



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:30 AM UTC

PDB ID : 4Z0L / pdb_00004z0l
Title : The murine cyclooxygenase-2 complexed with a nido-dicarbaborate-containing indomethacin derivative
Authors : Xu, S.; Neumann, W.; Banerjee, S.; Hey-Hawkins, E.; Marnett, L.J.
Deposited on : 2015-03-26
Resolution : 2.29 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 types of validation reports are described at

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

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

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

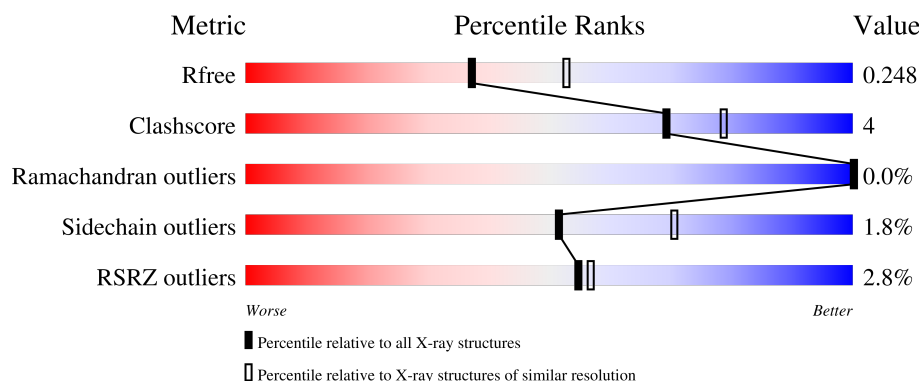
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

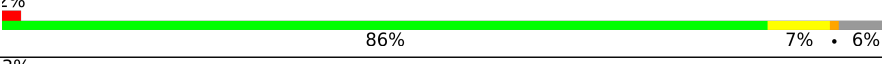
The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	587	
1	B	587	
1	C	587	
1	D	587	
2	E	2	

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

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 19280 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	551	Total	C	N	O	S	0	1	0
			4473	2885	751	812	25			
1	B	551	Total	C	N	O	S	0	1	0
			4473	2885	751	812	25			
1	C	551	Total	C	N	O	S	0	1	0
			4473	2885	751	812	25			
1	D	551	Total	C	N	O	S	0	1	0
			4473	2885	751	812	25			

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



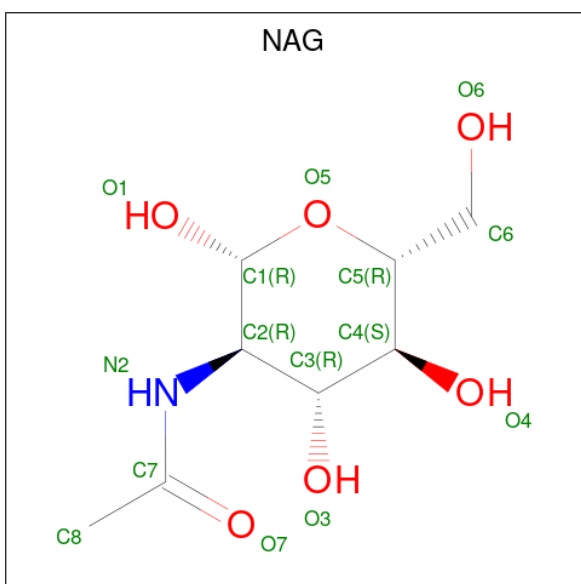
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



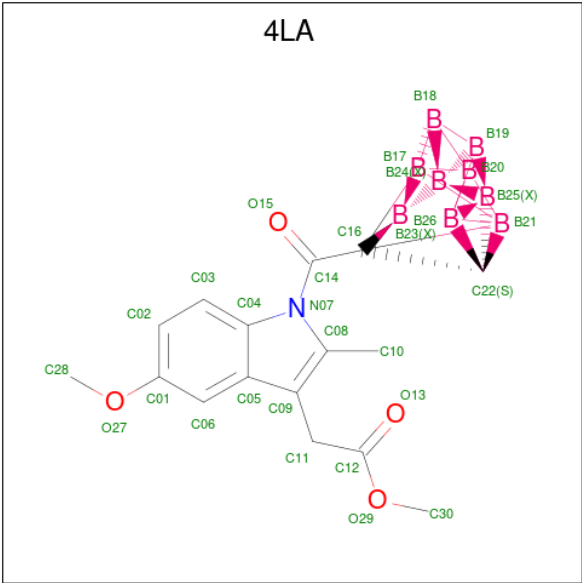
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).



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

- Molecule 5 is (R)-7-{[5-methoxy-2-methyl-3-(methoxycarbonylmethyl)-1H-indolyl]carbonyl}-7,8-dicarba-nido-dodeca-hydroundecaborate (CCD ID: 4LA) (formula: C₁₆H₁₄B₉NO₄).



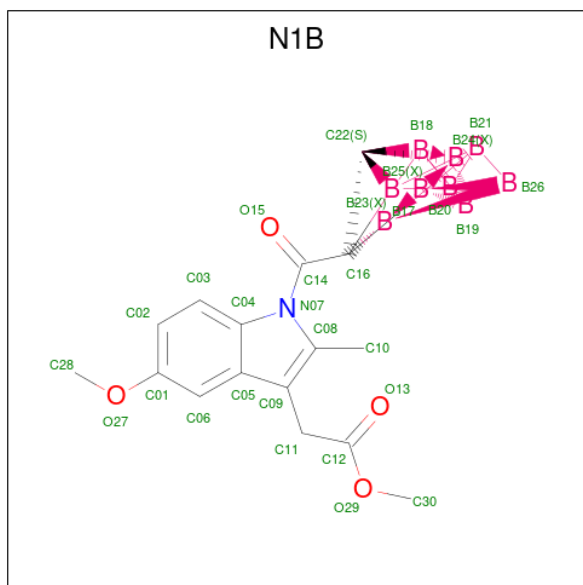
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 30	B 9	C 16	N 1	O 4	0	1
5	B	1	Total 30	B 9	C 16	N 1	O 4	0	1
5	C	1	Total 30	B 9	C 16	N 1	O 4	0	1

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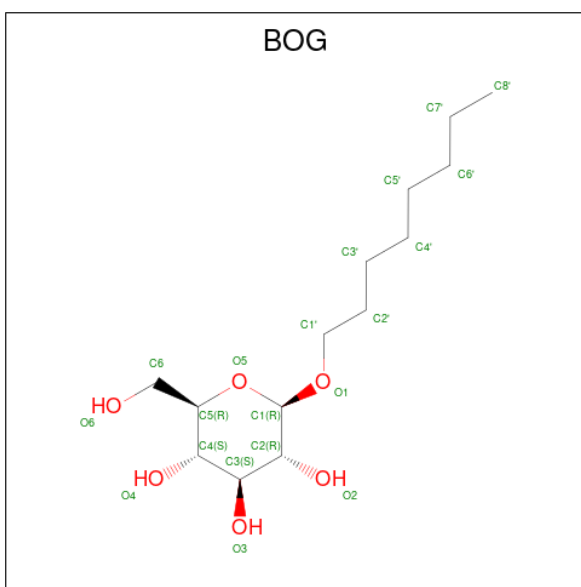
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	B	C	N	O	0	1
			30	9	16	1	4		

- Molecule 6 is (S)-7-[[5-methoxy-2-methyl-3-(methoxycarbonylmethyl)-1H-indolyl]carbonyl]-7,8-dicarba-nido-dodeca-hydrundecaborate (CCD ID: N1B) (formula: $C_{16}H_{14}B_9NO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	B	C	N	O	0	1
			30	9	16	1	4		
6	B	1	Total	B	C	N	O	0	1
			30	9	16	1	4		
6	C	1	Total	B	C	N	O	0	1
			30	9	16	1	4		
6	D	1	Total	B	C	N	O	0	1
			30	9	16	1	4		

- Molecule 7 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	162	Total	O	0	0
			162	162		
8	B	153	Total	O	0	0
			153	153		
8	C	162	Total	O	0	0
			162	162		
8	D	175	Total	O	0	0
			175	175		

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.

Chain A:

87% 4% 6% 6%

Amino acids shown (from left to right): A33, G51, E67, N68, L75, L81, V103, N104, I112, M113, K114, Y115, Y122, D173, S174, K175, V181, E186, Q203, H207, K215, R216, L230, N231, H232, D239, D268, T269, Q270, Q289, E290, V291, F292, I337, K358, E364, E380, Y385.

Chain B:

Amino Acid	Frequency
ARG	2%
LEU	86%
ASP	86%
ASP	86%
ILE	86%
ASN	86%
PRO	86%
THR	86%
VAL	86%
LEU	86%
LEU	86%
ILE	86%
LYS	86%
ARG	86%
ARG	86%
SER	86%
SER	86%
THR	86%
GLU	86%
LEU	86%
ILE	86%
LYS	86%
THR	86%
ALA	86%
ALA	86%
THR	86%
THR	86%
ILE	86%
ASN	86%
ALA	86%
ALA	86%
SER	86%
SER	86%
THR	86%
SER	86%
THR	86%
ASP	7%
PRO	7%
GLN	7%
GLN	7%
PRO	7%
THR	7%
LYS	7%
THR	7%
ALA	7%
ALA	7%
THR	7%
THR	7%
ILE	7%
ASN	7%
ALA	7%
ALA	7%
SER	7%
SER	7%
THR	7%
SER	7%
THR	7%
ASP	6%
PRO	6%
GLN	6%
GLN	6%
PRO	6%
THR	6%
LYS	6%
THR	6%
ALA	6%
ALA	6%
THR	6%
THR	6%
ILE	6%
ASN	6%
ALA	6%
ALA	6%
SER	6%
SER	6%
THR	6%
SER	6%
THR	6%

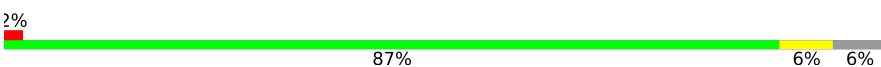
Chain C:

86% 3% 7% 6%

A33 A385 H386 V387 D399 Y409 M410 M411 S412 T416 H417 G418 L419 F422 Y466 L472 G483 E484 K485 E486 M487 A493 D497 L498 D499 V500 E520 E524 P528 Q543 F556 V592 GLN ASP PRO GLN PRO THR THR ALA THR ILE ASN ALA

ALA
SER
HIS
SER
ARG
LEU
ASP
ASP
ILE
ASN
PRO
THR
VAL
LEU
ILE
LYS
ARG
ARG
SER
THR
GLU
LEU

- Molecule 1: Prostaglandin G/H synthase 2

Chain D:  2% 87% 6% 6%

A33 M43 M44 M68 L80 T88 V103 I112 M113 K114 Y122 I123 I124 D125 W139 D173 S174 K175 Q203 H207 H214 H232 H239 K253 D268 I274 E281 N282 L283 V291 L294 V295 P296 G297 R307 K360 Y385

P389 L408 Y409 L419 V434 I442 K473 E484 D497 I498 M499 V500 P528 Q543 S566 V582 GLN ASP PRO GLN PRO THR LYS THR ALA THR ILE ASN ALA ALA SER HIS SER ARG LEU ASP ASP ILE ASN PRO THR VAL LEU ILE LYS ARG ARG

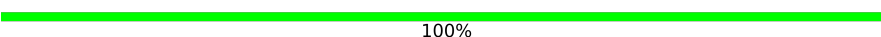
SER
THR
GLU
LEU

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

Chain E:  50% 50%

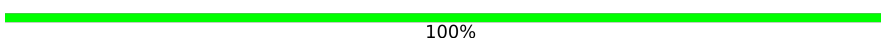
NAG1
NAG2

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

Chain F:  100%

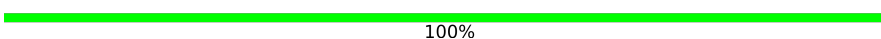
NAG1
NAG2

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

Chain G:  100%

NAG1
NAG2

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

Chain H:  100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	180.94Å 135.01Å 124.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 2.29 49.60 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.60-2.29) 87.6 (49.60-2.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.210 , 0.250 0.212 , 0.248	Depositor DCC
R_{free} test set	4057 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19280	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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 48.16 % 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 8.9572e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: N1B, BOG, NAG, 4LA, HEM

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	0.29	0/4603	0.72	0/6241
1	B	0.29	0/4603	0.71	0/6241
1	C	0.36	2/4603 (0.0%)	0.76	6/6241 (0.1%)
1	D	0.29	0/4603	0.71	0/6241
All	All	0.31	2/18412 (0.0%)	0.73	6/24964 (0.0%)

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	C	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	484	GLU	C-N	5.73	1.43	1.33
1	C	483	GLY	C-N	-5.37	1.26	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	483	GLY	O-C-N	-13.63	104.98	122.70
1	C	483	GLY	CA-C-N	9.34	139.38	121.54
1	C	483	GLY	C-N-CA	9.34	139.38	121.54
1	C	484	GLU	O-C-N	5.43	129.81	122.59
1	C	484	GLU	CA-C-N	-5.25	113.13	122.42
1	C	484	GLU	C-N-CA	-5.25	113.13	122.42

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	483	GLY	Mainchain,Peptide
1	C	484	GLU	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4473	0	4378	22	0
1	B	4473	0	4378	25	0
1	C	4473	0	4378	41	0
1	D	4473	0	4378	23	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	43	0	30	2	0
3	B	43	0	30	3	0
3	C	43	0	30	0	0
3	D	43	0	30	4	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
4	C	28	0	26	0	0
4	D	28	0	26	0	0
5	A	30	0	14	2	0
5	B	30	0	14	1	0
5	C	30	0	14	5	0
5	D	30	0	14	2	0
6	A	30	0	14	2	0
6	B	30	0	14	1	0
6	C	30	0	14	3	0
6	D	30	0	14	3	0
7	A	20	0	28	1	0
7	B	20	0	28	0	0
7	C	40	0	56	3	0
7	D	20	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	162	0	0	3	0
8	B	153	0	0	5	0
8	C	162	0	0	3	0
8	D	175	0	0	4	0
All	All	19280	0	18086	130	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 (130) 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:C:294:LEU:CD2	1:C:295:VAL:HG23	1.74	1.16
1:C:294:LEU:HD23	1:C:295:VAL:CG2	1.89	1.03
1:C:294:LEU:HD23	1:C:295:VAL:HG23	1.02	0.99
1:C:484:GLU:OE2	1:C:487:MET:N	2.07	0.88
1:C:294:LEU:CD2	1:C:295:VAL:CG2	2.48	0.86
3:B:701:HEM:HMB1	3:B:701:HEM:HBB2	1.64	0.80
1:D:88:THR:HG23	7:D:708:BOG:H4'1	1.65	0.76
6:D:707[B]:N1B:H4	6:D:707[B]:N1B:C22	2.20	0.72
1:B:137:LYS:O	8:B:801:HOH:O	2.08	0.71
1:D:294:LEU:HD13	1:D:409:TYR:CE2	2.25	0.70
3:B:701:HEM:HBB2	3:B:701:HEM:CMB	2.23	0.69
1:C:417:HIS:O	8:C:801:HOH:O	2.11	0.68
1:C:294:LEU:HA	1:C:409:TYR:CD1	2.34	0.63
1:C:289:GLN:HG2	1:C:292:PHE:CE1	2.35	0.62
1:A:207:HIS:NE2	8:A:809:HOH:O	2.31	0.62
1:D:207:HIS:NE2	8:D:805:HOH:O	2.31	0.61
1:D:274:ILE:HD12	1:D:291:VAL:HG12	1.84	0.59
1:C:294:LEU:HA	1:C:409:TYR:CE1	2.36	0.59
1:D:43:ASN:O	8:D:801:HOH:O	2.17	0.59
1:B:274:ILE:HD12	1:B:291:VAL:HG12	1.84	0.59
1:C:179:GLU:OE2	8:C:802:HOH:O	2.16	0.59
1:C:387:TRP:HZ2	5:C:706[A]:4LA:H12	1.68	0.59
1:B:41:CYS:O	8:B:802:HOH:O	2.17	0.58
1:C:274:ILE:HD12	1:C:291:VAL:HG12	1.85	0.58
1:A:511:LYS:O	8:A:801:HOH:O	2.17	0.58
1:C:410:ASN:OD1	1:C:412:SER:OG	2.22	0.58
1:B:497:ASP:OD1	1:B:498:ILE:N	2.37	0.57
1:B:579:SER:OG	1:B:581:ASN:OD1	2.22	0.57
1:D:389:PRO:HB2	1:D:434:VAL:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:HG11	1:D:112:ILE:HD12	1.87	0.56
1:D:214:HIS:NE2	3:D:701:HEM:O2A	2.40	0.55
1:B:110:SER:OG	8:B:803:HOH:O	2.17	0.54
1:C:520:GLU:OE2	8:C:803:HOH:O	2.18	0.54
1:B:389:PRO:HB2	1:B:434:VAL:HA	1.90	0.54
1:C:497:ASP:OD1	1:C:498:ILE:N	2.40	0.54
1:C:543:GLN:HB2	8:D:909:HOH:O	2.08	0.53
1:D:294:LEU:CD1	1:D:409:TYR:CE2	2.92	0.53
1:D:173:ASP:OD2	1:D:175:LYS:HB3	2.08	0.52
1:D:497:ASP:HB3	1:D:500:VAL:HG23	1.90	0.52
1:A:216:ARG:NH1	2:E:2:NAG:O7	2.42	0.52
1:C:114:LYS:HZ2	1:C:365:LEU:HD22	1.74	0.52
3:D:701:HEM:CMC	3:D:701:HEM:HBC2	2.39	0.52
1:A:203:GLN:N	3:A:701:HEM:HBC2	2.25	0.52
1:C:173:ASP:OD2	1:C:175:LYS:HB3	2.11	0.51
1:B:497:ASP:HB3	1:B:500:VAL:HG23	1.93	0.51
1:C:486:GLU:OE1	7:C:708:BOG:O4	2.18	0.51
1:C:387:TRP:CZ2	5:C:706[A]:4LA:H12	2.46	0.51
1:C:294:LEU:CG	1:C:295:VAL:HG23	2.38	0.51
1:C:294:LEU:HB2	1:C:409:TYR:CZ	2.45	0.51
1:B:124:ILE:HD11	1:B:528:PRO:HB2	1.93	0.50
1:B:103:VAL:HG11	1:B:112:ILE:HD12	1.92	0.50
1:A:68:ASN:N	1:A:68:ASN:OD1	2.45	0.50
1:B:44:ARG:NH2	1:B:125:ASP:OD1	2.44	0.50
1:C:88:THR:HG23	7:C:709:BOG:H4'1	1.93	0.50
1:A:410:ASN:OD1	1:A:412:SER:OG	2.30	0.50
6:C:707[B]:N1B:C16	6:C:707[B]:N1B:H4	2.42	0.50
1:D:497:ASP:OD1	1:D:498:ILE:N	2.45	0.50
5:A:706[A]:4LA:H4	5:A:706[A]:4LA:C16	2.42	0.49
1:B:473:LYS:NZ	1:B:473:LYS:HB3	2.27	0.49
6:C:707[B]:N1B:C16	6:C:707[B]:N1B:C10	2.91	0.49
1:C:289:GLN:HG3	1:C:291:VAL:H	1.78	0.48
1:C:387:TRP:HZ2	6:C:707[B]:N1B:H12	1.77	0.48
5:C:706[A]:4LA:C16	5:C:706[A]:4LA:H4	2.43	0.48
1:C:349:VAL:HG11	5:C:706[A]:4LA:C22	2.42	0.48
6:A:707[B]:N1B:H4	6:A:707[B]:N1B:C16	2.43	0.48
1:C:114:LYS:NZ	1:C:114:LYS:HB2	2.29	0.48
5:C:706[A]:4LA:C16	5:C:706[A]:4LA:C10	2.92	0.48
1:A:473:LYS:NZ	1:A:473:LYS:HB3	2.28	0.48
5:A:706[A]:4LA:C16	5:A:706[A]:4LA:C10	2.92	0.48
1:A:497:ASP:HB3	1:A:500:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:473:LYS:NZ	1:D:473:LYS:HB3	2.30	0.47
1:B:207:HIS:NE2	8:B:809:HOH:O	2.36	0.47
1:C:289:GLN:HG2	1:C:292:PHE:CD1	2.50	0.47
1:D:294:LEU:HD11	1:D:408:LEU:HG	1.95	0.47
1:B:295:VAL:HG12	1:B:297:GLY:H	1.80	0.47
1:B:410:ASN:OD1	1:B:412:SER:OG	2.27	0.47
1:D:114:LYS:HB2	1:D:114:LYS:NZ	2.31	0.46
6:A:707[B]:N1B:C16	6:A:707[B]:N1B:C10	2.93	0.46
1:C:294:LEU:HB2	1:C:409:TYR:CE1	2.51	0.46
1:A:104:ASN:HB3	1:A:358:LYS:HD3	1.98	0.46
1:C:484:GLU:OE2	1:C:486:GLU:N	2.49	0.45
1:A:543:GLN:HB2	8:B:884:HOH:O	2.16	0.45
1:B:183:LEU:HD22	1:B:442:ILE:HD12	1.98	0.45
1:C:497:ASP:HB3	1:C:500:VAL:HG23	1.99	0.45
1:A:67:GLU:OE2	8:A:802:HOH:O	2.21	0.45
1:A:289:GLN:HG3	1:A:291:VAL:H	1.82	0.45
1:C:68:ASN:OD1	1:C:68:ASN:N	2.49	0.45
1:D:124:ILE:HD11	1:D:528:PRO:HB2	1.99	0.45
1:B:68:ASN:OD1	1:B:68:ASN:N	2.49	0.45
1:D:68:ASN:N	1:D:68:ASN:OD1	2.50	0.44
1:B:353:SER:HA	5:B:706[A]:4LA:C01	2.47	0.44
1:A:456:ARG:NH2	1:A:502:GLU:OE2	2.48	0.44
1:C:124:ILE:HD11	1:C:528:PRO:HB2	1.99	0.44
3:D:701:HEM:HBC2	3:D:701:HEM:HMC1	1.99	0.44
7:A:708:BOG:H4'1	7:A:708:BOG:H1'1	1.77	0.44
1:C:346:GLU:OE2	1:C:360:LYS:HD2	2.17	0.44
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.52	0.44
1:C:294:LEU:HD21	1:C:295:VAL:CG2	2.43	0.44
5:D:706[A]:4LA:C16	5:D:706[A]:4LA:H4	2.48	0.44
1:A:114:LYS:HB2	1:A:114:LYS:NZ	2.32	0.44
1:B:346:GLU:OE2	1:B:360:LYS:HD2	2.17	0.44
1:B:353:SER:HA	6:B:707[B]:N1B:C01	2.48	0.44
3:B:701:HEM:HMB1	3:B:701:HEM:CBB	2.41	0.44
1:A:173:ASP:OD2	1:A:175:LYS:HB3	2.17	0.43
1:A:230:LEU:HD13	1:A:337:ILE:HG12	1.99	0.43
1:C:472:LEU:HD11	1:C:524:GLU:HB2	2.01	0.43
6:D:707[B]:N1B:H4	6:D:707[B]:N1B:C16	2.49	0.43
1:C:103:VAL:HG11	1:C:112:ILE:HD12	2.00	0.43
1:D:295:VAL:HG12	1:D:297:GLY:H	1.84	0.43
1:A:497:ASP:OD1	1:A:498:ILE:N	2.52	0.43
1:D:543:GLN:HB2	8:D:907:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:706[A]:4LA:C16	5:D:706[A]:4LA:C10	2.97	0.42
3:A:701:HEM:HBB2	3:A:701:HEM:HHC	2.01	0.42
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.55	0.42
1:B:132:VAL:HG13	1:B:133:HIS:CD2	2.54	0.42
6:D:707[B]:N1B:C16	6:D:707[B]:N1B:C10	2.98	0.42
1:C:380:GLU:HG2	1:C:466:TYR:CE1	2.54	0.42
1:D:203:GLN:HB2	3:D:701:HEM:HMC3	2.02	0.42
1:B:391:LEU:HB2	1:B:441:PRO:HG3	2.01	0.42
1:B:397:ILE:HD11	1:B:407:PHE:HE1	1.85	0.42
1:D:307:ARG:CZ	1:D:419:LEU:HD12	2.49	0.42
1:A:289:GLN:HG2	1:A:292:PHE:CE1	2.55	0.42
1:B:114:LYS:NZ	1:B:114:LYS:HB2	2.35	0.42
1:C:91:TYR:CD2	7:C:709:BOG:H3'2	2.55	0.41
1:A:103:VAL:HG11	1:A:112:ILE:HD12	2.02	0.41
1:A:181:VAL:HG21	1:A:491:LEU:HD21	2.02	0.41
1:C:229:ASP:HB3	1:D:139:TRP:CZ2	2.56	0.41
1:D:44:ARG:NH2	1:D:125:ASP:OD1	2.54	0.41
1:C:556:PHE:HD1	1:C:556:PHE:HA	1.82	0.41
1:A:389:PRO:HB2	1:A:434:VAL:HA	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	550/587 (94%)	532 (97%)	18 (3%)	0	100	100
1	B	550/587 (94%)	533 (97%)	17 (3%)	0	100	100
1	C	550/587 (94%)	533 (97%)	16 (3%)	1 (0%)	43	55
1	D	550/587 (94%)	534 (97%)	16 (3%)	0	100	100
All	All	2200/2348 (94%)	2132 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	484	GLU

