



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:32 am BST

PDB ID : 5V8K
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

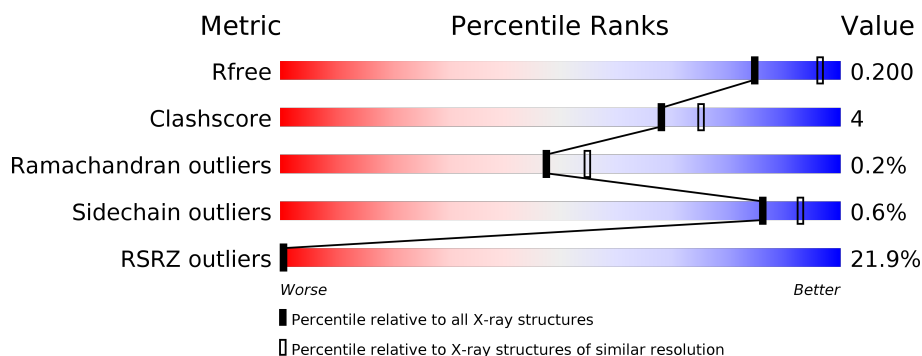
1 Overall quality at a glance ⓘ

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>21%</div> <div>93%</div> <div>7%</div> </div>
2	B	25	<div> <div>44%</div> <div>84%</div> <div>16%</div> </div>

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

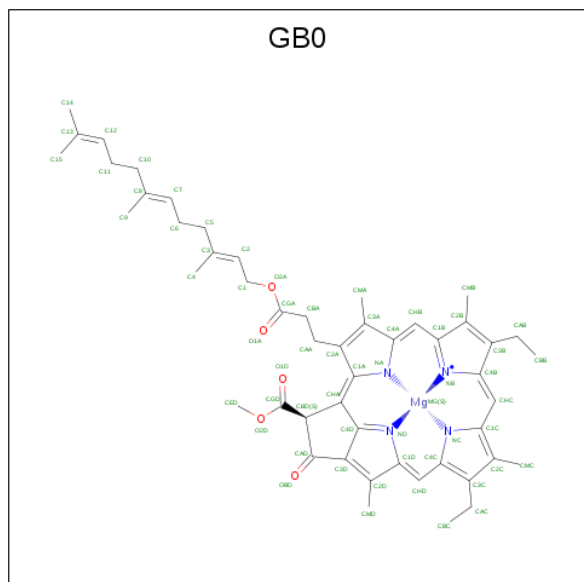
There are 3 discrepancies between the modelled and reference sequences:

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.

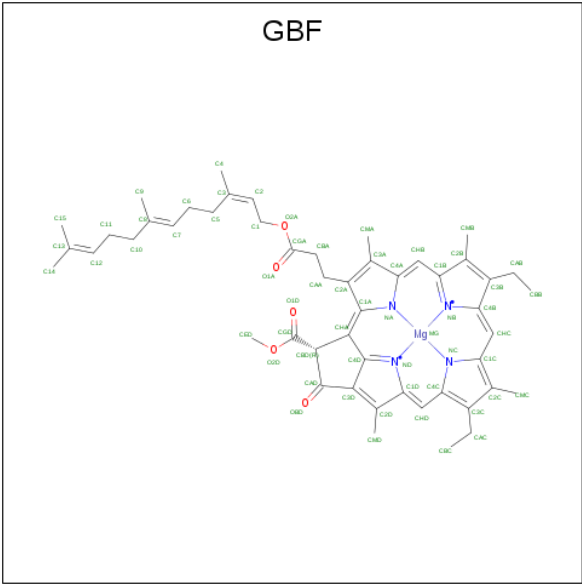
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	B	25	429	160	209	30	30	0	0	0

- Molecule 3 is Bacteriochlorophyll g' (three-letter code: 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 (three-letter code: GBF) (formula: C₅₀H₅₈MgN₄O₅).



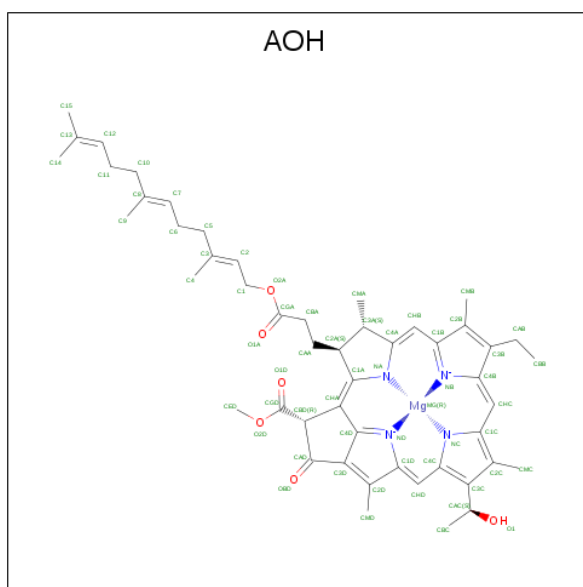
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	Mg	N	O	0	0
			113	50	53	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			87	40	37	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			75	35	30	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			114	50	54	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			100	45	45	1	4	5		
4	A	1	Total	C	H	Mg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

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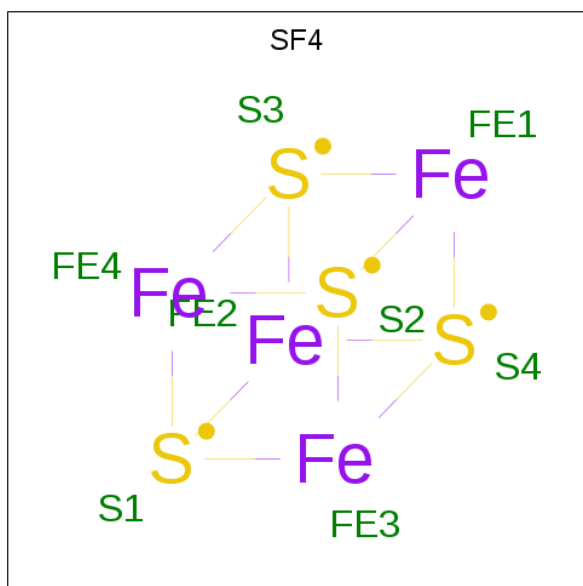
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	Mg	N	O	0	0
			75	35	30	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			112	50	52	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			73	35	28	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			112	50	52	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			87	40	37	1	4	5		
4	A	1	Total	C	H	Mg	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 (three-letter code: AOH) (formula: C₅₀H₆₀MgN₄O₆).



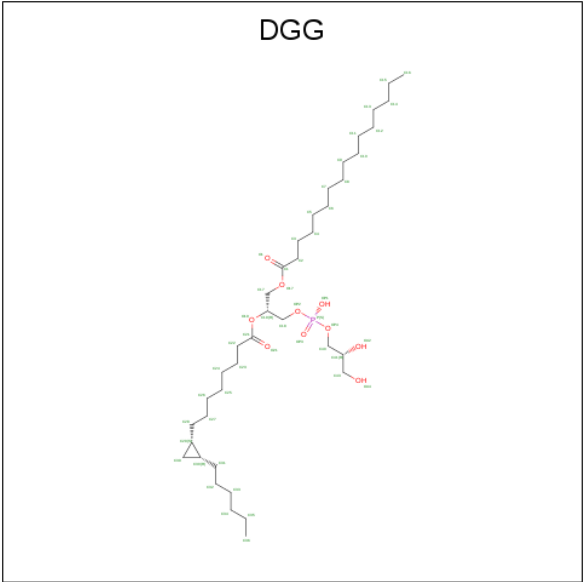
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	Mg	N	O	0	0
			113	50	52	1	4	6		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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)-OCT ANAL-1-YL]-3-[HEXADECANAL-1-YL]-GLYCEROL (three-letter code: DGG) (formula: C₃₉H₇₅O₁₀P).

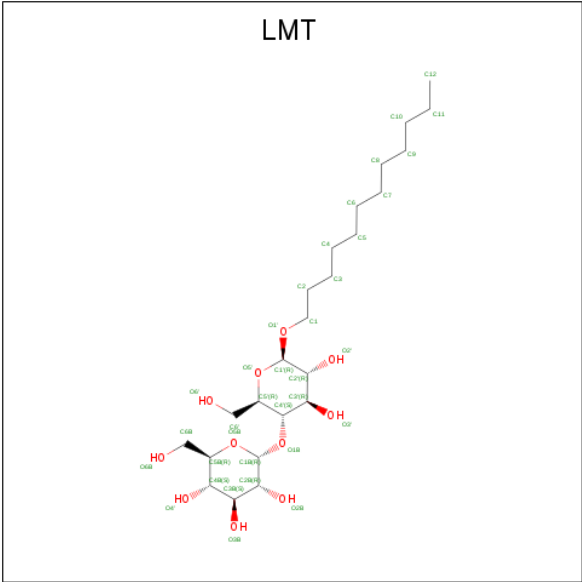


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	O	P	0	0
			88	30	47	10	1		
7	A	1	Total	C	H	O	P	0	0
			93	33	49	10	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

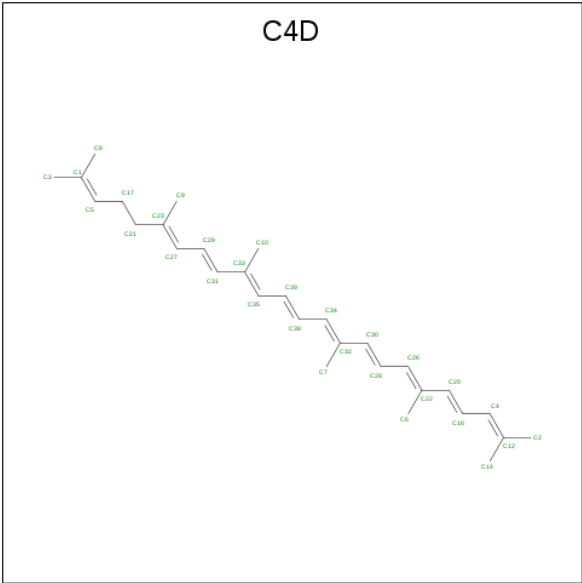
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Ca	0	0
			2	2		

- Molecule 9 is DODECYL-BETA-D-MALTOSE (three-letter code: 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 (three-letter code: C4D) (formula: C₃₀H₄₂).



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

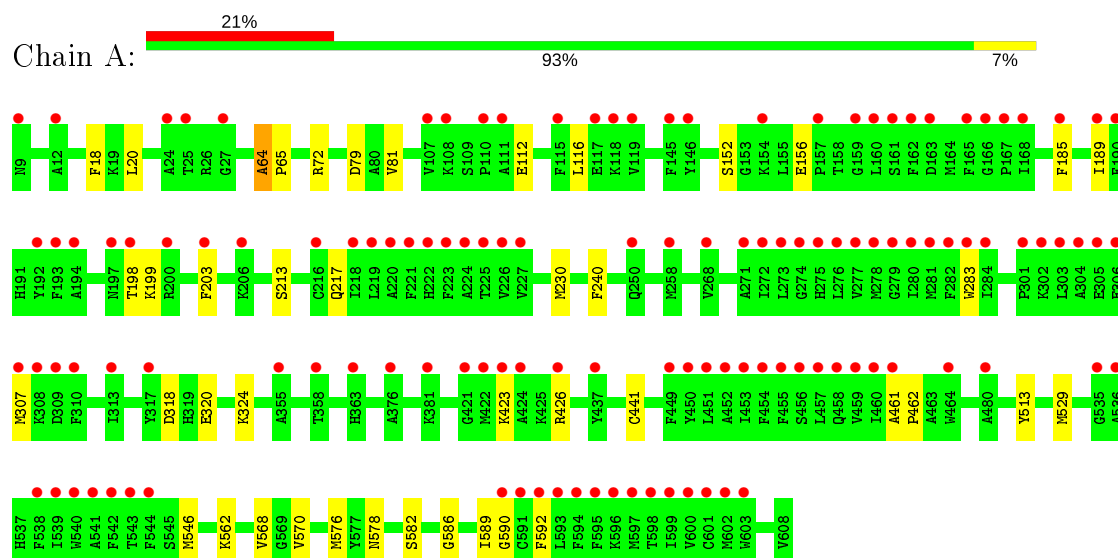
- Molecule 11 is water.

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

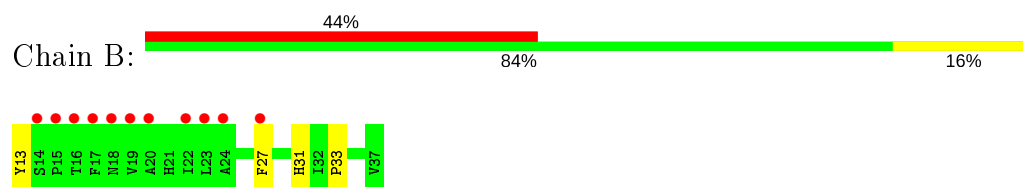
3 Residue-property plots [i](#)

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

- Molecule 1: 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 47.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.08-2.20) 98.2 (47.69-2.20)	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 0.173 , 0.200	Depositor DCC
R_{free} test set	2938 reflections (4.78%)	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)	0.47 , 79.7	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GBF, DGG, SF4, LMT, AOH, C4D, GB0, CA

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	0.55	0/4835	0.65	5/6562 (0.1%)
2	B	0.47	0/232	0.45	0/317
All	All	0.55	0/5067	0.65	5/6879 (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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	64	ALA	C-N-CD	-14.34	89.04	120.60
1	A	529	MET	CG-SD-CE	-6.99	89.02	100.20
1	A	64	ALA	C-N-CA	5.30	144.26	122.00
1	A	72	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	A	72	ARG	NE-CZ-NH1	-5.16	117.72	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	ALA	Mainchain,Peptide

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	33	0
2	B	220	209	209	3	0
3	A	120	100	0	0	0
4	A	1340	1066	0	1	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	44	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 44 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%)	47	55
2	B	23/25 (92%)	23 (100%)	0	0	100	100
All	All	621/625 (99%)	607 (98%)	13 (2%)	1 (0%)	47	55

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%)	460 (99%)	3 (1%)	86	93
2	B	23/23 (100%)	23 (100%)	0	100	100
All	All	486/499 (97%)	483 (99%)	3 (1%)	86	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	423	LYS
1	A	441	CYS
1	A	513	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1018	1	43,58,68	2.80	17 (39%)	32,95,107	6.43	16 (50%)
4	GBF	A	1004	-	43,58,68	2.83	18 (41%)	32,95,107	6.26	15 (46%)
4	GBF	A	1025	-	35,53,68	2.99	17 (48%)	23,89,107	7.47	14 (60%)
4	GBF	A	1007	-	53,68,68	2.34	14 (26%)	44,107,107	5.55	19 (43%)
4	GBF	A	1006	-	35,53,68	2.89	14 (40%)	23,89,107	7.15	13 (56%)
4	GBF	A	1008	-	48,63,68	2.50	18 (37%)	38,101,107	5.65	18 (47%)
4	GBF	A	1012	-	48,63,68	2.59	15 (31%)	38,101,107	5.84	20 (52%)
4	GBF	A	1023	-	53,68,68	2.42	16 (30%)	44,107,107	5.34	17 (38%)
4	GBF	A	1028	11	53,68,68	2.51	15 (28%)	44,107,107	5.34	20 (45%)
6	SF4	A	1029	1	0,12,12	0.00	-	-	-	-
4	GBF	A	1009	-	35,53,68	3.17	15 (42%)	23,89,107	7.32	15 (65%)
4	GBF	A	1011	11	53,68,68	2.44	15 (28%)	44,107,107	5.55	18 (40%)
4	GBF	A	1021	-	53,68,68	2.35	16 (30%)	44,107,107	5.44	20 (45%)
4	GBF	A	1013	-	48,63,68	2.69	17 (35%)	38,101,107	5.93	19 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DGG	A	1030	-	40,40,50	0.93	2 (5%)	43,46,59	1.21	4 (9%)
4	GBF	A	1017	11	53,68,68	2.52	16 (30%)	44,107,107	5.49	19 (43%)
4	GBF	B	103	-	53,68,68	2.73	16 (30%)	44,107,107	5.58	22 (50%)
3	GB0	A	1005	-	53,68,68	2.55	15 (28%)	44,107,107	5.38	22 (50%)
4	GBF	A	1022	-	35,53,68	2.94	15 (42%)	23,89,107	7.33	14 (60%)
4	GBF	A	1010	1	35,53,68	3.04	15 (42%)	23,89,107	7.39	17 (73%)
4	GBF	B	102	-	35,53,68	3.13	14 (40%)	23,89,107	7.65	15 (65%)
4	GBF	A	1014	1	35,53,68	2.90	14 (40%)	23,89,107	8.03	15 (65%)
9	LMT	A	1034	-	36,36,36	0.71	0	47,47,47	1.20	6 (12%)
4	GBF	A	1015	-	53,68,68	2.40	16 (30%)	44,107,107	5.87	17 (38%)
4	GBF	A	1020	-	53,68,68	2.54	16 (30%)	44,107,107	5.54	17 (38%)
9	LMT	A	1035	-	36,36,36	0.85	1 (2%)	47,47,47	1.08	4 (8%)
4	GBF	A	1016	-	35,53,68	3.10	15 (42%)	23,89,107	7.76	15 (65%)
4	GBF	A	1024	-	43,58,68	2.62	17 (39%)	32,95,107	6.39	18 (56%)
4	GBF	A	1027	-	43,58,68	2.85	16 (37%)	32,95,107	7.29	19 (59%)
10	C4D	B	101	-	29,29,29	0.76	0	33,34,34	1.66	10 (30%)
4	GBF	A	1019	11	53,68,68	2.51	16 (30%)	44,107,107	5.18	20 (45%)
4	GBF	A	1026	8	53,68,68	2.36	16 (30%)	44,107,107	5.56	18 (40%)
4	GBF	A	1002	11	53,68,68	2.44	17 (32%)	44,107,107	5.33	19 (43%)
7	DGG	A	1031	-	43,43,50	1.02	2 (4%)	46,49,59	1.21	4 (8%)
5	AOH	A	1003	11	57,69,69	1.82	10 (17%)	53,109,109	2.25	20 (37%)
3	GB0	A	1001	-	53,68,68	2.35	17 (32%)	44,107,107	5.60	20 (45%)

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	1018	1	1/1/11/15	8/21/77/89	-
4	GBF	A	1004	-	1/1/11/15	10/21/77/89	-
4	GBF	A	1007	-	1/1/15/15	12/33/89/89	-
4	GBF	A	1006	-	1/1/9/15	8/13/71/89	-
4	GBF	A	1008	-	1/1/13/15	10/27/83/89	-
4	GBF	A	1012	-	1/1/13/15	13/27/83/89	-
4	GBF	A	1023	-	1/1/15/15	7/33/89/89	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GBF	A	1028	11	1/1/15/15	11/33/89/89	-
6	SF4	A	1029	1	-	-	0/6/5/5
4	GBF	A	1009	-	1/1/9/15	7/13/71/89	-
4	GBF	A	1011	11	1/1/15/15	8/33/89/89	-
4	GBF	A	1021	-	1/1/15/15	15/33/89/89	-
4	GBF	A	1013	-	1/1/13/15	13/27/83/89	-
7	DGG	A	1030	-	-	15/45/45/59	-
4	GBF	A	1017	11	1/1/15/15	6/33/89/89	-
4	GBF	B	103	-	1/1/15/15	13/33/89/89	-
7	DGG	A	1031	-	-	18/48/48/59	-
4	GBF	A	1022	-	1/1/9/15	5/13/71/89	-
4	GBF	A	1010	1	1/1/9/15	7/13/71/89	-
4	GBF	B	102	-	1/1/9/15	8/13/71/89	-
4	GBF	A	1014	1	1/1/9/15	5/13/71/89	-
9	LMT	A	1034	-	-	10/21/61/61	0/2/2/2
4	GBF	A	1015	-	1/1/15/15	8/33/89/89	-
4	GBF	A	1020	-	1/1/15/15	12/33/89/89	-
9	LMT	A	1035	-	-	7/21/61/61	0/2/2/2
4	GBF	A	1016	-	1/1/9/15	8/13/71/89	-
4	GBF	A	1024	-	1/1/11/15	6/21/77/89	-
4	GBF	A	1027	-	1/1/11/15	10/21/77/89	-
3	GB0	A	1005	-	-	9/33/89/89	-
10	C4D	B	101	-	-	0/31/31/31	-
4	GBF	A	1019	11	1/1/15/15	10/33/89/89	-
4	GBF	A	1026	8	1/1/15/15	13/33/89/89	-
4	GBF	A	1002	11	1/1/15/15	8/33/89/89	-
4	GBF	A	1025	-	1/1/9/15	6/13/71/89	-
5	AOH	A	1003	11	3/3/21/21	6/31/111/111	-
3	GB0	A	1001	-	1/1/15/15	6/33/89/89	-

The worst 5 of 473 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1009	GBF	C1D-C2D	9.84	1.64	1.42
4	A	1016	GBF	C1D-C2D	9.66	1.64	1.42
4	B	102	GBF	C1D-C2D	9.62	1.64	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	103	GBF	C1D-C2D	9.53	1.64	1.42
4	A	1013	GBF	C1D-C2D	9.37	1.63	1.42

The worst 5 of 559 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1011	GBF	C1C-C2C-C3C	-28.85	86.92	107.00
4	B	103	GBF	C1C-C2C-C3C	-28.83	86.94	107.00
4	A	1016	GBF	C1C-C2C-C3C	-28.53	87.15	107.00
4	A	1017	GBF	C1C-C2C-C3C	-28.20	87.37	107.00
4	A	1009	GBF	C1C-C2C-C3C	-28.06	87.48	107.00

5 of 31 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1018	GBF	NA
4	A	1004	GBF	NA
4	A	1007	GBF	NA
4	A	1006	GBF	NA
4	A	1008	GBF	NA

5 of 318 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1018	GBF	C3A-C2A-CAA-CBA
4	A	1018	GBF	C2B-C3B-CAB-CBB
4	A	1018	GBF	C4B-C3B-CAB-CBB
4	A	1018	GBF	C2C-C3C-CAC-CBC
4	A	1018	GBF	C4C-C3C-CAC-CBC

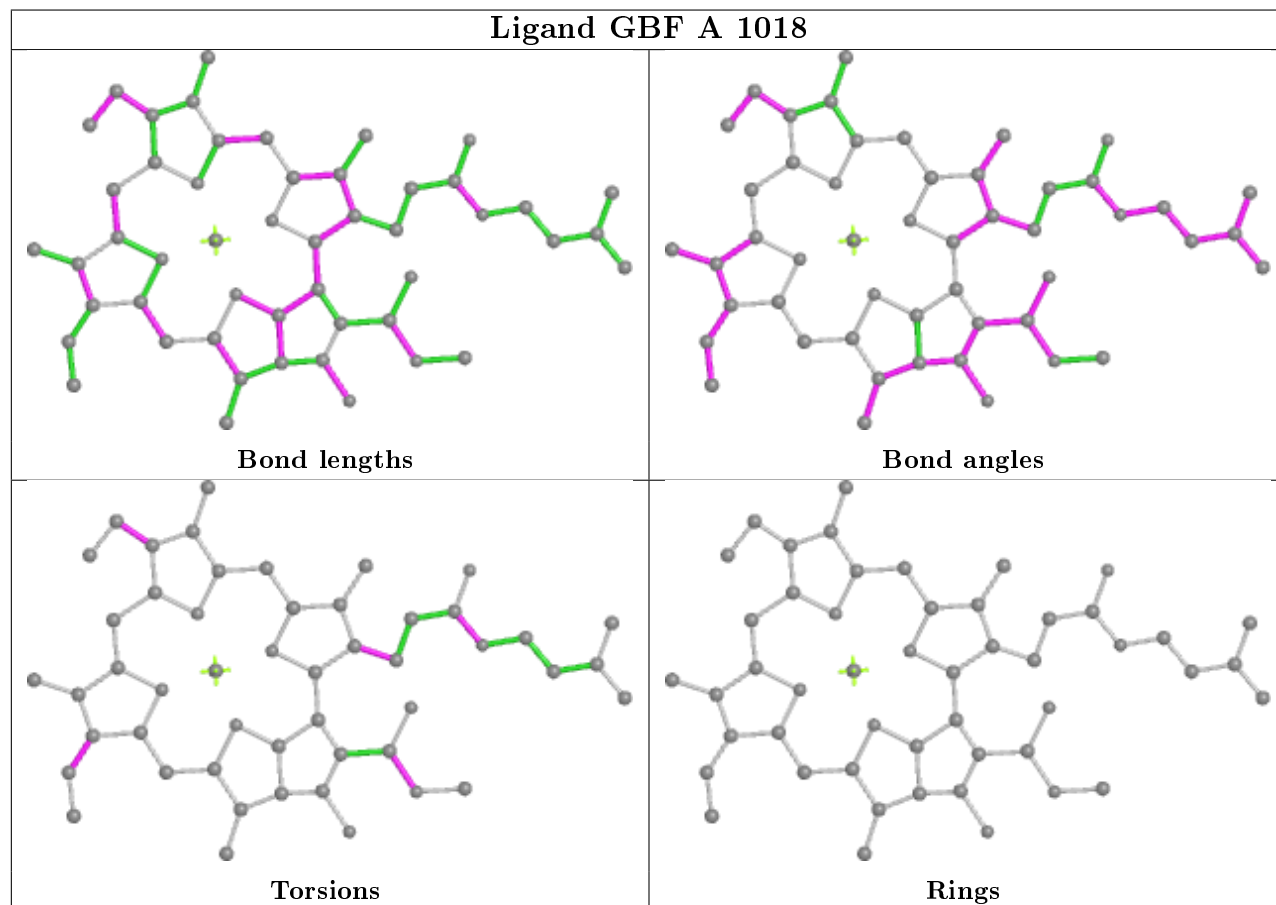
There are no ring outliers.

