



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 11:10 AM BST

PDB ID : 4FM5
Title : X-ray structure of des-methylflurbiprofen bound to murine COX-2
Authors : Xu, S.; Banerjee, S.; Windsor, M.A.; Marnett, L.J.
Deposited on : 2012-06-15
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

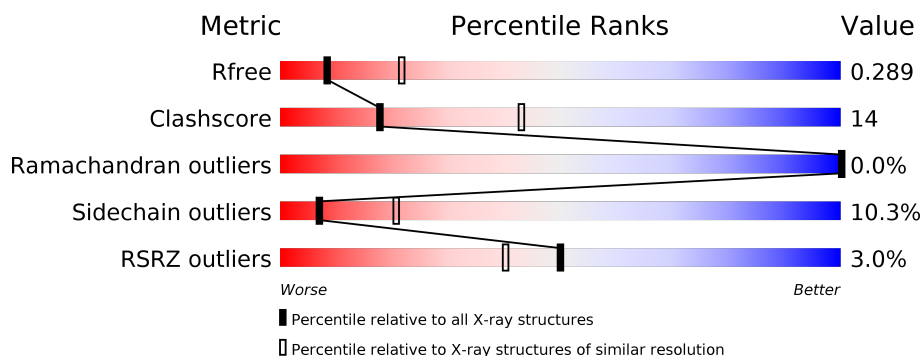
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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.



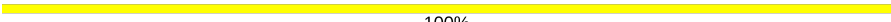
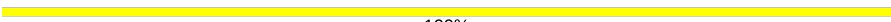
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	604	 2% 68% 20% • 9%
1	B	604	 4% 66% 20% • 9%
1	C	604	 3% 69% 19% • • 9%
1	D	604	 2% 66% 20% 5% 9%
2	E	2	 100%
2	F	2	 50% 50%

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	G	2	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18554 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

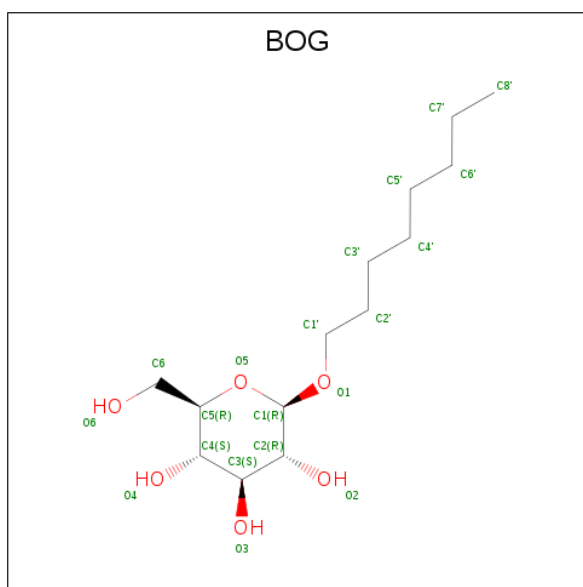
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



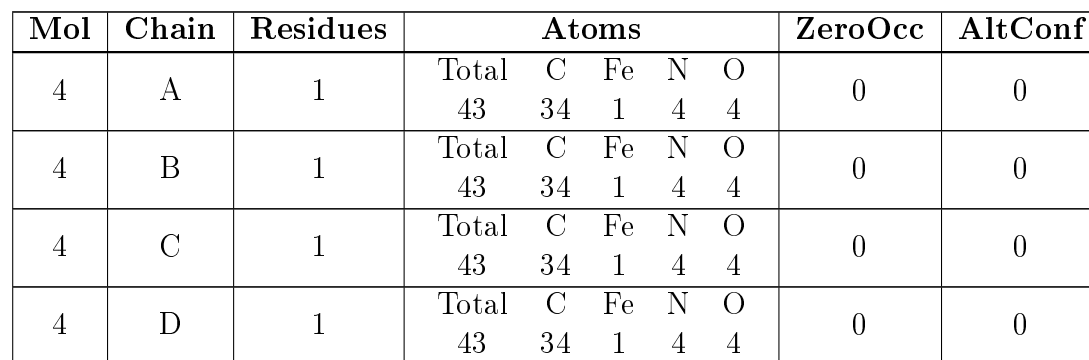
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		
3	C	1	Total	C	O	0	0
			20	14	6		
3	C	1	Total	C	O	0	0
			20	14	6		
3	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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- Chemical structure of DF0 (2-(2-fluorophenyl)-3-phenylpropanoic acid) is shown. The structure features a central benzene ring (C1-C6) with a fluorine atom (F) at C1. A phenyl ring (C7-C12) is attached at C2, and a propanoic acid chain (C3-C5) is attached at C3. The carboxylic acid group consists of C5 double-bonded to O and single-bonded to OH (O1).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	F	O	0	0
			17	14	1	2		
5	B	1	Total	C	F	O	0	0
			17	14	1	2		
5	C	1	Total	C	F	O	0	0
			17	14	1	2		
5	D	1	Total	C	F	O	0	0
			17	14	1	2		

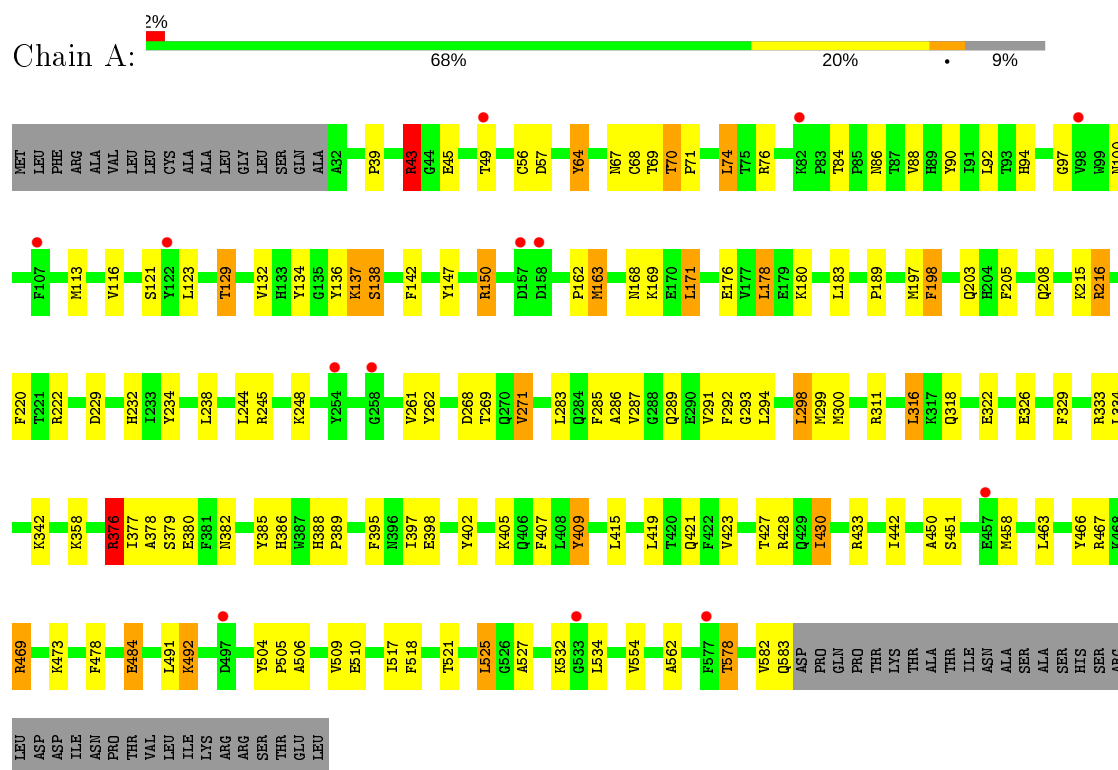
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	63	Total	O	0	0
			63	63		
6	B	39	Total	O	0	0
			39	39		
6	C	37	Total	O	0	0
			37	37		
6	D	47	Total	O	0	0
			47	47		

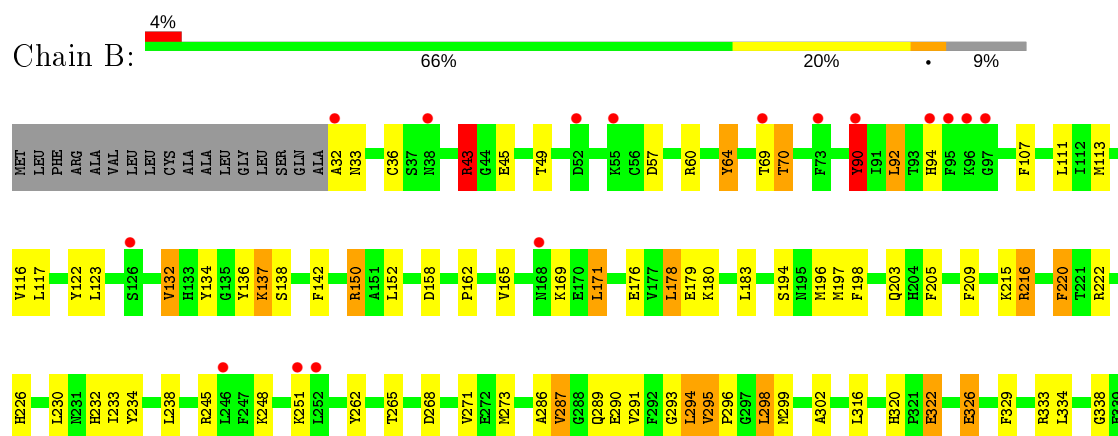
3 Residue-property plots

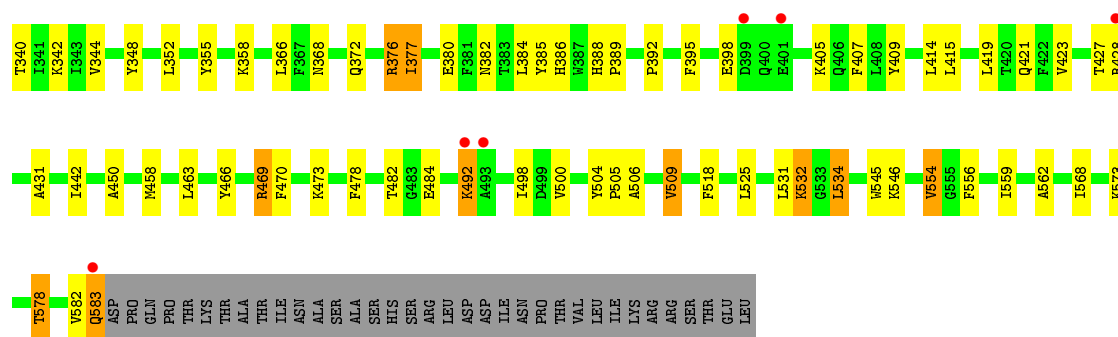
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Prostaglandin G/H synthase 2

