



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:20 AM UTC

PDB ID : 1Q4G / pdb_00001q4g
Title : 2.0 Angstrom Crystal Structure of Ovine Prostaglandin H2 Synthase-1, in complex with alpha-methyl-4-biphenylacetic acid
Authors : Gupta, K.; Selinsky, B.S.; Kaub, C.J.; Katz, A.K.; Loll, P.J.
Deposited on : 2003-08-03
Resolution : 2.00 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

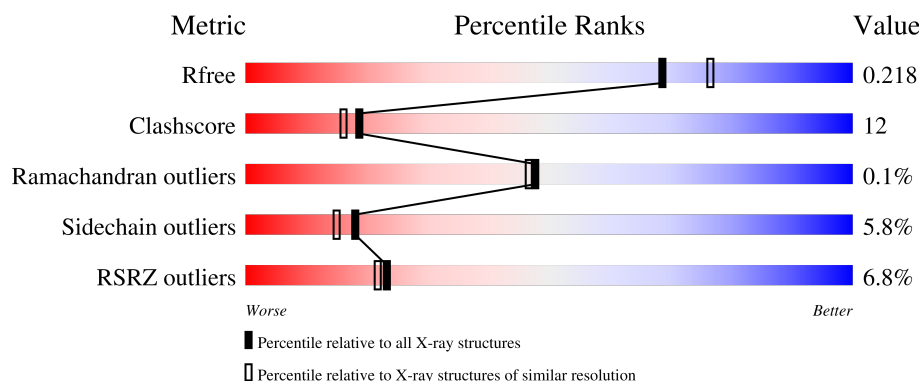
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	553	7% 76% 19% 5%
1	B	553	6% 76% 21% .
2	C	2	50% 50%
2	F	2	50% 50%
3	D	4	25% 75%

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Mol	Chain	Length	Quality of chain
3	G	4	
4	E	5	
5	H	5	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	GOL	A	758	-	X	-	-
9	GOL	A	759	-	X	-	-
9	GOL	B	1758	-	X	-	-
9	GOL	B	1759	-	X	-	-
9	GOL	B	1760	-	X	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10336 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	2	0
			4504	2918	762	795	29			
1	B	553	Total	C	N	O	S	0	2	0
			4504	2918	762	795	29			

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



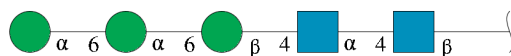
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



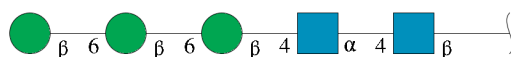
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



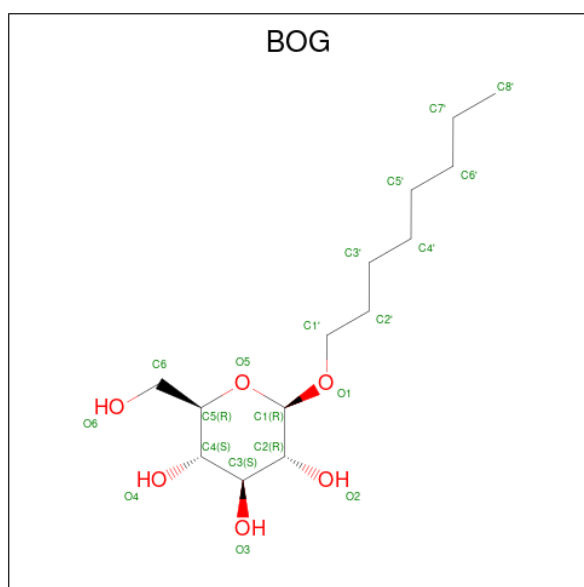
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



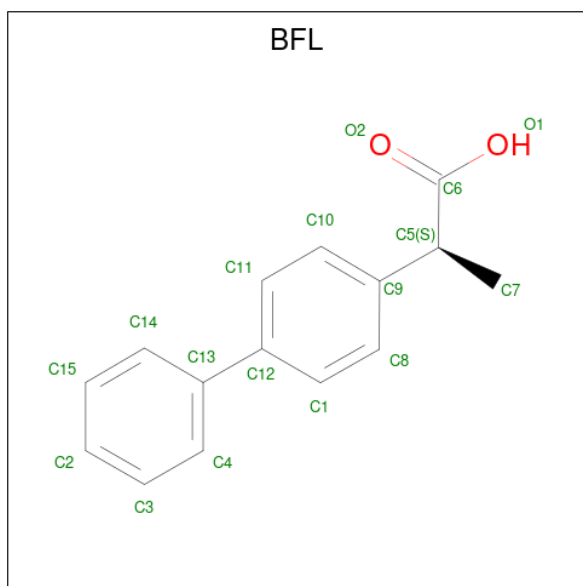
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



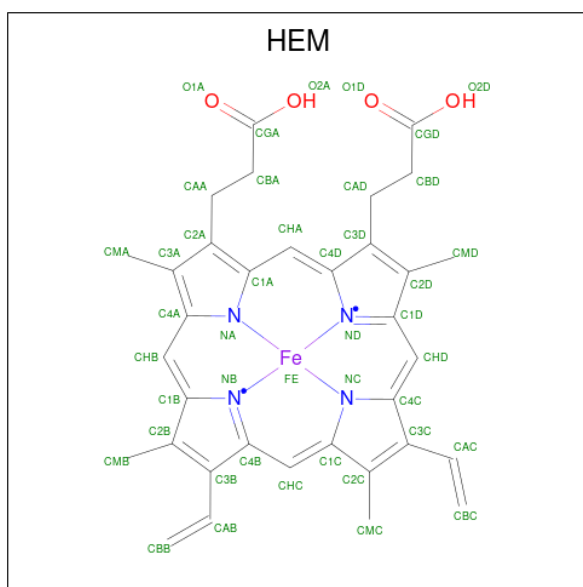
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	14	6		
6	A	1	Total	C	O	0	0
			20	14	6		
6	A	1	Total	C	O	0	0
			20	14	6		
6	A	1	Total	C	O	0	0
			20	14	6		
6	B	1	Total	C	O	0	0
			20	14	6		
6	B	1	Total	C	O	0	0
			20	14	6		
6	B	1	Total	C	O	0	0
			20	14	6		
6	B	1	Total	C	O	0	0
			20	14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

- Molecule 7 is 2-(1,1'-BIPHENYL-4-YL)PROPANOIC ACID (CCD ID: BFL) (formula: $C_{15}H_{14}O_2$).



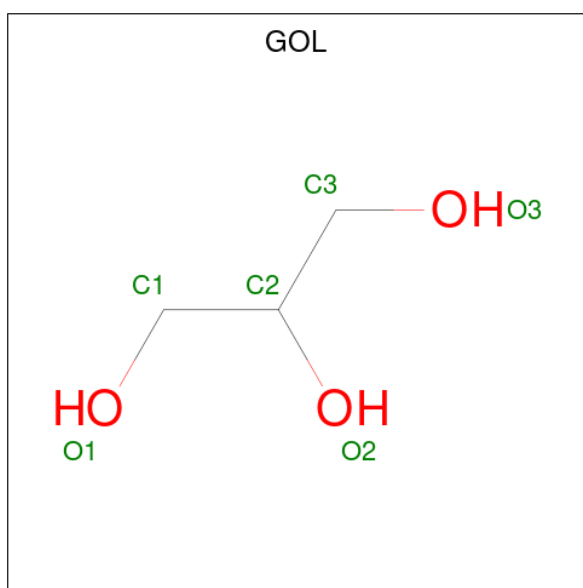
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			17	15	2		
7	B	1	Total	C	O	0	0
			17	15	2		

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total 86	C 68	Fe 2	N 8	O 8	0	1
8	B	1	Total 86	C 68	Fe 2	N 8	O 8	0	1

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		

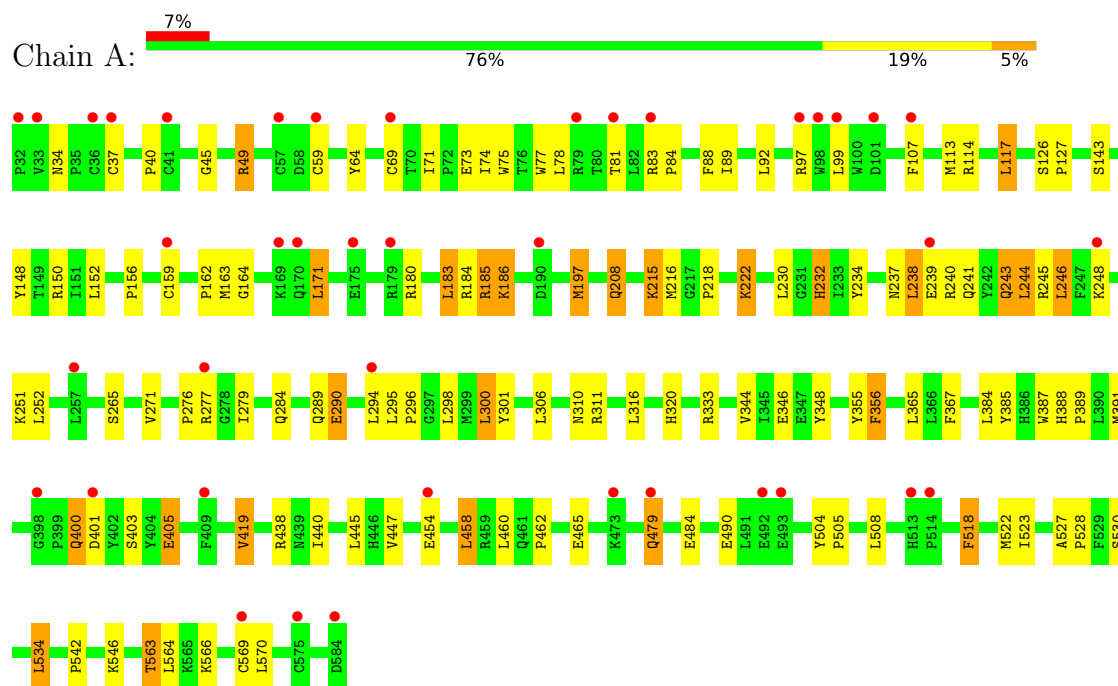
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	321	Total	O	0	0
			321	321		
10	B	333	Total	O	0	0
			333	333		

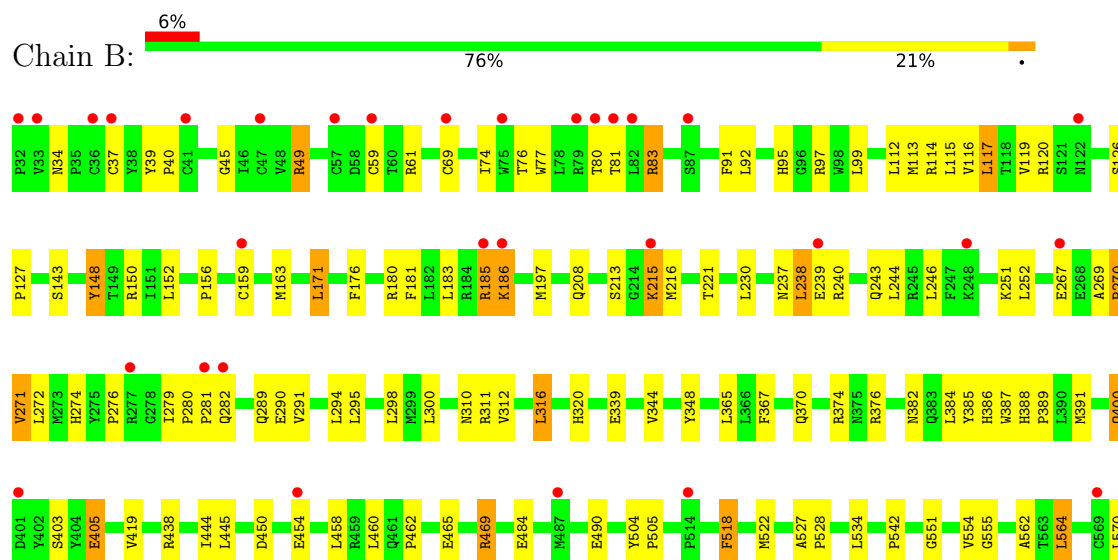
3 Residue-property plots

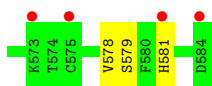
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Prostaglandin G/H synthase 1



• Molecule 1: Prostaglandin G/H synthase 1





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

Chain C: 50% 50%



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

Chain F: 50% 50%



- Molecule 3: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 25% 75%



- Molecule 3: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 25% 25% 50%



- Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 40% 60%



- Molecule 5: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 20% 20% 60%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.15Å 203.86Å 223.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.68 – 2.00 43.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (43.68-2.00) 94.8 (43.68-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.231 0.203 , 0.218	Depositor DCC
R_{free} test set	10694 reflections (7.42%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10336	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: BFL, GOL, HEM, NAG, NDG, BOG, MAN, BMA

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	0.40	0/4643	0.91	12/6302 (0.2%)
1	B	0.42	0/4643	0.91	9/6302 (0.1%)
All	All	0.41	0/9286	0.91	21/12604 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	TYR	N-CA-C	-8.80	97.45	110.48
1	B	148	TYR	N-CA-C	-7.63	99.18	110.48
1	B	251	LYS	N-CA-C	7.18	119.79	110.53
1	B	419	VAL	N-CA-C	6.37	116.53	110.42
1	A	73	GLU	N-CA-C	-6.25	101.27	110.52
1	B	143	SER	N-CA-C	6.05	120.83	112.90
1	A	185	ARG	N-CA-C	-6.05	104.88	112.93
1	A	143	SER	N-CA-C	6.00	120.76	112.90
1	A	197	MET	N-CA-C	-5.87	104.88	111.28
1	A	419	VAL	N-CA-C	5.83	116.02	110.42
1	A	251	LYS	N-CA-C	5.69	117.87	110.53
1	B	269	ALA	CA-C-N	5.64	126.89	119.84
1	B	269	ALA	C-N-CA	5.64	126.89	119.84
1	B	45	GLY	N-CA-C	-5.63	104.87	112.14
1	A	346	GLU	N-CA-C	5.45	119.77	113.18
1	A	356	PHE	N-CA-C	-5.42	106.17	112.89
1	B	185	ARG	N-CA-C	-5.33	104.83	112.13
1	A	569	CYS	N-CA-C	5.18	117.67	111.71
1	A	208	GLN	N-CA-C	-5.11	106.89	113.23
1	A	45	GLY	N-CA-C	-5.08	105.58	112.14
1	B	197	MET	N-CA-C	-5.07	105.76	111.28

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	4504	0	4403	109	0
1	B	4504	0	4403	104	0
2	C	28	0	24	3	0
2	F	28	0	24	1	0
3	D	50	0	43	5	0
3	G	50	0	43	4	0
4	E	61	0	51	7	0
5	H	61	0	51	7	0
6	A	80	0	112	2	0
6	B	80	0	112	6	0
7	A	17	0	13	1	0
7	B	17	0	13	0	0
8	A	86	0	60	4	0
8	B	86	0	60	4	0
9	A	12	0	8	1	0
9	B	18	0	12	1	0
10	A	321	0	0	7	0
10	B	333	0	0	7	0
All	All	10336	0	9432	227	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 12.