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	493/525 (94%)	485 (98%)	8 (2%)	55	73
1	B	493/525 (94%)	484 (98%)	9 (2%)	51	70
1	C	493/525 (94%)	483 (98%)	10 (2%)	48	67
1	D	493/525 (94%)	485 (98%)	8 (2%)	55	73
All	All	1972/2100 (94%)	1937 (98%)	35 (2%)	51	70

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	114	LYS
1	A	232	HIS
1	A	239	ASP
1	A	385	TYR
1	A	419	LEU
1	A	422	PHE
1	A	484	GLU
1	B	68	ASN
1	B	80	LEU
1	B	114	LYS
1	B	232	HIS
1	B	239	ASP
1	B	385	TYR
1	B	419	LEU
1	B	422	PHE
1	B	442	ILE
1	C	68	ASN
1	C	80	LEU

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Mol	Chain	Res	Type
1	C	114	LYS
1	C	232	HIS
1	C	294	LEU
1	C	385	TYR
1	C	419	LEU
1	C	422	PHE
1	C	485	LYS
1	C	556	PHE
1	D	68	ASN
1	D	80	LEU
1	D	114	LYS
1	D	232	HIS
1	D	239	ASP
1	D	385	TYR
1	D	442	ILE
1	D	484	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	101	ASN
1	A	356	HIS
1	A	445	GLN
1	A	461	GLN
1	B	39	ASN
1	B	90	HIS
1	C	90	HIS
1	C	105	ASN
1	C	214	HIS
1	C	374	GLN
1	C	461	GLN
1	D	39	ASN
1	D	571	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	0.31	0	17,19,21	0.50	0
2	NAG	E	2	2	14,14,15	1.03	0	17,19,21	1.35	3 (17%)
2	NAG	F	1	1,2	14,14,15	0.30	0	17,19,21	0.44	0
2	NAG	F	2	2	14,14,15	0.28	0	17,19,21	0.45	0
2	NAG	G	1	1,2	14,14,15	0.30	0	17,19,21	0.45	0
2	NAG	G	2	2	14,14,15	0.25	0	17,19,21	0.40	0
2	NAG	H	1	1,2	14,14,15	0.32	0	17,19,21	0.46	0
2	NAG	H	2	2	14,14,15	0.24	0	17,19,21	0.44	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	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	3.43	116.79	112.19
2	E	2	NAG	C6-C5-C4	-2.60	106.63	113.02
2	E	2	NAG	O3-C3-C4	-2.03	105.58	110.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

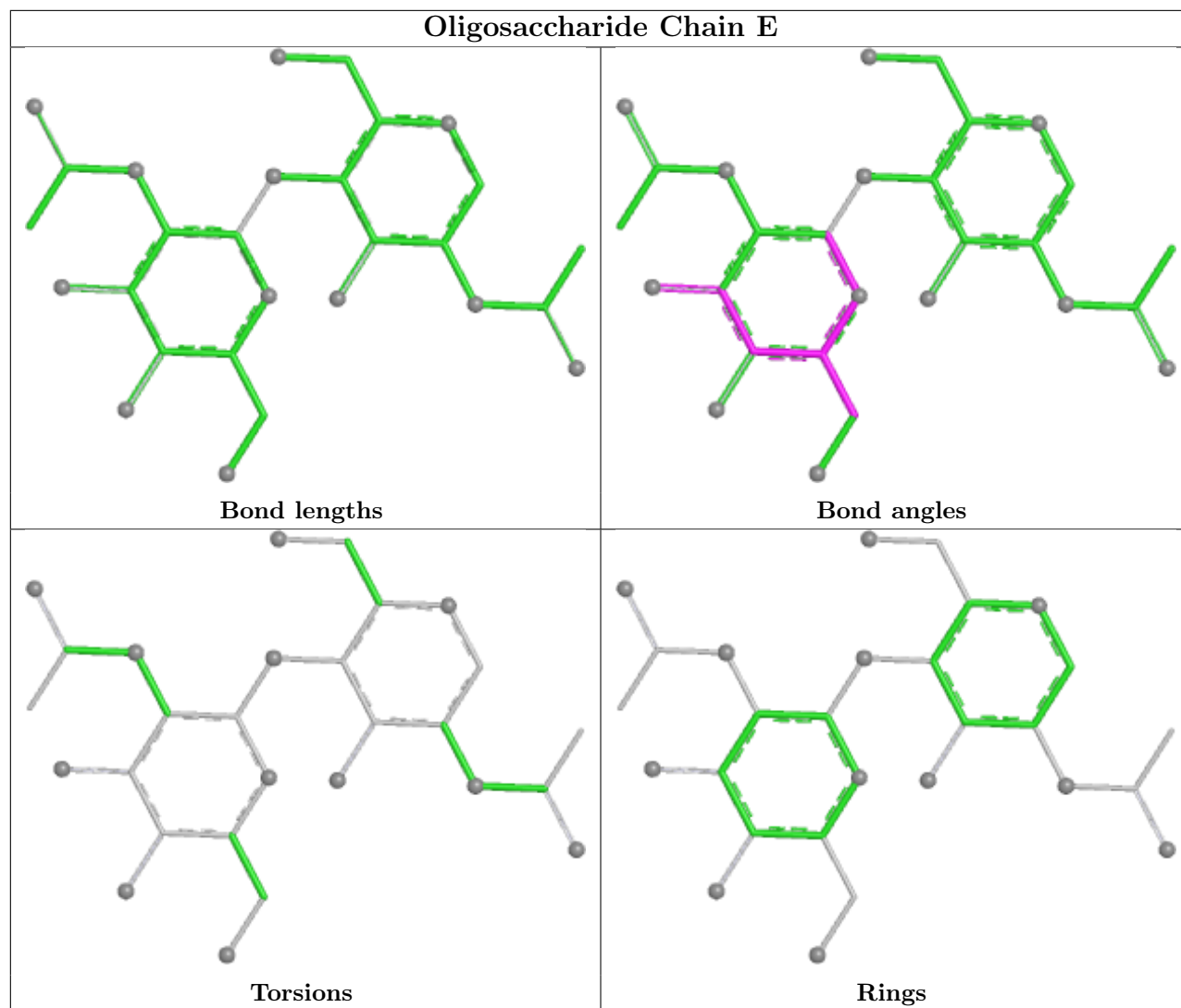
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C1-C2-N2-C7

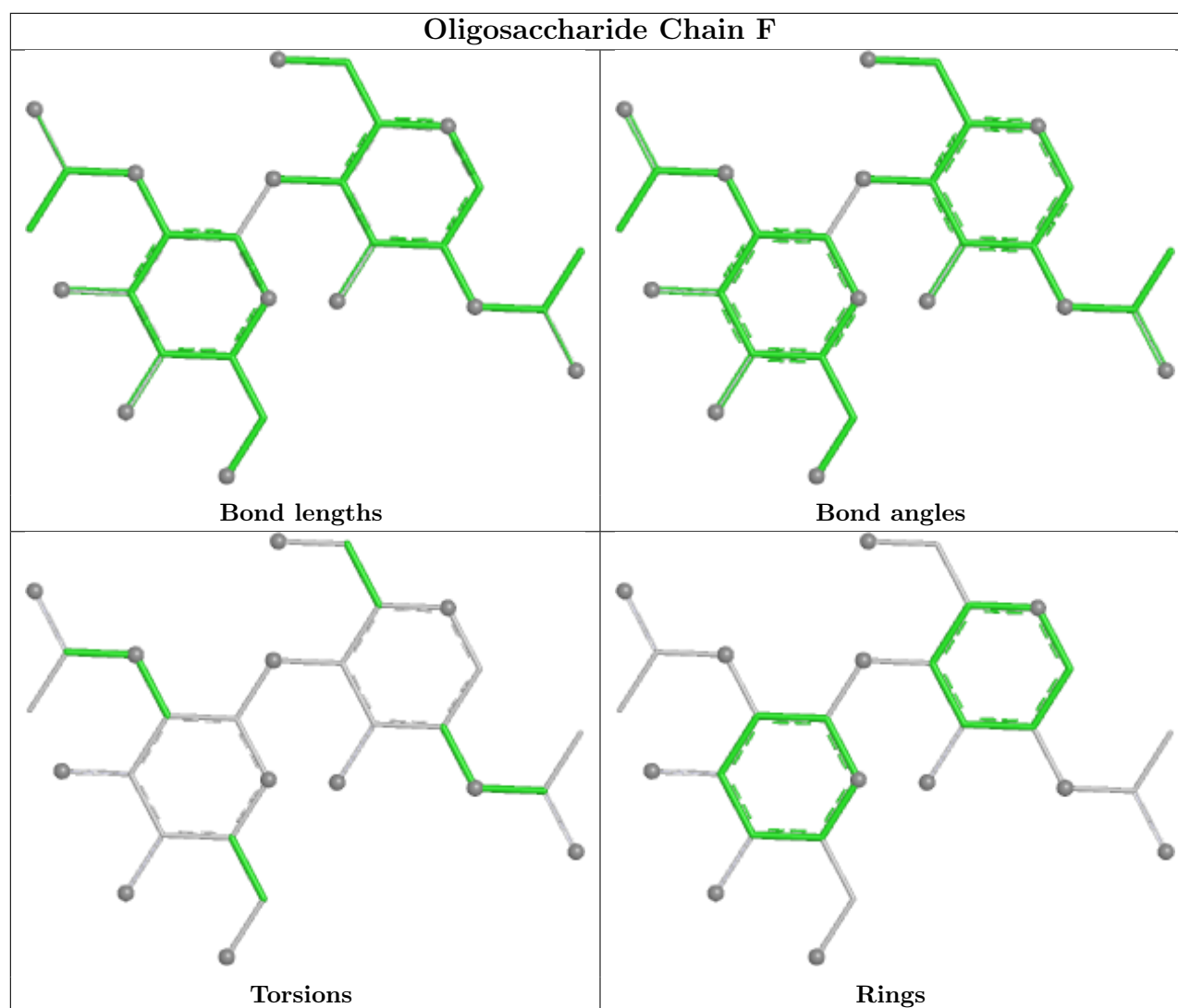
There are no ring outliers.

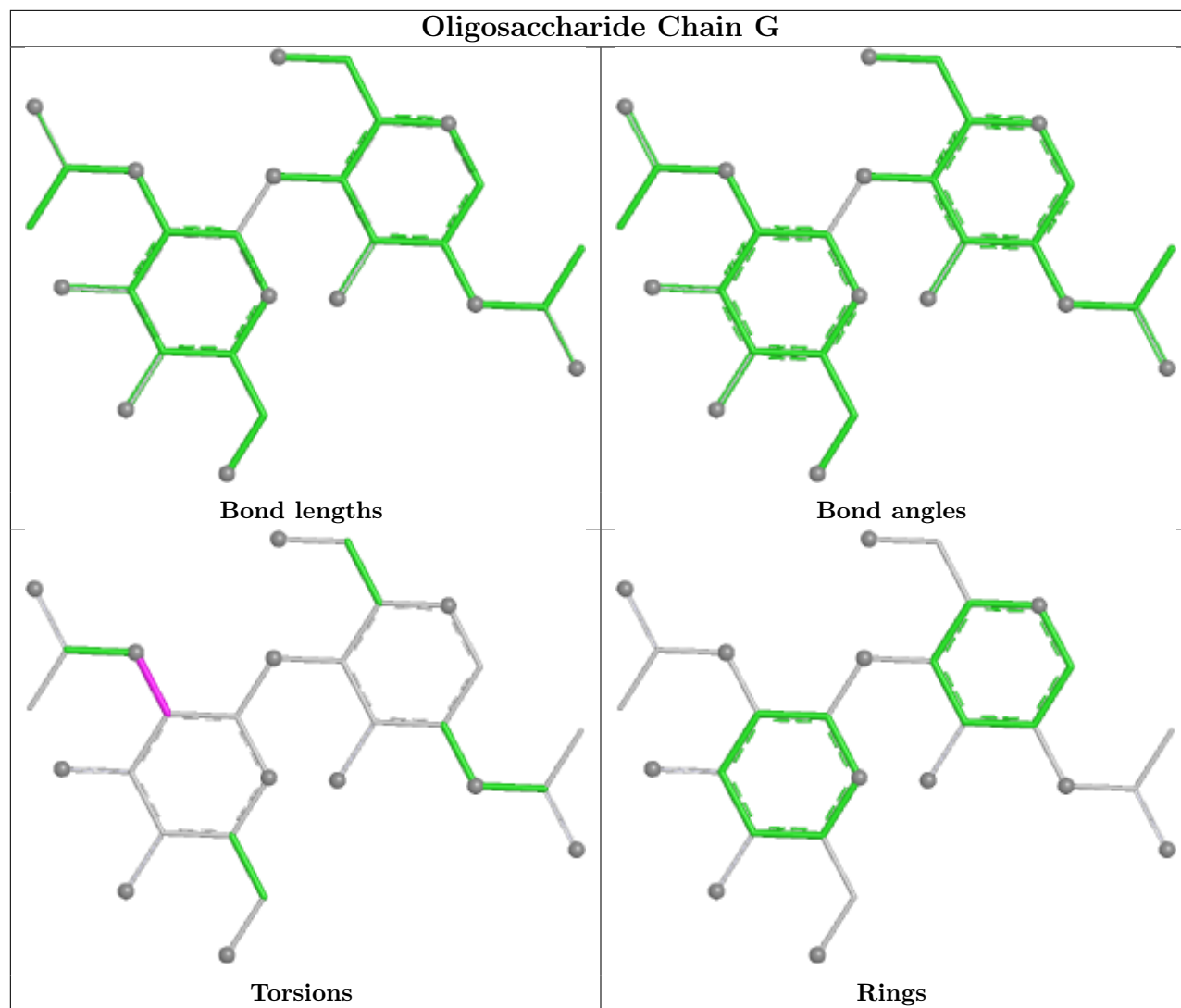
1 monomer is involved in 1 short contact:

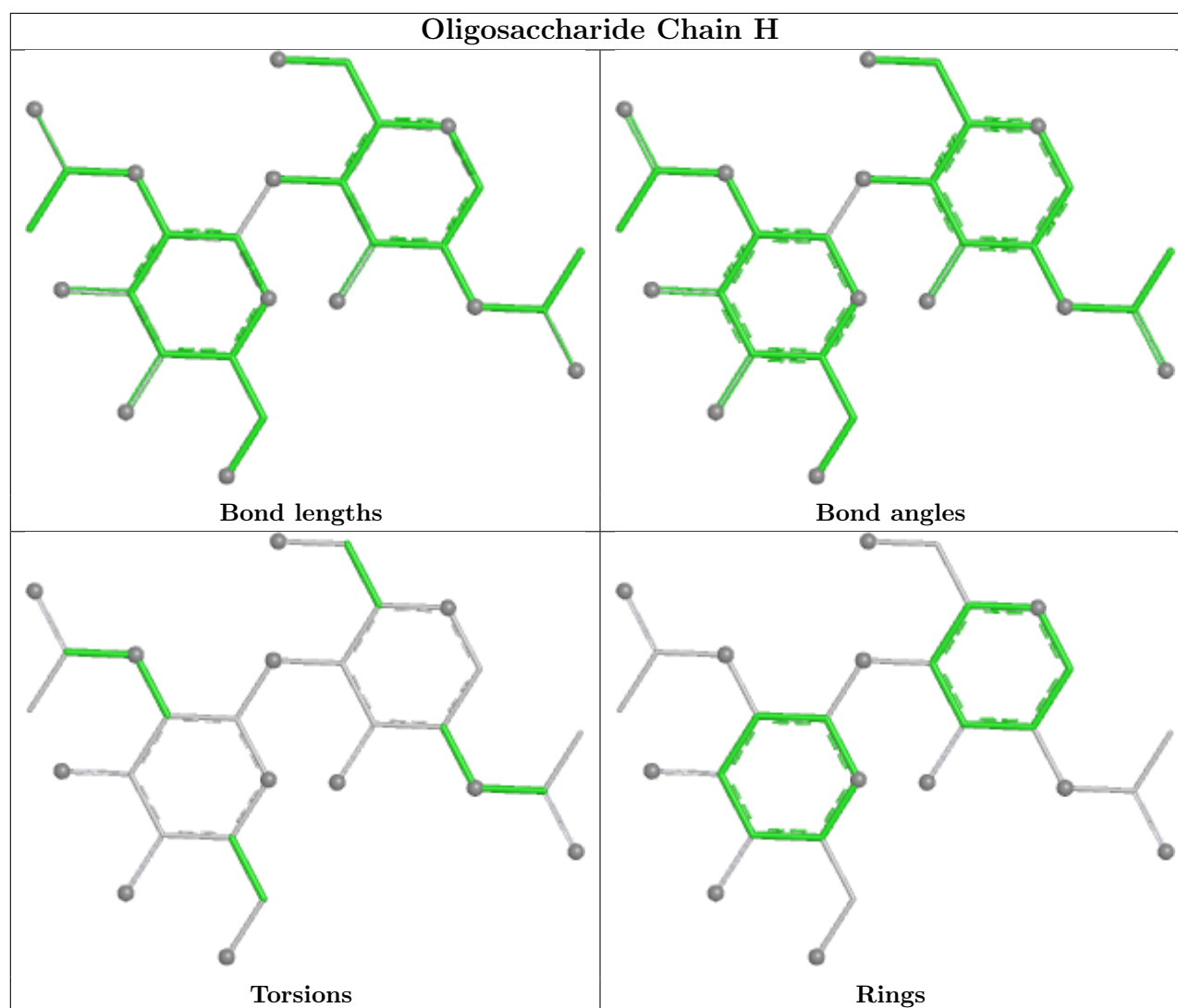
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0

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](#)

25 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	$\# Z > 2$
7	BOG	A	708	-	20,20,20	1.06	1 (5%)	25,25,25	1.07	2 (8%)
5	4LA	A	706[A]	-	37,46,46	1.93	6 (16%)	89,124,124	2.29	16 (17%)
4	NAG	C	705	1	14,14,15	0.26	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BOG	C	709	-	20,20,20	1.03	1 (5%)	25,25,25	1.12	2 (8%)
7	BOG	B	708	-	20,20,20	1.04	1 (5%)	25,25,25	1.15	2 (8%)
5	4LA	D	706[A]	-	37,46,46	1.98	6 (16%)	89,124,124	2.29	15 (16%)
4	NAG	A	702	1	14,14,15	0.31	0	17,19,21	0.35	0
4	NAG	D	702	1	14,14,15	0.31	0	17,19,21	0.33	0
6	N1B	A	707[B]	-	37,46,46	1.93	6 (16%)	89,124,124	2.33	17 (19%)
7	BOG	C	708	-	20,20,20	1.05	1 (5%)	25,25,25	1.05	3 (12%)
6	N1B	C	707[B]	-	37,46,46	1.87	6 (16%)	89,124,124	2.28	14 (15%)
4	NAG	B	705	1	14,14,15	0.27	0	17,19,21	0.44	0
3	HEM	C	701	1	50,50,50	2.09	20 (40%)	67,82,82	1.81	19 (28%)
4	NAG	D	705	1	14,14,15	0.20	0	17,19,21	0.42	0
3	HEM	D	701	1	50,50,50	2.18	20 (40%)	67,82,82	1.82	18 (26%)
3	HEM	A	701	1	50,50,50	2.24	21 (42%)	67,82,82	1.85	18 (26%)
4	NAG	B	702	1	14,14,15	0.30	0	17,19,21	0.36	0
5	4LA	B	706[A]	-	37,46,46	1.91	5 (13%)	89,124,124	2.36	17 (19%)
7	BOG	D	708	-	20,20,20	1.27	2 (10%)	25,25,25	1.13	2 (8%)
3	HEM	B	701	1,8	50,50,50	2.16	20 (40%)	67,82,82	1.80	17 (25%)
4	NAG	A	705	1	14,14,15	0.20	0	17,19,21	0.42	0
6	N1B	D	707[B]	-	37,46,46	1.98	6 (16%)	89,124,124	2.30	15 (16%)
6	N1B	B	707[B]	-	37,46,46	1.92	5 (13%)	89,124,124	2.35	17 (19%)
5	4LA	C	706[A]	-	37,46,46	1.88	5 (13%)	89,124,124	2.29	17 (19%)
4	NAG	C	702	1	14,14,15	0.31	0	17,19,21	0.37	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
7	BOG	A	708	-	-	3/11/31/31	0/1/1/1
5	4LA	A	706[A]	-	-	4/12/314/314	0/2/17/17
4	NAG	C	705	1	-	0/6/23/26	0/1/1/1
7	BOG	C	709	-	-	0/11/31/31	0/1/1/1
7	BOG	B	708	-	-	4/11/31/31	0/1/1/1
5	4LA	D	706[A]	-	-	6/12/314/314	0/2/17/17
4	NAG	A	702	1	-	2/6/23/26	0/1/1/1
4	NAG	D	702	1	-	2/6/23/26	0/1/1/1
6	N1B	A	707[B]	-	-	6/12/314/314	0/2/17/17