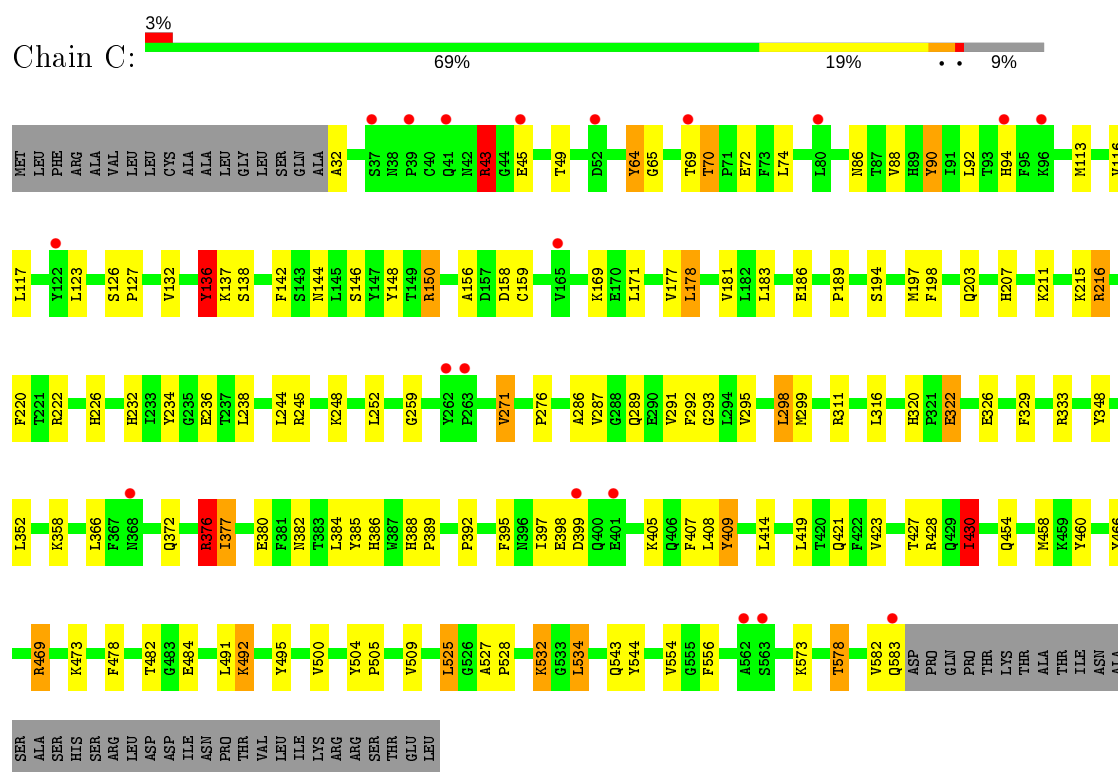


• Molecule 1: Prostaglandin G/H synthase 2

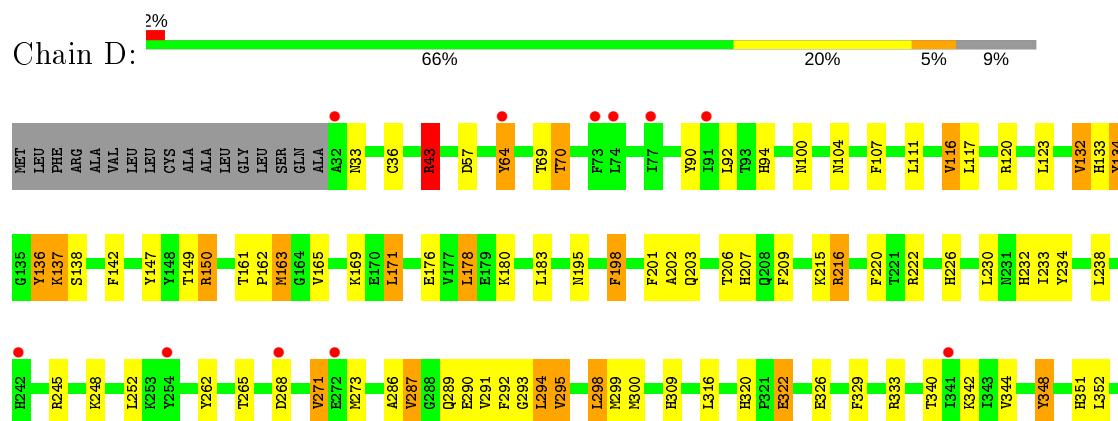


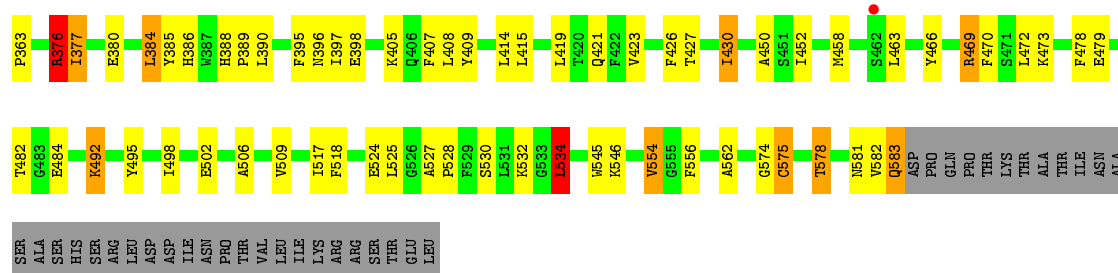


• Molecule 1: Prostaglandin G/H synthase 2



• Molecule 1: Prostaglandin G/H synthase 2





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50%  50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	181.63 Å 135.70 Å 125.15 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 2.81 49.86 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.86-2.81) 98.5 (49.86-2.81)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.240 , 0.290 0.240 , 0.289	Depositor DCC
R_{free} test set	3752 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18554	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6881e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, BOG, DF0, NAG

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	0.74	3/4601 (0.1%)	0.82	7/6239 (0.1%)
1	B	0.76	5/4601 (0.1%)	0.81	4/6239 (0.1%)
1	C	0.74	3/4601 (0.1%)	0.82	4/6239 (0.1%)
1	D	0.85	16/4601 (0.3%)	0.83	7/6239 (0.1%)
All	All	0.77	27/18404 (0.1%)	0.82	22/24956 (0.1%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	147	TYR	CE1-CZ	-11.20	1.24	1.38
1	D	348	TYR	CE1-CZ	-10.52	1.24	1.38
1	D	348	TYR	CG-CD2	-9.67	1.26	1.39
1	D	147	TYR	CG-CD2	-9.19	1.27	1.39
1	D	147	TYR	CG-CD1	-9.03	1.27	1.39

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	43	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	C	43	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	467	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	534	LEU	CA-CB-CG	6.15	129.45	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4474	0	4375	105	0
1	B	4474	0	4375	134	0
1	C	4474	0	4376	114	0
1	D	4474	0	4375	134	0
2	E	28	0	25	1	0
2	F	28	0	25	4	0
2	G	28	0	25	11	0
2	H	28	0	25	2	0
3	A	40	0	56	2	0
3	B	20	0	28	0	0
3	C	40	0	56	1	0
3	D	20	0	28	0	0
4	A	43	0	30	2	0
4	B	43	0	30	2	0
4	C	43	0	30	1	0
4	D	43	0	30	3	0
5	A	17	0	10	1	0
5	B	17	0	10	1	0
5	C	17	0	10	1	0
5	D	17	0	10	1	0
6	A	63	0	0	24	0
6	B	39	0	0	11	0
6	C	37	0	0	9	0
6	D	47	0	0	17	0
All	All	18554	0	17929	493	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 14.

The worst 5 of 493 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)
1:D:294:LEU:CD2	1:D:295:VAL:CG2	1.79	1.57
1:C:144:ASN:HD21	2:G:1:NAG:C1	0.90	1.55
1:D:294:LEU:HD23	1:D:295:VAL:CG2	1.15	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:LEU:CD2	1:D:295:VAL:HG22	1.39	1.47
3:A:701:BOG:H8'1	6:A:831:HOH:O	1.27	1.32

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/604 (91%)	527 (96%)	23 (4%)	0	100	100
1	B	550/604 (91%)	526 (96%)	24 (4%)	0	100	100
1	C	550/604 (91%)	523 (95%)	26 (5%)	1 (0%)	47	76
1	D	550/604 (91%)	524 (95%)	26 (5%)	0	100	100
All	All	2200/2416 (91%)	2100 (96%)	99 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	397	ILE

5.3.2 Protein sidechains [i](#)

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	493/537 (92%)	442 (90%)	51 (10%)	7	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	493/537 (92%)	443 (90%)	50 (10%)	7	21
1	C	493/537 (92%)	440 (89%)	53 (11%)	6	19
1	D	493/537 (92%)	443 (90%)	50 (10%)	7	21
All	All	1972/2148 (92%)	1768 (90%)	204 (10%)	7	21

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	532	LYS
1	C	169	LYS
1	D	385	TYR
1	B	554	VAL
1	C	64	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	86	ASN
1	C	144	ASN
1	C	445	GLN
1	B	583	GLN
1	D	86	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	1,2	14,14,15	0.93	1 (7%)	17,19,21	1.76	5 (29%)
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.61	0
2	NAG	F	1	1,2	14,14,15	0.68	0	17,19,21	1.50	2 (11%)
2	NAG	F	2	2	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	G	1	1,2	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.61	0
2	NAG	H	1	1,2	14,14,15	0.62	0	17,19,21	1.33	2 (11%)
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.62	0

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
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	-2.92	1.39	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	O5-C5-C6	4.15	113.71	107.20
2	H	1	NAG	C1-O5-C5	3.90	117.48	112.19
2	E	1	NAG	C1-C2-N2	-3.83	103.95	110.49
2	E	1	NAG	C1-O5-C5	3.46	116.88	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	C1-C2-N2	-2.59	106.06	110.49

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

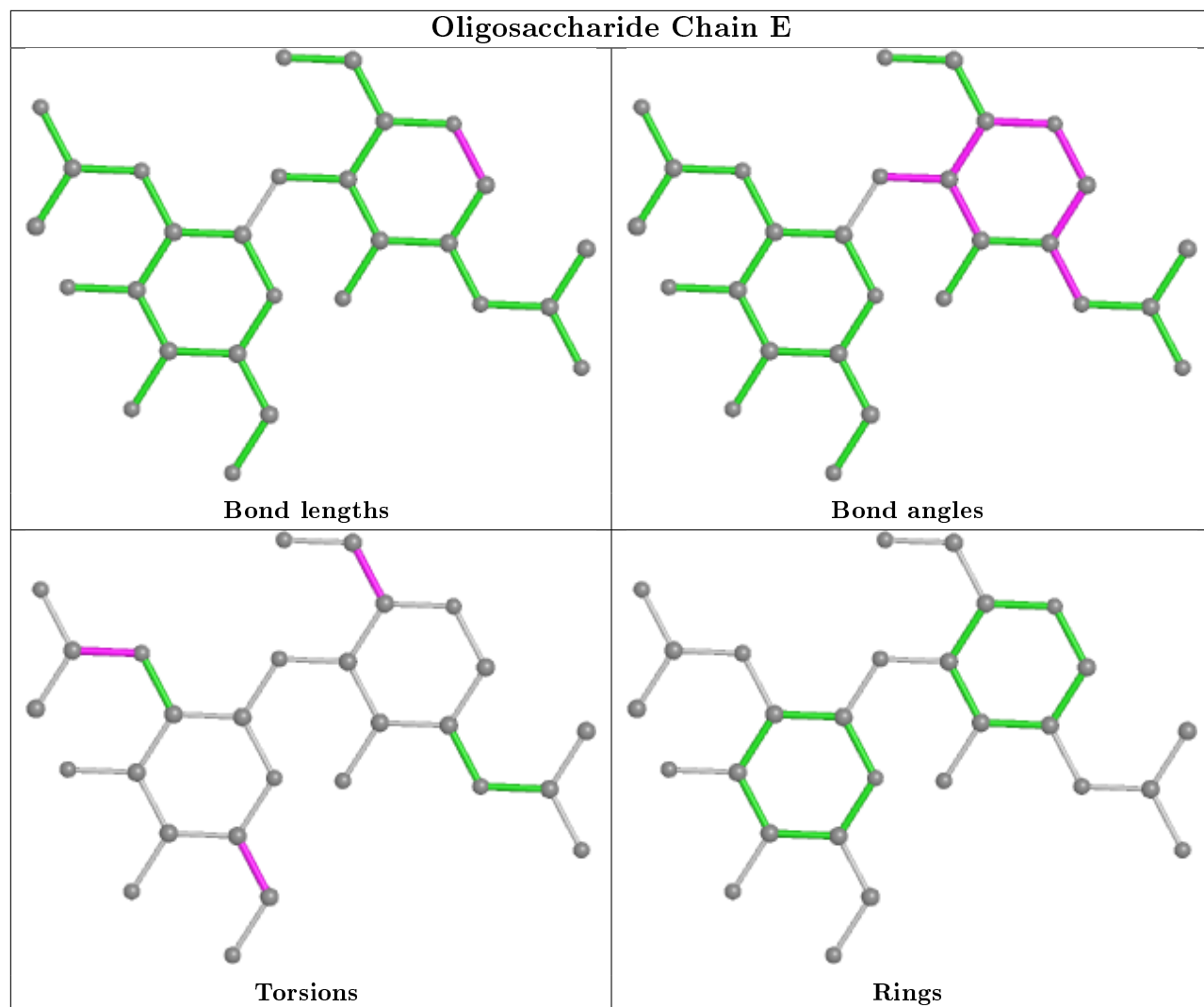
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6

