



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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

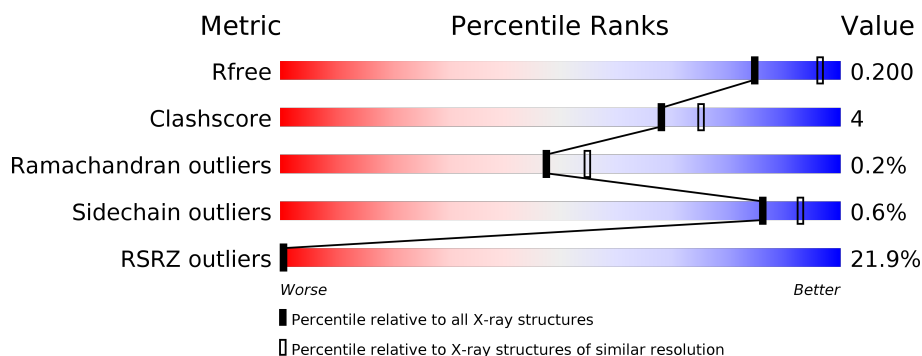
# 1 Overall quality at a glance

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  $\geq 3$ , 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> <div></div> <div>93%</div> <div>7%</div> </div> </div>
2	B	25	<div> <div>44%</div> <div> <div></div> <div>84%</div> <div>16%</div> </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

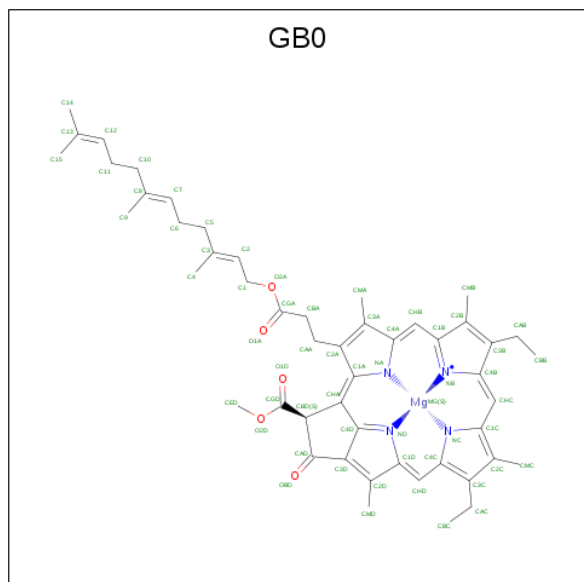
There are 3 discrepancies between the modelled and reference sequences:

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.

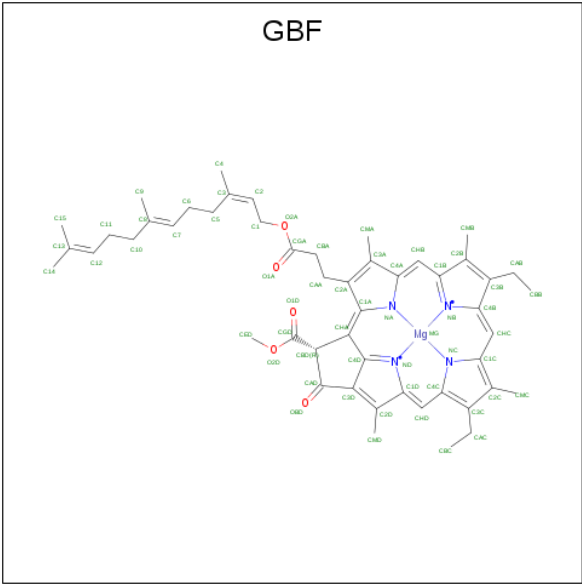
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	B	25	429	160	209	30	30	0	0	0

- 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		

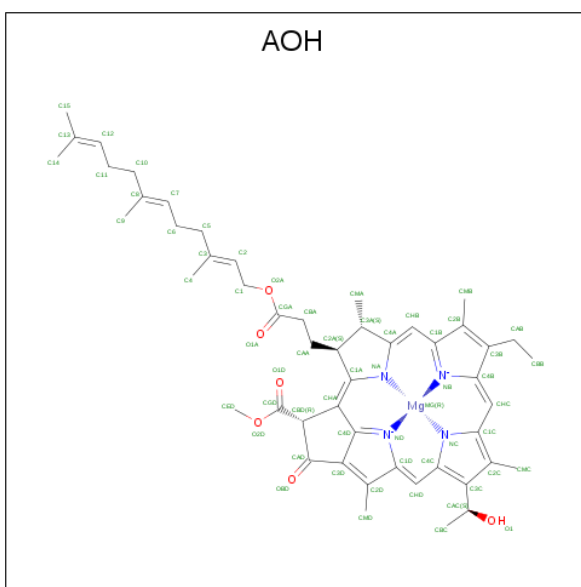
- Molecule 4 is Bacteriochlorophyll g (three-letter code: GBF) (formula: C<sub>50</sub>H<sub>58</sub>MgN<sub>4</sub>O<sub>5</sub>).



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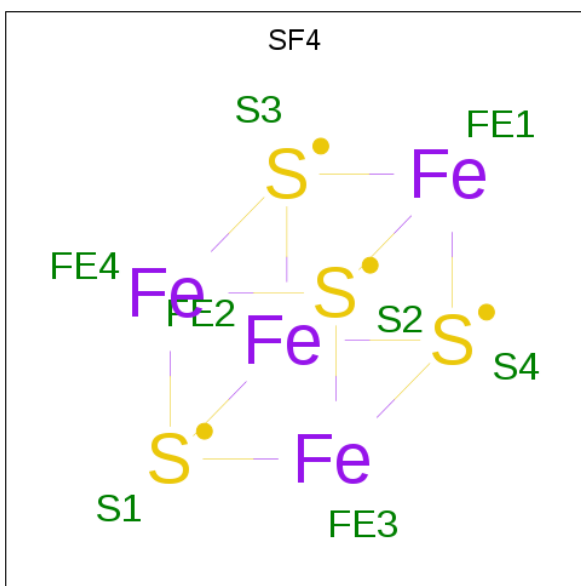
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	Mg	N	O	0	0
			75	35	30	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			112	50	52	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			73	35	28	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			112	50	52	1	4	5		
4	A	1	Total	C	H	Mg	N	O	0	0
			87	40	37	1	4	5		
4	A	1	Total	C	H	Mg	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
			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: C<sub>50</sub>H<sub>60</sub>MgN<sub>4</sub>O<sub>6</sub>).



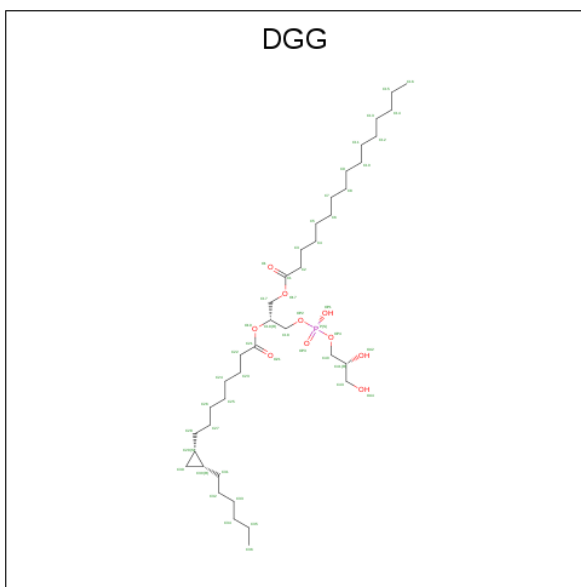
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	Mg	N	O	0	0
			113	50	52	1	4	6		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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: C<sub>39</sub>H<sub>75</sub>O<sub>10</sub>P).

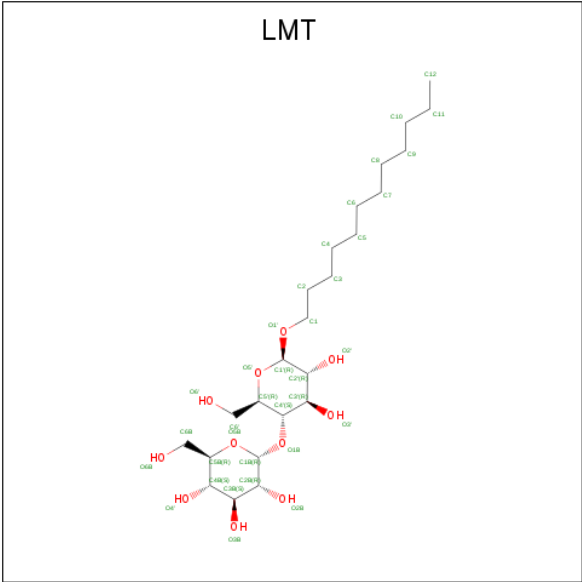


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	O	P	0	0
			88	30	47	10	1		
7	A	1	Total	C	H	O	P	0	0
			93	33	49	10	1		

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

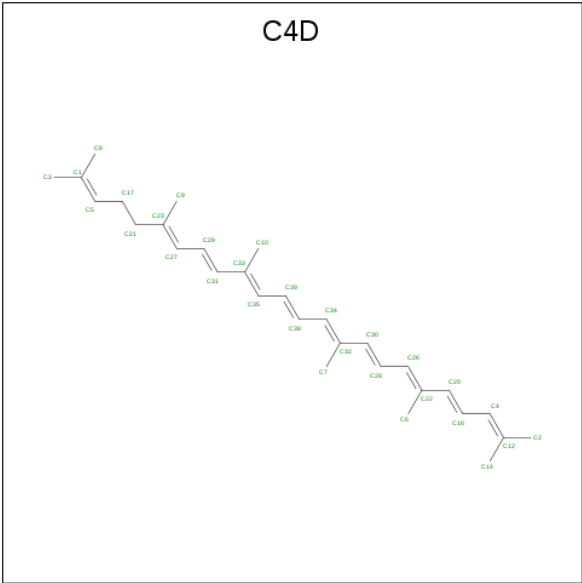
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Ca	0	0
			2	2		

- Molecule 9 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



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: C<sub>30</sub>H<sub>42</sub>).



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

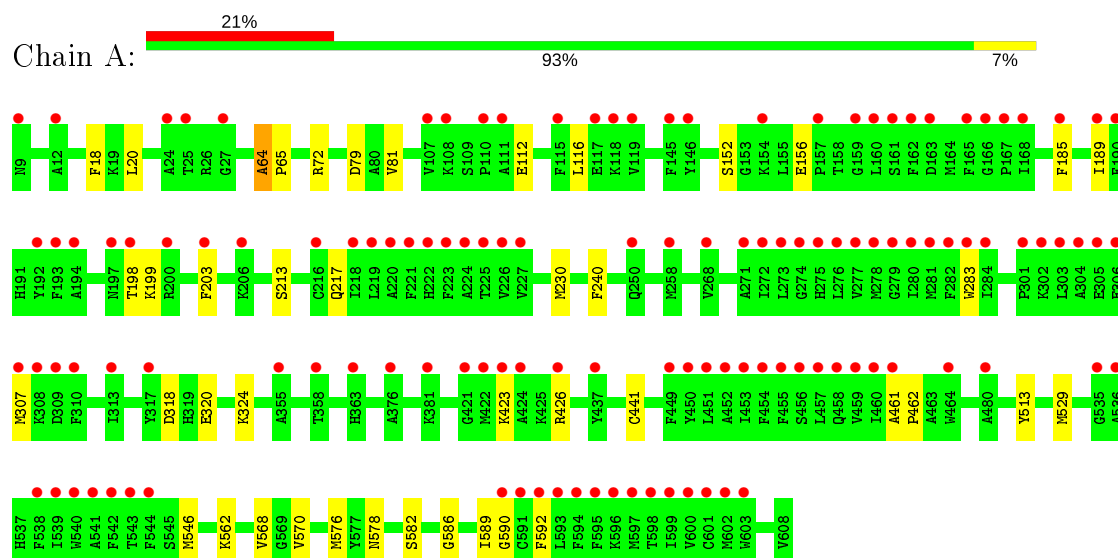
- Molecule 11 is water.

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

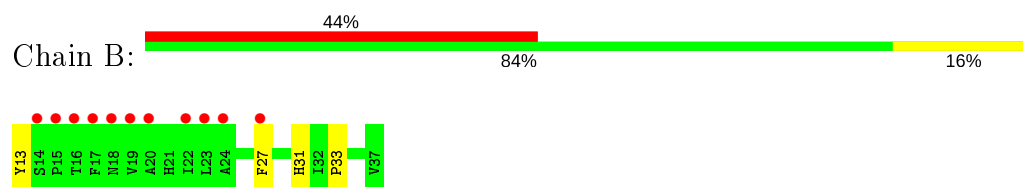
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.47 , 79.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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.

All (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
1:A:79:ASP:OD1	1:A:81:VAL:HG23	1.94	0.67
1:A:283:TRP:CE2	7:A:1031:DGG:H162	2.31	0.65
1:A:81:VAL:HG21	9:A:1034:LMT:O2'	1.98	0.64
1:A:18:PHE:HZ	7:A:1030:DGG:H252	1.65	0.60
7:A:1030:DGG:HC21	7:A:1030:DGG:H251	1.82	0.59
1:A:592:PHE:CD2	7:A:1030:DGG:HC71	2.38	0.58
4:A:1025:GBF:CGA	7:A:1031:DGG:H121	2.34	0.57
9:A:1034:LMT:H52	9:A:1035:LMT:C4	2.33	0.56
9:A:1034:LMT:H61	9:A:1035:LMT:C6	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PHE:CE2	7:A:1030:DGG:H252	2.45	0.51
1:A:576:MET:SD	2:B:33:PRO:HB2	2.51	0.51
1:A:320:GLU:O	1:A:324:LYS:HG3	2.12	0.49
1:A:283:TRP:CD2	7:A:1031:DGG:H162	2.47	0.49
1:A:582:SER:OG	7:A:1030:DGG:H402	2.12	0.49
1:A:426:ARG:NH2	11:A:1109:HOH:O	2.46	0.48
9:A:1034:LMT:C6	9:A:1035:LMT:H61	2.28	0.47
1:A:546:MET:HE3	1:A:586:GLY:HA2	1.96	0.46
9:A:1035:LMT:H82	9:A:1035:LMT:H52	1.78	0.46
1:A:213:SER:O	1:A:217:GLN:HG3	2.16	0.46
1:A:582:SER:HB3	7:A:1030:DGG:H402	1.98	0.44
2:B:13:TYR:N	11:B:201:HOH:O	2.50	0.44
1:A:112:GLU:O	1:A:116:LEU:HG	2.18	0.44
1:A:546:MET:HE1	1:A:590:GLY:N	2.33	0.43
1:A:546:MET:HE1	1:A:589:ILE:HG22	2.00	0.43
7:A:1031:DGG:H101	7:A:1031:DGG:H131	1.66	0.43
1:A:562:LYS:HD2	1:A:578:ASN:HA	2.00	0.43
1:A:20:LEU:H	1:A:20:LEU:HD23	1.84	0.42
1:A:198:THR:HG22	1:A:199:LYS:N	2.34	0.42
1:A:568:VAL:O	1:A:568:VAL:HG22	2.18	0.42
1:A:230:MET:HA	1:A:240:PHE:CD2	2.54	0.42
2:B:27:PHE:O	2:B:31:HIS:ND1	2.50	0.42
1:A:318:ASP:C	1:A:318:ASP:OD1	2.59	0.41
1:A:152:SER:OG	1:A:156:GLU:OE2	2.26	0.41
1:A:199:LYS:HD3	1:A:199:LYS:HA	1.93	0.41
1:A:546:MET:CE	1:A:590:GLY:N	2.83	0.41
1:A:185:PHE:CZ	1:A:189:ILE:HD11	2.56	0.41
1:A:203:PHE:HB2	1:A:307:MET:CE	2.50	0.40
1:A:461:ALA:HB3	1:A:462:PRO:HD3	2.03	0.40
1:A:568:VAL:HG13	1:A:570:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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	-

All (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
4	A	1010	GBF	C1D-C2D	9.22	1.63	1.42
4	A	1004	GBF	C1D-C2D	9.01	1.63	1.42
4	A	1018	GBF	C1D-C2D	8.96	1.62	1.42
4	A	1011	GBF	C1D-C2D	8.66	1.62	1.42
4	A	1006	GBF	C1D-C2D	8.64	1.62	1.42
4	A	1019	GBF	C1D-C2D	8.62	1.62	1.42
4	A	1025	GBF	C1D-C2D	8.60	1.62	1.42
4	A	1023	GBF	C1D-C2D	8.55	1.61	1.42
4	A	1008	GBF	C1D-C2D	8.54	1.61	1.42
4	A	1014	GBF	C1D-C2D	8.52	1.61	1.42
4	A	1012	GBF	C1D-C2D	8.50	1.61	1.42
4	A	1022	GBF	C1D-C2D	8.49	1.61	1.42
4	A	1015	GBF	C1D-C2D	8.47	1.61	1.42
4	A	1027	GBF	C1D-C2D	8.26	1.61	1.42
4	A	1020	GBF	C1D-C2D	8.16	1.61	1.42
3	A	1005	GB0	C1D-C2D	8.12	1.61	1.42
4	A	1024	GBF	C1D-C2D	8.07	1.60	1.42
4	A	1021	GBF	C1D-C2D	8.07	1.60	1.42
4	A	1017	GBF	C1D-C2D	8.04	1.60	1.42
4	A	1028	GBF	C1D-C2D	7.95	1.60	1.42
4	A	1007	GBF	C1D-C2D	7.68	1.60	1.42
4	A	1026	GBF	C1D-C2D	7.55	1.59	1.42
5	A	1003	AOH	C3C-CAC	-7.33	1.47	1.52
3	A	1001	GB0	C1D-C2D	7.15	1.58	1.42
4	A	1002	GBF	C1D-C2D	7.02	1.58	1.42
4	A	1027	GBF	C1A-CHA	7.01	1.51	1.38
3	A	1005	GB0	C1A-CHA	6.99	1.51	1.38
4	A	1024	GBF	C1A-CHA	6.78	1.51	1.38
4	A	1025	GBF	C1A-CHA	6.78	1.51	1.38
4	B	103	GBF	C1A-CHA	6.73	1.51	1.38
4	A	1028	GBF	C1A-CHA	6.69	1.51	1.38
4	B	102	GBF	C1A-CHA	6.67	1.51	1.38
4	A	1014	GBF	C1A-CHA	6.67	1.51	1.38
4	A	1004	GBF	C1A-CHA	6.59	1.50	1.38
4	A	1008	GBF	C1A-CHA	6.58	1.50	1.38
4	A	1016	GBF	C1A-CHA	6.51	1.50	1.38
4	A	1013	GBF	C1A-CHA	6.45	1.50	1.38
4	A	1017	GBF	C1A-CHA	6.41	1.50	1.38
4	A	1020	GBF	C1A-CHA	6.39	1.50	1.38
4	A	1011	GBF	C1A-CHA	6.35	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1021	GBF	C1A-CHA	6.21	1.50	1.38
4	A	1009	GBF	C1A-CHA	6.17	1.50	1.38
4	A	1023	GBF	C1A-CHA	6.04	1.49	1.38
4	A	1010	GBF	C1A-CHA	5.99	1.49	1.38
4	A	1018	GBF	C1A-CHA	5.97	1.49	1.38
4	B	103	GBF	C2A-C3A	5.95	1.55	1.37
4	A	1015	GBF	C1A-CHA	5.91	1.49	1.38
4	A	1019	GBF	C1A-CHA	5.89	1.49	1.38
4	A	1002	GBF	C1A-CHA	5.87	1.49	1.38
4	A	1006	GBF	C1A-CHA	5.83	1.49	1.38
4	A	1027	GBF	C2A-C3A	5.79	1.54	1.37
4	A	1013	GBF	C2A-C3A	5.76	1.54	1.37
4	A	1007	GBF	C1A-CHA	5.69	1.49	1.38
4	A	1002	GBF	C4A-C3A	5.64	1.55	1.42
4	A	1028	GBF	C2A-C3A	5.56	1.54	1.37
3	A	1005	GB0	C2A-C3A	5.55	1.54	1.37
4	A	1012	GBF	C1A-CHA	5.52	1.48	1.38
4	A	1025	GBF	C2A-C3A	5.49	1.53	1.37
4	A	1019	GBF	C2A-C3A	5.49	1.53	1.37
4	A	1017	GBF	C2A-C3A	5.48	1.53	1.37
3	A	1001	GB0	C1A-CHA	5.46	1.48	1.38
4	A	1009	GBF	C2A-C3A	5.45	1.53	1.37
4	A	1027	GBF	C4D-CHA	-5.44	1.38	1.45
4	A	1018	GBF	C2A-C3A	5.43	1.53	1.37
4	B	103	GBF	O2D-CGD	5.42	1.46	1.33
4	A	1013	GBF	O2D-CGD	5.40	1.46	1.33
4	A	1016	GBF	C2A-C3A	5.39	1.53	1.37
4	A	1002	GBF	C2A-C3A	5.39	1.53	1.37
4	A	1009	GBF	O2D-CGD	5.37	1.46	1.33
4	A	1014	GBF	C2A-C3A	5.37	1.53	1.37
4	A	1022	GBF	C1A-CHA	5.37	1.48	1.38
4	A	1004	GBF	C2A-C3A	5.36	1.53	1.37
4	A	1015	GBF	C2A-C3A	5.34	1.53	1.37
4	A	1016	GBF	O2D-CGD	5.31	1.46	1.33
4	A	1028	GBF	O2D-CGD	5.30	1.46	1.33
4	A	1021	GBF	C2A-C3A	5.29	1.53	1.37
4	B	102	GBF	O2D-CGD	5.22	1.45	1.33
4	A	1017	GBF	OBD-CAD	5.19	1.29	1.22
4	A	1012	GBF	C4D-CHA	-5.17	1.38	1.45
4	A	1019	GBF	C4D-ND	5.16	1.39	1.35
4	A	1012	GBF	C2A-C3A	5.14	1.52	1.37
4	A	1010	GBF	C2A-C3A	5.14	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	102	GBF	C2A-C3A	5.13	1.52	1.37
4	A	1018	GBF	C4D-ND	5.12	1.39	1.35
4	A	1010	GBF	O2D-CGD	5.12	1.45	1.33
4	A	1027	GBF	OBD-CAD	5.10	1.29	1.22
4	A	1002	GBF	OBD-CAD	5.09	1.29	1.22
4	A	1027	GBF	C4D-ND	5.09	1.39	1.35
4	A	1006	GBF	C2A-C3A	5.09	1.52	1.37
4	A	1020	GBF	C2A-C3A	5.08	1.52	1.37
4	A	1011	GBF	C2A-C3A	5.07	1.52	1.37
4	A	1022	GBF	C4D-CHA	-5.05	1.38	1.45
4	A	1010	GBF	C4D-CHA	-5.02	1.38	1.45
4	A	1008	GBF	C2A-C3A	5.02	1.52	1.37
4	A	1012	GBF	O2D-CGD	5.00	1.45	1.33
4	A	1026	GBF	C1A-C2A	5.00	1.53	1.42
3	A	1005	GB0	C4D-CHA	-4.97	1.38	1.45
4	A	1019	GBF	O2D-CGD	4.95	1.45	1.33
4	A	1014	GBF	C4D-CHA	-4.94	1.38	1.45
4	A	1026	GBF	C1A-CHA	4.93	1.47	1.38
4	A	1022	GBF	C2A-C3A	4.93	1.52	1.37
4	B	102	GBF	C4D-CHA	-4.93	1.38	1.45
4	A	1007	GBF	C2A-C3A	4.92	1.52	1.37
4	A	1024	GBF	C2A-C3A	4.88	1.52	1.37
4	A	1009	GBF	C4D-CHA	-4.87	1.39	1.45
4	B	103	GBF	OBD-CAD	4.85	1.29	1.22
4	A	1017	GBF	O2D-CGD	4.84	1.45	1.33
4	A	1002	GBF	O2D-CGD	4.82	1.45	1.33
4	A	1012	GBF	C4D-ND	4.80	1.39	1.35
4	B	103	GBF	C4D-ND	4.79	1.39	1.35
4	A	1019	GBF	OBD-CAD	4.75	1.28	1.22
4	A	1023	GBF	C2A-C3A	4.75	1.51	1.37
5	A	1003	AOH	O2D-CGD	4.75	1.44	1.33
4	A	1016	GBF	C4D-ND	4.75	1.39	1.35
4	A	1013	GBF	C4D-CHA	-4.74	1.39	1.45
3	A	1001	GB0	C2A-C3A	4.73	1.51	1.37
4	B	102	GBF	OBD-CAD	4.72	1.28	1.22
4	A	1004	GBF	C1A-C2A	4.71	1.53	1.42
3	A	1005	GB0	O2D-CGD	4.69	1.44	1.33
4	A	1020	GBF	OBD-CAD	4.69	1.28	1.22
4	A	1026	GBF	O2D-CGD	4.65	1.44	1.33
4	A	1026	GBF	C2A-C3A	4.64	1.51	1.37
4	A	1009	GBF	C4D-ND	4.59	1.39	1.35
4	A	1025	GBF	C4D-CHA	-4.58	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1009	GBF	OBD-CAD	4.58	1.28	1.22
4	A	1015	GBF	C4D-ND	4.54	1.39	1.35
4	A	1015	GBF	OBD-CAD	4.51	1.28	1.22
4	A	1024	GBF	C4D-CHA	-4.50	1.39	1.45
4	A	1017	GBF	C1A-C2A	4.47	1.52	1.42
4	A	1028	GBF	C4D-ND	4.45	1.39	1.35
5	A	1003	AOH	OBD-CAD	4.42	1.28	1.22
4	A	1026	GBF	OBD-CAD	4.40	1.28	1.22
4	A	1017	GBF	C4D-ND	4.40	1.39	1.35
4	A	1006	GBF	OBD-CAD	4.38	1.28	1.22
4	A	1025	GBF	OBD-CAD	4.36	1.28	1.22
4	B	102	GBF	C4D-ND	4.36	1.39	1.35
4	A	1002	GBF	C1A-C2A	4.35	1.52	1.42
4	A	1015	GBF	O2A-CGA	4.35	1.46	1.33
4	A	1006	GBF	O2D-CGD	4.35	1.43	1.33
4	B	103	GBF	C4A-C3A	4.34	1.52	1.42
4	A	1020	GBF	C4D-CHA	-4.34	1.39	1.45
4	A	1007	GBF	C4D-CHA	-4.33	1.39	1.45
4	A	1020	GBF	C1A-C2A	4.33	1.52	1.42
4	A	1016	GBF	OBD-CAD	4.32	1.28	1.22
4	A	1023	GBF	C4D-CHA	-4.32	1.39	1.45
4	A	1014	GBF	O2D-CGD	4.32	1.43	1.33
4	A	1022	GBF	C4A-C3A	4.32	1.52	1.42
4	A	1028	GBF	OBD-CAD	4.32	1.28	1.22
4	A	1024	GBF	OBD-CAD	4.32	1.28	1.22
4	A	1012	GBF	OBD-CAD	4.29	1.28	1.22
4	A	1027	GBF	O2A-CGA	4.27	1.45	1.33
4	A	1018	GBF	O2D-CGD	4.26	1.43	1.33
3	A	1005	GB0	O2A-CGA	4.25	1.45	1.33
4	B	103	GBF	O2A-CGA	4.24	1.45	1.33
4	A	1020	GBF	O2D-CGD	4.22	1.43	1.33
4	A	1007	GBF	O2A-CGA	4.22	1.45	1.33
4	A	1011	GBF	O2D-CGD	4.22	1.43	1.33
4	A	1004	GBF	C4D-CHA	-4.22	1.39	1.45
4	A	1026	GBF	C4A-C3A	4.21	1.52	1.42
4	A	1025	GBF	O2D-CGD	4.21	1.43	1.33
4	A	1018	GBF	O2A-CGA	4.21	1.45	1.33
3	A	1001	GB0	O2A-CGA	4.20	1.45	1.33
4	A	1023	GBF	O2D-CGD	4.20	1.43	1.33
4	A	1020	GBF	C4A-C3A	4.19	1.52	1.42
4	A	1020	GBF	C3D-C4D	4.18	1.44	1.40
4	A	1016	GBF	C4D-CHA	-4.17	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1020	GBF	O2A-CGA	4.17	1.45	1.33
7	A	1031	DGG	O17-C1	4.17	1.45	1.33
4	A	1006	GBF	C4D-CHA	-4.17	1.39	1.45
3	A	1005	GB0	C4A-C3A	4.16	1.52	1.42
4	A	1011	GBF	C4D-CHA	-4.14	1.39	1.45
4	A	1004	GBF	C4D-ND	4.14	1.38	1.35
4	A	1022	GBF	C4D-ND	4.14	1.38	1.35
4	A	1028	GBF	C1A-C2A	4.13	1.51	1.42
4	A	1018	GBF	OBD-CAD	4.12	1.28	1.22
4	A	1012	GBF	O2A-CGA	4.11	1.45	1.33
4	A	1024	GBF	O2A-CGA	4.11	1.45	1.33
3	A	1001	GB0	OBD-CAD	4.11	1.28	1.22
4	A	1017	GBF	C4D-CHA	-4.11	1.39	1.45
3	A	1005	GB0	C1A-C2A	4.10	1.51	1.42
4	A	1020	GBF	C4D-ND	4.09	1.38	1.35
4	A	1011	GBF	OBD-CAD	4.09	1.28	1.22
3	A	1001	GB0	C1A-C2A	4.07	1.51	1.42
4	A	1022	GBF	O2D-CGD	4.06	1.43	1.33
4	B	103	GBF	C4D-CHA	-4.06	1.40	1.45
4	A	1004	GBF	OBD-CAD	4.05	1.28	1.22
5	A	1003	AOH	C4D-CHA	-4.04	1.40	1.45
4	A	1028	GBF	O2A-CGA	4.04	1.45	1.33
4	A	1019	GBF	O2A-CGA	4.02	1.45	1.33
4	A	1007	GBF	O2D-CGD	4.01	1.43	1.33
4	A	1022	GBF	OBD-CAD	4.01	1.27	1.22
4	A	1019	GBF	C4A-C3A	4.01	1.51	1.42
4	A	1024	GBF	O2D-CGD	4.01	1.43	1.33
4	A	1010	GBF	OBD-CAD	3.99	1.27	1.22
4	A	1021	GBF	O2D-CGD	3.98	1.42	1.33
4	A	1004	GBF	O2D-CGD	3.97	1.42	1.33
4	A	1025	GBF	C4D-ND	3.97	1.38	1.35
4	A	1022	GBF	C1A-C2A	3.96	1.51	1.42
4	A	1023	GBF	OBD-CAD	3.95	1.27	1.22
4	A	1004	GBF	C4A-C3A	3.95	1.51	1.42
4	A	1017	GBF	O2A-CGA	3.95	1.44	1.33
7	A	1031	DGG	O19-C21	3.93	1.45	1.34
4	A	1021	GBF	O2A-CGA	3.92	1.44	1.33
4	A	1010	GBF	C4A-C3A	3.92	1.51	1.42
4	A	1023	GBF	C1A-C2A	3.89	1.51	1.42
4	A	1004	GBF	O2A-CGA	3.88	1.44	1.33
4	A	1007	GBF	OBD-CAD	3.87	1.27	1.22
4	B	103	GBF	C1A-C2A	3.85	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1023	GBF	O2A-CGA	3.84	1.44	1.33
4	A	1011	GBF	O2A-CGA	3.84	1.44	1.33
4	A	1007	GBF	C1A-C2A	3.83	1.51	1.42
4	A	1006	GBF	C4D-ND	3.83	1.38	1.35
4	A	1028	GBF	C4A-C3A	3.82	1.51	1.42
4	A	1011	GBF	C4A-C3A	3.80	1.51	1.42
4	A	1006	GBF	C4A-C3A	3.80	1.51	1.42
3	A	1005	GB0	OBD-CAD	3.79	1.27	1.22
4	A	1018	GBF	C4D-CHA	-3.79	1.40	1.45
4	A	1013	GBF	C4D-ND	3.79	1.38	1.35
4	A	1023	GBF	C4D-ND	3.79	1.38	1.35
4	A	1008	GBF	C4A-C3A	3.79	1.51	1.42
3	A	1001	GB0	O2D-CGD	3.78	1.42	1.33
4	A	1025	GBF	C1A-C2A	3.76	1.51	1.42
4	A	1009	GBF	C1A-C2A	3.74	1.51	1.42
4	A	1021	GBF	C1A-C2A	3.74	1.51	1.42
4	A	1014	GBF	OBD-CAD	3.72	1.27	1.22
4	A	1006	GBF	C1A-C2A	3.72	1.51	1.42
4	A	1013	GBF	O2A-CGA	3.72	1.44	1.33
4	A	1019	GBF	C4D-CHA	-3.72	1.40	1.45
4	A	1011	GBF	C3C-C2C	3.71	1.48	1.37
4	A	1008	GBF	C4D-ND	3.70	1.38	1.35
4	A	1028	GBF	C3C-C2C	3.69	1.48	1.37
4	A	1015	GBF	O2D-CGD	3.68	1.42	1.33
4	A	1013	GBF	C3C-C2C	3.68	1.48	1.37
4	A	1013	GBF	C1A-C2A	3.68	1.50	1.42
4	A	1010	GBF	C3C-C2C	3.68	1.48	1.37
4	A	1015	GBF	C4D-CHA	-3.66	1.40	1.45
4	A	1008	GBF	O2D-CGD	3.65	1.42	1.33
4	A	1019	GBF	C1A-C2A	3.65	1.50	1.42
4	A	1008	GBF	O2A-CGA	3.64	1.44	1.33
4	A	1026	GBF	C3C-C2C	3.63	1.48	1.37
4	A	1026	GBF	C4D-ND	3.62	1.38	1.35
4	A	1007	GBF	C4A-C3A	3.62	1.50	1.42
4	A	1007	GBF	C4D-ND	3.61	1.38	1.35
4	B	102	GBF	C3C-C2C	3.61	1.48	1.37
3	A	1005	GB0	C3C-C2C	3.60	1.48	1.37
4	A	1011	GBF	C1A-C2A	3.60	1.50	1.42
5	A	1003	AOH	CAB-C3B	-3.60	1.45	1.52
4	A	1008	GBF	C1A-C2A	3.60	1.50	1.42
3	A	1001	GB0	C3C-C2C	3.59	1.48	1.37
4	A	1002	GBF	O2A-CGA	3.59	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1016	GBF	C3C-C2C	3.59	1.48	1.37
4	A	1006	GBF	C3C-C2C	3.58	1.48	1.37
4	A	1016	GBF	C1A-C2A	3.57	1.50	1.42
4	A	1010	GBF	C4D-ND	3.57	1.38	1.35
4	A	1008	GBF	C4D-CHA	-3.54	1.40	1.45
4	A	1009	GBF	C3C-C2C	3.54	1.48	1.37
4	A	1002	GBF	C3C-C2C	3.54	1.48	1.37
4	A	1017	GBF	C3C-C2C	3.54	1.48	1.37
4	A	1010	GBF	C1A-C2A	3.52	1.50	1.42
4	A	1021	GBF	C4A-C3A	3.52	1.50	1.42
4	A	1011	GBF	C4D-ND	3.52	1.38	1.35
3	A	1001	GB0	C4A-C3A	3.51	1.50	1.42
7	A	1030	DGG	O19-C21	3.48	1.44	1.34
4	A	1017	GBF	C4A-C3A	3.48	1.50	1.42
4	A	1021	GBF	C3D-C4D	3.47	1.43	1.40
4	A	1027	GBF	O2D-CGD	3.47	1.41	1.33
4	A	1008	GBF	OBD-CAD	3.46	1.27	1.22
4	A	1023	GBF	C3C-C2C	3.46	1.47	1.37
3	A	1001	GB0	C4D-CHA	-3.43	1.40	1.45
4	A	1013	GBF	OBD-CAD	3.42	1.27	1.22
4	A	1009	GBF	C4A-C3A	3.42	1.50	1.42
4	A	1027	GBF	C1A-C2A	3.41	1.50	1.42
4	B	103	GBF	C3D-C4D	3.41	1.43	1.40
3	A	1001	GB0	C3D-C4D	3.39	1.43	1.40
4	A	1028	GBF	C1B-CHB	3.39	1.50	1.41
4	B	103	GBF	C3C-C2C	3.37	1.47	1.37
4	A	1013	GBF	C1C-CHC	3.37	1.50	1.41
4	A	1014	GBF	C4D-ND	3.35	1.38	1.35
4	A	1022	GBF	C3C-C2C	3.35	1.47	1.37
3	A	1005	GB0	CBB-CAB	-3.35	1.27	1.50
4	A	1014	GBF	C3C-C2C	3.33	1.47	1.37
4	A	1018	GBF	C4A-C3A	3.33	1.50	1.42
4	B	102	GBF	C4A-C3A	3.30	1.50	1.42
4	A	1008	GBF	C3C-C2C	3.30	1.47	1.37
4	A	1012	GBF	C3C-C2C	3.29	1.47	1.37
4	A	1027	GBF	C3C-C2C	3.29	1.47	1.37
4	A	1027	GBF	C4A-C3A	3.28	1.50	1.42
4	A	1015	GBF	C1A-C2A	3.27	1.50	1.42
4	A	1018	GBF	C3D-C4D	3.27	1.43	1.40
4	A	1021	GBF	C1C-CHC	3.26	1.50	1.41
3	A	1001	GB0	C4D-ND	3.26	1.38	1.35
4	A	1024	GBF	C4A-C3A	3.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1014	GBF	C1B-CHB	3.23	1.50	1.41
4	A	1012	GBF	C4A-C3A	3.23	1.49	1.42
4	A	1021	GBF	C4D-CHA	-3.23	1.41	1.45
4	A	1004	GBF	C3D-C4D	3.23	1.43	1.40
4	A	1013	GBF	C4A-C3A	3.22	1.49	1.42
4	B	103	GBF	C1B-CHB	3.22	1.49	1.41
4	A	1004	GBF	C3C-C2C	3.22	1.47	1.37
4	B	102	GBF	C1A-C2A	3.21	1.49	1.42
4	A	1021	GBF	C3C-C2C	3.20	1.47	1.37
4	A	1002	GBF	CBB-CAB	-3.20	1.28	1.50
4	A	1019	GBF	C3C-C2C	3.19	1.47	1.37
4	A	1018	GBF	C1B-CHB	3.17	1.49	1.41
4	B	102	GBF	C1C-CHC	3.17	1.49	1.41
4	A	1007	GBF	C3C-C2C	3.17	1.47	1.37
4	A	1006	GBF	C1B-CHB	3.16	1.49	1.41
4	A	1020	GBF	C1B-CHB	3.16	1.49	1.41
4	A	1024	GBF	C1A-C2A	3.15	1.49	1.42
4	A	1016	GBF	C4A-C3A	3.14	1.49	1.42
4	A	1012	GBF	C1A-C2A	3.14	1.49	1.42
4	A	1014	GBF	C1A-C2A	3.13	1.49	1.42
4	A	1009	GBF	C1C-CHC	3.11	1.49	1.41
4	A	1028	GBF	C4D-CHA	-3.11	1.41	1.45
4	A	1026	GBF	C4D-CHA	-3.10	1.41	1.45
4	A	1021	GBF	C4D-ND	3.10	1.38	1.35
4	A	1015	GBF	C4A-C3A	3.09	1.49	1.42
4	A	1014	GBF	C4A-C3A	3.09	1.49	1.42
3	A	1001	GB0	CBB-CAB	-3.07	1.29	1.50
4	A	1015	GBF	C3C-C2C	3.06	1.46	1.37
4	A	1021	GBF	OBD-CAD	3.05	1.26	1.22
4	A	1004	GBF	CAB-C3B	-3.04	1.46	1.52
4	A	1023	GBF	CBB-CAB	-3.03	1.29	1.50
4	A	1015	GBF	C1B-CHB	3.02	1.49	1.41
4	B	102	GBF	C1B-CHB	3.01	1.49	1.41
4	A	1012	GBF	C1B-CHB	3.01	1.49	1.41
4	A	1022	GBF	C1B-CHB	3.00	1.49	1.41
3	A	1005	GB0	C1B-CHB	2.99	1.49	1.41
4	A	1026	GBF	O2A-CGA	2.99	1.42	1.33
4	A	1010	GBF	C1C-CHC	2.99	1.49	1.41
4	A	1009	GBF	C4C-CHD	2.99	1.49	1.41
4	A	1009	GBF	C1B-CHB	2.97	1.49	1.41
3	A	1005	GB0	C4D-ND	2.97	1.37	1.35
4	A	1023	GBF	C4A-C3A	2.97	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	GBF	C1B-CHB	2.96	1.49	1.41
4	B	102	GBF	C4C-CHD	2.96	1.49	1.41
4	A	1025	GBF	C3C-C2C	2.96	1.46	1.37
7	A	1030	DGG	O17-C1	2.96	1.42	1.33
4	A	1026	GBF	CBB-CAB	-2.95	1.30	1.50
5	A	1003	AOH	CBB-CAB	-2.95	1.30	1.50
4	A	1025	GBF	C4A-C3A	2.95	1.49	1.42
4	A	1019	GBF	C1B-CHB	2.95	1.49	1.41
4	A	1018	GBF	C1C-CHC	2.95	1.49	1.41
4	A	1017	GBF	C3D-C4D	2.93	1.43	1.40
4	A	1016	GBF	C1B-CHB	2.93	1.49	1.41
4	A	1018	GBF	C1A-C2A	2.92	1.49	1.42
4	A	1016	GBF	C1C-CHC	2.92	1.49	1.41
5	A	1003	AOH	C1B-CHB	2.91	1.49	1.41
4	A	1010	GBF	C1B-CHB	2.91	1.49	1.41
4	A	1004	GBF	CBB-CAB	-2.90	1.30	1.50
3	A	1005	GB0	C1C-CHC	2.88	1.49	1.41
4	A	1002	GBF	C4D-ND	2.88	1.37	1.35
4	A	1008	GBF	CBB-CAB	-2.88	1.30	1.50
3	A	1001	GB0	C1C-NC	-2.87	1.32	1.35
4	A	1024	GBF	CBB-CAB	-2.86	1.31	1.50
4	A	1028	GBF	C1C-CHC	2.86	1.48	1.41
4	A	1020	GBF	C3C-C2C	2.84	1.46	1.37
4	A	1015	GBF	C1C-CHC	2.83	1.48	1.41
4	A	1022	GBF	C1C-CHC	2.82	1.48	1.41
4	A	1012	GBF	C1C-CHC	2.81	1.48	1.41
4	A	1025	GBF	C1B-NB	-2.81	1.32	1.35
4	A	1018	GBF	C3C-C2C	2.80	1.46	1.37
4	A	1007	GBF	C1C-CHC	2.80	1.48	1.41
4	A	1007	GBF	CBB-CAB	-2.79	1.31	1.50
4	A	1025	GBF	CBB-CAB	-2.79	1.31	1.50
4	A	1025	GBF	C3D-C4D	2.79	1.42	1.40
4	A	1018	GBF	CAB-C3B	-2.77	1.47	1.52
4	A	1023	GBF	C1B-CHB	2.77	1.48	1.41
4	A	1014	GBF	CBB-CAB	-2.77	1.31	1.50
4	A	1017	GBF	C1B-CHB	2.76	1.48	1.41
4	B	103	GBF	CBB-CAB	-2.75	1.31	1.50
4	A	1015	GBF	CBB-CAB	-2.75	1.31	1.50
4	A	1011	GBF	C1B-CHB	2.75	1.48	1.41
4	A	1027	GBF	CAB-C3B	-2.74	1.47	1.52
4	A	1027	GBF	C1C-NC	-2.74	1.32	1.35
4	A	1018	GBF	CBB-CAB	-2.73	1.31	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1010	GBF	C4C-CHD	2.73	1.48	1.41
4	A	1024	GBF	C3C-C2C	2.73	1.45	1.37
4	A	1026	GBF	C3D-C4D	2.73	1.42	1.40
4	A	1028	GBF	C4C-CHD	2.73	1.48	1.41
4	A	1014	GBF	C3D-C4D	2.70	1.42	1.40
4	A	1006	GBF	CBB-CAB	-2.70	1.32	1.50
4	A	1011	GBF	CBB-CAB	-2.70	1.32	1.50
4	A	1021	GBF	C4C-CHD	2.70	1.48	1.41
4	A	1007	GBF	C1B-CHB	2.69	1.48	1.41
4	A	1016	GBF	C4C-CHD	2.69	1.48	1.41
4	A	1019	GBF	CBB-CAB	-2.69	1.32	1.50
4	B	103	GBF	C1C-CHC	2.68	1.48	1.41
4	A	1028	GBF	CBB-CAB	-2.68	1.32	1.50
4	A	1020	GBF	CBB-CAB	-2.68	1.32	1.50
4	A	1024	GBF	C4D-ND	2.67	1.37	1.35
4	A	1024	GBF	C1B-CHB	2.64	1.48	1.41
4	B	102	GBF	CBB-CAB	-2.64	1.32	1.50
4	A	1002	GBF	CAB-C3B	-2.64	1.47	1.52
4	A	1013	GBF	CBB-CAB	-2.63	1.32	1.50
4	A	1023	GBF	C1C-CHC	2.62	1.48	1.41
3	A	1001	GB0	C1C-CHC	2.61	1.48	1.41
4	A	1021	GBF	C1B-CHB	2.61	1.48	1.41
4	A	1016	GBF	CBB-CAB	-2.61	1.32	1.50
4	A	1008	GBF	C4C-CHD	2.60	1.48	1.41
4	B	103	GBF	C4C-CHD	2.59	1.48	1.41
4	A	1009	GBF	CBB-CAB	-2.59	1.32	1.50
4	A	1012	GBF	CBB-CAB	-2.59	1.32	1.50
4	A	1008	GBF	C1B-CHB	2.58	1.48	1.41
4	A	1020	GBF	C1C-CHC	2.58	1.48	1.41
4	A	1006	GBF	C1C-CHC	2.57	1.48	1.41
4	A	1017	GBF	CBB-CAB	-2.56	1.33	1.50
4	A	1010	GBF	CBB-CAB	-2.56	1.33	1.50
4	A	1009	GBF	C3D-C4D	2.54	1.42	1.40
5	A	1003	AOH	C4D-ND	2.54	1.37	1.35
4	A	1010	GBF	C3D-C4D	2.53	1.42	1.40
4	A	1004	GBF	C1B-CHB	2.53	1.48	1.41
5	A	1003	AOH	O2A-CGA	2.53	1.40	1.33
4	A	1024	GBF	C1C-CHC	2.52	1.48	1.41
4	A	1027	GBF	CBB-CAB	-2.51	1.33	1.50
4	A	1011	GBF	C1C-CHC	2.50	1.48	1.41
4	A	1019	GBF	C1C-CHC	2.50	1.47	1.41
4	A	1016	GBF	C3D-C4D	2.49	1.42	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1023	GBF	CAB-C3B	-2.49	1.47	1.52
4	A	1022	GBF	CBB-CAB	-2.49	1.33	1.50
4	A	1026	GBF	C1C-CHC	2.48	1.47	1.41
4	A	1013	GBF	C1B-CHB	2.48	1.47	1.41
4	A	1002	GBF	C4C-NC	2.48	1.37	1.35
4	A	1012	GBF	C4C-CHD	2.47	1.47	1.41
4	A	1017	GBF	C1C-CHC	2.47	1.47	1.41
4	A	1025	GBF	CAB-C3B	-2.46	1.47	1.52
4	A	1014	GBF	C1C-CHC	2.44	1.47	1.41
4	A	1022	GBF	CAA-C2A	2.44	1.56	1.52
4	A	1013	GBF	C4C-CHD	2.43	1.47	1.41
4	A	1021	GBF	CBB-CAB	-2.42	1.34	1.50
3	A	1001	GB0	C1B-CHB	2.40	1.47	1.41
4	A	1027	GBF	C1C-CHC	2.37	1.47	1.41
4	A	1024	GBF	C3D-C4D	2.37	1.42	1.40
4	A	1008	GBF	C3D-C4D	2.37	1.42	1.40
4	A	1004	GBF	C1C-CHC	2.36	1.47	1.41
4	A	1015	GBF	C4C-CHD	2.36	1.47	1.41
5	A	1003	AOH	C1A-CHA	2.36	1.48	1.38
4	A	1026	GBF	CAB-C3B	-2.35	1.48	1.52
4	A	1025	GBF	C1C-CHC	2.35	1.47	1.41
4	A	1002	GBF	C4D-CHA	-2.34	1.42	1.45
4	A	1008	GBF	C1C-CHC	2.33	1.47	1.41
4	A	1013	GBF	C3D-C4D	2.33	1.42	1.40
4	A	1026	GBF	C1B-CHB	2.26	1.47	1.41
4	A	1006	GBF	C4C-CHD	2.26	1.47	1.41
4	A	1023	GBF	C4C-CHD	2.24	1.47	1.41
4	A	1027	GBF	C1B-CHB	2.23	1.47	1.41
4	A	1004	GBF	C1C-NC	-2.21	1.33	1.35
4	A	1025	GBF	C1B-CHB	2.21	1.47	1.41
4	A	1004	GBF	C4C-CHD	2.20	1.47	1.41
4	A	1018	GBF	C4C-CHD	2.18	1.47	1.41
4	A	1024	GBF	C1C-NC	-2.18	1.33	1.35
4	A	1019	GBF	C3D-C4D	2.16	1.42	1.40
4	A	1015	GBF	CAB-C3B	-2.16	1.48	1.52
4	A	1002	GBF	C1C-NC	-2.15	1.33	1.35
9	A	1035	LMT	O5'-C5'	-2.15	1.39	1.44
4	A	1022	GBF	C4C-CHD	2.13	1.46	1.41
4	A	1019	GBF	C4C-CHD	2.10	1.46	1.41
4	A	1024	GBF	CAB-C3B	-2.09	1.48	1.52
4	A	1025	GBF	C4C-CHD	2.07	1.46	1.41
4	A	1008	GBF	C1C-NC	-2.06	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1013	GBF	CAB-C3B	-2.05	1.48	1.52
3	A	1005	GB0	CAA-C2A	2.05	1.55	1.52
4	A	1008	GBF	CAB-C3B	-2.05	1.48	1.52
4	A	1017	GBF	C4C-CHD	2.04	1.46	1.41
4	A	1020	GBF	C1C-NC	-2.03	1.33	1.35
4	A	1002	GBF	C1C-CHC	2.02	1.46	1.41
3	A	1001	GB0	C4C-CHD	2.02	1.46	1.41
4	A	1011	GBF	C1B-NB	-2.02	1.33	1.35