All (227) 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:185:ARG:HH21	1:A:438:ARG:NH1	1.56	1.02
1:A:59:CYS:SG	1:A:69[B]:CYS:HB2	2.01	1.01
1:B:163:MET:HE3	1:B:171:LEU:HD21	1.43	0.99
1:A:59:CYS:SG	1:A:69[B]:CYS:CB	2.53	0.96
1:B:215:LYS:HE2	1:B:215:LYS:H	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HE2	1:A:215:LYS:H	1.35	0.89
1:B:237:ASN:ND2	1:B:239:GLU:HG3	1.88	0.89
1:A:563:THR:HG22	1:A:566:LYS:H	1.35	0.88
2:C:1:NAG:H61	2:C:2:NDG:H8C1	1.57	0.86
1:B:215:LYS:H	1:B:215:LYS:CE	1.91	0.82
1:A:163:MET:HE3	1:A:171:LEU:HD21	1.61	0.82
4:E:2:NDG:H4	4:E:3:BMA:O2	1.81	0.80
1:B:237:ASN:HD22	1:B:239:GLU:HG3	1.43	0.80
1:A:215:LYS:H	1:A:215:LYS:CE	1.98	0.76
1:B:216:MET:HG2	5:H:2:NDG:H8C1	1.71	0.73
5:H:4:BMA:O2	5:H:4:BMA:H62	1.88	0.73
1:A:185:ARG:HH21	1:A:438:ARG:HH11	1.34	0.73
1:A:185:ARG:HH21	1:A:438:ARG:HH12	1.37	0.71
1:A:387:TRP:HB2	8:A:801[A]:HEM:HAC	1.71	0.71
1:A:391:MET:HG3	8:A:801[A]:HEM:HAB	1.72	0.71
1:B:276:PRO:HD2	1:B:279:ILE:HD12	1.73	0.71
1:B:294:LEU:HG	1:B:295:LEU:HG	1.72	0.70
1:B:208:GLN:NE2	1:B:230:LEU:H	1.90	0.70
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.57	0.69
1:A:391:MET:HG3	8:A:801[B]:HEM:HAB	1.75	0.69
3:D:2:NAG:H4	3:D:3:BMA:O2	1.93	0.69
1:B:113:MET:HE3	1:B:117:LEU:HD13	1.77	0.67
1:B:387:TRP:HB2	8:B:1601[A]:HEM:HAC	1.77	0.67
1:A:208:GLN:NE2	1:A:230:LEU:H	1.93	0.66
1:B:83:ARG:NH1	6:B:1751:BOG:H3	2.10	0.65
1:A:40:PRO:HB3	2:C:1:NAG:H62	1.78	0.65
1:B:462:PRO:HG2	1:B:465:GLU:HG2	1.79	0.65
1:A:114:ARG:HD3	1:A:365:LEU:O	1.96	0.65
1:B:387:TRP:HB2	8:B:1601[B]:HEM:HAC	1.78	0.64
1:A:49:ARG:O	1:B:320:HIS:HD2	1.80	0.64
1:A:387:TRP:HB2	8:A:801[B]:HEM:HAC	1.79	0.64
5:H:4:BMA:H62	5:H:5:BMA:O2	1.98	0.64
1:B:208:GLN:HE21	1:B:230:LEU:H	1.44	0.63
1:A:216:MET:HE1	10:A:1062:HOH:O	1.98	0.63
1:B:156:PRO:HB2	1:B:159:CYS:SG	2.37	0.63
1:B:180:ARG:O	1:B:438:ARG:NH1	2.31	0.63
1:A:150:ARG:HD3	1:A:152:LEU:O	1.99	0.62
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.39	0.62
1:A:113:MET:HE3	1:A:117:LEU:HD13	1.81	0.61
1:B:150:ARG:HD3	1:B:152:LEU:O	1.99	0.61
1:B:243:GLN:OE1	1:B:270:PRO:HD2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HD23	6:A:754:BOG:H3'1	1.81	0.60
1:A:563:THR:HG21	10:A:1065:HOH:O	2.01	0.60
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.83	0.60
1:A:215:LYS:HG2	1:A:216:MET:H	1.66	0.60
1:B:554:VAL:HG13	1:B:555:GLY:N	2.16	0.60
1:B:518:PHE:CD1	1:B:522:MET:HG2	2.37	0.60
1:B:216:MET:HE1	10:B:1767:HOH:O	2.01	0.60
1:B:450:ASP:O	1:B:454:GLU:HG3	2.01	0.60
1:A:163:MET:HE1	10:A:913:HOH:O	2.02	0.60
1:A:215:LYS:HD2	1:A:222:LYS:NZ	2.16	0.60
1:A:185:ARG:NH2	1:A:438:ARG:NH1	2.40	0.59
1:B:267:GLU:OE1	1:B:282:GLN:HG2	2.03	0.59
1:A:479:GLN:HE21	1:A:479:GLN:C	2.11	0.59
1:B:115:LEU:HD21	6:B:1752:BOG:H2	1.84	0.59
1:A:294:LEU:HG	1:A:295:LEU:HG	1.84	0.58
4:E:2:NDG:O7	4:E:2:NDG:H3	2.02	0.58
1:A:180:ARG:HD3	1:A:490:GLU:OE2	2.02	0.58
1:B:183:LEU:HD13	1:B:445:LEU:HD22	1.85	0.58
1:A:454:GLU:HG3	1:A:458:LEU:HD22	1.86	0.58
1:A:320:HIS:HD2	1:B:49:ARG:O	1.86	0.57
1:A:64:TYR:HB2	1:A:69[B]:CYS:SG	2.44	0.56
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.86	0.56
5:H:2:NDG:O7	5:H:2:NDG:H3	2.04	0.56
1:A:403:SER:OG	1:A:405:GLU:HG2	2.06	0.56
1:B:311:ARG:NH2	1:B:570:LEU:HD23	2.20	0.56
1:B:208:GLN:HE22	1:B:230:LEU:HD12	1.71	0.56
1:A:518:PHE:HE2	1:A:523:ILE:HD11	1.71	0.55
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.87	0.55
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.87	0.55
1:A:530[B]:SER:O	1:A:534:LEU:HD22	2.07	0.55
1:B:185:ARG:NH2	1:B:438:ARG:NH1	2.55	0.54
1:B:405:GLU:CD	1:B:405:GLU:H	2.15	0.54
1:B:163:MET:HE1	10:B:2028:HOH:O	2.07	0.54
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.90	0.54
1:A:186:LYS:HB2	1:A:186:LYS:NZ	2.23	0.54
1:B:237:ASN:ND2	1:B:240:ARG:H	2.06	0.54
1:B:339:GLU:HG2	1:B:562:ALA:HB2	1.90	0.54
1:A:97:ARG:HG2	1:A:356:PHE:CE2	2.43	0.54
1:B:99:LEU:HD23	6:B:1753:BOG:H3'1	1.90	0.54
1:A:241:GLN:HE21	1:A:245:ARG:HH11	1.54	0.53
1:A:563:THR:HG23	10:A:832:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HG2	1:A:216:MET:N	2.23	0.53
4:E:2:NDG:H4	4:E:3:BMA:HO2	1.72	0.53
1:B:554:VAL:HG13	1:B:555:GLY:H	1.71	0.53
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.91	0.53
1:B:40:PRO:HB3	2:F:1:NAG:H62	1.90	0.53
1:A:180:ARG:O	1:A:438:ARG:NH1	2.42	0.53
1:A:162:PRO:O	1:A:163:MET:HE2	2.08	0.52
1:B:186:LYS:HB2	1:B:186:LYS:NZ	2.24	0.52
1:B:237:ASN:ND2	1:B:239:GLU:CG	2.67	0.52
1:B:403:SER:OG	1:B:405:GLU:HG2	2.09	0.52
1:A:238:LEU:HD13	5:H:2:NDG:H6C2	1.91	0.52
1:A:239:GLU:CD	1:A:239:GLU:H	2.17	0.52
1:A:276:PRO:HD2	1:A:279:ILE:HD12	1.92	0.52
1:B:215:LYS:HE2	1:B:215:LYS:N	2.14	0.52
1:B:367:PHE:CD2	1:B:542:PRO:HG3	2.45	0.52
1:A:530[A]:SER:O	1:A:534:LEU:HD22	2.08	0.52
10:A:1117:HOH:O	2:C:2:NDG:H3	2.09	0.52
1:A:290:GLU:CD	1:A:290:GLU:H	2.18	0.52
1:A:185:ARG:HG2	1:A:185:ARG:NH1	2.24	0.52
1:A:344:VAL:O	1:A:348:TYR:HB3	2.10	0.51
1:A:208:GLN:HE22	1:A:230:LEU:HD12	1.76	0.51
1:A:215:LYS:HD2	1:A:222:LYS:HZ2	1.74	0.51
1:A:218:PRO:HB3	1:A:454:GLU:OE2	2.10	0.51
1:B:290:GLU:H	1:B:290:GLU:CD	2.17	0.51
4:E:2:NDG:C4	4:E:3:BMA:O2	2.55	0.51
1:B:150:ARG:CD	1:B:152:LEU:O	2.58	0.50
1:A:208:GLN:HE21	1:A:230:LEU:H	1.60	0.50
1:A:310:ASN:HB3	9:A:758:GOL:O1	2.12	0.50
1:B:83:ARG:HH22	6:B:1751:BOG:H5	1.75	0.50
1:A:185:ARG:NH2	1:A:438:ARG:HH11	2.06	0.50
1:B:74:ILE:HG12	10:B:1877:HOH:O	2.12	0.50
1:B:176:PHE:CZ	1:B:180:ARG:HG3	2.47	0.50
1:A:244:LEU:HD13	1:A:271:VAL:HG11	1.93	0.50
3:D:2:NAG:C4	3:D:3:BMA:O2	2.60	0.49
1:B:391:MET:HG3	8:B:1601[B]:HEM:CBB	2.42	0.49
1:A:241:GLN:NE2	1:A:245:ARG:HH11	2.10	0.49
1:A:150:ARG:CD	1:A:152:LEU:O	2.61	0.49
1:A:388:HIS:N	1:A:389:PRO:CD	2.76	0.49
1:A:218:PRO:HB3	1:A:454:GLU:CD	2.38	0.49
1:A:400:GLN:OE1	3:D:3:BMA:H62	2.11	0.49
4:E:2:NDG:O7	4:E:2:NDG:C3	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TRP:O	1:A:81:THR:HG23	2.14	0.48
1:B:49:ARG:HG3	10:B:1763:HOH:O	2.14	0.48
3:G:2:NAG:H4	3:G:3:BMA:O2	2.14	0.48
1:B:237:ASN:HD21	1:B:239:GLU:CD	2.22	0.47
1:B:83:ARG:NH1	1:B:83:ARG:HG3	2.29	0.47
1:A:246:LEU:HD13	1:A:248:LYS:HB3	1.96	0.47
1:B:113:MET:HE3	1:B:117:LEU:CD1	2.44	0.47
1:A:197:MET:HE3	1:A:301:TYR:OH	2.15	0.47
1:A:384:LEU:C	1:A:384:LEU:HD23	2.40	0.47
1:B:344:VAL:HA	1:B:348:TYR:HB3	1.96	0.47
1:B:444:ILE:HG21	8:B:1601[B]:HEM:HBB2	1.96	0.47
1:B:579:SER:OG	1:B:581:HIS:HD2	1.98	0.47
1:B:311:ARG:NH2	10:B:1907:HOH:O	2.47	0.47
1:B:374:ARG:HD2	10:B:1942:HOH:O	2.14	0.47
1:B:240:ARG:NH1	1:B:271:VAL:HG13	2.30	0.46
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.79	0.46
1:A:546:LYS:HE3	10:B:1818:HOH:O	2.15	0.46
1:B:388:HIS:N	1:B:389:PRO:CD	2.79	0.46
1:A:311:ARG:NH2	10:A:975:HOH:O	2.48	0.46
1:A:243:GLN:CD	5:H:5:BMA:H62	2.41	0.46
1:B:59:CYS:SG	1:B:69[B]:CYS:SG	3.13	0.46
1:B:91:PHE:O	1:B:95:HIS:HD2	1.99	0.45
1:A:237:ASN:ND2	1:A:240:ARG:H	2.14	0.45
1:B:310:ASN:HB3	9:B:1759:GOL:O2	2.16	0.45
1:B:213:SER:OG	1:B:215:LYS:HE3	2.16	0.45
1:A:71:ILE:HD13	6:A:753:BOG:H3	1.97	0.45
1:B:77:TRP:O	1:B:81:THR:HG23	2.17	0.45
1:A:265:SER:HA	1:A:284:GLN:O	2.17	0.44
1:B:126:SER:HA	1:B:127:PRO:C	2.42	0.44
4:E:2:NDG:O3	4:E:3:BMA:C1	2.65	0.44
1:A:183:LEU:HD22	1:A:184:ARG:O	2.18	0.44
1:A:162:PRO:C	1:A:163:MET:HE2	2.43	0.44
1:B:181:PHE:HZ	1:B:490:GLU:HG2	1.82	0.44
1:A:74:ILE:HG23	1:A:75:TRP:N	2.33	0.44
1:A:215:LYS:HE2	1:A:215:LYS:N	2.17	0.44
1:A:230:LEU:HA	1:A:232:HIS:CE1	2.53	0.44
1:A:344:VAL:HA	1:A:348:TYR:HB3	2.00	0.44
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.57	0.44
1:B:274:HIS:HD2	1:B:291:VAL:HG12	1.82	0.44
1:B:469:ARG:O	1:B:469:ARG:NE	2.46	0.44
5:H:2:NDG:O7	5:H:2:NDG:C3	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:CYS:HB3	1:A:164:GLY:O	2.18	0.43
1:A:400:GLN:CA	1:A:400:GLN:HE21	2.29	0.43
1:B:400:GLN:OE1	3:G:3:BMA:H62	2.18	0.43
1:B:272:LEU:HD13	1:B:272:LEU:C	2.42	0.43
1:A:542:PRO:O	1:B:61:ARG:NH1	2.50	0.43
1:B:579:SER:OG	1:B:581:HIS:CD2	2.72	0.43
1:A:306:LEU:HD23	1:A:306:LEU:C	2.43	0.43
1:B:344:VAL:O	1:B:348:TYR:HB3	2.19	0.43
1:A:162:PRO:HB2	1:A:171:LEU:HD13	1.99	0.43
1:B:384:LEU:HG	1:B:522:MET:SD	2.58	0.43
1:A:400:GLN:HE21	1:A:401:ASP:H	1.65	0.43
1:B:119:VAL:HG12	6:B:1751:BOG:H62	2.00	0.43
1:A:107:PHE:CD1	1:A:107:PHE:C	2.96	0.43
1:B:215:LYS:HG2	1:B:216:MET:H	1.84	0.43
1:B:280:PRO:HA	1:B:281:PRO:HD3	1.87	0.43
1:B:400:GLN:OE1	3:G:3:BMA:C6	2.66	0.43
1:A:311:ARG:NH2	1:A:570:LEU:HD23	2.34	0.43
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.54	0.43
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.53	0.42
3:D:3:BMA:O6	3:D:4:BMA:H62	2.18	0.42
1:A:518:PHE:HE2	1:A:523:ILE:CD1	2.32	0.42
1:B:83:ARG:HH12	6:B:1751:BOG:H3	1.81	0.42
1:B:382:ASN:OD1	1:B:386:HIS:HE1	2.02	0.42
1:A:355:TYR:CE1	7:A:701:BFL:H5	2.54	0.42
1:A:277:ARG:HD2	1:A:277:ARG:HA	1.84	0.42
1:B:215:LYS:HG2	1:B:216:MET:N	2.33	0.42
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.55	0.42
1:A:300:LEU:HD21	1:A:419:VAL:HG13	2.02	0.42
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.35	0.42
1:B:148:TYR:CZ	1:B:221:THR:HB	2.55	0.42
1:A:88:PHE:O	1:A:92:LEU:HD13	2.20	0.42
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.55	0.42
1:B:564:LEU:HD13	1:B:578:VAL:HG22	2.02	0.42
1:B:114:ARG:HD3	1:B:365:LEU:O	2.20	0.41
1:B:238:LEU:HD12	4:E:1:NAG:H4	2.02	0.41
1:B:581:HIS:CD2	1:B:581:HIS:O	2.73	0.41
1:B:384:LEU:C	1:B:384:LEU:HD23	2.45	0.41
3:G:2:NAG:C4	3:G:3:BMA:O2	2.68	0.41
1:A:126:SER:HA	1:A:127:PRO:C	2.45	0.41
1:B:116:VAL:O	1:B:120:ARG:HB2	2.21	0.41
1:B:320:HIS:CE1	1:B:551:GLY:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.61	0.41
1:A:183:LEU:HG	1:A:445:LEU:HD22	2.01	0.41
1:A:295:LEU:HA	1:A:296:PRO:HD3	1.96	0.41
1:A:367:PHE:O	1:B:370:GLN:NE2	2.43	0.41
1:A:389:PRO:HG3	1:A:440:ILE:HG12	2.03	0.41
1:B:83:ARG:HH11	1:B:83:ARG:CG	2.33	0.41
1:B:112:LEU:O	1:B:116:VAL:HG23	2.20	0.41
1:A:83:ARG:HD3	10:A:944:HOH:O	2.21	0.41
1:B:39:TYR:N	1:B:40:PRO:CD	2.83	0.41
1:B:312:VAL:HG12	1:B:316:LEU:HD22	2.03	0.41
1:B:554:VAL:CG1	1:B:555:GLY:N	2.84	0.41
1:A:387:TRP:C	1:A:389:PRO:HD2	2.46	0.41
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.57	0.40
1:B:59:CYS:HB3	1:B:69[B]:CYS:SG	2.61	0.40
1:B:320:HIS:HE1	1:B:551:GLY:O	2.04	0.40
3:D:2:NAG:O3	3:D:3:BMA:C1	2.69	0.40
1:B:76:THR:O	1:B:80:THR:HG23	2.22	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	553/553 (100%)	537 (97%)	16 (3%)	0	100	100
1	B	553/553 (100%)	535 (97%)	17 (3%)	1 (0%)	43	42
All	All	1106/1106 (100%)	1072 (97%)	33 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/488 (100%)	460 (94%)	30 (6%)	17	14
1	B	490/488 (100%)	463 (94%)	27 (6%)	19	17
All	All	980/976 (100%)	923 (94%)	57 (6%)	18	15

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	78	LEU
1	A	117	LEU
1	A	171	LEU
1	A	183	LEU
1	A	186	LYS
1	A	215	LYS
1	A	222	LYS
1	A	232	HIS
1	A	238	LEU
1	A	243	GLN
1	A	244	LEU
1	A	246	LEU
1	A	252	LEU
1	A	289	GLN
1	A	290	GLU
1	A	298	LEU
1	A	300	LEU
1	A	316	LEU
1	A	385	TYR
1	A	400	GLN
1	A	405	GLU
1	A	458	LEU
1	A	460	LEU
1	A	479	GLN
1	A	484	GLU
1	A	518	PHE

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Mol	Chain	Res	Type
1	A	534	LEU
1	A	563	THR
1	A	564	LEU
1	B	49	ARG
1	B	83	ARG
1	B	92	LEU
1	B	117	LEU
1	B	171	LEU
1	B	186	LYS
1	B	215	LYS
1	B	238	LEU
1	B	244	LEU
1	B	246	LEU
1	B	252	LEU
1	B	271	VAL
1	B	289	GLN
1	B	298	LEU
1	B	300	LEU
1	B	316	LEU
1	B	376	ARG
1	B	385	TYR
1	B	400	GLN
1	B	405	GLU
1	B	458	LEU
1	B	460	LEU
1	B	469	ARG
1	B	484	GLU
1	B	518	PHE
1	B	534	LEU
1	B	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	95	HIS
1	A	134	HIS
1	A	203	GLN
1	A	204	HIS
1	A	208	GLN
1	A	237	ASN
1	A	241	GLN

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Mol	Chain	Res	Type
1	A	255	GLN
1	A	274	HIS
1	A	320	HIS
1	A	375	ASN
1	A	386	HIS
1	A	400	GLN
1	A	443	HIS
1	A	479	GLN
1	A	513	HIS
1	A	571	ASN
1	B	42	GLN
1	B	56	GLN
1	B	95	HIS
1	B	134	HIS
1	B	203	GLN
1	B	208	GLN
1	B	237	ASN
1	B	274	HIS
1	B	320	HIS
1	B	375	ASN
1	B	386	HIS
1	B	479	GLN
1	B	571	ASN
1	B	581	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

22 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	0.68	0	17,19,21	0.67	0
2	NDG	C	2	2	14,14,15	0.60	0	17,19,21	0.93	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.50	0	17,19,21	0.72	1 (5%)
3	NAG	D	2	3	14,14,15	0.66	0	17,19,21	0.74	1 (5%)
3	BMA	D	3	3	11,11,12	0.74	0	15,15,17	1.02	1 (6%)
3	BMA	D	4	3	11,11,12	0.61	0	15,15,17	0.88	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.75	0	17,19,21	1.03	1 (5%)
4	NDG	E	2	4	14,14,15	0.92	1 (7%)	17,19,21	1.67	3 (17%)
4	BMA	E	3	4	11,11,12	0.84	0	15,15,17	1.56	2 (13%)
4	MAN	E	4	4	11,11,12	0.65	0	15,15,17	0.75	1 (6%)
4	MAN	E	5	4	11,11,12	0.55	0	15,15,17	0.71	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.65	0	17,19,21	0.91	1 (5%)
2	NDG	F	2	2	14,14,15	0.65	0	17,19,21	0.79	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.56	0	17,19,21	0.64	0
3	NAG	G	2	3	14,14,15	0.63	0	17,19,21	0.78	1 (5%)
3	BMA	G	3	3	11,11,12	0.67	0	15,15,17	1.02	1 (6%)
3	BMA	G	4	3	11,11,12	0.60	0	15,15,17	0.87	1 (6%)
5	NAG	H	1	1,5	14,14,15	0.72	0	17,19,21	0.90	1 (5%)
5	NDG	H	2	5	14,14,15	0.77	1 (7%)	17,19,21	1.39	2 (11%)
5	BMA	H	3	5	11,11,12	0.53	0	15,15,17	0.63	0
5	BMA	H	4	5	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
5	BMA	H	5	5	11,11,12	0.66	0	15,15,17	0.80	1 (6%)

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	-	2/6/23/26	0/1/1/1
2	NDG	C	2	2	-	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	D	4	3	-	2/2/19/22	1/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NDG	E	2	4	-	1/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
4	MAN	E	5	4	-	2/2/19/22	1/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NDG	F	2	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	1/1/1/1
3	BMA	G	4	3	-	2/2/19/22	1/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NDG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	BMA	H	4	5	-	2/2/19/22	0/1/1/1
5	BMA	H	5	5	-	1/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NDG	C1-C2	2.42	1.55	1.52
5	H	2	NDG	C1-C2	2.32	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	BMA	C1-O5-C5	4.79	118.61	112.19
4	E	2	NDG	C1-O5-C5	4.46	118.16	112.19
5	H	2	NDG	C1-O5-C5	3.88	117.38	112.19
4	E	2	NDG	C4-C3-C2	-3.43	106.00	111.02
3	G	3	BMA	C1-O5-C5	3.35	116.67	112.19
5	H	4	BMA	C1-O5-C5	3.33	116.65	112.19
3	D	3	BMA	C1-O5-C5	3.29	116.59	112.19
3	D	4	BMA	C1-O5-C5	3.07	116.30	112.19
3	G	4	BMA	C1-O5-C5	3.06	116.28	112.19
4	E	3	BMA	C1-C2-C3	2.85	113.80	109.64
5	H	2	NDG	C4-C3-C2	-2.83	106.87	111.02
5	H	5	BMA	C1-O5-C5	2.70	115.80	112.19
4	E	5	MAN	C1-O5-C5	2.62	115.69	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NDG	C3-C4-C5	-2.49	105.71	110.23
4	E	4	MAN	C1-O5-C5	2.48	115.52	112.19
2	F	1	NAG	C2-N2-C7	-2.44	119.63	122.90
2	C	2	NDG	C2-N2-C7	-2.33	119.78	122.90
5	H	1	NAG	C2-N2-C7	-2.19	119.97	122.90
3	D	1	NAG	C2-N2-C7	-2.14	120.03	122.90
2	F	2	NDG	C2-N2-C7	-2.10	120.09	122.90
4	E	1	NAG	C2-N2-C7	-2.09	120.11	122.90
3	D	2	NAG	C2-N2-C7	-2.04	120.16	122.90
3	G	2	NAG	C2-N2-C7	-2.04	120.17	122.90

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NDG	C8-C7-N2-C2
2	C	2	NDG	O7-C7-N2-C2
4	E	2	NDG	C3-C2-N2-C7
3	D	2	NAG	O5-C5-C6-O6
3	G	4	BMA	C4-C5-C6-O6
3	G	4	BMA	O5-C5-C6-O6
3	D	4	BMA	C4-C5-C6-O6
2	F	2	NDG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	2	NDG	O5-C5-C6-O6
5	H	4	BMA	O5-C5-C6-O6
2	F	2	NDG	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
3	D	4	BMA	O5-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
4	E	4	MAN	C4-C5-C6-O6
4	E	5	MAN	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	E	5	MAN	O5-C5-C6-O6
5	H	5	BMA	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	3	BMA	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
5	H	2	NDG	C3-C2-N2-C7
2	C	2	NDG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C4-C5-C6-O6
5	H	4	BMA	C4-C5-C6-O6
3	D	2	NAG	O7-C7-N2-C2
2	F	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2