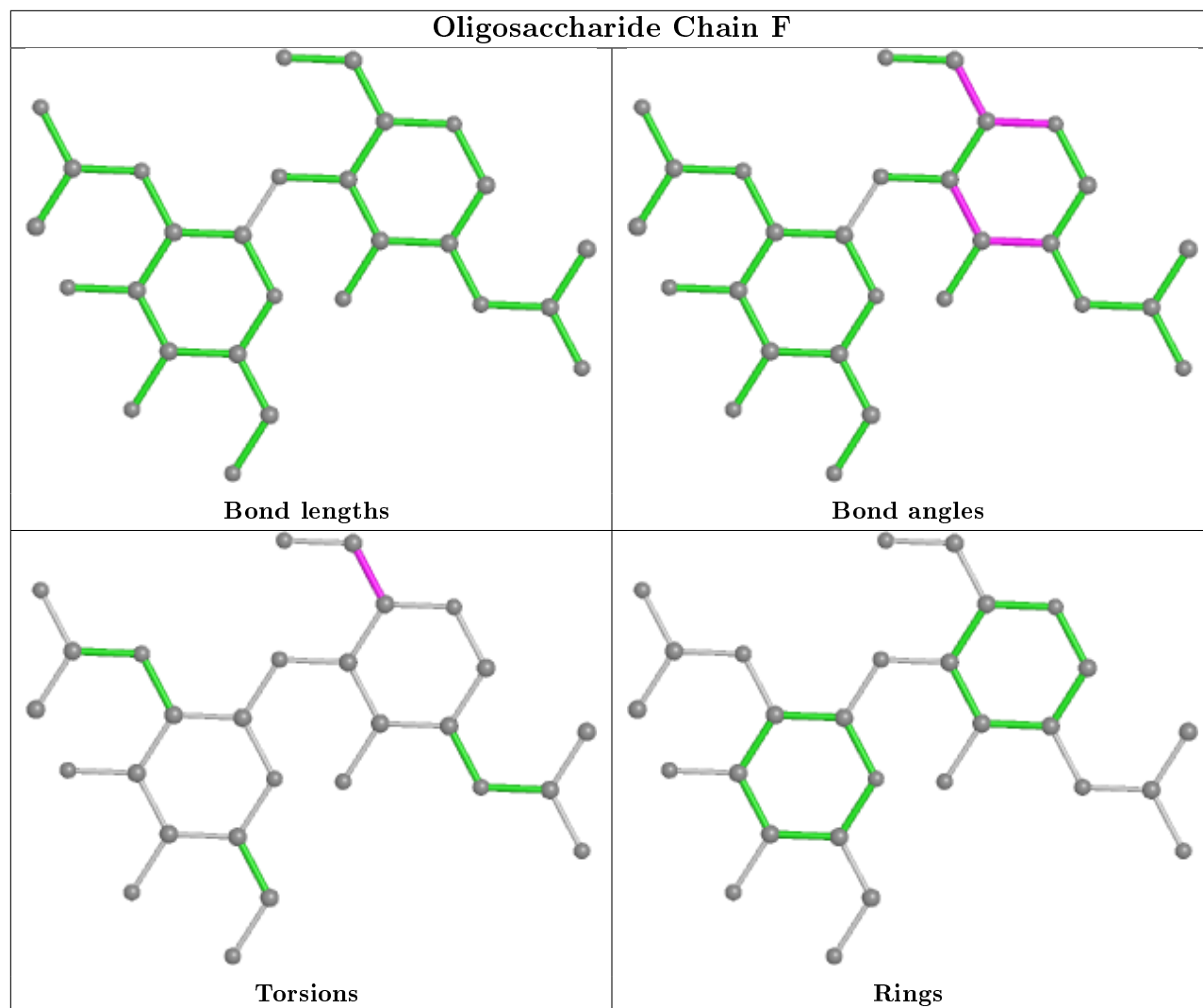
There are no ring outliers.

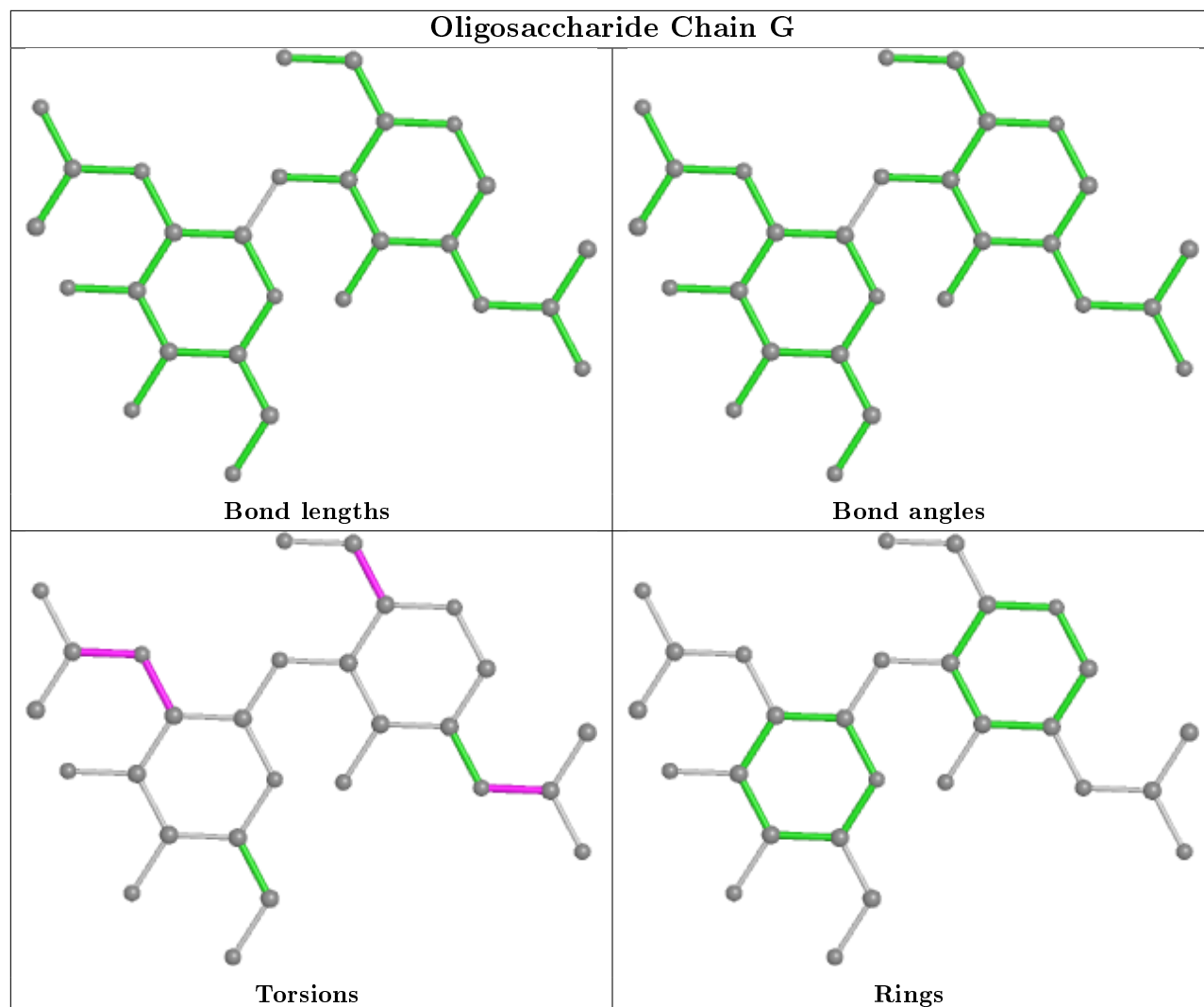
6 monomers are involved in 18 short contacts:

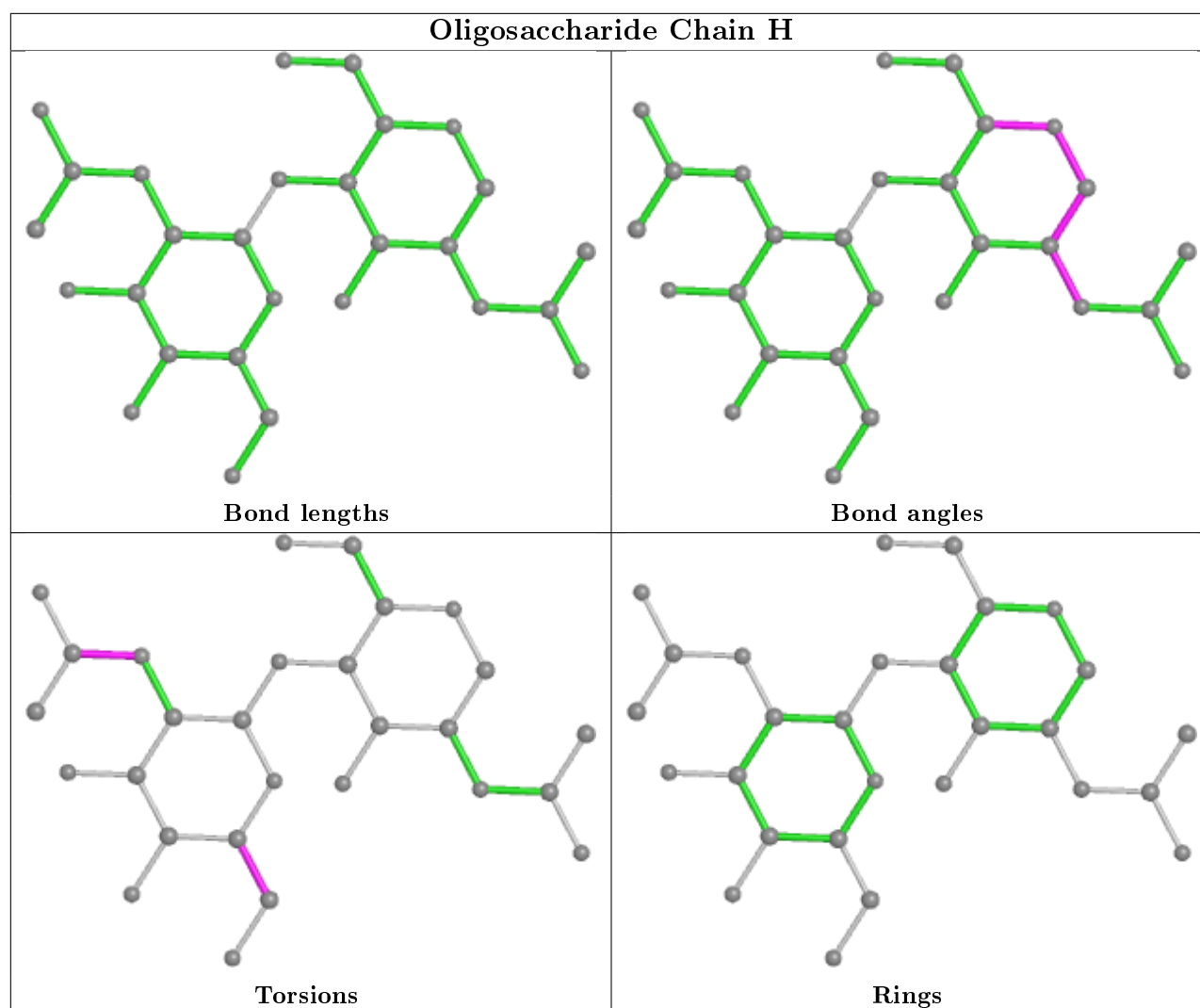
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
2	G	1	NAG	2	0
2	F	2	NAG	4	0
2	H	2	NAG	2	0
2	F	1	NAG	1	0
2	G	2	NAG	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BOG	A	701	-	20,20,20	0.39	0	25,25,25	2.13	6 (24%)
5	DF0	A	706	-	15,18,18	1.67	1 (6%)	20,24,24	1.44	3 (15%)
3	BOG	B	701	-	20,20,20	0.58	0	25,25,25	1.59	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	A	705	1	27,50,50	2.46	9 (33%)	17,82,82	3.00	6 (35%)
5	DF0	B	705	-	15,18,18	1.84	1 (6%)	20,24,24	1.15	2 (10%)
4	HEM	C	705	1	27,50,50	2.34	8 (29%)	17,82,82	3.44	7 (41%)
5	DF0	D	705	-	15,18,18	1.85	1 (6%)	20,24,24	1.09	1 (5%)
3	BOG	D	701	-	20,20,20	0.47	0	25,25,25	0.59	0
3	BOG	A	702	-	20,20,20	0.49	0	25,25,25	1.23	4 (16%)
3	BOG	C	702	-	20,20,20	0.75	1 (5%)	25,25,25	1.63	5 (20%)
4	HEM	B	704	1	27,50,50	2.48	9 (33%)	17,82,82	3.16	9 (52%)
4	HEM	D	704	1	27,50,50	2.44	9 (33%)	17,82,82	2.91	6 (35%)
5	DF0	C	706	-	15,18,18	1.52	1 (6%)	20,24,24	1.12	2 (10%)
3	BOG	C	701	-	20,20,20	0.46	0	25,25,25	0.59	0