All (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
3	A	1005	GB0	C1C-C2C-C3C	-27.93	87.57	107.00
4	A	1014	GBF	C1C-C2C-C3C	-27.76	87.68	107.00
4	A	1010	GBF	C1C-C2C-C3C	-27.69	87.73	107.00
4	A	1006	GBF	C1C-C2C-C3C	-27.61	87.78	107.00
3	A	1001	GB0	C1C-C2C-C3C	-27.58	87.81	107.00
4	A	1012	GBF	C1C-C2C-C3C	-27.57	87.81	107.00
4	A	1004	GBF	C1C-C2C-C3C	-27.54	87.84	107.00
4	A	1015	GBF	C1C-C2C-C3C	-27.46	87.89	107.00
4	A	1028	GBF	C1C-C2C-C3C	-27.43	87.91	107.00
4	A	1002	GBF	C1C-C2C-C3C	-27.31	88.00	107.00
4	A	1007	GBF	C1C-C2C-C3C	-27.29	88.01	107.00
4	A	1022	GBF	C1C-C2C-C3C	-27.22	88.06	107.00
4	A	1020	GBF	C1C-C2C-C3C	-27.21	88.07	107.00
4	A	1008	GBF	C1C-C2C-C3C	-27.20	88.07	107.00
4	A	1023	GBF	C1C-C2C-C3C	-27.14	88.11	107.00
4	B	102	GBF	C1C-C2C-C3C	-27.12	88.13	107.00
4	A	1025	GBF	C1C-C2C-C3C	-26.65	88.46	107.00
4	A	1013	GBF	C1C-C2C-C3C	-26.58	88.50	107.00
4	A	1026	GBF	C1C-C2C-C3C	-26.51	88.55	107.00
4	A	1018	GBF	C1C-C2C-C3C	-26.42	88.61	107.00
4	A	1021	GBF	C1C-C2C-C3C	-26.24	88.74	107.00
4	A	1027	GBF	C1C-C2C-C3C	-25.84	89.02	107.00
4	A	1024	GBF	C1C-C2C-C3C	-25.64	89.16	107.00
4	A	1019	GBF	C1C-C2C-C3C	-24.88	89.68	107.00
4	A	1027	GBF	CAA-C2A-C1A	-23.79	101.62	127.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1015	GBF	CAA-C2A-C1A	-17.18	108.82	127.48
4	A	1014	GBF	CAA-C2A-C1A	-16.71	109.33	127.48
4	B	102	GBF	CMC-C2C-C1C	-15.46	104.70	128.46
4	A	1024	GBF	CMC-C2C-C1C	-14.84	105.66	128.46
4	A	1020	GBF	CMC-C2C-C1C	-14.48	106.21	128.46
4	A	1013	GBF	CAA-C2A-C1A	-14.40	111.83	127.48
4	A	1021	GBF	CMC-C2C-C1C	-13.97	107.00	128.46
4	A	1025	GBF	CMC-C2C-C1C	-13.94	107.04	128.46
4	A	1016	GBF	CAA-C2A-C1A	-13.71	112.58	127.48
4	A	1022	GBF	CMC-C2C-C1C	-13.63	107.52	128.46
4	A	1018	GBF	CAA-C2A-C1A	-13.59	112.71	127.48
4	A	1023	GBF	CMC-C2C-C1C	-13.43	107.82	128.46
4	A	1026	GBF	CMC-C2C-C1C	-13.40	107.87	128.46
4	A	1012	GBF	CMC-C2C-C1C	-13.27	108.06	128.46
3	A	1001	GB0	CAA-C2A-C1A	-13.14	113.20	127.48
4	A	1018	GBF	CMC-C2C-C1C	-12.68	108.98	128.46
4	A	1019	GBF	CMC-C2C-C1C	-12.65	109.02	128.46
4	A	1015	GBF	CMC-C2C-C1C	-12.38	109.43	128.46
4	A	1009	GBF	CMC-C2C-C1C	-12.33	109.51	128.46
4	A	1026	GBF	CAA-C2A-C1A	-12.28	114.13	127.48
4	A	1004	GBF	CMC-C2C-C1C	-12.25	109.64	128.46
4	B	103	GBF	CMC-C2C-C1C	-12.23	109.67	128.46
4	A	1011	GBF	CAA-C2A-C1A	-12.22	114.20	127.48
4	A	1010	GBF	CMC-C2C-C1C	-12.20	109.72	128.46
4	A	1027	GBF	CMC-C2C-C1C	-12.19	109.73	128.46
3	A	1001	GB0	CMC-C2C-C1C	-12.15	109.79	128.46
4	A	1007	GBF	CMC-C2C-C1C	-12.13	109.82	128.46
4	A	1014	GBF	CMC-C2C-C1C	-12.12	109.84	128.46
4	A	1008	GBF	CMC-C2C-C1C	-11.97	110.07	128.46
4	A	1016	GBF	CMC-C2C-C1C	-11.81	110.32	128.46
4	A	1013	GBF	CMC-C2C-C1C	-11.71	110.46	128.46
4	A	1017	GBF	CMC-C2C-C1C	-11.42	110.91	128.46
4	A	1028	GBF	CMC-C2C-C1C	-11.16	111.32	128.46
4	B	102	GBF	CAA-C2A-C1A	-11.15	115.36	127.48
3	A	1005	GB0	CAA-C2A-C1A	-11.15	115.37	127.48
4	A	1006	GBF	CMC-C2C-C1C	-10.75	111.95	128.46
4	A	1011	GBF	CMC-C2C-C1C	-10.02	113.07	128.46
4	A	1002	GBF	CMC-C2C-C1C	-9.57	113.75	128.46
4	A	1025	GBF	CAA-C2A-C1A	-9.49	117.17	127.48
4	A	1006	GBF	CAA-C2A-C1A	-9.44	117.22	127.48
4	A	1021	GBF	CAA-C2A-C1A	-9.18	117.50	127.48
4	A	1017	GBF	CAA-C2A-C1A	-8.77	117.95	127.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1024	GBF	CAA-C2A-C1A	-8.65	118.08	127.48
4	A	1007	GBF	OBD-CAD-CBD	-8.57	113.66	125.89
4	A	1002	GBF	CMA-C3A-C2A	-8.54	108.85	124.94
4	A	1028	GBF	CAA-C2A-C1A	-8.42	118.33	127.48
4	A	1023	GBF	OBD-CAD-CBD	-8.35	113.96	125.89
4	A	1025	GBF	OBD-CAD-CBD	-8.34	113.98	125.89
4	B	103	GBF	CAA-C2A-C1A	-8.33	118.43	127.48
4	A	1019	GBF	CAA-C2A-C1A	-8.32	118.44	127.48
4	A	1020	GBF	CAA-C2A-C1A	-8.28	118.48	127.48
4	A	1009	GBF	CAA-C2A-C1A	-8.20	118.57	127.48
4	A	1026	GBF	CMA-C3A-C2A	-8.19	109.50	124.94
4	A	1015	GBF	OBD-CAD-CBD	-7.99	114.48	125.89
4	A	1012	GBF	CMA-C3A-C2A	-7.96	109.93	124.94
4	A	1002	GBF	CMD-C2D-C3D	7.95	139.56	124.68
4	A	1021	GBF	OBD-CAD-CBD	-7.91	114.59	125.89
4	B	102	GBF	OBD-CAD-CBD	-7.88	114.64	125.89
4	A	1024	GBF	CMA-C3A-C2A	-7.76	110.32	124.94
4	A	1027	GBF	CMC-C2C-C3C	-7.75	110.33	124.94
4	A	1018	GBF	CMC-C2C-C3C	-7.71	110.40	124.94
4	A	1022	GBF	CAA-C2A-C1A	-7.68	119.13	127.48
4	A	1010	GBF	OBD-CAD-CBD	-7.59	115.04	125.89
4	A	1023	GBF	CMA-C3A-C2A	-7.59	110.63	124.94
3	A	1005	GB0	CMC-C2C-C1C	-7.56	116.84	128.46
4	A	1013	GBF	OBD-CAD-CBD	-7.45	115.25	125.89
4	A	1007	GBF	CMD-C2D-C3D	7.41	138.55	124.68
4	A	1002	GBF	OBD-CAD-CBD	-7.40	115.32	125.89
4	B	103	GBF	OBD-CAD-CBD	-7.39	115.34	125.89
4	A	1004	GBF	OBD-CAD-CBD	-7.36	115.37	125.89
4	A	1014	GBF	OBD-CAD-CBD	-7.36	115.38	125.89
4	A	1024	GBF	CMC-C2C-C3C	-7.19	111.39	124.94
4	A	1025	GBF	CMC-C2C-C3C	-7.14	111.48	124.94
3	A	1005	GB0	OBD-CAD-CBD	-7.14	115.70	125.89
4	A	1026	GBF	CMC-C2C-C3C	-7.10	111.56	124.94
4	A	1022	GBF	CMA-C3A-C2A	-7.10	111.56	124.94
4	A	1010	GBF	CAA-C2A-C1A	-7.09	119.77	127.48
4	A	1012	GBF	OBD-CAD-CBD	-7.08	115.78	125.89
4	A	1024	GBF	OBD-CAD-CBD	-7.08	115.78	125.89
4	A	1020	GBF	CMC-C2C-C3C	-7.07	111.61	124.94
4	A	1017	GBF	CMA-C3A-C2A	-7.00	111.74	124.94
4	A	1007	GBF	CAA-C2A-C1A	-6.98	119.89	127.48
4	A	1009	GBF	OBD-CAD-CBD	-6.94	115.98	125.89
4	A	1004	GBF	CMC-C2C-C3C	-6.93	111.88	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1008	GBF	CAA-C2A-C1A	-6.89	119.99	127.48
4	A	1019	GBF	CMC-C2C-C3C	-6.89	111.96	124.94
4	A	1016	GBF	OBD-CAD-CBD	-6.85	116.10	125.89
4	A	1019	GBF	CMA-C3A-C2A	-6.83	112.06	124.94
4	A	1019	GBF	OBD-CAD-CBD	-6.83	116.14	125.89
4	A	1028	GBF	O2D-CGD-CBD	6.81	123.37	111.27
4	A	1022	GBF	OBD-CAD-CBD	-6.77	116.22	125.89
4	A	1020	GBF	OBD-CAD-CBD	-6.74	116.27	125.89
4	A	1022	GBF	CMC-C2C-C3C	-6.73	112.25	124.94
4	A	1006	GBF	CMA-C3A-C2A	-6.69	112.33	124.94
4	B	103	GBF	CMA-C3A-C2A	-6.65	112.41	124.94
4	A	1006	GBF	OBD-CAD-CBD	-6.65	116.40	125.89
4	A	1020	GBF	CMD-C2D-C3D	6.63	137.09	124.68
4	A	1027	GBF	OBD-CAD-CBD	-6.63	116.42	125.89
4	A	1021	GBF	CMD-C2D-C3D	6.62	137.06	124.68
4	A	1011	GBF	CMA-C3A-C2A	-6.61	112.48	124.94
4	A	1004	GBF	CMA-C3A-C2A	-6.58	112.54	124.94
4	A	1007	GBF	CMA-C3A-C2A	-6.57	112.55	124.94
4	A	1024	GBF	CMD-C2D-C3D	6.49	136.83	124.68
4	A	1017	GBF	CMD-C2D-C3D	6.48	136.80	124.68
3	A	1005	GB0	CMA-C3A-C2A	-6.47	112.75	124.94
4	A	1010	GBF	CMA-C3A-C2A	-6.42	112.84	124.94
4	A	1027	GBF	O2D-CGD-CBD	6.37	122.59	111.27
4	A	1018	GBF	OBD-CAD-CBD	-6.31	116.88	125.89
4	A	1011	GBF	OBD-CAD-CBD	-6.30	116.89	125.89
4	A	1014	GBF	O2D-CGD-CBD	6.28	122.43	111.27
4	A	1011	GBF	CMD-C2D-C3D	6.26	136.39	124.68
4	A	1007	GBF	CMC-C2C-C3C	-6.26	113.14	124.94
3	A	1001	GB0	CMD-C2D-C3D	6.23	136.34	124.68
4	A	1008	GBF	OBD-CAD-CBD	-6.23	116.99	125.89
4	A	1021	GBF	CMA-C3A-C2A	-6.21	113.22	124.94
4	A	1009	GBF	CMA-C3A-C2A	-6.21	113.23	124.94
4	A	1012	GBF	CMC-C2C-C3C	-6.20	113.25	124.94
4	A	1010	GBF	O2D-CGD-CBD	6.19	122.27	111.27
4	A	1015	GBF	CMC-C2C-C3C	-6.17	113.31	124.94
4	A	1023	GBF	CAA-C2A-C1A	-6.12	120.83	127.48
4	A	1014	GBF	CMD-C2D-C3D	6.07	136.04	124.68
4	A	1015	GBF	CMD-C2D-C3D	6.07	136.04	124.68
4	A	1026	GBF	CMD-C2D-C3D	6.02	135.93	124.68
4	A	1028	GBF	CMA-C3A-C2A	-6.01	113.61	124.94
4	B	102	GBF	CMC-C2C-C3C	-5.97	113.68	124.94
4	A	1028	GBF	CMD-C2D-C3D	5.97	135.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1007	GBF	O2D-CGD-CBD	5.97	121.88	111.27
4	A	1014	GBF	CMC-C2C-C3C	-5.92	113.78	124.94
4	A	1002	GBF	CAA-C2A-C3A	-5.91	110.27	127.25
4	B	102	GBF	CMA-C3A-C2A	-5.91	113.81	124.94
3	A	1001	GB0	OBD-CAD-CBD	-5.90	117.46	125.89
4	A	1028	GBF	OBD-CAD-CBD	-5.87	117.51	125.89
3	A	1005	GB0	CMD-C2D-C3D	5.83	135.59	124.68
4	A	1018	GBF	CMA-C3A-C2A	-5.81	113.99	124.94
4	A	1004	GBF	CAA-C2A-C3A	-5.79	110.62	127.25
4	A	1021	GBF	CMC-C2C-C3C	-5.73	114.14	124.94
4	A	1010	GBF	CAA-C2A-C3A	-5.72	110.80	127.25
4	A	1012	GBF	CAA-C2A-C3A	-5.72	110.82	127.25
4	A	1016	GBF	O2D-CGD-CBD	5.70	121.39	111.27
4	A	1008	GBF	CMC-C2C-C3C	-5.67	114.25	124.94
4	A	1002	GBF	CAA-C2A-C1A	-5.65	121.34	127.48
4	A	1007	GBF	CAA-C2A-C3A	-5.65	111.02	127.25
4	A	1019	GBF	CMD-C2D-C3D	5.63	135.21	124.68
4	A	1013	GBF	CMA-C3A-C2A	-5.62	114.34	124.94
4	A	1025	GBF	CAA-C2A-C3A	-5.62	111.10	127.25
4	A	1008	GBF	CMA-C3A-C2A	-5.61	114.36	124.94
4	A	1025	GBF	CMA-C3A-C2A	-5.61	114.37	124.94
4	A	1020	GBF	CMA-C3A-C2A	-5.60	114.38	124.94
4	A	1013	GBF	CMC-C2C-C3C	-5.60	114.38	124.94
4	A	1011	GBF	CAA-C2A-C3A	-5.58	111.22	127.25
4	A	1004	GBF	CAA-C2A-C1A	-5.55	121.45	127.48
4	A	1017	GBF	CMC-C2C-C3C	-5.54	114.49	124.94
5	A	1003	AOH	OBD-CAD-C3D	-5.54	118.79	127.98
4	A	1002	GBF	CBC-CAC-C3C	5.53	126.36	112.27
4	A	1019	GBF	CAA-C2A-C3A	-5.52	111.37	127.25
4	A	1017	GBF	CAA-C2A-C3A	-5.50	111.45	127.25
4	A	1018	GBF	O2D-CGD-CBD	5.48	121.00	111.27
3	A	1001	GB0	CMC-C2C-C3C	-5.46	114.64	124.94
4	A	1014	GBF	CAA-C2A-C3A	-5.45	111.59	127.25
4	A	1022	GBF	CAA-C2A-C3A	-5.44	111.61	127.25
4	A	1008	GBF	CAA-C2A-C3A	-5.42	111.66	127.25
4	B	103	GBF	O2D-CGD-CBD	5.38	120.83	111.27
4	A	1021	GBF	CAA-C2A-C3A	-5.38	111.79	127.25
4	A	1016	GBF	CMC-C2C-C3C	-5.37	114.82	124.94
4	A	1008	GBF	CMD-C2D-C3D	5.37	134.72	124.68
4	A	1020	GBF	CAA-C2A-C3A	-5.35	111.88	127.25
4	A	1024	GBF	CAA-C2A-C3A	-5.34	111.91	127.25
4	A	1010	GBF	CMC-C2C-C3C	-5.34	114.88	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	GB0	CAA-C2A-C3A	-5.32	111.97	127.25
4	A	1004	GBF	CMD-C2D-C3D	5.30	134.59	124.68
4	A	1027	GBF	CMD-C2D-C3D	5.27	134.53	124.68
5	A	1003	AOH	O2D-CGD-CBD	5.27	120.62	111.27
4	A	1023	GBF	CAA-C2A-C3A	-5.09	112.61	127.25
4	A	1009	GBF	CMC-C2C-C3C	-5.09	115.35	124.94
4	A	1018	GBF	CMD-C2D-C3D	5.08	134.19	124.68
4	A	1017	GBF	OBD-CAD-CBD	-5.07	118.64	125.89
4	A	1023	GBF	CMC-C2C-C3C	-5.07	115.38	124.94
4	A	1026	GBF	OBD-CAD-CBD	-5.07	118.65	125.89
4	A	1016	GBF	CMA-C3A-C2A	-5.04	115.45	124.94
4	A	1006	GBF	CAA-C2A-C3A	-5.01	112.85	127.25
4	B	102	GBF	CAA-C2A-C3A	-5.00	112.87	127.25
4	B	103	GBF	CAA-C2A-C3A	-5.00	112.89	127.25
4	A	1012	GBF	CAA-C2A-C1A	-4.90	122.16	127.48
5	A	1003	AOH	C2A-C1A-CHA	-4.86	116.65	126.36
4	A	1015	GBF	OBD-CAD-C3D	4.86	136.04	127.98
4	A	1015	GBF	CMA-C3A-C2A	-4.85	115.81	124.94
4	B	102	GBF	O2D-CGD-CBD	4.82	119.84	111.27
3	A	1001	GB0	CMA-C3A-C2A	-4.81	115.88	124.94
4	A	1027	GBF	CBC-CAC-C3C	4.80	124.49	112.27
3	A	1005	GB0	CAA-C2A-C3A	-4.79	113.48	127.25
4	A	1013	GBF	O2D-CGD-CBD	4.78	119.77	111.27
4	A	1025	GBF	O2D-CGD-CBD	4.77	119.74	111.27
4	A	1021	GBF	CBC-CAC-C3C	4.76	124.39	112.27
7	A	1031	DGG	O19-C21-C22	4.75	121.73	111.50
4	A	1024	GBF	O2D-CGD-CBD	4.71	119.64	111.27
4	A	1017	GBF	O2D-CGD-CBD	4.70	119.62	111.27
4	A	1020	GBF	O2D-CGD-CBD	4.70	119.62	111.27
4	A	1004	GBF	O2D-CGD-CBD	4.69	119.61	111.27
4	A	1016	GBF	CAA-C2A-C3A	-4.69	113.78	127.25
4	A	1028	GBF	CAA-C2A-C3A	-4.64	113.92	127.25
4	A	1025	GBF	CMD-C2D-C3D	4.60	133.29	124.68
4	A	1012	GBF	O2D-CGD-CBD	4.60	119.43	111.27
4	A	1022	GBF	CMD-C2D-C3D	4.59	133.26	124.68
4	A	1028	GBF	CMC-C2C-C3C	-4.55	116.36	124.94
4	A	1012	GBF	OBD-CAD-C3D	4.55	135.53	127.98
4	A	1016	GBF	OBD-CAD-C3D	4.54	135.52	127.98
4	B	103	GBF	CMD-C2D-C3D	4.52	133.14	124.68
4	A	1010	GBF	CMD-C2D-C3D	4.52	133.13	124.68
4	A	1023	GBF	CMD-C2D-C3D	4.50	133.09	124.68
4	A	1026	GBF	C4-C3-C5	4.49	122.83	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1014	GBF	O2D-CGD-O1D	-4.44	115.16	123.84
4	A	1009	GBF	O2D-CGD-CBD	4.43	119.13	111.27
4	A	1016	GBF	CBC-CAC-C3C	4.42	123.53	112.27
4	A	1007	GBF	C9-C8-C10	4.41	122.69	115.27
3	A	1001	GB0	C1-C2-C3	-4.40	118.44	126.04
4	A	1008	GBF	O2D-CGD-O1D	-4.39	115.26	123.84
4	A	1017	GBF	C9-C8-C10	4.35	122.59	115.27
4	A	1008	GBF	CBC-CAC-C3C	4.31	123.26	112.27
4	A	1020	GBF	OBD-CAD-C3D	4.31	135.14	127.98
3	A	1005	GB0	O2A-CGA-O1A	-4.28	112.80	123.59
4	A	1004	GBF	CBC-CAC-C3C	4.25	123.10	112.27
4	A	1021	GBF	C4-C3-C5	4.23	122.38	115.27
4	A	1009	GBF	OBD-CAD-C3D	4.22	135.00	127.98
4	B	102	GBF	OBD-CAD-C3D	4.22	135.00	127.98
4	A	1011	GBF	CBC-CAC-C3C	4.20	122.97	112.27
4	A	1015	GBF	O2D-CGD-CBD	4.20	118.73	111.27
4	A	1013	GBF	OBD-CAD-C3D	4.18	134.92	127.98
4	A	1016	GBF	CMD-C2D-C3D	4.18	132.50	124.68
4	B	103	GBF	C9-C8-C10	4.17	122.29	115.27
4	A	1019	GBF	CBC-CAC-C3C	4.17	122.90	112.27
4	A	1012	GBF	CBC-CAC-C3C	4.17	122.88	112.27
4	A	1022	GBF	O2D-CGD-CBD	4.16	118.65	111.27
3	A	1001	GB0	CBC-CAC-C3C	4.16	122.85	112.27
4	A	1015	GBF	CAA-C2A-C3A	-4.14	115.34	127.25
4	A	1014	GBF	CBC-CAC-C3C	4.13	122.78	112.27
4	A	1009	GBF	CAA-C2A-C3A	-4.13	115.39	127.25
4	B	103	GBF	CMC-C2C-C3C	-4.12	117.18	124.94
4	A	1007	GBF	CBC-CAC-C3C	4.12	122.76	112.27
4	A	1012	GBF	CMD-C2D-C3D	4.11	132.36	124.68
4	A	1017	GBF	CBC-CAC-C3C	4.11	122.73	112.27
3	A	1001	GB0	OBD-CAD-C3D	4.06	134.73	127.98
5	A	1003	AOH	C1B-C2B-C3B	-4.05	104.17	107.00
3	A	1005	GB0	OBD-CAD-C3D	4.04	134.69	127.98
3	A	1005	GB0	CMC-C2C-C3C	-4.04	117.33	124.94
4	A	1013	GBF	CBC-CAC-C3C	4.01	122.49	112.27
5	A	1003	AOH	O2A-CGA-O1A	-4.00	113.51	123.59
4	A	1024	GBF	OBD-CAD-C3D	3.98	134.60	127.98
4	A	1025	GBF	OBD-CAD-C3D	3.98	134.59	127.98
4	A	1015	GBF	CBC-CAC-C3C	3.97	122.38	112.27
4	A	1018	GBF	O2D-CGD-O1D	-3.96	116.10	123.84
4	A	1026	GBF	C6-C7-C8	-3.95	118.16	127.66
4	A	1027	GBF	CAA-C2A-C3A	-3.94	115.92	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1024	GBF	CBC-CAC-C3C	3.90	122.21	112.27
4	A	1025	GBF	CBC-CAC-C3C	3.88	122.16	112.27
4	A	1023	GBF	CBC-CAC-C3C	3.88	122.16	112.27
4	A	1011	GBF	CMC-C2C-C3C	-3.88	117.63	124.94
4	B	103	GBF	OBD-CAD-C3D	3.87	134.41	127.98
4	A	1006	GBF	CMC-C2C-C3C	-3.86	117.66	124.94
4	A	1013	GBF	CMD-C2D-C3D	3.86	131.90	124.68
4	A	1006	GBF	CMD-C2D-C3D	3.86	131.90	124.68
4	A	1010	GBF	OBD-CAD-C3D	3.85	134.38	127.98
4	A	1019	GBF	OBD-CAD-C3D	3.85	134.38	127.98
4	A	1008	GBF	O2D-CGD-CBD	3.85	118.11	111.27
4	A	1010	GBF	CBC-CAC-C3C	3.83	122.03	112.27
4	A	1027	GBF	O2D-CGD-O1D	-3.82	116.37	123.84
4	A	1009	GBF	CMD-C2D-C3D	3.80	131.79	124.68
4	A	1007	GBF	O2D-CGD-O1D	-3.80	116.42	123.84
4	A	1014	GBF	CAA-CBA-CGA	-3.79	106.31	112.67
4	A	1004	GBF	O2D-CGD-O1D	-3.79	116.43	123.84
4	A	1013	GBF	CAA-C2A-C3A	-3.77	116.40	127.25
4	A	1028	GBF	O2D-CGD-O1D	-3.76	116.49	123.84
5	A	1003	AOH	C9-C8-C10	3.76	121.59	115.27
7	A	1030	DGG	O19-C21-O21	-3.74	114.66	123.70
4	A	1015	GBF	O2D-CGD-O1D	-3.74	116.53	123.84
4	A	1008	GBF	OBD-CAD-C3D	3.74	134.18	127.98
4	A	1002	GBF	CMC-C2C-C3C	-3.72	117.93	124.94
4	B	103	GBF	CBC-CAC-C3C	3.71	121.72	112.27
7	A	1030	DGG	O19-C21-C22	3.70	119.47	111.50
4	A	1004	GBF	OBD-CAD-C3D	3.69	134.10	127.98
3	A	1005	GB0	CBC-CAC-C3C	3.69	121.66	112.27
4	A	1006	GBF	O2D-CGD-O1D	-3.68	116.64	123.84
4	A	1028	GBF	CBC-CAC-C3C	3.65	121.58	112.27
4	A	1025	GBF	O2D-CGD-O1D	-3.65	116.70	123.84
4	A	1009	GBF	CBC-CAC-C3C	3.65	121.56	112.27
4	A	1026	GBF	CAA-C2A-C3A	-3.64	116.77	127.25
4	A	1026	GBF	O2D-CGD-CBD	3.64	117.73	111.27
4	A	1026	GBF	CBC-CAC-C3C	3.63	121.52	112.27
4	A	1008	GBF	C4-C3-C5	3.62	121.36	115.27
4	A	1020	GBF	O2D-CGD-O1D	-3.61	116.79	123.84
4	A	1024	GBF	O2D-CGD-O1D	-3.55	116.89	123.84
4	A	1002	GBF	O2D-CGD-O1D	-3.55	116.90	123.84
4	A	1014	GBF	OBD-CAD-C3D	3.50	133.80	127.98
3	A	1005	GB0	O2D-CGD-CBD	3.49	117.47	111.27
5	A	1003	AOH	C3A-C4A-CHB	-3.49	118.53	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1020	GBF	CBC-CAC-C3C	3.48	121.13	112.27
4	A	1007	GBF	C6-C7-C8	-3.48	119.29	127.66
4	A	1011	GBF	O2D-CGD-CBD	3.44	117.39	111.27
4	B	102	GBF	CMD-C2D-C3D	3.44	131.11	124.68
4	A	1006	GBF	CBC-CAC-C3C	3.43	121.00	112.27
4	A	1018	GBF	CAA-C2A-C3A	-3.41	117.45	127.25
4	A	1006	GBF	OBD-CAD-C3D	3.39	133.61	127.98
4	A	1022	GBF	O2D-CGD-O1D	-3.38	117.23	123.84
4	A	1023	GBF	O2D-CGD-CBD	3.37	117.26	111.27
4	A	1002	GBF	O2D-CGD-CBD	3.35	117.21	111.27
4	A	1013	GBF	CBA-CAA-C2A	3.31	118.19	112.60
4	A	1018	GBF	CBC-CAC-C3C	3.29	120.66	112.27
4	A	1019	GBF	C1-C2-C3	-3.28	120.36	126.04
3	A	1001	GB0	C9-C8-C10	3.28	120.79	115.27
4	A	1022	GBF	CBC-CAC-C3C	3.25	120.55	112.27
4	A	1027	GBF	CMA-C3A-C2A	-3.23	118.86	124.94
4	A	1024	GBF	CMB-C2B-C1B	-3.23	123.51	128.46
4	A	1017	GBF	O2D-CGD-O1D	-3.22	117.54	123.84
7	A	1031	DGG	O17-C1-C2	3.21	121.99	111.91
3	A	1001	GB0	C4-C3-C5	3.19	120.64	115.27
4	A	1006	GBF	O2D-CGD-CBD	3.18	116.92	111.27
4	A	1027	GBF	CAA-CBA-CGA	-3.15	105.10	113.82
4	B	103	GBF	CMB-C2B-C1B	-3.13	123.65	128.46
4	A	1013	GBF	CED-O2D-CGD	3.13	123.02	115.94
5	A	1003	AOH	O2D-CGD-O1D	-3.13	117.72	123.84
5	A	1003	AOH	C1B-CHB-C4A	-3.12	123.94	130.12
4	A	1028	GBF	CMB-C2B-C1B	-3.11	123.68	128.46
4	A	1019	GBF	C9-C8-C10	3.11	120.50	115.27
4	A	1021	GBF	OBD-CAD-C3D	3.10	133.13	127.98
4	A	1027	GBF	CBA-CAA-C2A	3.10	117.82	112.60
4	B	102	GBF	CBC-CAC-C3C	3.09	120.15	112.27
4	A	1012	GBF	O2D-CGD-O1D	-3.07	117.84	123.84
4	A	1023	GBF	OBD-CAD-C3D	3.07	133.07	127.98
4	A	1023	GBF	C4-C3-C5	3.06	120.42	115.27
7	A	1030	DGG	O17-C1-C2	3.05	121.48	111.91
4	A	1002	GBF	C4-C3-C5	3.05	120.39	115.27
4	A	1014	GBF	CMA-C3A-C2A	-3.04	119.22	124.94
4	A	1002	GBF	C1-C2-C3	-3.01	120.83	126.04
4	A	1028	GBF	OBD-CAD-C3D	3.01	132.97	127.98
10	B	101	C4D	C16-C4-C12	-2.98	123.03	127.30
4	A	1024	GBF	CMB-C2B-C3B	2.95	130.50	124.94
4	A	1021	GBF	O2D-CGD-CBD	2.94	116.48	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	AOH	CMD-C2D-C3D	2.93	130.16	124.68
4	A	1017	GBF	OBD-CAD-C3D	2.93	132.84	127.98
4	A	1017	GBF	CMB-C2B-C1B	-2.92	123.98	128.46
9	A	1035	LMT	O5'-C1'-O1'	-2.91	103.09	109.97
4	A	1026	GBF	CED-O2D-CGD	2.91	122.51	115.94
4	A	1011	GBF	CMB-C2B-C1B	-2.90	124.01	128.46
10	B	101	C4D	C10-C33-C31	2.90	122.64	118.08
4	A	1023	GBF	C1-C2-C3	-2.90	121.03	126.04
4	A	1027	GBF	OBD-CAD-C3D	2.89	132.78	127.98
3	A	1001	GB0	C1B-C2B-C3B	2.88	109.00	107.00
5	A	1003	AOH	C4-C3-C5	2.88	120.11	115.27
4	A	1010	GBF	CMB-C2B-C1B	-2.87	124.06	128.46
5	A	1003	AOH	C4A-NA-C1A	2.86	108.03	106.30
4	A	1026	GBF	O2A-CGA-CBA	2.85	120.86	111.91
4	A	1007	GBF	CMB-C2B-C1B	-2.85	124.08	128.46
4	A	1026	GBF	OBD-CAD-C3D	2.84	132.69	127.98
4	A	1019	GBF	C6-C7-C8	-2.83	120.83	127.66
4	A	1009	GBF	CED-O2D-CGD	2.83	122.34	115.94
4	A	1013	GBF	C10-C8-C9	2.83	120.85	114.60
4	A	1018	GBF	C1-O2A-CGA	2.81	123.82	116.44
10	B	101	C4D	C7-C32-C30	2.80	122.48	118.08
3	A	1005	GB0	C6-C7-C8	-2.80	120.92	127.66
4	A	1026	GBF	O2A-CGA-O1A	-2.79	116.55	123.59
4	A	1011	GBF	OBD-CAD-C3D	2.79	132.61	127.98
5	A	1003	AOH	C4C-C3C-C2C	-2.79	104.33	106.92
4	A	1015	GBF	O2A-CGA-CBA	2.78	120.64	111.91
5	A	1003	AOH	C3A-C2A-C1A	-2.78	97.17	101.34
3	A	1005	GB0	CMB-C2B-C1B	-2.78	124.19	128.46
4	A	1012	GBF	CAA-CBA-CGA	-2.77	106.14	113.82
5	A	1003	AOH	OBD-CAD-CBD	2.77	129.85	125.89
4	A	1027	GBF	O2A-CGA-CBA	2.77	120.59	111.91
4	A	1013	GBF	C4-C3-C5	2.76	119.92	115.27
3	A	1005	GB0	O2A-CGA-CBA	2.76	120.57	111.91
4	A	1015	GBF	C4-C3-C5	2.76	119.91	115.27
9	A	1034	LMT	O2'-C2'-C1'	-2.75	103.35	110.05
4	A	1028	GBF	O2A-CGA-O1A	-2.74	116.67	123.59
4	A	1007	GBF	O2A-CGA-CBA	2.74	120.50	111.91
4	A	1012	GBF	O2A-CGA-O1A	-2.73	116.69	123.59
10	B	101	C4D	C9-C23-C21	2.73	119.87	115.27
4	A	1020	GBF	C1-C2-C3	-2.73	121.32	126.04
4	A	1021	GBF	CMB-C2B-C1B	-2.73	124.27	128.46
4	A	1007	GBF	C4-C3-C2	-2.73	116.67	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1009	GBF	O1D-CGD-CBD	-2.72	118.92	124.48
4	A	1004	GBF	C1-C2-C3	-2.71	122.36	126.75
4	A	1011	GBF	C4-C3-C5	2.71	119.83	115.27
4	A	1018	GBF	C1-C2-C3	-2.71	122.37	126.75
4	A	1016	GBF	O2D-CGD-O1D	-2.68	118.60	123.84
4	A	1008	GBF	C1-C2-C3	-2.67	121.43	126.04
4	A	1019	GBF	C11-C12-C13	-2.67	118.63	127.75
4	A	1020	GBF	C15-C13-C14	2.67	120.49	114.60
4	A	1027	GBF	C1-C2-C3	-2.66	122.44	126.75
9	A	1035	LMT	O3'-C3'-C2'	-2.66	104.19	110.35
4	A	1019	GBF	O2D-CGD-CBD	2.66	116.00	111.27
3	A	1001	GB0	O2A-CGA-O1A	-2.66	116.88	123.59
4	A	1024	GBF	C1-C2-C3	-2.66	122.45	126.75
4	A	1010	GBF	O2D-CGD-O1D	-2.66	118.65	123.84
4	A	1010	GBF	O1D-CGD-CBD	-2.64	119.08	124.48
9	A	1034	LMT	O5'-C1'-O1'	-2.63	103.75	109.97
10	B	101	C4D	C28-C26-C22	-2.63	123.56	127.31
9	A	1035	LMT	C1B-O1B-C4'	-2.61	111.51	117.96
4	A	1014	GBF	CMB-C2B-C1B	-2.60	124.46	128.46
4	A	1021	GBF	C15-C13-C14	2.59	120.33	114.60
9	A	1034	LMT	C1B-O1B-C4'	-2.59	111.56	117.96
7	A	1031	DGG	O17-C1-O1	-2.59	117.06	123.59
4	A	1018	GBF	OBD-CAD-C3D	2.58	132.26	127.98
4	A	1020	GBF	O2A-CGA-CBA	2.57	119.96	111.91
4	A	1027	GBF	CBB-CAB-C3B	2.56	131.39	113.39
4	A	1007	GBF	O2A-CGA-O1A	-2.55	117.15	123.59
4	A	1007	GBF	C9-C8-C7	-2.54	117.16	123.68
4	B	103	GBF	C4-C3-C5	2.54	119.54	115.27
3	A	1001	GB0	C6-C7-C8	-2.53	121.56	127.66
4	A	1016	GBF	CMB-C2B-C1B	-2.53	124.58	128.46
4	A	1015	GBF	CMB-C2B-C1B	-2.51	124.60	128.46
3	A	1005	GB0	CMB-C2B-C3B	2.51	129.68	124.94
4	B	103	GBF	C6-C7-C8	-2.50	121.63	127.66
4	A	1021	GBF	C11-C12-C13	-2.50	119.20	127.75
4	A	1012	GBF	CBB-CAB-C3B	2.50	130.97	113.39
4	A	1028	GBF	O2A-CGA-CBA	2.48	119.69	111.91
4	A	1027	GBF	C5-C3-C4	2.46	120.03	114.60
3	A	1005	GB0	C6-C5-C3	-2.46	104.90	112.98
4	A	1023	GBF	CBB-CAB-C3B	2.45	130.66	113.39
4	A	1006	GBF	CMB-C2B-C1B	-2.44	124.71	128.46
4	A	1013	GBF	CBB-CAB-C3B	2.44	130.57	113.39
9	A	1034	LMT	C6'-C5'-C4'	-2.44	106.24	113.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1017	GBF	C14-C13-C12	-2.44	115.61	122.65
4	A	1020	GBF	C6-C7-C8	-2.43	121.80	127.66
4	B	103	GBF	O2D-CGD-O1D	-2.43	119.09	123.84
4	A	1025	GBF	CMB-C2B-C1B	-2.42	124.74	128.46
4	A	1011	GBF	O2D-CGD-O1D	-2.42	119.11	123.84
4	A	1009	GBF	CMB-C2B-C1B	-2.40	124.77	128.46
3	A	1001	GB0	O2A-CGA-CBA	2.39	119.41	111.91
4	A	1019	GBF	C4-C3-C5	2.38	119.28	115.27
3	A	1005	GB0	CBA-CAA-C2A	2.38	116.62	112.60
4	A	1011	GBF	CMB-C2B-C3B	2.38	129.42	124.94
7	A	1030	DGG	O17-C1-O1	-2.37	117.62	123.59
5	A	1003	AOH	C11-C10-C8	2.36	120.75	112.98
4	B	103	GBF	C11-C12-C13	-2.36	119.67	127.75
4	A	1021	GBF	O2D-CGD-O1D	-2.36	119.22	123.84
4	A	1007	GBF	C4-C3-C5	2.36	119.24	115.27
3	A	1005	GB0	O2D-CGD-O1D	-2.34	119.25	123.84
4	A	1004	GBF	C5-C3-C4	2.33	119.75	114.60
4	A	1013	GBF	O1D-CGD-CBD	-2.33	119.71	124.48
4	A	1016	GBF	CBB-CAB-C3B	2.33	129.77	113.39
4	A	1002	GBF	C11-C10-C8	-2.32	105.33	112.98
10	B	101	C4D	C14-C12-C2	2.32	119.73	114.60
4	A	1028	GBF	C4-C3-C5	2.31	119.15	115.27
4	A	1022	GBF	OBD-CAD-C3D	2.30	131.81	127.98
3	A	1001	GB0	C11-C12-C13	-2.30	119.88	127.75
5	A	1003	AOH	C6-C7-C8	-2.30	122.12	127.66
4	B	103	GBF	O2A-CGA-O1A	-2.30	117.79	123.59
4	A	1027	GBF	C1B-C2B-C3B	-2.30	105.40	107.00
4	A	1020	GBF	CBB-CAB-C3B	2.30	129.55	113.39
4	A	1008	GBF	CBB-CAB-C3B	2.29	129.54	113.39
4	A	1021	GBF	CBB-CAB-C3B	2.29	129.53	113.39
4	B	103	GBF	CMB-C2B-C3B	2.29	129.26	124.94
4	A	1022	GBF	CBB-CAB-C3B	2.29	129.50	113.39
4	A	1019	GBF	O2A-CGA-O1A	-2.29	117.82	123.59
3	A	1005	GB0	C1-C2-C3	-2.28	122.10	126.04
4	A	1008	GBF	CED-O2D-CGD	-2.28	110.79	115.94
4	A	1019	GBF	C15-C13-C14	2.27	119.62	114.60
4	A	1002	GBF	CMB-C2B-C1B	-2.27	124.97	128.46
4	A	1026	GBF	C15-C13-C14	2.26	119.61	114.60
4	B	102	GBF	CAA-CBA-CGA	-2.26	108.88	112.67
4	A	1023	GBF	O2A-CGA-O1A	-2.24	117.93	123.59
4	A	1012	GBF	O2A-CGA-CBA	2.24	118.92	111.91
4	A	1012	GBF	C1-C2-C3	-2.23	122.19	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1011	GBF	O2A-CGA-O1A	-2.23	117.97	123.59
4	A	1002	GBF	C15-C13-C14	2.22	119.51	114.60
4	A	1013	GBF	O2A-CGA-O1A	-2.21	118.02	123.59
4	A	1010	GBF	CBA-CAA-C2A	-2.21	108.41	112.48
4	A	1011	GBF	O2A-CGA-CBA	2.21	118.83	111.91
7	A	1031	DGG	C17-O17-C1	2.20	125.28	117.12
4	A	1015	GBF	CBB-CAB-C3B	2.20	128.90	113.39
4	B	103	GBF	C15-C13-C14	2.20	119.47	114.60
4	A	1028	GBF	CBA-CAA-C2A	2.20	116.31	112.60
4	A	1021	GBF	CMB-C2B-C3B	2.19	129.08	124.94
4	A	1013	GBF	O2A-CGA-CBA	2.19	118.79	111.91
4	A	1012	GBF	C1-O2A-CGA	2.19	122.19	116.44
4	A	1016	GBF	O1D-CGD-CBD	-2.19	120.00	124.48
4	A	1017	GBF	C15-C13-C14	2.19	119.43	114.60
5	A	1003	AOH	C10-C11-C12	-2.18	104.71	111.88
4	A	1012	GBF	C10-C8-C9	2.18	119.42	114.60
4	A	1008	GBF	C4-C3-C2	-2.18	118.09	123.68
4	A	1028	GBF	CBB-CAB-C3B	2.17	128.70	113.39
5	A	1003	AOH	C5-C6-C7	-2.17	104.74	111.88
4	A	1010	GBF	CBB-CAB-C3B	2.17	128.68	113.39
4	A	1009	GBF	CBB-CAB-C3B	2.17	128.67	113.39
4	A	1024	GBF	O2A-CGA-O1A	-2.17	118.12	123.59
4	A	1028	GBF	C11-C12-C13	-2.17	120.35	127.75
4	A	1024	GBF	O2A-CGA-CBA	2.16	118.70	111.91
3	A	1005	GB0	C15-C13-C14	2.16	119.38	114.60
4	B	102	GBF	O2D-CGD-O1D	-2.15	119.63	123.84
4	A	1019	GBF	CBB-CAB-C3B	2.15	128.54	113.39
4	B	103	GBF	O1D-CGD-CBD	-2.15	120.08	124.48
4	A	1021	GBF	C1-C2-C3	-2.15	122.32	126.04
4	A	1017	GBF	C6-C7-C8	-2.15	122.48	127.66
10	B	101	C4D	C38-C34-C32	-2.14	124.25	127.31
4	A	1018	GBF	CBB-CAB-C3B	2.13	128.39	113.39
10	B	101	C4D	C10-C33-C35	-2.13	119.94	122.92
3	A	1001	GB0	CED-O2D-CGD	2.13	120.75	115.94
4	B	102	GBF	CBB-CAB-C3B	2.13	128.35	113.39
4	A	1021	GBF	O2A-CGA-O1A	-2.12	118.23	123.59
4	A	1028	GBF	O1D-CGD-CBD	-2.12	120.14	124.48
4	B	102	GBF	CMB-C2B-C1B	-2.12	125.21	128.46
9	A	1035	LMT	C1-O1'-C1'	-2.12	110.33	113.84
4	A	1023	GBF	C6-C7-C8	-2.10	122.59	127.66
4	A	1012	GBF	C4-C3-C5	2.10	118.81	115.27
4	A	1026	GBF	CBB-CAB-C3B	2.10	128.17	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1004	GBF	CBB-CAB-C3B	2.09	128.10	113.39
9	A	1034	LMT	O5'-C5'-C4'	2.09	114.15	109.75
3	A	1005	GB0	C9-C8-C7	-2.08	118.33	123.68
4	A	1023	GBF	C15-C13-C14	2.08	119.19	114.60
10	B	101	C4D	C6-C22-C20	2.07	121.34	118.08
9	A	1034	LMT	C1'-O5'-C5'	2.07	117.75	113.69
4	A	1011	GBF	CBB-CAB-C3B	2.07	127.94	113.39
10	B	101	C4D	C20-C22-C26	-2.06	115.78	118.94
4	A	1008	GBF	O2A-CGA-O1A	-2.05	118.41	123.59
4	A	1017	GBF	CBB-CAB-C3B	2.05	127.85	113.39
5	A	1003	AOH	CBB-CAB-C3B	2.05	127.81	113.39
4	A	1018	GBF	C5-C3-C4	2.05	119.12	114.60
4	A	1002	GBF	C4D-C3D-CAD	-2.05	104.50	107.81
4	A	1015	GBF	O2A-CGA-O1A	-2.05	118.43	123.59
4	A	1010	GBF	CED-O2D-CGD	2.04	120.56	115.94
4	A	1025	GBF	CBB-CAB-C3B	2.04	127.77	113.39
4	A	1002	GBF	C3D-CAD-CBD	2.04	110.30	107.61
4	B	103	GBF	O2A-CGA-CBA	2.04	118.29	111.91
4	A	1022	GBF	CMB-C2B-C1B	-2.03	125.34	128.46
3	A	1001	GB0	CBB-CAB-C3B	2.03	127.68	113.39
4	A	1002	GBF	C14-C13-C12	-2.02	116.80	122.65
4	A	1017	GBF	C1-O2A-CGA	2.01	121.71	116.44
4	A	1014	GBF	CBB-CAB-C3B	2.00	127.50	113.39
4	A	1019	GBF	CMB-C2B-C1B	-2.00	125.39	128.46
4	A	1024	GBF	CBB-CAB-C3B	2.00	127.47	113.39

