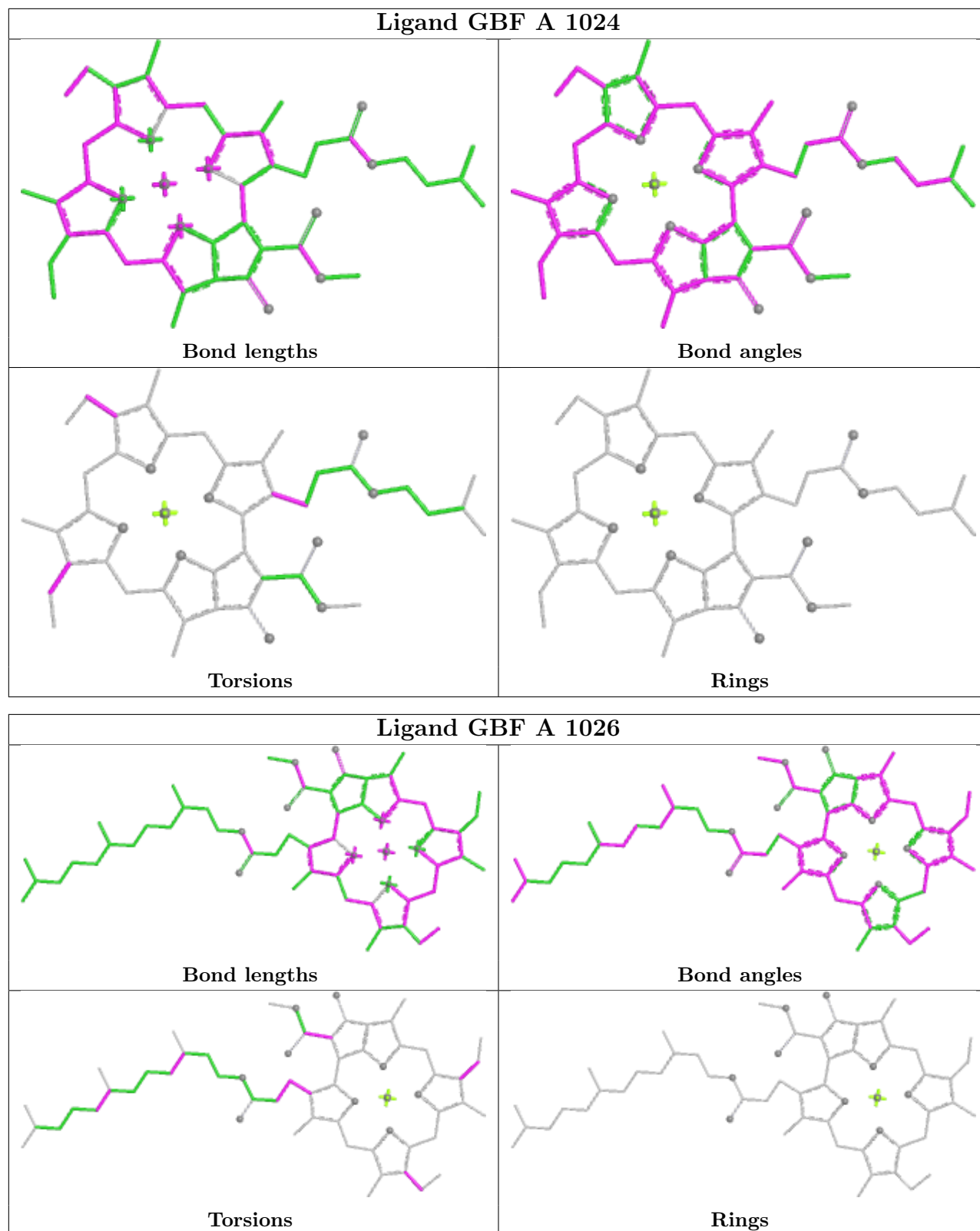
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1030	DGG	9	0

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.

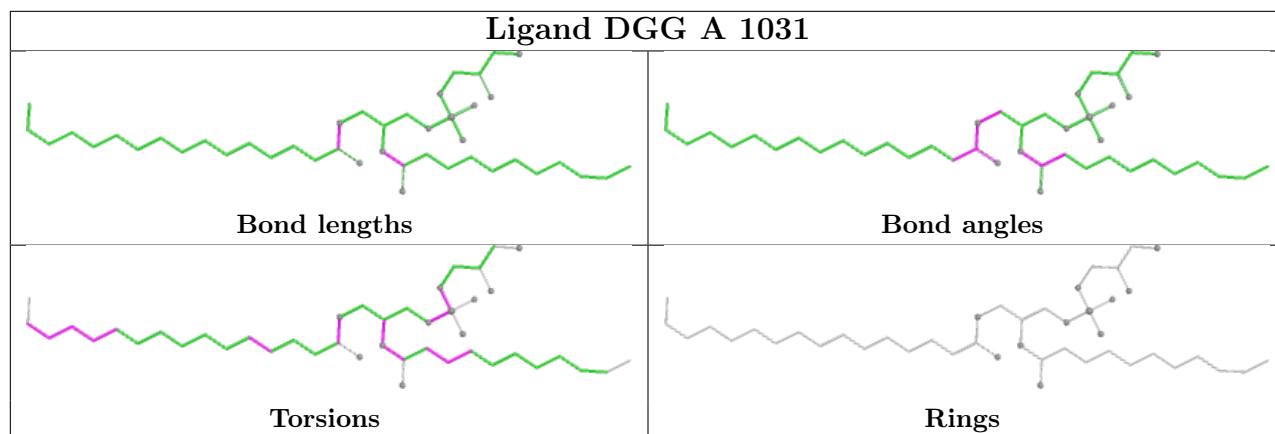




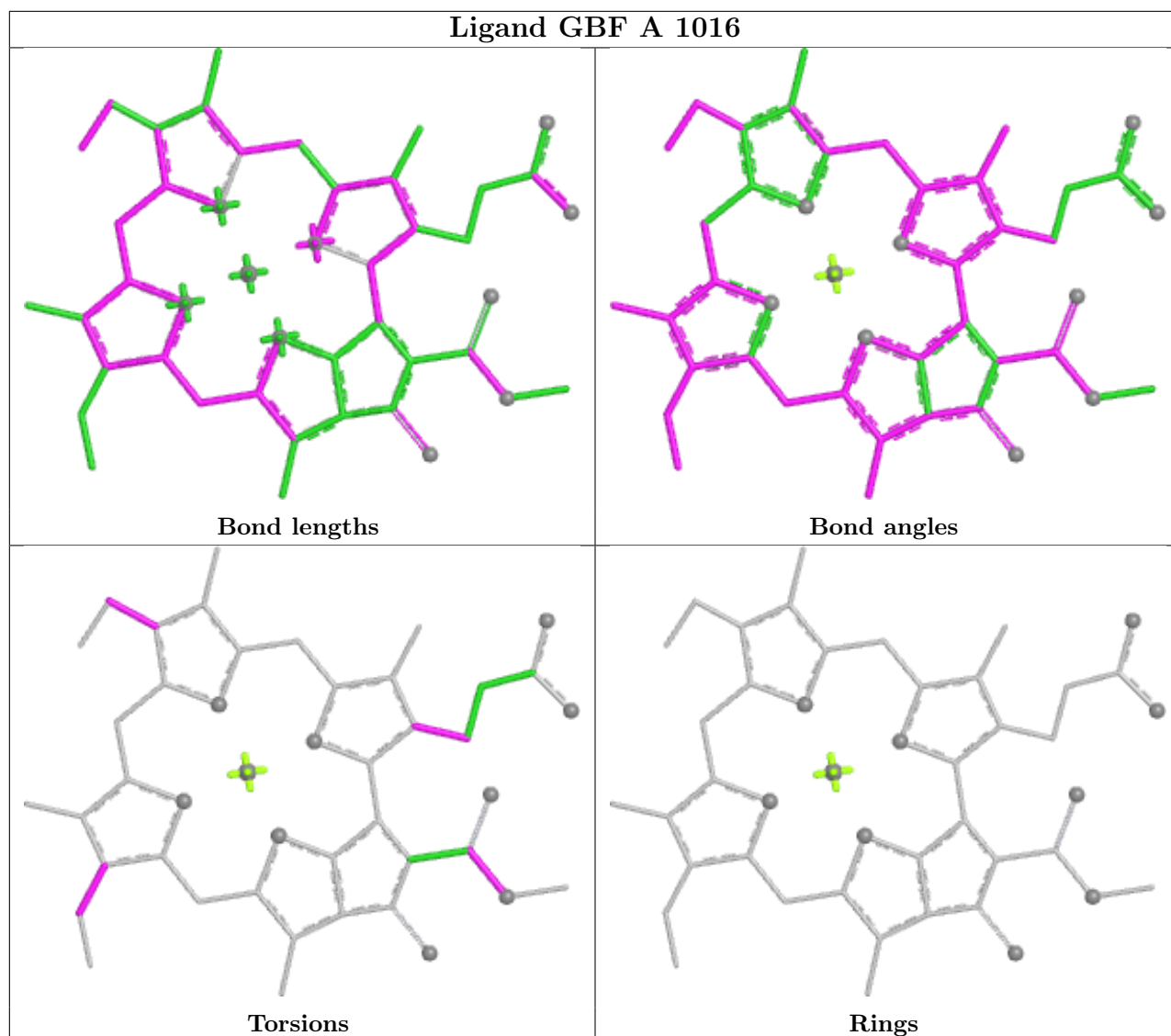




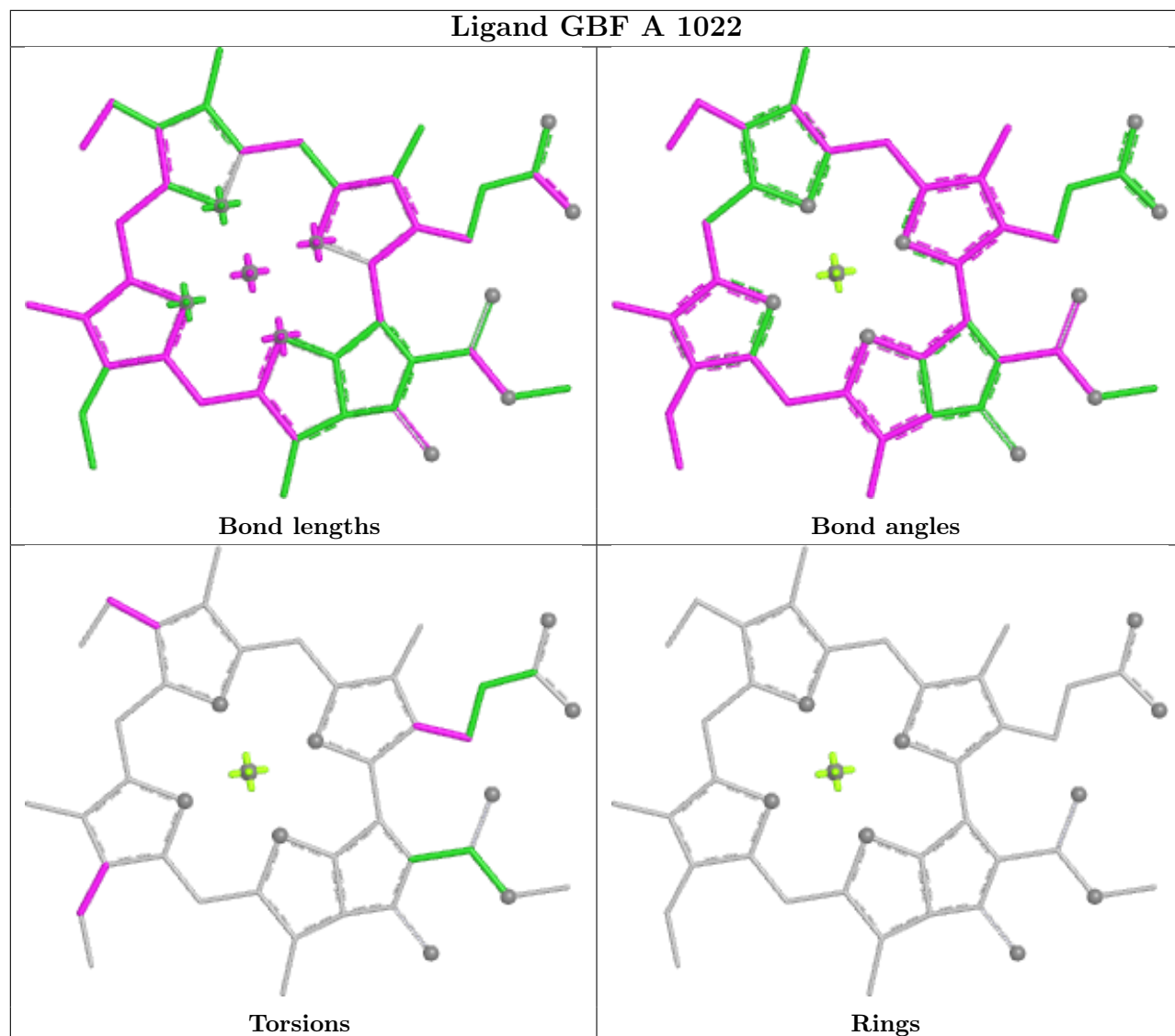
Ligand DGG A 1031

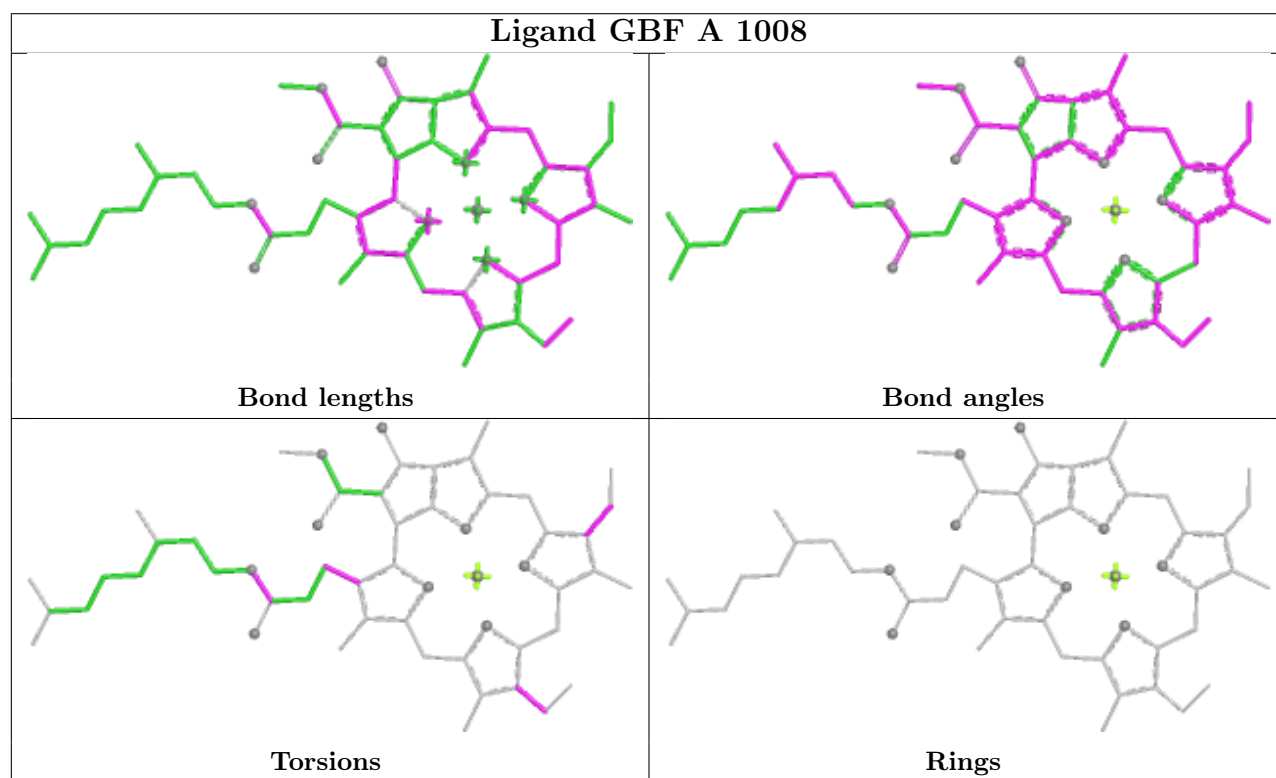
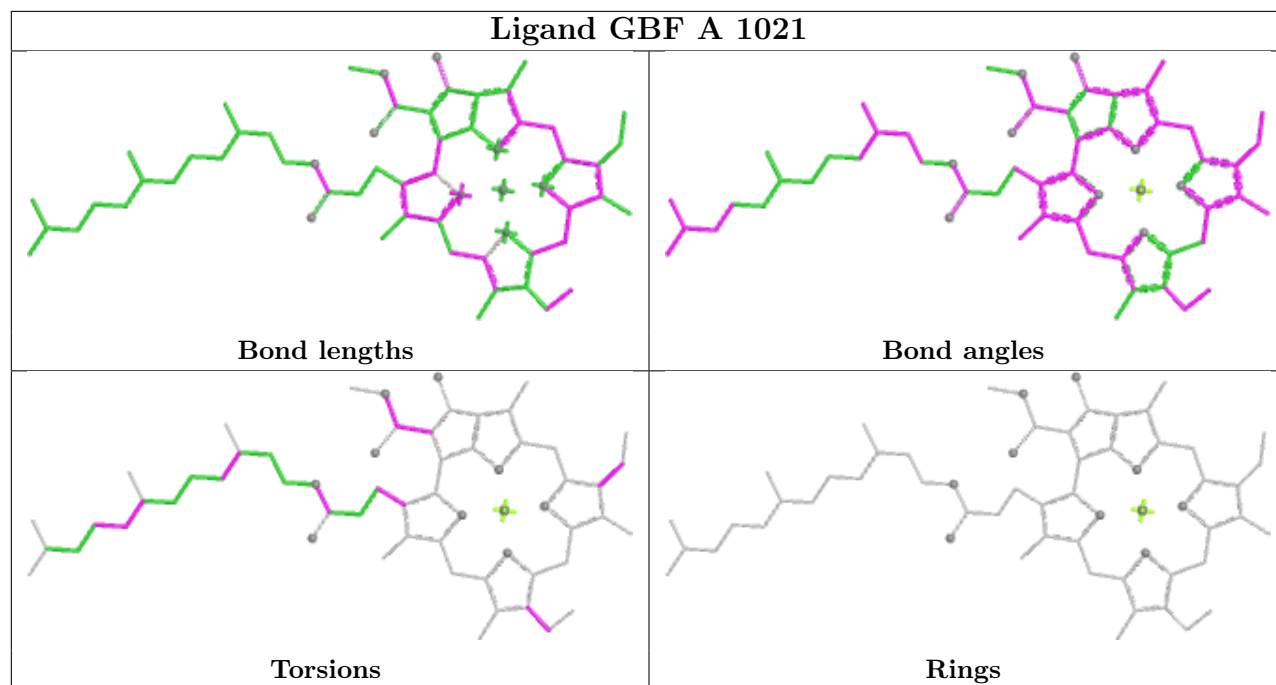