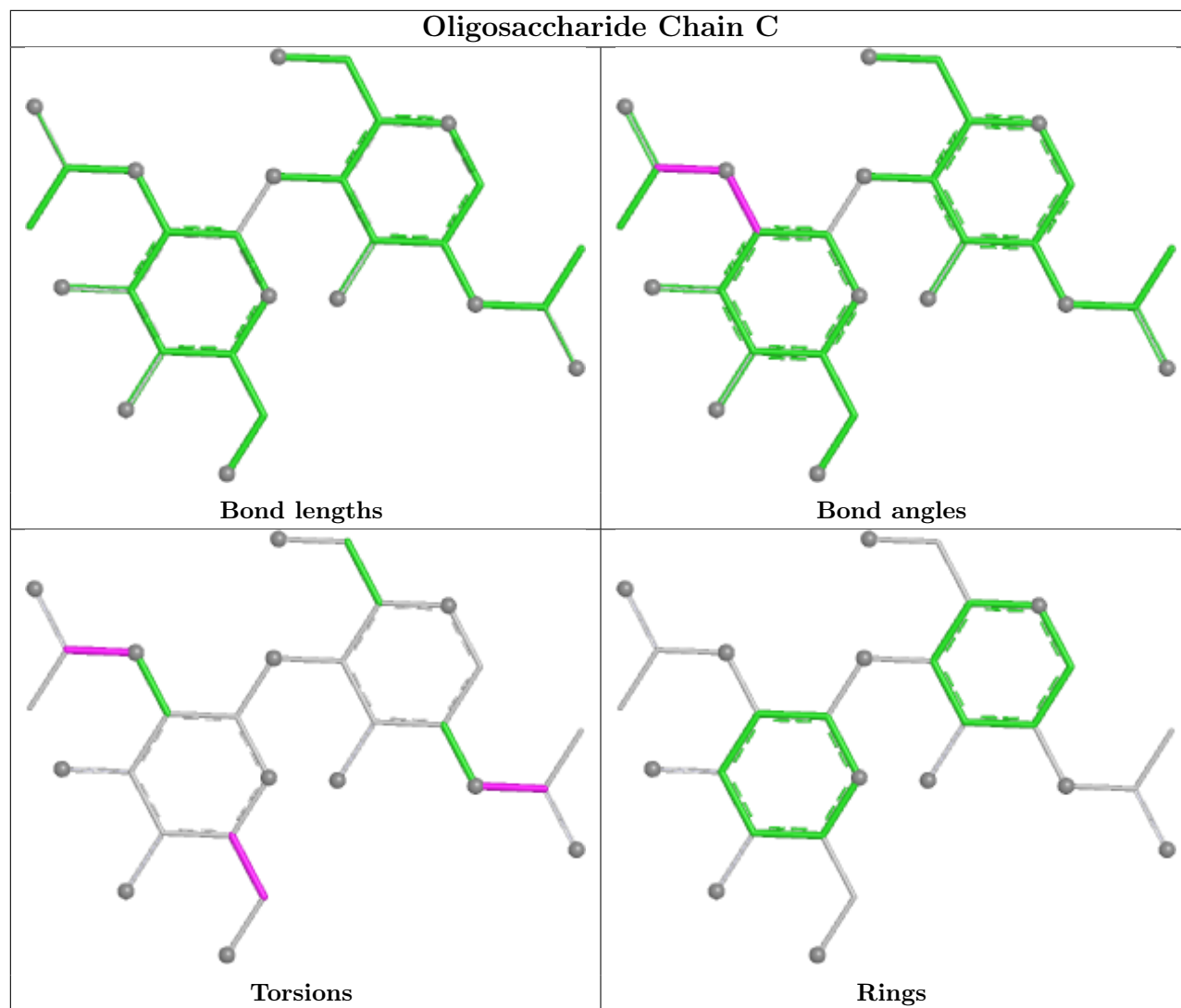
All (6) ring outliers are listed below:

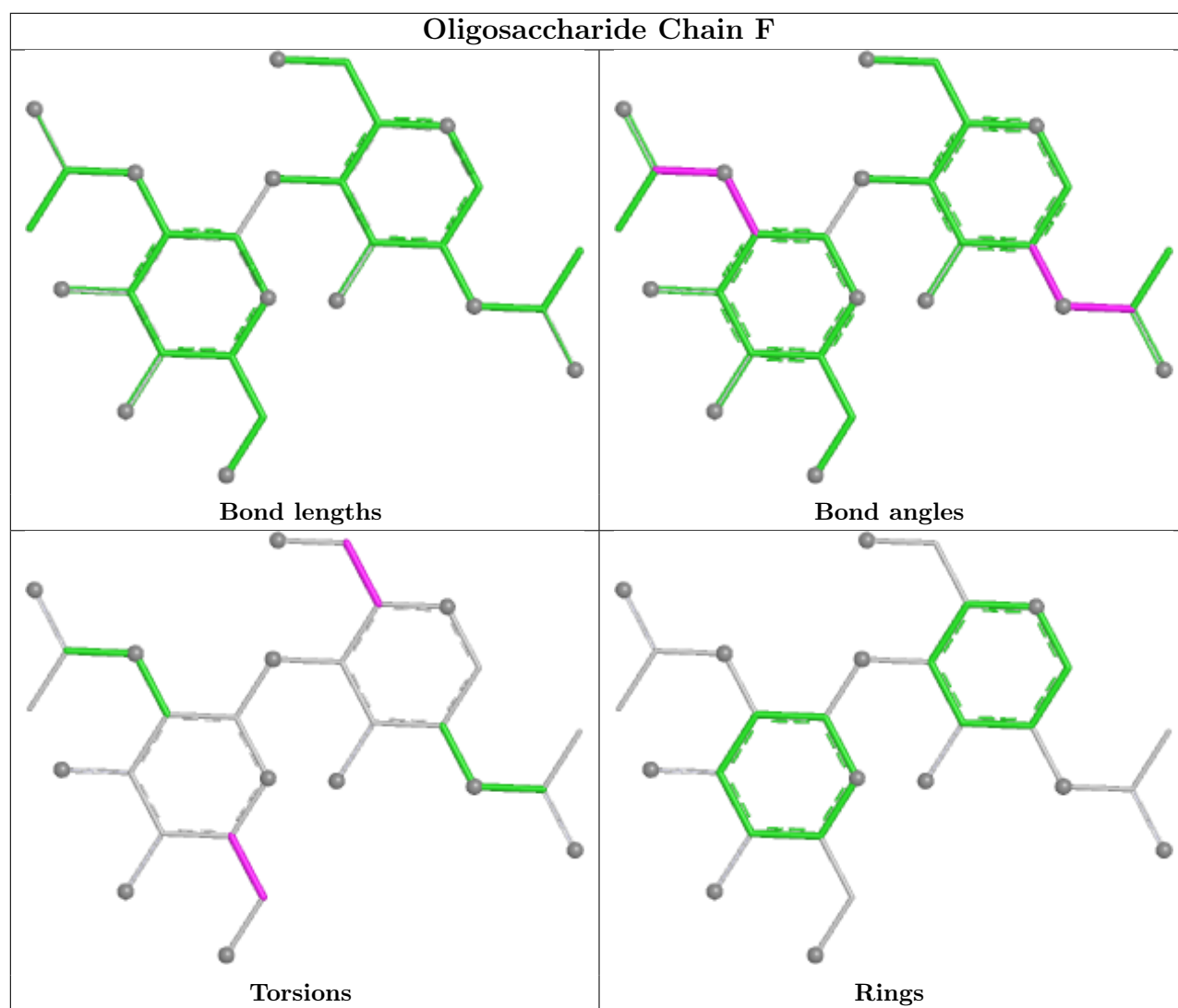
Mol	Chain	Res	Type	Atoms
5	H	5	BMA	C1-C2-C3-C4-C5-O5
4	E	5	MAN	C1-C2-C3-C4-C5-O5
3	D	4	BMA	C1-C2-C3-C4-C5-O5
3	G	4	BMA	C1-C2-C3-C4-C5-O5
3	D	3	BMA	C1-C2-C3-C4-C5-O5
3	G	3	BMA	C1-C2-C3-C4-C5-O5

14 monomers are involved in 27 short contacts:

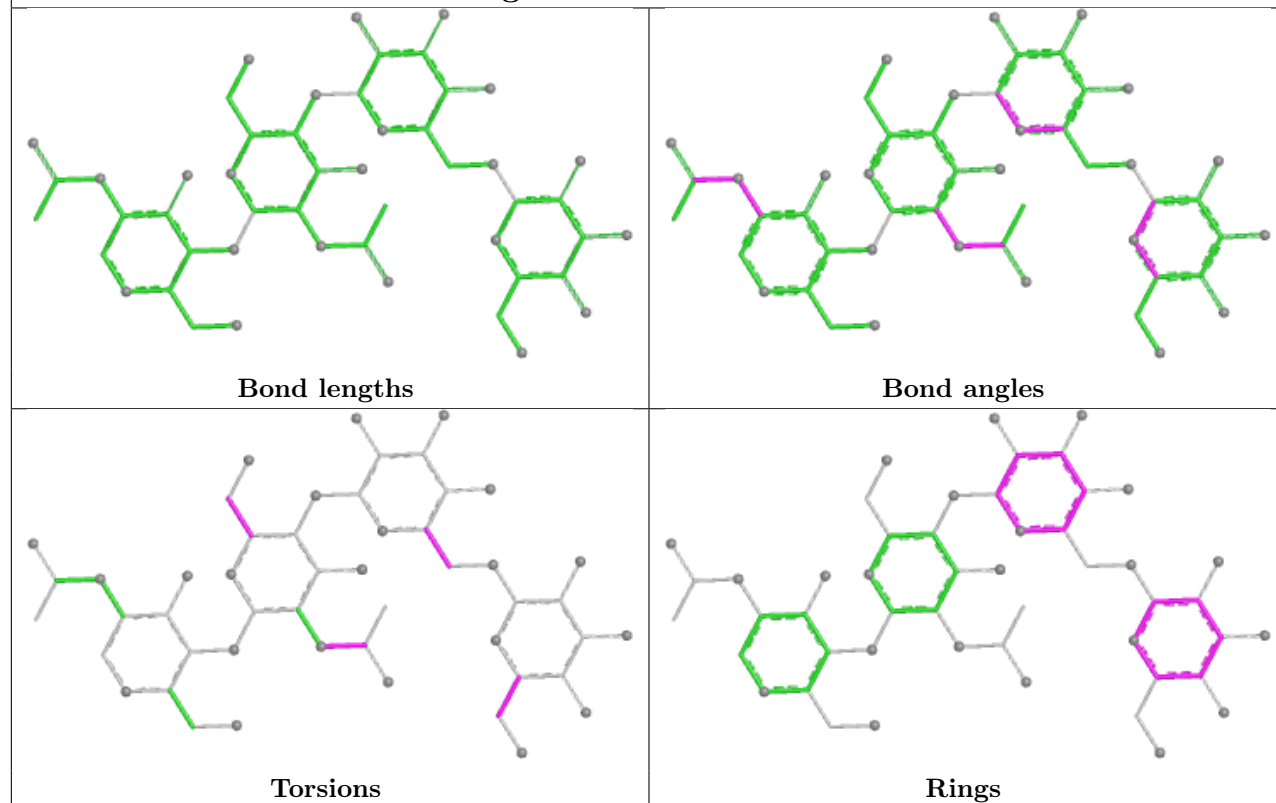
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NDG	2	0
3	G	3	BMA	4	0
3	D	4	BMA	1	0
4	E	1	NAG	1	0
5	H	4	BMA	2	0
2	C	1	NAG	2	0
2	F	1	NAG	1	0
3	G	2	NAG	2	0
3	D	2	NAG	3	0
3	D	3	BMA	5	0
5	H	5	BMA	2	0
4	E	3	BMA	4	0
4	E	2	NDG	6	0
5	H	2	NDG	4	0

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

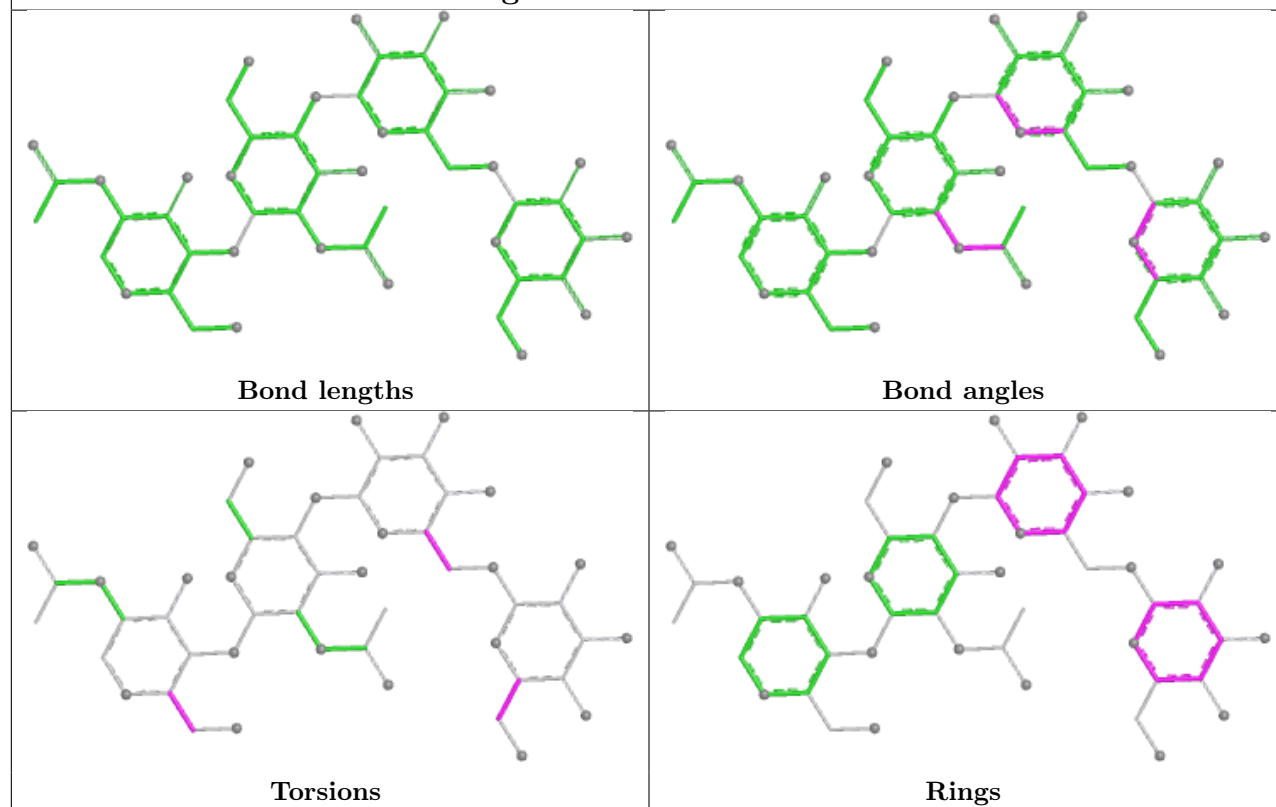




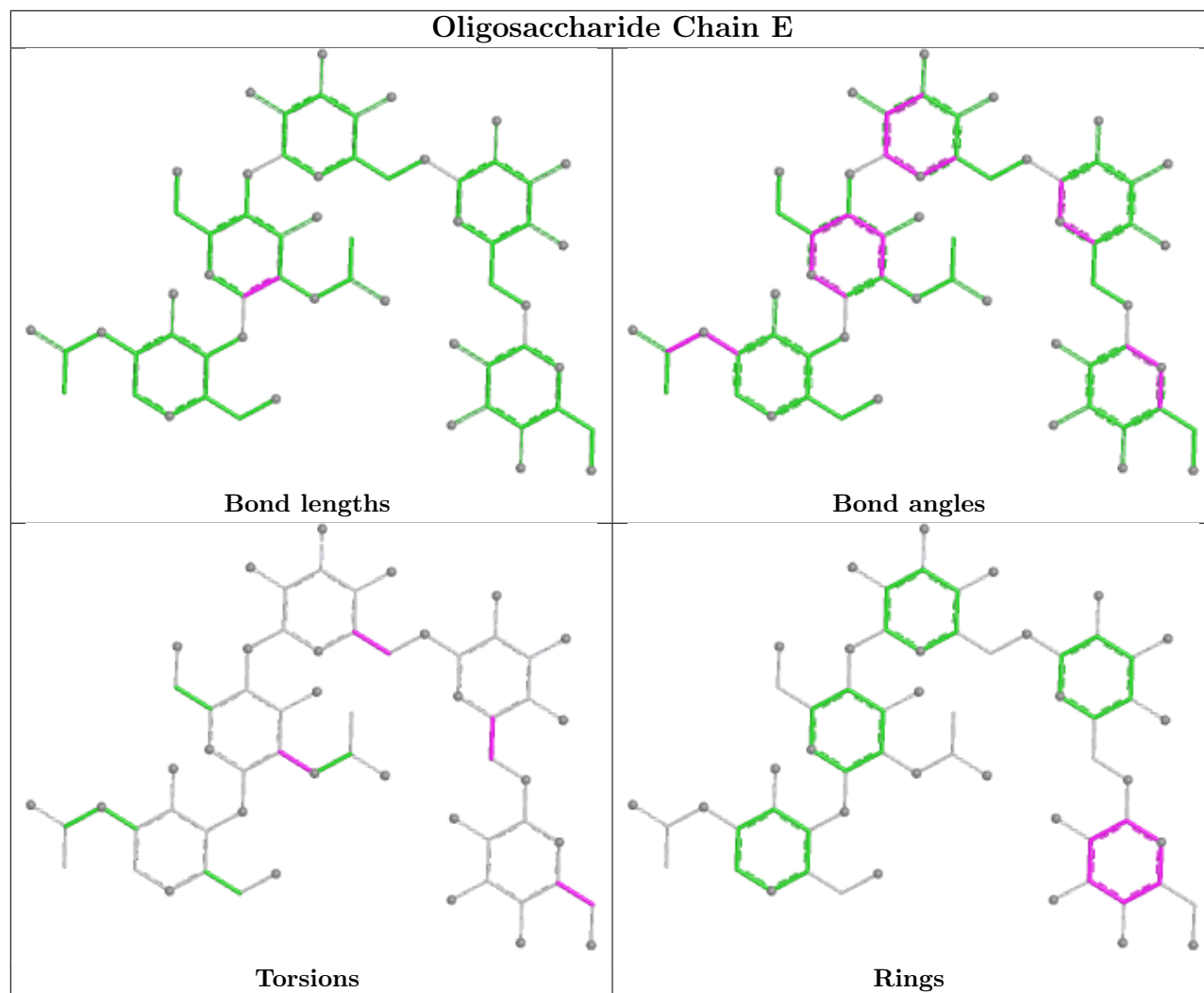
Oligosaccharide Chain D

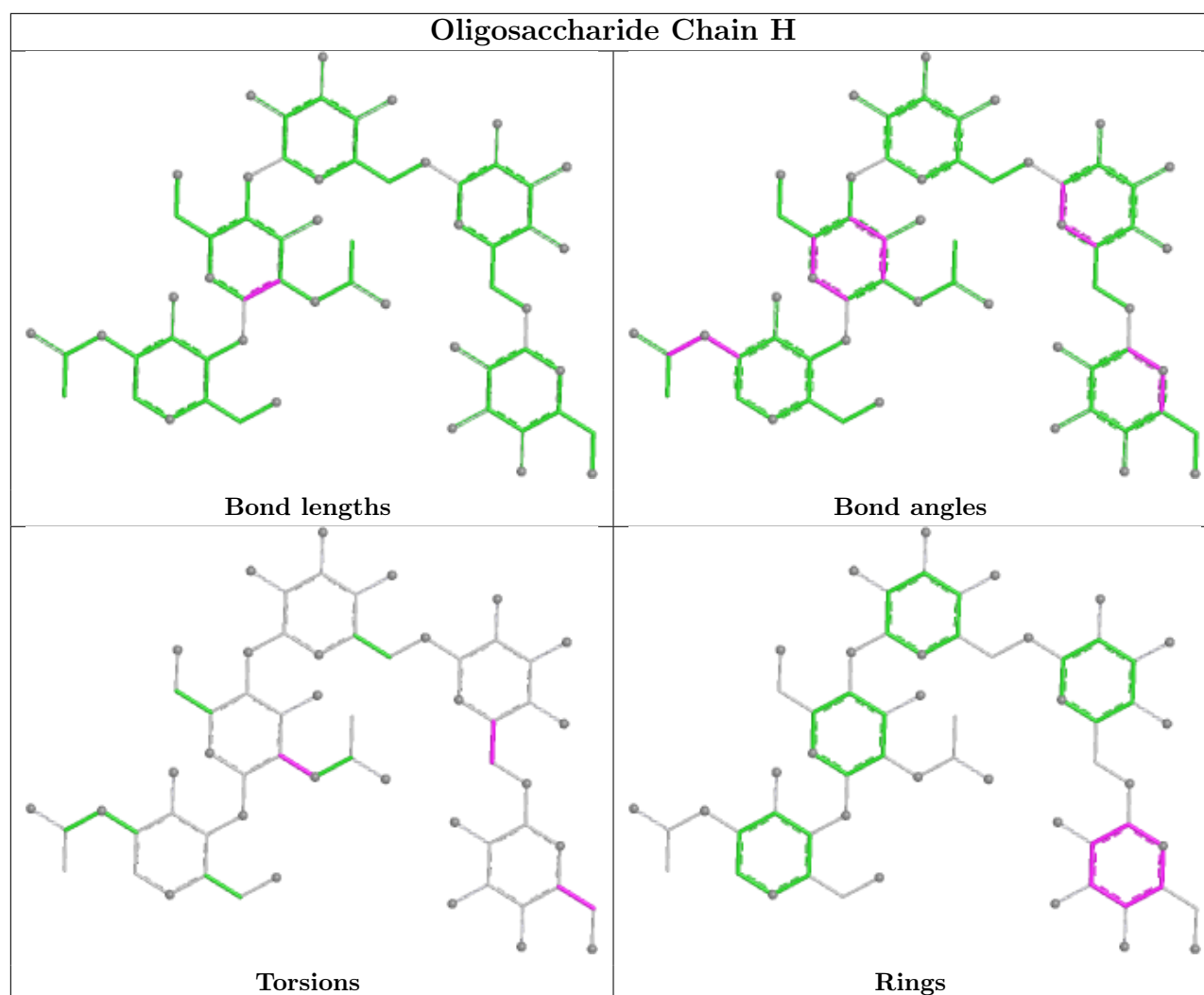


Oligosaccharide Chain G



Oligosaccharide Chain E





5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
8	HEM	A	801[A]	1	50,50,50	2.02	8 (16%)	67,82,82	5.95	41 (61%)
6	BOG	A	752	-	20,20,20	1.81	6 (30%)	25,25,25	0.89	2 (8%)
9	GOL	A	758	-	5,5,5	4.78	5 (100%)	5,5,5	6.05	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	B	1759	-	5,5,5	4.82	5 (100%)	5,5,5	6.09	3 (60%)
8	HEM	A	801[B]	1	50,50,50	1.97	8 (16%)	67,82,82	6.31	41 (61%)
7	BFL	B	1701	-	18,18,18	2.26	9 (50%)	24,24,24	1.25	4 (16%)
6	BOG	B	1751	-	20,20,20	1.69	7 (35%)	25,25,25	0.77	1 (4%)
9	GOL	B	1760	-	5,5,5	4.75	5 (100%)	5,5,5	6.17	3 (60%)
9	GOL	A	759	-	5,5,5	4.74	5 (100%)	5,5,5	6.14	3 (60%)
8	HEM	B	1601[A]	1	50,50,50	2.08	7 (14%)	67,82,82	5.63	36 (53%)
8	HEM	B	1601[B]	1	50,50,50	2.00	7 (14%)	67,82,82	5.38	36 (53%)
6	BOG	B	1752	-	20,20,20	1.73	6 (30%)	25,25,25	0.92	2 (8%)
6	BOG	B	1750	-	20,20,20	1.75	6 (30%)	25,25,25	0.92	2 (8%)
7	BFL	A	701	-	18,18,18	2.24	10 (55%)	24,24,24	1.29	4 (16%)
9	GOL	B	1758	-	5,5,5	4.85	5 (100%)	5,5,5	6.06	3 (60%)
6	BOG	A	753	-	20,20,20	1.71	6 (30%)	25,25,25	0.88	2 (8%)
6	BOG	A	751	-	20,20,20	1.70	7 (35%)	25,25,25	0.84	1 (4%)
6	BOG	B	1753	-	20,20,20	1.73	6 (30%)	25,25,25	0.91	2 (8%)
6	BOG	A	754	-	20,20,20	1.73	6 (30%)	25,25,25	0.93	2 (8%)

