



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:31 AM BST

PDB ID : 3NT1
Title : High resolution structure of naproxen:COX-2 complex.
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Marnett, L.J.
Deposited on : 2010-07-02
Resolution : 1.73 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

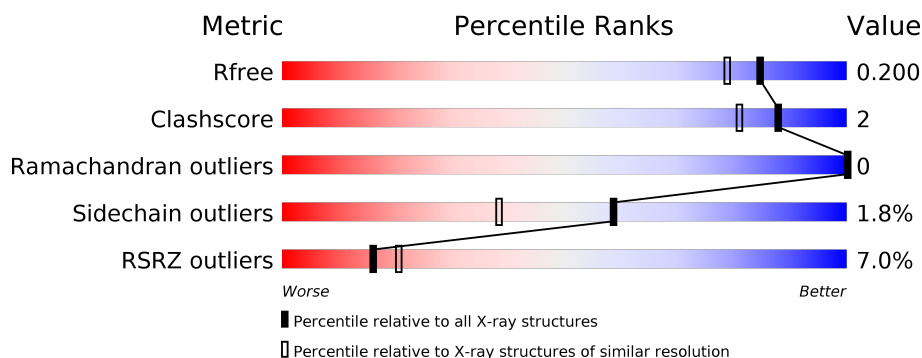
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	587	<div> <div>6%</div> <div> <div></div> <div>89%</div> <div>• 6%</div> </div> </div>
1	B	587	<div> <div>7%</div> <div> <div></div> <div>88%</div> <div>5% 6%</div> </div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	661	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10338 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-endoperoxide synthase 2.

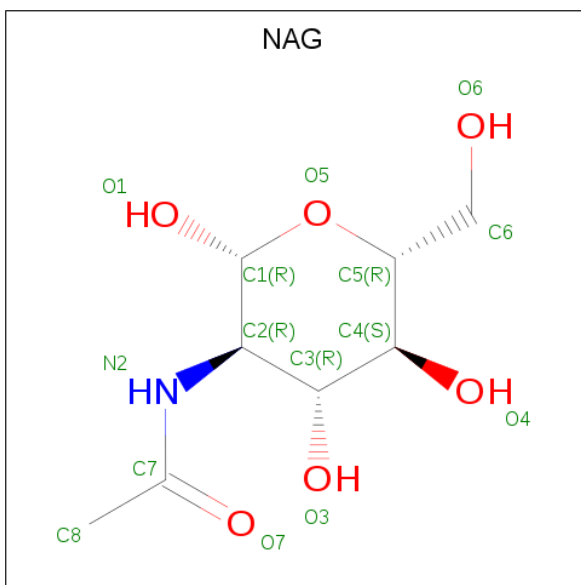
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	3	0
			4499	2899	756	819	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

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



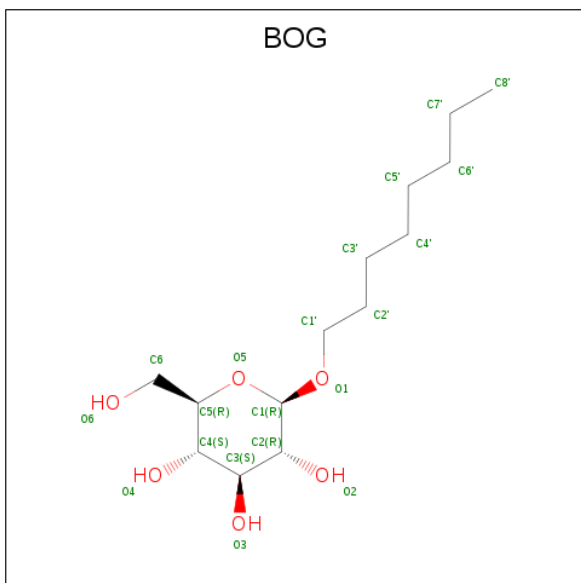
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



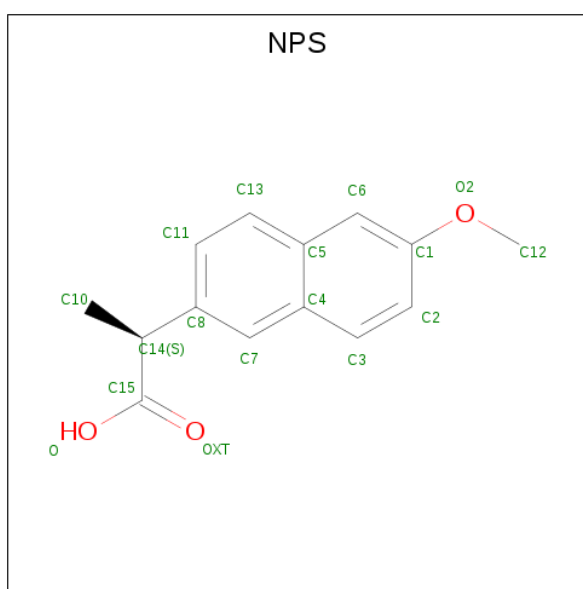
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



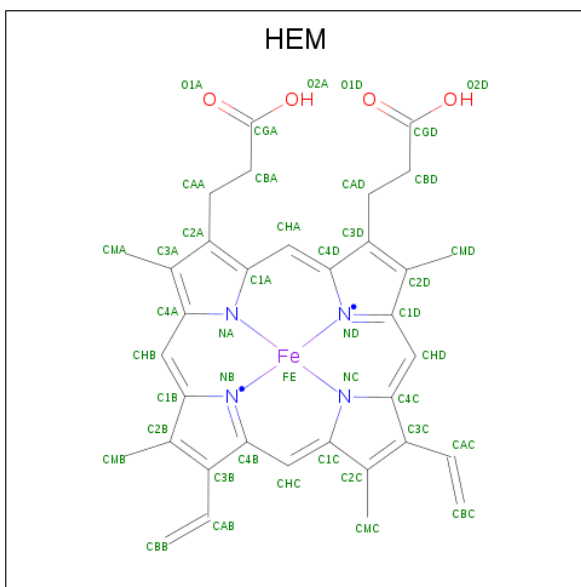
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is (2S)-2-(6-methoxynaphthalen-2-yl)propanoic acid (three-letter code: NPS) (formula: C₁₄H₁₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			17	14	3		
5	B	1	Total	C	O	0	0
			17	14	3		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Cl 1 1	0	0
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	527	Total O 527 527	0	0
8	B	524	Total O 524 524	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.30 Å 133.23 Å 181.27 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.73 28.51 – 1.73	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-1.73) 98.2 (28.51-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.73 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.167 , 0.186 0.182 , 0.200	Depositor DCC
R_{free} test set	7592 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10338	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.34	0/4629	0.51	0/6276
1	B	0.34	0/4601	0.52	0/6239
All	All	0.34	0/9230	0.51	0/12515

There are no bond length outliers.

There are no bond angle outliers.

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	4499	0	4396	17	0
1	B	4474	0	4373	18	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	60	0	84	3	0
4	B	20	0	28	0	0
5	A	17	0	13	0	0
5	B	17	0	13	0	0
6	A	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	43	0	30	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	527	0	0	0	0
8	B	524	0	0	1	0
All	All	10338	0	9069	36	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 2.