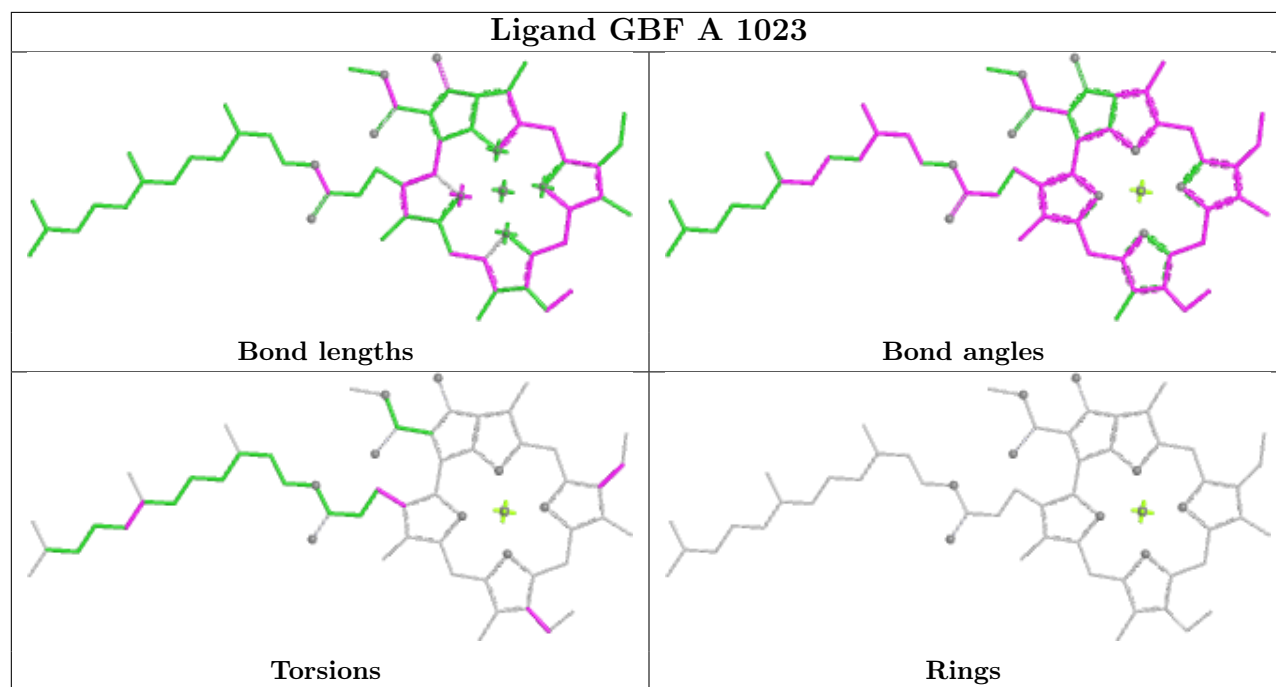
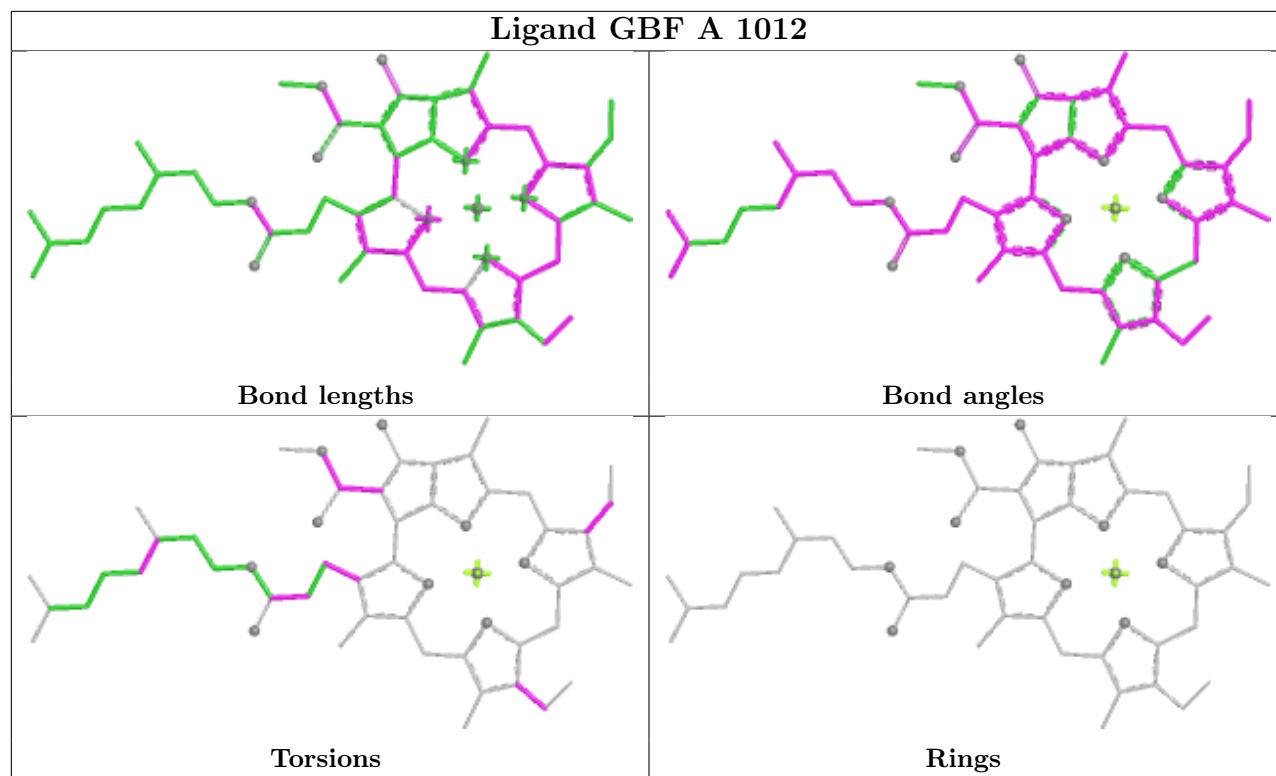
Ligand GBF A 1016



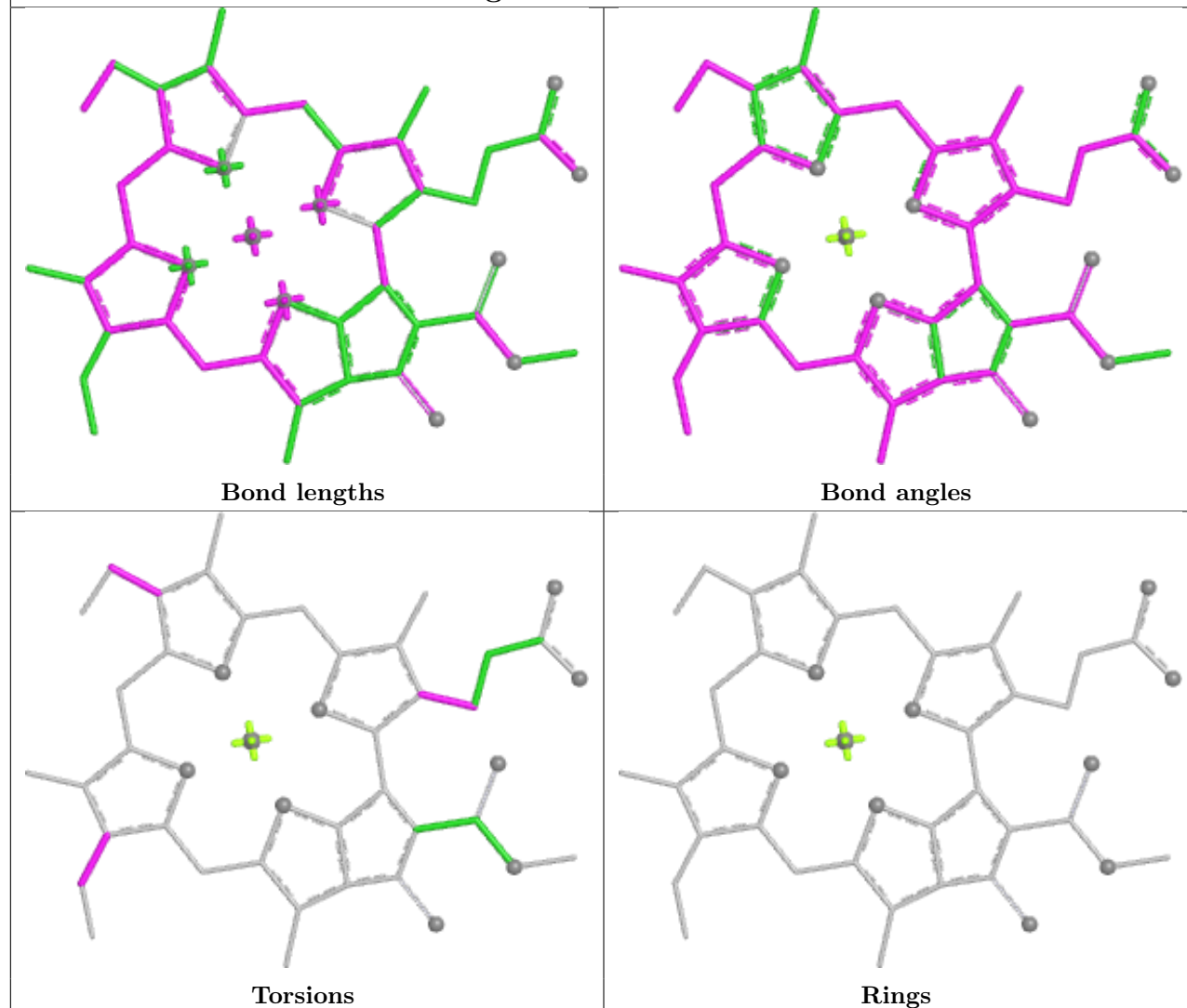
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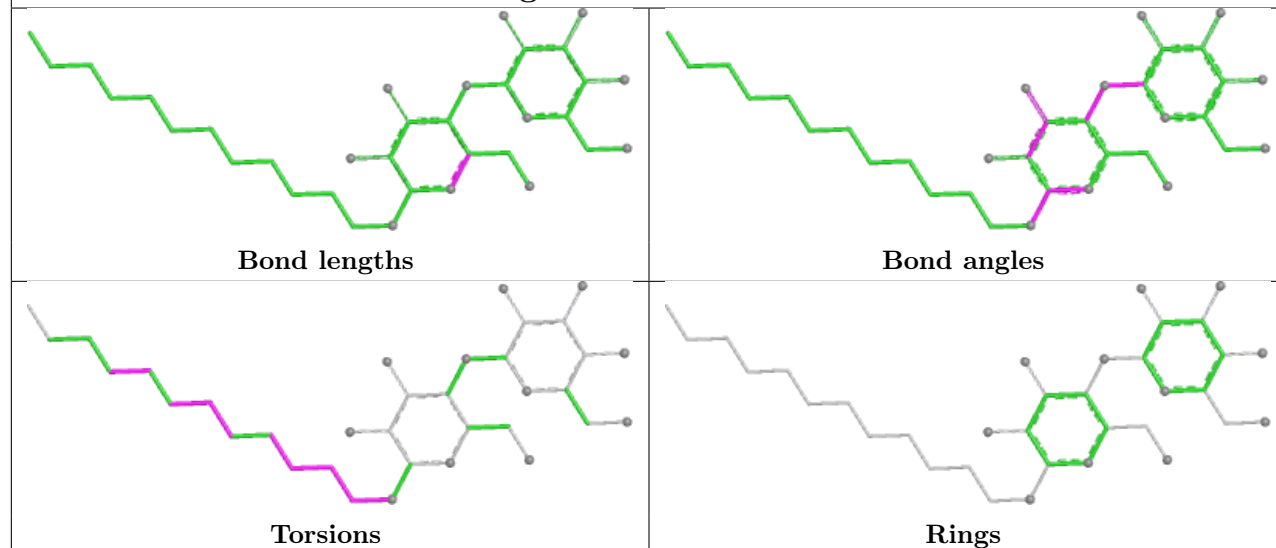




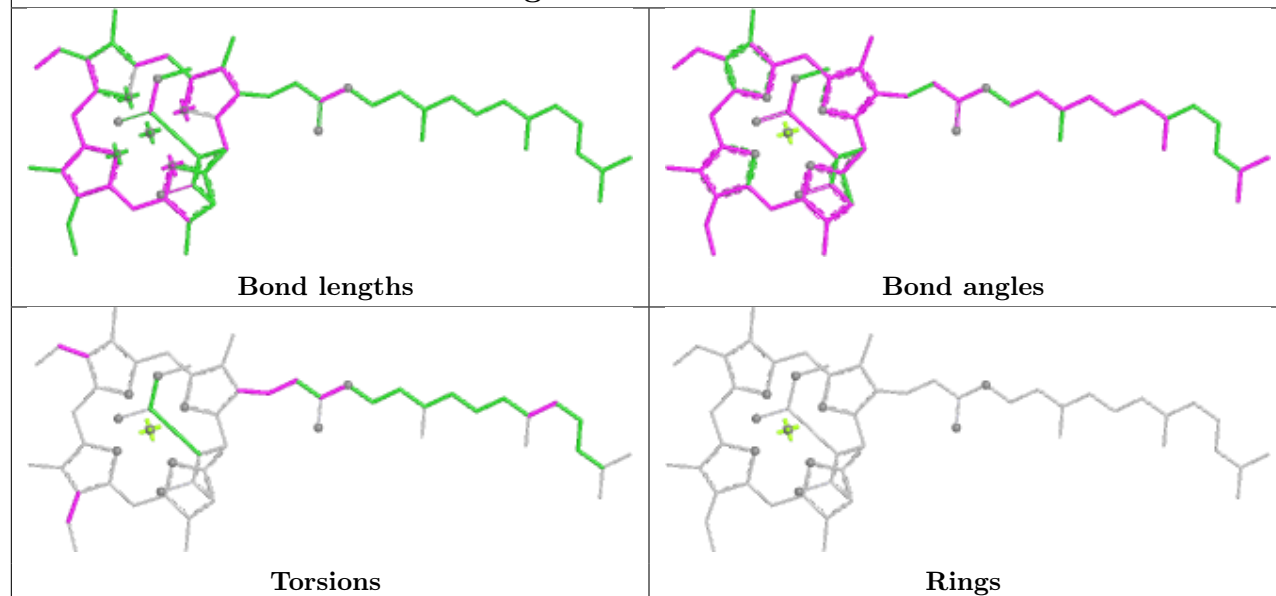
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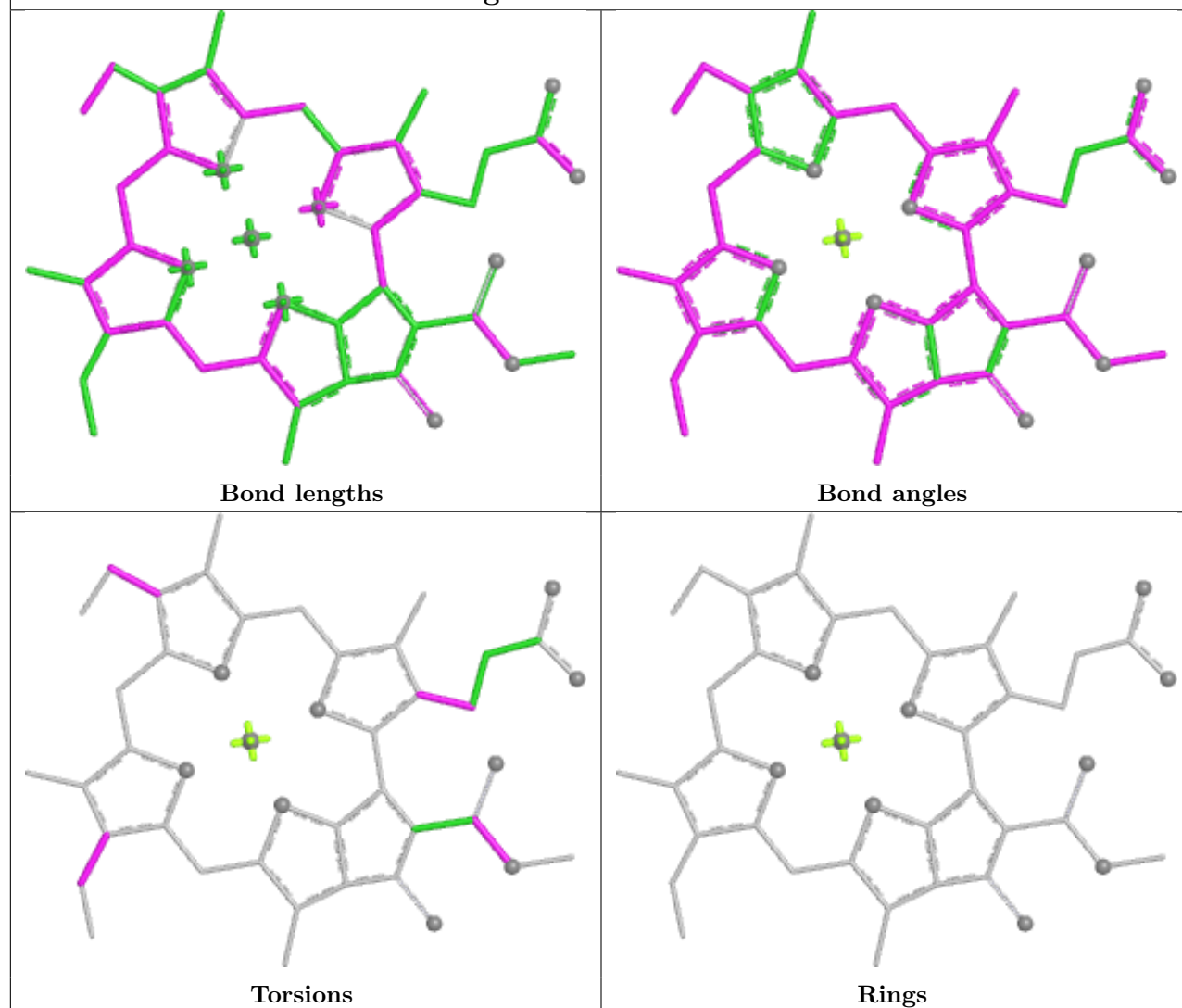
Ligand LMT A 1035