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BOG	C	708	-	-	1/11/31/31	0/1/1/1
6	N1B	C	707[B]	-	-	6/12/314/314	0/2/17/17
4	NAG	B	705	1	-	2/6/23/26	0/1/1/1
3	HEM	C	701	1	-	1/14/54/54	-
4	NAG	D	705	1	-	1/6/23/26	0/1/1/1
3	HEM	D	701	1	-	2/14/54/54	-
3	HEM	A	701	1	-	2/14/54/54	-
4	NAG	B	702	1	-	2/6/23/26	0/1/1/1
5	4LA	B	706[A]	-	-	6/12/314/314	0/2/17/17
7	BOG	D	708	-	-	5/11/31/31	0/1/1/1
3	HEM	B	701	1,8	-	0/14/54/54	-
4	NAG	A	705	1	-	0/6/23/26	0/1/1/1
6	N1B	D	707[B]	-	-	6/12/314/314	0/2/17/17
6	N1B	B	707[B]	-	-	5/12/314/314	0/2/17/17
5	4LA	C	706[A]	-	-	7/12/314/314	0/2/17/17
4	NAG	C	702	1	-	2/6/23/26	0/1/1/1

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	706[A]	4LA	C14-N07	6.75	1.44	1.34
6	D	707[B]	N1B	C14-N07	6.75	1.44	1.34
5	C	706[A]	4LA	C14-N07	6.49	1.44	1.34
6	C	707[B]	N1B	C14-N07	6.21	1.43	1.34
6	B	707[B]	N1B	C14-N07	5.22	1.42	1.34
5	A	706[A]	4LA	C14-N07	5.21	1.42	1.34
6	A	707[B]	N1B	C14-N07	5.21	1.42	1.34
5	B	706[A]	4LA	C14-N07	5.11	1.42	1.34
6	A	707[B]	N1B	C08-N07	-5.00	1.30	1.40
5	A	706[A]	4LA	C08-N07	-4.97	1.30	1.40
3	D	701	HEM	C1B-NB	-4.89	1.31	1.40
3	B	701	HEM	C1B-NB	-4.80	1.31	1.40
3	C	701	HEM	C1B-NB	-4.80	1.32	1.40
3	D	701	HEM	C4D-ND	-4.74	1.32	1.40
3	A	701	HEM	C4D-ND	-4.72	1.32	1.40
6	B	707[B]	N1B	C08-N07	-4.64	1.31	1.40
5	B	706[A]	4LA	C08-N07	-4.61	1.31	1.40
3	A	701	HEM	C1B-NB	-4.61	1.32	1.40
5	B	706[A]	4LA	C05-C04	-4.60	1.34	1.41
6	C	707[B]	N1B	C08-N07	-4.58	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	HEM	C4D-ND	-4.54	1.32	1.40
5	B	706[A]	4LA	C04-N07	-4.54	1.33	1.41
6	B	707[B]	N1B	C05-C04	-4.52	1.35	1.41
6	B	707[B]	N1B	C04-N07	-4.52	1.33	1.41
3	A	701	HEM	C3C-C4C	-4.44	1.38	1.46
3	D	701	HEM	FE-NB	4.43	2.08	1.94
6	A	707[B]	N1B	C04-N07	-4.42	1.34	1.41
3	A	701	HEM	FE-NB	4.41	2.08	1.94
5	A	706[A]	4LA	C04-N07	-4.41	1.34	1.41
3	B	701	HEM	C1C-C2C	-4.39	1.36	1.45
3	D	701	HEM	C3C-C4C	-4.32	1.38	1.46
5	D	706[A]	4LA	C08-N07	-4.32	1.31	1.40
6	D	707[B]	N1B	C08-N07	-4.31	1.31	1.40
3	C	701	HEM	FE-NB	4.30	2.08	1.94
5	C	706[A]	4LA	C08-N07	-4.24	1.32	1.40
3	C	701	HEM	C4D-ND	-4.03	1.33	1.40
3	D	701	HEM	C1C-C2C	-3.99	1.37	1.45
5	A	706[A]	4LA	B26-B21	-3.98	1.73	1.86
5	B	706[A]	4LA	B26-B21	-3.96	1.73	1.86
5	D	706[A]	4LA	C04-N07	-3.91	1.34	1.41
6	D	707[B]	N1B	C04-N07	-3.91	1.34	1.41
6	C	707[B]	N1B	B18-B17	-3.91	1.73	1.86
6	A	707[B]	N1B	B18-B17	-3.90	1.73	1.86
5	D	706[A]	4LA	B26-B21	-3.88	1.73	1.86
5	C	706[A]	4LA	B26-B21	-3.88	1.73	1.86
6	B	707[B]	N1B	B18-B17	-3.87	1.73	1.86
6	D	707[B]	N1B	B18-B17	-3.85	1.73	1.86
3	A	701	HEM	C1D-ND	-3.82	1.31	1.38
3	C	701	HEM	FE-ND	-3.81	1.83	1.94
3	B	701	HEM	C4B-NB	-3.78	1.31	1.38
3	A	701	HEM	C1C-C2C	-3.78	1.37	1.45
6	A	707[B]	N1B	C05-C04	-3.75	1.36	1.41
3	C	701	HEM	C1A-C2A	-3.74	1.37	1.44
3	A	701	HEM	C1A-C2A	-3.67	1.37	1.44
5	A	706[A]	4LA	C05-C04	-3.67	1.36	1.41
3	C	701	HEM	C1C-C2C	-3.62	1.38	1.45
3	B	701	HEM	FE-NB	3.61	2.06	1.94
3	A	701	HEM	FE-ND	-3.60	1.83	1.94
3	B	701	HEM	FE-ND	-3.56	1.83	1.94
3	D	701	HEM	C1D-ND	-3.54	1.31	1.38
3	C	701	HEM	C4B-NB	-3.49	1.32	1.38
3	B	701	HEM	C1D-ND	-3.48	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	701	HEM	FE-ND	-3.38	1.84	1.94
3	B	701	HEM	C1A-C2A	-3.37	1.37	1.44
3	B	701	HEM	FE-NC	3.37	2.06	1.95
3	D	701	HEM	C4B-NB	-3.36	1.32	1.38
3	C	701	HEM	C1D-ND	-3.35	1.32	1.38
3	D	701	HEM	C1A-C2A	-3.34	1.37	1.44
3	A	701	HEM	C4B-NB	-3.28	1.32	1.38
6	D	707[B]	N1B	C05-C04	-3.28	1.36	1.41
3	A	701	HEM	C4C-NC	-3.27	1.33	1.39
5	D	706[A]	4LA	C05-C04	-3.24	1.36	1.41
3	C	701	HEM	C3C-C4C	-3.22	1.40	1.46
3	D	701	HEM	C4A-NA	-3.18	1.33	1.39
3	D	701	HEM	O2D-CGD	-3.10	1.20	1.30
3	B	701	HEM	C1C-NC	-3.10	1.33	1.39
6	C	707[B]	N1B	C04-N07	-3.04	1.36	1.41
3	A	701	HEM	C1C-NC	-3.04	1.33	1.39
3	C	701	HEM	FE-NC	2.98	2.05	1.95
3	A	701	HEM	C1B-C2B	-2.97	1.38	1.44
3	D	701	HEM	C1B-C2B	-2.94	1.38	1.44
3	B	701	HEM	C3C-C4C	-2.94	1.40	1.46
3	A	701	HEM	C4A-NA	-2.89	1.34	1.39
7	D	708	BOG	O2-C2	-2.86	1.35	1.43
3	C	701	HEM	O2D-CGD	-2.83	1.21	1.30
3	B	701	HEM	C4C-NC	-2.77	1.34	1.39
3	B	701	HEM	O2D-CGD	-2.73	1.21	1.30
3	C	701	HEM	C1C-NC	-2.72	1.34	1.39
3	B	701	HEM	C1B-C2B	-2.66	1.39	1.44
3	D	701	HEM	C4C-NC	-2.64	1.34	1.39
3	C	701	HEM	C1B-C2B	-2.61	1.39	1.44
3	C	701	HEM	C2A-C3A	-2.60	1.32	1.38
3	A	701	HEM	O2D-CGD	-2.60	1.22	1.30
5	C	706[A]	4LA	C04-N07	-2.60	1.37	1.41
3	A	701	HEM	C2A-C3A	-2.57	1.32	1.38
3	B	701	HEM	C2A-C3A	-2.55	1.32	1.38
7	D	708	BOG	O3-C3	-2.50	1.36	1.43
3	A	701	HEM	C1A-NA	-2.44	1.35	1.39
3	A	701	HEM	FE-NC	2.41	2.03	1.95
7	A	708	BOG	O2-C2	-2.41	1.37	1.43
3	D	701	HEM	C1A-NA	-2.41	1.35	1.39
3	C	701	HEM	C4A-NA	-2.41	1.35	1.39
6	C	707[B]	N1B	C05-C04	-2.39	1.37	1.41
3	B	701	HEM	C1A-NA	-2.39	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	708	BOG	O2-C2	-2.38	1.37	1.43
7	C	709	BOG	O2-C2	-2.34	1.37	1.43
3	B	701	HEM	C3D-C2D	-2.34	1.31	1.36
7	B	708	BOG	O2-C2	-2.33	1.37	1.43
3	D	701	HEM	FE-NC	2.33	2.02	1.95
3	B	701	HEM	C4A-NA	-2.30	1.35	1.39
3	D	701	HEM	C3B-C2B	-2.30	1.32	1.37
3	D	701	HEM	C1C-NC	-2.29	1.35	1.39
3	A	701	HEM	C4A-C3A	-2.29	1.37	1.43
3	B	701	HEM	CHA-C1A	-2.28	1.34	1.39
3	D	701	HEM	C4A-C3A	-2.28	1.37	1.43
3	B	701	HEM	C4A-C3A	-2.27	1.37	1.43
5	A	706[A]	4LA	O29-C30	-2.27	1.40	1.45
6	A	707[B]	N1B	O29-C30	-2.25	1.40	1.45
3	D	701	HEM	C2A-C3A	-2.25	1.33	1.38
3	C	701	HEM	C1A-NA	-2.20	1.35	1.39
3	A	701	HEM	CHB-C4A	-2.17	1.34	1.39
3	A	701	HEM	CHA-C1A	-2.16	1.34	1.39
5	C	706[A]	4LA	C05-C04	-2.11	1.38	1.41
3	C	701	HEM	C3D-C2D	-2.11	1.32	1.36
5	D	706[A]	4LA	O29-C12	2.10	1.39	1.33
3	A	701	HEM	C3B-C2B	-2.09	1.32	1.37
3	D	701	HEM	C3D-C2D	-2.08	1.32	1.36
6	D	707[B]	N1B	O29-C12	2.06	1.39	1.33
6	C	707[B]	N1B	O29-C30	-2.04	1.40	1.45
3	C	701	HEM	C4C-NC	-2.02	1.35	1.39
3	C	701	HEM	C4A-C3A	-2.02	1.38	1.43
3	C	701	HEM	C3B-C2B	-2.00	1.33	1.37

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	706[A]	4LA	B25-B26-B21	14.90	106.24	91.02
6	C	707[B]	N1B	B24-B18-B17	14.86	106.20	91.02
5	C	706[A]	4LA	B25-B26-B21	14.79	106.13	91.02
6	B	707[B]	N1B	B24-B18-B17	14.74	106.09	91.02
6	A	707[B]	N1B	B24-B18-B17	14.73	106.07	91.02
6	D	707[B]	N1B	B24-B18-B17	14.72	106.06	91.02
5	D	706[A]	4LA	B25-B26-B21	14.69	106.03	91.02
5	A	706[A]	4LA	B25-B26-B21	14.50	105.84	91.02
6	D	707[B]	N1B	B17-B18-C22	9.11	59.77	54.90
5	D	706[A]	4LA	B21-B26-C22	9.10	59.77	54.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	707[B]	N1B	B17-B18-C22	9.09	59.76	54.90
6	A	707[B]	N1B	B17-B18-C22	9.06	59.75	54.90
5	B	706[A]	4LA	B21-B26-C22	9.02	59.72	54.90
5	A	706[A]	4LA	B21-B26-C22	8.94	59.68	54.90
6	C	707[B]	N1B	B17-B18-C22	8.84	59.63	54.90
5	C	706[A]	4LA	B21-B26-C22	8.83	59.62	54.90
3	B	701	HEM	CHC-C4B-NB	6.10	130.99	124.42
3	D	701	HEM	CHC-C4B-NB	4.85	129.64	124.42
5	B	706[A]	4LA	C04-N07-C08	4.83	111.74	107.80
5	A	706[A]	4LA	O29-C12-C11	4.79	120.95	111.28
6	A	707[B]	N1B	O29-C12-C11	4.78	120.94	111.28
5	B	706[A]	4LA	O29-C12-C11	4.77	120.91	111.28
6	B	707[B]	N1B	O29-C12-C11	4.76	120.89	111.28
6	B	707[B]	N1B	C04-N07-C08	4.76	111.68	107.80
5	C	706[A]	4LA	O29-C12-C11	4.66	120.68	111.28
5	C	706[A]	4LA	B23-C16-B17	-4.65	60.45	64.70
3	D	701	HEM	CHD-C4C-NC	4.59	129.46	124.45
6	B	707[B]	N1B	B23-C16-B21	-4.47	60.61	64.70
5	B	706[A]	4LA	B23-C16-B17	-4.47	60.61	64.70
6	C	707[B]	N1B	O29-C12-C11	4.42	120.21	111.28
3	C	701	HEM	CHC-C4B-NB	4.41	129.17	124.42
3	A	701	HEM	CHB-C1B-NB	4.37	129.78	124.37
6	A	707[B]	N1B	B23-C16-B21	-4.35	60.72	64.70
6	D	707[B]	N1B	B23-C16-B21	-4.31	60.76	64.70
6	C	707[B]	N1B	B23-C16-B21	-4.28	60.79	64.70
5	D	706[A]	4LA	B23-C16-B17	-4.24	60.83	64.70
5	A	706[A]	4LA	B23-C16-B17	-4.21	60.86	64.70
5	D	706[A]	4LA	O29-C12-C11	4.07	119.50	111.28
3	A	701	HEM	C3B-C4B-NB	-4.06	106.55	109.47
3	C	701	HEM	CHA-C4D-ND	4.05	129.37	124.37
6	D	707[B]	N1B	O29-C12-C11	4.04	119.44	111.28
5	B	706[A]	4LA	C10-C08-N07	4.04	128.12	122.07
3	A	701	HEM	CHA-C4D-ND	4.03	129.36	124.37
6	B	707[B]	N1B	C10-C08-N07	4.01	128.08	122.07
3	A	701	HEM	CHD-C4C-NC	3.97	128.78	124.45
3	C	701	HEM	CHA-C4D-C3D	-3.94	117.97	125.23
7	B	708	BOG	C1'-O1-C1	3.88	120.31	113.68
3	B	701	HEM	CHD-C1D-ND	3.83	128.54	124.42
3	C	701	HEM	CHB-C1B-NB	3.79	129.06	124.37
6	D	707[B]	N1B	C10-C08-N07	3.76	127.71	122.07
6	A	707[B]	N1B	C04-N07-C08	3.76	110.86	107.80
3	D	701	HEM	CHB-C1B-NB	3.75	129.00	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	706[A]	4LA	C10-C08-N07	3.75	127.69	122.07
3	A	701	HEM	C1B-NB-C4B	3.68	109.56	105.21
7	C	709	BOG	C1'-O1-C1	3.67	119.95	113.68
6	C	707[B]	N1B	C04-N07-C08	3.61	110.74	107.80
5	A	706[A]	4LA	C04-N07-C08	3.60	110.74	107.80
3	A	701	HEM	CHC-C4B-NB	3.60	128.30	124.42
3	B	701	HEM	C1B-NB-C4B	3.55	109.42	105.21
3	A	701	HEM	CHA-C4D-C3D	-3.53	118.73	125.23
6	A	707[B]	N1B	C10-C08-N07	3.51	127.33	122.07
3	D	701	HEM	CHA-C4D-C3D	-3.50	118.78	125.23
5	A	706[A]	4LA	C10-C08-N07	3.47	127.27	122.07
3	B	701	HEM	CHA-C4D-ND	3.47	128.66	124.37
6	A	707[B]	N1B	B25-B23-C16	-3.33	97.97	107.30
3	C	701	HEM	C1B-NB-C4B	3.33	109.16	105.21
7	A	708	BOG	C1'-O1-C1	3.31	119.33	113.68
6	D	707[B]	N1B	C04-N07-C08	3.30	110.49	107.80
5	D	706[A]	4LA	C04-N07-C08	3.25	110.45	107.80
3	C	701	HEM	O2D-CGD-O1D	-3.24	114.99	123.33
5	C	706[A]	4LA	C04-N07-C08	3.24	110.44	107.80
3	C	701	HEM	CHD-C1D-ND	3.24	127.91	124.42
5	D	706[A]	4LA	B24-B23-C16	-3.23	98.26	107.30
3	D	701	HEM	CHA-C4D-ND	3.22	128.35	124.37
3	B	701	HEM	CHA-C4D-C3D	-3.20	119.32	125.23
5	A	706[A]	4LA	B24-B23-C16	-3.19	98.38	107.30
5	B	706[A]	4LA	B24-B23-C16	-3.18	98.39	107.30
6	D	707[B]	N1B	B25-B23-C16	-3.17	98.44	107.30
7	D	708	BOG	C1'-O1-C1	3.09	118.96	113.68
5	C	706[A]	4LA	C03-C04-C05	-3.07	118.52	121.95
3	A	701	HEM	O2D-CGD-O1D	-3.04	115.52	123.33
6	B	707[B]	N1B	B25-B23-C16	-3.00	98.90	107.30
3	D	701	HEM	C3B-C4B-NB	-2.99	107.32	109.47
6	A	707[B]	N1B	B23-B25-B24	2.97	111.05	102.63
3	B	701	HEM	CHB-C1B-NB	2.96	128.02	124.37
6	C	707[B]	N1B	B25-B23-C16	-2.93	99.10	107.30
5	C	706[A]	4LA	B24-B23-C16	-2.91	99.16	107.30
5	B	706[A]	4LA	B23-B24-B25	2.89	110.84	102.63
6	A	707[B]	N1B	B24-B18-B20	2.86	107.73	103.71
6	D	707[B]	N1B	B23-B25-B24	2.85	110.72	102.63
5	D	706[A]	4LA	C04-C05-C09	-2.84	104.79	107.38
3	D	701	HEM	C1B-NB-C4B	2.84	108.57	105.21
3	A	701	HEM	O2D-CGD-CBD	2.84	122.97	114.00
3	B	701	HEM	CHD-C1D-C2D	-2.84	120.55	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	HEM	CHA-C1A-NA	2.81	128.96	123.86
3	C	701	HEM	C3B-C4B-NB	-2.80	107.45	109.47
6	D	707[B]	N1B	B24-B18-B20	2.80	107.65	103.71
3	A	701	HEM	C4A-CHB-C1B	-2.80	119.67	126.25
6	D	707[B]	N1B	C04-C05-C09	-2.80	104.83	107.38
6	C	707[B]	N1B	C03-C04-C05	-2.79	118.83	121.95
6	C	707[B]	N1B	B23-B25-B24	2.78	110.52	102.63
6	B	707[B]	N1B	B23-B25-B24	2.78	110.51	102.63
5	B	706[A]	4LA	B25-B26-B20	2.77	107.61	103.71
5	D	706[A]	4LA	B23-B24-B25	2.77	110.48	102.63
7	C	708	BOG	C1-O5-C5	-2.74	108.36	113.72
5	D	706[A]	4LA	C10-C08-C09	-2.74	123.78	128.07
6	D	707[B]	N1B	C10-C08-C09	-2.73	123.80	128.07
3	B	701	HEM	C1A-CHA-C4D	-2.73	119.84	126.25
6	B	707[B]	N1B	B24-B18-B20	2.73	107.54	103.71
5	D	706[A]	4LA	B25-B26-B20	2.72	107.54	103.71
3	C	701	HEM	O2D-CGD-CBD	2.72	122.59	114.00
6	C	707[B]	N1B	B24-B18-B20	2.71	107.52	103.71
5	C	706[A]	4LA	C10-C08-N07	2.70	126.11	122.07
6	C	707[B]	N1B	C10-C08-N07	2.70	126.11	122.07
3	D	701	HEM	CHD-C1D-ND	2.67	127.30	124.42
3	A	701	HEM	C1A-CHA-C4D	-2.67	119.98	126.25
3	D	701	HEM	C4C-CHD-C1D	-2.66	120.37	126.02
3	A	701	HEM	C4C-NC-C1C	2.66	110.15	105.82
5	C	706[A]	4LA	B25-B26-B20	2.65	107.44	103.71
3	A	701	HEM	CHD-C1D-ND	2.64	127.26	124.42
3	B	701	HEM	C4A-CHB-C1B	-2.63	120.05	126.25
5	A	706[A]	4LA	B25-B26-B20	2.63	107.41	103.71
5	C	706[A]	4LA	C04-C05-C09	-2.63	104.98	107.38
5	A	706[A]	4LA	C10-C08-C09	-2.62	123.97	128.07
5	A	706[A]	4LA	B23-B24-B25	2.60	110.01	102.63
3	D	701	HEM	O2D-CGD-O1D	-2.60	116.64	123.33
5	C	706[A]	4LA	B23-B24-B25	2.60	109.99	102.63
5	A	706[A]	4LA	C05-C09-C08	-2.59	105.87	108.13
3	D	701	HEM	C1C-CHC-C4B	-2.58	120.54	126.02
6	A	707[B]	N1B	C10-C08-C09	-2.58	124.03	128.07
3	B	701	HEM	O2D-CGD-O1D	-2.57	116.72	123.33
5	B	706[A]	4LA	B18-B20-B26	2.55	108.98	106.77
7	A	708	BOG	C1-O5-C5	-2.54	108.75	113.72
7	C	709	BOG	C1-O5-C5	-2.54	108.77	113.72
6	A	707[B]	N1B	C05-C09-C08	-2.54	105.92	108.13
6	B	707[B]	N1B	C10-C08-C09	-2.52	124.13	128.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	706[A]	4LA	C05-C09-C08	-2.51	105.94	108.13
7	C	708	BOG	O1-C1-C2	2.49	112.06	108.27
5	B	706[A]	4LA	C10-C08-C09	-2.49	124.17	128.07
3	C	701	HEM	C1A-CHA-C4D	-2.48	120.40	126.25
6	B	707[B]	N1B	C05-C09-C08	-2.48	105.96	108.13
6	C	707[B]	N1B	B26-B20-B18	2.48	108.93	106.77
5	A	706[A]	4LA	B19-B26-C22	2.48	109.46	103.28
6	A	707[B]	N1B	B26-B20-B18	2.46	108.91	106.77
6	B	707[B]	N1B	B26-B20-B18	2.46	108.91	106.77
5	C	706[A]	4LA	B18-B20-B26	2.46	108.91	106.77
6	B	707[B]	N1B	B19-B18-C22	2.44	109.35	103.28
6	A	707[B]	N1B	C30-O29-C12	-2.42	108.30	116.07
3	A	701	HEM	CHA-C1A-NA	2.42	128.25	123.86
3	D	701	HEM	C3D-C4D-ND	2.41	112.82	110.17
5	A	706[A]	4LA	C30-O29-C12	-2.41	108.34	116.07
5	C	706[A]	4LA	B19-B26-C22	2.41	109.29	103.28
6	D	707[B]	N1B	B19-B18-C22	2.41	109.28	103.28
3	C	701	HEM	CAC-C3C-C4C	2.41	130.57	124.82
3	C	701	HEM	C4A-CHB-C1B	-2.40	120.60	126.25
5	D	706[A]	4LA	B19-B26-C22	2.40	109.27	103.28
3	B	701	HEM	CAD-CBD-CGD	2.39	120.01	113.67
3	D	701	HEM	C1A-CHA-C4D	-2.39	120.62	126.25
3	A	701	HEM	CHB-C1B-C2B	-2.38	120.17	126.95
5	D	706[A]	4LA	B18-B20-B26	2.38	108.84	106.77
6	C	707[B]	N1B	B19-B18-C22	2.37	109.20	103.28
5	A	706[A]	4LA	B18-B20-B26	2.34	108.80	106.77
5	D	706[A]	4LA	B25-B26-B19	2.34	60.08	56.04
6	D	707[B]	N1B	B24-B18-B19	2.34	60.08	56.04
5	A	706[A]	4LA	B25-B26-B19	2.33	60.07	56.04
3	D	701	HEM	CHB-C1B-C2B	-2.33	120.33	126.95
6	C	707[B]	N1B	C04-C05-C09	-2.32	105.27	107.38
3	C	701	HEM	C4C-CHD-C1D	-2.31	121.10	126.02
6	D	707[B]	N1B	B26-B20-B18	2.31	108.78	106.77
3	B	701	HEM	CAC-C3C-C4C	2.31	130.34	124.82
5	B	706[A]	4LA	C30-O29-C12	-2.31	108.66	116.07
6	B	707[B]	N1B	B24-B18-B19	2.31	60.03	56.04
6	A	707[B]	N1B	B19-B18-C22	2.31	109.03	103.28
6	C	707[B]	N1B	B24-B18-B19	2.31	60.03	56.04
6	B	707[B]	N1B	C30-O29-C12	-2.30	108.69	116.07
6	A	707[B]	N1B	B24-B18-B19	2.30	60.01	56.04
3	A	701	HEM	C4C-CHD-C1D	-2.29	121.15	126.02
5	B	706[A]	4LA	B25-B26-B19	2.29	60.00	56.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	706[A]	4LA	B19-B26-C22	2.29	108.98	103.28
5	C	706[A]	4LA	B25-B26-B19	2.28	59.99	56.04
7	B	708	BOG	C1-O5-C5	-2.25	109.32	113.72
7	C	708	BOG	C1'-O1-C1	2.25	117.53	113.68
3	C	701	HEM	C3D-C4D-ND	2.24	112.63	110.17
7	D	708	BOG	O5-C1-O1	-2.21	104.82	110.04
3	B	701	HEM	C4C-CHD-C1D	-2.21	121.32	126.02
3	A	701	HEM	O2A-CGA-CBA	2.20	120.97	114.00
5	B	706[A]	4LA	O29-C12-O13	-2.17	116.71	123.20
6	B	707[B]	N1B	O29-C12-O13	-2.17	116.73	123.20
3	D	701	HEM	CBD-CAD-C3D	-2.17	106.55	112.53
3	D	701	HEM	C4A-CHB-C1B	-2.16	121.17	126.25
5	C	706[A]	4LA	C30-O29-C12	-2.15	109.17	116.07
3	C	701	HEM	CHB-C1B-C2B	-2.14	120.88	126.95
3	B	701	HEM	C3B-C4B-NB	-2.13	107.94	109.47
3	C	701	HEM	CHA-C1A-NA	2.11	127.68	123.86
5	B	706[A]	4LA	B23-C16-B21	-2.10	112.73	115.58
6	B	707[B]	N1B	B23-C16-B17	-2.09	112.74	115.58
3	C	701	HEM	CBB-CAB-C3B	-2.08	117.13	127.53
5	C	706[A]	4LA	B23-C16-B21	-2.06	112.78	115.58
6	A	707[B]	N1B	B25-B26-B21	-2.06	105.86	110.74
3	B	701	HEM	O2D-CGD-CBD	2.06	120.50	114.00
5	C	706[A]	4LA	C12-C11-C09	-2.05	108.53	113.49
3	A	701	HEM	CBD-CAD-C3D	-2.05	106.86	112.53
3	C	701	HEM	CHD-C4C-NC	2.05	126.68	124.45
3	C	701	HEM	C4C-NC-C1C	2.04	109.15	105.82
3	D	701	HEM	CHA-C1A-NA	2.04	127.56	123.86
6	D	707[B]	N1B	C05-C09-C08	-2.03	106.36	108.13
3	D	701	HEM	CHC-C1C-NC	2.03	126.66	124.45
6	A	707[B]	N1B	C04-C05-C09	-2.02	105.53	107.38
5	D	706[A]	4LA	C05-C09-C08	-2.02	106.37	108.13
5	A	706[A]	4LA	B24-B18-B17	-2.01	105.98	110.74
3	B	701	HEM	CHC-C4B-C3B	-2.00	121.07	125.07