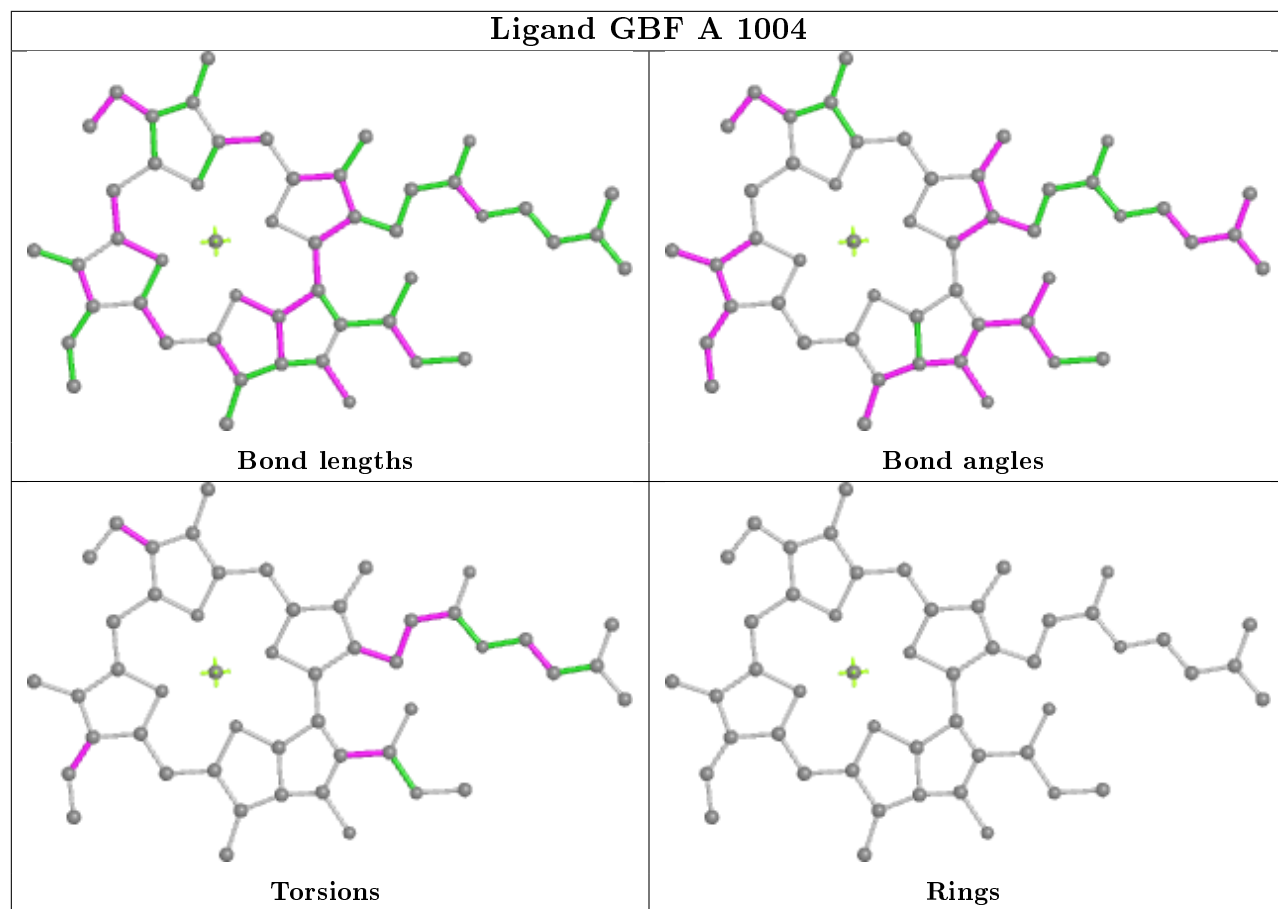
5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1025	GBF	1	0
7	A	1030	DGG	9	0
9	A	1034	LMT	6	0
9	A	1035	LMT	6	0
7	A	1031	DGG	4	0

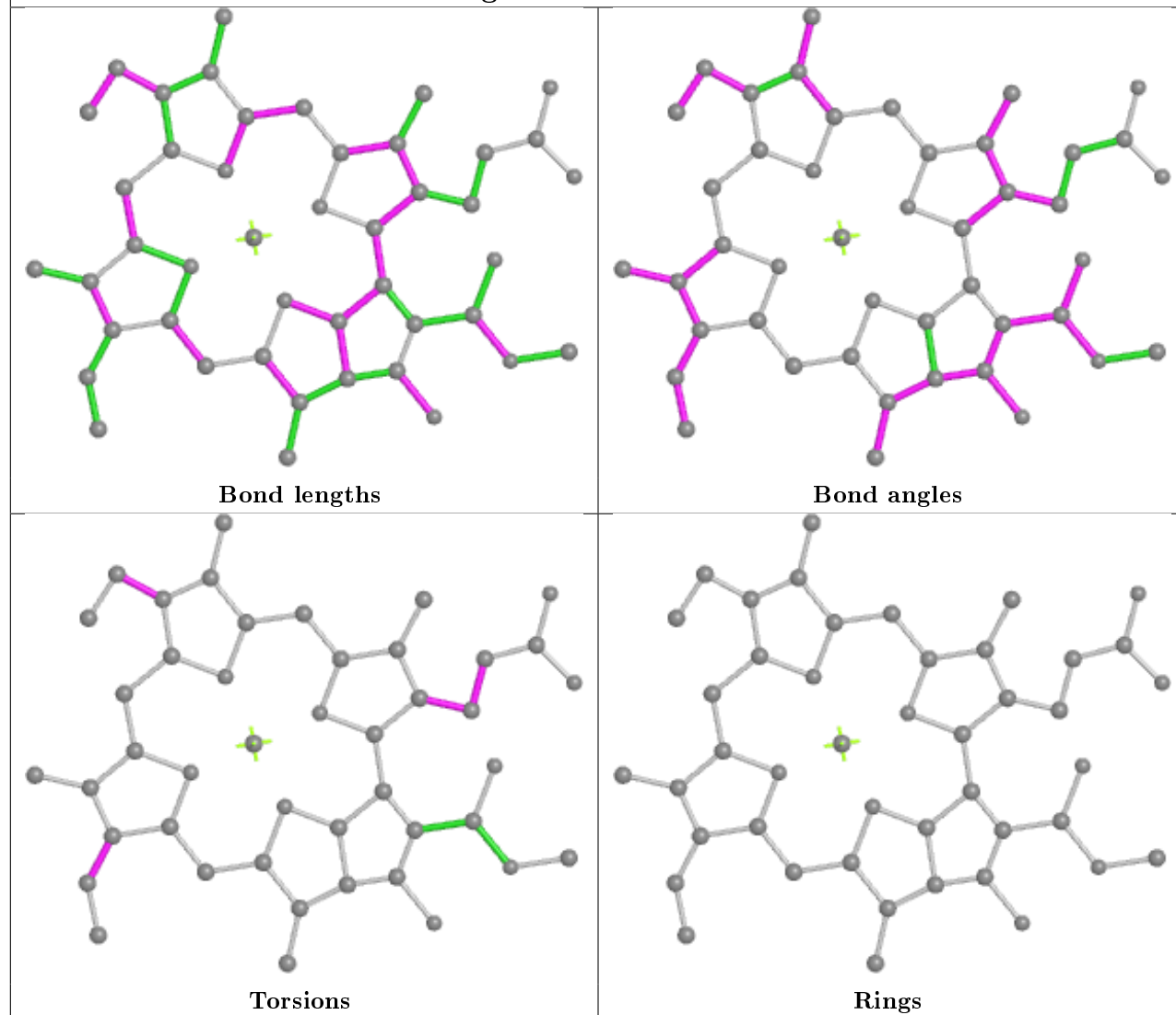
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

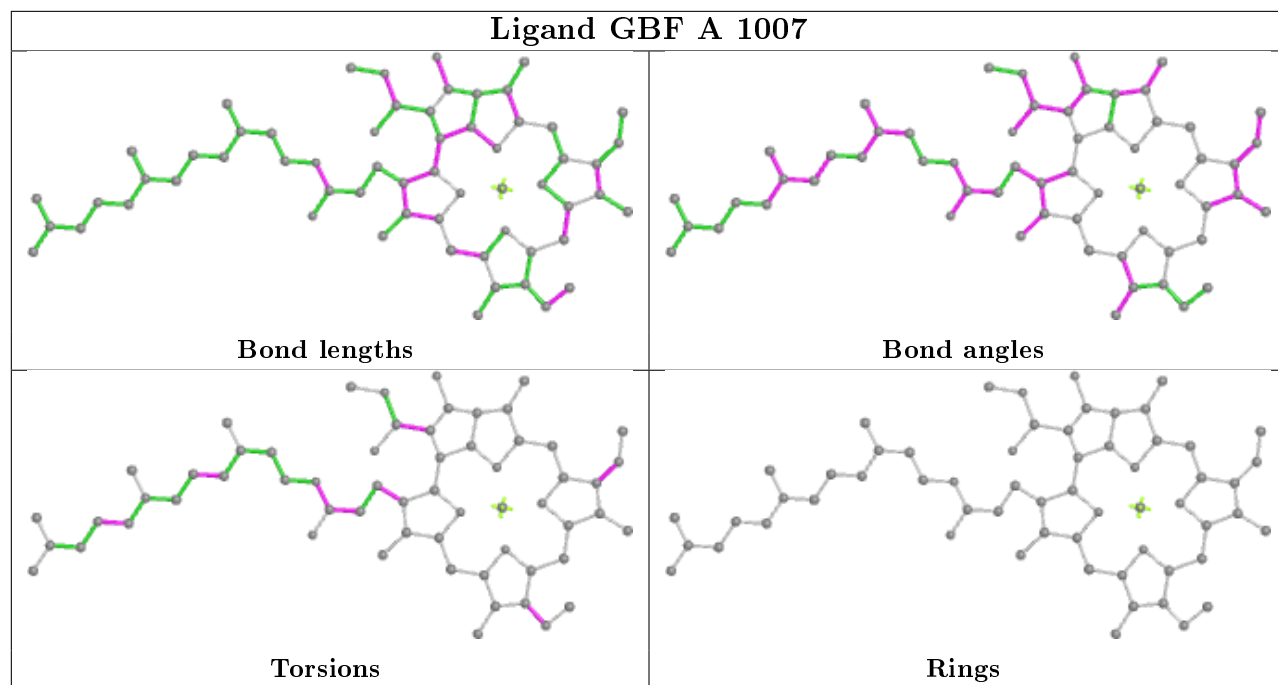
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



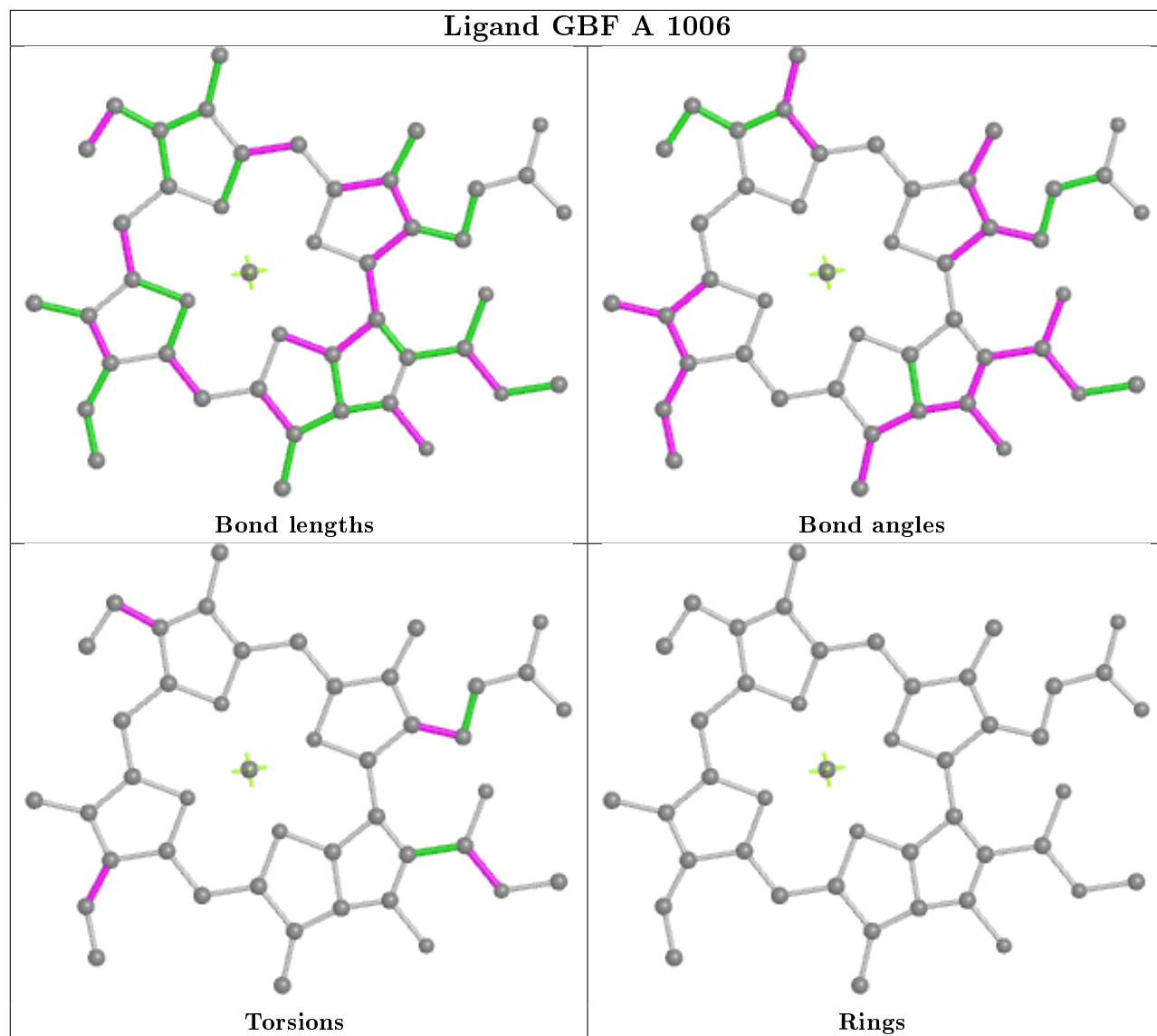


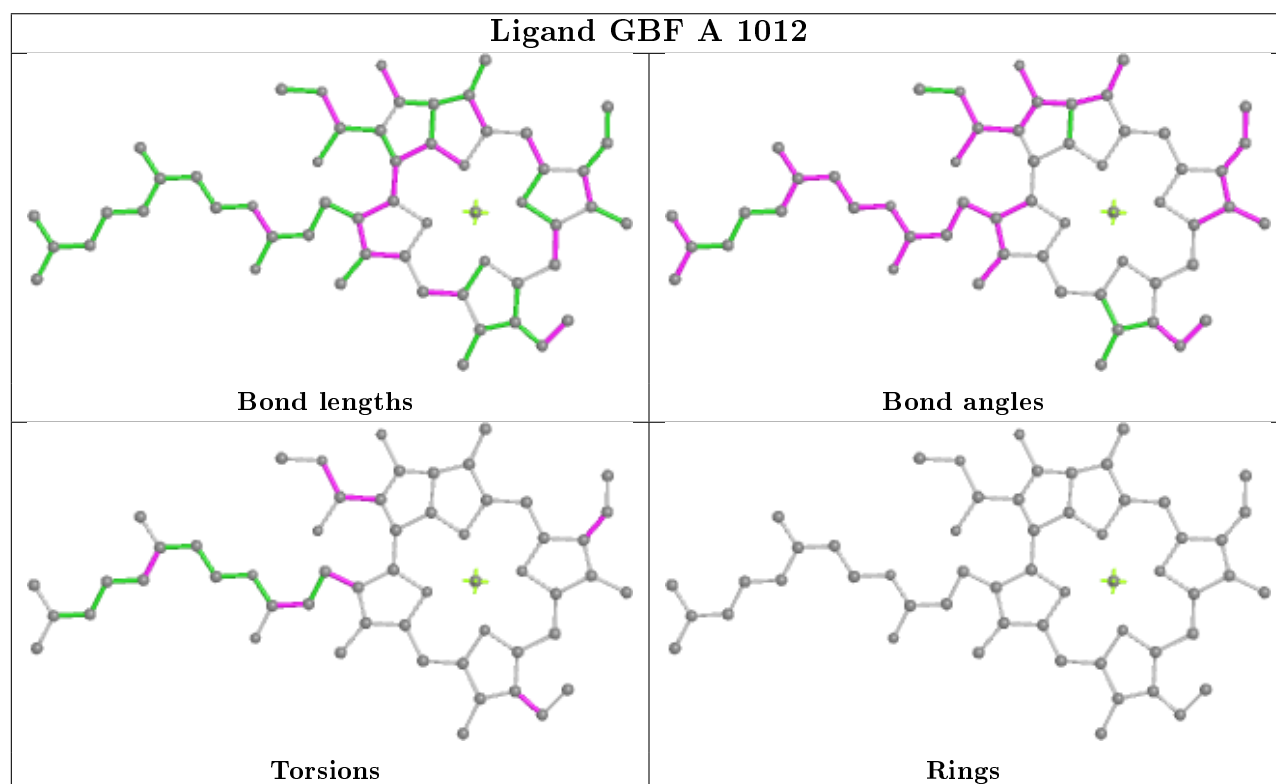
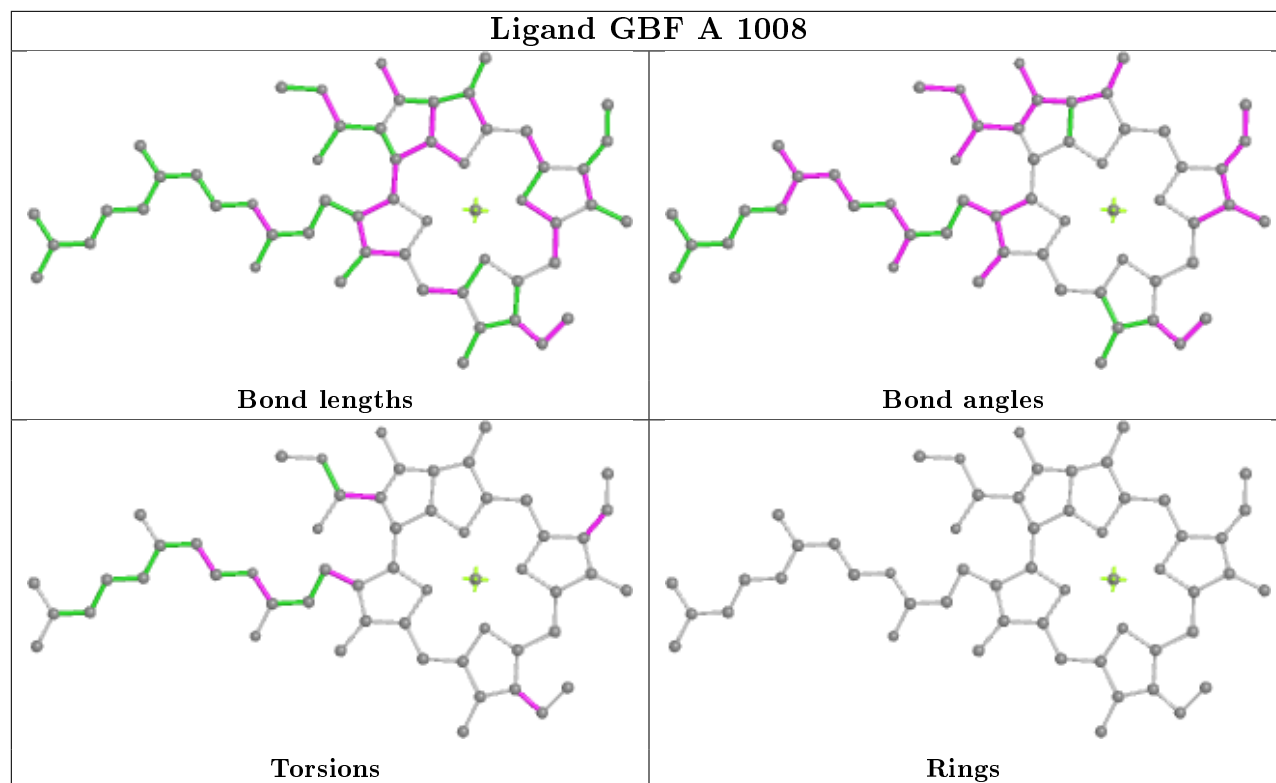
Ligand GBF A 1025

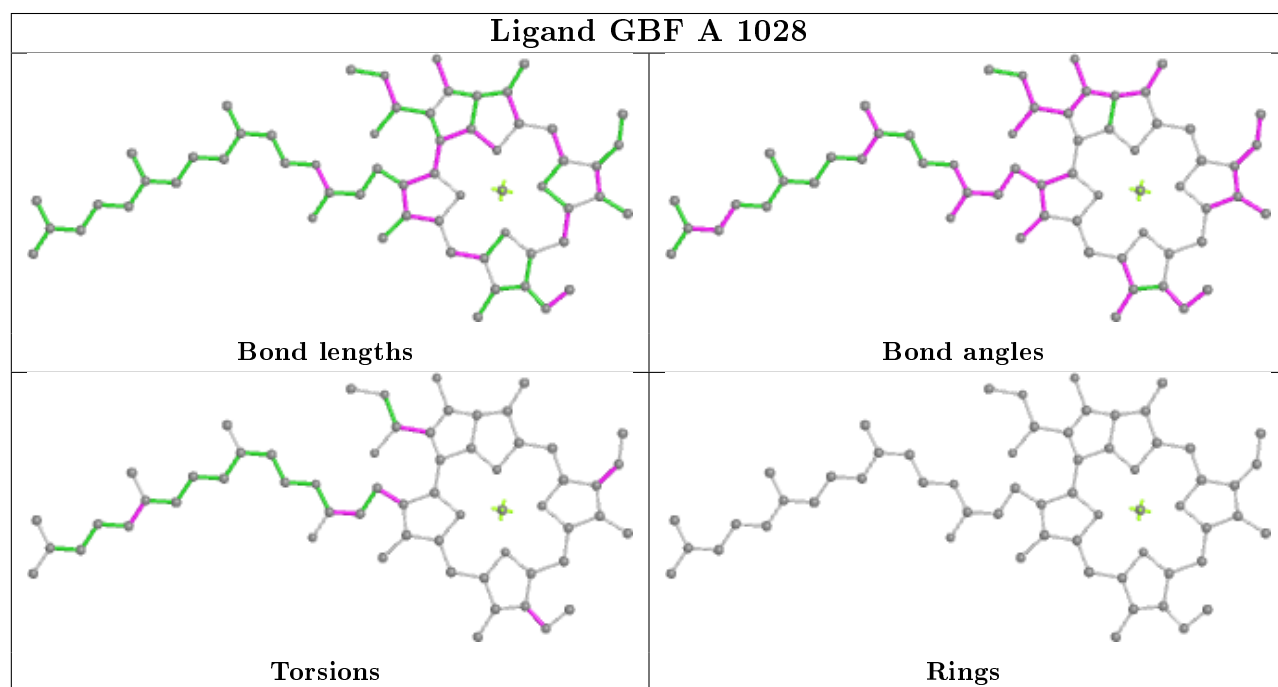
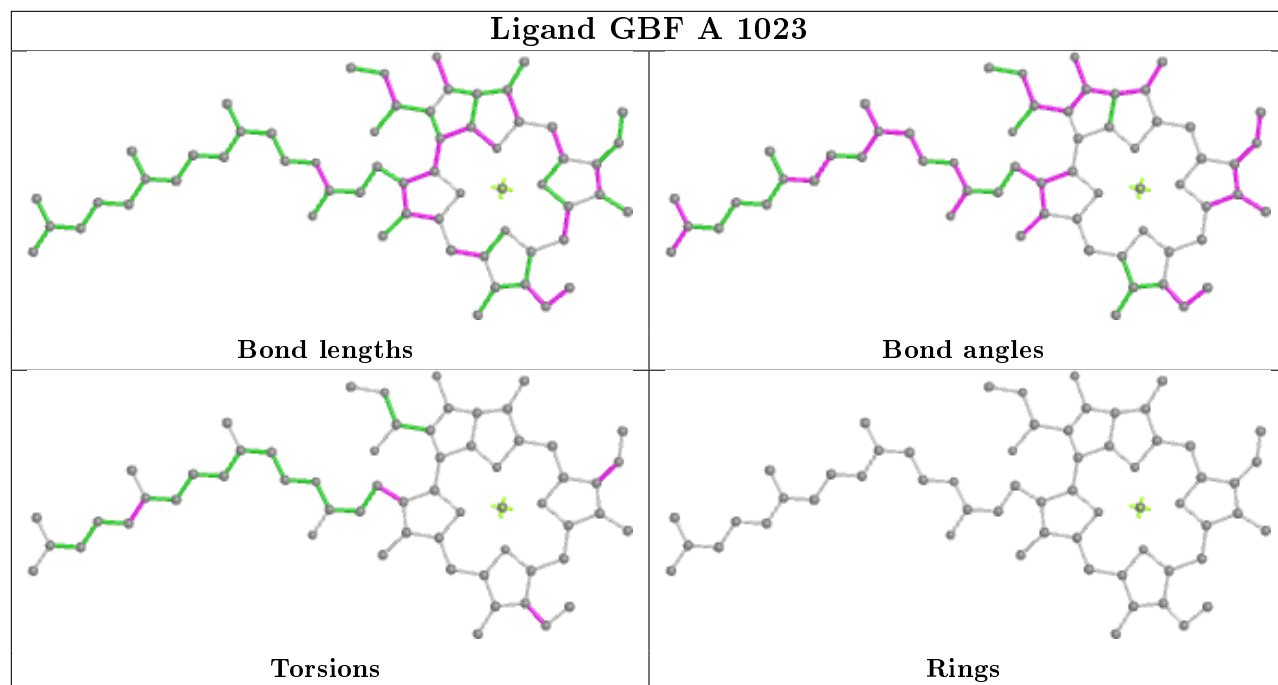