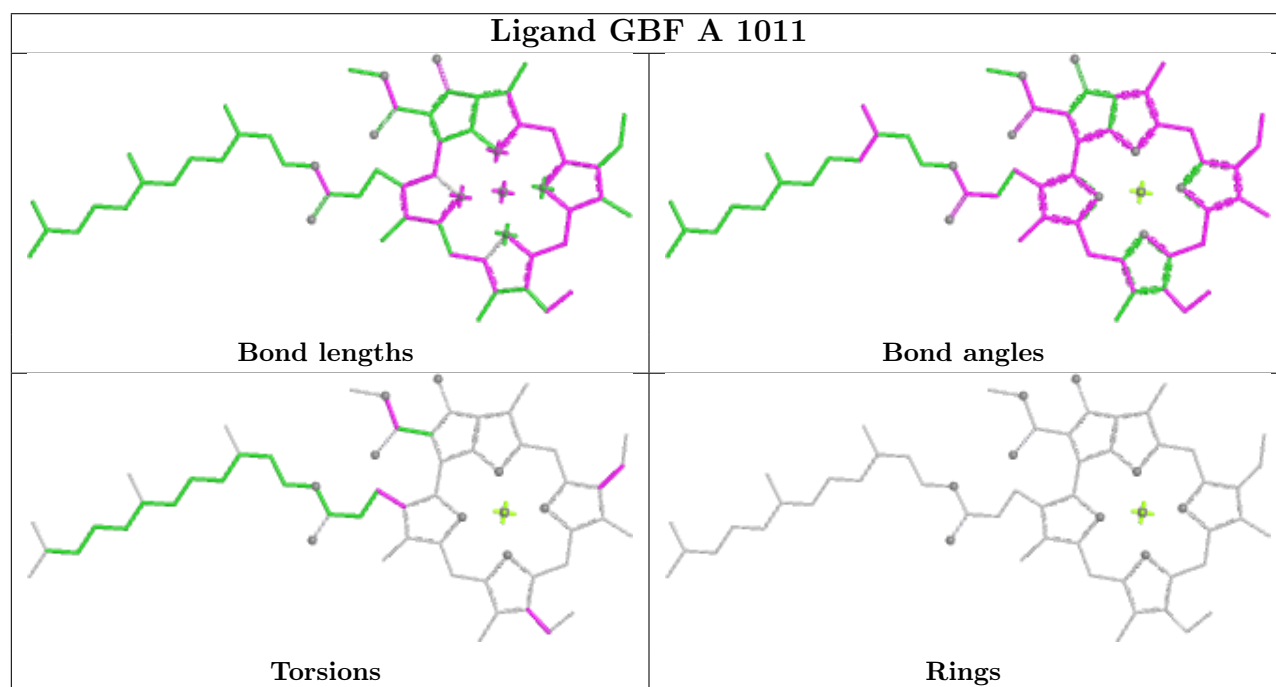
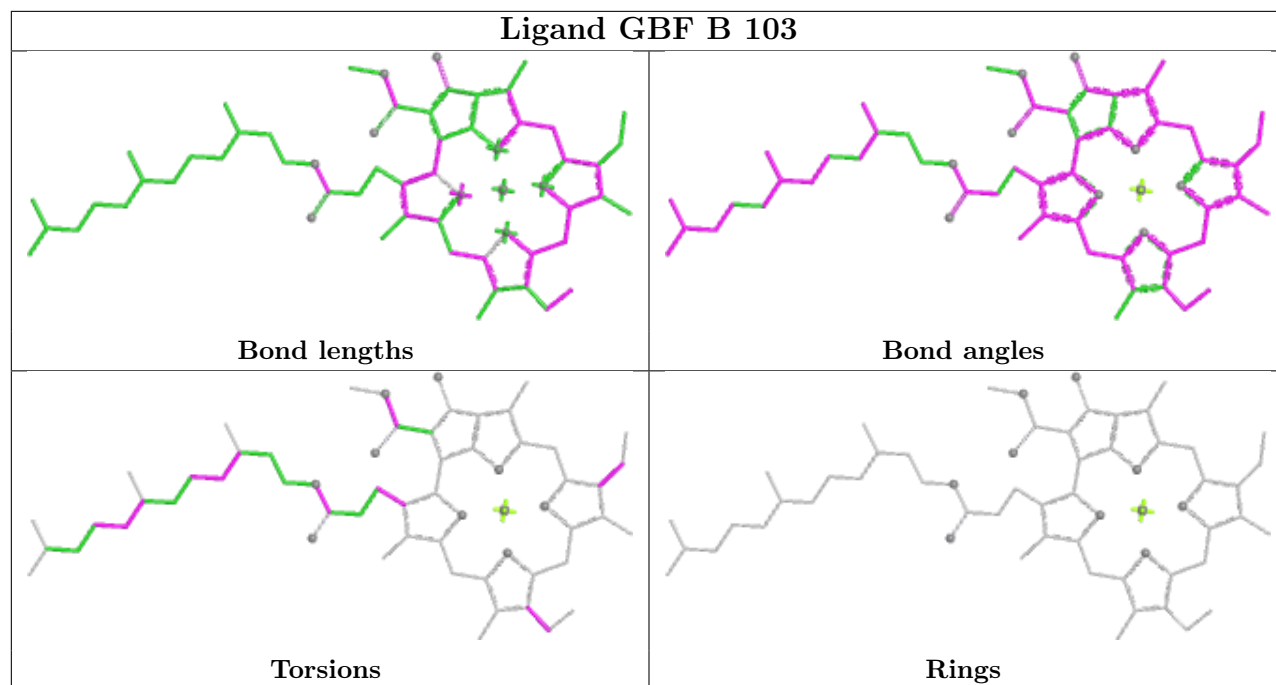