All (36) 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:A:283:LEU:HD21	1:A:415:LEU:HD12	1.48	0.95
1:A:87:ASN:HD22	4:A:620:BOG:H62	1.37	0.89
1:A:581[B]:ASN:HD22	1:A:582:VAL:N	1.88	0.72
1:A:283:LEU:CD2	1:A:415:LEU:HD12	2.21	0.69
1:B:382:ASN:HD21	6:B:619:HEM:HAD2	1.57	0.68
1:A:271:VAL:HG22	1:A:286:ALA:HB1	1.78	0.65
1:B:81:LEU:HD22	1:B:82:LEU:HD12	1.78	0.65
1:A:271:VAL:CG2	1:A:286:ALA:HB1	2.32	0.59
1:B:375:ASN:ND2	8:B:832:HOH:O	2.21	0.58
1:A:87:ASN:HD22	4:A:620:BOG:C6	2.12	0.58
1:B:274:ILE:HD12	1:B:291:VAL:HG12	1.88	0.55
1:B:581:ASN:HD22	1:B:582:VAL:N	2.07	0.52
1:A:120:ARG:HG3	1:A:531:LEU:HD12	1.91	0.52
1:A:500:VAL:HG12	1:A:500:VAL:O	2.09	0.51
1:B:196:MET:CE	1:B:431:ALA:HB2	2.41	0.51
1:B:382:ASN:O	1:B:386:HIS:HD2	1.94	0.51
1:A:87:ASN:ND2	4:A:620:BOG:H62	2.16	0.50
1:A:270:GLN:HE21	1:A:270:GLN:N	2.09	0.50
1:B:180:LYS:HD2	1:B:494:LEU:HD11	1.94	0.49
1:B:167:GLY:HA3	1:B:500:VAL:HG21	1.96	0.47
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.96	0.47
1:A:500:VAL:CG1	1:A:500:VAL:O	2.63	0.47
1:B:194:SER:O	1:B:430:ILE:HD12	2.15	0.47
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.97	0.46
1:A:216:ARG:NH1	2:C:2:NAG:O7	2.49	0.46
1:A:382:ASN:O	1:A:386:HIS:HD2	1.99	0.45
1:A:269:THR:HB	1:A:271:VAL:HG13	1.99	0.45
1:A:388:HIS:N	1:A:389:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:O	1:B:82:LEU:HD13	2.19	0.42
1:B:404:PHE:O	1:B:408:LEU:HD13	2.20	0.42
1:B:388:HIS:N	1:B:389:PRO:CD	2.83	0.41
1:B:463:LEU:HD22	1:B:506:ALA:CB	2.50	0.41
1:B:382:ASN:HD22	1:B:382:ASN:C	2.24	0.41
1:B:167:GLY:CA	1:B:500:VAL:HG21	2.51	0.41
1:B:216:ARG:NH1	2:D:1:NAG:O4	2.54	0.41
6:A:619:HEM:HBB2	6:A:619:HEM:HHC	2.04	0.40

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	553/587 (94%)	542 (98%)	11 (2%)	0	100	100
1	B	550/587 (94%)	539 (98%)	11 (2%)	0	100	100
All	All	1103/1174 (94%)	1081 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	496/525 (94%)	486 (98%)	10 (2%)	55	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	493/525 (94%)	485 (98%)	8 (2%)	62	44
All	All	989/1050 (94%)	971 (98%)	18 (2%)	59	38

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	101	ASN
1	A	232	HIS
1	A	267	LYS
1	A	270	GLN
1	A	271	VAL
1	A	282	ASN
1	A	289	GLN
1	A	385	TYR
1	A	484	GLU
1	B	232	HIS
1	B	289	GLN
1	B	382	ASN
1	B	385	TYR
1	B	405	LYS
1	B	473	LYS
1	B	484	GLU
1	B	581	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	270	GLN
1	A	282	ASN
1	A	369	GLN
1	A	421	GLN
1	B	101	ASN
1	B	369	GLN
1	B	382	ASN
1	B	386	HIS
1	B	388	HIS
1	B	581	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 ⓘ

4 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	C	1	1,2	14,14,15	0.55	0	17,19,21	0.91	1 (5%)
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	1.00	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.58	0	17,19,21	0.84	1 (5%)
2	NAG	D	2	2	14,14,15	0.50	0	17,19,21	1.32	3 (17%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C2-N2-C7	3.12	127.34	122.90
2	C	1	NAG	C1-O5-C5	2.71	115.86	112.19
2	C	2	NAG	C4-C3-C2	2.28	114.36	111.02
2	D	2	NAG	C8-C7-N2	2.24	119.89	116.10
2	D	1	NAG	C1-O5-C5	2.21	115.19	112.19
2	D	2	NAG	O5-C1-C2	-2.03	108.08	111.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

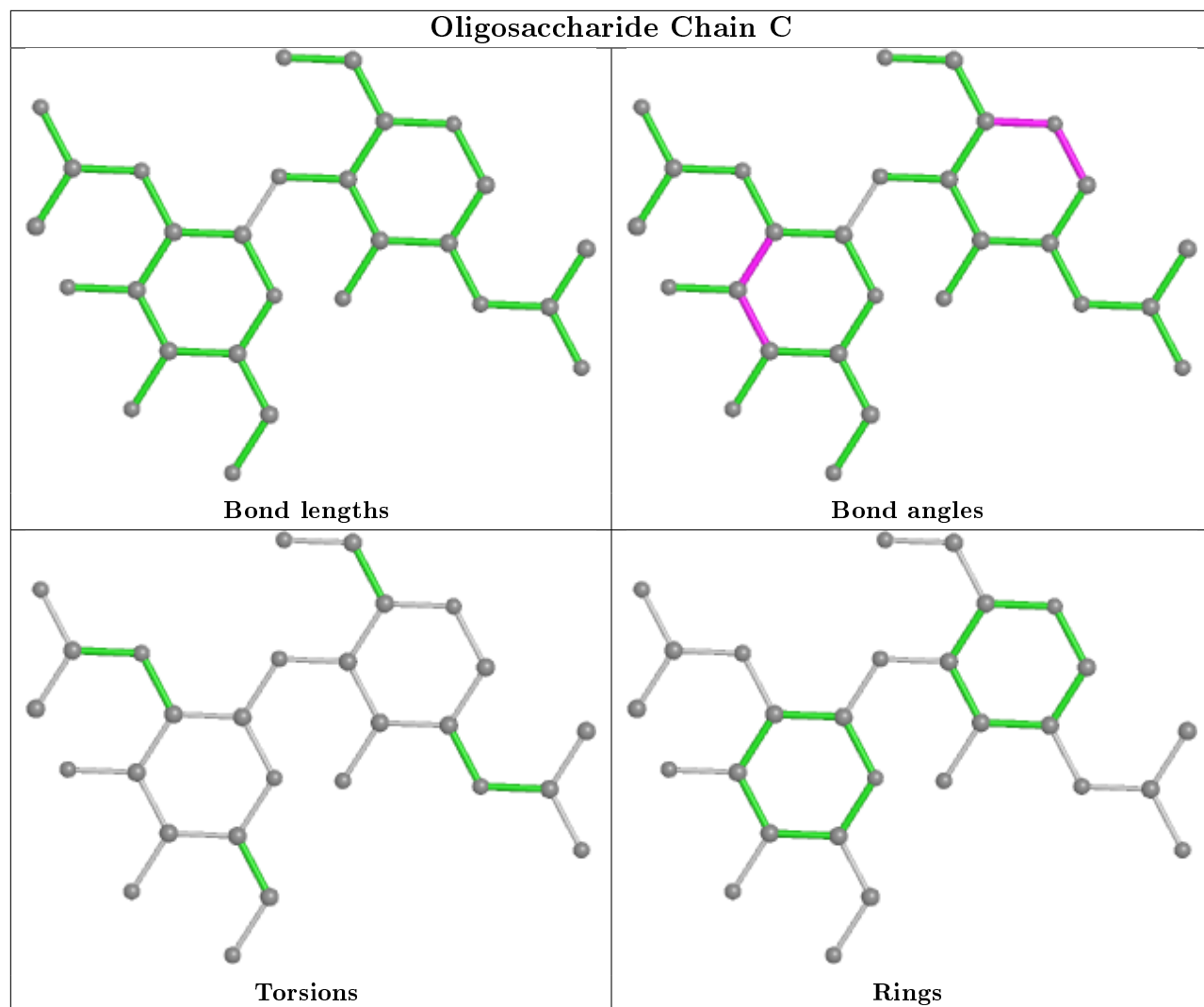
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C1-C2-N2-C7