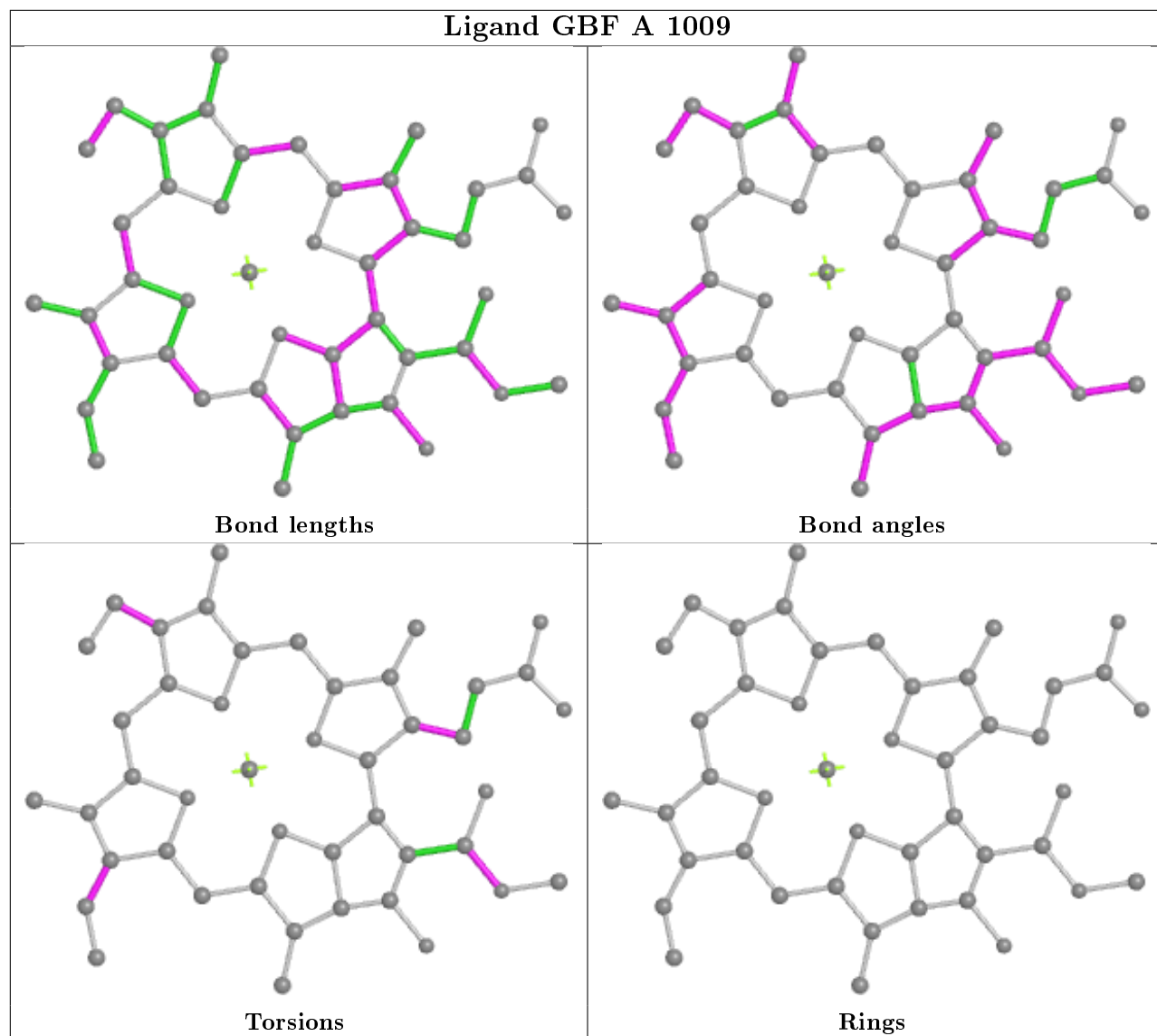
Ligand GBF A 1006

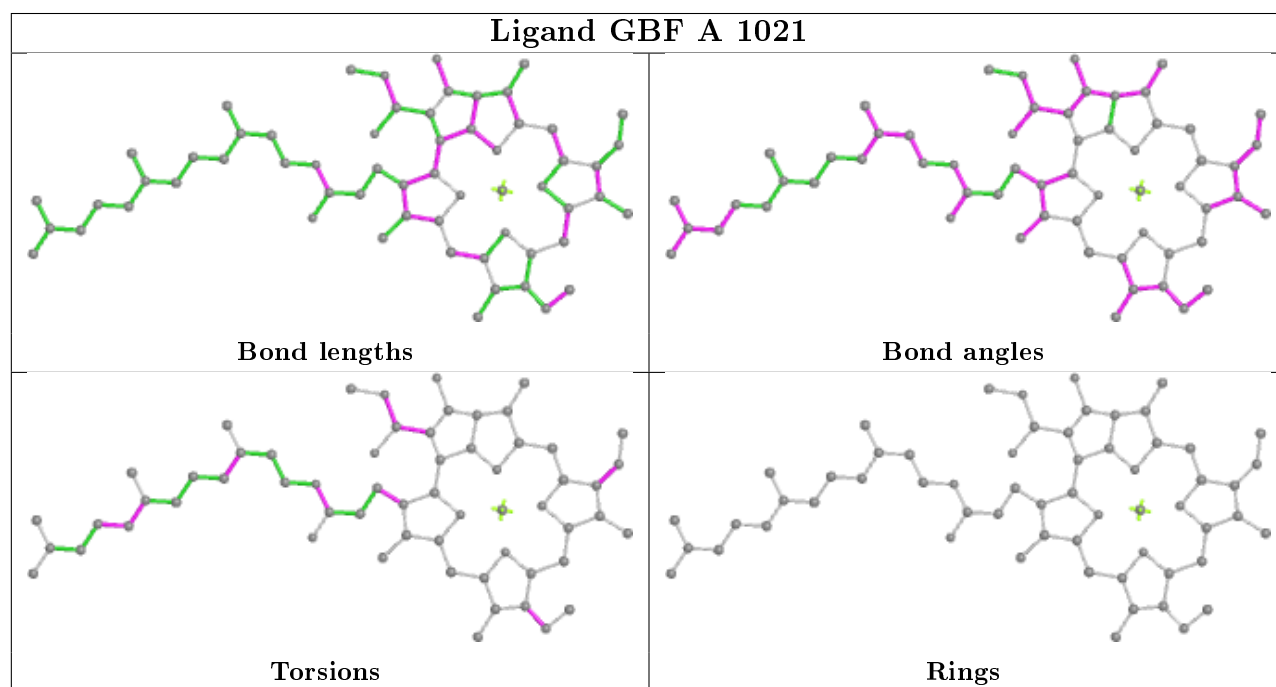
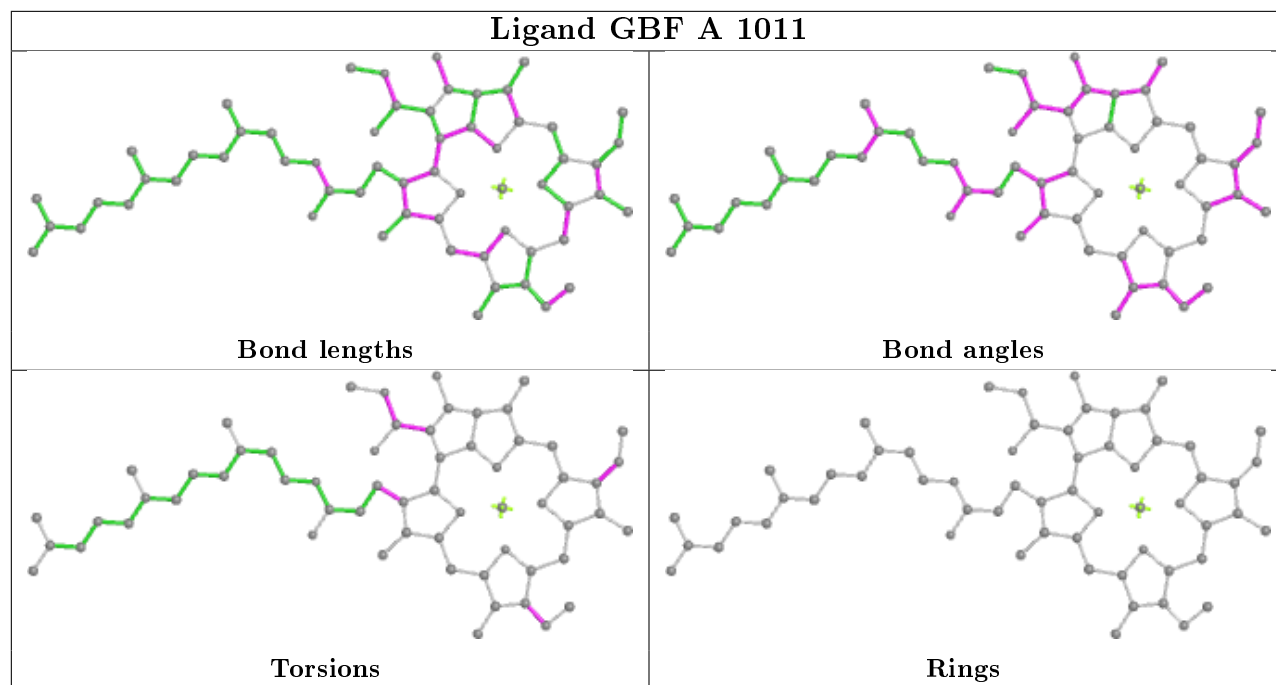


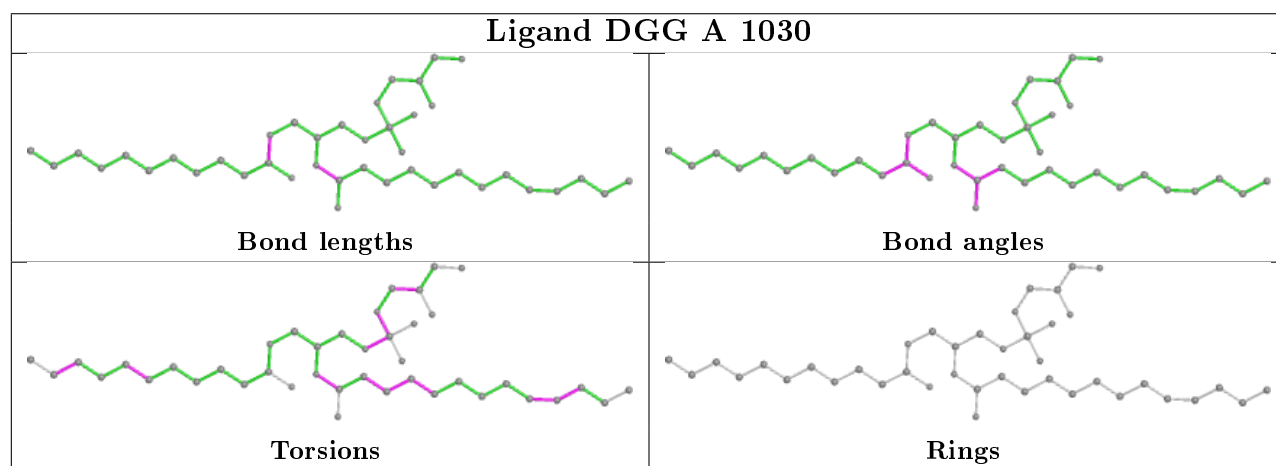
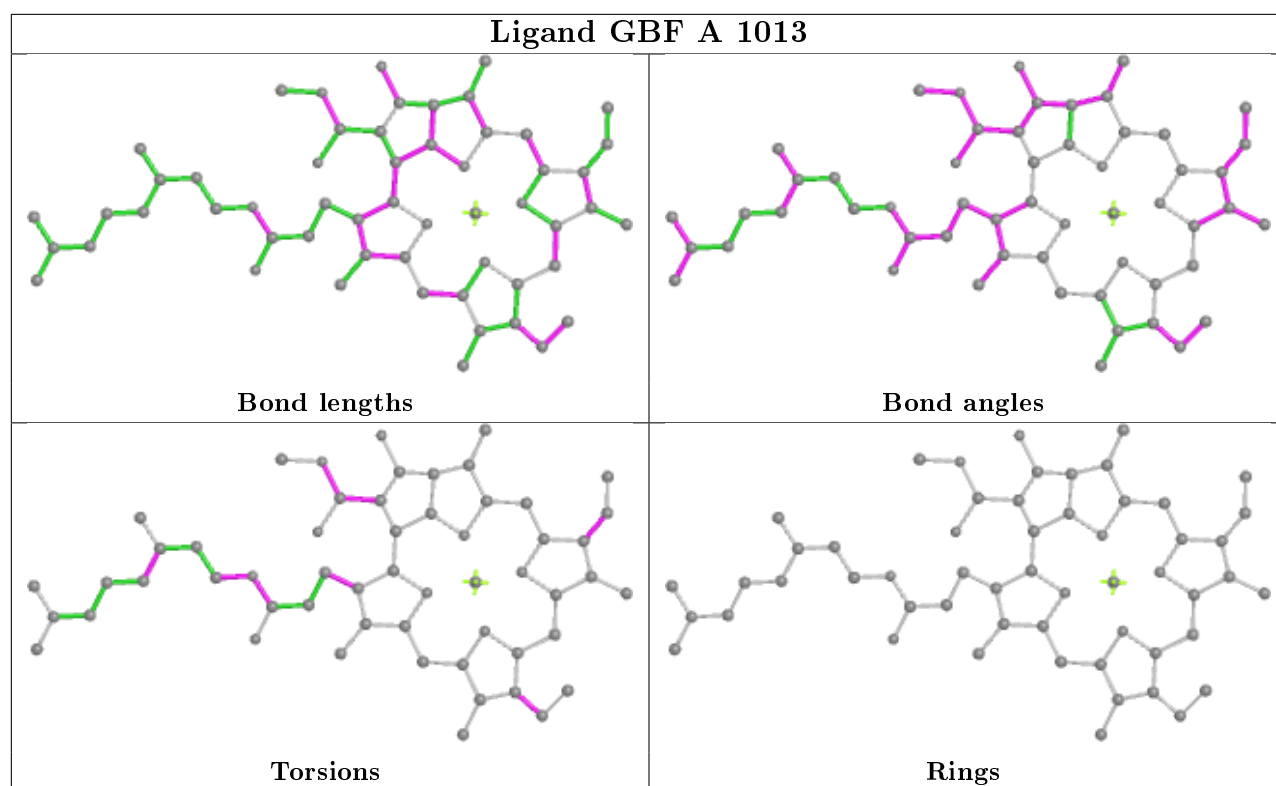


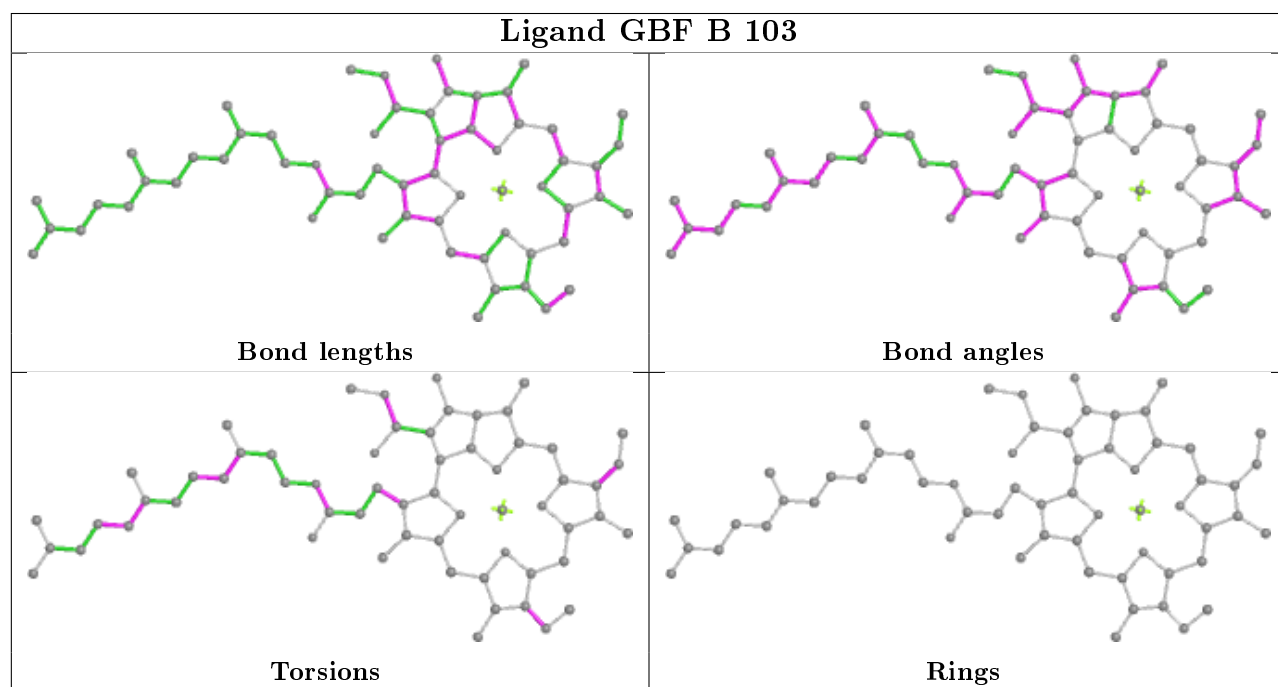
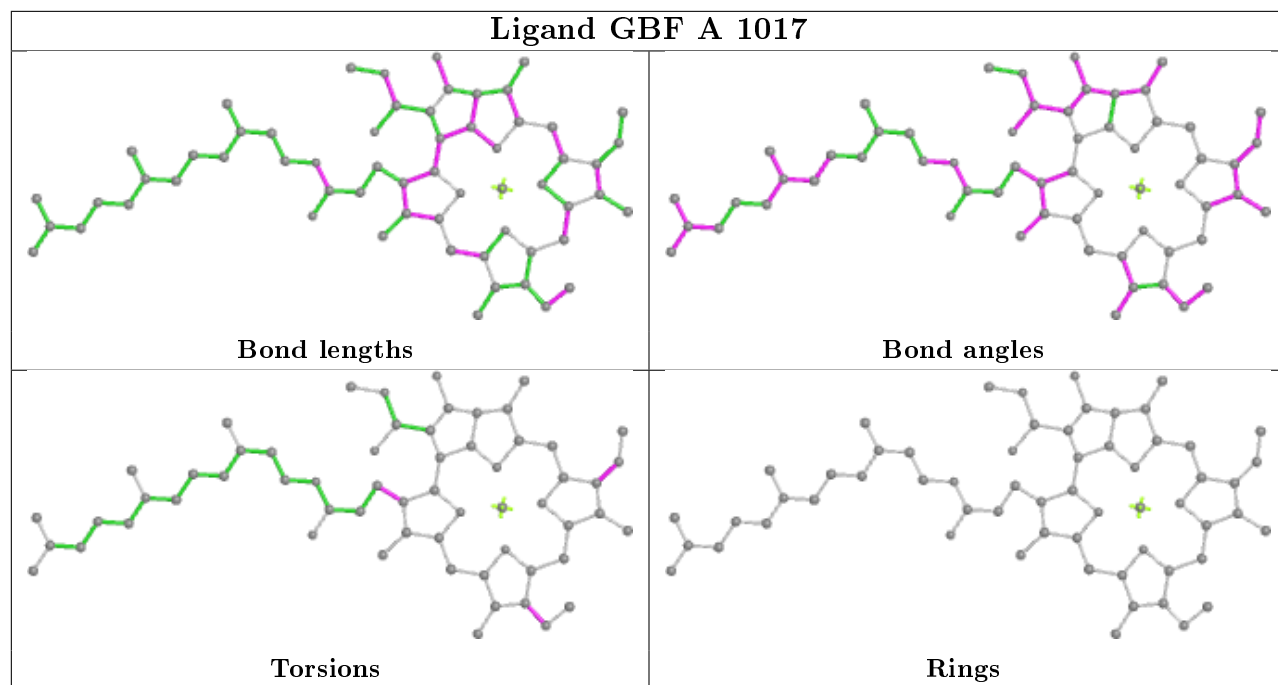