Ligand GB0 A 1005

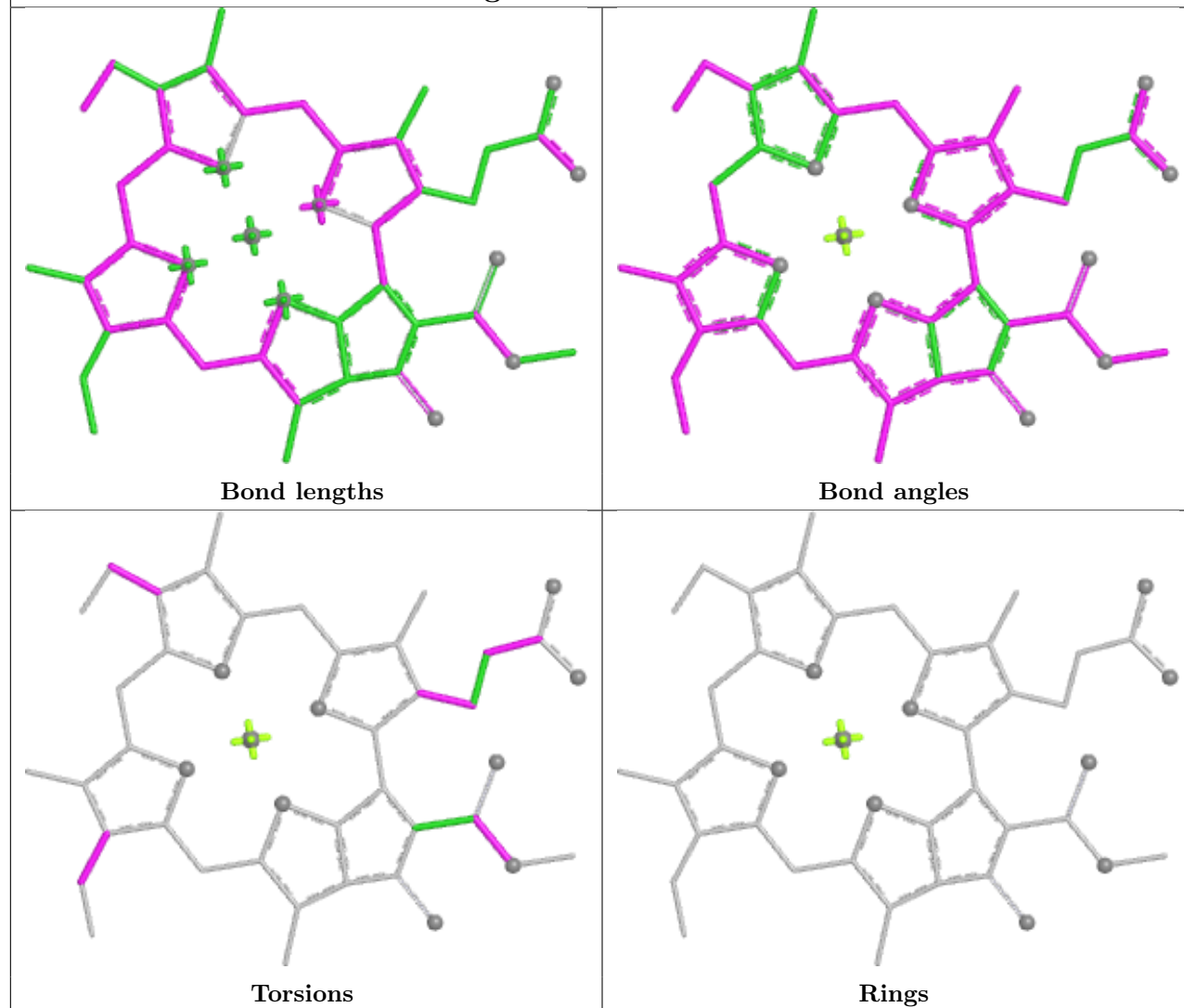


Ligand GBF A 1009

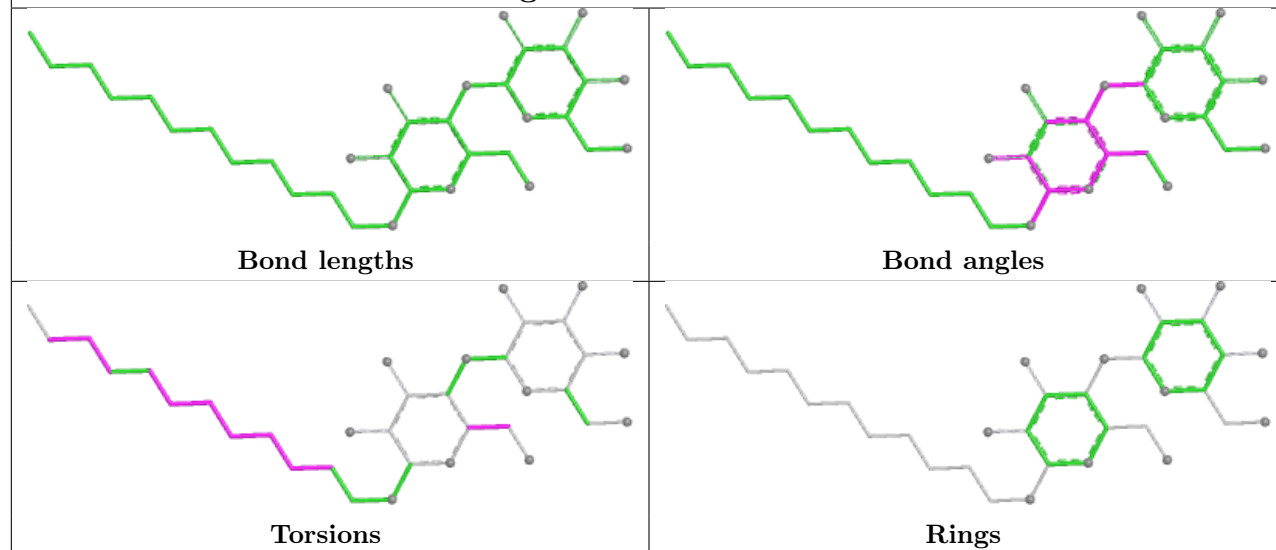


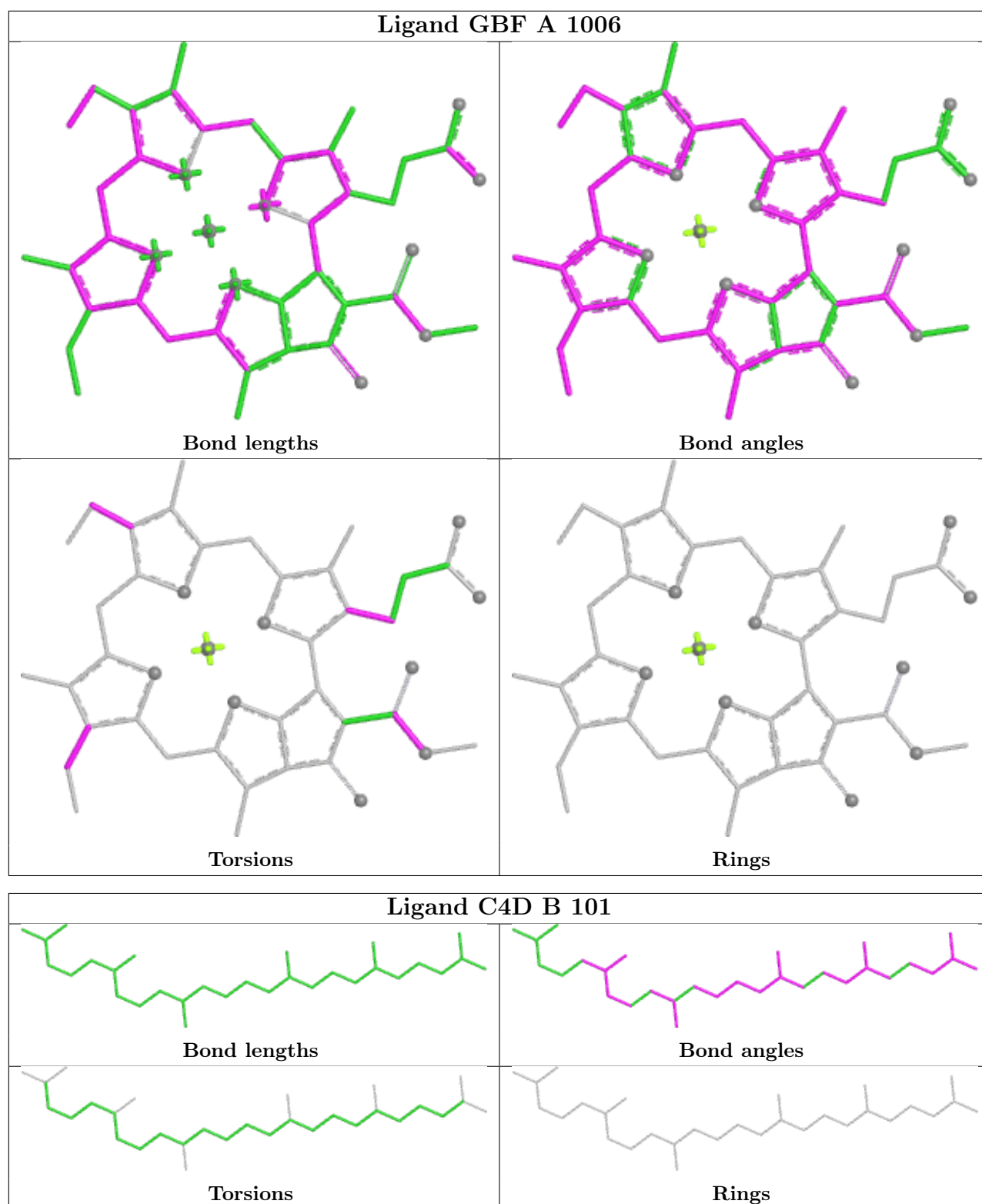


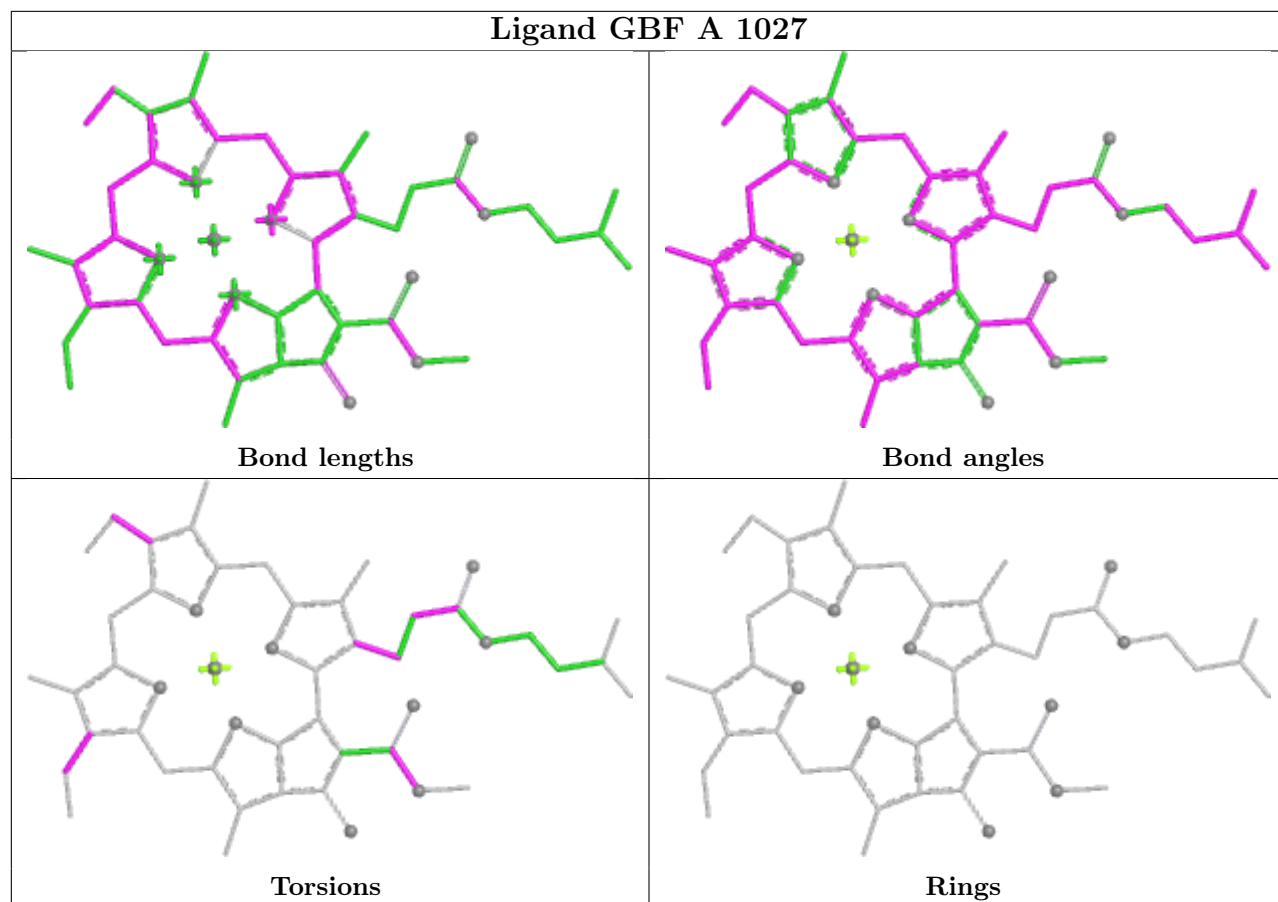
Ligand GBF A 1010



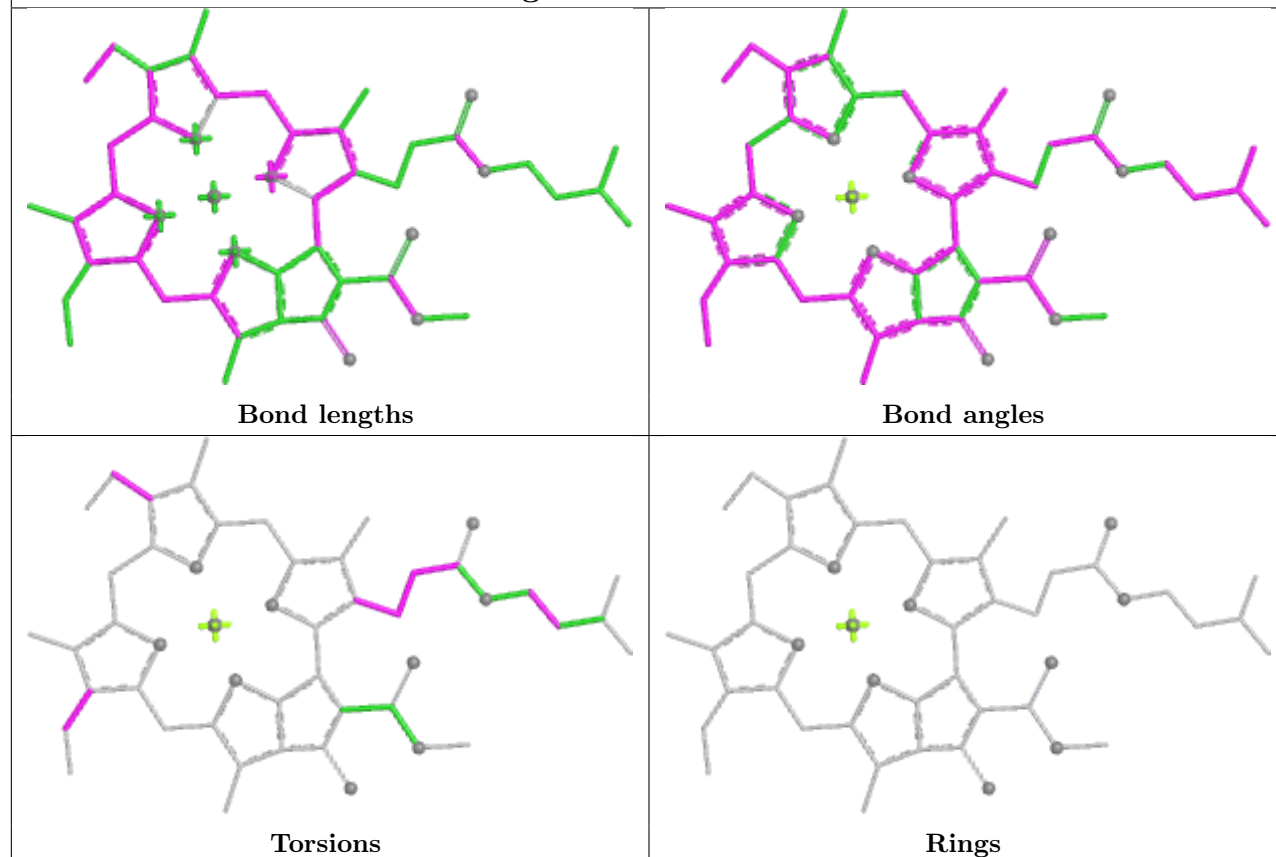
Ligand LMT A 1034



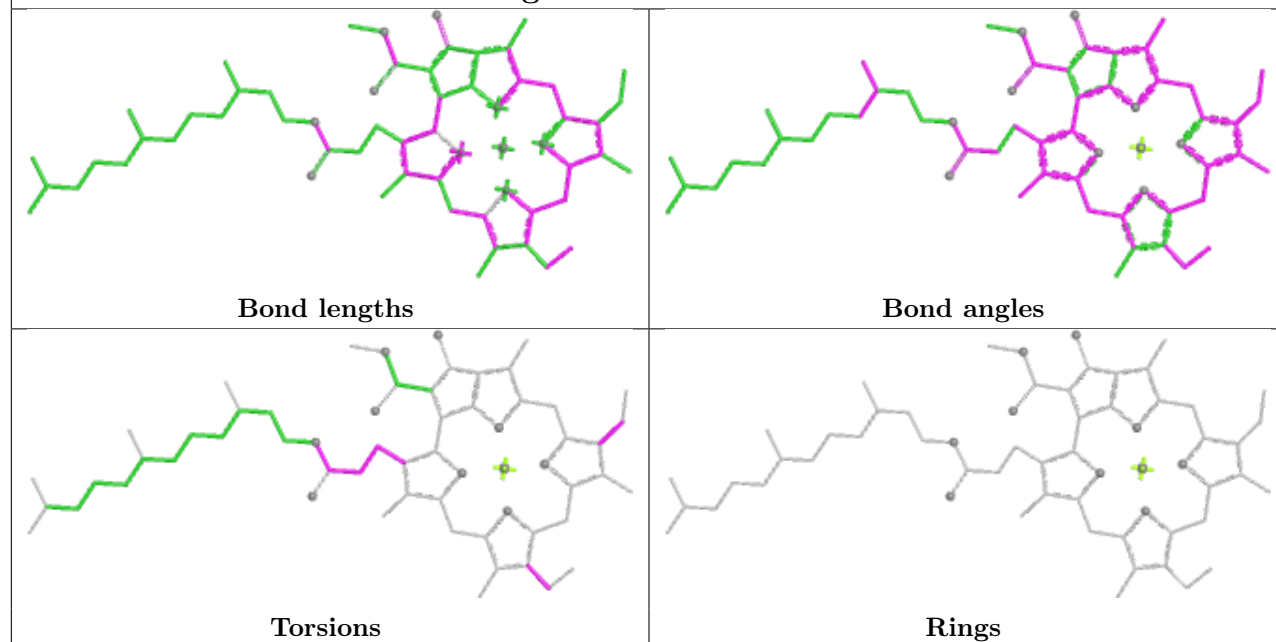


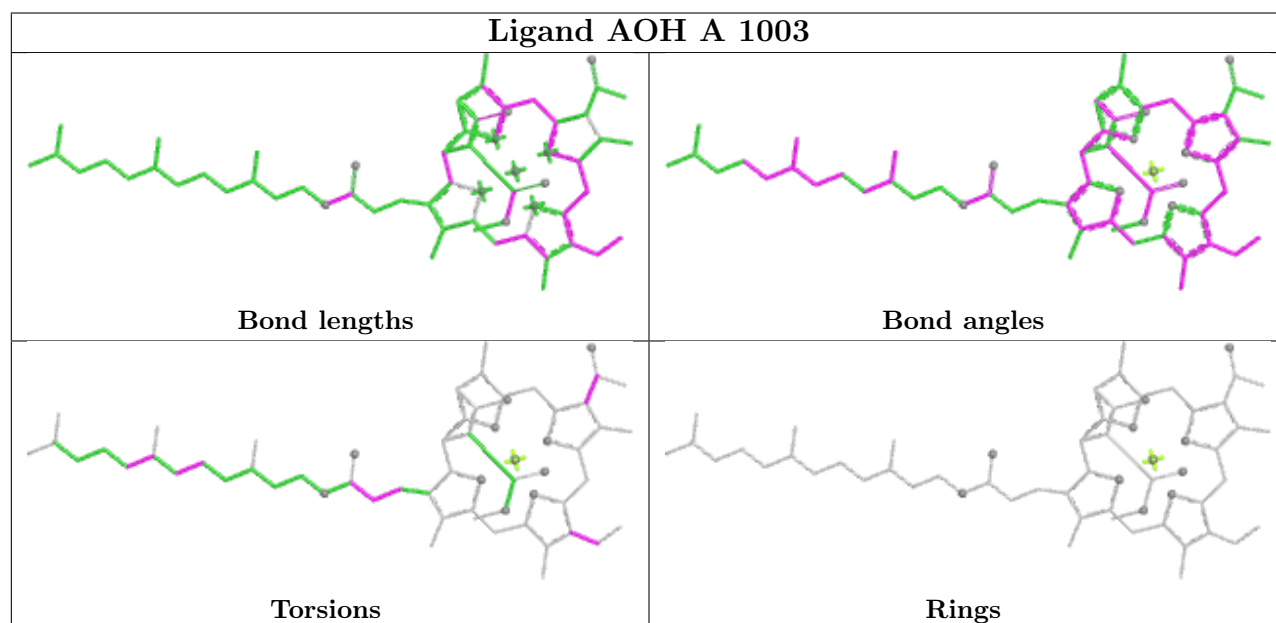
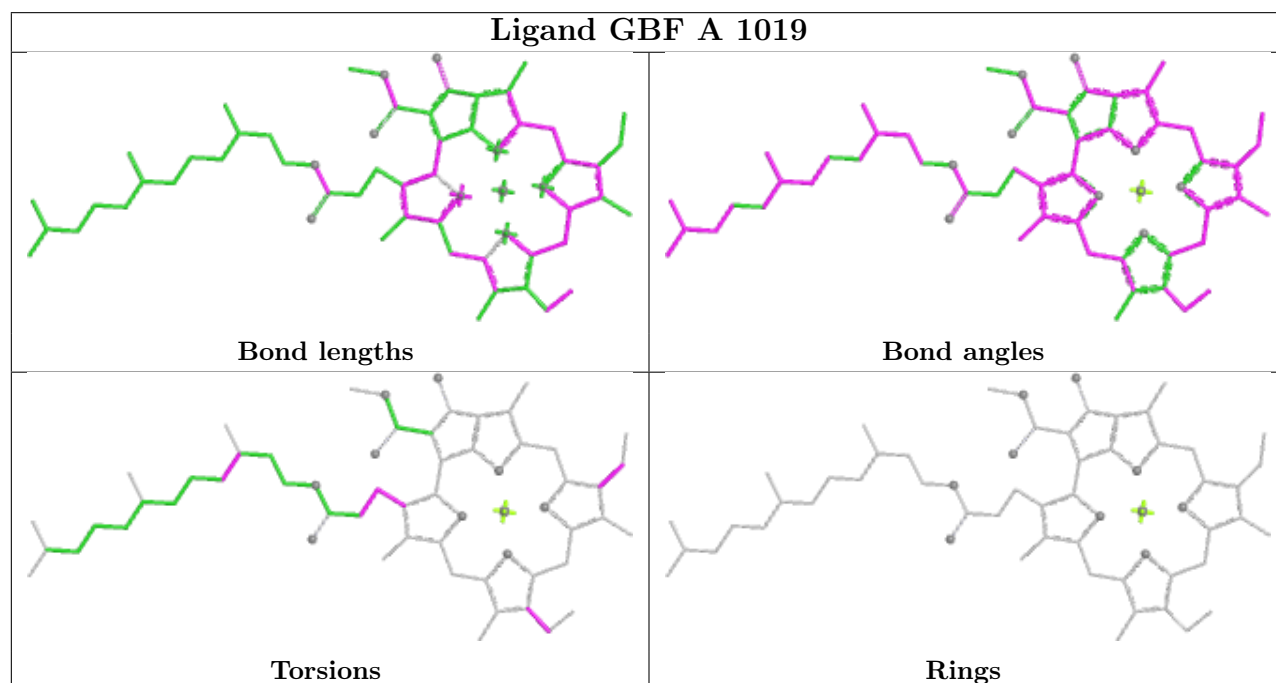
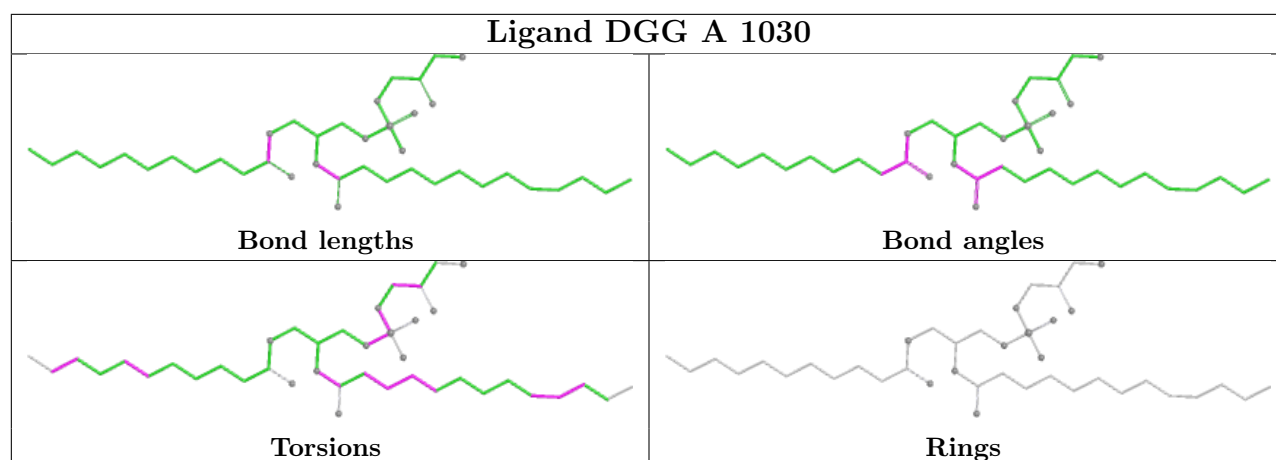


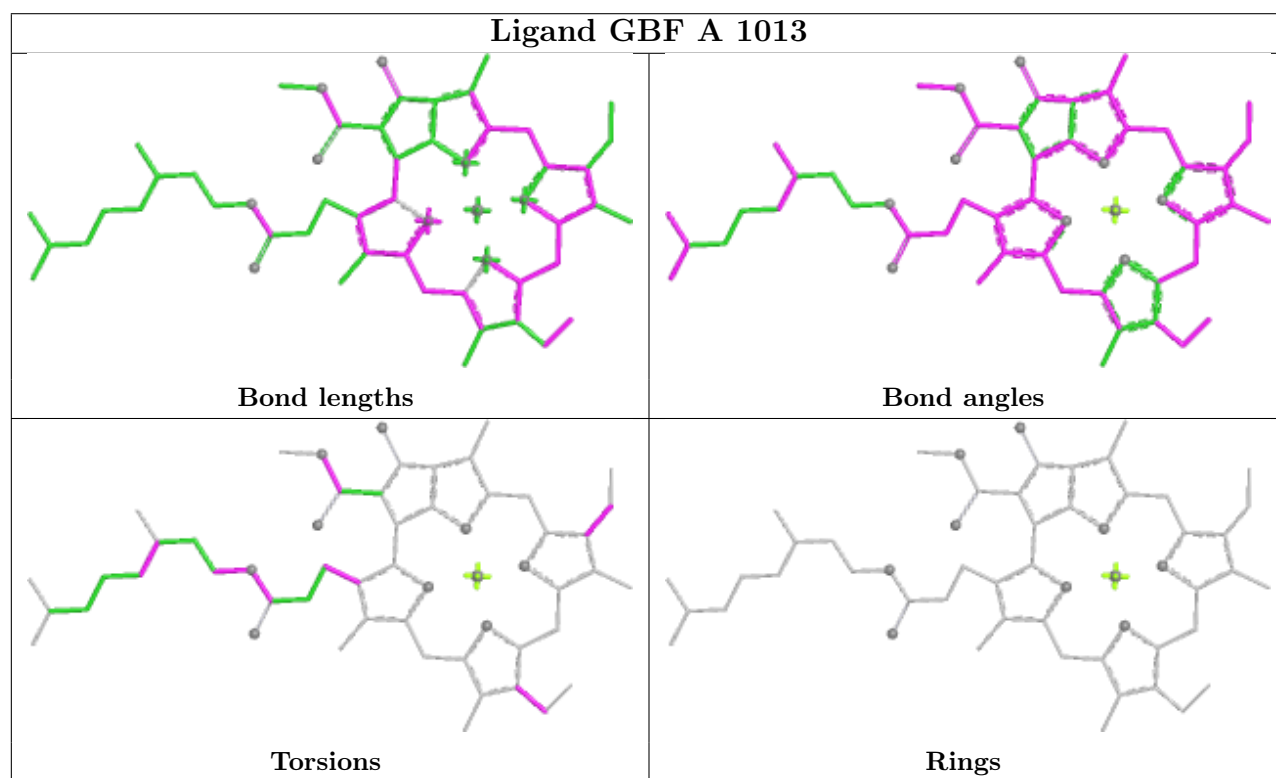
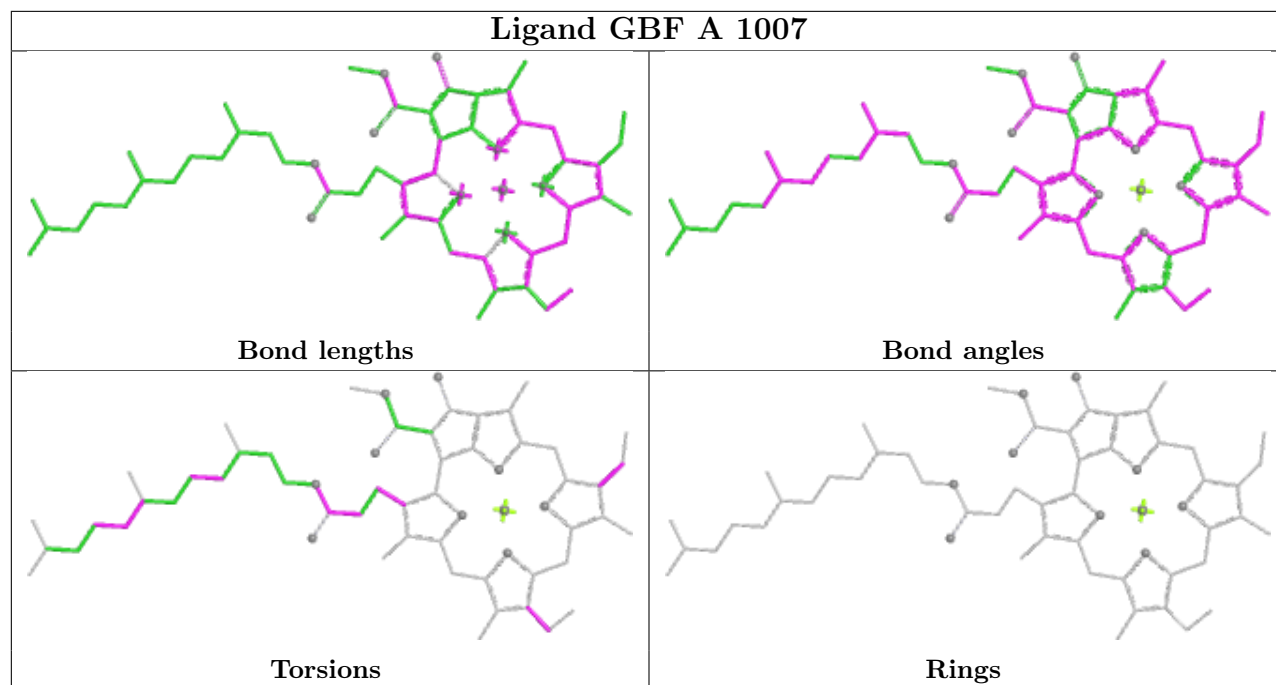
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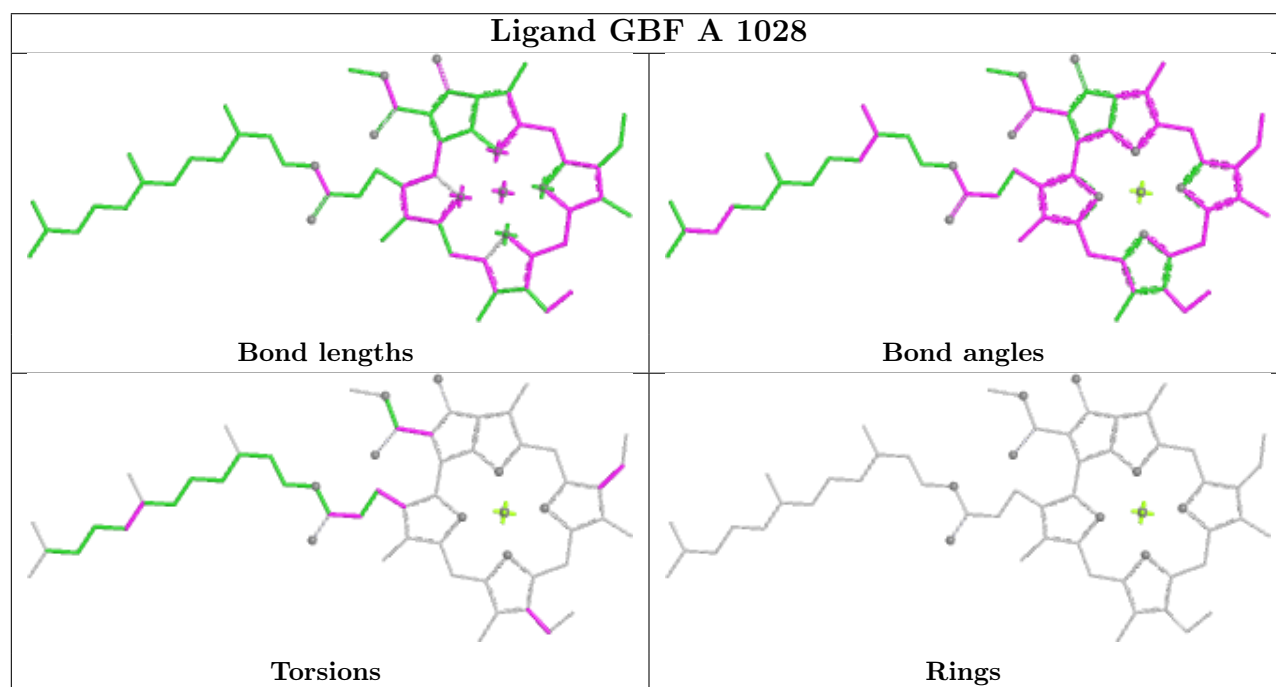
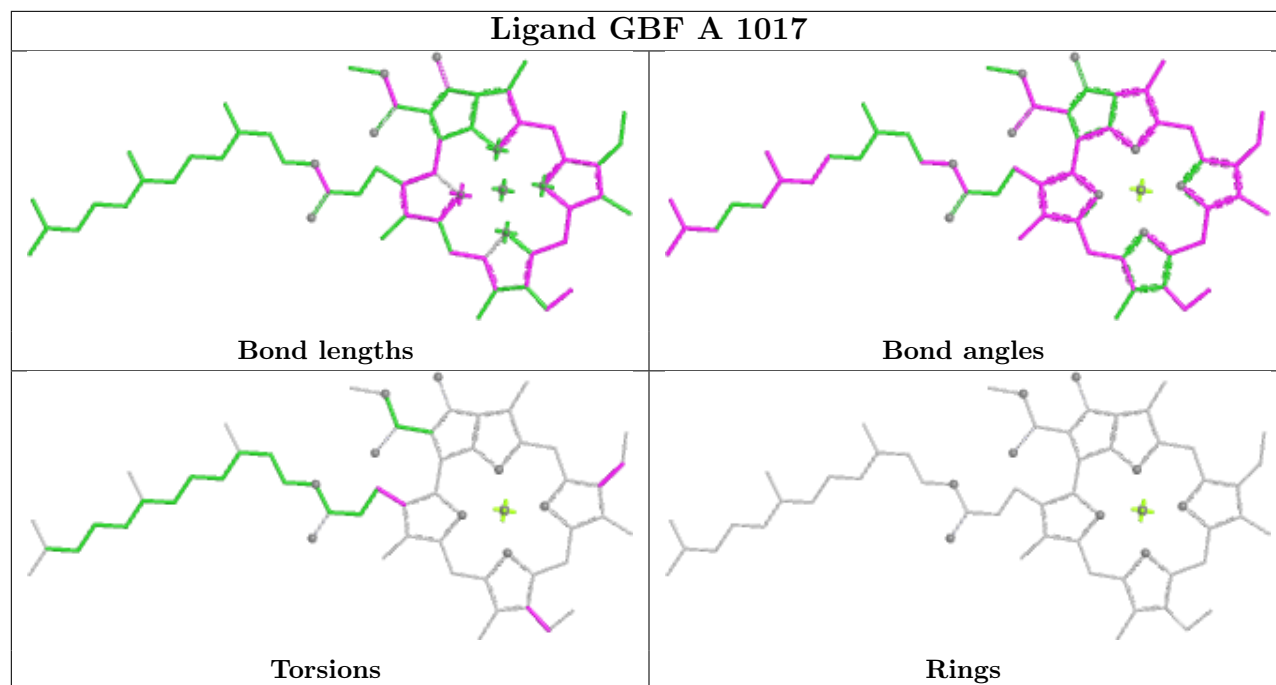