All (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
4	A	1012	GBF	NA
4	A	1023	GBF	NA
4	A	1028	GBF	NA
4	A	1009	GBF	NA
4	A	1011	GBF	NA
4	A	1021	GBF	NA
4	A	1013	GBF	NA
4	A	1017	GBF	NA

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Mol	Chain	Res	Type	Atom
4	B	103	GBF	NA
4	A	1025	GBF	NA
4	A	1022	GBF	NA
4	A	1010	GBF	NA
4	B	102	GBF	NA
4	A	1014	GBF	NA
4	A	1015	GBF	NA
4	A	1020	GBF	NA
4	A	1016	GBF	NA
4	A	1024	GBF	NA
4	A	1027	GBF	NA
4	A	1019	GBF	NA
4	A	1026	GBF	NA
4	A	1002	GBF	NA
5	A	1003	AOH	ND
5	A	1003	AOH	NA
5	A	1003	AOH	NB
3	A	1001	GB0	NA

All (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
4	A	1004	GBF	C1A-C2A-CAA-CBA
4	A	1004	GBF	C2B-C3B-CAB-CBB
4	A	1004	GBF	C4B-C3B-CAB-CBB
4	A	1004	GBF	C2C-C3C-CAC-CBC
4	A	1004	GBF	C4C-C3C-CAC-CBC
4	A	1007	GBF	C3A-C2A-CAA-CBA
4	A	1007	GBF	C2B-C3B-CAB-CBB
4	A	1007	GBF	C4B-C3B-CAB-CBB
4	A	1007	GBF	C2C-C3C-CAC-CBC
4	A	1007	GBF	C4C-C3C-CAC-CBC
4	A	1007	GBF	CHA-CBD-CGD-O1D
4	A	1006	GBF	C1A-C2A-CAA-CBA
4	A	1006	GBF	C2B-C3B-CAB-CBB
4	A	1006	GBF	C4B-C3B-CAB-CBB
4	A	1006	GBF	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
4	A	1006	GBF	C4C-C3C-CAC-CBC
4	A	1008	GBF	C1A-C2A-CAA-CBA
4	A	1008	GBF	C2B-C3B-CAB-CBB
4	A	1008	GBF	C4B-C3B-CAB-CBB
4	A	1008	GBF	C2C-C3C-CAC-CBC
4	A	1008	GBF	C4C-C3C-CAC-CBC
4	A	1012	GBF	C1A-C2A-CAA-CBA
4	A	1012	GBF	C2B-C3B-CAB-CBB
4	A	1012	GBF	C4B-C3B-CAB-CBB
4	A	1012	GBF	C2C-C3C-CAC-CBC
4	A	1012	GBF	C4C-C3C-CAC-CBC
4	A	1023	GBF	C1A-C2A-CAA-CBA
4	A	1023	GBF	C2B-C3B-CAB-CBB
4	A	1023	GBF	C4B-C3B-CAB-CBB
4	A	1023	GBF	C2C-C3C-CAC-CBC
4	A	1023	GBF	C4C-C3C-CAC-CBC
4	A	1028	GBF	C2B-C3B-CAB-CBB
4	A	1028	GBF	C4B-C3B-CAB-CBB
4	A	1028	GBF	C2C-C3C-CAC-CBC
4	A	1028	GBF	C4C-C3C-CAC-CBC
4	A	1028	GBF	CHA-CBD-CGD-O1D
4	A	1009	GBF	C1A-C2A-CAA-CBA
4	A	1009	GBF	C2B-C3B-CAB-CBB
4	A	1009	GBF	C4B-C3B-CAB-CBB
4	A	1009	GBF	C2C-C3C-CAC-CBC
4	A	1009	GBF	C4C-C3C-CAC-CBC
4	A	1011	GBF	C2B-C3B-CAB-CBB
4	A	1011	GBF	C4B-C3B-CAB-CBB
4	A	1011	GBF	C2C-C3C-CAC-CBC
4	A	1011	GBF	C4C-C3C-CAC-CBC
4	A	1021	GBF	C1A-C2A-CAA-CBA
4	A	1021	GBF	C2B-C3B-CAB-CBB
4	A	1021	GBF	C4B-C3B-CAB-CBB
4	A	1021	GBF	C2C-C3C-CAC-CBC
4	A	1021	GBF	C4C-C3C-CAC-CBC
7	A	1031	DGG	C18-OP2-P-OP1
7	A	1031	DGG	C18-OP2-P-OP3
7	A	1031	DGG	C18-OP2-P-OP4
7	A	1031	DGG	C40-OP4-P-OP1
7	A	1031	DGG	C40-OP4-P-OP2
7	A	1031	DGG	C40-OP4-P-OP3
4	A	1013	GBF	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
4	A	1013	GBF	C3A-C2A-CAA-CBA
4	A	1013	GBF	C2B-C3B-CAB-CBB
4	A	1013	GBF	C4B-C3B-CAB-CBB
4	A	1013	GBF	C2C-C3C-CAC-CBC
4	A	1013	GBF	C4C-C3C-CAC-CBC
7	A	1030	DGG	C40-OP4-P-OP1
7	A	1030	DGG	OP4-C40-C41-O42
4	A	1017	GBF	C1A-C2A-CAA-CBA
4	A	1017	GBF	C3A-C2A-CAA-CBA
4	A	1017	GBF	C2B-C3B-CAB-CBB
4	A	1017	GBF	C4B-C3B-CAB-CBB
4	A	1017	GBF	C2C-C3C-CAC-CBC
4	A	1017	GBF	C4C-C3C-CAC-CBC
4	B	103	GBF	C1A-C2A-CAA-CBA
4	B	103	GBF	C2B-C3B-CAB-CBB
4	B	103	GBF	C4B-C3B-CAB-CBB
4	B	103	GBF	C2C-C3C-CAC-CBC
4	B	103	GBF	C4C-C3C-CAC-CBC
4	B	103	GBF	CBD-CGD-O2D-CED
4	A	1025	GBF	C3A-C2A-CAA-CBA
4	A	1025	GBF	C2B-C3B-CAB-CBB
4	A	1025	GBF	C4B-C3B-CAB-CBB
4	A	1025	GBF	C2C-C3C-CAC-CBC
4	A	1025	GBF	C4C-C3C-CAC-CBC
4	A	1022	GBF	C1A-C2A-CAA-CBA
4	A	1022	GBF	C2B-C3B-CAB-CBB
4	A	1022	GBF	C4B-C3B-CAB-CBB
4	A	1022	GBF	C2C-C3C-CAC-CBC
4	A	1022	GBF	C4C-C3C-CAC-CBC
4	A	1010	GBF	C1A-C2A-CAA-CBA
4	A	1010	GBF	C2B-C3B-CAB-CBB
4	A	1010	GBF	C4B-C3B-CAB-CBB
4	A	1010	GBF	C2C-C3C-CAC-CBC
4	A	1010	GBF	C4C-C3C-CAC-CBC
4	A	1010	GBF	CBD-CGD-O2D-CED
4	A	1010	GBF	O1D-CGD-O2D-CED
4	B	102	GBF	C3A-C2A-CAA-CBA
4	B	102	GBF	C2B-C3B-CAB-CBB
4	B	102	GBF	C4B-C3B-CAB-CBB
4	B	102	GBF	C2C-C3C-CAC-CBC
4	B	102	GBF	C4C-C3C-CAC-CBC
4	B	102	GBF	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
4	A	1014	GBF	C1A-C2A-CAA-CBA
4	A	1014	GBF	C2B-C3B-CAB-CBB
4	A	1014	GBF	C4B-C3B-CAB-CBB
4	A	1014	GBF	C2C-C3C-CAC-CBC
4	A	1014	GBF	C4C-C3C-CAC-CBC
4	A	1015	GBF	C1A-C2A-CAA-CBA
4	A	1015	GBF	C3A-C2A-CAA-CBA
4	A	1015	GBF	C2B-C3B-CAB-CBB
4	A	1015	GBF	C4B-C3B-CAB-CBB
4	A	1015	GBF	C2C-C3C-CAC-CBC
4	A	1015	GBF	C4C-C3C-CAC-CBC
4	A	1020	GBF	C3A-C2A-CAA-CBA
4	A	1020	GBF	C2B-C3B-CAB-CBB
4	A	1020	GBF	C4B-C3B-CAB-CBB
4	A	1020	GBF	C2C-C3C-CAC-CBC
4	A	1020	GBF	C4C-C3C-CAC-CBC
4	A	1016	GBF	C2B-C3B-CAB-CBB
4	A	1016	GBF	C4B-C3B-CAB-CBB
4	A	1016	GBF	C2C-C3C-CAC-CBC
4	A	1016	GBF	C4C-C3C-CAC-CBC
4	A	1024	GBF	C1A-C2A-CAA-CBA
4	A	1024	GBF	C2B-C3B-CAB-CBB
4	A	1024	GBF	C4B-C3B-CAB-CBB
4	A	1024	GBF	C2C-C3C-CAC-CBC
4	A	1024	GBF	C4C-C3C-CAC-CBC
4	A	1027	GBF	C1A-C2A-CAA-CBA
4	A	1027	GBF	C3A-C2A-CAA-CBA
4	A	1027	GBF	C2B-C3B-CAB-CBB
4	A	1027	GBF	C4B-C3B-CAB-CBB
4	A	1027	GBF	C2C-C3C-CAC-CBC
4	A	1027	GBF	C4C-C3C-CAC-CBC
4	A	1019	GBF	C2B-C3B-CAB-CBB
4	A	1019	GBF	C4B-C3B-CAB-CBB
4	A	1019	GBF	C2C-C3C-CAC-CBC
4	A	1019	GBF	C4C-C3C-CAC-CBC
4	A	1026	GBF	C1A-C2A-CAA-CBA
4	A	1026	GBF	C2B-C3B-CAB-CBB
4	A	1026	GBF	C4B-C3B-CAB-CBB
4	A	1026	GBF	C2C-C3C-CAC-CBC
4	A	1026	GBF	C4C-C3C-CAC-CBC
4	A	1002	GBF	C2B-C3B-CAB-CBB
4	A	1002	GBF	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
4	A	1002	GBF	C2C-C3C-CAC-CBC
4	A	1002	GBF	C4C-C3C-CAC-CBC
3	A	1005	GB0	C1A-C2A-CAA-CBA
3	A	1005	GB0	C3A-C2A-CAA-CBA
3	A	1005	GB0	C2B-C3B-CAB-CBB
3	A	1005	GB0	C4B-C3B-CAB-CBB
3	A	1005	GB0	C2C-C3C-CAC-CBC
3	A	1005	GB0	C4C-C3C-CAC-CBC
5	A	1003	AOH	C2B-C3B-CAB-CBB
5	A	1003	AOH	C4B-C3B-CAB-CBB
3	A	1001	GB0	C2B-C3B-CAB-CBB
3	A	1001	GB0	C4B-C3B-CAB-CBB
3	A	1001	GB0	C2C-C3C-CAC-CBC
3	A	1001	GB0	C4C-C3C-CAC-CBC
4	A	1018	GBF	CBD-CGD-O2D-CED
4	A	1009	GBF	CBD-CGD-O2D-CED
4	A	1013	GBF	CBD-CGD-O2D-CED
4	B	103	GBF	O1D-CGD-O2D-CED
4	B	102	GBF	O1D-CGD-O2D-CED
4	A	1006	GBF	CBD-CGD-O2D-CED
4	A	1016	GBF	CBD-CGD-O2D-CED
7	A	1031	DGG	O21-C21-O19-C19
3	A	1005	GB0	CBA-CGA-O2A-C1
7	A	1031	DGG	C22-C21-O19-C19
4	A	1009	GBF	O1D-CGD-O2D-CED
4	A	1021	GBF	C4-C3-C5-C6
4	A	1026	GBF	C4-C3-C5-C6
4	A	1018	GBF	O1D-CGD-O2D-CED
9	A	1034	LMT	O5'-C5'-C6'-O6'
4	A	1013	GBF	O1D-CGD-O2D-CED
4	A	1021	GBF	C2-C3-C5-C6
4	A	1007	GBF	C3-C5-C6-C7
4	A	1021	GBF	C8-C10-C11-C12
4	B	103	GBF	C8-C10-C11-C12
4	A	1020	GBF	C8-C10-C11-C12
7	A	1030	DGG	C5-C6-C7-C8
4	A	1006	GBF	O1D-CGD-O2D-CED
7	A	1030	DGG	C29-C30-C31-C32
7	A	1030	DGG	C21-C22-C23-C24
9	A	1034	LMT	C4'-C5'-C6'-O6'
7	A	1031	DGG	C10-C11-C12-C13
4	A	1026	GBF	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	A	1031	DGG	C21-C22-C23-C24
7	A	1031	DGG	C2-C1-O17-C17
4	A	1002	GBF	C2A-CAA-CBA-CGA
4	A	1027	GBF	CBD-CGD-O2D-CED
4	A	1013	GBF	O1A-CGA-O2A-C1
4	A	1007	GBF	C8-C10-C11-C12
4	A	1016	GBF	O1D-CGD-O2D-CED
4	A	1021	GBF	O1A-CGA-O2A-C1
7	A	1030	DGG	C40-OP4-P-OP2
4	A	1011	GBF	CBD-CGD-O2D-CED
5	A	1003	AOH	C2A-CAA-CBA-CGA
9	A	1035	LMT	O1'-C1-C2-C3
9	A	1034	LMT	C2-C3-C4-C5
9	A	1035	LMT	C2-C3-C4-C5
4	A	1012	GBF	CBD-CGD-O2D-CED
4	A	1013	GBF	CBA-CGA-O2A-C1
7	A	1031	DGG	O1-C1-O17-C17
7	A	1030	DGG	C22-C21-O19-C19
7	A	1031	DGG	C22-C23-C24-C25
7	A	1031	DGG	C12-C13-C14-C15
7	A	1030	DGG	C28-C29-C30-C31
9	A	1034	LMT	C5-C6-C7-C8
9	A	1035	LMT	C2-C1-O1'-C1'
7	A	1031	DGG	C11-C12-C13-C14
4	A	1020	GBF	C4-C3-C5-C6
4	A	1020	GBF	C2-C3-C5-C6
9	A	1035	LMT	C4-C5-C6-C7
3	A	1005	GB0	O1A-CGA-O2A-C1
7	A	1030	DGG	O21-C21-O19-C19
9	A	1034	LMT	C4-C5-C6-C7
7	A	1030	DGG	C22-C23-C24-C25
9	A	1034	LMT	C6-C7-C8-C9
7	A	1030	DGG	OP4-C40-C41-C43
3	A	1005	GB0	C2A-CAA-CBA-CGA
9	A	1035	LMT	C7-C8-C9-C10
4	A	1012	GBF	O1D-CGD-O2D-CED
4	B	103	GBF	C3-C5-C6-C7
4	A	1021	GBF	CBD-CGD-O2D-CED
4	A	1011	GBF	O1D-CGD-O2D-CED
4	A	1027	GBF	O1D-CGD-O2D-CED
9	A	1034	LMT	C1-C2-C3-C4
4	A	1023	GBF	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
4	A	1021	GBF	C11-C10-C8-C9
4	A	1023	GBF	C11-C10-C8-C7
4	A	1008	GBF	O1A-CGA-O2A-C1
4	A	1021	GBF	O1D-CGD-O2D-CED
4	A	1012	GBF	C4-C3-C5-C6
4	B	103	GBF	O1A-CGA-O2A-C1
7	A	1031	DGG	C13-C14-C15-C16
4	A	1013	GBF	C2-C1-O2A-CGA
4	A	1021	GBF	C11-C10-C8-C7
7	A	1031	DGG	C3-C4-C5-C6
9	A	1034	LMT	C9-C10-C11-C12
4	A	1012	GBF	C2-C3-C5-C6
7	A	1031	DGG	C17-C19-O19-C21
4	A	1016	GBF	CAD-CBD-CGD-O2D
4	A	1019	GBF	CAD-CBD-CGD-O2D
4	A	1026	GBF	CAD-CBD-CGD-O2D
4	A	1002	GBF	CAD-CBD-CGD-O2D
4	A	1007	GBF	CHA-CBD-CGD-O2D
4	A	1012	GBF	CHA-CBD-CGD-O1D
4	A	1028	GBF	CHA-CBD-CGD-O2D
4	A	1021	GBF	CBA-CGA-O2A-C1
4	A	1012	GBF	CAD-CBD-CGD-O1D
4	A	1028	GBF	CAD-CBD-CGD-O1D
4	A	1004	GBF	C2A-CAA-CBA-CGA
4	A	1007	GBF	C1A-C2A-CAA-CBA
4	A	1006	GBF	C3A-C2A-CAA-CBA
4	A	1028	GBF	C1A-C2A-CAA-CBA
4	A	1028	GBF	C3A-C2A-CAA-CBA
4	A	1011	GBF	C1A-C2A-CAA-CBA
4	A	1016	GBF	C1A-C2A-CAA-CBA
4	A	1019	GBF	C1A-C2A-CAA-CBA
4	A	1026	GBF	C3A-C2A-CAA-CBA
4	A	1002	GBF	C1A-C2A-CAA-CBA
3	A	1001	GB0	C1A-C2A-CAA-CBA
9	A	1035	LMT	C1-C2-C3-C4
4	A	1007	GBF	O1A-CGA-O2A-C1
7	A	1030	DGG	C23-C24-C25-C26
7	A	1030	DGG	C18-OP2-P-OP4
4	A	1026	GBF	C11-C10-C8-C7
9	A	1034	LMT	C3-C4-C5-C6
4	A	1004	GBF	O2A-C1-C2-C3
4	A	1019	GBF	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
4	A	1020	GBF	C11-C10-C8-C9
4	A	1019	GBF	C2A-CAA-CBA-CGA
4	B	103	GBF	C4-C3-C5-C6
4	B	103	GBF	C11-C10-C8-C9
5	A	1003	AOH	C11-C10-C8-C9
4	A	1002	GBF	C11-C10-C8-C9
4	A	1015	GBF	CAA-CBA-CGA-O2A
4	A	1028	GBF	C11-C10-C8-C9
4	A	1019	GBF	C2-C3-C5-C6
4	A	1026	GBF	C2A-CAA-CBA-CGA
4	A	1015	GBF	O1A-CGA-O2A-C1
4	A	1004	GBF	CAD-CBD-CGD-O2D
4	A	1021	GBF	CAD-CBD-CGD-O2D
4	A	1026	GBF	C11-C10-C8-C9
4	B	103	GBF	C11-C10-C8-C7
4	A	1027	GBF	CAA-CBA-CGA-O2A
4	A	1008	GBF	O2A-C1-C2-C3
4	A	1019	GBF	O2A-C1-C2-C3
3	A	1001	GB0	O2A-C1-C2-C3
4	A	1008	GBF	CHA-CBD-CGD-O1D
4	A	1008	GBF	CHA-CBD-CGD-O2D
4	A	1012	GBF	CHA-CBD-CGD-O2D
4	A	1011	GBF	CHA-CBD-CGD-O2D
4	A	1013	GBF	CHA-CBD-CGD-O2D
4	B	102	GBF	CHA-CBD-CGD-O2D
4	A	1020	GBF	CHA-CBD-CGD-O1D
4	A	1020	GBF	CHA-CBD-CGD-O2D
4	A	1004	GBF	CAA-CBA-CGA-O2A
4	A	1007	GBF	CAA-CBA-CGA-O2A
5	A	1003	AOH	CAA-CBA-CGA-O2A
9	A	1034	LMT	C11-C10-C9-C8
4	A	1013	GBF	C4-C3-C5-C6
5	A	1003	AOH	C5-C6-C7-C8
4	A	1012	GBF	CAA-CBA-CGA-O2A
4	A	1018	GBF	CBA-CGA-O2A-C1
7	A	1030	DGG	C11-C10-C9-C8
4	A	1027	GBF	CAA-CBA-CGA-O1A
4	A	1025	GBF	C2A-CAA-CBA-CGA
4	A	1028	GBF	CAA-CBA-CGA-O2A
4	A	1004	GBF	CAA-CBA-CGA-O1A
7	A	1030	DGG	C18-OP2-P-OP3
4	A	1008	GBF	CAD-CBD-CGD-O1D