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
3	BOG	A	701	-	-	8/11/31/31	0/1/1/1
5	DF0	A	706	-	-	0/6/8/8	0/2/2/2
3	BOG	B	701	-	-	7/11/31/31	0/1/1/1
4	HEM	A	705	1	-	0/6/54/54	-
5	DF0	B	705	-	-	0/6/8/8	0/2/2/2
4	HEM	C	705	1	-	3/6/54/54	-
5	DF0	D	705	-	-	0/6/8/8	0/2/2/2
3	BOG	D	701	-	-	7/11/31/31	0/1/1/1
3	BOG	A	702	-	-	6/11/31/31	0/1/1/1
3	BOG	C	702	-	-	4/11/31/31	0/1/1/1
4	HEM	B	704	1	-	3/6/54/54	-
4	HEM	D	704	1	-	0/6/54/54	-
5	DF0	C	706	-	-	0/6/8/8	0/2/2/2
3	BOG	C	701	-	-	9/11/31/31	0/1/1/1

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	705	DF0	C1-C	6.58	1.48	1.39
5	D	705	DF0	C1-C	6.56	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	704	HEM	C1A-NA	6.20	1.48	1.36
5	A	706	DF0	C1-C	6.13	1.47	1.39
4	C	705	HEM	C4A-NA	6.07	1.48	1.36

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	705	HEM	C1D-C2D-C3D	-9.49	100.39	107.00
4	B	704	HEM	C1D-C2D-C3D	-9.37	100.47	107.00
4	A	705	HEM	C1D-C2D-C3D	-8.49	101.09	107.00
4	D	704	HEM	C1D-C2D-C3D	-8.00	101.43	107.00
3	A	701	BOG	O1-C1-C2	-6.62	97.97	108.30

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	BOG	C2-C1-O1-C1'
3	A	701	BOG	O5-C1-O1-C1'
3	B	701	BOG	C2-C1-O1-C1'
3	B	701	BOG	O5-C1-O1-C1'
4	C	705	HEM	C1A-C2A-CAA-CBA

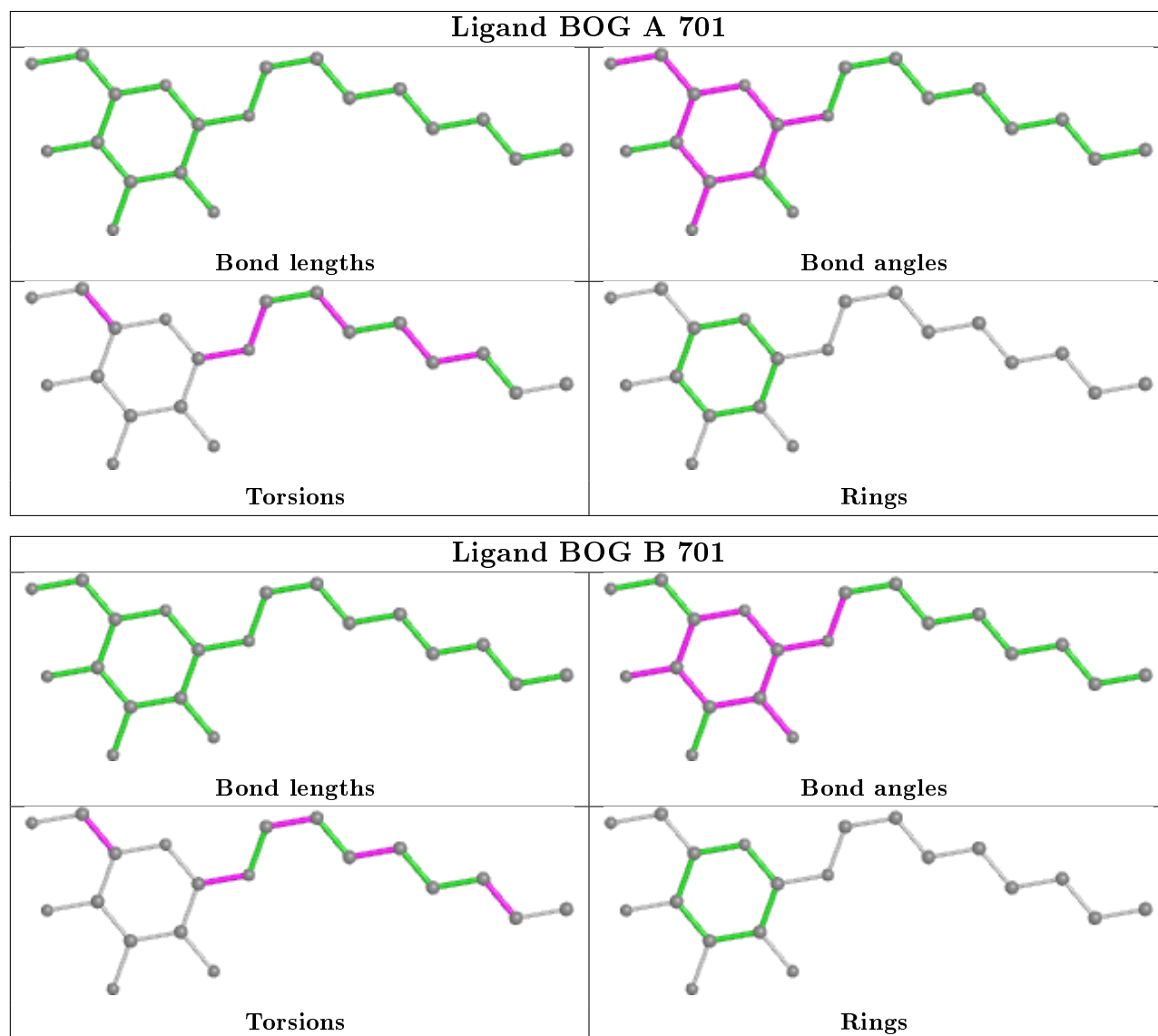
There are no ring outliers.

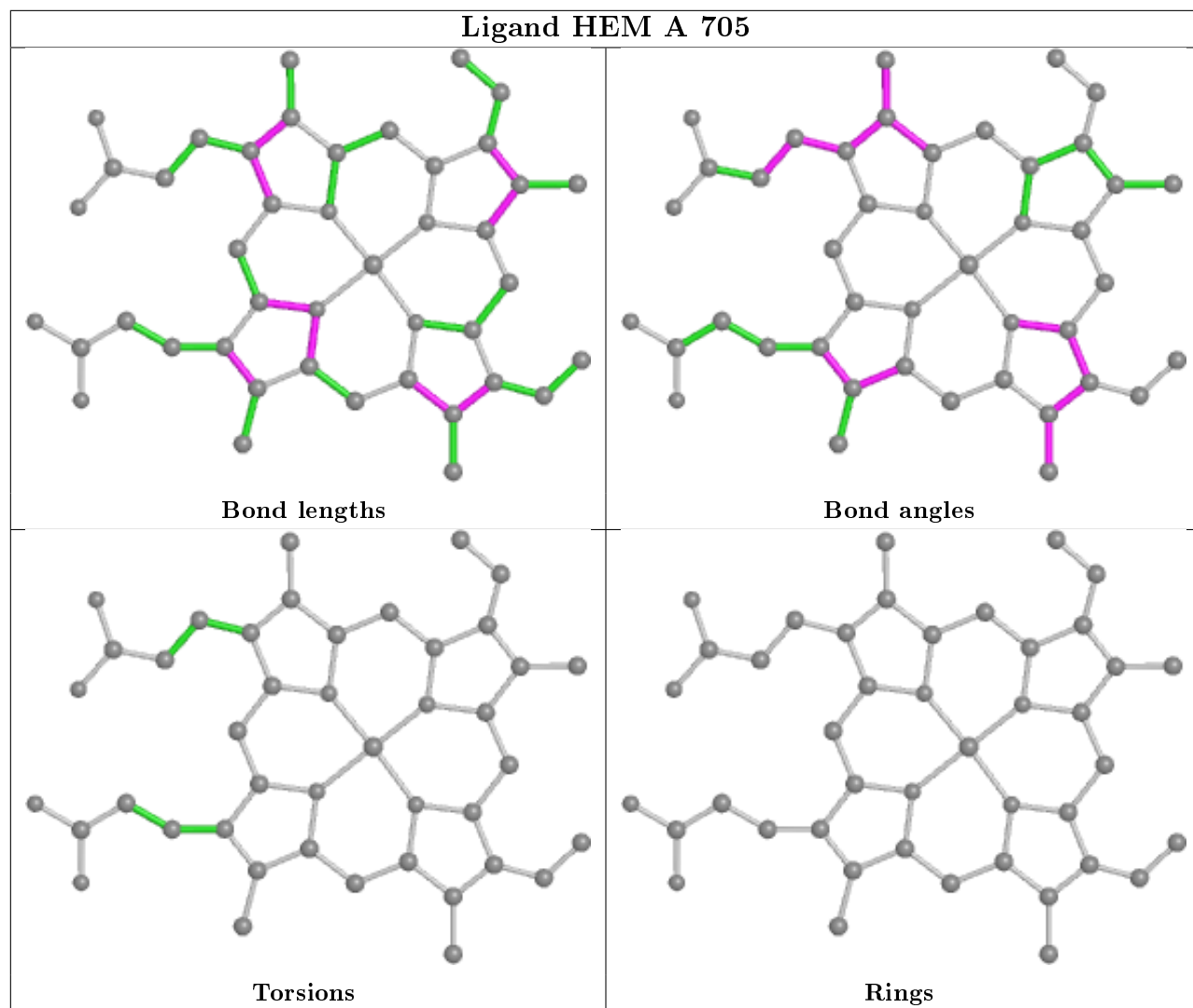
10 monomers are involved in 15 short contacts:

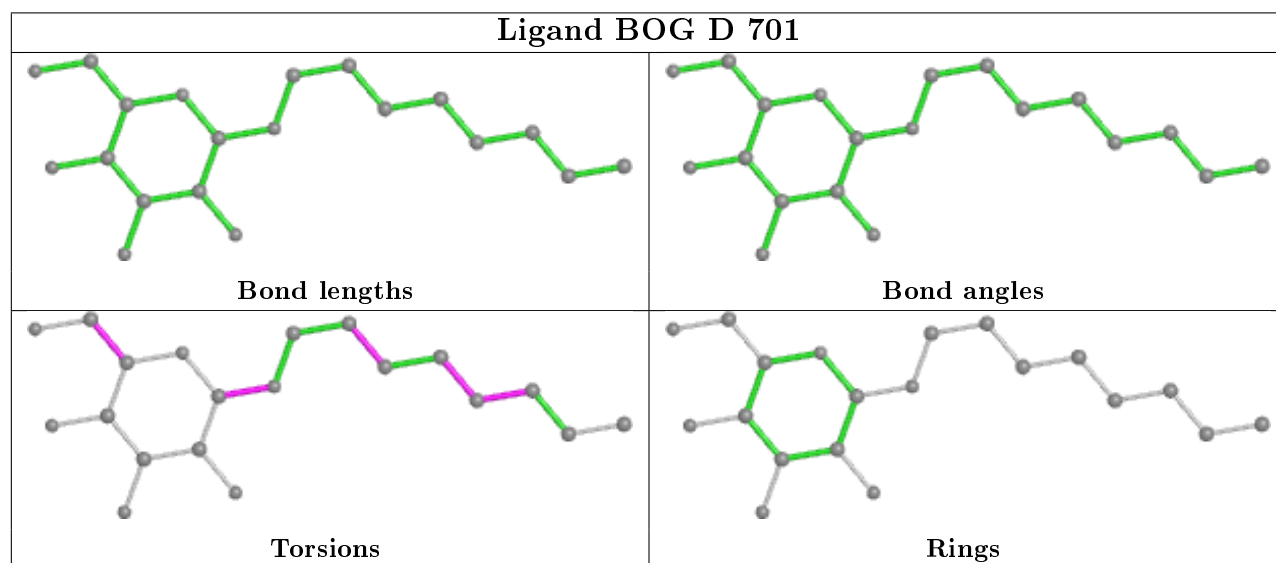
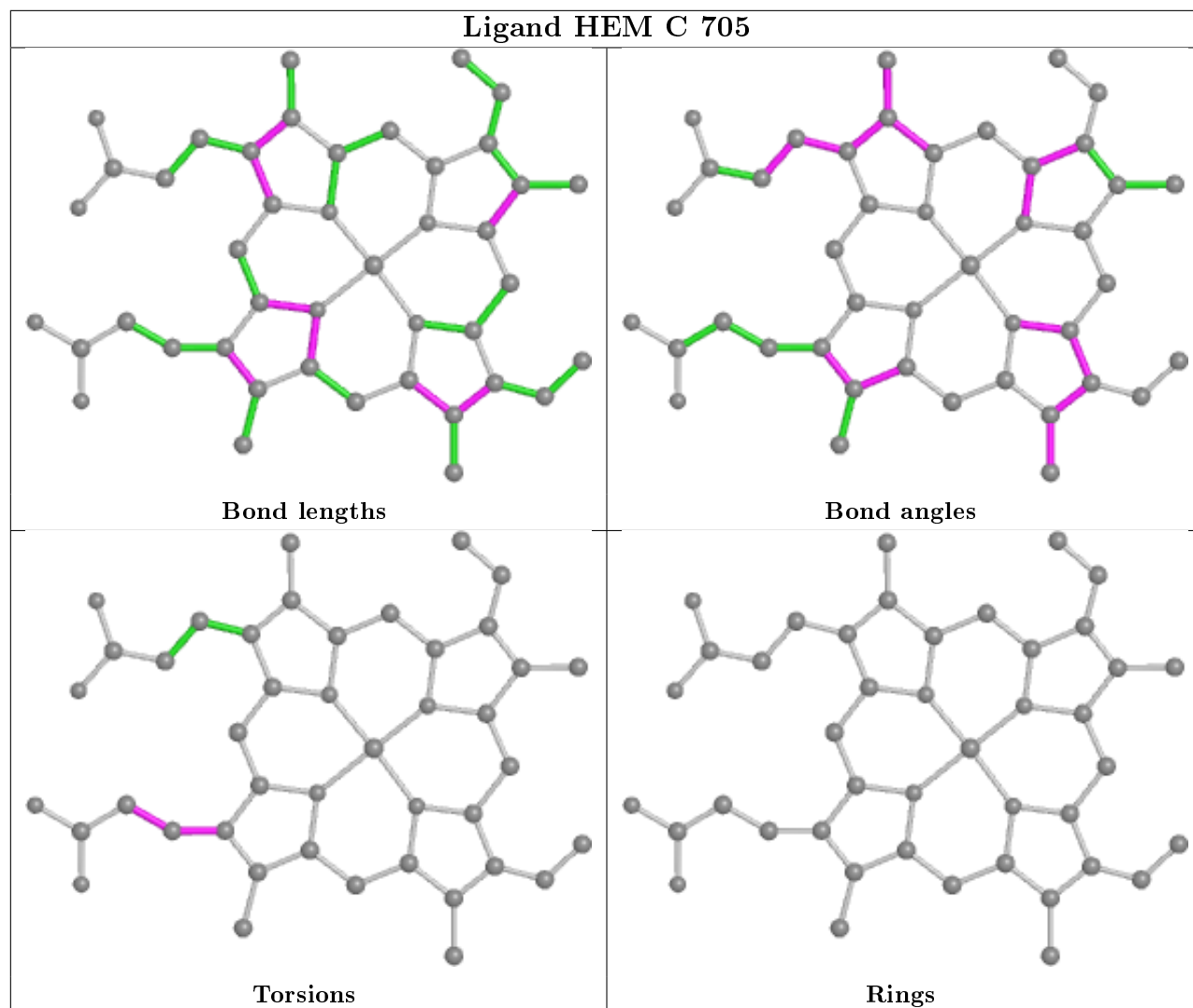
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	BOG	2	0
5	A	706	DF0	1	0
4	A	705	HEM	2	0
5	B	705	DF0	1	0
4	C	705	HEM	1	0
5	D	705	DF0	1	0
3	C	702	BOG	1	0
4	B	704	HEM	2	0
4	D	704	HEM	3	0
5	C	706	DF0	1	0