Ligand GBF A 1009

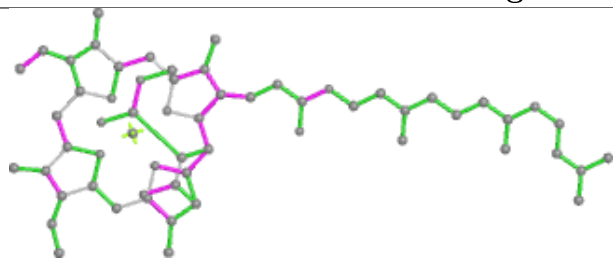




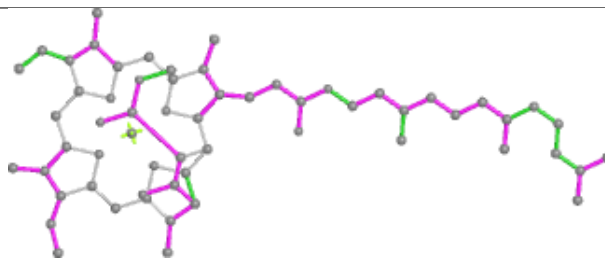




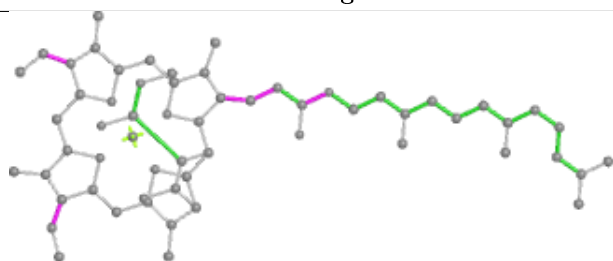
Ligand GB0 A 1005



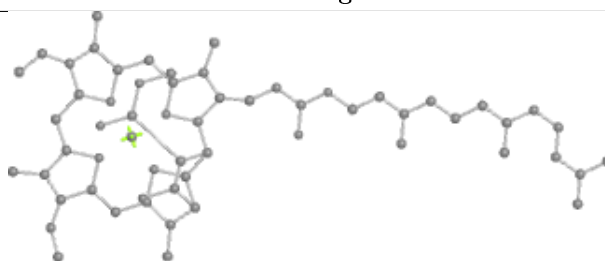
Bond lengths



Bond angles

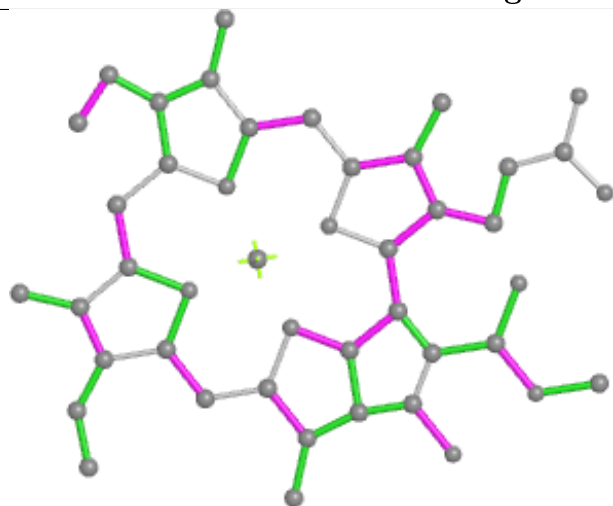


Torsions

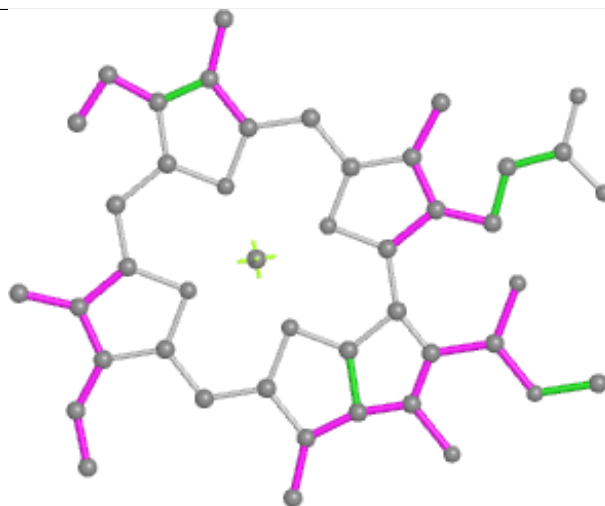


Rings

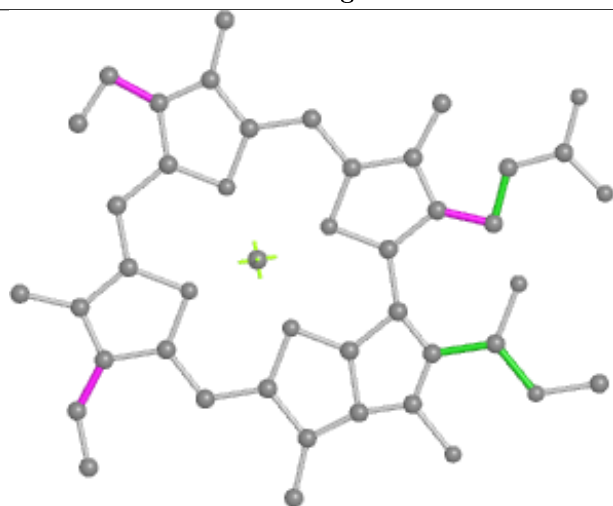
Ligand GBF A 1022



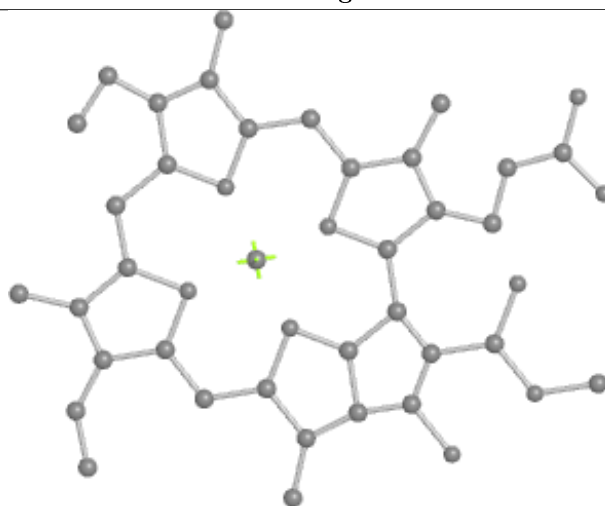
Bond lengths



Bond angles

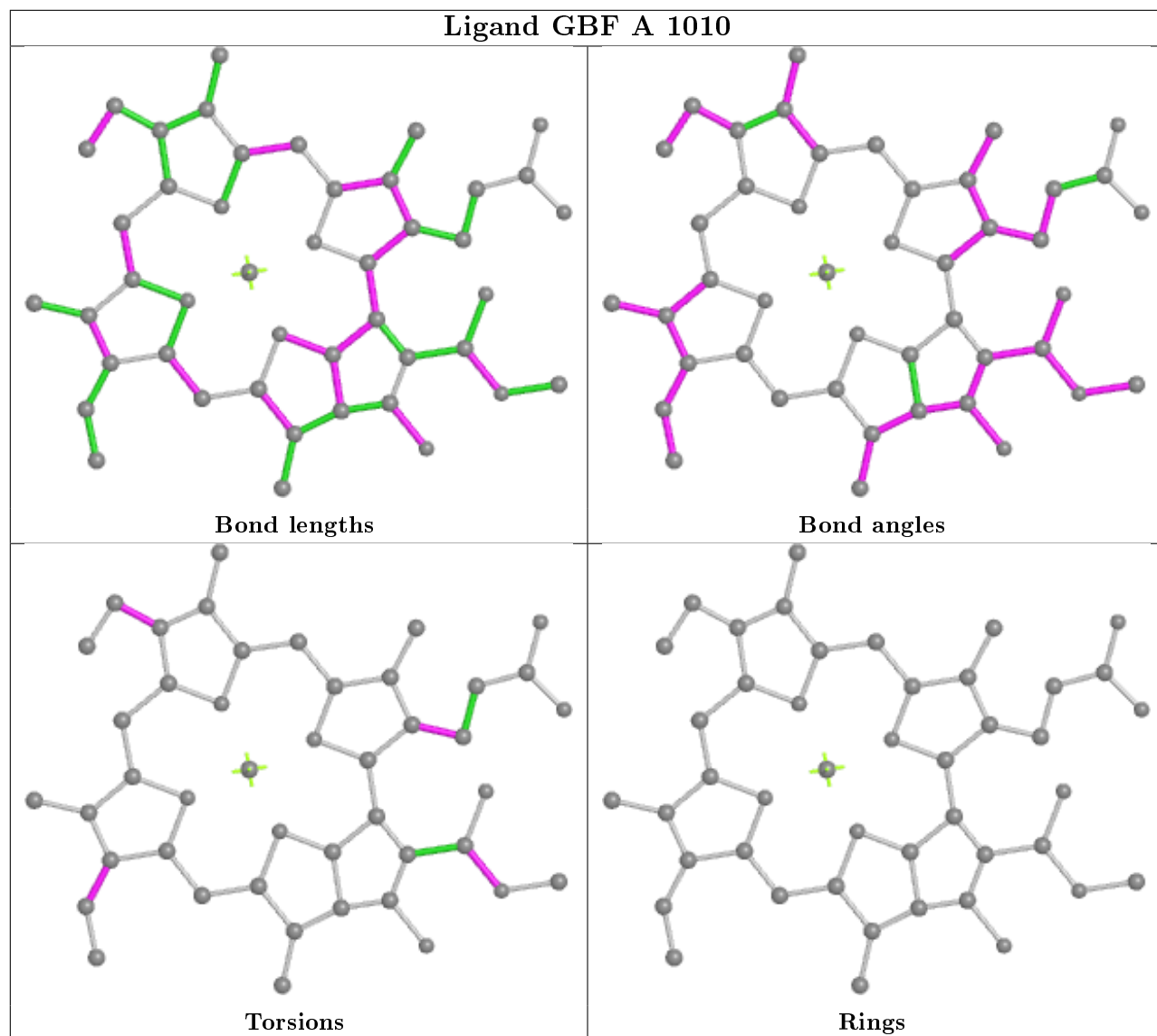


Torsions

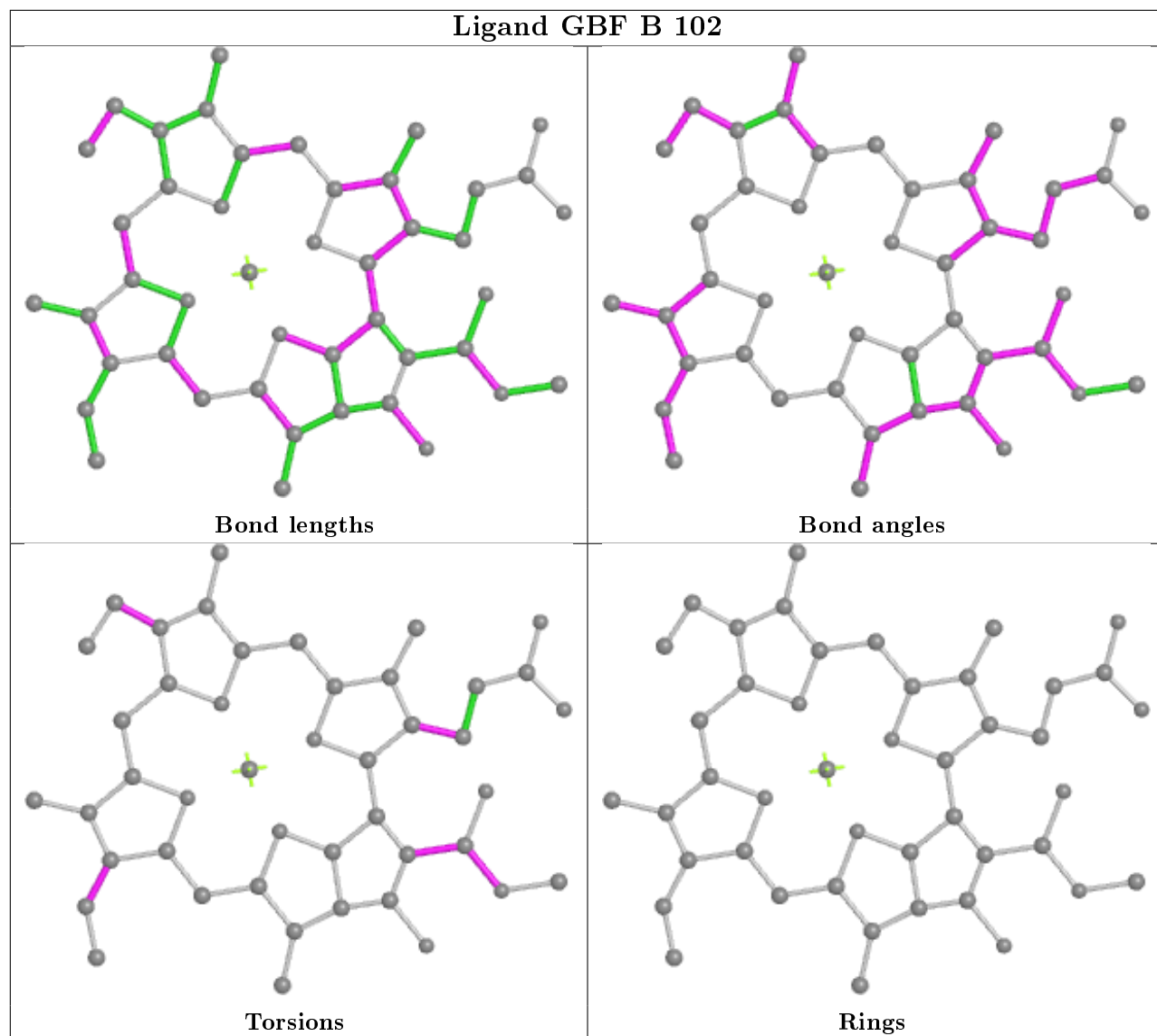


Rings

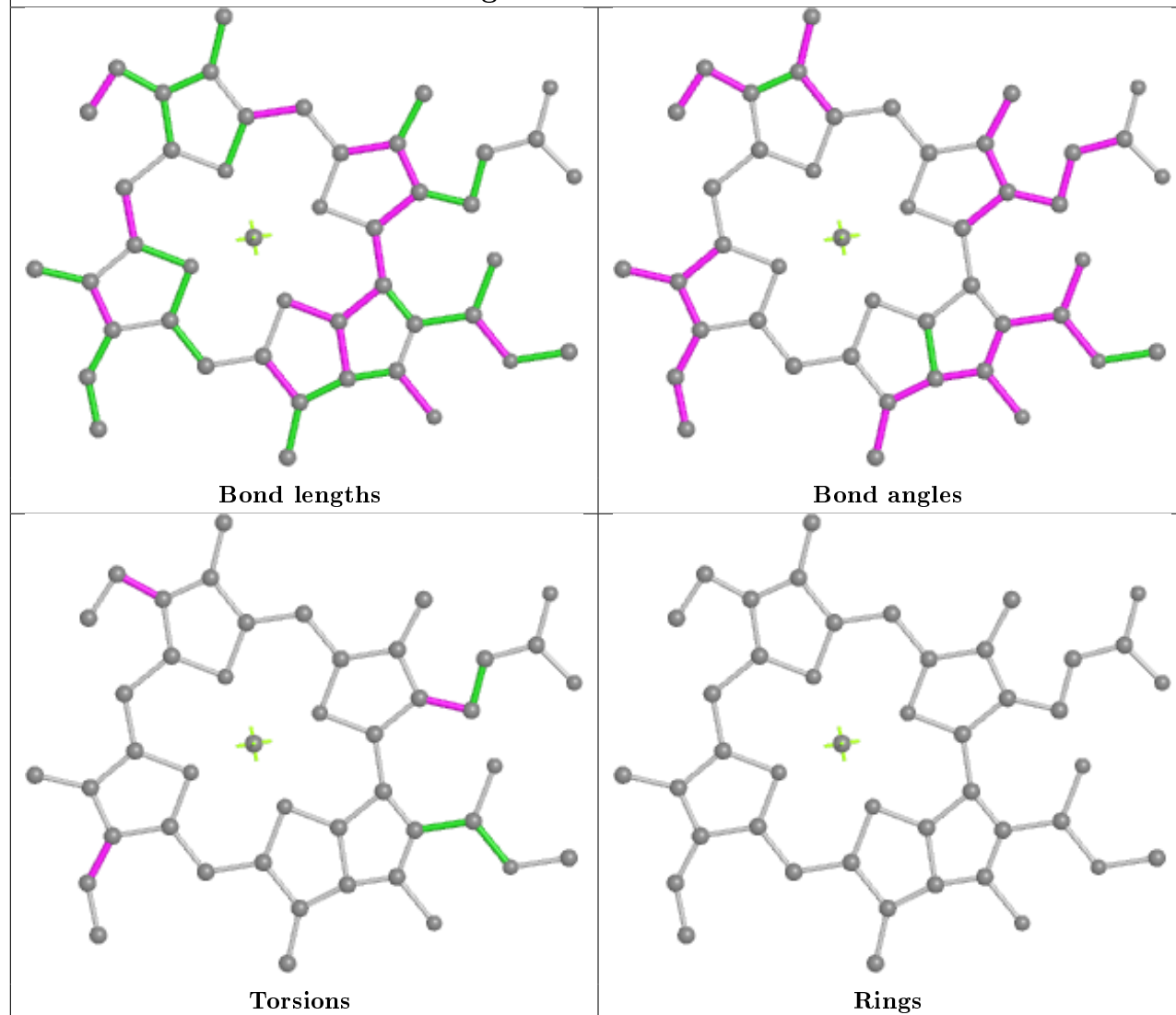
Ligand GBF A 1010



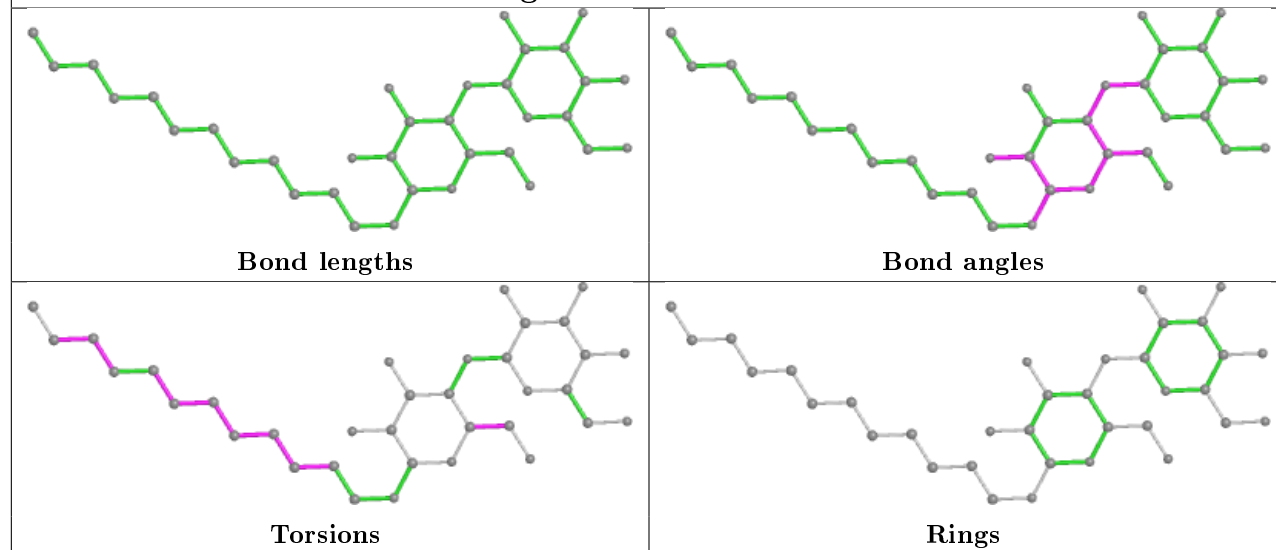
Ligand GBF B 102

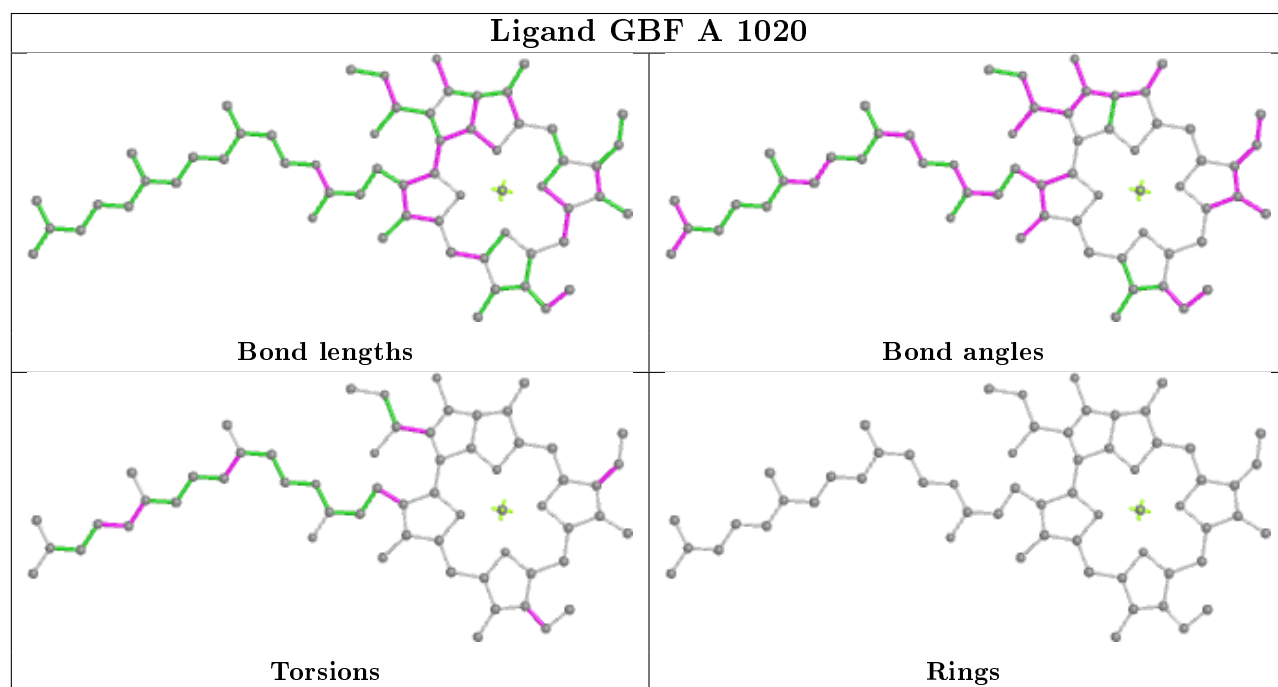
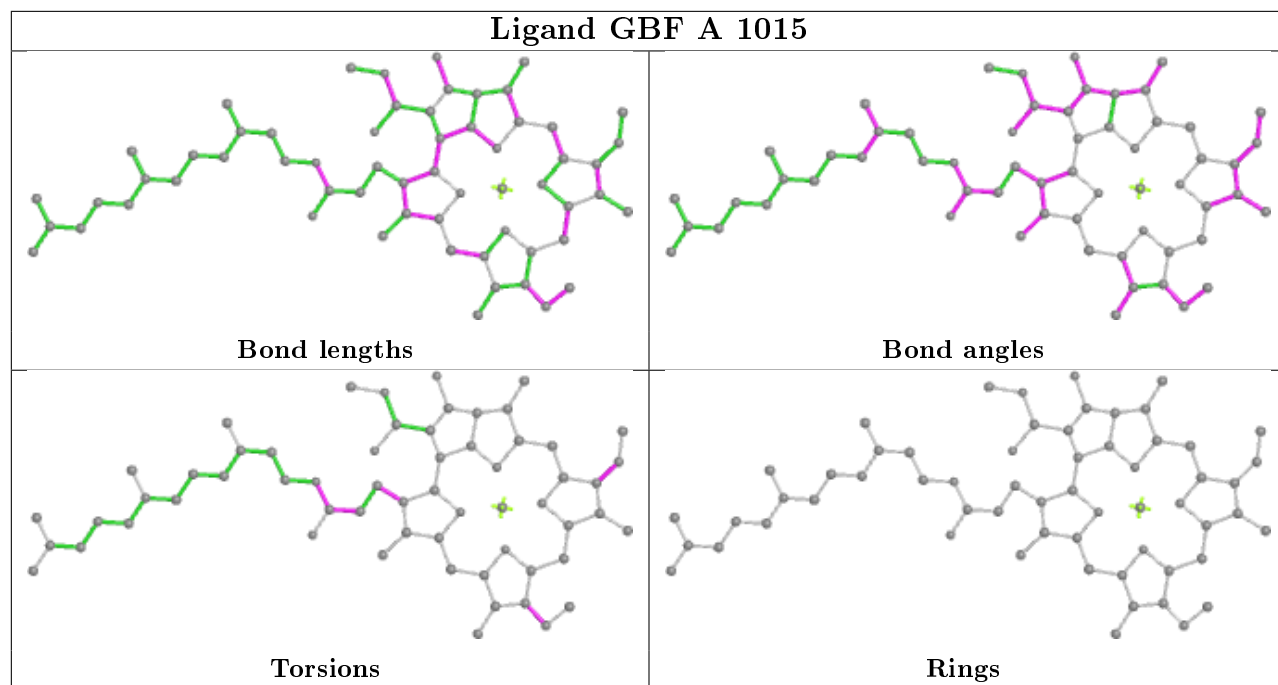