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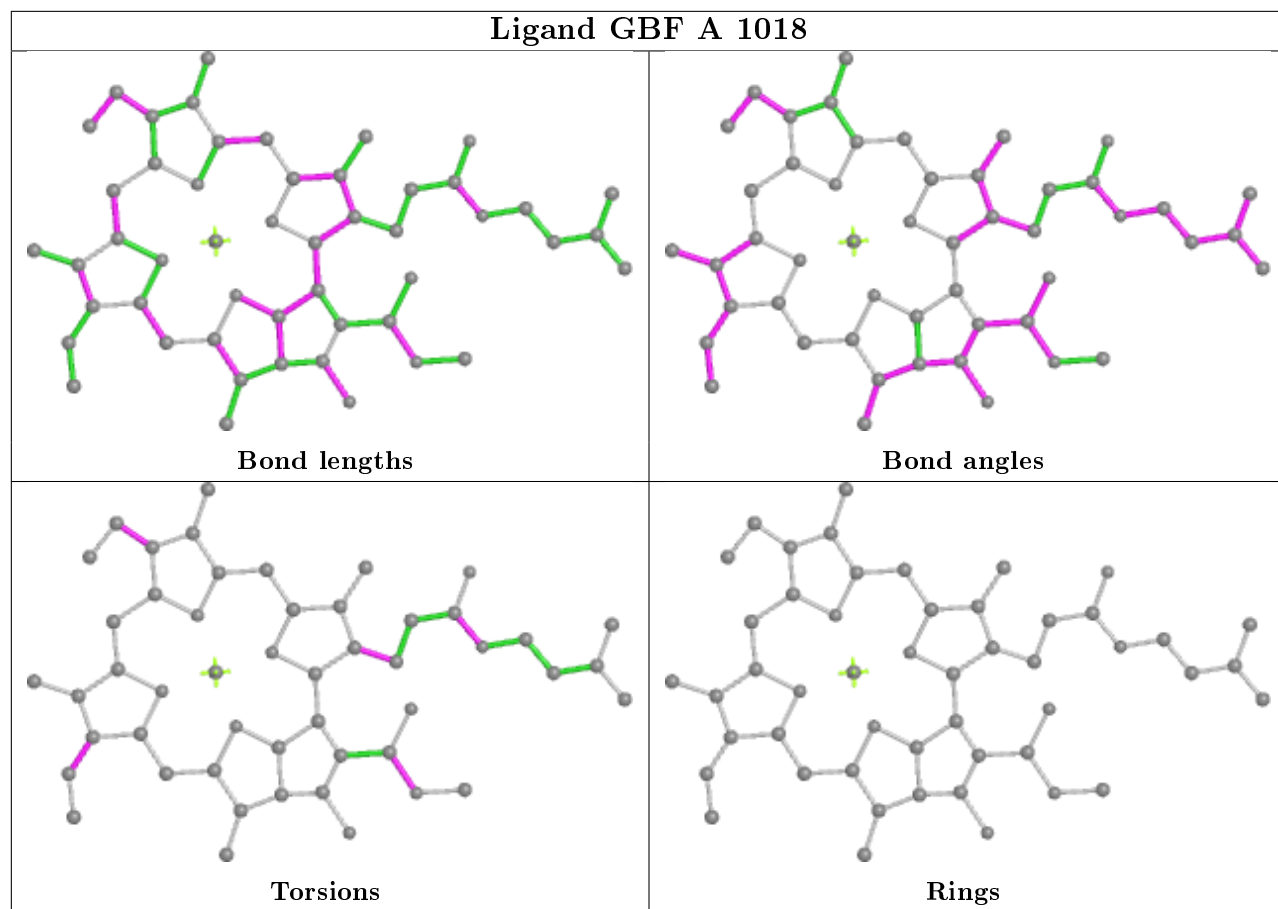
Mol	Chain	Res	Type	Atoms
4	A	1020	GBF	CAD-CBD-CGD-O1D
4	A	1024	GBF	CAD-CBD-CGD-O1D
9	A	1035	LMT	C5-C6-C7-C8
4	A	1026	GBF	C8-C10-C11-C12

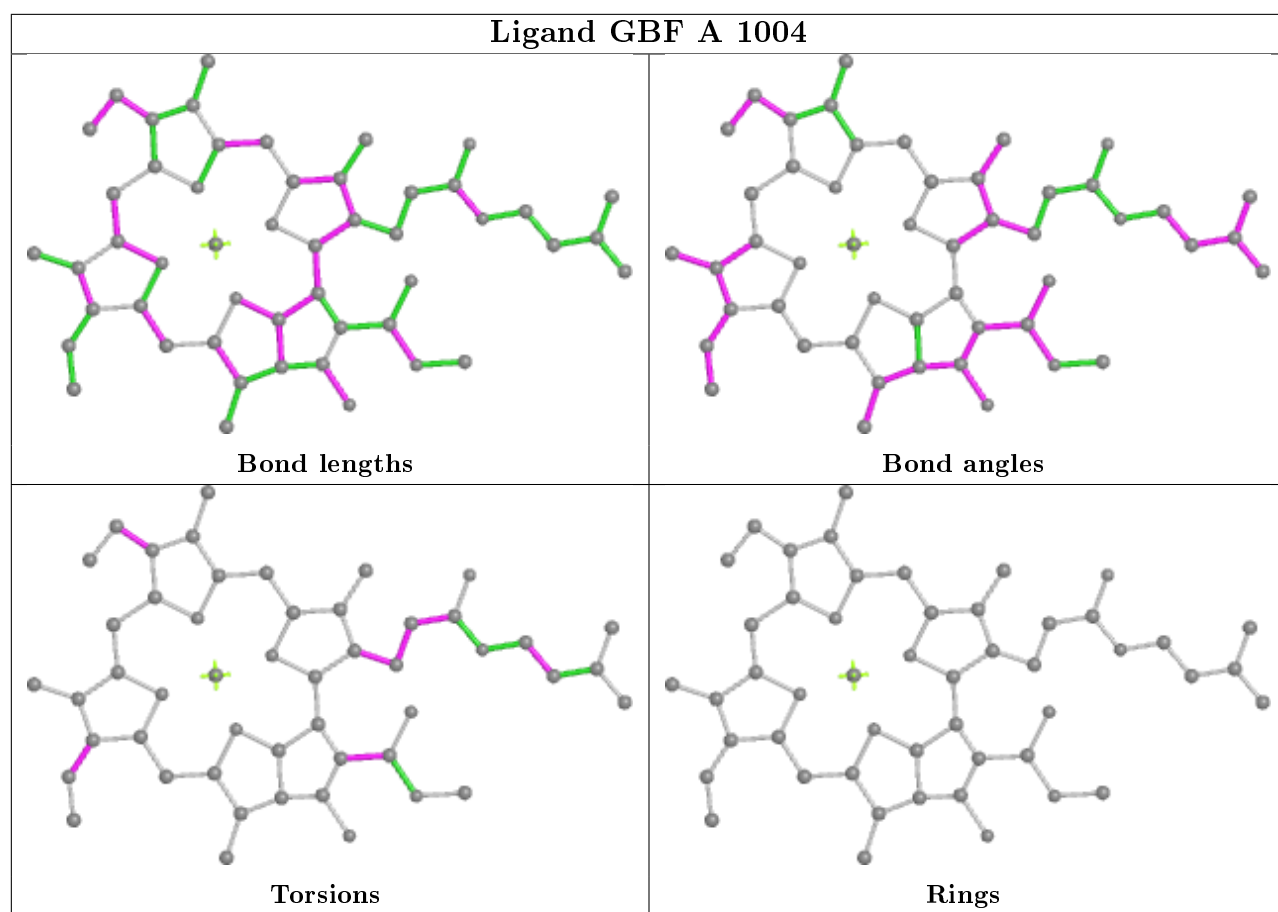
There are no ring outliers.

5 monomers are involved in 20 short contacts:

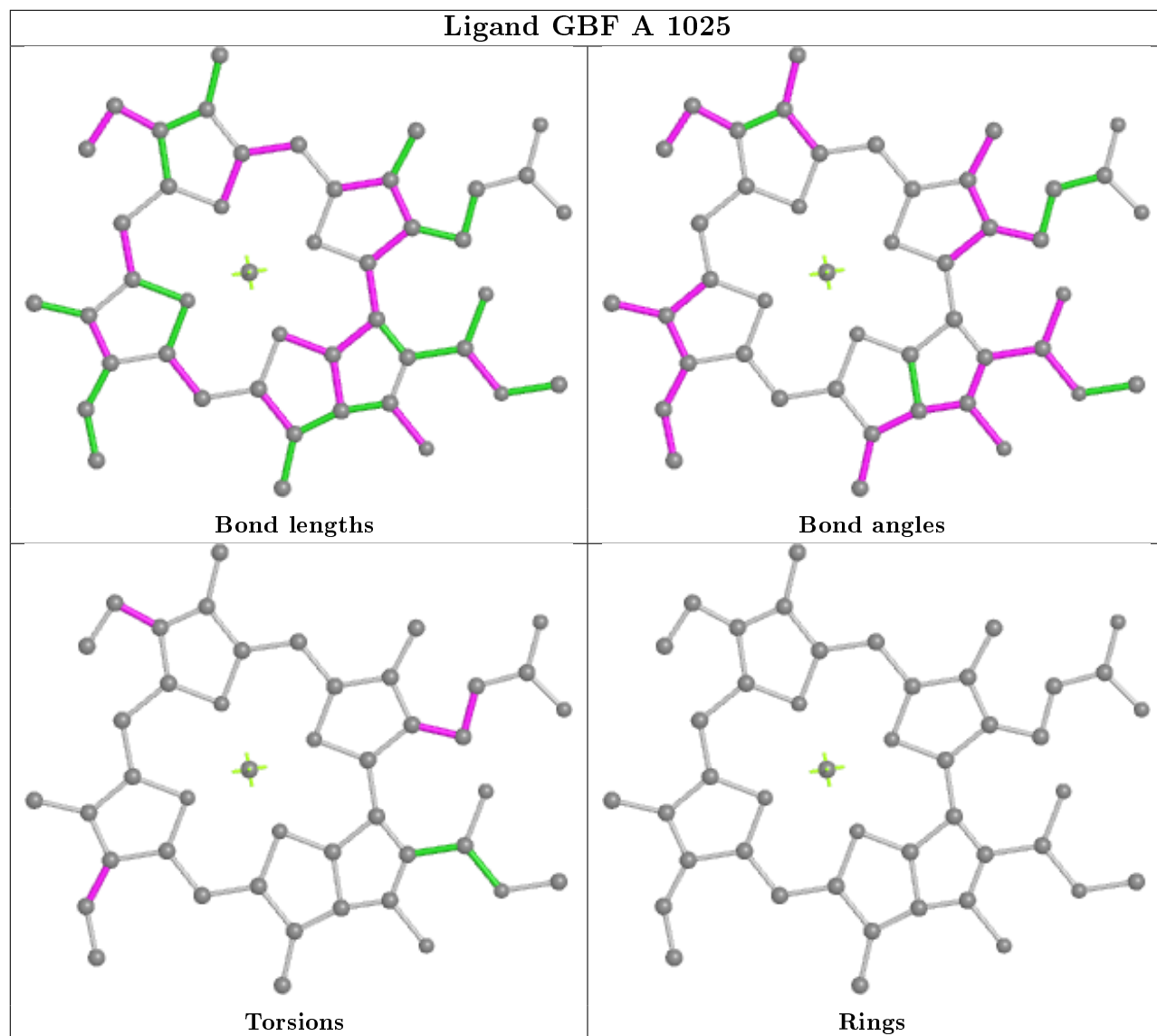
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1025	GBF	1	0
7	A	1030	DGG	9	0
9	A	1034	LMT	6	0
9	A	1035	LMT	6	0
7	A	1031	DGG	4	0

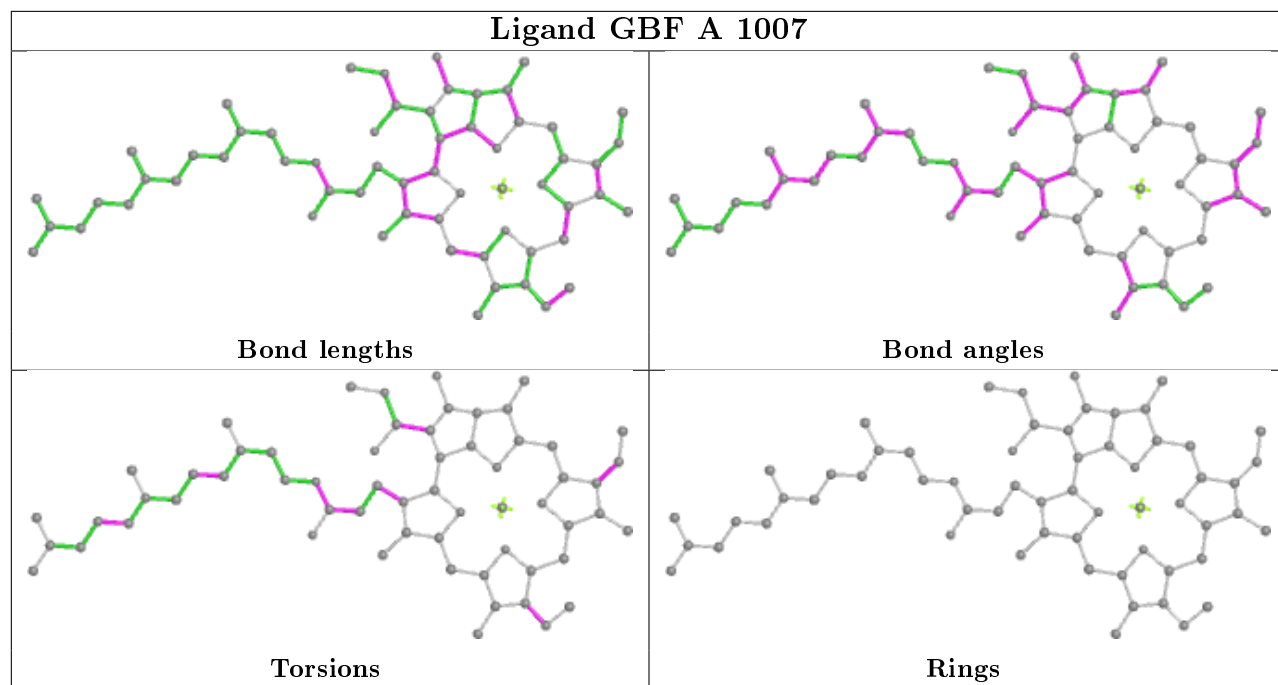
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



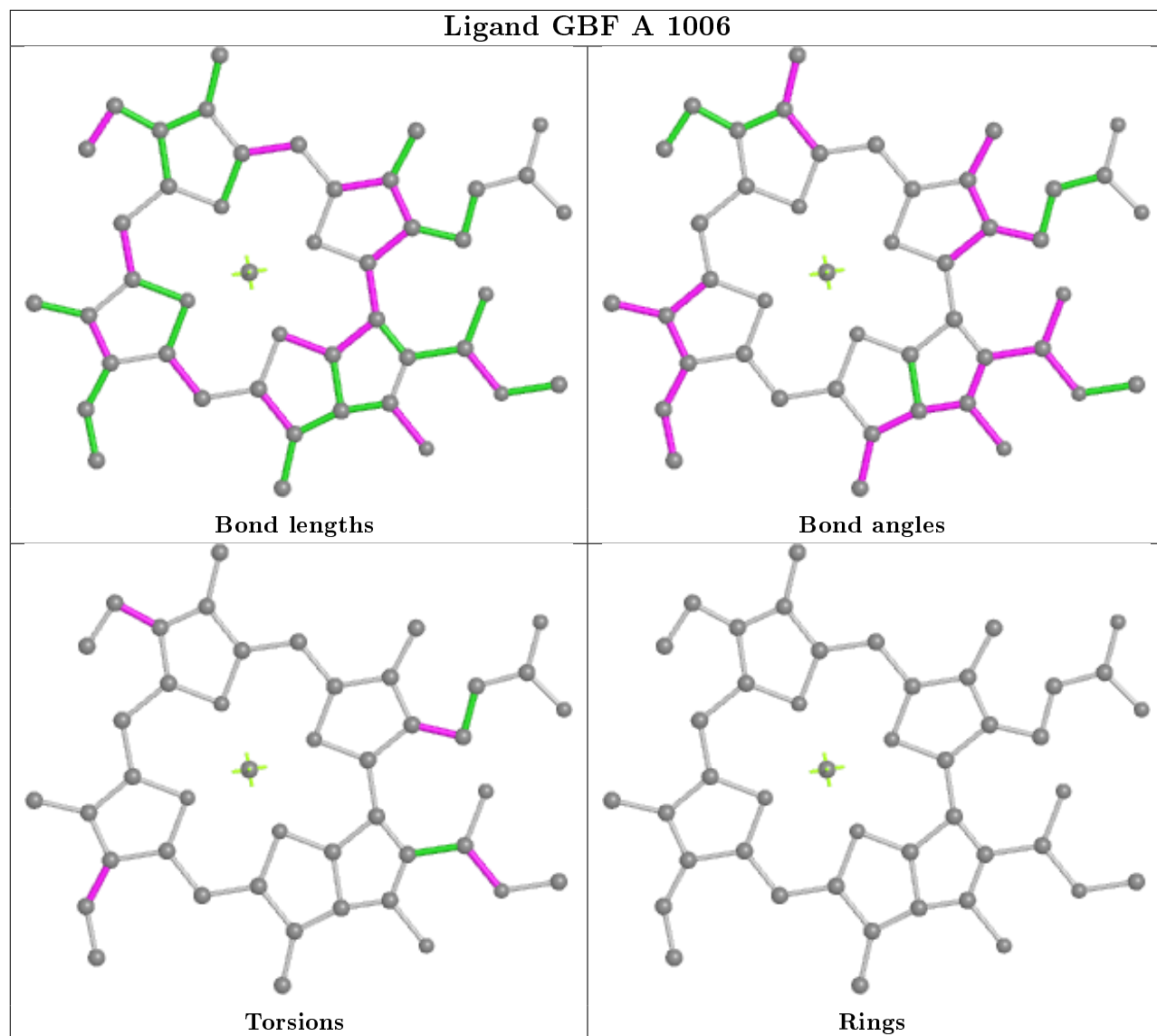


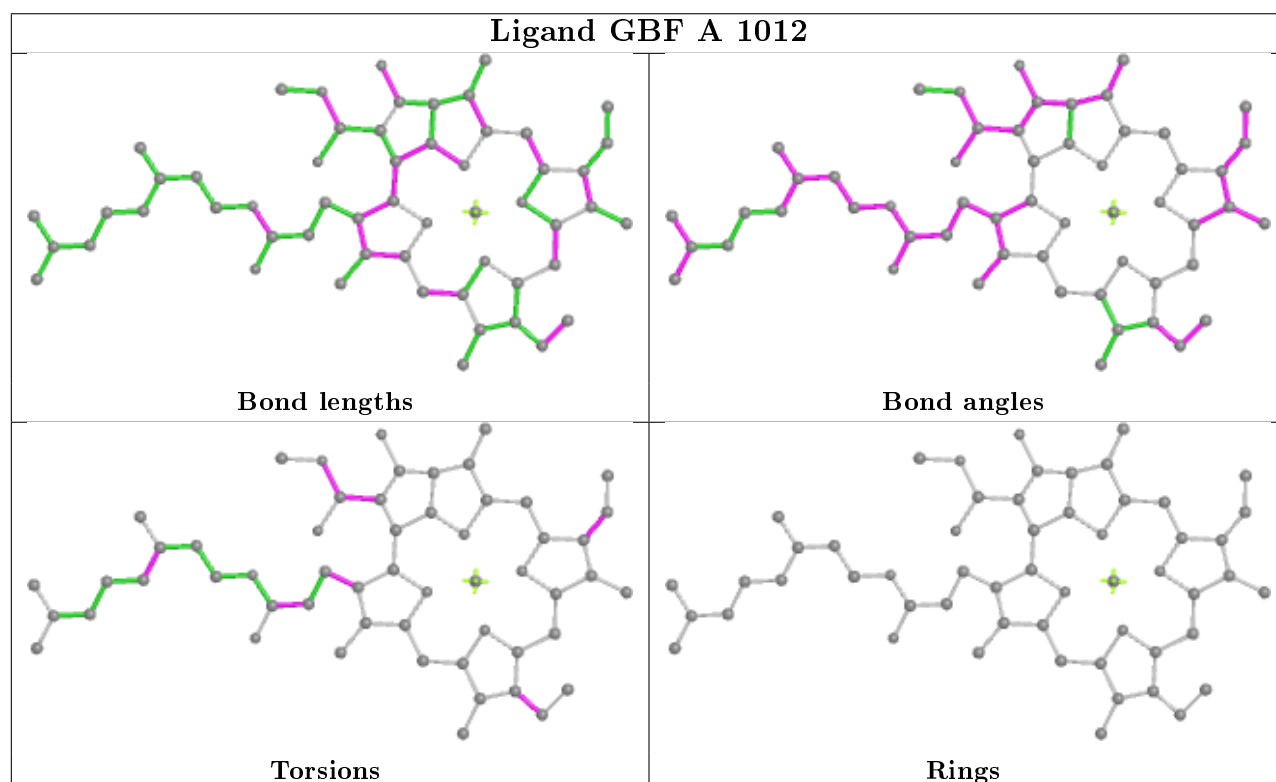
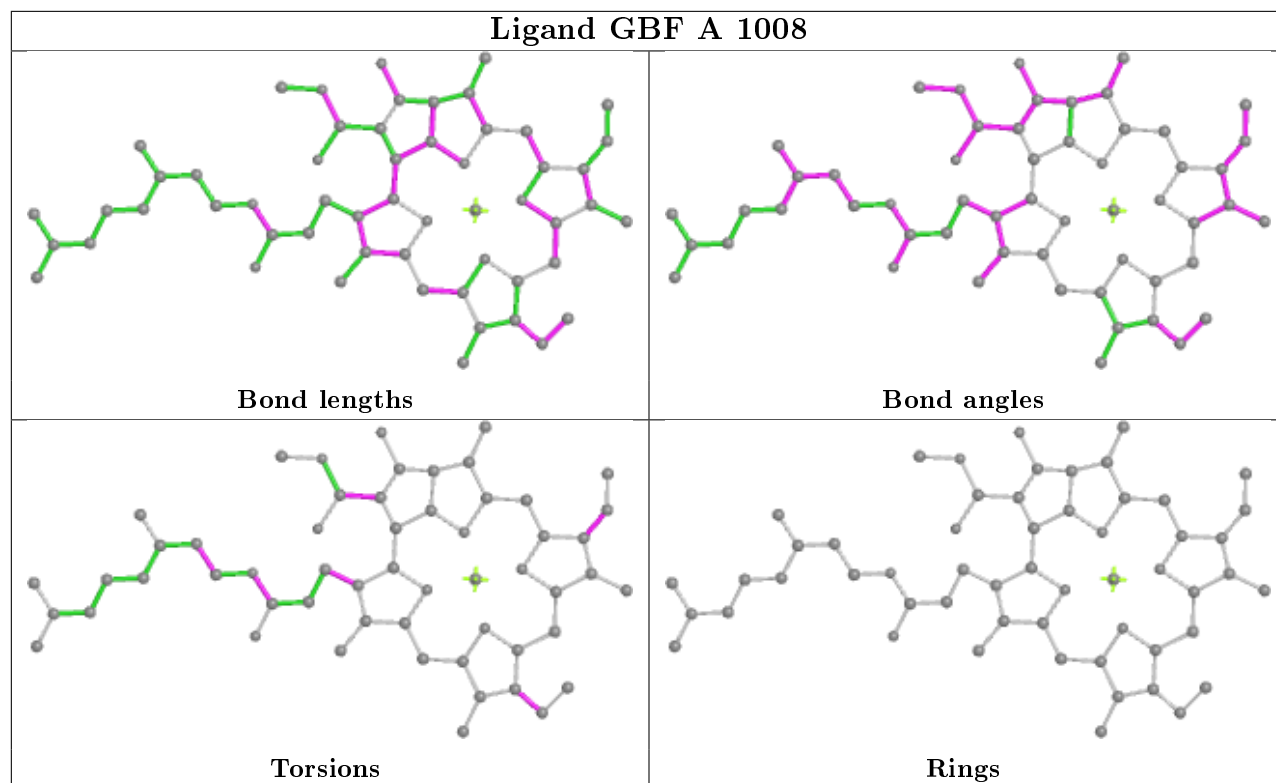
## Ligand GBF A 1025

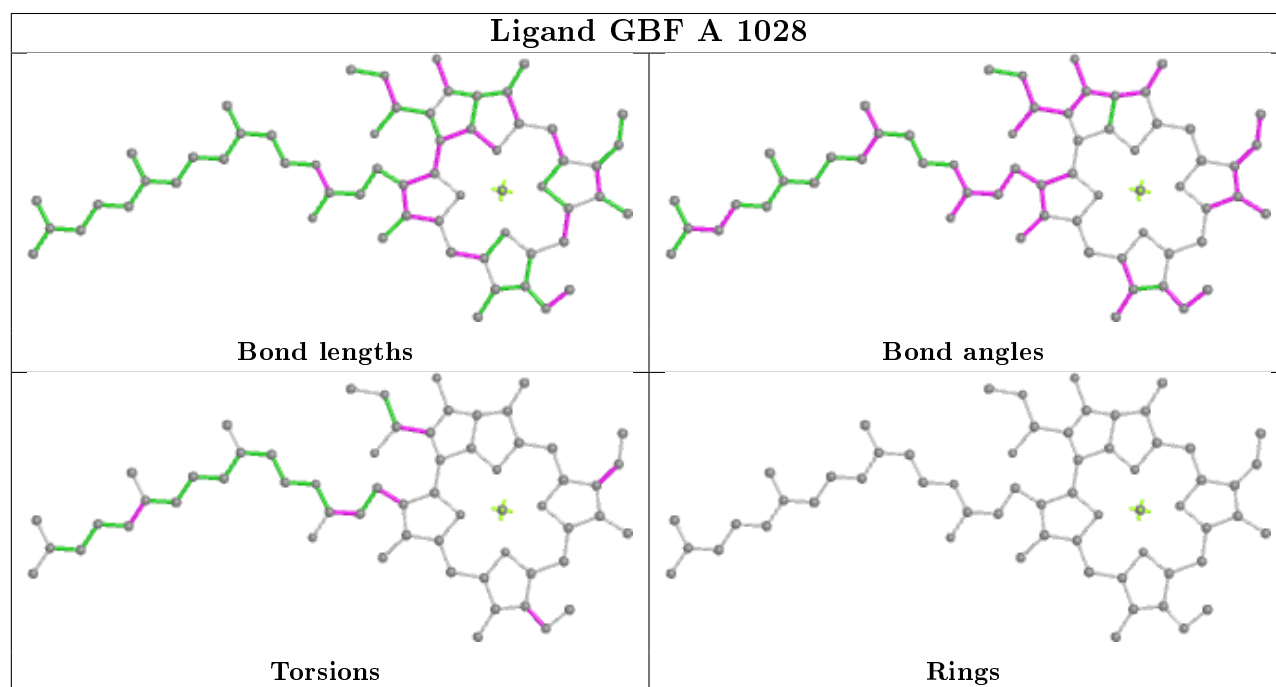
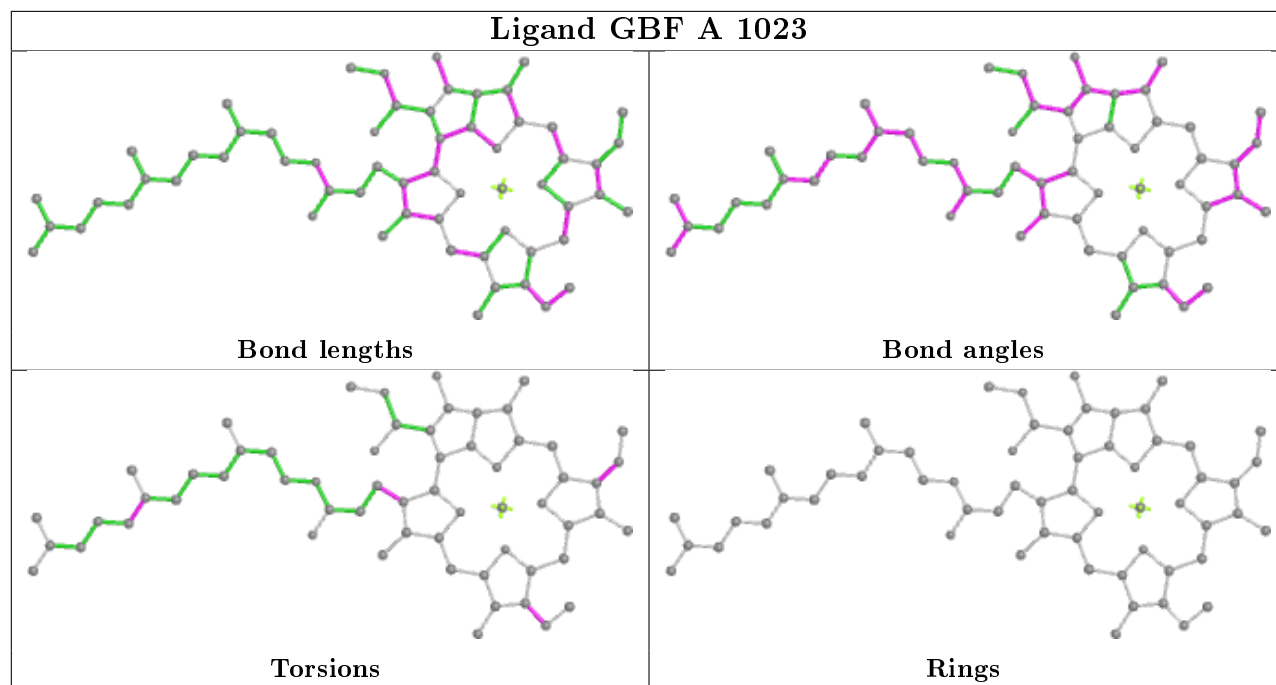