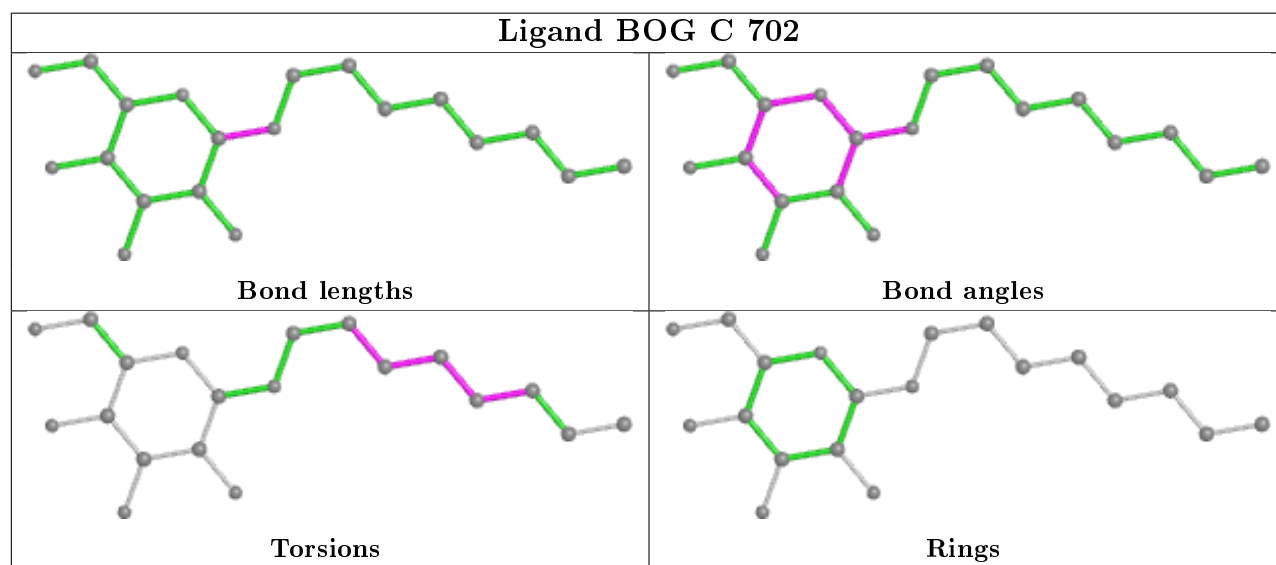
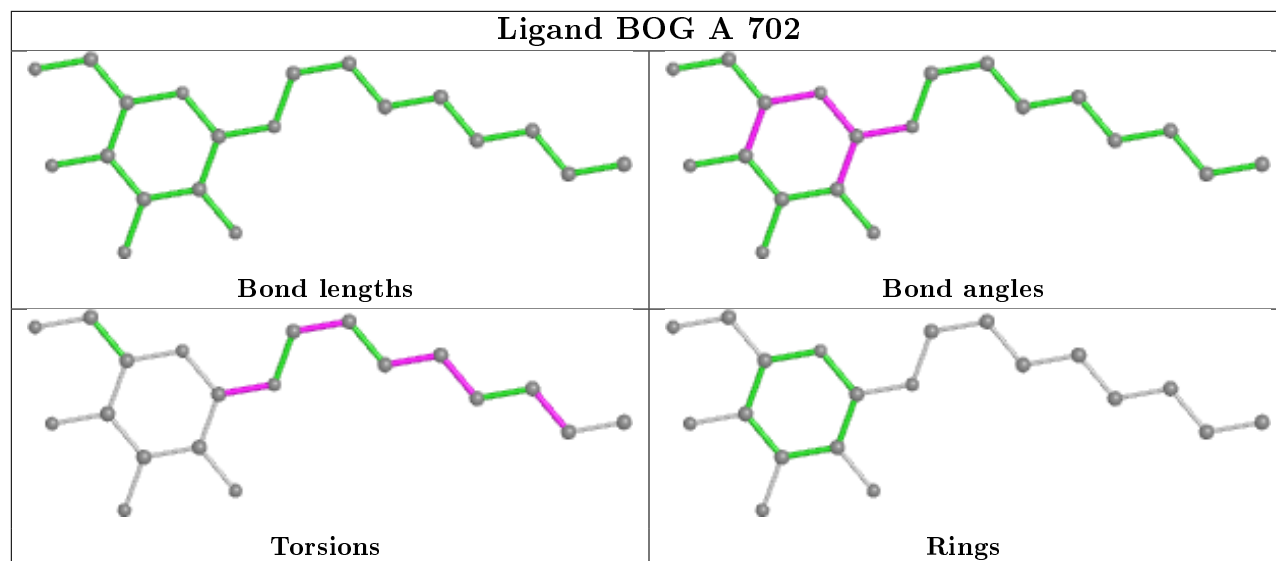
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

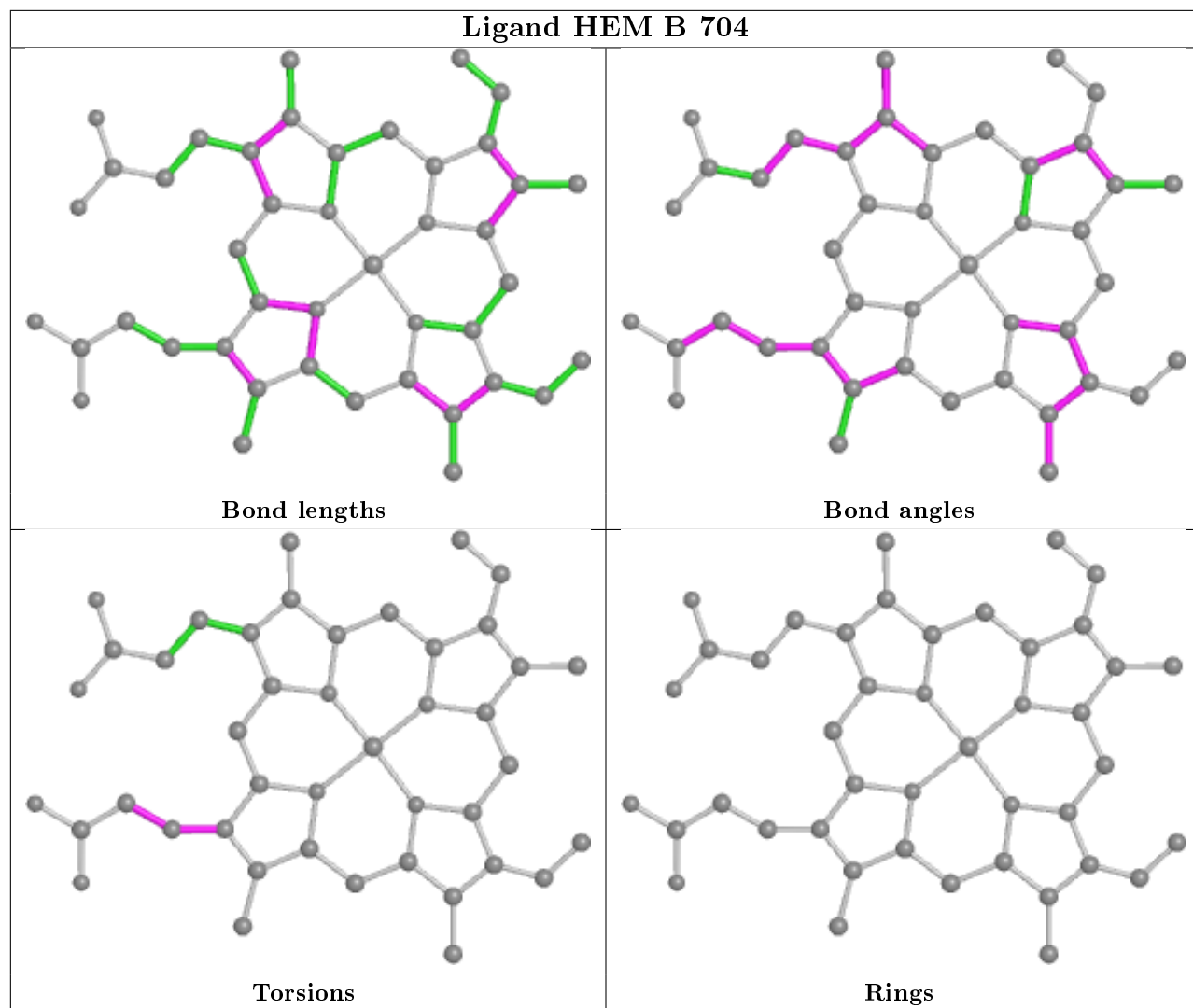
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