Ligand GBF A 1014

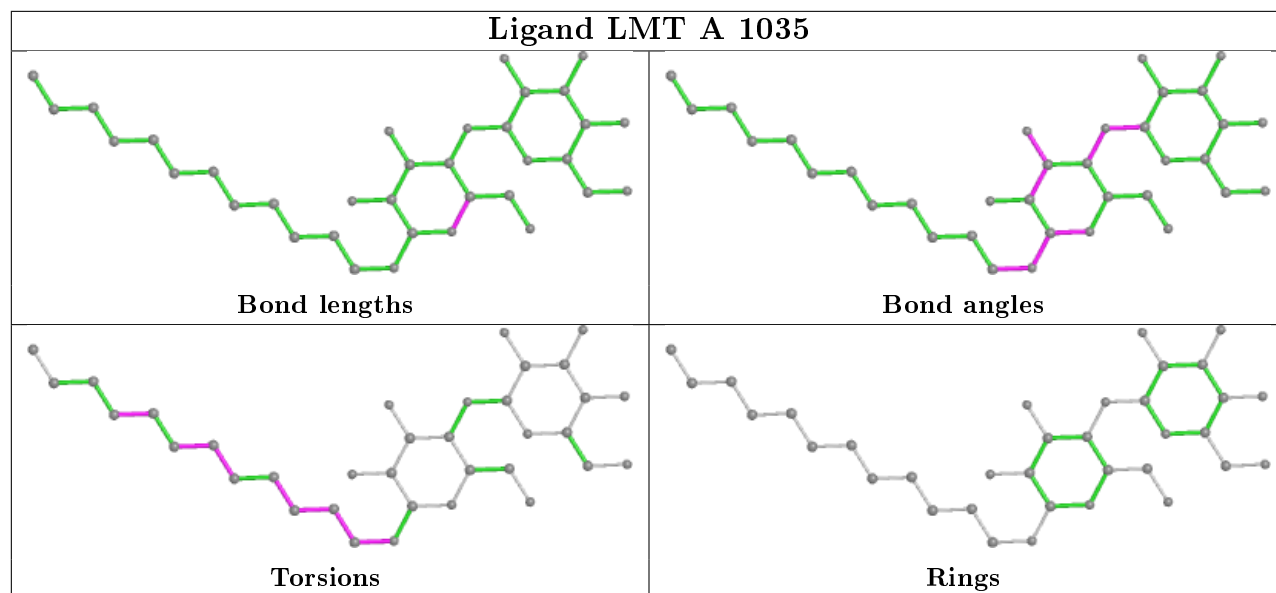


Ligand LMT A 1034

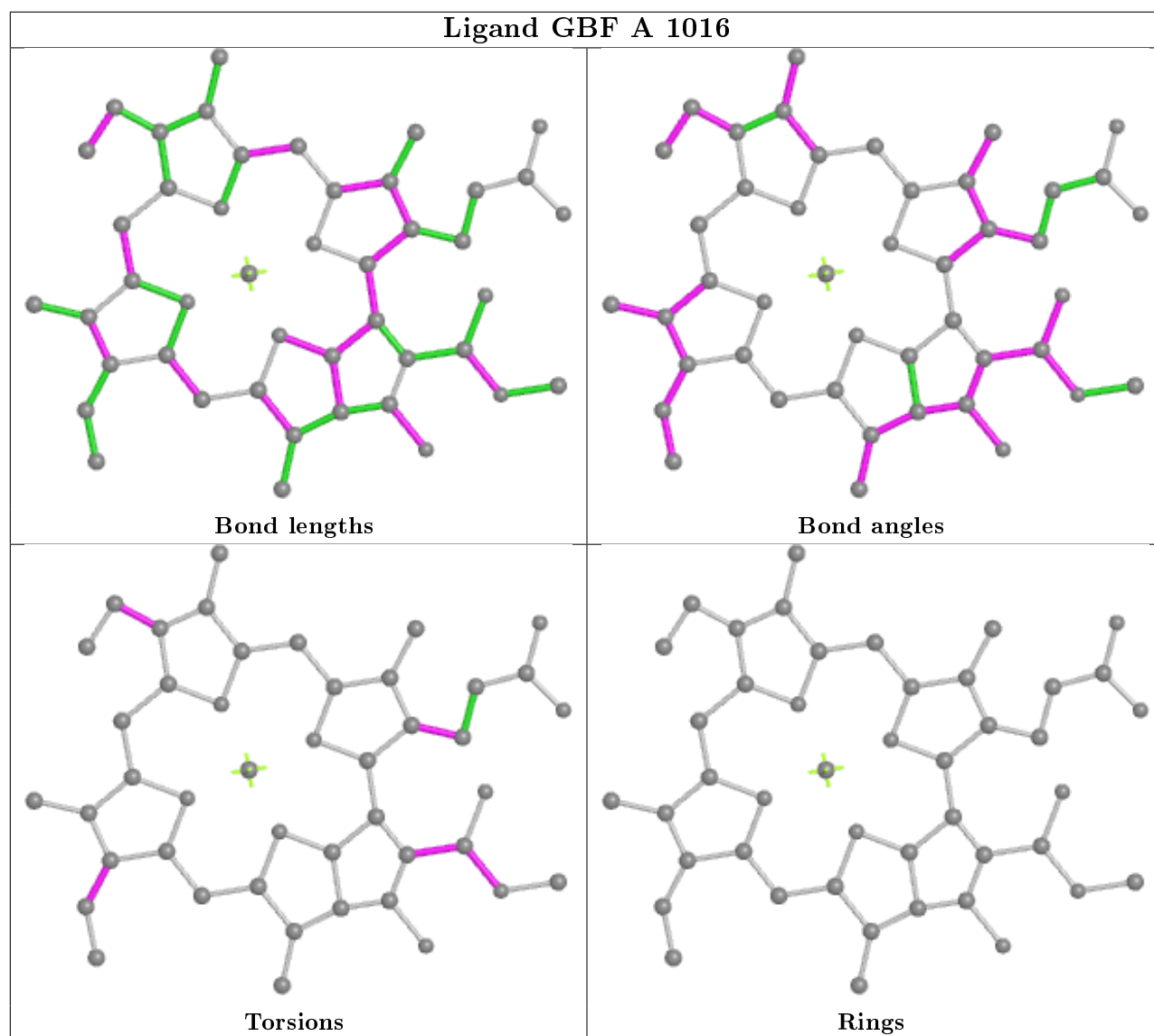


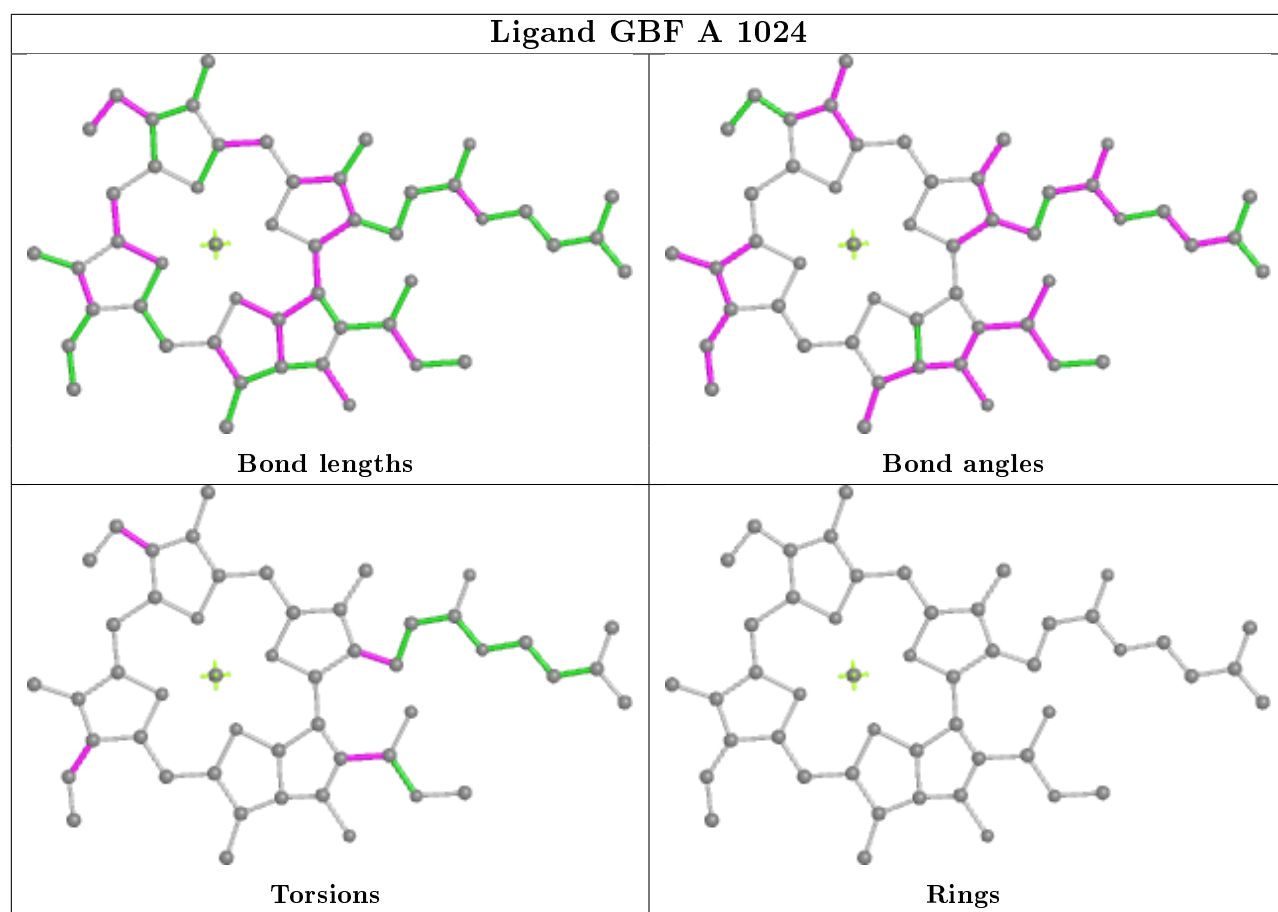


Ligand LMT A 1035

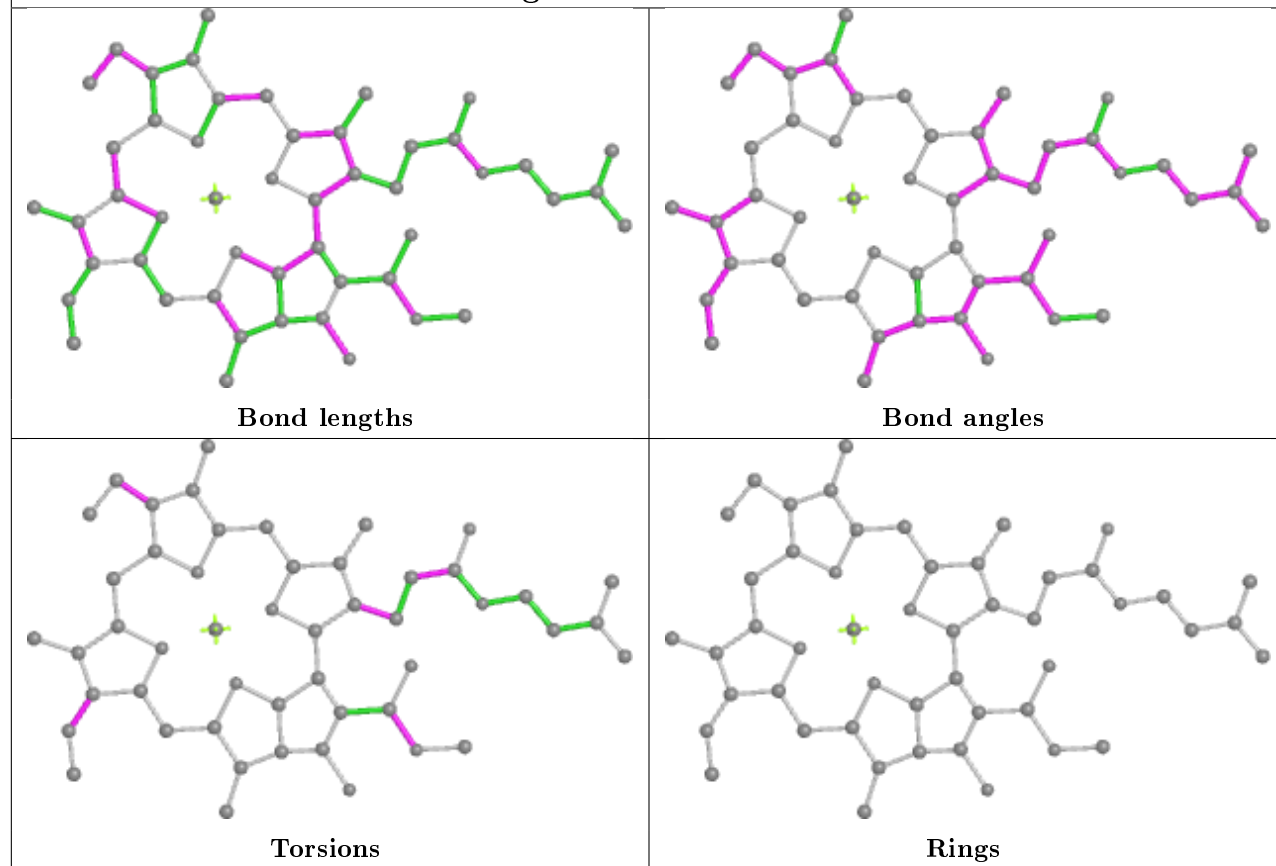


Ligand GBF A 1016

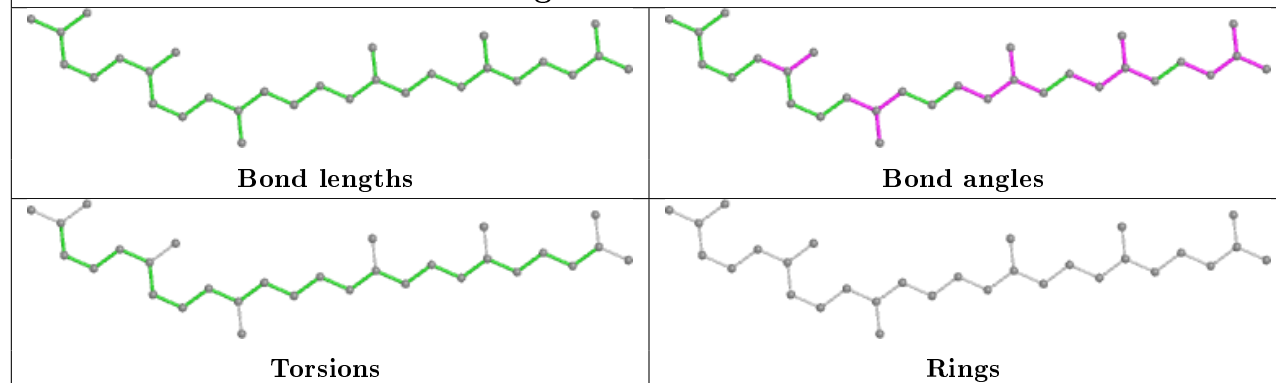


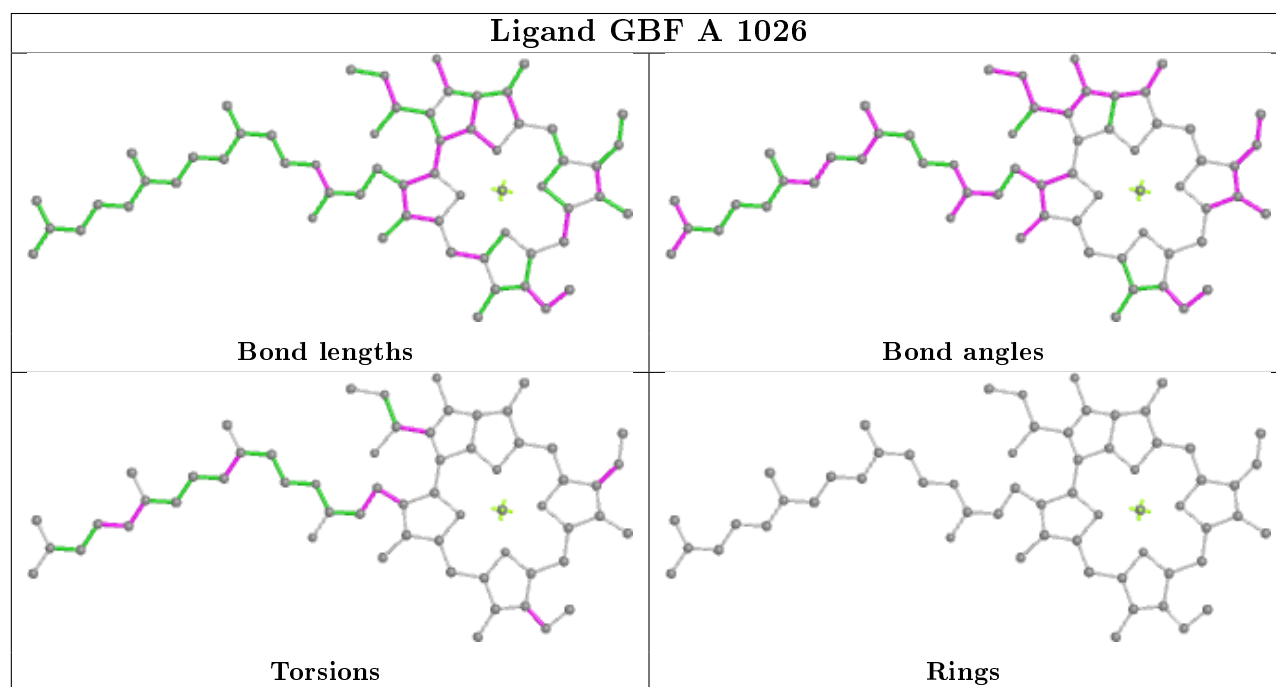
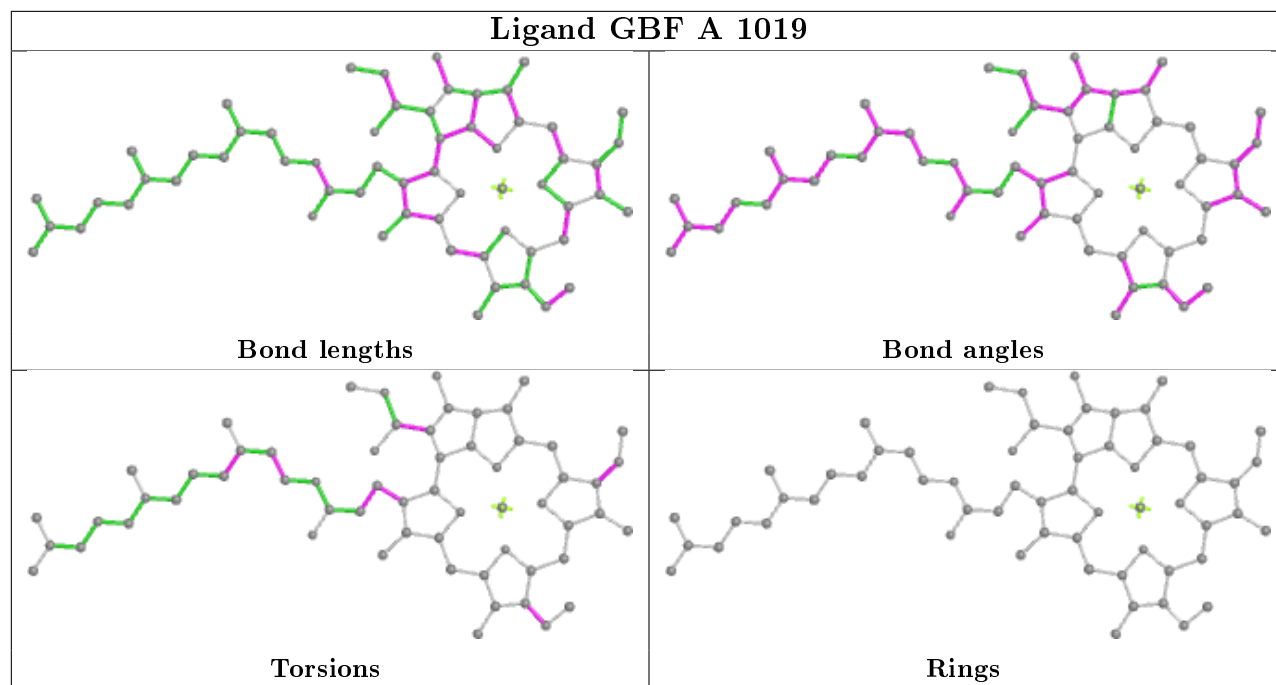


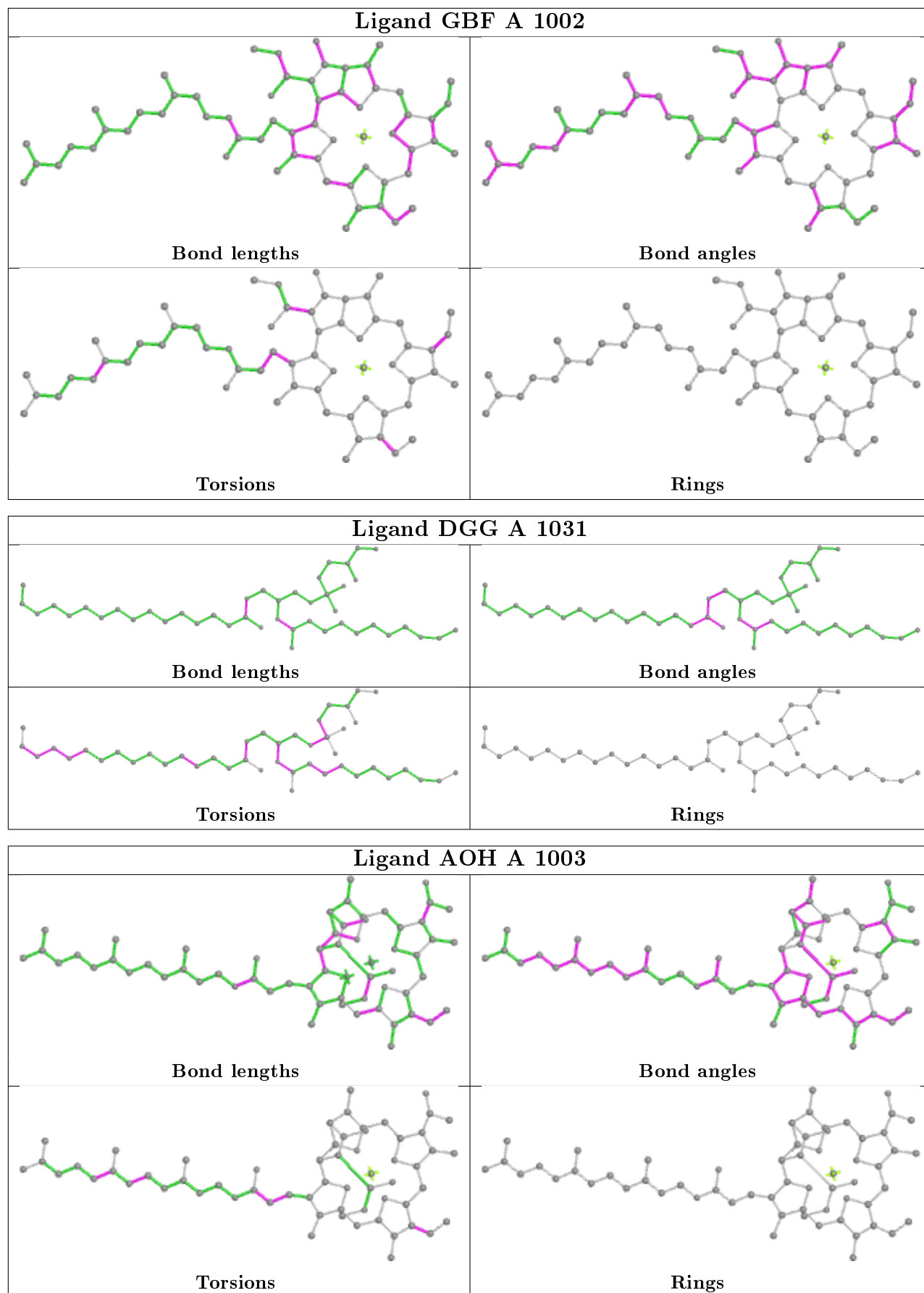
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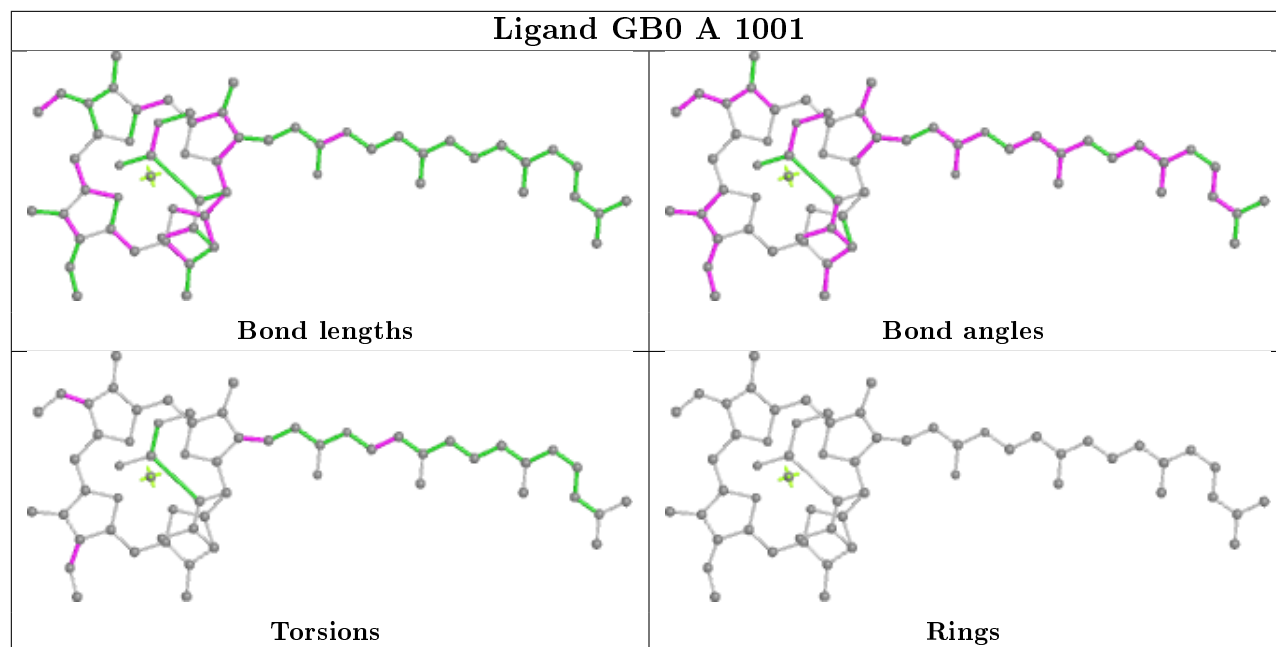


Ligand C4D B 101









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%)	0.82	126 (21%) 1 1	31, 47, 81, 147	0
2	B	25/25 (100%)	1.94	11 (44%) 0 0	77, 87, 92, 99	0
All	All	625/625 (100%)	0.86	137 (21%) 0 0	31, 48, 88, 147	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	VAL	6.0
1	A	595	PHE	5.9
1	A	198	THR	5.8
1	A	278	MET	5.7
1	A	457	LEU	5.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