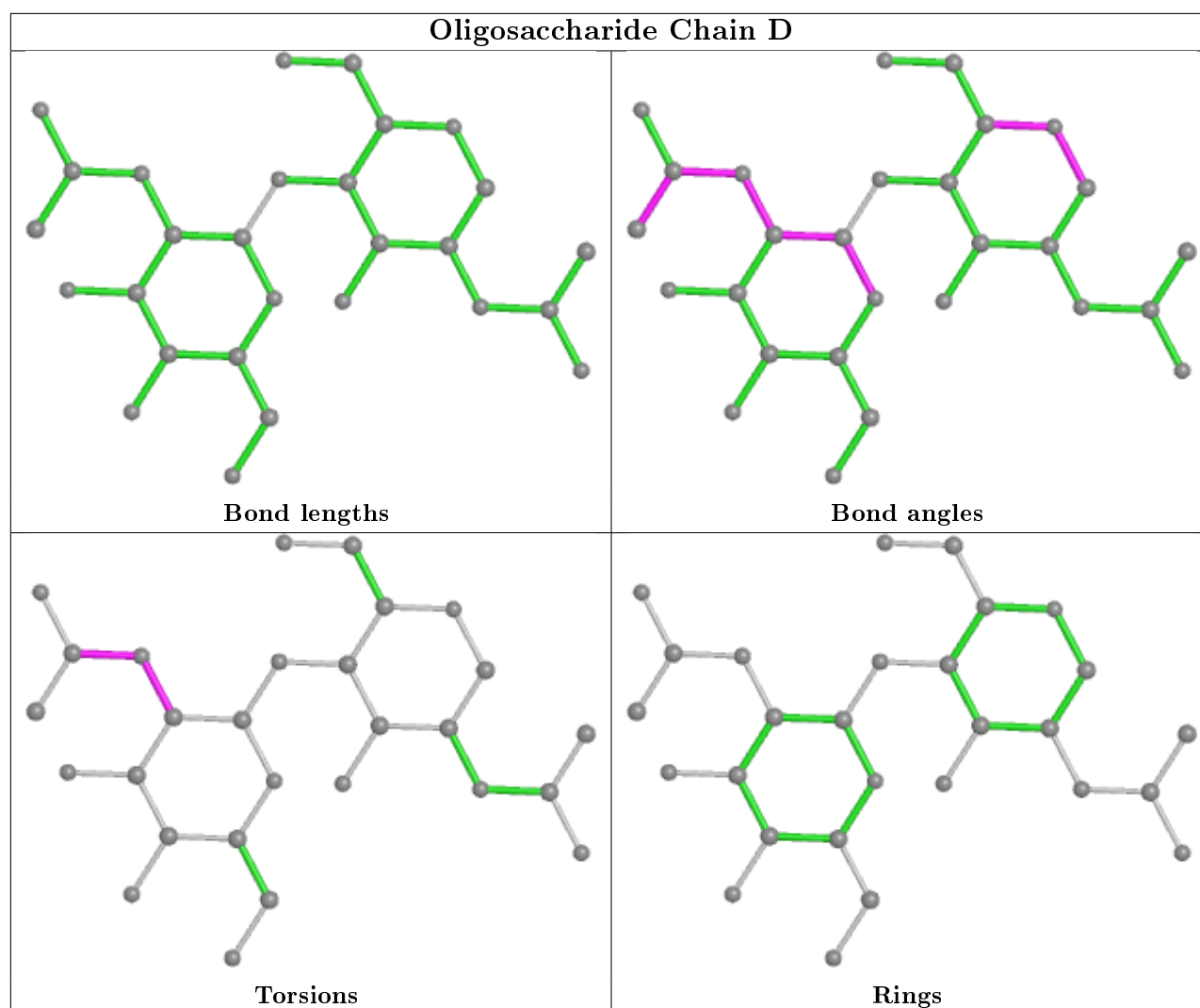
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
2	D	1	NAG	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 oligosaccharide.





5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\# Z > 2$
3	NAG	B	681	1	14,14,15	0.52	0	17,19,21	0.82	0
4	BOG	A	620	-	20,20,20	0.81	1 (5%)	25,25,25	1.60	4 (16%)
5	NPS	B	4	-	15,18,18	1.04	0	21,25,25	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BOG	B	3	-	20,20,20	0.76	1 (5%)	25,25,25	0.86	2 (8%)
3	NAG	A	681	1	14,14,15	0.47	0	17,19,21	1.01	1 (5%)
5	NPS	A	5	-	15,18,18	1.04	0	21,25,25	0.73	0
3	NAG	A	661	1	14,14,15	0.77	0	17,19,21	1.09	1 (5%)
6	HEM	A	619	1,8	27,50,50	2.17	5 (18%)	17,82,82	1.46	2 (11%)
6	HEM	B	619	1,8	27,50,50	2.15	6 (22%)	17,82,82	1.52	3 (17%)
4	BOG	A	6	-	20,20,20	0.72	1 (5%)	25,25,25	0.83	1 (4%)
3	NAG	B	9	1	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
4	BOG	A	3	-	20,20,20	0.62	1 (5%)	25,25,25	0.90	1 (4%)

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	NAG	B	681	1	-	0/6/23/26	0/1/1/1
4	BOG	A	620	-	-	5/11/31/31	0/1/1/1
5	NPS	B	4	-	-	0/6/10/10	0/2/2/2
4	BOG	B	3	-	-	6/11/31/31	0/1/1/1
3	NAG	A	681	1	-	0/6/23/26	0/1/1/1
5	NPS	A	5	-	-	0/6/10/10	0/2/2/2
3	NAG	A	661	1	1/1/5/7	6/6/23/26	0/1/1/1
6	HEM	A	619	1,8	-	0/6/54/54	-
6	HEM	B	619	1,8	-	0/6/54/54	-
4	BOG	A	6	-	-	3/11/31/31	0/1/1/1
3	NAG	B	9	1	-	2/6/23/26	0/1/1/1
4	BOG	A	3	-	-	6/11/31/31	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	619	HEM	C3D-C2D	5.21	1.53	1.37
6	B	619	HEM	C3D-C2D	5.17	1.53	1.37
6	A	619	HEM	C3B-C2B	-5.07	1.33	1.40
6	B	619	HEM	C3B-C2B	-4.66	1.33	1.40
6	A	619	HEM	C3C-C2C	-4.54	1.34	1.40
6	B	619	HEM	C3C-C2C	-4.50	1.34	1.40
6	B	619	HEM	C3C-CAC	3.59	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	619	HEM	C3C-CAC	3.55	1.55	1.47
6	B	619	HEM	C3B-CAB	3.31	1.54	1.47
6	A	619	HEM	C3B-CAB	3.18	1.54	1.47
4	A	620	BOG	O1-C1	2.89	1.45	1.40
6	B	619	HEM	CAA-C2A	2.24	1.55	1.52
4	A	6	BOG	O1-C1	2.16	1.43	1.40
4	B	3	BOG	O1-C1	2.11	1.43	1.40
4	A	3	BOG	O1-C1	2.01	1.43	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	620	BOG	O1-C1-C2	4.73	115.68	108.30
4	A	620	BOG	O5-C1-O1	-4.16	100.12	109.97
6	B	619	HEM	CBD-CAD-C3D	-3.46	106.11	112.48
6	A	619	HEM	CBD-CAD-C3D	-3.13	106.71	112.48
4	A	3	BOG	C1'-O1-C1	-3.09	108.71	113.84
4	A	620	BOG	O5-C5-C4	2.91	114.98	109.69
6	A	619	HEM	C1D-C2D-C3D	-2.85	105.02	107.00
3	A	681	NAG	C1-O5-C5	2.56	115.66	112.19
3	A	661	NAG	O5-C5-C4	-2.47	104.82	110.83
3	B	9	NAG	O5-C5-C6	2.41	110.99	107.20
6	B	619	HEM	C1D-C2D-C3D	-2.39	105.33	107.00
4	B	3	BOG	O5-C5-C4	2.29	113.86	109.69
4	B	3	BOG	O1-C1-C2	-2.17	104.92	108.30
4	A	6	BOG	O5-C5-C4	2.10	113.51	109.69
4	A	620	BOG	C1'-O1-C1	2.04	117.22	113.84
6	B	619	HEM	CBA-CAA-C2A	-2.00	108.80	112.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	661	NAG	C1