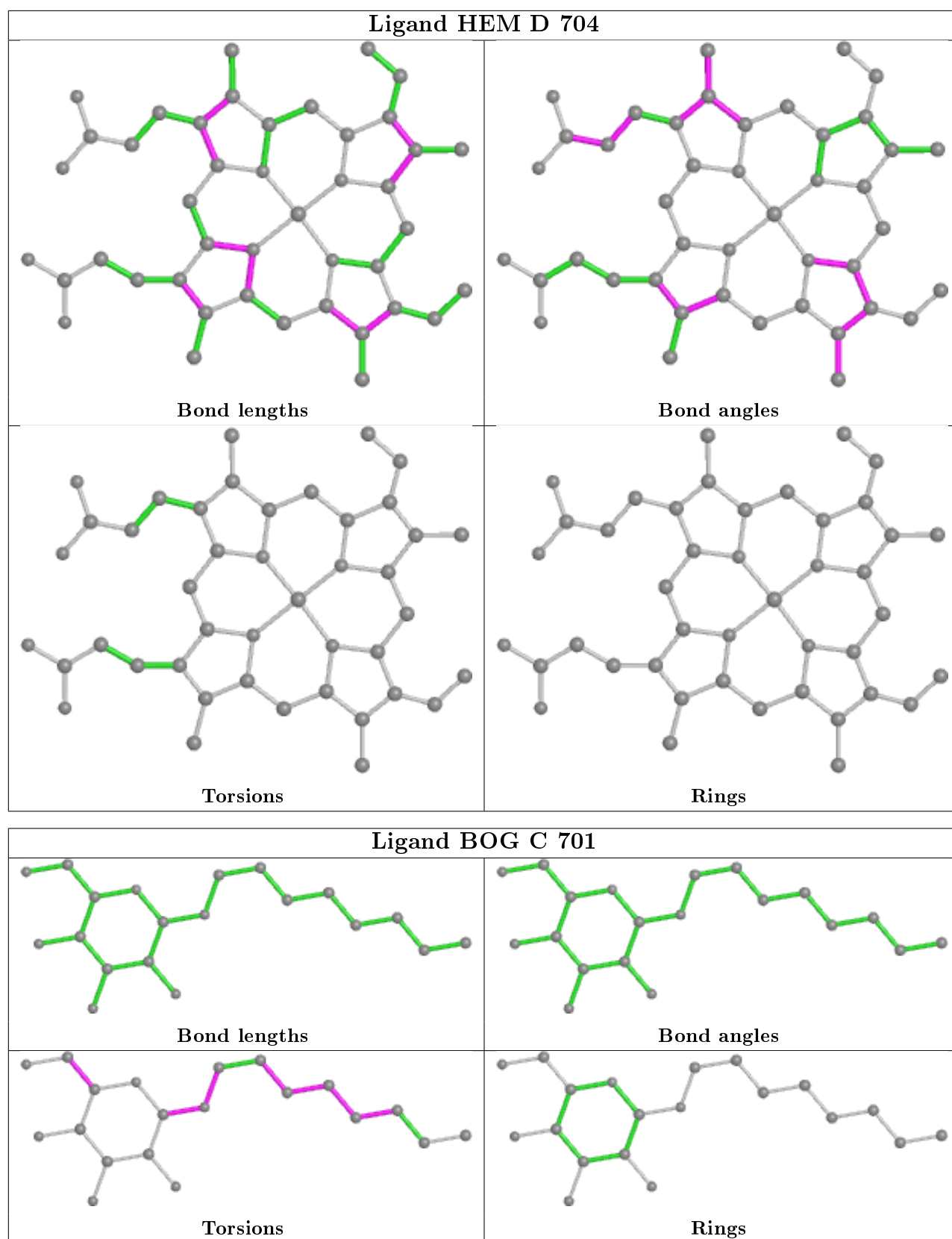












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	552/604 (91%)	-0.10	13 (2%) 59 49	24, 44, 67, 110	0
1	B	552/604 (91%)	0.00	22 (3%) 38 28	27, 43, 68, 90	0
1	C	552/604 (91%)	-0.15	19 (3%) 45 35	26, 43, 66, 110	0
1	D	552/604 (91%)	-0.13	12 (2%) 62 52	24, 42, 67, 101	0
All	All	2208/2416 (91%)	-0.09	66 (2%) 50 40	24, 43, 67, 110	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	583	GLN	6.3
1	B	52	ASP	5.2
1	C	583	GLN	5.1
1	D	242	HIS	4.5
1	C	399	ASP	4.3

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

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

6.3 Carbohydrates [i](#)

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

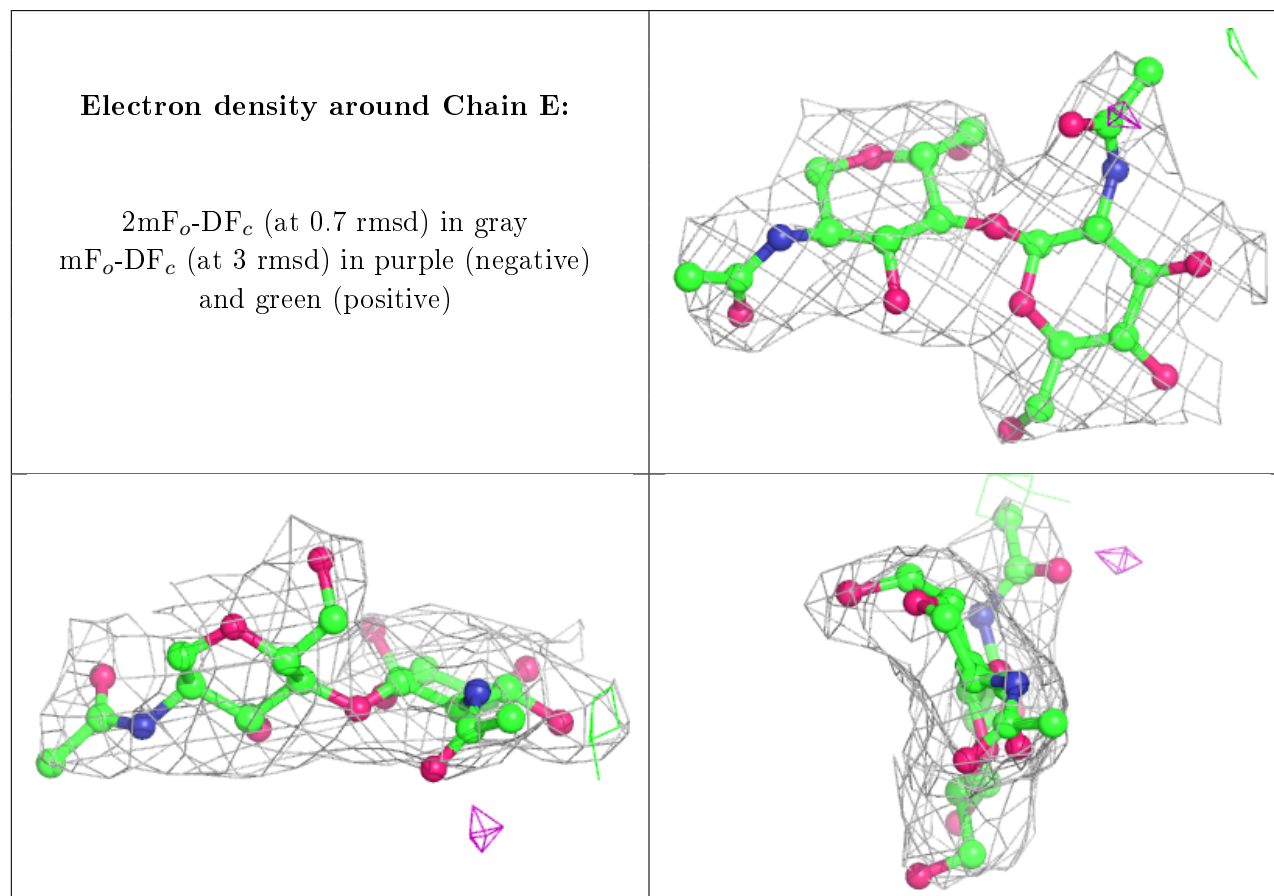
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	2	14/15	0.85	0.21	38,43,47,48	0
2	NAG	G	2	14/15	0.89	0.14	47,57,64,65	0

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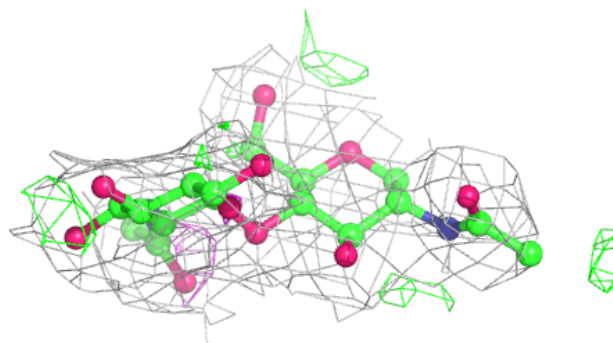
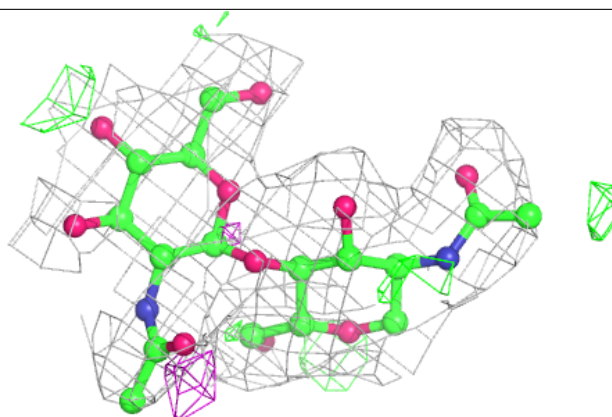
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	E	2	14/15	0.90	0.20	62,71,78,82	0
2	NAG	F	1	14/15	0.91	0.14	34,38,40,43	0
2	NAG	H	2	14/15	0.91	0.14	50,59,63,64	0
2	NAG	H	1	14/15	0.92	0.14	32,38,41,41	0
2	NAG	E	1	14/15	0.94	0.15	36,39,44,47	0
2	NAG	G	1	14/15	0.94	0.16	28,35,37,39	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

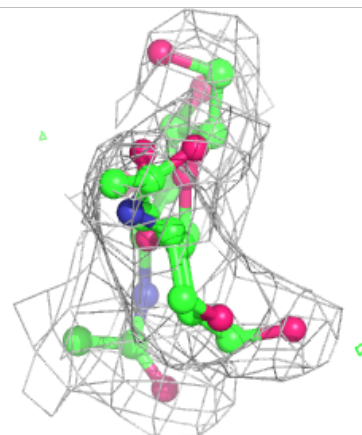
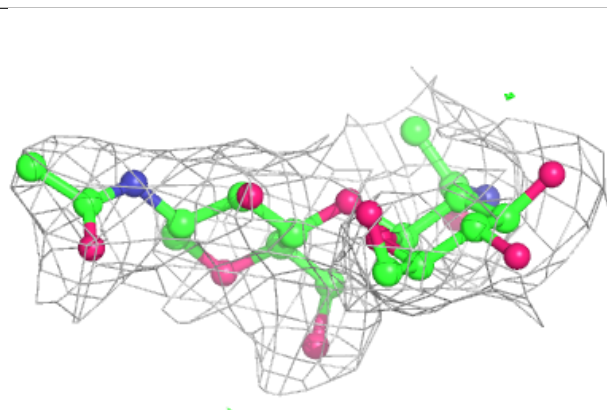
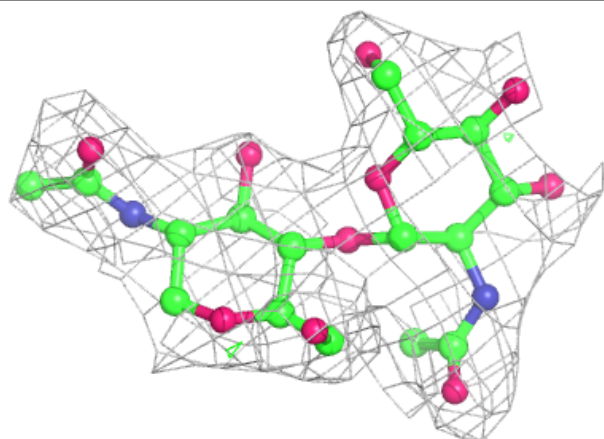