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	HEM	C2C-C3C-CAC-CBC
5	B	706[A]	4LA	O15-C14-C16-B21
6	A	707[B]	N1B	O15-C14-C16-B17
7	B	708	BOG	C2-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
7	B	708	BOG	O5-C1-O1-C1'
7	D	708	BOG	C2'-C1'-O1-C1
5	C	706[A]	4LA	C11-C12-O29-C30
6	C	707[B]	N1B	C11-C12-O29-C30
4	C	702	NAG	O5-C5-C6-O6
5	A	706[A]	4LA	O13-C12-O29-C30
5	B	706[A]	4LA	O13-C12-O29-C30
5	C	706[A]	4LA	O13-C12-O29-C30
6	A	707[B]	N1B	O13-C12-O29-C30
6	B	707[B]	N1B	O13-C12-O29-C30
6	C	707[B]	N1B	O13-C12-O29-C30
5	A	706[A]	4LA	C11-C12-O29-C30
5	B	706[A]	4LA	C11-C12-O29-C30
6	A	707[B]	N1B	C11-C12-O29-C30
6	B	707[B]	N1B	C11-C12-O29-C30
4	B	702	NAG	O5-C5-C6-O6
4	A	702	NAG	O5-C5-C6-O6
4	D	702	NAG	O5-C5-C6-O6
4	B	702	NAG	C4-C5-C6-O6
4	C	702	NAG	C4-C5-C6-O6
4	A	702	NAG	C4-C5-C6-O6
4	D	702	NAG	C4-C5-C6-O6
5	B	706[A]	4LA	C06-C01-O27-C28
6	B	707[B]	N1B	C06-C01-O27-C28
5	B	706[A]	4LA	C02-C01-O27-C28
6	B	707[B]	N1B	C02-C01-O27-C28
6	D	707[B]	N1B	C06-C01-O27-C28
5	D	706[A]	4LA	C06-C01-O27-C28
7	A	708	BOG	C4'-C5'-C6'-C7'
5	D	706[A]	4LA	C02-C01-O27-C28
6	D	707[B]	N1B	C02-C01-O27-C28
7	D	708	BOG	O5-C5-C6-O6
7	C	708	BOG	C4'-C5'-C6'-C7'
3	D	701	HEM	C2B-C3B-CAB-CBB
3	A	701	HEM	C4C-C3C-CAC-CBC
4	B	705	NAG	C4-C5-C6-O6
7	A	708	BOG	C3'-C4'-C5'-C6'
7	B	708	BOG	O5-C5-C6-O6
5	D	706[A]	4LA	C11-C12-O29-C30
6	D	707[B]	N1B	C11-C12-O29-C30
5	C	706[A]	4LA	C02-C01-O27-C28
7	D	708	BOG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
5	C	706[A]	4LA	C06-C01-O27-C28
5	D	706[A]	4LA	C09-C11-C12-O29
6	D	707[B]	N1B	C09-C11-C12-O29
4	B	705	NAG	O5-C5-C6-O6
7	D	708	BOG	C5'-C6'-C7'-C8'
5	D	706[A]	4LA	C09-C11-C12-O13
6	D	707[B]	N1B	C09-C11-C12-O13
5	A	706[A]	4LA	C09-C11-C12-O29
6	A	707[B]	N1B	C09-C11-C12-O29
5	D	706[A]	4LA	O13-C12-O29-C30
6	D	707[B]	N1B	O13-C12-O29-C30
5	C	706[A]	4LA	O15-C14-N07-C08
6	A	707[B]	N1B	O15-C14-N07-C08
6	C	707[B]	N1B	C02-C01-O27-C28
5	A	706[A]	4LA	C09-C11-C12-O13
6	A	707[B]	N1B	C09-C11-C12-O13
3	D	701	HEM	C4B-C3B-CAB-CBB
6	C	707[B]	N1B	C06-C01-O27-C28
4	D	705	NAG	C4-C5-C6-O6
7	D	708	BOG	C3'-C4'-C5'-C6'
6	C	707[B]	N1B	C09-C11-C12-O29
7	A	708	BOG	O1-C1'-C2'-C3'
6	C	707[B]	N1B	C09-C11-C12-O13
5	B	706[A]	4LA	C09-C11-C12-O29
5	C	706[A]	4LA	C09-C11-C12-O29
6	B	707[B]	N1B	C09-C11-C12-O29
7	B	708	BOG	O1-C1'-C2'-C3'
3	C	701	HEM	CAD-CBD-CGD-O2D
5	C	706[A]	4LA	C09-C11-C12-O13

There are no ring outliers.

15 monomers are involved in 33 short contacts:

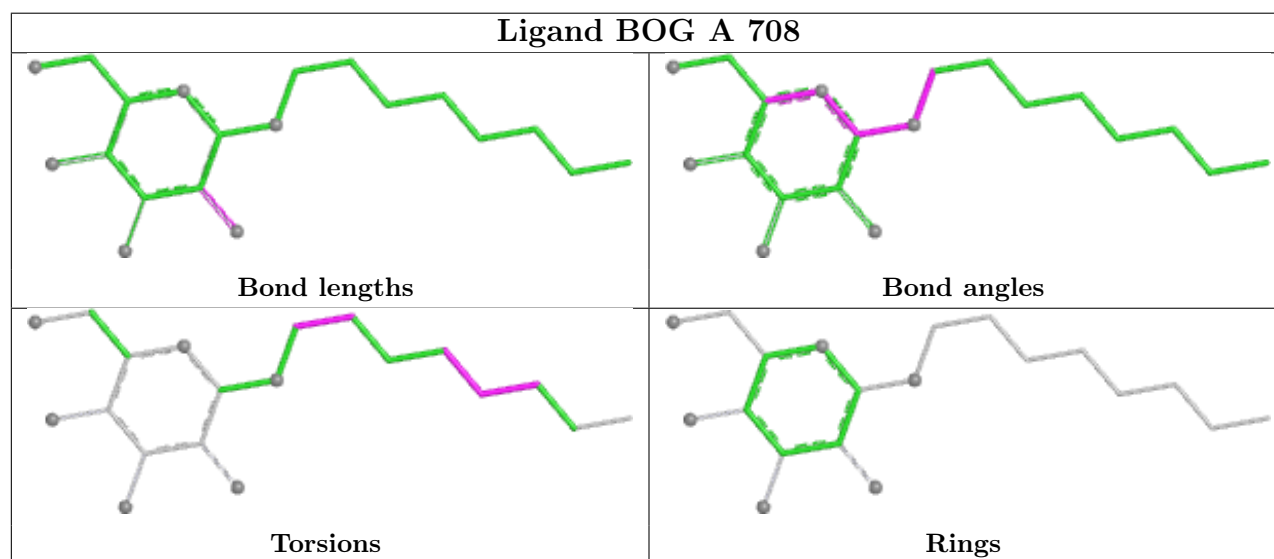
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	708	BOG	1	0
5	A	706[A]	4LA	2	0
7	C	709	BOG	2	0
5	D	706[A]	4LA	2	0
6	A	707[B]	N1B	2	0
7	C	708	BOG	1	0
6	C	707[B]	N1B	3	0
3	D	701	HEM	4	0

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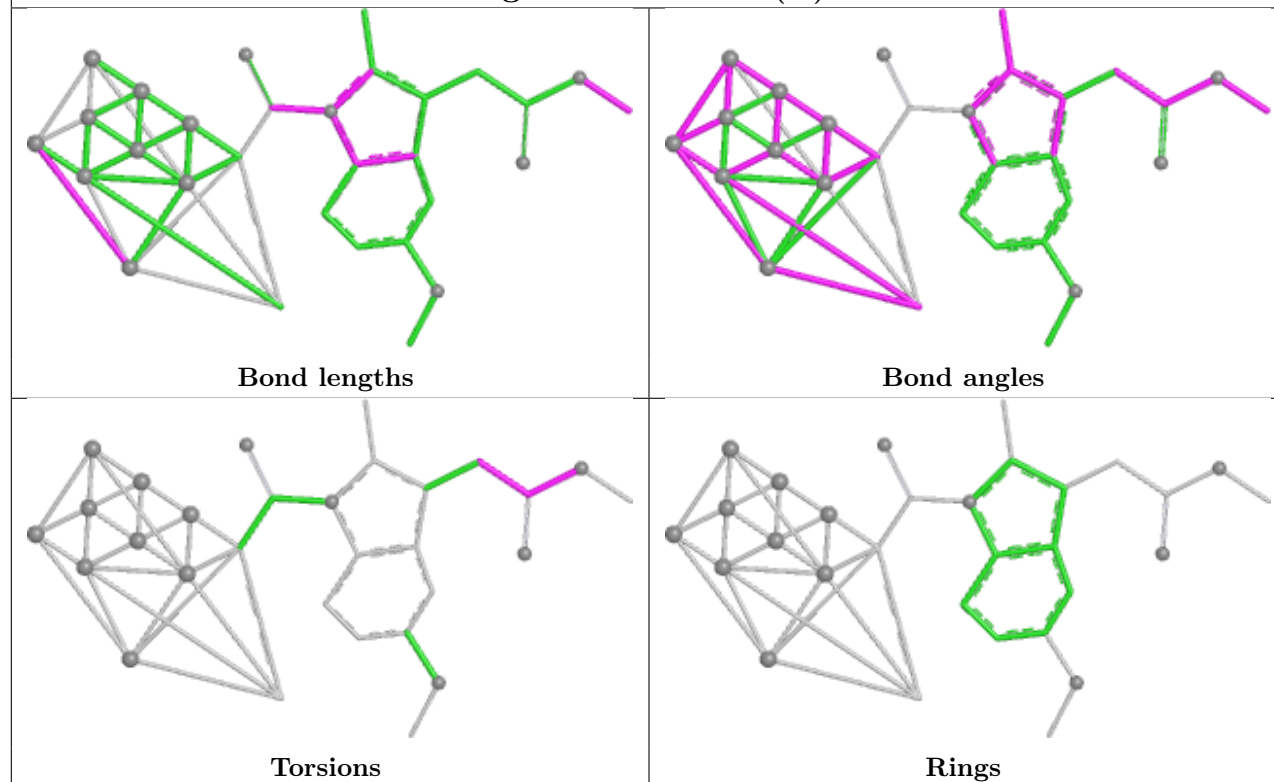
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	HEM	2	0
5	B	706[A]	4LA	1	0
7	D	708	BOG	1	0
3	B	701	HEM	3	0
6	D	707[B]	N1B	3	0
6	B	707[B]	N1B	1	0
5	C	706[A]	4LA	5	0

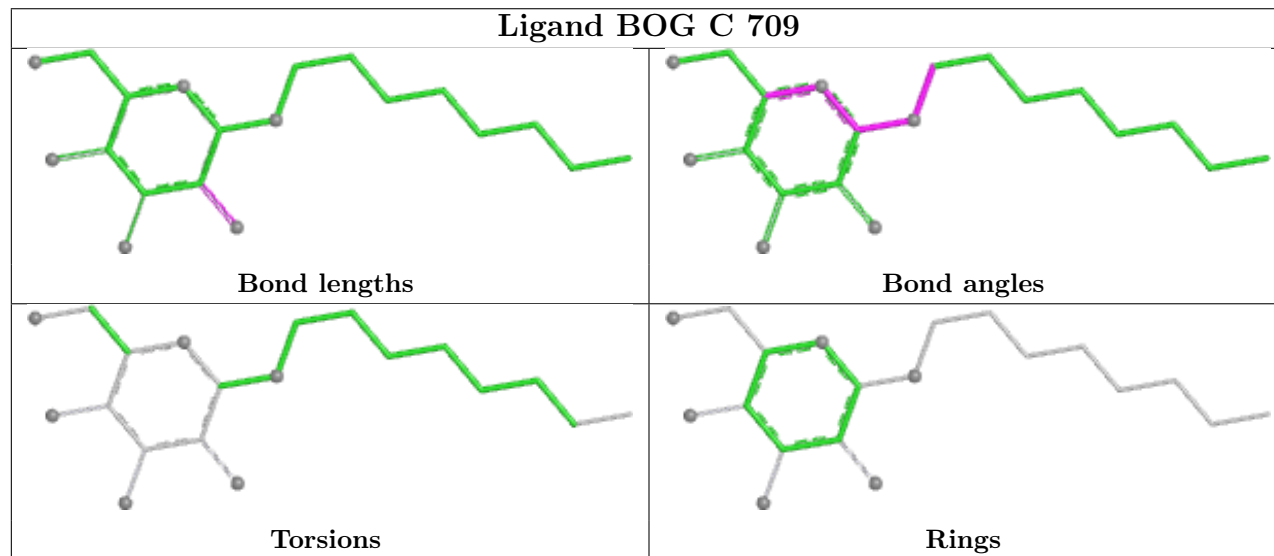
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