Ligand GBF A 1015

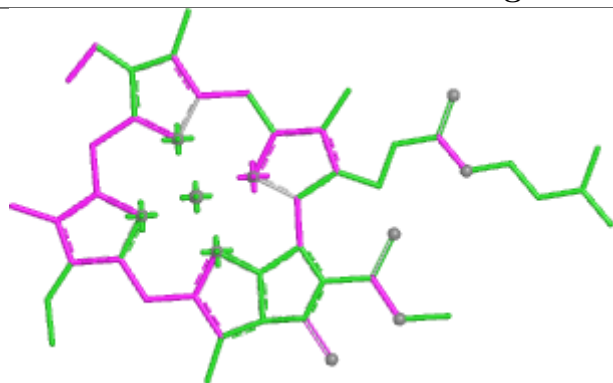




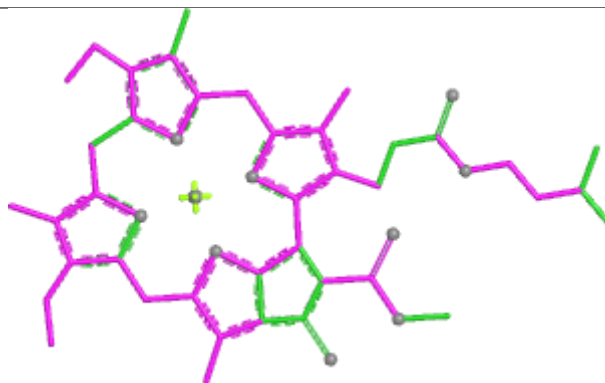




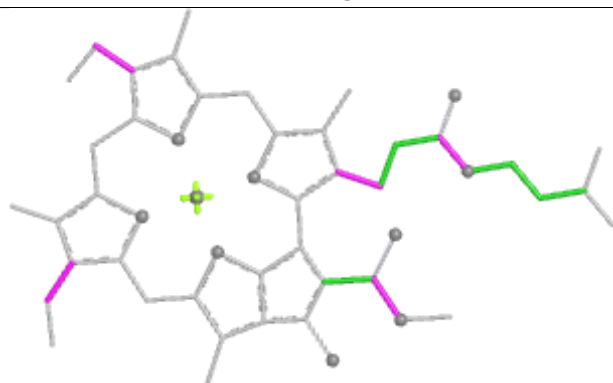
Ligand GBF A 1018



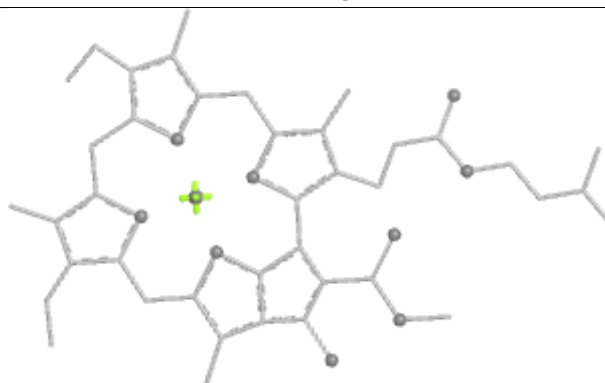
Bond lengths



Bond angles

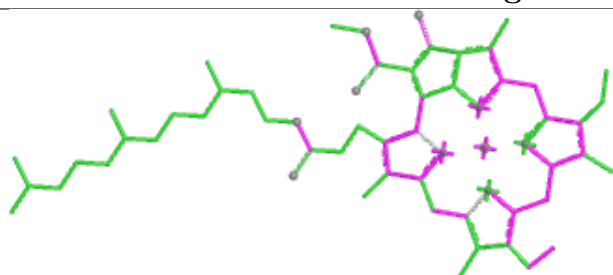


Torsions

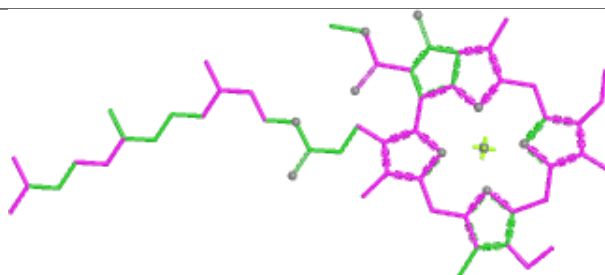


Rings

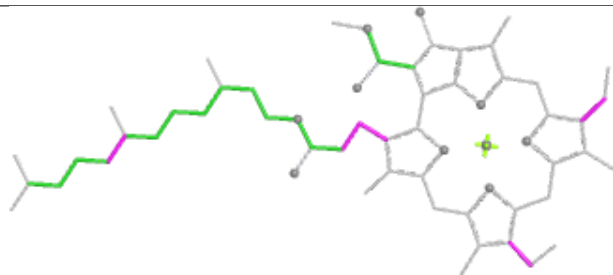
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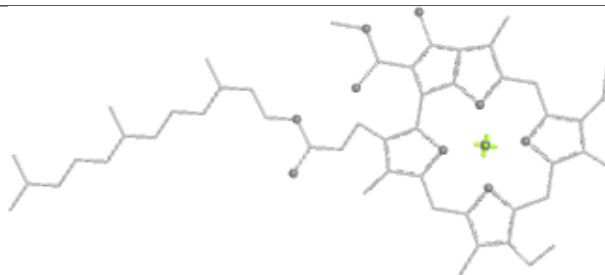
Bond lengths



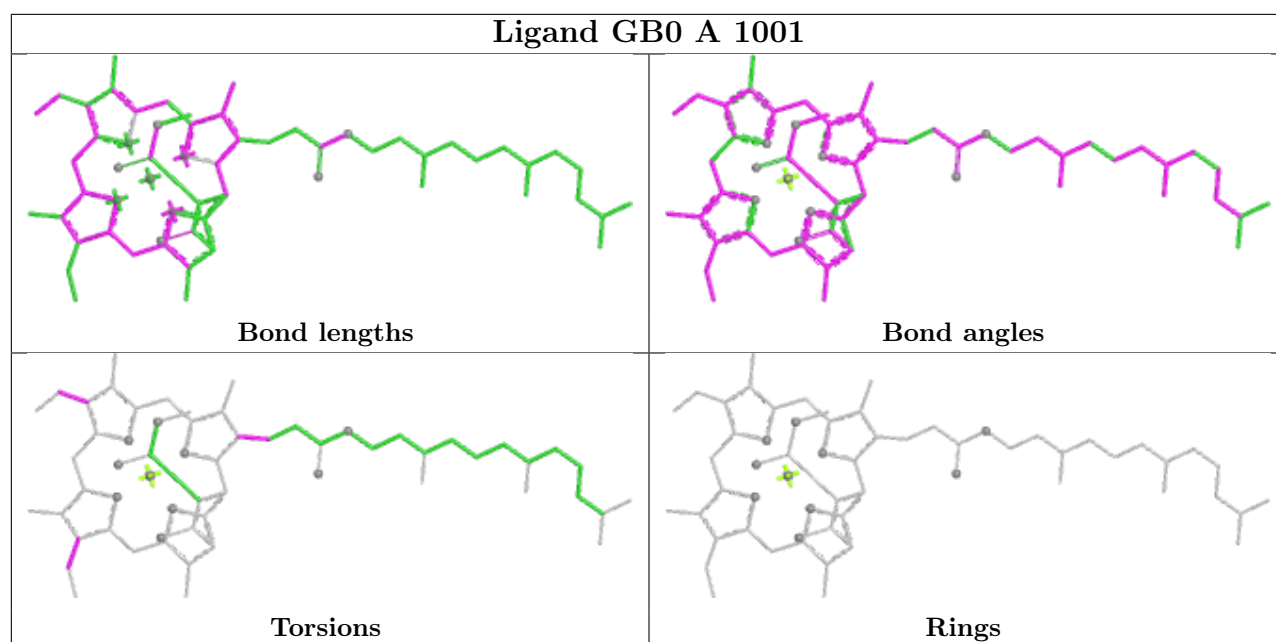
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	600/600 (100%)	-0.13	13 (2%) 62 59	29, 47, 80, 148	0
2	B	25/25 (100%)	1.57	6 (24%) 2 1	72, 77, 87, 92	0
All	All	625/625 (100%)	-0.06	19 (3%) 52 49	29, 48, 83, 148	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	PRO	4.9
1	A	304	ALA	4.8
1	A	305	GLU	4.5
1	A	303	LEU	4.5
2	B	24	ALA	3.4

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](#)

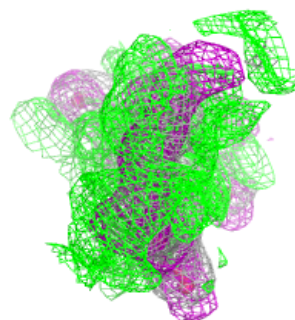
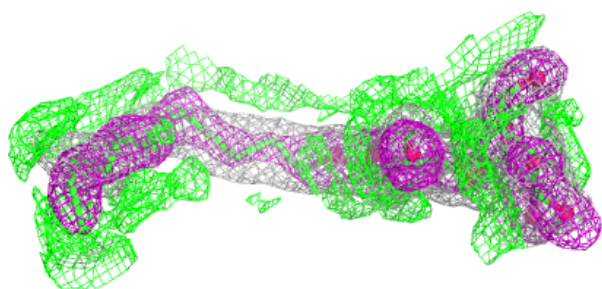
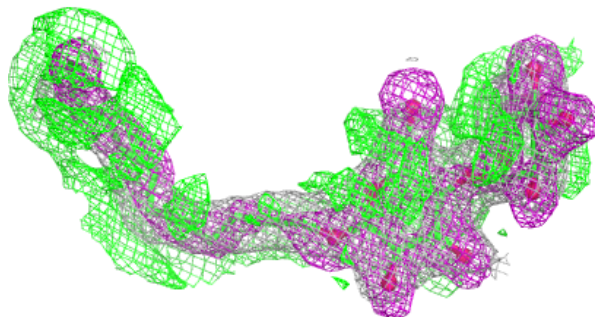
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
9	LMT	A	1034	35/35	0.78	0.14	20,20,20,20	0
4	GBF	B	103	60/60	0.79	0.15	68,82,96,98	0
7	DGG	A	1031	44/50	0.80	0.18	73,95,109,115	0
7	DGG	A	1030	41/50	0.82	0.17	56,73,102,102	0
9	LMT	A	1035	35/35	0.82	0.13	20,20,20,20	0
4	GBF	B	102	45/60	0.83	0.17	69,97,105,109	0
4	GBF	A	1009	45/60	0.84	0.17	70,98,105,110	0
4	GBF	A	1028	60/60	0.86	0.13	46,61,75,77	0
4	GBF	A	1010	45/60	0.90	0.12	54,66,103,105	0
4	GBF	A	1013	55/60	0.91	0.12	49,61,77,85	0
4	GBF	A	1016	45/60	0.91	0.10	53,67,97,107	0
4	GBF	A	1012	55/60	0.91	0.14	61,71,93,97	0
10	C4D	B	101	30/30	0.91	0.10	39,58,65,69	0
4	GBF	A	1007	60/60	0.93	0.11	38,57,95,97	0
4	GBF	A	1011	60/60	0.94	0.11	49,61,77,79	0
4	GBF	A	1014	45/60	0.94	0.09	50,58,83,102	0
4	GBF	A	1008	55/60	0.94	0.10	43,51,81,83	0
4	GBF	A	1018	50/60	0.94	0.10	41,50,79,79	0
4	GBF	A	1027	50/60	0.95	0.08	36,47,75,81	0
4	GBF	A	1002	60/60	0.95	0.09	25,33,57,67	0
4	GBF	A	1006	45/60	0.95	0.10	43,53,80,94	0
3	GB0	A	1005	60/60	0.95	0.09	35,47,90,91	0
5	AOH	A	1003	61/61	0.95	0.08	26,37,56,58	0
4	GBF	A	1019	60/60	0.95	0.10	43,52,94,96	0
4	GBF	A	1021	60/60	0.95	0.09	35,43,92,98	0
4	GBF	A	1022	45/60	0.95	0.08	36,45,67,90	0
4	GBF	A	1023	60/60	0.95	0.08	35,42,57,60	0
4	GBF	A	1024	50/60	0.95	0.09	41,49,82,85	0
4	GBF	A	1025	45/60	0.96	0.09	43,51,86,103	0
4	GBF	A	1026	60/60	0.96	0.08	27,38,75,77	0
4	GBF	A	1017	60/60	0.96	0.08	40,53,60,63	0
8	CA	A	1032	1/1	0.96	0.05	39,39,39,39	0
8	CA	A	1033	1/1	0.96	0.22	84,84,84,84	0
4	GBF	A	1015	60/60	0.96	0.08	39,48,53,57	0
4	GBF	A	1004	50/60	0.96	0.08	39,47,56,58	0
4	GBF	A	1020	60/60	0.96	0.08	33,43,65,72	0
3	GB0	A	1001	60/60	0.97	0.06	25,33,39,42	0
6	SF4	A	1029	8/8	0.99	0.08	38,42,42,43	8

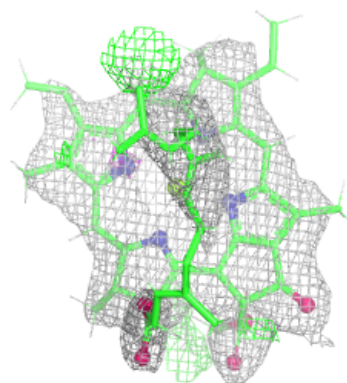
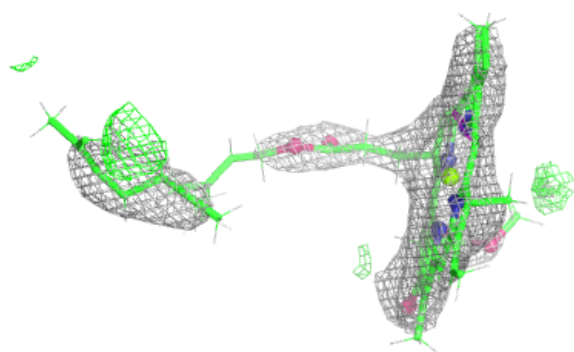
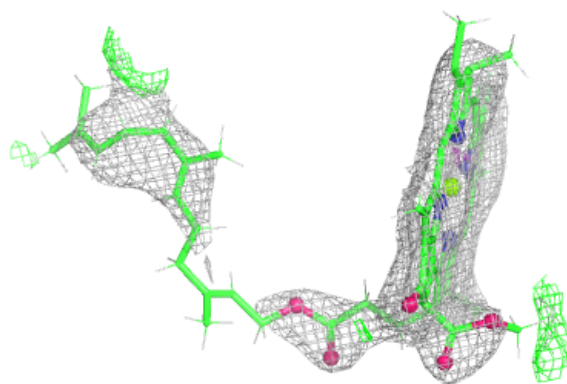
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 1034:

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

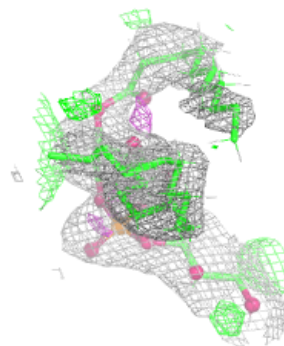
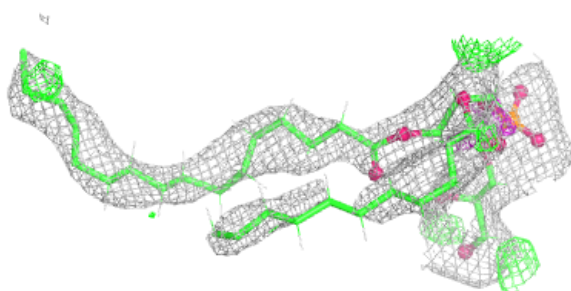
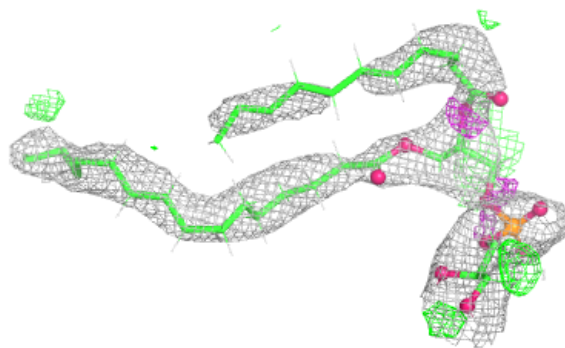
**Electron density around GBF B 103:**