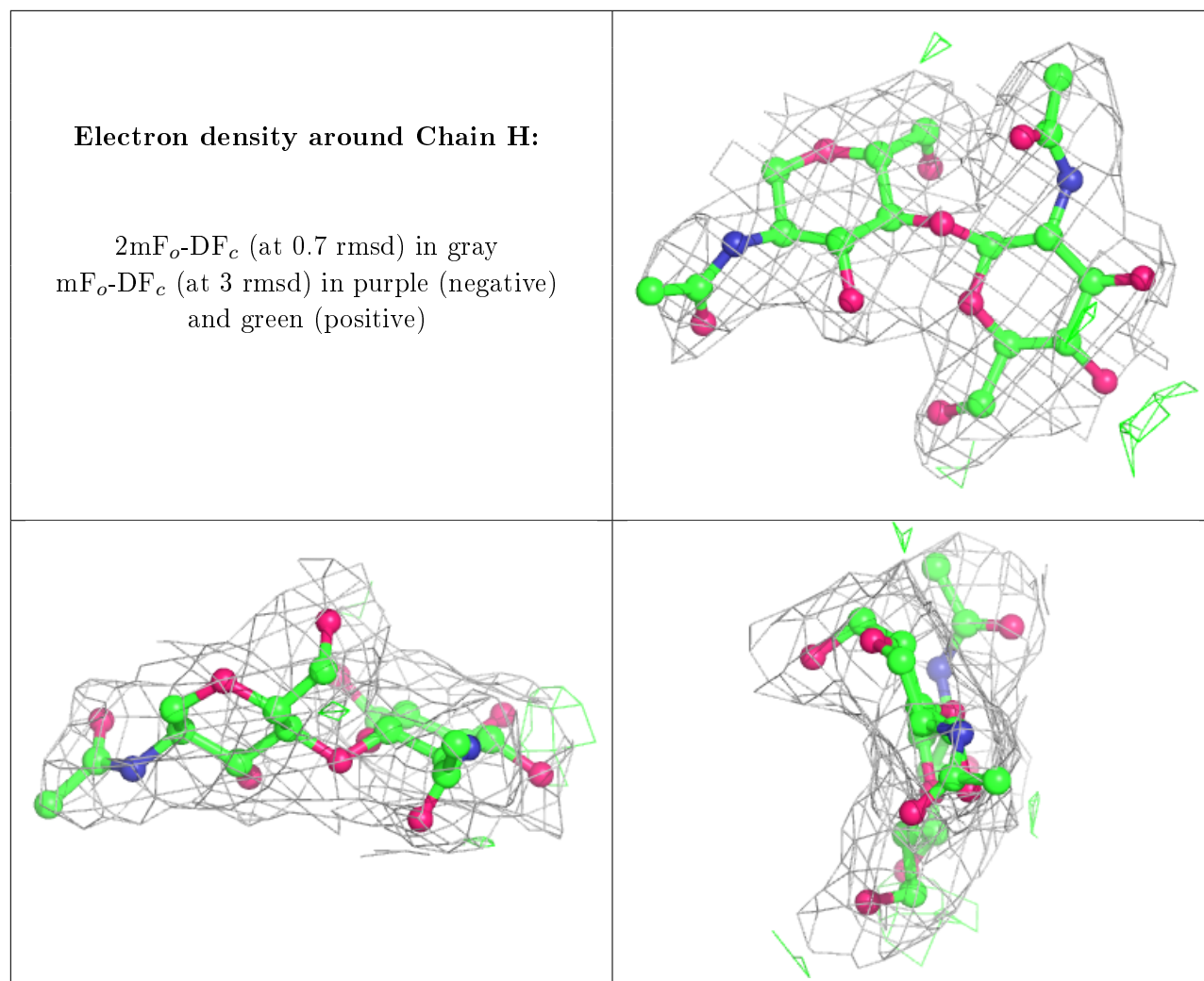
Electron density around Chain F:

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

**Electron density around Chain G:**

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





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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

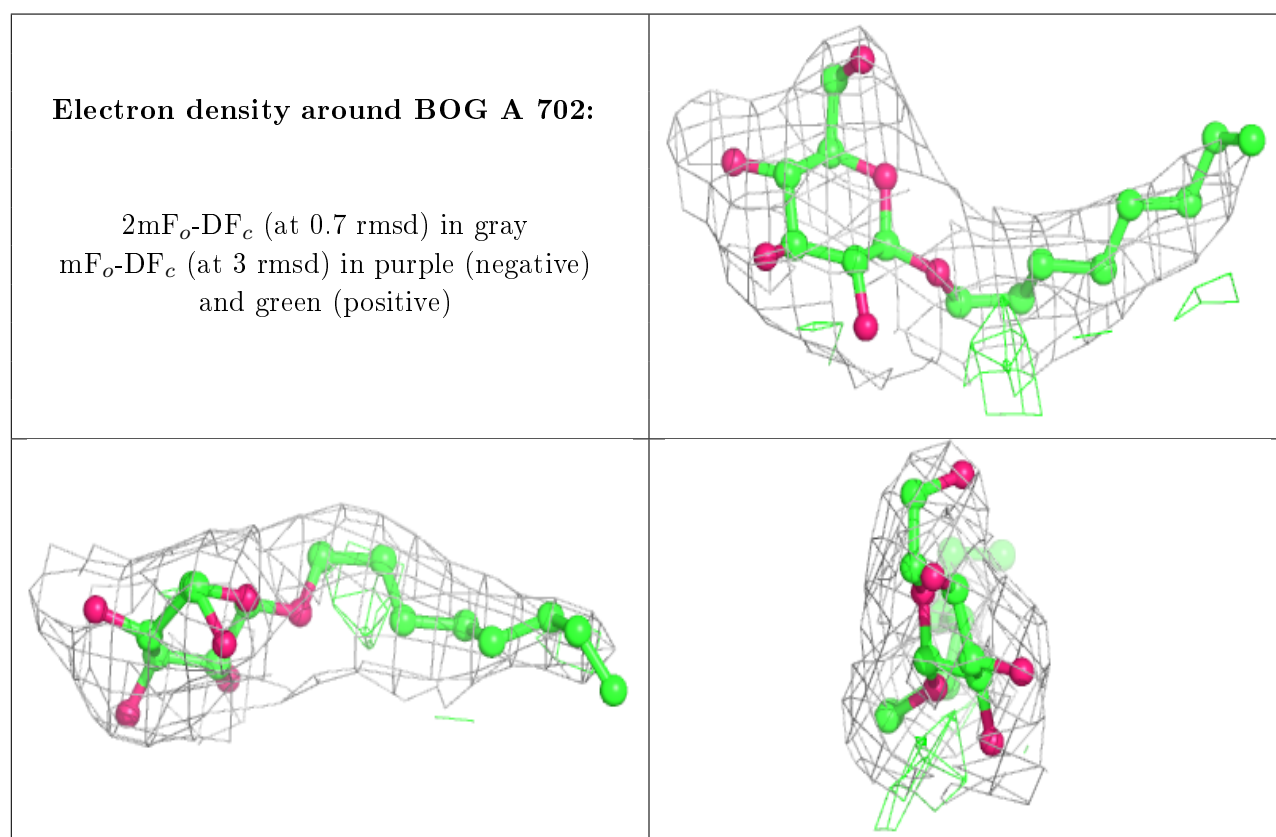
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BOG	A	702	20/20	0.81	0.26	58,66,73,74	0
5	DF0	D	705	17/17	0.86	0.26	34,37,44,45	0
3	BOG	D	701	20/20	0.90	0.21	40,45,50,50	0
3	BOG	B	701	20/20	0.90	0.20	55,61,68,69	0
3	BOG	C	702	20/20	0.90	0.30	54,62,67,69	0
3	BOG	A	701	20/20	0.91	0.19	53,58,70,70	0
3	BOG	C	701	20/20	0.91	0.23	47,53,59,62	0
5	DF0	B	705	17/17	0.92	0.19	37,46,52,53	0
5	DF0	C	706	17/17	0.93	0.27	41,43,48,48	0

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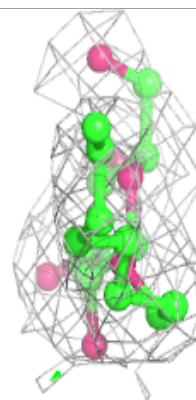
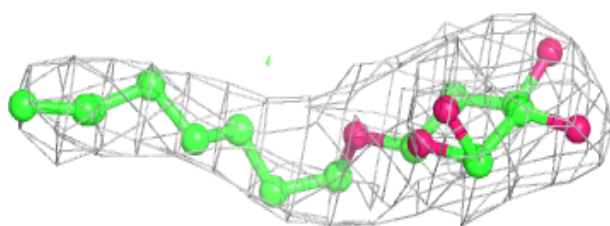
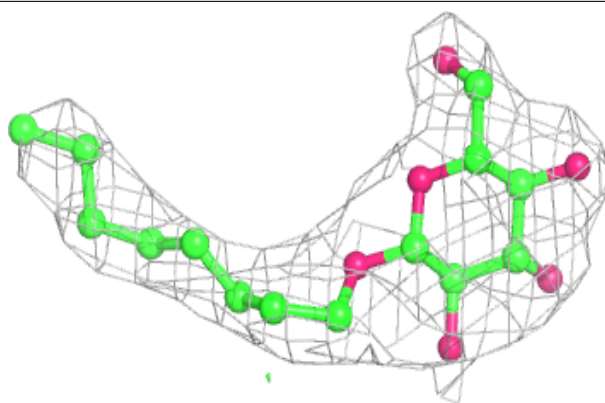
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	HEM	A	705	43/43	0.94	0.20	30,47,69,92	0
4	HEM	D	704	43/43	0.94	0.21	35,47,78,93	0
5	DF0	A	706	17/17	0.94	0.16	47,49,54,54	0
4	HEM	C	705	43/43	0.94	0.20	37,44,58,60	0
4	HEM	B	704	43/43	0.96	0.16	33,44,59,67	0

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

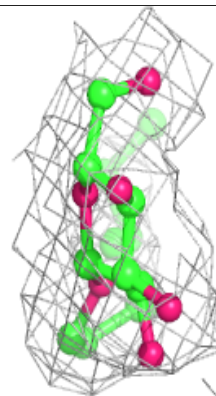
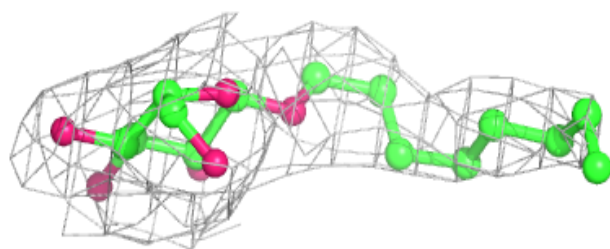
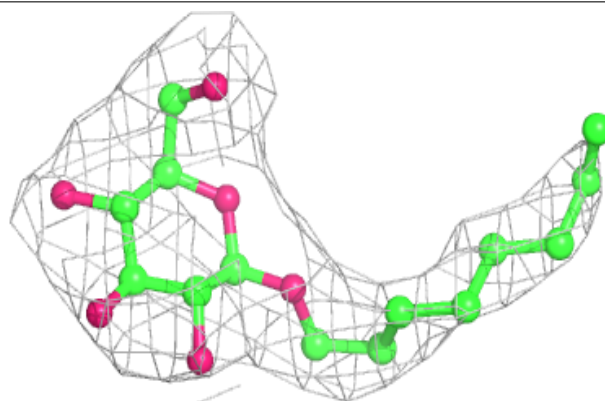


Electron density around BOG D 701:

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

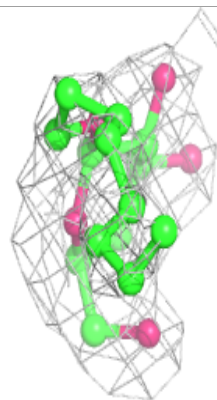
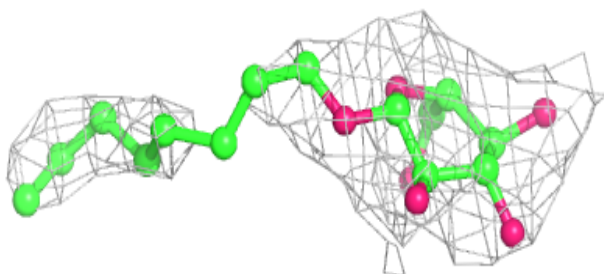
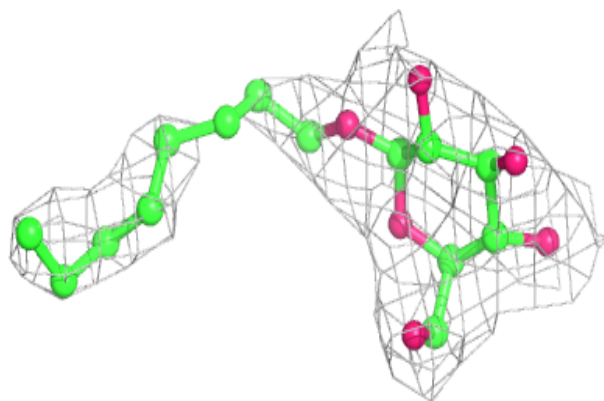
**Electron density around BOG B 701:**