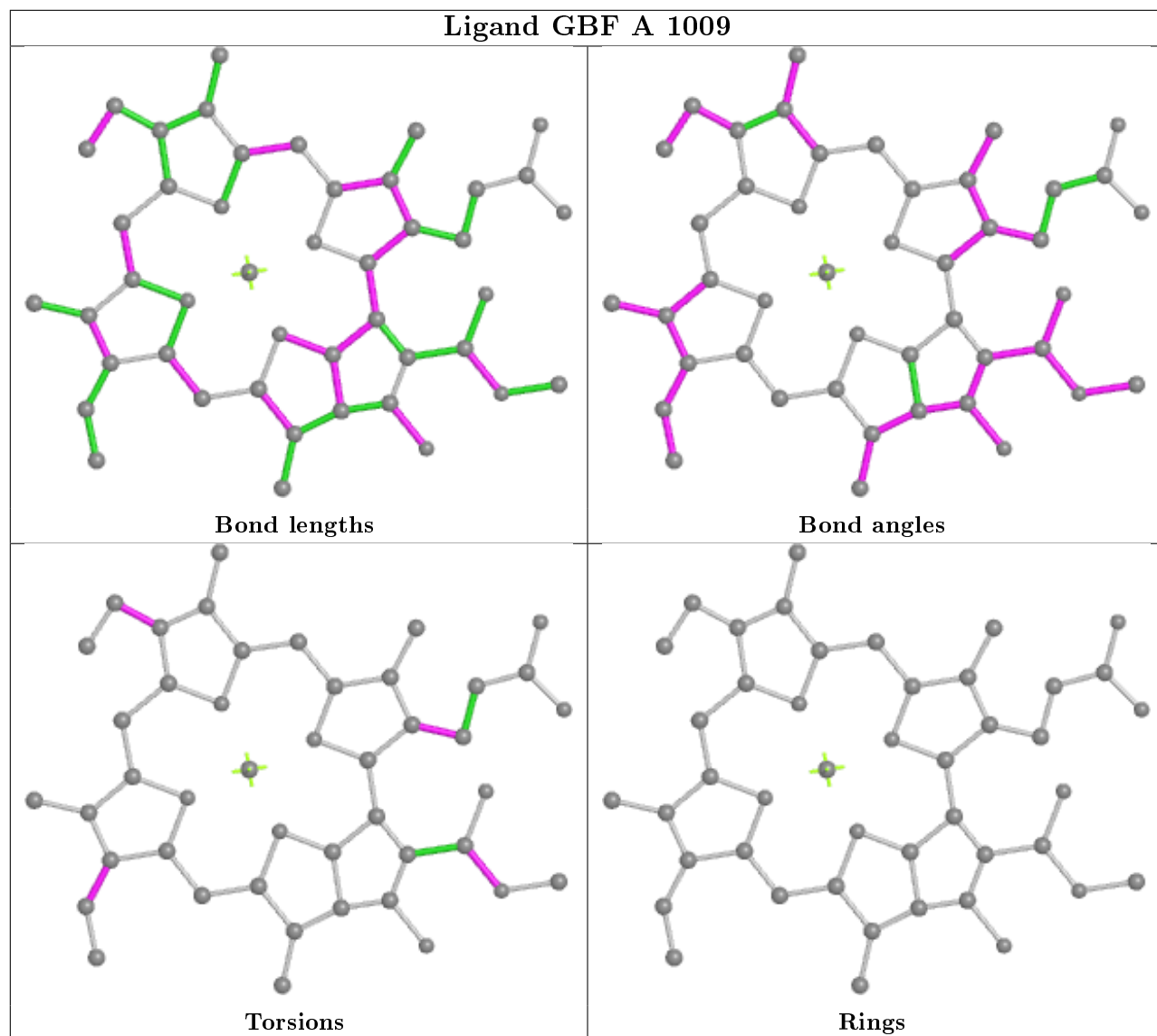
## Ligand GBF A 1006

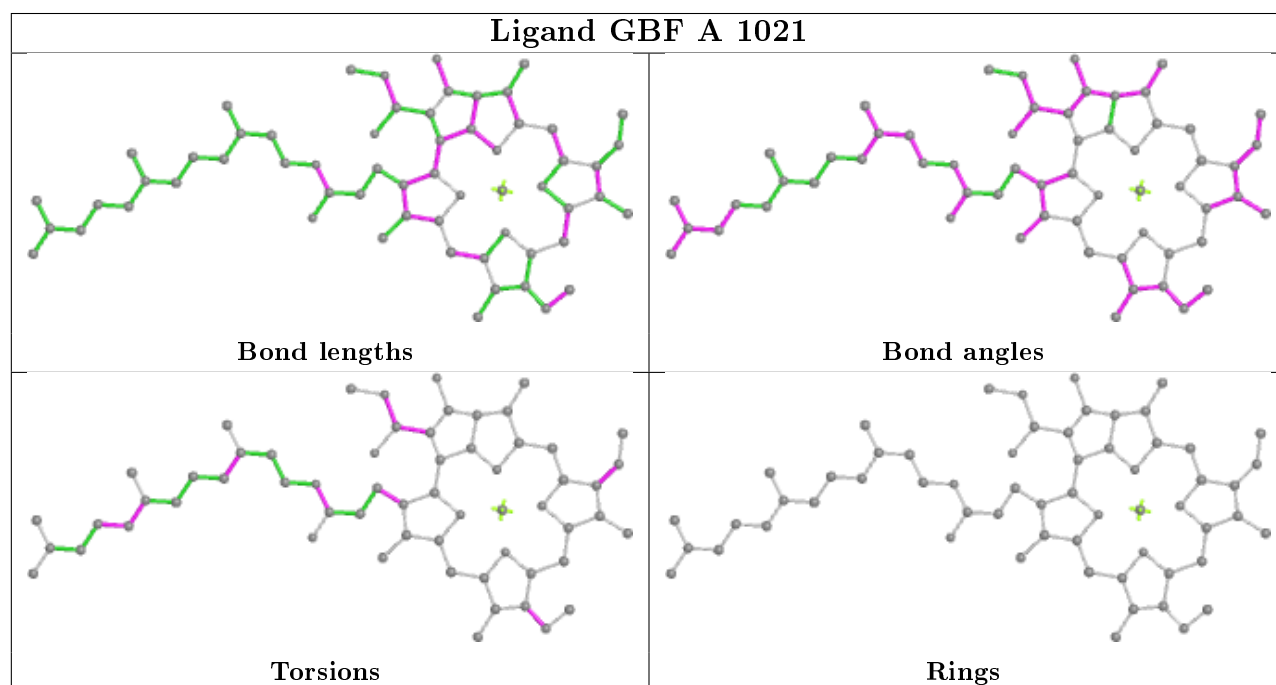
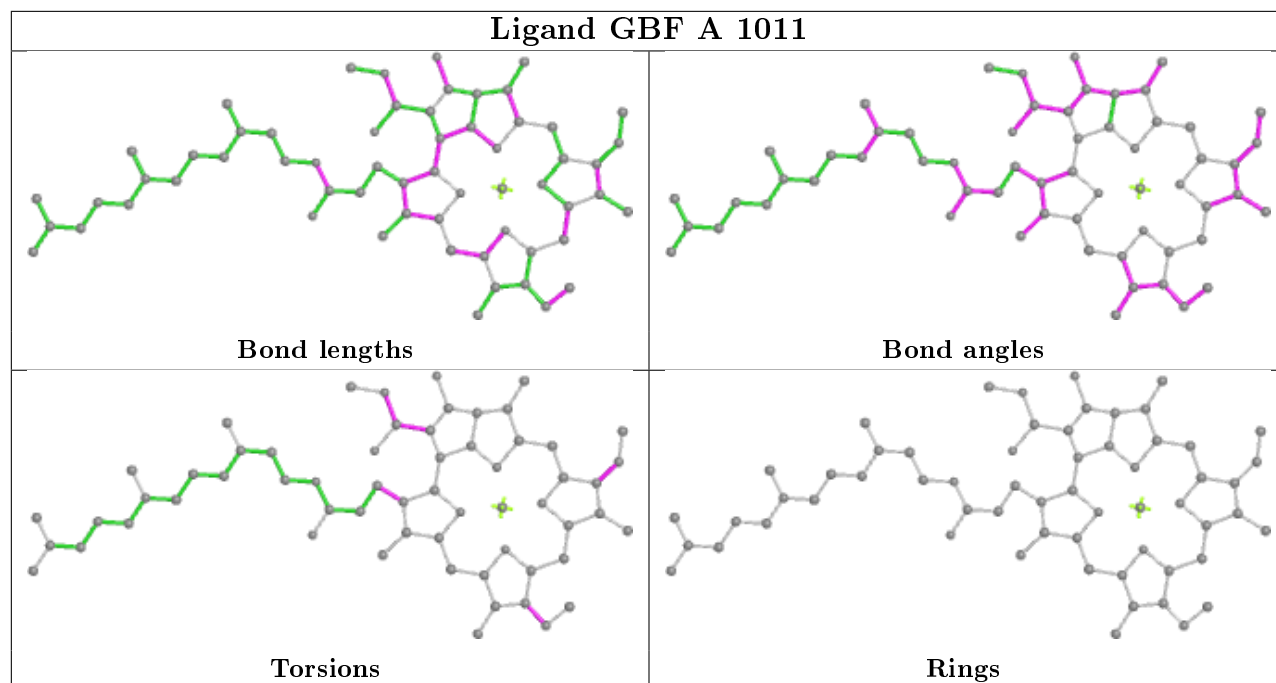


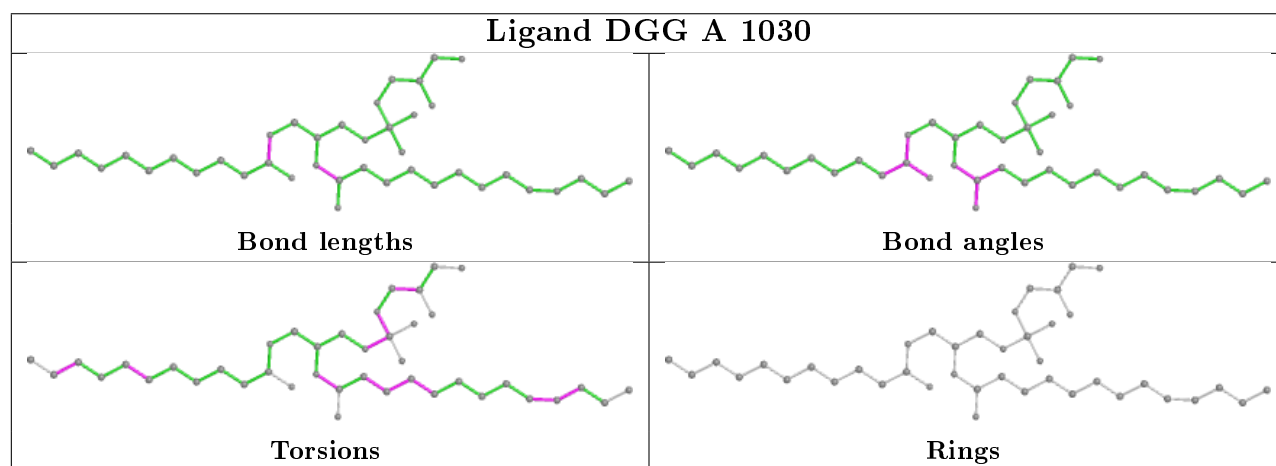
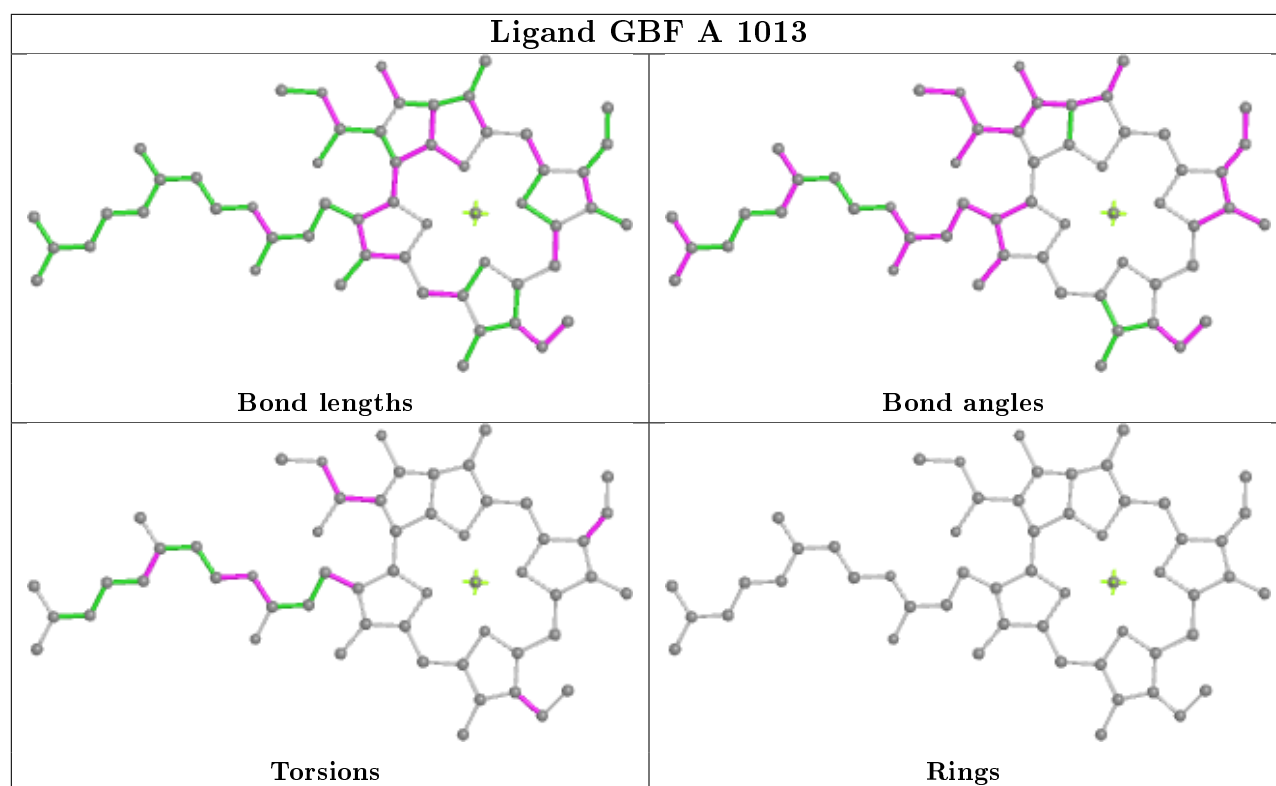


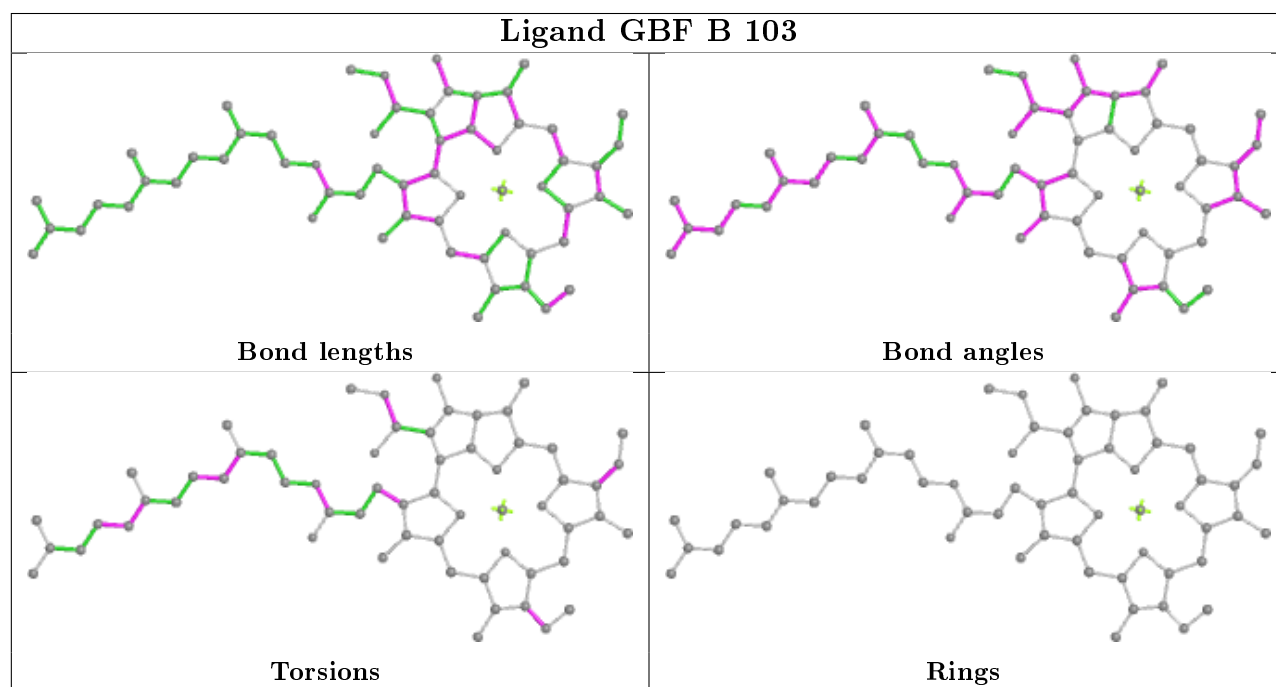
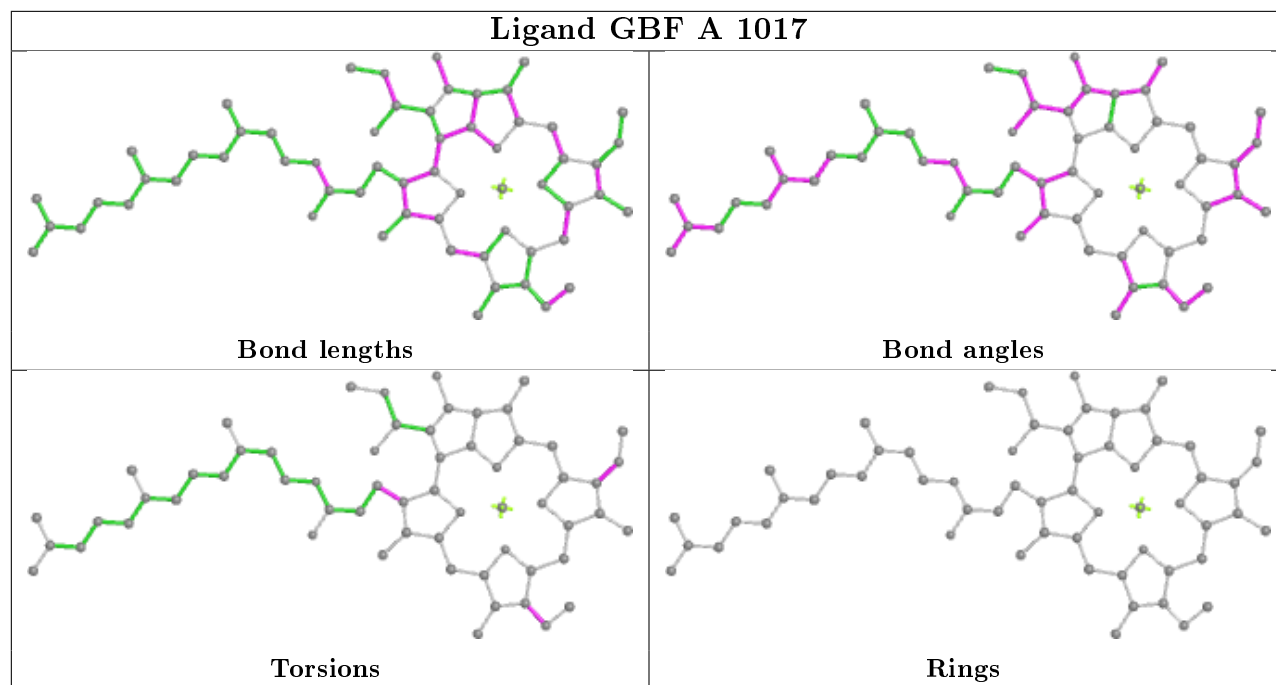


## Ligand GBF A 1009

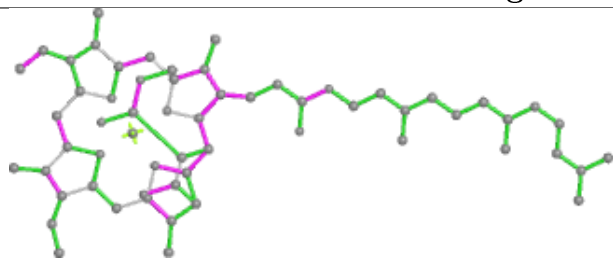




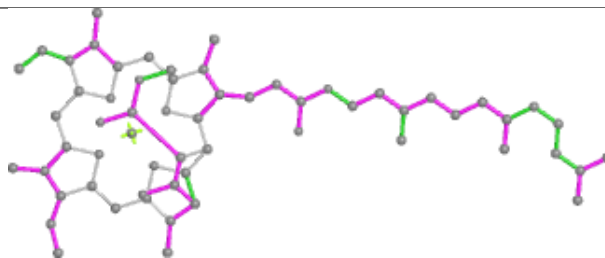




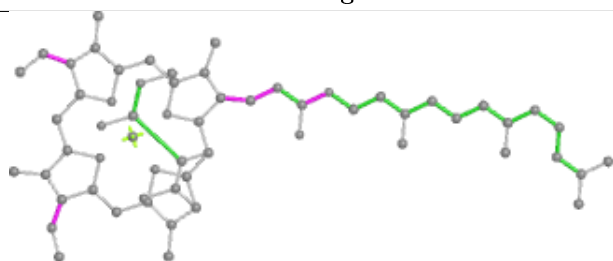
## Ligand GB0 A 1005



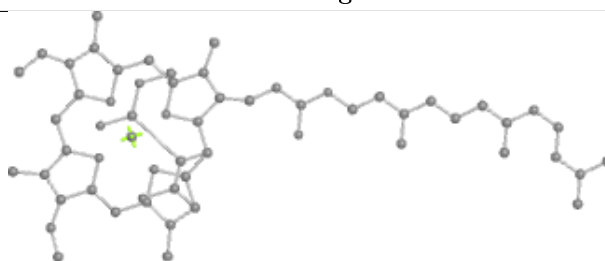
Bond lengths



Bond angles

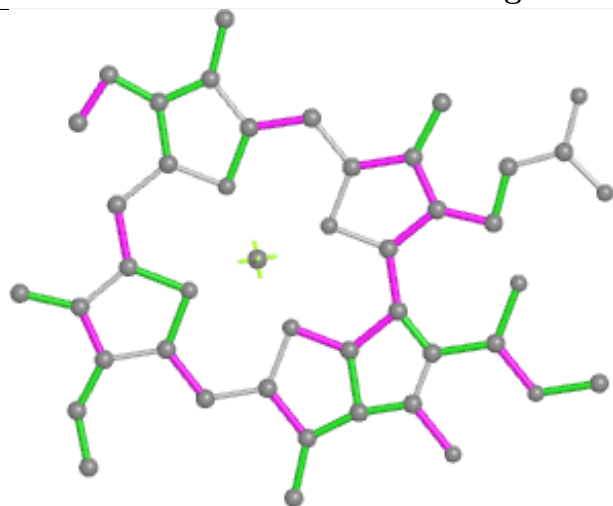


Torsions

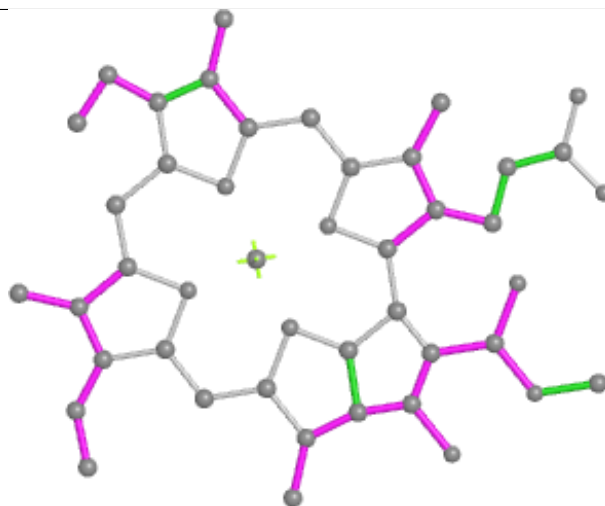


Rings

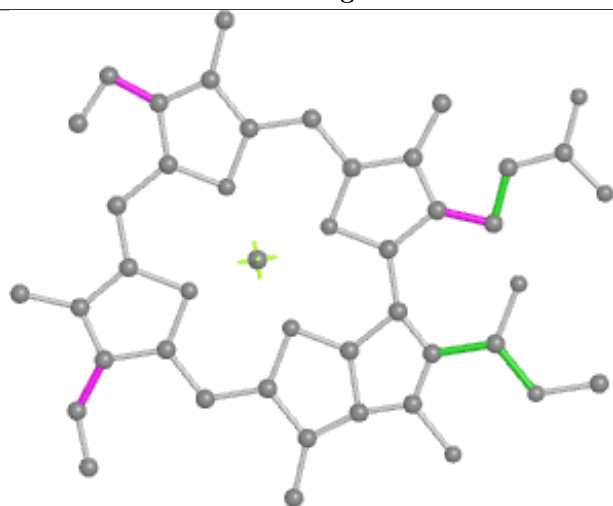
## Ligand GBF A 1022



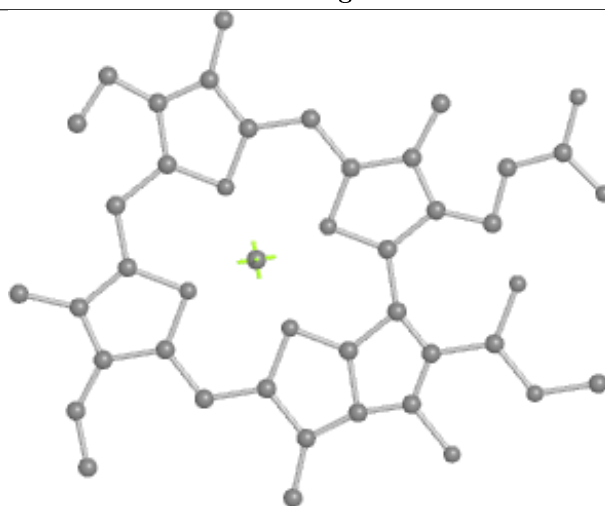
Bond lengths



Bond angles

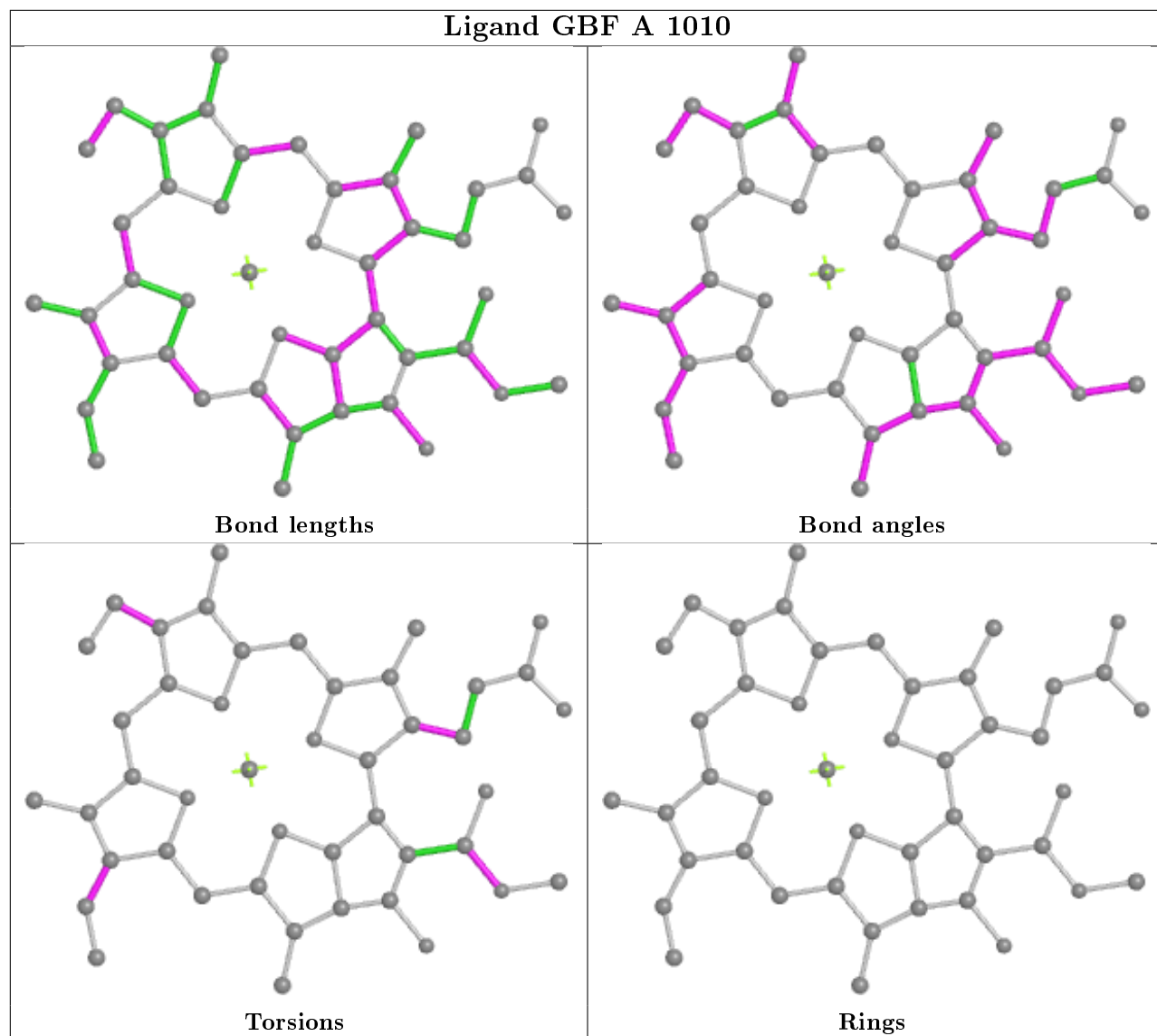


Torsions

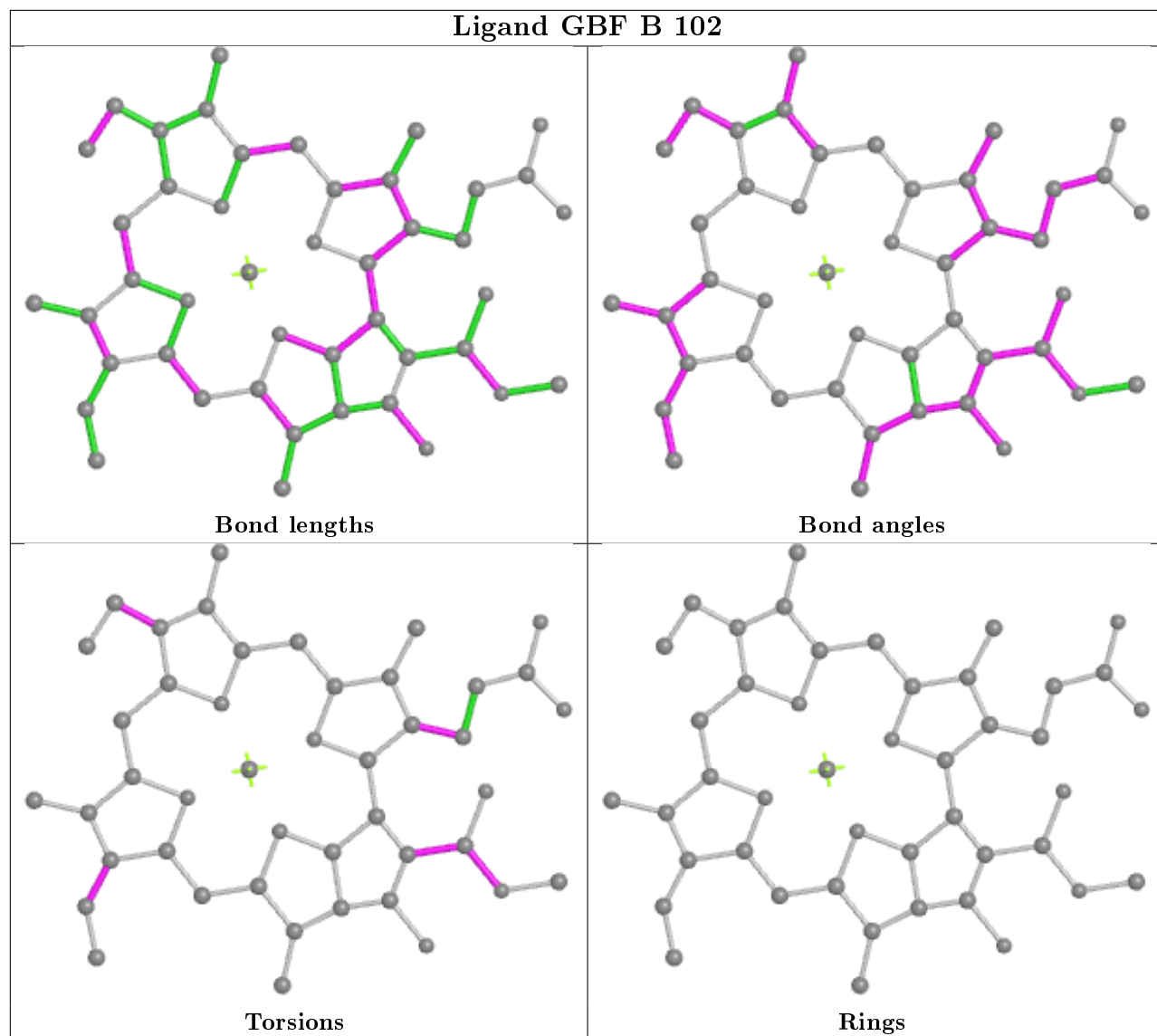


Rings

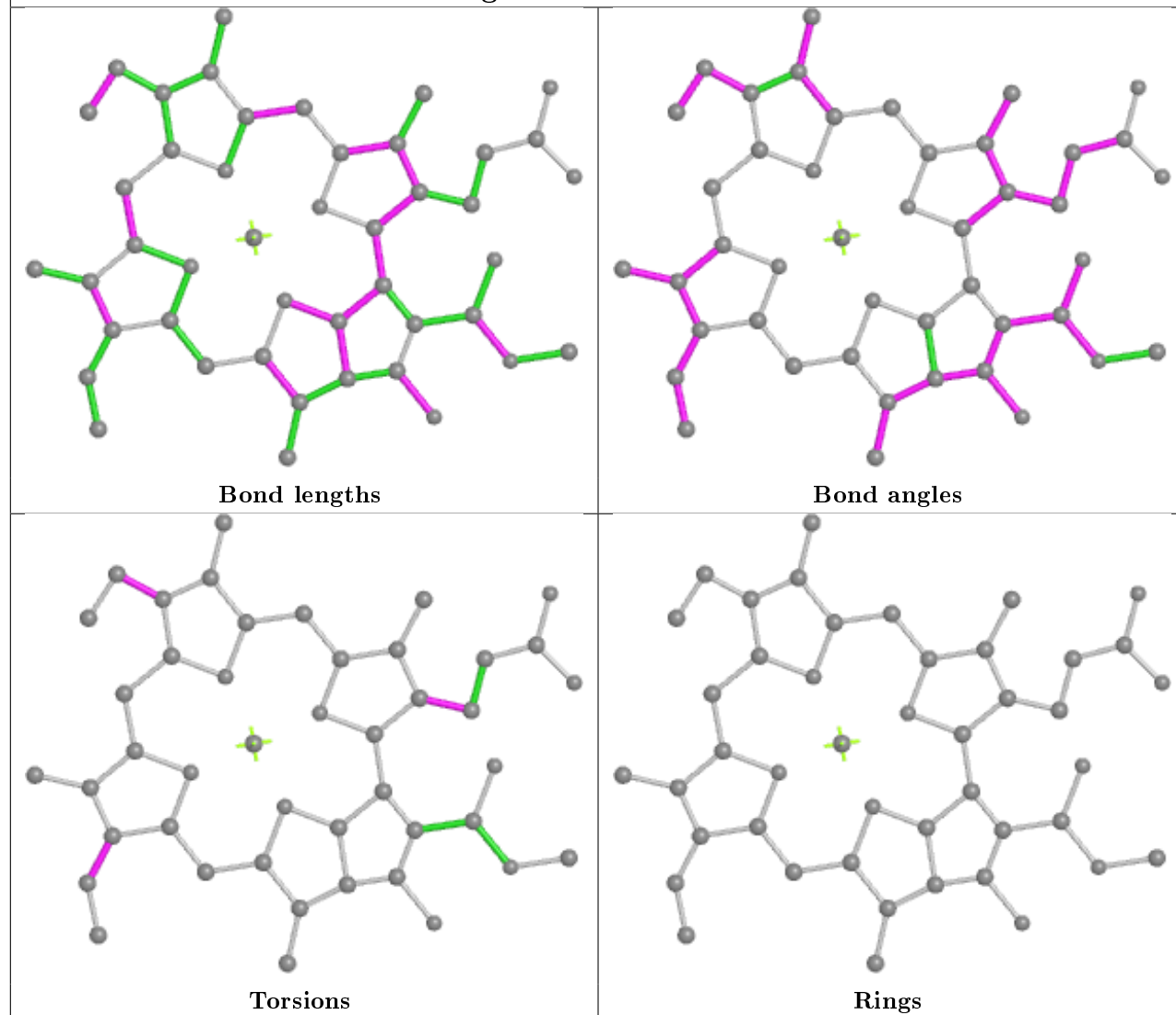
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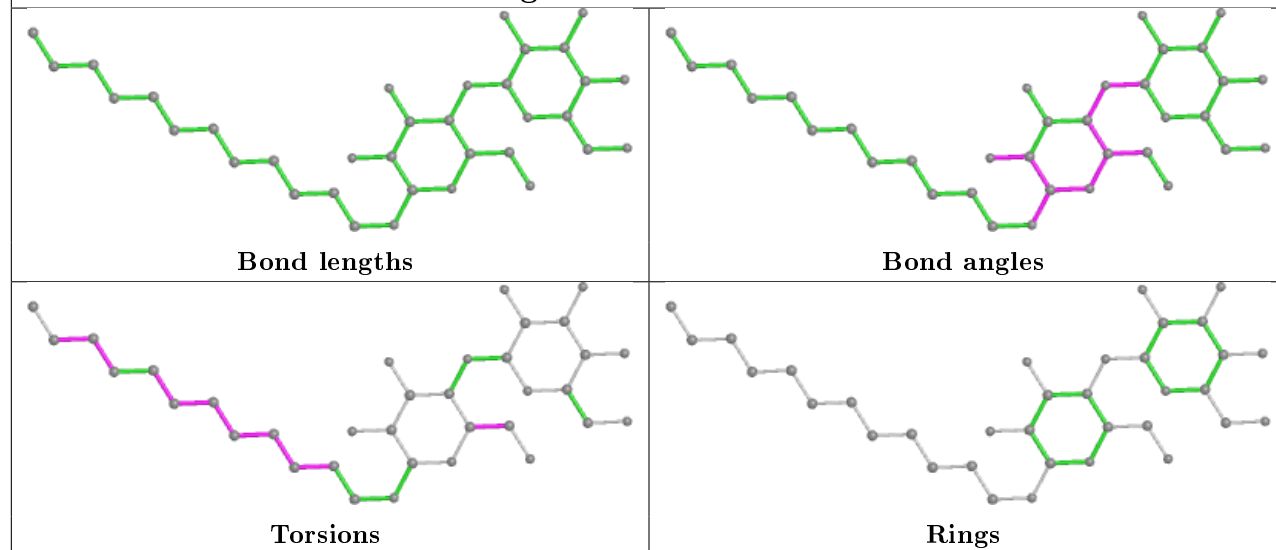
## Ligand GBF B 102