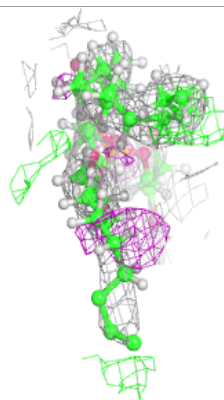
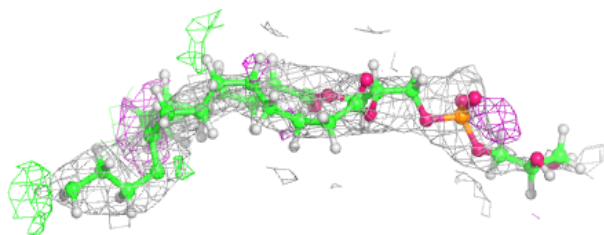
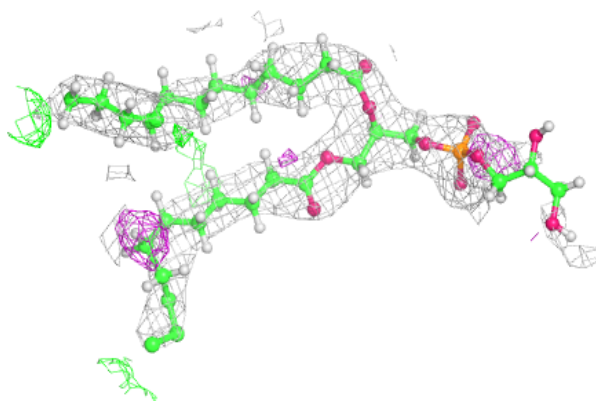
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	DGG	A	1030	41/50	0.65	0.33	56,73,102,102	0
7	DGG	A	1031	44/50	0.71	0.27	73,95,109,115	0
4	GBF	B	102	45/60	0.76	0.40	69,97,105,109	0
10	C4D	B	101	30/30	0.77	0.25	39,58,65,69	0
4	GBF	B	103	60/60	0.80	0.32	68,82,96,98	0
9	LMT	A	1035	35/35	0.81	0.34	20,20,20,20	0
4	GBF	A	1009	45/60	0.84	0.21	70,98,105,110	0
4	GBF	A	1016	45/60	0.86	0.23	53,67,97,107	0
9	LMT	A	1034	35/35	0.87	0.38	20,20,20,20	0
4	GBF	A	1013	55/60	0.87	0.16	49,61,77,85	0
4	GBF	A	1028	60/60	0.88	0.39	46,61,75,77	0
4	GBF	A	1010	45/60	0.90	0.21	54,66,103,105	0
4	GBF	A	1011	60/60	0.90	0.15	49,61,77,79	0
4	GBF	A	1018	50/60	0.91	0.17	41,50,79,79	0
4	GBF	A	1017	60/60	0.92	0.17	40,53,60,63	0
4	GBF	A	1007	60/60	0.92	0.15	38,57,95,97	0
4	GBF	A	1002	60/60	0.92	0.29	25,33,57,67	0
5	AOH	A	1003	61/61	0.92	0.22	26,37,56,58	0
4	GBF	A	1019	60/60	0.93	0.19	43,52,94,96	0
8	CA	A	1033	1/1	0.93	0.11	84,84,84,84	0
8	CA	A	1032	1/1	0.94	0.17	39,39,39,39	0
4	GBF	A	1027	50/60	0.94	0.13	36,47,75,81	0
4	GBF	A	1021	60/60	0.94	0.23	35,43,92,98	0
4	GBF	A	1012	55/60	0.94	0.21	61,71,93,97	0
4	GBF	A	1014	45/60	0.94	0.15	50,58,83,102	0
4	GBF	A	1006	45/60	0.94	0.13	43,53,80,94	0
4	GBF	A	1022	45/60	0.94	0.13	36,45,67,90	0
4	GBF	A	1008	55/60	0.95	0.18	43,51,81,83	0
4	GBF	A	1004	50/60	0.95	0.19	39,47,56,58	0
4	GBF	A	1020	60/60	0.95	0.34	33,43,65,72	0
4	GBF	A	1026	60/60	0.95	0.19	27,38,75,77	0
4	GBF	A	1023	60/60	0.95	0.16	35,42,57,60	0
4	GBF	A	1025	45/60	0.95	0.13	43,51,86,103	0
4	GBF	A	1024	50/60	0.95	0.12	41,49,82,85	0
4	GBF	A	1015	60/60	0.96	0.17	39,48,53,57	0
3	GB0	A	1001	60/60	0.96	0.26	25,33,39,42	0
3	GB0	A	1005	60/60	0.96	0.32	35,47,90,91	0
6	SF4	A	1029	8/8	0.99	0.14	38,42,42,43	8

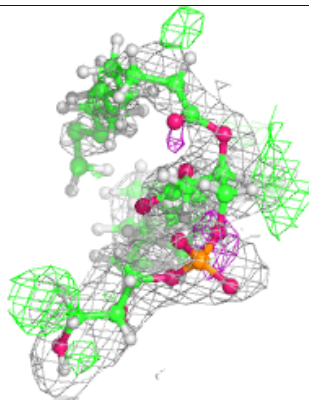
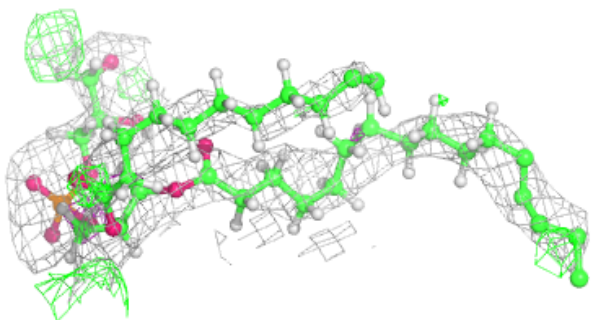
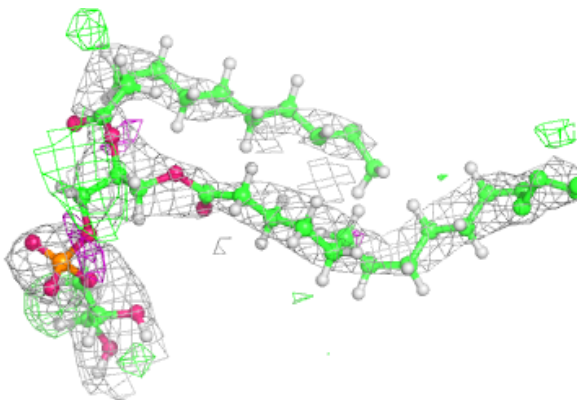
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

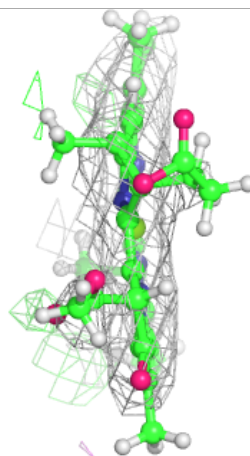
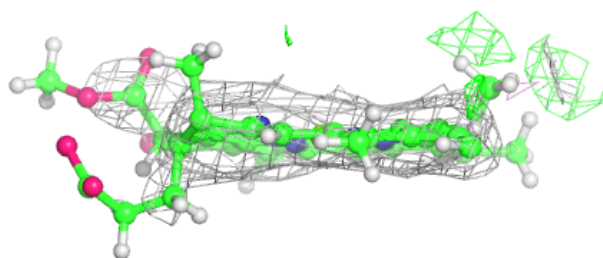
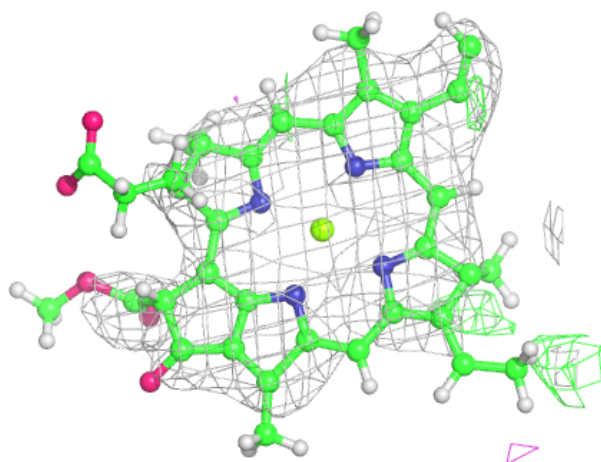
**Electron density around DGG A 1031:**

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



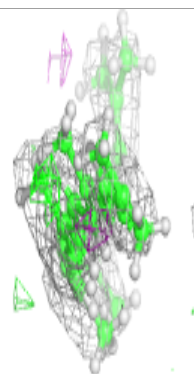
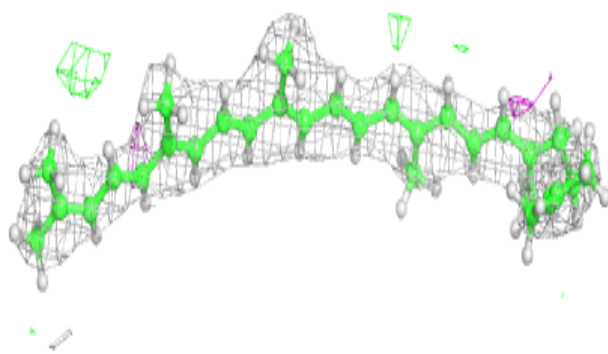
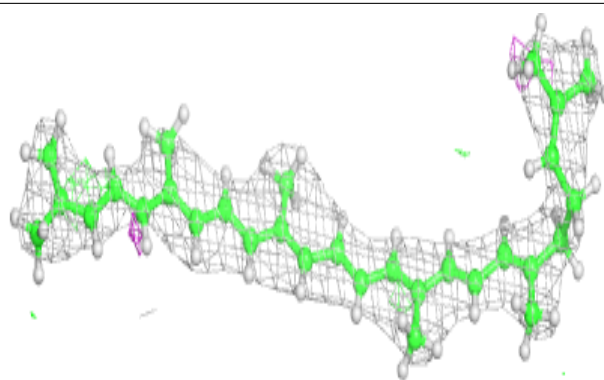
Electron density around GBF B 102:

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

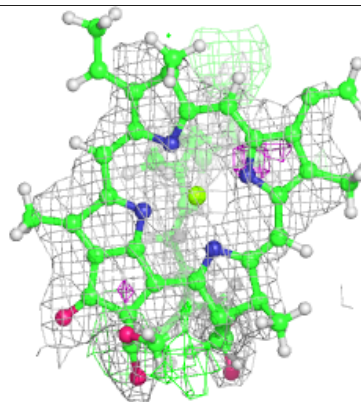
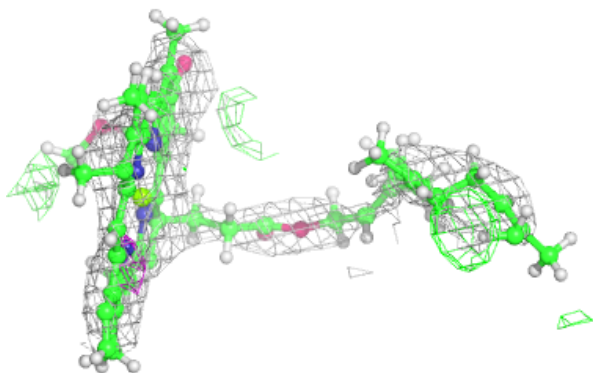
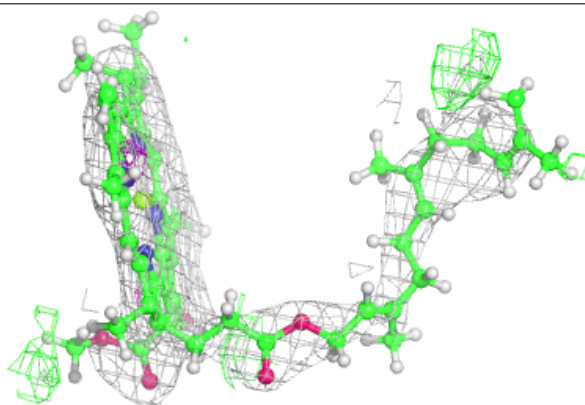


Electron density around C4D B 101:

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

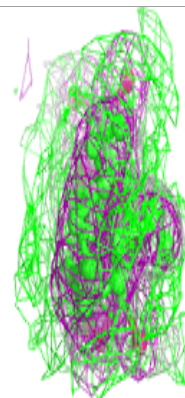
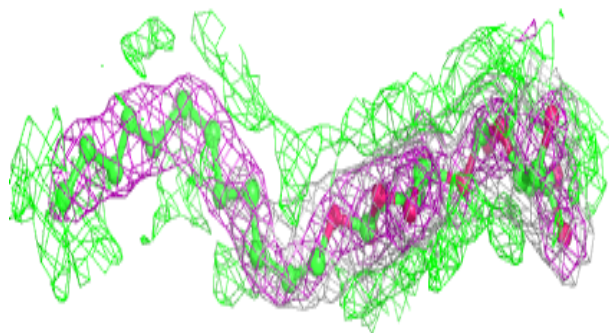
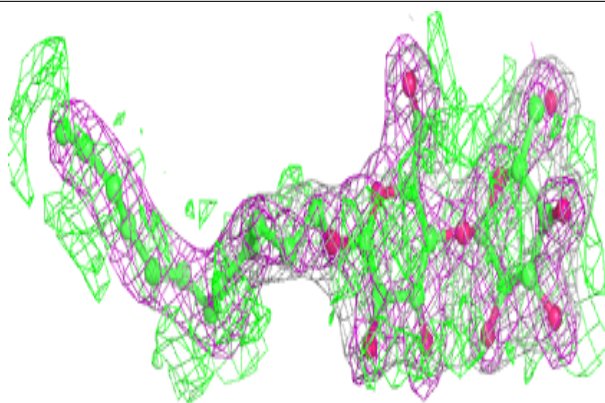
**Electron density around GBF B 103:**

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



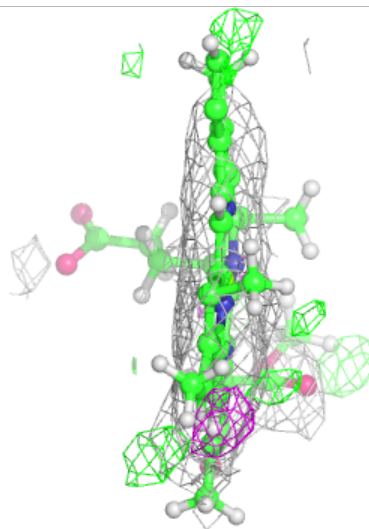
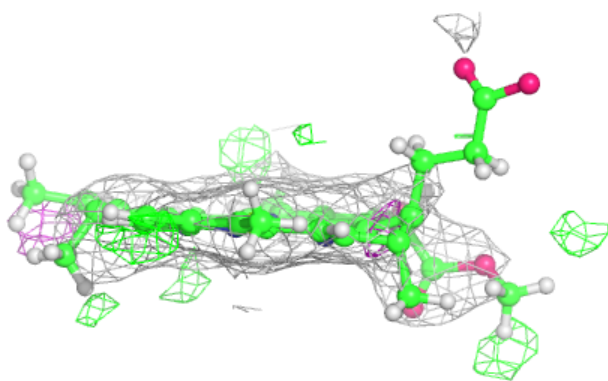
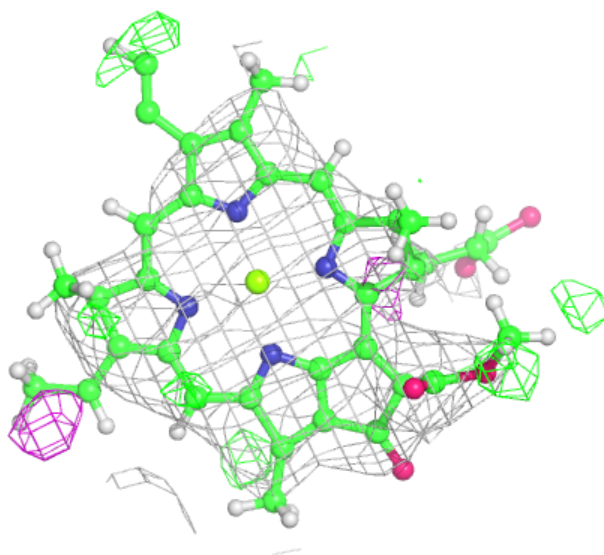
Electron density around LMT A 1035:

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



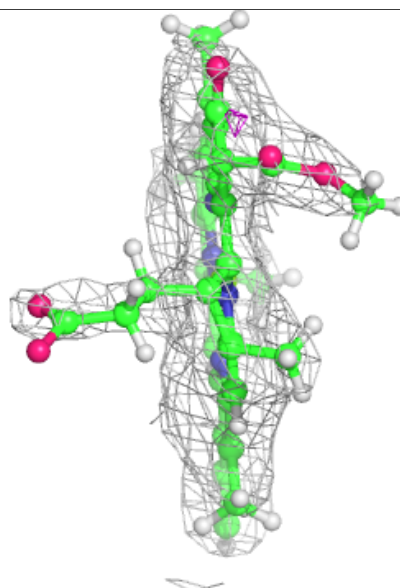
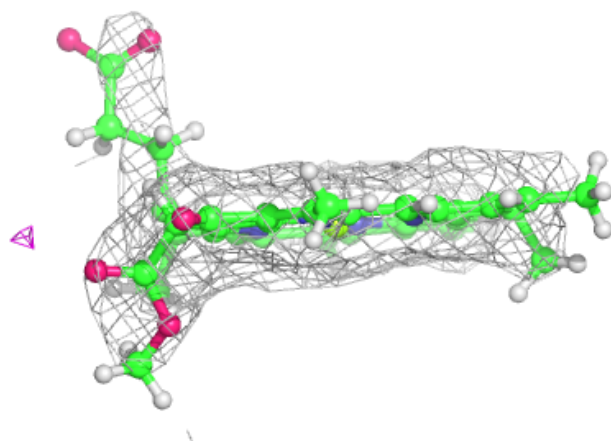
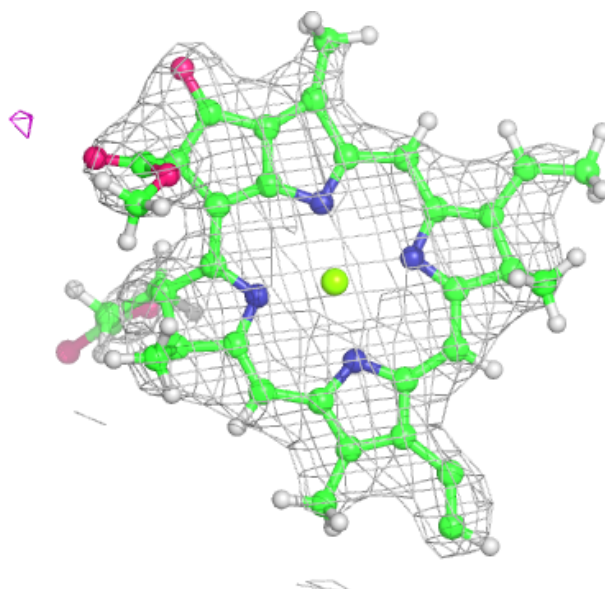
Electron density around GBF A 1009:

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



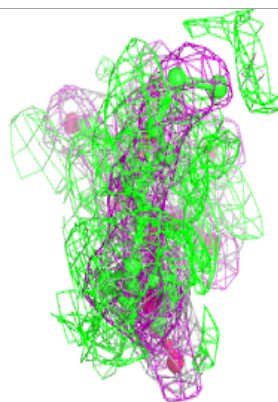
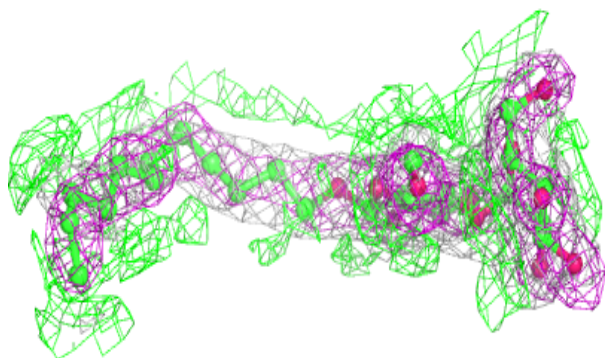
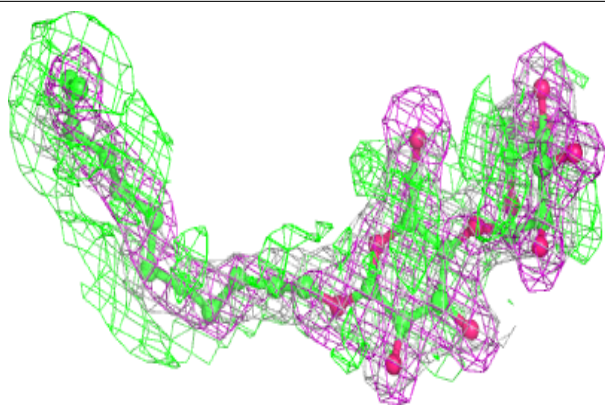
Electron density around GBF A 1016:

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

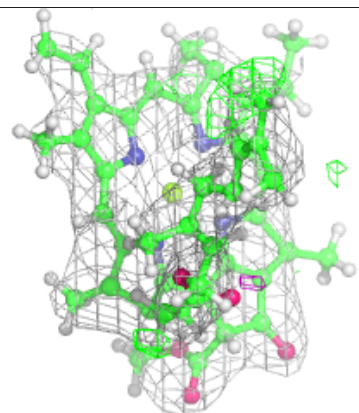
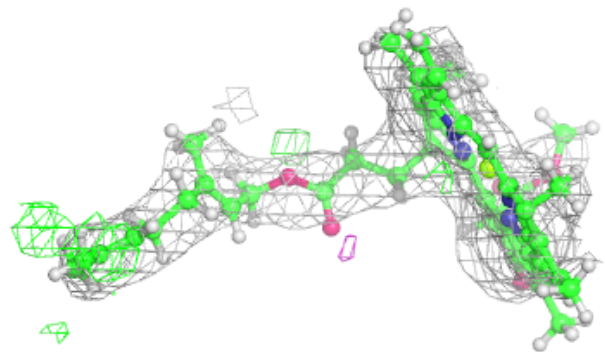
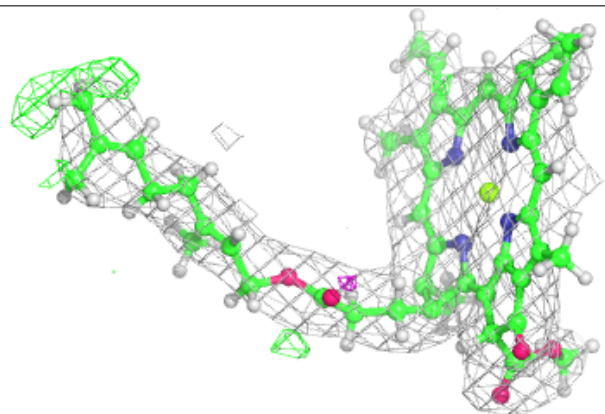


Electron density around LMT A 1034:

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

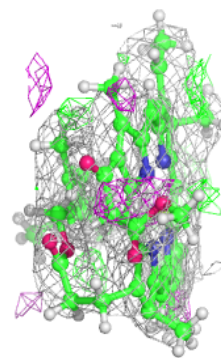
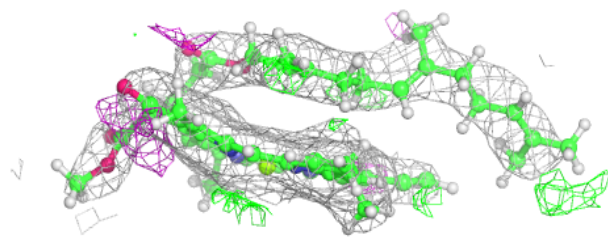
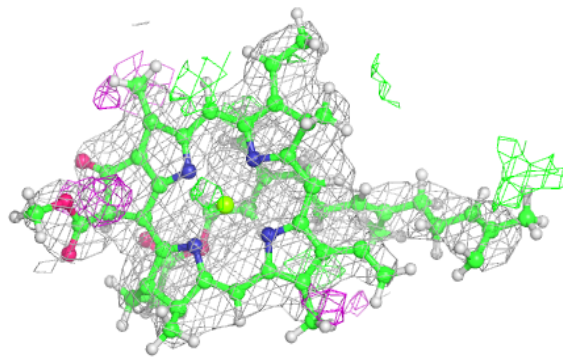
**Electron density around GBF A 1013:**