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

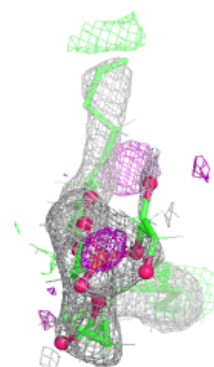
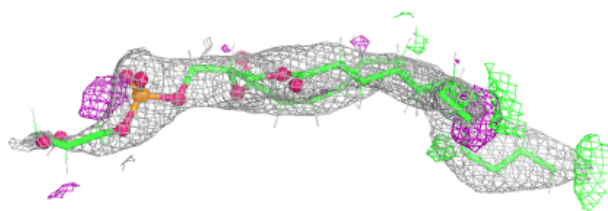
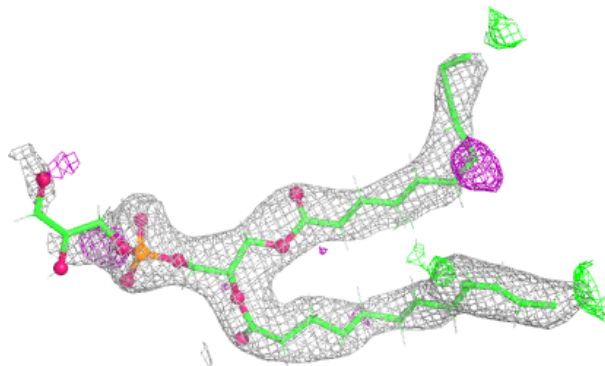


Electron density around DGG A 1031:

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

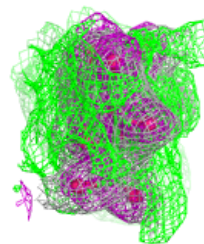
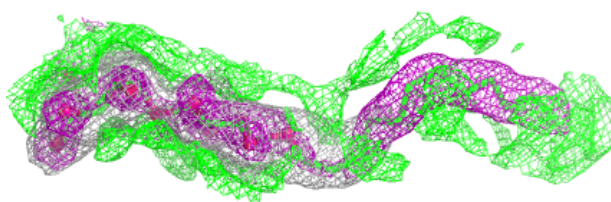
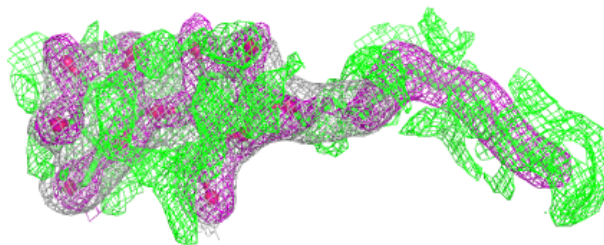
**Electron density around DGG A 1030:**

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



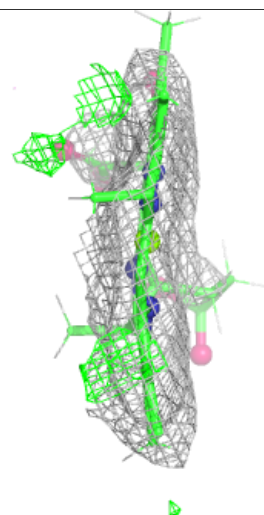
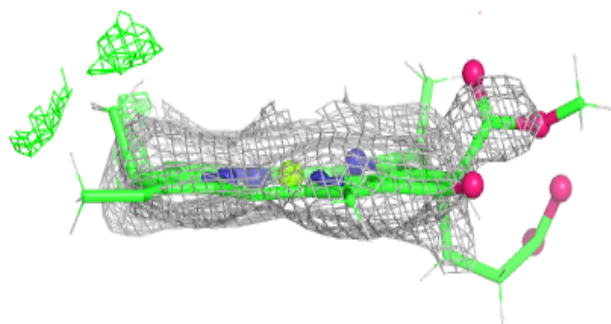
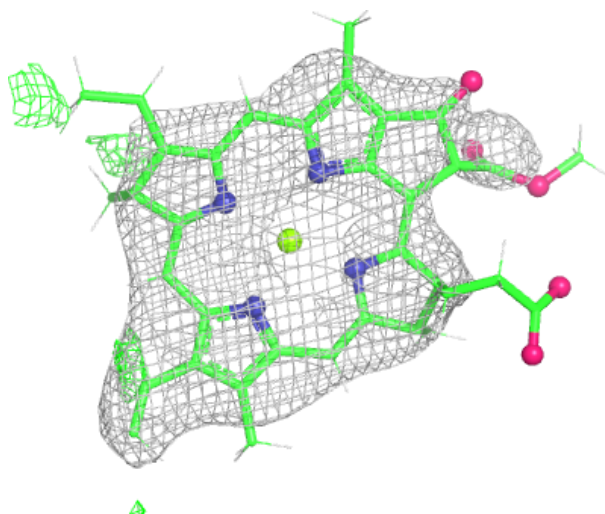
Electron density around LMT A 1035:

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



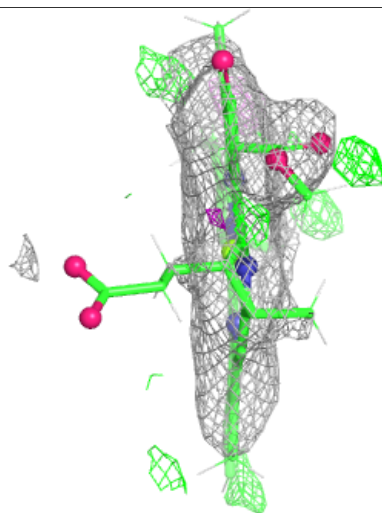
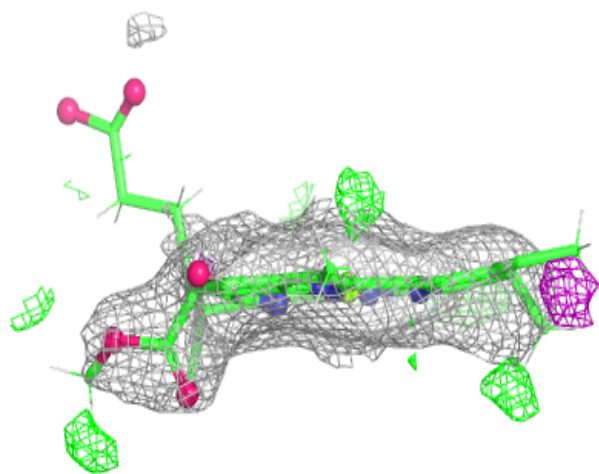
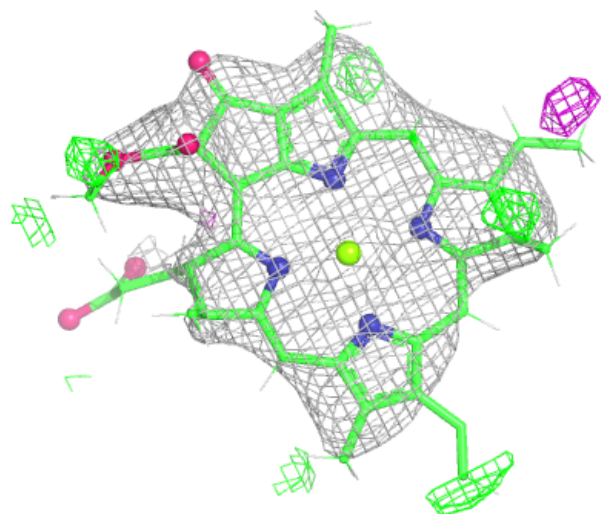
Electron density around GBF B 102:

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



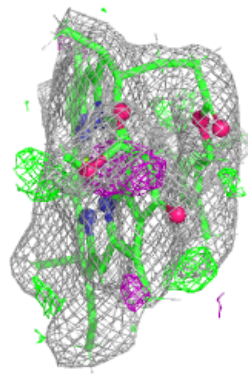
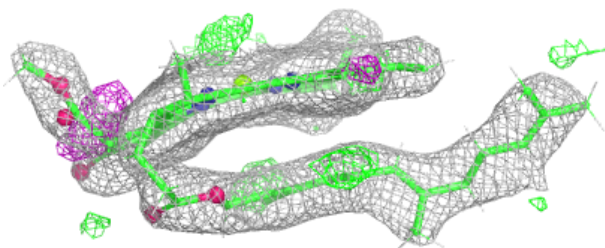
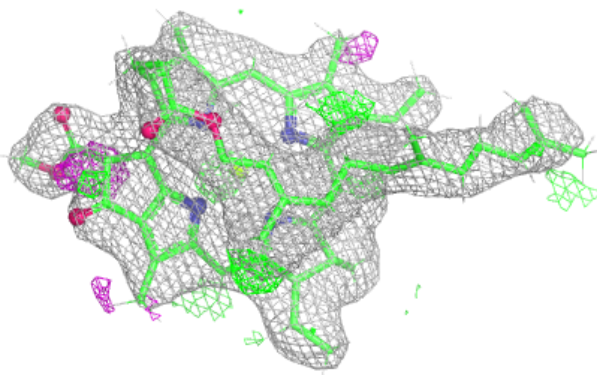
Electron density around GBF A 1009:

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



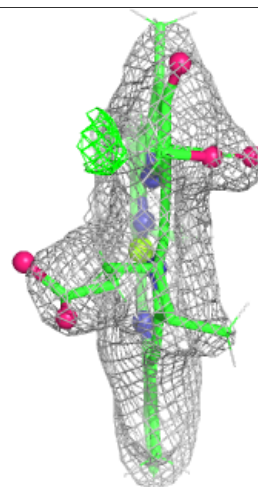
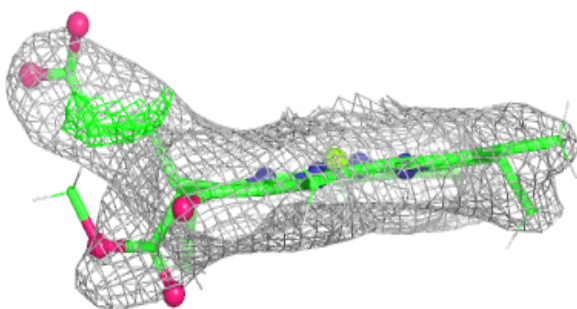
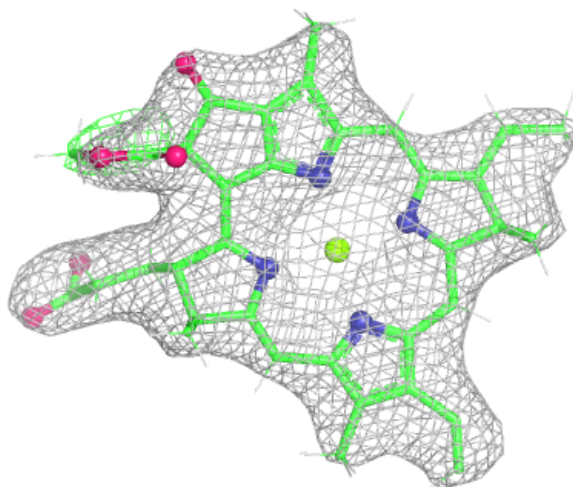
Electron density around GBF A 1028:

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



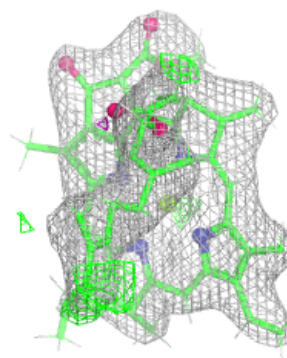
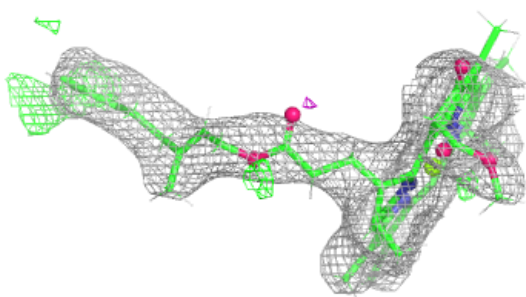
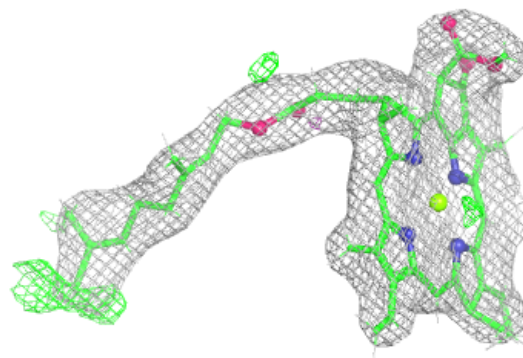
Electron density around GBF A 1010:

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



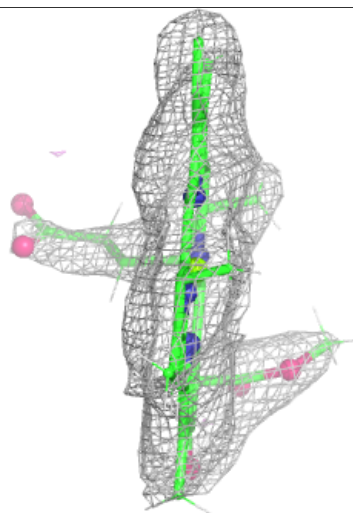
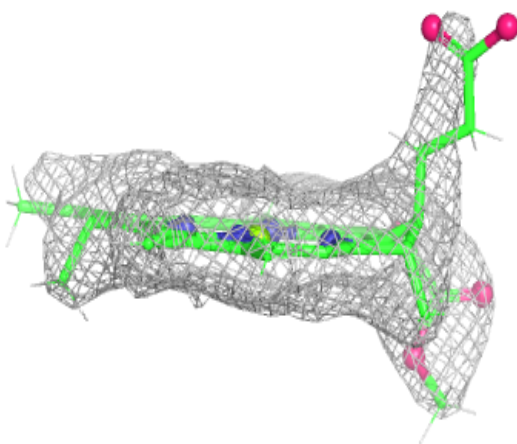
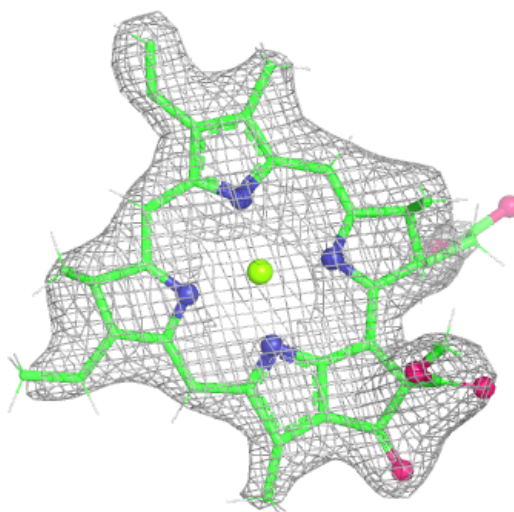
Electron density around GBF A 1013:

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



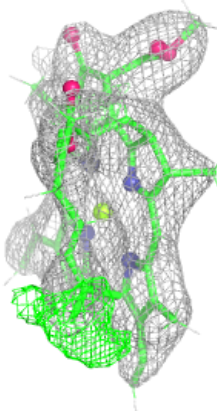
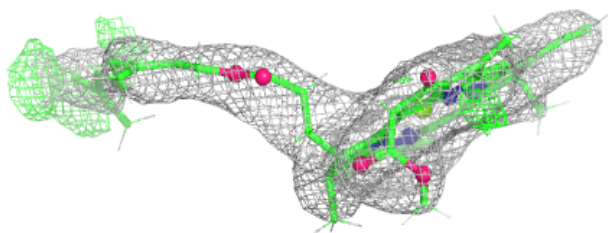
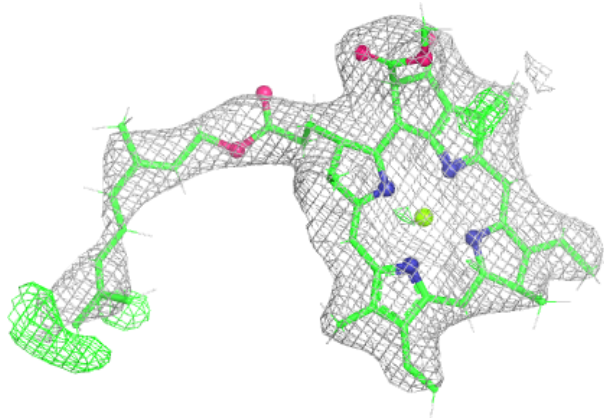
Electron density around GBF A 1016:

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

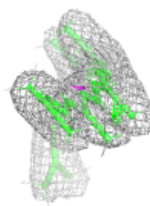
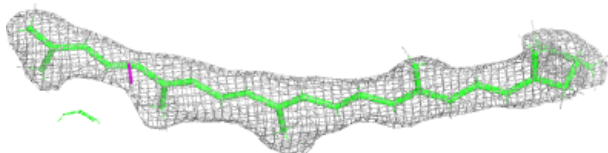
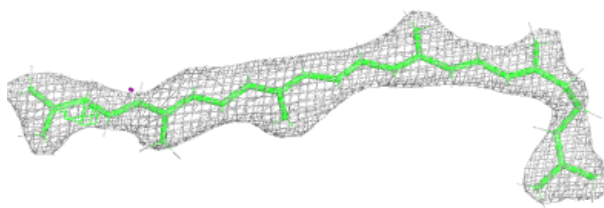


Electron density around GBF A 1012:

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

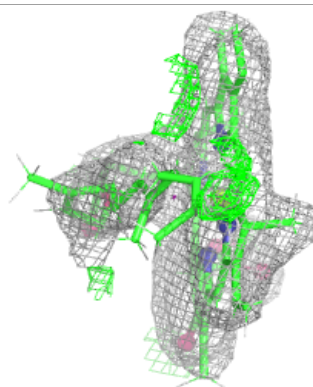
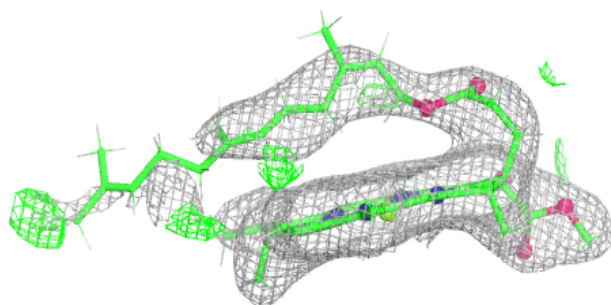
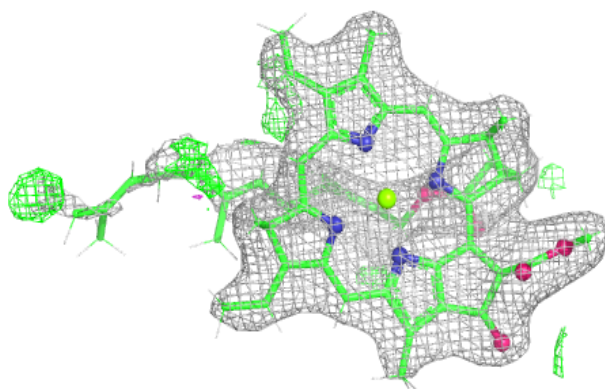
**Electron density around C4D B 101:**