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
8	HEM	A	801[A]	1	-	3/14/54/54	-
6	BOG	A	752	-	-	4/11/31/31	0/1/1/1
9	GOL	A	758	-	-	2/4/4/4	-
9	GOL	B	1759	-	-	2/4/4/4	-
8	HEM	A	801[B]	1	-	4/14/54/54	-
7	BFL	B	1701	-	-	0/12/12/12	0/2/2/2
6	BOG	B	1751	-	-	6/11/31/31	0/1/1/1
9	GOL	B	1760	-	-	3/4/4/4	-
9	GOL	A	759	-	-	2/4/4/4	-
8	HEM	B	1601[A]	1	-	4/14/54/54	-
8	HEM	B	1601[B]	1	-	4/14/54/54	-
6	BOG	B	1752	-	-	4/11/31/31	0/1/1/1
6	BOG	B	1750	-	-	3/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BFL	A	701	-	-	0/12/12/12	0/2/2/2
9	GOL	B	1758	-	-	2/4/4/4	-
6	BOG	A	753	-	-	2/11/31/31	0/1/1/1
6	BOG	A	751	-	-	4/11/31/31	0/1/1/1
6	BOG	B	1753	-	-	8/11/31/31	0/1/1/1
6	BOG	A	754	-	-	6/11/31/31	0/1/1/1

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1758	GOL	C3-C2	-8.35	1.19	1.51
9	B	1759	GOL	C3-C2	-8.17	1.20	1.51
9	A	758	GOL	C3-C2	-7.99	1.21	1.51
9	B	1760	GOL	C3-C2	-7.92	1.21	1.51
9	A	759	GOL	C3-C2	-7.91	1.21	1.51
8	B	1601[A]	HEM	FE-NC	7.15	2.18	1.95
8	B	1601[A]	HEM	FE-ND	6.91	2.16	1.94
8	A	801[B]	HEM	FE-NA	6.43	2.16	1.95
8	A	801[A]	HEM	FE-NA	6.29	2.15	1.95
8	B	1601[B]	HEM	FE-ND	6.14	2.13	1.94
8	A	801[A]	HEM	FE-ND	6.09	2.13	1.94
8	B	1601[B]	HEM	FE-NC	5.69	2.13	1.95
8	B	1601[B]	HEM	FE-NB	5.48	2.11	1.94
8	A	801[A]	HEM	FE-NC	5.23	2.12	1.95
8	A	801[B]	HEM	FE-ND	5.17	2.10	1.94
8	B	1601[A]	HEM	FE-NB	5.10	2.10	1.94
8	A	801[B]	HEM	FE-NC	4.83	2.11	1.95
8	A	801[A]	HEM	CBB-CAB	4.80	1.53	1.30
8	A	801[B]	HEM	CBB-CAB	4.79	1.53	1.30
8	B	1601[B]	HEM	CBB-CAB	4.74	1.53	1.30
8	B	1601[A]	HEM	CBB-CAB	4.71	1.53	1.30
9	B	1760	GOL	O1-C1	4.68	1.62	1.42
9	A	759	GOL	O1-C1	4.60	1.61	1.42
9	B	1758	GOL	O1-C1	4.50	1.61	1.42
8	B	1601[A]	HEM	CBC-CAC	4.44	1.51	1.30
9	B	1759	GOL	O1-C1	4.43	1.61	1.42
8	B	1601[B]	HEM	CBC-CAC	4.42	1.51	1.30
8	A	801[B]	HEM	CBC-CAC	4.36	1.51	1.30
8	A	801[A]	HEM	CBC-CAC	4.35	1.51	1.30
9	A	758	GOL	O1-C1	4.35	1.60	1.42
6	A	752	BOG	O5-C1	3.89	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	801[B]	HEM	FE-NB	3.87	2.06	1.94
8	B	1601[B]	HEM	FE-NA	3.82	2.07	1.95
6	A	753	BOG	O5-C1	3.73	1.51	1.41
6	B	1750	BOG	O5-C1	3.72	1.51	1.41
6	A	752	BOG	O5-C5	3.71	1.53	1.44
6	B	1751	BOG	O5-C1	3.69	1.51	1.41
6	B	1752	BOG	O5-C1	3.67	1.51	1.41
6	A	754	BOG	O5-C1	3.67	1.51	1.41
6	B	1753	BOG	O5-C1	3.62	1.51	1.41
8	A	801[A]	HEM	FE-NB	3.61	2.06	1.94
6	A	751	BOG	O5-C1	3.60	1.51	1.41
6	A	754	BOG	O5-C5	3.52	1.53	1.44
6	A	753	BOG	O5-C5	3.50	1.52	1.44
9	A	758	GOL	C1-C2	-3.46	1.38	1.51
6	B	1750	BOG	O5-C5	3.46	1.52	1.44
7	B	1701	BFL	C14-C13	3.46	1.46	1.39
6	B	1753	BOG	O5-C5	3.45	1.52	1.44
9	A	759	GOL	O3-C3	3.44	1.56	1.42
9	B	1760	GOL	O3-C3	3.40	1.56	1.42
7	A	701	BFL	C10-C9	3.39	1.44	1.39
6	B	1752	BOG	O5-C5	3.35	1.52	1.44
6	B	1751	BOG	O5-C5	3.32	1.52	1.44
7	A	701	BFL	C11-C12	3.31	1.46	1.39
9	A	758	GOL	O3-C3	3.30	1.56	1.42
7	A	701	BFL	C14-C13	3.30	1.46	1.39
9	B	1759	GOL	O3-C3	3.28	1.56	1.42
6	A	751	BOG	O5-C5	3.24	1.52	1.44
7	B	1701	BFL	C11-C12	3.24	1.45	1.39
7	B	1701	BFL	C10-C9	3.22	1.44	1.39
7	B	1701	BFL	O1-C6	-3.17	1.20	1.30
9	B	1759	GOL	O2-C2	-3.15	1.34	1.43
9	B	1758	GOL	O3-C3	3.14	1.55	1.42
9	B	1758	GOL	C1-C2	-3.02	1.40	1.51
9	B	1759	GOL	C1-C2	-3.01	1.40	1.51
9	A	759	GOL	C1-C2	-3.00	1.40	1.51
7	A	701	BFL	O1-C6	-2.98	1.21	1.30
9	B	1758	GOL	O2-C2	-2.98	1.34	1.43
9	B	1760	GOL	C1-C2	-2.91	1.40	1.51
9	A	758	GOL	O2-C2	-2.91	1.34	1.43
6	A	752	BOG	C3'-C2'	-2.85	1.37	1.51
9	B	1760	GOL	O2-C2	-2.84	1.35	1.43
6	A	754	BOG	C3'-C2'	-2.84	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1753	BOG	C3'-C2'	-2.84	1.37	1.51
9	A	759	GOL	O2-C2	-2.81	1.35	1.43
6	B	1750	BOG	C3'-C2'	-2.81	1.37	1.51
6	A	753	BOG	C3'-C2'	-2.80	1.37	1.51
6	B	1751	BOG	C3'-C2'	-2.76	1.38	1.51
6	B	1752	BOG	C3'-C2'	-2.74	1.38	1.51
7	B	1701	BFL	C11-C10	2.73	1.43	1.38
6	A	751	BOG	C3'-C2'	-2.73	1.38	1.51
7	B	1701	BFL	C3-C4	2.70	1.43	1.38
7	A	701	BFL	C15-C14	2.65	1.43	1.38
7	A	701	BFL	C11-C10	2.64	1.43	1.38
7	B	1701	BFL	O2-C6	2.62	1.29	1.22
7	B	1701	BFL	C15-C14	2.61	1.43	1.38
7	A	701	BFL	C3-C4	2.61	1.43	1.38
6	A	752	BOG	C4-C3	2.51	1.58	1.52
6	B	1752	BOG	C4-C3	2.50	1.58	1.52
6	B	1750	BOG	C4-C3	2.50	1.58	1.52
7	A	701	BFL	O2-C6	2.49	1.29	1.22
6	A	751	BOG	C4-C3	2.46	1.58	1.52
6	B	1753	BOG	C4-C3	2.42	1.58	1.52
6	A	754	BOG	C4-C3	2.38	1.58	1.52
6	A	753	BOG	C4-C3	2.37	1.58	1.52
8	A	801[B]	HEM	CAB-C3B	2.37	1.53	1.47
8	A	801[A]	HEM	CAB-C3B	2.37	1.53	1.47
6	B	1751	BOG	C4-C3	2.34	1.58	1.52
6	A	752	BOG	C1-C2	2.33	1.59	1.52
6	B	1752	BOG	C1-C2	2.32	1.59	1.52
8	B	1601[A]	HEM	FE-NA	2.32	2.02	1.95
6	B	1751	BOG	C7'-C6'	-2.29	1.37	1.51
6	A	751	BOG	C7'-C6'	-2.28	1.37	1.51
6	A	752	BOG	C7'-C6'	-2.27	1.37	1.51
6	B	1752	BOG	C7'-C6'	-2.25	1.37	1.51
6	A	753	BOG	C7'-C6'	-2.25	1.37	1.51
6	B	1753	BOG	C7'-C6'	-2.25	1.37	1.51
6	B	1750	BOG	C7'-C6'	-2.24	1.37	1.51
8	B	1601[B]	HEM	CAB-C3B	2.23	1.53	1.47
6	A	754	BOG	C7'-C6'	-2.22	1.37	1.51
8	B	1601[A]	HEM	CAB-C3B	2.22	1.53	1.47
6	A	751	BOG	C1-C2	2.22	1.59	1.52
7	A	701	BFL	C1-C12	2.22	1.43	1.39
6	B	1750	BOG	C1-C2	2.18	1.58	1.52
6	A	754	BOG	C1-C2	2.16	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1753	BOG	C1-C2	2.16	1.58	1.52
7	B	1701	BFL	C1-C12	2.14	1.43	1.39
6	A	751	BOG	C4-C5	-2.08	1.48	1.53
6	A	753	BOG	C1-C2	2.08	1.58	1.52
8	A	801[A]	HEM	CMB-C2B	2.07	1.55	1.50
7	A	701	BFL	C4-C13	2.03	1.43	1.39
8	A	801[B]	HEM	CMB-C2B	2.02	1.54	1.50
6	B	1751	BOG	C1-C2	2.02	1.58	1.52
6	B	1751	BOG	C4-C5	-2.00	1.48	1.53