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

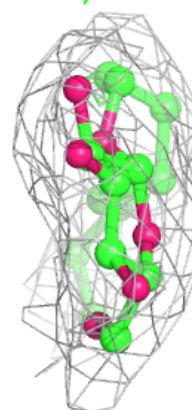
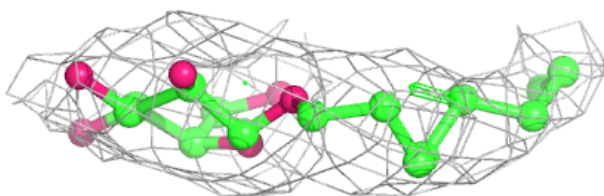
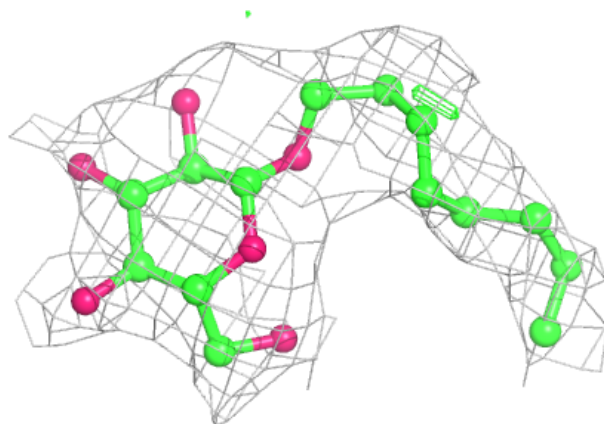


Electron density around BOG C 702:

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

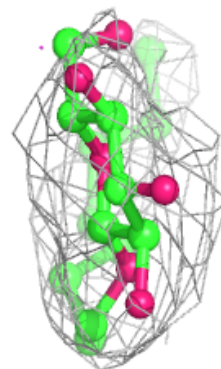
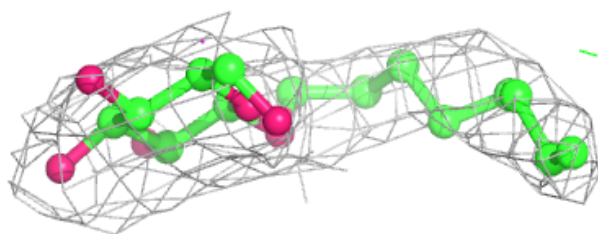
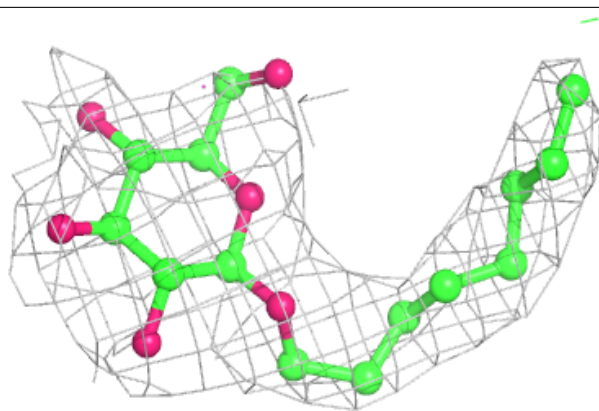
**Electron density around BOG A 701:**

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



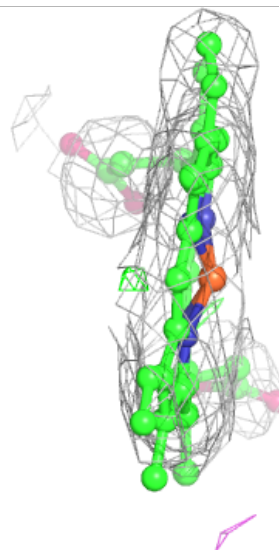
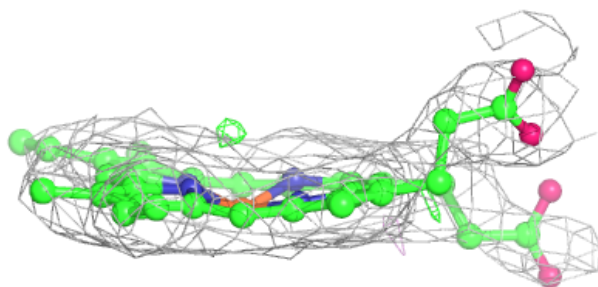
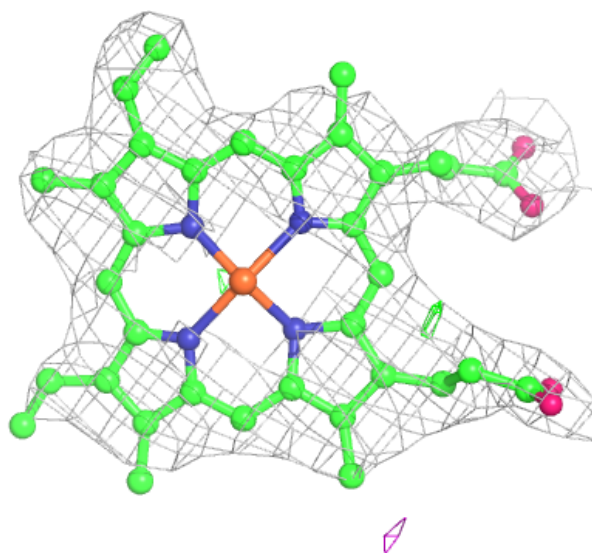
Electron density around BOG C 701:

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



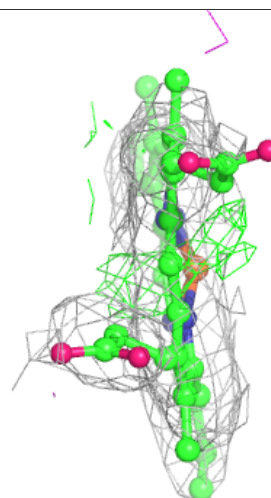
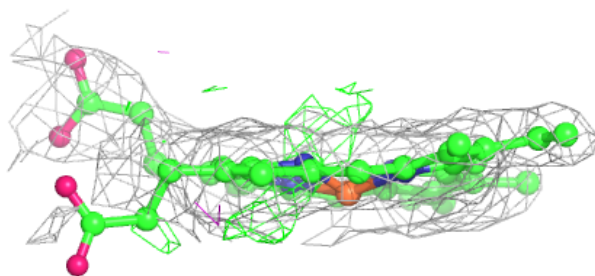
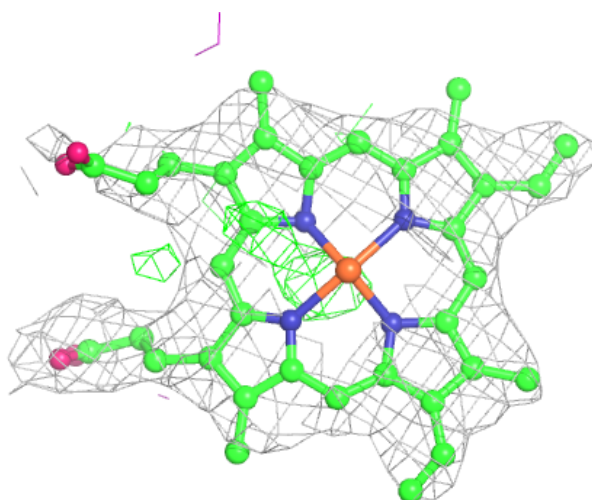
Electron density around HEM A 705:

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



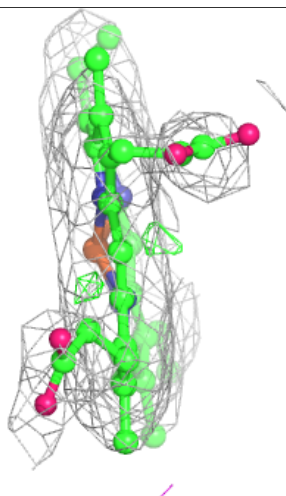
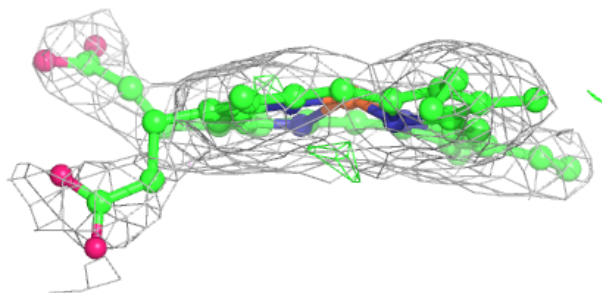
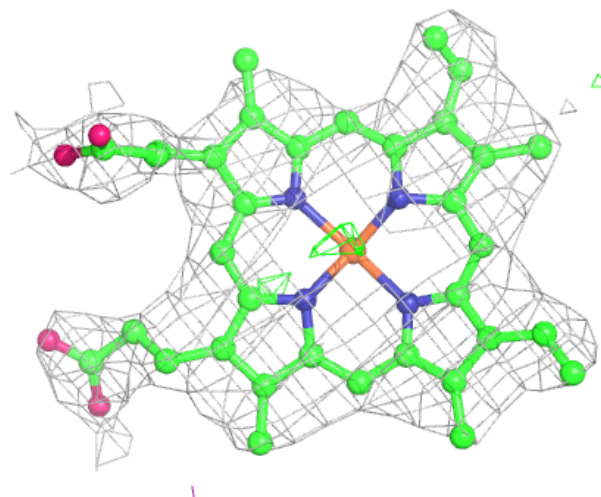
Electron density around HEM D 704:

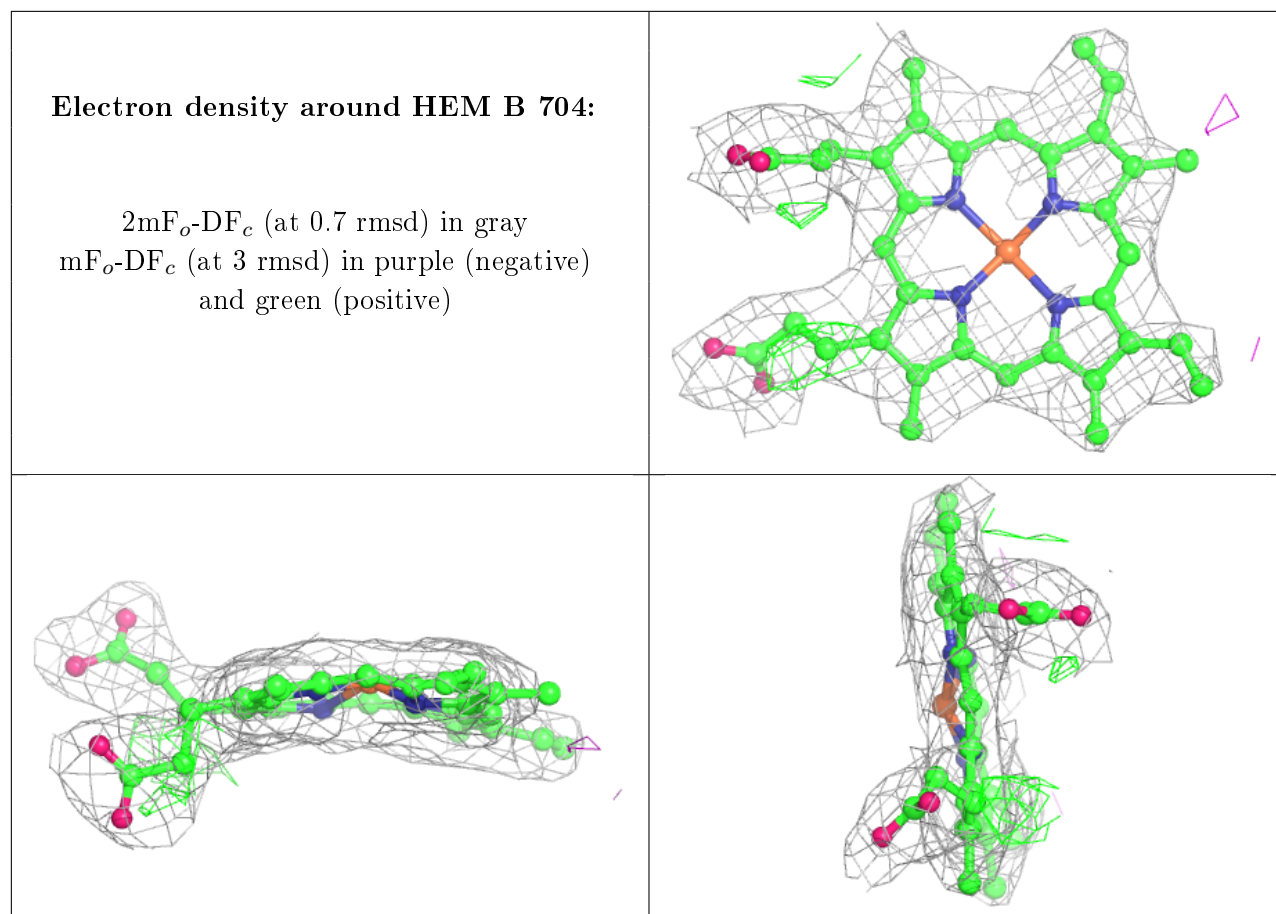
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 705:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.