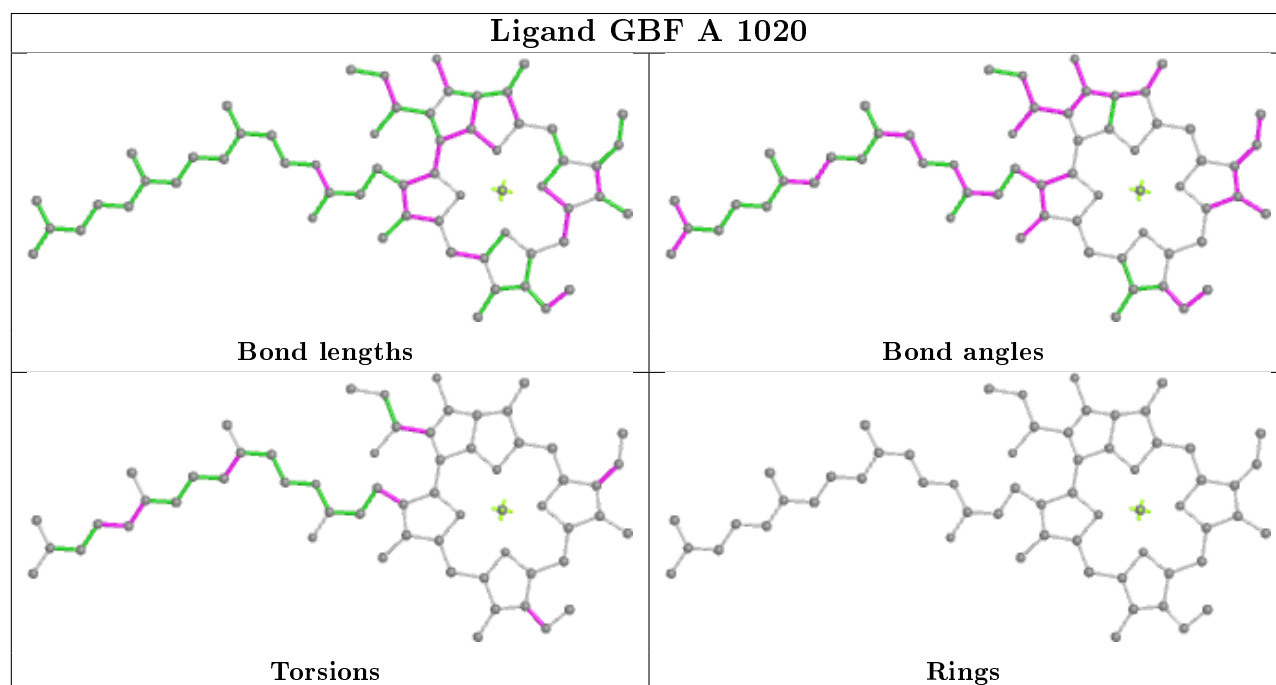
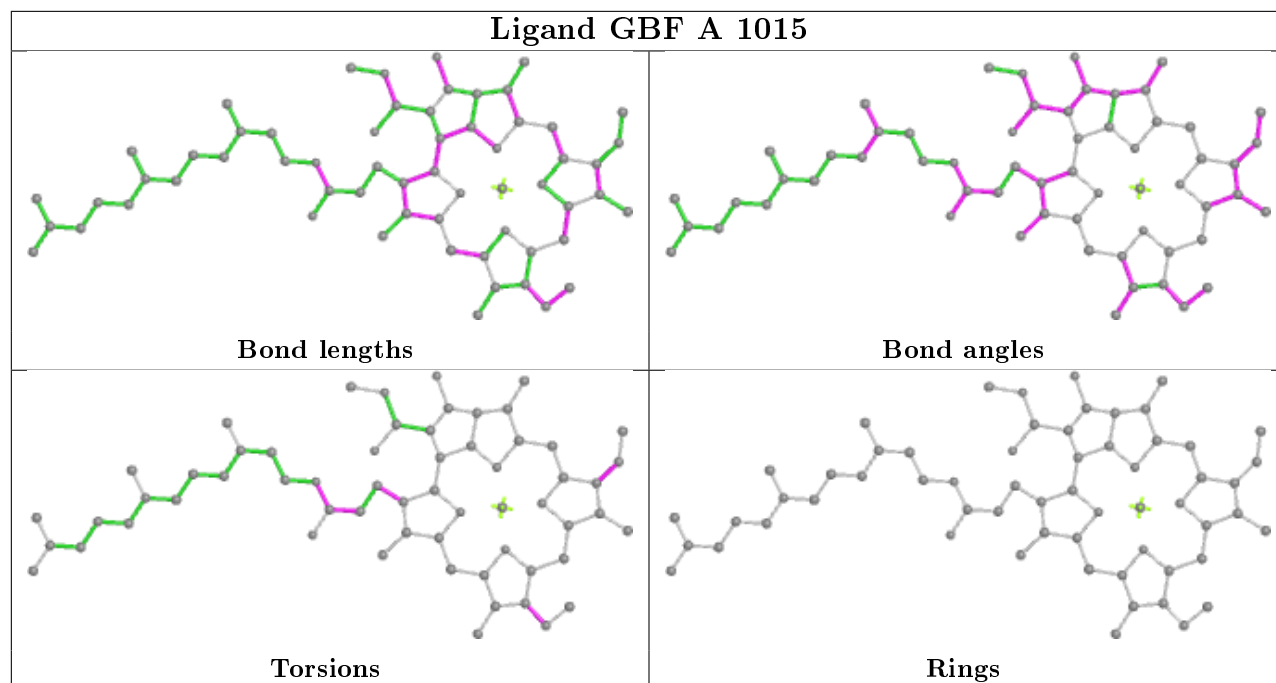


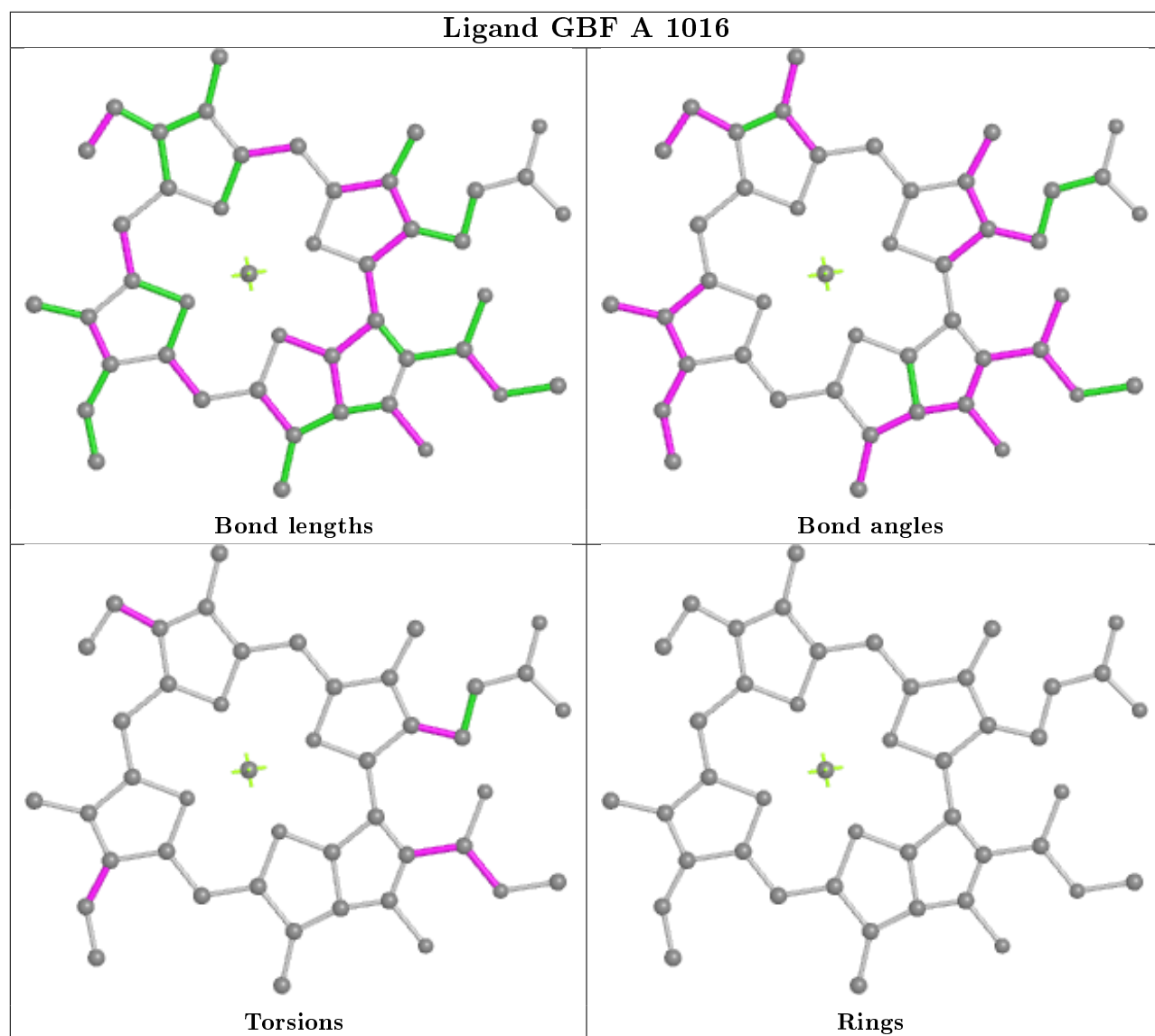
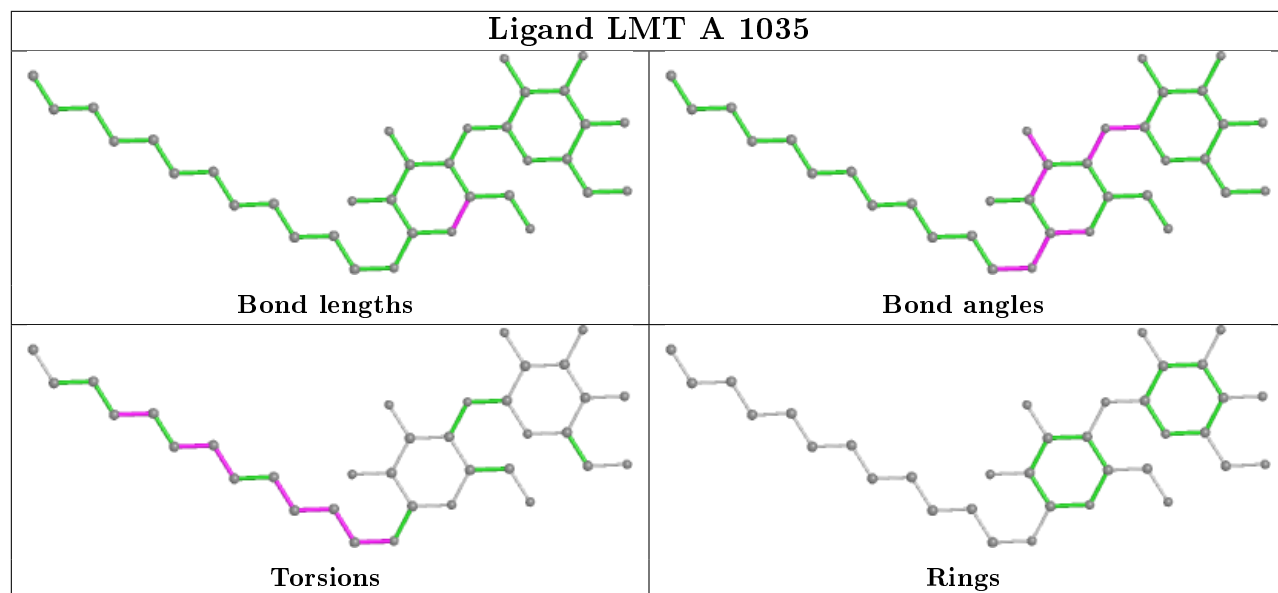
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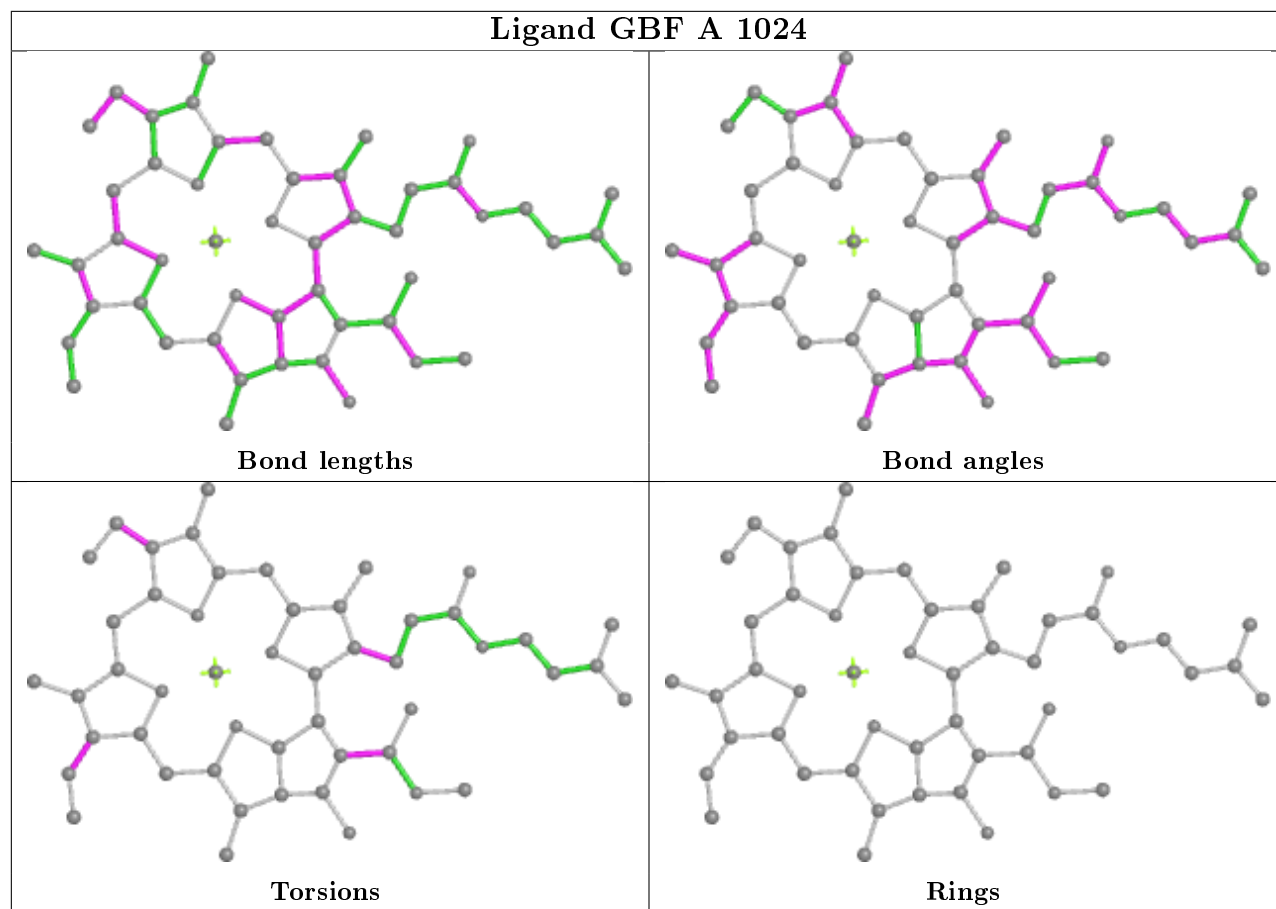


## Ligand LMT A 1034

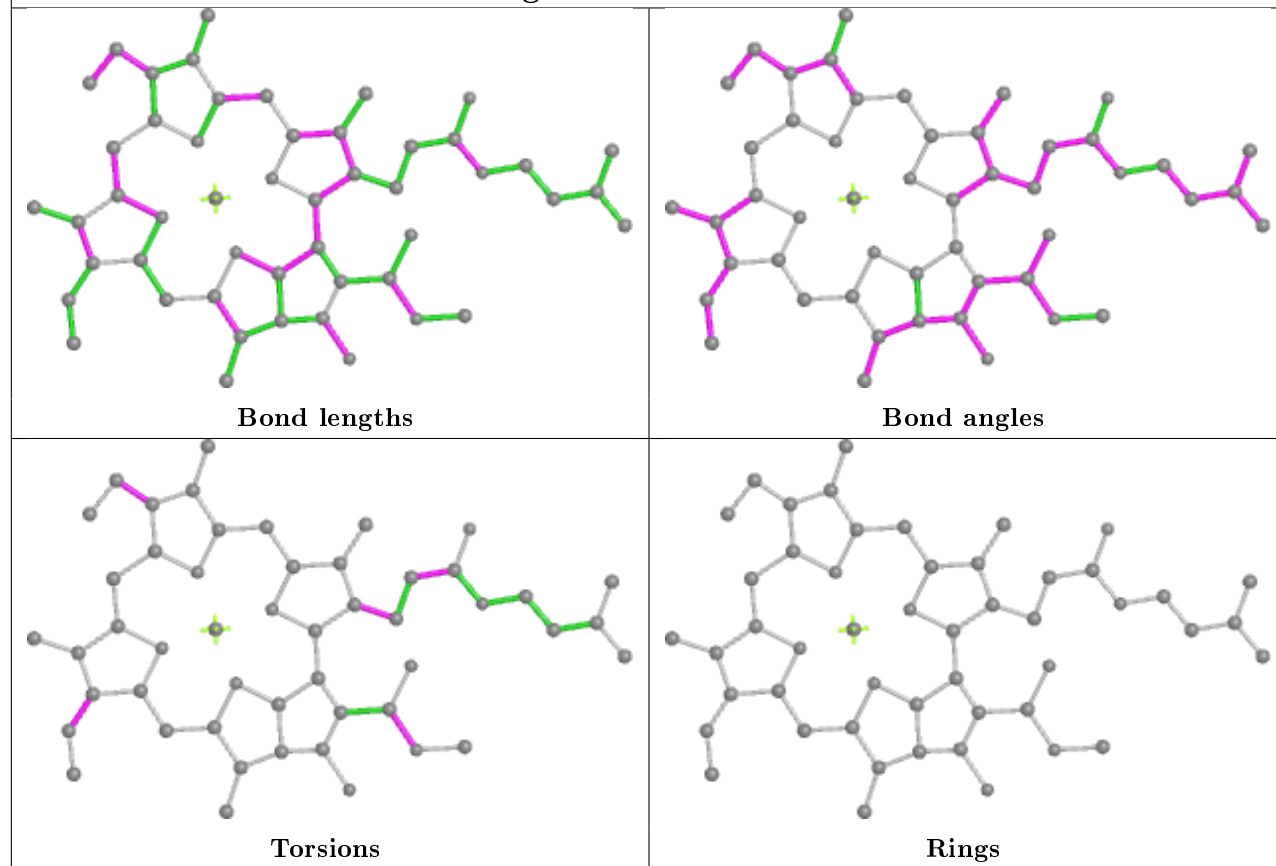




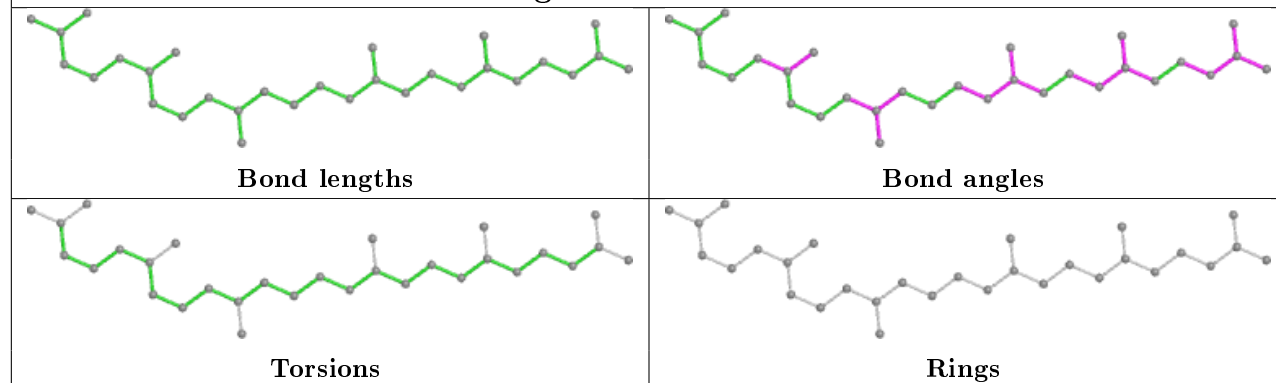


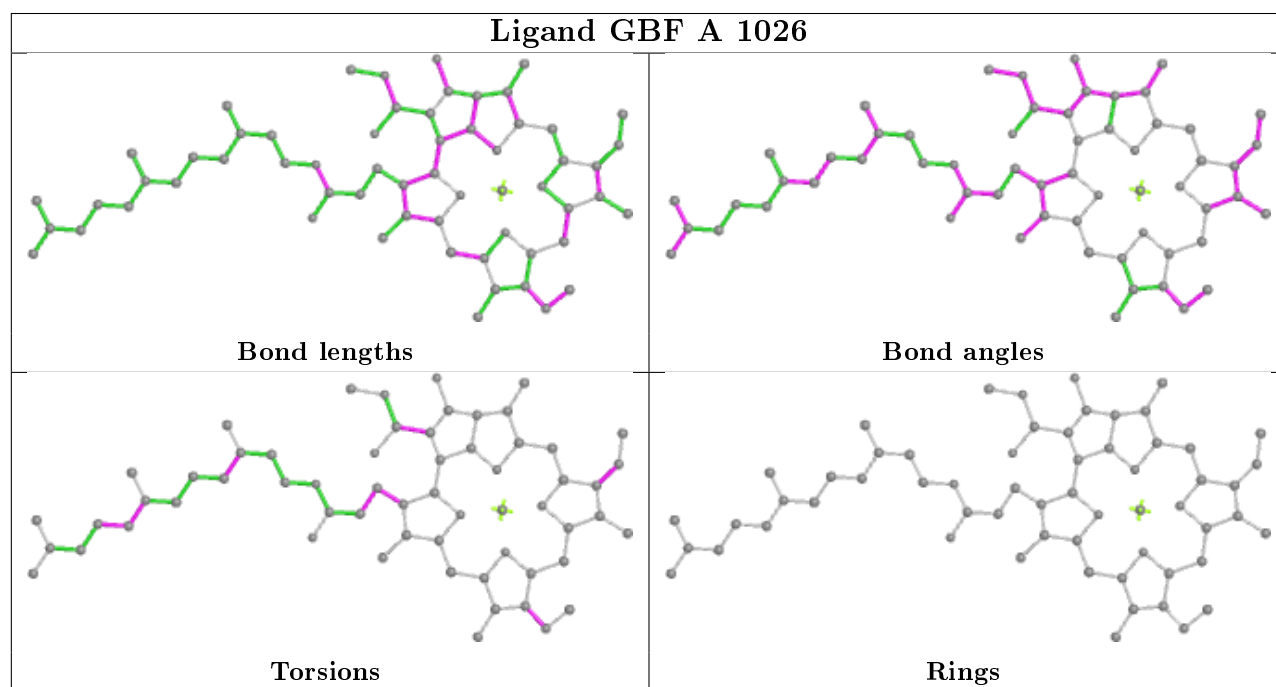
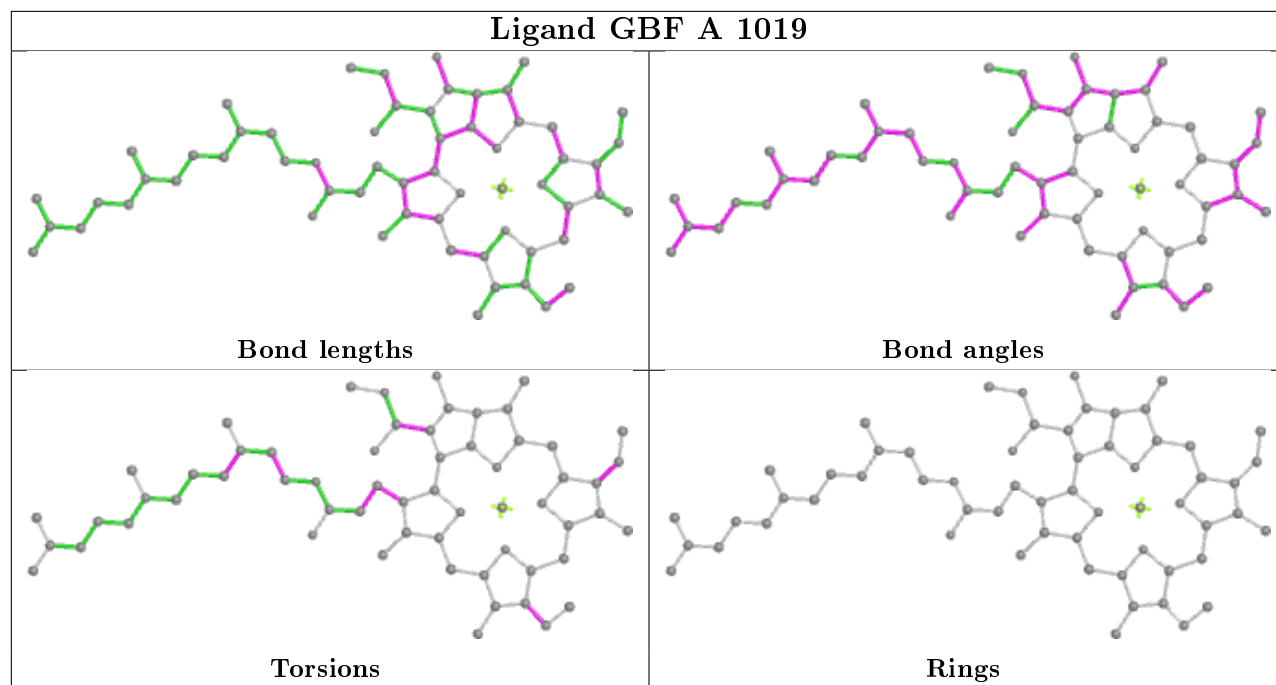


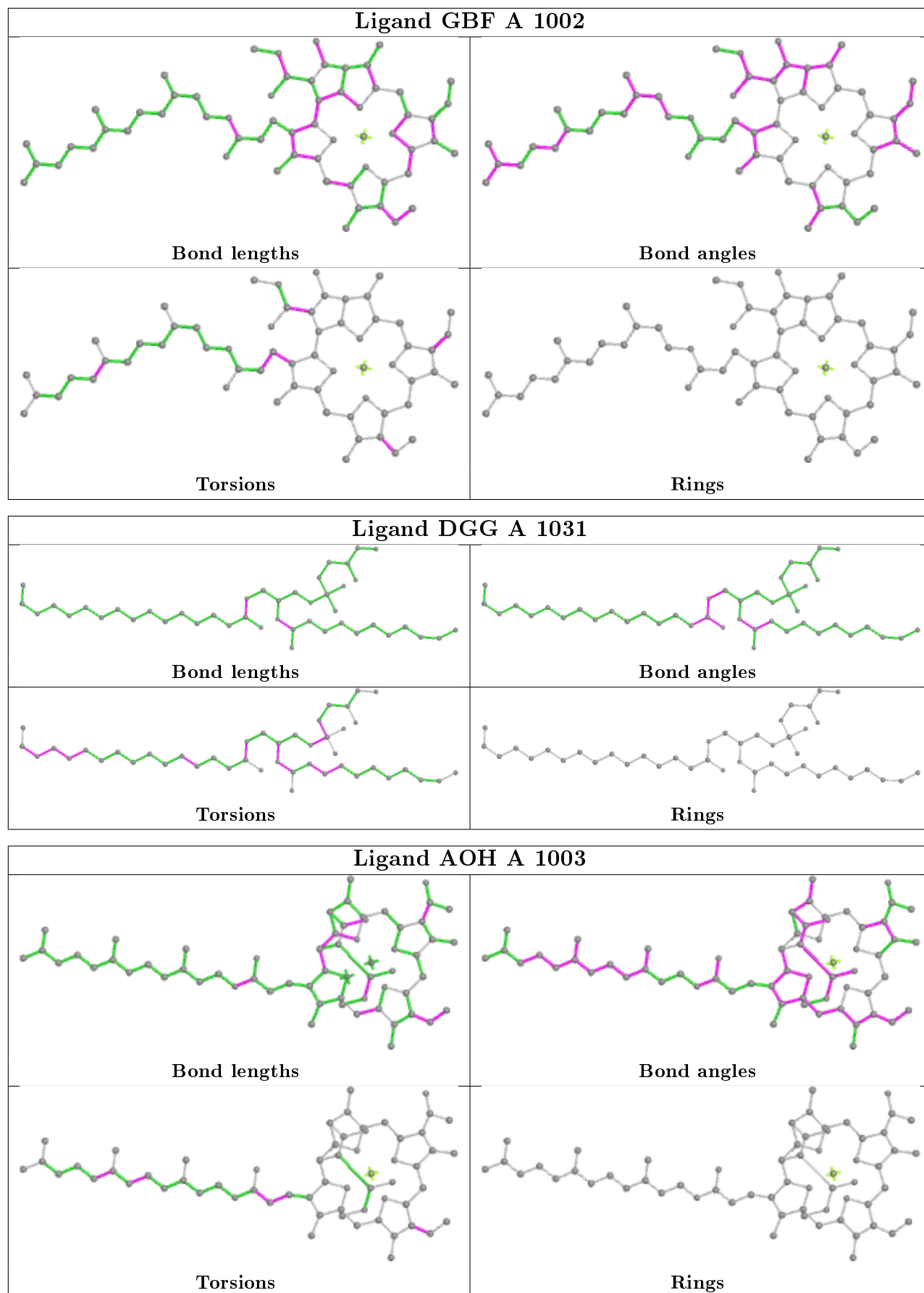
## Ligand GBF A 1027

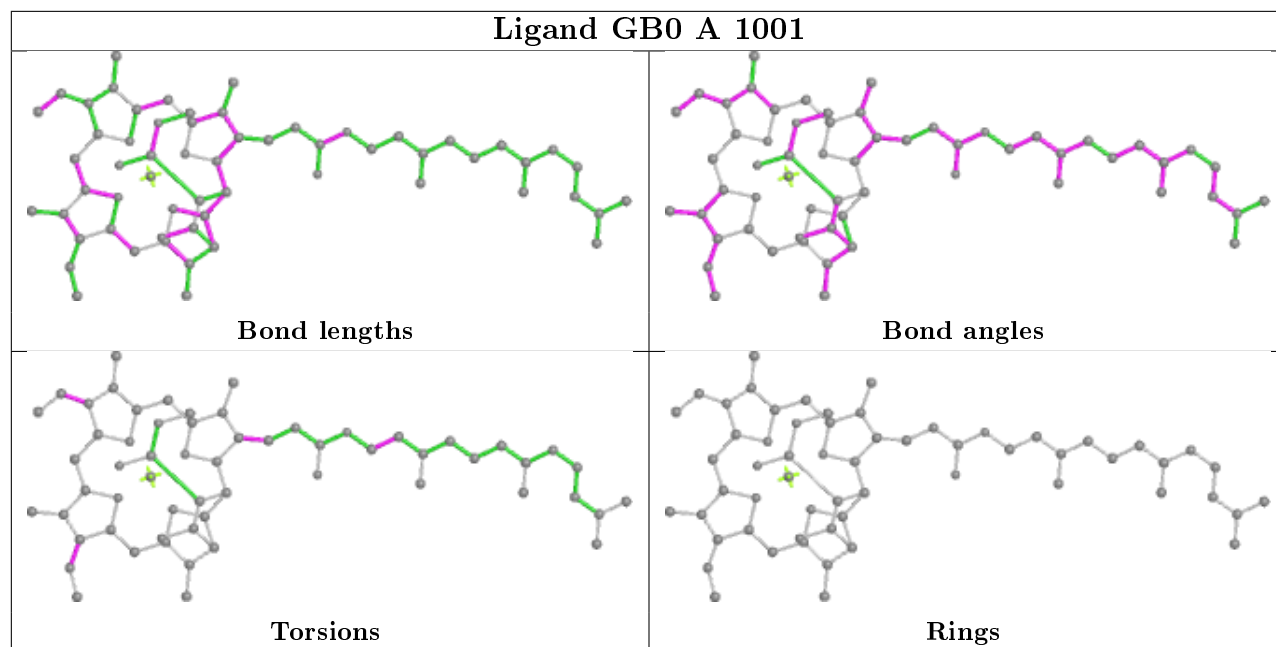


## Ligand C4D B 101









## 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	600/600 (100%)	0.82	126 (21%)  	31, 47, 81, 147	0
2	B	25/25 (100%)	1.94	11 (44%)  	77, 87, 92, 99	0
All	All	625/625 (100%)	0.86	137 (21%)  	31, 48, 88, 147	0

All (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
1	A	304	ALA	5.2
1	A	599	ILE	5.2
1	A	279	GLY	5.1
1	A	281	MET	5.0
1	A	310	PHE	5.0
1	A	453	ILE	4.9
1	A	280	ILE	4.9
1	A	301	PRO	4.9
1	A	165	PHE	4.9
1	A	454	PHE	4.9
1	A	223	PHE	4.8
1	A	303	LEU	4.7
1	A	273	LEU	4.6
1	A	197	ASN	4.6
2	B	17	PHE	4.6
2	B	14	SER	4.5
2	B	16	THR	4.5
1	A	276	LEU	4.3
1	A	305	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	302	LYS	4.3
1	A	460	ILE	4.2
1	A	193	PHE	4.2
1	A	107	VAL	4.1
1	A	168	ILE	4.1
1	A	274	GLY	4.1
1	A	206	LYS	4.0
2	B	24	ALA	4.0
1	A	596	LYS	3.9
1	A	593	LEU	3.9
1	A	461	ALA	3.9
2	B	15	PRO	3.9
1	A	220	ALA	3.9
1	A	166	GLY	3.8
2	B	23	LEU	3.8
1	A	145	PHE	3.8
1	A	108	LYS	3.8
1	A	592	PHE	3.7
1	A	119	VAL	3.7
1	A	540	TRP	3.7
1	A	591	CYS	3.7
1	A	437	TYR	3.7
1	A	160	LEU	3.6
1	A	459	VAL	3.6
1	A	594	PHE	3.6
1	A	422	MET	3.6
1	A	219	LEU	3.6
1	A	275	HIS	3.6
1	A	309	ASP	3.6
1	A	307	MET	3.6
2	B	22	ILE	3.6
1	A	452	ALA	3.5
1	A	598	THR	3.5
2	B	19	VAL	3.5
1	A	283	TRP	3.4
1	A	284	ILE	3.4
1	A	363	HIS	3.4
1	A	455	PHE	3.4
1	A	282	PHE	3.4
1	A	226	VAL	3.4
1	A	456	SER	3.4
2	B	18	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	601	CYS	3.4
1	A	163	ASP	3.3
1	A	602	MET	3.3
1	A	258	MET	3.3
1	A	423	LYS	3.3
1	A	271	ALA	3.2
1	A	544	PHE	3.2
1	A	161	SER	3.1
1	A	538	PHE	3.1
1	A	539	ILE	3.1
1	A	192	TYR	3.1
1	A	190	PHE	3.1
1	A	600	VAL	3.0
1	A	167	PRO	3.0
1	A	597	MET	3.0
1	A	110	PRO	3.0
1	A	358	THR	3.0
1	A	117	GLU	3.0
1	A	480	ALA	3.0
1	A	222	HIS	2.9
1	A	216	CYS	2.9
1	A	376	ALA	2.9
1	A	221	PHE	2.9
1	A	194	ALA	2.8
2	B	20	ALA	2.8
1	A	536	ALA	2.8
1	A	272	ILE	2.7
1	A	451	LEU	2.7
2	B	27	PHE	2.6
1	A	224	ALA	2.6
1	A	227	VAL	2.6
1	A	426	ARG	2.6
1	A	154	LYS	2.6
1	A	200	ARG	2.5
1	A	603	TRP	2.5
1	A	355	ALA	2.5
1	A	9	ASN	2.4
1	A	146	TYR	2.4
1	A	308	LYS	2.4
1	A	12	ALA	2.4
1	A	189	ILE	2.4
1	A	541	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	225	THR	2.3
1	A	381	LYS	2.3
1	A	306	GLU	2.3
1	A	458	GLN	2.3
1	A	185	PHE	2.3
1	A	543	THR	2.3
1	A	424	ALA	2.3
1	A	268	VAL	2.3
1	A	542	PHE	2.3
1	A	203	PHE	2.2
1	A	27	GLY	2.2
1	A	313	ILE	2.2
1	A	115	PHE	2.2
1	A	111	ALA	2.2
1	A	590	GLY	2.2
1	A	24	ALA	2.2
1	A	25	THR	2.2
1	A	317	TYR	2.1
1	A	450	TYR	2.1
1	A	157	PRO	2.1
1	A	464	TRP	2.1
1	A	535	GLY	2.1
1	A	218	ILE	2.1
1	A	250	GLN	2.0
1	A	421	GLY	2.0
1	A	162	PHE	2.0
1	A	449	PHE	2.0
1	A	159	GLY	2.0
1	A	118	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	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

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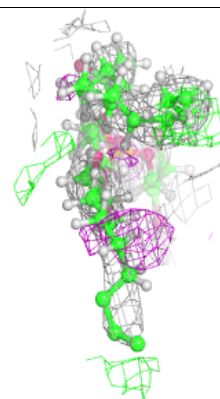
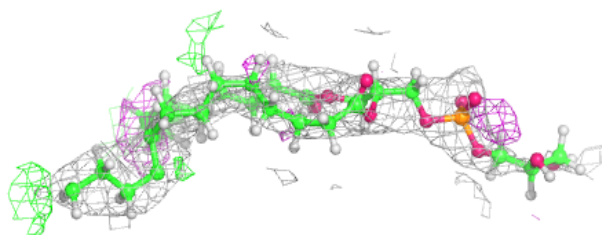
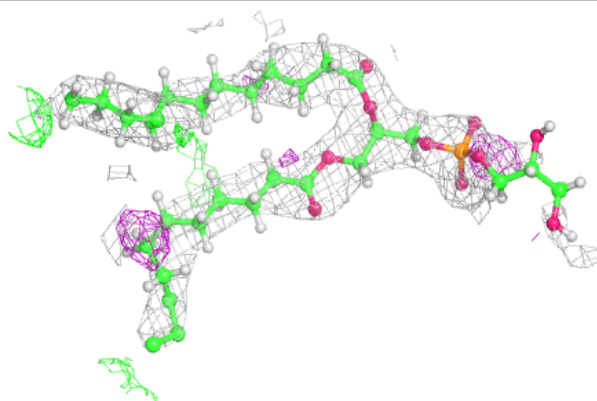
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SF4	A	1029	8/8	0.99	0.14	38,42,42,43	8

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.