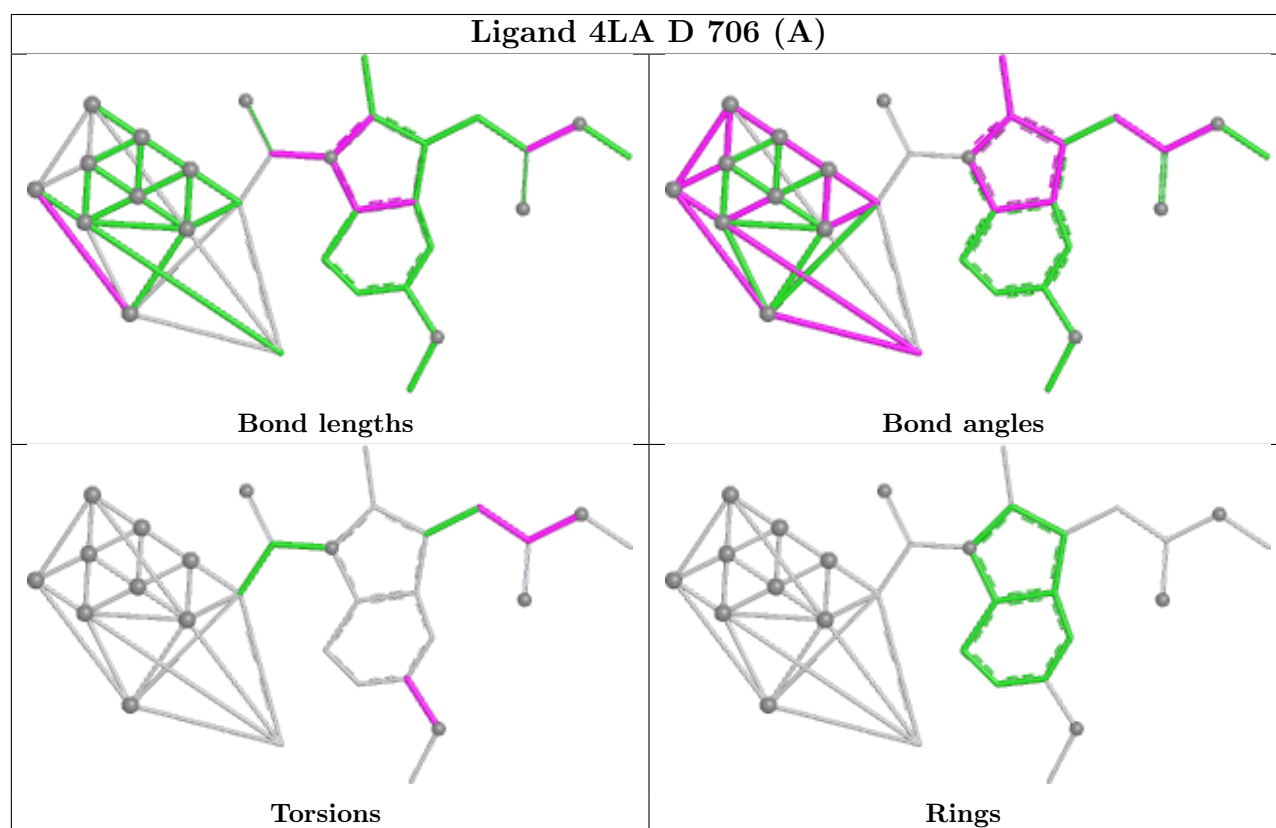
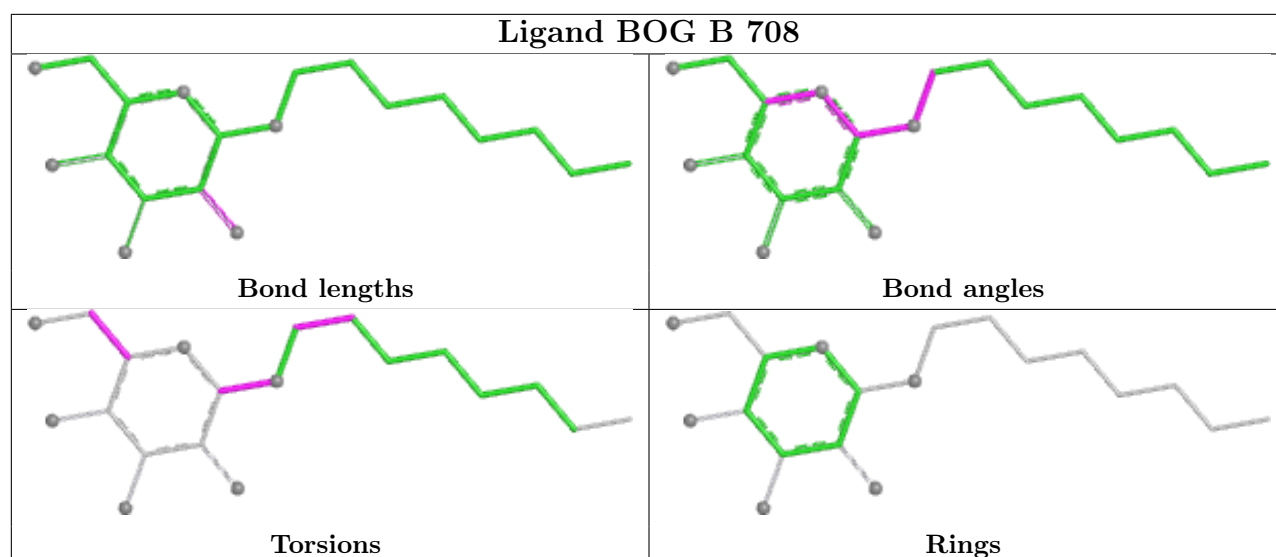


Ligand 4LA A 706 (A)

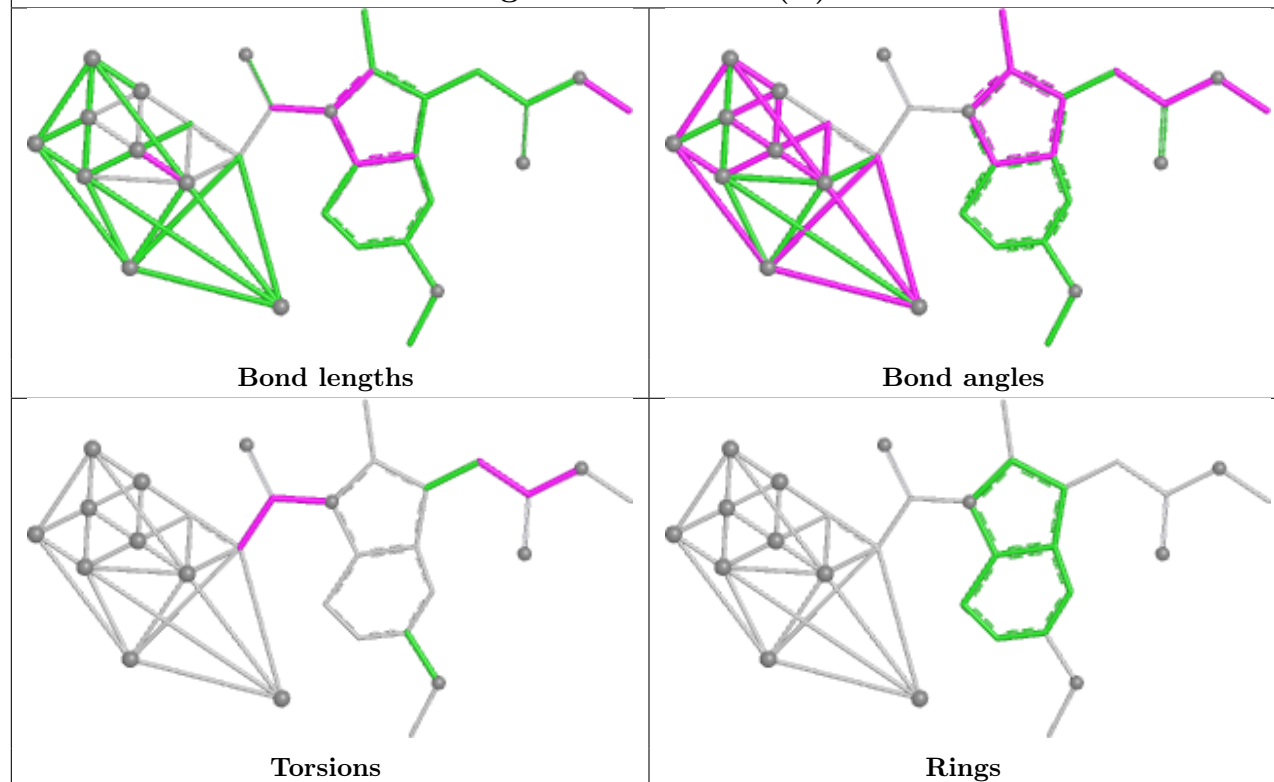


Ligand BOG C 709

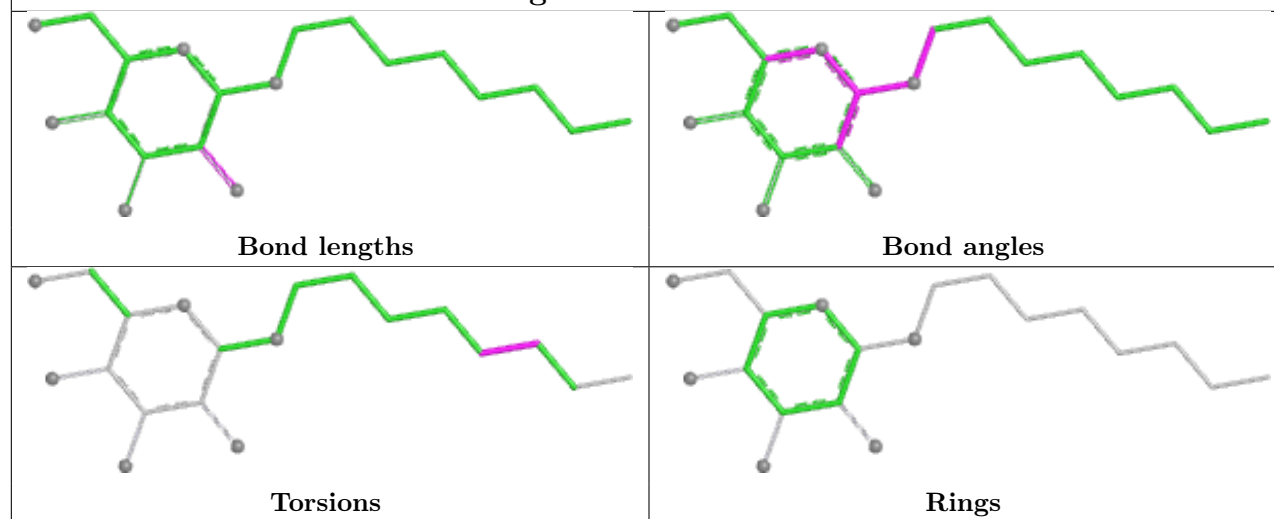


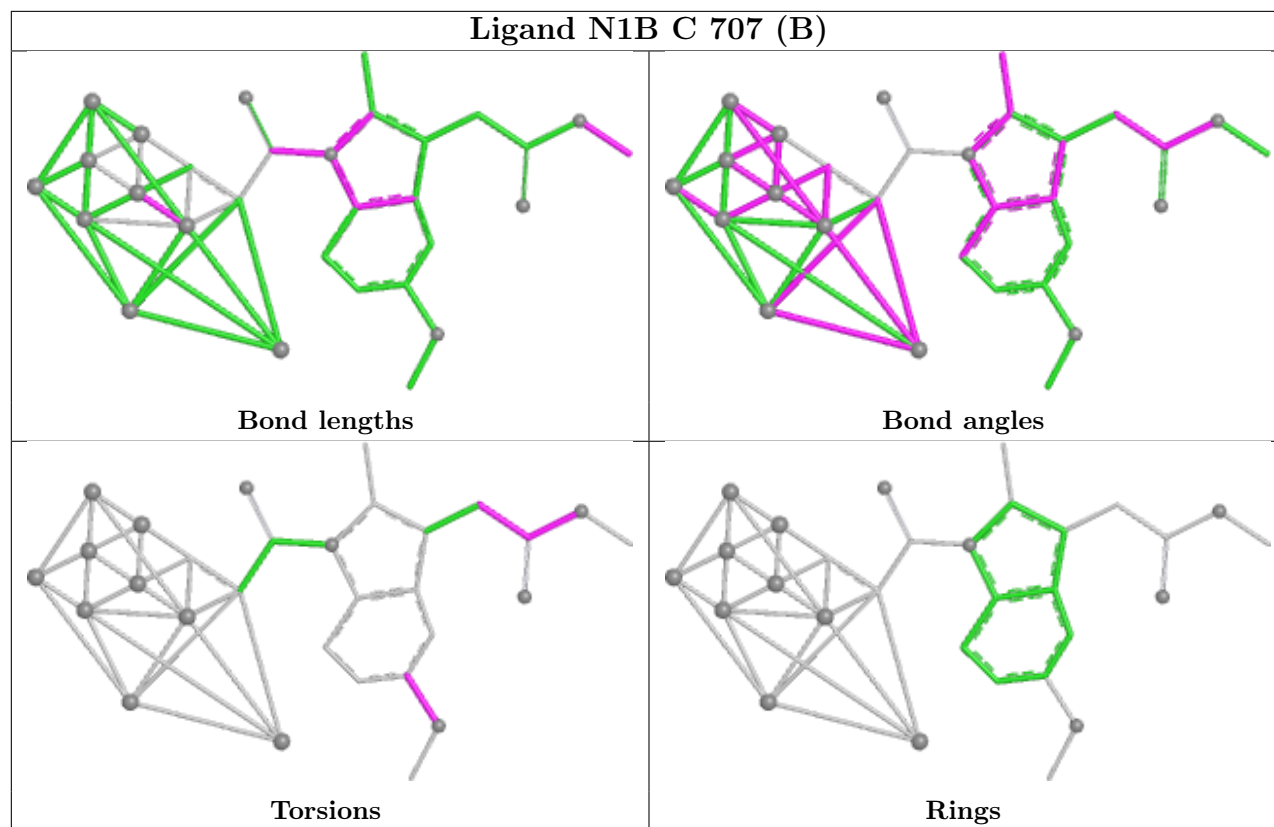


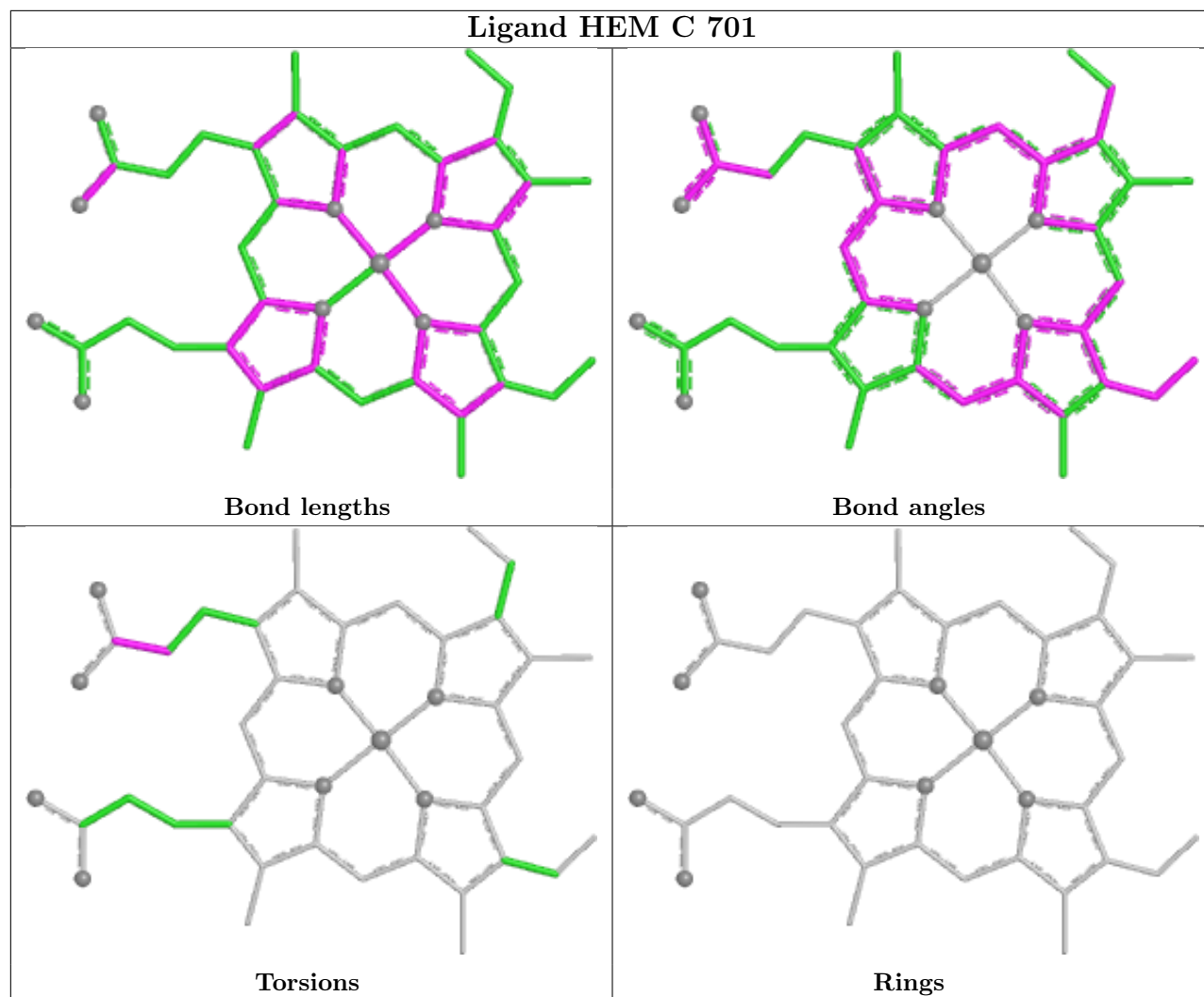
Ligand N1B A 707 (B)