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	620	BOG	O5-C1-O1-C1'
3	A	661	NAG	C3-C2-N2-C7
3	A	661	NAG	O7-C7-N2-C2
3	A	661	NAG	C8-C7-N2-C2
3	A	661	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	9	NAG	O5-C5-C6-O6
3	A	661	NAG	C4-C5-C6-O6
3	B	9	NAG	C4-C5-C6-O6
4	A	3	BOG	O1-C1'-C2'-C3'
4	B	3	BOG	C3'-C4'-C5'-C6'
4	B	3	BOG	C2'-C3'-C4'-C5'
4	B	3	BOG	C2-C1-O1-C1'
4	B	3	BOG	C4'-C5'-C6'-C7'
4	B	3	BOG	O5-C1-O1-C1'
3	A	661	NAG	C1-C2-N2-C7
4	A	6	BOG	C3'-C4'-C5'-C6'
4	A	3	BOG	C1'-C2'-C3'-C4'
4	A	620	BOG	C4'-C5'-C6'-C7'
4	B	3	BOG	C1'-C2'-C3'-C4'
4	A	620	BOG	O5-C5-C6-O6
4	A	620	BOG	C2-C1-O1-C1'
4	A	3	BOG	C4'-C5'-C6'-C7'
4	A	3	BOG	C3'-C4'-C5'-C6'
4	A	620	BOG	C2'-C3'-C4'-C5'
4	A	3	BOG	C2'-C3'-C4'-C5'
4	A	6	BOG	C4'-C5'-C6'-C7'
4	A	6	BOG	C5'-C6'-C7'-C8'
4	A	3	BOG	C2'-C1'-O1-C1

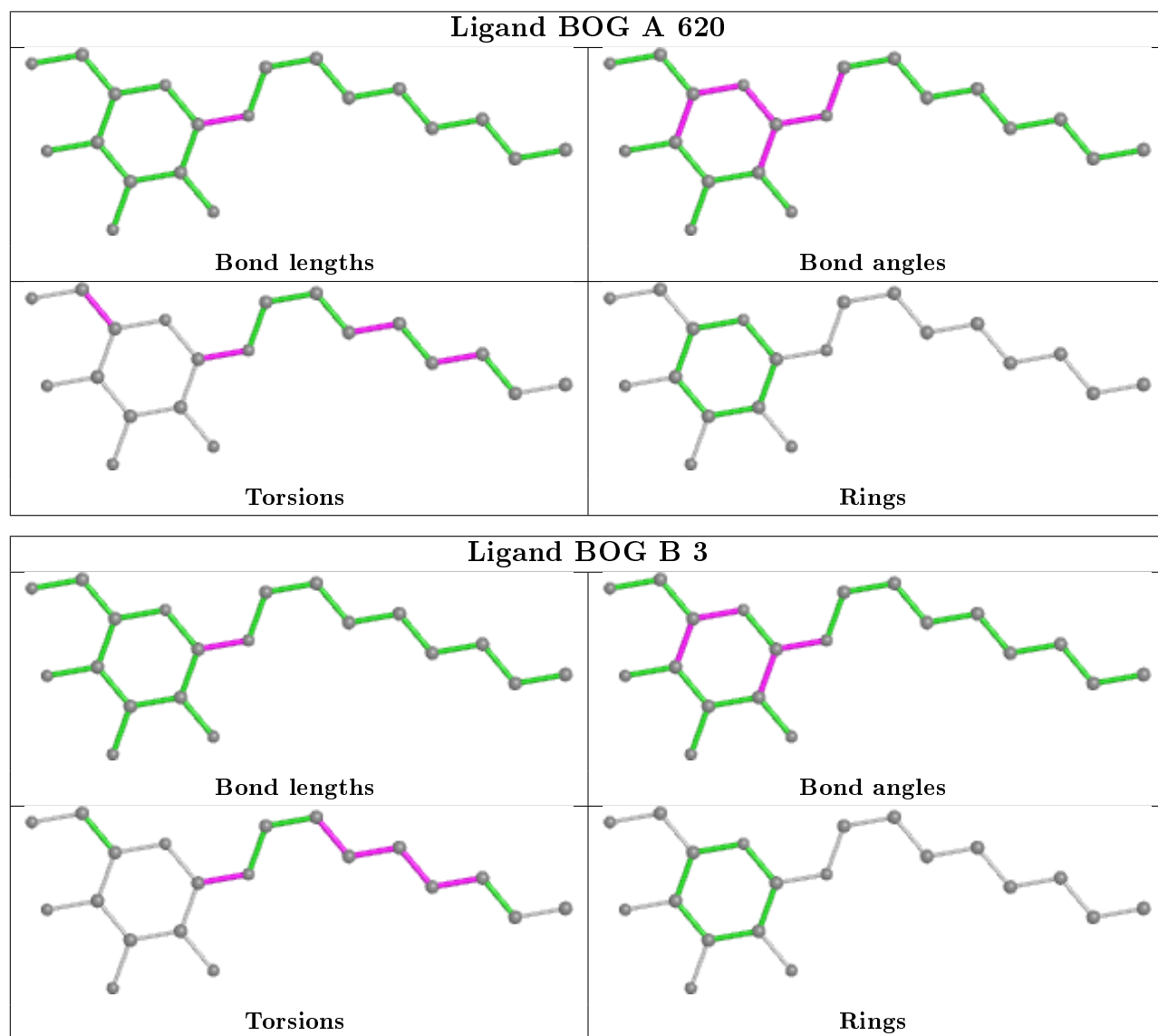
There are no ring outliers.

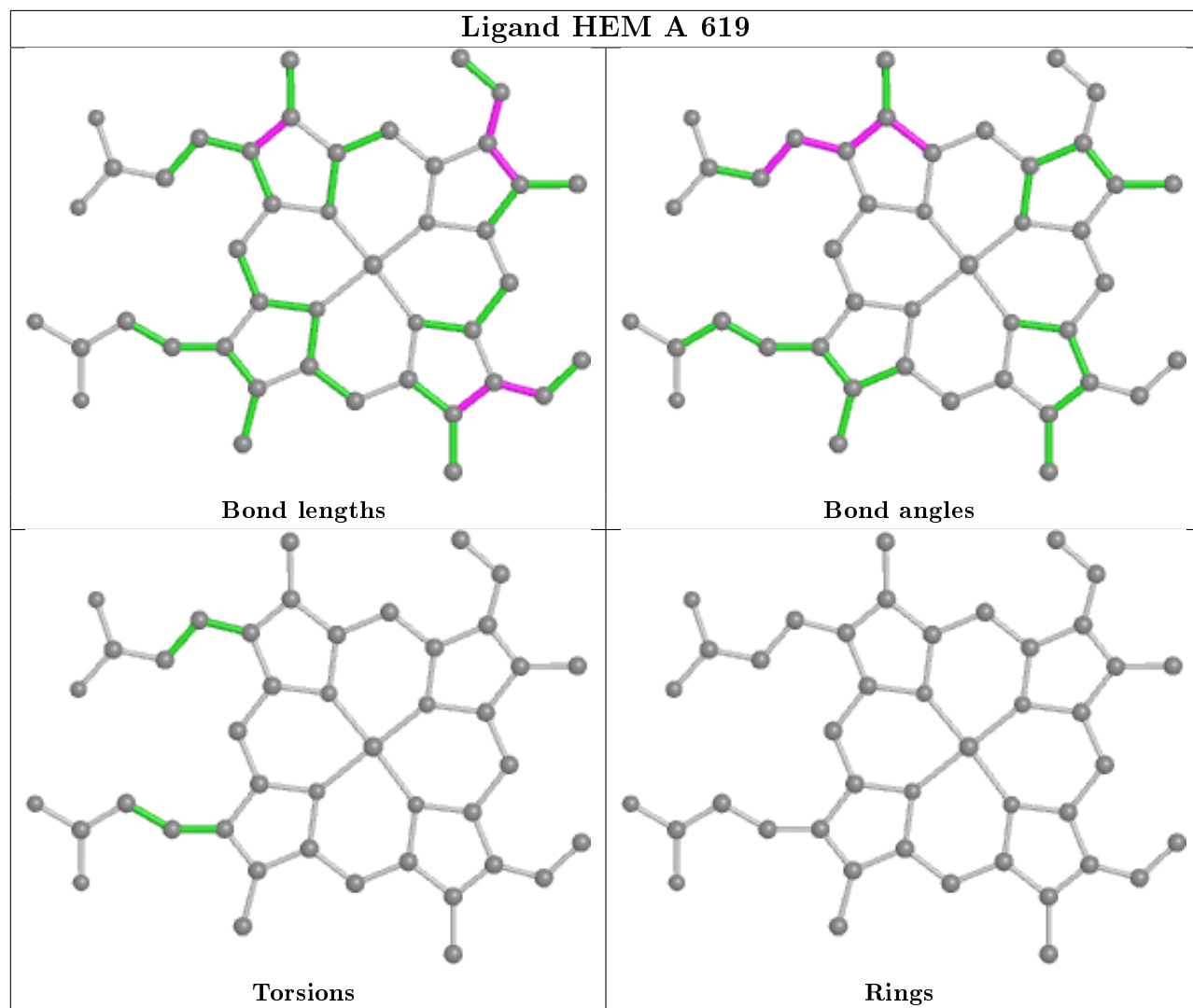
3 monomers are involved in 5 short contacts:

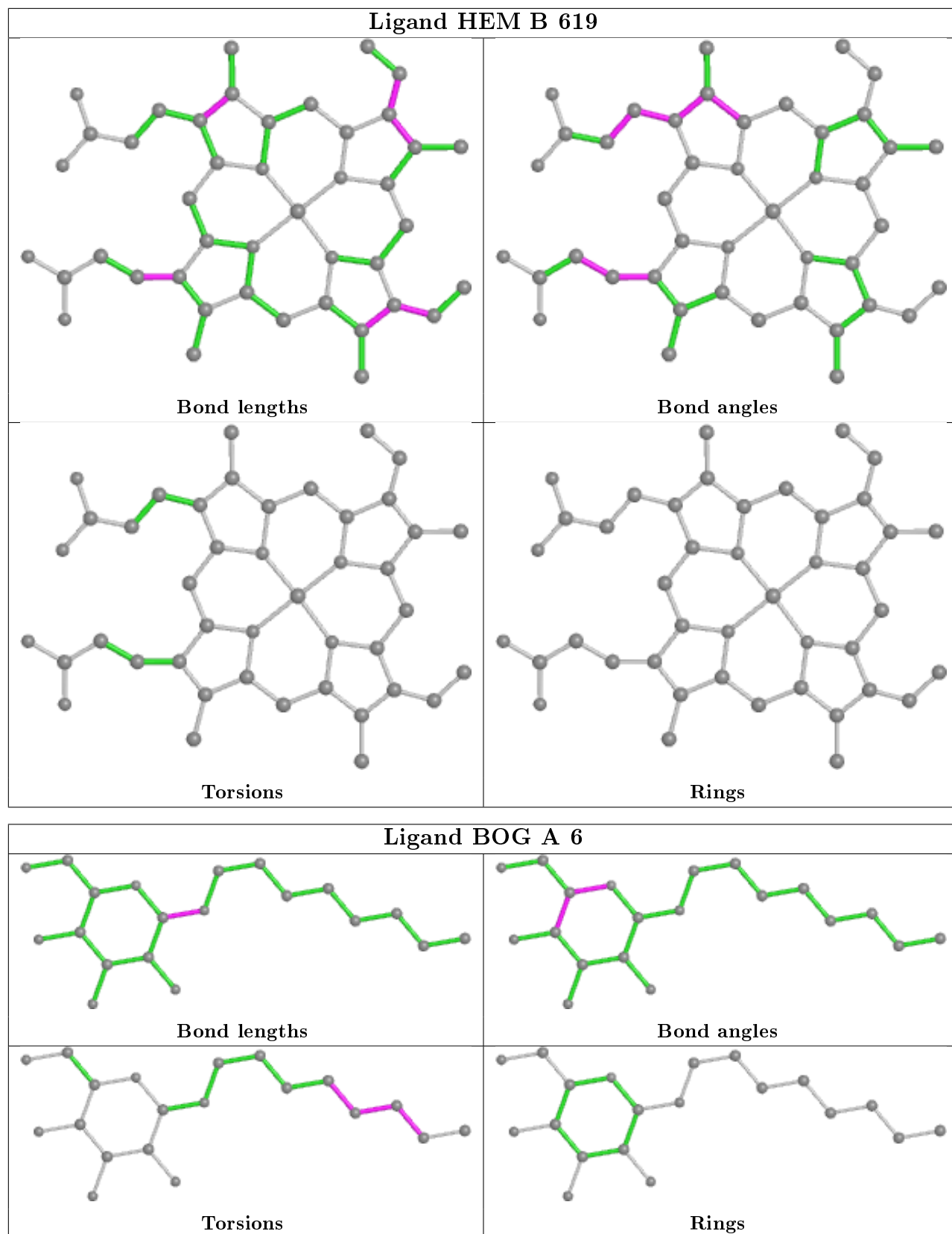
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	620	BOG	3	0
6	A	619	HEM	1	0
6	B	619	HEM	1	0

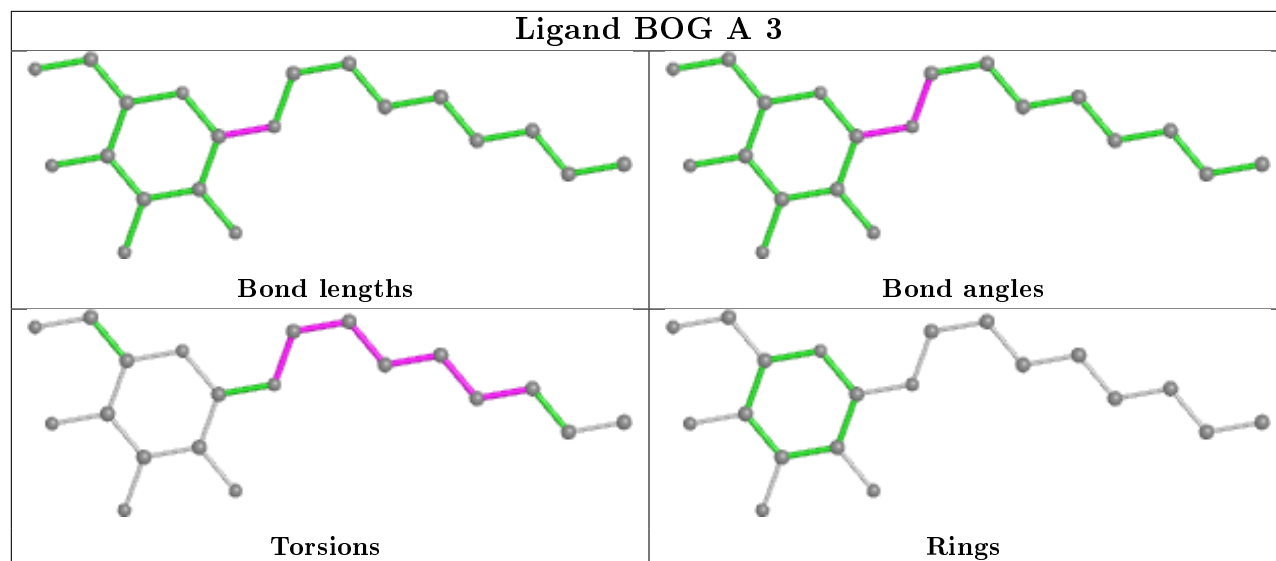
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	552/587 (94%)	0.27	36 (6%)	18 23	16, 25, 40, 50	0
1	B	552/587 (94%)	0.28	41 (7%)	14 19	16, 25, 41, 55	0
All	All	1104/1174 (94%)	0.28	77 (6%)	16 21	16, 25, 40, 55	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	PHE	6.7
1	A	81	LEU	6.5
1	B	81	LEU	5.2
1	A	75	LEU	4.9
1	A	583	GLN	4.7
1	B	75	LEU	4.5
1	B	583	GLN	4.4
1	A	74	PHE	4.3
1	A	169	LYS	3.9
1	B	33	ALA	3.9
1	B	77	ARG	3.9
1	A	80	LEU	3.8
1	B	169	LYS	3.6
1	B	577	PHE	3.5
1	A	506	ALA	3.3
1	B	82	LEU	3.3
1	B	122	TYR	3.3
1	A	503	LEU	3.3
1	A	77	ARG	3.2
1	A	107	PHE	3.2
1	B	503	LEU	3.2
1	A	33	ALA	3.1
1	A	507	LEU	3.0
1	B	409	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	82	LEU	2.9
1	B	215	LYS	2.9
1	B	107	PHE	2.8
1	B	78	ILE	2.7
1	A	463	LEU	2.7
1	A	96	PHE	2.7
1	A	122	TYR	2.7
1	B	405	LYS	2.7
1	A	305	TRP	2.6
1	B	65	TYR	2.6
1	A	65	TYR	2.6
1	A	505	PRO	2.6
1	B	98	GLY	2.5
1	A	215	LYS	2.5
1	A	53	ASP	2.5
1	B	170	GLU	2.5
1	A	399	ASP	2.5
1	B	399	ASP	2.5
1	B	564	ILE	2.5
1	A	98	GLY	2.5
1	A	470	PHE	2.5
1	B	305	TRP	2.5
1	B	182	LEU	2.4
1	B	73	GLU	2.4
1	A	158	ASP	2.4
1	B	463	LEU	2.4
1	A	466	TYR	2.4
1	A	54	GLN	2.4
1	B	101	ASN	2.4
1	B	505	PRO	2.3
1	B	387	TRP	2.3
1	A	387	TRP	2.3
1	B	508	LEU	2.3
1	B	496	SER	2.2
1	A	130	TYR	2.2
1	A	108	LEU	2.2
1	B	390	LEU	2.2
1	B	539	ILE	2.2
1	A	214	HIS	2.1
1	B	295	VAL	2.1
1	B	53	ASP	2.1
1	A	300	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	142	PHE	2.1
1	B	214	HIS	2.1
1	B	54	GLN	2.1
1	B	105	ASN	2.1
1	B	301	TYR	2.1
1	B	201	PHE	2.1
1	B	506	ALA	2.1
1	A	409	TYR	2.0
1	A	508	LEU	2.0
1	A	501	MET	2.0
1	A	105	ASN	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 ⓘ