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	801[B]	HEM	CHA-C4D-ND	-15.52	105.17	124.37
8	A	801[B]	HEM	CHD-C1D-ND	-15.49	107.76	124.42
8	A	801[A]	HEM	CHD-C1D-ND	-13.69	109.69	124.42
8	B	1601[B]	HEM	CHC-C4B-NB	-13.45	109.95	124.42
8	B	1601[A]	HEM	CHC-C4B-NB	-13.21	110.20	124.42
8	A	801[B]	HEM	CHD-C4C-NC	-13.18	110.11	124.45
8	A	801[A]	HEM	C4C-CHD-C1D	12.92	153.48	126.02
8	A	801[B]	HEM	C4C-CHD-C1D	12.88	153.39	126.02
8	A	801[A]	HEM	CHD-C4C-NC	-12.87	110.44	124.45
8	A	801[B]	HEM	CHC-C4B-NB	-12.76	110.69	124.42
8	A	801[B]	HEM	C1A-CHA-C4D	12.70	156.12	126.25
8	A	801[A]	HEM	CHB-C1B-NB	-12.65	108.72	124.37
8	B	1601[A]	HEM	CHC-C1C-NC	-12.48	110.87	124.45
8	B	1601[A]	HEM	CHD-C4C-NC	-12.47	110.88	124.45
8	A	801[B]	HEM	C4A-CHB-C1B	12.43	155.47	126.25
8	A	801[A]	HEM	C4A-CHB-C1B	12.34	155.26	126.25
8	B	1601[B]	HEM	CHD-C4C-NC	-12.30	111.06	124.45
8	A	801[B]	HEM	CHB-C1B-NB	-12.26	109.21	124.37
8	B	1601[B]	HEM	CHC-C1C-NC	-12.21	111.16	124.45
8	A	801[A]	HEM	CHC-C4B-NB	-12.14	111.36	124.42
8	A	801[B]	HEM	CHC-C1C-NC	-12.07	111.31	124.45
8	A	801[B]	HEM	C1C-CHC-C4B	11.96	151.44	126.02
8	B	1601[A]	HEM	C4C-CHD-C1D	11.92	151.35	126.02
8	B	1601[B]	HEM	C4C-CHD-C1D	11.67	150.82	126.02
8	B	1601[A]	HEM	C1C-CHC-C4B	11.65	150.79	126.02
8	B	1601[B]	HEM	C1C-CHC-C4B	11.63	150.74	126.02
8	A	801[A]	HEM	CHC-C1C-NC	-11.52	111.91	124.45
8	B	1601[A]	HEM	CHB-C1B-NB	-11.45	110.21	124.37
8	B	1601[A]	HEM	CHD-C1D-ND	-11.39	112.17	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1601[B]	HEM	CHD-C1D-ND	-11.34	112.22	124.42
8	A	801[A]	HEM	CHA-C4D-ND	-11.31	110.38	124.37
9	B	1760	GOL	O3-C3-C2	11.25	161.01	110.38
9	A	759	GOL	O3-C3-C2	11.17	160.65	110.38
8	B	1601[A]	HEM	C3B-C2B-C1B	-11.07	98.10	106.41
9	B	1759	GOL	O3-C3-C2	11.07	160.20	110.38
9	B	1758	GOL	O3-C3-C2	11.03	160.03	110.38
8	B	1601[A]	HEM	C4A-CHB-C1B	11.01	152.14	126.25
8	A	801[A]	HEM	C1C-CHC-C4B	10.93	149.26	126.02
8	A	801[A]	HEM	C3B-C2B-C1B	-10.88	98.25	106.41
9	A	758	GOL	O3-C3-C2	10.82	159.07	110.38
8	A	801[A]	HEM	C1A-CHA-C4D	10.79	151.61	126.25
8	B	1601[B]	HEM	CHB-C1B-NB	-10.68	111.16	124.37
8	B	1601[B]	HEM	C4A-CHB-C1B	10.45	150.83	126.25
8	A	801[B]	HEM	CHB-C4A-NA	-9.59	106.46	123.86
8	A	801[B]	HEM	CHA-C1A-NA	-9.52	106.60	123.86
8	B	1601[B]	HEM	C1A-CHA-C4D	8.88	147.13	126.25
8	B	1601[A]	HEM	C1A-CHA-C4D	8.87	147.12	126.25
8	B	1601[A]	HEM	CHC-C4B-C3B	8.61	142.25	125.07
8	A	801[A]	HEM	CHA-C1A-NA	-8.43	108.58	123.86
8	A	801[A]	HEM	CHD-C4C-C3C	8.39	139.35	125.21
8	B	1601[B]	HEM	CHA-C4D-ND	-8.34	114.05	124.37
8	A	801[B]	HEM	CHD-C4C-C3C	8.33	139.26	125.21
8	A	801[B]	HEM	C3B-C2B-C1B	-8.28	100.19	106.41
8	B	1601[B]	HEM	C3B-C2B-C1B	-8.24	100.22	106.41
8	A	801[A]	HEM	CHB-C4A-NA	-8.23	108.93	123.86
8	B	1601[B]	HEM	CHC-C4B-C3B	7.97	140.97	125.07
8	A	801[B]	HEM	CHC-C4B-C3B	7.95	140.93	125.07
8	B	1601[A]	HEM	CHA-C4D-ND	-7.93	114.56	124.37
8	B	1601[B]	HEM	CHB-C4A-NA	-7.72	109.86	123.86
8	B	1601[A]	HEM	CHB-C4A-NA	-7.62	110.04	123.86
8	B	1601[A]	HEM	CHD-C4C-C3C	7.61	138.05	125.21
8	A	801[A]	HEM	CHC-C4B-C3B	7.61	140.27	125.07
8	B	1601[B]	HEM	CHD-C4C-C3C	7.53	137.90	125.21
8	B	1601[A]	HEM	CHA-C4D-C3D	7.51	139.08	125.23
9	A	758	GOL	O2-C2-C3	7.39	139.79	109.18
8	A	801[A]	HEM	C2B-C1B-NB	7.21	118.13	109.84
8	B	1601[B]	HEM	CHA-C4D-C3D	7.21	138.52	125.23
9	A	759	GOL	O2-C2-C3	7.14	138.73	109.18
9	B	1760	GOL	O2-C2-C3	7.12	138.64	109.18
9	B	1759	GOL	O2-C2-C3	7.09	138.53	109.18
8	B	1601[A]	HEM	CHA-C1A-NA	-7.03	111.11	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	801[A]	HEM	CHA-C4D-C3D	7.01	138.14	125.23
9	B	1758	GOL	O2-C2-C3	6.97	138.05	109.18
8	B	1601[A]	HEM	C2B-C1B-NB	6.95	117.83	109.84
8	B	1601[A]	HEM	C4B-C3B-C2B	6.88	113.60	107.28
8	A	801[B]	HEM	C2D-C1D-ND	6.86	117.83	109.90
8	A	801[B]	HEM	CHA-C4D-C3D	6.82	137.81	125.23
8	A	801[A]	HEM	CHA-C1A-C2A	6.73	140.03	125.30
8	A	801[B]	HEM	CHA-C1A-C2A	6.68	139.92	125.30
8	B	1601[A]	HEM	CHD-C1D-C2D	6.66	135.54	125.03
8	B	1601[B]	HEM	CHA-C1A-NA	-6.63	111.84	123.86
8	B	1601[B]	HEM	CHD-C1D-C2D	6.56	135.38	125.03
8	A	801[A]	HEM	C1D-C2D-C3D	-6.49	100.15	106.98
8	A	801[B]	HEM	C4D-ND-C1D	-6.34	97.70	105.21
8	A	801[A]	HEM	C4B-C3B-C2B	6.26	113.03	107.28
8	A	801[B]	HEM	CHC-C1C-C2C	6.14	138.25	125.49
8	B	1601[B]	HEM	C2B-C1B-NB	5.86	116.58	109.84
8	A	801[B]	HEM	CMB-C2B-C3B	5.58	141.92	128.43
8	A	801[A]	HEM	CHC-C1C-C2C	5.51	136.95	125.49
8	B	1601[A]	HEM	C1D-C2D-C3D	-5.49	101.21	106.98
8	A	801[A]	HEM	C2D-C1D-ND	5.39	116.13	109.90
8	A	801[B]	HEM	C2B-C1B-NB	5.36	116.00	109.84
8	A	801[B]	HEM	C3D-C4D-ND	5.32	116.00	110.17
8	A	801[B]	HEM	C1D-C2D-C3D	-5.19	101.52	106.98
8	A	801[A]	HEM	CHD-C1D-C2D	5.12	133.11	125.03
8	A	801[A]	HEM	CMB-C2B-C3B	5.08	140.72	128.43
8	A	801[B]	HEM	CHD-C1D-C2D	5.08	133.04	125.03
8	B	1601[B]	HEM	C1D-C2D-C3D	-5.00	101.72	106.98
8	A	801[B]	HEM	CMB-C2B-C1B	-4.99	117.24	125.03
8	A	801[B]	HEM	C4B-C3B-C2B	4.97	111.85	107.28
8	B	1601[B]	HEM	CHC-C1C-C2C	4.85	135.57	125.49
8	A	801[A]	HEM	CMA-C3A-C2A	4.81	135.83	125.62
8	B	1601[A]	HEM	CHC-C1C-C2C	4.81	135.49	125.49
8	B	1601[A]	HEM	CHA-C1A-C2A	4.54	135.24	125.30
8	B	1601[B]	HEM	CAA-CBA-CGA	4.51	125.62	113.67
8	B	1601[A]	HEM	CMB-C2B-C3B	4.48	139.26	128.43
8	B	1601[B]	HEM	C4B-C3B-C2B	4.44	111.36	107.28
8	B	1601[A]	HEM	C3A-C4A-NA	4.22	116.91	110.14
8	B	1601[B]	HEM	CHA-C1A-C2A	4.18	134.46	125.30
8	B	1601[A]	HEM	C4A-C3A-C2A	-4.16	102.05	106.82
8	B	1601[A]	HEM	C4D-C3D-C2D	4.15	112.94	106.89
8	A	801[A]	HEM	C4A-C3A-C2A	-4.10	102.12	106.82
8	B	1601[A]	HEM	C4A-NA-C1A	-4.09	99.16	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1601[B]	HEM	C4A-NA-C1A	-3.90	99.46	105.82
8	B	1601[B]	HEM	C4A-C3A-C2A	-3.76	102.50	106.82
8	A	801[B]	HEM	CHB-C4A-C3A	3.67	138.08	127.43
8	B	1601[B]	HEM	C3A-C4A-NA	3.65	115.99	110.14
8	B	1601[A]	HEM	CMA-C3A-C2A	3.58	133.23	125.62
9	B	1760	GOL	O1-C1-C2	3.57	126.43	110.38
8	A	801[A]	HEM	C3A-C4A-NA	3.53	115.80	110.14
9	B	1758	GOL	O1-C1-C2	3.52	126.24	110.38
8	B	1601[A]	HEM	C3D-C4D-ND	-3.52	106.31	110.17
8	B	1601[B]	HEM	C4D-C3D-C2D	3.51	112.00	106.89
8	B	1601[A]	HEM	CAD-C3D-C4D	-3.49	118.62	124.70
9	A	759	GOL	O1-C1-C2	3.47	126.02	110.38
9	B	1759	GOL	O1-C1-C2	3.44	125.87	110.38
8	A	801[B]	HEM	O1D-CGD-CBD	-3.43	112.22	123.09
8	A	801[B]	HEM	O2A-CGA-O1A	-3.35	114.72	123.33
9	A	758	GOL	O1-C1-C2	3.25	124.99	110.38
8	A	801[B]	HEM	C4A-NA-C1A	-3.24	100.54	105.82
8	B	1601[B]	HEM	C2A-C1A-NA	3.20	113.70	110.15
8	B	1601[A]	HEM	C2A-C1A-NA	3.15	113.65	110.15
8	B	1601[B]	HEM	CAD-C3D-C4D	-3.14	119.22	124.70
8	A	801[B]	HEM	CBB-CAB-C3B	3.08	142.94	127.53
8	A	801[B]	HEM	C3A-C4A-NA	3.07	115.06	110.14
6	A	754	BOG	C1'-O1-C1	3.06	118.90	113.68
8	A	801[B]	HEM	C2A-C1A-NA	2.99	113.47	110.15
8	A	801[A]	HEM	CMB-C2B-C1B	-2.99	120.36	125.03
8	A	801[A]	HEM	CBB-CAB-C3B	2.97	142.39	127.53
6	B	1750	BOG	C1'-O1-C1	2.91	118.65	113.68
8	A	801[A]	HEM	C4D-ND-C1D	-2.90	101.78	105.21
6	A	753	BOG	C1'-O1-C1	2.88	118.59	113.68
8	A	801[B]	HEM	O2D-CGD-CBD	2.85	122.99	114.00
6	A	752	BOG	C1'-O1-C1	2.84	118.53	113.68
8	A	801[B]	HEM	CMA-C3A-C2A	2.79	131.54	125.62
8	A	801[B]	HEM	CHB-C1B-C2B	2.74	134.75	126.95
8	B	1601[B]	HEM	CMB-C2B-C3B	2.74	135.07	128.43
8	A	801[A]	HEM	C4D-C3D-C2D	2.74	110.88	106.89
6	B	1752	BOG	C1'-O1-C1	2.74	118.36	113.68
8	A	801[B]	HEM	CBA-CAA-C2A	2.73	120.08	112.53
6	B	1753	BOG	C1'-O1-C1	2.72	118.33	113.68
6	A	751	BOG	O1-C1-C2	2.71	112.39	108.27
8	A	801[A]	HEM	CHB-C4A-C3A	2.70	135.26	127.43
8	B	1601[A]	HEM	C3B-C4B-NB	-2.68	107.54	109.47
8	A	801[A]	HEM	C4A-NA-C1A	-2.68	101.45	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	701	BFL	O2-C6-C5	-2.67	112.98	122.86
6	B	1752	BOG	O1-C1-C2	2.67	112.32	108.27
8	A	801[A]	HEM	C1B-NB-C4B	-2.58	102.15	105.21
8	B	1601[B]	HEM	C3D-C4D-ND	-2.58	107.34	110.17
6	B	1753	BOG	O1-C1-C2	2.54	112.13	108.27
7	B	1701	BFL	O2-C6-C5	-2.53	113.51	122.86
8	A	801[A]	HEM	CAA-C2A-C1A	-2.52	120.01	124.94
6	B	1750	BOG	O1-C1-C2	2.49	112.06	108.27
8	A	801[B]	HEM	CMD-C2D-C1D	2.45	128.87	125.03
8	A	801[B]	HEM	CAA-CBA-CGA	2.44	120.14	113.67
7	A	701	BFL	C1-C8-C9	-2.43	118.76	121.18
6	B	1751	BOG	O1-C1-C2	2.42	111.94	108.27
8	A	801[B]	HEM	C4A-C3A-C2A	-2.42	104.05	106.82
8	B	1601[B]	HEM	O2A-CGA-O1A	-2.41	117.13	123.33
8	B	1601[B]	HEM	CMA-C3A-C2A	2.38	130.68	125.62
7	A	701	BFL	O1-C6-C5	2.37	124.27	114.25
6	A	754	BOG	O1-C1-C2	2.36	111.85	108.27
8	A	801[A]	HEM	CMA-C3A-C4A	-2.34	121.86	125.42
7	B	1701	BFL	O1-C6-C5	2.31	124.03	114.25
8	B	1601[B]	HEM	C1B-NB-C4B	-2.28	102.51	105.21
8	A	801[A]	HEM	CMD-C2D-C1D	2.27	128.58	125.03
8	B	1601[A]	HEM	CAA-CBA-CGA	2.25	119.64	113.67
7	B	1701	BFL	C1-C8-C9	-2.24	118.94	121.18
8	B	1601[B]	HEM	CHB-C4A-C3A	2.23	133.89	127.43
8	A	801[A]	HEM	CAA-CBA-CGA	2.20	119.51	113.67
8	A	801[A]	HEM	O2A-CGA-O1A	-2.19	117.71	123.33
7	A	701	BFL	C8-C1-C12	2.18	123.93	121.12
8	B	1601[A]	HEM	C3C-C2C-C1C	-2.17	104.99	107.05
8	A	801[A]	HEM	CHB-C1B-C2B	2.17	133.10	126.95
8	B	1601[B]	HEM	C2D-C1D-ND	2.15	112.39	109.90
6	A	752	BOG	O1-C1-C2	2.13	111.51	108.27
7	B	1701	BFL	C8-C1-C12	2.12	123.84	121.12
8	B	1601[A]	HEM	C1B-NB-C4B	-2.09	102.73	105.21
8	B	1601[A]	HEM	C2D-C1D-ND	2.04	112.26	109.90
6	A	753	BOG	O1-C1-C2	2.02	111.34	108.27
8	A	801[A]	HEM	CAB-C3B-C2B	-2.01	121.90	128.43

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	801[A]	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	B	1601[A]	HEM	C2B-C3B-CAB-CBB
8	B	1601[B]	HEM	C2B-C3B-CAB-CBB
9	A	758	GOL	C1-C2-C3-O3
9	A	759	GOL	O1-C1-C2-O2
9	A	759	GOL	C1-C2-C3-O3
9	B	1758	GOL	C1-C2-C3-O3
9	B	1759	GOL	C1-C2-C3-O3
9	B	1760	GOL	C1-C2-C3-O3
6	A	754	BOG	O5-C5-C6-O6
6	B	1753	BOG	O5-C5-C6-O6
9	A	758	GOL	O1-C1-C2-O2
6	B	1753	BOG	C4-C5-C6-O6
6	A	754	BOG	C4-C5-C6-O6
6	B	1751	BOG	C2-C1-O1-C1'
9	B	1758	GOL	O1-C1-C2-O2
9	B	1759	GOL	O1-C1-C2-O2
9	B	1760	GOL	O1-C1-C2-O2
6	B	1752	BOG	C2'-C3'-C4'-C5'
6	A	751	BOG	C3'-C4'-C5'-C6'
6	A	754	BOG	C1'-C2'-C3'-C4'
6	B	1752	BOG	C1'-C2'-C3'-C4'
8	A	801[B]	HEM	C2C-C3C-CAC-CBC
8	B	1601[A]	HEM	C2C-C3C-CAC-CBC
8	B	1601[B]	HEM	C2C-C3C-CAC-CBC
8	A	801[A]	HEM	C4C-C3C-CAC-CBC
8	B	1601[B]	HEM	C4B-C3B-CAB-CBB
6	B	1752	BOG	O1-C1'-C2'-C3'
6	B	1751	BOG	C3'-C4'-C5'-C6'
6	A	752	BOG	C2'-C3'-C4'-C5'
6	B	1751	BOG	O1-C1'-C2'-C3'
6	B	1753	BOG	C1'-C2'-C3'-C4'
6	A	753	BOG	C2'-C3'-C4'-C5'
6	B	1750	BOG	C3'-C4'-C5'-C6'
6	A	754	BOG	C3'-C4'-C5'-C6'
6	B	1750	BOG	C1'-C2'-C3'-C4'
6	B	1751	BOG	O5-C1-O1-C1'
6	A	754	BOG	C2'-C3'-C4'-C5'
6	B	1753	BOG	C2-C1-O1-C1'
6	B	1750	BOG	O1-C1'-C2'-C3'
6	B	1752	BOG	C3'-C4'-C5'-C6'
6	A	751	BOG	C2'-C3'-C4'-C5'
8	A	801[A]	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
6	A	751	BOG	C1'-C2'-C3'-C4'
8	A	801[B]	HEM	C4C-C3C-CAC-CBC
8	B	1601[A]	HEM	C4B-C3B-CAB-CBB
8	B	1601[A]	HEM	C4C-C3C-CAC-CBC
8	B	1601[B]	HEM	C4C-C3C-CAC-CBC
6	B	1753	BOG	C3'-C4'-C5'-C6'
6	A	752	BOG	C3'-C4'-C5'-C6'
6	B	1753	BOG	C2'-C3'-C4'-C5'
6	B	1751	BOG	C1'-C2'-C3'-C4'
6	A	752	BOG	C2-C1-O1-C1'
6	B	1753	BOG	O1-C1'-C2'-C3'
6	A	753	BOG	O1-C1'-C2'-C3'
9	B	1760	GOL	O1-C1-C2-C3
6	B	1753	BOG	O5-C1-O1-C1'
6	B	1751	BOG	C2'-C3'-C4'-C5'
6	A	754	BOG	O1-C1'-C2'-C3'
6	A	752	BOG	O5-C1-O1-C1'
6	A	751	BOG	O1-C1'-C2'-C3'
8	A	801[B]	HEM	C2B-C3B-CAB-CBB
8	A	801[B]	HEM	CAD-CBD-CGD-O1D

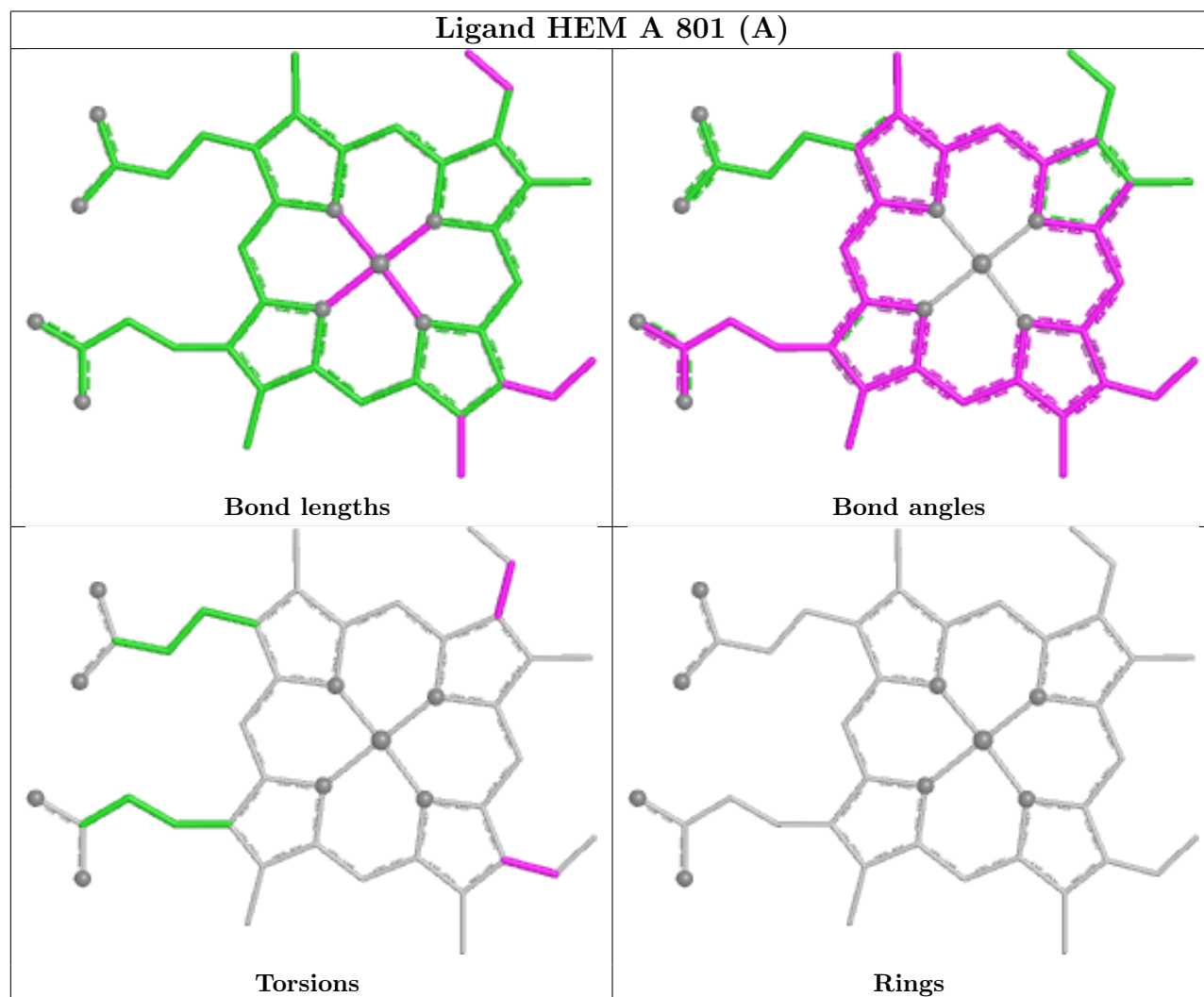
There are no ring outliers.

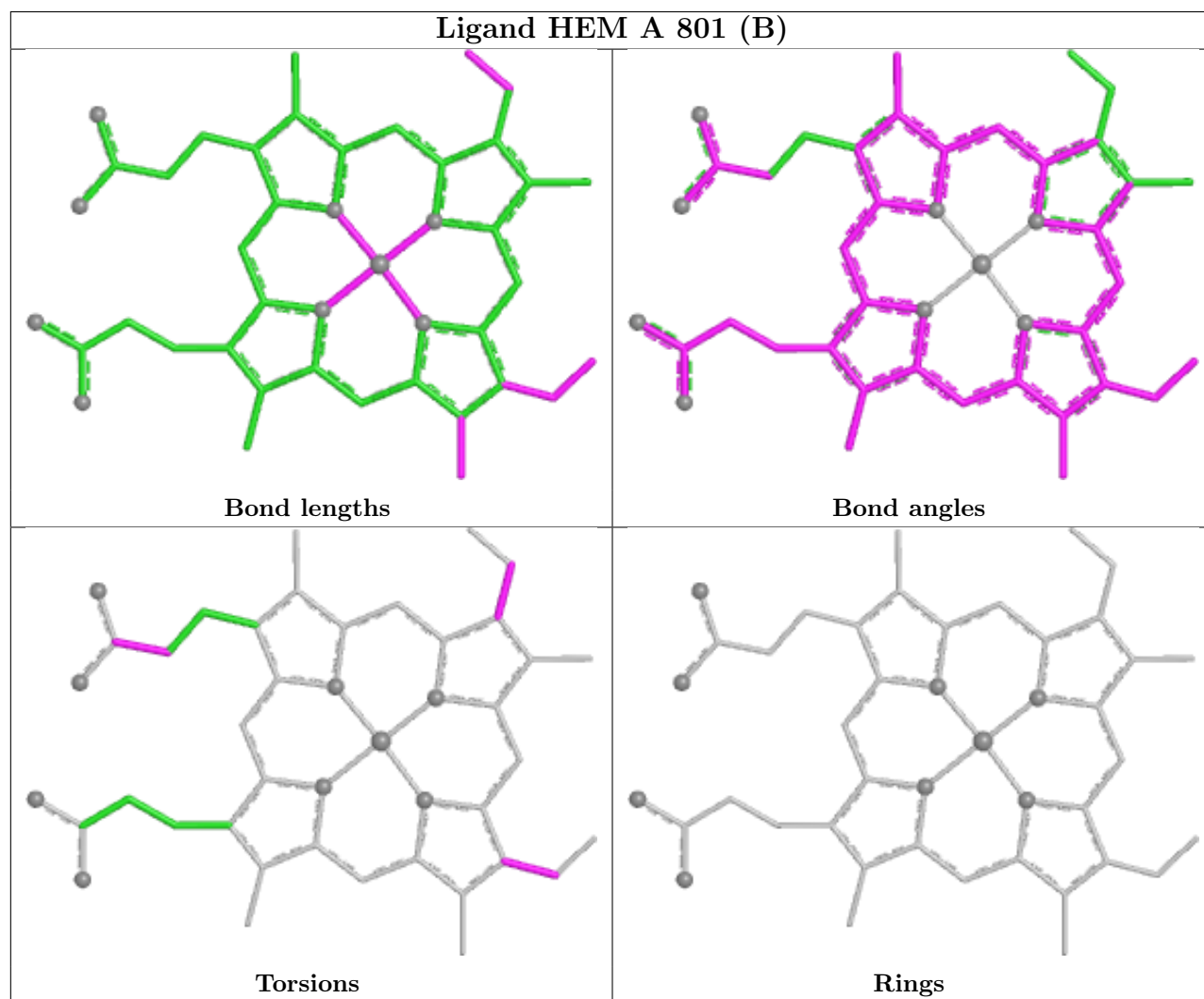
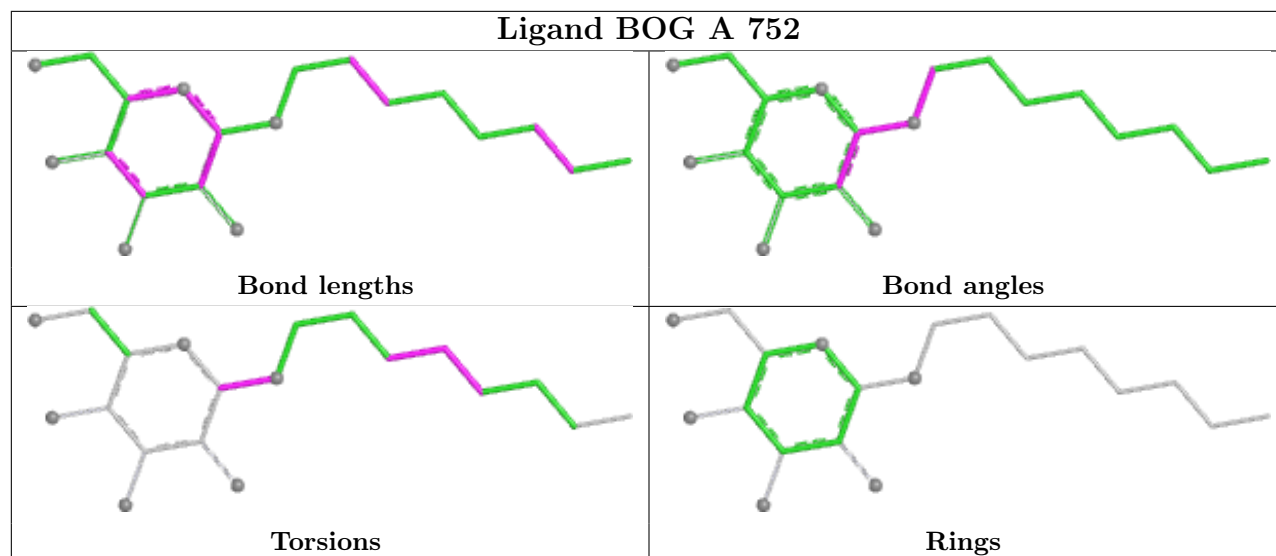
12 monomers are involved in 19 short contacts:

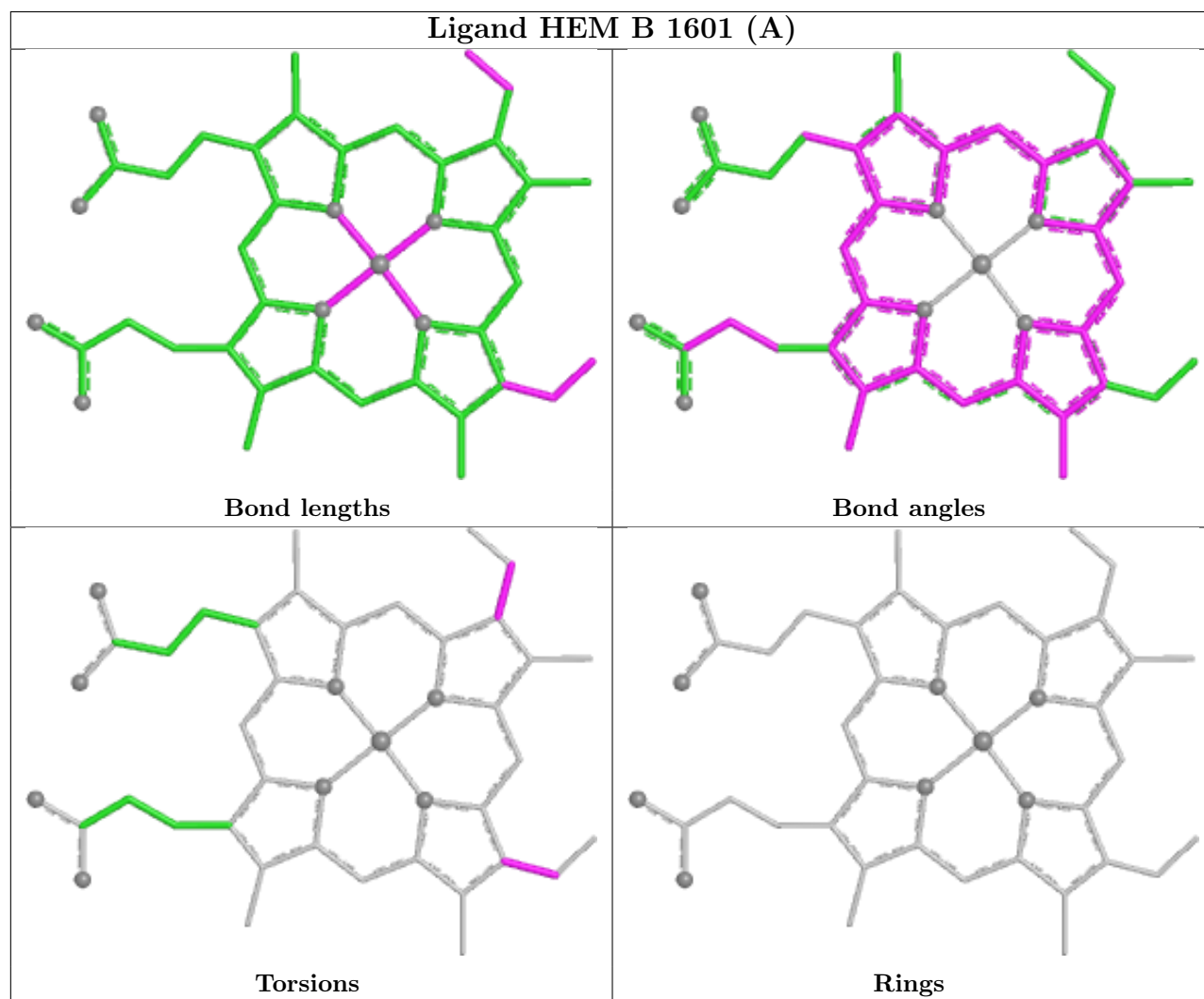
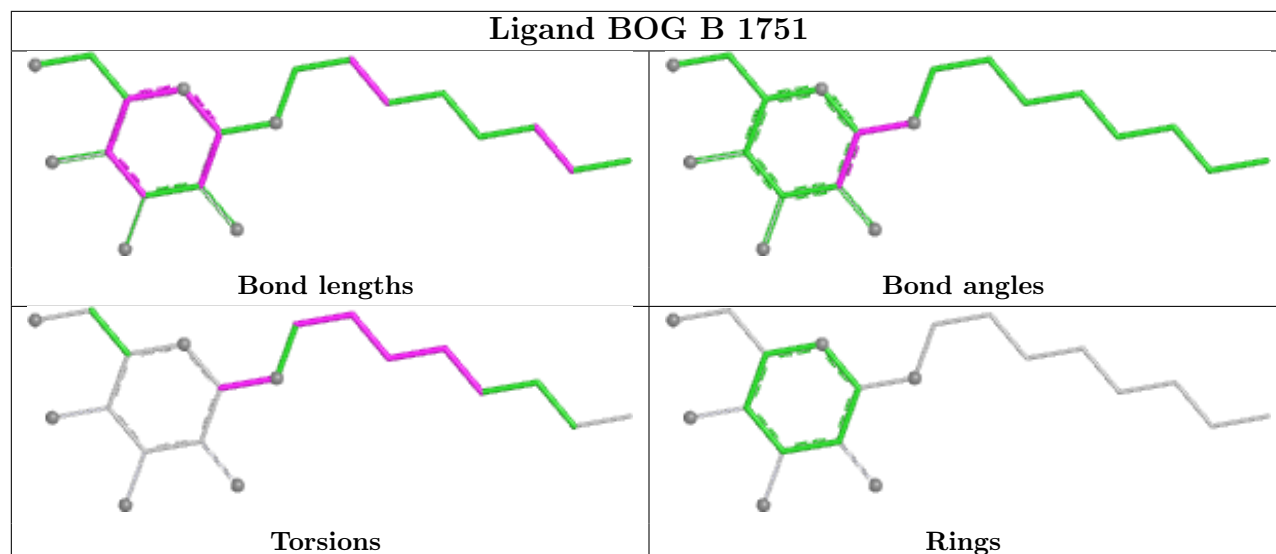
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	801[A]	HEM	2	0
9	A	758	GOL	1	0
9	B	1759	GOL	1	0
8	A	801[B]	HEM	2	0
6	B	1751	BOG	4	0
8	B	1601[A]	HEM	1	0
8	B	1601[B]	HEM	3	0
6	B	1752	BOG	1	0
7	A	701	BFL	1	0
6	A	753	BOG	1	0
6	B	1753	BOG	1	0
6	A	754	BOG	1	0

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

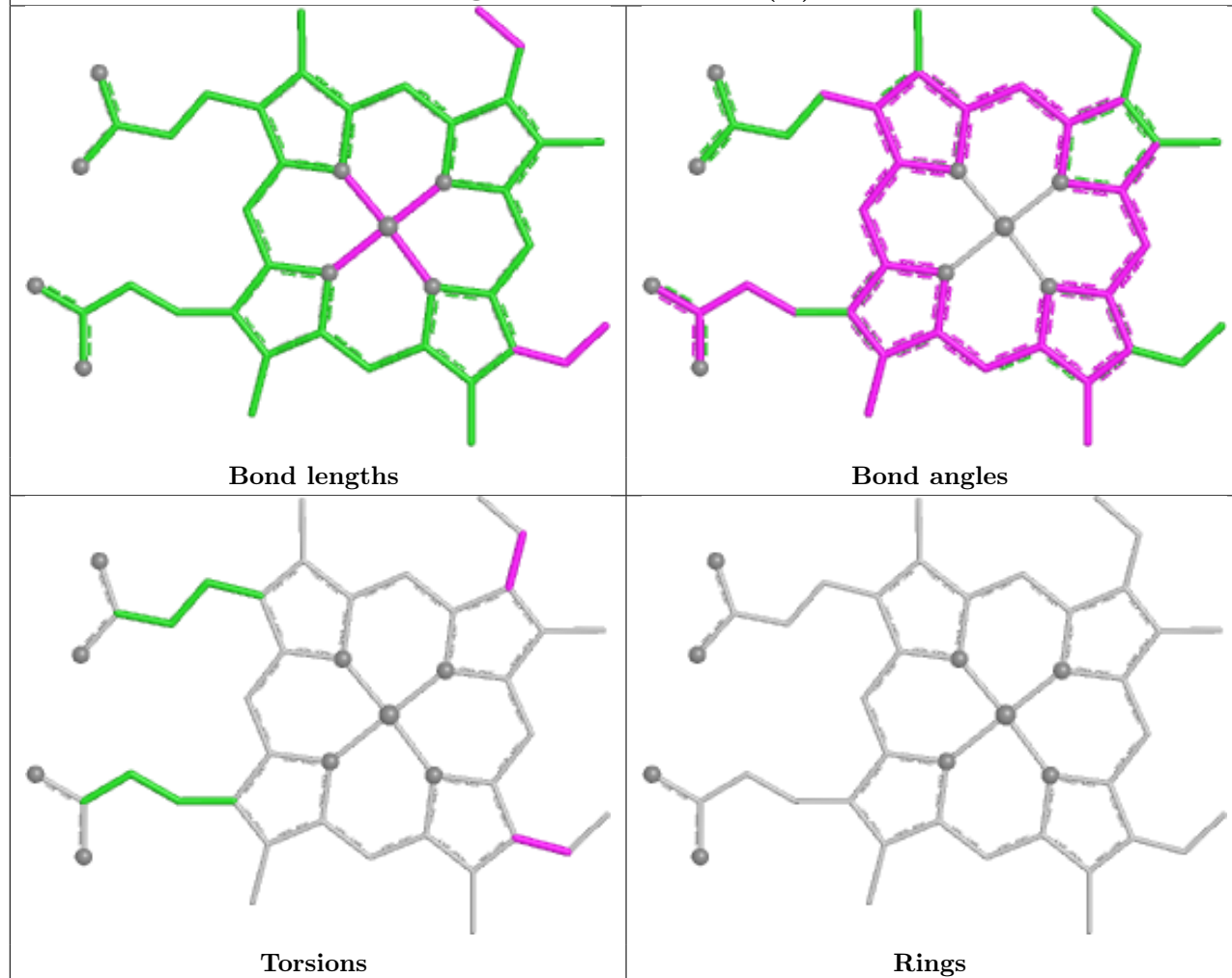
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



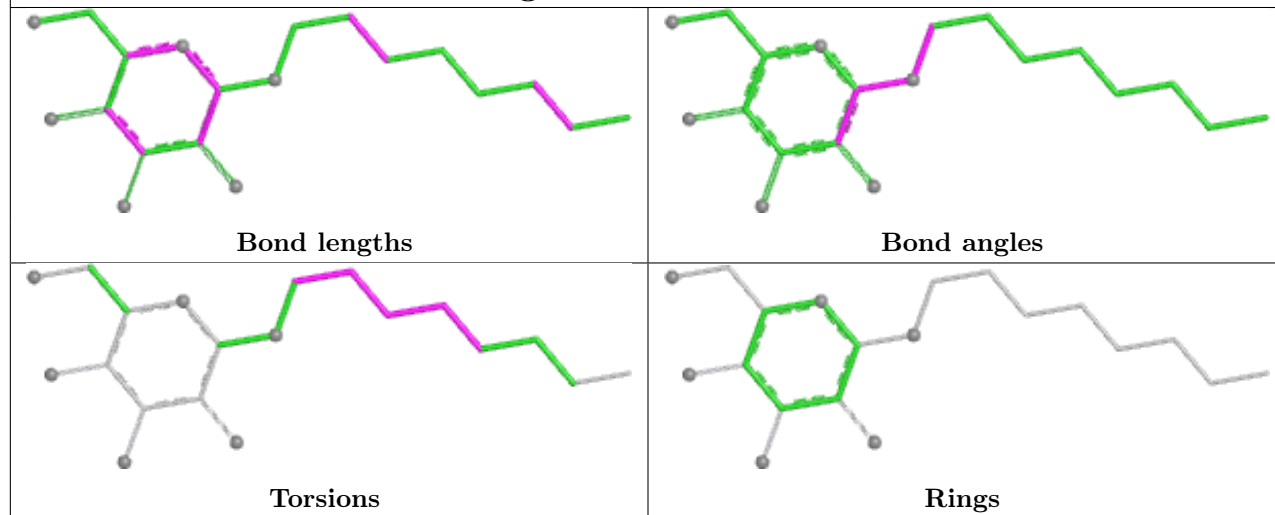


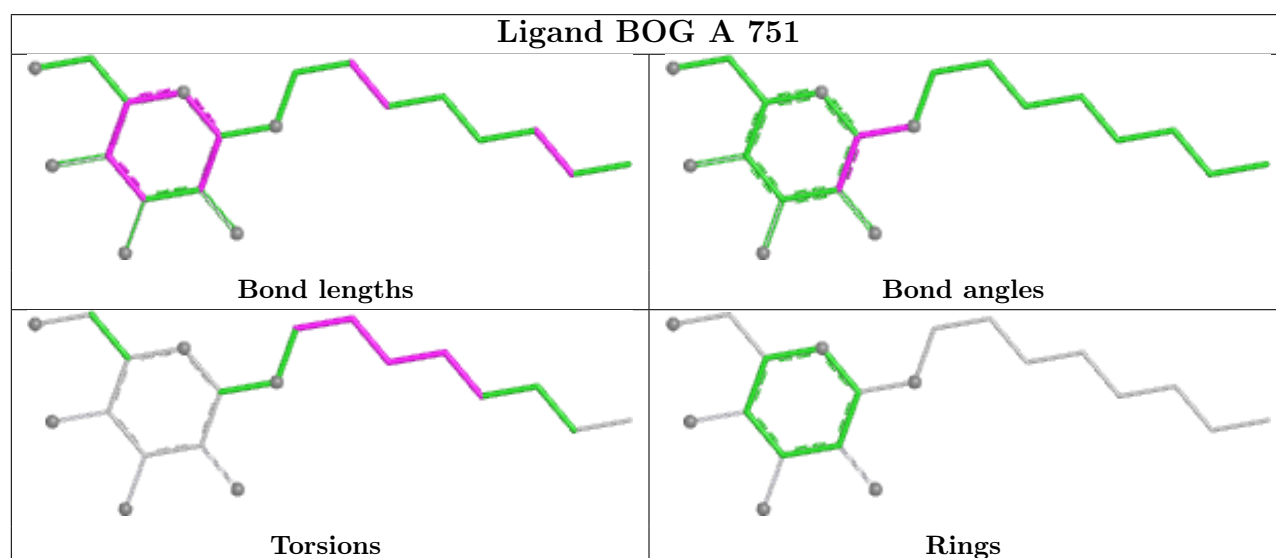
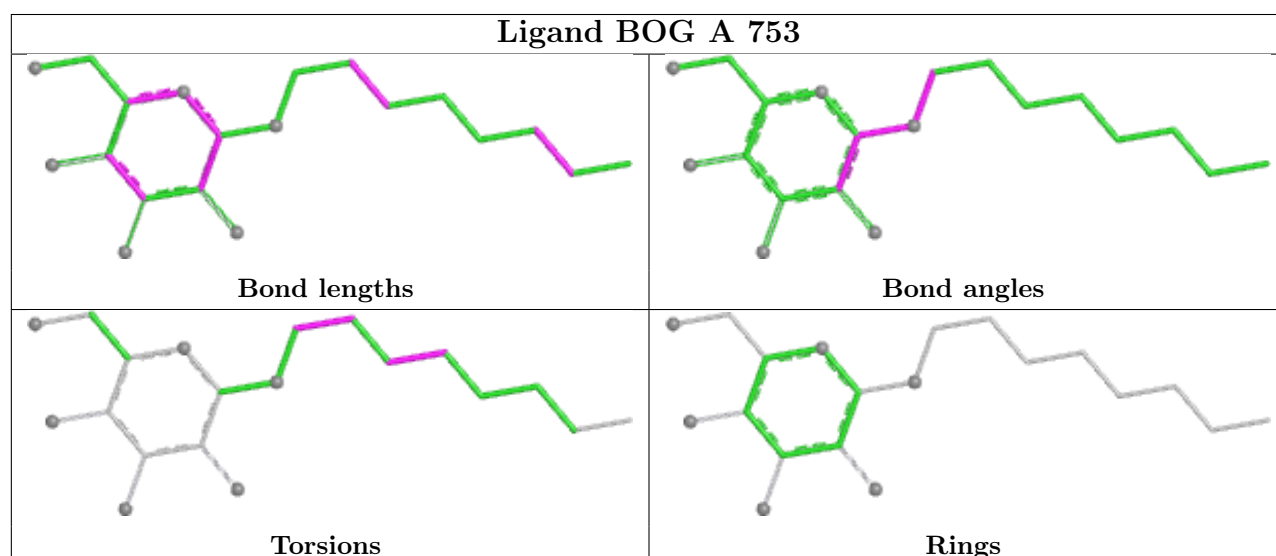
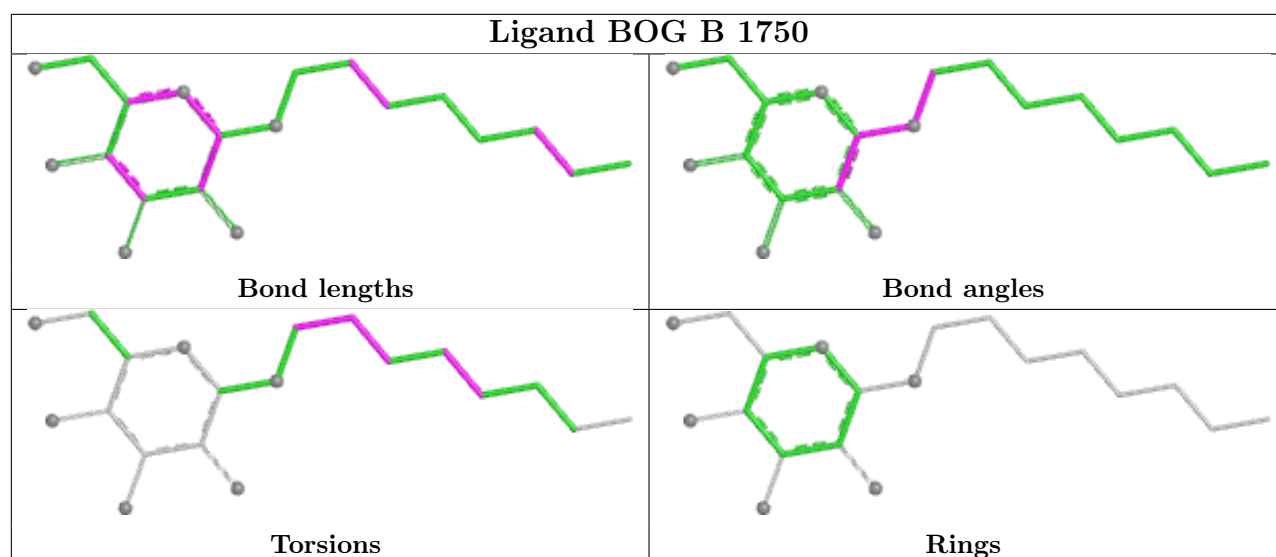