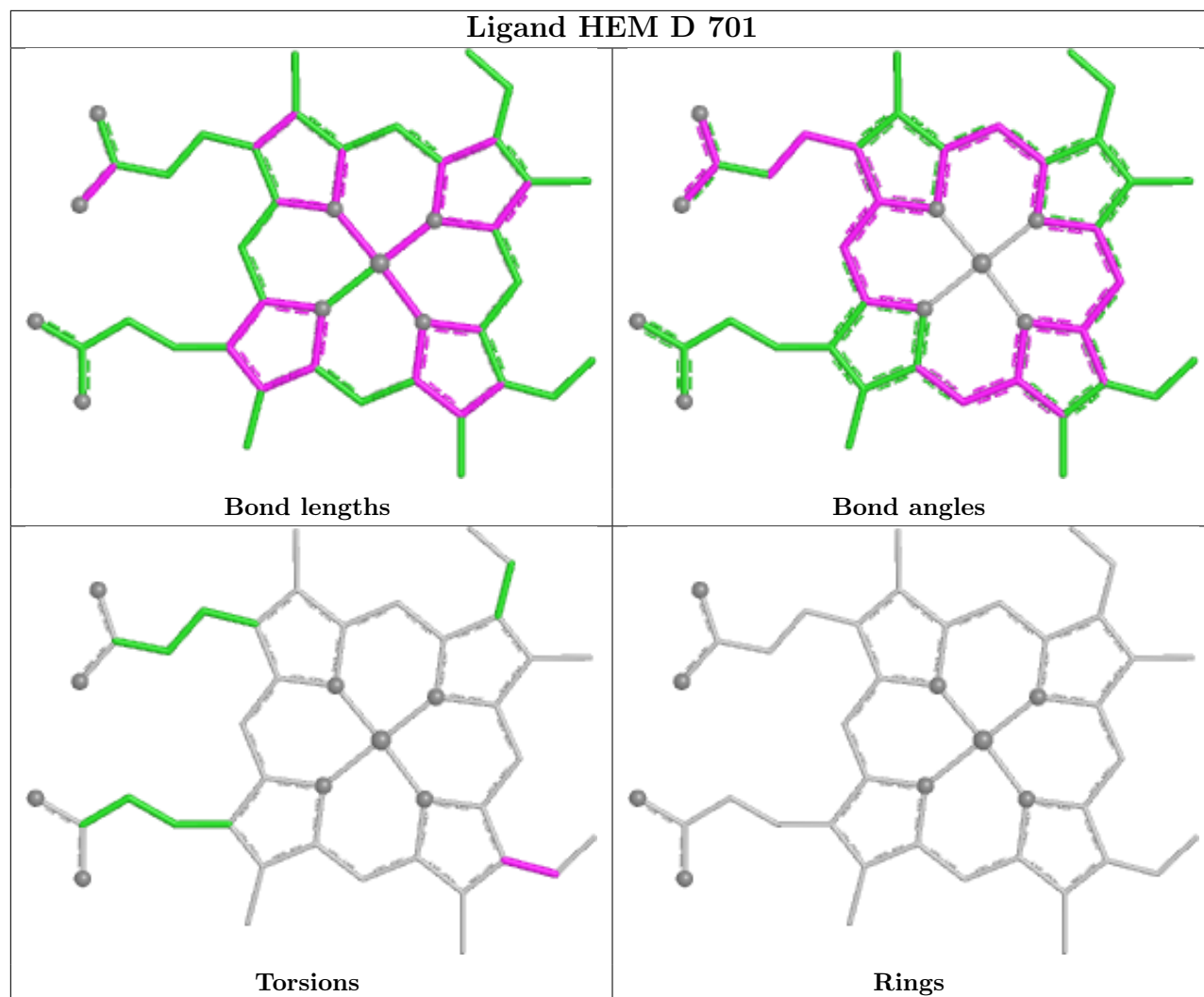


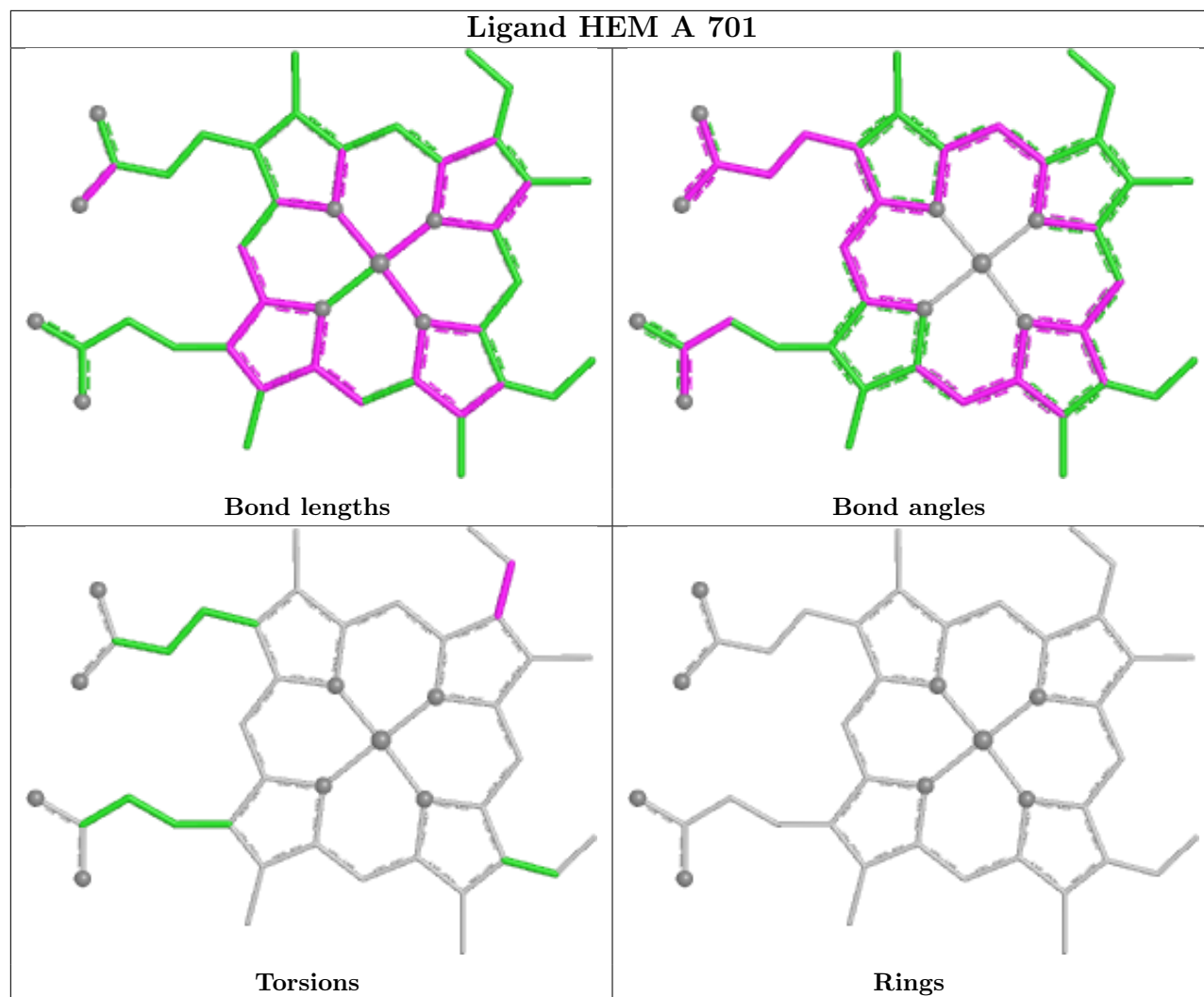
Ligand BOG C 708



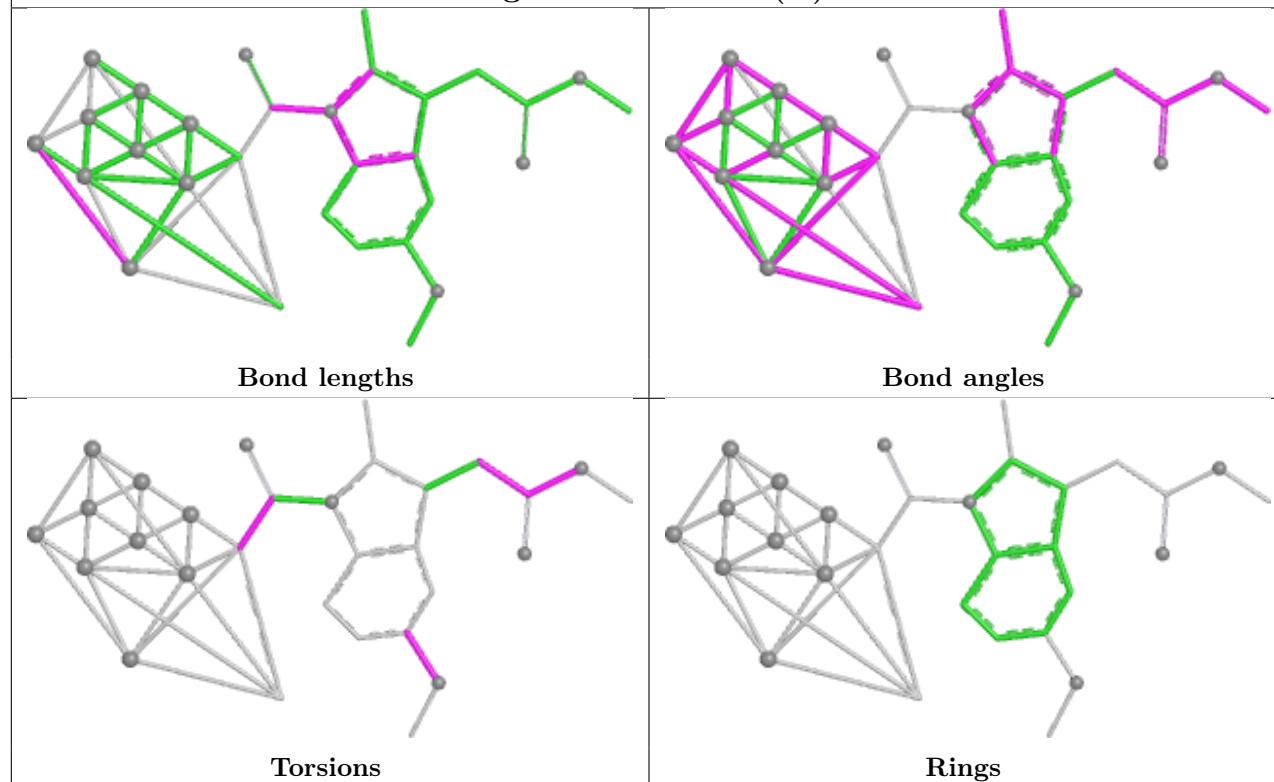




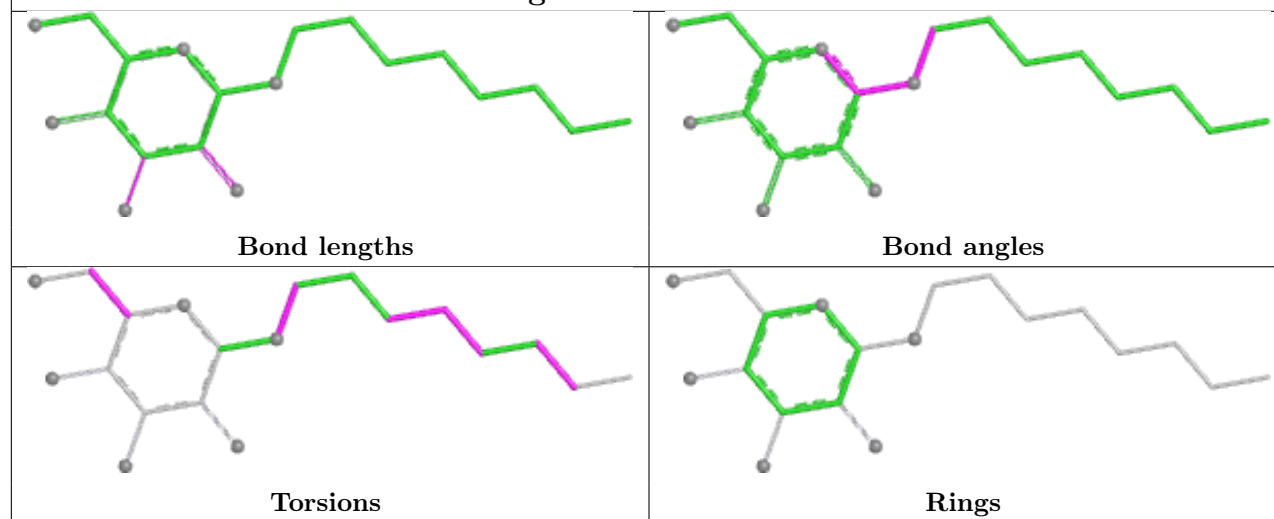


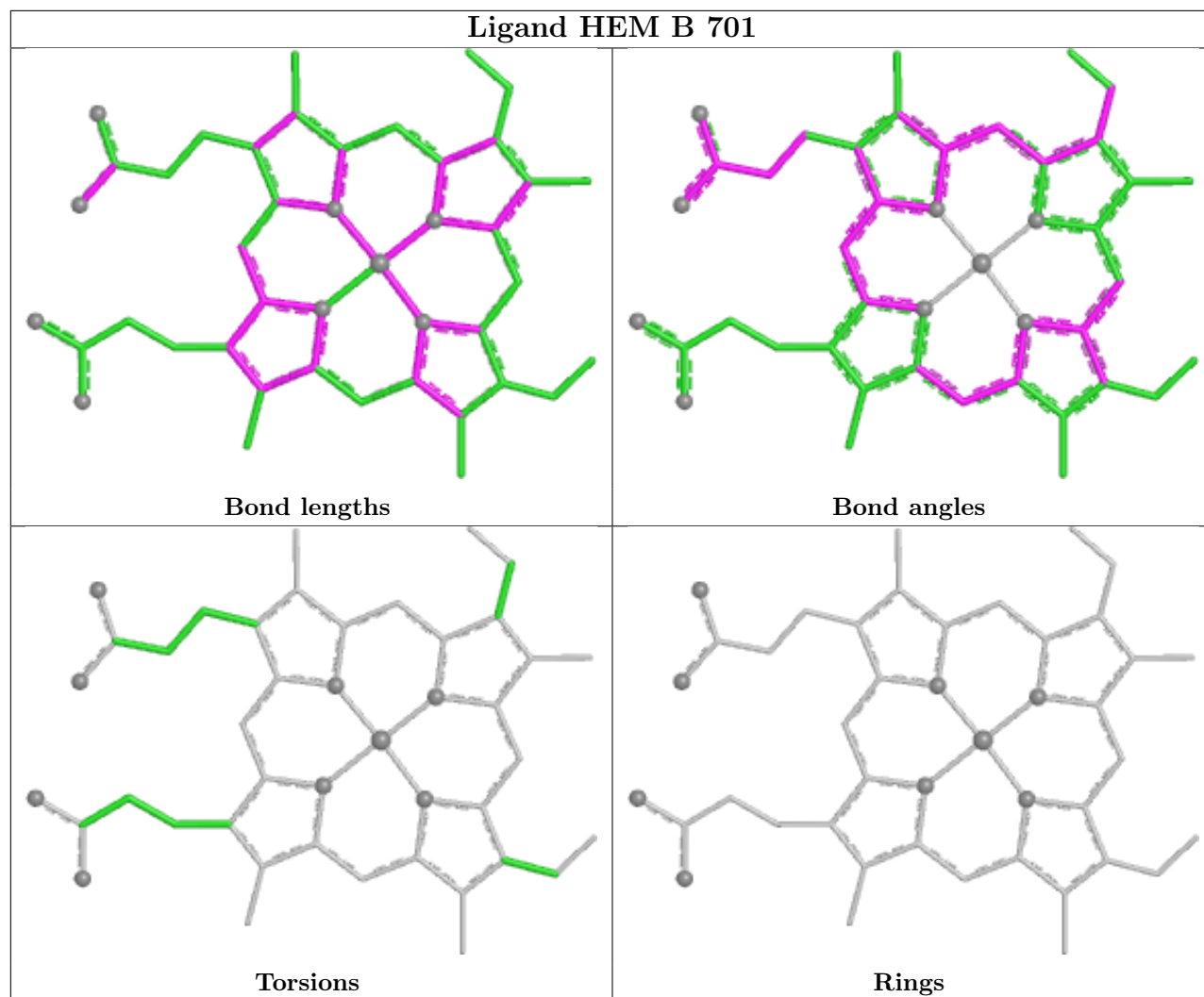


Ligand 4LA B 706 (A)

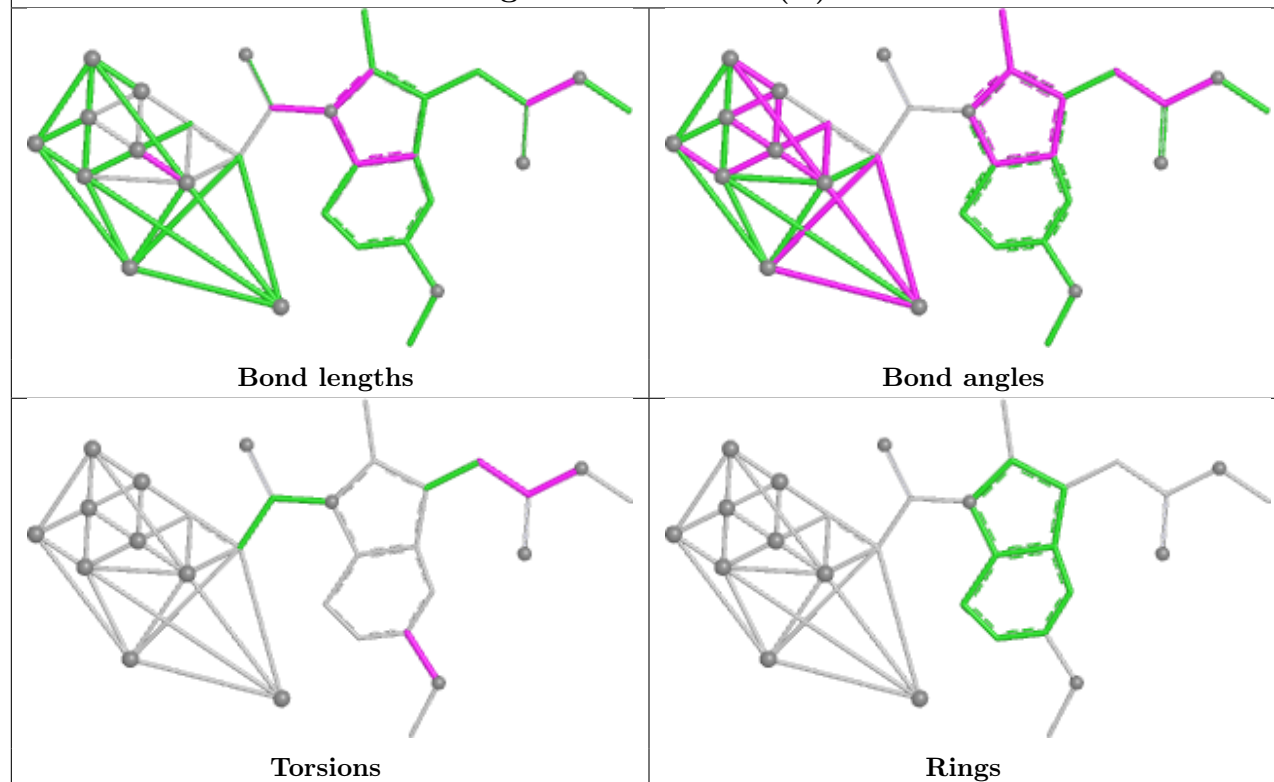


Ligand BOG D 708

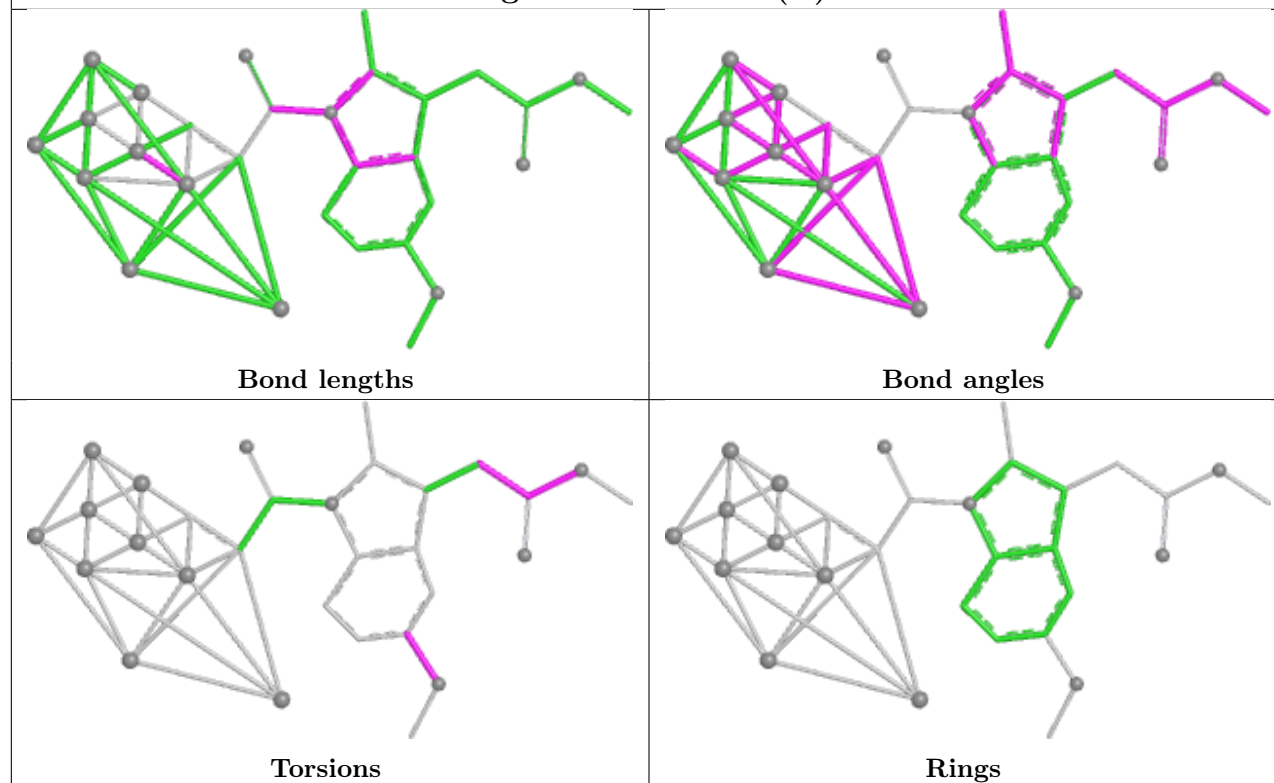


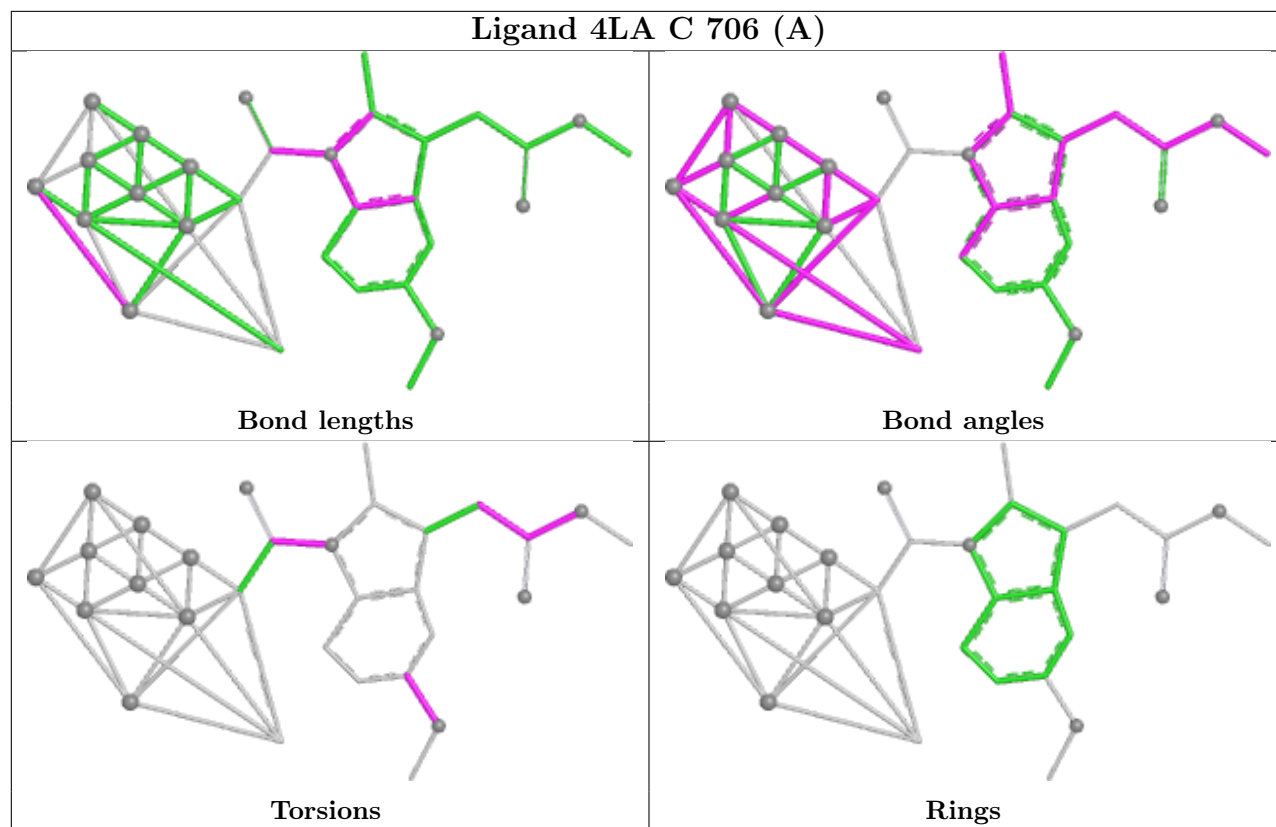


Ligand N1B D 707 (B)



Ligand N1B B 707 (B)





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	551/587 (93%)	0.47	21 (3%)	44 46	27, 52, 77, 95	1 (0%)
1	B	551/587 (93%)	0.43	12 (2%)	62 64	26, 50, 76, 97	1 (0%)
1	C	551/587 (93%)	0.39	15 (2%)	56 58	24, 49, 73, 99	1 (0%)
1	D	551/587 (93%)	0.34	14 (2%)	58 60	24, 47, 73, 102	1 (0%)
All	All	2204/2348 (93%)	0.41	62 (2%)	55 57	24, 50, 75, 102	4 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	ASP	4.0
1	C	399	ASP	3.9
1	C	75	LEU	3.3
1	B	122	TYR	3.3
1	C	122	TYR	3.0
1	A	413	ILE	3.0
1	D	122	TYR	2.9
1	D	268	ASP	2.9
1	C	107	PHE	2.9
1	B	360	LYS	2.8
1	A	122	TYR	2.8
1	C	33	ALA	2.7
1	D	409	TYR	2.7
1	B	239	ASP	2.7
1	A	186	GLU	2.7
1	A	364	GLU	2.7
1	A	115	TYR	2.7
1	B	115	TYR	2.7
1	D	281	GLU	2.6
1	C	409	TYR	2.6
1	D	360	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	283	LEU	2.5
1	A	33	ALA	2.5
1	A	51	GLY	2.5
1	C	74	PHE	2.5
1	A	409	TYR	2.5
1	C	239	ASP	2.5
1	B	33	ALA	2.5
1	D	566	SER	2.4
1	B	409	TYR	2.4
1	B	165	VAL	2.4
1	A	239	ASP	2.3
1	A	397	ILE	2.3
1	D	282	ASN	2.3
1	D	497	ASP	2.3
1	A	555	GLY	2.3
1	C	294	LEU	2.3
1	C	81	LEU	2.3
1	D	253	LYS	2.3
1	B	107	PHE	2.2
1	A	270	GLN	2.2
1	A	402	TYR	2.2
1	C	419	LEU	2.2
1	D	294	LEU	2.2
1	B	268	ASP	2.2
1	B	499	ASP	2.2
1	B	281	GLU	2.2
1	C	169	LYS	2.2
1	A	75	LEU	2.1
1	A	414	LEU	2.1
1	C	112	ILE	2.1
1	D	239	ASP	2.1
1	A	215	LYS	2.1
1	A	416	GLU	2.1
1	A	269	THR	2.1
1	A	81	LEU	2.1
1	C	416	GLU	2.1
1	D	295	VAL	2.1
1	C	493	ALA	2.1
1	A	268	ASP	2.1
1	B	169	LYS	2.0
1	D	123	LEU	2.0

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

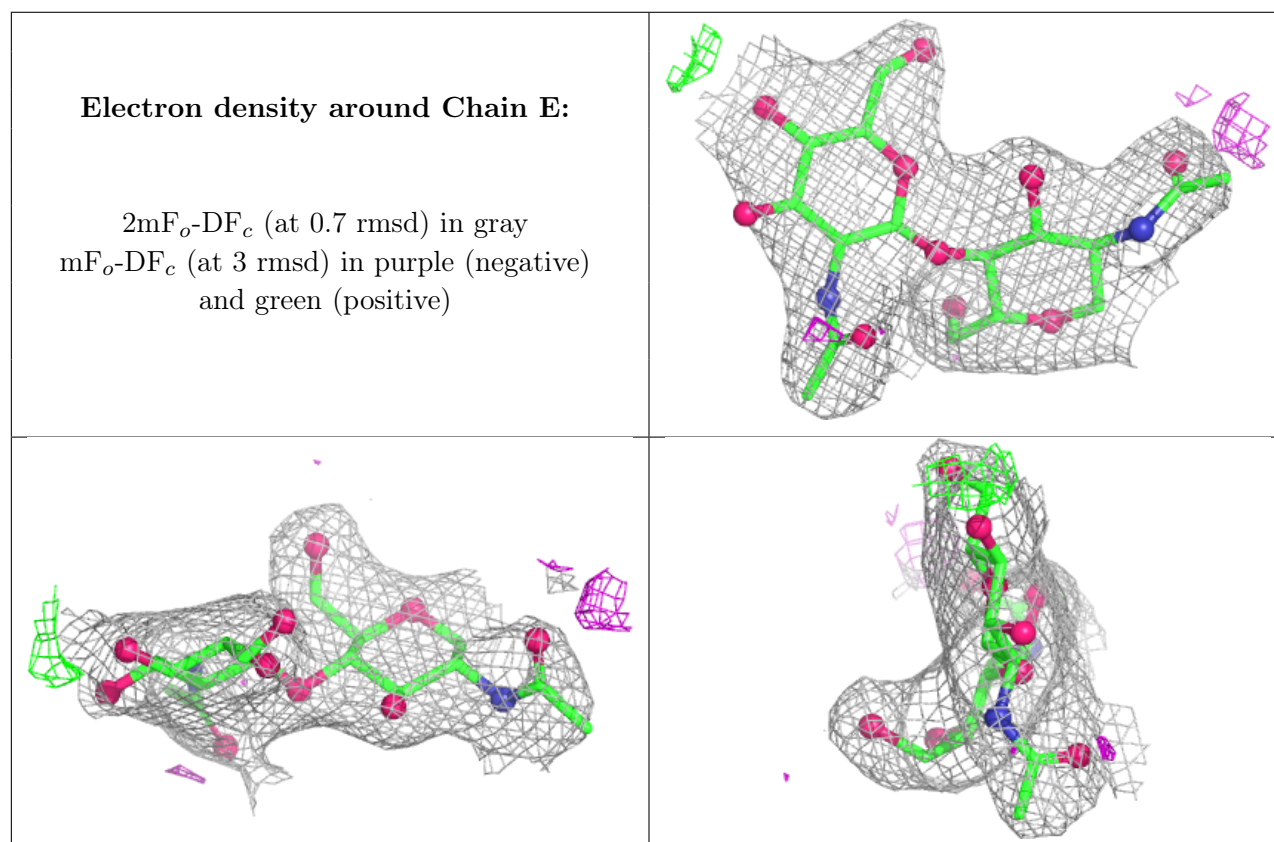
There are no non-standard protein/DNA/RNA residues in this entry.