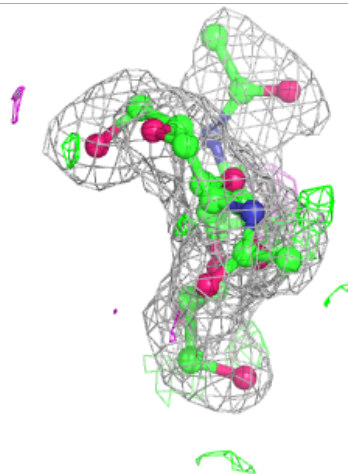
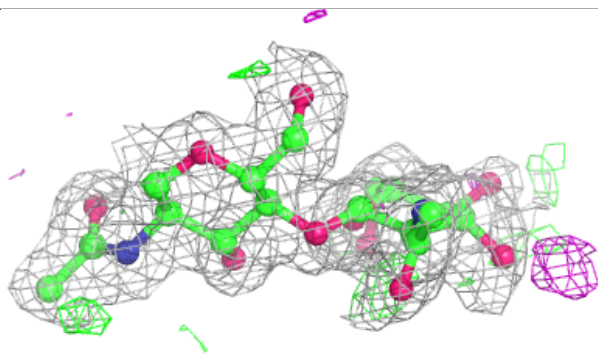
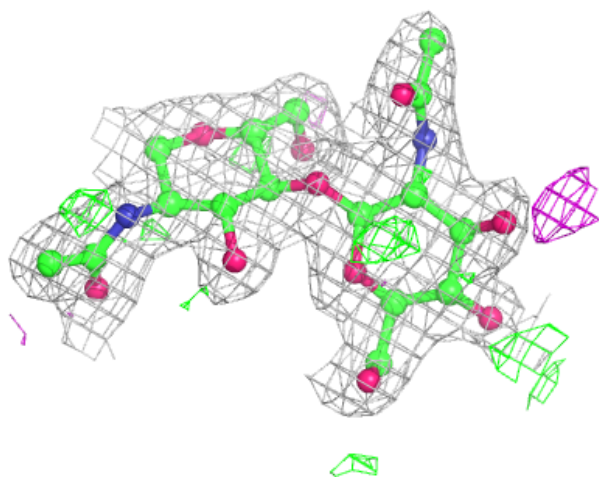
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

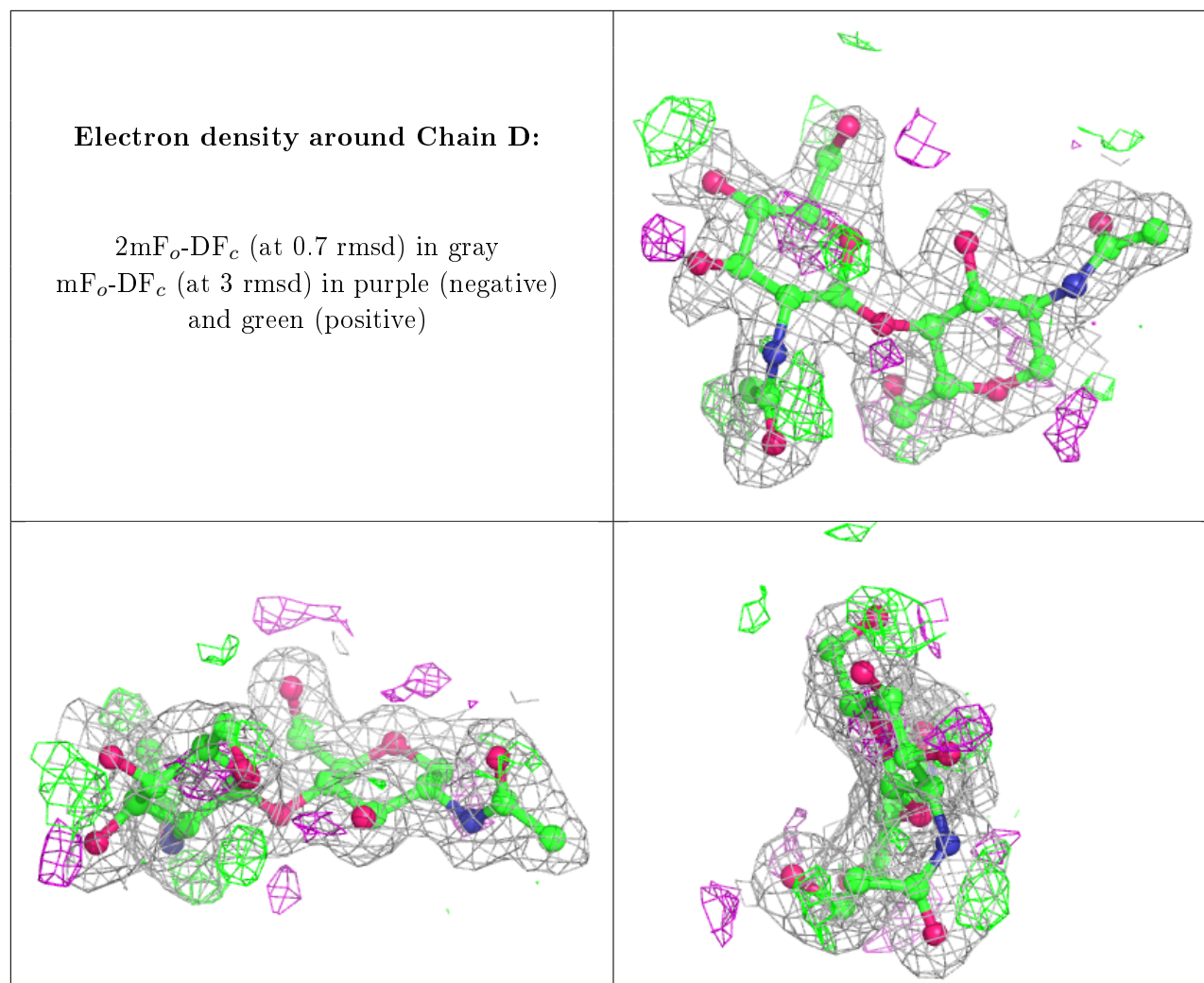
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.75	0.28	38,42,44,45	0
2	NAG	C	2	14/15	0.83	0.23	35,38,40,40	0
2	NAG	C	1	14/15	0.91	0.10	22,27,29,31	0
2	NAG	D	1	14/15	0.95	0.08	22,26,28,33	0

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 C:

$2mF_o-DF_c$ (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.