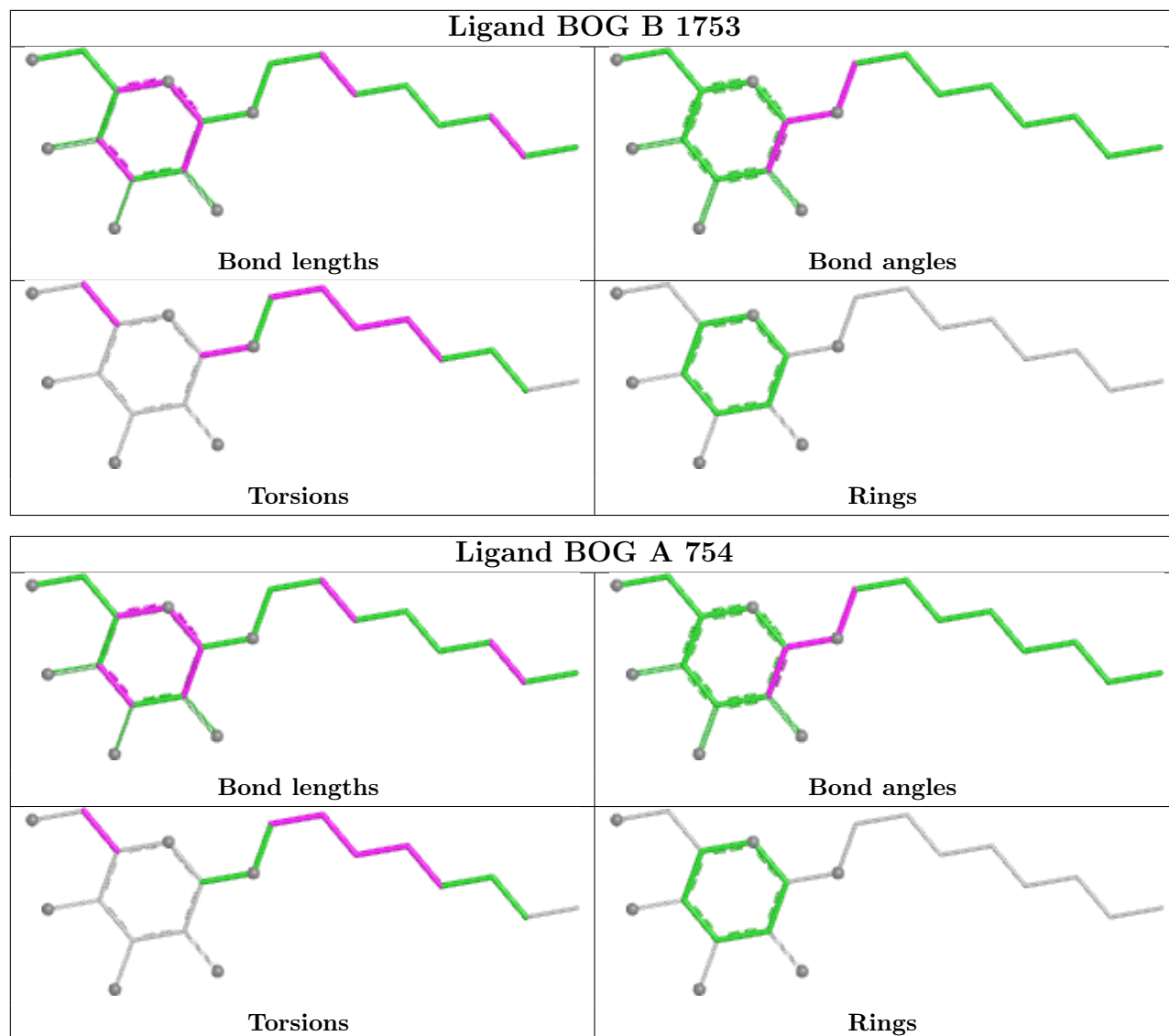
Ligand HEM B 1601 (B)



Ligand BOG B 1752







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	553/553 (100%)	0.50	40 (7%)	21 20	19, 41, 55, 65	2 (0%)
1	B	553/553 (100%)	0.46	35 (6%)	26 24	18, 41, 54, 66	2 (0%)
All	All	1106/1106 (100%)	0.48	75 (6%)	23 22	18, 41, 55, 66	4 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	584	ASP	6.9
1	A	36	CYS	6.1
1	B	36	CYS	5.9
1	A	575	CYS	5.2
1	A	107	PHE	4.9
1	B	32	PRO	4.5
1	B	575	CYS	4.5
1	A	32	PRO	4.3
1	A	98	TRP	4.3
1	A	492	GLU	4.1
1	B	82	LEU	3.9
1	B	569	CYS	3.9
1	A	409	PHE	3.9
1	B	454	GLU	3.8
1	B	239	GLU	3.8
1	A	159	CYS	3.7
1	A	493	GLU	3.7
1	B	159	CYS	3.7
1	A	479	GLN	3.6
1	B	33	VAL	3.6
1	B	81	THR	3.5
1	A	514	PRO	3.5
1	A	83	ARG	3.3
1	B	87	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	179	ARG	3.3
1	B	282	GLN	3.2
1	A	584	ASP	3.2
1	B	75	TRP	3.1
1	A	569	CYS	3.1
1	B	37	CYS	3.0
1	B	581	HIS	3.0
1	A	59	CYS	3.0
1	A	97	ARG	2.9
1	B	277	ARG	2.9
1	A	248	LYS	2.8
1	B	573	LYS	2.8
1	A	513	HIS	2.8
1	A	69[A]	CYS	2.8
1	B	79	ARG	2.8
1	B	57	CYS	2.7
1	A	175	GLU	2.7
1	A	454	GLU	2.7
1	B	267	GLU	2.6
1	A	277	ARG	2.6
1	A	79	ARG	2.6
1	B	69[A]	CYS	2.6
1	A	294	LEU	2.6
1	A	239	GLU	2.5
1	B	215	LYS	2.5
1	A	57	CYS	2.5
1	B	487	MET	2.5
1	A	33	VAL	2.4
1	A	190	ASP	2.4
1	B	281	PRO	2.4
1	B	41	CYS	2.4
1	A	170	GLN	2.3
1	A	99	LEU	2.3
1	A	169	LYS	2.3
1	A	41	CYS	2.2
1	B	80	THR	2.2
1	A	257	LEU	2.2
1	A	401	ASP	2.2
1	A	37	CYS	2.1
1	B	59	CYS	2.1
1	B	248	LYS	2.1
1	B	122	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	101	ASP	2.1
1	B	185	ARG	2.1
1	A	473	LYS	2.1
1	B	186	LYS	2.1
1	B	401	ASP	2.0
1	A	81	THR	2.0
1	B	514	PRO	2.0
1	A	398	GLY	2.0
1	B	47	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	D	4	11/12	0.25	0.20	89,90,91,91	0
5	BMA	H	4	11/12	0.31	0.32	84,86,88,90	0
4	MAN	E	4	11/12	0.43	0.21	86,88,90,91	0
3	BMA	D	3	11/12	0.46	0.19	78,81,85,88	0
5	BMA	H	3	11/12	0.50	0.18	70,73,78,81	0
3	BMA	G	4	11/12	0.50	0.18	81,82,82,83	0
5	BMA	H	5	11/12	0.51	0.25	90,91,92,92	0
4	MAN	E	5	11/12	0.55	0.20	92,93,93,94	0
4	BMA	E	3	11/12	0.55	0.22	71,74,79,83	0
3	BMA	G	3	11/12	0.58	0.17	69,71,76,79	0
2	NDG	C	2	14/15	0.64	0.20	72,74,75,75	0
2	NDG	F	2	14/15	0.78	0.17	68,70,71,71	0
4	NDG	E	2	14/15	0.81	0.17	53,56,60,65	0
5	NDG	H	2	14/15	0.83	0.16	53,56,60,65	0
2	NAG	C	1	14/15	0.84	0.14	57,61,63,68	0
3	NAG	D	2	14/15	0.85	0.14	63,66,69,74	0
2	NAG	F	1	14/15	0.86	0.15	59,62,64,66	0
3	NAG	G	2	14/15	0.90	0.12	54,55,59,64	0
3	NAG	D	1	14/15	0.94	0.12	50,53,56,60	0

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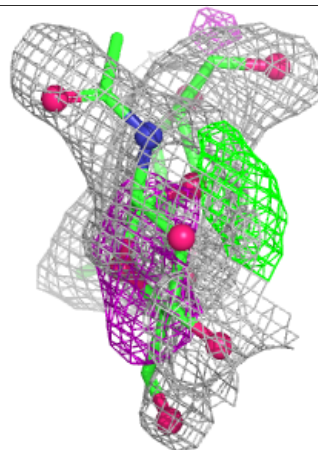
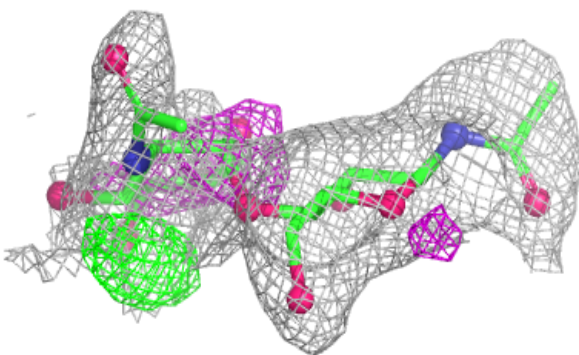
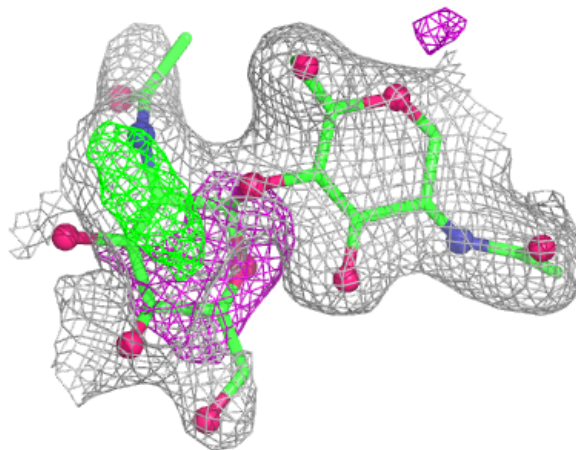
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	E	1	14/15	0.94	0.11	37,38,42,47	0
3	NAG	G	1	14/15	0.95	0.08	43,45,49,50	0
5	NAG	H	1	14/15	0.95	0.10	36,37,41,47	0

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.

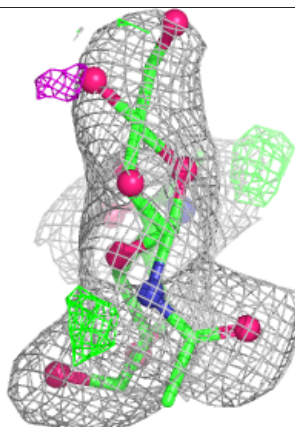
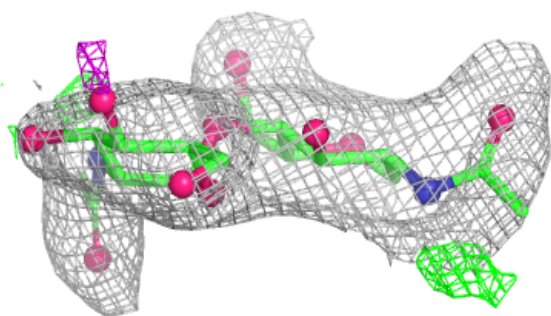
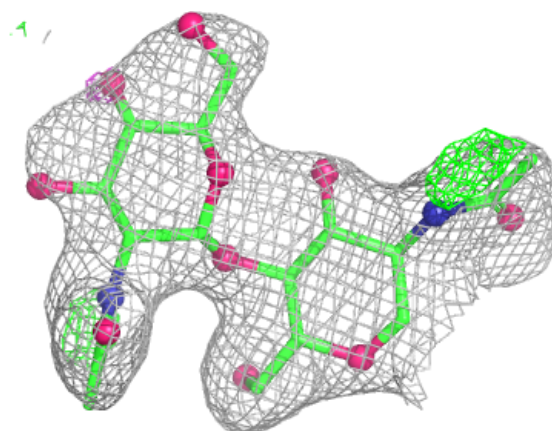
Electron density around Chain C:

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

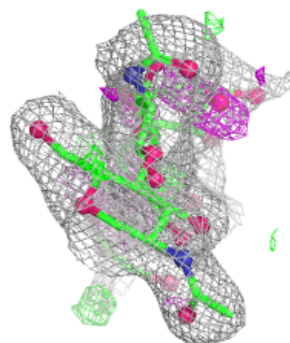
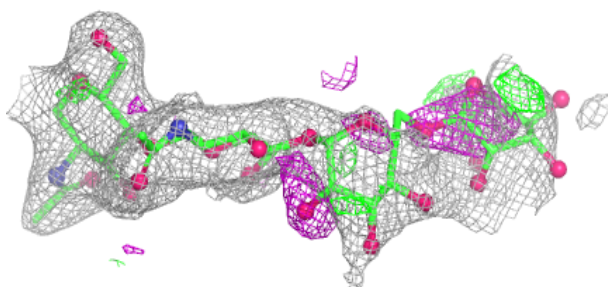
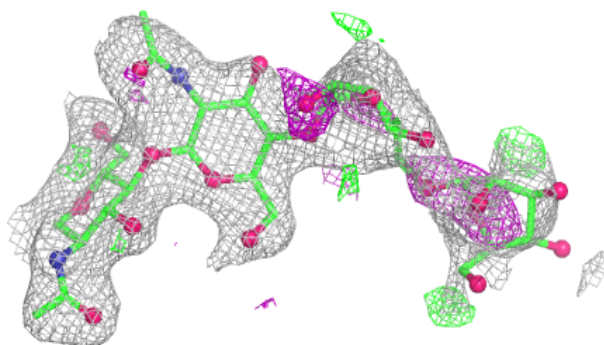


Electron density around Chain F:

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

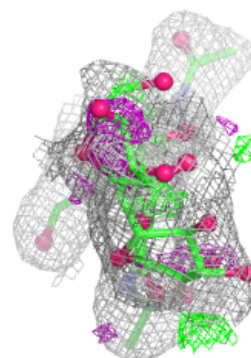
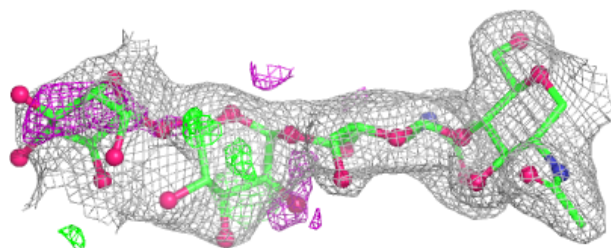
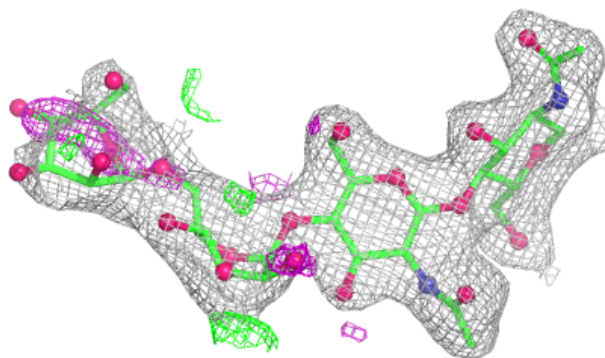
**Electron density around Chain D:**

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

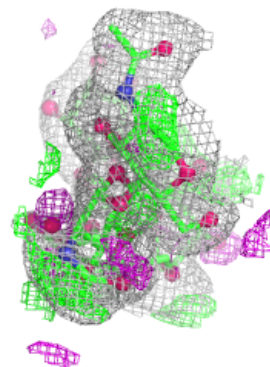
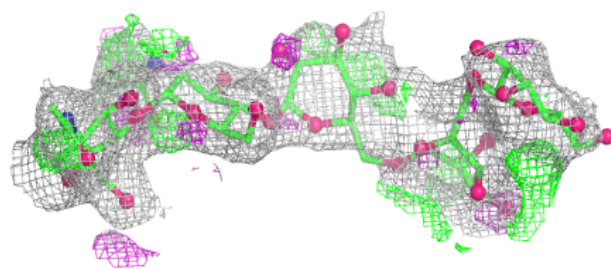
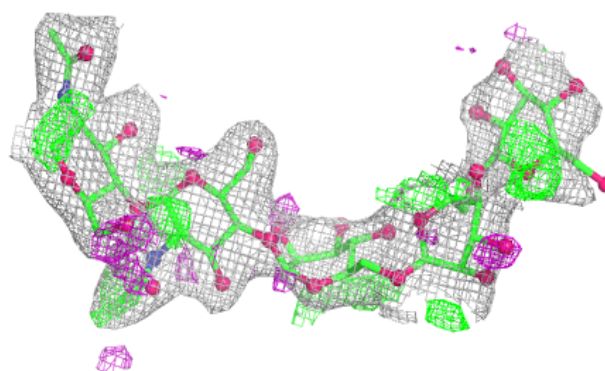


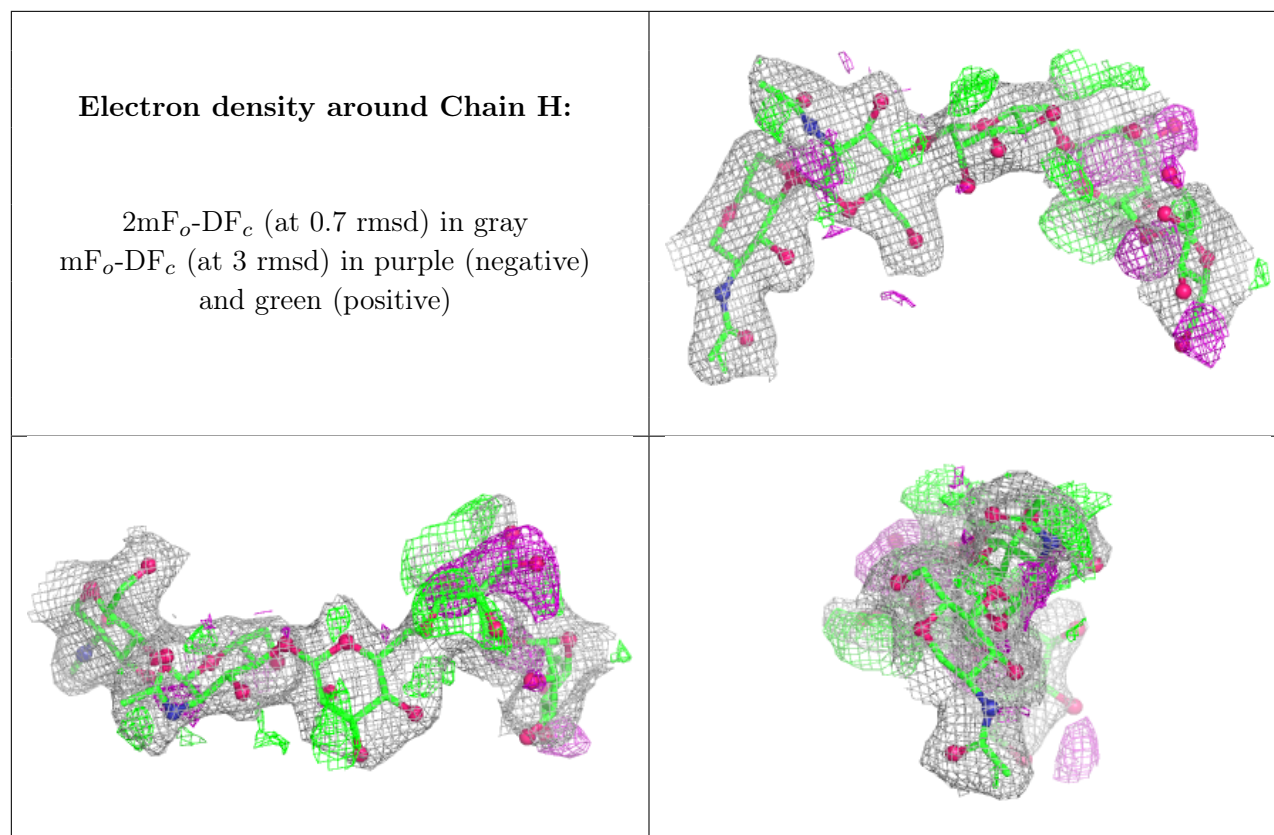
Electron density around Chain G:

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

**Electron density around Chain E:**

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BOG	A	752	20/20	0.51	0.38	96,104,105,105	0
6	BOG	B	1752	20/20	0.58	0.36	112,113,113,113	0
6	BOG	A	754	20/20	0.65	0.31	103,105,106,106	0
6	BOG	B	1750	20/20	0.67	0.28	91,91,94,94	0
9	GOL	B	1760	6/6	0.72	0.28	78,79,79,79	0
6	BOG	B	1753	20/20	0.73	0.32	101,103,104,104	0
9	GOL	B	1759	6/6	0.77	0.23	50,53,56,59	0
9	GOL	A	758	6/6	0.79	0.26	57,60,61,61	0
6	BOG	A	753	20/20	0.81	0.27	73,80,82,82	0
9	GOL	B	1758	6/6	0.84	0.33	79,82,82,83	0
6	BOG	B	1751	20/20	0.85	0.20	76,78,78,78	0
9	GOL	A	759	6/6	0.86	0.21	77,77,77,77	0
7	BFL	B	1701	17/17	0.87	0.17	52,53,57,57	0
7	BFL	A	701	17/17	0.87	0.18	51,53,57,58	0

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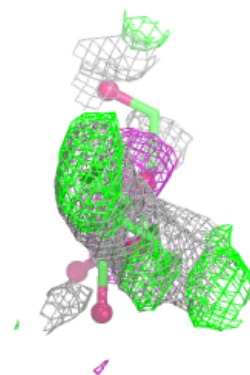
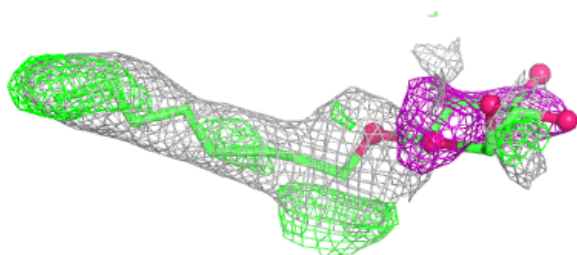
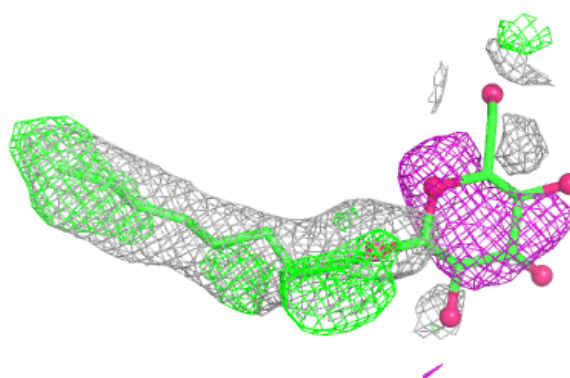
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BOG	A	751	20/20	0.89	0.18	70,71,73,73	0
8	HEM	A	801[B]	43/43	0.93	0.13	39,41,46,48	43
8	HEM	B	1601[A]	43/43	0.93	0.12	40,41,47,49	43
8	HEM	B	1601[B]	43/43	0.93	0.12	40,42,47,49	43
8	HEM	A	801[A]	43/43	0.93	0.13	41,42,48,50	43

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.

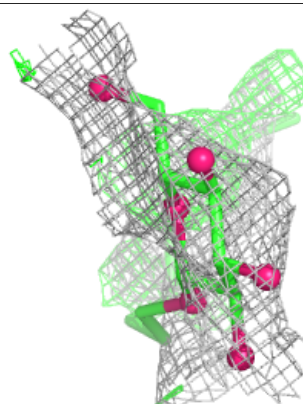
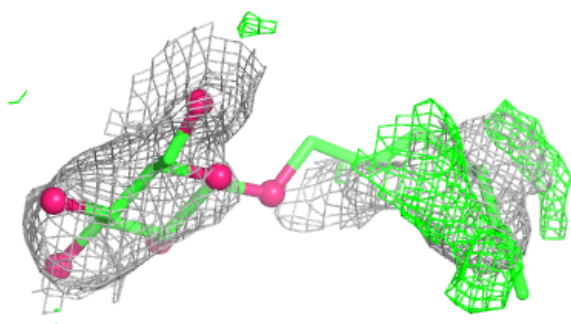
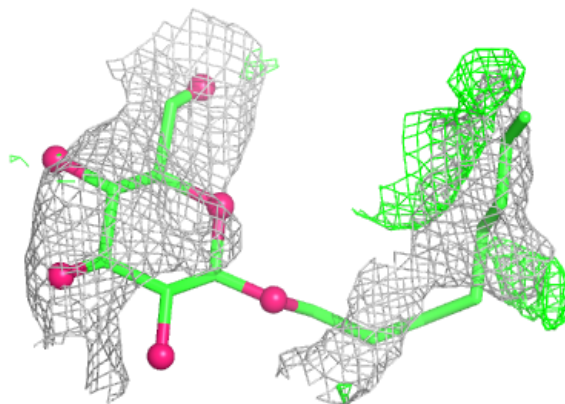
Electron density around BOG A 752:

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

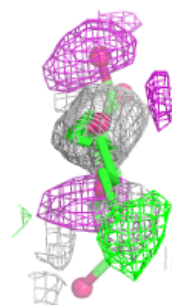
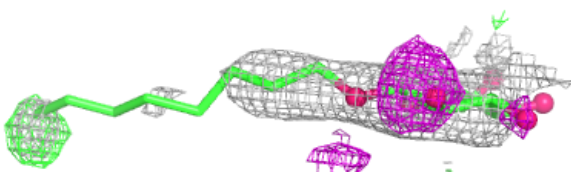
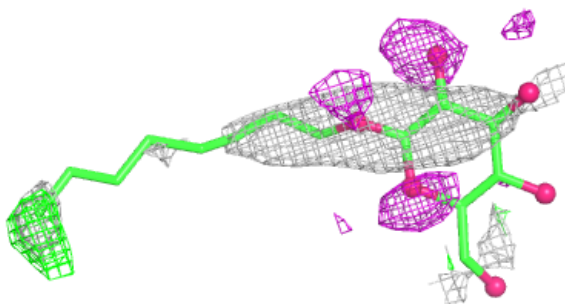


Electron density around BOG B 1752:

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

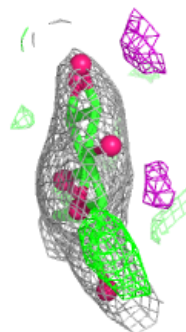
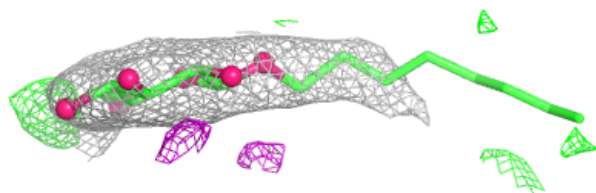
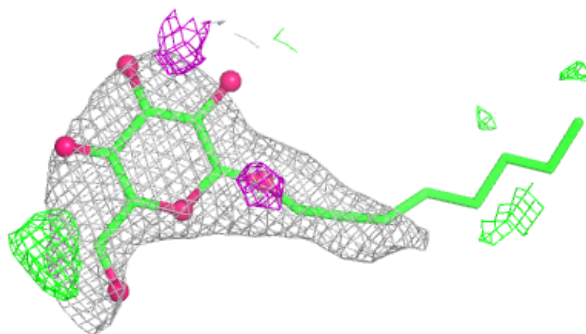
**Electron density around BOG A 754:**

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

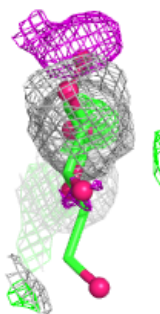
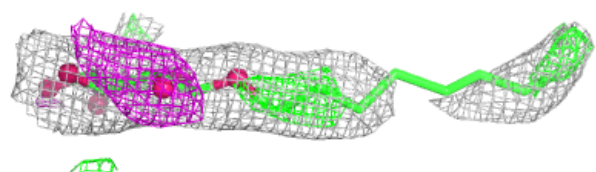
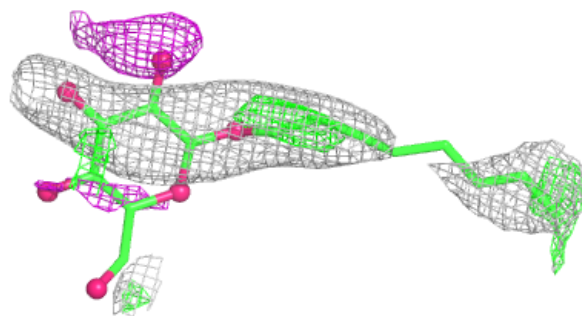


Electron density around BOG B 1750:

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

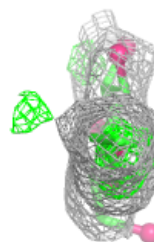
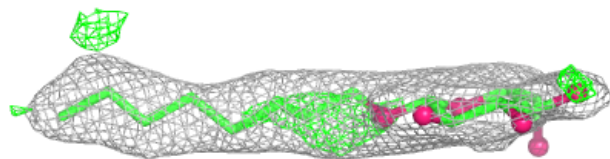
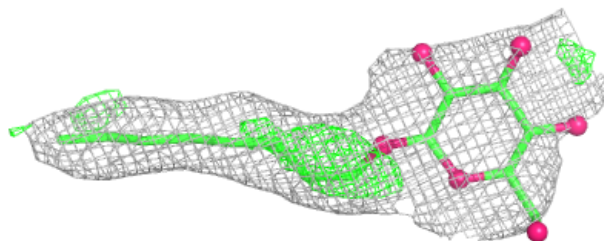
**Electron density around BOG B 1753:**

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

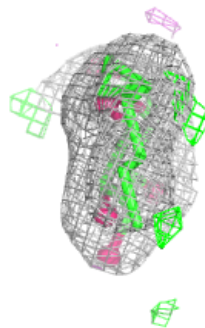
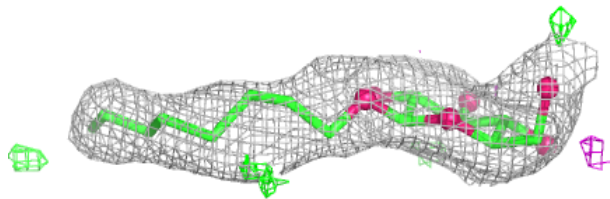
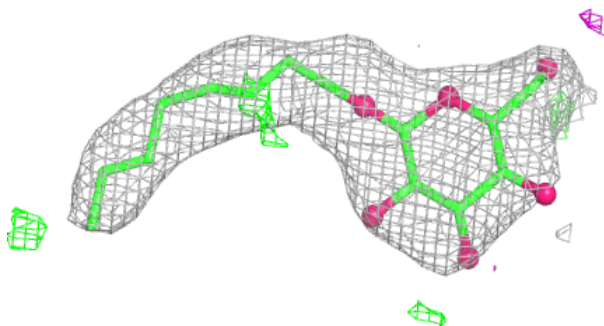


Electron density around BOG A 753:

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

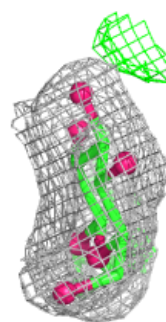
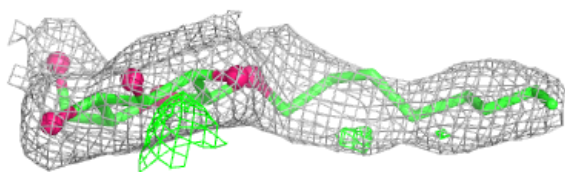
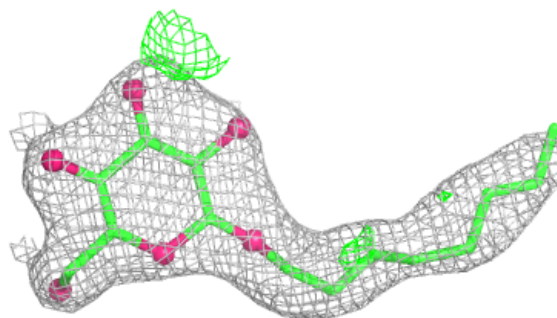
**Electron density around BOG B 1751:**

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



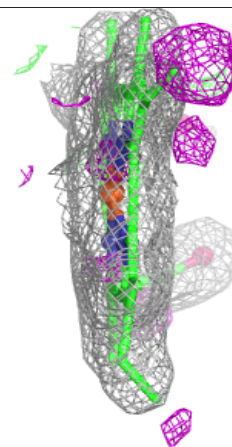
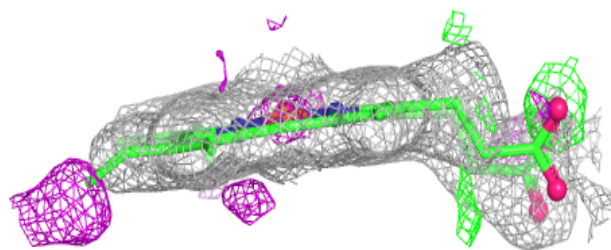
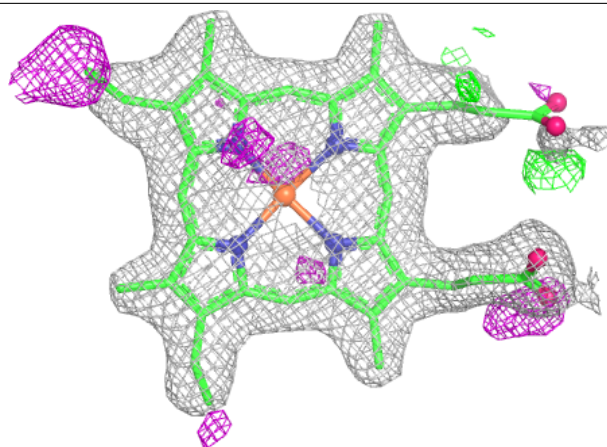
Electron density around BOG A 751:

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



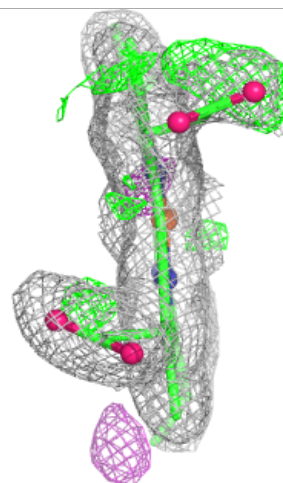
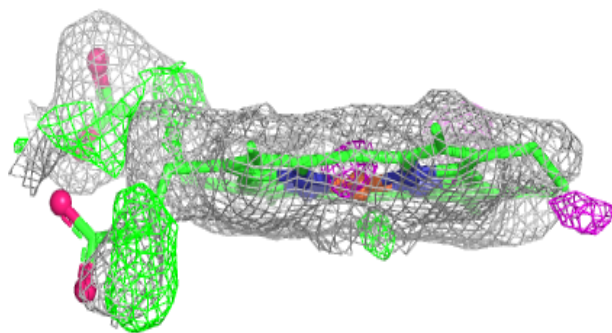
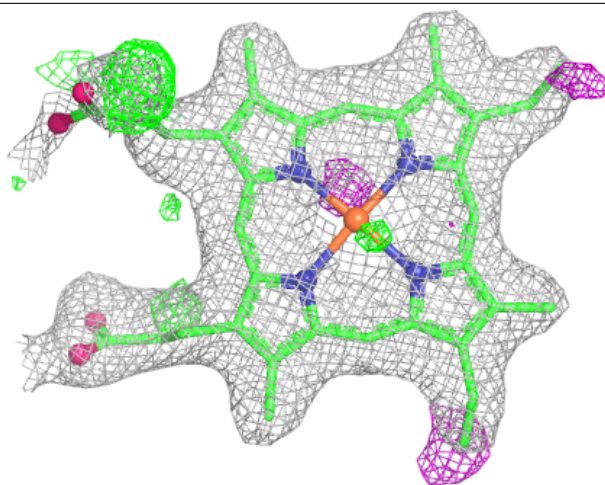
Electron density around HEM A 801 (B):

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



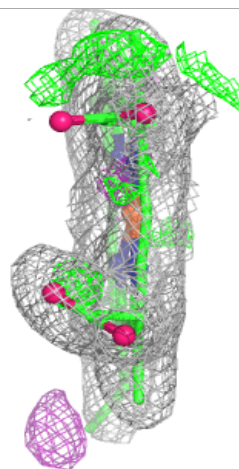
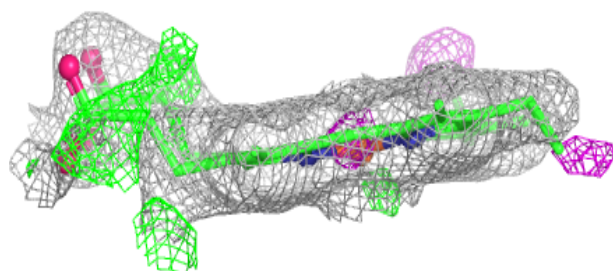
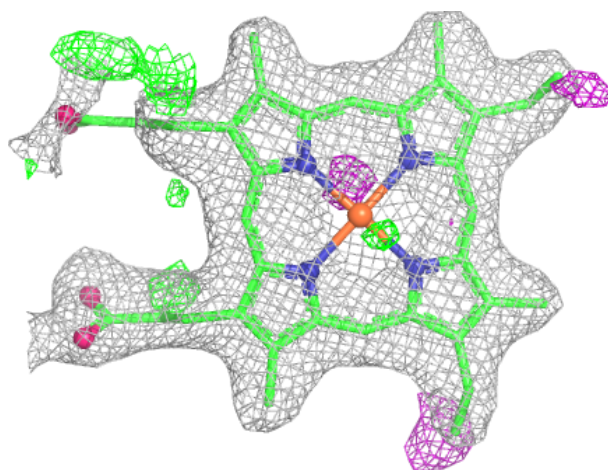
Electron density around HEM B 1601 (A):

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



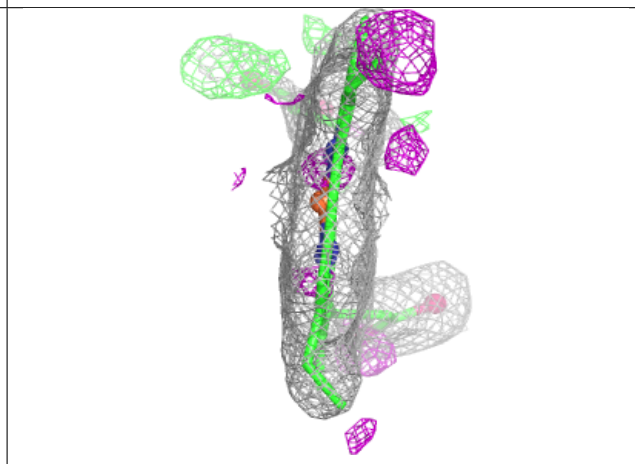
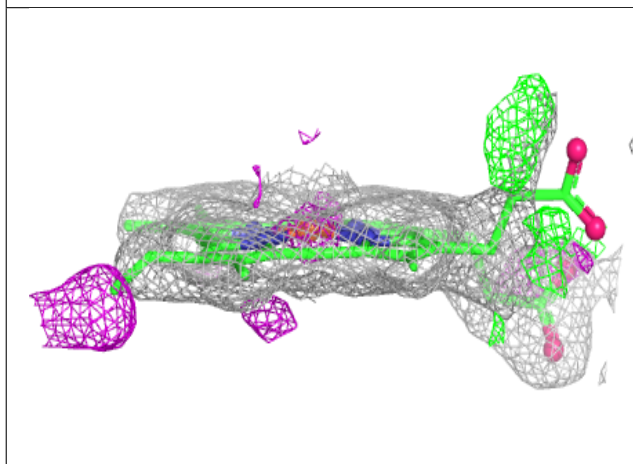
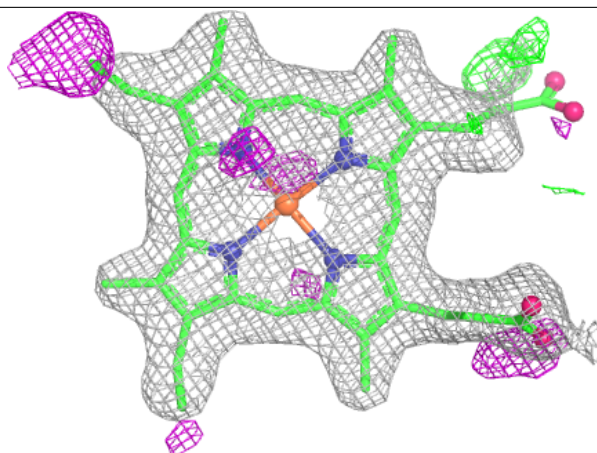
Electron density around HEM B 1601 (B):

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



Electron density around HEM A 801 (A):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.