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



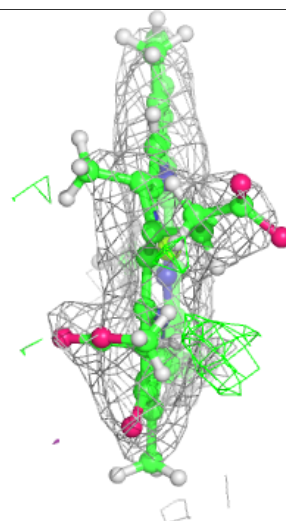
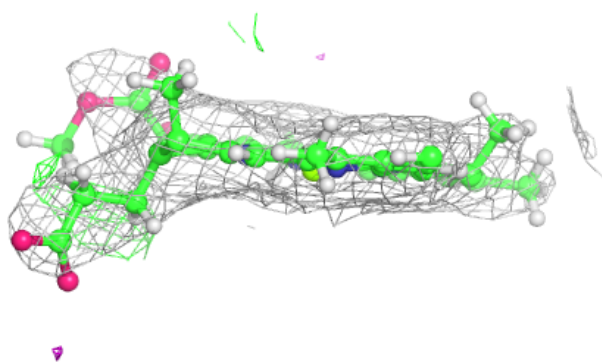
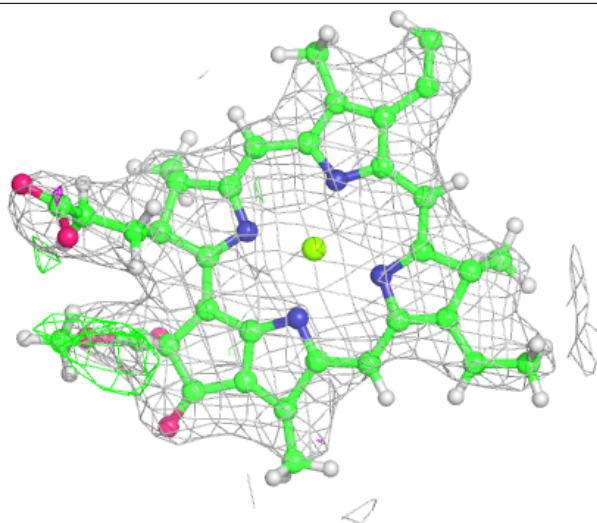
Electron density around GBF A 1028:

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



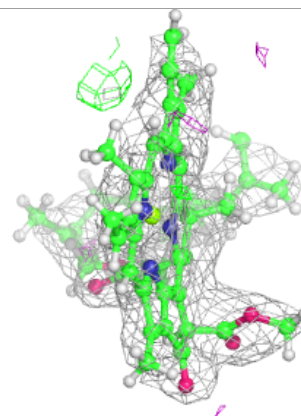
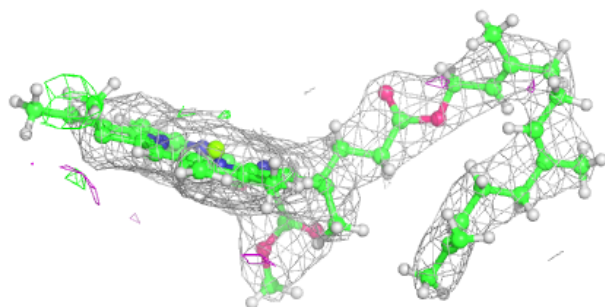
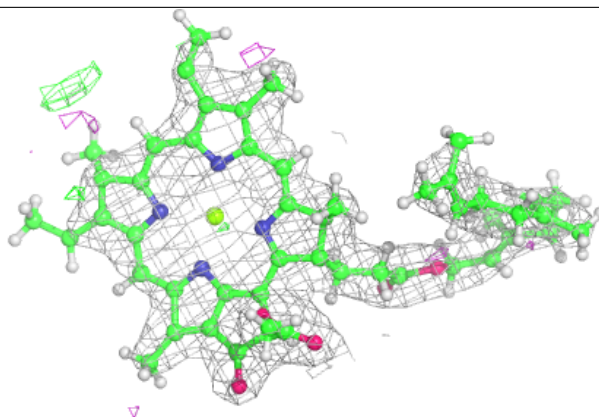
Electron density around GBF A 1010:

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



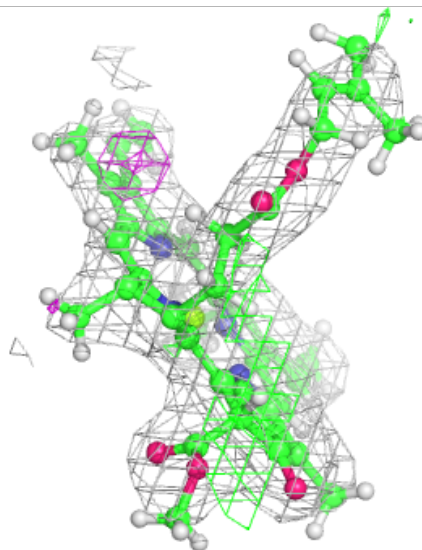
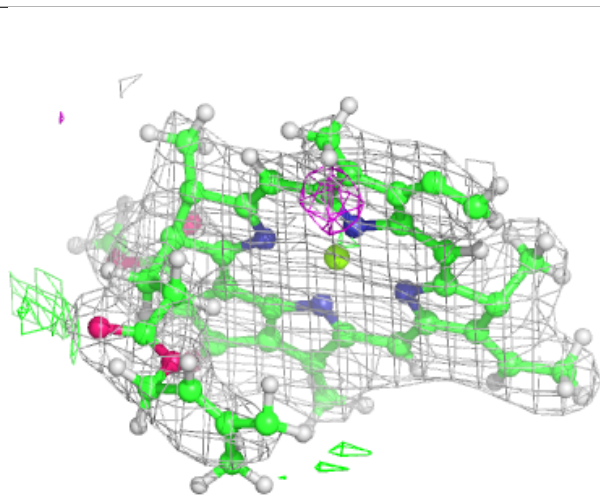
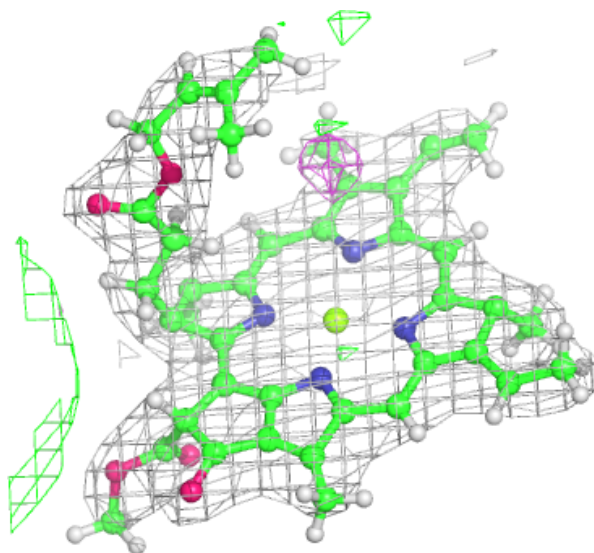
Electron density around GBF A 1011:

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



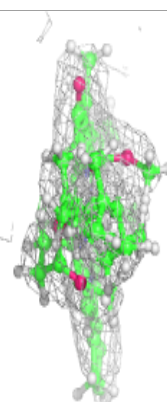
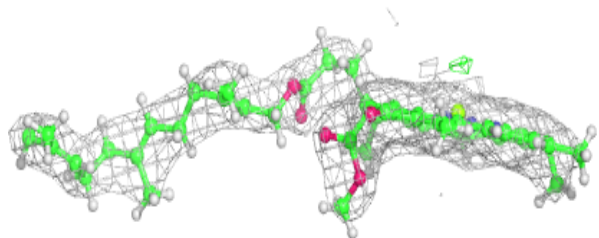
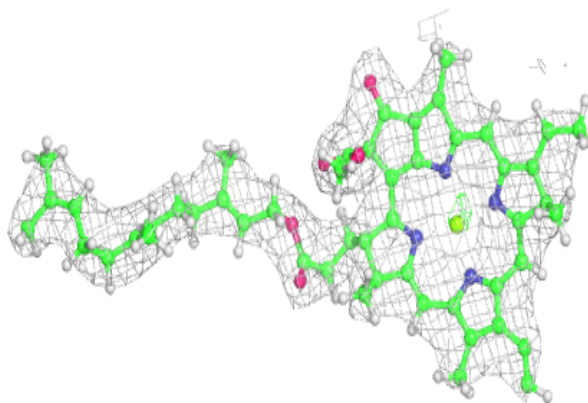
Electron density around GBF A 1018:

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

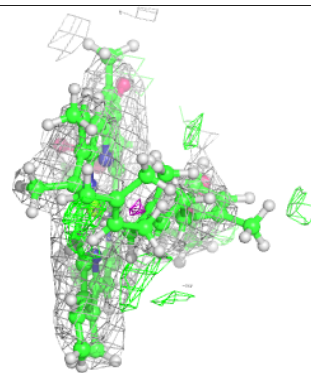
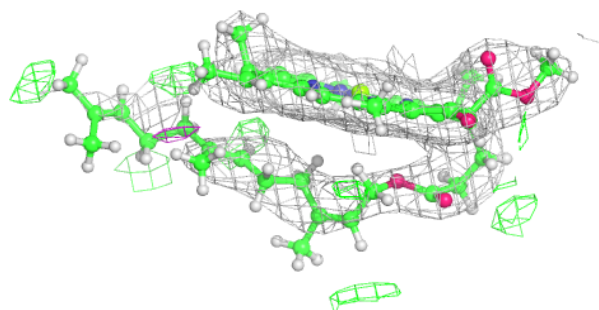
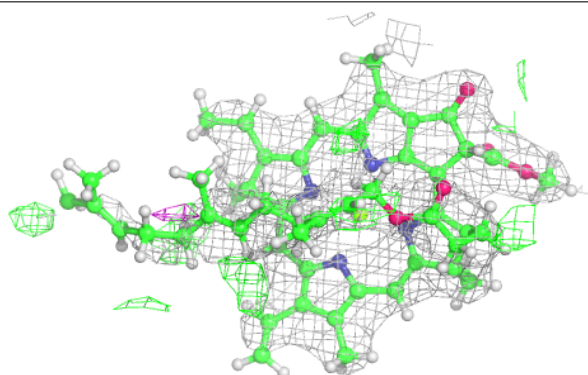


Electron density around GBF A 1017:

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

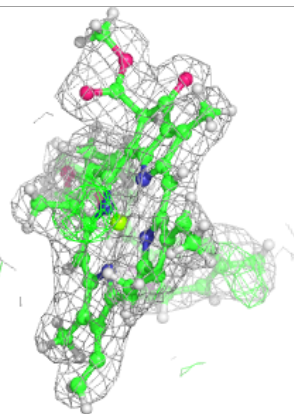
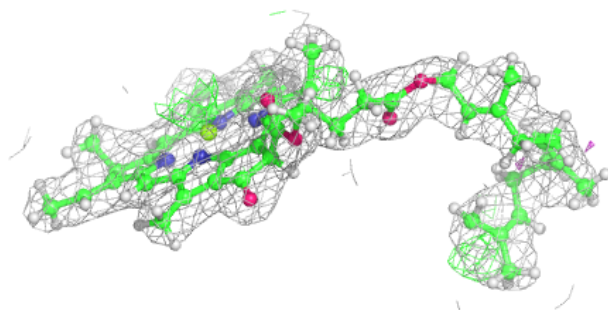
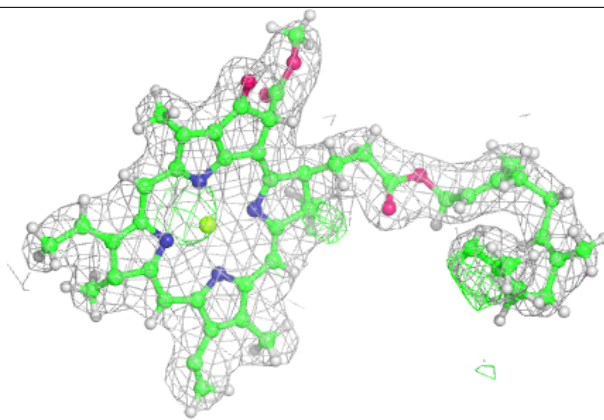
**Electron density around GBF A 1007:**

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



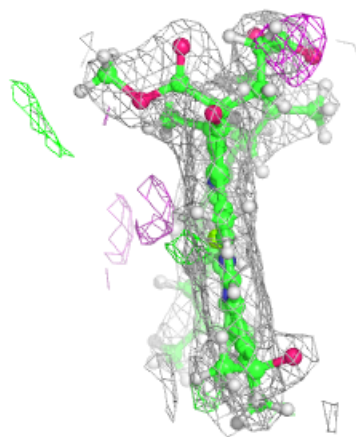
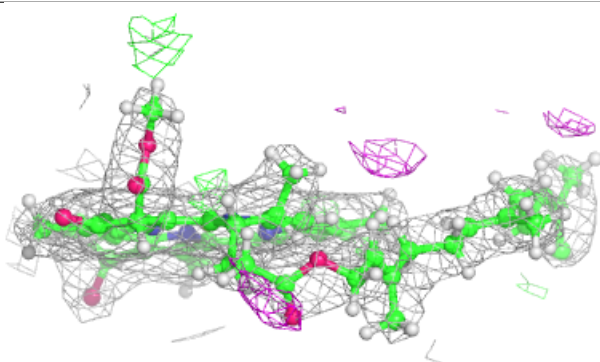
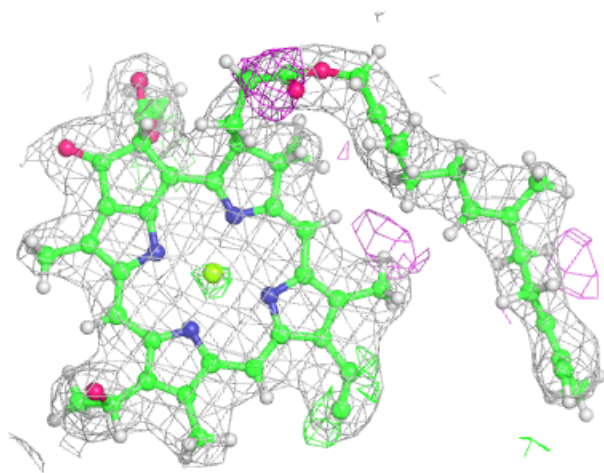
Electron density around GBF A 1002:

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



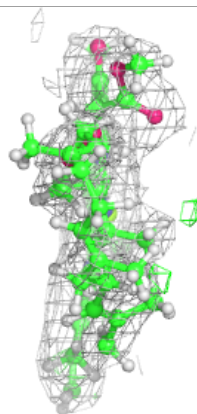
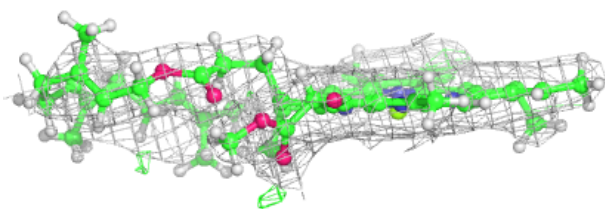
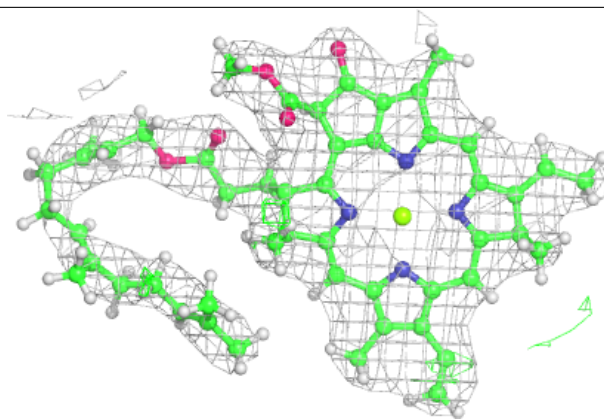
Electron density around AOH A 1003:

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



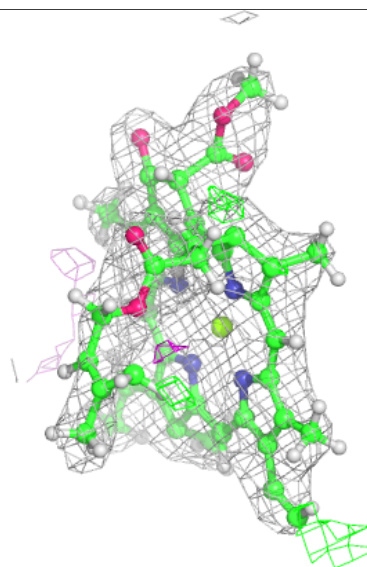
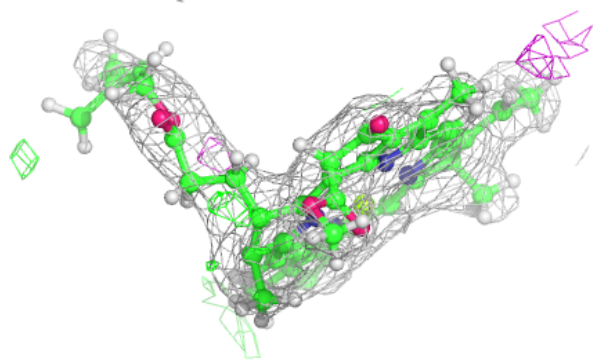
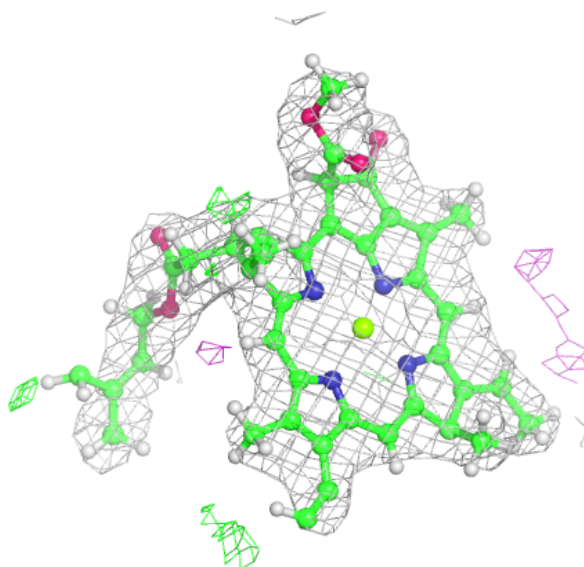
Electron density around GBF A 1019:

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



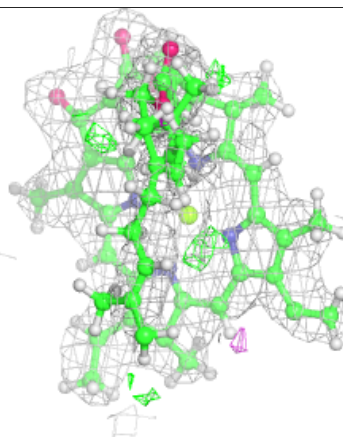
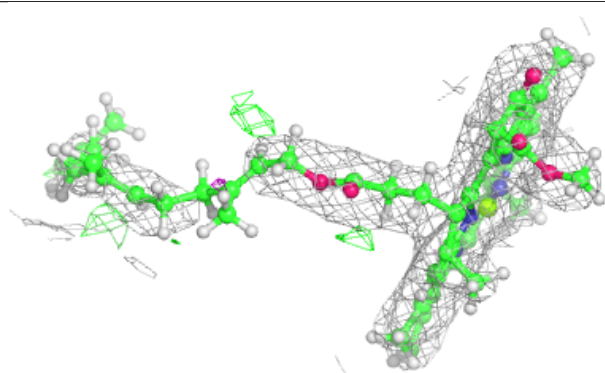
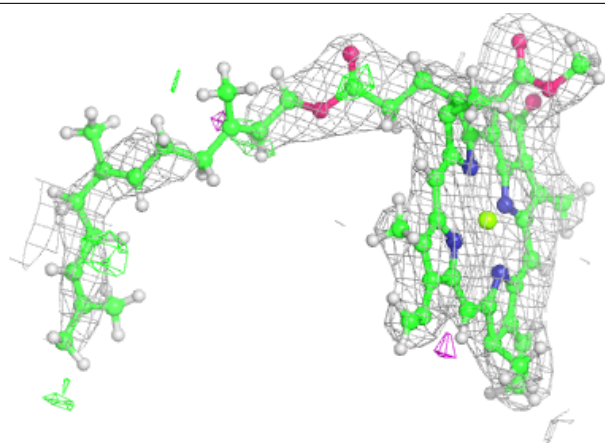
Electron density around GBF A 1027:

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



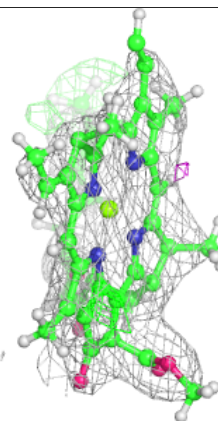
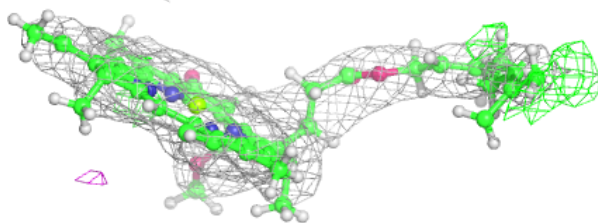
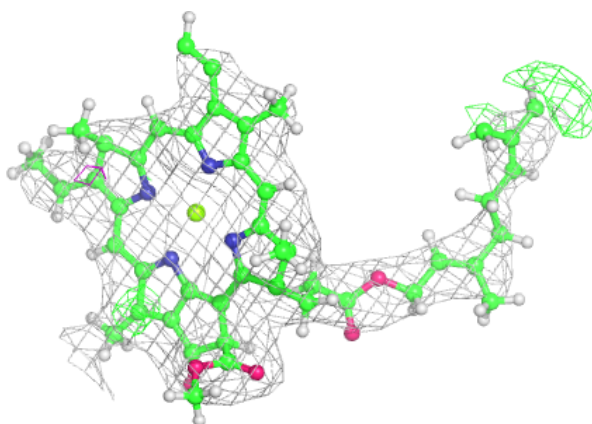
Electron density around GBF A 1021:

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



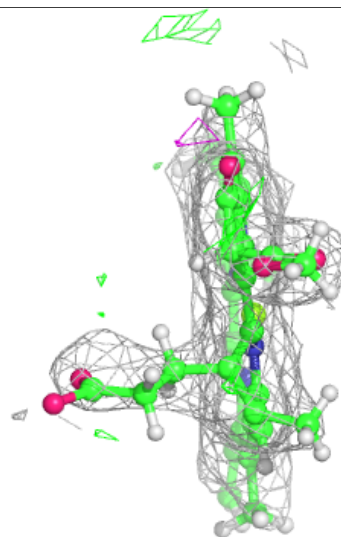
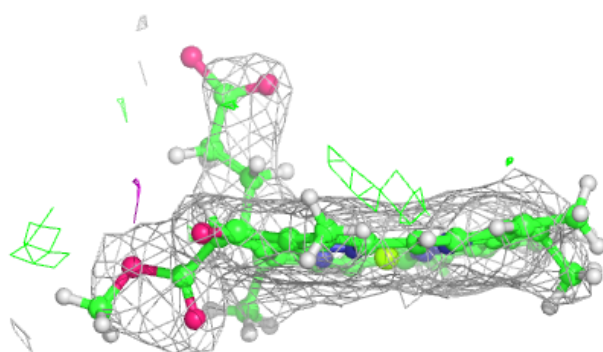
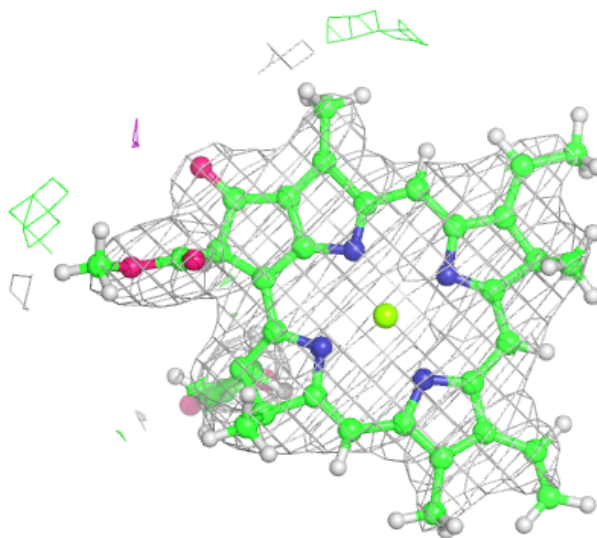
Electron density around GBF A 1012:

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



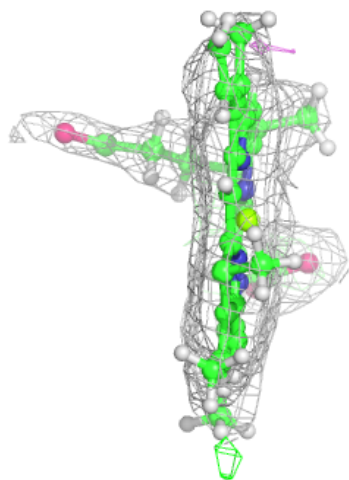
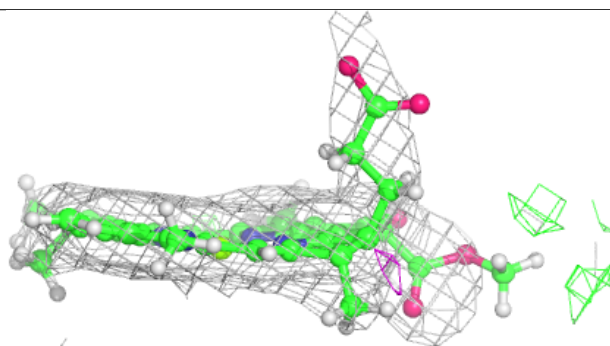
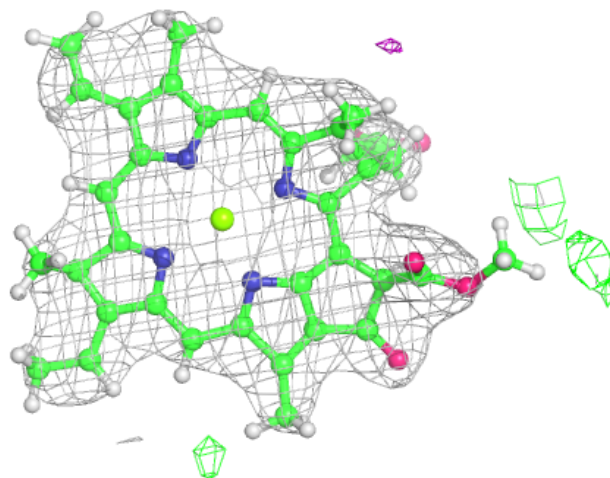
Electron density around GBF A 1014:

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



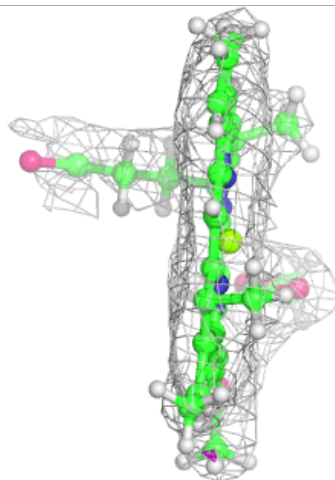
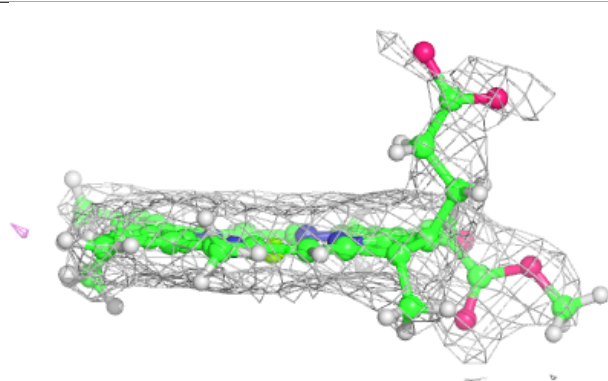
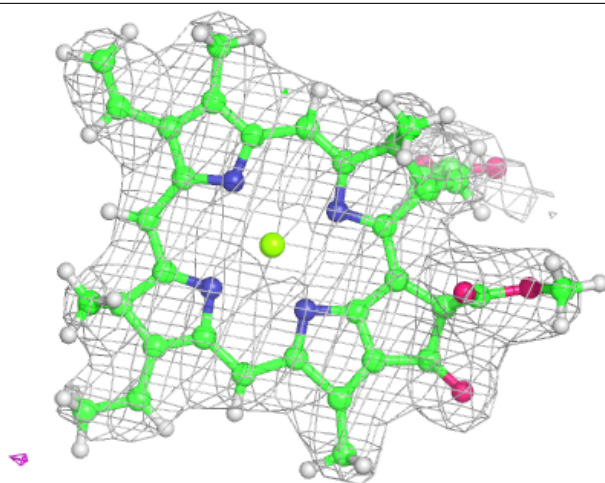
Electron density around GBF A 1006:

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



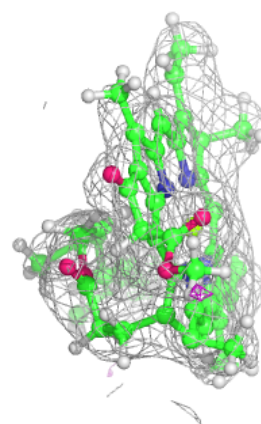
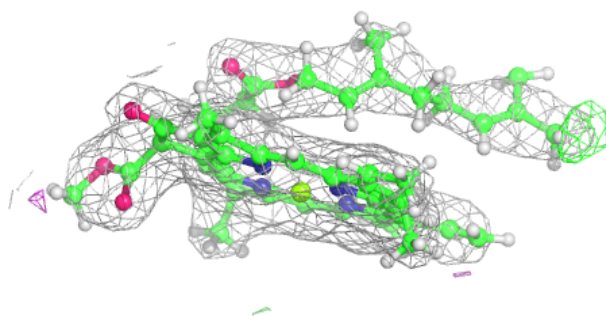
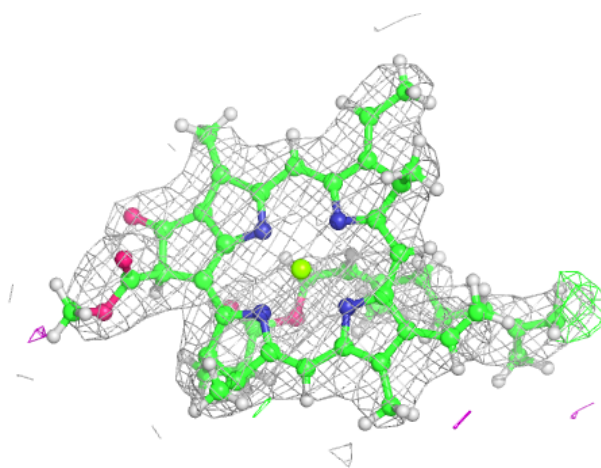
Electron density around GBF A 1022:

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



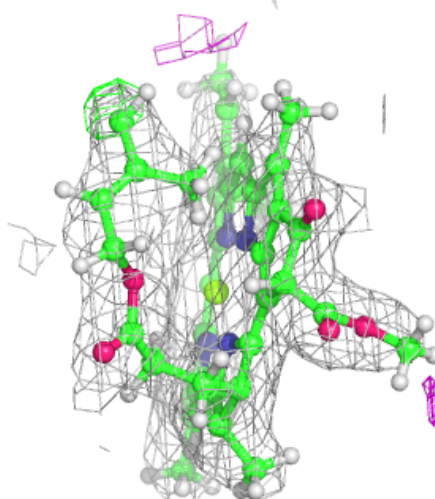
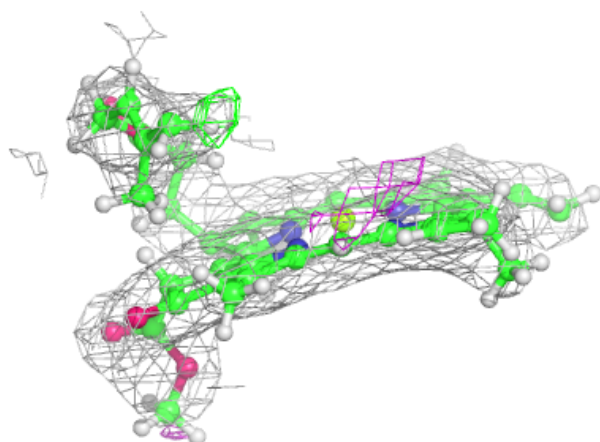
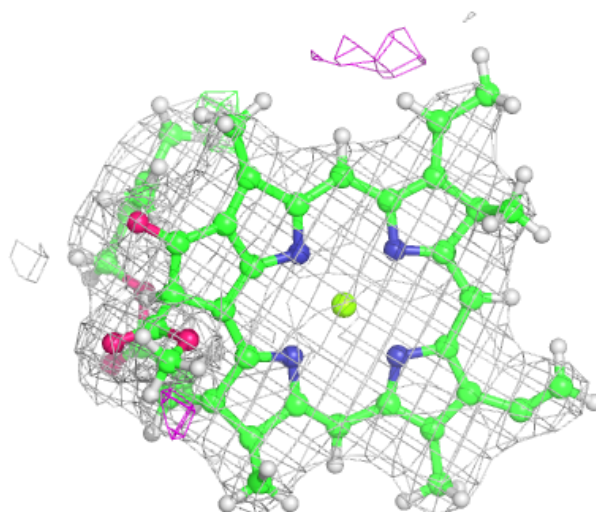
Electron density around GBF A 1008:

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



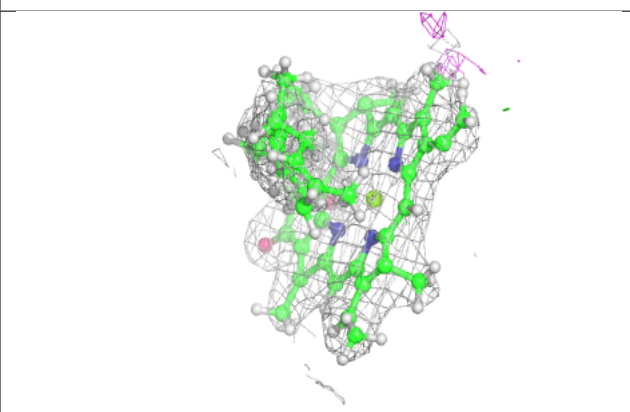
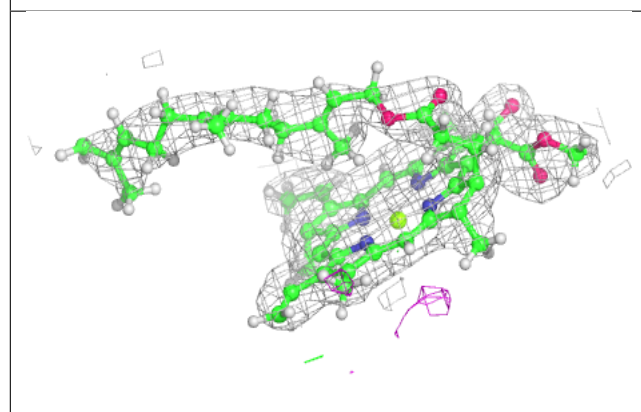
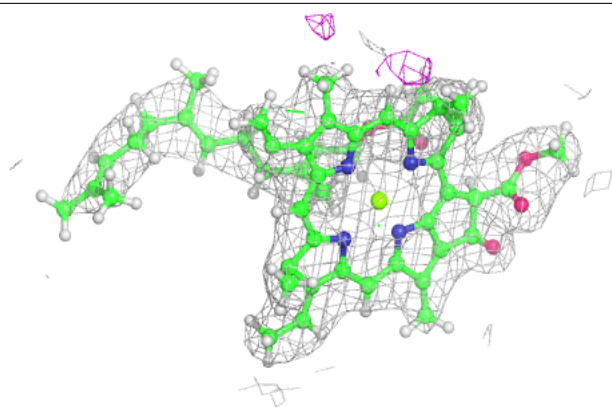
Electron density around GBF A 1004:

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

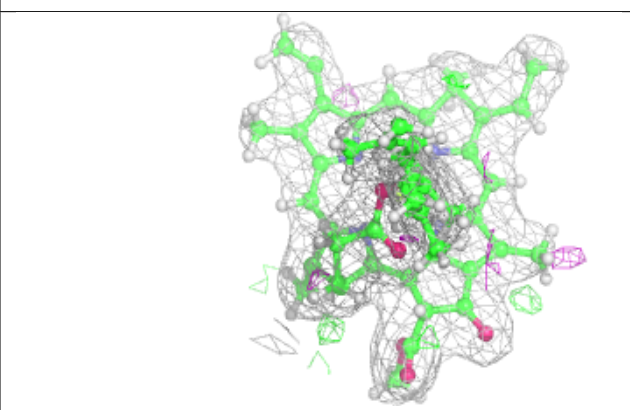
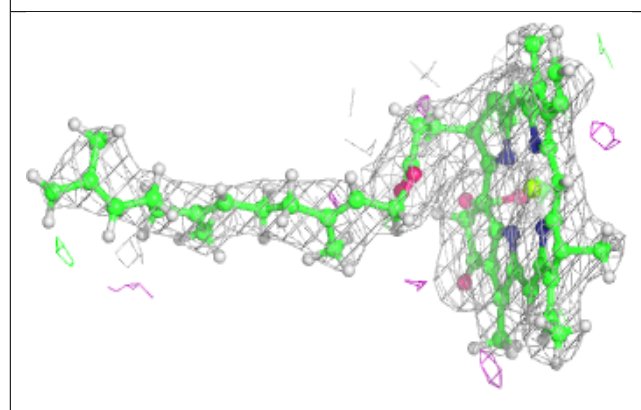
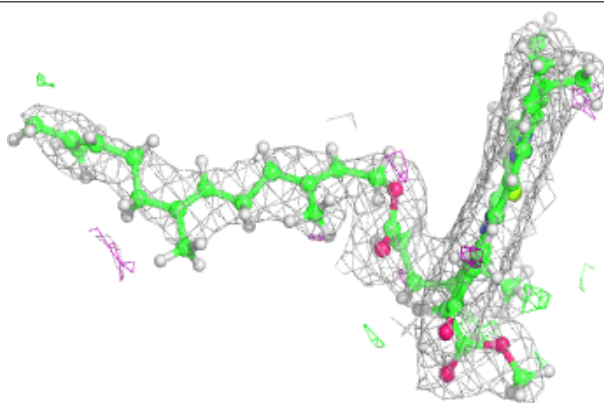


Electron density around GBF A 1020:

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

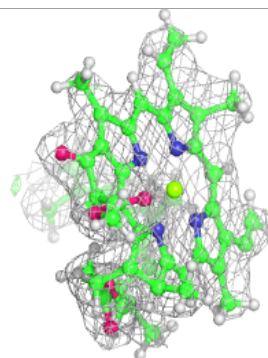
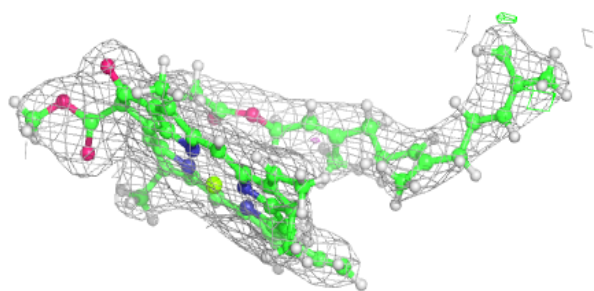
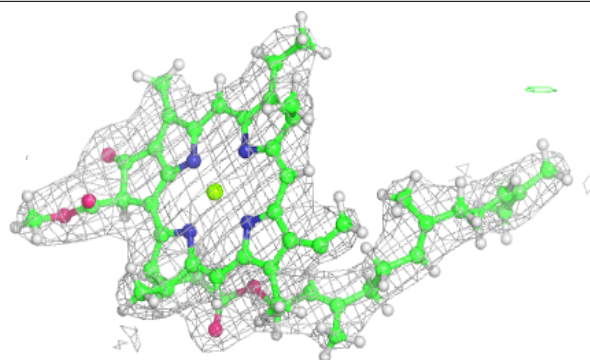
**Electron density around GBF A 1026:**

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



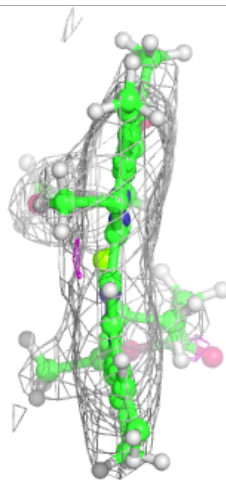
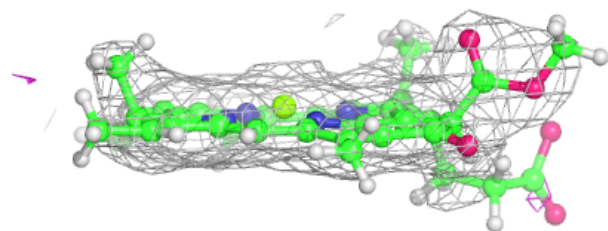
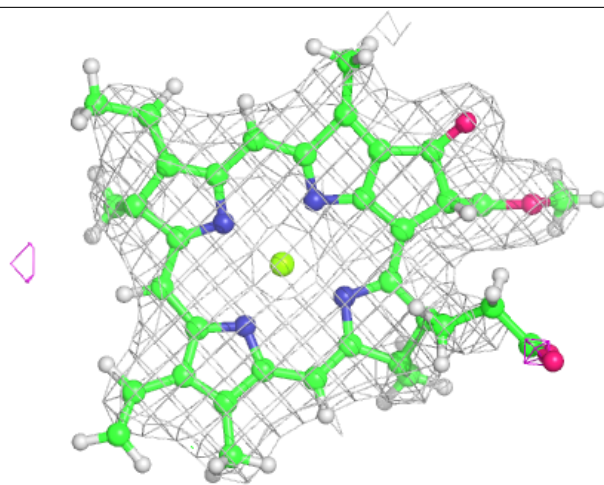
Electron density around GBF A 1023:

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



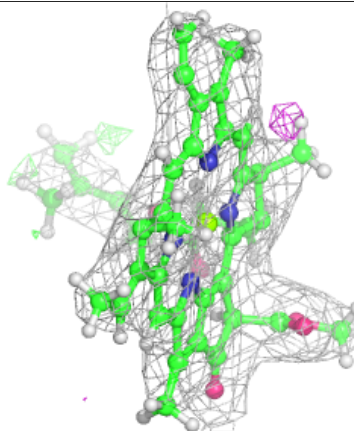
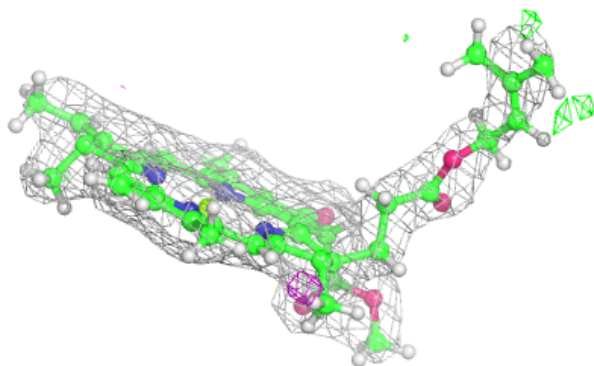
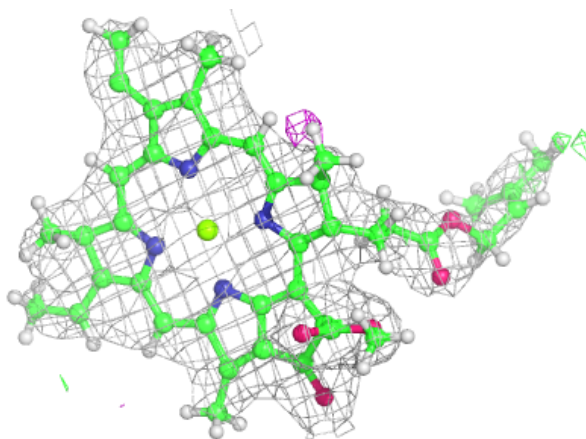
Electron density around GBF A 1025:

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

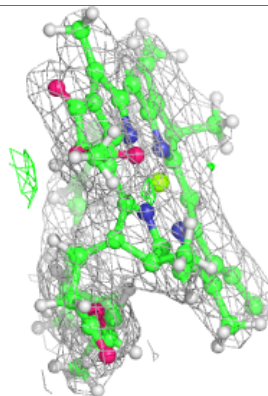
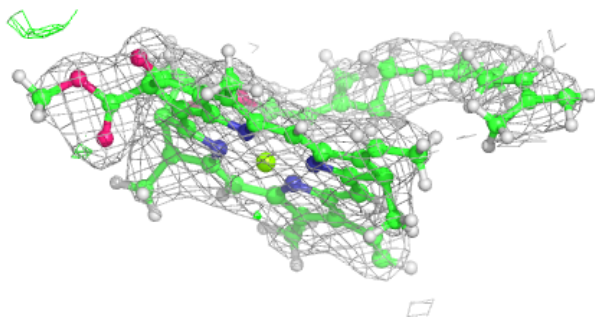
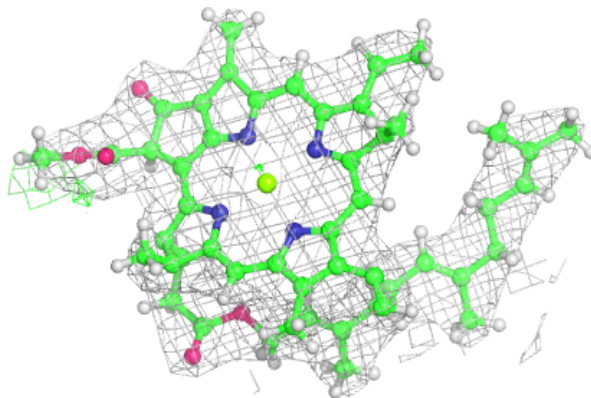


Electron density around GBF A 1024:

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

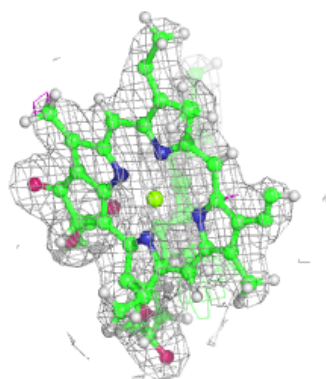
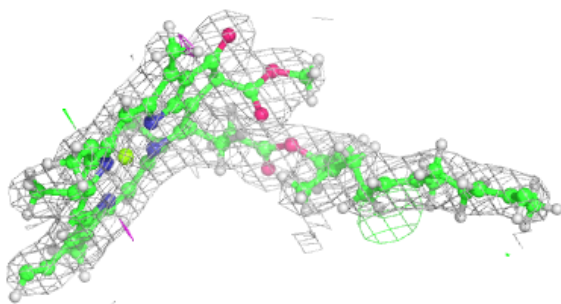
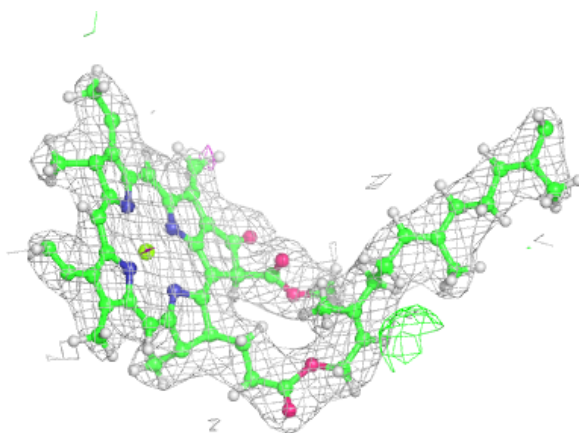
**Electron density around GBF A 1015:**

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



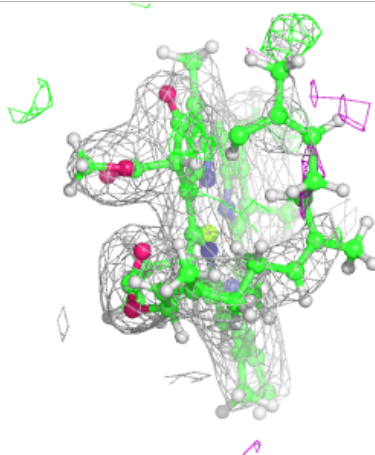
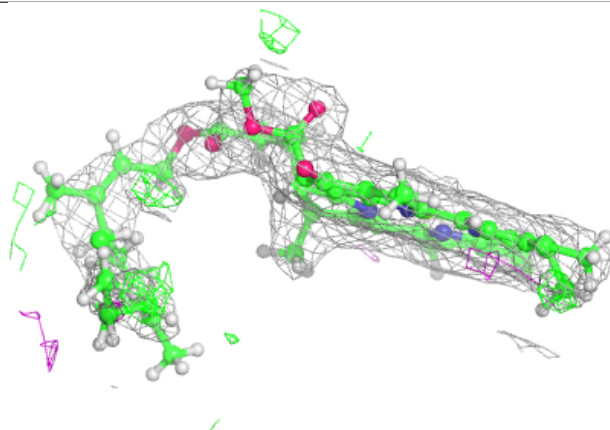
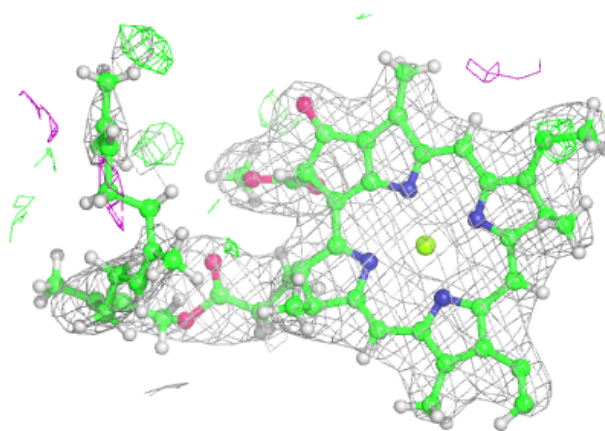
Electron density around GB0 A 1001:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.