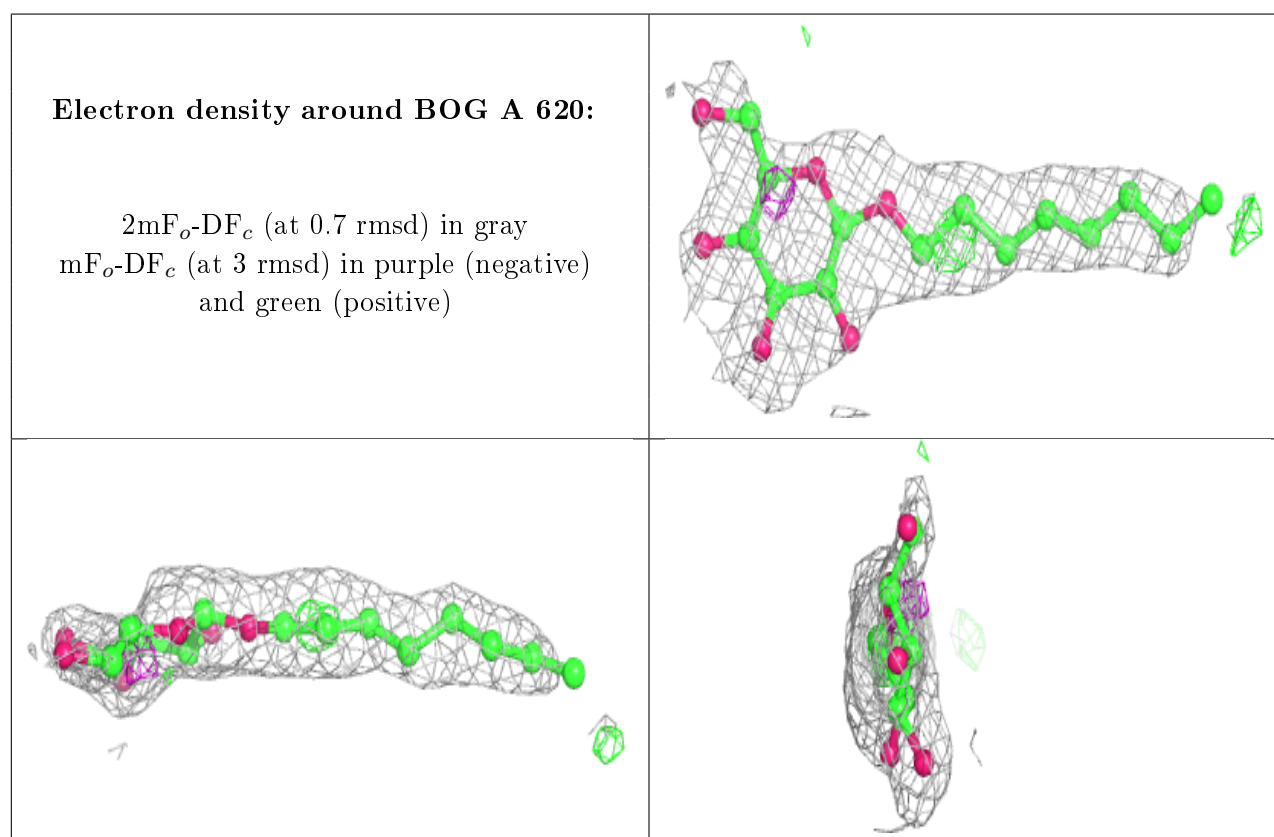
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BOG	A	620	20/20	0.65	0.25	54,58,59,59	0
3	NAG	A	661	14/15	0.70	0.30	38,44,46,47	0
3	NAG	B	9	14/15	0.82	0.29	37,42,45,45	0
4	BOG	A	6	20/20	0.84	0.14	41,42,46,46	0
4	BOG	B	3	20/20	0.84	0.14	43,45,50,50	0
3	NAG	A	681	14/15	0.86	0.20	32,35,38,38	0
3	NAG	B	681	14/15	0.89	0.23	33,36,38,39	0
4	BOG	A	3	20/20	0.92	0.11	30,33,43,43	0
6	HEM	A	619	43/43	0.93	0.11	26,28,38,41	0

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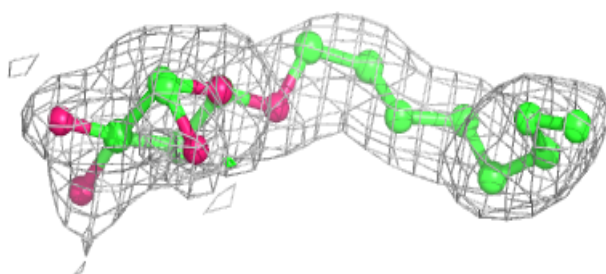
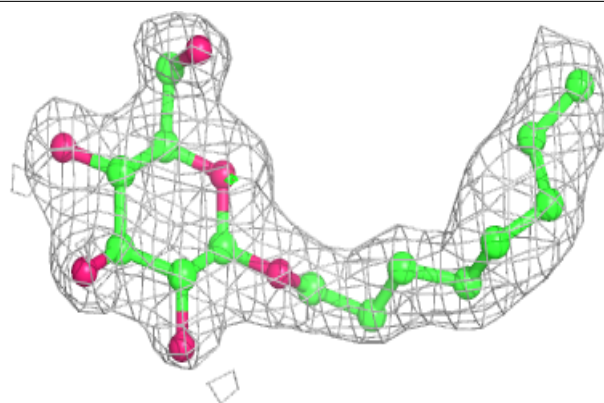
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	HEM	B	619	43/43	0.94	0.11	26,28,37,42	0
5	NPS	A	5	17/17	0.96	0.13	20,21,23,24	0
5	NPS	B	4	17/17	0.97	0.10	20,21,24,25	0
7	CL	B	1	1/1	0.99	0.03	26,26,26,26	0
7	CL	A	1	1/1	0.99	0.04	25,25,25,25	0

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.