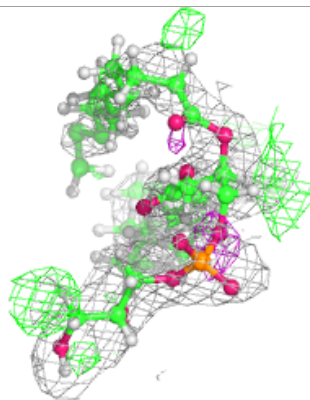
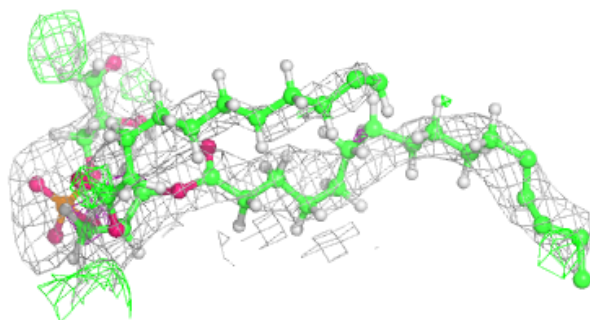
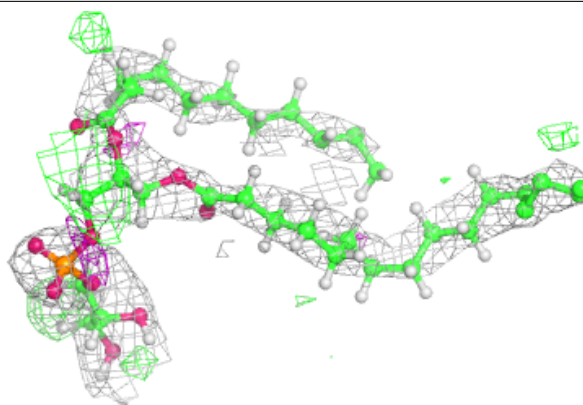
**Electron density around DGG A 1030:**

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mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



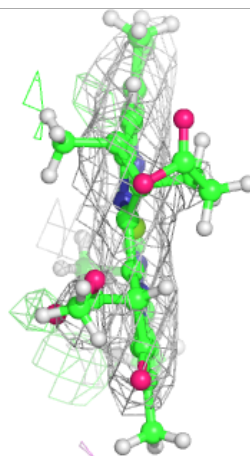
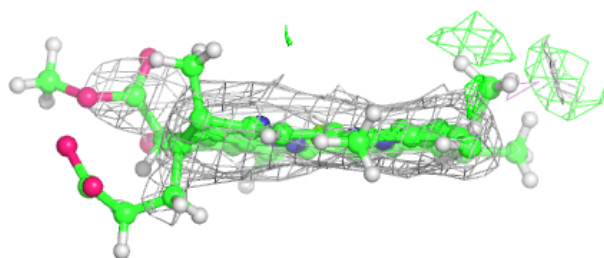
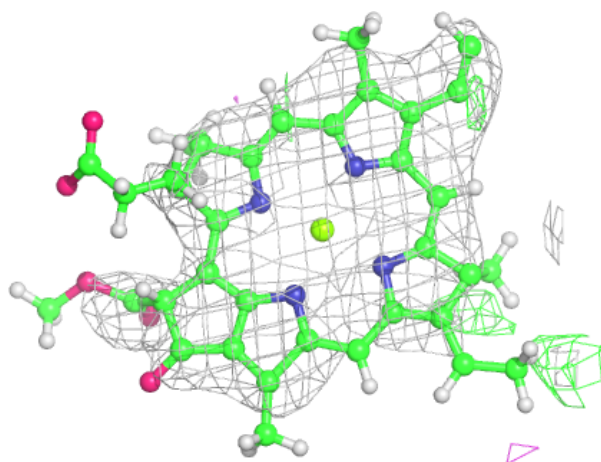
**Electron density around DGG A 1031:**

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and green (positive)



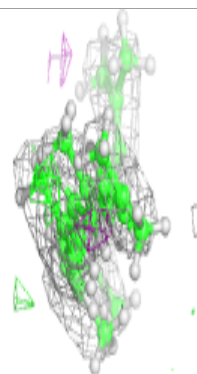
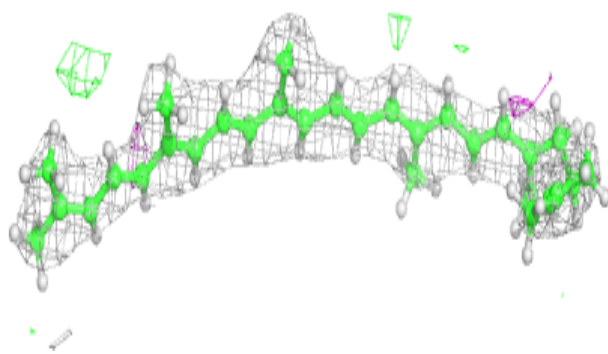
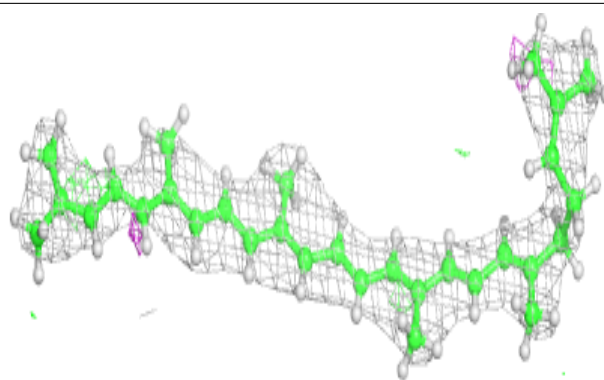
**Electron density around GBF B 102:**

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and green (positive)

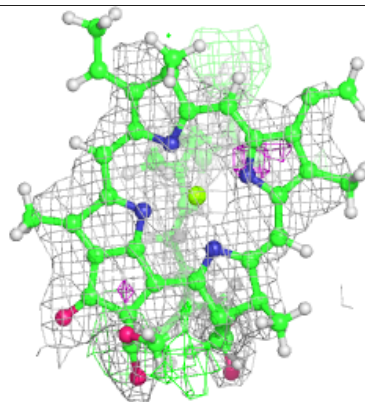
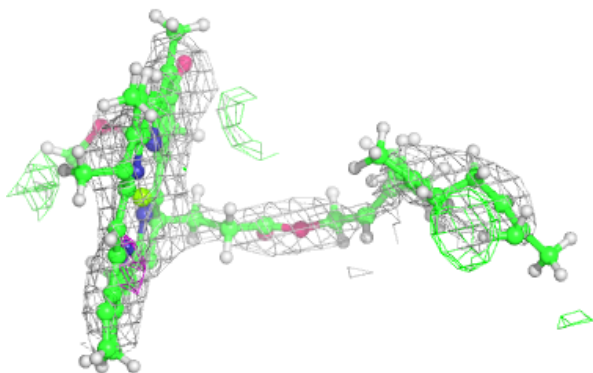
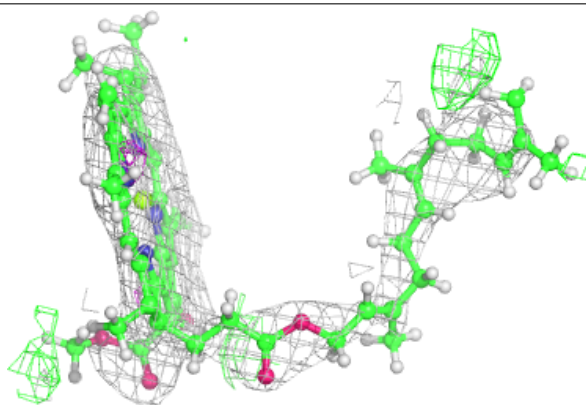


**Electron density around C4D B 101:**

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and green (positive)

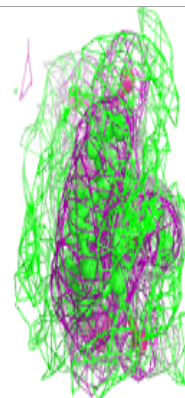
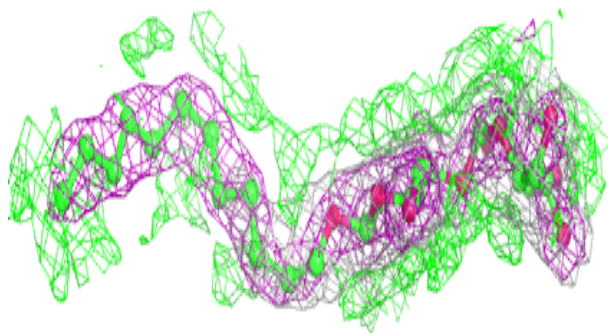
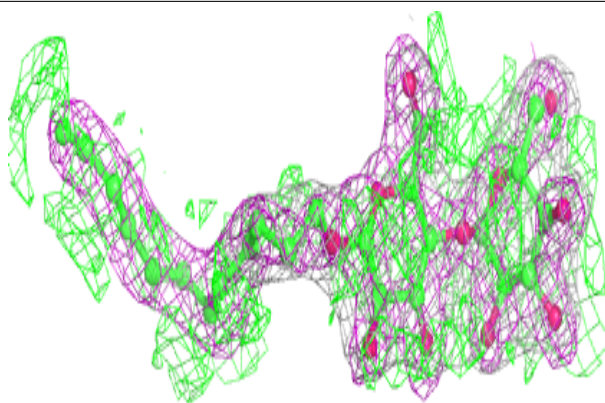
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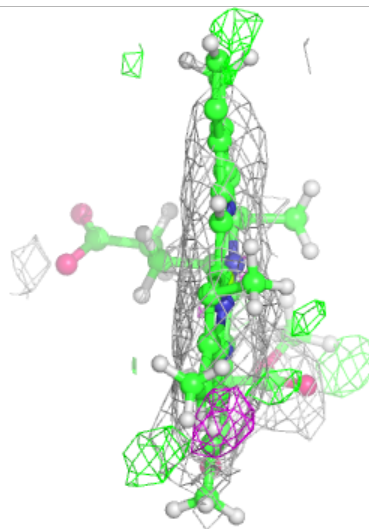
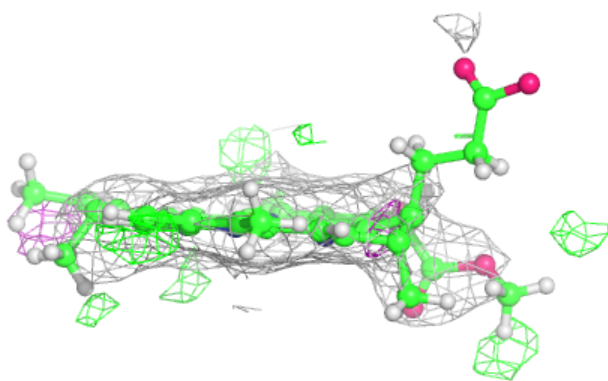
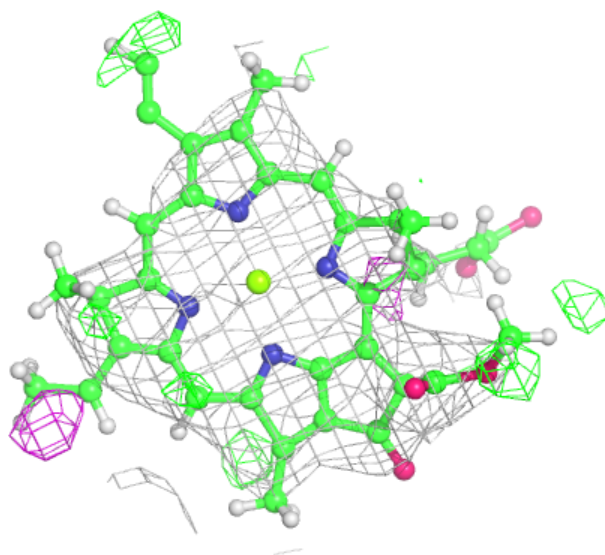
**Electron density around LMT A 1035:**

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and green (positive)



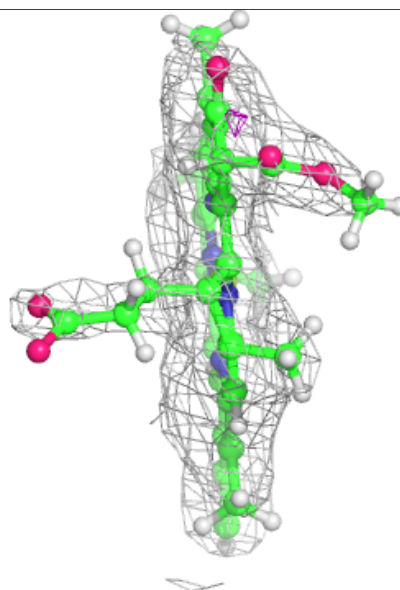
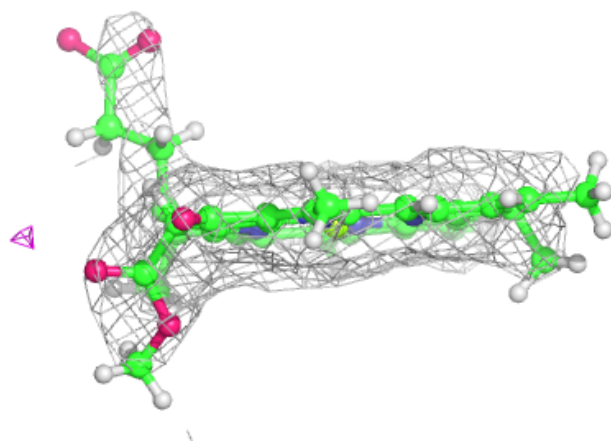
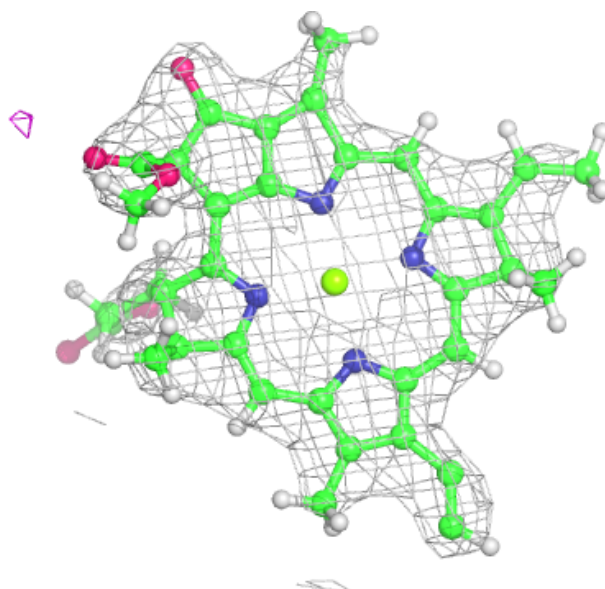
**Electron density around GBF A 1009:**

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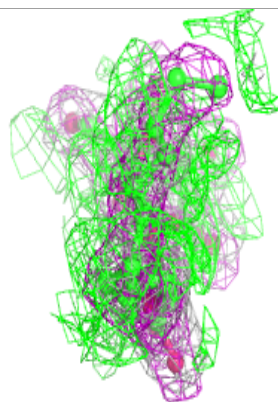
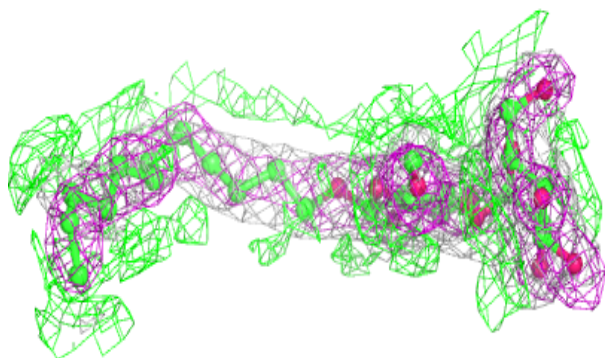
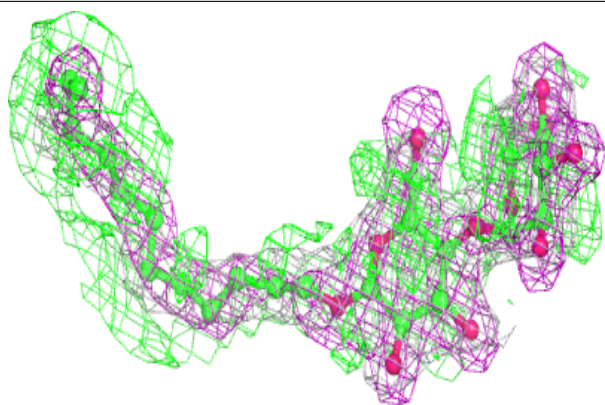
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and green (positive)

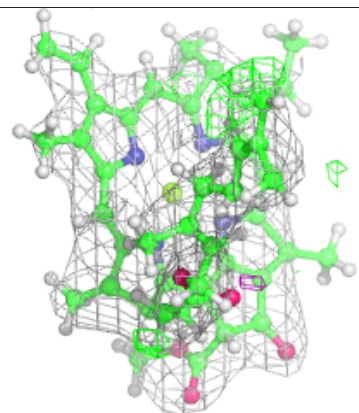
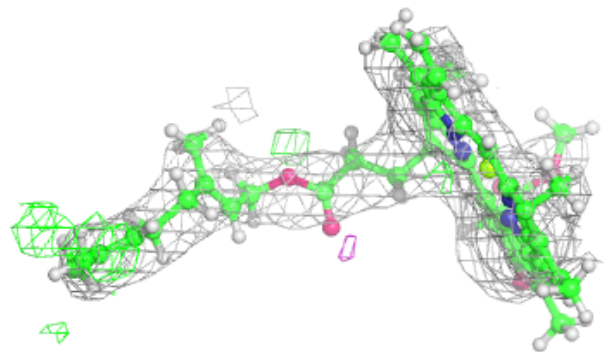
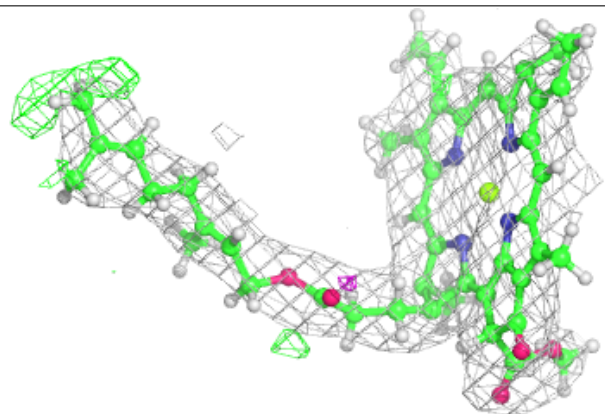


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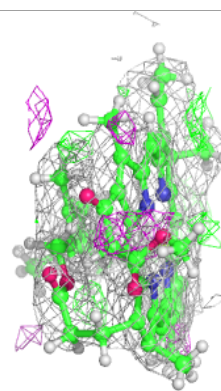
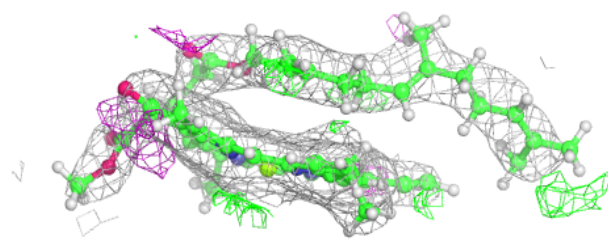
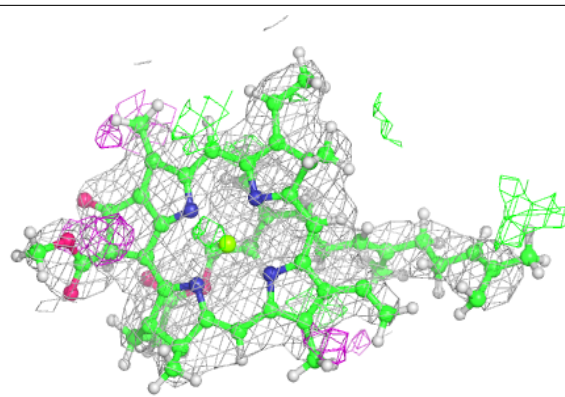
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and green (positive)



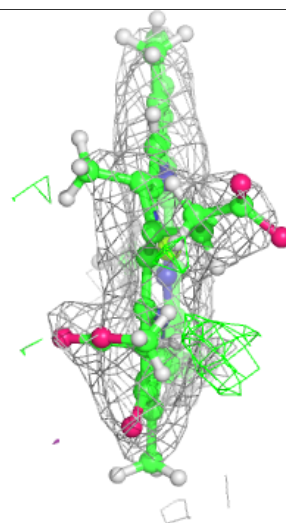
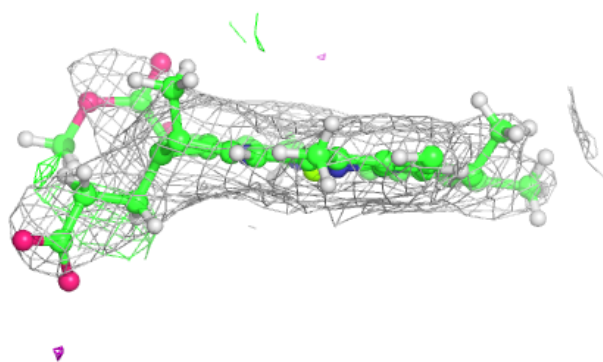
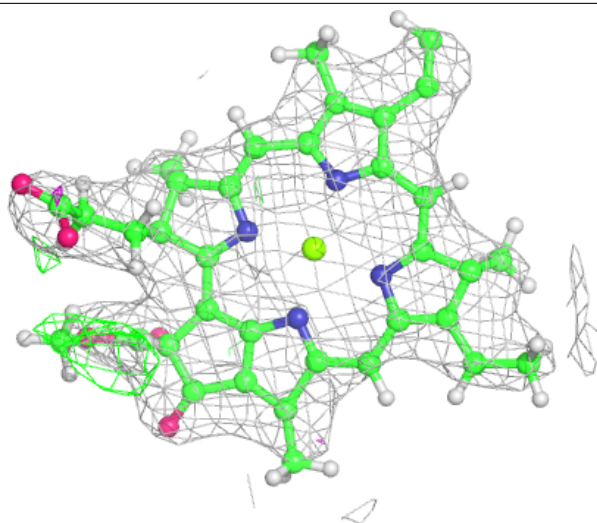
**Electron density around GBF A 1028:**

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and green (positive)



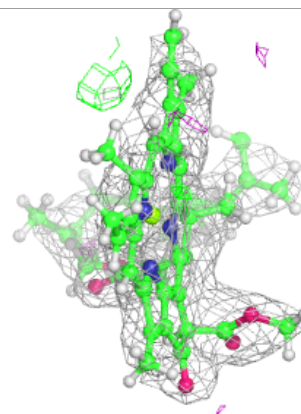
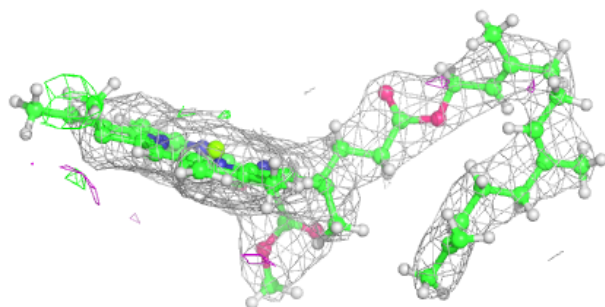
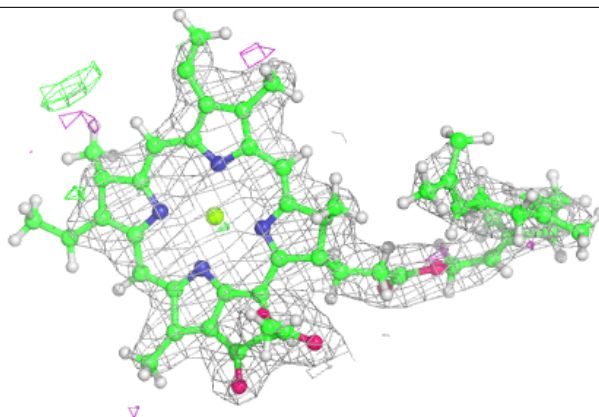
**Electron density around GBF A 1010:**

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



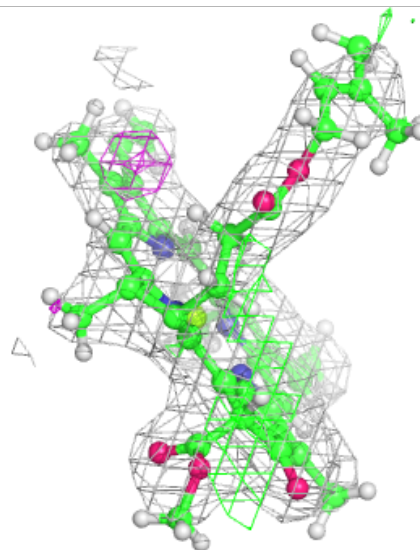
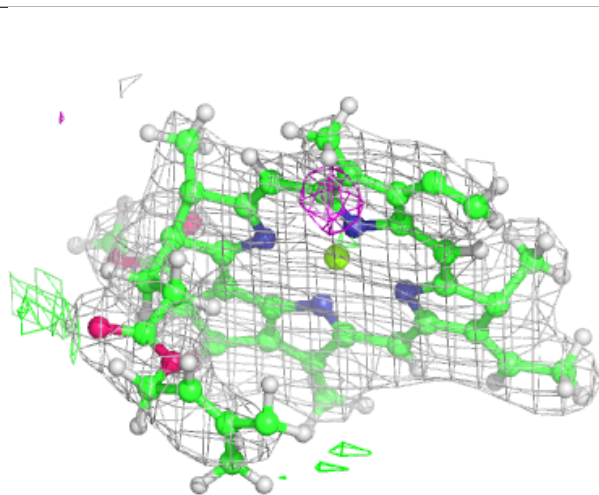
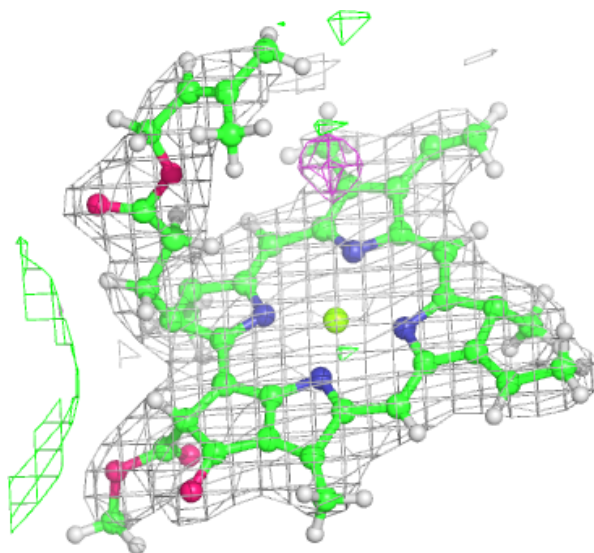
**Electron density around GBF A 1011:**

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



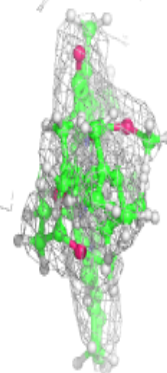
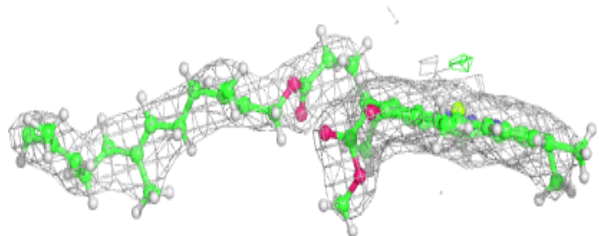
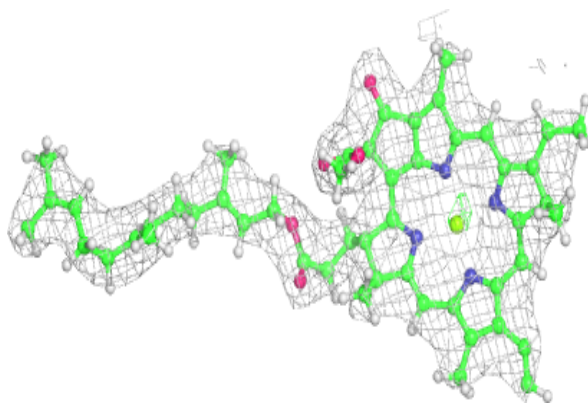
**Electron density around GBF A 1018:**

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

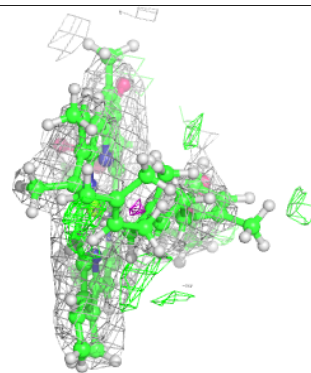
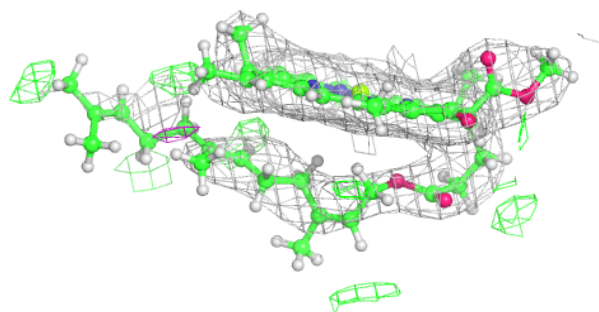
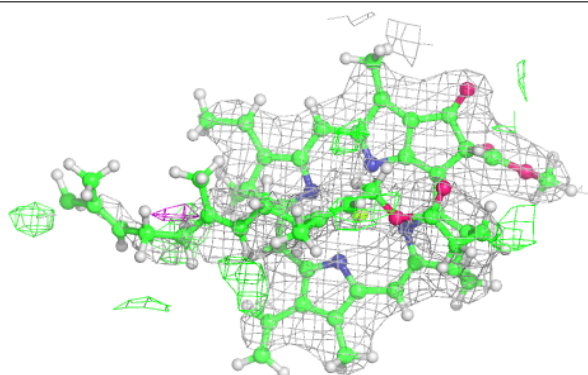


**Electron density around GBF A 1017:**

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

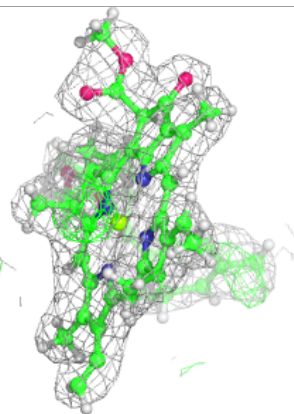
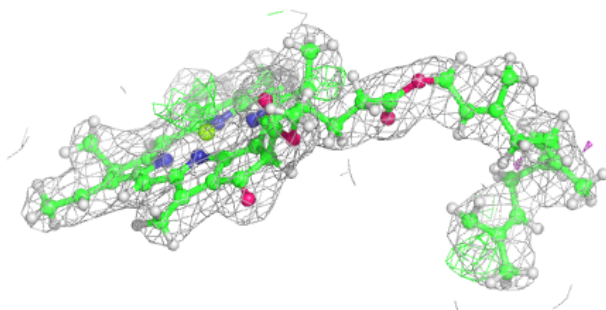
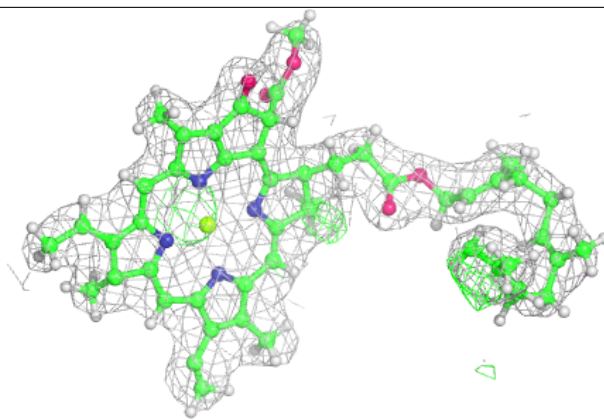
**Electron density around GBF A 1007:**

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



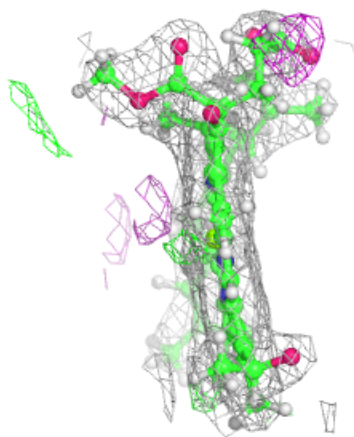
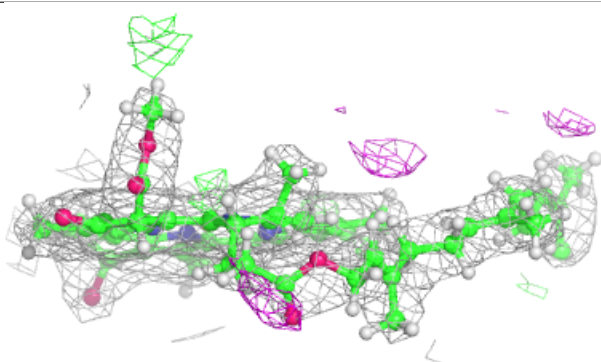
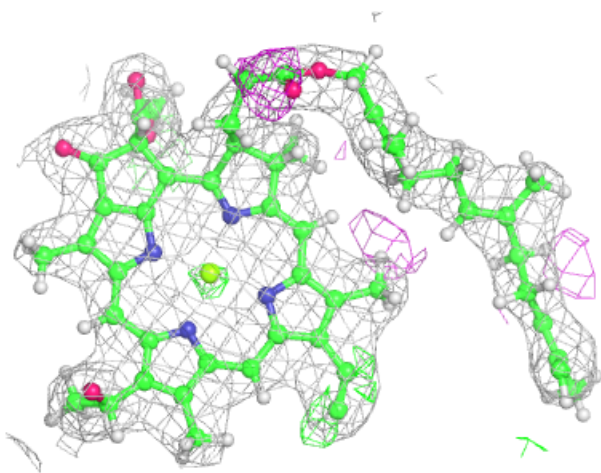
**Electron density around GBF A 1002:**