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.

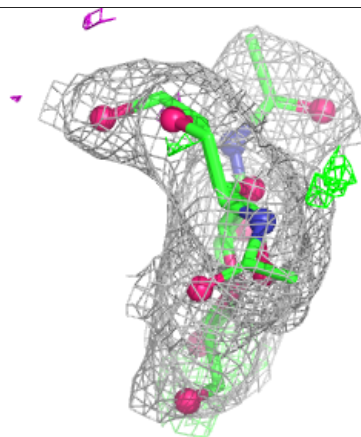
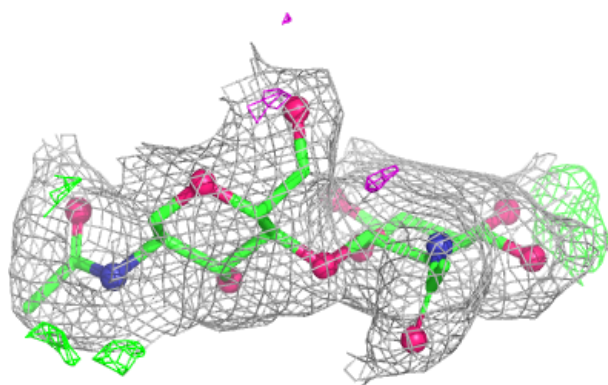
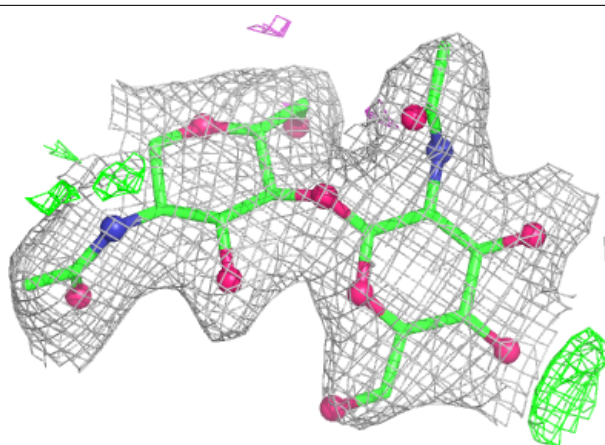
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.83	0.12	67,70,76,76	0
2	NAG	F	2	14/15	0.85	0.12	62,67,73,75	0
2	NAG	H	2	14/15	0.85	0.11	61,66,72,75	0
2	NAG	G	2	14/15	0.87	0.11	64,68,72,73	0
2	NAG	H	1	14/15	0.93	0.09	40,49,54,60	0
2	NAG	F	1	14/15	0.93	0.08	45,48,56,62	0
2	NAG	G	1	14/15	0.94	0.07	37,45,55,62	0
2	NAG	E	1	14/15	0.94	0.08	35,49,54,62	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.



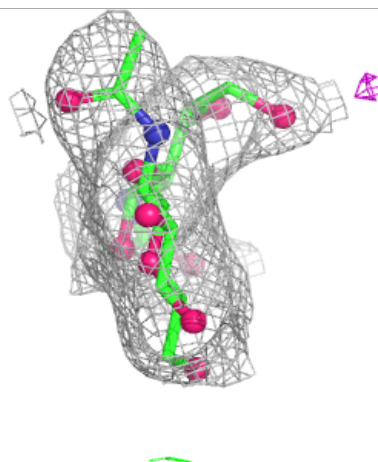
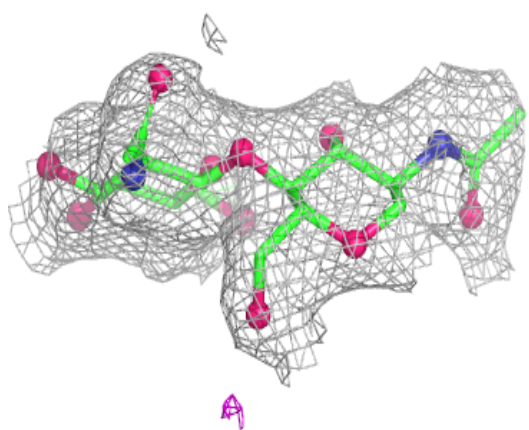
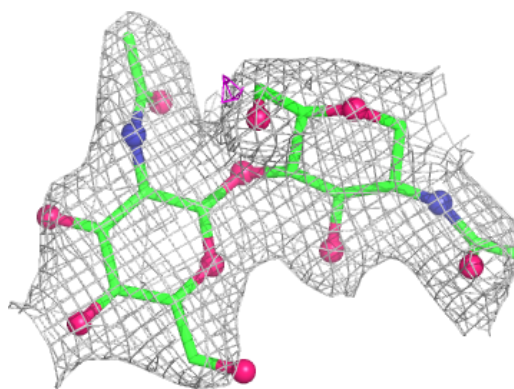
Electron density around Chain F:

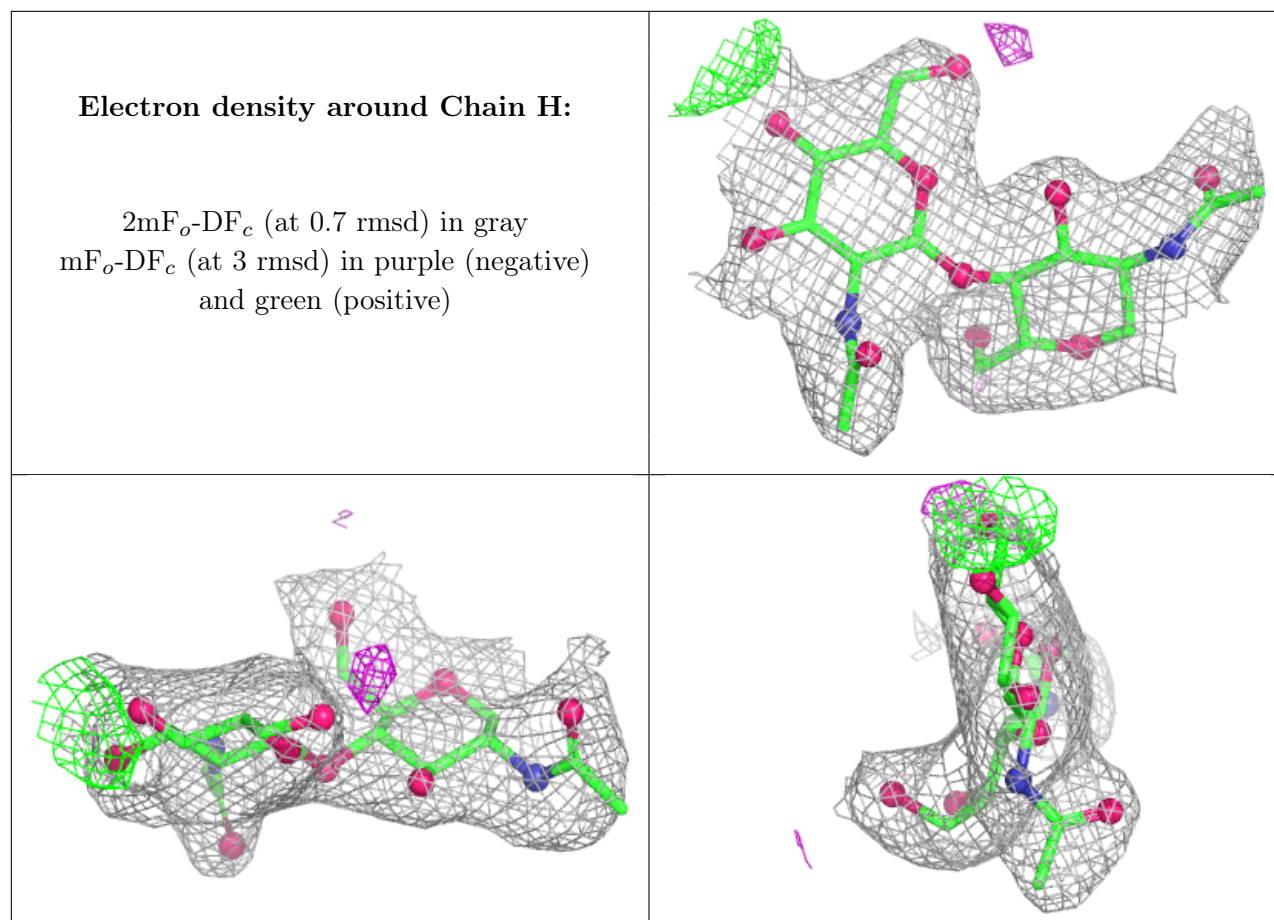
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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 [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.

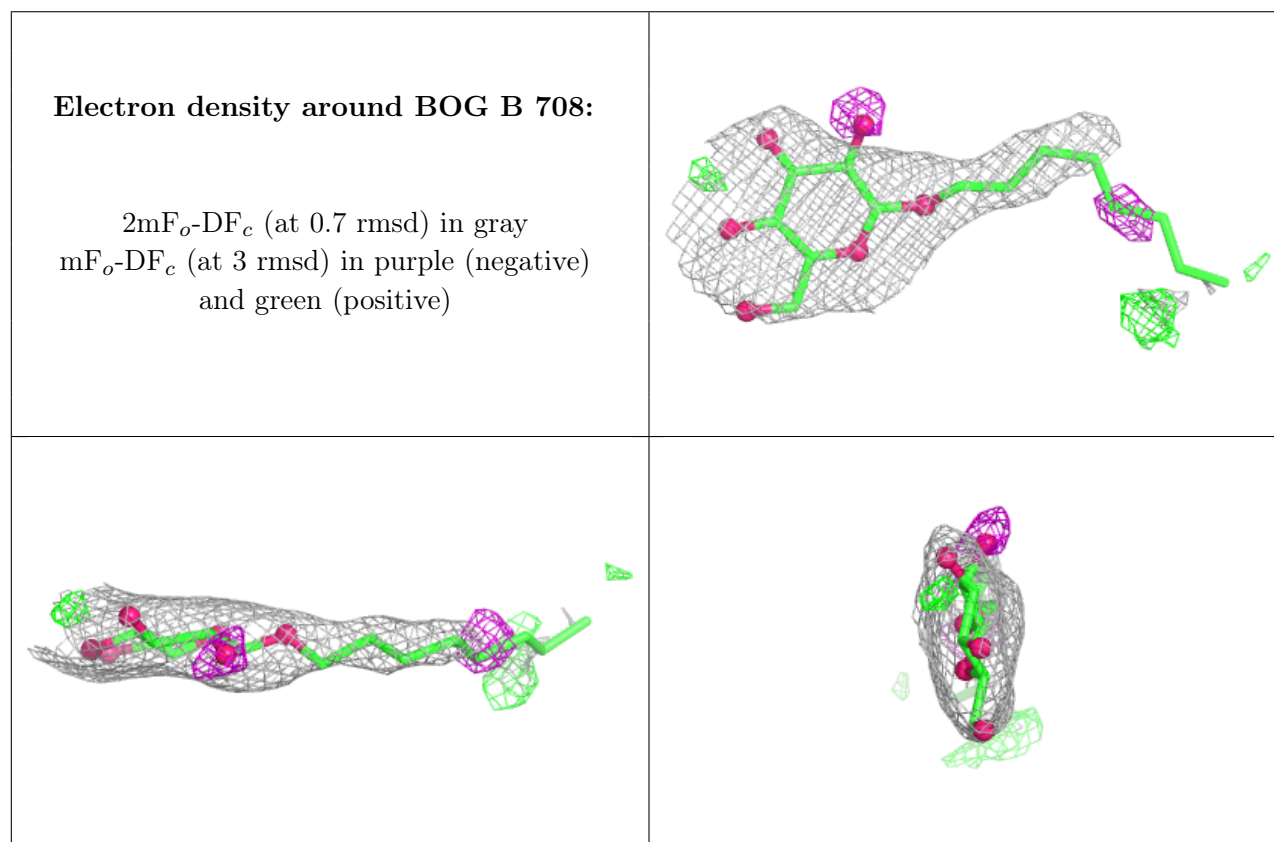
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	BOG	B	708	20/20	0.67	0.22	68,84,104,105	0
4	NAG	C	702	14/15	0.70	0.17	66,76,79,83	0
4	NAG	A	702	14/15	0.72	0.17	69,81,84,85	0
4	NAG	D	702	14/15	0.78	0.18	82,86,91,94	0
4	NAG	A	705	14/15	0.78	0.13	62,76,80,80	0
7	BOG	C	709	20/20	0.78	0.15	64,75,79,81	0
4	NAG	C	705	14/15	0.80	0.12	61,69,76,79	0
4	NAG	B	702	14/15	0.80	0.16	85,92,98,98	0
4	NAG	B	705	14/15	0.83	0.11	70,74,78,79	0
4	NAG	D	705	14/15	0.83	0.12	70,76,78,80	0
7	BOG	D	708	20/20	0.83	0.15	67,77,82,83	0
6	N1B	B	707[B]	30/30	0.87	0.16	40,48,56,60	30

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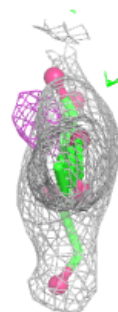
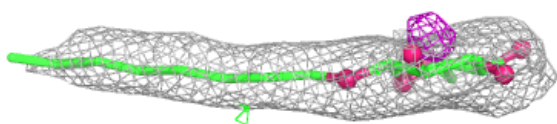
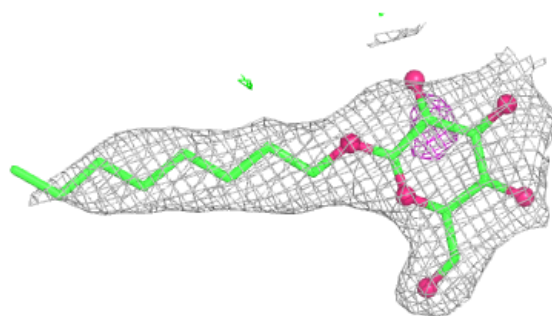
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	4LA	B	706[A]	30/30	0.88	0.16	41,48,56,60	30
7	BOG	C	708	20/20	0.92	0.11	47,56,58,59	0
6	N1B	C	707[B]	30/30	0.92	0.13	40,49,57,61	30
5	4LA	C	706[A]	30/30	0.92	0.13	40,49,57,61	30
5	4LA	D	706[A]	30/30	0.93	0.12	32,47,58,68	30
6	N1B	D	707[B]	30/30	0.93	0.12	32,47,58,68	30
5	4LA	A	706[A]	30/30	0.93	0.12	45,48,54,56	30
6	N1B	A	707[B]	30/30	0.94	0.11	44,48,54,56	30
7	BOG	A	708	20/20	0.95	0.09	48,52,67,69	0
3	HEM	D	701	43/43	0.96	0.09	30,41,64,77	0
3	HEM	A	701	43/43	0.96	0.10	35,44,64,76	0
3	HEM	B	701	43/43	0.97	0.08	35,43,66,75	0
3	HEM	C	701	43/43	0.97	0.08	37,41,59,71	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.

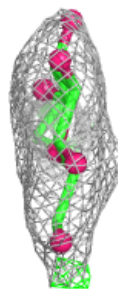
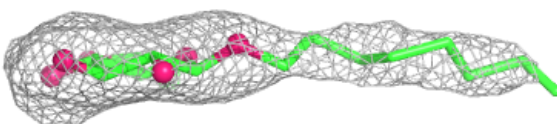


Electron density around BOG C 709:

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

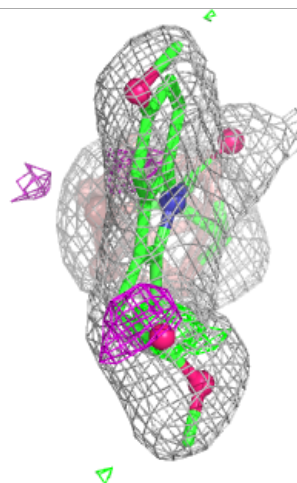
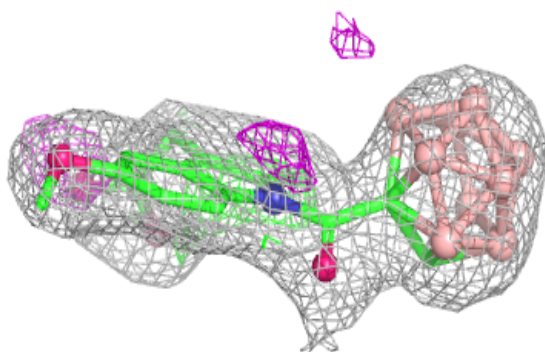
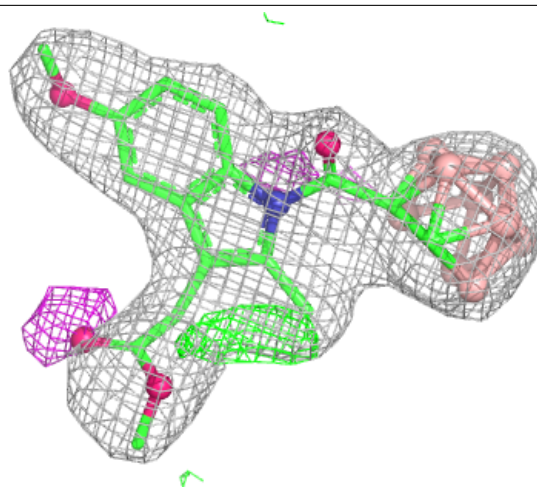
**Electron density around BOG D 708:**

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



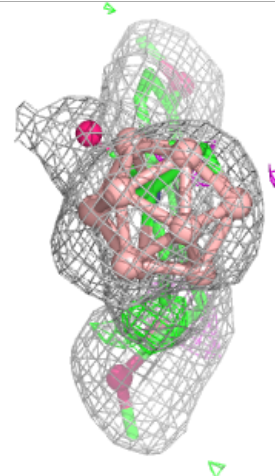
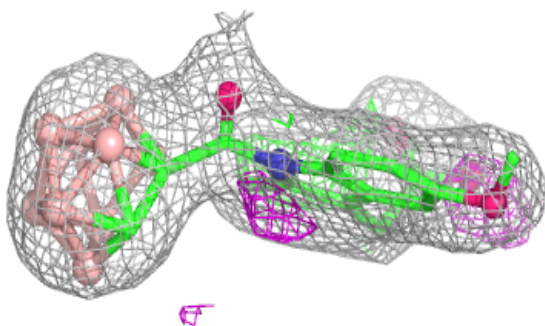
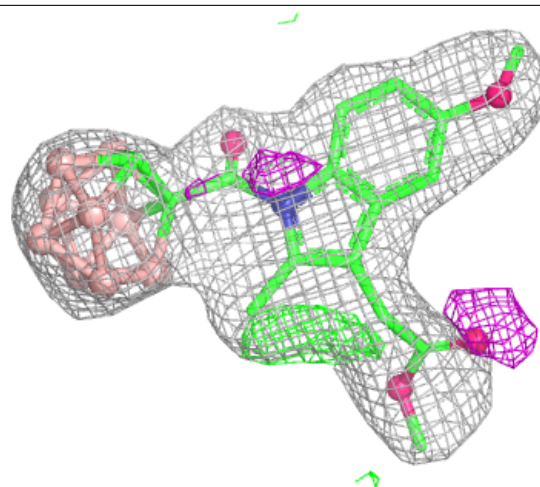
Electron density around N1B B 707 (B):