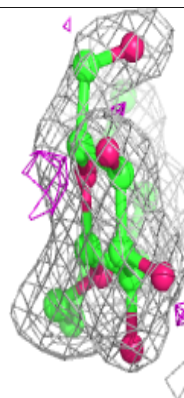
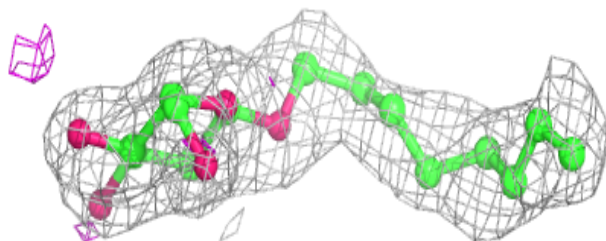
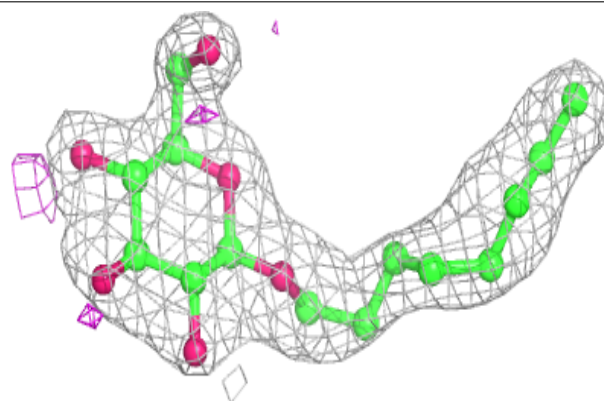


Electron density around BOG A 6:

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

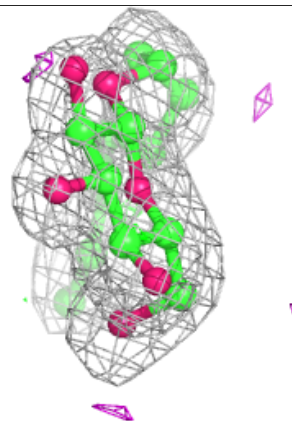
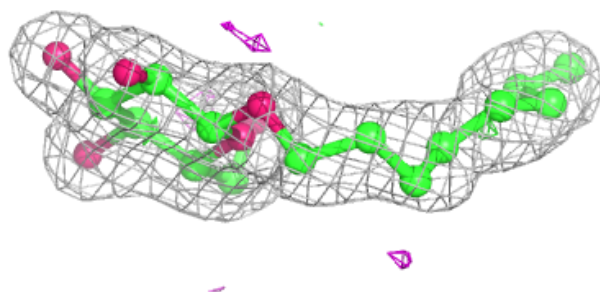
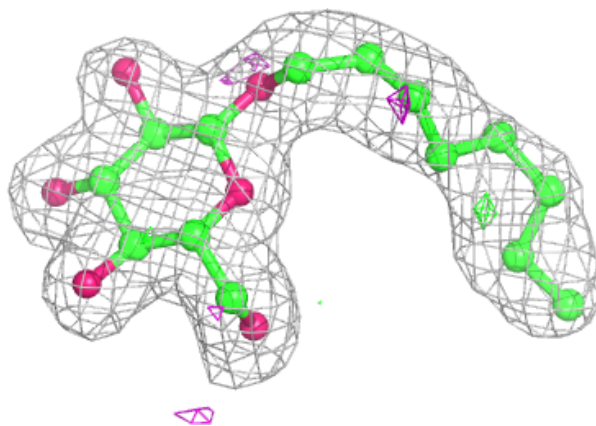
**Electron density around BOG B 3:**

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



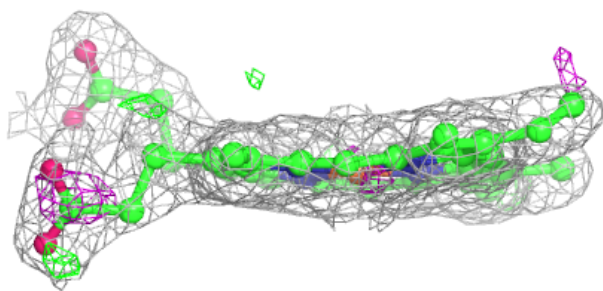
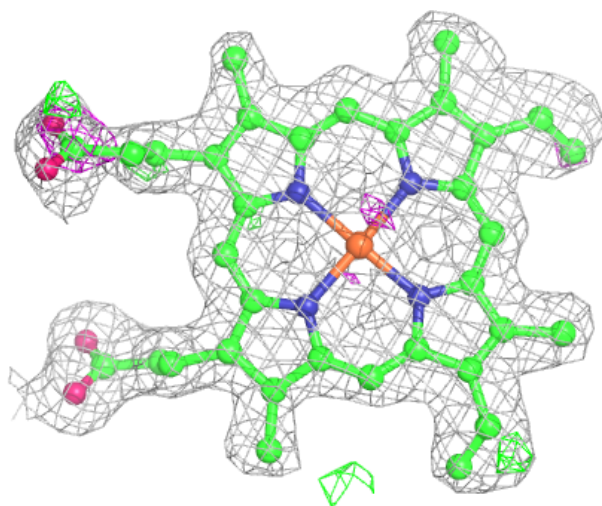
Electron density around BOG A 3:

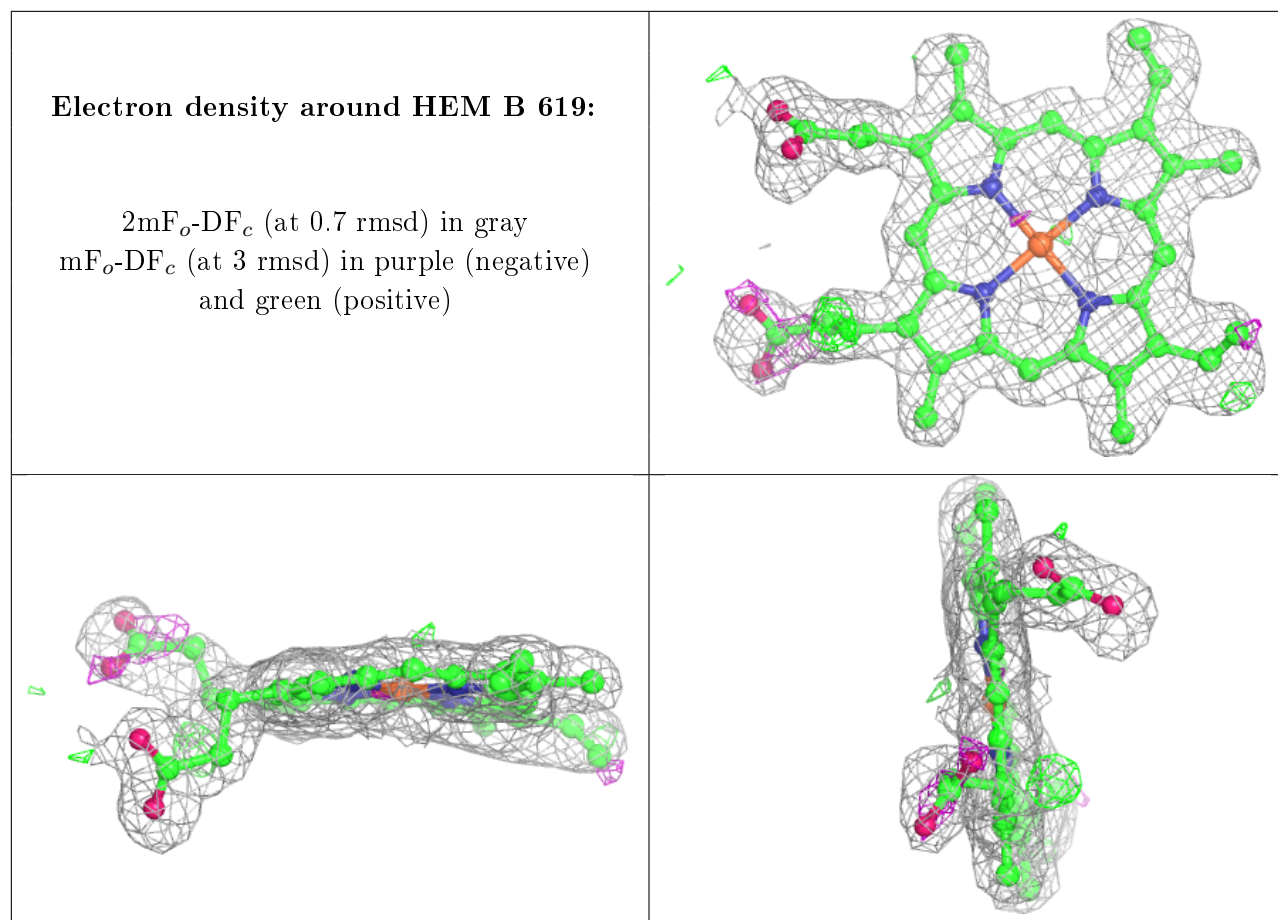
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 619:

$2mF_o-DF_c$ (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.