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



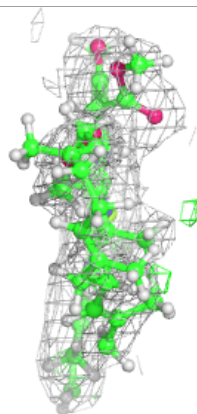
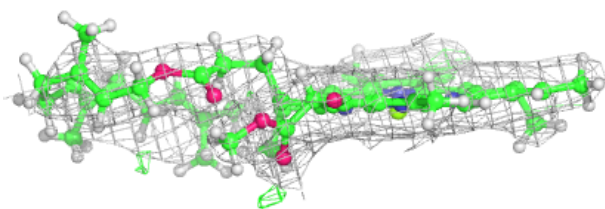
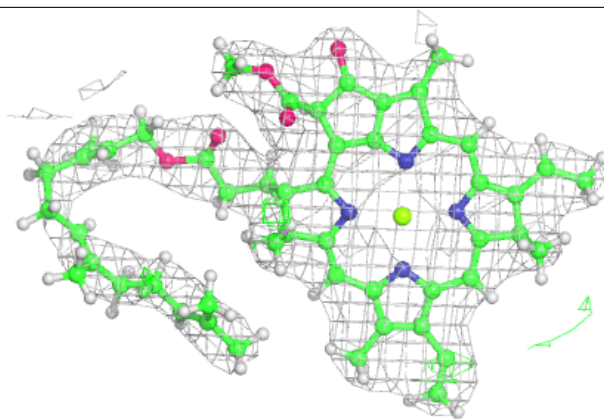
**Electron density around AOH A 1003:**

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



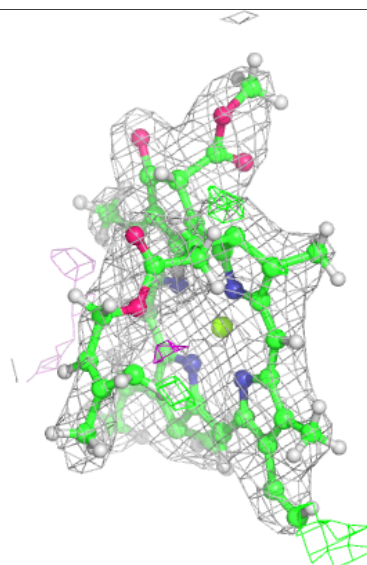
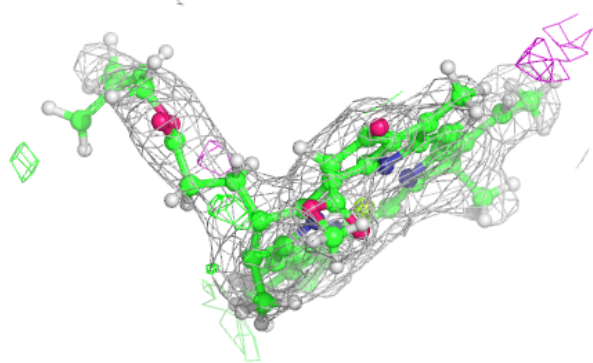
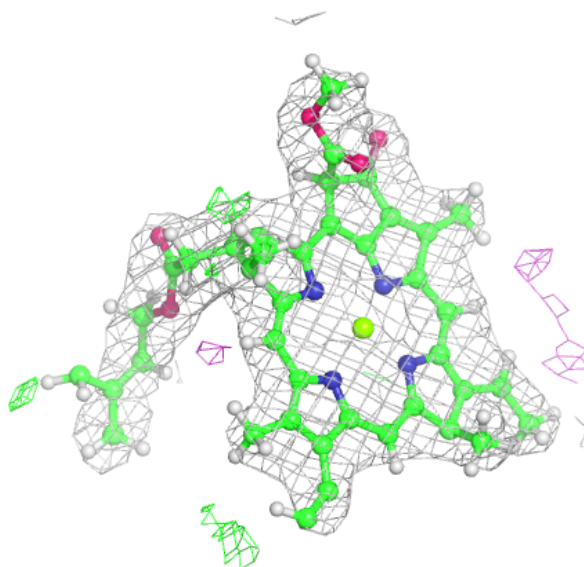
**Electron density around GBF A 1019:**

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



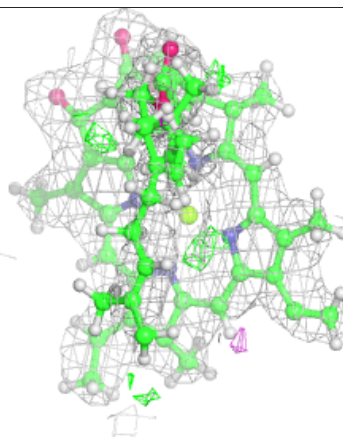
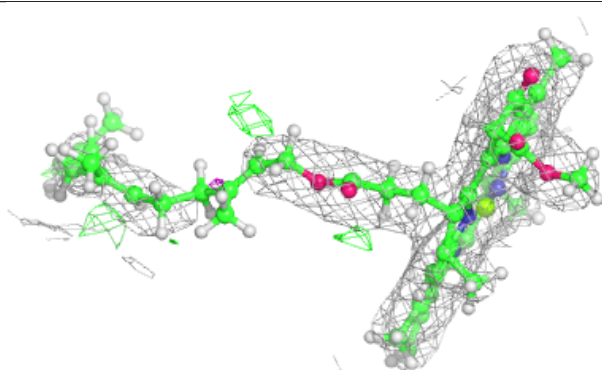
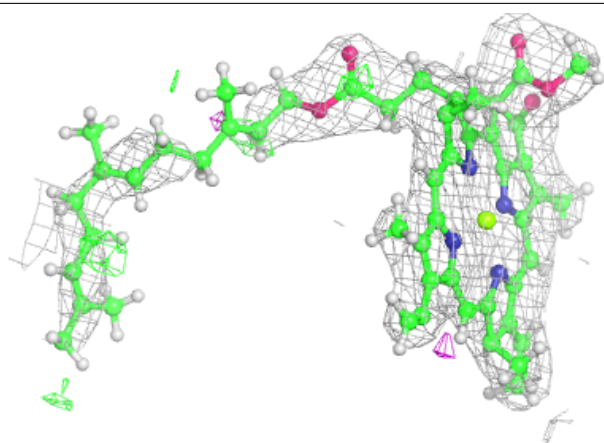
**Electron density around GBF A 1027:**

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



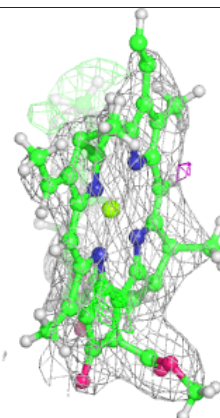
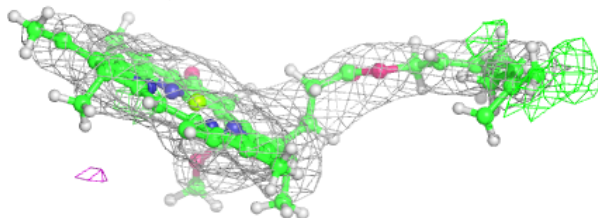
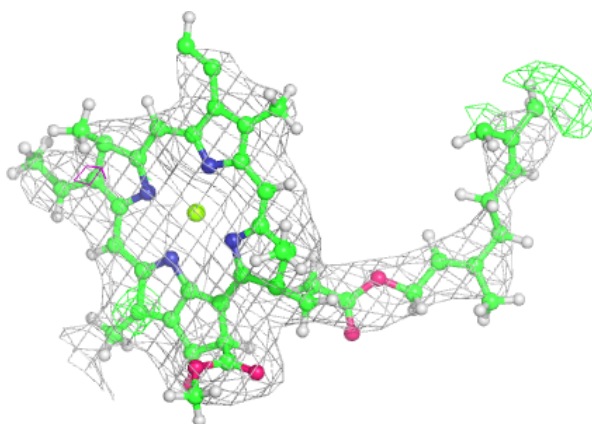
**Electron density around GBF A 1021:**

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



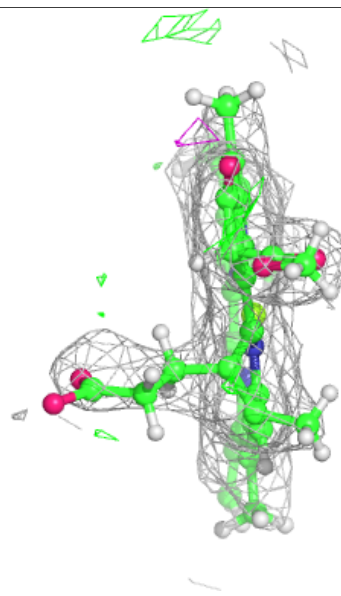
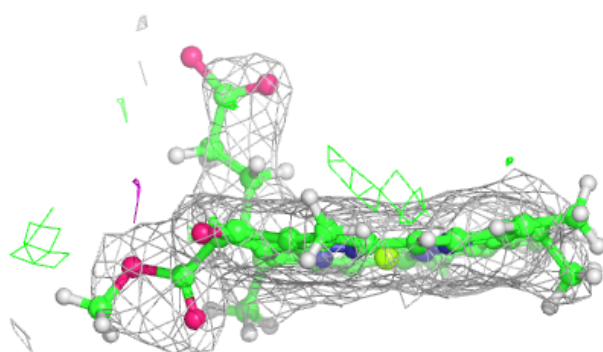
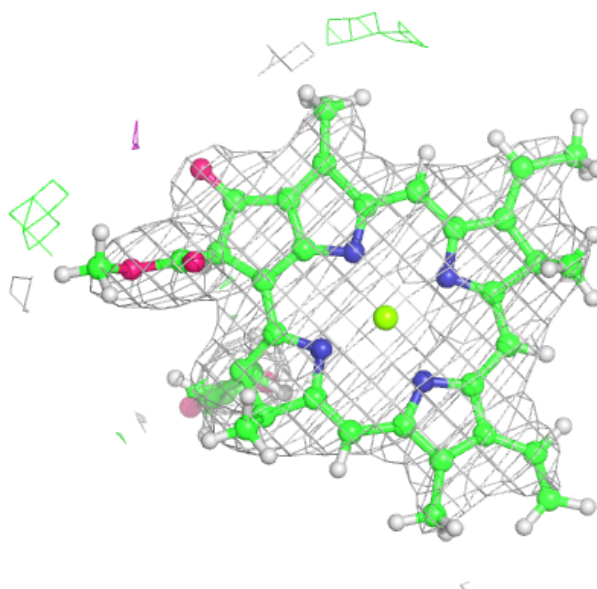
**Electron density around GBF A 1012:**

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



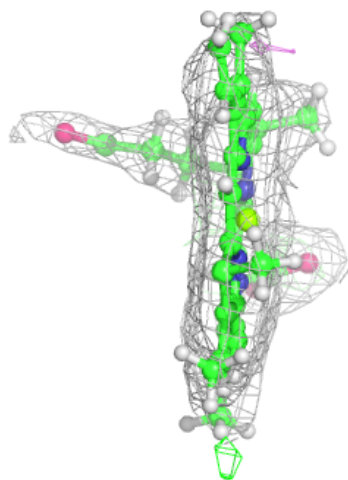
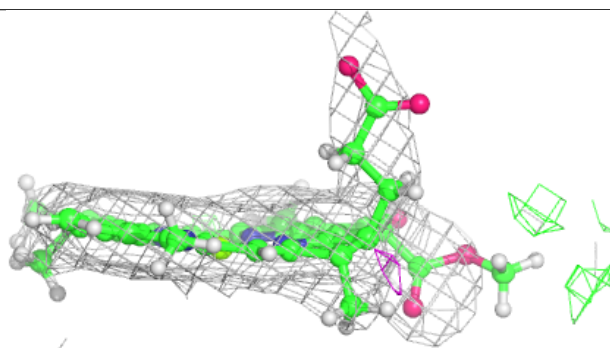
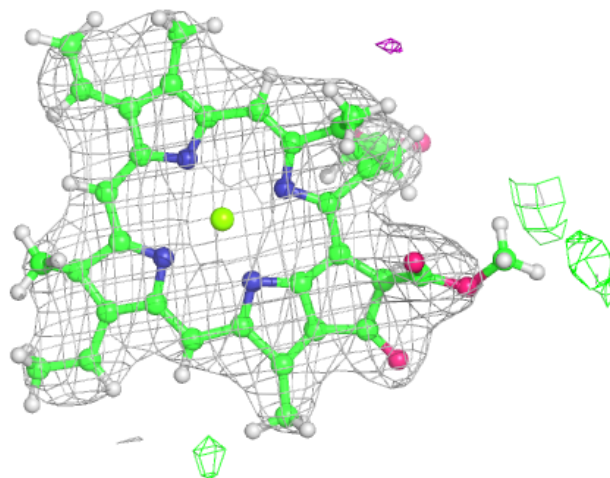
**Electron density around GBF A 1014:**

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



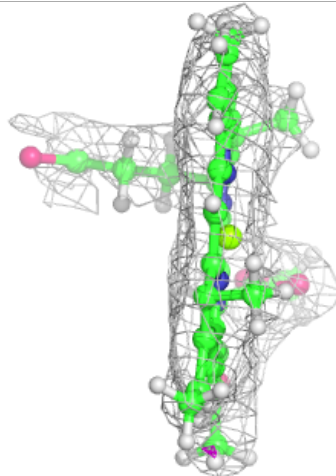
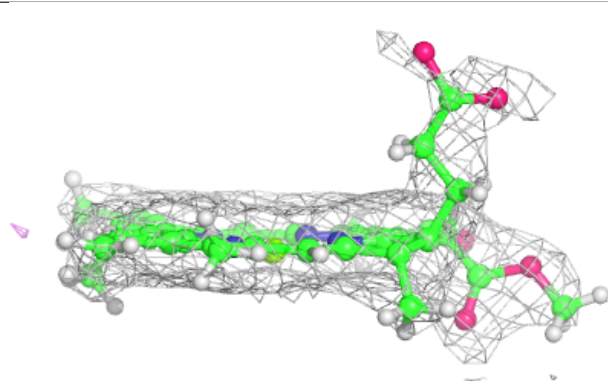
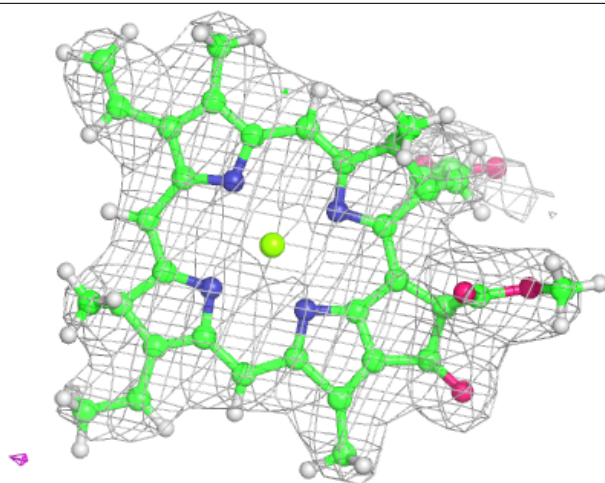
**Electron density around GBF A 1006:**

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



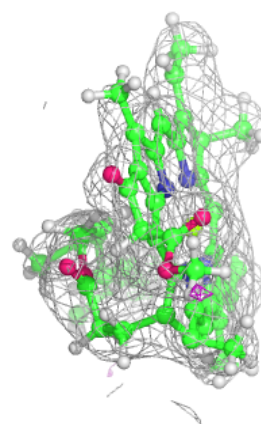
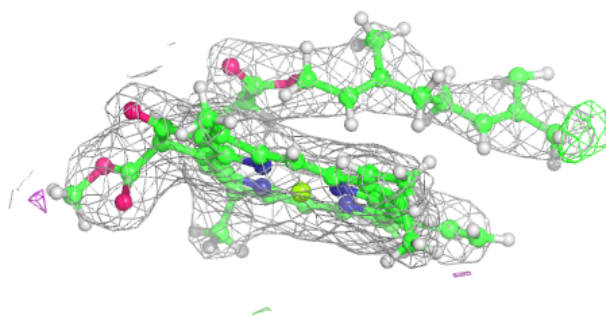
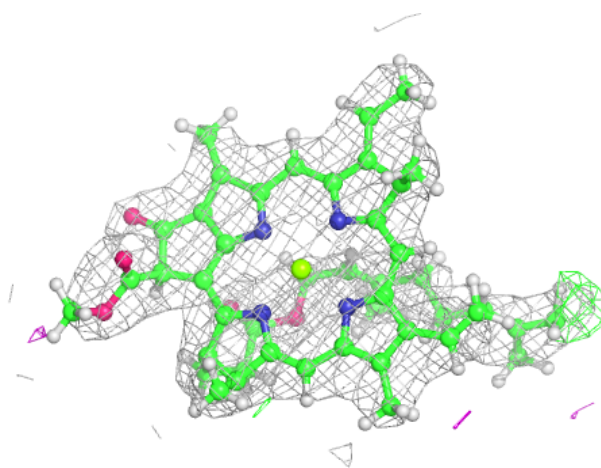
**Electron density around GBF A 1022:**

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



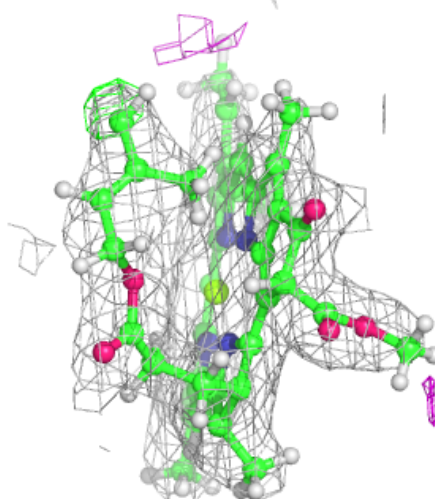
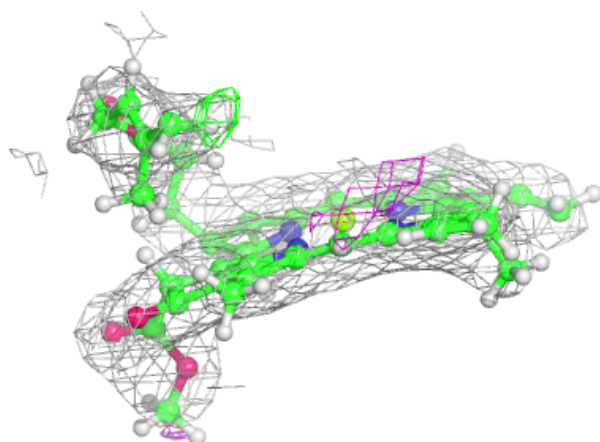
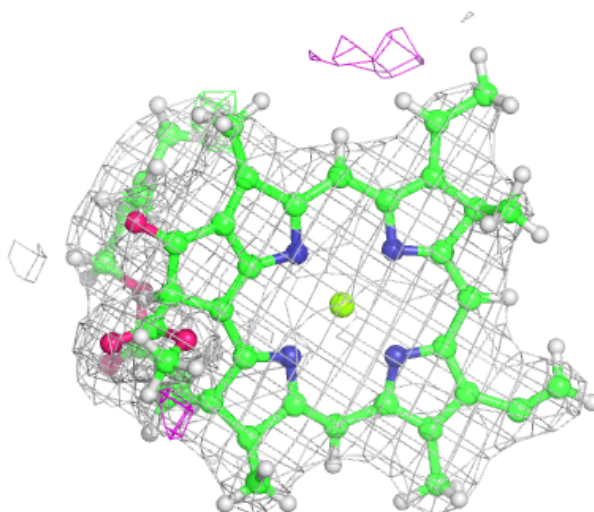
**Electron density around GBF A 1008:**

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



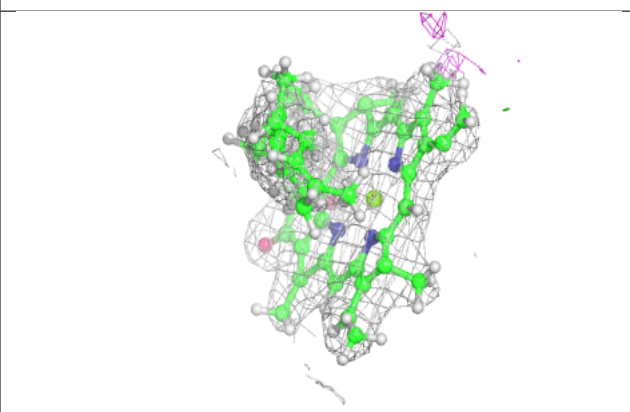
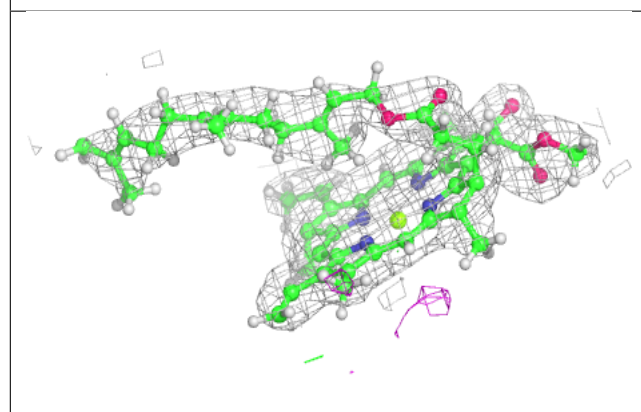
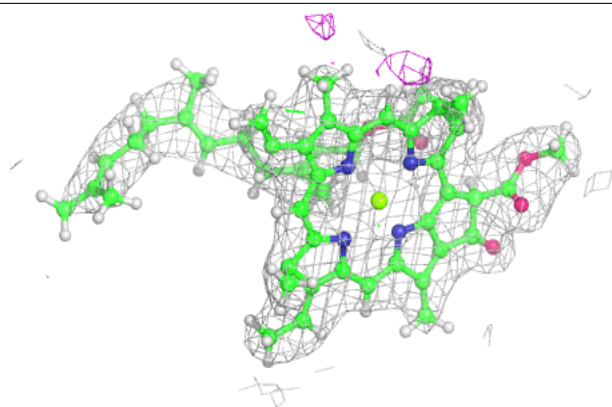
**Electron density around GBF A 1004:**

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

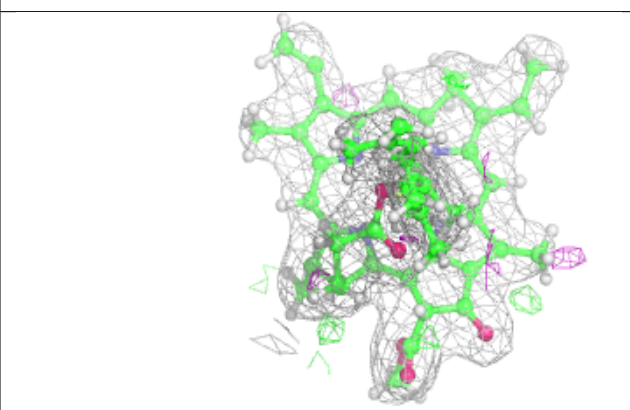
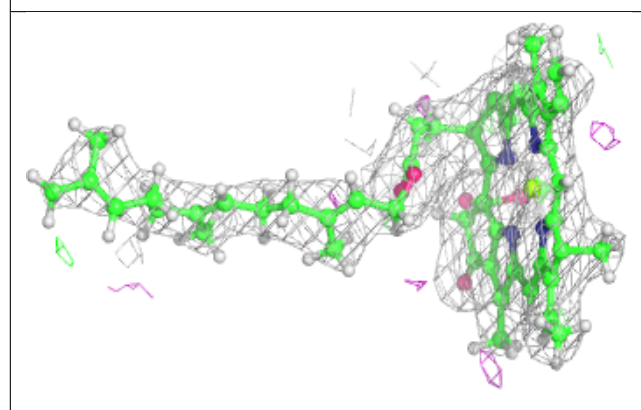
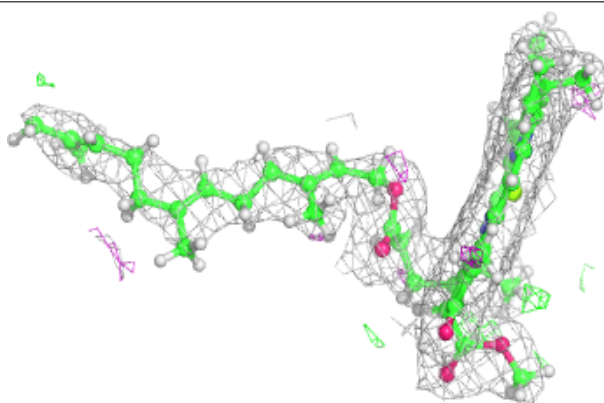


**Electron density around GBF A 1020:**

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

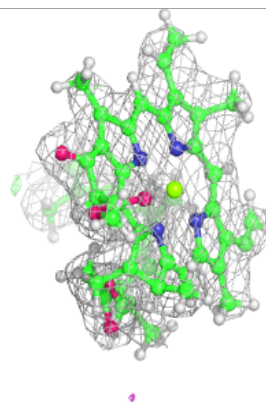
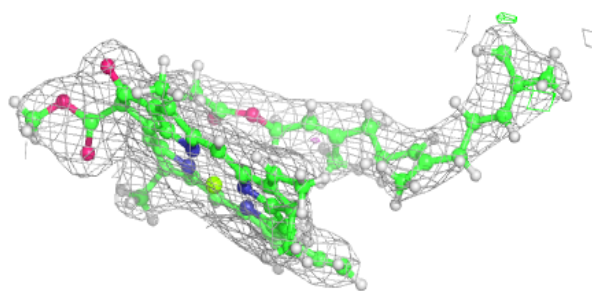
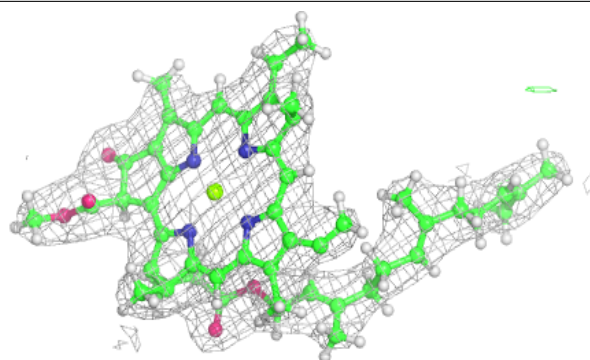
**Electron density around GBF A 1026:**

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



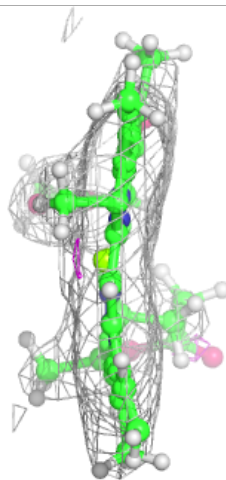
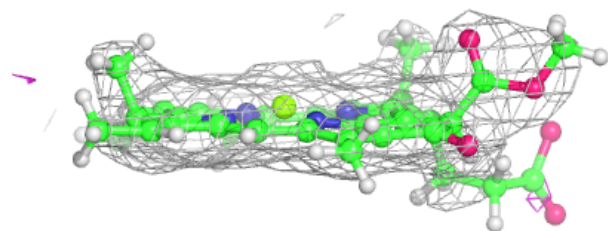
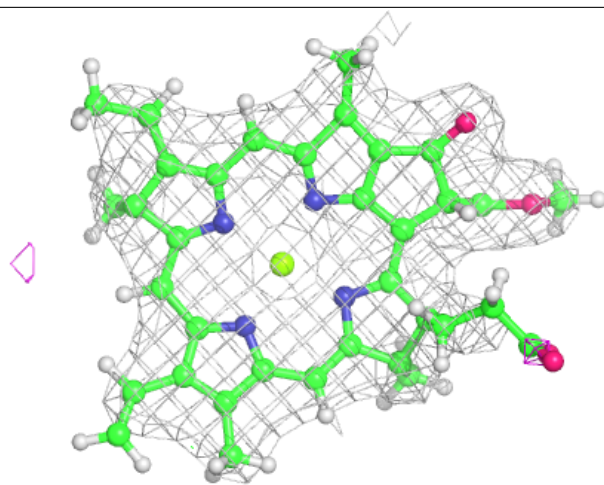
**Electron density around GBF A 1023:**

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



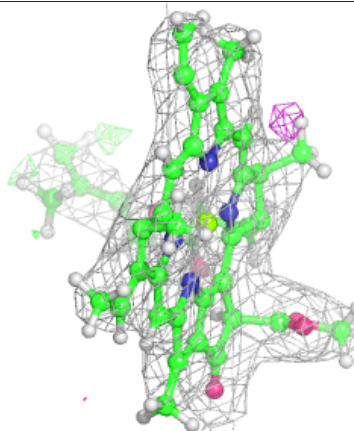
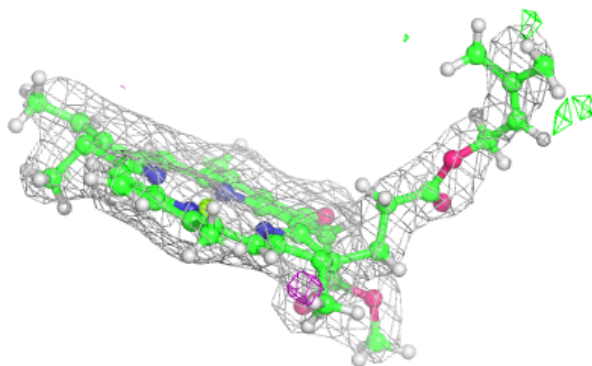
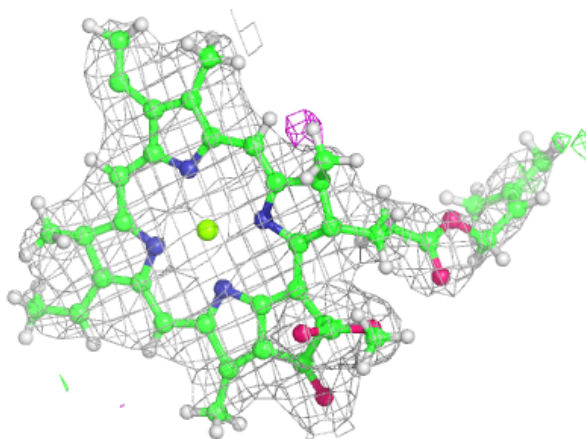
**Electron density around GBF A 1025:**

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

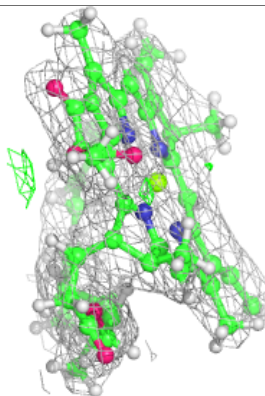
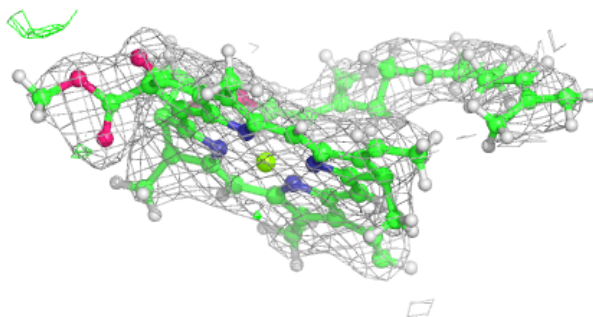
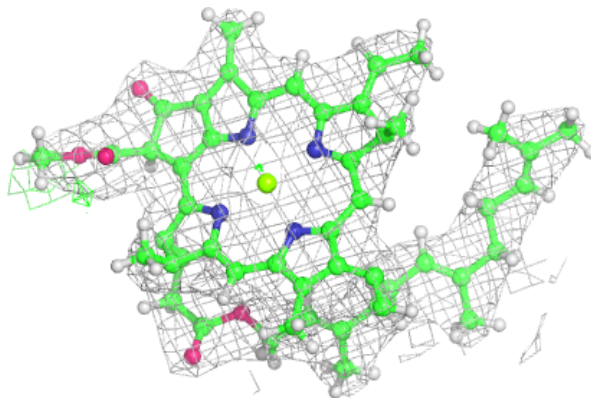


**Electron density around GBF A 1024:**

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

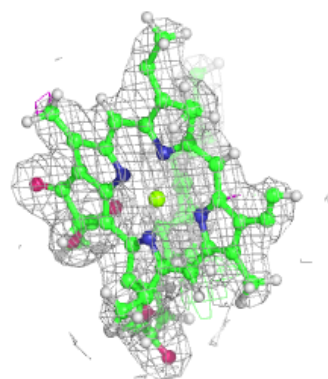
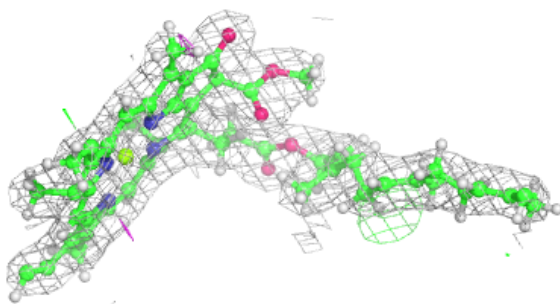
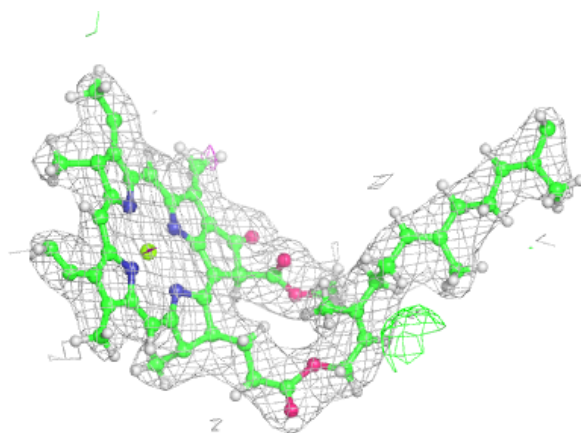
**Electron density around GBF A 1015:**

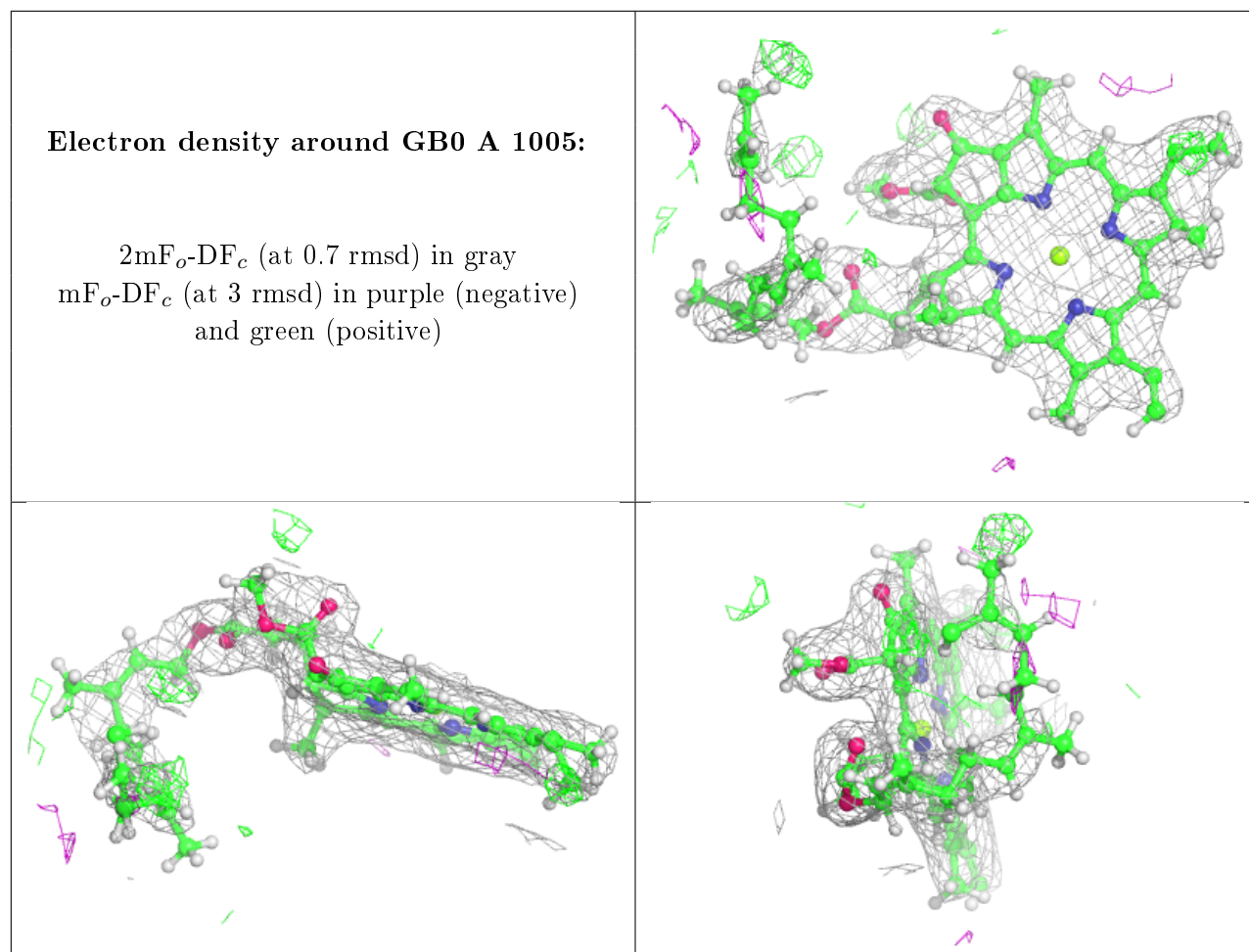
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.