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



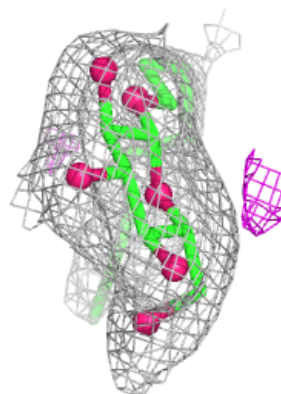
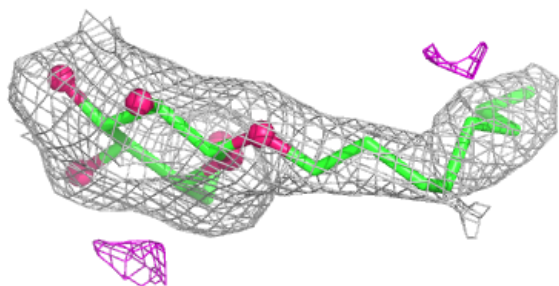
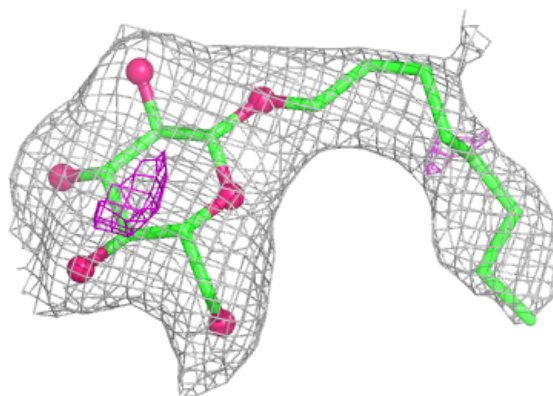
Electron density around 4LA B 706 (A):

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



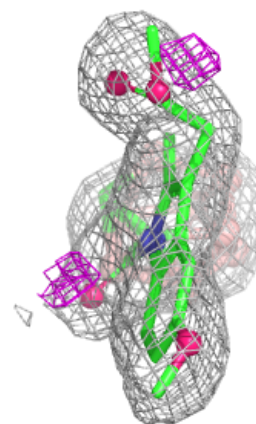
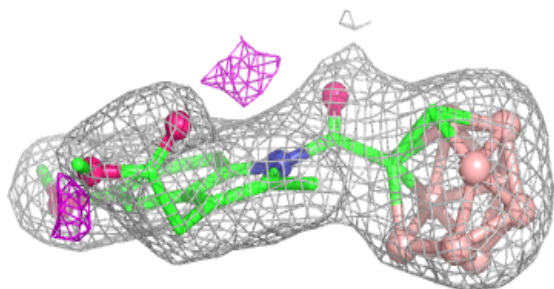
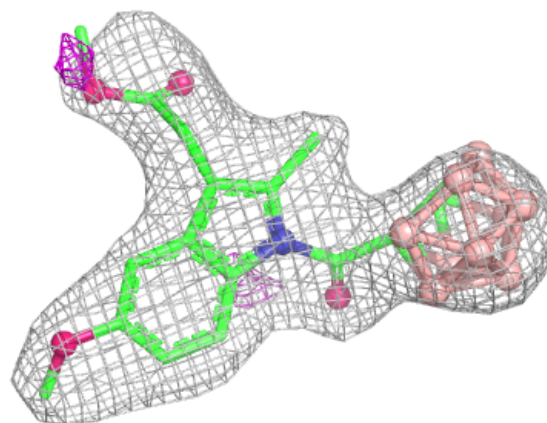
Electron density around BOG C 708:

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



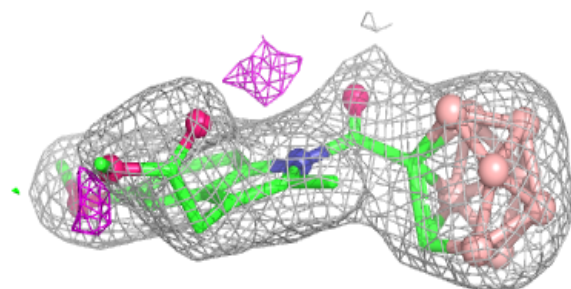
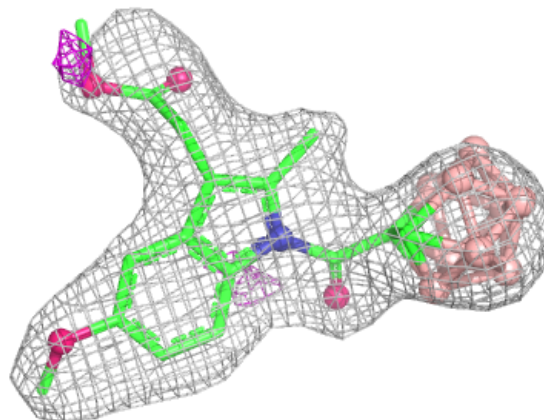
Electron density around N1B C 707 (B):

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



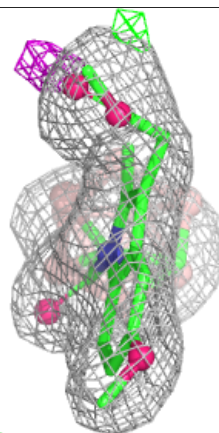
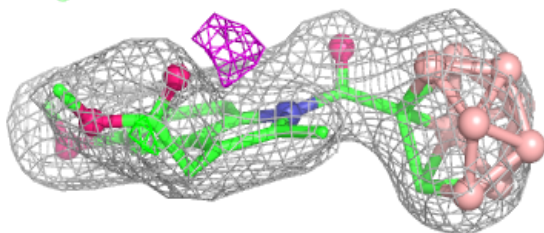
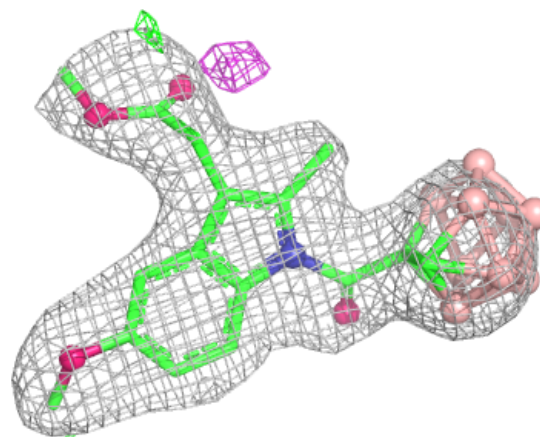
Electron density around 4LA C 706 (A):

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



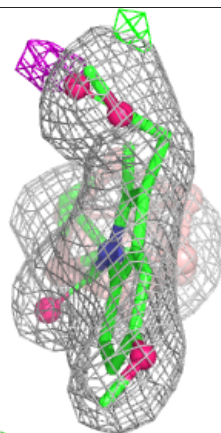
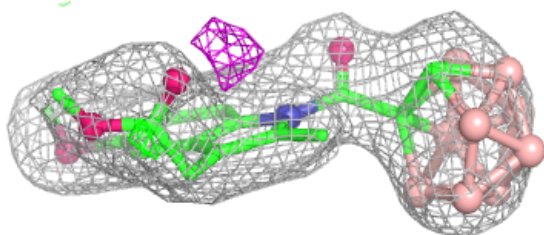
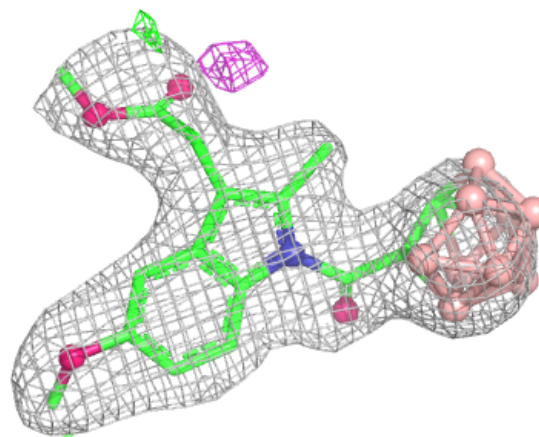
Electron density around 4LA D 706 (A):

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



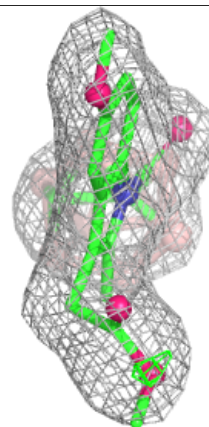
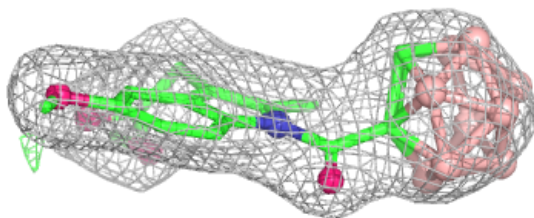
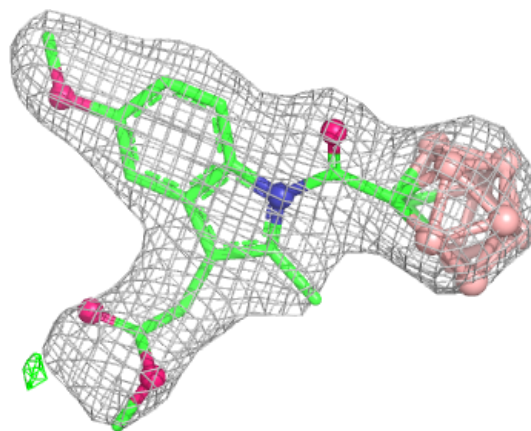
Electron density around N1B D 707 (B):

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



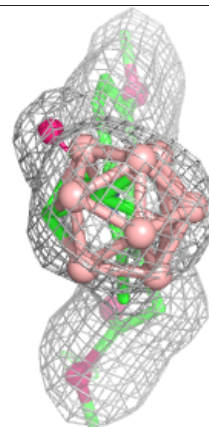
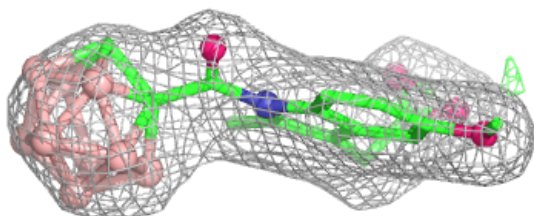
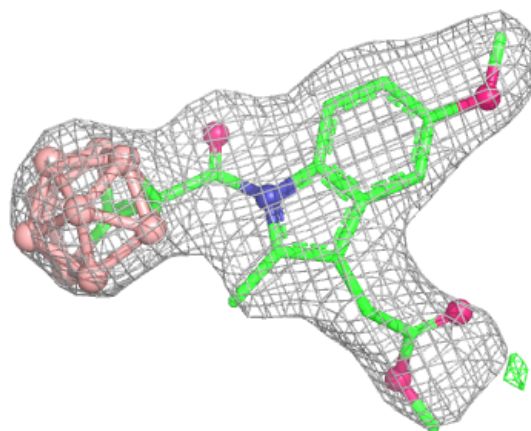
Electron density around 4LA A 706 (A):

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

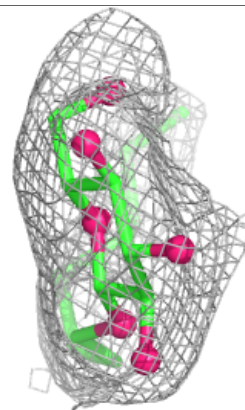
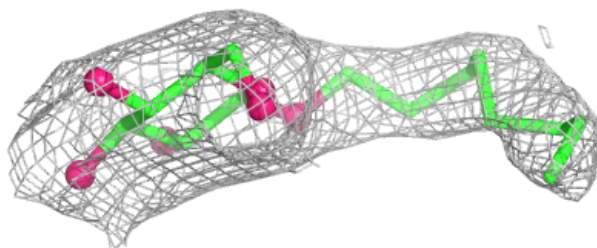
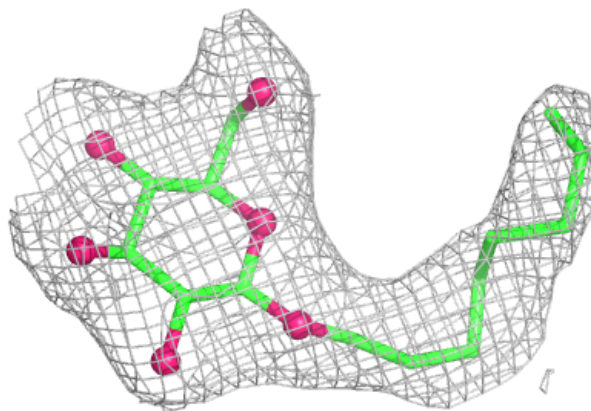


Electron density around N1B A 707 (B):

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

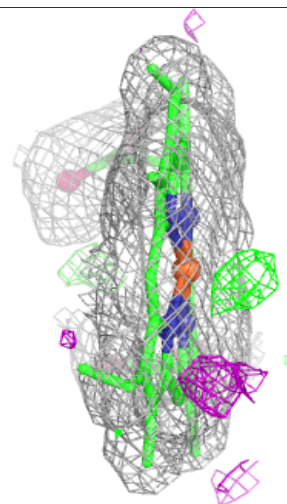
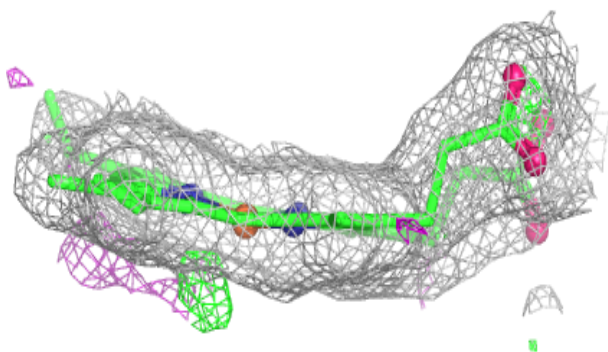
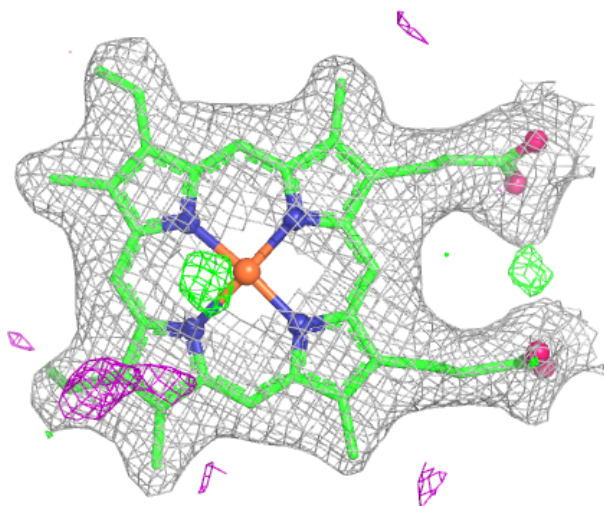
**Electron density around BOG A 708:**

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



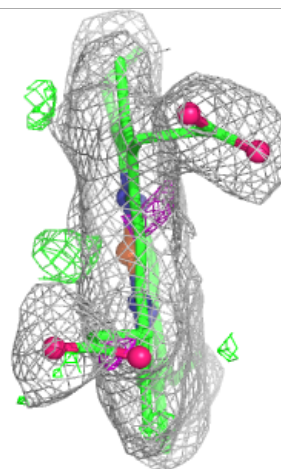
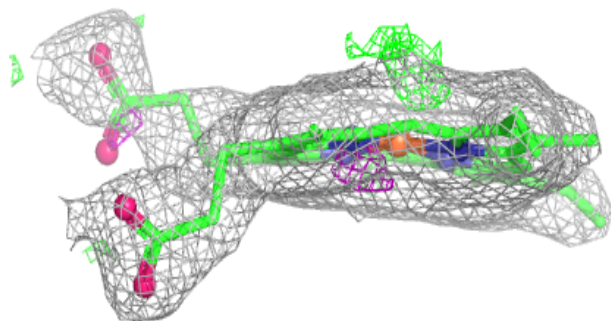
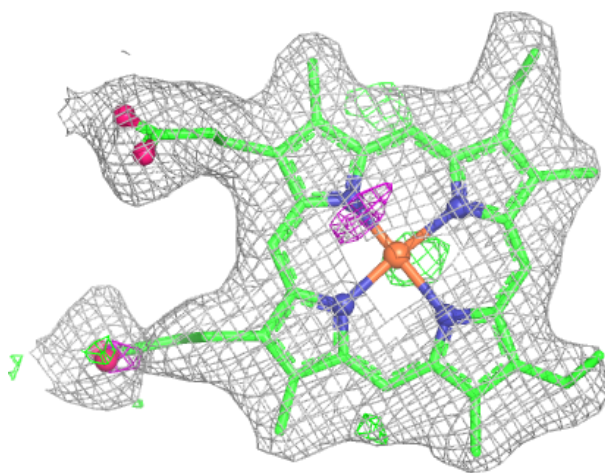
Electron density around HEM D 701:

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



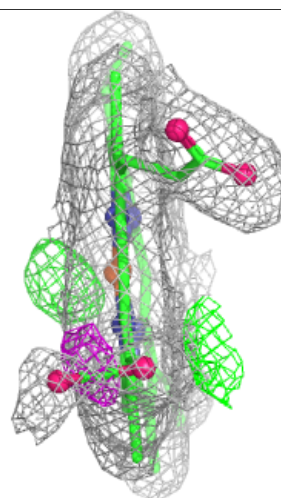
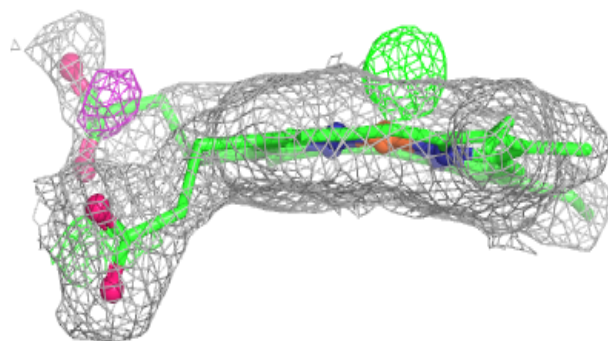
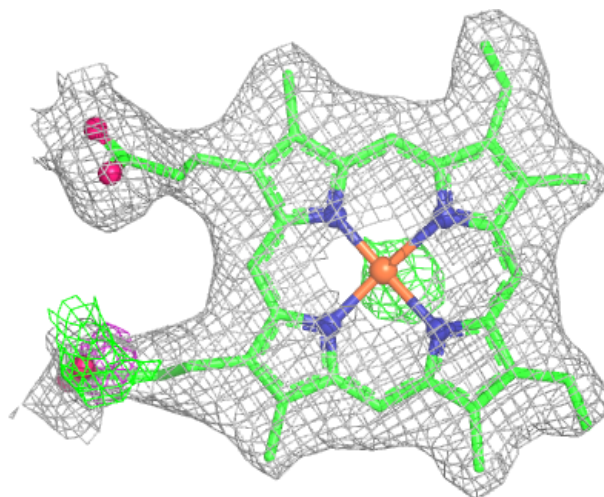
Electron density around HEM A 701:

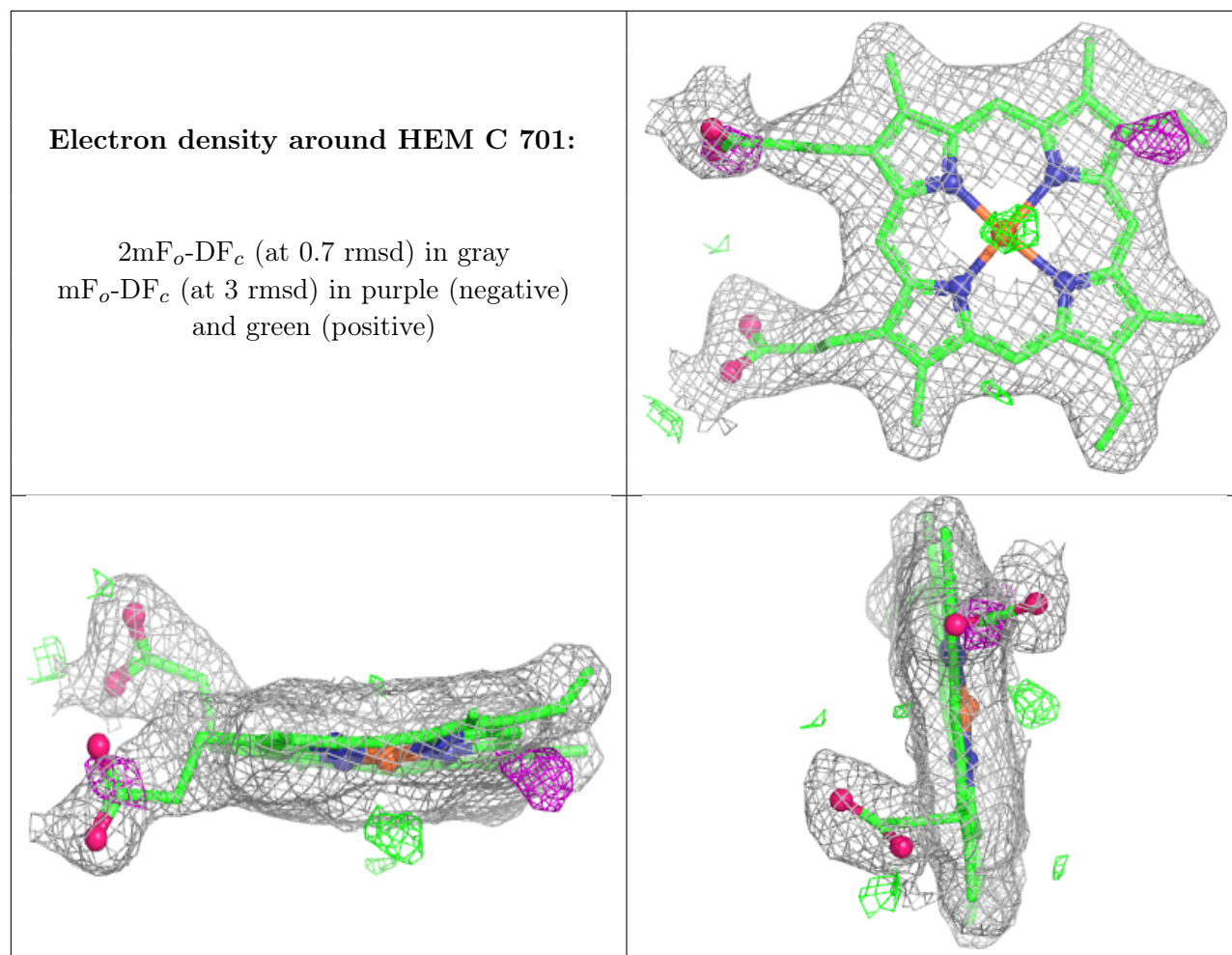
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.