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

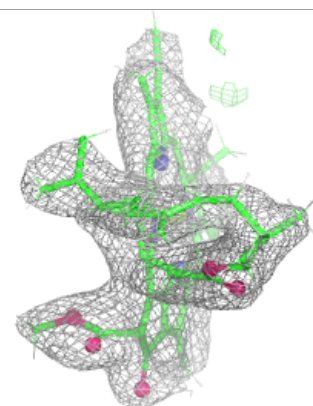
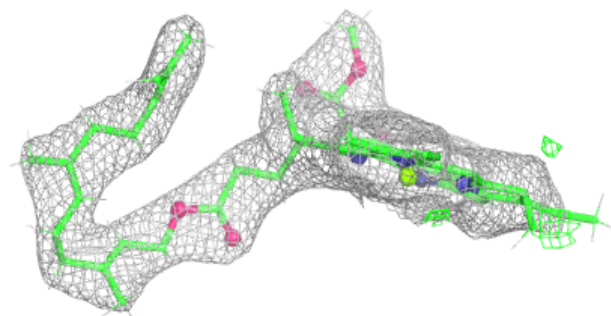
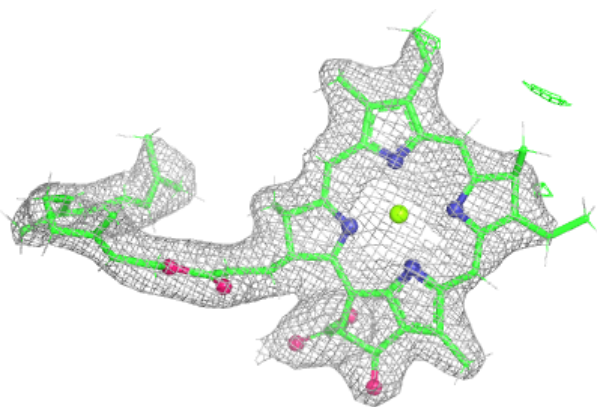


Electron density around GBF A 1007:

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

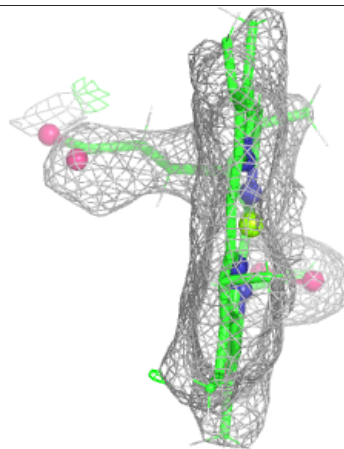
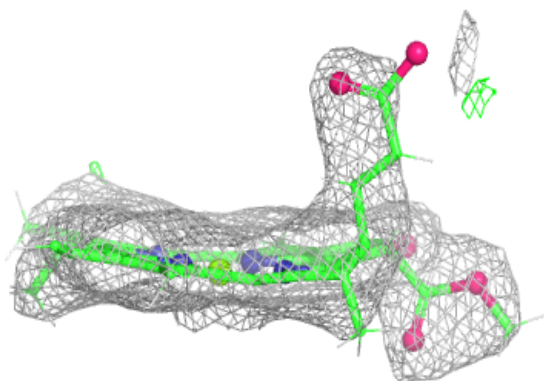
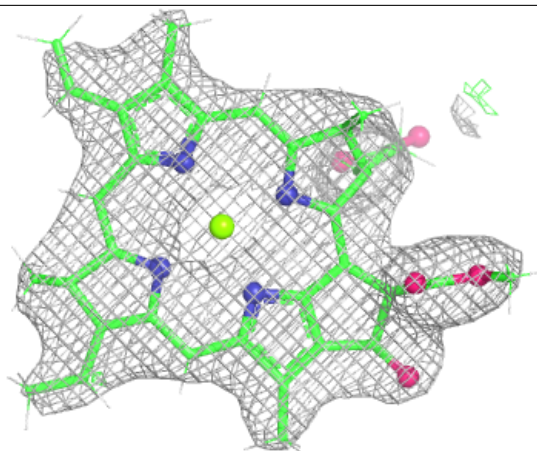
**Electron density around GBF A 1011:**

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

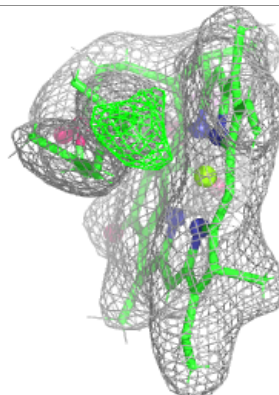
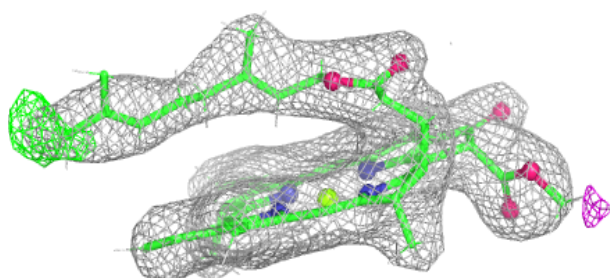
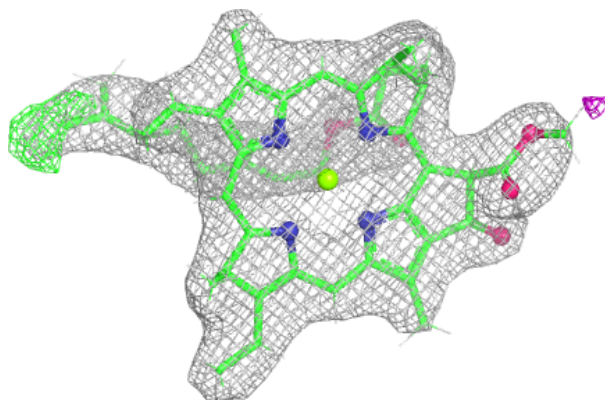


Electron density around GBF A 1014:

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

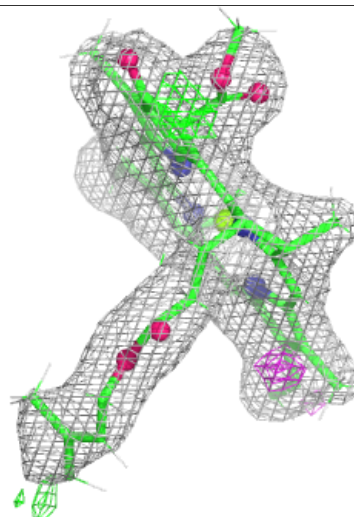
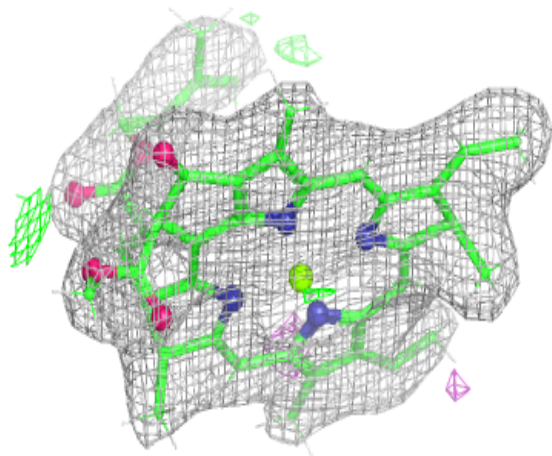
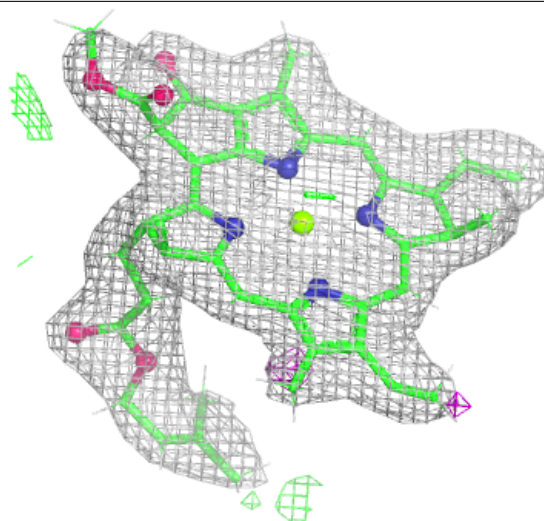
**Electron density around GBF A 1008:**

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



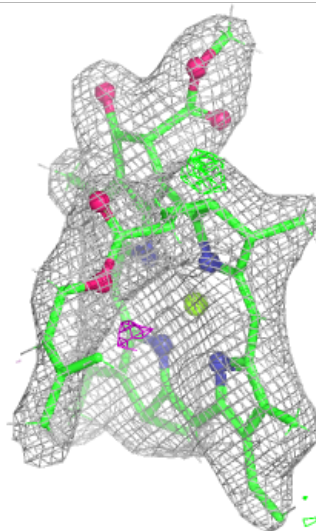
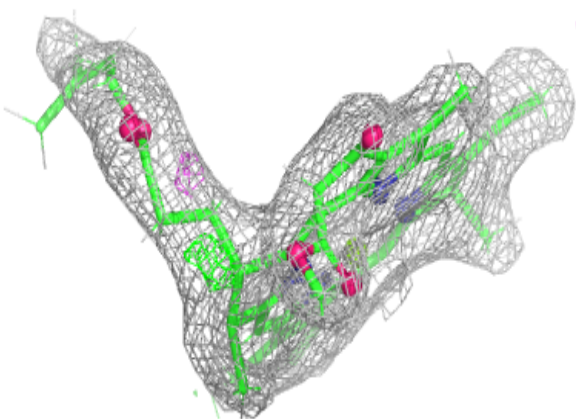
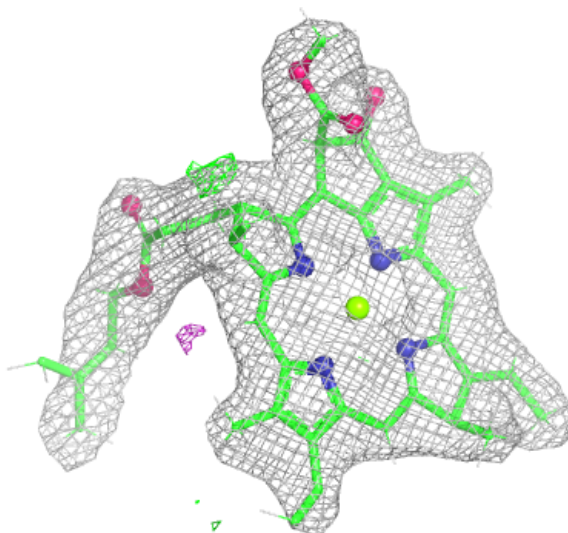
Electron density around GBF A 1018:

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



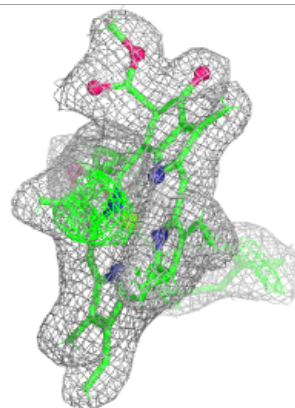
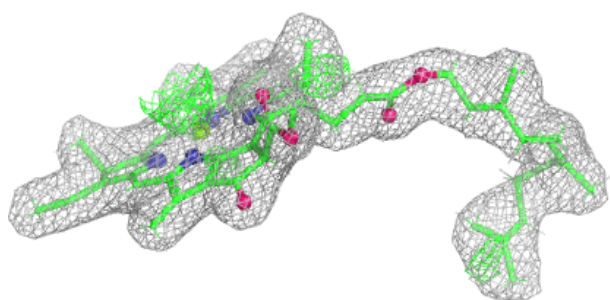
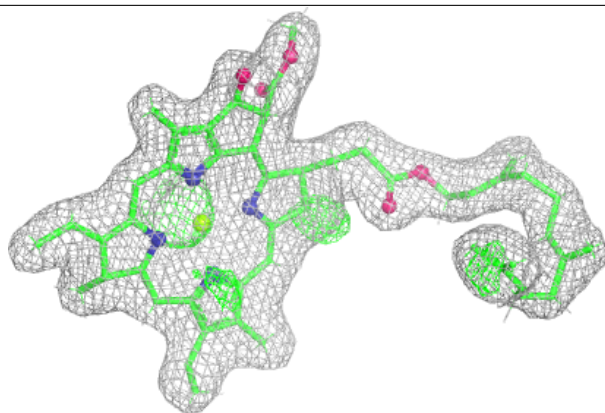
Electron density around GBF A 1027:

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

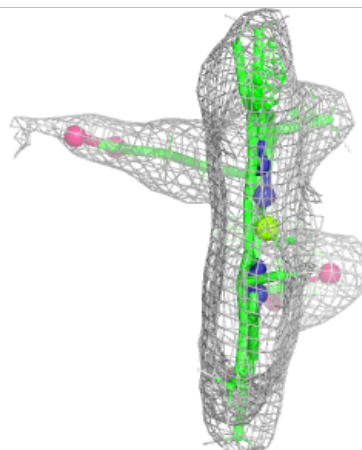
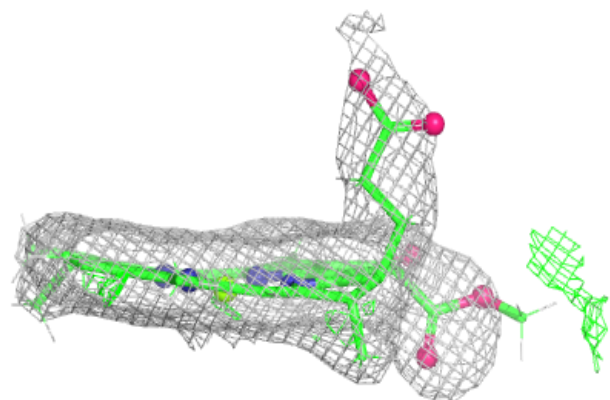
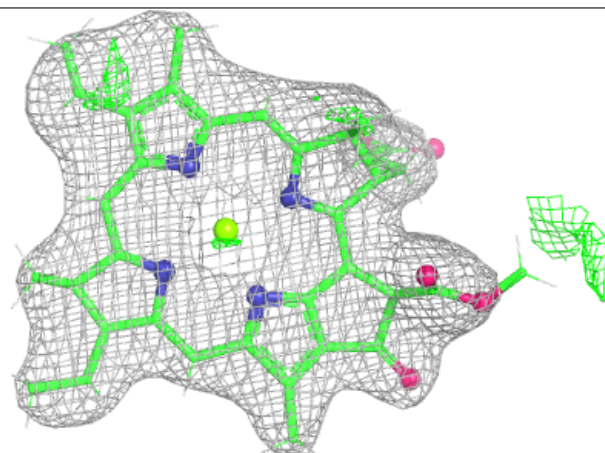


Electron density around GBF A 1002:

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

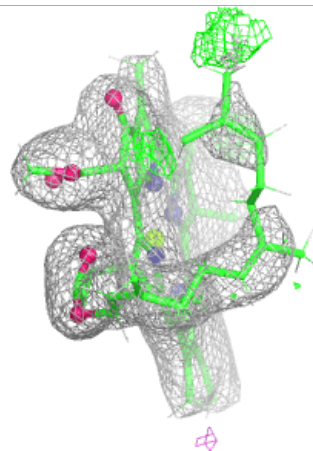
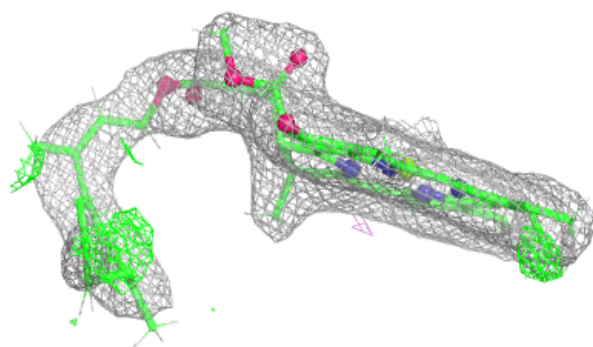
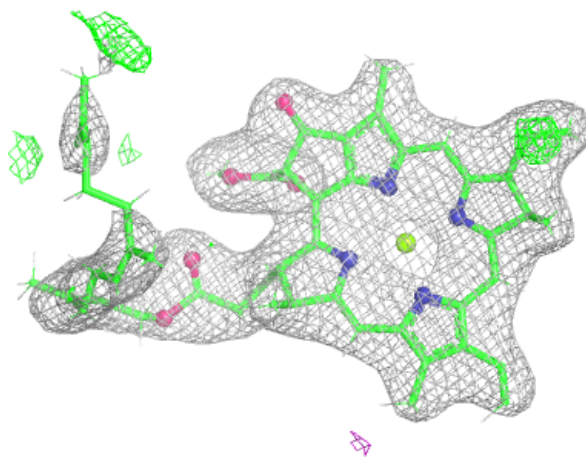
**Electron density around GBF A 1006:**

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



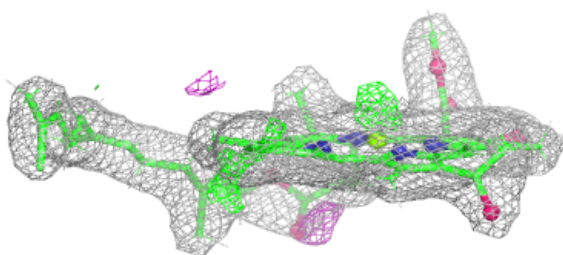
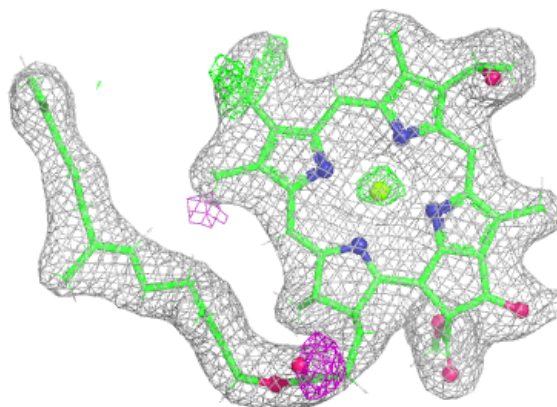
Electron density around GB0 A 1005:

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

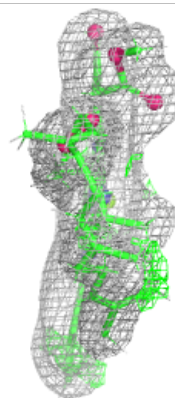
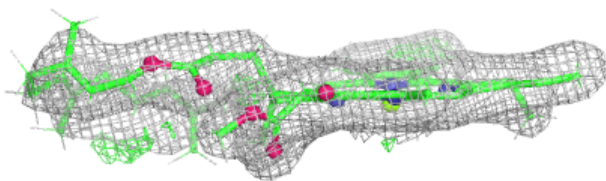
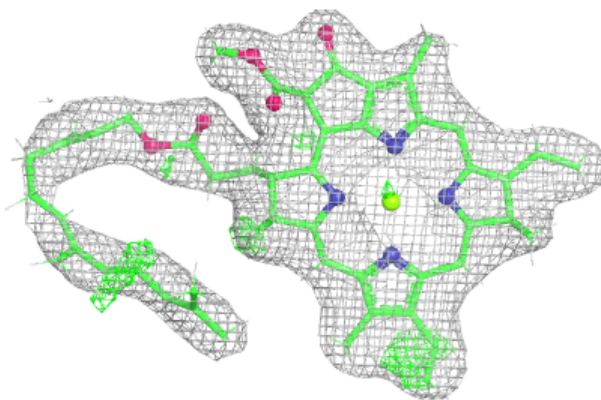


Electron density around AOH A 1003:

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

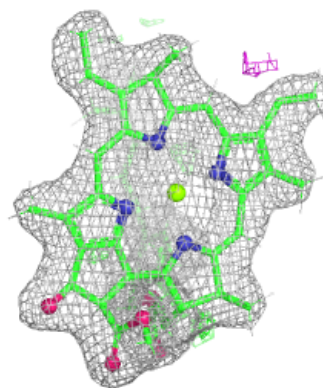
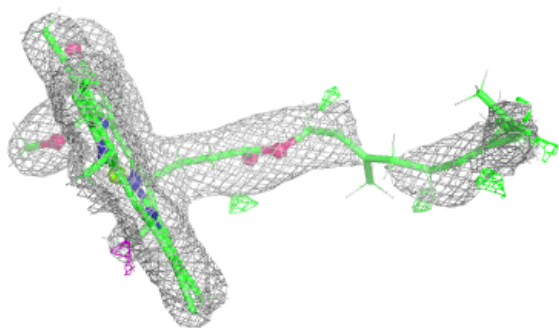
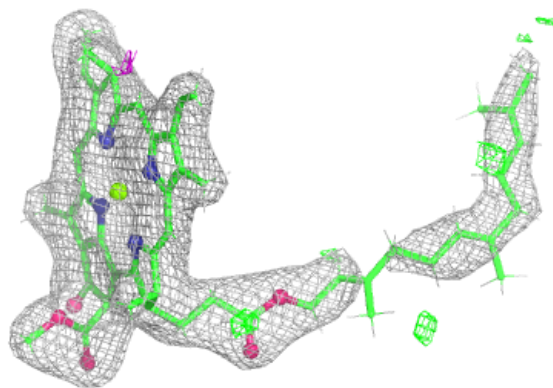
**Electron density around GBF A 1019:**

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



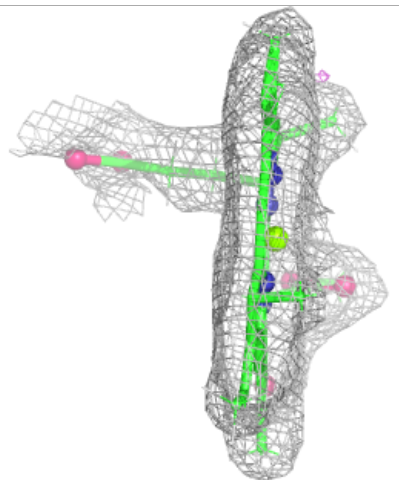
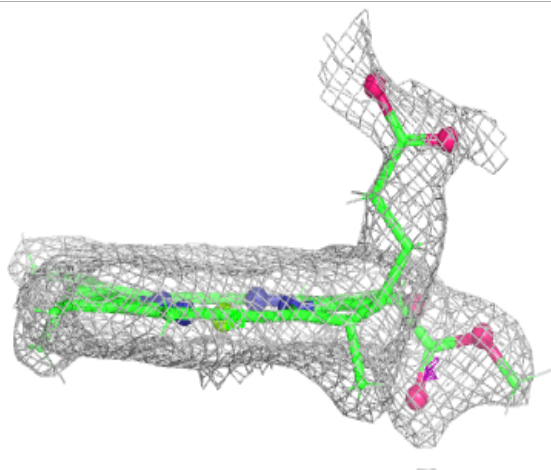
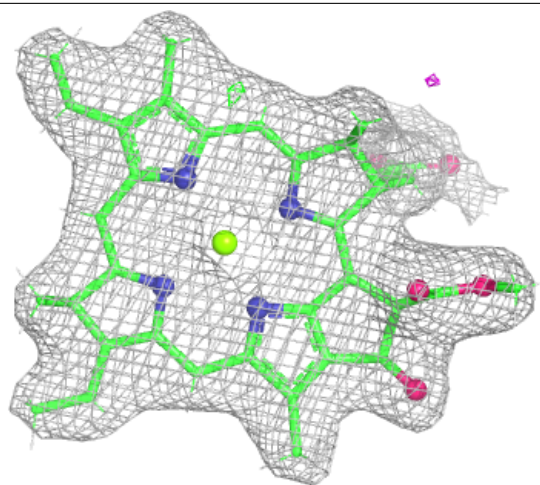
Electron density around GBF A 1021:

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



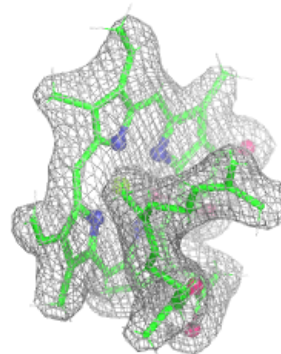
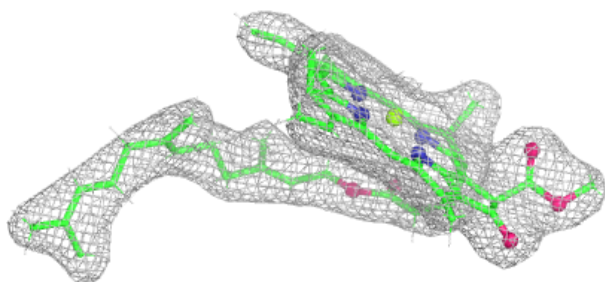
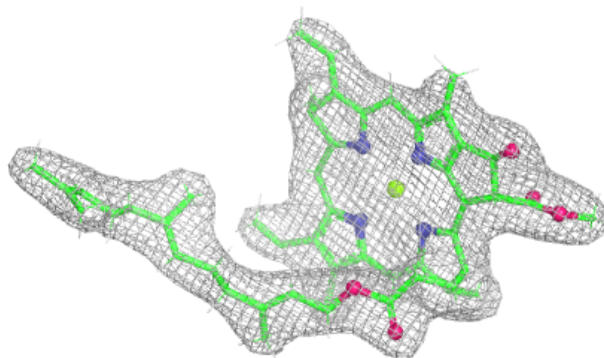
Electron density around GBF A 1022:

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

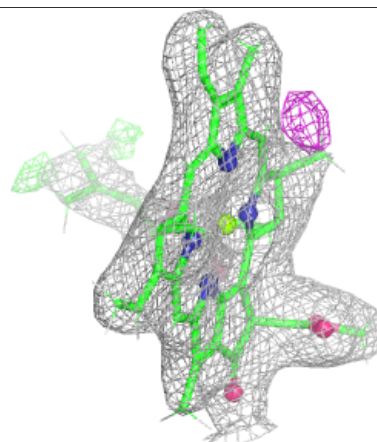
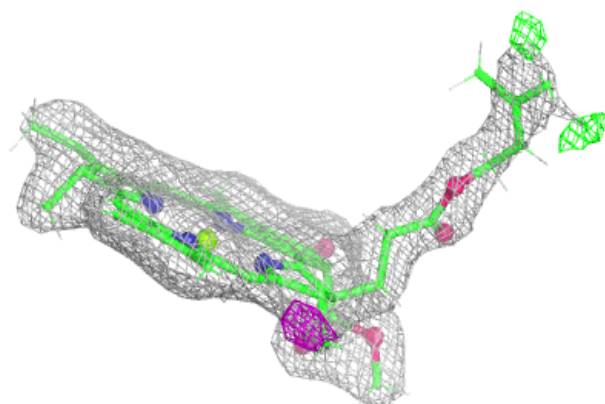
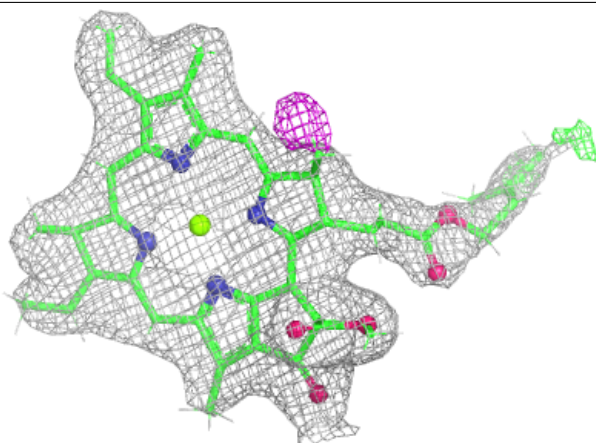


Electron density around GBF A 1023:

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

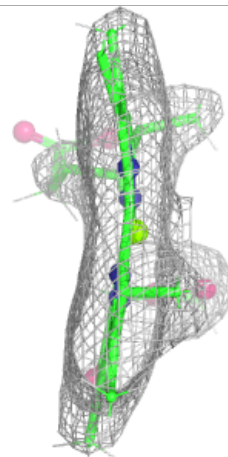
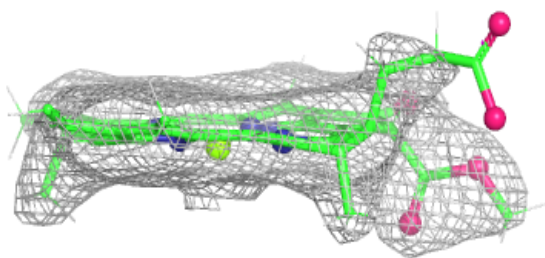
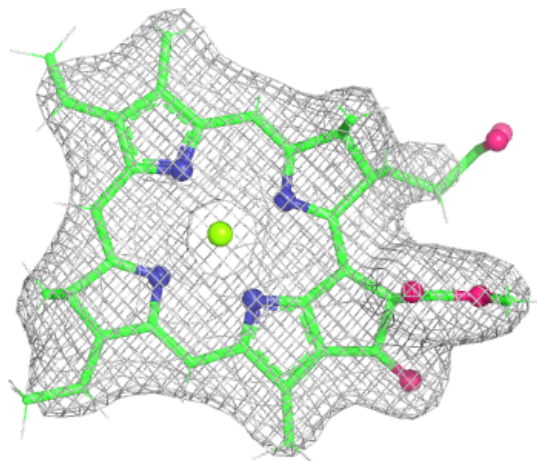
**Electron density around GBF A 1024:**

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



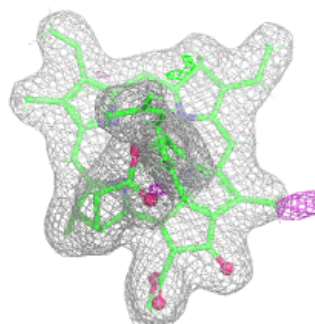
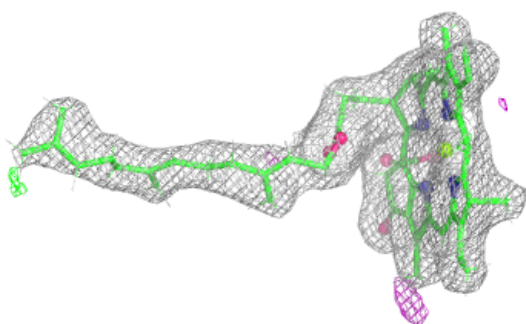
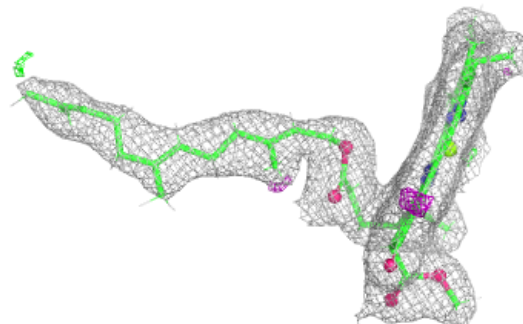
Electron density around GBF A 1025:

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

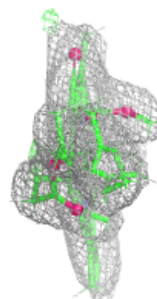
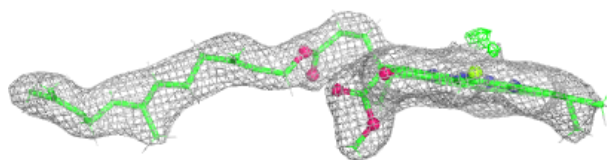
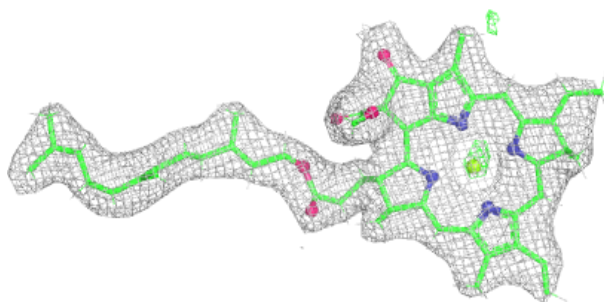


Electron density around GBF A 1026:

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

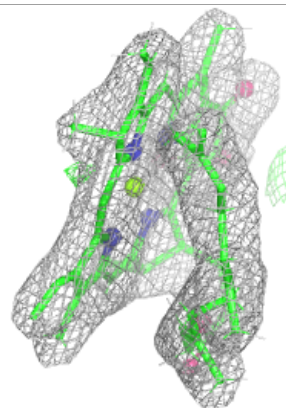
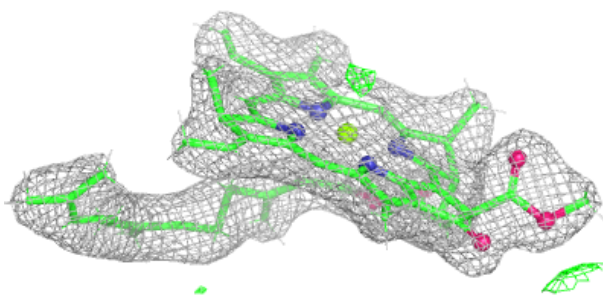
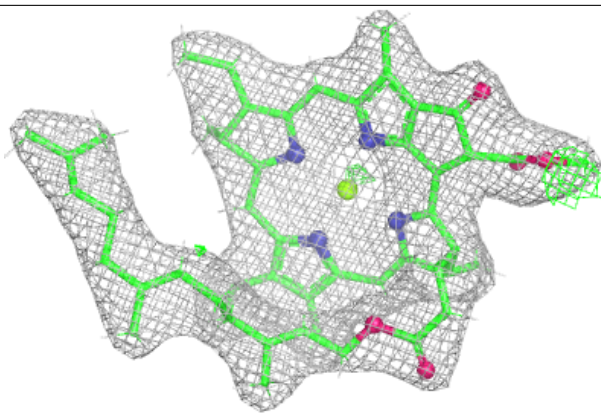
**Electron density around GBF A 1017:**

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



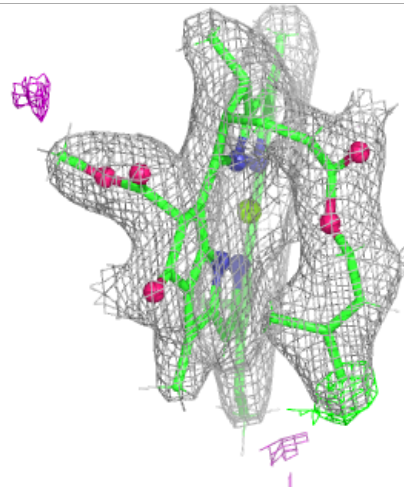
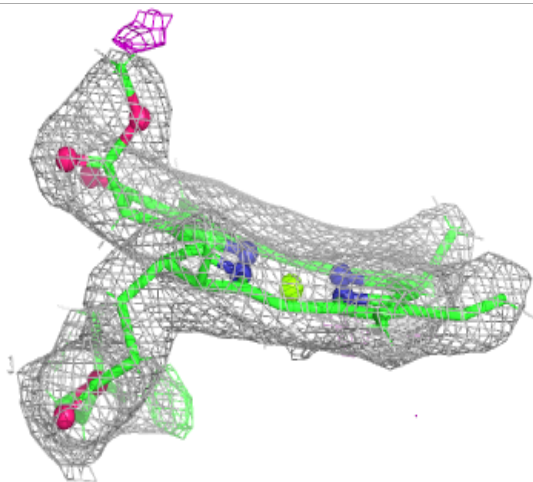
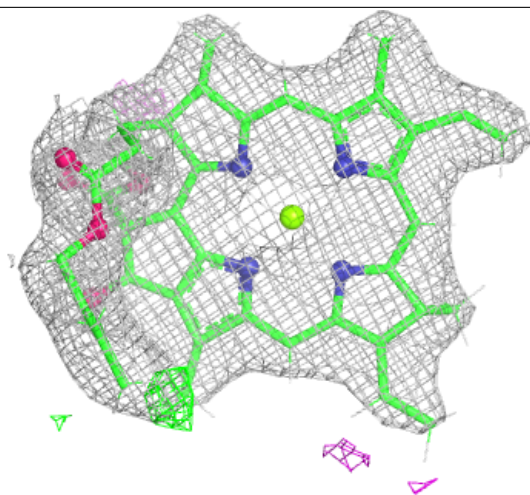
Electron density around GBF A 1015:

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



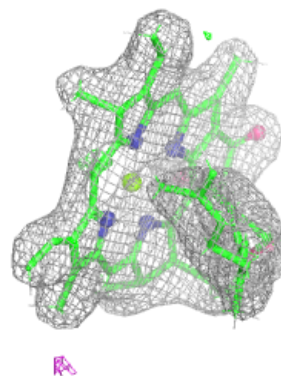
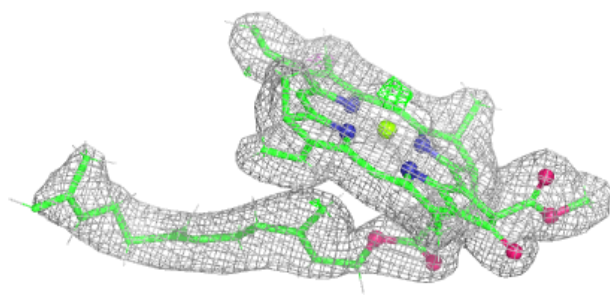
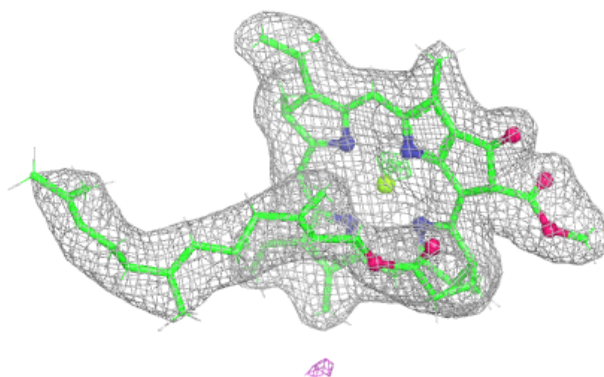
Electron density around GBF A 1004:

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

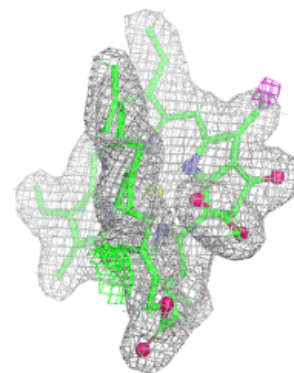
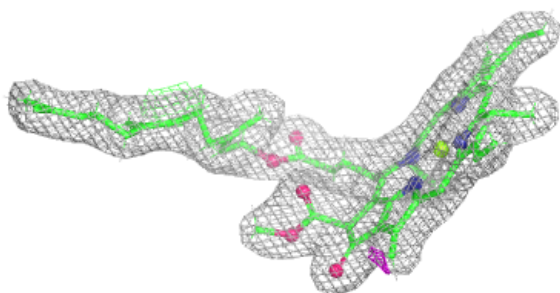
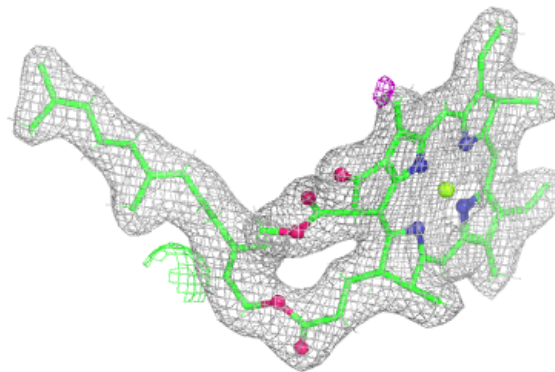


Electron density around GBF A 1020:

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

**Electron density around GB0 A 1001:**

$2mF_o-DF_c$ (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.